SUPPORTING INFORMATION FOR

The search for the optimal methodology for predicting fluorinated cathinone drugs NMR chemical shifts

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For better comparison of results, the data in Tables S1-S21 are given with four dessimal places.

Table S1. Theoretical chemical shifts (in ppm) of *S*-cathinone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	B3LYP											B3P86											Exp.[b]
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	140.8253	141.1187	142.1132	141.2558	142.6706	141.2401	142.4580	141.2248	142.4660	141.2699	142.4982	138.6291	138.8962	139.9644	139.0633	140.4390	139.0716	140.2763	139.0583	140.4139	139.0996	140.3400	**132.3**
C2	136.2269	135.9719	136.4747	135.7308	136.2765	135.7409	136.6568	135.7508	136.5509	135.7199	136.6695	135.2377	134.9625	135.5217	134.7575	135.3722	134.7904	135.6745	134.8016	135.6927	134.7703	135.7073	**129.3**
C3	135.1175	135.9997	136.5970	136.2776	137.0283	136.2581	137.1773	136.2382	137.1068	136.2944	137.2567	134.1100	135.0070	135.6838	135.3367	136.1793	135.3392	136.3177	135.3195	136.3582	135.3783	136.4260	**128.9**
C4	139.5081	141.4069	142.0273	142.1559	142.7598	142.1096	143.6598	142.0627	143.4039	142.1973	143.8635	138.5201	140.4040	141.0979	141.1919	141.9076	141.1684	142.7638	141.1223	142.6155	141.2580	142.9883	**135.2**
C5	133.7356	135.1468	135.8072	135.7648	136.6783	135.7244	136.7579	135.6834	136.6669	135.8014	136.8845	132.7560	134.1915	134.9326	134.8676	135.8685	134.8485	135.9395	134.8072	135.9564	134.9294	136.0934	**128.9**
C6	134.6077	136.1580	137.1964	136.9035	138.4376	136.8551	138.8833	136.8062	138.6601	136.9477	139.1613	133.5373	135.0402	136.1159	135.8046	137.3816	135.7798	137.7856	135.7329	137.6741	135.8718	138.0706	**129.3**
C7	213.1205	216.8948	218.5279	218.4139	219.1379	218.3225	224.2807	218.2301	223.2978	218.4987	224.9571	211.1221	214.6643	216.3245	216.1126	216.8356	216.0508	221.8637	215.9665	221.0143	216.2142	222.5295	**198.1**
C8	57.6817	58.2515	58.8301	58.4304	59.1286	58.4144	59.8120	58.3983	59.6436	58.4442	59.8637	56.1564	56.7270	57.3522	56.9392	57.6140	56.9473	58.3206	56.9335	58.2764	56.9754	58.4000	**51.9**
C9	23.8951	24.0979	24.0782	24.2701	24.3789	24.2537	24.2138	24.2373	24.1439	24.2841	24.1358	23.6267	23.8131	23.8150	24.0234	24.1504	24.0295	23.9608	24.0138	24.0072	24.0617	23.9181	**16.6**
H2	8.7076	8.6201	8.6182	8.5677	8.5770	8.5707	8.5616	8.5737	8.5635	8.5647	8.5679	8.7654	8.6782	8.6749	8.6267	8.6421	8.6311	8.6164	8.6336	8.6239	8.6238	8.6227	**7.89**
H3	7.6873	7.8135	7.8560	7.8587	7.9231	7.8559	7.9353	7.8531	7.9254	7.8611	7.9536	7.7335	7.8655	7.9137	7.9131	7.9842	7.9116	7.9961	7.9084	7.9921	7.9156	8.0160	**7.48**
H4	7.7138	7.8998	7.9473	7.9739	8.0378	7.9694	8.0767	7.9649	8.0597	7.9778	8.0998	7.7591	7.9492	8.0025	8.0250	8.0959	8.0219	8.1334	8.0170	8.1224	8.0290	8.1579	**7.67**
H5	7.5854	7.7439	7.7856	7.8123	7.8814	7.8081	7.8874	7.8038	7.8763	7.8161	7.9091	7.6285	7.7941	7.8413	7.8654	7.9418	7.8625	7.9464	7.8577	7.9411	7.8694	7.9696	**7.48**
H6	8.0664	8.2348	8.3286	8.3115	8.4634	8.3068	8.4902	8.3020	8.4737	8.3157	8.5281	8.1510	8.3149	8.4093	8.3896	8.5467	8.3864	8.5698	8.3815	8.5585	8.3937	8.6090	**7.89**
H8	4.3181	4.5117	4.5771	4.5955	4.6934	4.5903	4.7435	4.5850	4.7285	4.6002	4.7547	4.3554	4.5430	4.6098	4.6230	4.7219	4.6195	4.7699	4.6141	4.7604	4.6275	4.7810	**5.06**
H(9A-9C)	1.2628	1.2693	1.2570	1.2644	1.2462	1.2646	1.2837	1.2647	1.2759	1.2641	1.2941	1.2622	1.2714	1.2597	1.2669	1.2499	1.2686	1.2875	1.2684	1.2854	1.2666	1.2997	**1.46**
Nuclei	B3PW91											B98											
C1	138.8583	139.2634	140.2055	139.4648	140.8278	139.4536	140.6563	139.4345	140.6904	139.4785	140.7308	139.7533	140.0127	140.9971	140.1901	141.5967	140.1916	141.3447	140.1909	141.3776	140.1916	141.3965	**132.3**
C2	135.3457	135.1166	135.6034	134.9091	135.5260	134.9261	135.8212	134.9346	135.7428	134.8952	135.8542	135.0205	134.7603	135.2595	134.5642	135.1609	134.5909	135.4929	134.6153	135.4137	134.5410	135.5146	**129.3**
C3	134.2150	135.1321	135.7282	135.4488	136.2803	135.4360	136.4129	135.4143	136.3570	135.4627	136.5229	133.9800	134.8313	135.4365	135.1484	135.9584	135.1457	136.0817	135.1405	136.0327	135.1529	136.1718	**128.9**
C4	138.5536	140.4351	141.0538	141.1932	141.8977	141.1559	142.7401	141.1092	142.5010	141.2301	142.9633	138.2677	140.0924	140.7232	140.8570	141.5400	140.8291	142.3968	140.7984	142.1665	140.8851	142.6033	**135.2**
C5	132.8749	134.3258	134.9856	134.9794	135.9719	134.9459	136.0339	134.9034	135.9563	135.0130	136.1898	132.6440	134.0126	134.6748	134.6637	135.6283	134.6404	135.6832	134.6144	135.6148	134.6878	135.8202	**128.9**
C6	133.5564	135.0682	136.0929	135.8173	137.3888	135.7780	137.7789	135.7295	137.5762	135.8562	138.0721	133.5603	135.0172	136.0512	135.7683	137.3297	135.7388	137.7470	135.7063	137.5513	135.7986	138.0253	**129.3**
C7	211.2345	214.9126	216.4394	216.3942	217.0783	216.3133	222.1336	216.2231	221.1772	216.4728	222.8074	209.6080	213.2785	214.8703	214.7988	215.5126	214.7267	220.6274	214.6518	219.6493	214.8691	221.3005	**198.1**
C8	56.1416	56.7863	57.3308	57.0265	57.6794	57.0160	58.3723	56.9969	58.2284	57.0387	58.4702	57.8371	58.3960	58.9229	58.6261	59.2562	58.6266	59.9113	58.6248	59.7630	58.6280	59.9789	**51.9**
C9	23.2995	23.4921	23.4641	23.6856	23.8209	23.6773	23.6585	23.6604	23.6105	23.6955	23.6201	24.0738	24.2442	24.2280	24.4424	24.5710	24.4437	24.4148	24.4427	24.3678	24.4435	24.3504	**16.6**
H2	8.7455	8.6492	8.6508	8.5955	8.6125	8.5994	8.5911	8.6030	8.5944	8.5919	8.5945	8.7273	8.6387	8.6404	8.5880	8.6033	8.5913	8.5900	8.5947	8.5943	8.5852	8.5934	**7.89**
H3	7.7355	7.8649	7.9122	7.9130	7.9823	7.9109	7.9968	7.9083	7.9887	7.9152	8.0144	7.7139	7.8436	7.8923	7.8924	7.9627	7.8898	7.9763	7.8873	7.9686	7.8951	7.9929	**7.48**
H4	7.7604	7.9478	7.9996	8.0234	8.0923	8.0196	8.1319	8.0155	8.1169	8.0271	8.1540	7.7389	7.9264	7.9805	8.0030	8.0738	7.9988	8.1132	7.9946	8.0986	8.0072	8.1345	**7.67**
H5	7.6323	7.7943	7.8415	7.8657	7.9403	7.8621	7.9477	7.8581	7.9383	7.8693	7.9682	7.6153	7.7767	7.8254	7.8487	7.9240	7.8447	7.9316	7.8407	7.9228	7.8527	7.9516	**7.48**
H6	8.1353	8.2964	8.3929	8.3712	8.5269	8.3675	8.5517	8.3633	8.5366	8.3749	8.5883	8.0983	8.2621	8.3632	8.3395	8.5012	8.3352	8.5300	8.3309	8.5160	8.3439	8.5659	**7.89**
H8	4.3391	4.5245	4.5867	4.6037	4.7000	4.5996	4.7475	4.5950	4.7341	4.6078	4.7558	4.3121	4.4971	4.5653	4.5782	4.6807	4.5735	4.7301	4.5689	4.7174	4.5828	4.7367	**5.06**
H(9A-9C)	1.2393	1.2440	1.2348	1.2403	1.2214	1.2412	1.2605	1.2418	1.2547	1.2396	1.2707	1.2628	1.2679	1.2561	1.2646	1.2425	1.2651	1.2827	1.2656	1.2775	1.2644	1.2917	**1.46**
Nuclei	B971											B972											
C1	139.3668	139.6203	140.6194	139.8139	141.2045	139.8074	140.9658	139.8009	140.9977	139.8265	141.0245	136.2011	136.5636	137.4979	136.8490	138.1950	136.8262	137.9832	136.8026	138.0149	136.8679	138.0587	**132.3**
C2	134.7335	134.4769	134.9685	134.2892	134.8710	134.3083	135.1926	134.3267	135.1149	134.2773	135.2199	132.7378	132.4726	132.9764	132.3428	132.9077	132.3518	133.2020	132.3584	133.1234	132.3302	133.2372	**129.3**
C3	133.7868	134.6485	135.2523	134.9762	135.7812	134.9656	135.9011	134.9542	135.8516	134.9919	135.9975	131.4508	132.2816	132.8829	132.6572	133.4196	132.6372	133.5413	132.6146	133.4882	132.6718	133.6496	**128.9**
C4	138.0264	139.8611	140.4886	140.6350	141.3172	140.5992	142.1573	140.5623	141.9297	140.6747	142.3692	135.7289	137.4949	138.1201	138.2925	138.9202	138.2498	139.7447	138.2039	139.5130	138.3280	139.9635	**135.2**
C5	132.4519	133.8304	134.4901	134.4930	135.4509	134.4616	135.5030	134.4296	135.4341	134.5287	135.6460	130.1376	131.4779	132.1397	132.1733	133.0909	132.1338	133.1440	132.0918	133.0709	132.2059	133.2975	**128.9**
C6	133.3169	134.7711	135.7951	135.5240	137.0798	135.4865	137.4853	135.4485	137.2904	135.5653	137.7705	130.9745	132.3968	133.4204	133.1931	134.6581	133.1486	135.0359	133.1011	134.8414	133.2303	135.3301	**129.3**
C7	209.5647	213.1855	214.8007	214.7002	215.4329	214.6216	220.4742	214.5414	219.5180	214.7804	221.1535	206.8457	210.4219	211.9064	211.9682	212.6127	211.8770	217.5295	211.7841	216.5826	212.0507	218.1821	**198.1**
C8	57.7265	58.2750	58.7985	58.5120	59.1268	58.5048	59.7750	58.4973	59.6271	58.5247	59.8507	55.1581	55.7377	56.2702	56.0631	56.6448	56.0424	57.2738	56.0199	57.1336	56.0790	57.3700	**51.9**
C9	24.0602	24.2414	24.2110	24.4464	24.5613	24.4397	24.4057	24.4326	24.3568	24.4588	24.3561	22.9112	23.0714	23.0947	23.3318	23.4303	23.3169	23.2872	23.2996	23.2442	23.3414	23.2495	**16.6**
H2	8.7243	8.6383	8.6373	8.5886	8.6019	8.5916	8.5876	8.5947	8.5919	8.5861	8.5910	8.7315	8.6331	8.6379	8.5812	8.5939	8.5849	8.5751	8.5883	8.5786	8.5774	8.5789	**7.89**
H3	7.7162	7.8450	7.8936	7.8943	7.9640	7.8915	7.9769	7.8888	7.9693	7.8972	7.9936	7.7297	7.8563	7.9038	7.9072	7.9738	7.9045	7.9880	7.9015	7.9801	7.9096	8.0056	**7.48**
H4	7.7381	7.9244	7.9786	8.0014	8.0717	7.9970	8.1100	7.9927	8.0957	8.0058	8.1313	7.7592	7.9432	7.9952	8.0211	8.0874	8.0169	8.1269	8.0123	8.1121	8.0250	8.1489	**7.67**
H5	7.6183	7.7795	7.8279	7.8520	7.9266	7.8478	7.9339	7.8436	7.9250	7.8563	7.9540	7.6260	7.7866	7.8340	7.8603	7.9316	7.8562	7.9394	7.8519	7.9303	7.8641	7.9600	**7.48**
H6	8.1046	8.2659	8.3652	8.3423	8.5029	8.3379	8.5305	8.3334	8.5165	8.3469	8.5668	8.1126	8.2739	8.3712	8.3519	8.5021	8.3477	8.5266	8.3432	8.5118	8.3557	8.5628	**7.89**
H8	4.3073	4.4912	4.5602	4.5725	4.6750	4.5677	4.7227	4.5630	4.7105	4.5774	4.7293	4.3032	4.4875	4.5500	4.5696	4.6648	4.5649	4.7112	4.5600	4.6978	4.5739	4.7196	**5.06**
H(9A-9C)	1.2601	1.2651	1.2519	1.2624	1.2392	1.2627	1.2787	1.2629	1.2734	1.2626	1.2881	1.2330	1.2369	1.2275	1.2369	1.2122	1.2373	1.2487	1.2374	1.2433	1.2364	1.2585	**1.46**
Nuclei	BHandH											BHandHLYP											
C1	140.7900	140.8037	141.6669	140.8704	141.6145	140.8560	141.7805	140.8602	141.8228	140.8539	141.8556	141.1171	141.1608	142.1665	141.2867	142.6574	141.2763	142.2570	141.2692	142.3474	141.2967	142.3026	**132.3**
C2	139.8520	139.5078	140.0370	139.2844	140.0285	139.2876	140.2157	139.3094	140.1387	139.2511	140.2632	138.4651	138.1194	138.6237	137.9139	138.4568	137.9263	138.8215	137.9414	138.7531	137.9020	138.8546	**129.3**
C3	137.6264	138.4636	139.1356	138.7861	139.5302	138.7578	139.6936	138.7477	139.6604	138.7826	139.7988	135.8460	136.5613	137.1206	136.8464	137.5469	136.8305	137.6018	136.8170	137.5868	136.8609	137.6939	**128.9**
C4	143.0358	144.9714	145.7407	145.8009	146.5450	145.7432	147.4860	145.7036	147.2467	145.8248	147.7143	141.1052	142.8817	143.4877	143.6434	144.2454	143.6011	145.1539	143.5602	144.9192	143.6829	145.3761	**135.2**
C5	136.0333	137.4978	138.2288	138.2151	138.9592	138.1625	139.2297	138.1282	139.1671	138.2349	139.3922	134.3312	135.6287	136.2583	136.2769	137.1461	136.2387	137.1451	136.2027	137.1023	136.3127	137.2901	**128.9**
C6	138.1993	139.8168	141.0135	140.6705	141.4146	140.6070	142.8049	140.5619	142.6034	140.7011	143.1192	136.5140	138.0273	139.0442	138.8189	140.3431	138.7721	140.8083	138.7275	140.6056	138.8625	141.1129	**129.3**
C7	212.8064	216.4928	217.9637	218.0078	218.7519	217.9138	223.7319	217.8367	222.6782	218.0660	224.4378	210.6877	214.6185	216.1623	216.2870	216.7511	216.1923	222.3118	216.0988	221.2162	216.3765	223.0179	**198.1**
C8	52.2103	52.7223	53.2241	52.9270	53.6711	52.9038	54.1728	52.8991	54.0206	52.9189	54.2992	54.0698	54.5440	55.0296	54.7668	55.3089	54.7532	55.9335	54.7420	55.8045	54.7796	56.0002	**51.9**
C9	23.7954	23.9568	23.9549	24.1768	24.9209	24.1497	23.9612	24.1415	23.9699	24.1728	23.9342	23.0867	23.1824	23.1563	23.3736	23.4862	23.3604	23.2341	23.3498	23.2281	23.3858	23.1797	**16.6**
H2	9.0253	8.9355	8.9432	8.8872	8.8060	8.8908	8.8801	8.8937	8.8889	8.8849	8.8820	8.9165	8.8237	8.8210	8.7720	8.7873	8.7754	8.7696	8.7787	8.7731	8.7687	8.7741	**7.89**
H3	7.8340	7.9670	8.0146	8.0164	7.9352	8.0146	8.0995	8.0119	8.0921	8.0191	8.1175	7.7948	7.9211	7.9658	7.9703	8.0338	7.9678	8.0496	7.9652	8.0413	7.9726	8.0666	**7.48**
H4	7.8857	8.0796	8.1330	8.1582	8.0770	8.1547	8.2729	8.1504	8.2572	8.1625	8.2959	7.8613	8.0490	8.1007	8.1275	8.1932	8.1233	8.2394	8.1190	8.2226	8.1314	8.2617	**7.67**
H5	7.7305	7.9054	7.9544	7.9827	7.9015	7.9791	8.0671	7.9747	8.0578	7.9871	8.0894	7.6891	7.8523	7.8959	7.9266	7.9952	7.9226	8.0051	7.9184	7.9950	7.9304	8.0261	**7.48**
H6	8.3497	8.5217	8.6360	8.6080	8.5268	8.6036	8.8077	8.5983	8.7937	8.6132	8.8476	8.1969	8.3722	8.4722	8.4571	8.6192	8.4525	8.6514	8.4476	8.6335	8.4615	8.6887	**7.89**
H8	4.2510	4.4387	4.5024	4.5240	4.4428	4.5201	4.6762	4.5153	4.6604	4.5287	4.6812	4.1446	4.3394	4.4111	4.4282	4.5318	4.4232	4.5868	4.4182	4.5698	4.4330	4.5958	**5.06**
H(9A-9C)	1.3172	1.3331	1.3256	1.3340	1.2527	1.3347	1.3551	1.3345	1.3499	1.3344	1.3694	1.2723	1.2766	1.2573	1.2738	1.2475	1.2743	1.2833	1.2746	1.2768	1.2732	1.2919	**1.46**

[a] methyl protons shifts are averaged

[b] according to [1]

Table S1. Cont. I

Nuclei	BLYP											BMK										Exp. [b]
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	140.0008	140.3683	141.3039	140.6035	142.0894	140.8626	141.8008	140.6593	142.0242	140.9858	141.9234	157.0784	157.0702	158.3945	157.2660	158.9781	157.2403	158.6759	157.4251	158.6446	157.4531	158.6634	**132.3**
C2	133.9448	133.6447	134.0766	133.4261	134.0154	133.7173	134.1921	133.5465	134.2950	133.7770	134.3021	151.4917	150.9931	151.6608	150.6842	151.5855	150.6859	151.8182	150.8993	151.6666	150.8441	151.7994	**129.3**
C3	133.9152	134.7866	135.3654	135.1017	135.9361	135.3628	135.9210	135.1615	136.0449	135.4807	136.0995	150.5844	151.3877	152.2060	151.6976	152.8034	151.6654	152.8665	151.8439	152.7272	151.8895	152.9296	**128.9**
C4	137.8141	139.6912	140.2799	140.4807	141.1420	140.7147	141.8197	140.4863	141.7704	140.8849	142.1274	155.2394	157.1059	157.9473	157.8918	158.8961	157.8320	159.7389	157.9830	159.3932	158.1095	159.9292	**135.2**
C5	132.6375	133.9841	134.6247	134.6206	135.6171	134.8614	135.5244	134.6403	135.6300	135.0184	135.7469	149.0282	150.4597	151.3652	151.1421	152.4616	151.0864	152.4024	151.2416	152.2617	151.3565	152.5332	**128.9**
C6	132.6868	134.1712	135.1418	134.9195	136.5241	135.1542	136.7155	134.9269	136.6950	135.3233	137.1029	149.9685	151.5472	152.6620	152.2428	154.1469	152.1815	154.5533	152.3316	154.2295	152.4625	154.7860	**129.3**
C7	214.5100	217.9083	219.5856	219.3667	220.3224	219.5574	224.8885	219.2853	224.2709	219.8129	225.6245	228.1863	232.2298	234.2164	233.9949	234.8284	233.8820	240.8416	233.9786	239.6087	234.2633	241.5538	**198.1**
C8	60.6156	61.2053	61.7518	61.3723	62.3232	61.6435	62.7931	61.4512	62.8592	61.7414	62.9468	63.2096	63.7660	64.2123	64.0095	64.5723	63.9803	65.2734	64.1620	64.9635	64.1995	65.2948	**51.9**
C9	24.4872	24.6944	24.6521	24.8814	25.1237	25.1480	24.8059	24.9529	24.9135	25.2553	24.8356	26.3023	26.3592	26.4049	26.5944	26.8249	26.5643	26.8104	26.7449	26.5908	26.7832	26.6566	**16.6**
H2	8.5158	8.4307	8.4298	8.3775	8.3831	8.4284	8.5412	8.3869	8.3753	8.4293	8.5613	9.0875	8.9952	8.9827	8.9475	8.9621	8.9469	8.9514	8.9464	8.9539	8.9385	8.9587	**7.89**
H3	7.5687	7.6870	7.7291	7.7299	7.7949	7.7749	7.9752	7.7275	7.8009	7.7873	8.0044	8.1001	8.2370	8.2860	8.2973	8.3648	8.2909	8.3847	8.2845	8.3761	8.2937	8.4017	**7.48**
H4	7.5692	7.7482	7.7946	7.8209	7.8839	7.8642	8.0893	7.8149	7.9084	7.8800	8.1232	8.1086	8.3007	8.3556	8.3882	8.4576	8.3803	8.5012	8.3723	8.4858	8.3861	8.5231	**7.67**
H5	7.4706	7.6184	7.6596	7.6830	7.7521	7.7268	7.9259	7.6779	7.7502	7.7418	7.9581	7.9923	8.1637	8.2143	8.2469	8.3232	8.2391	8.3246	8.2313	8.3180	8.2446	8.3496	**7.48**
H6	7.9240	8.0839	8.1763	8.1562	8.3012	8.1995	8.4960	8.1503	8.3144	8.2154	8.5461	8.5033	8.6774	8.7771	8.7609	8.9353	8.7525	8.9656	8.7440	8.9501	8.7593	8.9924	**7.89**
H8	4.4254	4.6097	4.6787	4.6930	4.7910	4.7353	5.0085	4.6852	4.8303	4.7530	5.0325	4.3182	4.4823	4.5714	4.5858	4.6946	4.5772	4.7413	4.5684	4.7248	4.5843	4.7419	**5.06**
H(9A-9C)	1.2563	1.2616	1.2535	1.2555	1.2444	1.3036	1.4520	1.2592	1.2795	1.3099	1.4757	1.2762	1.2947	1.2476	1.2943	1.2424	1.2912	1.2789	1.2881	1.2691	1.2877	1.2879	**1.46**
Nuclei	BP86											CAM-B3LYP											
C1	137.2123	137.7375	138.6925	137.9160	139.2776	137.9105	139.2400	137.9004	139.2466	137.9166	139.4585	142.5310	142.7350	143.7443	142.9133	144.3153	142.9034	144.0549	142.8946	144.0960	142.9250	144.1185	**132.3**
C2	132.5697	132.4233	132.8637	132.1798	132.7165	132.2026	133.0004	132.2205	132.9176	132.1534	133.1847	138.9249	138.6454	139.1151	138.4380	139.0090	138.4541	139.3610	138.4708	139.2770	138.4251	139.3951	**129.3**
C3	132.5824	133.6467	134.2352	133.9533	134.7484	133.9449	134.9143	133.9311	134.8451	133.9561	135.1788	137.2388	138.0368	138.5893	138.3191	139.0883	138.3072	139.1693	138.2957	139.1283	138.3323	139.2661	**128.9**
C4	136.4983	138.5341	139.1251	139.3003	139.9369	139.2658	140.7576	139.2253	140.5224	139.3277	141.1385	142.0050	143.8208	144.4098	144.5620	145.2380	144.5245	146.0548	144.4865	145.8266	144.5995	146.2719	**135.2**
C5	131.3428	132.8941	133.5383	133.5265	134.4773	133.4977	134.5597	133.4636	134.4730	133.5485	134.8656	135.8035	137.1812	137.8065	137.8273	138.7704	137.7931	138.7848	137.7590	138.7198	137.8616	138.9318	**128.9**
C6	131.2429	132.8146	133.7720	133.5283	135.0135	133.4938	135.3616	133.4538	135.1617	133.5557	135.8098	137.1487	138.6788	139.6785	139.4410	141.0372	139.3997	141.4276	139.3586	141.2255	139.4822	141.7265	**129.3**
C7	211.5059	214.8691	216.5117	216.1501	217.0579	216.0852	221.7054	216.0145	220.8962	216.2068	222.4997	215.0587	219.0132	220.6480	220.6603	221.3163	220.5702	226.6816	220.4798	225.6588	220.7474	227.4067	**198.1**
C8	58.7125	59.3741	59.9780	59.5452	60.2948	59.5419	61.0255	59.5336	60.8838	59.5437	61.2865	56.2265	56.8152	57.31600	57.0423	57.6401	57.0325	58.3340	57.0231	58.1853	57.0537	58.4162	**51.9**
C9	24.2157	24.5400	24.4392	24.7264	24.7771	24.7212	24.6223	24.7111	24.5453	24.7266	24.7498	23.6281	23.7215	23.6032	23.8957	23.9758	23.8868	23.6936	23.8785	23.6678	23.9066	23.6296	**16.6**
H2	8.5695	8.4885	8.4755	8.4399	8.4351	8.4438	8.4165	8.4474	8.4188	8.4357	8.4348	8.8348	8.7384	8.7323	8.6821	8.6980	8.6858	8.6717	8.6895	8.6772	8.6787	8.6750	**7.89**
H3	7.6104	7.7395	7.7761	7.7868	7.8455	7.7850	7.8572	7.7829	7.8487	7.7880	7.8881	7.7687	7.8920	7.9366	7.9384	8.0042	7.9360	8.0163	7.9337	8.0092	7.9406	8.0328	**7.48**
H4	7.6080	7.7961	7.8368	7.8719	7.9292	7.8685	7.9647	7.8647	7.9500	7.8747	8.0000	7.8136	7.9957	8.0466	8.0704	8.1377	8.0664	8.1762	8.0624	8.1619	8.0741	8.1976	**7.67**
H5	7.5096	7.6686	7.7040	7.7380	7.8011	7.7349	7.8051	7.7314	7.7954	7.7406	7.8390	7.6732	7.8322	7.8759	7.9031	7.9741	7.8992	7.9799	7.8953	7.9713	7.9067	8.0002	**7.48**
H6	8.0080	8.1658	8.2460	8.2372	8.3724	8.2340	8.3961	8.2304	8.3823	8.2399	8.4470	8.1724	8.3383	8.4361	8.4160	8.5796	8.4117	8.6008	8.4074	8.5864	8.4200	8.6367	**7.89**
H8	4.4728	4.6561	4.7089	4.7345	4.8187	4.7308	4.8656	4.7267	4.8549	4.7377	4.8889	4.2588	4.4530	4.5272	4.5386	4.6481	4.5337	4.6947	4.5290	4.6812	4.5431	4.7025	**5.06**
H(9A-9C)	1.2634	1.2703	1.2538	1.2664	1.2408	1.2676	1.2843	1.2686	1.2781	1.2649	1.3102	1.2887	1.2937	1.2782	1.2894	1.2699	1.2900	1.3053	1.2906	1.2999	1.2888	1.3141	**1.46**
Nuclei	HF											LC-BLYP											
C1	139.6607	139.6241	140.5073	139.7386	141.1358	139.7228	140.3960	139.7095	140.5014	139.7550	140.4472	146.4335	146.5179	147.6341	146.6803	148.0758	146.6491	147.8623	146.6450	147.9135	146.6925	147.9311	**132.3**
C2	139.7984	139.4288	139.9138	139.1784	139.7397	139.1944	140.1865	139.2106	140.0876	139.1628	140.2275	144.7320	144.3466	144.9226	144.1597	144.7668	144.1492	145.1320	144.1664	145.0434	144.1523	145.1667	**129.3**
C3	134.4250	134.9332	135.3717	135.1214	135.7122	135.1101	135.6168	135.0993	135.6227	135.1320	135.6838	142.1299	142.8151	143.4593	143.1146	143.8898	143.0766	143.9553	143.0658	143.9162	143.1331	144.0489	**128.9**
C4	141.5127	143.1664	143.7409	143.8266	144.3848	143.7923	145.4481	143.7575	145.1784	143.8574	145.6624	147.6194	149.3801	150.0864	150.1640	150.9007	150.0982	151.7095	150.0594	151.4692	150.2086	151.9257	**135.2**
C5	132.7479	133.8752	134.3900	134.4341	135.2114	134.4006	135.0696	134.3675	135.0473	134.4654	135.1978	140.5883	141.9218	142.6663	142.6176	143.6025	142.5552	143.5941	142.5199	143.5281	142.6593	143.7354	**128.9**
C6	137.3230	138.8285	139.8520	139.5756	141.0917	139.5349	141.6945	139.4938	141.4667	139.6122	141.9954	142.6364	144.1986	145.2422	145.0634	146.6612	144.9903	147.0472	144.9440	146.8187	145.1157	147.3843	**129.3**
C7	204.0791	208.4010	209.7219	210.2412	210.3651	210.1321	216.6742	210.0239	215.3200	210.3447	217.4306	220.5659	224.7425	226.5075	226.5077	227.0605	226.3879	232.8670	226.2944	231.7605	226.6021	233.6017	**198.1**
C8	49.2972	49.7513	50.10233	49.9877	50.4171	49.9708	50.9385	49.9550	50.7898	50.0040	50.9852	54.1861	54.8077	55.3009	55.1233	55.5711	55.0839	56.3632	55.0716	56.1971	55.1429	56.4986	**51.9**
C9	21.2779	21.2889	21.3256	21.4018	21.6008	21.3951	21.3176	21.3886	21.3283	21.4073	21.2542	23.0604	23.0011	22.8780	23.1812	23.2319	23.1468	22.8636	23.1401	22.8449	23.1968	22.8209	**16.6**
H2	9.0113	8.9084	8.9225	8.8476	8.8805	8.8521	8.8727	8.8562	8.8780	8.8433	8.8776	9.0197	8.9088	8.9008	8.8536	8.8714	8.8559	8.8279	8.8598	8.8344	8.8505	8.8307	**7.89**
H3	7.7722	7.9034	7.9510	7.9542	8.0226	7.9515	8.0327	7.9485	8.0256	7.9568	8.0503	7.8991	8.0182	8.0640	8.0644	8.1298	8.0611	8.1404	8.0592	8.1338	8.0666	8.1584	**7.48**
H4	7.9257	8.1238	8.1821	8.2047	8.2795	8.2003	8.3311	8.1957	8.3131	8.2088	8.3554	7.9699	8.1484	8.2018	8.2225	8.2920	8.2175	8.3290	8.2141	8.3149	8.2262	8.3519	**7.67**
H5	7.6612	7.8325	7.8798	7.9100	7.9832	7.9056	7.9890	7.9010	7.9801	7.9141	8.0111	7.8118	7.9715	8.0163	8.0447	8.1154	8.0397	8.1198	8.0362	8.1112	8.0485	8.1422	**7.48**
H6	8.1910	8.3879	8.5069	8.4811	8.6641	8.4762	8.7054	8.4708	8.6863	8.4858	8.7438	8.3497	8.5153	8.6125	8.5986	8.7648	8.5928	8.7774	8.5886	8.7621	8.6031	8.8160	**7.89**
H8	3.7932	3.9963	4.0749	4.0889	4.2068	4.0837	4.2644	4.0782	4.2449	4.0940	4.2755	4.2365	4.4266	4.5107	4.5102	4.6300	4.5045	4.6671	4.5005	4.6545	4.5144	4.6714	**5.06**
H(9A-9C)	1.2245	1.2212	1.2012	1.2143	1.1835	1.2151	1.2120	1.2156	1.2084	1.2135	1.2179	1.3196	1.3261	1.3013	1.3288	1.2974	1.3278	1.3291	1.3283	1.3226	1.3288	1.3428	**1.46**
Nuclei	M06											M06-2X											
C1	137.2959	137.3554	138.4171	137.4923	138.9580	137.4704	138.5981	137.4571	138.6818	137.5283	138.6701	155.6275	155.9009	156.9075	156.0514	157.4126	156.0648	157.2600	156.0794	157.3208	156.0318	157.3499	**132.3**
C2	136.5335	136.2154	136.8128	136.0226	136.7106	136.0245	137.0622	136.0341	136.9781	136.0356	137.1015	151.4273	151.0547	151.6292	150.7995	151.4974	150.8357	151.8029	150.8733	151.7298	150.7588	151.8539	**129.3**
C3	135.1423	135.9375	136.6414	136.2724	137.1957	136.2436	137.2891	136.2225	137.2479	136.3141	137.3932	151.0502	151.9890	152.7074	152.3393	153.3074	152.3410	153.4136	152.3437	153.3577	152.3311	153.5464	**128.9**
C4	140.0619	141.9249	142.6688	142.7534	143.5556	142.6967	144.4568	142.6470	144.2048	142.8215	144.6728	155.3691	157.4042	158.1928	158.2595	159.1718	158.2320	160.0440	158.2051	159.7819	158.2788	160.3034	**135.2**
C5	133.7830	135.1241	135.8828	135.8084	136.8851	135.7578	136.9213	135.7148	136.8526	135.8708	137.0784	149.2161	150.8315	151.6534	151.6083	152.7942	151.5836	152.8538	151.5599	152.7641	151.6253	153.0395	**128.9**
C6	134.9534	136.3969	137.5431	137.1869	138.8668	137.1302	139.3202	137.0809	139.1081	137.2551	139.5808	149.9291	151.6010	152.7472	152.4542	154.2425	152.4233	154.6584	152.3935	154.4281	152.4772	155.0182	**129.3**
C7	211.8406	215.2956	216.9132	216.7621	217.4900	216.6671	222.4224	216.5795	221.4975	216.8664	223.0986	229.7447	233.9967	235.6542	235.7261	236.2097	235.6524	242.3668	235.5784	241.1884	235.7887	243.2011	**198.1**
C8	52.8747	53.2467	53.8660	53.4339	54.1741	53.4124	54.7537	53.3989	54.6422	53.4689	54.8089	58.7148	59.4172	59.8416	59.6916	60.2084	59.6971	60.8882	59.7036	60.7442	59.6800	61.0113	**51.9**
C9	23.0447	23.1511	23.2516	23.3616	23.6421	23.3374	23.3825	23.3212	23.3548	23.3994	23.2646	23.9249	24.1047	24.1395	24.2659	24.4907	24.2748	24.2687	24.2853	24.2333	24.2513	24.2742	**16.6**
H2	8.7512	8.6609	8.6715	8.6034	8.6311	8.6070	8.6197	8.6111	8.6229	8.6006	8.6211	9.2802	9.1886	9.1985	9.1464	9.1715	9.1474	9.1485	9.1482	9.1502	9.1456	9.1507	**7.89**
H3	7.7290	7.8605	7.9182	7.9091	7.9847	7.9062	8.0087	7.9039	7.9997	7.9124	8.0239	8.3146	8.4542	8.5107	8.5107	8.5830	8.5064	8.6077	8.5018	8.5990	8.5149	8.6241	**7.48**
H4	7.7271	7.9142	7.9722	7.9893	8.0638	7.9849	8.1078	7.9811	8.0923	7.9940	8.1271	8.3275	8.5115	8.5712	8.5902	8.6676	8.5846	8.7022	8.5786	8.6880	8.5957	8.7226	**7.67**
H5	7.6099	7.7613	7.8077	7.8258	7.9064	7.8220	7.9111	7.8188	7.9019	7.8299	7.9330	8.2207	8.3887	8.4443	8.4680	8.5505	8.4621	8.5574	8.4560	8.5479	8.4736	8.5777	**7.48**
H6	8.2120	8.3595	8.4583	8.4280	8.5875	8.4239	8.6102	8.4204	8.5960	8.4325	8.6377	8.7846	8.9450	9.0544	9.0307	9.2019	9.0243	9.2249	9.0175	9.2078	9.0369	9.2584	**7.89**
H8	4.3173	4.4907	4.5604	4.5643	4.6615	4.5597	4.7141	4.5558	4.7015	4.5691	4.7190	4.3313	4.4998	4.5882	4.5830	4.6998	4.5770	4.7401	4.5707	4.7269	4.5887	4.7387	**5.06**
H(9A-9C)	1.2282	1.2336	1.2288	1.2254	1.2159	1.2260	1.2527	1.2271	1.2472	1.2254	1.2588	1.3024	1.3171	1.2932	1.3225	1.2915	1.3209	1.3196	1.3189	1.3130	1.3241	1.3313	**1.46**

[a] methyl protons shifts are averaged.
[b] according to [1]

Table S1. Cont. II

Nuclei	mpW1LYP											mpW1PW91										Exp. [b]
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	141.0342	141.2018	142.2062	141.3909	142.7682	141.3738	142.5034	141.3586	142.5431	141.4060	142.5316	138.6123	138.9367	139.9004	139.1359	140.4726	139.1208	140.2891	139.1120	140.3310	139.1501	140.3635	**132.3**
C2	136.5712	136.2480	136.7437	136.0646	136.5628	136.0727	136.9360	136.0825	136.8566	136.0552	136.9356	135.5123	135.2465	135.7476	135.0433	135.6626	135.0551	135.9587	135.0729	135.8806	135.0313	135.9935	**129.3**
C3	135.2922	136.0945	136.6809	136.4259	137.1313	136.4047	137.2405	136.3849	137.2017	136.4441	137.3054	134.1948	135.0691	135.6794	135.3887	136.2267	135.3706	136.3463	135.3583	136.2928	135.4048	136.4542	**128.9**
C4	139.8121	141.6490	142.2651	142.4565	143.0279	142.4082	143.9036	142.3612	143.6753	142.4996	144.0935	138.6609	140.5055	141.1447	141.2669	141.9961	141.2241	142.8310	141.1865	142.5896	141.3062	143.0524	**135.2**
C5	133.8731	135.2167	135.8655	135.8953	136.7635	135.8526	136.8064	135.8113	136.7455	135.9336	136.9199	132.8276	134.2451	134.9216	134.9075	135.9091	134.8686	135.9608	134.8349	135.8839	134.9436	136.1148	**128.9**
C6	135.0215	136.5242	137.5638	137.3309	138.8439	137.2802	139.2725	137.2308	139.0769	137.3769	139.5398	133.7434	135.2291	136.2642	135.9808	137.5791	135.9363	137.9612	135.8972	137.7571	136.0221	138.2449	**129.3**
C7	212.7896	216.5521	218.2073	218.1660	218.8608	218.0707	224.0122	217.9763	223.0407	218.2542	224.6910	210.5451	214.1999	215.7470	215.7025	216.3588	215.6163	221.4381	215.5352	220.4681	215.7832	222.1179	**198.1**
C8	57.2880	57.7809	58.3419	58.0122	58.6472	57.9945	59.2999	57.9784	59.1614	58.0273	59.3411	55.3732	55.9792	56.5080	56.2213	56.8479	56.2066	57.5282	56.1975	57.3885	56.2346	57.6104	**51.9**
C9	23.9827	24.1263	24.0870	24.3578	24.4178	24.3393	24.2158	24.3223	24.1785	24.3737	24.1241	23.2444	23.4084	23.3817	23.6004	23.7479	23.5872	23.5654	23.5798	23.5213	23.6123	23.5222	**16.6**
H2	8.7489	8.6605	8.6613	8.6118	8.6199	8.6152	8.6059	8.6182	8.6110	8.6085	8.6078	8.8014	8.7046	8.7044	8.6495	8.6693	8.6532	8.6457	8.6570	8.6489	8.6462	8.6493	**7.89**
H3	7.7005	7.8243	7.8712	7.8742	7.9367	7.8718	7.9499	7.8690	7.9431	7.8764	7.9641	7.7652	7.8956	7.9431	7.9436	8.0138	7.9412	8.0281	7.9390	8.0201	7.9460	8.0459	**7.48**
H4	7.7326	7.9164	7.9688	7.9953	8.0581	7.9912	8.0985	7.9867	8.0844	7.9991	8.1177	7.7958	7.9838	8.0363	8.0592	8.1297	8.0553	8.1694	8.0514	8.1544	8.0631	8.1917	**7.67**
H5	7.5990	7.7542	7.7998	7.8269	7.8940	7.8230	7.9012	7.8187	7.8931	7.8304	7.9189	7.6621	7.8243	7.8714	7.8954	7.9713	7.8916	7.9784	7.8879	7.9690	7.8992	7.9993	**7.48**
H6	8.0848	8.2546	8.3549	8.3372	8.4915	8.3327	8.5200	8.3279	8.5061	8.3413	8.5539	8.1779	8.3413	8.4388	8.4164	8.5768	8.4124	8.6011	8.4085	8.5856	8.4204	8.6376	**7.89**
H8	4.2822	4.4764	4.5504	4.5671	4.6677	4.5621	4.7195	4.5567	4.7067	4.5717	4.7267	4.3100	4.4975	4.5629	4.5772	4.6769	4.5728	4.7245	4.5686	4.7105	4.5816	4.7329	**5.06**
H(9A-9C)	1.2707	1.2763	1.2671	1.2756	1.2551	1.2760	1.2935	1.2762	1.2889	1.2750	1.3001	1.2444	1.2499	1.2376	1.2455	1.2266	1.2462	1.2646	1.2470	1.2588	1.2450	1.2740	**1.46**
Nuclei	O3LYP											OLYP										
C1	135.1298	135.7941	136.8990	137.1851	138.6909	137.1408	138.8350	137.0946	139.0824	137.2250	139.0466	133.4154	135.1976	136.3781	136.5446	138.2528	136.4952	138.1930	136.4354	138.2937	136.5787	138.3629	**132.3**
C2	130.8375	130.5900	131.1366	130.5372	131.1953	130.5526	131.4195	130.5629	131.3300	130.5165	131.4237	128.3780	128.2293	128.8305	128.2004	128.8119	128.2119	128.9986	128.2176	128.9409	128.1803	129.0023	**129.3**
C3	130.1313	130.9364	131.5863	131.3459	132.1467	131.3330	132.2784	131.3149	132.2405	131.3521	132.3755	128.3085	129.1167	129.8028	129.5149	130.3482	129.5013	130.4791	129.4822	130.4315	129.5185	130.5601	**128.9**
C4	133.9955	135.6723	136.3030	136.2758	136.8721	136.2491	137.5391	136.2163	137.2948	136.2933	137.7039	131.7901	133.2935	133.9159	133.8829	134.4648	133.8558	135.1522	133.8236	134.9464	133.9000	135.3058	**135.2**
C5	128.8432	130.1185	130.8263	130.7387	131.6875	130.7109	131.7084	130.6778	131.6267	130.7582	131.8354	127.0665	128.2306	128.9497	128.8078	129.7167	128.7811	129.7754	128.7491	129.6966	128.8243	129.8930	**128.9**
C6	129.1493	130.5079	131.5112	130.9596	132.3989	130.9294	132.5915	130.8934	132.3475	130.9799	132.7887	126.8794	127.9107	128.8769	128.4412	129.7331	128.4102	129.9626	128.3755	129.7905	128.4624	130.1804	**129.3**
C7	206.1988	209.8236	211.4728	212.3073	213.0453	212.2010	218.0244	212.0922	217.3854	212.4047	218.7989	205.1073	209.3827	211.0521	211.7448	212.8612	211.6346	217.4570	211.5141	216.7439	211.8364	218.1218	**198.1**
C8	55.6096	56.2735	56.9423	56.9217	57.7363	56.8940	58.5171	56.8626	58.4216	56.9433	58.5731	56.3992	57.3951	58.2424	57.9871	58.5470	57.9641	59.2467	57.9346	59.1116	57.9993	59.3518	**51.9**
C9	22.6084	22.7550	22.8398	22.8855	23.0696	22.8803	22.9350	22.8699	22.8634	22.8836	22.8281	22.5893	22.6735	22.8199	22.8846	22.9567	22.8769	22.8869	22.8639	22.8335	22.8833	22.8002	**16.6**
H2	8.6475	8.5299	8.5250	8.3790	8.3915	8.3855	8.3516	8.3914	8.3309	8.3723	8.3440	8.5235	8.3157	8.3131	8.1774	8.1714	8.1835	8.1623	8.1900	8.1533	8.1715	8.1599	**7.89**
H3	7.7140	7.8322	7.8804	7.8784	7.9446	7.8762	7.9571	7.8737	7.9496	7.8803	7.9739	7.6611	7.7706	7.8193	7.8125	7.8790	7.8104	7.8925	7.8082	7.8851	7.8141	7.9075	**7.48**
H4	7.7270	7.9014	7.9531	7.9744	8.0369	7.9708	8.0711	7.9669	8.0575	7.9775	8.0923	7.6575	7.8248	7.8747	7.8914	7.9546	7.8880	7.9890	7.8844	7.9760	7.8942	8.0082	**7.67**
H5	7.6096	7.7574	7.8045	7.8197	7.8889	7.8164	7.8933	7.8126	7.8837	7.8228	7.9119	7.5557	7.6892	7.7360	7.7479	7.8167	7.7447	7.8243	7.7413	7.8157	7.7506	7.8413	**7.48**
H6	8.0423	8.1961	8.2875	8.2302	8.3668	8.2276	8.3710	8.2244	8.3499	8.2326	8.3991	7.9638	8.0720	8.1513	8.1099	8.2480	8.1071	8.2606	8.1044	8.2453	8.1123	8.2874	**7.89**
H8	4.3630	4.5397	4.6063	4.6154	4.6998	4.6123	4.7315	4.6087	4.7191	4.6182	4.7418	4.4310	4.5931	4.6442	4.6469	4.7477	4.6440	4.7809	4.6410	4.7660	4.6494	4.7914	**5.06**
H(9A-9C)	1.2058	1.2073	1.1967	1.1763	1.1583	1.1771	1.1871	1.1775	1.1742	1.1753	1.1854	1.1958	1.1699	1.1710	1.1489	1.1194	1.1497	1.1570	1.1505	1.1491	1.1478	1.1552	**1.46**
Nuclei	OPBE											OPW91										
C1	131.0265	133.0024	133.8530	134.0591	135.4874	134.0341	135.6518	133.9909	135.9319	134.0778	135.8999	131.2953	133.2412	134.1193	134.3212	135.7114	134.2861	135.8983	134.2333	136.1872	134.3361	136.1512	**132.3**
C2	127.0529	126.9788	127.5161	126.8443	127.5003	126.8685	127.6077	126.8747	127.5473	126.8167	127.6398	127.2720	127.1969	127.7305	127.0667	127.7100	127.0810	127.8212	127.0781	127.7622	127.0353	127.8551	**129.3**
C3	126.8965	127.8196	128.4631	128.1500	129.0240	128.1470	129.1639	128.1262	129.1127	128.1478	129.2854	127.0924	128.0159	128.6528	128.3507	129.2093	128.3378	129.3493	128.3078	129.2998	128.3446	129.4724	**128.9**
C4	130.3007	131.8372	132.4563	132.3525	133.0338	132.3356	133.6349	132.3008	133.3981	132.3632	133.8132	130.5086	132.0576	132.6642	132.5769	133.2485	132.5497	133.8486	132.5055	133.6127	132.5837	134.0287	**135.2**
C5	125.6936	126.9653	127.6571	127.4894	128.4656	127.4728	128.5115	127.4382	128.4104	127.4999	128.6611	125.8887	127.1645	127.8475	127.6918	128.6562	127.6650	128.6995	127.6215	128.5989	127.6984	128.8503	**128.9**
C6	125.2037	126.2920	127.2454	126.7787	128.1479	126.7584	128.3078	126.7200	128.0816	126.7932	128.5328	125.4325	126.5316	127.4728	127.0197	128.3837	126.9891	128.5412	126.9418	128.3114	127.0305	128.7673	**129.3**
C7	202.6468	206.9020	208.2465	208.9005	209.7081	208.8190	214.3683	208.7189	213.8875	208.9722	215.0932	202.9971	207.2491	208.6136	209.2756	210.0457	209.1835	214.7402	209.0731	214.2731	209.3437	215.4739	**198.1**
C8	54.3177	55.4974	56.0919	56.0480	56.5343	56.0424	57.3986	56.0186	57.2414	56.0484	57.5269	54.4940	55.6567	56.2715	56.2202	56.6862	56.2046	57.5646	56.1715	57.3905	56.2167	57.6928	**51.9**
C9	21.6593	21.8576	21.9356	22.0012	22.1197	22.0047	22.0287	21.9905	21.9367	21.9932	21.9700	21.7269	21.9284	22.0045	22.0764	22.1894	22.0697	22.0997	22.0464	22.0035	22.0645	22.0418	**16.6**
H2	8.5335	8.3176	8.3344	8.2006	8.2179	8.2058	8.1899	8.2104	8.1645	8.1949	8.1858	8.5364	8.3232	8.3369	8.2046	8.2234	8.2092	8.1931	8.2136	8.1669	8.1986	8.1884	**7.89**
H3	7.7195	7.8371	7.8841	7.8799	7.9484	7.8780	7.9614	7.8754	7.9526	7.8810	7.9794	7.7185	7.8358	7.8825	7.8791	7.9465	7.8766	7.9595	7.8738	7.9507	7.8798	7.9774	**7.48**
H4	7.7162	7.8884	7.9355	7.9538	8.0186	7.9507	8.0505	7.9468	8.0367	7.9560	8.0725	7.7159	7.8881	7.9349	7.9541	8.0179	7.9502	8.0499	7.9462	8.0360	7.9559	8.0717	**7.67**
H5	7.6107	7.7520	7.7984	7.8115	7.8833	7.8084	7.8878	7.8046	7.8779	7.8136	7.9071	7.6102	7.7516	7.7974	7.8115	7.8825	7.8077	7.8868	7.8037	7.8769	7.8132	7.9060	**7.48**
H6	8.0215	8.1222	8.2076	8.1606	8.3055	8.1578	8.3056	8.1543	8.2863	8.1625	8.3345	8.0213	8.1237	8.2072	8.1620	8.3067	8.1586	8.3060	8.1549	8.2870	8.1636	8.3347	**7.89**
H8	4.4592	4.6036	4.6495	4.6504	4.7507	4.6477	4.7755	4.6443	4.7631	4.6522	4.7884	4.4564	4.6030	4.6478	4.6505	4.7502	4.6471	4.7746	4.6435	4.7625	4.6520	4.7873	**5.06**
H(9A-9C)	1.1460	1.1223	1.1210	1.1055	1.0744	1.1069	1.1117	1.1074	1.0961	1.1037	1.1103	1.1488	1.1255	1.1239	1.1090	1.0778	1.1096	1.1147	1.1099	1.0985	1.1069	1.1131	**1.46**
Nuclei	PBE											PBE0										
C1	136.7513	137.2600	138.3042	137.4553	138.9532	137.4372	138.9785	137.4302	138.9681	137.4910	139.0764	138.2012	138.5127	139.5094	138.6963	140.0322	138.6779	139.9544	138.6618	139.9361	138.7170	139.9691	**132.3**
C2	132.5052	132.3390	132.8232	132.0845	132.7741	132.0967	133.0604	132.1196	132.9792	132.0911	133.1068	135.2288	134.9792	135.4801	134.7726	135.3757	134.7796	135.7523	134.7887	135.6181	134.7692	135.7329	**129.3**
C3	132.6372	133.6617	134.2990	133.9470	134.9104	133.9283	135.0679	133.9204	135.0016	133.9819	135.1931	134.0341	134.9259	135.5415	135.2413	136.0740	135.2185	136.2738	135.1973	136.1631	135.2659	136.3262	**128.9**
C4	136.5241	138.5195	139.1607	139.2613	140.0826	139.2167	140.8704	139.1824	140.6447	139.3206	141.1075	138.4771	140.3412	140.9834	141.1017	141.8289	141.0536	142.7285	141.0069	142.4336	141.1498	142.8949	**135.2**
C5	131.3872	132.9060	133.5967	133.5206	134.6386	133.4815	134.7143	133.4528	134.6301	133.5751	134.8802	132.6595	134.0946	134.7788	134.7574	135.7539	134.7131	135.8862	134.6704	135.7518	134.8024	135.9842	**128.9**
C6	131.2741	132.8032	133.8222	133.4888	135.1651	133.4447	135.4864	133.4110	135.2973	133.5482	135.7907	133.5401	135.0434	136.0586	135.7906	137.3685	135.7407	137.8195	135.6927	137.5601	135.8404	138.0490	**129.3**
C7	211.6949	214.9651	216.7136	216.2158	217.3470	216.1408	221.8839	216.0762	221.0911	216.3045	222.5420	210.2895	213.8793	215.4720	215.3444	216.0413	215.2559	221.1317	215.1685	220.1251	215.4304	221.7474	**198.1**
C8	58.1047	58.7464	59.4234	58.9045	59.7953	58.8904	60.5456	58.8873	60.3982	58.9359	60.6861	55.1079	55.7049	56.2148	55.9298	56.5205	55.9112	57.2875	55.8943	57.0906	55.9503	57.3145	**51.9**
C9	24.1834	24.4833	24.4146	24.6524	24.8524	24.6368	24.6942	24.6323	24.6253	24.6852	24.6857	23.2759	23.4659	23.4095	23.6560	23.7694	23.6375	23.6511	23.6211	23.5509	23.6767	23.5581	**16.6**
H2	8.5961	8.5158	8.5082	8.4631	8.4710	8.4666	8.4492	8.4706	8.4531	8.4605	8.4521	8.7988	8.7070	8.7031	8.6539	8.6690	8.6571	8.6484	8.6603	8.6491	8.6505	8.6496	**7.89**
H3	7.6377	7.7646	7.8111	7.8084	7.8799	7.8062	7.8916	7.8043	7.8840	7.8112	7.9086	7.7628	7.8923	7.9398	7.9398	8.0089	7.9372	8.0271	7.9345	8.0164	7.9419	8.0419	**7.48**
H4	7.6318	7.8172	7.8683	7.8895	7.9601	7.8856	7.9947	7.8821	7.9811	7.8939	8.0159	7.7895	7.9765	8.0297	8.0517	8.1214	8.0474	8.1645	8.0431	8.1471	8.0553	8.1839	**7.67**
H5	7.5411	7.6979	7.7432	7.7638	7.8399	7.7601	7.8440	7.7569	7.8353	7.7679	7.8634	7.6611	7.8246	7.8717	7.8961	7.9707	7.8920	7.9820	7.8878	7.9699	7.8996	8.0001	**7.48**
H6	8.0408	8.1972	8.2882	8.2644	8.4162	8.2607	8.4379	8.2575	8.4255	8.2686	8.4745	8.1829	8.3447	8.4401	8.4192	8.5776	8.4149	8.6050	8.4105	8.5869	8.4229	8.6391	**7.89**
H8	4.4695	4.6530	4.7200	4.7291	4.8300	4.7248	4.8763	4.7209	4.8663	4.7338	4.8854	4.3100	4.4948	4.5634	4.5735	4.6745	4.5689	4.7259	4.5642	4.7097	4.5775	4.7308	**5.06**
H(9A-9C)	1.2601	1.2686	1.2634	1.2624	1.2513	1.2631	1.2953	1.2642	1.2897	1.2625	1.3078	1.2475	1.2543	1.2384	1.2501	1.2269	1.2505	1.2691	1.2508	1.2605	1.2495	1.2761	**1.46**

[a] methyl protons shifts are averaged.

[b] according to [1]

Table S1. Cont. III

Nuclei	TPSS											VSXC											Exp. [b]
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	133.8442	134.0013	135.0500	134.1846	135.5449	134.1779	135.4490	134.1829	135.2870	134.2018	135.4839	131.8630	131.8201	132.5994	131.8494	133.0134	131.8494	132.5912	131.8476	132.6286	131.8510	132.6464	**132.3**
C2	129.7258	129.4226	129.9822	129.2635	129.8220	129.2795	130.1188	129.3068	130.4474	129.2592	130.1285	128.2191	127.9849	128.4680	127.8363	128.3483	127.8481	128.6974	127.8579	128.6064	127.8268	128.7563	**129.3**
C3	129.0139	129.8376	130.5298	130.1956	131.0042	130.1821	131.1596	130.1799	131.3140	130.2187	131.2465	127.6097	128.5474	129.1598	128.9497	129.7362	128.9297	129.8926	128.9073	129.8152	128.9699	130.0119	**128.9**
C4	133.1384	134.9400	135.6481	135.7572	136.4277	135.7174	137.2675	135.6885	136.7813	135.8050	137.4731	131.6101	133.6166	134.2496	134.5120	135.1815	134.4637	136.0626	134.4128	135.8257	134.5589	136.3174	**135.2**
C5	127.8274	129.1132	129.8553	129.7810	130.7328	129.7481	130.8124	129.7262	130.8637	129.8226	130.9365	126.2933	127.6959	128.3507	128.4083	129.3093	128.3687	129.4309	128.3266	129.3303	128.4474	129.5846	**128.9**
C6	128.3912	129.7722	130.8179	130.5395	132.0240	130.4999	132.4127	130.4715	131.6034	130.5875	132.6809	128.2563	129.7579	130.6719	130.5283	131.9028	130.4849	132.2921	130.4394	132.1502	130.5710	132.6015	**129.3**
C7	206.9645	209.9849	211.6685	211.2862	212.1700	211.2187	216.7444	211.1615	211.6882	211.3603	217.3713	201.6393	204.3358	205.5812	205.4655	206.0483	205.4042	209.9511	205.3399	209.1835	205.5248	210.5908	**198.1**
C8	57.7397	58.1997	58.8346	58.4262	59.1327	58.4186	59.8509	58.4224	60.0947	58.4442	59.9257	61.1191	61.5554	61.9503	61.7409	62.3010	61.7330	62.5766	61.7230	62.5028	61.7500	62.6167	**51.9**
C9	24.4235	24.6244	24.6726	24.8798	25.0225	24.8686	24.9032	24.8692	26.7931	24.9012	24.8649	29.6427	30.3368	30.6408	30.7648	31.0815	30.7403	31.4702	30.7138	31.2833	30.7897	31.5540	**16.6**
H2	8.5827	8.5037	8.5081	8.4600	8.4712	8.4628	8.4482	8.4662	8.5759	8.4577	8.4476	8.6673	8.5980	8.5978	8.5599	8.5645	8.5623	8.5696	8.5648	8.5792	8.5576	8.5937	**7.89**
H3	7.5564	7.6830	7.7356	7.7341	7.8063	7.7314	7.8188	7.7293	7.8445	7.7370	7.8327	7.6100	7.7387	7.7798	7.7870	7.8500	7.7845	7.8657	7.7820	7.8605	7.7893	7.8910	**7.48**
H4	7.5750	7.7603	7.8180	7.8403	7.9119	7.8359	7.9501	7.8321	7.9466	7.8448	7.9686	7.6333	7.8181	7.8627	7.8943	7.9549	7.8901	7.9975	7.8860	7.9845	7.8982	8.0266	**7.67**
H5	7.4652	7.6220	7.6733	7.6951	7.7710	7.6910	7.7759	7.6875	7.8031	7.6993	7.7916	7.5455	7.7080	7.7530	7.7799	7.8482	7.7759	7.8668	7.7719	7.8576	7.7837	7.8942	**7.48**
H6	7.9314	8.0967	8.1960	8.1773	8.3328	8.1727	8.3612	8.1687	8.2807	8.1819	8.3967	8.1437	8.2938	8.3904	8.3715	8.5062	8.3668	8.5790	8.3623	8.5555	8.3759	8.6251	**7.89**
H8	4.3217	4.5075	4.5827	4.5961	4.7010	4.5910	4.7496	4.5865	4.7253	4.6012	4.7564	4.3672	4.5380	4.5649	4.6109	4.6585	4.6069	4.7531	4.6030	4.7434	4.6146	4.8027	**5.06**
H(9A-9C)	1.2656	1.2748	1.2692	1.2756	1.2597	1.2759	1.3039	1.2766	1.4402	1.2758	1.3120	1.4571	1.4976	1.4877	1.5067	1.4874	1.5064	1.5441	1.5062	1.5359	1.5070	1.5702	**1.46**
Nuclei	wB97											wB97X											
C1	138.9705	139.0197	140.0068	139.1625	140.4868	139.1535	140.1516	139.1436	140.2312	139.1714	140.2229	140.2155	140.3084	141.3213	140.4667	141.8248	140.4591	141.5429	140.4506	141.5522	140.4748	141.5816	**132.3**
C2	136.6575	136.2946	136.8147	136.0943	136.7084	136.1044	136.9927	136.1139	136.9108	136.0853	137.0272	137.2285	136.9071	137.4167	136.7108	137.3120	136.7236	137.6435	136.7355	137.5011	136.7000	137.6605	**129.3**
C3	134.5888	135.2845	135.8971	135.5728	136.3757	135.5553	136.4057	135.5371	136.3680	135.5895	136.4973	135.3963	136.1180	136.7238	136.4125	137.2120	136.3974	137.2926	136.3814	137.1922	136.4277	137.3720	**128.9**
C4	139.4400	141.1178	141.7949	141.8441	142.6123	141.8013	143.3418	141.7574	143.1161	141.8847	143.5445	140.0391	141.7475	142.4062	142.4828	143.2269	142.4422	144.0152	142.4003	143.7276	142.5223	144.2101	**135.2**
C5	133.1924	134.4554	135.1411	135.1011	136.0762	135.0613	136.0438	135.0208	135.9804	135.1389	136.1835	133.9880	135.2740	135.9624	135.9272	136.9054	135.8897	136.9280	135.8512	136.8025	135.9638	137.0543	**128.9**
C6	134.9408	136.3657	137.3591	137.1218	138.6749	137.0741	139.0346	137.0258	138.8231	137.1675	139.3267	135.4709	136.9142	137.8818	137.6807	139.2069	137.6354	139.6104	137.5894	139.3375	137.7249	139.8960	**129.3**
C7	209.7234	213.4973	215.0558	215.1119	215.5978	215.0217	220.8345	214.9294	219.8564	215.1965	221.5673	211.5808	215.3541	216.9529	216.9591	217.5146	216.8716	222.8061	216.7816	221.7555	217.0417	223.4911	**198.1**
C8	54.1575	54.7096	55.1072	54.9796	55.3878	54.9629	56.0014	54.9454	55.8774	54.9958	56.0883	55.0869	55.6353	56.0384	55.9282	56.3257	55.9134	57.0159	55.8973	56.8122	55.9432	57.1003	**51.9**
C9	23.0304	23.0822	23.0706	23.2375	23.4247	23.2247	23.1200	23.2115	23.0955	23.2504	23.0824	23.2890	23.3915	23.3054	23.5633	23.6703	23.5527	23.4270	23.5413	23.3322	23.5749	23.3699	**16.6**
H2	8.8754	8.7780	8.7788	8.7239	8.7523	8.7268	8.7205	8.7296	8.7227	8.7214	8.7220	8.8561	8.7629	8.7593	8.7093	8.7318	8.7124	8.7030	8.7155	8.7036	8.7066	8.7042	**7.89**
H3	7.8286	7.9509	7.9985	7.9956	8.0683	7.9931	8.0773	7.9905	8.0702	7.9980	8.0945	7.8057	7.9299	7.9757	7.9765	8.0468	7.9741	8.0584	7.9717	8.0484	7.9788	8.0736	**7.48**
H4	7.8892	8.0683	8.1232	8.1395	8.2158	8.1355	8.2505	8.1314	8.2363	8.1433	8.2724	7.8598	8.0416	8.0947	8.1150	8.1885	8.1111	8.2255	8.1071	8.2086	8.1188	8.2454	**7.67**
H5	7.7387	7.9005	7.9484	7.9711	8.0490	7.9670	8.0543	7.9627	8.0452	7.9750	8.0756	7.7192	7.8817	7.9296	7.9546	8.0313	7.9506	8.0382	7.9465	8.0264	7.9586	8.0580	**7.48**
H6	8.2757	8.4306	8.5306	8.5066	8.6767	8.5020	8.6891	8.4972	8.6724	8.5111	8.7252	8.2414	8.4011	8.4930	8.4761	8.6406	8.4718	8.6590	8.4674	8.6404	8.4805	8.6924	**7.89**
H8	4.1547	4.3318	4.4162	4.4109	4.5350	4.4064	4.5637	4.4018	4.5507	4.4152	4.5680	4.1869	4.3690	4.4494	4.4475	4.5678	4.4433	4.6053	4.4389	4.5906	4.4518	4.6075	**5.06**
H(9A-9C)	1.3053	1.3152	1.2873	1.3135	1.2822	1.3134	1.3112	1.3133	1.3047	1.3137	1.3214	1.2881	1.2965	1.2698	1.2976	1.2638	1.2977	1.2978	1.2977	1.2881	1.2977	1.3076	**1.46**

Nuclei	X3LYP											Exp. [b]
C1	140.8852	141.1026	142.1042	141.2902	142.6957	141.2794	142.4537	141.2661	142.4859	141.3047	142.4969	**132.3**
C2	136.4292	136.1319	136.6277	135.9444	136.4839	135.9591	136.8407	135.9709	136.7578	135.9342	136.8544	**129.3**
C3	135.2808	136.1196	136.7103	136.4511	137.2000	136.4361	137.3155	136.4180	137.2689	136.4686	137.3973	**128.9**
C4	139.7313	141.5961	142.2127	142.4020	143.0129	142.3602	143.8816	142.3148	143.6477	142.4447	144.0869	**135.2**
C5	133.8833	135.2574	135.9107	135.9339	136.8450	135.8976	136.8922	135.8581	136.8239	135.9717	137.0217	**128.9**
C6	134.8463	136.3615	137.3970	137.1614	138.7037	137.1175	139.1228	137.0699	138.9223	137.2068	139.4046	**129.3**
C7	213.1079	216.8393	218.4861	218.4173	219.1506	218.3302	224.2621	218.2396	223.2992	218.5029	224.9437	**198.1**
C8	57.4488	57.9664	58.5355	58.1925	58.8685	58.1814	59.5343	58.1673	59.3900	58.2070	59.5961	**51.9**
C9	23.9811	24.1449	24.1040	24.3733	24.4676	24.3613	24.2637	24.3462	24.2188	24.3886	24.1893	**16.6**
H2	8.7269	8.6390	8.6403	8.5912	8.6001	8.5945	8.5847	8.5973	8.5894	8.5880	8.5879	**7.89**
H3	7.6938	7.8179	7.8651	7.8679	7.9316	7.8654	7.9447	7.8624	7.9375	7.8702	7.9605	**7.48**
H4	7.7213	7.9055	7.9580	7.9845	8.0482	7.9803	8.0880	7.9756	8.0736	7.9884	8.1086	**7.67**
H5	7.5928	7.7494	7.7957	7.8227	7.8912	7.8187	7.8982	7.8142	7.8896	7.8264	7.9174	**7.48**
H6	8.0788	8.2461	8.3451	8.3276	8.4809	8.3232	8.5087	8.3182	8.4946	8.3318	8.5441	**7.89**
H8	4.3086	4.5009	4.5730	4.5903	4.6894	4.5853	4.7409	4.5798	4.7281	4.5950	4.7494	**5.06**
H(9A-9C)	1.2676	1.2729	1.2646	1.2724	1.2531	1.2728	1.2921	1.2727	1.2870	1.2720	1.3003	**1.46**

[a] methyl protons shifts are averaged
[b] according to [1]

Table S2. Theoretical chemical shifts (in ppm) of *(R,S)*-4-trifluoromethylmethcathinone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R												S										Exp. [b]
	B3LYP												B3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	146.0958	146.2278	147.5491	147.4218	150.8969	147.4088	149.3403	147.4036	150.1234	147.4439	149.4787	143.7395	145.7960	147.3774	146.9694	148.8010	146.9053	149.1986	146.8200	149.2962	147.0435	149.3862	**137.3**
C2	136.8518	136.8850	137.3336	136.6336	136.9960	136.6497	137.5933	136.6663	137.3168	136.6170	137.2877	136.2761	136.6236	137.4407	136.5876	137.0038	136.6803	137.6513	136.6725	137.5525	136.5896	137.4512	**136.5**
C3	132.8796	133.6062	134.4412	133.8049	134.5903	133.7929	135.2838	133.7797	134.7280	133.8132	134.6689	132.9055	133.5539	135.2064	133.6654	134.4225	133.9503	135.0151	133.9312	134.9607	133.6718	134.6523	**130.8**
C4	142.3544	142.0621	142.1229	141.9755	141.5681	141.9652	142.4924	141.9541	142.2121	141.9828	142.6772	142.6200	142.0044	141.9670	141.8279	141.7753	141.8344	142.2976	141.8412	142.1390	141.8214	142.4337	**127.3**
C5	131.4105	132.7894	133.5620	133.4888	134.9076	133.4388	134.4074	133.3892	134.8464	133.5368	135.3018	131.7048	132.9037	132.9075	133.5558	135.0195	133.2113	134.4192	133.1803	134.3270	133.5927	135.0615	**130.8**
C6	133.4691	135.4594	136.3625	136.1167	137.0755	136.0603	137.4922	136.0018	137.2782	136.1648	138.1149	133.8854	135.8776	136.3245	136.7886	138.2473	136.6061	138.3767	136.5513	138.1476	136.8408	138.8067	**136.5**
C7	204.5842	209.4312	211.3479	213.3234	215.9221	213.1217	220.4917	212.9260	220.0350	213.5251	221.2874	209.0453	213.6104	215.6212	216.0451	217.3393	215.9749	222.2187	215.8303	221.2371	216.1784	222.8007	**196.6**
C8	65.8330	66.8466	67.5195	67.3198	68.5992	67.3093	68.8908	67.2977	68.9990	67.3265	69.5579	60.1665	62.3074	63.0745	63.3374	64.1080	63.2096	65.0826	63.1315	64.9303	63.4088	65.3533	**61**
C9	22.6569	23.0280	23.1991	23.0523	23.1669	23.0342	23.3493	23.0146	23.2029	23.0644	23.4581	19.4003	19.7115	19.8109	19.9242	20.0244	19.8800	20.2392	19.8634	20.1865	19.9367	20.5768	**15.8**
C4``	135.4005	136.6305	137.6446	137.0660	138.4974	137.0394	138.2736	137.0127	138.3038	137.0896	138.3640	135.3118	136.6140	137.4461	137.0437	138.4421	137.0188	138.3427	136.9898	138.3026	137.0685	138.3762	**123.2**
C8`	36.5261	37.3149	37.5781	37.7206	38.0154	37.6956	38.1934	37.6683	38.1390	37.7409	38.6069	32.0616	32.1937	32.3459	32.2980	32.5680	32.2988	32.5977	32.2892	32.5480	32.3053	32.6500	**31.8**
H2	8.6052	8.6146	8.5856	8.4711	8.3202	8.4741	8.4332	8.4764	8.3584	8.4672	8.4261	8.7001	8.5167	8.4998	8.4210	8.4000	8.4331	8.3692	8.4400	8.3608	8.4145	8.3618	**8.24**
H3	7.9718	8.0737	8.1407	8.0983	8.1938	8.0967	8.2022	8.0949	8.1979	8.0997	8.2362	7.9848	8.0780	8.1283	8.1112	8.2056	8.1027	8.2137	8.1011	8.2041	8.1126	8.2318	**7.92**
H5	7.8793	8.0287	8.0888	8.0863	8.1664	8.0819	8.1917	8.0773	8.1666	8.0902	8.2052	7.8774	8.0030	8.0728	8.0579	8.1628	8.0603	8.1579	8.0567	8.1467	8.0608	8.1834	**7.92**
H6	8.1154	8.3540	8.4200	8.4248	8.4907	8.4167	8.5647	8.4084	8.5175	8.4319	8.6196	7.9490	8.1142	8.1606	8.1938	8.3447	8.1855	8.3213	8.1818	8.3005	8.1973	8.3707	**8.24**
H8	4.4118	4.5372	4.5645	4.6145	4.6975	4.6051	4.7529	4.5960	4.7108	4.6240	4.7854	4.5748	4.7197	4.7805	4.7820	4.9106	4.7826	4.9151	4.7794	4.8977	4.7847	4.9481	**5.17**
H(9A-9C)	1.3239	1.3479	1.3163	1.2910	1.2079	1.2933	1.2482	1.2951	1.2224	1.2881	1.2659	1.4062	1.4238	1.3898	1.4403	1.4015	1.4393	1.4116	1.4383	1.4010	1.4412	1.4350	**1.59**
H(8`A-8`C)	2.5446	2.4696	2.4496	2.4722	2.4554	2.4730	2.4371	2.4740	2.4437	2.4714	2.4186	2.9695	2.7936	2.7376	2.6984	2.6624	2.7085	2.5658	2.7149	2.5721	2.6928	2.5380	**2.8**
Nuclei	B3P86											B3P86											
C1	143.5720	143.7526	145.1950	144.9447	146.9265	144.9906	146.4144	145.0104	146.3991	144.9405	146.7483	141.6240	143.3605	144.8846	144.5601	146.0812	144.5129	146.7846	144.4437	147.1002	144.6486	146.9466	**137.3**
C2	135.8551	135.9006	136.4528	135.8101	136.2449	135.8453	136.4673	135.8577	136.4585	135.8197	136.4479	135.3794	135.6635	136.5493	135.6941	136.1456	135.7119	136.8061	135.7083	136.8259	135.7215	136.6451	**136.5**
C3	131.8409	132.5775	133.4990	132.8437	133.8578	132.8532	133.9416	132.8401	133.9682	132.8781	134.0354	131.8583	132.5262	134.2026	132.7017	133.5319	132.7150	134.0763	132.7061	134.1347	132.7332	133.7972	**130.8**
C4	140.7715	140.5654	140.6963	140.5344	140.4704	140.5402	141.2965	140.5255	141.2687	140.5742	141.4100	140.9951	140.5161	140.5894	140.4288	140.4812	140.4529	140.9976	140.4553	140.9280	140.4499	141.1352	**127.3**
C5	130.4888	131.8254	132.5909	132.4914	133.7124	132.4665	133.8940	132.4203	133.9397	132.5597	134.0753	130.6891	131.8834	132.0165	132.5559	134.0699	132.5370	133.4953	132.4959	133.5095	132.6175	134.0913	**130.8**
C6	132.5391	134.4862	135.4902	135.2618	136.7598	135.2167	137.0919	135.1503	137.0432	135.3493	137.4008	132.9247	134.9130	135.4670	135.8477	137.5078	135.8142	137.5199	135.7576	137.3824	135.9222	137.9901	**136.5**
C7	202.7303	207.2866	209.1382	210.5354	211.8480	210.4208	217.0332	210.2835	215.9685	210.6864	218.0446	206.6078	211.0529	213.0049	213.4903	214.5194	213.3713	219.4874	213.2296	218.6808	213.6460	219.9852	**196.6**
C8	64.2834	65.3255	66.0463	65.9429	66.8854	65.9531	67.3948	65.9394	67.2557	65.9748	68.1720	58.8172	60.5420	61.2735	61.5378	62.2615	61.4952	63.2346	61.4312	63.2428	61.6220	63.5164	**61**
C9	22.4523	22.7713	23.0334	22.9264	23.2633	22.9308	23.1789	22.9135	23.2319	22.9666	23.3202	19.2595	19.6026	19.7315	19.8572	20.0569	19.8676	20.2141	19.8558	20.2862	19.8911	20.6180	**15.8**
C4``	132.3434	133.4327	134.4391	133.8453	135.2457	133.8445	135.0789	133.8215	135.1512	133.8895	135.1585	132.2800	133.4280	134.2350	133.8368	135.1804	133.8349	135.0820	133.8108	135.1608	133.8823	135.1227	**123.2**
C8`	35.9329	36.6681	36.9118	37.0081	37.3997	37.0081	37.6077	36.9863	37.6627	37.0524	38.0829	31.2144	31.4571	31.6577	31.6149	31.9357	31.6278	31.9411	31.6185	31.9663	31.6465	32.0080	**31.8**
H2	8.6821	8.6848	8.6524	8.5563	8.5205	8.5567	8.5299	8.5556	8.5431	8.5575	8.5179	8.7368	8.5872	8.5803	8.4935	8.4975	8.5006	8.4425	8.5060	8.4314	8.4881	8.4397	**8.24**
H3	8.0231	8.1280	8.1963	8.1538	8.2563	8.1532	8.2744	8.1508	8.2729	8.1556	8.2937	8.0339	8.1321	8.1879	8.1663	8.2642	8.1659	8.2748	8.1636	8.2710	8.1679	8.2911	**7.92**
H5	7.9280	8.0809	8.1428	8.1404	8.2366	8.1369	8.2466	8.1316	8.2427	8.1450	8.2723	7.9210	8.0563	8.1308	8.1122	8.2236	8.1102	8.2186	8.1064	8.2131	8.1153	8.2431	**7.92**
H6	8.2040	8.4370	8.4993	8.4887	8.6145	8.4808	8.6497	8.4713	8.6493	8.4977	8.6830	8.0127	8.1939	8.2472	8.2747	8.4444	8.2719	8.4062	8.2671	8.3859	8.2785	8.4597	**8.24**
H8	4.4450	4.5701	4.5932	4.6175	4.6853	4.6098	4.7297	4.6009	4.7249	4.6265	4.7616	4.6258	4.7697	4.8328	4.8341	4.9626	4.8319	4.9687	4.8279	4.9542	4.8373	5.0038	**5.17**
H(9A-9C)	1.3433	1.3656	1.3330	1.3264	1.2873	1.3278	1.2945	1.3276	1.2953	1.3263	1.3059	1.4207	1.4365	1.4015	1.4494	1.4212	1.4500	1.4180	1.4488	1.4111	1.4503	1.4473	**1.59**
H(8`A-8`C)	2.5241	2.4423	2.4317	2.4510	2.4262	2.4546	2.4102	2.4563	2.4110	2.4488	2.3981	2.9048	2.7459	2.6925	2.6514	2.6165	2.6576	2.5126	2.6621	2.5239	2.6469	2.4886	**2.8**
Nuclei	B3PW91											B3PW91											
C1	143.9680	145.2861	145.3030	145.3252	147.6021	145.3151	147.8816	145.3012	148.1122	145.3430	147.8471	141.9101	143.7628	145.7481	145.1440	147.2658	145.1036	147.4325	145.0195	147.4892	145.1993	147.5528	**137.3**
C2	135.9436	136.0575	136.4438	135.8229	136.5065	135.8446	136.6622	135.8598	136.5815	135.8054	136.6329	135.4997	135.7925	136.6812	135.8193	136.3557	135.9145	136.8678	135.9002	136.8027	135.8177	136.7097	**136.5**
C3	131.9691	132.7466	133.5595	132.9686	134.1950	132.9630	134.0521	132.9487	134.0196	132.9752	134.1507	131.9865	132.6536	134.3275	132.8146	133.6765	133.0543	134.1660	133.0184	134.1271	132.8187	133.9040	**130.8**
C4	140.7482	140.4245	140.6506	140.5439	140.8105	140.5398	141.0441	140.5257	140.8604	140.5490	141.2257	140.9748	140.4917	140.4641	140.3675	140.3322	140.3821	140.8723	140.3857	140.7350	140.3606	141.0332	**127.3**
C5	130.6038	131.9409	132.7115	132.6639	134.3345	132.6241	134.0533	132.5742	133.9549	132.7039	134.2242	130.8127	132.0709	132.0575	132.7307	134.1535	132.4250	133.6524	132.4074	133.5700	132.7644	134.2519	**130.8**
C6	132.4390	134.1915	135.3335	135.1221	136.9534	135.0729	136.5202	135.0147	136.2969	135.1700	136.9657	132.8861	134.8788	135.2846	135.7770	137.2374	135.6212	137.3589	135.5782	137.1594	135.8226	137.8301	**136.5**
C7	202.9996	208.5381	209.4049	211.3573	212.8967	211.1744	218.8219	210.9795	217.9146	211.5349	219.4046	206.7552	211.3682	213.4772	213.8868	215.1902	213.8014	220.0464	213.6466	219.0113	214.0138	220.5442	**196.6**
C8	64.0681	65.3873	65.6926	65.6411	66.8256	65.6323	67.4513	65.6169	67.3379	65.6527	68.1075	58.7625	60.5900	61.3971	61.6676	62.5814	61.5804	63.4137	61.5102	63.2651	61.7238	63.6836	**61**
C9	22.1615	22.4308	22.6684	22.5791	23.1523	22.5677	22.8212	22.5480	22.7617	22.5911	22.9949	18.9729	19.3137	19.4310	19.5605	19.7581	19.5429	19.8692	19.5310	19.8398	19.5655	20.2492	**15.8**
C4``	132.5359	133.6842	134.5991	134.0738	135.7815	134.0572	135.2910	134.0317	135.2703	134.0917	135.3721	132.4868	133.6715	134.4351	134.0758	135.4233	134.0667	135.3131	134.0402	135.2933	134.0939	135.3553	**123.2**
C8`	35.8894	36.6726	36.8915	37.0969	37.7509	37.0774	37.5509	37.0465	37.4996	37.1156	37.9989	31.2628	31.5298	31.6068	31.6487	31.8819	31.6491	31.9461	31.6393	31.9031	31.6544	32.0201	**31.8**
H2	8.6365	8.5362	8.6282	8.5114	8.4952	8.5151	8.4216	8.5182	8.4029	8.5076	8.4374	8.7058	8.5482	8.5258	8.4427	8.4052	8.4530	8.3930	8.4594	8.3897	8.4377	8.3904	**8.24**
H3	8.0172	8.1150	8.1918	8.1483	8.2689	8.1473	8.2619	8.1458	8.2532	8.1494	8.2814	8.0305	8.1268	8.1807	8.1606	8.2559	8.1544	8.2688	8.1534	8.2613	8.1619	8.2844	**7.92**
H5	7.9208	8.0597	8.1377	8.1348	8.2465	8.1309	8.2353	8.1266	8.2249	8.1385	8.2621	7.9218	8.0540	8.1231	8.1109	8.2138	8.1114	8.2148	8.1081	8.2052	8.1136	8.2390	**7.92**
H6	8.1761	8.3482	8.4880	8.4820	8.6315	8.4751	8.5890	8.4674	8.5650	8.4882	8.6385	7.9955	8.1748	8.2163	8.2504	8.3924	8.2408	8.3765	8.2379	8.3583	8.2540	8.4298	**8.24**
H8	4.4236	4.4987	4.5816	4.6259	4.7307	4.6179	4.7435	4.6092	4.7237	4.6336	4.7789	4.5969	4.7399	4.8013	4.8026	4.9260	4.8017	4.9359	4.7985	4.9185	4.8056	4.9711	**5.17**
H(9A-9C)	1.3002	1.2899	1.2925	1.2687	1.2434	1.2713	1.2102	1.2736	1.1993	1.2663	1.2309	1.3803	1.3980	1.3654	1.4121	1.3646	1.4111	1.3828	1.4106	1.3759	1.4131	1.4087	**1.59**
H(8`A-8`C)	2.4962	2.4531	2.3965	2.4192	2.4050	2.4208	2.3919	2.4225	2.3951	2.4181	2.3742	2.8737	2.7158	2.6490	2.6190	2.5669	2.6257	2.4850	2.6309	2.4968	2.6145	2.4595	**2.8**
Nuclei	B98											B98											
C1	144.6817	144.7735	146.1060	146.0230	149.6033	146.0491	147.3430	146.0726	147.2536	146.0020	147.6851	142.6920	144.7148	146.4355	145.7596	147.5403	145.7132	147.9368	145.6463	148.0281	145.8144	148.0860	**137.3**
C2	135.6236	135.6313	136.1341	135.4960	135.9251	135.5317	136.1963	135.5637	136.1119	135.4642	136.1530	135.1384	135.4310	136.2726	135.4219	135.8823	135.5307	136.4802	135.5367	136.4127	135.4105	136.2879	**136.5**
C3	131.6876	132.3770	133.2050	132.6082	133.5093	132.6142	133.5992	132.6174	133.5457	132.6044	133.6544	131.6892	132.3271	134.0012	132.4781	133.2729	132.7411	133.8363	132.7295	133.8100	132.4740	133.5023	**130.8**
C4	141.6154	141.3650	141.4455	141.3519	141.0444	141.3518	142.0639	141.3495	141.9398	141.3547	142.1758	141.8162	141.2600	141.2835	141.1553	141.1883	141.1616	141.6483	141.1817	141.5148	141.1389	141.8200	**127.3**
C5	130.2933	131.5703	132.3049	132.2867	133.6565	132.2545	133.6606	132.2200	133.5991	132.3193	133.8638	130.4845	131.6904	131.6722	132.3505	133.8536	132.0417	133.2371	132.0316	133.1625	132.3744	133.8898	**130.8**
C6	132.4618	134.4024	135.3078	135.0616	136.0082	135.0166	136.9583	134.9685	136.8119	135.1059	137.2407	132.8518	134.7326	135.1926	135.6895	137.2053	135.5422	137.2615	135.5088	137.0579	135.7259	137.7069	**136.5**
C7	201.1408	205.8480	207.6423	209.5337	212.2712	209.3659	215.7906	209.1983	214.5722	209.6972	216.9081	205.0936	209.8308	211.8380	212.1990	213.4128	212.1126	218.4306	211.9741	217.4175	212.3241	218.9937	**196.6**
C8	65.7063	66.6959	67.3740	67.2385	68.5057	67.2520	68.7663	67.2626	68.5520	67.2290	69.4477	60.3977	62.2464	63.0208	63.2563	64.0443	63.1691	64.9719	63.1136	64.8262	63.3072	65.2120	**61**
C9	22.9529	23.2852	23.4567	23.3273	23.4646	23.3284	23.6497	23.3281	23.6182	23.3294	23.7704	19.8640	20.1672	20.2357	20.3492	20.5006	20.3405	20.6538	20.3434	20.6259	20.3453	20.9937	**15.8**
C4``	131.0991	132.1915	133.1530	132.6219	134.0294	132.6150	133.8547	132.6050	133.8345	132.6305	133.9201	131.0280	132.1772	133.0081	132.6015	133.9668	132.5942	133.8516	132.5833	133.8355	132.6114	133.8933	**123.2**
C8`	36.7268	37.4157	37.6378	37.8586	38.1851	37.8462	38.3927	37.8330	38.3535	37.8739	38.8230	32.0654	32.2381	32.3594	32.4189	32.7073	32.4289	32.7601	32.4320	32.7196	32.4158	32.8078	**31.8**
H2	8.6441	8.6517	8.6308	8.5158	8.3593	8.5168	8.5091	8.5178	8.5190	8.5148	8.4932	8.7072	8.5485	8.5236	8.4503	8.4357	8.4627	8.4090	8.4693	8.4055	8.4449	8.4001	**8.24**
H3	7.9998	8.1033	8.1757	8.1321	8.2308	8.1304	8.2526	8.1287	8.2470	8.1338	8.2697	8.0053	8.1066	8.1633	8.1390	8.2376	8.1316	8.2493	8.1304	8.2422	8.1408	8.2636	**7.92**
H5	7.9012	8.0534	8.1195	8.1160	8.2066	8.1113	8.2243	8.1068	8.2162	8.1206	8.2476	7.9013	8.0357	8.1096	8.0907	8.2008	8.0918	8.1947	8.0886	8.1858	8.0938	8.2207	**7.92**
H6	8.1436	8.3798	8.4472	8.4483	8.5180	8.4387	8.6085	8.4293	8.6011	8.4575	8.6467	7.9678	8.1483	8.1982	8.2259	8.3865	8.2182	8.3604	8.2151	8.3422	8.2296	8.4109	**8.24**
H8	4.3980	4.5187	4.5470	4.5861	4.6789	4.5767	4.6807	4.5674	4.6676	4.5951	4.7251	4.5626	4.7149	4.7791	4.7785	4.9063	4.7780	4.9132	4.7749	4.8986	4.7817	4.9452	**5.17**
H(9A-9C)	1.3259	1.3503	1.3226	1.2975	1.2035	1.2992	1.2865	1.3008	1.2849	1.2959	1.2883	1.4079	1.4295	1.3903	1.4348	1.3950	1.4357	1.4034	1.4358	1.3962	1.4355	1.4262	**1.59**
H(8`A-8`C)	2.5205	2.4463	2.4312	2.4500	2.4376	2.4522	2.4215	2.4545	2.4191	2.4483	2.4039	2.9109	2.7459	2.6877	2.6567	2.6175	2.6650	2.5240	2.6709	2.5362	2.6520	2.4964	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S2. Cont. I

Nuclei	R											S										Exp. [b]
	B971											B971										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	144.2075	144.3591	145.7057	145.6369	147.5389	145.6525	146.9067	145.6650	148.2176	145.6256	147.2579	142.2795	144.2596	145.9794	145.3233	147.0026	145.2669	147.4501	145.1910	147.5471	145.3890	147.6230	**137.3**
C2	135.3519	135.3692	135.8806	135.2827	135.7053	135.3069	135.9694	135.3296	135.9961	135.2643	135.9354	134.8588	135.1644	136.0033	135.1678	135.6057	135.2651	136.2203	135.1808	136.1514	135.1677	136.0256	**136.5**
C3	131.4605	132.1526	132.9895	132.4070	133.3759	132.4041	133.4077	132.4002	133.4151	132.4151	133.4842	131.4602	132.1101	133.7921	132.2743	133.0533	132.5150	133.6344	132.2705	133.6083	132.2817	133.2870	**130.8**
C4	141.2443	140.9936	141.0677	140.9785	140.8811	140.9707	141.6898	140.9638	141.3802	140.9931	141.7994	141.4387	140.8943	140.9208	140.7992	140.8381	140.7977	141.2840	140.8233	141.1513	140.7941	141.4602	**127.3**
C5	130.0816	131.3751	132.0828	132.0707	133.2556	132.0314	133.4231	131.9920	133.4091	132.1143	133.6009	130.2704	131.4714	131.4519	132.1340	133.6427	131.8341	132.9971	132.0717	132.9231	132.1689	133.6781	**130.8**
C6	132.2808	134.2107	135.1262	134.8825	136.3871	134.8299	136.7643	134.7775	135.9994	134.9387	137.0603	132.6477	134.5407	134.9971	135.5047	137.0565	135.3573	137.0861	135.4135	136.8802	135.5523	137.5353	**136.5**
C7	201.0262	205.7073	207.5076	209.2633	210.3800	209.0943	215.4862	208.9267	216.0420	209.4319	216.5760	204.9786	209.6701	211.6953	212.0392	213.2059	211.9402	218.1699	211.7602	217.1879	212.1755	218.7518	**196.6**
C8	65.6623	66.6670	67.3459	67.2469	68.2192	67.2521	68.6790	67.2540	68.6676	67.2449	69.3882	60.3706	62.1546	62.9077	63.1588	63.9241	63.0675	64.8290	63.0412	64.6869	63.2195	65.0725	**61**
C9	22.9552	23.2943	23.4615	23.3548	23.7034	23.3509	23.6587	23.3479	23.4768	23.3656	23.7827	19.8902	20.2028	20.2527	20.3861	20.5451	20.3727	20.6956	20.3825	20.6663	20.3927	21.0396	**15.8**
C4``	131.6640	132.7636	133.7194	133.2007	134.5849	133.1856	134.4193	133.1694	134.4087	133.2207	134.4927	131.5899	132.7409	133.5724	133.1730	134.5328	133.1581	134.4092	133.1396	134.3927	133.1941	134.4597	**123.2**
C8`	36.7351	37.4122	37.6112	37.8308	38.1771	37.8156	38.3455	37.8001	38.2754	37.8519	38.7827	32.0021	32.1890	32.2975	32.3668	32.6529	32.3705	32.6872	32.3642	32.6414	32.3738	32.7349	**31.8**
H2	8.6491	8.6497	8.6282	8.5164	8.4883	8.5169	8.5141	8.5176	8.4221	8.5164	8.4969	8.7055	8.5528	8.5254	8.4536	8.4437	8.4660	8.4133	8.4663	8.4090	8.4484	8.4025	**8.24**
H3	7.9994	8.1013	8.1731	8.1301	8.2318	8.1282	8.2495	8.1263	8.2380	8.1323	8.2660	8.0056	8.1052	8.1620	8.1377	8.2349	8.1309	8.2462	8.1342	8.2392	8.1398	8.2599	**7.92**
H5	7.9003	8.0509	8.1166	8.1137	8.2102	8.1087	8.2230	8.1039	8.2122	8.1187	8.2454	7.9011	8.0338	8.1080	8.0891	8.1986	8.0906	8.1928	8.0828	8.1841	8.0925	8.2176	**7.92**
H6	8.1485	8.3825	8.4473	8.4436	8.5681	8.4342	8.6089	8.4250	8.5633	8.4532	8.6430	7.9689	8.1514	8.2007	8.2287	8.3914	8.2215	8.3646	8.2213	8.3462	8.2326	8.4141	**8.24**
H8	4.3968	4.5154	4.5426	4.5752	4.6358	4.5654	4.6770	4.556	4.7126	4.5852	4.7102	4.5661	4.7165	4.7811	4.7819	4.9077	4.7813	4.9154	4.7752	4.9015	4.7855	4.9468	**5.17**
H(9A-9C)	1.3297	1.3507	1.3232	1.3023	1.2710	1.3037	1.2883	1.3052	1.2216	1.3012	1.2929	1.4115	1.4317	1.3906	1.4369	1.3996	1.4377	1.4056	1.4361	1.3982	1.4379	1.4284	**1.59**
H(8`A-8`C)	2.5158	2.4418	2.4283	2.4478	2.4235	2.4500	2.4132	2.4522	2.4135	2.4461	2.3968	2.9000	2.7383	2.6806	2.6506	2.6110	2.6584	2.5169	2.6611	2.5297	2.6463	2.4890	**2.8**
Nuclei	B972											B972											
C1	141.3855	142.3892	142.6458	144.0881	146.1903	144.0786	145.1463	144.0602	145.6156	144.0857	145.1997	139.2872	141.1596	143.1121	142.6886	144.9073	142.6729	144.8268	142.5969	144.8243	142.7317	144.9164	**137.3**
C2	133.3133	133.3116	133.6241	133.2395	133.6732	133.2458	133.8190	133.2490	133.7363	133.2290	133.8277	132.8890	133.1052	133.9686	133.1724	133.6384	133.2749	134.0936	133.2673	134.0359	133.1689	133.9361	**136.5**
C3	129.3416	130.0366	130.7900	130.3404	131.2218	130.3330	130.9522	130.3216	130.9365	130.3423	131.0885	129.3427	129.9137	131.6207	130.1127	130.9233	130.4156	131.3943	130.3947	131.3549	130.1163	131.1310	**130.8**
C4	138.0491	137.7117	137.9532	137.6000	137.4100	137.5910	138.2767	137.5815	138.0382	137.6058	138.4388	138.2617	137.7042	137.6890	137.6250	137.5017	137.6159	138.0254	137.6182	137.9058	137.6202	138.2148	**127.3**
C5	127.9135	129.1809	130.0590	129.8632	131.1212	129.8155	131.5741	129.7668	131.4328	129.9052	131.7024	128.1482	129.3461	129.2693	130.0892	131.3822	129.7056	130.8910	129.6712	130.8140	130.1251	131.5082	**130.8**
C6	129.7716	131.4533	132.5446	132.0478	133.2631	131.9830	133.8612	131.9177	133.5469	132.1071	134.2333	130.2562	132.0857	132.5268	132.9957	134.2870	132.8131	134.4372	132.7650	134.2634	133.0421	134.9004	**136.5**
C7	199.0631	204.4435	205.6649	208.3211	209.7781	208.1668	214.4876	208.0065	213.6878	208.4576	215.1195	202.6406	207.2108	209.1752	209.7820	211.0719	209.7166	215.7680	209.5671	214.7083	209.9037	216.2767	**196.6**
C8	62.7897	63.9111	64.1399	64.8318	65.6221	64.8026	66.0819	64.7684	66.1193	64.8523	66.7284	57.6874	59.4758	60.3520	60.6579	61.5790	60.5674	62.3296	60.4982	62.1533	60.7085	62.5668	**61**
C9	21.8674	22.0407	22.2262	22.2335	22.4502	22.2185	22.5155	22.2016	22.4381	22.2442	22.6756	18.7458	18.9793	19.1654	19.2809	19.4503	19.2506	19.5379	19.2381	19.4995	19.2853	19.8791	**15.8**
C4``	129.4413	130.5130	131.4344	130.9910	132.2841	130.966	132.0755	130.9390	132.0703	131.0098	132.1693	129.3960	130.5030	131.2850	130.9692	132.2407	130.9560	132.1348	130.9280	132.1129	130.9874	132.1811	**123.2**
C8`	35.6477	36.3949	36.6433	36.7863	37.0730	36.7590	37.1996	36.7303	37.1493	36.8084	37.6152	31.1859	31.3739	31.4675	31.5248	31.7044	31.5167	31.7547	31.5044	31.7281	31.5335	31.8377	**31.8**
H2	8.6067	8.5252	8.5911	8.3672	8.3300	8.3688	8.3874	8.3707	8.3491	8.3661	8.3995	8.6854	8.5157	8.4972	8.4018	8.3519	8.4108	8.3573	8.4164	8.3585	8.3980	8.3561	**8.24**
H3	8.0032	8.1022	8.1800	8.1296	8.2266	8.1278	8.2537	8.1258	8.2431	8.1312	8.2715	8.0166	8.1106	8.1666	8.1470	8.2384	8.1391	8.2514	8.1372	8.2444	8.1487	8.2674	**7.92**
H5	7.9050	8.045	8.1215	8.1076	8.2027	8.1035	8.2074	8.0992	8.1953	8.1113	8.2349	7.9065	8.0348	8.1013	8.0949	8.1935	8.0926	8.1931	8.0890	8.1839	8.0980	8.2209	**7.92**
H6	8.1439	8.3337	8.4722	8.3718	8.5033	8.3646	8.5646	8.3578	8.5167	8.3789	8.6071	7.9730	8.1461	8.1857	8.2199	8.3505	8.2067	8.3393	8.2029	8.3246	8.2243	8.3945	**8.24**
H8	4.3871	4.4813	4.5705	4.5491	4.6507	4.5431	4.6925	4.5372	4.6505	4.5552	4.7232	4.5562	4.6946	4.7520	4.7551	4.8727	4.7534	4.8817	4.7499	4.8662	4.7583	4.9184	**5.17**
H(9A-9C)	1.2754	1.2659	1.2574	1.2224	1.1629	1.2224	1.2011	1.2223	1.1893	1.2223	1.2197	1.3619	1.3777	1.3519	1.3944	1.3429	1.3918	1.3661	1.3905	1.3611	1.3959	1.3893	**1.59**
H(8`A-8`C)	2.4868	2.4414	2.3923	2.4466	2.4064	2.4474	2.3965	2.4480	2.4041	2.4455	2.3780	2.8679	2.7102	2.6407	2.6152	2.5576	2.6209	2.4852	2.6252	2.4982	2.6116	2.4598	**2.8**
Nuclei	BHandH											BHandH											
C1	145.7019	146.1416	147.4184	146.3886	148.1155	146.3524	147.3162	146.3373	147.6906	146.3969	147.6156	144.4298	145.6978	146.4805	146.3536	147.0977	146.3011	147.8321	146.2675	147.4549	146.3736	148.0981	**137.3**
C2	140.0914	140.0917	140.6887	139.9711	140.3671	139.9699	140.7074	139.9870	140.6668	139.9424	140.7223	139.8089	139.9586	140.5869	139.8854	140.6295	139.8787	140.9162	139.8905	140.8450	139.8621	140.7983	**136.5**
C3	135.1669	135.8248	136.7648	136.0532	136.9621	136.0308	137.0385	136.0266	137.0481	136.0443	137.1305	135.2159	135.8456	136.9134	136.0259	136.7700	136.0056	137.3482	136.0037	137.3164	136.0151	137.1778	**130.8**
C4	144.3785	144.1738	144.2765	144.3037	144.2332	144.2821	145.1007	144.2789	144.9043	144.2944	145.2415	144.5924	144.1848	144.3847	144.1940	144.9381	144.1799	144.8271	144.1849	144.7566	144.1773	144.9655	**127.3**
C5	133.5573	134.9149	135.5938	135.6558	136.9209	135.5972	136.9760	135.5575	136.8891	135.6814	137.1467	133.6557	134.9210	135.5246	135.6503	136.3944	135.5956	136.5549	135.5594	136.4748	135.6721	137.0131	**130.8**
C6	137.0738	139.0908	140.1712	140.1104	141.8547	140.0418	142.3276	139.9908	142.0316	140.1446	142.6903	137.3760	139.5800	140.6540	140.6656	141.4097	140.5955	142.6329	140.5427	142.5034	140.7010	143.0654	**136.5**
C7	204.0156	208.7373	210.4711	211.2602	212.2504	211.0847	217.1069	210.9305	216.2432	211.3998	218.0467	208.0179	212.2447	213.7490	214.5364	215.2805	214.3847	220.1811	214.2517	218.9100	214.6508	220.8594	**196.6**
C8	60.4414	61.6304	62.3870	62.1025	63.0298	62.0653	63.5103	62.0464	63.4181	62.1076	64.2768	54.5559	55.9472	56.4343	56.7013	57.4454	56.6451	58.1501	56.6069	57.8360	56.7247	58.4949	**61**
C9	22.0777	22.3139	22.6589	22.5481	23.0631	22.5254	22.9624	22.5211	22.8939	22.5399	23.1241	18.8080	19.1580	19.3069	19.3513	20.0954	19.3326	19.7545	19.3319	19.7168	19.3382	20.1267	**15.8**
C4``	121.6910	122.7021	123.6414	123.0950	124.3794	123.0623	124.2265	123.0477	124.2202	123.0957	124.3285	121.6363	122.6689	123.5830	123.0738	123.8179	123.0408	124.2025	123.0258	124.1798	123.0752	124.3124	**123.2**
C8`	33.7954	34.5397	34.8533	34.9118	35.2617	34.8763	35.4701	34.8593	35.4575	34.9158	35.9810	28.5695	28.9934	29.3575	29.2580	30.0021	29.2316	29.6683	29.2230	29.7441	29.2525	29.8112	**31.8**
H2	9.0057	8.9629	8.9413	8.9192	8.8889	8.9238	8.9061	8.9273	8.8857	8.9156	8.8945	9.0260	8.8929	8.9231	8.8116	8.7304	8.8171	8.7802	8.8218	8.8242	8.8074	8.7699	**8.24**
H3	8.1943	8.2934	8.3585	8.3254	8.4285	8.3245	8.4458	8.3229	8.4376	8.3271	8.4634	8.2008	8.2949	8.3656	8.3287	8.2475	8.3277	8.4401	8.3259	8.4335	8.3306	8.4581	**7.92**
H5	8.0848	8.2389	8.3013	8.3132	8.4069	8.3097	8.4200	8.3053	8.4074	8.3176	8.4457	8.0768	8.2189	8.2948	8.2855	8.2043	8.2825	8.3999	8.2786	8.3921	8.2894	8.4191	**7.92**
H6	8.3966	8.6212	8.6906	8.7261	8.8708	8.7209	8.9171	8.7147	8.8824	8.7319	8.9501	8.2073	8.4147	8.5275	8.5145	8.4333	8.5097	8.6930	8.5041	8.6950	8.5199	8.7394	**8.24**
H8	4.2120	4.3340	4.3352	4.4212	4.4816	4.4160	4.5274	4.4100	4.4996	4.4273	4.5511	4.4806	4.6494	4.7236	4.7331	4.6519	4.7289	4.8821	4.7238	4.8739	4.7382	4.9150	**5.17**
H(9A-9C)	1.4175	1.4308	1.4026	1.4227	1.3902	1.4249	1.4035	1.4261	1.3909	1.4214	1.4185	1.4962	1.5077	1.4956	1.5142	1.4330	1.5146	1.4951	1.5141	1.5055	1.5149	1.5141	**1.59**
H(8`A-8`C)	2.5808	2.4999	2.4871	2.4733	2.4554	2.4757	2.4253	2.4772	2.4358	2.4723	2.4148	2.9111	2.7427	2.7071	2.6666	2.5854	2.6714	2.5240	2.6754	2.5577	2.6634	2.4974	**2.8**
Nuclei	BHandHLYP											BHandHLYP											
C1	146.3121	146.5525	147.8583	147.5581	149.6920	147.5636	148.8377	147.5762	148.8568	147.5629	149.1315	144.5727	146.2680	147.5969	147.0512	148.7082	147.0176	149.2967	146.9576	149.6938	147.1096	149.4106	**137.3**
C2	138.6016	138.5440	138.9688	138.4261	138.6517	138.4425	138.9710	138.4597	138.8978	138.4079	138.9527	138.2358	138.3538	139.0367	138.2429	138.5840	138.3388	139.1401	138.3425	139.0524	138.2358	139.0093	**136.5**
C3	134.0359	134.5814	135.4061	134.8426	135.7194	134.8359	135.7277	134.8308	135.7014	134.8477	135.8105	134.0221	134.5913	136.0934	134.7087	135.4762	134.9262	135.9861	134.9094	135.9923	134.7123	135.7178	**130.8**
C4	143.3617	143.0291	143.0714	142.9946	142.8299	142.9786	143.6807	142.9666	143.5511	143.0103	143.8002	143.6072	142.9649	142.9717	142.8616	142.8169	142.8712	143.3124	142.8798	143.1200	142.8558	143.4747	**127.3**
C5	132.4297	133.7007	134.4084	134.4248	135.6855	134.3750	135.7269	134.3301	135.6828	134.4760	135.9161	132.5700	133.7586	133.8833	134.4954	135.8406	134.2125	135.3448	134.1841	135.3066	134.5392	135.8925	**130.8**
C6	135.0266	136.9881	137.8564	137.7174	138.9615	137.6586	139.4531	137.5982	139.2987	137.7662	139.7559	135.4225	137.3313	137.8061	138.3083	139.7084	138.1463	139.7508	138.1015	139.4898	138.3567	140.2118	**136.5**
C7	202.2642	207.3002	209.0695	210.7544	212.0678	210.5655	217.6680	210.3940	216.3727	210.9595	218.7321	206.5494	211.1452	213.0417	213.5723	214.5673	213.4765	220.1641	213.3257	219.1680	213.7160	220.7486	**196.6**
C8	61.2143	62.1854	62.8092	62.7125	63.5015	62.7099	64.0602	62.7051	63.8792	62.7082	64.7152	55.94815	57.7045	58.2737	58.6126	59.2881	58.5194	60.2216	58.4596	60.2070	58.6723	60.4896	**61**
C9	21.9019	22.1062	22.2853	22.1853	22.3814	22.1790	22.2770	22.1722	22.2756	22.1860	22.4002	18.7855	18.9103	18.9455	19.0174	19.1544	18.9986	19.2691	18.9937	19.3062	19.0233	19.5690	**15.8**
C4``	123.9654	125.0152	125.9444	125.4484	126.7633	125.4255	126.5959	125.4050	126.5890	125.4698	126.6896	123.8961	124.9998	125.7652	125.4378	126.7161	125.4060	126.5830	125.3840	126.5836	125.4603	126.6635	**123.2**
C8`	34.7861	35.5022	35.7539	35.8991	36.2723	35.8756	36.4696	35.8554	36.4359	35.9233	36.8786	30.4947	30.6543	30.8775	30.8773	31.1566	30.8681	31.1523	30.8589	31.0884	30.8866	31.2586	**31.8**
H2	8.8567	8.8305	8.8027	8.7110	8.6532	8.7124	8.6791	8.7133	8.6834	8.7084	8.6655	8.9189	8.7319	8.7245	8.6412	8.6292	8.6511	8.5762	8.6575	8.5492	8.6348	8.5765	**8.24**
H3	8.1220	8.2200	8.2888	8.2508	8.3540	8.2492	8.3733	8.2475	8.3663	8.2524	8.3905	8.1292	8.2227	8.2764	8.2587	8.3548	8.2509	8.3688	8.2494	8.3604	8.2604	8.3892	**7.92**
H5	8.0237	8.1724	8.2333	8.2391	8.3279	8.2346	8.3400	8.2299	8.3304	8.2433	8.3642	8.0164	8.1491	8.2265	8.2122	8.3137	8.2165	8.3169	8.2125	8.3064	8.2152	8.3365	**7.92**
H6	8.2177	8.4560	8.5295	8.5355	8.6677	8.5257	8.7093	8.5161	8.6953	8.5451	8.7449	8.0753	8.2606	8.3234	8.3532	8.5113	8.3435	8.4914	8.3391	8.4606	8.3574	8.5415	**8.24**
H8	4.1304	4.2693	4.3064	4.3494	4.4440	4.3382	4.4773	4.3279	4.4595	4.3612	4.5127	4.3324	4.4933	4.5642	4.5666	4.6951	4.5658	4.7150	4.5619	4.6908	4.5700	4.7434	**5.17**
H(9A-9C)	1.3112	1.3272	1.2928	1.2892	1.2274	1.2915	1.2550	1.2928	1.2511	1.2856	1.2615	1.3879	1.3911	1.3550	1.4030	1.3627	1.4023	1.3722	1.4017	1.3572	1.4034	1.3945	**1.59**
H(8`A-8`C)	2.4762	2.4107	2.3942	2.4187	2.3854	2.4212	2.3850	2.4232	2.3815	2.4161	2.3726	2.8760	2.7046	2.6627	2.6264	2.5905	2.6340	2.4950	2.6392	2.4953	2.6217	2.4699	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S2. Cont. II

Nuclei	R											S										Exp. [b]
	BLYP											BLYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	145.5691	146.6600	146.5234	146.9367	150.1369	147.1375	148.8278	146.9070	149.3222	147.4258	148.8749	142.3549	144.8625	146.5583	146.0678	144.9821	146.2450	148.1781	145.9637	148.3966	146.5221	148.6549	**137.3**
C2	134.8518	134.8129	135.1590	134.5621	135.1393	134.8472	135.5103	134.6733	135.6288	134.9242	135.5643	134.0693	134.4932	135.3458	134.5644	134.2789	134.9297	135.6398	134.7370	135.7384	134.9340	135.4918	**136.5**
C3	131.4357	132.1595	132.9628	132.3380	133.2580	132.6124	133.7236	132.4254	133.8579	132.7081	133.9167	131.5325	132.1094	133.8333	132.2584	134.1568	132.8854	133.6138	132.6908	133.7752	132.6272	133.1362	**130.8**
C4	141.1003	140.5808	140.7358	140.5463	140.1739	140.8348	140.8203	140.6570	140.8153	140.8911	141.0651	141.4410	140.6641	140.5575	140.4714	141.0576	140.7536	140.7729	140.5828	140.8429	140.8233	140.9911	**127.3**
C5	130.0199	131.3508	132.2481	132.1327	133.5020	132.3692	132.8747	132.1393	132.9537	132.5242	133.0940	130.5351	131.6260	131.4128	132.2051	133.5053	132.1044	132.8535	131.8921	132.9563	132.5977	133.7610	**130.8**
C6	131.6964	133.3553	134.4573	134.2296	135.4201	134.4561	135.5383	134.2152	135.4683	134.6318	136.0571	132.1611	134.0348	134.4695	134.9687	136.5949	135.0698	136.4976	134.8343	136.4925	135.3806	137.0076	**136.5**
C7	205.7569	211.4352	212.4165	214.5902	216.9674	214.6727	221.0058	214.3064	220.4511	215.1569	221.6868	210.5147	214.9191	216.9136	217.1238	220.8124	217.3423	222.6570	217.0251	222.0130	217.6115	223.4084	**196.6**
C8	69.8760	71.0382	71.3826	71.3041	72.7011	71.5240	72.9912	71.2975	73.1469	71.7501	73.7169	63.7503	66.2861	67.0905	67.4097	69.7838	67.5360	69.1487	67.2701	69.1714	67.8525	69.5429	**61**
C9	23.4060	23.6195	23.8880	23.8593	24.0973	24.1246	24.1549	23.9272	24.2462	24.2331	24.4374	20.0665	20.5318	20.6228	20.7449	24.4284	20.9752	21.0816	20.7764	21.1883	21.1222	21.5539	**15.8**
C4``	145.4983	146.8369	147.8684	147.3069	148.9554	147.5568	148.4956	147.3451	148.6634	147.6977	148.6336	145.3895	146.7787	147.6522	147.278	148.7094	147.5324	148.5749	147.3205	148.7378	147.6660	148.6777	**123.2**
C8`	38.2168	38.9589	39.1759	39.3452	39.6889	39.5998	39.6660	39.3915	39.8168	39.7275	40.1541	33.7079	33.6516	33.7261	33.7350	39.6742	34.0300	33.8693	33.8437	34.0401	34.1004	33.9740	**31.8**
H2	8.3554	8.2819	8.3764	8.2361	8.1263	8.2907	8.3818	8.2505	8.1905	8.2806	8.4140	8.5076	8.3168	8.3026	8.2185	8.4154	8.2812	8.3608	8.2437	8.1909	8.2666	8.3486	**8.24**
H3	7.8140	7.9069	7.9837	7.9340	8.0257	7.9805	8.2049	7.9342	8.0294	7.9898	8.2364	7.8399	7.9321	7.9693	7.9560	8.0747	7.9947	8.2254	7.9484	8.0520	8.0123	8.2511	**7.92**
H5	7.7255	7.8572	7.9348	7.9219	8.0051	7.9664	8.1931	7.9180	8.0155	7.9796	8.2325	7.7377	7.8518	7.9232	7.9007	8.0759	7.9507	8.1703	7.9026	7.9954	7.9584	8.2073	**7.92**
H6	7.9764	8.1608	8.2937	8.2825	8.3485	8.3271	8.5690	8.2772	8.3701	8.3364	8.6281	7.8114	7.9514	7.9975	8.0197	8.4505	8.0613	8.3163	8.0133	8.1340	8.0776	8.3721	**8.24**
H8	4.6194	4.6944	4.7506	4.8193	4.8680	4.8646	5.0681	4.8159	4.8746	4.8737	5.1169	4.7461	4.8766	4.9368	4.9331	4.6286	4.9824	5.2265	4.9348	5.0468	4.9903	5.2715	**5.17**
H(9A-9C)	1.3404	1.3295	1.3398	1.2971	1.2421	1.3455	1.4513	1.3013	1.2742	1.3511	1.4842	1.4264	1.4565	1.4351	1.4715	1.1906	1.5191	1.6285	1.4732	1.4541	1.5276	1.6614	**1.59**
H(8`A-8`C)	2.6100	2.5494	2.4979	2.5243	2.5074	2.5719	2.6623	2.5274	2.5006	2.5804	2.6514	3.0578	2.8675	2.8083	2.7722	2.4494	2.8320	2.8056	2.7941	2.6486	2.8207	2.7846	**2.8**
Nuclei	BMK											BMK										
C1	162.1489	162.5844	164.0500	162.8924	164.7003	162.8385	164.6408	163.0004	164.4061	163.1095	164.8594	160.7828	162.4101	163.3813	163.4015	165.2813	163.3225	165.7581	163.4575	165.9039	163.6403	165.9851	**137.3**
C2	152.3702	152.2294	152.7678	152.0151	152.5796	152.0178	152.8191	152.2305	152.6988	152.1734	152.7628	151.8865	151.8126	152.7096	151.5887	152.2296	151.5814	152.9402	151.7879	152.7907	151.7593	152.6803	**136.5**
C3	147.8971	148.4038	149.3231	148.5730	149.7972	148.5473	149.9162	148.7329	149.7496	148.7594	149.9594	148.0229	148.6432	150.4182	148.6456	149.7140	148.6269	150.2574	148.8214	150.1445	148.8257	149.8594	**130.8**
C4	159.0221	158.5621	158.7661	158.5116	158.7354	158.4984	159.4333	158.6965	159.2265	158.6858	159.5007	159.1598	158.5656	158.6943	158.3245	158.4583	158.3194	159.2047	158.5265	158.9527	158.4919	159.0710	**127.3**
C5	146.0877	147.5663	148.5303	148.2203	149.7341	148.1654	149.7982	148.3220	149.6452	148.4346	149.8943	146.3633	147.4663	147.8095	148.1460	149.9241	148.0908	149.3408	148.2454	149.1755	148.3594	149.8800	**130.8**
C6	149.0518	150.9702	152.2328	151.9767	154.0266	151.9029	154.1714	152.0399	153.9111	152.2074	154.4901	149.2994	151.3630	152.1414	152.4473	154.4305	152.3715	154.3431	152.5048	153.9915	152.6789	154.8513	**136.5**
C7	218.1751	223.5815	225.5580	226.4561	227.5627	226.2518	233.9701	226.2629	232.4177	226.8165	234.9721	222.5340	227.6432	229.3304	230.2334	231.3661	230.0458	237.6187	230.0707	236.4269	230.5746	238.2951	**196.6**
C8	71.0752	72.3742	73.2350	72.8705	73.9673	72.8224	74.7292	72.9859	74.4130	73.0782	75.4659	65.4191	66.9836	67.6768	67.9199	68.9170	67.8480	69.8369	67.9883	69.6498	68.1509	70.0932	**61**
C9	24.9257	25.6319	25.7358	25.7424	26.2413	25.7301	26.1534	25.9288	26.0751	25.9163	26.1278	22.1002	22.2767	22.5169	22.2221	22.6719	22.2080	22.7122	22.4067	22.6142	22.3983	22.9474	**15.8**
C4``	133.4438	134.4888	135.5976	134.8604	136.4792	134.8234	136.2765	134.9974	136.1624	135.0570	136.3210	133.5024	134.5926	135.5943	134.9543	136.6883	134.9171	136.3798	135.0911	136.2708	135.1513	136.5088	**123.2**
C8`	38.7377	39.4936	39.7790	39.7515	40.2471	39.7212	40.6929	39.9021	40.5525	39.9415	41.1304	33.7908	34.0582	34.3832	34.0967	34.5972	34.0830	34.5047	34.2798	34.2266	34.2705	34.5456	**31.8**
H2	9.0938	9.0679	9.0203	9.0076	8.9904	9.0107	8.9552	9.0134	8.9764	8.9946	8.9485	9.1036	8.9442	8.9687	8.8526	8.8601	8.8557	8.7947	8.8586	8.7737	8.8400	8.7949	**8.24**
H3	8.3639	8.4823	8.5545	8.5126	8.6249	8.5082	8.6455	8.5038	8.6435	8.5073	8.6603	8.4197	8.5279	8.5564	8.5588	8.6498	8.5542	8.6598	8.5496	8.6512	8.5536	8.6696	**7.92**
H5	8.2970	8.4347	8.5028	8.5103	8.6171	8.5025	8.6208	8.4947	8.6129	8.5082	8.6483	8.2686	8.4352	8.5235	8.4782	8.5585	8.4723	8.6358	8.4667	8.6315	8.4744	8.5928	**7.92**
H6	8.5066	8.7584	8.8206	8.8510	9.0074	8.8438	9.0154	8.8363	9.0131	8.8482	9.0489	8.3681	8.5747	8.6555	8.6234	8.7797	8.6150	8.8028	8.6070	8.7854	8.6219	8.8427	**8.24**
H8	4.3221	4.4690	4.4853	4.5567	4.6355	4.5479	4.6679	4.5392	4.6508	4.5556	4.6909	4.5449	4.7461	4.7948	4.8057	4.9302	4.7996	4.9372	4.7937	4.9324	4.8021	4.9774	**5.17**
H(9A-9C)	1.3300	1.3666	1.3216	1.3614	1.3173	1.3599	1.3135	1.3581	1.3190	1.3532	1.3277	1.3839	1.3991	1.3852	1.4013	1.3618	1.3973	1.3694	1.3935	1.3694	1.3957	1.4017	**1.59**
H(8`A-8`C)	2.4630	2.3876	2.3792	2.3941	2.3517	2.3895	2.3552	2.3851	2.3522	2.3891	2.3391	2.8009	2.6649	2.6226	2.5759	2.5284	2.5773	2.4350	2.5789	2.4500	2.5651	2.4140	**2.8**
Nuclei	BP86											BP86										
C1	142.2646	143.7967	143.7179	143.7733	145.7769	143.7983	146.0836	143.8174	146.3697	143.7525	145.7449	139.6980	141.9170	143.7007	143.1322	144.9804	143.0756	145.3484	142.9928	145.3536	143.1845	145.7628	**137.3**
C2	133.4166	133.6634	134.0556	133.4064	133.7486	133.4468	134.1792	133.4774	134.1360	133.3638	134.2001	132.7981	133.3000	134.2243	133.3792	133.8505	133.4653	134.5457	133.3793	134.4621	133.3713	134.4826	**136.5**
C3	129.9889	130.8670	131.7557	131.1277	132.0521	131.1244	132.1394	131.1151	132.1198	131.1244	132.3793	130.0666	130.8531	132.5427	130.9799	131.7302	131.2312	132.3693	130.9784	132.3287	130.9727	132.0978	**130.8**
C4	139.0519	138.7900	138.9600	138.8747	138.7182	138.8678	139.3814	138.8577	139.1809	138.8752	139.7657	139.3303	138.9119	138.8678	138.7574	138.6913	138.7803	139.2332	138.7839	139.1107	138.7379	139.5171	**127.3**
C5	128.7014	130.1207	130.8447	130.7991	132.0480	130.7576	132.2340	130.7136	132.0726	130.8338	132.5371	129.0444	130.3500	130.2439	130.8983	132.4032	130.6124	131.7364	130.8457	131.6537	130.9162	132.6390	**130.8**
C6	130.4160	132.2124	133.3640	133.0818	134.5452	133.0422	134.5088	132.9948	134.2449	133.1140	135.4175	130.8009	132.8271	133.2622	133.7618	135.2945	133.6170	135.4010	133.6702	135.2012	133.7971	136.0261	**136.5**
C7	202.8078	208.1644	208.9623	210.7829	212.2899	210.5886	217.7502	210.4063	216.9637	210.9661	217.7314	206.9460	211.4050	213.3954	213.5283	214.8867	213.4545	219.0973	213.2805	218.2467	213.6352	219.7694	**196.6**
C8	67.8843	69.3335	69.6779	69.5409	70.4242	69.5564	71.1584	69.5625	71.0890	69.5238	72.0440	62.1863	64.1865	64.9372	65.24985	66.0652	65.1540	66.9231	65.1273	66.7453	65.2981	67.3638	**61**
C9	23.1337	23.5410	23.8162	23.6945	23.8770	23.6902	23.9562	23.6814	23.8516	23.6956	24.3512	19.9182	20.5341	20.5499	20.7715	20.8608	20.7498	21.1238	20.7608	21.0535	20.7678	21.7281	**15.8**
C4``	140.7811	142.0861	143.0219	142.4585	143.8858	142.4472	143.6876	142.4300	143.6671	142.4641	143.9114	140.7074	142.0443	142.8261	142.4413	143.8188	142.4363	143.7000	142.4092	143.6774	142.4486	143.8700	**123.2**
C8`	37.4868	38.2791	38.3911	38.6410	38.8798	38.6135	39.0726	38.5858	39.0160	38.6614	39.6960	32.5485	32.8078	32.8375	32.8627	33.0371	32.8736	33.0995	32.8666	33.0724	32.8547	33.2815	**31.8**
H2	8.4331	8.3442	8.4264	8.3297	8.2787	8.3317	8.2600	8.3330	8.2368	8.3267	8.3138	8.5262	8.3879	8.3556	8.2859	8.2521	8.2977	8.2452	8.2991	8.2436	8.2799	8.2446	**8.24**
H3	7.8575	7.9549	8.0224	7.9896	8.0803	7.9887	8.0902	7.9873	8.0801	7.9900	8.1270	7.8812	7.9805	8.0200	8.0076	8.0899	8.0039	8.1031	8.0061	8.0957	8.0078	8.1278	**7.92**
H5	7.7646	7.8998	7.9692	7.9747	8.0619	7.9707	8.0684	7.9664	8.0567	7.9780	8.1086	7.7716	7.8999	7.9566	7.9521	8.0500	7.9539	8.0466	7.9474	8.0375	7.9538	8.0845	**7.92**
H6	8.0653	8.2205	8.3463	8.3520	8.4613	8.3423	8.4633	8.3328	8.4265	8.3602	8.5319	7.8580	8.0294	8.0571	8.0981	8.2366	8.0917	8.2198	8.0922	8.2031	8.1006	8.2827	**8.24**
H8	4.6570	4.7066	4.7715	4.8202	4.8879	4.8100	4.9403	4.8004	4.9108	4.8291	4.9488	4.8048	4.9410	4.9862	4.9950	5.1087	4.9956	5.1146	4.9905	5.1012	4.9967	5.1640	**5.17**
H(9A-9C)	1.3727	1.3650	1.3627	1.3466	1.2958	1.3502	1.2795	1.3530	1.2690	1.3425	1.3488	1.4586	1.4897	1.4414	1.4989	1.4497	1.4992	1.4660	1.4986	1.4581	1.4988	1.5069	**1.59**
H(8`A-8`C)	2.5962	2.5441	2.4807	2.5028	2.4656	2.5068	2.4540	2.5104	2.4587	2.4991	2.4517	2.9894	2.8226	2.7466	2.7223	2.6666	2.7314	2.5717	2.7352	2.5855	2.7161	2.5566	**2.8**
Nuclei	CAM-B3LYP											CAM-B3LYP										
C1	147.8331	148.0612	149.4087	149.2392	151.3209	149.2575	151.9757	149.2753	152.0486	149.2236	147.1352	145.9561	147.7934	149.4617	148.9977	150.7759	148.9300	151.3446	148.8625	151.5034	149.0634	151.4483	**137.3**
C2	139.2196	139.2384	139.6705	139.1519	139.4930	139.1691	139.8694	139.1859	139.7962	139.1372	139.8883	138.8272	139.0516	139.8200	138.9926	139.3951	138.9981	139.9546	139.0053	139.8833	138.9896	139.7938	**136.5**
C3	135.1057	135.7619	136.5895	136.0205	136.9854	136.0164	137.1114	136.0119	137.0757	136.0265	137.2358	135.1182	135.7316	137.3113	135.8616	136.6664	135.8587	137.1937	135.8568	137.1705	135.8666	136.9149	**130.8**
C4	144.5181	144.2000	144.2052	144.1235	143.9978	144.1154	144.5894	144.1087	144.4582	144.1343	145.3632	144.7712	144.1513	144.0841	144.0023	143.9868	144.0138	144.3978	144.0256	144.2495	143.9939	144.5629	**127.3**
C5	133.6120	134.9268	135.5905	135.6077	136.8241	135.5668	137.0138	135.5271	136.9540	135.6488	136.9963	133.7704	135.0168	135.0367	135.7448	137.1757	135.7078	136.6219	135.6700	136.5454	135.7810	137.1885	**130.8**
C6	135.8297	137.8172	138.7028	138.5346	139.9659	138.4736	139.6822	138.4129	139.4975	138.5938	141.6518	136.2466	138.2289	138.5649	139.1705	140.6843	139.1237	140.6353	139.0757	140.4194	139.2158	141.1226	**136.5**
C7	206.4300	211.4112	213.2687	214.9491	216.2792	214.7938	223.3939	214.6410	222.3086	215.1017	222.4203	210.6466	215.3777	217.4653	218.0053	219.1690	217.8558	224.5036	217.7056	223.4555	218.1473	225.0595	**196.6**
C8	64.0416	65.1055	65.7587	65.6972	66.6293	65.6893	67.3170	65.6799	67.1138	65.7048	64.9357	58.4519	60.2829	61.0035	61.3035	62.0728	61.2406	63.0518	61.1782	62.9527	61.3651	63.3456	**61**
C9	22.0749	22.3373	22.5065	22.4375	22.7481	22.4276	22.4563	22.4183	22.4207	22.4492	19.7576	19.0778	19.2606	19.2650	19.4223	19.5949	19.4204	19.6547	19.4187	19.6569	19.4260	20.0096	**15.8**
C4``	133.2084	134.3677	135.3027	134.8064	136.2040	134.7870	136.0491	134.7677	136.0203	134.8266	136.0181	133.1468	134.3508	135.1315	134.7907	136.1580	134.7701	136.0284	134.7496	136.0058	134.8120	136.1044	**123.2**
C8`	35.5599	36.3294	36.5371	36.7112	37.1211	36.6937	37.2322	36.6767	37.1742	36.7298	34.6845	30.9234	31.1677	31.2719	31.3452	31.6371	31.3411	31.6285	31.3371	31.5700	31.3512	31.7430	**31.8**
H2	8.7541	8.7416	8.7094	8.6099	8.5657	8.6103	8.4853	8.6108	8.4831	8.6095	8.7927	8.8263	8.6455	8.6136	8.5409	8.5265	8.5479	8.4657	8.5551	8.4567	8.5345	8.4655	**8.24**
H3	8.0855	8.1815	8.2482	8.2081	8.3088	8.2066	8.3223	8.2052	8.3163	8.2094	8.3547	8.0960	8.1845	8.2363	8.2195	8.3165	8.2179	8.3224	8.2164	8.3152	8.2209	8.3416	**7.92**
H5	7.9899	8.1376	8.1985	8.1994	8.2908	8.1949	8.3011	8.1906	8.2928	8.2036	8.3570	7.9879	8.1159	8.1919	8.1726	8.2760	8.1697	8.2766	8.1669	8.2677	8.1754	8.2950	**7.92**
H6	8.1943	8.4319	8.5003	8.4945	8.6252	8.4855	8.6137	8.4768	8.6024	8.5031	8.6860	8.0430	8.2250	8.2698	8.3093	8.4683	8.3054	8.4327	8.3016	8.4114	8.3128	8.4834	**8.24**
H8	4.2721	4.4091	4.4398	4.4757	4.5583	4.4663	4.6372	4.4575	4.6259	4.4851	4.7466	4.4692	4.6298	4.6984	4.7032	4.8365	4.6997	4.8419	4.6962	4.8222	4.7064	4.8725	**5.17**
H(9A-9C)	1.3399	1.3586	1.3274	1.3196	1.2759	1.3203	1.2273	1.3210	1.2204	1.3184	1.3342	1.4178	1.4252	1.3830	1.4396	1.4032	1.4390	1.4036	1.4386	1.3956	1.4401	1.4273	**1.59**
H(8`A-8`C)	2.5511	2.4741	2.4620	2.4842	2.4579	2.4863	2.4505	2.4884	2.4491	2.4821	2.6052	2.9352	2.7654	2.7099	2.6729	2.6362	2.6780	2.5375	2.6833	2.5448	2.6681	2.5119	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S2. Cont. III

Nuclei	R											S										Exp. [b]
	HF											HF										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	145.4746	146.5190	146.8081	148.1520	151.2446	148.1657	149.9183	148.1803	149.2436	148.1389	148.9112	143.6786	145.7401	147.3630	147.0208	149.5293	146.8994	149.2120	146.7746	149.3477	147.0185	149.3030	**137.3**
C2	138.9119	138.7196	139.0655	138.3417	138.5966	138.3530	138.9051	138.3649	139.0067	138.3299	139.1089	138.8085	138.6264	139.0274	138.3491	138.4108	138.3730	138.7497	138.3986	138.6921	138.2557	138.7611	**136.5**
C3	133.7396	134.1385	134.6703	134.3730	135.9521	134.3812	135.8562	134.3905	135.7851	134.3651	136.0240	133.6502	134.2448	135.4236	134.4395	135.0940	134.4163	135.4077	134.3939	135.4077	134.1925	135.4770	**130.8**
C4	142.9631	142.5000	142.7296	142.2208	141.7357	142.2070	142.7203	142.1933	142.8021	142.2332	143.1391	143.3113	142.4814	142.3291	142.2447	141.9375	142.2711	142.4787	142.2990	142.3183	142.2539	142.6305	**127.3**
C5	131.6479	133.0547	133.7854	133.9384	134.7111	133.8946	134.5910	133.8499	134.4060	133.9787	134.3032	131.5261	132.9037	133.2407	133.6819	135.2673	133.6346	134.8526	133.5850	134.8091	134.0013	134.9857	**130.8**
C6	134.6762	136.3087	137.3819	136.6846	137.0557	136.6094	137.7254	136.5345	137.8490	136.7549	138.4447	135.2713	136.7389	137.0688	137.4040	138.3842	137.3945	138.5285	137.3856	138.3316	137.5778	138.8358	**136.5**
C7	196.0598	202.2945	203.2985	206.6321	208.5341	206.4672	215.2152	206.3000	212.7757	206.7860	214.8933	200.0583	205.2035	206.9481	208.1492	209.0586	207.9511	215.2860	207.7494	213.8542	208.1908	216.0633	**196.6**
C8	54.9908	55.9707	56.2601	56.7627	57.7256	56.7493	58.2795	56.7370	57.7262	56.7751	58.3544	50.2906	52.0564	52.7875	52.9453	53.9336	52.8697	54.7243	52.7950	54.5739	53.0302	54.9440	**61**
C9	20.4042	20.3340	20.4915	20.3608	20.5307	20.3519	20.3589	20.3440	20.3836	20.3690	20.4682	17.6736	17.4625	17.5321	17.4770	17.7311	17.4769	17.6417	17.4788	17.6565	17.4987	17.8176	**15.8**
C4``	108.7244	109.6737	110.4984	110.0621	111.2233	110.0421	111.0795	110.0222	111.0150	110.0803	111.0350	108.6816	109.6465	110.3873	110.0293	111.2293	110.0076	111.1109	109.9863	111.0926	110.0610	111.2125	**123.2**
C8`	32.7295	33.4363	33.6903	33.7315	34.0331	33.7143	34.1806	33.6972	34.1361	33.7471	34.5396	29.0093	29.1671	29.3364	29.3551	29.5595	29.3505	29.5823	29.3454	29.5540	29.3565	29.6888	**31.8**
H2	8.9162	8.7901	8.8751	8.5939	8.4989	8.5946	8.5536	8.5951	8.6229	8.5932	8.6514	9.0182	8.7587	8.7178	8.6319	8.5604	8.6448	8.5441	8.6580	8.5400	8.6267	8.5518	**8.24**
H3	8.1230	8.2340	8.3167	8.2754	8.3768	8.2733	8.3920	8.2710	8.3826	8.2774	8.4025	8.1222	8.2263	8.2942	8.2701	8.3959	8.2676	8.4001	8.2649	8.3926	8.2868	8.4192	**7.92**
H5	8.0282	8.1810	8.2525	8.2516	8.3780	8.2475	8.3880	8.2432	8.3761	8.2555	8.4121	8.0301	8.1769	8.2554	8.2448	8.3374	8.2413	8.3450	8.2375	8.3357	8.2365	8.3702	**7.92**
H6	8.1362	8.3677	8.5034	8.4340	8.5255	8.4249	8.5758	8.4155	8.5966	8.4426	8.6649	8.0488	8.2411	8.3015	8.3304	8.4696	8.3282	8.4581	8.3256	8.4385	8.3439	8.5005	**8.24**
H8	3.6783	3.8283	3.9138	3.9154	4.0206	3.9071	4.0652	3.8983	4.0697	3.9233	4.1272	3.8749	4.0599	4.1336	4.1480	4.2705	4.1448	4.2835	4.1412	4.2628	4.1494	4.3130	**5.17**
H(9A-9C)	1.2042	1.1823	1.1829	1.1259	1.0558	1.1257	1.0896	1.1254	1.1005	1.1262	1.1176	1.2983	1.2622	1.2253	1.2714	1.2111	1.2725	1.2298	1.2739	1.2244	1.2736	1.2426	**1.59**
H(8`A-8`C)	2.3078	2.2838	2.2303	2.2973	2.2624	2.2980	2.2685	2.2986	2.2566	2.2968	2.2503	2.6969	2.5346	2.4798	2.4585	2.4026	2.4636	2.3393	2.4688	2.3469	2.4520	2.3189	**2.8**
Nuclei	**LC-BLYP**																						
C1	152.0509	152.2904	153.7367	153.3601	155.5681	153.3670	154.9437	153.3954	154.4339	153.3288	155.2680	150.5045	152.2031	153.7908	153.2534	155.8212	153.1622	156.0226	153.0608	156.1468	153.3303	156.1618	**137.3**
C2	144.7125	144.6312	145.1272	144.5499	144.8944	144.5365	145.2491	144.5496	145.1530	144.5447	145.2395	144.4802	144.5126	145.2941	144.4095	144.8488	144.5040	145.2713	144.3999	145.1959	144.4110	145.2848	**136.5**
C3	140.2145	140.7752	141.7113	141.0557	142.0498	141.0254	142.1229	141.0212	141.9892	141.0660	142.2143	140.2499	140.7596	142.3781	140.8962	141.8768	141.1074	142.3066	140.8601	142.2860	140.9090	142.3933	**130.8**
C4	149.2071	148.8173	148.8841	148.7901	148.6545	148.7528	149.4392	148.7442	149.3874	148.8102	149.5669	149.4608	148.7676	148.8184	148.6584	148.5160	148.6472	148.9934	148.6594	148.8377	148.6557	149.1307	**127.3**
C5	138.5876	139.8632	140.5990	140.6264	141.8705	140.5611	141.8918	140.5236	141.8563	140.6714	142.0907	138.6374	139.9495	140.1075	140.7741	142.1180	140.4431	141.7181	140.6653	141.6278	140.8194	141.8604	**130.8**
C6	141.0535	143.0445	144.0231	143.8824	145.2947	143.7857	145.6579	143.7183	145.6385	143.9589	145.9777	141.4719	143.4938	143.9739	144.4883	145.8383	144.2965	145.9051	144.3790	145.6901	144.5358	146.2724	**136.5**
C7	211.6896	216.8845	218.8796	220.4281	221.7615	220.2641	227.5203	220.1231	225.8335	220.5608	228.6578	215.6685	220.5967	222.6674	223.3869	224.7998	223.2342	230.4409	223.0210	229.2955	223.5507	231.1013	**196.6**
C8	61.8066	62.9317	63.6984	63.6108	64.5342	63.5680	65.1152	63.5513	64.7959	63.6317	65.8516	56.0740	57.7256	58.4200	58.7387	59.6991	58.6176	60.5826	58.5785	60.4712	58.8057	60.9407	**61**
C9	21.1661	21.2770	21.5524	21.4751	21.7877	21.4332	21.6156	21.4196	21.6205	21.4987	21.7354	18.4099	18.4575	18.5392	18.5549	18.8782	18.5245	18.8809	18.5270	18.8811	18.5621	19.2427	**15.8**
C4``	132.5172	133.5825	134.5684	134.0496	135.3951	134.0033	135.2576	133.9839	135.2137	134.0758	135.3557	132.4788	133.5691	134.4274	134.0437	135.3697	133.9815	135.2416	133.9748	135.2063	134.0714	135.3360	**123.2**
C8`	33.6857	34.4375	34.7733	34.9029	35.3193	34.8597	35.5481	34.8435	35.4453	34.9260	36.0715	28.9840	29.3256	29.5147	29.5678	29.7478	29.5398	29.8261	29.5348	29.7508	29.5815	29.9991	**31.8**
H2	8.9592	8.9238	8.8891	8.8020	8.7486	8.7999	8.7505	8.7999	8.8006	8.8037	8.7371	9.0153	8.8275	8.8032	8.7157	8.6572	8.7274	8.6098	8.7322	8.6016	8.7088	8.6148	**8.24**
H3	8.2581	8.3475	8.4141	8.3755	8.4752	8.3732	8.4903	8.3724	8.4872	8.3768	8.5094	8.2680	8.3511	8.4017	8.3845	8.4819	8.3733	8.4866	8.3809	8.4799	8.3859	8.5050	**7.92**
H5	8.1636	8.3101	8.3726	8.3761	8.4648	8.3705	8.4731	8.3664	8.4673	8.3806	8.4990	8.1630	8.2921	8.3734	8.3499	8.4461	8.3581	8.4547	8.3435	8.4460	8.3527	8.4792	**7.92**
H6	8.3451	8.5831	8.6564	8.6531	8.7830	8.6429	8.8104	8.6347	8.8269	8.6622	8.8478	8.2072	8.4014	8.4562	8.4867	8.6272	8.4762	8.6044	8.4795	8.5835	8.4901	8.6475	**8.24**
H8	4.1559	4.3070	4.3311	4.3813	4.4678	4.3707	4.5064	4.3622	4.5124	4.3908	4.5393	4.3917	4.5685	4.6440	4.6477	4.7849	4.6466	4.7928	4.6400	4.7697	4.6512	4.8243	**5.17**
H(9A-9C)	1.3604	1.3752	1.3412	1.3433	1.2926	1.3421	1.3021	1.3426	1.3118	1.3437	1.3127	1.4296	1.4287	1.3910	1.4345	1.3876	1.4341	1.3963	1.4339	1.3899	1.4351	1.4191	**1.59**
H(8`A-8`C)	2.5416	2.4622	2.4501	2.4737	2.4486	2.4749	2.4370	2.4774	2.4232	2.4715	2.4263	2.8817	2.7085	2.6604	2.6308	2.5674	2.6366	2.4814	2.6403	2.4851	2.6266	2.4583	**2.8**
Nuclei	**M06**																						
C1	142.5304	142.5214	143.9959	143.5563	145.9436	143.5938	145.2542	143.6307	145.5188	143.5248	145.5315	140.8593	142.5937	144.5792	144.0367	145.8867	143.8832	146.3241	143.8079	146.4972	144.1042	146.2943	**137.3**
C2	137.3881	137.3101	137.8151	137.1436	137.6404	137.1585	137.9385	137.1789	137.8754	137.1414	137.9348	137.0441	137.2283	137.7575	136.6347	137.2838	137.1287	138.3154	137.1180	138.2547	136.6642	137.7695	**136.5**
C3	133.9825	134.3636	135.3553	134.5515	135.7811	134.5292	135.8873	134.5159	135.8726	134.5880	135.9711	134.5832	134.8735	135.7514	132.8369	133.9725	135.0082	136.1351	135.0026	136.1164	132.8791	134.1329	**130.8**
C4	140.3342	140.0366	140.1713	140.0494	139.9833	140.0193	140.7589	139.9992	140.5818	140.0946	140.8758	140.4119	139.6902	139.8023	139.7549	139.8604	139.5337	140.1577	139.5367	140.0045	139.7794	140.5695	**127.3**
C5	130.4780	131.8510	133.0096	132.7277	134.2279	132.6652	134.2392	132.6119	134.1416	132.8026	134.4146	130.5129	131.8350	132.8544	134.3366	135.5591	132.5786	133.7689	132.5373	133.6953	134.3885	135.7114	**130.8**
C6	133.6983	135.5708	136.5678	136.3975	137.6546	136.3241	138.0807	136.2581	137.8349	136.4818	138.3952	133.7133	135.6859	136.7150	137.3373	138.9866	136.6725	138.6820	136.6123	138.4382	137.4152	139.6779	**136.5**
C7	203.3427	208.0439	210.0199	211.2717	212.6612	211.1231	217.6004	210.9825	216.6066	211.4269	218.4942	207.5557	211.9284	213.7581	214.1467	215.1908	214.0737	219.9951	213.9362	219.0198	214.2939	220.3471	**196.6**
C8	61.1980	62.2855	63.0763	62.9953	64.0262	62.9770	64.5450	62.9621	64.4476	63.0228	65.3182	54.5954	56.2359	57.0974	57.3333	58.2781	57.1446	59.0542	57.0811	58.9330	57.4050	59.4515	**61**
C9	21.6160	22.0167	22.4473	22.2890	22.6669	22.2353	22.7136	22.1942	22.5978	22.3590	22.8140	19.1901	19.2771	19.4926	19.4542	19.8770	19.4422	19.9670	19.4291	19.9423	19.4856	20.4634	**15.8**
C4``	125.7597	126.7920	127.9093	127.2691	128.8332	127.2418	128.6555	127.2213	128.6480	127.3085	128.7376	125.5460	126.7182	127.8794	127.7747	129.2811	127.1786	128.7081	127.1476	128.6869	127.8217	129.2054	**123.2**
C8`	37.0450	37.6940	37.8835	37.8772	38.3973	37.8448	38.6069	37.8202	38.5778	37.9226	39.0934	31.5291	31.7000	31.8863	31.8182	32.2538	31.8472	32.4883	31.8311	32.3995	31.8623	32.6089	**31.8**
H2	8.7069	8.6784	8.6928	8.6053	8.5454	8.6073	8.5479	8.6098	8.5343	8.6039	8.5372	8.7807	8.6012	8.5696	8.4457	8.4404	8.5036	8.4665	8.5093	8.4619	8.4427	8.4200	**8.24**
H3	8.0158	8.0988	8.2272	8.1377	8.2827	8.1368	8.2910	8.1364	8.2841	8.1391	8.3061	7.9920	8.0946	8.2076	8.2048	8.2973	8.1316	8.2916	8.1305	8.2844	8.2068	8.3249	**7.92**
H5	7.9494	8.0972	8.1803	8.1686	8.2684	8.1645	8.2725	8.1608	8.2623	8.1730	8.2960	7.9197	8.0617	8.1458	8.0756	8.2233	8.1348	8.2328	8.1318	8.2227	8.0796	8.2598	**7.92**
H6	8.2234	8.4837	8.5504	8.5152	8.6199	8.5047	8.6524	8.4954	8.6194	8.5265	8.6775	8.0120	8.1807	8.2580	8.2738	8.4318	8.2652	8.4178	8.2609	8.3913	8.2799	8.4899	**8.24**
H8	4.4104	4.5520	4.6020	4.6273	4.6777	4.6180	4.6910	4.6096	4.6575	4.6370	4.7194	4.5352	4.7033	4.7593	4.7525	4.8737	4.7515	4.8659	4.7494	4.8444	4.7564	4.9040	**5.17**
H(9A-9C)	1.3045	1.3201	1.3096	1.2974	1.2497	1.2984	1.2666	1.2998	1.2614	1.2969	1.2714	1.3986	1.4265	1.3984	1.4181	1.3894	1.4393	1.4093	1.4389	1.4028	1.4199	1.4150	**1.59**
H(8`A-8`C)	2.5039	2.4289	2.4185	2.4392	2.4200	2.4398	2.4123	2.4409	2.4141	2.4391	2.3982	2.9118	2.7517	2.6818	2.6405	2.5916	2.6543	2.5092	2.6599	2.5172	2.6379	2.4728	**2.8**
Nuclei	**M06-2X**																						
C1	160.7812	161.0469	162.5455	161.6717	163.2331	161.5936	163.0308	162.1862	162.9763	161.7362	163.3570	159.4780	161.2884	163.1285	162.8746	164.9031	162.8708	165.0996	162.8652	165.2939	162.8691	165.3736	**137.3**
C2	152.3716	152.4344	152.8979	152.2272	152.6934	152.2499	153.0785	152.3390	153.0188	152.1973	153.1001	152.1224	152.2293	153.1677	152.2015	152.6835	152.2268	153.2056	152.2531	153.1595	152.1711	153.0350	**136.5**
C3	148.0777	149.1088	149.5307	148.9264	149.9379	148.9295	150.0878	148.9831	150.0285	148.9164	150.1950	148.3996	148.8696	150.7241	148.9722	149.7604	148.9863	150.2854	149.0018	150.2481	148.9523	150.0513	**130.8**
C4	157.0834	156.7269	156.8402	156.7636	156.8158	156.7870	157.5708	156.7323	157.4212	156.7358	157.7244	157.2275	156.6756	156.6273	156.5684	156.5103	156.5882	157.1793	156.6098	157.0072	156.5437	157.2822	**127.3**
C5	146.2865	147.4241	148.6402	148.5356	149.9022	148.5156	149.9231	148.4517	149.8325	148.5489	150.1218	146.0862	147.5102	147.7038	148.2411	149.9800	148.2162	149.3829	148.1923	149.2666	148.2584	150.0473	**130.8**
C6	149.2115	151.2168	152.5585	152.3737	154.3147	152.3414	154.5563	152.1990	154.3608	152.3992	154.9380	149.3500	151.6799	152.2678	152.7029	154.6092	152.6622	154.6326	152.6226	154.3948	152.7349	155.1715	**136.5**
C7	219.8379	225.1136	227.1287	228.2419	229.1118	228.0337	235.1503	228.2818	233.7990	228.4332	236.2713	223.2667	228.5162	230.4809	231.5768	232.6758	231.4403	238.7422	231.3023	237.5446	231.6985	239.5725	**196.6**
C8	66.6877	67.8725	68.6463	68.4731	69.4288	68.4435	70.0657	68.5768	69.8849	68.4932	70.8457	60.9160	62.6250	63.4930	63.7820	64.7141	63.7606	65.5453	63.7390	65.4520	63.7952	65.9087	**61**
C9	22.7187	23.0614	23.2458	23.2276	23.6788	23.2358	23.5684	23.2017	23.5225	23.2166	23.7532	20.1129	20.1977	20.4014	20.3278	20.6954	20.3490	20.7794	20.3710	20.7796	20.3011	21.1513	**15.8**
C4``	128.9729	130.1874	131.0653	130.5257	131.9061	130.5242	131.7423	130.5161	131.7167	130.5206	131.8568	129.0341	130.2231	130.9361	130.7024	132.0283	130.6988	131.9000	130.6959	131.8685	130.6991	132.0710	**123.2**
C8`	36.1583	36.8117	37.0490	37.1950	37.5165	37.1919	37.7409	37.2318	37.6971	37.1907	38.2470	30.6328	31.0950	31.0595	31.1086	31.3260	31.1080	31.3212	31.1094	31.2246	31.1036	31.5266	**31.8**
H2	9.2752	9.2781	9.2443	9.2079	9.2051	9.2147	9.1892	9.1728	9.2001	9.2015	9.1779	9.3141	9.1632	9.1533	9.0260	9.0085	9.0261	8.9735	9.0261	8.9598	9.0263	8.9697	**8.24**
H3	8.6139	8.7129	8.7869	8.7471	8.8480	8.7444	8.8596	8.7387	8.8539	8.7497	8.8756	8.6388	8.7165	8.7880	8.7413	8.8344	8.7380	8.8518	8.7344	8.8449	8.7446	8.8630	**7.92**
H5	8.5057	8.6790	8.7242	8.7320	8.8378	8.7265	8.8434	8.7173	8.8343	8.7374	8.8672	8.5500	8.6753	8.7083	8.7291	8.8526	8.7238	8.8247	8.7182	8.8128	8.7342	8.8646	**7.92**
H6	8.7790	9.0052	9.1051	9.1177	9.2838	9.1126	9.3018	9.0803	9.2876	9.1227	9.3349	8.6506	8.8368	8.8660	8.9036	9.0820	8.8958	9.0507	8.8877	9.0256	8.9113	9.1112	**8.24**
H8	4.2826	4.4385	4.4624	4.5326	4.6216	4.5267	4.6533	4.4977	4.6336	4.5388	4.6780	4.5967	4.7305	4.7817	4.7824	4.9132	4.7762	4.9131	4.7698	4.8896	4.7884	4.9457	**5.17**
H(9A-9C)	1.3663	1.3956	1.3572	1.3769	1.3484	1.3786	1.3512	1.3596	1.3525	1.3755	1.3638	1.4344	1.4359	1.4105	1.4346	1.4038	1.4314	1.4037	1.4281	1.3976	1.4377	1.4301	**1.59**
H(8`A-8`C)	2.4903	2.4194	2.4092	2.4158	2.3835	2.4115	2.3883	2.4317	2.3857	2.4201	2.3743	2.7768	2.6286	2.5753	2.5515	2.5055	2.5519	2.4360	2.5522	2.4378	2.5513	2.4113	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S2. Cont. IV

Nuclei	R											S										Exp. [b]
	mpW1LYP											mpW1LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	146.3011	146.4224	147.7951	147.6820	151.2162	147.6958	149.5841	147.7119	148.8340	147.6710	149.5731	144.0082	145.9547	147.5148	147.1335	148.8614	147.0617	149.2721	146.9772	149.4582	147.2103	149.4472	**137.3**
C2	137.1269	137.0834	137.5504	136.9264	137.2035	136.9488	137.5009	136.9726	137.4156	136.9040	137.4474	136.5419	136.8143	137.6048	136.8271	137.1730	136.9147	137.8074	136.9065	137.7305	136.8297	137.5980	**136.5**
C3	133.0432	133.6785	134.5277	133.9494	134.7771	133.9381	134.6612	133.9284	134.7983	133.9577	134.7653	133.0462	133.6460	135.2918	133.8145	134.5268	134.0843	135.1048	134.0604	135.0811	133.8225	134.7247	**130.8**
C4	142.6891	142.3187	142.3565	142.2937	141.8367	142.2759	142.8151	142.2594	142.7725	142.3083	142.9353	142.9332	142.2438	142.2003	142.1354	142.0510	142.1359	142.5366	142.1420	142.3943	142.1308	142.6653	**127.3**
C5	131.5256	132.8272	133.5462	133.5849	134.9095	133.5293	135.2277	133.4752	134.8319	133.6353	135.2839	131.8034	132.9444	132.9679	133.6763	135.1049	133.3379	134.4725	133.3099	134.4118	133.7163	135.1008	**130.8**
C6	133.8544	135.8080	136.7082	136.4859	137.3352	136.4220	137.9905	136.3589	138.1817	136.5439	138.3712	134.2310	136.1799	136.6053	137.1577	138.5996	136.9769	138.6820	136.9226	138.4679	137.2117	139.1059	**136.5**
C7	204.1435	208.9718	210.8713	212.8431	215.5762	212.6436	220.2740	212.4482	217.9395	213.0320	220.9021	208.7698	213.2274	215.2815	215.7249	216.9554	215.6428	221.8605	215.4967	220.9247	215.8621	222.4402	**196.6**
C8	65.3405	66.3268	67.0108	66.8427	68.0810	66.8366	68.2723	66.8328	68.1115	66.8481	68.9293	59.7565	61.7690	62.4885	62.8117	63.5389	62.6898	64.4543	62.6146	64.3535	62.8823	64.7146	**61**
C9	22.6898	23.0014	23.1882	23.0516	23.1193	23.0335	23.2111	23.0178	23.2603	23.0672	23.3444	19.4329	19.6698	19.7280	19.8989	19.9691	19.8615	20.1344	19.8467	20.1180	19.9107	20.4549	**15.8**
C4``	133.5566	134.7311	135.7328	135.2303	136.6214	135.2016	136.3970	135.1742	136.4256	135.2554	136.4626	133.4548	134.6985	135.5224	135.1936	136.5468	135.1632	136.4269	135.1339	136.4140	135.2205	136.4564	**123.2**
C8`	36.3421	37.0508	37.2997	37.5198	37.8215	37.4840	37.9658	37.4509	37.9881	37.5518	38.3753	31.8478	31.9274	32.0924	32.1118	32.3621	32.1074	32.3640	32.0964	32.3328	32.1213	32.4094	**31.8**
H2	8.6559	8.6549	8.6278	8.5206	8.3551	8.5219	8.4612	8.5226	8.5169	8.5189	8.4695	8.7476	8.5595	8.5464	8.4689	8.4508	8.4808	8.4134	8.4878	8.4037	8.4620	8.4033	**8.24**
H3	7.9953	8.0939	8.1639	8.1243	8.2189	8.1227	8.2453	8.1206	8.2355	8.1256	8.2588	8.0058	8.0969	8.1508	8.1352	8.2304	8.1259	8.2369	8.1245	8.2303	8.1365	8.2532	**7.92**
H5	7.9041	8.0501	8.1136	8.1125	8.1920	8.1082	8.2021	8.1034	8.2032	8.1165	8.2269	7.8973	8.0223	8.0976	8.0831	8.1850	8.0860	8.1827	8.0823	8.1743	8.0857	8.2025	**7.92**
H6	8.1307	8.3666	8.4338	8.4377	8.5030	8.4278	8.6044	8.4175	8.5882	8.4466	8.6391	7.9691	8.1345	8.1869	8.2218	8.3751	8.2137	8.3504	8.2100	8.3302	8.2251	8.3959	**8.24**
H8	4.3551	4.4794	4.5126	4.5575	4.6447	4.5475	4.7145	4.5370	4.6436	4.5664	4.7365	4.5303	4.6786	4.7462	4.7476	4.8759	4.7482	4.8822	4.7450	4.8668	4.7502	4.9096	**5.17**
H(9A-9C)	1.3321	1.3540	1.3262	1.3040	1.2099	1.3061	1.2486	1.3077	1.2890	1.3019	1.2667	1.4215	1.4330	1.4003	1.4518	1.4141	1.4514	1.4203	1.4506	1.4112	1.4523	1.4402	**1.59**
H(8`A-8`C)	2.5558	2.4799	2.4688	2.4871	2.4716	2.4893	2.4473	2.4913	2.4542	2.4852	2.4278	2.9797	2.7985	2.7509	2.7098	2.6741	2.7196	2.5777	2.7260	2.5857	2.7040	2.5459	**2.8**
Nuclei	mpW1PW91											mpW1PW91											
C1	143.6775	143.7517	145.0712	145.0383	147.0466	145.0375	147.4508	145.0422	147.5493	145.0398	146.9032	141.7344	143.5002	145.1332	144.8167	146.6312	144.7477	147.1214	144.6821	147.2314	144.8781	147.2352	**137.3**
C2	136.0542	136.0919	136.5570	135.9437	136.3200	135.9637	136.7277	135.9875	136.6637	135.9216	136.5838	135.6181	135.8562	136.7006	135.8799	136.3768	135.8791	136.9015	135.8845	136.8364	135.8801	136.7516	**136.5**
C3	131.9531	132.6848	133.5226	132.9283	133.8886	132.9196	134.0313	132.9157	134.0011	132.9344	134.0480	131.9585	132.6033	134.2436	132.7719	133.6291	132.7639	134.1271	132.7614	134.0917	132.7784	133.8757	**130.8**
C4	140.7326	140.5294	140.6108	140.5113	140.4711	140.4968	141.0862	140.4896	140.9295	140.5250	141.3562	140.9263	140.4248	140.4138	140.3268	140.3470	140.3314	140.8255	140.3419	140.6750	140.3225	140.9882	**127.3**
C5	130.5628	131.8435	132.5777	132.5599	133.8610	132.5118	133.9579	132.4705	133.8692	132.6067	134.1525	130.7440	131.9721	132.0038	132.6590	134.1172	132.6195	133.5873	132.5853	133.5021	132.6959	134.1599	**130.8**
C6	132.6202	134.5827	135.5253	135.2716	136.7450	135.2185	136.6493	135.1701	136.4412	135.3201	137.3994	133.0360	135.0018	135.4098	135.9117	137.4654	135.8608	137.4920	135.8146	137.2809	135.9591	137.9659	**136.5**
C7	202.2625	206.7780	208.5712	210.3873	211.7261	210.1980	218.0071	210.0218	216.9703	210.5764	217.9186	206.0032	210.5726	212.5449	213.0801	214.2283	212.9380	219.2496	212.7991	218.2288	213.2122	219.7443	**196.6**
C8	63.1677	64.1978	64.8164	64.7550	65.6257	64.7497	66.4081	64.7473	66.2313	64.7573	67.0008	57.9642	59.6631	60.4091	60.6813	61.4932	60.6183	62.4089	60.5602	62.2899	60.7395	62.6802	**61**
C9	22.0834	22.4018	22.5994	22.4665	22.7324	22.4602	22.6398	22.4596	22.5781	22.4708	22.8588	18.9157	19.2074	19.2625	19.4196	19.6241	19.4114	19.7309	19.4086	19.7091	19.4264	20.1124	**15.8**
C4``	130.1889	131.2662	132.1970	131.6747	133.0433	131.6527	132.8682	131.6363	132.8445	131.6945	132.9589	130.1341	131.2651	132.0161	131.6691	132.9895	131.6468	132.8908	131.6297	132.8706	131.6892	132.9353	**123.2**
C8`	35.5524	36.2834	36.4651	36.6650	37.0422	36.6365	37.2069	36.6156	37.1572	36.6948	37.6786	30.8808	31.1456	31.2562	31.2890	31.5810	31.2816	31.5853	31.2802	31.5300	31.2961	31.6619	**31.8**
H2	8.7045	8.7154	8.6873	8.5759	8.5386	8.5780	8.4913	8.5801	8.4848	8.5738	8.5357	8.7643	8.6062	8.5877	8.5029	8.4874	8.5092	8.4460	8.5159	8.4386	8.4976	8.4443	**8.24**
H3	8.0587	8.1621	8.2311	8.1896	8.2951	8.1881	8.3063	8.1867	8.2989	8.1912	8.3303	8.0691	8.1663	8.2190	8.1995	8.2980	8.1981	8.3080	8.1968	8.3004	8.2011	8.3249	**7.92**
H5	7.9630	8.1147	8.1778	8.1763	8.2724	8.1720	8.2797	8.1679	8.2701	8.1806	8.3060	7.9605	8.0949	8.1640	8.1533	8.2582	8.1504	8.2570	8.1477	8.2472	8.1562	8.2802	**7.92**
H6	8.2149	8.4502	8.5198	8.5109	8.6446	8.5024	8.6424	8.4942	8.6249	8.5195	8.7010	8.0374	8.2199	8.2609	8.2983	8.4549	8.2948	8.4233	8.2913	8.4024	8.3020	8.4774	**8.24**
H8	4.3734	4.5005	4.5323	4.5682	4.6533	4.5586	4.7151	4.5495	4.6974	4.5780	4.7166	4.5651	4.7101	4.7707	4.7748	4.9019	4.7718	4.9077	4.7688	4.8883	4.7779	4.9417	**5.17**
H(9A-9C)	1.3071	1.3334	1.2996	1.2790	1.2333	1.2818	1.2077	1.2844	1.2005	1.2762	1.2596	1.3921	1.4050	1.3646	1.4166	1.3764	1.4160	1.3836	1.4157	1.3759	1.4175	1.4105	**1.59**
H(8`A-8`C)	2.4970	2.4170	2.4027	2.4228	2.3920	2.4256	2.3878	2.4283	2.3876	2.4203	2.3751	2.8634	2.7056	2.6488	2.6124	2.5680	2.6174	2.4766	2.6225	2.4862	2.6082	2.4514	**2.8**
Nuclei	O3LYP											O3LYP											
C1	141.1836	142.7400	144.7813	144.2184	146.2802	144.1968	145.4808	144.2640	145.5812	144.2797	145.6497	138.4959	141.4472	142.5593	142.6679	145.9405	142.7270	144.7837	142.6883	144.7861	142.6851	144.9676	**137.3**
C2	131.4397	131.4889	132.2644	131.8082	132.4821	131.8138	132.5709	131.7208	132.6034	131.7954	132.5734	131.1540	131.4322	132.2584	131.3754	131.9766	131.5291	132.3676	131.5305	132.3173	131.3604	132.3268	**136.5**
C3	127.8612	128.3961	129.3971	129.1794	130.7180	129.1803	130.3909	128.7868	130.7892	129.1598	130.5140	127.8400	128.5426	130.3396	128.4583	129.7865	128.8913	129.8068	128.8782	129.7650	128.4543	129.9043	**130.8**
C4	136.4132	135.8351	135.8460	135.7653	135.7374	135.7520	136.4750	135.7540	136.3443	135.7729	136.5459	136.7030	135.9339	136.0357	135.8282	135.4494	135.7963	136.1345	135.8003	136.0338	135.8155	136.2511	**127.3**
C5	126.3016	127.6143	128.3374	127.8450	128.5701	127.8035	129.0516	128.1224	128.5556	127.8864	129.1458	126.6645	127.6228	127.5737	128.6440	129.3611	128.1325	129.3505	128.1013	129.2848	128.6690	129.4945	**130.8**
C6	127.6592	129.2225	129.8546	129.9015	130.9261	129.8395	131.4597	129.9361	131.1426	129.9494	131.7250	128.3326	129.8832	130.5409	130.8174	131.5342	130.6026	132.2011	130.5537	132.0382	130.8568	132.4289	**136.5**
C7	199.3378	205.1848	207.8598	208.9941	210.4109	208.8298	215.0291	208.7695	214.2122	209.1941	215.6717	202.7281	207.7227	208.9774	210.0470	212.5723	210.0386	215.7368	209.9072	214.7938	210.1540	216.4382	**196.6**
C8	63.5509	64.9998	65.7170	65.6909	66.5746	65.6872	67.2126	65.6604	67.0719	65.6939	67.8575	58.5365	60.8631	61.7113	62.0574	63.1139	61.9868	63.8450	61.9390	63.6432	62.0893	64.0165	**61**
C9	21.5536	21.7932	21.9663	22.0544	22.2615	22.0402	22.4359	22.0265	22.3402	22.0696	22.5836	18.1798	18.5075	18.7628	18.7014	18.7680	18.6811	19.0418	18.6763	18.9601	18.6957	19.2949	**15.8**
C4``	131.5244	132.6294	133.6082	133.0271	134.3315	133.0045	134.2651	133.0784	134.1496	133.0490	134.3169	131.4658	132.6230	133.4807	133.1078	134.5097	133.1175	134.3494	133.0933	134.3222	133.1178	134.4127	**123.2**
C8`	35.8915	36.6320	36.9704	37.1226	37.4695	37.1121	37.5623	37.0969	37.5134	37.1135	37.9350	31.4810	31.5404	31.7444	31.7522	32.0722	31.7475	31.9705	31.7311	31.9701	31.7574	32.0236	**31.8**
H2	8.4038	8.2843	8.2386	8.1853	8.1710	8.1874	8.2206	8.1783	8.2093	8.1791	8.2247	8.5333	8.3098	8.3603	8.2130	8.1123	8.2214	8.2048	8.2238	8.2033	8.2108	8.2060	**8.24**
H3	7.9446	8.0359	8.1015	8.0532	8.1753	8.0498	8.1909	8.0622	8.1861	8.0574	8.2043	7.9626	8.0515	8.1131	8.0909	8.1821	8.0837	8.1932	8.0819	8.1874	8.0923	8.2114	**7.92**
H5	7.8530	7.9763	8.0267	8.0293	8.1306	8.0252	8.1438	8.0134	8.1375	8.0331	8.1626	7.8517	7.9709	8.0477	8.0283	8.1193	8.0243	8.1255	8.0208	8.1167	8.0313	8.1494	**7.92**
H6	8.0516	8.2251	8.2627	8.2720	8.3793	8.2645	8.4188	8.2678	8.3941	8.2782	8.4440	7.8868	8.0207	8.0821	8.0984	8.1882	8.0807	8.2094	8.0754	8.1959	8.1035	8.2483	**8.24**
H8	4.4518	4.5459	4.5421	4.5785	4.6535	4.5722	4.6637	4.5690	4.6572	4.5863	4.6845	4.5975	4.7281	4.7930	4.7909	4.9096	4.7872	4.9084	4.7828	4.8946	4.7947	4.9488	**5.17**
H(9A-9C)	1.2134	1.2014	1.1623	1.1786	1.1372	1.1794	1.1808	1.1769	1.1655	1.1764	1.1943	1.3130	1.3368	1.3465	1.3564	1.2868	1.3547	1.3468	1.3530	1.3430	1.3577	1.3596	**1.59**
H(8`A-8`C)	2.5244	2.4849	2.4681	2.4873	2.4562	2.4877	2.4515	2.4888	2.4546	2.4874	2.4316	2.9203	2.7421	2.6837	2.6580	2.6204	2.6641	2.5362	2.6674	2.5484	2.6547	2.5105	**2.8**
Nuclei	OLYP											OLYP											
C1	139.9602	142.1202	143.6629	142.8443	145.6409	142.8247	144.2168	142.8022	144.5979	142.8634	144.3219	137.5022	140.9341	142.4201	141.6150	144.5011	141.6107	143.4280	141.5952	143.4745	141.6043	143.5978	**137.3**
C2	129.0985	129.3943	129.9739	129.5799	129.9603	129.5878	130.2659	129.5894	130.1611	129.5609	130.2586	128.9770	129.3066	130.0189	129.3003	129.7427	129.3070	130.0958	129.3077	130.0390	129.2849	130.0356	**136.5**
C3	125.8183	126.4055	127.2472	127.1042	127.6922	127.1051	127.9839	127.0979	127.9494	127.0884	128.1240	126.0334	127.0496	128.5779	126.9285	127.7588	126.9213	127.7943	126.9084	127.7484	126.9263	127.8950	**130.8**
C4	134.2360	133.5218	133.6917	133.6468	133.2511	133.6439	134.1973	133.6367	133.9875	133.6421	134.3242	134.6346	133.6249	133.8060	133.5807	133.2260	133.5856	133.8951	133.5864	133.7881	133.5683	134.0106	**127.3**
C5	124.3149	125.5415	126.4757	125.8444	127.1774	125.8037	127.2441	125.7596	127.1354	125.8787	127.3730	124.5820	125.2320	125.5470	126.1307	127.2817	126.1017	127.3451	126.0673	127.2851	126.1494	127.4852	**130.8**
C6	125.3481	126.8775	127.7206	127.6594	128.8246	127.6058	129.2498	127.5467	129.0188	127.7001	129.5341	125.9976	127.2141	127.7780	128.2067	129.2784	128.1507	129.7985	128.0911	129.6341	128.2533	130.0248	**136.5**
C7	198.7061	205.0031	207.1463	207.8294	210.2832	207.6757	213.9628	207.5229	213.0854	207.9863	214.3909	202.7830	207.5159	209.6461	209.4435	211.3523	209.3617	214.4687	209.2687	213.6168	209.5061	215.2012	**196.6**
C8	64.9955	66.4933	67.2492	67.1658	68.3192	67.1364	68.6159	67.1031	68.7169	67.1901	69.2892	59.5164	62.4587	63.1159	63.4829	64.6565	63.4329	65.3533	63.3772	65.1734	63.5208	65.4493	**61**
C9	21.6882	21.9650	22.1779	22.2783	22.5195	22.2700	22.8023	22.2556	22.6416	22.2747	22.8138	18.1987	18.5447	18.7225	18.7771	18.9690	18.7657	19.2330	18.7499	19.1542	18.7801	19.4739	**15.8**
C4``	134.9145	136.0601	137.1334	136.5354	137.9918	136.5107	137.7975	136.4810	137.8046	136.5518	137.8754	134.8717	136.0092	137.0114	136.6086	138.0035	136.5871	137.8419	136.5598	137.8153	136.6195	137.8932	**123.2**
C8`	36.56895	37.3427	37.6131	37.6993	38.1818	37.6821	38.1865	37.6607	38.0949	37.7101	38.4667	32.0509	32.1657	32.5010	32.4185	32.6442	32.4111	32.5601	32.3981	32.5506	32.4164	32.6271	**31.8**
H2	8.2078	8.0715	8.0687	8.0362	7.9736	8.0380	8.0739	8.0395	8.0420	8.0331	8.0802	8.3185	8.0821	8.0927	8.0542	7.9924	8.0540	8.0721	8.0541	8.0658	8.0544	8.0741	**8.24**
H3	7.8553	7.9389	8.0214	7.9735	8.0756	7.9711	8.1007	7.9688	8.0917	7.9756	8.1183	7.8838	7.9638	8.0429	8.0096	8.0974	8.0079	8.1147	8.0062	8.1089	8.0108	8.1313	**7.92**
H5	7.7659	7.8612	7.9345	7.9375	8.0374	7.9337	8.0587	7.9298	8.0401	7.9408	8.0724	7.7686	7.8814	7.9500	7.9330	8.0250	7.9297	8.0352	7.9263	8.0263	7.9358	8.0582	**7.92**
H6	7.9547	8.0913	8.1664	8.1673	8.2311	8.1615	8.2965	8.1557	8.2613	8.1723	8.3396	7.7916	7.8770	7.9503	7.9601	8.0659	7.9547	8.0863	7.9494	8.0709	7.9650	8.1261	**8.24**
H8	4.5622	4.5888	4.6023	4.6465	4.6517	4.6426	4.7084	4.6387	4.6846	4.6494	4.7477	4.6763	4.7899	4.8584	4.8610	4.9696	4.8566	4.9758	4.8521	4.9592	4.8648	5.0184	**5.17**
H(9A-9C)	1.2077	1.1908	1.1787	1.1926	1.1536	1.1923	1.1937	1.1919	1.1875	1.1923	1.2043	1.2884	1.3277	1.3136	1.3578	1.3099	1.3553	1.3597	1.3528	1.3542	1.3599	1.3702	**1.59**
H(8`A-8`C)	2.5653	2.5334	2.5139	2.5254	2.5139	2.5265	2.5013	2.5274	2.5009	2.5239	2.4674	2.9743	2.7841	2.7578	2.7126	2.6563	2.7171	2.5832	2.7214	2.5934	2.7079	2.5580	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S2. Cont. V

Nuclei	R											S										Exp. [b]
	OPBE											OPBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.1705	139.3531	140.8748	140.1631	142.5639	140.1575	141.3810	140.0883	141.7297	140.1583	141.3492	134.7067	138.4686	139.9807	138.9365	142.0073	138.9275	140.8309	138.9022	141.0985	138.9391	141.1038	**137.3**
C2	127.7617	128.1200	128.6511	128.2188	128.7282	128.2367	128.9618	128.2383	128.7878	128.1968	129.1422	127.6513	128.0267	128.7495	128.0062	128.4535	128.0240	128.8323	128.0236	128.7275	127.9840	128.7912	**136.5**
C3	124.3807	125.1126	125.8983	125.7515	126.4788	125.7607	126.6838	125.7624	126.4959	125.7388	127.6591	124.5553	125.2614	127.0954	125.4862	126.3248	125.4873	126.3989	125.4706	126.3649	125.4812	126.5224	**130.8**
C4	131.9388	131.4820	131.5975	131.4504	131.3346	131.4539	132.1930	131.4423	131.9240	131.4422	132.3309	132.2005	131.4977	131.5545	131.4104	131.0407	131.4272	131.7672	131.4263	131.5951	131.3905	131.8913	**127.3**
C5	122.9812	124.2328	125.0742	124.4322	125.7634	124.4046	125.8959	124.3546	125.9314	124.4526	125.4455	123.2533	124.2950	124.2296	124.8077	125.9186	124.7943	126.0436	124.7630	125.9272	124.8168	126.2206	**130.8**
C6	123.8307	125.4372	126.2114	126.0669	127.3200	126.0241	127.7150	125.9679	127.5633	126.1029	127.7894	124.4203	125.7670	126.1452	126.6426	127.6163	126.6054	128.1281	126.5500	127.8906	126.6723	128.3575	**136.5**
C7	196.3849	202.5087	204.5290	205.1428	207.0013	205.0151	210.8618	204.8288	209.9772	205.2541	211.1105	199.1310	204.5085	206.3201	206.2041	208.2288	206.1145	211.4903	206.0087	210.7194	206.2851	212.1782	**196.6**
C8	62.4709	64.0302	64.6985	64.7424	65.6816	64.7349	66.1331	64.6974	66.1717	64.7445	66.8068	57.8242	60.1799	61.0203	61.1110	62.3348	61.0769	62.9027	61.0240	62.7872	61.1368	63.1085	**61**
C9	20.9292	21.2927	21.4056	21.5100	21.7296	21.5111	21.9116	21.4904	21.8147	21.5036	22.0506	17.5730	17.9159	18.0716	18.1348	18.2682	18.1374	18.5028	18.1220	18.4151	18.1267	18.8048	**15.8**
C4``	130.5332	131.6387	132.5622	131.9557	133.3215	131.9477	133.1551	131.9164	133.1932	131.9577	133.0760	130.5203	131.6580	132.4534	132.0497	133.3431	132.0441	133.1826	132.0205	133.1696	132.0504	133.2688	**123.2**
C8`	35.5134	36.3454	36.5158	36.5901	36.9518	36.5905	37.0128	36.5812	36.9266	36.5865	37.3636	30.8398	31.0922	31.1927	31.2282	31.3990	31.2324	31.3836	31.2195	31.3509	31.2200	31.4215	**31.8**
H2	8.2340	8.1148	8.1032	8.0690	8.0346	8.0708	8.1186	8.0754	8.0832	8.0668	8.1358	8.3339	8.1013	8.1121	8.0860	8.0136	8.0874	8.0969	8.0880	8.0770	8.0840	8.0950	**8.24**
H3	7.9047	7.9952	8.0729	8.0251	8.1370	8.0227	8.1625	8.0185	8.1460	8.0265	8.1810	7.9349	8.0361	8.0896	8.0694	8.1477	8.0682	8.1620	8.0661	8.1617	8.0699	8.1809	**7.92**
H5	7.8140	7.9193	7.9869	7.9902	8.0903	7.9866	8.1083	7.9824	8.0863	7.9928	8.1279	7.8184	7.9310	8.0002	7.9874	8.0758	7.9847	8.0903	7.9813	8.0770	7.9893	8.1156	**7.92**
H6	8.0050	8.1449	8.2105	8.2001	8.2963	8.1943	8.3508	8.1895	8.3179	8.2050	8.3699	7.8118	7.9244	7.9694	8.0103	8.1006	8.0054	8.1403	7.9997	8.1090	8.0143	8.1780	**8.24**
H8	4.5750	4.6169	4.6163	4.6535	4.6849	4.6492	4.7248	4.6435	4.6925	4.6569	4.7507	4.7071	4.8224	4.8825	4.8870	4.9836	4.8835	5.0029	4.8793	4.9746	4.8898	5.0476	**5.17**
H(9A-9C)	1.1645	1.1520	1.1319	1.1511	1.1078	1.1516	1.1496	1.1519	1.1411	1.1500	1.1631	1.2584	1.2784	1.2604	1.3115	1.2451	1.3101	1.3038	1.3080	1.2913	1.3119	1.3163	**1.59**
H(8`A-8`C)	2.4882	2.4560	2.4281	2.4490	2.4167	2.4506	2.4058	2.4512	2.4095	2.4467	2.3784	2.8231	2.6613	2.5976	2.5866	2.5173	2.5908	2.4581	2.5944	2.4688	2.5822	2.4318	**2.8**
Nuclei	OPW91											OPW91										
C1	137.4597	139.6571	141.1765	140.4597	142.8571	140.4439	141.6692	140.3742	142.0279	140.4515	141.8930	134.9688	138.7552	140.2125	139.1782	142.2827	139.1624	141.0945	139.1309	141.3464	139.1755	141.3625	**137.3**
C2	127.9797	128.3398	128.8650	128.4443	128.9343	128.4521	129.1728	128.4444	129.0010	128.4183	129.2461	127.8652	128.2436	128.9631	128.2357	128.6605	128.2429	129.0418	128.2332	128.9504	128.2106	129.0047	**136.5**
C3	124.6039	125.3315	126.1131	125.9782	126.6927	125.9772	126.8985	125.9676	126.7142	125.9618	127.1807	124.7724	125.4850	127.3195	125.7202	126.5414	125.7113	126.6139	125.6857	126.5796	125.7104	126.7402	**130.8**
C4	132.1909	131.7183	131.8284	131.6944	131.5594	131.6888	132.4210	131.6689	132.1531	131.6818	132.5623	132.4606	131.7467	131.8184	131.6700	131.2796	131.6759	132.0098	131.6652	131.8362	131.6463	132.1379	**127.3**
C5	123.1962	124.4561	125.2948	124.6617	125.9811	124.6247	126.1113	124.5671	126.1427	124.6781	126.1629	123.4743	124.5119	124.4563	125.0520	126.1344	125.0281	126.2586	124.9869	126.1569	125.0563	126.4370	**130.8**
C6	124.0524	125.6614	126.4310	126.3037	127.5409	126.2513	127.9385	126.1856	127.7829	126.3356	128.1599	124.6525	125.9973	126.3809	126.8753	127.8433	126.8264	128.3623	126.7596	128.1099	126.9030	128.5956	**136.5**
C7	196.7274	202.8832	204.9061	205.5281	207.3817	205.3903	211.2558	205.2026	210.3858	205.6361	211.9283	199.5026	204.9103	206.7634	206.6519	208.6291	206.5552	211.8811	206.4436	211.2017	206.7273	212.5726	**196.6**
C8	62.6493	64.2129	64.8810	64.9221	65.8580	64.9033	66.3094	64.8572	66.3503	64.9210	67.0023	57.9751	60.3483	61.1057	61.2786	62.4953	61.2347	63.0688	61.1727	62.9503	61.3009	63.2711	**61**
C9	20.9903	21.3587	21.4686	21.5829	21.7945	21.5740	21.9756	21.5458	21.8774	21.5726	22.0940	17.6485	17.9941	18.1352	18.2188	18.3457	18.2106	18.5830	18.1850	18.4931	18.2079	18.8831	**15.8**
C4``	131.0411	132.1581	133.0850	132.4847	133.8494	132.4664	133.6815	132.4269	133.7194	132.4833	133.7333	131.0250	132.1776	132.9708	132.5794	133.8715	132.5634	133.7093	132.5303	133.6927	132.5760	133.7972	**123.2**
C8`	35.5788	36.4142	36.5880	36.6695	37.0215	36.6598	37.0840	36.6392	37.0002	36.6620	37.4600	30.9369	31.1884	31.3183	31.3166	31.4965	31.3104	31.4770	31.2881	31.4411	31.3047	31.5220	**31.8**
H2	8.2376	8.1163	8.1047	8.0719	8.0358	8.0731	8.1200	8.0769	8.0843	8.0694	8.1283	8.3398	8.1037	8.1179	8.0926	8.0157	8.0928	8.0997	8.0927	8.0780	8.0907	8.0982	**8.24**
H3	7.9051	7.9951	8.0727	8.0259	8.1364	8.0228	8.1619	8.0188	8.1458	8.0269	8.1820	7.9350	8.0360	8.0904	8.0608	8.1473	8.0588	8.1617	8.0567	8.1527	8.0609	8.1805	**7.92**
H5	7.8149	7.9194	7.9869	7.9911	8.0901	7.9869	8.1081	7.9825	8.0864	7.9933	8.1347	7.8193	7.9314	8.0022	7.9941	8.0760	7.9907	8.0907	7.9870	8.0786	7.9956	8.1160	**7.92**
H6	8.0050	8.1444	8.2103	8.2020	8.2966	8.1956	8.3515	8.1905	8.3180	8.2065	8.3823	7.8141	7.9258	7.9756	8.0220	8.1020	8.0163	8.1416	8.0104	8.1176	8.0256	8.1797	**8.24**
H8	4.5746	4.6164	4.6158	4.6549	4.6853	4.6499	4.7254	4.6444	4.6935	4.6578	4.7597	4.7034	4.8187	4.8824	4.8952	4.9811	4.8910	5.0002	4.8866	4.9819	4.8976	5.0449	**5.17**
H(9A-9C)	1.1663	1.1536	1.1336	1.1534	1.1093	1.1531	1.1514	1.1530	1.1427	1.1521	1.1644	1.2598	1.2794	1.2615	1.3158	1.2465	1.3136	1.3056	1.3111	1.2943	1.3162	1.3181	**1.59**
H(8`A-8`C)	2.4892	2.4573	2.4298	2.4510	2.4185	2.4519	2.4075	2.4523	2.4114	2.4485	2.3848	2.8285	2.6667	2.6107	2.5893	2.5237	2.5929	2.4635	2.5963	2.4721	2.5846	2.4377	**2.8**
Nuclei	PBE											PBE										
C1	141.8631	143.3996	143.4023	143.4628	145.4879	143.4561	145.4178	143.4610	145.1279	143.4874	145.5867	139.2708	141.5219	143.4102	142.7731	144.9146	142.7178	145.2630	142.6372	145.2443	142.8538	145.4659	**137.3**
C2	133.4186	133.6311	134.0721	133.4133	133.9799	133.4308	134.2150	133.4581	134.1386	133.4134	134.2237	132.7759	133.2763	134.2330	133.3136	133.9525	133.3935	134.3866	133.3136	134.5231	133.3361	134.3976	**136.5**
C3	129.9155	130.7528	131.7007	131.0070	132.1694	130.9925	132.2060	130.9890	132.1564	131.0382	132.3163	129.9508	130.7042	132.5348	130.8157	131.7360	131.0657	131.8477	130.8099	132.3223	130.8405	131.9693	**130.8**
C4	138.7860	138.5046	138.7194	138.5600	138.5740	138.5476	139.3123	138.5468	139.2036	138.5901	139.4665	139.0345	138.5902	138.6141	138.4166	138.5086	138.4027	139.0528	138.4375	138.8754	138.4305	139.1911	**127.3**
C5	128.6033	129.9779	130.7274	130.5997	131.9005	130.5547	132.1191	130.5201	132.0328	130.6600	132.3177	128.9825	130.2494	130.1344	130.7821	132.4342	130.4568	132.3849	130.7224	131.6757	130.8339	132.5415	**130.8**
C6	130.4794	132.2379	133.4645	133.0987	134.7677	133.0463	134.9776	133.0030	134.8855	133.1652	135.3860	130.8938	132.8695	133.3564	133.7717	135.4639	133.6211	135.7114	133.6776	135.3592	133.8387	136.0397	**136.5**
C7	202.7985	208.0403	208.9232	210.4607	212.0494	210.2892	216.8047	210.1344	215.5850	210.6467	217.5814	206.9804	211.3922	213.4617	213.4967	215.0791	213.4114	219.1548	213.2492	218.3341	213.6333	219.6605	**196.6**
C8	67.3143	68.7236	69.1465	68.9770	70.1078	68.9677	70.6698	68.9674	70.4564	69.0017	71.4631	61.7677	63.6266	64.4232	64.6359	65.6899	64.5404	66.4416	64.5187	66.2891	64.7123	66.7519	**61**
C9	23.0003	23.3850	23.7083	23.5481	23.9889	23.5356	23.9528	23.5348	23.9301	23.5790	24.1831	19.8407	20.3930	20.4366	20.5729	20.8750	20.5480	21.0490	20.5636	21.0175	20.5992	21.5615	**15.8**
C4``	140.2034	141.4730	142.4538	141.8314	143.4051	141.8084	143.2287	141.7959	143.2013	141.8707	143.3096	140.1262	141.4196	142.2762	141.7968	143.3315	141.7792	143.1634	141.7603	143.1858	141.8365	143.2506	**123.2**
C8`	37.1014	37.8421	37.9986	38.1066	38.5774	38.0827	38.7418	38.0703	38.7064	38.1476	39.2237	32.0004	32.2555	32.3336	32.2971	32.6181	32.2950	32.6818	32.2939	32.6459	32.3228	32.7231	**31.8**
H2	8.4576	8.36777	8.4586	8.3482	8.3212	8.3499	8.3239	8.3521	8.3407	8.3470	8.3269	8.5525	8.4135	8.3882	8.3033	8.2705	8.3149	8.2537	8.3155	8.2691	8.2991	8.2561	**8.24**
H3	7.8848	7.9803	8.0583	8.0121	8.1140	8.0105	8.1296	8.0094	8.1247	8.0141	8.1479	7.9054	8.0006	8.0563	8.0246	8.1188	8.0195	8.1278	8.0227	8.1255	8.0264	8.1434	**7.92**
H5	7.7893	7.9230	8.0029	7.9940	8.0932	7.9897	8.1043	7.9859	8.0962	7.9987	8.1286	7.8007	7.9300	7.9901	7.9773	8.0868	7.9748	8.0862	7.9724	8.0702	7.9806	8.1082	**7.92**
H6	8.0993	8.2516	8.3867	8.3644	8.4865	8.3568	8.5054	8.3498	8.5034	8.3723	8.5446	7.8842	8.0572	8.0908	8.1210	8.2687	8.1127	8.2628	8.1145	8.2356	8.1251	8.3036	**8.24**
H8	4.6410	4.6918	4.7669	4.7880	4.8517	4.7797	4.8908	4.7723	4.8667	4.7968	4.9231	4.8068	4.9481	5.0044	5.0002	5.1266	4.9997	5.1330	4.9949	5.1207	5.0035	5.1702	**5.17**
H(9A-9C)	1.3709	1.3634	1.3719	1.3478	1.3212	1.3499	1.3256	1.3521	1.3321	1.3463	1.3428	1.4738	1.4982	1.4579	1.5012	1.4642	1.5010	1.4814	1.5004	1.4734	1.5026	1.5081	**1.59**
H(8`A-8`C)	2.6087	2.5568	2.5036	2.5160	2.4922	2.5187	2.4795	2.5218	2.4777	2.5141	2.4579	2.9833	2.8192	2.7537	2.7177	2.6688	2.7251	2.5838	2.7291	2.5962	2.7134	2.5525	**2.8**
Nuclei	PBE0											PBE0										
C1	143.1162	143.2977	144.6404	144.4795	146.4414	144.4926	146.0592	144.5049	145.8510	144.4668	146.4097	141.2941	143.0511	144.9279	144.3102	145.9402	144.2352	146.6936	144.1611	146.7784	144.3820	146.7562	**137.3**
C2	135.7837	135.8343	136.3252	135.7455	136.1677	135.7541	136.4962	135.7638	136.3403	135.7395	136.4205	135.3588	135.6224	136.5017	135.6393	136.0947	135.6335	136.7346	135.6301	136.6126	135.6483	136.5231	**136.5**
C3	131.6955	132.4336	133.2786	132.6861	133.6635	132.6700	133.8245	132.6552	133.7000	132.7038	133.8625	131.6976	132.3612	134.0368	132.5253	133.3429	132.5124	133.9498	132.5011	133.8595	132.5405	133.6333	**130.8**
C4	140.4830	140.3056	140.3817	140.2842	140.2185	140.2648	141.0889	140.2484	140.9088	140.3066	141.1465	140.6735	140.2088	140.2282	140.1177	140.1591	140.1166	140.6777	140.1178	140.4656	140.1222	140.7939	**127.3**
C5	130.3075	131.6292	132.3294	132.2917	133.5018	132.2427	133.7261	132.1957	133.6056	132.3419	133.8592	130.4918	131.7197	131.7438	132.3989	133.8730	132.3544	133.3835	132.3116	133.2385	132.4437	133.9130	**130.8**
C6	132.4835	134.4432	135.3932	135.1955	136.6965	135.1265	137.0785	135.0599	136.9046	135.2644	137.3019	132.8916	134.8800	135.3198	135.7838	137.3947	135.7280	137.4465	135.6732	137.1697	135.8389	137.8655	**136.5**
C7	201.8665	206.4072	208.1892	209.6696	210.9568	209.5261	216.1894	209.3836	214.8901	209.8082	217.2456	205.6493	210.1743	212.2659	212.6673	213.7386	212.5198	218.8237	212.3722	217.7955	212.8082	219.2669	**196.6**
C8	63.0753	64.1043	64.7522	64.6963	65.6215	64.6796	66.2128	64.6630	65.9330	64.7132	66.9059	57.7716	59.4213	60.1473	60.3870	61.1355	60.3198	62.1586	60.2544	61.9990	60.4531	62.3768	**61**
C9	22.0745	22.3894	22.5854	22.5293	22.8504	22.5097	22.8273	22.4922	22.7550	22.5512	22.8925	18.9014	19.2082	19.3020	19.4057	19.5967	19.3927	19.7945	19.3813	19.7137	19.4206	20.1343	**15.8**
C4``	129.7474	130.8239	131.7444	131.2173	132.5619	131.1911	132.4830	131.1666	132.4014	131.2449	132.5118	129.6964	130.8170	131.5870	131.2078	132.5042	131.1808	132.4835	131.1554	132.4061	131.2360	132.4783	**123.2**
C8`	35.4674	36.1857	36.3689	36.5170	36.8975	36.4923	37.1587	36.4697	37.0542	36.5433	37.5564	30.6234	30.9137	31.0079	31.0525	31.3470	31.0410	31.3975	31.0315	31.2792	31.0670	31.4143	**31.8**
H2	8.7147	8.7173	8.6873	8.5885	8.5507	8.5882	8.5652	8.5880	8.5746	8.5887	8.5435	8.7671	8.6127	8.5951	8.5129	8.5049	8.5191	8.4552	8.5256	8.4426	8.5069	8.4483	**8.24**
H3	8.0553	8.1585	8.2263	8.1848	8.2844	8.1830	8.3080	8.1812	8.2993	8.1862	8.3227	8.0640	8.1588	8.2150	8.1916	8.2875	8.1900	8.3027	8.1883	8.2923	8.1929	8.3153	**7.92**
H5	7.9549	8.1064	8.1682	8.1671	8.2608	8.1625	8.2776	8.1578	8.2669	8.1713	8.2985	7.9550	8.0876	8.1567	8.1456	8.2534	8.1424	8.2505	8.1393	8.2379	8.1482	8.2733	**7.92**
H6	8.2264	8.4572	8.5229	8.5125	8.6393	8.5038	8.6750	8.4954	8.6680	8.5206	8.7022	8.0392	8.2228	8.2684	8.3016	8.4654	8.2978	8.4308	8.2938	8.4058	8.3049	8.4818	**8.24**
H8	4.3669	4.4939	4.5180	4.5458	4.6122	4.5371	4.6572	4.5289	4.6431	4.5540	4.6881	4.5682	4.7145	4.7804	4.7826	4.9085	4.7792	4.9194	4.7757	4.8970	4.7854	4.9494	**5.17**
H(9A-9C)	1.3197	1.3409	1.3074	1.3001	1.2578	1.3004	1.2731	1.3008	1.2705	1.2995	1.2751	1.4057	1.4160	1.3801	1.4268	1.3902	1.4261	1.3951	1.4257	1.3842	1.4273	1.4190	**1.59**
H(8`A-8`C)	2.5034	2.4217	2.4093	2.4310	2.4023	2.4333	2.3945	2.4355	2.3886	2.4285	2.3771	2.8635	2.7056	2.6441	2.6150	2.5714	2.6197	2.4795	2.6245	2.4852	2.6105	2.4508	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S2. Cont. VI

Nuclei	R											S										Exp. [b]
	TPSS											TPSS										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	138.4874	138.6401	140.0652	139.8115	141.6833	139.8518	140.8491	139.8948	140.4265	139.7736	141.1525	136.2205	138.0809	139.8089	139.1643	140.5853	139.0922	141.1900	139.0319	140.0996	139.2438	141.3795	**137.3**
C2	130.3555	130.3455	130.9630	130.3380	130.7904	130.3579	131.0082	130.3877	130.8814	130.3281	130.9656	129.7085	130.0618	130.9902	130.1591	130.5676	130.1582	131.2788	130.1690	131.3032	130.1707	131.0704	**136.5**
C3	126.7618	127.4477	128.3735	127.7101	128.7284	127.7024	128.8162	127.7054	128.1883	127.7275	128.8928	126.7542	127.3701	129.1561	127.6033	128.4227	127.5966	128.9720	127.6013	128.7547	127.6200	128.6506	**130.8**
C4	135.5994	135.2656	135.4261	135.2439	135.1511	135.2340	136.0274	135.2371	135.7502	135.2659	136.1231	135.8288	135.1965	135.3258	135.1133	135.1747	135.1233	135.6693	135.1449	136.2418	135.1145	135.8311	**127.3**
C5	125.6556	126.8716	127.6285	127.4992	128.6210	127.4593	128.8274	127.4318	127.9136	127.5486	128.9717	125.9826	127.0144	127.1185	127.6052	129.1010	127.5779	128.4905	127.5616	128.7153	127.6414	129.1349	**130.8**
C6	127.4328	129.1977	130.1831	129.9871	131.4172	129.9253	131.8798	129.8768	130.3684	130.0588	132.1768	127.7647	129.5289	130.1358	130.5039	132.1055	130.4562	132.1868	130.4187	131.5510	130.5585	132.6150	**136.5**
C7	198.5920	202.7828	204.5831	205.7343	207.1045	205.6224	211.3801	205.5167	206.3109	205.8452	212.3667	202.5104	206.5448	208.5961	208.6571	209.7881	208.5301	214.0975	208.4147	208.9620	208.7876	214.5995	**196.6**
C8	65.8155	66.7612	67.5340	67.3893	68.3695	67.3846	68.7561	67.3888	67.6305	67.4014	69.4876	60.8765	62.5968	63.3482	63.5790	64.3286	63.5196	65.1597	63.4720	65.1064	63.6461	65.3912	**61**
C9	23.6237	23.8996	24.1677	24.1003	24.4389	24.0875	24.5658	24.0866	24.1551	24.1238	24.6959	20.5688	21.0214	21.1212	21.2722	21.4782	21.2648	21.7195	21.2684	23.2193	21.2896	22.1093	**15.8**
C4``	137.7788	138.8875	139.9522	139.3580	140.7821	139.3391	140.6054	139.3315	139.8609	139.3859	140.6586	137.7230	138.8767	139.7854	139.3487	140.7126	139.3287	140.6145	139.3199	140.3854	139.3780	140.6202	**123.2**
C8`	37.5430	38.1648	38.4275	38.4800	38.8830	38.4626	39.0889	38.4571	38.5831	38.5075	39.5229	33.1386	33.1916	33.4054	33.3412	33.6585	33.3418	33.6704	33.3534	35.2137	33.3509	33.6757	**31.8**
H2	8.4831	8.4885	8.4688	8.3752	8.3439	8.3732	8.3901	8.3725	8.2124	8.3783	8.3726	8.5639	8.4194	8.4047	8.3249	8.3289	8.3317	8.2944	8.3392	8.4499	8.3189	8.2746	**8.24**
H3	7.8383	7.9432	8.0169	7.9713	8.0724	7.9691	8.0931	7.9676	7.8059	7.9738	8.1075	7.8492	7.9458	8.0094	7.9788	8.0799	7.9772	8.0911	7.9762	8.0896	7.9807	8.1012	**7.92**
H5	7.7486	7.8970	7.9648	7.9568	8.0557	7.9518	8.0732	7.9475	7.7857	7.9620	8.0916	7.7600	7.8918	7.9556	7.9473	8.0616	7.9444	8.0474	7.9419	8.0555	7.9505	8.0756	**7.92**
H6	7.9880	8.2148	8.2769	8.2724	8.3956	8.2628	8.4566	8.2542	8.0936	8.2825	8.4864	7.8034	7.9859	8.0380	8.0684	8.2400	8.0645	8.2144	8.0610	8.1738	8.0725	8.2631	**8.24**
H8	4.5160	4.6256	4.6486	4.6692	4.7290	4.6608	4.7842	4.6536	4.4786	4.6781	4.8076	4.6565	4.8048	4.8679	4.8726	4.9986	4.8689	5.0142	4.8657	5.0024	4.8764	5.0440	**5.17**
H(9A-9C)	1.3674	1.3877	1.3661	1.3612	1.3285	1.3608	1.3535	1.3611	1.1729	1.3623	1.3613	1.4597	1.4867	1.4510	1.4999	1.4790	1.4994	1.4828	1.4994	1.6613	1.5010	1.5074	**1.59**
H(8`A-8`C)	2.5573	2.4706	2.4641	2.4810	2.4598	2.4838	2.4370	2.4869	2.3032	2.4784	2.4181	2.9545	2.7853	2.7366	2.6999	2.6676	2.7052	2.5726	2.7113	2.8641	2.6954	2.5405	**2.8**
Nuclei	VSXC											VSXC										
C1	135.5320	136.1083	136.8637	136.2826	137.4077	136.2774	137.1255	136.2699	137.0028	136.2885	137.1077	135.7904	137.5107	138.1956	137.8330	139.2979	137.9754	139.3047	137.9630	139.6696	137.8585	139.4916	**137.3**
C2	129.3157	129.4736	129.9493	129.4494	129.8698	129.4551	129.8004	129.4584	130.1343	129.4454	130.2937	129.1972	129.3664	129.9198	128.9784	129.4637	129.3870	130.2399	129.3877	130.1862	128.9796	129.7951	**136.5**
C3	125.2117	125.7702	126.6038	125.9248	126.9657	125.9213	125.6262	125.9150	127.0602	125.9296	127.0892	126.2216	126.6147	127.5239	124.5753	125.5735	126.7396	127.8493	126.7316	127.7586	124.5965	125.7305	**130.8**
C4	135.3713	135.1595	135.2035	135.2960	135.2445	135.2872	135.9584	135.2767	135.8365	135.3064	136.1458	135.2871	134.8722	134.9284	135.3574	135.2907	134.9218	135.4560	134.9153	135.2984	135.3635	136.0927	**127.3**
C5	121.9823	123.5127	124.3640	124.3347	125.4634	124.2878	128.0607	124.2388	125.4072	124.3807	125.6829	121.5537	122.8415	123.6747	125.8259	126.9191	123.5476	124.7157	123.5007	124.5929	125.8586	126.9858	**130.8**
C6	127.7647	129.5771	130.5541	130.5765	132.0581	130.5182	132.5500	130.4575	132.2802	130.6335	132.8392	128.0349	130.1858	131.1601	131.3995	132.9642	131.1499	133.0889	131.0905	132.8624	131.4521	133.5690	**136.5**
C7	192.2113	196.2843	197.5772	198.3240	199.2710	198.2056	202.9130	198.0847	202.1073	198.4373	203.6553	194.1043	198.2719	199.6023	200.2182	201.2591	200.1943	204.9444	200.0763	204.2310	200.3315	205.5324	**196.6**
C8	71.3941	72.2540	72.8585	72.5622	73.4140	72.5483	73.7226	72.5321	73.6227	72.5767	74.3146	63.7285	64.8944	65.5445	65.5908	66.5560	65.4844	66.8116	65.4488	66.7643	65.6271	67.3515	**61**
C9	26.9127	27.8221	28.1721	28.4757	29.0419	28.4366	29.3216	28.3957	29.2968	28.5146	29.4164	28.2922	28.3244	28.2994	28.3788	28.5289	28.4052	28.4778	28.4007	28.4742	28.3840	28.7185	**15.8**
C4``	135.5317	136.7335	137.6571	137.2377	138.6073	137.2117	138.3820	137.1832	138.3972	137.2640	138.5237	135.7401	136.9252	137.8376	137.2008	138.5060	137.3761	138.5740	137.3505	138.5691	137.2248	138.4294	**123.2**
C8`	40.5707	40.9800	41.1265	41.1967	41.3611	41.1869	41.4015	41.1749	41.2908	41.2076	41.7454	35.5106	35.8394	36.1088	36.2260	36.5003	36.1191	36.4555	36.0951	36.2952	36.2453	36.8886	**31.8**
H2	8.7582	8.7052	8.7087	8.6706	8.6653	8.6728	8.6045	8.6752	8.6636	8.6684	8.6626	8.7140	8.5943	8.6061	8.4823	8.4696	8.5515	8.5281	8.5536	8.5220	8.4797	8.4460	**8.24**
H3	7.9427	8.0319	8.1219	8.0555	8.1795	8.0546	8.1119	8.0537	8.1835	8.0563	8.1992	7.9927	8.0899	8.1784	7.9874	8.0670	8.1147	8.2500	8.1138	8.2470	7.9891	8.0908	**7.92**
H5	7.7953	7.9388	7.9985	8.0111	8.1090	8.0069	8.1888	8.0027	8.1059	8.0151	8.1415	7.8402	7.9674	8.0357	8.0601	8.1881	8.0319	8.1306	8.0277	8.1157	8.0635	8.2126	**7.92**
H6	8.1822	8.3666	8.4536	8.4649	8.6205	8.4589	8.6981	8.4531	8.6426	8.4705	8.6960	7.8519	8.0504	8.1544	8.1973	8.3615	8.1500	8.3438	8.1435	8.3146	8.2031	8.4172	**8.24**
H8	4.4313	4.4994	4.5225	4.5633	4.6386	4.5590	4.6539	4.5548	4.6453	4.5674	4.6896	4.7033	4.8678	4.9239	4.9588	5.0770	4.9551	5.1062	4.9498	5.0899	4.9646	5.1360	**5.17**
H(9A-9C)	1.6030	1.6168	1.6077	1.6168	1.6004	1.6169	1.6244	1.6171	1.6161	1.6166	1.6302	1.7817	1.7716	1.7670	1.7683	1.7542	1.7863	1.7833	1.7851	1.7721	1.7694	1.7810	**1.59**
H(8`A-8`C)	2.7295	2.6787	2.6488	2.6592	2.6160	2.6602	2.5999	2.6614	2.6029	2.6582	2.5741	2.8584	2.7230	2.6927	2.6715	2.6207	2.6910	2.6028	2.6921	2.5929	2.6699	2.5358	**2.8**
Nuclei	wB97											wB97										
C1	143.9410	144.0359	145.4039	144.9644	147.0502	145.0037	146.2819	145.0327	145.8015	144.9159	146.5497	142.7671	144.3174	145.9622	145.4512	147.5684	137.3985	147.5404	145.2738	147.6441	145.5026	147.7260	**137.3**
C2	136.6884	136.6565	137.1174	136.5369	136.9387	136.5406	137.2677	136.5439	137.2066	136.5339	137.2596	136.4760	136.5383	137.3048	136.4391	136.8418	129.3931	137.2952	136.4387	137.2511	136.4397	137.1025	**136.5**
C3	132.8553	133.3920	134.2739	133.6457	134.6750	133.6380	134.6782	133.6282	134.5420	133.6513	134.7684	132.8922	133.3673	135.0791	133.5222	134.3936	128.0421	134.8855	133.4979	134.8784	133.5325	134.5769	**130.8**
C4	141.4346	141.0833	141.1483	141.0269	140.9689	141.0102	141.6927	140.9950	141.6451	141.0450	141.8132	141.6206	141.0401	141.0423	140.9044	140.8447	130.0193	141.3475	140.9196	141.2085	140.9026	141.4248	**127.3**
C5	131.3432	132.5448	133.2637	133.2367	134.4359	133.1949	134.4607	133.1525	134.4295	133.2770	134.6278	131.3341	132.5796	132.6244	133.2789	134.6998	128.0424	134.1661	133.1945	134.0689	133.3183	134.7169	**130.8**
C6	133.6351	135.5124	136.4089	136.2730	137.6498	136.1982	138.0148	136.1261	138.0013	136.3488	138.3322	134.0044	135.9014	136.2252	136.7447	138.1142	129.3273	138.1065	136.6595	137.8836	136.7918	138.5940	**136.5**
C7	201.4912	206.1891	208.0118	209.3481	210.6130	209.2325	215.6752	209.1082	214.0834	209.4485	216.7392	204.6947	209.3963	211.3874	212.1390	213.3397	212.0885	218.5298	211.7964	217.4508	212.2863	219.1963	**196.6**
C8	61.5724	62.4646	63.1724	63.0682	63.9439	63.0540	64.3441	63.0374	64.1035	63.0797	64.9694	56.1153	57.5729	58.2689	58.5246	59.4252	50.0648	60.1639	58.3778	60.0598	58.5781	60.4430	**61**
C9	21.7679	21.8798	22.0516	22.0084	22.3096	21.9907	22.1547	21.9738	22.1655	22.0276	22.2617	19.3435	19.4051	19.5094	19.4841	19.7597	13.2611	19.7753	19.4630	19.7773	19.4894	20.1203	**15.8**
C4``	130.8539	131.8504	132.7873	132.2680	133.5885	132.2444	133.4289	132.2197	133.3886	132.2905	133.5129	130.7582	131.8047	132.5348	132.2228	133.5296	137.4366	133.4132	132.1711	133.3861	132.2466	133.4794	**123.2**
C8`	35.2078	35.7488	36.0278	36.1523	36.5421	36.1366	36.6761	36.1195	36.6219	36.1669	37.1152	30.4674	30.8523	30.9043	30.9239	31.1102	22.9410	31.0977	30.9223	31.0190	30.9349	31.2156	**31.8**
H2	8.8346	8.8195	8.7758	8.6849	8.6395	8.6820	8.6672	8.6800	8.7144	8.6890	8.6583	8.8685	8.7172	8.6770	8.5838	8.5466	7.6951	8.5093	8.6015	8.5033	8.5791	8.5095	**8.24**
H3	8.1537	8.2420	8.3086	8.2688	8.3737	8.2677	8.3885	8.2665	8.3819	8.2699	8.4066	8.1681	8.2591	8.2999	8.2873	8.3846	7.2220	8.3890	8.2842	8.3816	8.2890	8.4090	**7.92**
H5	8.0502	8.1961	8.2583	8.2574	8.3538	8.2528	8.3642	8.2481	8.3571	8.2619	8.3892	8.0530	8.1792	8.2620	8.2294	8.3280	7.2027	8.3537	8.2237	8.3453	8.2323	8.3536	**7.92**
H6	8.2797	8.5178	8.5808	8.5700	8.6914	8.5605	8.7237	8.5515	8.7404	8.5797	8.7629	8.1381	8.3239	8.3574	8.3934	8.5333	7.2635	8.5225	8.3864	8.5007	8.3979	8.5686	**8.24**
H8	4.1375	4.2899	4.3068	4.3473	4.4211	4.3379	4.4707	4.3289	4.4686	4.3566	4.5007	4.3612	4.5170	4.5838	4.5799	4.7095	3.6580	4.7190	4.5738	4.6969	4.5835	4.7461	**5.17**
H(9A-9C)	1.3569	1.3751	1.3377	1.3396	1.2951	1.3386	1.3076	1.3379	1.3211	1.3410	1.3171	1.4204	1.4276	1.3839	1.4227	1.3801	1.5219	1.3913	1.4217	1.3864	1.4240	1.4149	**1.59**
H(8`A-8`C)	2.4966	2.4144	2.4057	2.4316	2.4125	2.4342	2.3962	2.4364	2.3811	2.4289	2.3832	2.8146	2.6459	2.5928	2.5660	2.5155	1.7253	2.4374	2.5758	2.4440	2.5629	2.4184	**2.8**
Nuclei	wB97X											wB97X										
C1	145.1605	145.2874	146.6458	146.2848	148.3997	146.3204	147.6708	146.3479	147.1264	146.2434	147.9985	143.8236	145.5472	147.2426	146.6171	148.8015	146.5265	148.8718	146.4389	148.9067	146.6848	148.9849	**137.3**
C2	137.3527	137.3402	137.8108	137.2594	137.6597	137.2669	138.0192	137.2733	137.8915	137.2526	137.9936	137.1254	137.2618	138.0227	137.1496	137.5673	137.2629	138.0379	137.1566	137.9270	137.1482	137.8498	**136.5**
C3	133.4276	134.0238	134.8776	134.2799	135.2601	134.2719	135.3172	134.2621	135.1310	134.2870	135.3986	133.4658	133.9831	135.6436	134.1299	134.9988	134.3788	135.4826	134.1097	135.4033	134.1392	135.2111	**130.8**
C4	142.5545	142.2510	142.3196	142.2159	142.1420	142.2011	142.9238	142.1872	142.8146	142.2330	143.0259	142.7516	142.1904	142.2084	142.0818	142.0167	142.1031	142.5045	142.1003	142.3048	142.0766	142.6323	**127.3**
C5	131.9459	133.1669	133.8635	133.8409	135.0437	133.8000	135.1225	133.7590	135.0464	133.8817	135.2819	131.9543	133.1935	133.2524	133.9199	135.3126	133.6154	134.8390	133.8397	134.6845	133.9584	135.3864	**130.8**
C6	134.1955	136.0773	136.9789	136.8241	138.2192	136.7529	138.6486	136.6834	138.5467	136.8956	138.9343	134.6000	136.5057	136.8422	137.3690	138.7164	137.2164	138.7678	137.2920	138.4934	137.4094	139.2412	**136.5**
C7	203.2519	208.0315	209.8243	211.2359	212.5253	211.1137	217.7110	210.9856	216.0652	211.3471	218.8212	206.6854	211.4650	213.5088	214.1355	215.3861	213.9920	220.6343	213.7946	219.4764	214.2880	221.2353	**196.6**
C8	62.6717	63.5832	64.2841	64.1815	65.0810	64.1711	65.5597	64.1578	65.1930	64.1901	66.2196	57.1385	58.6964	59.4150	59.6548	60.5813	59.5586	61.3892	59.5134	61.2155	59.7154	61.6555	**61**
C9	21.9214	22.1150	22.2952	22.2375	22.5337	22.2185	22.4488	22.2000	22.3983	22.2583	22.5383	19.3739	19.5137	19.5802	19.5944	19.8483	19.5884	19.8823	19.5835	19.8211	19.5987	20.2115	**15.8**
C4``	130.8431	131.8615	132.8010	132.2791	133.6047	132.2571	133.4769	132.2343	133.3792	132.3004	133.5480	130.7294	131.7941	132.5116	132.2220	133.5289	132.1959	133.4436	132.1749	133.3557	132.2444	133.5004	**123.2**
C8`	35.4871	36.0765	36.3435	36.4510	36.8380	36.4354	37.0124	36.4189	36.8840	36.4666	37.4685	30.6384	30.9820	31.0644	31.1112	31.2987	31.1161	31.3580	31.1143	31.2203	31.1159	31.4703	**31.8**
H2	8.8025	8.7887	8.7493	8.6612	8.6140	8.6590	8.6421	8.6575	8.6888	8.6642	8.6248	8.8443	8.6875	8.6457	8.5670	8.5201	8.5812	8.4874	8.5855	8.4797	8.5604	8.4859	**8.24**
H3	8.1223	8.2163	8.2830	8.2437	8.3449	8.2423	8.3620	8.2409	8.3538	8.2452	8.3780	8.1326	8.2233	8.2703	8.2554	8.3515	8.2458	8.3578	8.2526	8.3479	8.2570	8.3762	**7.92**
H5	8.0155	8.1643	8.2254	8.2272	8.3216	8.2227	8.3340	8.2182	8.3251	8.2316	8.3568	8.0247	8.1525	8.2358	8.2048	8.3026	8.2165	8.3159	8.1997	8.3041	8.2075	8.3260	**7.92**
H6	8.2495	8.4895	8.5515	8.5406	8.6641	8.5313	8.7017	8.5225	8.7140	8.5502	8.7358	8.0998	8.2925	8.3290	8.3625	8.5004	8.3545	8.4880	8.3573	8.4645	8.3659	8.5363	**8.24**
H8	4.1938	4.3388	4.3570	4.3972	4.4693	4.3883	4.5119	4.3798	4.5145	4.4064	4.5381	4.3991	4.5576	4.6261	4.6256	4.7504	4.6262	4.7598	4.6204	4.7354	4.6286	4.7870	**5.17**
H(9A-9C)	1.3393	1.3564	1.3216	1.3226	1.2759	1.3221	1.2923	1.3218	1.2993	1.3234	1.2983	1.4088	1.4216	1.3744	1.4202	1.3715	1.4218	1.3834	1.4207	1.3753	1.4207	1.4035	**1.59**
H(8`A-8`C)	2.5051	2.4246	2.4155	2.4403	2.4174	2.4428	2.4029	2.4451	2.3851	2.4378	2.3878	2.8360	2.6696	2.6170	2.5932	2.5394	2.6002	2.4591	2.6032	2.4647	2.5894	2.4357	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S2. Cont. VII

Nuclei	R											S										Exp. [b]
	X3LYP											X3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	146.1048	146.2369	147.6127	147.5146	151.0595	147.5332	148.8151	147.5504	149.9356	147.5056	149.1366	143.8300	145.7814	147.3530	146.9782	148.7186	146.9158	149.1537	146.8328	149.3218	147.0535	149.3399	**137.3**
C2	137.0373	137.0277	137.5002	136.8751	137.2093	136.9037	137.4856	136.9291	137.5213	136.8525	137.4389	136.4594	136.7592	137.5642	136.7741	137.1681	136.8676	137.8025	136.8601	137.7223	136.7767	137.6064	**136.5**
C3	133.0047	133.6828	134.5301	133.9479	134.8150	133.9424	134.8864	133.9338	134.8679	133.9566	134.9368	133.0208	133.6394	135.2851	133.8048	134.5558	134.0777	135.1303	134.0542	135.0993	133.8121	134.7673	**130.8**
C4	142.5362	142.2018	142.2431	142.1747	141.7671	142.1630	142.8068	142.1483	142.4849	142.1886	142.9070	142.7859	142.1419	142.1046	142.0293	141.9873	142.0372	142.4740	142.0451	142.3292	142.0244	142.6163	**127.3**
C5	131.5122	132.8420	133.5624	133.5930	134.9355	133.5433	134.9424	133.4904	134.9801	133.6434	135.1484	131.8062	132.9622	132.9776	133.6789	135.1498	133.3494	134.5121	133.3253	134.4438	133.7176	135.1577	**130.8**
C6	133.7279	135.7001	136.6102	136.3878	137.3022	136.3306	138.2601	136.2695	137.5618	136.4449	138.5382	134.1213	136.0951	136.5285	137.0664	138.5591	136.8965	138.6351	136.8452	138.4184	137.1194	139.0739	**136.5**
C7	204.4817	209.2686	211.1566	213.1239	215.8606	212.9312	219.4265	212.7378	219.7934	213.3125	220.5408	209.0137	213.4876	215.5325	215.9775	217.2252	215.8995	222.1035	215.7551	221.1703	216.1138	222.6794	**196.6**
C8	65.6184	66.6266	67.3076	67.1501	68.4234	67.1504	68.6635	67.1486	68.6197	67.1554	69.3636	59.9737	62.0021	62.7278	63.0537	63.8054	62.9386	64.7375	62.8647	64.6262	63.1237	65.0136	**61**
C9	22.6919	23.0326	23.2213	23.0869	23.1937	23.0748	23.3540	23.0607	23.2188	23.1026	23.4795	19.4270	19.7103	19.7755	19.9555	20.0612	19.9248	20.2351	19.9112	20.2107	19.9669	20.5801	**15.8**
C4``	134.5945	135.7800	136.7805	136.2700	137.7026	136.2481	137.5154	136.2227	137.4899	136.2941	137.5760	134.5034	135.7578	136.5792	136.2420	137.6319	136.2196	137.5040	136.1925	137.4868	136.2677	137.5454	**123.2**
C8`	36.4173	37.1488	37.3817	37.6027	37.9307	37.5728	38.1275	37.5408	38.0390	37.6343	38.5586	31.8764	31.9835	32.1379	32.1549	32.4329	32.1572	32.4332	32.1484	32.3981	32.1635	32.4900	**31.8**
H2	8.6344	8.6361	8.6084	8.5004	8.3388	8.5018	8.4863	8.5023	8.4090	8.4986	8.4717	8.7230	8.5409	8.5275	8.4504	8.4342	8.4626	8.3974	8.4693	8.3881	8.4438	8.3880	**8.24**
H3	7.9838	8.0829	8.1528	8.1130	8.2066	8.1113	8.2292	8.1091	8.2183	8.1144	8.2454	7.9957	8.0863	8.1412	8.1241	8.2188	8.1158	8.2269	8.1142	8.2199	8.1255	8.2432	**7.92**
H5	7.8904	8.0376	8.1010	8.0999	8.1817	8.0954	8.2002	8.0904	8.1874	8.1041	8.2229	7.8876	8.0119	8.0866	8.0724	8.1770	8.0747	8.1726	8.0707	8.1638	8.0752	8.1952	**7.92**
H6	8.1295	8.3641	8.4302	8.4344	8.4969	8.4246	8.5909	8.4140	8.5554	8.4433	8.6264	7.9604	8.1272	8.1788	8.2132	8.3675	8.2051	8.3427	8.2013	8.3225	8.2165	8.3898	**8.24**
H8	4.3939	4.5153	4.5467	4.5924	4.6784	4.5824	4.6910	4.5717	4.7180	4.6015	4.7345	4.5641	4.7106	4.7778	4.7787	4.9072	4.7792	4.9140	4.7757	4.8986	4.7815	4.9439	**5.17**
H(9A-9C)	1.3332	1.3553	1.3274	1.3051	1.2139	1.3072	1.2925	1.3086	1.2352	1.3030	1.2952	1.4181	1.4326	1.4000	1.4522	1.4153	1.4518	1.4221	1.4507	1.4129	1.4528	1.4438	**1.59**
H(8`A-8`C)	2.5536	2.4759	2.4648	2.4823	2.4686	2.4845	2.4511	2.4864	2.4494	2.4805	2.4328	2.9749	2.7962	2.7470	2.7065	2.6712	2.7163	2.5736	2.7224	2.5818	2.7010	2.5432	**2.8**

[a] methyl protons shifts are averaged

[b] according to [2]

Table S3. Theoretical chemical shifts (in ppm) of *(R,S)*-3-fluoromethcathinone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S										Exp. [b]
	B3LYP											B3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	145.9125	146.4378	146.4912	146.3710	147.9538	146.3708	146.9562	146.3695	147.1512	146.3678	146.9965	144.5358	145.5782	146.1256	145.9704	147.3342	145.9419	147.2635	145.9147	147.1982	145.9972	147.3747	**134.46**
C2	122.9260	122.3003	122.7525	121.8359	122.3217	121.8605	122.7793	121.8852	122.7064	121.8107	122.7318	122.4060	122.0652	122.5169	121.7563	122.2625	121.7710	122.8409	121.7860	122.7190	121.7412	122.8223	**115.52**
C3	173.9878	174.3260	175.0099	174.3733	175.3361	174.3667	175.2414	174.3598	175.2239	174.3780	175.2902	174.1815	174.4177	175.1129	174.4036	175.3334	174.3972	175.2330	174.3906	175.2220	174.4083	175.2751	**162.83**
C4	125.5986	127.1790	127.8855	127.9137	128.3905	127.8643	129.5774	127.8149	129.2812	127.9588	129.7748	125.8762	127.0814	127.7667	127.5997	128.1588	127.5657	128.9174	127.5310	128.7210	127.6297	129.0948	**122.41**
C5	134.9964	136.9996	137.6291	137.9445	138.8915	137.8832	139.0197	137.8214	138.8955	138.0008	139.1862	135.1978	137.0408	137.7110	137.9261	138.8510	137.8705	138.8594	137.8142	138.7663	137.9770	139.0276	**131.43**
C6	128.9977	130.9805	132.4300	132.1085	133.6801	132.0337	134.3057	131.9596	133.9950	132.1790	134.7081	129.2939	131.5219	132.8127	132.6150	134.3602	132.5486	134.6859	132.4815	134.4831	132.6760	135.0257	**125.17**
C7	203.7081	209.3132	210.1408	211.9227	212.8230	211.7560	217.8151	211.5884	216.7697	212.0766	218.5808	208.7432	213.1237	214.5711	215.3499	216.1919	215.2135	220.9591	215.0765	219.9013	215.4780	221.5020	**196.61**
C8	65.7615	66.9869	67.4023	67.3686	68.1466	67.3491	68.5355	67.3279	68.3865	67.3842	69.2181	60.1689	62.1821	62.5942	63.0877	63.8787	63.0292	64.6529	62.9715	64.3784	63.1421	64.9851	**59.97**
C9	22.9207	23.1873	23.5297	23.4084	23.6757	23.3908	23.7957	23.3734	23.7131	23.4239	23.9365	19.5719	19.9819	20.0777	20.1398	20.4102	20.1253	20.5600	20.1110	20.4657	20.1521	20.9193	**15.26**
C8`	36.4904	37.3464	37.5061	37.6810	38.0283	37.6565	38.2354	37.6311	38.1780	37.7017	38.6712	32.0251	32.2650	32.6135	32.4119	32.7000	32.3979	32.7740	32.3836	32.7822	32.4230	32.8216	**31.09**
H2	8.2255	8.1131	8.2462	8.0580	8.09478	8.0611	8.1523	8.0643	8.1429	8.0550	8.1549	8.2965	8.1093	8.1864	8.0062	8.0578	8.0115	8.0358	8.0167	8.0461	8.0008	8.0364	**7.66**
H4	7.3391	7.5398	7.6288	7.6203	7.7378	7.6153	7.7867	7.6103	7.7670	7.6247	7.8114	7.3521	7.5331	7.6255	7.5964	7.7169	7.5921	7.7487	7.5878	7.7332	7.6001	7.7719	**7.33**
H5	7.4816	7.6920	7.7462	7.7871	7.8655	7.7812	7.8824	7.7752	7.8679	7.7925	7.9089	7.4810	7.6739	7.7262	7.7642	7.8413	7.7588	7.8462	7.7533	7.8345	7.7690	7.8708	**7.45**
H6	7.8000	7.9984	8.1341	8.1125	8.2458	8.1048	8.3087	8.0972	8.2827	8.1197	8.3510	7.6283	7.8139	7.9279	7.9126	8.0785	7.9068	8.0769	7.9010	8.0644	7.9177	8.1193	**7.57**
H8	4.3672	4.4656	4.5210	4.5488	4.6239	4.5421	4.6709	4.5354	4.6545	4.5552	4.6968	4.5097	4.6815	4.7418	4.7560	4.8756	4.7515	4.8938	4.7469	4.8801	4.7600	4.9230	**4.92**
H(9A-9C)	1.3188	1.3068	1.3225	1.2998	1.2629	1.3001	1.2906	1.3005	1.2800	1.2994	1.3118	1.3894	1.4246	1.4101	1.4498	1.4220	1.4482	1.4406	1.4464	1.4323	1.4513	1.4655	**1.44**
H(8`A-8`C)	2.521	2.47031	2.4174	2.4506	2.4187	2.4514	2.4028	2.4523	2.4032	2.4496	2.3861	2.9624	2.7956	2.7637	2.7148	2.6725	2.7189	2.5876	2.7229	2.6029	2.7107	2.5545	**2.64**
F3	-131.1490	-134.4920	-136.9050	-135.7630	-139.2430	-135.6910	-138.8130	-135.6180	-138.7680	-135.8310	-138.7900	-130.9960	-134.3940	-137.0130	-135.7940	-139.3040	-135.7270	-138.9380	-135.6590	-138.8820	-135.8570	-138.8960	**-114.23**
Nuclei	B3P86											B3P86											
C1	143.5882	143.8857	144.2601	143.9944	145.4860	144.0184	144.6761	144.0202	144.7972	144.0161	144.6223	142.5032	143.3389	143.9361	143.7927	145.0846	143.7838	145.0234	143.7552	144.9969	143.8483	145.1531	**134.46**
C2	122.0500	121.4140	121.9484	120.9786	121.5496	121.0264	121.9407	121.0521	121.9662	120.9775	121.8958	121.6059	121.2313	121.7336	120.9810	121.5467	121.0160	122.0953	121.0302	122.0647	120.9924	122.0967	**115.52**
C3	171.4766	171.7572	172.4534	171.8562	172.8205	171.8722	172.7552	171.8663	172.8432	171.8848	172.8132	171.5989	171.7923	172.5273	171.8492	172.7903	171.8669	172.6872	171.8624	172.7898	171.8762	172.7509	**162.83**
C4	124.7383	126.3386	127.1703	127.1465	127.7289	127.1190	128.8825	127.0698	128.7318	127.2163	129.0989	124.9692	126.2742	127.0621	126.8523	127.5412	126.8407	128.2740	126.8062	128.2031	126.9060	128.4801	**122.41**
C5	134.1190	136.0923	136.8360	137.1175	138.1511	137.0776	138.2932	137.0156	138.2758	137.1994	138.4696	134.2869	136.1384	136.9160	137.0534	138.0822	137.0204	138.0830	136.9648	138.1060	137.1283	138.2758	**131.43**
C6	127.7437	129.7963	131.1240	130.8021	132.4588	130.7549	132.9204	130.6858	132.8108	130.8906	133.4203	128.0255	130.2460	131.5499	131.2899	133.1034	131.2477	133.4157	131.1830	133.3543	131.3732	133.7598	**125.17**
C7	201.9099	206.8478	207.9904	209.5808	210.2942	209.4481	215.2960	209.2939	214.2210	209.7511	215.8620	206.3180	210.5062	211.9865	212.7171	213.5157	212.6075	218.1374	212.4759	217.1507	212.8653	218.6886	**196.61**
C8	64.1947	65.4630	65.8606	65.8682	66.6991	65.8672	67.0646	65.8435	66.9744	65.9125	67.8105	58.7228	60.4363	60.8267	61.3178	62.0716	61.2816	62.8455	61.2251	62.6601	61.3983	63.1673	**59.97**
C9	22.7475	23.0717	23.3242	23.2283	23.6105	23.2337	23.6256	23.2170	23.6953	23.2667	23.8703	19.4531	19.8849	19.9864	20.0966	20.4037	20.1003	20.5372	20.0831	20.5704	20.1379	20.9405	**15.26**
C8`	35.8781	36.6414	36.8568	37.0306	37.3127	37.0303	37.5686	37.0080	37.6041	37.0752	38.0187	31.2493	31.5208	31.9177	31.6781	32.0171	31.6880	32.0895	31.6758	32.2063	31.7119	32.1736	**31.09**
H2	8.2745	8.1793	8.2813	8.1109	8.1549	8.1156	8.1944	8.1185	8.2075	8.1077	8.2042	8.3112	8.1470	8.2209	8.0493	8.1095	8.0566	8.0849	8.0618	8.1072	8.0432	8.0875	**7.66**
H4	7.3557	7.5607	7.6556	7.6463	7.7696	7.6427	7.8178	7.6373	7.8047	7.6509	7.8419	7.3607	7.5493	7.6483	7.6231	7.7505	7.6202	7.7815	7.6155	7.7723	7.6270	7.8060	**7.33**
H5	7.5209	7.7338	7.7950	7.8329	7.9161	7.8283	7.9352	7.8219	7.9277	7.8384	7.9625	7.5202	7.7209	7.7789	7.8106	7.8950	7.8066	7.8993	7.8007	7.8943	7.8156	7.9253	**7.45**
H6	7.8758	8.0757	8.2047	8.1846	8.3140	8.1788	8.3726	8.1712	8.3643	8.1913	8.4241	7.6910	7.8848	8.0037	7.9751	8.1504	7.9710	8.1467	7.9649	8.1448	7.9801	8.1911	**7.57**
H8	4.4009	4.4924	4.5542	4.5758	4.6402	4.5712	4.6993	4.5650	4.6918	4.5814	4.7239	4.5720	4.7356	4.8033	4.8046	4.9268	4.8020	4.9412	4.7974	4.9366	4.8082	4.9727	**4.92**
H(9A-9C)	1.3389	1.3452	1.3394	1.3236	1.2953	1.3256	1.3051	1.3258	1.3092	1.3229	1.3403	1.4048	1.4431	1.4244	1.4604	1.4333	1.4604	1.4511	1.4585	1.4512	1.4617	1.4785	**1.44**
H(8`A-8`C)	2.4988	2.4477	2.3928	2.4185	2.3931	2.4210	2.3678	2.4216	2.3713	2.4175	2.3530	2.9054	2.7426	2.7200	2.6666	2.6266	2.6725	2.5336	2.6764	2.5595	2.6621	2.5055	**2.64**
F3	-123.8480	-126.8610	-129.2580	-127.9970	-131.2570	-127.9330	-130.7960	-127.8690	-130.7610	-128.0560	-130.7680	-123.9030	-126.9660	-129.4040	-128.0530	-131.3380	-127.9940	-130.9330	-127.9350	-130.8970	-128.1080	-130.8890	**-114.23**
Nuclei	B3PW91											B3PW91											
C1	143.8800	144.4147	145.4722	144.3995	146.2931	144.4034	145.1105	144.3978	145.5447	144.3973	145.1306	142.7315	143.8074	144.2290	144.1743	145.4535	144.1473	145.5161	144.1157	145.4085	144.2081	145.6977	**134.46**
C2	122.1447	121.5756	122.0735	121.1515	122.0417	121.1830	122.1122	121.2053	122.0772	121.1240	122.0749	121.7362	121.4309	121.8580	121.1399	121.7072	121.1604	122.2245	121.1730	122.1307	121.1241	122.2513	**115.52**
C3	171.5748	171.8425	172.5139	171.9060	173.1870	171.9073	172.7796	171.8997	172.7815	171.9067	172.9125	171.6836	171.9096	172.5674	171.9623	172.8953	171.9643	172.7360	171.9574	172.7937	171.9621	172.8561	**162.83**
C4	124.7719	126.4292	127.0364	127.2002	128.0962	127.1580	128.8928	127.1074	128.5317	127.2421	129.0779	124.9875	126.2657	126.9872	126.8378	127.5108	126.8124	128.2019	126.7769	128.0256	126.8618	128.3806	**122.41**
C5	134.2338	136.2477	136.9376	137.2244	138.5703	137.1700	138.3662	137.1070	138.2394	137.2776	138.5637	134.3858	136.2471	136.9390	137.1454	138.1528	137.0978	138.1519	137.0409	138.0629	137.1916	138.3314	**131.43**
C6	127.6758	129.6648	130.6611	130.7720	132.6653	130.7089	132.8829	130.6376	132.5347	130.8346	133.2961	128.0141	130.1811	131.4346	131.2282	133.0315	131.1721	133.3189	131.1059	133.1252	131.2819	133.6088	**125.17**
C7	202.0718	207.4183	209.0569	209.9610	211.1159	209.8061	215.7742	209.6417	214.8888	210.1096	216.4884	206.4108	210.8306	212.1503	213.0297	213.7709	212.9022	218.6056	212.7666	217.4713	213.1539	219.1794	**196.61**
C8	63.9750	65.2393	65.7508	65.6534	66.7534	65.6399	66.8360	65.6163	66.8245	65.6670	67.5695	58.6675	60.5171	60.8101	61.3625	62.1253	61.3082	62.9717	61.2481	62.6815	61.4201	63.3178	**59.97**
C9	22.4502	22.7145	22.8333	22.9525	23.5657	22.9430	23.3193	22.9254	23.2343	22.9634	23.4981	19.1804	19.5801	19.6279	19.7626	20.0693	19.7521	20.1999	19.7340	20.1209	19.7756	20.5623	**15.26**
C8`	35.8422	36.7074	36.8658	37.0444	37.6935	37.0291	37.5500	37.0040	37.4984	37.0605	38.0013	31.2940	31.5836	31.9173	31.7595	32.0797	31.7558	32.1105	31.7423	32.1322	31.7634	32.1905	**31.09**
H2	8.2403	8.1215	8.1517	8.0665	8.1219	8.0706	8.1519	8.0744	8.1204	8.0629	8.1604	8.2833	8.0990	8.1864	8.0124	8.0735	8.0191	8.0316	8.0250	8.0587	8.0056	8.0376	**7.66**
H4	7.3561	7.5583	7.6532	7.6420	7.7789	7.6376	7.8139	7.6329	7.7939	7.6463	7.8374	7.3610	7.5461	7.6437	7.6203	7.7448	7.6167	7.7721	7.6128	7.7638	7.6238	7.7990	**7.33**
H5	7.5260	7.7362	7.7925	7.8341	7.9320	7.8288	7.9354	7.8231	7.9202	7.8392	7.9619	7.5242	7.7192	7.7774	7.8094	7.8917	7.8047	7.8997	7.7996	7.8879	7.8140	7.9205	**7.45**
H6	7.8568	8.0468	8.1242	8.1588	8.3049	8.1520	8.3452	8.1453	8.3011	8.1652	8.3959	7.6747	7.8589	7.9798	7.9551	8.1278	7.9504	8.1225	7.9450	8.1138	7.9594	8.1595	**7.57**
H8	4.3822	4.4758	4.5140	4.5605	4.6465	4.5544	4.6815	4.5483	4.6513	4.5667	4.7074	4.5456	4.7034	4.7694	4.7755	4.8955	4.7721	4.9137	4.7681	4.9035	4.7787	4.9401	**4.92**
H(9A-9C)	1.3011	1.2890	1.2558	1.2813	1.2589	1.2826	1.2670	1.2836	1.2547	1.2803	1.2891	1.3711	1.4019	1.3884	1.4242	1.3969	1.4232	1.4187	1.4220	1.4115	1.4251	1.4380	**1.44**
H(8`A-8`C)	2.4674	2.4163	2.3862	2.3971	2.3791	2.3987	2.3498	2.4000	2.3588	2.3959	2.3304	2.8744	2.7115	2.6894	2.6415	2.5988	2.6465	2.5082	2.6510	2.5310	2.6365	2.4757	**2.64**
F3	-123.2020	-126.4690	-128.8900	-127.6170	-129.7320	-127.5520	-130.4150	-127.4870	-130.3890	-127.6770	-130.1910	-123.2340	-126.3520	-128.8000	-127.4490	-130.7460	-127.3900	-130.5610	-127.3300	-130.3050	-127.5050	-130.2930	**-114.23**
Nuclei	B98											B98											
C1	144.6912	145.1473	145.2484	145.1160	146.6617	145.1308	145.7032	145.1429	145.8633	145.1039	145.7376	143.5207	144.4784	144.9860	144.8610	146.2082	144.8492	146.1736	144.8363	146.0946	144.8771	146.3230	**134.46**
C2	121.8392	121.1925	121.6495	120.7723	121.3222	120.8136	121.7340	120.8523	121.6761	120.7355	121.6994	121.3720	121.0411	121.4894	120.7551	121.3064	120.7868	121.8401	120.8168	121.7380	120.7278	121.8371	**115.52**
C3	171.3798	171.6392	172.2889	171.7095	172.6763	171.7205	172.5821	171.7290	172.5866	171.7014	172.6373	171.5646	171.6951	172.3690	171.7571	172.6945	171.7685	172.5796	171.7776	172.5921	171.7486	172.6330	**162.83**
C4	124.5512	126.0897	126.8377	126.8573	127.4027	126.8258	128.5411	126.7921	128.2839	126.8894	128.7456	124.7334	125.9597	126.6672	126.5323	127.1662	126.5153	127.8641	126.4952	127.7038	126.5497	128.0437	**122.41**
C5	133.9957	135.9330	136.5648	136.9065	137.8988	136.8625	138.0162	136.8159	137.9178	136.9503	138.1891	134.1576	135.9511	136.6379	136.8545	137.8258	136.8161	137.8101	136.7747	137.7441	136.8929	137.9858	**131.43**
C6	127.7600	129.6454	131.0479	130.7507	132.3478	130.6979	132.8888	130.6429	132.6290	130.8035	133.2983	128.0343	130.1734	131.4142	131.2223	132.9822	131.1747	133.2801	131.1239	133.1102	131.2694	133.6069	**125.17**
C7	200.3847	205.8210	206.6302	208.4239	209.2010	208.2766	214.2818	208.1271	213.1864	208.5658	215.0160	204.8815	209.2606	210.7400	211.5452	212.3559	211.4233	217.1974	211.2992	216.1094	211.6637	217.8036	**196.61**
C8	65.6444	66.8320	67.2503	67.2632	68.0685	67.2581	68.4263	67.2491	68.2684	67.2685	69.1043	60.3450	62.1437	62.4694	62.9801	63.7622	62.9409	64.5626	62.9005	64.2805	63.0214	64.8946	**59.97**
C9	23.1980	23.4234	23.7294	23.6797	24.0099	23.6790	24.0670	23.6758	24.0133	23.6828	24.2291	20.0207	20.3805	20.4020	20.5221	20.8130	20.5255	20.9448	20.5271	20.8729	20.5220	21.2988	**15.26**
C8`	36.6858	37.4599	37.6057	37.8314	38.1507	37.8240	38.3667	37.8133	38.3252	37.8400	38.8016	32.0806	32.3129	32.6647	32.5156	32.8281	32.5190	32.8955	32.5193	32.9209	32.5139	32.9413	**31.09**
H2	8.2422	8.1254	8.2502	8.0710	8.1142	8.0747	8.1700	8.0786	8.1688	8.0678	8.1716	8.2869	8.0982	8.1880	8.0133	8.0716	8.0189	8.0477	8.0244	8.0637	8.0080	8.0451	**7.66**
H4	7.3491	7.5528	7.6486	7.6371	7.7598	7.6324	7.8106	7.6277	7.7936	7.6418	7.8334	7.3601	7.5372	7.6372	7.6122	7.7387	7.6082	7.7714	7.6041	7.7584	7.6163	7.7929	**7.33**
H5	7.5101	7.7209	7.7802	7.8189	7.9020	7.8132	7.9211	7.8077	7.9093	7.8245	7.9448	7.5068	7.7030	7.7610	7.7958	7.8786	7.7905	7.8855	7.7852	7.8760	7.8010	7.9077	**7.45**
H6	7.8240	8.0213	8.1543	8.1379	8.2740	8.1307	8.3365	8.1236	8.3167	8.1451	8.3778	7.6446	7.8376	7.9585	7.9304	8.1040	7.9251	8.1030	7.9197	8.0932	7.9357	8.1447	**7.57**
H8	4.3568	4.4526	4.5088	4.5358	4.6085	4.5295	4.6622	4.5236	4.6511	4.5422	4.6846	4.5104	4.6782	4.7425	4.7482	4.8718	4.7442	4.8870	4.7403	4.8770	4.7521	4.9144	**4.92**
H(9A-9C)	1.3224	1.3104	1.3261	1.3036	1.2685	1.3046	1.2927	1.3056	1.2869	1.3030	1.3135	1.3935	1.4261	1.4092	1.4455	1.4167	1.4443	1.4350	1.4431	1.4301	1.4469	1.4568	**1.44**
H(8`A-8`C)	2.4937	2.4463	2.3982	2.4270	2.3963	2.4282	2.3810	2.4293	2.3827	2.4263	2.3622	2.9118	2.7469	2.7222	2.6733	2.6323	2.6777	2.5444	2.6821	2.5664	2.6694	2.5101	**2.64**
F3	-126.2150	-129.2130	-131.7250	-130.3470	-133.6920	-130.2830	-133.2670	-130.2190	-133.2300	-130.4070	-133.2220	-126.1000	-129.3280	-131.8480	-130.4130	-133.7870	-130.3550	-133.4210	-130.2950	-133.3780	-130.4680	-133.3550	**-114.23**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S3. Cont. I

Nuclei	R											S										Exp. [b]
	B971											B971										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	144.2858	144.6963	144.8810	144.7090	146.1990	144.7156	145.3255	144.7228	145.4535	144.7095	145.3479	143.1278	144.0596	144.5992	144.4695	145.8067	144.4484	145.7610	144.4287	145.6754	144.4977	145.9166	**134.46**
C2	121.5536	120.8971	121.3534	120.4829	121.0157	120.5166	121.4207	120.5498	121.3599	120.4572	121.3902	121.0799	120.7403	121.1826	120.4666	120.9980	120.4902	121.5306	120.5135	121.4243	120.4508	121.5318	**115.52**
C3	171.3009	171.5668	172.2221	171.6510	172.6078	171.6538	172.5198	171.6562	172.5233	171.6544	172.5803	171.4842	171.6233	172.2984	171.6936	172.6252	171.6972	172.5067	171.7001	172.5183	171.6963	172.5664	**162.83**
C4	124.3159	125.8533	126.5929	126.6316	127.1722	126.5925	128.2854	126.5526	128.0375	126.6747	128.4970	124.4899	125.7349	126.4358	126.3143	126.9410	126.2895	127.6345	126.2635	127.4750	126.3429	127.8216	**122.41**
C5	133.7740	135.7159	136.3600	136.7103	137.6949	136.6577	137.8185	136.6047	137.7197	136.7662	137.9956	133.9388	135.7465	136.4351	136.6619	137.6329	136.6155	137.6106	136.5684	137.5459	136.7113	137.7923	**131.43**
C6	127.5496	129.4609	130.8010	130.5367	132.1567	130.4780	132.6331	130.4187	132.3883	130.5982	133.0588	127.7907	129.9596	131.1729	131.0198	132.7763	130.9641	133.0736	130.9075	132.9085	131.0779	133.4019	**125.17**
C7	200.2828	205.5725	206.5032	208.2255	208.9531	208.0715	214.0194	207.9184	212.9210	208.3790	214.7353	204.7631	209.0909	210.6142	211.3822	212.2103	211.2531	216.9467	211.1230	215.8795	211.5108	217.5640	**196.61**
C8	65.6155	66.8022	67.2103	67.2219	68.0383	67.2073	68.3845	67.1914	68.2192	67.2404	69.0669	60.3135	62.0473	62.3658	62.8947	63.6702	62.8471	64.4461	62.8002	64.1686	62.9474	64.7738	**59.97**
C9	23.2095	23.4487	23.7131	23.6905	24.0412	23.6825	24.0738	23.6737	24.0266	23.7042	24.2534	20.0362	20.4070	20.4206	20.5640	20.8483	20.5581	20.9884	20.5527	20.9160	20.5765	21.3570	**15.26**
C8`	36.6917	37.4457	37.5883	37.8149	38.0991	37.7979	38.3371	37.7806	38.2887	37.8365	38.7686	32.0232	32.2662	32.6085	32.4612	32.7611	32.4576	32.8140	32.4530	32.8408	32.4699	32.8668	**31.09**
H2	8.2393	8.1270	8.2441	8.0716	8.1154	8.0752	8.1650	8.0788	8.1660	8.0685	8.1683	8.2815	8.1000	8.1852	8.0140	8.0699	8.0195	8.0481	8.0249	8.0638	8.0089	8.0458	**7.66**
H4	7.3460	7.5474	7.6433	7.6329	7.7543	7.6280	7.8043	7.6231	7.7877	7.6379	7.8269	7.3560	7.5329	7.6330	7.6084	7.7339	7.6041	7.7661	7.5999	7.7532	7.6127	7.7878	**7.33**
H5	7.5117	7.7212	7.7814	7.8202	7.9023	7.8143	7.9213	7.8086	7.9099	7.8261	7.9449	7.5092	7.7054	7.7628	7.7981	7.8805	7.7927	7.8864	7.7873	7.8773	7.8036	7.9085	**7.45**
H6	7.8296	8.0263	8.1533	8.1409	8.2748	8.1335	8.3348	8.1263	8.3168	8.1482	8.3769	7.6455	7.8396	7.9610	7.9337	8.1063	7.9280	8.1077	7.9223	8.0977	7.9394	8.1491	**7.57**
H8	4.3551	4.4487	4.5048	4.5324	4.6023	4.5263	4.6565	4.5204	4.6464	4.5389	4.6784	4.5121	4.6785	4.7453	4.7492	4.8719	4.7450	4.8880	4.7408	4.8778	4.7536	4.9154	**4.92**
H(9A-9C)	1.3229	1.3162	1.3247	1.3073	1.2754	1.3081	1.2934	1.3089	1.2888	1.3068	1.3160	1.3965	1.4286	1.4098	1.4487	1.4194	1.4472	1.4375	1.4459	1.4329	1.4504	1.4594	**1.44**
H(8`A-8`C)	2.4912	2.4428	2.3934	2.4220	2.3921	2.4230	2.3743	2.4241	2.3755	2.4215	2.3550	2.9037	2.7397	2.7169	2.6672	2.6257	2.6714	2.5384	2.6755	2.5602	2.6637	2.5047	**2.64**
F3	-126.8460	-129.8690	-132.3840	-131.0090	-134.3690	-130.9450	-133.9360	-130.8800	-133.8980	-131.0690	-133.8950	-126.7480	-129.9850	-132.5090	-131.0820	-134.4640	-131.0220	-134.0970	-130.9630	-134.0520	-131.1370	-134.0340	**-114.23**
Nuclei	B972											B972										
C1	141.2342	141.6506	142.7266	141.7299	143.2843	141.7305	142.4664	141.7293	142.9618	141.7258	143.1773	140.0113	141.1468	141.5287	141.5569	142.8076	141.5189	142.8883	141.4848	142.9386	141.5980	143.0817	**134.46**
C2	119.7317	119.1483	119.6658	118.8149	119.3431	118.8372	119.7074	118.8570	119.6937	118.7896	119.7506	119.3405	119.0263	119.4669	118.8013	119.3217	118.8137	119.7986	118.8249	119.7255	118.7869	119.8144	**115.52**
C3	168.2732	168.4793	169.1572	168.6101	169.4995	168.6044	169.4066	168.5960	169.4009	168.6113	169.4863	168.3917	168.5517	169.2157	168.6764	169.5422	168.6705	169.3844	168.6622	169.3884	168.6775	169.4549	**162.83**
C4	122.1892	123.7396	124.3607	124.5654	125.0699	124.5163	126.1100	124.4648	125.7655	124.6072	126.1425	122.3897	123.5421	124.2685	124.1675	124.7609	124.1365	125.4016	124.1012	125.2031	124.1894	125.5840	**122.41**
C5	131.5363	133.4137	134.0989	134.4183	135.3588	134.3592	135.4500	134.2977	135.3373	134.4699	135.6259	131.6632	133.3991	134.0780	134.3355	135.2487	134.2822	135.2475	134.2258	135.1627	134.3810	135.4358	**131.43**
C6	125.0627	126.9763	127.9602	128.1319	129.6026	128.0595	130.1473	127.9845	129.7780	128.1963	130.3129	125.4310	127.4217	128.6994	128.5016	130.1890	128.4427	130.4260	128.3792	130.2192	128.5499	130.7362	**125.17**
C7	198.1130	203.2735	204.9522	205.9151	206.7453	205.7587	211.5986	205.5999	210.9110	206.0594	212.9086	202.2824	206.6676	207.8990	208.9064	209.5861	208.7689	214.4033	208.6311	213.3890	209.0354	214.9807	**196.61**
C8	62.7055	63.8602	64.3230	64.2776	64.9739	64.2619	65.4325	64.2431	65.4239	64.2879	66.3446	57.6239	59.4402	59.7721	60.3181	61.0364	60.2576	61.8700	60.1978	61.6540	60.3764	62.2175	**59.97**
C9	22.1305	22.3749	22.5096	22.6434	22.8754	22.6258	22.9796	22.6063	22.8864	22.6564	23.0535	18.9733	19.2591	19.3543	19.4810	19.7298	19.4663	19.8374	19.4498	19.7701	19.4914	20.1871	**15.26**
C8`	35.6102	36.4027	36.5773	36.8090	37.1085	36.7901	37.2019	36.7683	37.1923	36.8224	37.6237	31.1992	31.4270	31.7695	31.6774	31.9475	31.6669	31.9423	31.6525	31.9351	31.6807	32.0059	**31.09**
H2	8.2202	8.1039	8.1362	8.0508	8.0874	8.0538	8.1218	8.0565	8.0850	8.0477	8.0643	8.2713	8.0721	8.1659	7.9914	8.0486	7.9978	8.0032	8.0034	8.0079	7.9843	7.9995	**7.66**
H4	7.3567	7.5561	7.6513	7.6433	7.7610	7.6384	7.8102	7.6332	7.7911	7.6478	7.8290	7.3656	7.5462	7.6429	7.6230	7.7433	7.6189	7.7684	7.6145	7.7539	7.6266	7.7903	**7.33**
H5	7.5304	7.7369	7.7933	7.8364	7.9152	7.8306	7.9316	7.8247	7.9164	7.8417	7.9510	7.5255	7.7139	7.7729	7.8059	7.8843	7.8008	7.8925	7.7953	7.8819	7.8105	7.9154	**7.45**
H6	7.8294	8.0190	8.1022	8.1371	8.2676	8.1296	8.3137	8.1218	8.2736	8.1440	8.3117	7.6512	7.8295	7.9511	7.9302	8.0965	7.9251	8.0904	7.9194	8.0760	7.9343	8.1266	**7.57**
H8	4.3502	4.4406	4.4870	4.5320	4.6055	4.5254	4.6441	4.5186	4.6161	4.5382	4.6478	4.5078	4.6585	4.7265	4.7353	4.8523	4.7313	4.8712	4.7269	4.8595	4.7386	4.8963	**4.92**
H(9A-9C)	1.2782	1.2679	1.2367	1.2621	1.2209	1.2623	1.2488	1.2623	1.2313	1.2618	1.2497	1.3582	1.3850	1.3772	1.4110	1.3811	1.4097	1.4012	1.4081	1.3940	1.4120	1.4219	**1.44**
H(8`A-8`C)	2.4578	2.4146	2.3838	2.3997	2.3632	2.4005	2.3560	2.4012	2.3627	2.3989	2.3495	2.8672	2.7056	2.6834	2.6429	2.5976	2.6471	2.5119	2.6510	2.5283	2.6383	2.4759	**2.64**
F3	-120.6790	-123.8960	-126.2360	-125.0220	-128.1940	-124.9590	-127.7520	-124.8970	-127.7220	-125.0820	-127.7200	-120.7160	-123.7860	-126.1710	-124.8600	-128.0700	-124.8020	-127.9050	-124.7440	-127.8710	-124.9140	-127.8630	**-114.23**
Nuclei	BHandH											BHandH										
C1	145.6360	145.6202	146.2594	145.4915	146.8219	145.4920	145.8942	145.5103	146.0198	145.4598	146.0408	144.8250	145.0762	145.8833	145.6125	146.3566	145.5754	146.5035	145.5557	146.3936	145.6175	146.6148	**134.46**
C2	125.5346	124.8614	125.3852	124.4017	124.9632	124.4203	125.3070	124.4573	125.2714	124.3538	125.3096	125.1931	124.6852	125.2900	124.4661	125.2102	124.4704	125.5203	124.4930	125.4125	124.4318	125.5282	**115.52**
C3	171.8732	171.9700	172.6046	172.0080	172.8208	171.9951	172.7345	172.0008	172.7559	171.9901	172.8083	171.9185	171.9893	172.6152	172.0294	172.7735	172.0161	172.7471	172.0215	172.7571	172.0120	172.8168	**162.83**
C4	128.1593	129.8441	130.6558	130.7021	131.3619	130.6394	132.4962	130.5948	132.2208	130.7320	132.7262	128.3774	129.8761	130.6155	130.4811	131.2252	130.4340	132.0262	130.4051	131.8519	130.4957	132.2546	**122.41**
C5	137.7618	139.7698	140.4697	140.8119	141.7707	140.7383	141.8522	140.6830	141.7474	140.8514	142.0546	137.8857	139.7969	140.4930	140.7560	141.5001	140.6878	141.7509	140.6375	141.6660	140.7909	141.9471	**131.43**
C6	131.8650	134.1148	135.4404	135.2854	137.1236	135.2039	137.6614	135.1406	137.4270	135.3330	138.0745	132.0987	134.5952	135.9847	135.7379	136.4820	135.6609	138.0145	135.6017	137.8882	135.7808	138.3869	**125.17**
C7	203.6138	208.5172	209.8103	210.9896	211.6240	210.8308	216.6493	210.6894	215.4270	211.1096	217.5301	207.9046	212.0671	213.4264	214.2911	215.0352	214.1425	219.7537	214.0124	218.5758	214.4019	220.3276	**196.61**
C8	60.4282	61.6949	62.2727	62.1198	62.9860	62.0891	63.4098	62.0761	63.2734	62.1183	64.1380	54.5800	55.8507	56.5007	56.7153	57.4594	56.6558	58.0038	56.6138	57.8144	56.7411	58.3269	**59.97**
C9	22.3805	22.6640	22.8450	22.9402	23.3623	22.9132	23.3034	22.9043	23.2689	22.9357	23.4993	18.9705	19.4038	19.6250	19.6671	20.4112	19.6428	19.9886	19.6365	20.0067	19.6602	20.4147	**15.26**
C8`	33.7019	34.5319	34.7480	34.8536	35.2051	34.8254	35.4138	34.8155	35.3360	34.8501	35.9159	28.6013	29.0694	29.3172	29.2263	29.9704	29.2005	29.6834	29.1938	29.7130	29.2211	29.8358	**31.09**
H2	8.5722	8.4795	8.5451	8.4246	8.4730	8.4286	8.5049	8.4318	8.5079	8.4219	8.5011	8.5877	8.4565	8.4984	8.3373	8.2561	8.3446	8.3818	8.3512	8.4001	8.3316	8.3840	**7.66**
H4	7.4985	7.7095	7.8085	7.7982	7.9259	7.7940	7.9763	7.7889	7.9578	7.8032	8.0012	7.5018	7.7017	7.7993	7.7806	7.6994	7.7770	7.9489	7.7725	7.9342	7.7850	7.9735	**7.33**
H5	7.6246	7.8443	7.9007	7.9466	8.0283	7.9415	8.0466	7.9355	8.0338	7.9525	8.0731	7.6234	7.8356	7.8898	7.9314	7.8502	7.9267	8.0222	7.9211	8.0126	7.9368	8.0471	**7.45**
H6	8.0335	8.2570	8.3730	8.3788	8.5362	8.3720	8.6047	8.3644	8.5771	8.3864	8.6503	7.8509	8.0823	8.1934	8.1739	8.0927	8.1690	8.3690	8.1633	8.3621	8.1795	8.4148	**7.57**
H8	4.1658	4.2674	4.3192	4.3652	4.4301	4.3592	4.5088	4.3524	4.4784	4.3720	4.5395	4.4307	4.6046	4.6688	4.6828	4.6016	4.6792	4.8401	4.6747	4.8222	4.6872	4.8693	**4.92**
H(9A-9C)	1.4018	1.4107	1.3957	1.4074	1.3829	1.4085	1.3982	1.4087	1.3961	1.4074	1.4174	1.4787	1.5148	1.4955	1.5189	1.4377	1.5194	1.5006	1.5190	1.5024	1.5196	1.5250	**1.44**
H(8`A-8`C)	2.5560	2.4887	2.4337	2.4585	2.4255	2.4613	2.3897	2.4632	2.3949	2.4568	2.3736	2.9080	2.7589	2.7052	2.6642	2.5829	2.6700	2.5306	2.6752	2.5535	2.6597	2.5073	**2.64**
F3	-111.9810	-114.6650	-116.6860	-115.6670	-118.3730	-115.6120	-118.0960	-115.5550	-118.0360	-115.7180	-118.1120	-112.0420	-114.7710	-116.8330	-115.7370	-116.0740	-115.6860	-118.1890	-115.6330	-118.1500	-115.7860	-118.1880	**-114.23**
Nuclei	BHandHLYP											BHandHLYP										
C1	145.9669	146.1759	146.2853	146.1113	147.5505	146.1200	146.5389	146.1313	146.5831	146.1038	146.5447	144.8879	145.5103	146.1158	146.0017	147.2410	145.9780	146.9278	145.9578	146.8892	146.0259	147.0243	**134.46**
C2	124.7515	124.0653	124.5461	123.6469	124.1741	123.6733	124.5921	123.7021	124.5316	123.6218	124.5706	124.3796	123.9052	124.4021	123.6341	124.1686	123.6521	124.6622	123.6725	124.5779	123.6171	124.6729	**115.52**
C3	171.7043	171.8078	172.3461	171.8437	172.6613	171.8422	172.5332	171.8432	172.5540	171.8447	172.5906	171.7888	171.8290	172.4188	171.8672	172.6522	171.8651	172.5289	171.8651	172.5561	171.8690	172.5864	**162.83**
C4	126.8528	128.3654	129.1479	129.1567	129.6354	129.1088	130.8346	129.0636	130.6113	129.2014	131.0509	127.1371	128.3244	129.0171	128.8473	129.4342	128.8162	130.1960	128.7867	130.0374	128.8755	130.4016	**122.41**
C5	136.1415	137.9845	138.5163	138.9472	139.8001	138.8900	139.8405	138.8351	139.7634	139.0011	140.0097	136.2629	137.9948	138.5973	138.8877	139.7198	138.8352	139.6727	138.7846	139.6227	138.9370	139.8503	**131.43**
C6	130.4116	132.4695	133.9130	133.6262	135.2232	133.5527	135.7764	133.4813	135.5814	133.6955	136.2221	130.7205	132.9798	134.2257	134.0284	135.8034	133.9634	136.1403	133.9004	135.9856	134.0893	136.5014	**125.17**
C7	201.8321	207.4006	208.2736	210.2494	210.7410	210.0807	216.5002	209.9158	215.1153	210.4091	217.2571	206.5177	210.9495	212.4315	213.3909	213.9546	213.2498	219.1800	213.1105	217.9581	213.5236	219.7995	**196.61**
C8	61.1863	62.2965	62.6692	62.6877	63.4497	62.6691	63.7555	62.6519	63.5794	62.7040	64.4069	55.9833	57.6105	58.0052	58.5002	59.2270	58.4476	59.8950	58.3984	59.6616	58.5510	60.2030	**59.97**
C9	22.1319	22.2439	22.5189	22.4257	22.7743	22.4127	22.6380	22.4021	22.6483	22.4376	22.8001	18.9225	19.1131	19.1758	19.2384	19.5320	19.2278	19.5100	19.2205	19.4920	19.2488	19.8200	**15.26**
C8`	34.7229	35.4951	35.6672	35.8743	36.1736	35.8529	36.3975	35.8339	36.3632	35.8942	36.8278	30.4753	30.7423	31.063	30.9170	31.2202	30.9040	31.3030	30.8934	31.3347	30.9286	31.4094	**31.09**
H2	8.4732	8.3531	8.4758	8.2941	8.3382	8.2976	8.3879	8.3009	8.4012	8.2908	8.3907	8.5140	8.3314	8.3985	8.2222	8.2799	8.2283	8.2660	8.2342	8.2819	8.2162	8.2679	**7.66**
H4	7.5023	7.7057	7.7988	7.7926	7.9095	7.7879	7.9669	7.7830	7.9483	7.7970	7.9897	7.5103	7.6957	7.7919	7.7705	7.8916	7.7665	7.9298	7.7623	7.9150	7.7741	7.9526	**7.33**
H5	7.6036	7.8161	7.8699	7.9168	7.9910	7.9111	8.0117	7.9054	7.9997	7.9221	8.0365	7.6006	7.8024	7.8543	7.8958	7.9708	7.8906	7.9797	7.8852	7.9693	7.9007	8.0032	**7.45**
H6	7.8862	8.1057	8.2423	8.2348	8.3728	8.2268	8.4463	8.2188	8.4310	8.2423	8.4902	7.7397	7.9492	8.0666	8.0466	8.2224	8.0407	8.2327	8.0347	8.2216	8.0519	8.2752	**7.57**
H8	4.0886	4.2077	4.2753	4.3124	4.3846	4.3052	4.4614	4.2981	4.4439	4.3194	4.4850	4.2755	4.4537	4.5253	4.5332	4.6547	4.5288	4.6820	4.5243	4.6690	4.5372	4.7086	**4.92**
H(9A-9C)	1.2996	1.2921	1.3009	1.2820	1.2498	1.2828	1.2651	1.2833	1.2665	1.2812	1.2869	1.3654	1.3916	1.3722	1.4072	1.3768	1.4061	1.3973	1.4048	1.3934	1.4082	1.4181	**1.44**
H(8`A-8`C)	2.4510	2.4053	2.3496	2.3879	2.3566	2.3890	2.3405	2.3899	2.3357	2.3869	2.3262	2.8661	2.7046	2.6760	2.6318	2.5854	2.6359	2.5109	2.6399	2.5281	2.6278	2.4822	**2.64**
F3	-115.0720	-118.0370	-120.2260	-119.1810	-122.0510	-119.1160	-121.7530	-119.0510	-121.7000	-119.2420	-121.7810	-115.1680	-118.1450	-120.3290	-119.2170	-122.1200	-119.1590	-121.8290	-119.1000	-121.7810	-119.2720	-121.8290	**-114.23**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S3. Cont. II

Nuclei	R											S										Exp. [b]
	BLYP											BLYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	145.5450	146.0429	147.1140	146.1068	147.7986	146.3885	146.6492	146.2085	147.2347	146.4667	146.8219	143.7828	144.7209	145.5672	145.4278	146.9795	145.6805	146.8743	145.4719	147.0441	145.8161	147.0664	**134.46**
C2	120.8047	120.1141	120.5513	119.6783	120.1736	119.9844	120.4482	119.8286	120.6128	120.0147	120.5020	120.1479	119.6918	120.1601	119.4918	120.0265	119.7882	120.4772	119.6229	120.5599	119.8378	120.5410	**115.52**
C3	175.9013	176.3257	177.0927	176.4452	177.6220	176.7175	177.3132	176.5274	177.4898	176.8136	177.4629	176.1113	176.4275	177.1619	176.5133	177.6627	176.7855	177.3261	176.5958	177.5168	176.8816	177.4729	**162.83**
C4	124.0175	125.5362	126.0703	126.2893	126.7806	126.5226	127.7623	126.2931	127.6290	126.6945	128.0567	124.4345	125.5186	126.0303	125.9745	126.5488	126.2213	127.0869	126.0057	127.0861	126.3668	127.3739	**122.41**
C5	133.4939	135.4708	136.1370	136.4608	137.5177	136.6797	137.4897	136.4362	137.5416	136.8800	137.7612	133.8536	135.6443	136.2784	136.5056	137.5472	136.7303	137.3589	136.4925	137.4573	136.9191	137.6361	**131.43**
C6	127.3335	129.2443	130.2486	130.3468	132.0288	130.5519	132.4283	130.2954	132.2771	130.7791	132.9242	127.7381	129.9027	131.0864	130.8943	132.6839	131.1099	132.7663	130.8629	132.7695	131.3161	133.1971	**125.17**
C7	204.3147	209.5974	211.3643	212.2138	213.3986	212.3424	217.6300	212.0072	217.0965	212.7173	218.5008	209.9855	213.7889	215.2206	215.8739	217.0497	216.0246	221.1931	215.7137	220.4874	216.3575	221.7907	**196.61**
C8	69.7467	70.9133	71.4699	71.3079	72.2357	71.5712	72.4406	71.3721	72.5974	71.6848	73.2670	63.4344	65.8959	66.5807	67.0939	68.0176	67.3157	68.6302	67.0757	68.5879	67.5108	69.0388	**59.97**
C9	23.7062	24.0257	24.1727	24.2581	24.6168	24.5176	24.6672	24.3164	24.7533	24.6398	24.9144	20.0844	20.7739	20.9191	21.0394	21.3485	21.3048	21.4163	21.1084	21.5141	21.4143	21.9134	**15.26**
C8`	38.1900	38.9597	39.1326	39.3487	39.7506	39.6097	39.7477	39.4076	39.8899	39.7268	40.2871	33.7250	33.8484	34.0039	33.8977	34.2370	34.1650	34.0793	33.9700	34.2737	34.2710	34.2020	**31.09**
H2	8.0144	7.9189	7.9482	7.8624	7.8961	7.9128	8.1257	7.8706	7.9334	7.9147	8.1393	8.1164	7.9489	7.9914	7.8300	7.8766	7.8827	8.0190	7.8427	7.8585	7.8803	8.0324	**7.66**
H4	7.1890	7.3809	7.4696	7.4593	7.5757	7.5022	7.7919	7.4526	7.6069	7.5187	7.8276	7.2020	7.3728	7.4591	7.4377	7.5578	7.4812	7.7564	7.4322	7.5764	7.4965	7.7911	**7.33**
H5	7.3549	7.5559	7.6077	7.6483	7.7289	7.6903	7.9148	7.6398	7.7335	7.7087	7.9524	7.3623	7.5446	7.5939	7.6255	7.7039	7.6680	7.8758	7.6179	7.6995	7.6853	7.9117	**7.45**
H6	7.6850	7.8736	7.9488	7.9791	8.1082	8.0197	8.3379	7.9677	8.1352	8.0407	8.3884	7.5195	7.6882	7.7795	7.7578	7.9182	7.8000	8.0791	7.7495	7.9004	7.8181	8.1330	**7.57**
H8	4.5761	4.6500	4.6786	4.7145	4.7859	4.7570	4.9873	4.7070	4.8028	4.7746	5.0235	4.6740	4.8401	4.8901	4.9038	5.0249	4.9471	5.2085	4.8978	5.0292	4.9630	5.2513	**4.92**
H(9A-9C)	1.3402	1.3303	1.3028	1.3212	1.2904	1.3686	1.4914	1.3236	1.3125	1.3764	1.5231	1.4094	1.4647	1.4498	1.4862	1.4612	1.5321	1.6498	1.4855	1.4752	1.5429	1.6882	**1.44**
H(8`A-8`C)	2.5822	2.5238	2.4953	2.5006	2.4750	2.5491	2.6267	2.5052	2.4680	2.5548	2.6184	3.0640	2.8899	2.8367	2.7907	2.7527	2.8426	2.8332	2.8020	2.6829	2.8417	2.8107	**2.64**
F3	-149.5110	-153.2650	-156.3110	-154.7170	-158.8230	-154.4270	-157.2910	-154.5530	-158.2730	-154.7280	-157.7550	-149.3510	-153.2220	-156.3260	-154.6670	-158.7980	-154.3830	-157.3990	-154.5130	-158.3430	-154.6730	-157.8360	**-114.23**
Nuclei	BMK											BMK										
C1	162.2400	162.1101	162.7462	162.1787	163.7432	162.1732	162.7329	162.3788	162.5499	162.3453	162.8250	161.3138	161.8189	162.6178	162.4354	163.8322	162.3810	163.7489	162.5443	163.5016	162.6573	163.8918	**134.46**
C2	136.7126	135.7407	136.3571	135.1216	135.9083	135.1421	136.2364	135.3741	136.0691	135.2636	136.1930	136.2628	135.4326	136.0286	135.0703	135.7132	135.0819	136.1680	135.3055	135.9639	135.2213	136.1478	**115.52**
C3	187.0301	187.0551	187.8408	187.0477	188.1962	187.0333	188.0420	187.2302	187.9469	187.2230	188.0648	187.2376	187.1687	187.9784	187.1390	188.2778	187.1240	188.1259	187.3205	188.0362	187.3149	188.1513	**162.83**
C4	139.5338	141.0867	141.9440	141.8030	142.6696	141.7419	143.7062	141.8918	143.3926	142.0227	143.8873	139.7892	141.0292	141.9252	141.5094	142.4656	141.4635	143.1447	141.6273	142.8800	141.7124	143.3050	**122.41**
C5	150.5620	152.5708	153.4546	153.6247	154.9031	153.5456	154.9676	153.6775	154.7813	153.8616	155.1400	150.7561	152.7680	153.5758	153.6700	154.9685	153.6018	154.8508	153.7437	154.7018	153.8949	155.0130	**131.43**
C6	143.3877	145.7280	147.0994	146.7575	148.8367	146.6701	149.2565	146.7941	148.9691	147.0018	149.6360	143.4992	146.0572	147.3665	147.2515	149.4923	147.1717	149.7664	147.3009	149.5231	147.4870	150.0856	**125.17**
C7	217.8060	223.4655	224.9383	226.4686	227.1939	226.2755	233.0517	226.2929	231.5604	226.8133	233.9788	222.3530	227.3456	229.0592	230.0127	231.0492	229.8346	236.7529	229.8700	235.3030	230.3458	237.5066	**196.61**
C8	71.2103	72.3800	73.0712	72.9676	74.0630	72.9310	74.4301	73.1053	74.0994	73.1633	75.0734	65.2856	66.6120	67.1563	67.8075	68.5986	67.7283	69.5166	67.8632	69.0652	68.0480	69.8209	**59.97**
C9	25.5376	25.8446	26.0318	25.9188	26.4894	25.8901	26.4426	26.0718	26.2908	26.1081	26.6342	22.3266	22.2570	22.4909	22.7080	22.9725	22.6732	23.0897	22.8502	22.9345	22.9034	23.4149	**15.26**
C8`	38.7669	39.4262	39.7117	39.8197	40.3008	39.7903	40.3722	39.9721	40.2640	40.0092	40.7922	33.7006	34.0446	34.4504	34.1208	34.6961	34.0997	34.6697	34.2891	34.6786	34.3014	34.7612	**31.09**
H2	8.5985	8.5179	8.5943	8.4278	8.4833	8.4281	8.5266	8.4285	8.5512	8.4179	8.5251	8.5848	8.4049	8.4853	8.3273	8.3863	8.3305	8.3735	8.3332	8.4009	8.3138	8.3733	**7.66**
H4	7.6493	7.8608	7.9448	7.9468	8.0661	7.9386	8.1039	7.9304	8.0859	7.9449	8.1322	7.6620	7.8408	7.9425	7.9230	8.0503	7.9150	8.0813	7.9070	8.0691	7.9209	8.1058	**7.33**
H5	7.8765	8.1019	8.1629	8.2055	8.2858	8.1960	8.3072	8.1865	8.2981	8.2048	8.3310	7.8678	8.0844	8.1336	8.1798	8.2616	8.1705	8.2654	8.1612	8.2551	8.1790	8.2876	**7.45**
H6	8.2070	8.4386	8.5498	8.5495	8.6971	8.5388	8.7420	8.5280	8.7421	8.5502	8.7907	8.0160	8.2064	8.3309	8.3395	8.5254	8.3290	8.5327	8.3183	8.5189	8.3395	8.5783	**7.57**
H8	4.2821	4.4049	4.4538	4.4832	4.5594	4.4734	4.6132	4.4638	4.6089	4.4829	4.6388	4.4973	4.6358	4.7186	4.7368	4.8600	4.7268	4.8923	4.7167	4.8668	4.7368	4.9222	**4.92**
H(9A-9C)	1.3069	1.3289	1.3147	1.3201	1.2859	1.3172	1.3085	1.3142	1.3133	1.3134	1.3258	1.3376	1.3959	1.3567	1.4192	1.3884	1.4140	1.4066	1.4088	1.3969	1.4144	1.4317	**1.44**
H(8`A-8`C)	2.4403	2.3909	2.3332	2.3812	2.3387	2.3786	2.3210	2.3761	2.3112	2.3741	2.3056	2.8178	2.6558	2.6295	2.5940	2.5372	2.5946	2.4500	2.5949	2.4707	2.5833	2.4236	**2.64**
F3	-124.0340	-127.1270	-129.6180	-128.2800	-131.6250	-128.2180	-131.2150	-128.1530	-131.1640	-128.3400	-131.1870	-123.9260	-127.2520	-129.7640	-128.3300	-131.6780	-128.2740	-131.2840	-128.2160	-131.2510	-128.3830	-131.2370	**-114.23**
Nuclei	BP86											BP86										
C1	142.6033	143.2892	144.3217	143.3129	144.8294	143.3161	144.1093	143.3149	144.3473	143.3051	144.2880	141.2102	142.3913	142.8955	142.7789	144.0934	142.7583	144.2034	142.7343	144.0933	142.7962	144.5179	**134.46**
C2	119.5132	118.9948	119.4330	118.5273	118.9749	118.5643	119.3960	118.5964	119.3473	118.4873	119.5119	118.9530	118.7496	119.1040	118.4438	118.9042	118.4690	119.5071	118.4896	119.3803	118.4158	119.6576	**115.52**
C3	172.4608	172.9866	173.7055	173.0692	174.0928	173.0730	174.0023	173.0716	173.9922	173.0606	174.2325	172.6041	173.0252	173.7451	173.0803	174.0764	173.0859	173.9418	173.0864	173.9453	173.0699	174.1650	**162.83**
C4	122.8492	124.5769	125.1420	125.3271	125.8172	125.2897	126.9376	125.2471	126.6421	125.3577	127.3199	123.0920	124.4730	125.1351	125.0277	125.6030	125.0052	126.3091	124.9769	126.1381	125.0431	126.6652	**122.41**
C5	132.3039	134.4559	135.1483	135.4396	136.4619	135.3882	136.6274	135.3316	136.4931	135.4832	136.9837	132.5764	134.5444	135.2681	135.4289	136.4465	135.3852	136.4384	135.3359	136.3593	135.4648	136.7926	**131.43**
C6	125.6950	127.6383	128.6236	128.6503	130.2114	128.5969	130.6655	128.5381	130.3845	128.6961	131.2615	125.9992	128.2203	129.3919	129.2180	130.9403	129.1674	131.2237	129.1109	131.0571	129.2602	131.7128	**125.17**
C7	201.4869	206.6192	208.2390	209.0105	209.9463	208.8668	214.4244	208.7193	213.5707	209.1433	215.2402	206.3315	210.3628	211.8523	212.3568	213.2823	212.2454	217.4302	212.1289	216.5301	212.4577	218.1117	**196.61**
C8	67.7583	69.1024	69.6319	69.4925	70.2735	69.4833	70.6802	69.4672	70.5751	69.4949	71.6087	62.0427	64.0265	64.2886	64.8784	65.6473	64.8306	66.4624	64.7787	66.1861	64.9206	66.9619	**59.97**
C9	23.4587	23.8784	23.9802	24.1183	24.3813	24.1120	24.5183	24.1003	24.4332	24.1189	24.8862	20.1385	20.7994	20.7668	21.0088	21.2511	21.0015	21.5039	20.9895	21.4011	21.0115	22.1254	**15.26**
C8`	37.4532	38.3350	38.4359	38.6311	38.8361	38.6206	39.0764	38.6051	39.0143	38.6360	39.7128	32.5953	32.8935	33.1929	33.0035	33.2356	33.0063	33.2521	33.0032	33.2824	32.9950	33.4517	**31.09**
H2	8.0460	7.9530	7.9729	7.8987	7.9248	7.9033	7.9680	7.9075	7.9548	7.8941	7.9863	8.1062	7.9414	8.0081	7.8573	7.8978	7.8638	7.8711	7.8698	7.8847	7.8505	7.8826	**7.66**
H4	7.1940	7.3974	7.4813	7.4806	7.5914	7.4767	7.6388	7.4724	7.6207	7.4840	7.6760	7.1971	7.3813	7.4684	7.4550	7.5689	7.4518	7.5995	7.4482	7.5860	7.4577	7.6351	**7.33**
H5	7.3836	7.5932	7.6394	7.6900	7.7639	7.6851	7.7826	7.6799	7.7686	7.6943	7.8221	7.3932	7.5853	7.6333	7.6731	7.7466	7.6689	7.7505	7.6643	7.7411	7.6767	7.7875	**7.45**
H6	7.7551	7.9399	7.9988	8.0409	8.1524	8.0354	8.2056	8.0298	8.1770	8.0457	8.2633	7.5562	7.7292	7.8336	7.8195	7.9743	7.8153	7.9668	7.8106	7.9591	7.8230	8.0215	**7.57**
H8	4.6102	4.6886	4.7066	4.7545	4.8085	4.7500	4.8491	4.7453	4.8359	4.7587	4.8868	4.7499	4.9016	4.9510	4.9712	5.0773	4.9680	5.0911	4.9645	5.0812	4.9737	5.1350	**4.92**
H(9A-9C)	1.3746	1.3642	1.3222	1.3541	1.3091	1.3560	1.3291	1.3576	1.3202	1.3518	1.3676	1.4508	1.4923	1.4616	1.5156	1.4781	1.5149	1.4991	1.5140	1.4923	1.5158	1.5398	**1.44**
H(8`A-8`C)	2.5693	2.5039	2.4639	2.4798	2.4397	2.4819	2.4190	2.4838	2.4247	2.4774	2.4119	2.9949	2.8241	2.7917	2.7480	2.6939	2.7534	2.5979	2.7585	2.6174	2.7424	2.5769	**2.64**
F3	-141.0370	-144.3320	-147.1730	-145.5650	-149.3730	-145.4950	-148.8330	-145.4250	-148.8150	-145.6310	-148.7520	-140.9280	-144.3630	-147.1850	-145.5720	-149.4050	-145.5060	-148.9800	-145.4390	-148.9300	-145.6350	-148.8910	**-114.23**
Nuclei	CAM-B3LYP											CAM-B3LYP										
C1	147.5356	147.8355	148.0266	147.8495	149.3617	147.8601	148.4435	147.8717	148.5998	147.8423	148.4144	146.3788	147.2835	147.7550	147.7021	148.9802	147.6764	148.8682	147.6547	148.7837	147.7335	149.0350	**134.46**
C2	125.3419	124.7113	125.1447	124.2638	124.8115	124.2955	125.2207	124.3274	125.1608	124.2361	125.1909	124.9277	124.5601	124.9831	124.2725	124.8107	124.2933	125.3385	124.3149	125.2347	124.2562	125.3523	**115.52**
C3	175.2350	175.4104	175.9761	175.4531	176.3474	175.4552	176.2406	175.4577	176.2474	175.4534	176.2969	175.3257	175.4458	176.0405	175.4756	176.3409	175.4775	176.2215	175.4799	176.2296	175.4758	176.2811	**162.83**
C4	127.7281	129.2396	129.9748	130.0025	130.5411	129.9608	131.6302	129.9196	131.3634	130.0440	131.8418	127.9995	129.1976	129.8916	129.7256	130.3720	129.7006	131.0401	129.6749	130.8844	129.7497	131.2249	**122.41**
C5	137.3892	139.3230	139.8977	140.3179	141.2561	140.2631	141.3314	140.2087	141.2302	140.3722	141.5022	137.5314	139.3463	139.9686	140.2385	141.1638	140.1900	141.1167	140.1415	141.0496	140.2861	141.2976	**131.43**
C6	131.2257	133.3580	134.7016	134.4471	136.1424	134.3790	136.5910	134.3108	136.3369	134.5135	137.0724	131.5278	133.8293	135.0818	134.9175	136.7818	134.8560	137.0470	134.7942	136.8772	134.9768	137.3859	**125.17**
C7	205.8158	211.3203	212.3152	214.2540	214.9544	214.0898	220.3783	213.9268	219.1675	214.4135	221.0775	210.5254	215.0693	216.5808	217.4571	218.2184	217.3208	223.2425	217.1839	222.0917	217.5892	223.8996	**196.61**
C8	63.9844	65.2551	65.6029	65.6396	66.4641	65.6224	66.8154	65.6052	66.6859	65.6570	67.5204	58.4440	60.2366	60.5256	61.1146	61.8719	61.0606	62.6313	61.0093	62.3592	61.1711	62.9887	**59.97**
C9	22.3327	22.5619	22.7611	22.7043	23.0742	22.6947	22.9898	22.6852	22.9701	22.7152	23.1866	19.2303	19.4890	19.4813	19.6125	19.9006	19.6045	19.9102	19.5981	19.8670	19.6232	20.2578	**15.26**
C8`	35.4863	36.2975	36.4201	36.6866	37.0001	36.6684	37.2088	36.6510	37.1430	36.7059	37.6692	30.9431	31.2277	31.5600	31.4215	31.7541	31.4134	31.8210	31.4050	31.8326	31.4304	31.9378	**31.09**
H2	8.3798	8.2664	8.3814	8.2018	8.2456	8.2053	8.2878	8.2089	8.2860	8.1983	8.2930	8.4262	8.2344	8.3139	8.1354	8.1963	8.1420	8.1687	8.1483	8.1867	8.1287	8.1656	**7.66**
H4	7.4469	7.6448	7.7395	7.7293	7.8500	7.7247	7.8996	7.7202	7.8822	7.7336	7.9211	7.4536	7.6353	7.7333	7.7082	7.8332	7.7043	7.8644	7.7005	7.8518	7.7117	7.8860	**7.33**
H5	7.5707	7.7782	7.8342	7.8767	7.9539	7.8711	7.9715	7.8656	7.9595	7.8819	7.9956	7.5711	7.7675	7.8212	7.8578	7.9361	7.8527	7.9405	7.8477	7.9316	7.8625	7.9629	**7.45**
H6	7.8683	8.0780	8.2089	8.2034	8.3425	8.1957	8.4017	8.1882	8.3774	8.2107	8.4461	7.7114	7.9097	8.0319	8.0073	8.1871	8.0019	8.1841	7.9963	8.1760	8.0122	8.2230	**7.57**
H8	4.2292	4.3359	4.4025	4.4390	4.5151	4.4322	4.5799	4.4257	4.5586	4.4456	4.6008	4.4120	4.5862	4.6603	4.6626	4.7906	4.6585	4.8082	4.6544	4.7987	4.6662	4.8353	**4.92**
H(9A-9C)	1.3314	1.3306	1.3316	1.3144	1.2856	1.3152	1.2974	1.3159	1.2948	1.3135	1.3232	1.3989	1.4252	1.4082	1.4443	1.4181	1.4431	1.4338	1.4420	1.4305	1.4452	1.4544	**1.44**
H(8`A-8`C)	2.5237	2.4766	2.4216	2.4512	2.4244	2.4524	2.4046	2.4537	2.4070	2.4499	2.3891	2.9298	2.7596	2.7397	2.6871	2.6470	2.6918	2.5606	2.6963	2.5813	2.6823	2.5287	**2.64**
F3	-121.3820	-124.6950	-127.0670	-125.9590	-129.1170	-125.8870	-128.7520	-125.8150	-128.6920	-126.0270	-128.7820	-121.4370	-124.7910	-127.1700	-126.0010	-129.1880	-125.9350	-128.8540	-125.8680	-128.7980	-126.0640	-128.8540	**-114.23**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S3. Cont. III

Nuclei	R											S										Exp. [b]
	HF											HF										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	145.1677	145.2378	146.1793	145.1951	146.5230	145.2415	146.2831	145.2879	146.5411	145.1504	146.2684	143.8874	144.9107	145.1291	145.1548	146.6395	145.1154	146.3722	145.0877	146.8385	145.2125	146.5032	**134.46**
C2	124.8548	124.2329	124.7641	123.8094	124.3650	123.8340	124.8109	123.8592	124.7478	123.7855	124.8079	124.6664	124.1659	124.7260	123.7863	124.4122	123.8105	124.7666	123.8347	124.6550	123.7618	124.7910	**115.52**
C3	167.1337	167.0098	167.5260	166.9284	167.6437	166.9374	167.5171	166.9470	167.5577	166.9190	167.5617	167.0818	167.0306	167.4573	166.9955	167.6886	166.9946	167.5593	166.9954	167.6231	166.9981	167.6129	**162.83**
C4	126.3184	127.7879	128.3536	128.5420	129.0127	128.4876	129.9189	128.4333	129.6154	128.5927	130.1142	126.7038	127.6162	128.3776	128.1090	128.5953	128.0889	129.2704	128.0654	128.9167	128.1196	129.4438	**122.41**
C5	135.8334	137.4527	137.9371	138.2817	138.9895	138.2389	138.9602	138.1962	138.9178	138.3215	139.1093	135.8066	137.4361	137.7994	138.2373	138.9137	138.1866	138.8311	138.1375	138.8328	138.2876	138.9885	**131.43**
C6	129.7535	131.8567	132.8318	133.0111	134.5804	132.9177	134.7522	132.8251	134.4567	133.0994	135.1656	130.2746	132.2328	133.5988	133.2539	134.7807	133.2069	135.0040	133.1539	134.6024	133.2868	135.3099	**125.17**
C7	195.8399	202.0153	203.5372	205.3507	205.4212	205.1916	212.9887	205.0320	211.3990	205.5006	213.7654	200.1574	205.1172	206.2747	207.6847	208.1644	207.5170	214.5301	207.3560	213.2937	207.8540	215.2728	**196.61**
C8	55.0095	56.0239	56.4212	56.2553	56.9002	56.2429	57.6872	56.2310	57.5214	56.2665	58.2199	50.3637	52.1147	52.4148	52.8310	53.5355	52.7807	54.3163	52.7345	54.2258	52.8847	54.6077	**59.97**
C9	20.5409	20.5028	20.6164	20.5360	20.8734	20.5232	20.5925	20.5111	20.5996	20.5481	20.6991	17.7127	17.6210	17.6828	17.6093	17.8513	17.6102	17.7197	17.6114	17.7151	17.6077	17.9090	**15.26**
C8`	32.6536	33.4069	33.5694	33.6973	34.0330	33.6772	34.1688	33.6578	34.1278	33.7159	34.5276	29.0067	29.1901	29.5101	29.4080	29.6885	29.3969	29.7184	29.3850	29.6688	29.4150	29.8130	**31.09**
H2	8.5518	8.4155	8.4613	8.3404	8.4137	8.3406	8.3611	8.3408	8.3577	8.3402	8.3658	8.6211	8.3563	8.4700	8.2623	8.3167	8.2704	8.2791	8.2771	8.2537	8.2526	8.2794	**7.66**
H4	7.5717	7.7846	7.8839	7.8760	7.9999	7.8708	8.0500	7.8652	8.0291	7.8811	8.0741	7.5798	7.7683	7.8722	7.8468	7.9725	7.8427	8.0088	7.8383	7.9874	7.8505	8.0328	**7.33**
H5	7.6227	7.8424	7.8973	7.9449	8.0244	7.9392	8.0380	7.9332	8.0261	7.9504	8.0619	7.6213	7.8329	7.8846	7.9311	8.0078	7.9255	8.0137	7.9197	8.0030	7.9365	8.0378	**7.45**
H6	7.7959	8.0473	8.1542	8.1962	8.3642	8.1857	8.3722	8.1750	8.3462	8.2062	8.4149	7.7020	7.9162	8.0530	8.0283	8.2023	8.0229	8.2021	8.0167	8.1679	8.0325	8.2407	**7.57**
H8	3.6366	3.7867	3.8521	3.9217	4.0280	3.9130	4.0563	3.9041	4.0325	3.9301	4.0811	3.8329	4.0130	4.0991	4.1004	4.2326	4.0960	4.2631	4.0910	4.2381	4.1042	4.2842	**4.92**
H(9A-9C)	1.1917	1.1740	1.1473	1.1559	1.1242	1.1553	1.1164	1.1545	1.1112	1.1565	1.1329	1.2684	1.2605	1.2550	1.2769	1.2348	1.2767	1.2445	1.2760	1.2304	1.2765	1.2586	**1.44**
H(8`A-8`C)	2.2784	2.2543	2.2224	2.2433	2.2059	2.2439	2.2257	2.2445	2.2237	2.2427	2.2162	2.6838	2.5215	2.4984	2.4642	2.4215	2.4678	2.3589	2.4711	2.3640	2.4603	2.3320	**2.64**
F3	-99.7310	-102.3540	-104.0890	-103.3870	-105.7190	-103.3210	-105.4830	-103.2540	-105.3970	-103.4480	-105.5420	-99.9537	-102.4910	-104.3720	-103.4150	-105.7580	-103.3690	-105.5650	-103.3200	-105.4340	-103.4530	-105.5770	**-114.23**
Nuclei	**LC-BLYP**																						
C1	151.6406	151.6150	152.1182	151.6273	153.2014	151.6051	149.9239	151.6087	151.8050	151.6298	152.0605	150.6311	151.4407	151.8398	151.8586	153.0937	151.7947	152.9477	151.7655	152.9773	151.9101	153.1198	**134.46**
C2	130.5572	129.8547	130.4105	129.4435	130.0664	129.4484	123.3853	129.4803	130.3267	129.4213	130.4315	130.2390	129.7777	130.2908	129.5014	130.0877	129.4945	130.5914	129.5158	130.4994	129.4922	130.6146	**115.52**
C3	179.0494	178.9660	179.5524	178.9789	179.7589	178.9566	175.4331	178.9615	179.6318	178.9829	179.7007	179.0746	178.9989	179.5800	179.0214	179.7698	178.9977	179.6790	179.0016	179.6788	179.0269	179.7371	**162.83**
C4	132.7367	134.2318	135.0568	135.0341	135.6405	134.9645	128.8534	134.9220	136.5643	135.0830	136.9680	132.9846	134.1607	135.0182	134.7493	135.4701	134.6991	136.1429	134.6738	135.9371	134.7773	136.3295	**122.41**
C5	142.6444	144.5170	145.1617	145.5629	146.5042	145.4777	139.0341	145.4195	146.3819	145.6259	146.6952	142.7457	144.5442	145.2217	145.5022	146.4054	145.4248	146.3535	145.3743	146.2703	145.5578	146.5303	**131.43**
C6	136.1743	138.5344	139.9181	139.7387	141.4675	139.6445	132.9154	139.5784	141.9509	139.8114	142.5261	136.5101	138.9208	140.3700	140.1268	142.0728	140.0378	142.3382	139.9738	142.1186	140.1909	142.6918	**125.17**
C7	211.2213	216.7556	218.0599	219.7660	220.5761	219.5580	218.1908	219.3757	224.4550	219.9444	226.8586	215.6172	220.4133	221.9804	223.0103	223.7365	222.8297	229.1980	222.6786	227.9504	223.1673	229.8745	**196.61**
C8	61.7675	63.0661	63.6132	63.5795	64.4141	63.5336	75.5767	63.5142	64.6026	63.6053	65.5012	56.0690	57.7378	58.0853	58.6359	59.3376	58.5505	60.1132	58.4958	59.8892	58.7036	60.5024	**59.97**
C9	21.3939	21.6030	21.8003	21.7764	22.1042	21.7442	30.4102	21.7399	22.0256	21.7900	22.1817	18.5296	18.6772	18.7286	18.8273	19.0770	18.7934	19.0073	18.7875	18.9893	18.8429	19.3517	**15.26**
C8`	33.5846	34.3905	34.6247	34.8135	35.1791	34.7680	45.4877	34.7497	35.2897	34.8392	35.8447	29.0279	29.3230	29.7330	29.6296	29.9390	29.5919	30.0597	29.5801	30.0124	29.6464	30.2415	**31.09**
H2	8.5744	8.4657	8.5518	8.3981	8.4359	8.4016	7.9211	8.4068	8.5218	8.3939	8.4885	8.6079	8.4037	8.4921	8.3033	8.3675	8.3101	8.3382	8.3177	8.3467	8.2953	8.3367	**7.66**
H4	7.6035	7.7991	7.8984	7.8840	8.0081	7.8783	7.8461	7.8741	8.0402	7.8884	8.0801	7.6063	7.7883	7.8903	7.8634	7.9913	7.8586	8.0222	7.8552	8.0079	7.8670	8.0457	**7.33**
H5	7.7110	7.9193	7.9730	8.0188	8.0931	8.0122	7.9710	8.0071	8.0989	8.0241	8.1344	7.7124	7.9120	7.9653	8.0056	8.0806	7.9995	8.0843	7.9948	8.0746	8.0104	8.1083	**7.45**
H6	8.0036	8.2305	8.3501	8.3565	8.5000	8.3477	8.2629	8.3407	8.5698	8.3638	8.6162	7.8616	8.0684	8.2025	8.1729	8.3589	8.1667	8.3548	8.1617	8.3402	8.1775	8.3952	**7.57**
H8	4.1114	4.2259	4.2904	4.3352	4.4194	4.3266	4.8855	4.3197	4.4795	4.3425	4.5201	4.3377	4.5163	4.6030	4.5967	4.7328	4.5916	4.7521	4.5879	4.7384	4.6004	4.7808	**4.92**
H(9A-9C)	1.3478	1.3562	1.3463	1.3476	1.3085	1.3476	1.3914	1.3493	1.3424	1.3466	1.3563	1.4109	1.4272	1.4135	1.4452	1.4151	1.4434	1.4286	1.4431	1.4235	1.4457	1.4511	**1.44**
H(8`A-8`C)	2.5108	2.4643	2.4127	2.4477	2.4101	2.4421	2.6377	2.4441	2.3757	2.4404	2.3745	2.8768	2.7011	2.6883	2.6296	2.5949	2.6338	2.5084	2.6393	2.5263	2.6244	2.4822	**2.64**
F3	-108.5750	-111.9820	-114.1030	-113.2930	-116.0980	-113.2200	-117.5970	-113.1470	-115.7710	-113.3620	-115.9000	-108.6240	-112.0630	-114.1980	-113.3260	-116.1750	-113.2580	-115.8890	-113.1890	-115.8250	-113.3900	-115.9390	**-114.23**
Nuclei	**M06**																						
C1	142.6100	142.7300	143.0454	142.7340	143.7952	142.7250	143.3688	142.7244	143.0681	142.7578	143.3211	141.5753	142.5015	142.9778	143.0204	144.3722	142.9669	144.4920	142.9269	144.4076	143.0943	144.6737	**134.46**
C2	122.8621	122.1289	122.8254	121.7371	122.3743	121.7508	122.8697	121.7726	122.7712	121.7391	122.8266	122.1978	121.7023	122.2692	121.4963	122.1744	121.4943	122.8413	121.5020	122.7016	121.5149	122.8658	**115.52**
C3	170.5734	170.8459	171.4345	170.9665	171.9071	170.9501	171.8655	170.9415	171.7854	170.9966	171.9210	170.7644	170.8909	171.6339	170.9578	171.9704	170.9443	171.8259	170.9386	171.8434	170.9851	171.8826	**162.83**
C4	125.6640	127.3094	128.2074	128.1692	128.9348	128.1068	130.0787	128.0522	129.8388	128.2430	130.2864	125.9065	127.1879	128.0140	127.7923	128.5669	127.7505	129.2452	127.7148	129.0687	127.8445	129.4364	**122.41**
C5	135.6887	137.5510	138.2569	138.5484	139.6022	138.4783	139.6833	138.4160	139.5531	138.6293	139.8671	135.8725	137.5786	138.3359	138.4620	139.5146	138.4005	139.4387	138.3463	139.3793	138.5343	139.6213	**131.43**
C6	128.9117	130.9149	132.4880	132.0695	134.1091	131.9866	134.5013	131.9118	134.4441	132.1630	134.9347	129.3042	131.3920	132.8302	132.4756	134.4064	132.4023	134.6565	132.3351	134.4766	132.5576	134.9979	**125.17**
C7	202.5219	207.4680	208.5314	210.0985	210.4038	209.9294	215.8172	209.7687	214.2685	210.2746	216.4449	207.0367	211.4372	212.7257	213.5404	214.3027	213.4054	218.9142	213.2798	217.8567	213.6852	219.5410	**196.61**
C8	61.2220	62.4204	62.9714	62.8873	63.7173	62.8533	64.2539	62.8266	64.0542	62.9341	64.9711	55.0945	56.4420	56.9674	57.2880	58.1503	57.2180	58.9305	57.1583	58.6774	57.3730	59.3588	**59.97**
C9	22.1763	22.5044	22.8687	22.8545	23.3921	22.8224	23.4598	22.7979	23.4809	22.8990	23.6035	19.4991	19.6749	19.8107	19.8576	20.2441	19.8327	20.2193	19.8162	20.1885	19.8969	20.6729	**15.26**
C8`	36.7689	37.4563	37.7123	37.8164	38.2128	37.7839	38.4849	37.7598	38.3566	37.8624	38.9626	31.7478	32.1694	32.5224	32.5253	32.9929	32.4927	33.1917	32.4677	33.1587	32.5701	33.2539	**31.09**
H2	8.2548	8.1658	8.2720	8.1141	8.1983	8.1170	8.2281	8.1205	8.2426	8.1120	8.2273	8.2324	8.0482	8.1325	7.9578	8.0248	7.9635	8.0244	7.9696	8.0327	7.9523	8.0153	**7.66**
H4	7.2524	7.4645	7.5576	7.5559	7.6784	7.5505	7.7436	7.5457	7.7161	7.5615	7.7627	7.2868	7.4768	7.5766	7.5517	7.6834	7.5475	7.7165	7.5437	7.7023	7.5563	7.7398	**7.33**
H5	7.5526	7.7659	7.8199	7.8661	7.9476	7.8601	7.9704	7.8547	7.9557	7.8724	7.9978	7.5369	7.7301	7.7898	7.8103	7.8940	7.8057	7.8868	7.8017	7.8806	7.8150	7.9090	**7.45**
H6	7.8636	8.0641	8.2300	8.1778	8.3636	8.1701	8.4193	8.1630	8.4189	8.1859	8.4537	7.6558	7.8449	7.9575	7.9519	8.1258	7.9453	8.1377	7.9391	8.1202	7.9586	8.1847	**7.57**
H8	4.3341	4.4115	4.4919	4.4913	4.5727	4.4847	4.6419	4.4790	4.6192	4.4983	4.6596	4.4942	4.6900	4.7345	4.7695	4.8867	4.7649	4.8906	4.7609	4.8810	4.7742	4.9283	**4.92**
H(9A-9C)	1.3114	1.3092	1.3133	1.2953	1.2992	1.2962	1.2903	1.2977	1.3150	1.2950	1.3185	1.4056	1.4366	1.4199	1.4455	1.4222	1.4450	1.4101	1.4449	1.4105	1.4464	1.4388	**1.44**
H(8`A-8`C)	2.5014	2.4361	2.3931	2.4129	2.3778	2.4140	2.3705	2.4156	2.3656	2.4124	2.3546	2.9241	2.7396	2.7165	2.6531	2.6143	2.6586	2.5127	2.6645	2.5340	2.6482	2.4863	**2.64**
F3	-124.9790	-128.3630	-130.3560	-128.9050	-132.1690	-128.8450	-131.7870	-128.7830	-131.8180	-128.9630	-131.7620	-124.9870	-128.4560	-130.3320	-128.9730	-132.1950	-128.9160	-131.8410	-128.8590	-131.8080	-129.0260	-131.8080	**-114.23**
Nuclei	**M06-2X**																						
C1	160.2039	160.4075	160.8616	160.3809	161.8509	160.4014	160.8912	160.4238	160.8117	160.3557	161.0333	159.5562	160.4489	160.8060	160.9398	162.3797	160.9052	162.2314	160.8799	162.1593	160.9778	162.4971	**134.46**
C2	136.2986	135.4893	136.0083	134.9546	135.5838	135.0088	135.9044	135.0640	135.8241	134.8968	135.9063	136.0353	135.4050	135.8346	135.0522	135.6519	135.0881	136.1343	135.1272	136.0198	135.0143	136.1769	**115.52**
C3	184.7965	184.9329	185.5597	184.9658	185.8905	184.9847	185.8255	185.0046	185.8016	184.9419	185.9159	184.9731	185.0160	185.6807	185.0134	185.9144	185.0350	185.8171	185.0576	185.8216	184.9867	185.9028	**162.83**
C4	139.5616	141.2328	142.0505	142.0631	142.7998	142.0346	143.9051	142.0075	143.6702	142.0835	144.1570	139.6623	141.0405	141.9051	141.6654	142.4562	141.6559	143.2040	141.6456	143.0062	141.6654	143.4178	**122.41**
C5	150.6292	152.8608	153.6432	154.0076	155.1735	153.9591	155.3006	153.9119	155.1651	154.0469	155.5351	150.6966	152.7864	153.6075	153.8244	154.9891	153.7859	154.9758	153.7477	154.8831	153.8532	155.2040	**131.43**
C6	143.3981	145.7620	147.1273	146.9508	148.9090	146.9007	149.3533	146.8517	149.1444	146.9916	149.8293	143.7814	146.2730	147.7056	147.4606	149.4805	147.4161	149.7934	147.3704	149.5889	147.4939	150.1576	**125.17**
C7	219.0157	224.7861	226.0210	227.7348	228.4245	227.5720	234.2341	227.4109	232.7365	227.8838	235.2505	223.0297	228.1750	229.6967	230.8889	231.7104	230.7365	237.4898	230.5890	236.1098	231.0318	238.3293	**196.61**
C8	66.6741	67.9547	68.5793	68.4286	69.4017	68.4237	69.7847	68.4195	69.5857	68.4263	70.5200	61.0495	62.6358	63.0376	63.5084	64.3313	63.4653	65.0479	63.4268	64.7912	63.5472	65.4736	**59.97**
C9	23.0147	23.3948	23.5897	23.6329	24.0432	23.6410	24.0607	23.6499	24.0373	23.6187	24.2702	20.2632	20.6357	20.6578	20.7707	21.0327	20.7823	20.9843	20.7953	20.9724	20.7539	21.3638	**15.26**
C8`	35.8732	36.6055	36.7501	36.9007	37.2623	36.9035	37.4137	36.9075	37.3413	36.8920	37.9308	30.7163	31.2212	31.4977	31.4763	31.7634	31.4863	31.8713	31.4960	31.8361	31.4581	32.0763	**31.09**
H2	8.7559	8.6567	8.7466	8.6032	8.6533	8.6056	8.7013	8.6076	8.7188	8.6010	8.6968	8.7460	8.5978	8.6819	8.5161	8.5704	8.5213	8.5683	8.5257	8.5773	8.5107	8.5663	**7.66**
H4	7.8487	8.0556	8.1525	8.1474	8.2738	8.1409	8.3223	8.1340	8.3035	8.1537	8.3453	7.8550	8.0357	8.1431	8.1120	8.2410	8.1068	8.2708	8.1012	8.2583	8.1169	8.2914	**7.33**
H5	8.1179	8.3327	8.3961	8.4380	8.5234	8.4305	8.5437	8.4228	8.5328	8.4451	8.5678	8.1000	8.3064	8.3681	8.4047	8.4891	8.3979	8.4957	8.3908	8.4860	8.4110	8.5179	**7.45**
H6	8.4358	8.6417	8.7621	8.7595	8.9095	8.7511	8.9642	8.7424	8.9568	8.7675	9.0065	8.2680	8.4624	8.5993	8.5640	8.7471	8.5577	8.7545	8.5507	8.7417	8.5697	8.7892	**7.57**
H8	4.2595	4.3525	4.4097	4.4474	4.5186	4.4399	4.5950	4.4320	4.5876	4.4548	4.6191	4.4926	4.6553	4.7343	4.7346	4.8691	4.7291	4.8908	4.7231	4.8800	4.7399	4.9125	**4.92**
H(9A-9C)	1.3628	1.3640	1.3646	1.3614	1.3332	1.3605	1.3528	1.3593	1.3556	1.3623	1.3705	1.4127	1.4357	1.4257	1.4525	1.4183	1.4507	1.4382	1.4484	1.4333	1.4542	1.4540	**1.44**
H(8`A-8`C)	2.4796	2.4391	2.3858	2.4208	2.3884	2.4206	2.3634	2.4200	2.3556	2.4212	2.3454	2.7754	2.6266	2.6214	2.5637	2.5257	2.5670	2.4591	2.5697	2.4796	2.5603	2.4208	**2.64**
F3	-120.2380	-123.3530	-125.7360	-124.5130	-127.6330	-124.4490	-127.2790	-124.3840	-127.2500	-124.5730	-127.2790	-120.2820	-123.4440	-125.8070	-124.5250	-127.6640	-124.4700	-127.2530	-124.4110	-127.2290	-124.5770	-127.2190	**-114.23**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S3. Cont. IV

Nuclei	R											S										Exp. [b]
	mpW1LYP											mpW1LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	146.0269	146.5336	146.5552	146.4909	147.9806	146.4894	147.0113	146.4898	147.1371	146.4900	146.9834	144.6962	145.5706	146.1755	146.0537	147.3805	146.0231	147.2167	145.9948	147.1868	146.0820	147.3103	**134.46**
C2	123.1094	122.3966	122.8616	121.9837	122.4212	122.0066	122.8751	122.0310	122.8154	121.9599	122.8045	122.5930	122.1596	122.6132	121.9150	122.3785	121.9277	122.9347	121.9421	122.8375	121.9013	122.9038	**115.52**
C3	173.8719	174.1228	174.7674	174.2263	175.1374	174.2176	175.0172	174.2103	175.0277	174.2323	175.0914	174.0539	174.2203	174.8994	174.3104	175.1895	174.3022	175.0255	174.2954	175.0429	174.3164	175.0544	**162.83**
C4	125.7145	127.2554	127.9629	128.0518	128.4834	128.0006	129.6503	127.9511	129.4103	128.0984	129.8091	126.0216	127.1831	127.8524	127.7447	128.2606	127.7090	129.0144	127.6743	128.8429	127.7761	129.1810	**122.41**
C5	135.1659	137.1062	137.7034	138.1091	138.9981	138.0457	139.0952	137.9839	139.0057	138.1672	139.2444	135.3594	137.1444	137.7962	138.0654	138.9359	138.0077	138.9419	137.9513	138.8780	138.1180	139.0963	**131.43**
C6	129.3751	131.3203	132.7943	132.5147	134.0992	132.4387	134.6438	132.3645	134.3996	132.5852	135.0376	129.6470	131.8580	133.1308	132.9678	134.7027	132.8986	135.0596	132.8304	134.8827	133.0310	135.3911	**125.17**
C7	203.3925	208.9937	209.8106	211.6811	212.4428	211.5115	217.5884	211.3437	216.4668	211.8405	218.3507	208.5264	212.8448	214.3763	215.1372	215.9496	214.9971	220.6988	214.8582	219.6652	215.2681	221.2491	**196.61**
C8	65.2746	66.4394	66.8668	66.8744	67.6480	66.8517	67.9858	66.8290	67.8159	66.8928	68.6348	59.8158	61.6502	62.0736	62.6041	63.3735	62.5446	64.0667	62.4872	63.8345	62.6592	64.3785	**59.97**
C9	22.9532	23.1223	23.4677	23.3996	23.6906	23.3798	23.7037	23.3614	23.6649	23.4162	23.8427	19.5881	19.9102	19.9859	20.1059	20.3504	20.0902	20.4529	20.0764	20.3931	20.1192	20.7932	**15.26**
C8`	36.2978	37.0995	37.2411	37.4892	37.7732	37.4625	38.0041	37.4372	37.9639	37.5126	38.4061	31.7987	32.0119	32.3518	32.2157	32.4757	32.1994	32.5335	32.1844	32.5666	32.2289	32.5799	**31.09**
H2	8.2878	8.1579	8.2983	8.1091	8.1475	8.1125	8.2029	8.1156	8.2062	8.1057	8.2112	8.3471	8.1610	8.2358	8.0657	8.1145	8.0714	8.0904	8.0769	8.1028	8.0599	8.0877	**7.66**
H4	7.3683	7.5679	7.6614	7.6532	7.7695	7.6486	7.8204	7.6436	7.8045	7.6575	7.8409	7.3835	7.5624	7.6599	7.6364	7.7557	7.6325	7.7818	7.6283	7.7691	7.6399	7.8012	**7.33**
H5	7.5006	7.7079	7.7648	7.8075	7.8833	7.8020	7.9013	7.7960	7.8907	7.8127	7.9241	7.4958	7.6858	7.7418	7.7768	7.8520	7.7718	7.8615	7.7664	7.8528	7.7814	7.8821	**7.45**
H6	7.8174	8.0129	8.1541	8.1340	8.2670	8.1266	8.3320	8.1190	8.3158	8.1409	8.3796	7.6446	7.8383	7.9561	7.9352	8.1029	7.9296	8.1121	7.9237	8.1021	7.9402	8.1507	**7.57**
H8	4.3146	4.4120	4.4746	4.5020	4.5746	4.4955	4.6290	4.4889	4.6197	4.5083	4.6551	4.4685	4.6448	4.7128	4.7216	4.8412	4.7173	4.8617	4.7127	4.8508	4.7254	4.8862	**4.92**
H(9A-9C)	1.3264	1.3108	1.3319	1.3086	1.2748	1.3093	1.2969	1.3097	1.2929	1.3077	1.3153	1.4020	1.4346	1.4218	1.4584	1.4295	1.4571	1.4517	1.4555	1.4467	1.4595	1.4718	**1.44**
H(8`A-8`C)	2.5322	2.4814	2.4318	2.4652	2.4344	2.4663	2.4167	2.4673	2.4176	2.4640	2.3937	2.9695	2.8027	2.7753	2.7261	2.6815	2.7305	2.5991	2.7346	2.6164	2.7219	2.5627	**2.64**
F3	-129.7380	-133.2440	-135.6320	-134.5300	-137.9270	-134.4580	-137.5450	-134.3840	-137.4910	-134.5980	-137.3580	-129.7840	-133.1640	-135.7430	-134.4050	-137.8460	-134.3380	-137.7110	-134.269	-137.6470	-134.4680	-137.6800	**-114.23**
Nuclei	mpW1PW91											mpW1PW91										
C1	143.5699	144.0168	144.0785	143.9817	145.5150	143.9824	144.6596	143.9894	144.8877	143.9806	144.6840	142.4669	143.4285	143.8758	143.8157	145.0827	143.7825	145.0818	143.7593	144.9713	143.8532	145.2597	**134.46**
C2	122.1983	121.5726	122.0392	121.1463	121.7251	121.1727	122.1109	121.2048	122.0571	121.1207	122.0754	121.8044	121.4455	121.8869	121.1662	121.7402	121.1808	122.2592	121.2022	122.1497	121.1531	122.2704	**115.52**
C3	170.8862	171.1532	171.7537	171.2210	172.1680	171.2172	172.0847	171.2188	172.0873	171.2242	172.1525	171.0089	171.1828	171.8372	171.2329	172.1499	171.2302	172.0433	171.2331	172.0483	171.2346	172.1087	**162.83**
C4	124.7842	126.3705	127.1434	127.1543	127.7398	127.1073	128.8626	127.0658	128.5580	127.1984	129.0738	124.9842	126.2508	126.9888	126.8254	127.5208	126.7952	128.2051	126.7692	128.0411	126.8513	128.3964	**122.41**
C5	134.2524	136.2287	136.8633	137.2128	138.2370	137.1532	138.3503	137.0993	138.2355	137.2683	138.5358	134.3880	136.2192	136.9194	137.1225	138.1335	137.0700	138.1147	137.0223	138.0412	137.1711	138.3068	**131.43**
C6	127.7955	129.7468	131.1644	130.8537	132.4713	130.7861	132.9556	130.7240	132.6762	130.9174	133.3944	128.1038	130.2639	131.5313	131.3161	133.1320	131.2546	133.3953	131.1974	133.2343	131.3723	133.7132	**125.17**
C7	201.4506	206.7343	207.4632	209.2834	210.0345	209.1252	215.0943	208.9740	214.0069	209.4327	215.7743	205.7263	210.1038	211.4586	212.3148	213.0760	212.1820	217.8610	212.0560	216.7366	212.4407	218.4680	**196.61**
C8	63.0839	64.3145	64.6607	64.7258	65.5397	64.7053	65.9089	64.6893	65.8029	64.7436	66.6321	57.9004	59.6130	59.9266	60.4530	61.2024	60.3939	61.9921	60.3435	61.7102	60.5123	62.3270	**59.97**
C9	22.3568	22.5873	22.8840	22.8205	23.1655	22.8063	23.1630	22.7976	23.1112	22.8334	23.3562	19.1018	19.4568	19.5101	19.6448	19.9454	19.6287	20.0374	19.6194	19.9779	19.6602	20.4051	**15.26**
C8`	35.5026	36.3104	36.4144	36.6456	36.9609	36.6251	37.1698	36.6103	37.1030	36.6644	37.6249	30.9155	31.1907	31.5390	31.3758	31.7148	31.3656	31.7582	31.3603	31.7703	31.3833	31.8402	**31.09**
H2	8.2991	8.1886	8.3132	8.1328	8.1738	8.1368	8.2183	8.1408	8.2071	8.1293	8.2200	8.3365	8.1549	8.2387	8.0645	8.1272	8.0712	8.0989	8.0776	8.1171	8.0577	8.0961	**7.66**
H4	7.3921	7.5973	7.6904	7.6812	7.8038	7.6768	7.8544	7.6723	7.8359	7.6857	7.8772	7.3996	7.5855	7.6837	7.6595	7.7858	7.6557	7.8182	7.6520	7.8049	7.6631	7.8404	**7.33**
H5	7.5608	7.7733	7.8309	7.8711	7.9535	7.8656	7.9731	7.8603	7.9599	7.8764	7.9981	7.5546	7.7498	7.8077	7.8398	7.9228	7.8349	7.9286	7.8301	7.9193	7.8446	7.9520	**7.45**
H6	7.8927	8.0902	8.2272	8.2042	8.3364	8.1975	8.3948	8.1909	8.3649	8.2109	8.4384	7.7148	7.9057	8.0277	8.0006	8.1767	7.9958	8.1718	7.9908	8.1651	8.0050	8.2104	**7.57**
H8	4.3334	4.4323	4.4938	4.5187	4.5864	4.5127	4.6447	4.5070	4.6226	4.5248	4.6677	4.5200	4.6792	4.7487	4.7481	4.8711	4.7448	4.8866	4.7414	4.8784	4.7513	4.9140	**4.92**
H(9A-9C)	1.3079	1.2964	1.3106	1.2870	1.2528	1.2882	1.2700	1.2894	1.2638	1.2861	1.2945	1.3817	1.4112	1.3957	1.4304	1.4022	1.4295	1.4205	1.4286	1.4170	1.4313	1.4424	**1.44**
H(8`A-8`C)	2.4705	2.4159	2.3645	2.3947	2.3647	2.3961	2.3462	2.3976	2.3513	2.3935	2.3302	2.8641	2.7030	2.6811	2.6308	2.5901	2.6360	2.5014	2.6409	2.5234	2.6258	2.4687	**2.64**
F3	-120.0560	-123.0390	-125.3950	-124.1620	-127.3090	-124.1000	-126.8840	-124.0360	-126.8480	-124.2210	-126.8620	-120.1080	-123.1640	-125.5300	-124.2430	-127.4320	-124.1850	-127.0530	-124.1260	-127.0160	-124.2990	-127.0170	**-114.23**
Nuclei	O3LYP											O3LYP										
C1	140.8997	141.9466	143.2729	142.4032	144.4207	142.3049	143.1195	142.1745	143.5932	142.4183	143.4379	139.0203	140.4638	141.9430	141.6630	143.3736	141.6465	142.9837	141.5765	143.1903	141.6575	143.0888	**134.46**
C2	117.9082	117.5570	118.1520	117.3237	117.8850	117.3477	118.1887	117.3620	118.1720	117.2906	118.1760	117.4220	117.1821	117.8195	117.0863	117.6912	117.1065	118.0262	117.1162	117.9728	117.0591	118.0140	**115.52**
C3	167.5165	167.7112	168.4244	167.8550	168.8211	167.8565	168.7431	167.8540	168.7252	167.8481	168.8048	167.7102	167.8453	168.5409	167.9755	168.9022	167.9768	168.7816	167.9752	168.7821	167.9682	168.8406	**162.83**
C4	120.3932	121.7407	122.2980	122.4581	122.8238	122.4457	123.9552	122.4384	123.5727	122.4812	124.0535	120.6586	121.6250	122.0982	122.0374	122.5064	122.0159	123.1802	122.0013	122.9548	122.0548	123.3653	**122.41**
C5	129.9513	131.7207	132.4390	132.6715	133.6148	132.6285	133.7702	132.5829	133.6330	132.7094	133.9281	130.1391	131.7960	132.4601	132.6642	133.5740	132.6214	133.5937	132.5764	133.5006	132.6990	133.7718	**131.43**
C6	123.0408	124.8626	125.8820	125.9817	127.3998	125.9424	127.9714	125.9083	127.6222	126.0322	128.2235	123.6577	125.5240	126.5029	126.2800	127.8225	126.2291	128.1629	126.1919	127.9056	126.3276	128.4425	**125.17**
C7	197.6897	203.5719	205.5736	206.6169	207.9554	206.3492	212.3594	206.0691	211.4753	206.7853	213.1635	201.9831	206.3849	208.2014	209.1385	210.1475	209.0303	214.3678	208.8806	213.5525	209.2214	214.8852	**196.61**
C8	63.3589	64.5386	65.2615	65.1762	66.1014	65.1096	66.3981	65.0214	66.5018	65.1945	67.1484	58.1496	60.4441	61.3149	61.6476	62.5796	61.5886	63.3277	61.5062	63.1529	61.6929	63.5679	**59.97**
C9	21.8183	22.0587	22.2184	22.3011	22.5583	22.3024	22.7288	22.3027	22.6200	22.3067	22.8473	18.4006	18.7140	18.8718	18.9018	19.1361	18.8951	19.3083	18.8851	19.2278	18.9034	19.5833	**15.26**
C8`	35.8881	36.6338	36.9019	37.1057	37.4549	37.0775	37.6035	37.0483	37.5427	37.1164	37.9353	31.5880	31.7215	31.9149	31.9045	32.1649	31.9002	32.1712	31.8977	32.1533	31.9038	32.2022	**31.09**
H2	8.0517	7.8936	7.9199	7.8228	7.8430	7.8353	7.9300	7.8501	7.8958	7.8176	7.9122	8.1796	7.9467	7.9398	7.7986	7.8379	7.8028	7.8504	7.8113	7.8388	7.7959	7.8536	**7.66**
H4	7.3263	7.5151	7.6090	7.6021	7.7162	7.5976	7.7700	7.5933	7.7461	7.6064	7.7887	7.3402	7.4960	7.5832	7.5650	7.6786	7.5613	7.7108	7.5577	7.6958	7.5683	7.7331	**7.33**
H5	7.5191	7.6984	7.7476	7.7823	7.8549	7.7791	7.8758	7.7759	7.8601	7.7864	7.8969	7.5075	7.6828	7.7325	7.7644	7.8379	7.7598	7.8474	7.7552	7.8359	7.7687	7.8693	**7.45**
H6	7.7403	7.9188	8.0045	8.0357	8.1619	8.0319	8.2349	8.0308	8.1820	8.0423	8.2510	7.5926	7.7537	7.8265	7.8111	7.9580	7.8063	7.9681	7.8036	7.9466	7.8162	8.0054	**7.57**
H8	4.4153	4.4962	4.5220	4.5699	4.6391	4.5679	4.6787	4.5680	4.6410	4.5750	4.6963	4.5712	4.7077	4.7652	4.7684	4.8911	4.7649	4.9133	4.7620	4.8966	4.7718	4.9427	**4.92**
H(9A-9C)	1.2189	1.2025	1.1806	1.2003	1.1616	1.2026	1.2011	1.2046	1.1947	1.1995	1.2124	1.3233	1.3611	1.3327	1.3666	1.3326	1.3645	1.3666	1.3635	1.3547	1.3689	1.3845	**1.44**
H(8`A-8`C)	2.4971	2.4632	2.4406	2.4534	2.4264	2.4531	2.4158	2.4519	2.4227	2.4528	2.3977	2.9315	2.7673	2.7104	2.6886	2.6373	2.6937	2.5630	2.6994	2.5772	2.6839	2.5298	**2.64**
F3	-125.4700	-128.6940	-131.2040	-129.8780	-133.1980	-129.8160	-132.6800	-129.7490	-132.6960	-129.9370	-132.6490	-125.2160	-128.7070	-131.2940	-129.9000	-133.3250	-129.8380	-132.9370	-129.7710	-132.8980	-129.9580	-132.8750	**-114.23**
Nuclei	OLYP											OLYP										
C1	139.7233	141.0789	141.6734	141.2583	143.3840	141.2435	142.5023	141.2258	142.5923	141.2664	142.5553	137.6104	139.4304	140.6371	140.4210	141.9170	140.4196	141.6925	140.4105	141.8243	140.4109	141.7913	**134.46**
C2	115.7645	115.4147	115.9344	115.1368	115.6978	115.1623	115.9635	115.1824	115.9629	115.1040	115.9375	115.2249	115.0273	115.6178	114.9025	115.4276	114.9246	115.7890	114.9412	115.7370	114.8729	115.7565	**115.52**
C3	166.6520	166.9005	167.6958	167.1236	168.0959	167.1200	168.0114	167.1108	168.0145	167.1179	168.0780	166.8854	167.1065	167.8640	167.2535	168.2360	167.2502	168.0977	167.2418	168.0981	167.2478	168.1533	**162.83**
C4	118.3116	119.5949	120.2884	120.3169	120.5159	120.2884	121.4317	120.2533	121.2532	120.3336	121.6372	118.6368	119.4496	119.9624	119.8574	120.3478	119.8289	120.9627	119.7957	120.7595	119.8761	121.1381	**122.41**
C5	127.8865	129.5987	130.4042	130.5497	131.4485	130.5032	131.6125	130.4505	131.5020	130.5844	131.7897	128.1770	129.7359	130.4447	130.5808	131.5174	130.5343	131.5406	130.4824	131.4396	130.6158	131.7131	**131.43**
C6	120.7979	122.6442	123.7878	123.8070	125.0823	123.7476	125.4938	123.6820	125.2820	123.8536	125.8314	121.5280	123.1048	124.2090	123.9342	125.5401	123.8771	125.7960	123.8149	125.5882	123.9796	126.0685	**125.17**
C7	196.6851	202.9787	204.1837	205.6074	206.7091	205.4542	210.7690	205.2967	210.0025	205.7460	211.4251	200.9576	205.3766	206.8862	207.7614	208.7224	207.6594	212.7123	207.5507	211.8864	207.8480	213.7177	**196.61**
C8	64.5964	65.8444	66.3688	66.3872	67.5527	66.3530	68.1551	66.3151	67.9491	66.4123	68.7145	59.1188	61.8546	62.7447	63.1433	63.9669	63.0966	64.7876	63.0433	64.6140	63.1775	65.0044	**59.97**
C9	21.9765	22.2709	22.4545	22.6141	22.8208	22.6015	22.9884	22.5835	22.9273	22.6178	23.1296	18.3905	18.8370	19.0529	19.1040	19.3001	19.0970	19.4960	19.0841	19.4420	19.1016	19.7940	**15.26**
C8`	36.5321	37.2950	37.6251	37.7477	38.0214	37.7321	38.0661	37.7104	38.0890	37.7531	38.4144	32.2384	32.3312	32.5297	32.4904	32.7767	32.4790	32.7546	32.4626	32.7295	32.4929	32.7534	**31.09**
H2	7.8759	7.7225	7.8156	7.6820	7.6960	7.6862	7.7447	7.6901	7.7479	7.6772	7.7508	8.0240	7.7734	7.8048	7.6596	7.7195	7.6617	7.7281	7.6639	7.7205	7.6574	7.7292	**7.66**
H4	7.2468	7.4439	7.5373	7.5281	7.6289	7.5239	7.6697	7.5196	7.6587	7.5316	7.6927	7.2578	7.4112	7.4984	7.4769	7.5908	7.4731	7.6214	7.4691	7.6068	7.4802	7.6423	**7.33**
H5	7.4574	7.6162	7.6798	7.7043	7.7760	7.6995	7.7946	7.6946	7.7831	7.7084	7.8168	7.4520	7.6143	7.6669	7.6933	7.7688	7.6885	7.7772	7.6837	7.7662	7.6973	7.7975	**7.45**
H6	7.6549	7.8627	7.9685	7.9801	8.0616	7.9749	8.0865	7.9693	8.0812	7.9844	8.1261	7.5289	7.6390	7.7270	7.7014	7.8599	7.6955	7.8629	7.6897	7.8444	7.7066	7.8986	**7.57**
H8	4.5165	4.6114	4.6292	4.6680	4.7021	4.6652	4.7091	4.6622	4.6990	4.6702	4.7402	4.6608	4.7777	4.8401	4.8411	4.9706	4.8368	4.9867	4.8324	4.9708	4.8448	5.0181	**4.92**
H(9A-9C)	1.2131	1.2018	1.1989	1.2076	1.1768	1.2078	1.2151	1.2077	1.2087	1.2071	1.2273	1.3168	1.3562	1.3465	1.3777	1.3507	1.3756	1.3820	1.3733	1.3739	1.3793	1.3991	**1.44**
H(8`A-8`C)	2.5388	2.5013	2.4785	2.4898	2.4672	2.4906	2.4613	2.4911	2.4605	2.4887	2.4354	2.9772	2.8106	2.7538	2.7281	2.6815	2.7321	2.6050	2.7360	2.6197	2.7241	2.5686	**2.64**
F3	-133.2410	-136.5690	-139.2300	-137.7280	-141.4070	-137.6610	-140.9120	-137.5930	-140.8340	-137.7910	-140.8320	-133.0170	-136.5700	-139.3360	-137.8530	-141.5280	-137.7890	-141.1350	-137.7240	-141.0970	-137.9130	-141.0540	**-114.23**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S3. Cont. V

Nuclei	R											S										Exp. [b]
	OPBE											OPBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.0168	138.5097	138.9262	138.8224	140.7563	138.8125	139.9428	138.7824	140.1179	138.8238	140.0850	135.3672	137.6783	138.1895	138.0126	139.3776	138.0216	139.3757	138.0099	139.4882	137.9961	139.5225	**134.46**
C2	114.6170	114.3904	114.8828	114.0743	114.6778	114.1109	114.8941	114.1297	114.8951	114.0345	114.9023	114.2576	114.1953	114.6619	113.9396	114.5080	113.9726	114.8059	113.9873	114.7495	113.9033	114.8074	**115.52**
C3	163.0652	163.4107	164.1167	163.5270	164.4693	163.5371	164.4137	163.5296	164.3919	163.5127	164.5182	163.2349	163.5035	164.2073	163.6022	164.5519	163.6116	164.4283	163.6033	164.4261	163.5888	164.5180	**162.83**
C4	117.0875	118.4716	119.1644	119.0733	119.4321	119.0586	120.3014	119.0262	120.0439	119.0835	120.5267	117.2011	118.1217	118.7728	118.6300	119.2379	118.6126	119.7559	118.5778	119.5598	118.6426	119.9561	**122.41**
C5	126.6629	128.4455	129.2158	129.2889	130.2429	129.2557	130.4292	129.2044	130.3007	129.3158	130.6388	126.8326	128.4577	129.1821	129.2747	130.2740	129.2405	130.2868	129.1887	130.1857	129.3024	130.4917	**131.43**
C6	118.9473	120.7741	121.8309	121.7446	123.0406	121.7025	123.4150	121.6435	123.1562	121.7812	123.7562	119.5104	121.0091	122.2007	121.8840	123.4734	121.8430	123.6469	121.7851	123.4558	121.9191	123.9365	**125.17**
C7	194.4087	200.3927	201.3265	202.9629	204.0112	202.8239	207.9731	202.6644	207.0787	203.0868	208.6560	197.8357	202.7029	203.7837	204.6315	205.5188	204.5407	209.6365	204.4296	208.8338	204.7102	210.0688	**196.61**
C8	62.0246	63.4759	63.8328	64.0390	64.9607	64.01308	65.6396	63.9678	65.5766	64.0562	66.2790	57.4808	59.8474	60.2403	60.6966	61.3470	60.6657	62.3193	60.6159	62.1121	60.7199	62.5834	**59.97**
C9	21.2184	21.5692	21.6964	21.7937	22.0246	21.7954	22.1798	21.7804	22.0714	21.7887	22.3487	17.8387	18.2469	18.3199	18.4106	18.5662	18.4149	18.7700	18.4018	18.6893	18.4017	19.1117	**15.26**
C8`	35.4607	36.2977	36.4862	36.6343	36.8947	36.6333	36.9156	36.6134	36.9219	36.6293	37.3065	30.9597	31.1232	31.3803	31.3230	31.6166	31.3250	31.5559	31.3095	31.5441	31.3168	31.5647	**31.09**
H2	7.8619	7.7166	7.8155	7.6603	7.6905	7.6655	7.7354	7.6701	7.7254	7.6549	7.7410	7.9540	7.6922	7.7799	7.6410	7.7078	7.6436	7.7010	7.6456	7.6926	7.6381	7.7040	**7.66**
H4	7.2666	7.4701	7.5590	7.5531	7.6586	7.5493	7.6975	7.5448	7.6779	7.5560	7.7235	7.2631	7.4306	7.5193	7.5021	7.6172	7.4985	7.6457	7.4942	7.6312	7.5048	7.6689	**7.33**
H5	7.5078	7.6769	7.7375	7.7622	7.8354	7.7579	7.8542	7.7528	7.8399	7.7656	7.8788	7.4993	7.6672	7.7222	7.7493	7.8266	7.7449	7.8326	7.7399	7.8217	7.7526	7.8554	**7.45**
H6	7.6973	7.8916	7.9919	7.9940	8.0938	7.9897	8.1090	7.9849	8.0766	7.9974	8.1508	7.5284	7.6456	7.7588	7.7358	7.8955	7.7304	7.8875	7.7244	7.8700	7.7403	7.9247	**7.57**
H8	4.5310	4.6254	4.6380	4.6769	4.7172	4.6748	4.7188	4.6723	4.6855	4.6786	4.7541	4.6902	4.8053	4.8724	4.8739	5.0018	4.8702	5.0121	4.8658	4.9970	4.8767	5.0472	**4.92**
H(9A-9C)	1.1719	1.1616	1.1564	1.1635	1.1255	1.1641	1.1665	1.1640	1.1637	1.1622	1.1815	1.2856	1.3043	1.2938	1.3335	1.2959	1.3320	1.3270	1.3298	1.3170	1.3343	1.3487	**1.44**
H(8`A-8`C)	2.4599	2.4252	2.3906	2.4107	2.3774	2.4119	2.3736	2.4124	2.3768	2.4087	2.3501	2.8429	2.6777	2.6358	2.6088	2.5655	2.6129	2.4825	2.6164	2.4962	2.6043	2.4468	**2.64**
F3	-122.6130	-125.4550	-127.8350	-126.4160	-129.6860	-126.3610	-129.1560	-126.3060	-129.1800	-126.4670	-129.0510	-122.4410	-125.5720	-127.9890	-126.5560	-129.8500	-126.5050	-129.4250	-126.4540	-129.4040	-126.6020	-129.3270	**-114.23**
Nuclei	OPW91											OPW91										
C1	137.2927	138.7921	139.2035	139.0741	141.0334	139.0551	140.2122	139.0181	140.3789	139.0716	140.3514	135.6218	137.9465	138.4497	138.2826	139.6367	138.2817	139.6226	138.2612	139.7359	138.2620	139.7679	**134.46**
C2	114.8303	114.6035	115.0905	114.2896	114.8811	114.3160	115.0991	114.3257	115.0998	114.2457	115.1094	114.4634	114.4014	114.8641	114.1493	114.7047	114.1720	115.0072	114.1778	114.9516	114.1090	115.0108	**115.52**
C3	163.4635	163.8083	164.5122	163.9322	164.8624	163.9321	164.8065	163.9150	164.7866	163.9140	164.9121	163.6352	163.9044	164.6060	164.0086	164.9492	164.0077	164.8252	163.9903	164.8239	163.9912	164.9169	**162.83**
C4	117.2951	118.6815	119.3705	119.3009	119.6251	119.2756	120.5032	119.2333	120.2527	119.3071	120.7313	117.4203	118.3352	118.9825	118.8493	119.4412	118.8217	119.9684	118.7779	119.7726	118.8581	120.1723	**122.41**
C5	126.8583	128.6464	129.4103	129.5007	130.4367	129.4571	130.6217	129.3963	130.4954	129.5239	130.8334	127.0353	128.6631	129.3828	129.4872	130.4718	129.4429	130.4861	129.3816	130.3856	129.5111	130.6930	**131.43**
C6	119.1957	121.0351	122.0933	122.0275	123.2987	121.9747	123.6819	121.9057	123.4265	122.0604	124.0270	119.7712	121.2773	122.4677	122.1625	123.7425	122.1109	123.9225	122.0434	123.7298	122.1942	124.2154	**125.17**
C7	194.7470	200.7723	201.7073	203.3291	204.3636	203.1806	208.3618	203.0130	207.4704	203.4495	209.0423	198.2213	203.0945	204.1684	205.0327	205.9047	204.9322	210.0310	204.8120	209.2232	205.1075	210.4680	**196.61**
C8	62.2071	63.6563	64.0081	64.2018	65.1534	64.1663	65.8205	64.1134	65.7476	64.2157	66.4583	57.6233	60.0248	60.4177	60.8806	61.5261	60.8394	62.4923	60.7799	62.2839	60.9006	62.7553	**59.97**
C9	21.2792	21.6330	21.7606	21.8706	22.0843	21.8624	22.2432	21.8382	22.1362	21.8615	22.4153	17.9107	18.3290	18.4025	18.4985	18.6462	18.4926	18.8517	18.4702	18.7720	18.4862	19.1928	**15.26**
C8`	35.5266	36.3700	36.5580	36.7130	36.9604	36.7014	36.9890	36.6718	36.9980	36.7049	37.3801	31.0590	31.2167	31.4730	31.4226	31.7084	31.4144	31.6513	31.3896	31.6400	31.4123	31.6650	**31.09**
H2	7.8669	7.7201	7.8191	7.6674	7.6929	7.6718	7.7382	7.6761	7.7293	7.6616	7.7437	7.9620	7.6970	7.7851	7.6464	7.7121	7.6482	7.7060	7.6501	7.6978	7.6432	7.7090	**7.66**
H4	7.2686	7.4718	7.5607	7.5557	7.6587	7.5512	7.6985	7.5465	7.6795	7.5582	7.7242	7.2659	7.4323	7.5210	7.5044	7.6183	7.5002	7.6472	7.4957	7.6326	7.5067	7.6703	**7.33**
H5	7.5077	7.6765	7.7370	7.7628	7.8343	7.7578	7.8535	7.7525	7.8393	7.7659	7.8779	7.4994	7.6671	7.7220	7.7499	7.8261	7.7449	7.8324	7.7397	7.8215	7.7530	7.8550	**7.45**
H6	7.6978	7.8929	7.9939	7.9989	8.0926	7.9939	8.1100	7.9886	8.0796	8.0020	8.1514	7.5322	7.6480	7.7612	7.7390	7.8976	7.7329	7.8906	7.7267	7.8730	7.7432	7.9278	**7.57**
H8	4.5305	4.6248	4.6386	4.6792	4.7153	4.6764	4.7179	4.6736	4.6861	4.6804	4.7528	4.6867	4.8012	4.8683	4.8708	4.9972	4.8664	5.0086	4.8618	4.9934	4.8733	5.0435	**4.92**
H(9A-9C)	1.1734	1.1630	1.1578	1.1659	1.1278	1.1659	1.1683	1.1656	1.1652	1.1644	1.1833	1.2862	1.3054	1.2954	1.3354	1.2975	1.3331	1.3287	1.3307	1.3188	1.3359	1.3503	**1.44**
H(8`A-8`C)	2.4610	2.4265	2.3921	2.4124	2.3795	2.4130	2.3757	2.4132	2.3785	2.4103	2.3525	2.8480	2.6819	2.6403	2.6141	2.5699	2.6176	2.4874	2.6209	2.5013	2.6094	2.4523	**2.64**
F3	-123.2130	-126.1040	-128.4990	-127.0830	-130.3850	-127.0270	-129.8500	-126.9710	-129.8680	-127.1360	-129.7490	-123.0400	-126.2170	-128.6490	-127.2210	-130.5370	-127.1690	-130.1110	-127.1170	-130.0890	-127.2690	-130.0160	**-114.23**
Nuclei	PBE											PBE										
C1	142.1816	142.8010	143.8198	142.8834	144.5207	142.8776	143.9094	142.8834	144.0984	142.9074	143.9127	140.7424	141.9216	142.4937	142.3319	143.7918	142.2972	143.9628	142.2757	143.8304	142.3862	144.1505	**134.46**
C2	119.2950	118.7283	119.2020	118.2285	118.8283	118.2562	119.2398	118.2946	119.1888	118.2203	119.2122	118.7147	118.4960	118.8862	118.1803	118.7819	118.1942	119.3915	118.2199	119.2629	118.1859	119.4026	**115.52**
C3	172.1464	172.6278	173.3848	172.7002	173.8707	172.6935	173.7994	172.6975	173.7890	172.7242	173.8899	172.3082	172.6943	173.4582	172.7298	173.8790	172.7254	173.7470	172.7317	173.7524	172.7516	173.8329	**162.83**
C4	122.6934	124.3511	124.9743	125.0895	125.7479	125.0427	126.8224	125.0067	126.5469	125.1513	127.0617	122.9119	124.2681	124.9736	124.7986	125.5432	124.7665	126.2227	124.7444	126.0613	124.8457	126.4363	**122.41**
C5	132.2849	134.3920	135.1418	135.3713	136.5603	135.3097	136.7276	135.2589	136.5974	135.4475	136.9403	132.5421	134.4790	135.2588	135.3430	136.5326	135.2895	136.5190	135.2460	136.4441	135.4107	136.7335	**131.43**
C6	125.6771	127.6409	128.6911	128.5688	130.3315	128.5053	130.7038	128.4524	130.4480	128.6465	131.1919	125.9574	128.1465	129.3617	129.1140	131.0219	129.0540	131.2761	129.0040	131.1183	129.1879	131.6187	**125.17**
C7	201.4517	206.3214	207.9921	208.8009	209.9020	208.6525	214.2617	208.5163	213.4149	208.9608	214.8731	206.3668	210.3182	211.9033	212.2804	213.4325	212.1598	217.4356	212.0495	216.5627	212.4127	217.9681	**196.61**
C8	67.1718	68.5140	69.1180	68.8732	69.8486	68.8510	70.2565	68.8390	70.1298	68.9111	71.0458	61.6156	63.4701	63.7948	64.2819	65.2151	64.2241	66.0027	64.17873	65.7294	64.3566	66.3598	**59.97**
C9	23.3212	23.7874	23.9124	23.9572	24.4157	23.9398	24.5298	23.9331	24.4525	23.9912	24.7904	20.0440	20.6474	20.6698	20.8257	21.2360	20.8085	21.4694	20.8028	21.3763	20.8607	21.9582	**15.26**
C8`	37.0709	37.8528	38.0432	38.1530	38.5274	38.1334	38.7413	38.1247	38.6798	38.1898	39.2159	32.0699	32.3535	32.7068	32.4432	32.8601	32.4358	32.8546	32.4386	32.8871	32.4667	32.9169	**31.09**
H2	8.0613	7.9709	8.0060	7.9085	7.9489	7.9124	7.9856	7.9168	7.9764	7.9054	7.9921	8.1252	7.9615	8.0342	7.8721	7.9248	7.8783	7.8974	7.8847	7.9129	7.8665	7.8947	**7.66**
H4	7.2105	7.4115	7.5061	7.4936	7.6170	7.4891	7.6646	7.4850	7.6478	7.4985	7.6872	7.2161	7.3988	7.4967	7.4693	7.5963	7.4656	7.6262	7.4622	7.6139	7.4735	7.6478	**7.33**
H5	7.4152	7.6204	7.6775	7.7144	7.8007	7.7091	7.8198	7.7042	7.8073	7.7202	7.8446	7.4218	7.6096	7.6685	7.6931	7.7793	7.6884	7.7834	7.6841	7.7750	7.6981	7.8059	**7.45**
H6	7.7882	7.9703	8.0440	8.0699	8.1952	8.0640	8.2411	8.0585	8.2170	8.0761	8.2863	7.5805	7.7575	7.8725	7.8436	8.0145	7.8389	8.0055	7.8346	7.9998	7.8485	8.0452	**7.57**
H8	4.5982	4.6739	4.6984	4.7382	4.8050	4.7335	4.8465	4.7295	4.8356	4.7435	4.8689	4.7599	4.9123	4.9777	4.9774	5.1006	4.9739	5.1117	4.9708	5.1039	4.9813	5.1413	**4.92**
H(9A-9C)	1.3755	1.3742	1.3462	1.3558	1.3275	1.3569	1.3428	1.3584	1.3355	1.3552	1.3707	1.4676	1.5049	1.4844	1.5225	1.4988	1.5215	1.5185	1.5210	1.5133	1.5241	1.5445	**1.44**
H(8`A-8`C)	2.5809	2.5203	2.4881	2.4883	2.4634	2.4898	2.4423	2.4919	2.4481	2.4875	2.4202	2.9909	2.8234	2.8026	2.7459	2.7059	2.7508	2.6109	2.7560	2.6322	2.7418	2.5746	**2.64**
F3	-138.7280	-142.0230	-144.8290	-143.2550	-147.0170	-143.1870	-146.4840	-143.1160	-146.4590	-143.3210	-146.4110	-138.6180	-142.0770	-144.8620	-143.3070	-147.0980	-143.2400	-146.6950	-143.1710	-146.6390	-143.3710	-146.6200	**-114.23**
Nuclei	PBE0											PBE0										
C1	143.1198	143.4402	143.7210	143.5364	145.0234	143.5338	144.2813	143.5337	144.2780	143.5419	144.2049	142.0685	142.9891	143.4758	143.4059	144.6630	143.3676	144.7287	143.3353	144.5476	143.4505	144.8343	**134.46**
C2	121.8507	121.2420	121.6941	120.8009	121.3653	120.8230	121.8101	120.8473	121.6886	120.7828	121.7174	121.4451	121.1106	121.5389	120.8391	121.3850	120.8485	121.9863	120.8609	121.8141	120.8343	121.9375	**115.52**
C3	170.5382	170.7930	171.4194	170.8673	171.7866	170.8584	171.8008	170.8514	171.7367	170.8786	171.8075	170.6486	170.8332	171.4838	170.8758	171.7737	170.8682	171.7516	170.8625	171.6988	170.8857	171.7619	**162.83**
C4	124.5260	126.1173	126.8865	126.9041	127.4816	126.8521	128.6626	126.8018	128.3526	126.9564	128.8241	124.7157	126.0193	126.7515	126.5880	127.2766	126.5523	128.0398	126.5170	127.8223	126.6232	128.1802	**122.41**
C5	134.0593	136.0273	136.6965	137.0363	138.0523	136.9715	138.2554	136.9083	138.0842	137.1008	138.3770	134.1915	136.0387	136.7471	136.9380	137.9472	136.8803	138.0112	136.8236	137.8814	136.9953	138.1465	**131.43**
C6	127.5835	129.6369	130.9138	130.6381	132.2739	130.5658	132.7945	130.4952	132.5243	130.7093	133.2195	127.8690	130.0621	131.3120	131.1004	132.9014	131.0341	133.2515	130.9684	133.0368	131.1650	133.5245	**125.17**
C7	201.0956	206.0865	207.1149	208.7983	209.5312	208.6395	214.5599	208.4828	213.3382	208.9524	215.1321	205.3965	209.6985	211.1075	211.8981	212.7064	211.7605	217.4540	211.6262	216.2948	212.0327	217.9863	**196.61**
C8	62.9977	64.2517	64.5885	64.6346	65.4442	64.6084	65.8894	64.5836	65.6717	64.6617	66.5520	57.6970	59.3578	59.6693	60.1920	60.9105	60.1298	61.7516	60.0719	61.4146	60.2570	62.0221	**59.97**
C9	22.3499	22.6729	22.8713	22.8296	23.1821	22.8100	23.2575	22.7919	23.1732	22.8511	23.4263	19.0803	19.4589	19.4902	19.6439	19.9135	19.6236	20.0860	19.6057	19.9729	19.6669	20.4182	**15.26**
C8`	35.4113	36.1702	36.3016	36.5288	36.8075	36.5039	37.0966	36.4810	36.9830	36.5557	37.4814	30.6707	30.9567	31.2958	31.1302	31.4530	31.1144	31.5755	31.0997	31.5332	31.1471	31.6022	**31.09**
H2	8.3010	8.2028	8.3059	8.1346	8.1748	8.1381	8.2203	8.1416	8.2233	8.1308	8.2234	8.3350	8.1625	8.2397	8.0678	8.1270	8.0742	8.1047	8.0803	8.1208	8.0609	8.1003	**7.66**
H4	7.3834	7.5862	7.6817	7.6721	7.7930	7.6673	7.8476	7.6625	7.8276	7.6764	7.8670	7.3888	7.5758	7.6742	7.6498	7.7752	7.6457	7.8116	7.6415	7.7958	7.6532	7.8309	**7.33**
H5	7.5550	7.7647	7.8243	7.8629	7.9435	7.8572	7.9680	7.8514	7.9533	7.8680	7.9899	7.5522	7.7484	7.8060	7.8379	7.9195	7.8327	7.9300	7.8275	7.9182	7.8424	7.9505	**7.45**
H6	7.8969	8.0970	8.2242	8.2086	8.3380	8.2015	8.3994	8.1944	8.3801	8.2149	8.4445	7.7110	7.9030	8.0242	7.9958	8.1712	7.9907	8.1717	7.9852	8.1628	8.0001	8.2087	**7.57**
H8	4.3272	4.4212	4.4835	4.5096	4.5742	4.5036	4.6369	4.4977	4.6185	4.5150	4.6586	4.5220	4.6815	4.7530	4.7491	4.8729	4.7454	4.8926	4.7416	4.8820	4.7521	4.9175	**4.92**
H(9A-9C)	1.3171	1.3205	1.3153	1.2999	1.2663	1.3007	1.2850	1.3015	1.2820	1.2988	1.3116	1.3929	1.4222	1.4036	1.4390	1.4077	1.4379	1.4305	1.4368	1.4245	1.4396	1.4507	**1.44**
H(8`A-8`C)	2.4766	2.4262	2.3704	2.3988	2.3690	2.4000	2.3524	2.4012	2.3501	2.3974	2.3322	2.8658	2.7045	2.6832	2.6303	2.5894	2.6351	2.5048	2.6398	2.5250	2.6251	2.4693	**2.64**
F3	-120.0200	-122.9510	-125.2790	-124.0450	-127.1820	-123.9840	-126.7530	-123.9230	-126.7200	-124.1020	-126.7350	-120.0800	-123.0690	-125.4230	-124.1240	-127.2910	-124.0670	-126.9120	-124.0090	-126.8770	-124.1770	-126.8760	**-114.23**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S3. Cont. VI

Nuclei	R											S										Exp. [b]
	TPSS																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	138.8059	139.0898	139.5919	139.2633	140.3810	139.2664	139.9486	139.2801	139.8093	139.2707	139.8094	137.5807	138.0367	139.0764	138.7925	140.1732	138.7671	140.0161	138.7539	139.8237	138.8281	140.0916	**134.46**
C2	117.0898	116.3926	116.9394	115.9959	116.4764	116.0269	116.9067	116.0692	116.5056	115.9775	116.8315	116.5199	116.0238	116.6111	115.8859	116.3977	115.9044	116.9415	115.9346	117.1755	115.8793	116.9047	**115.52**
C3	168.5071	168.7990	169.6005	168.9534	169.9650	168.9513	169.9108	168.9609	169.6089	168.9659	169.9557	168.6864	168.8675	169.6723	168.9756	169.9824	168.9754	169.8707	168.9866	169.8296	168.9862	169.9215	**162.83**
C4	120.1045	121.5549	122.3588	122.3538	122.9272	122.3127	124.0169	122.2828	122.7440	122.4037	124.2308	120.2817	121.5251	122.2233	122.0560	122.6607	122.0289	123.4415	122.0129	123.2082	122.0916	123.6365	**122.41**
C5	128.9155	130.7559	131.5414	131.7781	132.7862	131.7236	132.9510	131.6804	132.1792	131.8405	133.1007	129.1270	130.8671	131.6520	131.7543	132.7661	131.7072	132.7899	131.6711	132.7940	131.8090	132.9662	**131.43**
C6	122.9481	124.8260	126.0633	125.8027	127.5335	125.7443	127.8489	125.6976	126.1725	125.8688	128.3679	123.1349	125.3084	126.4565	126.2797	127.9647	126.2247	128.3259	126.1809	127.3450	126.3418	128.6562	**125.17**
C7	197.4897	201.9788	203.2574	204.5614	205.0734	204.4204	209.8003	204.2901	205.0794	204.7056	210.2600	201.9641	205.5398	207.3066	207.6437	208.6125	207.5293	212.6078	207.4257	207.9804	207.7624	213.0826	**196.61**
C8	65.6953	66.8552	67.3546	67.2991	68.1357	67.2804	68.5446	67.2724	67.5136	67.3268	69.2522	60.8248	62.3487	62.8990	63.3800	64.1895	63.3295	64.8370	63.2909	64.9267	63.4393	65.0940	**59.97**
C9	23.9076	24.2385	24.4947	24.4318	24.8941	24.4215	24.9472	24.4227	24.4925	24.4522	25.2171	20.7231	21.2301	21.3245	21.5131	21.8274	21.5005	22.0763	21.4997	23.4489	21.5363	22.4915	**15.26**
C8`	37.4869	38.1479	38.4201	38.5776	38.8327	38.5590	39.133	38.5518	38.6781	38.6061	39.5078	33.1142	33.3568	33.6821	33.3954	33.7048	33.3928	33.7628	33.4016	35.2615	33.4081	33.7999	**31.09**
H2	8.0852	7.9945	8.0901	7.9325	8.0086	7.9360	8.0214	7.9402	7.7784	7.9295	8.0315	8.1488	8.0103	8.0468	7.8888	7.9374	7.8946	7.9272	7.9010	8.0150	7.8835	7.9262	**7.66**
H4	7.1903	7.3893	7.4911	7.4780	7.6017	7.4732	7.6528	7.4688	7.3051	7.4830	7.6724	7.1988	7.3761	7.4792	7.4517	7.5797	7.4476	7.6142	7.4440	7.5614	7.4560	7.6328	**7.33**
H5	7.3552	7.5622	7.6283	7.6646	7.7514	7.6588	7.7711	7.6535	7.4905	7.6705	7.7919	7.3590	7.5515	7.6120	7.6409	7.7269	7.6357	7.7346	7.6310	7.7470	7.6462	7.7547	**7.45**
H6	7.6781	7.8717	7.9890	7.9830	8.1286	7.9762	8.1677	7.9700	7.8083	7.9899	8.2205	7.4937	7.7092	7.8091	7.7899	7.9591	7.7846	7.9671	7.7798	7.8947	7.7953	8.0078	**7.57**
H8	4.4745	4.5555	4.6040	4.6298	4.6976	4.6248	4.7397	4.6205	4.4454	4.6351	4.7627	4.6045	4.7682	4.8386	4.8432	4.9649	4.8391	4.9845	4.8356	4.9725	4.8473	5.0085	**4.92**
H(9A-9C)	1.3648	1.3728	1.3688	1.3606	1.3534	1.3613	1.3563	1.3626	1.1744	1.3603	1.3897	1.4408	1.4977	1.4703	1.5129	1.4866	1.5115	1.5132	1.5107	1.6725	1.5147	1.5371	**1.44**
H(8`A-8`C)	2.5368	2.4806	2.4340	2.4542	2.4272	2.4554	2.4076	2.4572	2.2734	2.4534	2.3836	2.9531	2.8059	2.7740	2.7196	2.6797	2.7240	2.5968	2.7290	2.8817	2.7158	2.5604	**2.64**
F3	-132.7610	-136.2000	-138.8700	-137.5020	-141.1170	-137.4290	-140.6060	-137.3560	-138.9140	-137.5710	-140.5450	-132.5580	-136.2530	-138.9790	-137.5790	-141.2260	-137.5090	-140.8040	-137.4380	-135.8180	-137.6450	-140.7380	**-114.23**
Nuclei	VSXC																						
C1	136.3307	136.2864	136.9028	136.1548	137.2539	136.1671	136.6742	136.1775	136.6870	136.1449	136.8382	136.2863	136.7108	137.6402	137.0135	138.2163	136.9798	137.8969	136.9488	137.8849	137.0523	138.0756	**134.46**
C2	114.3022	113.7629	114.1502	113.3732	113.7252	113.4016	114.1239	113.4278	114.0515	113.3479	114.1933	114.7622	114.1703	114.5041	113.8039	114.1621	113.8290	114.5435	113.8523	114.4710	113.7817	114.5265	**115.52**
C3	166.3069	166.7057	167.4257	166.8970	167.9094	166.8884	167.8189	166.8778	167.8042	166.9067	167.9013	165.6138	166.0033	166.7046	166.1989	167.1866	166.1900	167.0910	166.1789	167.0764	166.2090	167.1850	**162.83**
C4	118.1148	119.8138	120.4539	120.7250	121.3055	120.6716	122.3128	120.6162	122.0735	120.7772	122.5570	118.2844	119.8217	120.4022	120.5762	121.1664	120.5368	121.9950	120.4944	121.7780	120.6143	122.2183	**122.41**
C5	127.4791	129.5095	130.2304	130.5985	131.6175	130.5348	131.7214	130.4690	131.6228	130.6604	131.9236	127.4262	129.2999	129.9028	130.2602	131.2189	130.2088	131.2382	130.1541	131.1464	130.3096	131.4329	**131.43**
C6	123.0292	124.9919	126.0663	126.0647	127.6576	126.0015	128.1142	125.9362	127.8535	126.1261	128.4608	123.8719	126.0352	127.2339	127.1388	128.7805	127.0754	129.1759	127.0095	128.9842	127.2004	129.4534	**125.17**
C7	192.0244	196.0207	197.2558	198.1348	198.8965	198.0066	202.6570	197.8766	201.8931	198.2577	203.3608	192.8407	196.8027	198.2324	198.9390	199.8282	198.7978	203.5454	198.6585	202.6718	199.0789	204.3314	**196.61**
C8	71.7409	72.5868	73.1222	72.8179	73.6123	72.8129	73.8930	72.8049	73.8144	72.8231	74.5203	63.9006	64.9936	65.7007	65.6462	66.5943	65.6012	66.9548	65.5561	66.8125	65.6928	67.4158	**59.97**
C9	27.8470	28.7573	29.0954	29.5548	30.0731	29.4996	30.3676	29.4437	30.3289	29.6103	30.4871	28.7860	28.9261	29.0849	29.0553	29.2750	29.0454	29.2406	29.0344	29.2395	29.0675	29.4468	**15.26**
C8`	40.4195	40.7975	40.7781	40.9513	41.0897	40.9454	41.1784	40.9374	41.0912	40.9586	41.6289	35.4155	36.3399	36.5974	36.8641	37.2017	36.8313	37.4160	36.7971	37.3209	36.8972	37.8521	**31.09**
H2	8.2134	8.1231	8.1776	8.0764	8.1275	8.0791	8.1390	8.0819	8.1563	8.0737	8.1295	8.2284	8.1088	8.1211	8.0305	8.0750	8.0372	8.0690	8.0436	8.0792	8.0236	8.0591	**7.66**
H4	7.2051	7.3960	7.4902	7.4835	7.6012	7.4784	7.6457	7.4734	7.6338	7.4883	7.6673	7.2200	7.4073	7.5008	7.4880	7.6091	7.4834	7.6473	7.4789	7.6319	7.4923	7.6718	**7.33**
H5	7.4674	7.6754	7.7330	7.7775	7.8614	7.7716	7.8756	7.7656	7.8670	7.7832	7.9004	7.4446	7.6396	7.6945	7.7326	7.8143	7.7272	7.8241	7.7220	7.8131	7.7376	7.8462	**7.45**
H6	7.8523	8.0466	8.1462	8.1625	8.3141	8.1553	8.3579	8.1481	8.3448	8.1693	8.3919	7.5400	7.7386	7.8420	7.8464	8.0069	7.8401	8.0421	7.8339	8.0215	7.8523	8.0752	**7.57**
H8	4.3974	4.4948	4.5209	4.5791	4.6442	4.5733	4.6934	4.5676	4.6749	4.5847	4.7266	4.6276	4.7885	4.8608	4.8788	4.9951	4.8730	5.0355	4.8675	5.0171	4.8844	5.0639	**4.92**
H(9A-9C)	1.6028	1.6275	1.6151	1.6319	1.6077	1.6320	1.6341	1.6320	1.6330	1.6318	1.6445	1.7178	1.7227	1.7091	1.7330	1.7185	1.7323	1.7387	1.7317	1.7317	1.7338	1.7524	**1.44**
H(8`A-8`C)	2.7216	2.6729	2.6333	2.6461	2.6098	2.6478	2.5916	2.6497	2.5862	2.6444	2.5709	2.8282	2.7185	2.6641	2.6717	2.6195	2.6751	2.5848	2.6786	2.5962	2.6683	2.5437	**2.64**
F3	-133.2810	-136.7820	-139.4990	-138.0900	-141.7570	-138.0180	-141.2770	-137.9360	-141.2250	-138.1570	-141.2470	-134.0080	-137.6750	-140.4880	-139.0190	-142.7420	-138.9450	-142.2750	-138.8610	-142.2330	-139.0880	-142.2230	**-114.23**
Nuclei	wB97																						
C1	143.8884	143.7754	144.3011	143.7230	145.1388	143.7226	144.0079	143.7217	143.9586	143.7240	144.0913	143.0868	143.7292	144.1324	144.1072	145.3921	144.0526	145.2995	144.0106	145.4679	144.1802	145.5016	**134.46**
C2	123.3047	122.6459	123.1621	122.2304	122.8304	122.2552	123.1655	122.2792	123.0612	122.2075	123.1476	123.0749	122.6064	123.0585	122.3117	122.8698	122.3239	123.2791	122.3375	123.1970	122.3028	123.2931	**115.52**
C3	171.6610	171.6577	172.2588	171.6725	172.5210	171.6698	172.3794	171.6667	172.3812	171.6753	172.4364	171.6722	171.6725	172.2700	171.6959	172.5239	171.6917	172.3409	171.6874	172.3473	171.7010	172.4000	**162.83**
C4	125.5590	127.0034	127.7560	127.7463	128.3922	127.7004	129.3852	127.6537	129.1961	127.7901	129.5874	125.7034	126.8590	127.6546	127.4086	128.1276	127.3837	128.7101	127.3540	128.4843	127.4267	128.8729	**122.41**
C5	135.1939	136.9748	137.6055	137.9433	138.8839	137.8828	138.8851	137.8215	138.7827	138.0011	139.0641	135.2939	137.0103	137.6532	137.8973	138.8267	137.8450	138.7455	137.7911	138.6664	137.9460	138.9150	**131.43**
C6	128.7249	130.9092	132.1475	132.0136	133.7323	131.9461	134.2186	131.8779	134.0409	132.0781	134.6183	129.0338	131.2512	132.5567	132.3578	134.1699	132.2979	134.4117	132.2337	134.1653	132.4093	134.7131	**125.17**
C7	201.0619	206.0886	207.3362	208.7941	209.4820	208.6239	214.3985	208.4522	213.1530	208.9565	215.2764	204.5747	209.1359	210.5409	211.5926	212.3843	211.4335	217.5009	211.2786	216.4473	211.7522	218.2229	**196.61**
C8	61.5755	62.6237	63.1206	63.0390	63.8459	63.0179	64.1400	62.9952	63.9605	63.0589	64.7431	56.1541	57.5883	57.9147	58.3983	59.0916	58.3316	59.8257	58.2709	59.6675	58.4723	60.1584	**59.97**
C9	21.9065	22.1377	22.2844	22.2892	22.6479	22.2781	22.5363	22.2667	22.5441	22.3001	22.6948	19.4140	19.5878	19.6011	19.7258	19.9639	19.7112	19.9262	19.6974	19.9035	19.7417	20.2516	**15.26**
C8`	35.1209	35.7278	35.9043	36.0351	36.3575	36.0164	36.4784	35.9967	36.4261	36.0531	36.8959	30.5100	30.7786	31.1230	31.0115	31.3129	31.0012	31.3491	30.9876	31.2871	31.0171	31.5156	**31.09**
H2	8.4230	8.3351	8.4136	8.2701	8.3200	8.2745	8.3709	8.2788	8.3910	8.2659	8.3667	8.4514	8.2793	8.3597	8.1835	8.2441	8.1917	8.1994	8.1987	8.1955	8.1738	8.1974	**7.66**
H4	7.5006	7.6971	7.7936	7.7781	7.9051	7.7734	7.9507	7.7686	7.9350	7.7825	7.9739	7.4992	7.6802	7.7808	7.7528	7.8832	7.7489	7.9088	7.7448	7.8934	7.7563	7.9306	**7.33**
H5	7.6385	7.8475	7.9026	7.9438	8.0250	7.9382	8.0406	7.9324	8.0319	7.9492	8.0656	7.6372	7.8393	7.8930	7.9311	8.0127	7.9258	8.0181	7.9204	8.0072	7.9360	8.0412	**7.45**
H6	7.9237	8.1419	8.2495	8.2585	8.4057	8.2514	8.4696	8.2441	8.4635	8.2654	8.5119	7.7826	7.9791	8.1071	8.0800	8.2600	8.0753	8.2560	8.0698	8.2345	8.0835	8.2907	**7.57**
H8	4.0931	4.2075	4.2558	4.3046	4.3831	4.2977	4.4531	4.2907	4.4473	4.3114	4.4814	4.2823	4.4487	4.5285	4.5266	4.6574	4.5228	4.6820	4.5185	4.6664	4.5298	4.7045	**4.92**
H(9A-9C)	1.3404	1.3512	1.3385	1.3415	1.3122	1.3423	1.3335	1.3431	1.3361	1.3407	1.3531	1.3998	1.4195	1.4072	1.4335	1.4028	1.4334	1.4186	1.4329	1.4086	1.4333	1.4354	**1.44**
H(8`A-8`C)	2.4713	2.4291	2.3810	2.4046	2.3761	2.4057	2.3500	2.4067	2.3429	2.4037	2.3365	2.8007	2.6446	2.6318	2.5750	2.5446	2.5802	2.4603	2.5849	2.4743	2.5692	2.4288	**2.64**
F3	-113.6110	-117.0360	-119.2440	-118.3680	-121.2950	-118.2940	-120.9950	-118.2200	-120.9270	-118.4370	-121.0480	-113.6760	-117.1380	-119.3520	-118.4050	-121.3530	-118.3390	-121.1410	-118.2700	-121.0730	-118.4660	-121.1710	**-114.23**
Nuclei	wB97X																						
C1	145.0757	145.0547	145.5379	145.1077	146.5506	145.1027	145.4800	145.0974	145.2743	145.1125	145.4922	144.1861	144.9230	145.3717	145.3228	146.5831	145.2815	146.5366	145.2475	146.4295	145.3759	146.7158	**134.46**
C2	123.8370	123.1807	123.6696	122.7709	123.3544	122.7986	123.7407	122.8252	123.5677	122.7453	123.7022	123.5475	123.1357	123.5890	122.8537	123.4031	122.8700	123.8837	122.8867	123.7285	122.8412	123.8803	**115.52**
C3	172.4812	172.5210	173.1395	172.5546	173.4143	172.5537	173.3261	172.5520	173.2668	172.5567	173.3711	172.5182	172.5553	173.1668	172.5918	173.4298	172.5902	173.3425	172.5882	173.2834	172.5949	173.3887	**162.83**
C4	126.1181	127.5819	128.3415	128.3423	128.9544	128.2982	130.0033	128.2531	129.7630	128.3854	130.2091	126.2716	127.4409	128.2077	128.0042	128.7071	127.9775	129.3380	127.9475	129.1133	128.0270	129.4948	**122.41**
C5	135.8003	137.6105	138.2473	138.6080	139.5563	138.5481	139.6226	138.4872	139.4415	138.6660	139.7791	135.9075	137.6384	138.2976	138.5373	139.4744	138.4860	139.4392	138.4332	139.3088	138.5860	139.5983	**131.43**
C6	129.3481	131.4874	132.7164	132.5436	134.2351	132.4808	134.7542	132.4172	134.5627	132.6044	135.1839	129.6638	131.8726	133.1460	132.9668	134.7767	132.9080	135.0313	132.8458	134.7911	133.0196	135.3318	**125.17**
C7	202.7304	207.8177	209.0366	210.6501	211.3249	210.4728	216.3919	210.2950	214.9594	210.8197	217.1628	206.5991	211.0861	212.5382	213.5311	214.2935	213.3777	219.4465	213.2261	218.2232	213.6827	220.1295	**196.61**
C8	62.6761	63.7691	64.2047	64.1664	64.9656	64.1471	65.3262	64.1273	65.0736	64.1859	65.9302	57.1458	58.6871	58.9842	59.5211	60.2069	59.4622	60.9946	59.4068	60.6771	59.5843	61.3297	**59.97**
C9	22.1384	22.3762	22.5287	22.5236	22.8690	22.5163	22.8035	22.5078	22.7734	22.5318	22.9819	19.5078	19.6722	19.6759	19.8113	20.0432	19.8020	20.0370	19.7926	19.9392	19.8221	20.3619	**15.26**
C8`	35.3925	36.0358	36.1998	36.3571	36.6737	36.3381	36.8447	36.3191	36.7404	36.3767	37.2550	30.7290	30.9668	31.3358	31.2099	31.5193	31.1989	31.5582	31.1857	31.4807	31.2191	31.6731	**31.09**
H2	8.3948	8.3031	8.3888	8.2310	8.2787	8.2363	8.3308	8.2414	8.3566	8.2262	8.3323	8.4221	8.2480	8.3270	8.1543	8.2173	8.1617	8.1811	8.1683	8.1914	8.1465	8.1756	**7.66**
H4	7.4701	7.6675	7.7654	7.7523	7.8765	7.7477	7.9241	7.7429	7.9055	7.7569	7.9460	7.4739	7.6561	7.7551	7.7310	7.8593	7.7271	7.8910	7.7231	7.8749	7.7348	7.9115	**7.33**
H5	7.6120	7.8212	7.8772	7.9189	7.9989	7.9133	8.0174	7.9078	8.0058	7.9243	8.0403	7.6138	7.8130	7.8679	7.9054	7.9865	7.9003	7.9931	7.8951	7.9810	7.9104	8.0146	**7.45**
H6	7.9050	8.1194	8.2316	8.2387	8.3831	8.2312	8.4449	8.2237	8.4390	8.2460	8.4898	7.7597	7.9506	8.0758	8.0534	8.2329	8.0483	8.2323	8.0428	8.2195	8.0577	8.2671	**7.57**
H8	4.1493	4.2579	4.3151	4.3622	4.4378	4.3550	4.4993	4.3480	4.4881	4.3692	4.5274	4.3358	4.4931	4.5733	4.5704	4.7003	4.5664	4.7239	4.5622	4.7136	4.5739	4.7475	**4.92**
H(9A-9C)	1.3277	1.3372	1.3245	1.3221	1.2911	1.3238	1.3137	1.3253	1.3194	1.3206	1.3356	1.3927	1.4126	1.3942	1.4268	1.3969	1.4265	1.4126	1.4261	1.4068	1.4267	1.4304	**1.44**
H(8`A-8`C)	2.4780	2.4346	2.3835	2.4123	2.3823	2.4138	2.3583	2.4151	2.3485	2.4110	2.3414	2.8390	2.6697	2.6555	2.6009	2.5689	2.6059	2.4854	2.6104	2.5042	2.5958	2.4525	**2.64**
F3	-115.8910	-119.1010	-121.3360	-120.3230	-123.2980	-120.2550	-122.9770	-120.1860	-122.9300	-120.3860	-123.0060	-115.9500	-119.2000	-121.4440	-120.3750	-123.3770	-120.3130	-123.0450	-120.2480	-122.9930	-120.4340	-123.0530	**-114.23**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S3. Cont. VII

Nuclei	R											S										Exp. [b]
	X3LYP											X3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	145.8940	146.4306	146.4662	146.3956	147.9242	146.3998	146.9732	146.4011	147.0962	146.3953	146.9582	144.5867	145.5136	146.0930	145.9784	147.3288	145.9542	147.1933	145.9276	147.1459	146.0063	147.3097	**134.46**
C2	123.0375	122.3621	122.8136	121.9461	122.4226	121.9755	122.8617	122.0017	122.7982	121.9218	122.8035	122.5169	122.1240	122.5692	121.8724	122.3719	121.8915	122.9235	121.9077	122.8194	121.8583	122.9076	**115.52**
C3	173.9683	174.2327	174.8979	174.3326	175.2832	174.3305	175.1671	174.3254	175.1715	174.3384	175.2647	174.1357	174.3255	175.0102	174.4116	175.3309	174.4100	175.1574	174.4052	175.1689	174.4169	175.2023	**162.83**
C4	125.6972	127.2737	127.9767	128.0684	128.5422	128.0237	129.7045	127.9759	129.4570	128.1148	129.8775	126.0040	127.1940	127.8742	127.7610	128.3205	127.7315	129.0689	127.6986	128.8942	127.7919	129.2504	**122.41**
C5	135.1518	137.1236	137.7353	138.1279	139.0663	138.0707	139.1702	138.0103	139.0724	138.1856	139.3354	135.3487	137.1586	137.8258	138.0790	139.0006	138.0277	139.0063	137.9730	138.9364	138.1308	139.1774	**131.43**
C6	129.2079	131.1671	132.6227	132.3480	133.9589	132.2791	134.4980	132.2072	134.2474	132.4173	134.9089	129.4988	131.7189	132.9890	132.8206	134.5914	132.7581	134.9427	132.6921	134.7648	132.8828	135.2825	**125.17**
C7	203.6700	209.2273	210.0454	211.8819	212.6837	211.7197	217.7740	211.5557	216.6687	212.0391	218.5290	208.7411	213.0443	214.5616	215.3172	216.1501	215.1847	220.8595	215.0487	219.8258	215.4462	221.4208	**196.61**
C8	65.5438	66.7396	67.1559	67.1713	67.9742	67.1550	68.3138	67.1343	68.1395	67.1889	68.9925	59.9947	61.8769	62.2719	62.8214	63.6188	62.7678	64.3355	62.7118	64.0902	62.8764	64.6639	**59.97**
C9	22.9705	23.1692	23.5115	23.4457	23.7659	23.4323	23.7895	23.4156	23.7428	23.4619	23.9482	19.6027	19.9654	20.0344	20.1635	20.4457	20.1535	20.5622	20.1410	20.4948	20.1769	20.9242	**15.26**
C8`	36.3709	37.1931	37.3296	37.5740	37.8820	37.5541	38.1127	37.5309	38.0680	37.5966	38.5358	31.8426	32.0663	32.4101	32.2640	32.5525	32.2547	32.6038	32.2421	32.6340	32.2762	32.6621	**31.09**
H2	8.2605	8.1327	8.2705	8.0837	8.1222	8.0871	8.1762	8.0901	8.1785	8.0804	8.1857	8.3168	8.1335	8.2105	8.0407	8.0908	8.0464	8.0650	8.0516	8.0779	8.0351	8.0632	**7.66**
H4	7.3475	7.5472	7.6408	7.6329	7.7500	7.6282	7.8007	7.6230	7.7843	7.6372	7.8227	7.3620	7.5420	7.6399	7.6168	7.7370	7.6128	7.7633	7.6083	7.7502	7.6204	7.7841	**7.33**
H5	7.4902	7.6979	7.7560	7.7979	7.8752	7.7923	7.8936	7.7861	7.8826	7.8032	7.9174	7.4879	7.6791	7.7359	7.7705	7.8472	7.7655	7.8566	7.7598	7.8476	7.7753	7.8786	**7.45**
H6	7.8144	8.0087	8.1481	8.1283	8.2599	8.1210	8.3245	8.1133	8.3079	8.1353	8.3735	7.6367	7.8260	7.9445	7.9233	8.0913	7.9177	8.0987	7.9116	8.0889	7.9285	8.1386	**7.57**
H8	4.3520	4.4472	4.5076	4.5355	4.6068	4.5290	4.6609	4.5223	4.6516	4.5418	4.6880	4.5015	4.6738	4.7413	4.7512	4.8710	4.7469	4.8918	4.7421	4.8807	4.7552	4.9187	**4.92**
H(9A-9C)	1.3272	1.3126	1.3324	1.3104	1.2771	1.3112	1.2987	1.3113	1.2940	1.3097	1.3190	1.4001	1.4334	1.4207	1.4581	1.4303	1.4567	1.4530	1.4548	1.4478	1.4594	1.4750	**1.44**
H(8`A-8`C)	2.5285	2.4765	2.4277	2.4602	2.4300	2.4614	2.4121	2.4620	2.4130	2.4591	2.3905	2.9671	2.7987	2.7731	2.7234	2.6794	2.7278	2.5949	2.7317	2.6124	2.7193	2.5600	**2.64**
F3	-130.3030	-133.7990	-136.1940	-135.0750	-138.5060	-135.0030	-138.0860	-134.9300	-138.0360	-135.1430	-137.9040	-130.3350	-133.7010	-136.2980	-134.9270	-138.3970	-134.8610	-138.2210	-134.7930	-138.1630	-134.9900	-138.1850	**-114.23**

[a] methyl protons shifts are averaged

[b] according to [3]

Table S4. Theoretical chemical shifts (in ppm) of *(R,S)*-4-fluoro-α-pyrrolidinopentiophenone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S										Exp. [b]
	B3LYP											B3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.6595	141.0130	142.0566	141.4838	143.2056	141.4487	142.6536	141.4144	142.6775	141.5164	143.0299	139.6595	141.0131	142.0568	141.4838	143.2056	141.4487	142.6536	141.4144	142.6773	141.5164	143.0300	**133.8**
C2	139.5607	139.5533	140.0992	139.3810	139.9034	139.3881	140.3839	139.3950	140.2814	139.3726	140.3845	139.5607	139.5533	140.0993	139.3811	139.9034	139.3881	140.3839	139.3950	140.2813	139.3725	140.3845	**132.1**
C3	121.8992	122.6659	123.2367	122.8572	123.5136	122.8442	123.8248	122.8308	123.7329	122.8674	123.8998	121.8992	122.6660	123.2367	122.8571	123.5136	122.8442	123.8248	122.8308	123.7328	122.8674	123.8997	**115.8**
C4	176.3634	177.2400	177.9170	177.5979	178.3179	177.5726	178.9122	177.5470	178.7385	177.6202	179.0146	176.3634	177.2401	177.9169	177.5978	178.3179	177.5726	178.9122	177.5470	178.7385	177.6202	179.0144	**165.8**
C5	119.9425	121.2697	121.8855	121.8481	122.6291	121.8091	122.8607	121.7699	122.7343	121.8835	122.9906	119.9425	121.2697	121.8855	121.8481	122.6291	121.8091	122.8607	121.7699	122.7343	121.8835	122.9905	**115.8**
C6	135.8367	137.5847	138.5465	138.6062	140.0186	138.5384	140.6828	138.4705	140.3917	138.6689	140.9248	135.8368	137.5847	138.5464	138.6062	140.0186	138.5384	140.6828	138.4705	140.3918	138.6689	140.9249	**132.1**
C7	203.8262	208.9948	210.3970	211.6481	212.3534	211.4769	217.6027	211.3067	216.4065	211.8097	218.7711	203.8262	208.9948	210.3967	211.6481	212.3534	211.4769	217.6027	211.3067	216.4064	211.8097	218.7711	**198.9**
C8	66.4966	67.7258	68.4480	68.3496	69.0459	68.3005	69.8267	68.2525	69.6471	68.3953	70.1540	66.4967	67.7257	68.4479	68.3496	69.0459	68.3005	69.8267	68.2525	69.6470	68.3953	70.1539	**69.3**
C9	38.7755	38.3733	38.4550	38.1579	38.3135	38.1667	38.5364	38.1754	38.4611	38.1474	38.5718	38.7755	38.3732	38.4549	38.1578	38.3135	38.1667	38.5364	38.1754	38.4610	38.1474	38.5718	**31.5**
C10	19.9937	20.4460	20.7085	20.6771	21.1223	20.6584	21.0452	20.6393	21.0064	20.6931	21.1559	19.9937	20.4461	20.7085	20.6771	21.1223	20.6584	21.0452	20.6393	21.0065	20.6931	21.1559	**19.9**
C11	16.0946	16.2853	16.4075	16.3075	16.5083	16.3018	16.4979	16.2960	16.4791	16.3112	16.6477	16.0946	16.2853	16.4075	16.3075	16.5083	16.3018	16.4979	16.2960	16.4791	16.3112	16.6476	**14.3**
C1`	52.3223	53.1970	53.5209	53.6907	54.1936	53.6541	54.2321	53.6172	54.1877	53.7237	54.6654	56.8876	57.9796	58.3853	58.4297	58.9956	58.3966	59.1331	58.3636	59.0349	58.4600	59.3734	**50.6**
C2`	26.1592	26.6379	26.9310	26.8078	27.2269	26.7905	27.2729	26.7736	27.2316	26.8230	27.1130	25.7213	25.9896	26.3448	26.0758	26.6580	26.0646	26.5476	26.0537	26.5196	26.0853	26.3447	**23.8**
C3`	25.7214	25.9896	26.3449	26.0759	26.6580	26.0646	26.5476	26.0537	26.5196	26.0853	26.3449	26.1592	26.6379	26.9310	26.8079	27.2269	26.7905	27.2729	26.7736	27.2316	26.8230	27.1131	**23.8**
C4`	56.8875	57.9797	58.3854	58.4296	58.9956	58.3966	59.1331	58.3636	59.0349	58.4601	59.3733	52.3224	53.1971	53.5209	53.6908	54.1936	53.6541	54.2321	53.6172	54.1877	53.7237	54.6654	**50.6**
H2	8.6658	8.5221	8.5209	8.4446	8.4398	8.4493	8.4470	8.4539	8.4473	8.4398	8.4321	8.6658	8.5221	8.5209	8.4446	8.4398	8.4493	8.4470	8.4539	8.4473	8.4398	8.4321	**8.35**
H3	7.2988	7.4402	7.5270	7.4790	7.5943	7.4769	7.6101	7.4747	7.6007	7.4807	7.6258	7.2988	7.4402	7.5271	7.4790	7.5943	7.4769	7.6101	7.4747	7.6007	7.4807	7.6258	**7.06**
H5	7.1478	7.3279	7.4131	7.4001	7.5227	7.3956	7.5364	7.3911	7.5218	7.4041	7.5568	7.1478	7.3279	7.4131	7.4001	7.5227	7.3956	7.5364	7.3911	7.5218	7.4041	7.5568	**7.06**
H6	7.9815	8.1560	8.2289	8.2444	8.3759	8.2389	8.4114	8.2333	8.3880	8.2495	8.4315	7.9815	8.1560	8.2289	8.2445	8.3759	8.2389	8.4114	8.2333	8.3880	8.2495	8.4315	**8.35**
H8	4.6382	4.7005	4.7167	4.7308	4.8264	4.7285	4.8453	4.7263	4.8230	4.7330	4.8374	4.6382	4.7005	4.7167	4.7308	4.8264	4.7285	4.8453	4.7263	4.8230	4.7330	4.8374	**4.88**
H(9A-9B)	1.6769	1.6946	1.6718	1.7219	1.7054	1.7196	1.7129	1.7173	1.7075	1.7237	1.7365	1.6769	1.6946	1.6718	1.7219	1.7054	1.7196	1.7129	1.7173	1.7075	1.7237	1.7365	**2.05**
H(10A-10B)	1.4170	1.3092	1.2585	1.2423	1.1832	1.2464	1.1948	1.2505	1.1943	1.2381	1.1836	1.4170	1.3092	1.2585	1.2423	1.1832	1.2464	1.1949	1.2505	1.1943	1.2381	1.1835	**1.36**
H(11A-11C)	0.7806	0.7859	0.7568	0.7886	0.7603	0.7881	0.7593	0.7875	0.7566	0.7889	0.7528	0.7806	0.7859	0.7568	0.7886	0.7603	0.7881	0.7593	0.7875	0.7566	0.7889	0.7528	**0.77**
H(1`A)	2.7396	2.7448	2.7135	2.7304	2.6812	2.7311	2.6921	2.7318	2.6904	2.7295	2.6710	2.8685	2.8717	2.8592	2.8509	2.8194	2.8517	2.8290	2.8526	2.8282	2.8499	2.7949	**3.03**
H(1`B)	3.1966	3.2378	3.2732	3.2692	3.3388	3.2666	3.3209	3.2641	3.3137	3.2715	3.3213	2.8682	2.7242	2.7036	2.6902	2.6871	2.6914	2.6646	2.6927	2.6635	2.6889	2.6644	**3.23**
H(2`-3`A-2`-3`B)	1.6690	1.7354	1.7006	1.7713	1.7310	1.7687	1.7485	1.7660	1.7408	1.7737	1.7768	1.6690	1.7354	1.7006	1.7713	1.7310	1.7687	1.7485	1.7660	1.7408	1.7738	1.7768	**1.77**
H(4`A)	2.8682	2.7242	2.7036	2.6902	2.6871	2.6914	2.6646	2.6927	2.6635	2.6889	2.6644	3.1966	3.2378	3.2732	3.2692	3.3388	3.2666	3.3209	3.2641	3.3137	3.2715	3.3213	**3.03**
H(4`B)	2.8685	2.8718	2.8592	2.8509	2.8194	2.8517	2.8290	2.8526	2.8282	2.8499	2.7949	2.7396	2.7448	2.7135	2.7304	2.6812	2.7311	2.6921	2.7318	2.6904	2.7295	2.6710	**3.23**
Nuclei	B3P86											B3P86											
C1	137.0834	137.9700	138.7039	138.2940	140.4959	138.2856	139.9806	138.2578	139.9799	138.3478	140.2201	137.0834	137.9700	138.7039	138.2939	140.4957	138.2855	139.9806	138.2579	139.9799	138.3479	140.2200	**133.8**
C2	138.6697	138.6011	139.2492	138.4593	139.0695	138.4902	139.4613	138.4992	139.5061	138.4735	139.4640	138.6697	138.6011	139.2492	138.4593	139.0695	138.4902	139.4613	138.4995	139.5060	138.4735	139.4640	**132.1**
C3	121.0740	121.8419	122.4817	122.0957	122.8695	122.1028	123.1861	122.0878	123.2309	122.1325	123.2858	121.0740	121.8419	122.4817	122.0956	122.8695	122.1029	123.1861	122.0880	123.2309	122.1324	123.2858	**115.8**
C4	173.8519	174.6554	175.3491	175.0610	175.7802	175.0567	176.4157	175.0301	176.4015	175.1095	176.5441	173.8519	174.6554	175.3491	175.0611	175.7802	175.0566	176.4157	175.0301	176.4015	175.1096	176.5440	**165.8**
C5	119.1494	120.5275	121.2124	121.2172	122.1039	121.1955	122.3368	121.1515	122.3319	121.2823	122.4971	119.1494	120.5275	121.2124	121.2175	122.1039	121.1955	122.3368	121.1515	122.3319	121.2824	122.4971	**115.8**
C6	134.8903	136.7414	137.9127	137.8080	139.0992	137.7648	139.7068	137.6992	139.5516	137.8923	140.0277	134.8903	136.7414	137.9127	137.8081	139.0992	137.7650	139.7068	137.6993	139.5517	137.8924	140.0277	**132.1**
C7	201.9935	206.5379	207.6449	208.9027	210.1328	208.7685	215.1507	208.6149	213.8462	209.0759	216.1905	201.9935	206.5379	207.6449	208.9027	210.1328	208.7685	215.1507	208.6149	213.8463	209.0758	216.1905	**198.9**
C8	64.8034	65.9736	66.6913	66.5410	67.5554	66.5226	68.2240	66.4836	67.9231	66.6033	68.6619	64.8034	65.9736	66.6913	66.5410	67.5554	66.5226	68.2240	66.4836	67.9231	66.6033	68.6619	**69.3**
C9	37.6384	37.4660	37.7532	37.3213	37.5375	37.3547	37.6239	37.3657	37.5293	37.3326	37.7648	37.6384	37.4660	37.7532	37.3212	37.5375	37.3548	37.6239	37.3658	37.5293	37.3326	37.7648	**31.5**
C10	18.7463	19.2110	19.5410	19.4685	19.9226	19.4732	19.8038	19.4560	19.8274	19.5080	20.0120	18.7463	19.2110	19.5410	19.4685	19.9226	19.4733	19.8038	19.4559	19.8274	19.5080	20.0119	**19.9**
C11	15.6799	15.8487	16.0027	15.8858	16.1260	15.9043	16.0704	15.9010	16.1497	15.9122	16.2415	15.6799	15.8487	16.0027	15.8858	16.1261	15.9044	16.0704	15.9010	16.1496	15.9122	16.2414	**14.3**
C1`	51.2447	52.0577	52.3607	52.5446	53.1062	52.5338	53.0540	52.5013	53.0966	52.5988	53.5834	55.5720	56.5444	56.9649	57.0256	57.5965	57.0137	57.7967	56.9807	57.8796	57.0811	58.0295	**50.6**
C2`	24.9427	25.3436	25.6830	25.5269	25.9615	25.5347	25.9987	25.5209	26.0503	25.5637	25.8565	24.3771	24.5999	24.9475	24.7179	25.2484	24.7307	25.1836	24.7216	25.2911	24.7497	25.0495	**23.8**
C3`	24.3771	24.5999	24.9475	24.7179	25.2484	24.7307	25.1836	24.7217	25.2911	24.7496	25.0495	24.9427	25.3436	25.6830	25.5270	25.9615	25.5347	25.9987	25.5209	26.0503	25.5638	25.8565	**23.8**
C4`	55.5720	56.5444	56.9649	57.0254	57.5964	57.0137	57.7967	56.9808	57.8797	57.0812	58.0295	51.2447	52.0577	52.3607	52.5446	53.1061	52.5338	53.0540	52.5013	53.0967	52.5987	53.5835	**50.6**
H2	8.7356	8.6315	8.6671	8.5696	8.5174	8.5756	8.5132	8.5795	8.5326	8.5649	8.5091	8.7356	8.6315	8.6671	8.5696	8.5174	8.5756	8.5132	8.5795	8.5326	8.5650	8.5091	**8.35**
H3	7.3191	7.4609	7.5518	7.5063	7.6326	7.5051	7.6514	7.5020	7.6478	7.5087	7.6717	7.3191	7.4609	7.5518	7.5063	7.6326	7.5051	7.6514	7.5020	7.6478	7.5086	7.6717	**7.06**
H5	7.1598	7.3540	7.4469	7.4346	7.5590	7.4312	7.5697	7.4260	7.5622	7.4390	7.5920	7.1598	7.3540	7.4469	7.4346	7.5590	7.4312	7.5697	7.4260	7.5622	7.4390	7.5920	**7.06**
H6	8.0640	8.2389	8.3289	8.3344	8.4363	8.3300	8.4815	8.3236	8.4785	8.3398	8.5089	8.0640	8.2389	8.3289	8.3344	8.4363	8.3300	8.4815	8.3236	8.4785	8.3398	8.5089	**8.35**
H8	4.6400	4.7026	4.7244	4.7366	4.8022	4.7356	4.8453	4.7328	4.8505	4.7388	4.8420	4.6400	4.7026	4.7244	4.7366	4.8022	4.7356	4.8453	4.7328	4.8505	4.7388	4.8420	**4.88**
H(9A-9B)	1.7416	1.7883	1.7937	1.8184	1.7905	1.8182	1.7669	1.8161	1.7538	1.8196	1.8042	1.7416	1.7883	1.7937	1.8183	1.7905	1.8182	1.7669	1.8161	1.7538	1.8196	1.8042	**2.05**
H(10A-10B)	1.4033	1.2887	1.2417	1.2217	1.1482	1.2273	1.1635	1.2309	1.1803	1.2176	1.1520	1.4033	1.2887	1.2417	1.2217	1.1482	1.2273	1.1635	1.2310	1.1803	1.2176	1.1520	**1.36**
H(11A-11C)	0.7436	0.7503	0.7264	0.7554	0.7181	0.7563	0.7178	0.7554	0.7285	0.7558	0.7112	0.7436	0.7503	0.7264	0.7554	0.7181	0.7563	0.7178	0.7554	0.7285	0.7558	0.7112	**0.77**
H(1`A)	2.6954	2.7070	2.6878	2.6933	2.6530	2.6955	2.6625	2.6959	2.6647	2.6923	2.6372	2.8227	2.8243	2.8064	2.7807	2.8087	2.7945	2.8092	2.7940	2.8054	2.7646	**3.03**
H(1`B)	3.1996	3.2388	3.2707	3.2664	3.3284	3.2657	3.3054	3.2632	3.3068	3.2683	3.3052	2.9093	2.7544	2.7264	2.6975	2.7241	2.7016	2.6736	2.6950	2.6628	**3.23**
H(2`-3`A-2`-3`B)	1.6557	1.7151	1.6795	1.7495	1.7149	1.7483	1.7350	1.7453	1.7365	1.7520	1.7641	1.6557	1.7151	1.6795	1.7495	1.7149	1.7483	1.7350	1.7453	1.7365	1.7520	1.7640	**1.77**
H(4`A)	2.9093	2.7544	2.7264	2.6975	2.7241	2.7016	2.6736	2.7040	2.6611	2.6950	2.6629	3.1996	3.2388	3.2707	3.2664	3.3283	3.2656	3.3054	3.2632	3.3068	3.2683	3.3052	**3.03**
H(4`B)	2.8227	2.8243	2.8115	2.8064	2.7807	2.8087	2.7945	2.8092	2.7941	2.8054	2.7646	2.6954	2.7070	2.6878	2.6933	2.6530	2.6955	2.6625	2.6959	2.6647	2.6923	2.6372	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. I

Nuclei	R											S										Exp. [b]
	B3PW91											B3PW91										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.3240	138.3570	138.9423	139.0780	141.3135	139.0503	140.5015	139.0142	140.3718	139.1064	140.8683	137.3240	138.3570	138.9423	139.0780	140.9945	139.0503	140.5015	139.0142	140.3718	139.1064	140.8684	**133.8**
C2	138.7406	138.7359	139.3047	138.5884	139.5155	138.6032	139.5708	138.6087	139.5248	138.5765	139.5857	138.7406	138.7359	139.3048	138.5884	139.1965	138.6032	139.5708	138.6087	139.5248	138.5765	139.5857	**132.1**
C3	121.1602	121.9507	122.5047	122.2008	123.2602	122.1943	123.2452	122.1786	123.1838	122.2088	123.3490	121.1602	121.9508	122.5047	122.2008	122.9412	122.1943	123.2452	122.1786	123.1838	122.2088	123.3490	**115.8**
C4	173.8875	174.7119	175.3233	175.0897	176.1045	175.0726	176.3829	175.0466	176.2739	175.1079	176.5084	173.8875	174.7119	175.3233	175.0897	175.7855	175.0726	176.3829	175.0466	176.2739	175.1080	176.5085	**165.8**
C5	119.2614	120.6353	121.2374	121.2949	122.4633	121.2608	122.3700	121.2179	122.2743	121.3290	122.5313	119.2614	120.6353	121.2374	121.2949	122.1443	121.2608	122.3700	121.2179	122.2743	121.3291	122.5314	**115.8**
C6	134.8881	136.7480	137.8575	137.6742	139.3812	137.6161	139.6614	137.5494	139.4318	137.7317	139.9273	134.8881	136.7480	137.8575	137.6742	139.0622	137.6161	139.6615	137.5494	139.4318	137.7318	139.9274	**132.1**
C7	202.0068	206.7256	207.7025	209.5098	210.7621	209.3506	215.5636	209.1833	214.1346	209.6636	216.7030	202.0068	206.7255	207.7027	209.5098	210.4431	209.3506	215.5636	209.1833	214.1346	209.6636	216.7029	**198.9**
C8	64.7706	66.0246	66.6937	66.7619	68.0060	66.7169	68.3767	66.6643	67.9973	66.8079	68.7804	64.7706	66.0245	66.6937	66.7619	67.6870	66.7169	68.3767	66.6643	67.9973	66.8079	68.7804	**69.3**
C9	37.1523	37.0117	37.2475	36.7905	37.3749	36.8050	37.1661	36.8112	37.0112	36.7793	37.2445	37.1523	37.0117	37.2476	36.7905	37.0559	36.8050	37.1661	36.8112	37.0112	36.7794	37.2446	**31.5**
C10	18.7078	19.2020	19.4695	19.4349	20.2138	19.4228	19.7891	19.4020	19.7285	19.4488	19.9748	18.7078	19.2020	19.4696	19.4349	19.8948	19.4228	19.7891	19.4020	19.7285	19.4488	19.9748	**19.9**
C11	15.7083	15.8983	15.9801	15.9249	16.4664	15.9275	16.0952	15.9214	16.0810	15.9249	16.2589	15.7083	15.8984	15.9801	15.9249	16.1474	15.9275	16.0952	15.9214	16.0810	15.9250	16.2588	**14.3**
C1`	51.1668	51.9977	52.2339	52.5010	53.3444	52.4744	52.9853	52.4389	52.9389	52.5279	53.4848	55.5096	56.5041	56.8262	56.9997	57.5394	56.9736	57.7030	56.9391	57.6758	57.0268	57.9585	**50.6**
C2`	25.1909	25.6108	25.8728	25.7945	26.5286	25.7859	26.2348	25.7688	26.1945	25.8052	26.0679	24.6529	24.8754	25.1417	24.9807	25.5012	24.9798	25.4208	24.9700	25.4250	24.9834	25.2497	**23.8**
C3`	24.6529	24.8754	25.1416	24.9807	25.8202	24.9798	25.4208	24.9700	25.4250	24.9835	25.2498	25.1909	25.6108	25.8728	25.7945	26.2096	25.7859	26.2348	25.7688	26.1945	25.8052	26.0679	**23.8**
C4`	55.5096	56.5041	56.8263	56.9997	57.8584	56.9736	57.7030	56.9391	57.6758	57.0267	57.9585	51.1668	51.9977	52.2338	52.5010	53.0254	52.4744	52.9853	52.4389	52.9389	52.5279	53.4847	**50.6**
H2	8.7063	8.5916	8.6349	8.4920	8.4832	8.4975	8.4709	8.5026	8.4896	8.4870	8.4576	8.7063	8.5916	8.6349	8.4920	8.4677	8.4975	8.4709	8.5026	8.4896	8.4870	8.4575	**8.35**
H3	7.3201	7.4605	7.5499	7.5052	7.6405	7.5036	7.6437	7.5016	7.6363	7.5069	7.6603	7.3201	7.4605	7.5499	7.5052	7.6250	7.5036	7.6437	7.5016	7.6363	7.5069	7.6603	**7.06**
H5	7.1620	7.3498	7.4420	7.4265	7.5662	7.4225	7.5662	7.4181	7.5549	7.4305	7.5848	7.1620	7.3498	7.4420	7.4265	7.5507	7.4225	7.5662	7.4181	7.5549	7.4305	7.5848	**7.06**
H6	8.0473	8.2195	8.3070	8.2987	8.4277	8.2939	8.4532	8.2889	8.4474	8.3033	8.4728	8.0473	8.2195	8.3070	8.2987	8.4122	8.2939	8.4532	8.2889	8.4474	8.3033	8.4728	**8.35**
H8	4.6321	4.6900	4.7084	4.7159	4.8047	4.7146	4.8315	4.7131	4.8294	4.7173	4.8251	4.6321	4.6900	4.7084	4.7159	4.7892	4.7146	4.8315	4.7131	4.8294	4.7173	4.8252	**4.88**
H(9A-9B)	1.6981	1.7410	1.7540	1.7511	1.7538	1.7496	1.7252	1.7479	1.7130	1.7528	1.7506	1.6981	1.7410	1.7540	1.7511	1.7383	1.7496	1.7252	1.7479	1.7130	1.7528	1.7506	**2.05**
H(10A-10B)	1.3764	1.2627	1.2145	1.1925	1.1401	1.1975	1.1436	1.2023	1.1537	1.1878	1.1315	1.3764	1.2627	1.2145	1.1925	1.1246	1.1975	1.1436	1.2023	1.1537	1.1878	1.1314	**1.36**
H(11A-11C)	0.7339	0.7383	0.7137	0.7390	0.7204	0.7393	0.7072	0.7392	0.7126	0.7390	0.6984	0.7339	0.7383	0.7136	0.7390	0.7049	0.7393	0.7072	0.7392	0.7126	0.7390	0.6984	**0.77**
H(1`A)	2.6891	2.6965	2.6752	2.6813	2.6535	2.6829	2.6507	2.6842	2.6495	2.6800	2.6248	2.8185	2.8168	2.8044	2.8024	2.7725	2.8038	2.7885	2.8049	2.7837	2.8012	2.7537	**3.03**
H(1`B)	3.1751	3.2151	3.2483	3.2426	3.3187	3.2409	3.2853	3.2390	3.2822	3.2444	3.2835	2.8650	2.7239	2.6983	2.6825	2.6990	2.6853	2.6603	2.6878	2.6451	2.6802	2.6502	**3.23**
H(2`-3`A-2`-3`B)	1.6449	1.7030	1.6659	1.7420	1.7171	1.7401	1.7233	1.7380	1.7203	1.7439	1.7513	1.6449	1.7030	1.6659	1.7420	1.7016	1.7401	1.7233	1.7380	1.7203	1.7439	1.7513	**1.77**
H(4`A)	2.8650	2.7239	2.6982	2.6825	2.7145	2.6853	2.6603	2.6878	2.6451	2.6802	2.6502	3.1751	3.2151	3.2483	3.2426	3.3032	3.2409	3.2853	3.2390	3.2822	3.2444	3.2835	**3.03**
H(4`B)	2.8185	2.8168	2.8045	2.8024	2.7880	2.8038	2.7885	2.8049	2.7837	2.8012	2.7537	2.6891	2.6965	2.6752	2.6813	2.6380	2.6829	2.6507	2.6842	2.6495	2.6800	2.6247	**3.23**
Nuclei	B98											B98											
C1	138.2224	139.1640	139.9051	139.8882	141.7003	139.8842	141.1990	139.8762	141.1387	139.8933	141.5892	138.2225	139.1640	139.9050	139.8882	141.7003	139.8843	141.1989	139.8762	141.1387	139.8934	141.5892	**133.8**
C2	138.3975	138.3805	138.9375	138.2296	138.7920	138.2538	139.2215	138.2758	139.1629	138.2089	139.2303	138.3977	138.3805	138.9374	138.2296	138.7920	138.2538	139.2215	138.2758	139.1630	138.2088	139.2303	**132.1**
C3	120.9098	121.6403	122.1892	121.9083	122.6382	121.9116	122.9215	121.9121	122.8614	121.9068	123.0044	120.9098	121.6403	122.1891	121.9083	122.6382	121.9116	122.9215	121.9121	122.8615	121.9069	123.0044	**115.8**
C4	173.6926	174.4602	175.0884	174.8453	175.5834	174.8371	176.1492	174.8264	176.0280	174.8553	176.2539	173.6926	174.4602	175.0884	174.8453	175.5834	174.8371	176.1492	174.8264	176.0279	174.8553	176.2539	**165.8**
C5	118.9981	120.3027	120.8910	120.9799	121.8149	120.9557	122.0144	120.9289	121.9207	121.0050	122.1558	118.9980	120.3027	120.8911	120.9799	121.8149	120.9557	122.0144	120.9289	121.9207	121.0051	122.1558	**115.8**
C6	134.8559	136.6645	137.7541	137.6013	139.0072	137.5486	139.5986	137.4941	139.3624	137.6546	139.8326	134.8558	136.6645	137.7543	137.6013	139.0072	137.5486	139.5985	137.4941	139.3624	137.6545	139.8326	**132.1**
C7	200.4682	205.2187	206.3918	208.0300	208.8092	207.8906	214.1407	207.7481	212.7881	208.1635	215.3302	200.4686	205.2187	206.3918	208.0300	208.8092	207.8906	214.1407	207.7481	212.7880	208.1636	215.3302	**198.9**
C8	66.3871	67.6168	68.4226	68.2708	69.0696	68.2442	69.8409	68.2155	69.5502	68.2988	70.2427	66.3871	67.6168	68.4226	68.2708	69.0696	68.2442	69.8409	68.2155	69.5501	68.2989	70.2427	**69.3**
C9	38.4616	38.2575	38.5178	38.0095	38.2028	38.0334	38.4017	38.0552	38.2887	37.9894	38.4483	38.4616	38.2575	38.5178	38.0095	38.2028	38.0334	38.4017	38.0552	38.2886	37.9894	38.4483	**31.5**
C10	20.1212	20.5386	20.8234	20.7589	21.1975	20.7577	21.1155	20.7539	21.0819	20.7625	21.2510	20.1211	20.5386	20.8234	20.7589	21.1975	20.7577	21.1154	20.7539	21.0820	20.7625	21.2510	**19.9**
C11	16.3161	16.4561	16.5672	16.5007	16.7076	16.5122	16.6770	16.5215	16.6738	16.4920	16.8309	16.3162	16.4561	16.5671	16.5007	16.7075	16.5122	16.6770	16.5215	16.6738	16.4920	16.8309	**14.3**
C1`	52.4322	53.2094	53.4644	53.7262	54.1926	53.7098	54.1985	53.6905	54.1769	53.7438	54.6700	56.9107	57.8097	58.1546	58.3077	58.9077	58.2931	59.0087	58.2762	58.9647	58.3242	59.2359	**50.6**
C2`	26.3567	26.7481	27.0235	26.9415	27.3702	26.9430	27.3853	26.9422	27.3586	26.9426	27.2367	25.8357	26.0296	26.3025	26.1673	26.7228	26.1753	26.6111	26.1807	26.6224	26.1617	26.4450	**23.8**
C3`	25.8357	26.0296	26.3025	26.1673	26.7228	26.1753	26.6111	26.1807	26.6224	26.1617	26.4450	26.3566	26.7481	27.0234	26.9415	27.3702	26.9430	27.3852	26.9422	27.3587	26.9427	27.2367	**23.8**
C4`	56.9107	57.8097	58.1547	58.3077	58.9077	58.2931	59.0087	58.2762	58.9647	58.3241	59.2359	52.4323	53.2094	53.4643	53.7262	54.1926	53.7098	54.1985	53.6905	54.1769	53.7438	54.6700	**50.6**
H2	8.6894	8.5909	8.6224	8.4935	8.4821	8.4973	8.4850	8.5013	8.4994	8.4903	8.4675	8.6894	8.5909	8.6224	8.4935	8.4821	8.4973	8.4850	8.5013	8.4994	8.4902	8.4675	**8.35**
H3	7.3105	7.4535	7.5447	7.5015	7.6240	7.4994	7.6413	7.4973	7.6346	7.5037	7.6546	7.3105	7.4535	7.5447	7.5015	7.6240	7.4994	7.6413	7.4973	7.6346	7.5037	7.6546	**7.06**
H5	7.1523	7.3441	7.4354	7.4263	7.5528	7.4218	7.5657	7.4173	7.5546	7.4309	7.5834	7.1523	7.3441	7.4354	7.4263	7.5528	7.4218	7.5657	7.4173	7.5546	7.4309	7.5834	**7.06**
H6	8.0177	8.1926	8.2749	8.2771	8.4094	8.2712	8.4410	8.2654	8.4303	8.2831	8.4600	8.0177	8.1926	8.2749	8.2771	8.4094	8.2712	8.4410	8.2654	8.4303	8.2831	8.4600	**8.35**
H8	4.5931	4.6518	4.6646	4.6876	4.7858	4.6853	4.8089	4.6831	4.8002	4.6902	4.7991	4.5931	4.6518	4.6646	4.6876	4.7858	4.6853	4.8089	4.6831	4.8002	4.6902	4.7991	**4.88**
H(9A-9B)	1.6901	1.7360	1.7485	1.7400	1.7203	1.7377	1.7240	1.7356	1.7164	1.7426	1.7462	1.6901	1.7360	1.7485	1.7400	1.7203	1.7377	1.7240	1.7356	1.7164	1.7426	1.7462	**2.05**
H(10A-10B)	1.4152	1.2960	1.2444	1.2276	1.1642	1.2323	1.1763	1.2369	1.1845	1.2235	1.1606	1.4152	1.2960	1.2444	1.2276	1.1642	1.2323	1.1762	1.2369	1.1845	1.2235	1.1606	**1.36**
H(11A-11C)	0.7611	0.7656	0.7386	0.7672	0.7371	0.7669	0.7360	0.7668	0.7397	0.7677	0.7254	0.7611	0.7656	0.7386	0.7672	0.7371	0.7669	0.7360	0.7668	0.7397	0.7677	0.7254	**0.77**
H(1`A)	2.7078	2.7124	2.6914	2.6987	2.6511	2.6997	2.6647	2.7008	2.6644	2.6979	2.6436	2.8359	2.8334	2.8251	2.8174	2.7884	2.8186	2.8028	2.8200	2.8005	2.8165	2.7709	**3.03**
H(1`B)	3.1881	3.2199	3.2554	3.2500	3.3125	3.2475	3.2980	3.2452	3.2948	3.2527	3.2997	2.8681	2.7298	2.6956	2.6924	2.6978	2.6788	2.7002	2.6697	2.6937	2.6724	2.6724	**3.23**
H(2`-3`A-2`-3`B)	1.6629	1.7224	1.6860	1.7638	1.7243	1.7616	1.7439	1.7594	1.7405	1.7663	1.7711	1.6629	1.7224	1.6861	1.7638	1.7243	1.7616	1.7439	1.7594	1.7405	1.7662	1.7711	**1.77**
H(4`A)	2.8681	2.7298	2.7147	2.6956	2.6924	2.6978	2.6788	2.7002	2.6697	2.6937	2.6724	3.1881	3.2199	3.2554	3.2500	3.3125	3.2475	3.2980	3.2452	3.2948	3.2527	3.2997	**3.03**
H(4`B)	2.8359	2.8334	2.8251	2.8174	2.7884	2.8186	2.8028	2.8200	2.8005	2.8165	2.7709	2.7078	2.7124	2.6914	2.6987	2.6511	2.6997	2.6647	2.7008	2.6644	2.6979	2.6436	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. II

Nuclei	R											S											Exp. [b]
	B971											B971											
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.7896	138.7258	139.4757	139.3145	141.3703	139.2969	140.8309	139.2753	140.7248	139.3352	141.1889	137.7897	138.7257	139.4757	139.3145	141.3704	139.2969	140.8309	139.2753	140.7248	139.3352	141.1889	**133.8**
C2	138.1048	138.0869	138.6350	137.9511	138.5060	137.9671	138.9203	137.9828	138.8733	137.9418	138.9371	138.1048	138.0869	138.6351	137.9511	138.5061	137.9671	138.9203	137.9827	138.8733	137.9418	138.9372	**132.1**
C3	120.7076	121.4428	121.9913	121.7128	122.4280	121.7077	122.7193	121.7016	122.6649	121.7232	122.8145	120.7077	121.4429	121.9912	121.7128	122.4279	121.7077	122.7193	121.7016	122.6649	121.7232	122.8144	**115.8**
C4	173.5909	174.3695	174.9990	174.7694	175.4614	174.7530	176.0418	174.7363	175.9345	174.7910	176.1612	173.5907	174.3696	174.9991	174.7693	175.4613	174.7530	176.0419	174.7364	175.9345	174.7910	176.1611	**165.8**
C5	118.7920	120.1069	120.6911	120.8026	121.6266	120.7691	121.8331	120.7350	121.7422	120.8401	121.9820	118.7921	120.1070	120.6912	120.8026	121.6267	120.7691	121.8330	120.7351	121.7422	120.8401	121.9820	**115.8**
C6	134.5937	136.4061	137.4903	137.3977	138.7332	137.3391	139.3078	137.2814	139.0782	137.4601	139.5577	134.5937	136.4060	137.4904	137.3977	138.7332	137.3391	139.3077	137.2816	139.0782	137.4601	139.5577	**132.1**
C7	200.3690	205.0557	206.2416	207.7038	208.8030	207.5540	213.9618	207.4011	212.5592	207.8508	215.1135	200.3691	205.0558	206.2416	207.7038	208.8030	207.5540	213.9616	207.4011	212.5592	207.8508	215.1135	**198.9**
C8	66.2089	67.4207	68.2147	68.0185	69.0026	67.9848	69.6635	67.9509	69.3168	68.0569	70.0400	66.2089	67.4207	68.2147	68.0186	69.0027	67.9848	69.6636	67.9509	69.3168	68.0569	70.4000	**69.3**
C9	38.4612	38.2837	38.5360	38.0822	38.3178	38.1001	38.4549	38.1185	38.3110	38.0718	38.5001	38.4612	38.2837	38.5360	38.0822	38.3179	38.1001	38.4549	38.1184	38.3110	38.0718	38.5001	**31.5**
C10	20.1289	20.5580	20.8276	20.7907	21.2145	20.7818	21.1285	20.7727	21.0890	20.8054	21.2735	20.1289	20.5579	20.8276	20.7908	21.2145	20.7818	21.1285	20.7727	21.0890	20.8054	21.2735	**19.9**
C11	16.2682	16.4143	16.5169	16.4684	16.6720	16.4723	16.6310	16.4757	16.6242	16.4709	16.7883	16.2682	16.4142	16.5169	16.4685	16.6719	16.4723	16.6310	16.4756	16.6242	16.4709	16.7882	**14.3**
C1`	52.3575	53.1298	53.3760	53.6428	54.1294	53.6181	54.1018	53.5927	54.0746	53.6717	54.5739	56.8143	57.7040	58.0473	58.1961	58.7517	58.1727	58.8883	58.1489	58.8567	58.2244	59.1183	**50.6**
C2`	26.1707	26.5679	26.8437	26.7698	27.1862	26.7633	27.2121	26.7565	27.1781	26.7821	27.0715	25.6513	25.8535	26.1266	25.9996	26.5124	25.9994	26.4278	25.9984	26.4461	26.0053	26.2931	**23.8**
C3`	25.6512	25.8535	26.1266	25.9996	26.5125	25.9994	26.4279	25.9984	26.4461	26.0053	26.2931	26.1707	26.5680	26.8437	26.7698	27.1863	26.7633	27.2122	26.7565	27.1781	26.7821	27.0716	**23.8**
C4`	56.8144	57.7041	58.0473	58.1960	58.7517	58.1727	58.8883	58.1489	58.8567	58.2244	59.1183	52.3575	53.1298	53.3759	53.6428	54.1294	53.6182	54.1016	53.5925	54.0746	53.6717	54.5739	**50.6**
H2	8.6882	8.5915	8.6209	8.5103	8.4727	8.5144	8.4810	8.5188	8.5000	8.5071	8.4668	8.6882	8.5915	8.6209	8.5103	8.4727	8.5144	8.4811	8.5188	8.5000	8.5071	8.4668	**8.35**
H3	7.3085	7.4501	7.5415	7.4990	7.6202	7.4966	7.6384	7.4942	7.6316	7.5016	7.6522	7.3085	7.4502	7.5415	7.4990	7.6202	7.4966	7.6384	7.4942	7.6316	7.5016	7.6522	**7.06**
H5	7.1494	7.3412	7.4323	7.4259	7.5519	7.4211	7.5645	7.4163	7.5535	7.4308	7.5823	7.1494	7.3412	7.4323	7.4259	7.5519	7.4211	7.5645	7.4163	7.5535	7.4308	7.5823	**7.06**
H6	8.0262	8.1982	8.2822	8.2875	8.3973	8.2816	8.4362	8.2759	8.4293	8.2936	8.4567	8.0262	8.1982	8.2822	8.2875	8.3973	8.2816	8.4362	8.2759	8.4293	8.2936	8.4567	**8.35**
H8	4.5982	4.6556	4.6721	4.6947	4.7692	4.6923	4.8069	4.6900	4.8035	4.6974	4.7993	4.5982	4.6556	4.6721	4.6945	4.7692	4.6923	4.8069	4.6900	4.8035	4.6974	4.7993	**4.88**
H(9A-9B)	1.6969	1.7418	1.7519	1.7550	1.7355	1.7530	1.7286	1.7513	1.7184	1.7575	1.7500	1.6969	1.7418	1.7519	1.7550	1.7355	1.7530	1.7286	1.7513	1.7184	1.7575	1.7500	**2.05**
H(10A-10B)	1.4117	1.2931	1.2426	1.2275	1.1562	1.2319	1.1722	1.2362	1.1828	1.2238	1.1586	1.4117	1.2931	1.2426	1.2275	1.1562	1.2319	1.1722	1.2362	1.1828	1.2238	1.1586	**1.36**
H(11A-11C)	0.7557	0.7592	0.7327	0.7628	0.7269	0.7624	0.7273	0.7620	0.7328	0.7637	0.7178	0.7557	0.7592	0.7327	0.7628	0.7269	0.7624	0.7273	0.7620	0.7328	0.7637	0.7178	**0.77**
H(1`A)	2.6983	2.7040	2.6840	2.6920	2.6456	2.6929	2.6578	2.6938	2.6567	2.6916	2.6341	2.8264	2.8244	2.8168	2.8089	2.7828	2.8100	2.7961	2.8111	2.7921	2.8083	2.6730	**3.03**
H(1`B)	3.1922	3.2226	3.2567	3.2538	3.3131	3.2513	3.2981	3.2489	3.2952	3.2567	3.2988	2.8701	2.7333	2.7168	2.6954	2.7118	2.6975	2.6836	2.6997	2.6697	2.6938	2.6730	**3.23**
H(2`-3`A-2`-3`B)	1.6619	1.7208	1.6851	1.7611	1.7208	1.7585	1.7415	1.7560	1.7388	1.7639	1.7689	1.6619	1.7208	1.6851	1.7611	1.7208	1.7585	1.7415	1.7560	1.7388	1.7639	1.7689	**1.77**
H(4`A)	2.8701	2.7333	2.7168	2.6954	2.7118	2.6975	2.6836	2.6997	2.6697	2.6938	2.6730	3.1922	3.2226	3.2567	3.2538	3.3131	3.2513	3.2981	3.2489	3.2952	3.2567	3.2988	**3.03**
H(4`B)	2.8264	2.8244	2.8168	2.8089	2.7828	2.8100	2.7961	2.8111	2.7921	2.8083	2.7640	2.6983	2.7040	2.6840	2.6920	2.6456	2.6929	2.6578	2.6938	2.6567	2.6916	2.6341	**3.23**
Nuclei	B972											B972											
C1	134.7000	136.2436	137.1818	136.8329	138.4324	136.7985	137.8759	136.7628	137.7451	136.8625	138.2351	134.7000	136.2436	137.1818	136.8330	138.4324	136.7985	137.8759	136.7628	137.7451	136.8625	138.2351	**133.8**
C2	136.0990	136.0628	136.6204	135.9754	136.5157	135.9836	136.9002	135.9887	136.8502	135.9635	136.9116	136.0991	136.0628	136.6204	135.9755	136.5157	135.9836	136.9002	135.9887	136.8502	135.9635	136.9116	**132.1**
C3	118.5870	119.3172	119.9025	119.6168	120.2925	119.6024	120.5790	119.5852	120.5089	119.6260	120.6806	118.5870	119.3172	119.9024	119.6168	120.2924	119.6024	120.5789	119.5852	120.5089	119.6260	120.6806	**115.8**
C4	170.5548	171.2810	171.9148	171.6922	172.3497	171.6680	172.9154	171.6416	172.7991	171.7106	173.0415	170.5549	171.2810	171.9147	171.6921	172.3496	171.6680	172.9153	171.6416	172.7991	171.7107	173.0415	**165.8**
C5	116.7290	118.0016	118.6162	118.6724	119.4580	118.6330	119.6671	118.5914	119.5732	118.7054	119.8271	116.7289	118.0016	118.6162	118.6724	119.4580	118.6330	119.6671	118.5914	119.5732	118.7054	119.8271	**115.8**
C6	132.3207	133.8605	134.8157	134.8931	136.2813	134.8294	136.8581	134.7633	136.6544	134.9490	137.1200	132.3206	133.8605	134.8157	134.8932	136.2813	134.8294	136.8581	134.7633	136.6544	134.9490	137.1200	**132.1**
C7	197.9191	203.0510	204.3145	205.7374	206.2945	205.5739	211.3106	205.4087	209.9428	205.8898	212.4204	197.9188	203.0510	204.3144	205.7374	206.2946	205.5739	211.3106	205.4087	209.9428	205.8898	212.4204	**198.9**
C8	63.4911	64.8297	65.5365	65.6161	66.2773	65.5680	66.9467	65.5180	66.6397	65.6578	67.2902	63.4911	64.8297	65.5366	65.6161	66.2773	65.5680	66.9467	65.5180	66.6397	65.6578	67.2902	**69.3**
C9	36.4665	36.1386	36.2826	36.0589	36.2549	36.0665	36.4100	36.0714	36.3170	36.0469	36.4935	36.4665	36.1386	36.2827	36.0589	36.2549	36.0665	36.4101	36.0714	36.3170	36.0469	36.4935	**31.5**
C10	18.8488	19.2698	19.5409	19.6061	20.0211	19.5873	19.9147	19.5659	19.8801	19.6194	20.0861	18.8488	19.2698	19.5408	19.6061	20.0211	19.5873	19.9146	19.5659	19.8801	19.6194	20.0861	**19.9**
C11	15.8897	16.0176	16.1272	16.1216	16.2966	16.1158	16.2532	16.1079	16.2460	16.1230	16.4162	15.8897	16.0176	16.1271	16.1216	16.2966	16.1158	16.2531	16.1079	16.2460	16.1230	16.4162	**14.3**
C1`	50.3452	51.1497	51.4234	51.6980	52.1403	51.6664	52.1193	51.6323	52.0919	51.7233	52.5644	54.6924	55.6376	56.0022	56.1680	56.6754	56.1343	56.7805	56.0986	56.7295	56.1964	57.0279	**50.6**
C2`	25.1240	25.4950	25.7942	25.7589	26.1290	25.7426	26.1316	25.7238	26.1053	25.7704	25.9833	24.6170	24.8027	25.1396	24.9599	25.4611	24.9502	25.3578	24.9384	25.3545	24.9649	25.1771	**23.8**
C3`	24.6170	24.8027	25.1397	24.9600	25.4610	24.9502	25.3578	24.9383	25.3545	24.9650	25.1771	25.1242	25.4950	25.7941	25.7589	26.1290	25.7426	26.1315	25.7238	26.1053	25.7704	25.9833	**23.8**
C4`	54.6924	55.6376	56.0022	56.1680	56.6750	56.1343	56.7805	56.0986	56.7295	56.1964	57.0279	50.3452	51.1497	51.4235	51.6979	52.1403	51.6664	52.1192	51.6323	52.0919	51.7233	52.5644	**50.6**
H2	8.6882	8.5150	8.5284	8.4403	8.4433	8.4451	8.4562	8.4495	8.4736	8.4356	8.4447	8.6882	8.5150	8.5284	8.4403	8.4433	8.4451	8.4562	8.4495	8.4736	8.4356	8.4447	**8.35**
H3	7.3161	7.4512	7.5417	7.4954	7.6123	7.4933	7.6312	7.4909	7.6246	7.4972	7.6480	7.3161	7.4512	7.5417	7.4954	7.6123	7.4933	7.6312	7.4909	7.6246	7.4972	7.6480	**7.06**
H5	7.1578	7.3389	7.4289	7.4180	7.5411	7.4135	7.5577	7.4087	7.5460	7.4222	7.5769	7.1578	7.3389	7.4289	7.4180	7.5411	7.4135	7.5577	7.4087	7.5460	7.4222	7.5769	**7.06**
H6	8.0334	8.1775	8.2555	8.2618	8.3931	8.2564	8.4269	8.2508	8.4195	8.2668	8.4475	8.0334	8.1775	8.2555	8.2618	8.3931	8.2564	8.4269	8.2508	8.4195	8.2668	8.4475	**8.35**
H8	4.6059	4.6489	4.6756	4.6813	4.7723	4.6784	4.8012	4.6755	4.7908	4.6840	4.7938	4.6059	4.6489	4.6756	4.6813	4.7723	4.6784	4.8012	4.6755	4.7908	4.6840	4.7938	**4.88**
H(9A-9B)	1.6638	1.6691	1.6582	1.6982	1.6869	1.6966	1.6880	1.6946	1.6833	1.6995	1.7129	1.6638	1.6691	1.6582	1.6982	1.6870	1.6966	1.6880	1.6946	1.6833	1.6995	1.7129	**2.05**
H(10A-10B)	1.3756	1.2612	1.2159	1.1986	1.1370	1.2026	1.1556	1.2063	1.1622	1.1947	1.1443	1.3756	1.2612	1.2158	1.1986	1.1370	1.2027	1.1555	1.2063	1.1622	1.1947	1.1443	**1.36**
H(11A-11C)	0.7480	0.7466	0.7214	0.7531	0.7224	0.7525	0.7247	0.7518	0.7276	0.7536	0.7164	0.7480	0.7466	0.7214	0.7531	0.7224	0.7525	0.7247	0.7518	0.7276	0.7536	0.7164	**0.77**
H(1`A)	2.6909	2.6924	2.6690	2.6803	2.6344	2.6813	2.6467	2.6821	2.6463	2.6792	2.6221	2.8262	2.8279	2.8199	2.8132	2.7776	2.8142	2.7913	2.8150	2.7885	2.8122	2.7566	**3.03**
H(1`B)	3.1749	3.2131	3.2469	3.2467	3.3078	3.2444	3.2919	3.2419	3.2886	3.2488	3.2903	2.8410	2.7272	2.7113	2.6915	2.6918	2.6936	2.6671	2.6955	2.6562	2.6895	2.6608	**3.23**
H(2`-3`A-2`-3`B)	1.6437	1.7062	1.6731	1.7448	1.7011	1.7423	1.7207	1.7397	1.7165	1.7470	1.7477	1.6438	1.7062	1.6730	1.7448	1.7011	1.7423	1.7207	1.7397	1.7165	1.7470	1.7477	**1.77**
H(4`A)	2.8410	2.7272	2.7113	2.6915	2.6918	2.6936	2.6671	2.6955	2.6562	2.6895	2.6608	3.1749	3.2131	3.2469	3.2467	3.3078	3.2444	3.2919	3.2419	3.2886	3.2488	3.2903	**3.03**
H(4`B)	2.8262	2.8279	2.8199	2.8132	2.7776	2.8142	2.7912	2.8150	2.7884	2.8122	2.7566	2.6909	2.6924	2.6690	2.6803	2.6344	2.6813	2.6467	2.6821	2.6463	2.6792	2.6221	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. III

Nuclei	R											S										Exp. [b]
	BHandH											BHandH										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	138.6239	139.3098	140.1633	139.5276	141.1787	139.5165	140.0987	139.5222	140.2563	139.5071	140.4432	138.6239	139.3098	140.1633	139.5276	140.2717	139.5165	140.0987	139.5222	140.2563	139.5071	140.4431	**133.8**
C2	143.5738	143.4947	144.0312	143.3147	143.8526	143.3175	144.3129	143.3387	144.2043	143.2814	144.3448	143.5738	143.4947	144.0312	143.3147	144.0588	143.3175	144.3129	143.3387	144.2043	143.2814	144.3448	**132.1**
C3	123.6964	124.4238	125.0999	124.6746	125.3915	124.6516	125.6126	124.6467	125.5819	124.6660	125.6923	123.6964	124.4238	125.0999	124.6746	125.4187	124.6516	125.6126	124.6467	125.5819	124.6660	125.6922	**115.8**
C4	174.7958	175.5262	176.1958	175.9464	176.5287	175.9082	177.2561	175.8886	177.0899	175.9528	177.3931	174.7958	175.5262	176.1958	175.9464	176.6905	175.9083	177.2561	175.8886	177.0899	175.9529	177.3932	**165.8**
C5	121.4818	122.8933	123.6425	123.6703	124.5646	123.6119	124.8041	123.5718	124.7042	123.6956	124.9837	121.4818	122.8933	123.6425	123.6703	124.4144	123.6119	124.8041	123.5718	124.7042	123.6956	124.9838	**115.8**
C6	139.8395	141.7777	142.9069	142.9335	144.5142	142.8465	145.2948	142.7787	145.0237	142.9871	145.6621	139.8395	141.7777	142.9069	142.9335	143.6776	142.8465	145.2948	142.7787	145.0237	142.9870	145.6622	**132.1**
C7	204.1536	208.7473	209.9381	211.1734	211.8512	211.0273	216.7295	210.8976	215.6262	211.2809	217.9024	204.1536	208.7473	209.9381	211.1734	211.9175	211.0273	216.7295	210.8976	215.6262	211.2809	217.9027	**198.9**
C8	60.1105	61.2911	61.8318	61.8324	62.6666	61.7978	63.0997	61.7803	62.9850	61.8343	63.6345	60.1105	61.2911	61.8318	61.8324	62.5765	61.7978	63.0997	61.7803	62.9850	61.8343	63.6346	**69.3**
C9	36.0832	35.8942	36.0047	35.7106	36.0824	35.7146	36.0744	35.7361	36.0332	35.6765	36.3132	36.0832	35.8942	36.0047	35.7106	36.4547	35.7146	36.0744	35.7361	36.0332	35.6764	36.3132	**31.5**
C10	16.5118	16.9597	17.2604	17.2441	17.7611	17.2147	17.6352	17.2037	17.6119	17.2423	17.8191	16.5118	16.9597	17.2604	17.2441	17.9882	17.2147	17.6352	17.2037	17.6119	17.2423	17.8192	**19.9**
C11	15.0257	15.1517	15.3021	15.1736	15.4059	15.1626	15.3623	15.1698	15.3719	15.1539	15.5551	15.0257	15.1517	15.3021	15.1736	15.9177	15.1626	15.3623	15.1698	15.3718	15.1540	15.5550	**14.3**
C1`	48.2361	49.0965	49.3704	49.5476	50.1639	49.5114	50.0607	49.4936	50.0482	49.5517	50.5118	52.1815	53.1322	53.5867	53.6620	54.4061	53.6183	54.3625	53.5933	54.3033	53.6736	54.6277	**50.6**
C2`	21.6424	22.0034	22.3249	22.2037	22.6190	22.1811	22.6630	22.1771	22.6622	22.1954	22.6800	21.0763	21.2802	21.6706	21.4316	22.1757	21.4090	21.8657	21.4052	21.8725	21.4234	21.7951	**23.8**
C3`	21.0763	21.2802	21.6706	21.4316	21.9126	21.4090	21.8657	21.4052	21.8725	21.4234	21.7950	21.6424	22.0034	22.3249	22.2037	22.9478	22.1811	22.6630	22.1771	22.6622	22.1954	22.6801	**23.8**
C4`	52.1815	53.1322	53.5867	53.6620	54.2099	53.6183	54.3625	53.5933	54.3033	53.6736	54.6277	48.2361	49.0965	49.3704	49.5476	50.2917	49.5114	50.0607	49.4936	50.0482	49.5517	50.5119	**50.6**
H2	9.0187	8.9184	8.9416	8.8630	8.8530	8.8660	8.9011	8.8684	8.8933	8.8611	8.8800	9.0187	8.9184	8.9416	8.8630	8.7818	8.8660	8.9011	8.8684	8.8933	8.8612	8.8800	**8.35**
H3	7.4583	7.5981	7.6918	7.6419	7.7660	7.6406	7.7830	7.6384	7.7755	7.6441	7.7978	7.4583	7.5981	7.6918	7.6419	7.5607	7.6406	7.7830	7.6384	7.7755	7.6441	7.7978	**7.06**
H5	7.2809	7.4790	7.5747	7.5691	7.7003	7.5646	7.7181	7.5593	7.7066	7.5743	7.7422	7.2809	7.4790	7.5747	7.5691	7.4879	7.5646	7.7181	7.5593	7.7066	7.5743	7.7422	**7.06**
H6	8.2276	8.4076	8.5091	8.5190	8.6554	8.5119	8.7355	8.5042	8.7089	8.5268	8.7614	8.2276	8.4076	8.5091	8.5190	8.4378	8.5119	8.7355	8.5042	8.7089	8.5268	8.7614	**8.35**
H8	4.2707	4.3319	4.4006	4.3985	4.4661	4.3936	4.5556	4.3880	4.5270	4.4043	4.5618	4.2707	4.3319	4.4006	4.3985	4.3173	4.3936	4.5556	4.3880	4.5270	4.4043	4.5618	**4.88**
H(9A-9B)	1.7526	1.8039	1.7713	1.8251	1.8368	1.8248	1.8202	1.8236	1.8142	1.8264	1.8579	1.7526	1.8039	1.7713	1.8251	1.7438	1.8248	1.8202	1.8236	1.8142	1.8264	1.8579	**2.05**
H(10A-10B)	1.3693	1.2395	1.2010	1.1704	1.0883	1.1748	1.1128	1.1785	1.1147	1.1672	1.0936	1.3693	1.2395	1.2010	1.1704	1.0891	1.1748	1.1128	1.1785	1.1147	1.1672	1.0936	**1.36**
H(11A-11C)	0.7598	0.7638	0.7408	0.7704	0.7291	0.7705	0.7393	0.7696	0.7386	0.7715	0.7301	0.7598	0.7638	0.7408	0.7704	0.6892	0.7705	0.7393	0.7696	0.7386	0.7715	0.7301	**0.77**
H(1`A)	2.5811	2.5765	2.5597	2.5625	2.5141	2.5642	2.5321	2.5650	2.5320	2.5619	2.5148	2.7241	2.7319	2.7078	2.7181	2.6783	2.7204	2.6863	2.7218	2.6889	2.7169	2.6658	**3.03**
H(1`B)	3.0809	3.1130	3.1395	3.1381	3.1895	3.1372	3.1758	3.1354	3.1708	3.1400	3.1806	2.8917	2.7175	2.6455	2.6342	2.6346	2.6408	2.5366	2.6465	2.5450	2.6289	2.5331	**3.23**
H(2`-3`A-2`-3`B)	1.6289	1.6841	1.6486	1.7194	1.6743	1.7179	1.6955	1.7156	1.6898	1.7218	1.7223	1.6289	1.6841	1.6486	1.7194	1.6381	1.7179	1.6955	1.7156	1.6898	1.7218	1.7223	**1.77**
H(4`A)	2.8917	2.7175	2.6455	2.6342	2.6346	2.6408	2.5366	2.6465	2.5450	2.6289	2.5331	3.0809	3.1130	3.1395	3.1381	3.1895	3.1372	3.1758	3.1354	3.1708	3.1400	3.1806	**3.03**
H(4`B)	2.7241	2.7319	2.7078	2.7181	2.6782	2.7204	2.6863	2.7218	2.6889	2.7169	2.6658	2.5811	2.5765	2.5597	2.5625	2.5141	2.5642	2.5321	2.5650	2.5320	2.5619	2.5148	**3.23**
Nuclei	BHandHLYP											BHandHLYP										
C1	139.1995	139.9344	140.7124	140.2115	142.4073	140.1838	141.7706	140.1622	141.7596	140.2418	142.2408	139.1995	139.9344	140.7124	140.2116	142.4071	140.1838	141.7706	140.1622	141.7596	140.2418	142.2408	**133.8**
C2	142.1036	141.9531	142.4769	141.8156	142.2866	141.8255	142.7286	141.8377	142.6885	141.8061	142.7175	142.1036	141.9531	142.4769	141.8158	142.2866	141.8255	142.7286	141.8376	142.6885	141.8060	142.7175	**132.1**
C3	122.4961	123.1091	123.6312	123.3084	124.0035	123.2980	124.1932	123.2900	124.1687	123.3180	124.2908	122.4961	123.1091	123.6312	123.3085	124.0035	123.2980	124.1932	123.2900	124.1687	123.3180	124.2908	**115.8**
C4	174.5922	175.2566	175.8308	175.6409	176.2467	175.6172	176.8399	175.5962	176.7288	175.6628	176.9445	174.5922	175.2566	175.8308	175.6409	176.2467	175.6172	176.8399	175.5962	176.7286	175.6628	176.9445	**165.8**
C5	120.3085	121.5940	122.1677	122.2586	123.0862	122.2171	123.2268	122.1783	123.1489	122.2980	123.3912	120.3085	121.5940	122.1677	122.2586	123.0863	122.2171	123.2268	122.1783	123.1489	122.2981	123.3912	**115.8**
C6	138.1484	139.9784	141.0642	141.0829	142.1719	141.0196	142.8408	140.9569	142.5998	141.1408	143.0584	138.1484	139.9784	141.0642	141.0829	142.1720	141.0196	142.8408	140.9569	142.5997	141.1408	143.0584	**132.1**
C7	202.2649	207.2010	208.3379	209.8082	210.7606	209.6369	216.7690	209.4723	215.2774	209.9747	218.0633	202.2649	207.2010	208.3379	209.8079	210.7610	209.6369	216.7690	209.4723	215.2771	209.9744	218.0633	**198.9**
C8	61.8458	62.8304	63.5344	63.3115	63.9662	63.2792	64.8164	63.2505	64.5141	63.3431	65.2211	61.8458	62.8304	63.5344	63.3115	63.9662	63.2792	64.8164	63.2505	64.5142	63.3431	65.2211	**69.3**
C9	35.5682	35.2268	35.4409	35.0480	35.0587	35.0643	35.1701	35.0818	35.0932	35.0309	35.1967	35.5682	35.2268	35.4409	35.0480	35.0587	35.0643	35.1701	35.0817	35.0932	35.0307	35.1967	**31.5**
C10	18.3108	18.7220	18.9982	18.9799	19.3800	18.9644	19.2649	18.9513	19.2456	18.9941	19.3876	18.3108	18.7220	18.9982	18.9799	19.3800	18.9644	19.2650	18.9513	19.2456	18.9941	19.3876	**19.9**
C11	15.8988	16.0123	16.1497	16.0717	16.2865	16.0682	16.2351	16.0671	16.2477	16.0747	16.3848	15.8988	16.0123	16.1497	16.0717	16.2865	16.0682	16.2351	16.0670	16.2477	16.0746	16.3848	**14.3**
C1`	49.0619	49.8235	50.1189	50.3249	50.8251	50.2909	50.8340	50.2599	50.8225	50.3574	51.2993	53.3229	54.2124	54.5676	54.6856	55.2693	54.6539	55.3618	54.6254	55.3266	54.7162	55.6172	**50.6**
C2`	24.4347	24.7574	25.0607	24.9331	25.3432	24.9209	25.3584	24.9113	25.3395	24.9448	25.2085	23.8796	24.0140	24.3263	24.1401	24.7203	24.1309	24.5630	24.1244	24.5892	24.1486	24.4005	**23.8**
C3`	23.8796	24.0140	24.3263	24.1401	24.7203	24.1309	24.5630	24.1245	24.5892	24.1486	24.4005	24.4347	24.7574	25.0607	24.9331	25.3432	24.9209	25.3584	24.9113	25.3394	24.9449	25.2085	**23.8**
C4`	53.3229	54.2124	54.5676	54.6856	55.2692	54.6539	55.3618	54.6254	55.3266	54.7162	55.6172	49.0620	49.8235	50.1189	50.3249	50.8250	50.2909	50.8340	50.2599	50.8223	50.3574	51.2993	**50.6**
H2	8.9120	8.8065	8.8331	8.7485	8.6943	8.7536	8.6881	8.7581	8.7047	8.7432	8.6588	8.9120	8.8065	8.8331	8.7485	8.6943	8.7536	8.6881	8.7581	8.7047	8.7432	8.6588	**8.35**
H3	7.4376	7.5713	7.6590	7.6162	7.7362	7.6141	7.7545	7.6118	7.7469	7.6181	7.7692	7.4376	7.5713	7.6590	7.6162	7.7362	7.6141	7.7545	7.6118	7.7470	7.6181	7.7692	**7.06**
H5	7.2696	7.4607	7.5483	7.5438	7.6626	7.5393	7.6778	7.5346	7.6656	7.5480	7.6980	7.2696	7.4607	7.5483	7.5438	7.6626	7.5393	7.6778	7.5346	7.6656	7.5481	7.6980	**7.06**
H6	8.0935	8.2902	8.3789	8.4029	8.5310	8.3964	8.5708	8.3897	8.5558	8.4089	8.5892	8.0935	8.2902	8.3789	8.4029	8.5310	8.3964	8.5708	8.3897	8.5558	8.4089	8.5892	**8.35**
H8	4.2157	4.3089	4.3348	4.3694	4.4804	4.3657	4.5083	4.3619	4.4942	4.3727	4.4993	4.2157	4.3089	4.3348	4.3694	4.4804	4.3657	4.5083	4.3619	4.4942	4.3727	4.4993	**4.88**
H(9A-9B)	1.5615	1.6076	1.6122	1.6423	1.5807	1.6413	1.5917	1.6398	1.5810	1.6430	1.6082	1.5615	1.6076	1.6122	1.6423	1.5807	1.6413	1.5917	1.6397	1.5810	1.6430	1.6082	**2.05**
H(10A-10B)	1.3552	1.2326	1.1775	1.1688	1.1078	1.1731	1.1127	1.1772	1.1234	1.1646	1.1005	1.3552	1.2326	1.1775	1.1688	1.1078	1.1731	1.1127	1.1773	1.1234	1.1646	1.1005	**1.36**
H(11A-11C)	0.7791	0.7824	0.7529	0.7916	0.7546	0.7913	0.7544	0.7908	0.7581	0.7918	0.7460	0.7791	0.7824	0.7529	0.7916	0.7546	0.7913	0.7544	0.7908	0.7581	0.7918	0.7460	**0.77**
H(1`A)	2.5995	2.6032	2.5768	2.5918	2.5385	2.5929	2.5592	2.5940	2.5572	2.5906	2.5374	2.7413	2.7309	2.7180	2.7108	2.6715	2.7123	2.6963	2.7136	2.6903	2.7094	2.6678	**3.03**
H(1`B)	3.0093	3.0609	3.0950	3.0991	3.1584	3.0968	3.1477	3.0944	3.1427	3.1012	3.1491	2.7058	2.5710	2.5558	2.5295	2.5291	2.5317	2.5179	2.5339	2.5054	2.5275	2.5185	**3.23**
H(2`-3`A-2`-3`B)	1.5889	1.6489	1.6104	1.6887	1.6526	1.6860	1.6745	1.6833	1.6697	1.6913	1.7016	1.5889	1.6489	1.6104	1.6887	1.6526	1.6860	1.6745	1.6833	1.6697	1.6913	1.7016	**1.77**
H(4`A)	2.7058	2.5710	2.5558	2.5295	2.5291	2.5317	2.5179	2.5339	2.5054	2.5275	2.5185	3.0093	3.0609	3.0950	3.0991	3.1583	3.0968	3.1477	3.0944	3.1426	3.1012	3.1491	**3.03**
H(4`B)	2.7413	2.7309	2.7180	2.7108	2.6715	2.7123	2.6963	2.7136	2.6903	2.7094	2.6678	2.5995	2.6032	2.5768	2.5918	2.5385	2.5929	2.5592	2.5940	2.5572	2.5906	2.5374	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. IV

Nuclei	R											S										Exp. [b]
	BLYP											BLYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.4895	140.9405	141.8206	141.4766	143.2818	141.7006	142.4159	141.4678	142.7930	141.8949	142.8093	139.4895	140.9405	141.8206	141.4766	143.2818	141.7006	142.4159	141.4678	142.7930	141.8949	142.8094	**133.8**
C2	137.2308	137.2081	137.6806	137.0743	137.6665	137.3605	137.9679	137.1854	138.0635	137.4306	138.0853	137.2309	137.2081	137.6806	137.0743	137.6665	137.3603	137.9679	137.1854	138.0635	137.4306	138.0855	**132.1**
C3	120.6710	121.3939	121.9003	121.6308	122.3081	121.8979	122.4734	121.7025	122.5601	122.0037	122.6525	120.6710	121.3939	121.9003	121.6308	122.3081	121.8979	122.4734	121.7025	122.5601	122.0037	122.6525	**115.8**
C4	178.0035	178.9429	179.6390	179.3664	180.2338	179.6209	180.6154	179.4131	180.6222	179.7517	180.8326	178.0034	178.9429	179.6390	179.3664	180.2338	179.6209	180.6156	179.4131	180.6222	179.7517	180.8325	**165.8**
C5	118.8398	119.9843	120.5493	120.5733	121.3733	120.8158	121.4705	120.5966	121.5178	120.9702	121.6972	118.8397	119.9843	120.5493	120.5733	121.3733	120.8159	121.4705	120.5966	121.5178	120.9702	121.6971	**115.8**
C6	133.6979	135.3938	136.4105	136.4593	138.0034	136.6736	138.4632	136.4250	138.3361	136.8823	138.8461	133.6981	135.3938	136.4105	136.4593	138.0034	136.6735	138.4632	136.4250	138.3361	136.8823	138.8460	**132.1**
C7	204.1334	209.0563	210.3744	211.5288	212.6039	211.6372	216.8249	211.2867	216.1919	212.0555	217.9816	204.1331	209.0563	210.3744	211.5288	212.6039	211.6372	216.8248	211.2867	216.1919	212.0555	217.9816	**198.9**
C8	70.4568	71.7688	72.5312	72.3141	73.3438	72.5565	73.7788	72.3363	73.9759	72.7087	74.1628	70.4568	71.7688	72.5312	72.3141	73.3438	72.5565	73.7789	72.3363	73.9759	72.7087	74.1627	**69.3**
C9	41.7168	41.1992	41.3838	40.9811	41.3059	41.2750	41.4199	41.1056	41.5562	41.3276	41.5382	41.7169	41.1992	41.3838	40.9811	41.3059	41.2749	41.4200	41.1056	41.5562	41.3276	41.5381	**31.5**
C10	21.7869	22.2253	22.4724	22.4392	23.0090	22.7070	22.7239	22.5118	22.9092	22.8109	22.9318	21.7868	22.2253	22.4724	22.4392	23.0090	22.7070	22.7239	22.5118	22.9092	22.8109	22.9319	**19.9**
C11	16.4022	16.5324	16.6233	16.5596	16.8485	16.8378	16.6378	16.6535	16.8340	16.9219	16.8955	16.4022	16.5324	16.6233	16.5596	16.8485	16.8378	16.6376	16.6535	16.8340	16.9219	16.8955	**14.3**
C1`	55.2667	56.1003	56.3800	56.5748	57.2181	56.8253	57.0602	56.6135	57.2187	56.9632	57.5578	60.0092	61.1782	61.4954	61.6847	62.2799	61.9321	62.2641	61.7182	62.3281	62.0778	62.6144	**50.6**
C2`	27.7055	28.2445	28.4534	28.4560	28.9441	28.7232	28.8130	28.5280	28.9595	28.8289	28.7854	27.5071	27.7380	28.0254	27.8939	28.5101	28.1587	28.2147	27.9626	28.3738	28.2707	28.0968	**23.8**
C3`	27.5070	27.7380	28.0254	27.8939	28.5101	28.1587	28.2148	27.9626	28.3737	28.2707	28.0969	27.7054	28.2445	28.4534	28.4560	28.9441	28.7232	28.8130	28.5280	28.9595	28.8289	28.7855	**23.8**
C4`	60.0092	61.1782	61.4954	61.6847	62.2799	61.9321	62.2641	61.7182	62.3281	62.0778	62.6144	55.2668	56.1003	56.3800	56.5748	57.2181	56.8254	57.0603	56.6135	57.2187	56.9632	57.5579	**50.6**
H2	8.4452	8.2989	8.3074	8.2267	8.2222	8.2803	8.4224	8.2411	8.2440	8.2758	8.4302	8.4452	8.2989	8.3074	8.2267	8.2222	8.2803	8.4224	8.2411	8.2440	8.2758	8.4302	**8.35**
H3	7.1620	7.2929	7.3792	7.3253	7.4406	7.3718	7.6280	7.3255	7.4527	7.3814	7.6553	7.1620	7.2929	7.3792	7.3253	7.4406	7.3718	7.6280	7.3255	7.4527	7.3814	7.6554	**7.06**
H5	7.0215	7.1808	7.2686	7.2526	7.3763	7.2956	7.5610	7.2461	7.3794	7.3122	7.5916	7.0215	7.1808	7.2686	7.2526	7.3763	7.2956	7.5610	7.2461	7.3794	7.3122	7.5915	**7.06**
H6	7.8520	8.0113	8.0781	8.0933	8.2078	8.1366	8.4230	8.0872	8.2227	8.1523	8.4588	7.8520	8.0113	8.0781	8.0933	8.2078	8.1366	8.4230	8.0872	8.2227	8.1523	8.4588	**8.35**
H8	4.9708	4.9960	4.9983	5.0252	5.0872	5.0703	5.2706	5.0230	5.0792	5.0829	5.2755	4.9709	4.9960	4.9983	5.0252	5.0872	5.0703	5.2706	5.0230	5.0792	5.0829	5.2755	**4.88**
H(9A-9B)	1.7560	1.7720	1.7722	1.7894	1.8023	1.8367	1.9811	1.7910	1.8154	1.8445	2.0196	1.7560	1.7720	1.7722	1.7894	1.8023	1.8367	1.9811	1.7910	1.8154	1.8445	2.0196	**2.05**
H(10A-10B)	1.4824	1.3795	1.3272	1.3243	1.2591	1.3750	1.4434	1.3332	1.2740	1.3768	1.4433	1.4824	1.3795	1.3272	1.3243	1.2591	1.3749	1.4433	1.3332	1.2740	1.3768	1.4433	**1.36**
H(11A-11C)	0.7919	0.7932	0.7650	0.7981	0.7705	0.8451	0.9397	0.7996	0.7702	0.8538	0.9453	0.7919	0.7932	0.7650	0.7981	0.7705	0.8451	0.9397	0.7996	0.7702	0.8538	0.9453	**0.77**
H(1`A)	2.8436	2.8449	2.8146	2.8300	2.7849	2.8784	2.9602	2.8344	2.7940	2.8842	2.9459	2.9651	2.9764	2.9648	2.9564	2.9333	3.0052	3.1045	2.9614	2.9423	3.0104	3.0765	**3.03**
H(1`B)	3.3529	3.3857	3.4292	3.4166	3.4920	3.4617	3.6409	3.4143	3.4686	3.4742	3.6522	3.0272	2.8489	2.8478	2.8158	2.8289	2.8634	2.9652	2.8187	2.8098	2.8710	2.9711	**3.23**
H(2`-3`A-2`-3`B)	1.7331	1.7967	1.7585	1.8321	1.7907	1.8770	1.9768	1.8294	1.8035	1.8898	2.0158	1.7331	1.7967	1.7585	1.8321	1.7907	1.8769	1.9768	1.8294	1.8035	1.8898	2.0158	**1.77**
H(4`A)	3.0272	2.8489	2.8478	2.8158	2.8289	2.8634	2.9652	2.8187	2.8098	2.8710	2.9711	3.3529	3.3857	3.4292	3.4166	3.4920	3.4617	3.6409	3.4143	3.4686	3.4742	3.6522	**3.03**
H(4`B)	2.9651	2.9764	2.9648	2.9564	2.9333	3.0052	3.1045	2.9614	2.9423	3.0104	3.0765	2.8436	2.8449	2.8146	2.8300	2.7849	2.8784	2.9602	2.8344	2.7940	2.8842	2.9460	**3.23**
Nuclei	BMK											BMK										
C1	154.6534	155.3770	156.2661	155.4845	157.3071	155.4687	156.4807	155.6633	156.4569	155.6605	156.6331	154.6534	155.3770	156.2661	155.4846	157.3071	155.4687	156.4808	155.6633	156.4571	155.6605	156.6332	**133.8**
C2	155.3955	155.2632	155.9723	155.0000	155.7846	155.0032	156.0295	155.2173	155.9035	155.1585	155.9990	155.3955	155.2632	155.9723	155.0000	155.7845	155.0032	156.0293	155.2173	155.9035	155.1585	155.9990	**132.1**
C3	135.7205	136.4086	137.1308	136.6235	137.5562	136.5972	137.7878	136.7821	137.6260	136.8093	137.8595	135.7205	136.4086	137.1307	136.6234	137.5561	136.5972	137.7877	136.7821	137.6260	136.8093	137.8595	**115.8**
C4	189.5429	190.1910	190.9701	190.5526	191.4611	190.5142	192.0687	190.6869	191.8115	190.7506	192.1784	189.5429	190.1910	190.9700	190.5526	191.4611	190.5142	192.0687	190.6869	191.8114	190.7506	192.1784	**165.8**
C5	133.4889	134.8487	135.6048	135.5347	136.6482	135.4775	136.8252	135.6314	136.6085	135.7504	136.9992	133.4889	134.8487	135.6048	135.5347	136.6481	135.4775	136.8251	135.6314	136.6083	135.7504	136.9992	**115.8**
C6	151.2332	153.2462	154.6976	154.4747	156.4940	154.3799	157.1556	154.4968	156.7451	154.7267	157.5988	151.2332	153.2462	154.6975	154.4747	156.4940	154.3799	157.1557	154.4968	156.7454	154.7267	157.5988	**132.1**
C7	218.2075	223.1111	224.4657	225.7578	226.4957	225.5858	232.4885	225.6243	230.9674	226.0818	233.6134	218.2075	223.1111	224.4657	225.7578	226.4957	225.5858	232.4889	225.6243	230.9674	226.0818	233.6134	**198.9**
C8	71.9552	73.1264	73.9248	73.6017	74.6842	73.5600	75.3098	73.7290	75.0506	73.8024	75.6986	71.9552	73.1264	73.9249	73.6017	74.6842	73.5600	75.3097	73.7290	75.0506	73.8024	75.6986	**69.3**
C9	40.3028	40.3891	40.8734	40.3098	41.1107	40.3034	41.1837	40.5077	40.9816	40.4769	41.3861	40.3028	40.3891	40.8733	40.3098	41.1107	40.3034	41.1838	40.5077	40.9817	40.4769	41.3861	**31.5**
C10	21.6716	21.8649	22.1771	22.0249	22.6919	21.9982	22.4908	22.1830	22.3842	22.2121	22.5292	21.6716	21.8649	22.1771	22.0249	22.6919	21.9982	22.4909	22.1830	22.3843	22.2121	22.5292	**19.9**
C11	17.3061	17.3558	17.5267	17.3626	17.7488	17.3459	17.6638	17.5405	17.5702	17.5402	17.8322	17.3061	17.3558	17.5267	17.3627	17.7488	17.3459	17.6637	17.5405	17.5701	17.5402	17.8322	**14.3**
C1`	56.1424	56.8316	57.0621	57.1837	57.7854	57.1449	57.6152	57.3174	57.5088	57.3823	57.8793	60.6063	61.1573	61.6448	61.5063	62.1935	61.4670	62.2916	61.6396	62.1398	61.7055	62.4755	**50.6**
C2`	27.9938	28.1017	28.4391	28.2214	28.7603	28.1972	28.7515	28.3843	28.6356	28.4061	28.6534	27.3938	27.4030	27.7553	27.4792	28.0904	27.4554	27.9646	27.6433	27.8760	27.6637	27.9093	**23.8**
C3`	27.3938	27.4030	27.7552	27.4792	28.0903	27.4554	27.9647	27.6433	27.8760	27.6637	27.9093	27.9938	28.1017	28.4390	28.2213	28.7602	28.1972	28.7515	28.3843	28.6357	28.4061	28.6534	**23.8**
C4`	60.6063	61.1573	61.6448	61.5064	62.1937	61.4670	62.2914	61.6396	62.1399	61.7055	62.4755	56.1424	56.8316	57.0621	57.1838	57.7853	57.1449	57.6152	57.3174	57.5088	57.3823	57.8793	**50.6**
H2	9.0281	9.0099	9.0311	8.9772	8.9787	8.9761	8.9822	8.9750	8.9942	8.9687	8.9805	9.0281	9.0099	9.0311	8.9772	8.9787	8.9761	8.9822	8.9750	8.9941	8.9687	8.9805	**8.35**
H3	7.6171	7.7670	7.8548	7.8236	7.9447	7.8175	7.9730	7.8114	7.9625	7.8197	7.9954	7.6171	7.7670	7.8548	7.8236	7.9447	7.8175	7.9730	7.8114	7.9625	7.8197	7.9954	**7.06**
H5	7.4753	7.6779	7.7714	7.7700	7.9009	7.7615	7.9155	7.7530	7.9049	7.7685	7.9448	7.4753	7.6779	7.7714	7.7700	7.9008	7.7615	7.9155	7.7530	7.9049	7.7685	7.9448	**7.06**
H6	8.4133	8.5826	8.6802	8.6993	8.8327	8.6883	8.8889	8.6774	8.8682	8.7002	8.9186	8.4133	8.5826	8.6801	8.6993	8.8327	8.6883	8.8889	8.6774	8.8682	8.7002	8.9186	**8.35**
H8	4.4185	4.4927	4.5162	4.5629	4.6190	4.5545	4.6848	4.5462	4.6656	4.5615	4.6923	4.4185	4.4927	4.5162	4.5629	4.6190	4.5545	4.6848	4.5462	4.6656	4.5615	4.6923	**4.88**
H(9A-9B)	1.5971	1.6659	1.6759	1.7171	1.7479	1.7108	1.7421	1.7046	1.7346	1.7135	1.7968	1.5971	1.6659	1.6759	1.7171	1.7479	1.7108	1.7421	1.7046	1.7347	1.7135	1.7968	**2.05**
H(10A-10B)	1.3590	1.2180	1.1675	1.1566	1.0821	1.1572	1.0949	1.1579	1.1006	1.1464	1.0896	1.3590	1.2180	1.1674	1.1566	1.0821	1.1572	1.0950	1.1579	1.1006	1.1464	1.0896	**1.36**
H(11A-11C)	0.7078	0.7018	0.6697	0.7167	0.6735	0.7124	0.6766	0.7082	0.6783	0.7113	0.6762	0.7078	0.7018	0.6697	0.7167	0.6735	0.7124	0.6766	0.7082	0.6783	0.7113	0.6762	**0.77**
H(1`A)	2.6301	2.6339	2.6096	2.6281	2.5782	2.6256	2.5917	2.6230	2.5932	2.6210	2.5734	2.7678	2.7734	2.7516	2.7599	2.7104	2.7579	2.7352	2.7559	2.7374	2.7522	2.7047	**3.03**
H(1`B)	3.0373	3.0825	3.1037	3.1266	3.1785	3.1207	3.1629	3.1147	3.1598	3.1227	3.1748	2.7095	2.6167	2.5903	2.5819	2.5835	2.5809	2.5512	2.5798	2.5522	2.5733	2.5453	**3.23**
H(2`-3`A-2`-3`B)	1.6204	1.6842	1.6398	1.7230	1.6644	1.7172	1.6860	1.7116	1.6825	1.7189	1.7056	1.6204	1.6842	1.6398	1.7230	1.6644	1.7172	1.6860	1.7116	1.6825	1.7189	1.7056	**1.77**
H(4`A)	2.7095	2.6167	2.5903	2.5819	2.5835	2.5809	2.5512	2.5798	2.5522	2.5733	2.5453	3.0373	3.0825	3.1037	3.1266	3.1785	3.1207	3.1629	3.1147	3.1598	3.1227	3.1748	**3.03**
H(4`B)	2.7678	2.7734	2.7516	2.7599	2.7104	2.7579	2.7353	2.7559	2.7374	2.7522	2.7047	2.6301	2.6339	2.6096	2.6281	2.5782	2.6256	2.5917	2.6230	2.5932	2.6210	2.5734	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. V

Nuclei	R											S										Exp. [b]
	BP86																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.1786	137.4302	137.9541	138.0013	139.8617	137.9889	139.5122	137.9709	139.3793	138.0084	140.0217	136.1786	137.4302	137.9541	138.0013	139.8616	137.9889	139.5123	137.9709	139.3793	138.0085	140.0217	**133.8**
C2	135.9369	136.0084	136.5965	135.8244	136.3954	135.8439	136.7969	135.8582	136.7385	135.8011	136.9677	135.9369	136.0084	136.5965	135.8244	136.3953	135.8439	136.7969	135.8582	136.7385	135.8011	136.9676	**132.1**
C3	119.5269	120.4467	120.9587	120.6876	121.3566	120.6849	121.7048	120.6766	121.6379	120.6847	121.9711	119.5269	120.4467	120.9587	120.6876	121.3565	120.6849	121.7048	120.6766	121.6379	120.6848	121.9710	**115.8**
C4	174.5696	175.5902	176.2076	175.9912	176.7401	175.9767	177.2974	175.9567	177.1827	176.0000	177.5836	174.5696	175.5902	176.2076	175.9912	176.7401	175.9767	177.2974	175.9567	177.1827	176.0001	177.5836	**165.8**
C5	117.7171	119.1506	119.7207	119.7697	120.5353	119.7402	120.7953	119.7055	120.6965	119.7929	121.1037	117.7171	119.1506	119.7207	119.7697	120.5354	119.7402	120.7953	119.7055	120.6965	119.7929	121.1037	**115.8**
C6	132.3618	134.2536	135.3367	135.1946	136.5907	135.1390	137.1393	135.0789	136.9019	135.2426	137.5755	132.3618	134.2536	135.3367	135.1946	136.5909	135.1390	137.1393	135.0789	136.9019	135.2426	137.5755	**132.1**
C7	201.3079	205.8618	206.8684	208.2537	209.3563	208.1242	213.8087	207.9894	212.5909	208.3731	215.0760	201.3079	205.8618	206.8684	208.2537	209.3563	208.1242	213.8087	207.9894	212.5909	208.3732	215.0761	**198.9**
C8	68.1155	69.5553	70.3110	70.2031	71.1644	70.16753	71.9112	70.1279	71.5380	70.2338	72.4855	68.1155	69.5553	70.3110	70.2031	71.1644	70.1675	71.9112	70.1279	71.5380	70.2338	72.4856	**69.3**
C9	40.3458	40.2327	40.4918	39.9769	40.1549	39.9964	40.3724	40.0111	40.2032	39.9541	40.6324	40.3458	40.2327	40.4918	39.9769	40.1549	39.9964	40.3723	40.0111	40.2032	39.9540	40.6324	**31.5**
C10	20.2946	20.8624	21.1245	21.0746	21.4590	21.0670	21.3752	21.0543	21.3076	21.0770	21.7363	20.2946	20.8624	21.1245	21.0746	21.4590	21.0670	21.3752	21.0543	21.3076	21.0770	21.7363	**19.9**
C11	15.9373	16.2103	16.2545	16.2021	16.3361	16.2098	16.2955	16.2125	16.2756	16.1902	16.6361	15.9373	16.2100	16.2545	16.2021	16.3361	16.2098	16.2955	16.2125	16.2756	16.1901	16.6361	**14.3**
C1`	53.7507	54.6651	54.8659	55.1290	55.5805	55.1072	55.5538	55.0804	55.5136	55.1448	56.2217	58.2906	59.4655	59.7520	59.9494	60.4426	59.9283	60.6372	59.9023	60.6067	59.9648	61.0456	**50.6**
C2`	26.2286	26.8185	27.0524	27.0028	27.3646	26.9978	27.4093	26.9879	27.3628	27.0030	27.4314	25.8079	26.1594	26.3791	26.2600	26.7272	26.2630	26.6575	26.2604	26.6605	26.2520	26.6671	**23.8**
C3`	25.8079	26.1594	26.3791	26.2600	26.7272	26.2630	26.6576	26.2604	26.6605	26.2519	26.6670	26.2286	26.8185	27.0524	27.0027	27.3646	26.9978	27.4093	26.9879	27.3628	27.0030	27.4315	**23.8**
C4`	58.2906	59.4655	59.7520	59.9494	60.4426	59.9283	60.6372	59.9023	60.6067	59.9648	61.0455	53.7507	54.6651	54.8659	55.1290	55.5805	55.1072	55.5537	55.0804	55.5134	55.1448	56.2218	**50.6**
H2	8.5222	8.4073	8.4412	8.3257	8.2874	8.3303	8.2897	8.3345	8.3026	8.3211	8.2924	8.5222	8.4073	8.4412	8.3257	8.2874	8.3303	8.2897	8.3345	8.3026	8.3211	8.2924	**8.35**
H3	7.1721	7.3156	7.3926	7.3613	7.4701	7.3599	7.4869	7.3582	7.4789	7.3621	7.5176	7.1721	7.3156	7.3926	7.3613	7.4701	7.3599	7.4869	7.3582	7.4789	7.3621	7.5176	**7.06**
H5	7.0215	7.2046	7.2873	7.2785	7.3923	7.2749	7.4064	7.2710	7.3950	7.2815	7.4377	7.0215	7.2046	7.2873	7.2785	7.3923	7.2749	7.4064	7.2710	7.3950	7.2815	7.4377	**7.06**
H6	7.9345	8.0936	8.1585	8.1734	8.2683	8.1689	8.3003	8.1642	8.2934	8.1772	8.3329	7.9345	8.0936	8.1585	8.1734	8.2683	8.1689	8.3003	8.1642	8.2934	8.1772	8.3329	**8.35**
H8	4.9786	5.0072	4.9965	5.0223	5.0748	5.0222	5.0960	5.0218	5.0943	5.0220	5.1034	4.9786	5.0072	4.9965	5.0223	5.0748	5.0222	5.0960	5.0218	5.0943	5.0220	5.1034	**4.88**
H(9A-9B)	1.8488	1.8885	1.8978	1.9030	1.8797	1.9015	1.8704	1.8998	1.8573	1.9042	1.9128	1.8488	1.8885	1.8978	1.9030	1.8797	1.9015	1.8704	1.8998	1.8573	1.9042	1.9128	**2.05**
H(10A-10B)	1.4788	1.3707	1.3093	1.3055	1.2278	1.3108	1.2423	1.3156	1.2507	1.3001	1.2427	1.4788	1.3707	1.3093	1.3055	1.2278	1.3108	1.2423	1.3156	1.2507	1.3001	1.2427	**1.36**
H(11A-11C)	0.7611	0.7670	0.7306	0.7691	0.7268	0.7696	0.7253	0.7699	0.7295	0.7683	0.7306	0.7611	0.7670	0.7306	0.7691	0.7268	0.7696	0.7253	0.7699	0.7295	0.7683	0.7306	**0.77**
H(1`A)	2.7940	2.8077	2.7772	2.7956	2.7436	2.7973	2.7499	2.7988	2.7481	2.7935	2.7342	2.9160	2.9279	2.9077	2.9136	2.8800	2.9153	2.8907	2.9169	2.8878	2.9115	2.8660	**3.03**
H(1`B)	3.3743	3.4038	3.4287	3.4274	3.4813	3.4263	3.4567	3.4250	3.4547	3.4281	3.4648	3.0722	2.8996	2.8654	2.8446	2.8443	2.8486	2.8084	2.8523	2.7966	2.8406	2.8085	**3.23**
H(2`-3`A-2`-3`B)	1.7277	1.7852	1.7366	1.8209	1.7709	1.8195	1.7901	1.8179	1.7869	1.8218	1.8340	1.7277	1.7852	1.7366	1.8209	1.7709	1.8195	1.7901	1.8179	1.7869	1.8218	1.8340	**1.77**
H(4`A)	3.0722	2.8996	2.8654	2.8446	2.8443	2.8486	2.8083	2.8523	2.7966	2.8406	2.8085	3.3743	3.4038	3.4287	3.4274	3.4813	3.4263	3.4567	3.4249	3.4547	3.4281	3.4648	**3.03**
H(4`B)	2.9160	2.9279	2.9077	2.9135	2.8800	2.9153	2.8907	2.9169	2.8878	2.9115	2.8660	2.7940	2.8077	2.7772	2.7956	2.7436	2.7973	2.7499	2.7987	2.7481	2.7935	2.7342	**3.23**
Nuclei	CAM-B3LYP																						
C1	140.9266	141.9077	142.5773	142.5860	144.7771	142.5347	144.2091	142.4721	144.1884	142.6310	144.5927	140.9266	141.9077	142.5773	142.5860	144.7771	142.5347	144.2091	142.4721	144.1884	142.6311	144.5927	**133.8**
C2	142.4301	142.3674	142.8646	142.2220	142.7350	142.2354	143.1452	142.2494	143.0878	142.2115	143.1534	142.4302	142.3674	142.8647	142.2220	142.7350	142.2355	143.1452	142.2494	143.0878	142.2115	143.1534	**132.1**
C3	123.8296	124.5019	125.0076	124.7106	125.4095	124.7045	125.6498	124.6974	125.5900	124.7176	125.7386	123.8297	124.5019	125.0076	124.7106	125.4095	124.7045	125.6498	124.6974	125.5900	124.7176	125.7386	**115.8**
C4	177.7516	178.4670	179.0444	178.8161	179.4341	178.7999	180.0116	178.7844	179.8802	178.8335	180.1274	177.7516	178.4670	179.0445	178.8160	179.4341	178.7999	180.0116	178.7844	179.8802	178.8334	180.1274	**165.8**
C5	121.8071	123.1309	123.6904	123.7994	124.6335	123.7627	124.8019	123.7254	124.7039	123.8356	124.9632	121.8071	123.1309	123.6903	123.7994	124.6335	123.7627	124.8019	123.7254	124.7039	123.8356	124.9632	**115.8**
C6	138.5574	140.4016	141.5123	141.3473	142.6341	141.2957	143.1895	141.2504	142.9402	141.4012	143.4541	138.5573	140.4016	141.5124	141.3473	142.6341	141.2957	143.1895	141.2504	142.9402	141.4012	143.4541	**132.1**
C7	206.2278	211.3109	212.3833	214.3098	215.3800	214.1127	221.0719	213.9048	219.6673	214.4947	222.2973	206.2279	211.3109	212.3833	214.3098	215.3800	214.1126	221.0719	213.9048	219.6673	214.4946	222.2973	**198.9**
C8	64.5921	65.7432	66.3737	66.4216	67.3595	66.3724	68.0155	66.3227	67.7673	66.4708	68.4288	64.5920	65.7432	66.3736	66.4216	67.3595	66.3724	68.0155	66.3227	67.7673	66.4709	68.4288	**69.3**
C9	36.9478	36.6632	36.8498	36.3985	36.6277	36.4198	36.6461	36.4449	36.5829	36.3826	36.6973	36.9479	36.6632	36.8498	36.3985	36.6277	36.4198	36.6461	36.4449	36.5829	36.3826	36.6973	**31.5**
C10	18.7015	19.1547	19.3875	19.3798	19.8399	19.3691	19.7280	19.3600	19.6927	19.3928	19.8728	18.7015	19.1547	19.3877	19.3798	19.8399	19.3691	19.7280	19.3600	19.6927	19.3928	19.8728	**19.9**
C11	15.6830	15.8449	15.9294	15.8751	16.1201	15.8770	16.0640	15.8796	16.0619	15.8757	16.2245	15.6831	15.8449	15.9294	15.8751	16.1201	15.8770	16.0640	15.8796	16.0619	15.8757	16.2245	**14.3**
C1`	50.8424	51.6920	51.9176	52.2185	52.7669	52.1897	52.7350	52.1604	52.6956	52.2476	53.2350	55.1496	56.0994	56.4320	56.6051	57.1606	56.5753	57.2952	56.5453	57.2367	56.6353	57.5631	**50.6**
C2`	25.0081	25.3772	25.6412	25.5596	25.9829	25.5500	26.0119	25.5411	25.9771	25.5711	25.8584	24.4589	24.6447	24.9269	24.7551	25.2974	24.7521	25.2056	24.7489	25.2002	24.7595	25.0505	**23.8**
C3`	24.4590	24.6447	24.9269	24.7551	25.2974	24.7521	25.2056	24.7489	25.2002	24.7595	25.0505	25.0080	25.3772	25.6413	25.5596	25.9829	25.5500	26.0119	25.5411	25.9771	25.5711	25.8584	**23.8**
C4`	55.1496	56.0994	56.4319	56.6051	57.1606	56.5753	57.2952	56.5453	57.2367	56.6353	57.5631	50.8424	51.6920	51.9176	52.2185	52.7669	52.1897	52.7350	52.1604	52.6956	52.2475	53.2350	**50.6**
H2	8.8110	8.6933	8.7294	8.5958	8.5502	8.6033	8.5477	8.6122	8.5611	8.5891	8.5304	8.8110	8.6933	8.7294	8.5958	8.5502	8.6033	8.5477	8.6122	8.5611	8.5891	8.5304	**8.35**
H3	7.4020	7.5341	7.6236	7.5769	7.6964	7.5750	7.7136	7.5731	7.7065	7.5786	7.7287	7.4020	7.5341	7.6236	7.5769	7.6964	7.5750	7.7136	7.5731	7.7065	7.5787	7.7287	**7.06**
H5	7.2447	7.4318	7.5220	7.5115	7.6341	7.5072	7.6476	7.5030	7.6363	7.5156	7.6673	7.2447	7.4318	7.5220	7.5115	7.6341	7.5072	7.6476	7.5030	7.6363	7.5156	7.6673	**7.06**
H6	8.0643	8.2435	8.3388	8.3319	8.4473	8.3272	8.4891	8.3231	8.4735	8.3365	8.5103	8.0643	8.2435	8.3388	8.3319	8.4473	8.3272	8.4891	8.3231	8.4735	8.3365	8.5103	**8.35**
H8	4.4117	4.4875	4.5224	4.5293	4.6167	4.5270	4.6653	4.5250	4.6500	4.5314	4.6575	4.4117	4.4875	4.5223	4.5293	4.6167	4.5270	4.6653	4.5250	4.6500	4.5314	4.6575	**4.88**
H(9A-9B)	1.6498	1.6930	1.6991	1.7084	1.6888	1.7077	1.6717	1.7081	1.6678	1.7093	1.6955	1.6498	1.6930	1.6992	1.7084	1.6888	1.7077	1.6717	1.7081	1.6678	1.7093	1.6955	**2.05**
H(10A-10B)	1.3768	1.2583	1.2118	1.1889	1.1200	1.1937	1.1412	1.1987	1.1473	1.1841	1.1304	1.3768	1.2583	1.2118	1.1889	1.1200	1.1937	1.1412	1.1987	1.1473	1.1841	1.1304	**1.36**
H(11A-11C)	0.7876	0.7903	0.7657	0.7934	0.7565	0.7934	0.7583	0.7936	0.7608	0.7933	0.7499	0.7876	0.7903	0.7657	0.7934	0.7565	0.7934	0.7583	0.7936	0.7608	0.7933	0.7499	**0.77**
H(1`A)	2.7019	2.7060	2.6841	2.6921	2.6466	2.6933	2.6608	2.6946	2.6608	2.6910	2.6344	2.8328	2.8275	2.8147	2.8678	2.7833	2.8142	2.7969	2.8152	2.7949	2.8123	2.6344	**3.03**
H(1`B)	3.1157	3.1616	3.1954	3.1924	3.2559	3.1904	3.2396	3.1887	3.2361	3.1944	3.2401	2.8021	2.6732	2.6438	2.6969	2.6568	2.6379	2.6216	2.6393	2.6170	2.6352	2.3401	**3.23**
H(2`-3`A-2`-3`B)	1.6571	1.7174	1.6802	1.7585	1.7196	1.7559	1.7423	1.7532	1.7374	1.7609	1.7694	1.6571	1.7174	1.6802	1.7585	1.7196	1.7559	1.7423	1.7532	1.7374	1.7609	1.7694	**1.77**
H(4`A)	2.8021	2.6732	2.6438	2.6365	2.6568	2.6379	2.6216	2.6393	2.6170	2.6352	2.6152	3.1157	3.1616	3.1954	3.2485	3.2559	3.1904	3.2396	3.1887	3.2361	3.1944	2.6152	**3.03**
H(4`B)	2.8328	2.8275	2.8147	2.8132	2.7833	2.8142	2.7969	2.8152	2.7949	2.8123	2.7637	2.7018	2.7060	2.6841	2.7372	2.6466	2.6933	2.6608	2.6946	2.6608	2.6910	2.7637	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. VI

Nuclei	R											S										Exp. [b]
	HF											HF										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.4414	137.5014	138.4538	138.1924	139.8150	138.1346	138.8330	138.0750	138.9018	138.2468	139.1504	136.4413	137.5014	138.4538	138.1924	139.8150	138.1346	138.8330	138.0750	138.9018	138.2467	139.1504	**133.8**
C2	144.4173	144.1728	144.6114	143.8967	144.2996	143.9185	144.8354	143.9409	144.7479	143.8757	144.8310	144.4173	144.1728	144.6114	143.8966	144.2996	143.9185	144.8354	143.9410	144.7479	143.8756	144.8310	**132.1**
C3	120.4744	121.0412	121.5064	121.1750	121.7383	121.1678	121.7760	121.1606	121.7557	121.1812	121.8450	120.4744	121.0412	121.5064	121.1750	121.7383	121.1678	121.7758	121.1606	121.7557	121.1811	121.8450	**115.8**
C4	171.1128	171.6055	172.1010	171.8031	172.3125	171.7947	173.0265	171.7874	172.8557	171.8108	173.1462	171.1128	171.6055	172.1010	171.8031	172.3125	171.7947	173.0265	171.7874	172.8556	171.8109	173.1462	**165.8**
C5	117.8496	119.1488	119.7030	119.7919	120.5418	119.7519	120.5591	119.7121	120.4895	119.8285	120.7326	117.8497	119.1488	119.7030	119.7919	120.5418	119.7519	120.5591	119.7121	120.4895	119.8286	120.7326	**115.8**
C6	140.0136	141.4903	142.3589	142.3541	143.6752	142.3088	144.4959	142.2651	144.2248	142.3962	144.7347	140.0135	141.4903	142.3589	142.3541	143.6752	142.3088	144.4962	142.2651	144.2248	142.3963	144.7347	**132.1**
C7	196.4495	202.1767	203.4250	205.4842	205.5403	205.2643	212.4997	205.0429	210.7934	205.6921	213.6871	196.4499	202.1767	203.4250	205.4842	205.5403	205.2643	212.4997	205.0433	210.7933	205.6921	213.6871	**198.9**
C8	55.7145	56.6022	56.9914	57.2558	57.7427	57.2041	58.5143	57.1519	58.3197	57.3033	58.7602	55.7144	56.6022	56.9914	57.2558	57.7427	57.2041	58.5142	57.1519	58.3197	57.3033	58.7602	**69.3**
C9	31.1481	30.5519	30.6807	30.3496	30.5631	30.3610	30.5462	30.3731	30.5463	30.3374	30.5372	31.1481	30.5519	30.6807	30.3496	30.5631	30.3610	30.5462	30.3731	30.5463	30.3374	30.5372	**31.5**
C10	16.7291	17.0912	17.3419	17.3136	17.7681	17.3011	17.6649	17.2889	17.6541	17.3243	17.7400	16.7292	17.0912	17.3419	17.3136	17.7681	17.3011	17.6649	17.2889	17.6541	17.3243	17.7400	**19.9**
C11	15.7593	15.8051	15.9437	15.8378	16.0843	15.8359	16.0348	15.8345	16.0336	15.8389	16.1539	15.7593	15.8051	15.9437	15.8378	16.0843	15.8359	16.0347	15.8345	16.0337	15.8389	16.1539	**14.3**
C1`	44.6427	45.3307	45.6608	45.8037	46.3013	45.7713	46.3321	45.7393	46.3006	45.8335	46.6765	48.5403	49.4088	49.6458	49.8163	50.2686	49.7920	50.3671	49.7682	50.3017	49.8388	50.6134	**50.6**
C2`	22.8166	23.0703	23.2952	23.1618	23.5813	23.1542	23.5742	23.1472	23.5602	23.1685	23.4000	22.2001	22.2972	22.6394	22.3564	22.9166	22.3503	22.7594	22.3451	22.7610	22.3622	22.5826	**23.8**
C3`	22.2001	22.2972	22.6394	22.3564	22.9166	22.3503	22.7594	22.3451	22.7610	22.3623	22.5826	22.8167	23.0703	23.2952	23.1618	23.5813	23.1542	23.5741	23.1472	23.5603	23.1686	23.4000	**23.8**
C4`	48.5403	49.4088	49.6459	49.8163	50.2686	49.7920	50.3671	49.7682	50.3017	49.8388	50.6134	44.6427	45.3307	45.6608	45.8037	46.3013	45.7713	46.3320	45.7393	46.3005	45.8336	46.6765	**50.6**
H2	9.0786	8.9268	8.9429	8.8084	8.8374	8.8178	8.8458	8.8273	8.8538	8.7996	8.8299	9.0786	8.9268	8.9429	8.8084	8.8374	8.8178	8.8458	8.8273	8.8538	8.7996	8.8299	**8.35**
H3	7.4354	7.5749	7.6671	7.6176	7.7395	7.6155	7.7519	7.6132	7.7449	7.6195	7.7676	7.4354	7.5749	7.6671	7.6176	7.7395	7.6155	7.7519	7.6132	7.7449	7.6195	7.7676	**7.06**
H5	7.2468	7.4451	7.5351	7.5315	7.6597	7.5266	7.6705	7.5215	7.6586	7.5362	7.6954	7.2468	7.4451	7.5351	7.5315	7.6597	7.5266	7.6705	7.5215	7.6586	7.5362	7.6954	**7.06**
H6	8.1005	8.3206	8.4139	8.4235	8.5927	8.4182	8.6446	8.4128	8.6190	8.4287	8.6771	8.1005	8.3206	8.4139	8.4235	8.5927	8.4182	8.6446	8.4128	8.6190	8.4287	8.6771	**8.35**
H8	3.6317	3.7654	3.8157	3.8310	3.9676	3.8272	4.0131	3.8234	3.9840	3.8350	4.0129	3.6316	3.7654	3.8157	3.8310	3.9676	3.8272	4.0131	3.8234	3.9840	3.8350	4.0129	**4.88**
H(9A-9B)	1.3010	1.3077	1.2916	1.3310	1.3204	1.3300	1.3347	1.3288	1.3337	1.3319	1.3499	1.3011	1.3077	1.2916	1.3310	1.3204	1.3300	1.3347	1.3288	1.3337	1.3319	1.3499	**2.05**
H(10A-10B)	1.2641	1.1347	1.1014	1.0575	1.0030	1.0626	1.0110	1.0677	1.0121	1.0529	1.0039	1.2641	1.1347	1.1014	1.0575	1.0030	1.0626	1.0110	1.0677	1.0121	1.0529	1.0039	**1.36**
H(11A-11C)	0.7647	0.7639	0.7366	0.7661	0.7356	0.7661	0.7378	0.7660	0.7370	0.7664	0.7334	0.7647	0.7639	0.7366	0.7661	0.7356	0.7661	0.7378	0.7660	0.7369	0.7664	0.7334	**0.77**
H(1`A)	2.3641	2.3616	2.3365	2.3490	2.2936	2.3501	2.3189	2.3510	2.3168	2.3479	2.3034	2.5251	2.5114	2.4900	2.4891	3.2500	2.4901	2.4669	2.4909	2.4667	2.4882	2.4403	**3.03**
H(1`B)	2.7108	2.7752	2.8023	2.8177	2.8790	2.8150	2.8770	2.8121	2.8700	2.8205	2.8850	2.3756	2.2648	2.2718	2.2718	3.1235	2.2702	2.2526	2.2682	2.2516	2.2734	2.2573	**3.23**
H(2`-3`A-2`-3`B)	1.4360	1.5100	1.4737	1.5555	1.5080	1.5525	1.5289	1.5493	1.5214	1.5585	1.5547	1.4360	1.5100	1.4737	1.5555	1.5080	1.5525	1.5289	1.5493	1.5214	1.5585	1.5547	**1.77**
H(4`A)	2.3756	2.2648	2.2718	2.2718	2.2686	2.2702	2.2526	2.2682	2.2516	2.2734	2.2573	2.7108	2.7752	2.8023	2.8177	3.7226	2.8150	2.8770	2.8121	2.8699	2.8205	2.8850	**3.03**
H(4`B)	2.5251	2.5114	2.4900	2.4891	2.4394	2.4901	2.4669	2.4909	2.4667	2.4882	2.4403	2.3641	2.3616	2.3365	2.3490	3.1133	2.3501	2.3189	2.3510	2.3168	2.3479	2.3034	**3.23**
Nuclei	LC-BLYP											LC-BLYP										
C1	144.3308	145.4927	145.9944	145.9621	147.5542	145.9028	147.5626	145.8745	147.6800	146.0056	147.9719	144.3308	145.4927	145.9944	145.9622	147.5543	145.9028	147.5626	145.8746	147.6800	146.0056	147.9719	**133.8**
C2	148.6152	148.4676	149.0028	148.3230	148.8404	148.3132	149.2150	148.3305	149.1034	148.3145	149.1965	148.6152	148.4676	149.0029	148.3231	148.8407	148.3134	149.2150	148.3305	149.1034	148.3144	149.1965	**132.1**
C3	128.3178	128.9172	129.5180	129.1317	129.8023	129.0994	130.0812	129.0944	130.0300	129.1448	130.1620	128.3178	128.9172	129.5179	129.1316	129.8022	129.0994	130.0812	129.0944	130.0300	129.1448	130.1620	**115.8**
C4	181.9593	182.4590	183.1240	182.8206	183.3714	182.7772	183.9613	182.7607	183.7961	182.8441	184.0537	181.9593	182.4589	183.1240	182.8206	183.3713	182.7771	183.9613	182.7607	183.7961	182.8441	184.0537	**165.8**
C5	126.1620	127.4795	128.1520	128.2178	129.0591	128.1494	129.3479	128.1085	129.2485	128.2663	129.5150	126.1620	127.4795	128.1521	128.2178	129.0590	128.1492	129.3479	128.1085	129.2485	128.2664	129.5150	**115.8**
C6	144.4002	146.1413	147.4579	147.2869	148.8967	147.1981	149.0477	147.1351	148.7769	147.3519	149.3759	144.4002	146.1413	147.4579	147.2869	148.8966	147.1981	149.0477	147.1351	148.7769	147.3519	149.3759	**132.1**
C7	211.8618	217.4555	218.3176	220.4747	220.8255	220.2563	227.5439	220.0688	226.2474	220.6703	228.8976	211.8618	217.4554	218.3177	220.4747	220.8259	220.2563	227.5439	220.0688	226.2474	220.6702	228.8976	**198.9**
C8	62.4870	63.7764	64.1570	64.4288	65.1947	64.3660	65.8352	64.3316	65.6756	64.4723	66.4294	62.4870	63.7763	64.1570	64.4288	65.1947	64.3660	65.8352	64.3316	65.6756	64.4724	66.4294	**69.3**
C9	34.7784	34.4106	34.6278	34.2412	34.6042	34.2354	34.3458	34.2557	34.3082	34.2282	34.4958	34.7784	34.4106	34.6278	34.2412	34.6042	34.2354	34.3458	34.2557	34.3082	34.2283	34.4958	**31.5**
C10	16.5821	16.9598	17.2502	17.2282	17.7410	17.1911	17.5454	17.1812	17.5103	17.2458	17.7072	16.5821	16.9599	17.2502	17.2282	17.7410	17.1911	17.5454	17.1812	17.5103	17.2458	17.7072	**19.9**
C11	14.7041	14.7757	14.9360	14.8361	15.0888	14.8116	15.0340	14.8143	15.0234	14.8420	15.1917	14.7041	14.7758	14.9361	14.8361	15.0890	14.8115	15.0340	14.8143	15.0234	14.8421	15.1917	**14.3**
C1`	48.8010	49.6372	49.8785	50.1433	50.7500	50.0896	50.7271	50.0633	50.6647	50.1774	51.1918	52.7051	53.6090	53.9949	54.1344	54.6609	54.0789	54.8308	54.0513	54.7470	54.1705	55.1182	**50.6**
C2`	23.0101	23.2872	23.5583	23.4621	23.8479	23.4292	23.8490	23.4240	23.8258	23.4762	23.7763	22.3692	22.4486	22.8208	22.5763	23.0537	22.5459	23.0058	22.5430	23.0003	22.5881	22.8821	**23.8**
C3`	22.3692	22.4485	22.8208	22.5763	23.0537	22.5459	23.0058	22.5430	23.0003	22.5881	22.8821	23.0101	23.2872	23.5583	23.4621	23.8479	23.4293	23.8490	23.4240	23.8258	23.4761	23.7763	**23.8**
C4`	52.7051	53.6090	53.9949	54.1345	54.6610	54.0790	54.8308	54.0513	54.7469	54.1704	55.1181	48.8010	49.6372	49.8785	50.1433	50.7501	50.0895	50.7271	50.0633	50.6647	50.1774	51.1918	**50.6**
H2	9.0106	8.8554	8.9239	8.7786	8.7921	8.7835	8.7327	8.7896	8.7301	8.7725	8.7058	9.0106	8.8554	8.9239	8.7786	8.7921	8.7835	8.7327	8.7896	8.7301	8.7725	8.7058	**8.35**
H3	7.5456	7.6744	7.7676	7.7156	7.8350	7.7128	7.8538	7.7115	7.8461	7.7173	7.8696	7.5456	7.6744	7.7676	7.7156	7.8350	7.7128	7.8538	7.7115	7.8461	7.7172	7.8696	**7.06**
H5	7.3903	7.5763	7.6702	7.6619	7.7870	7.6561	7.8016	7.6518	7.7910	7.6665	7.8251	7.3903	7.5763	7.6702	7.6619	7.7870	7.6561	7.8016	7.6518	7.7910	7.6665	7.8251	**7.06**
H6	8.2180	8.3832	8.5114	8.4895	8.6346	8.4823	8.6528	8.4765	8.6305	8.4952	8.6741	8.2180	8.3832	8.5114	8.4895	8.6346	8.4823	8.6528	8.4765	8.6305	8.4952	8.6741	**8.35**
H8	4.2014	4.2699	4.3515	4.3370	4.4203	4.3314	4.5040	4.3275	4.4802	4.3412	4.5025	4.2014	4.2699	4.3515	4.3370	4.4203	4.3314	4.5040	4.3275	4.4802	4.3412	4.5025	**4.88**
H(9A-9B)	1.6373	1.6762	1.6736	1.7038	1.7253	1.7020	1.6446	1.7016	1.6394	1.7042	1.6801	1.6373	1.6762	1.6736	1.7038	1.7253	1.7020	1.6446	1.7016	1.6394	1.7042	1.6801	**2.05**
H(10A-10B)	1.3285	1.1875	1.1641	1.1190	1.0512	1.1224	1.0751	1.1274	1.0779	1.1147	1.0602	1.3285	1.1875	1.1641	1.1190	1.0512	1.1224	1.0751	1.1274	1.0779	1.1147	1.0602	**1.36**
H(11A-11C)	0.7838	0.7781	0.7632	0.7853	0.7488	0.7840	0.7460	0.7842	0.7463	0.7855	0.7370	0.7838	0.7782	0.7632	0.7853	0.7488	0.7840	0.7460	0.7842	0.7463	0.7855	0.7370	**0.77**
H(1`A)	2.6651	2.6587	2.6432	2.6437	2.5949	2.6441	2.6105	2.6461	2.6116	2.6423	2.5894	2.7943	2.7946	2.7650	2.7789	2.7365	2.7790	2.7481	2.7808	2.7503	2.7776	2.7269	**3.03**
H(1`B)	3.0078	3.0469	3.0820	3.0813	3.1389	3.0782	3.1224	3.0768	3.1178	3.0832	3.1257	2.7241	2.6071	2.6432	2.6437	2.5949	2.6441	2.6105	2.6461	2.6116	2.6423	2.5894	**3.23**
H(2`-3`A-2`-3`B)	1.6440	1.7039	1.6686	1.7445	1.6993	1.7408	1.7320	1.7388	1.7255	1.7470	1.7576	1.6440	1.7040	1.6686	1.7445	1.6993	1.7408	1.7320	1.7388	1.7255	1.7470	1.7576	**1.77**
H(4`A)	2.7241	2.6071	2.5460	2.5645	2.5576	2.5659	2.5280	2.5691	2.5289	2.5622	2.5276	3.0078	3.0469	3.0820	3.0813	3.1389	3.0782	3.1224	3.0768	3.1178	3.0832	3.1257	**3.03**
H(4`B)	2.7943	2.7946	2.7650	2.7788	2.7365	2.7790	2.7481	2.7808	2.7503	2.7776	2.7269	2.6651	2.6587	2.6432	2.6437	2.5949	2.6441	2.6105	2.6461	2.6116	2.6423	2.5894	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. VII

Nuclei	R											S										Exp. [b]
	M06											M06										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.8587	138.6854	139.8459	139.3176	141.4728	139.2641	140.3172	139.2203	140.4496	139.3850	140.6478	136.8587	138.6852	139.8458	139.3176	141.4728	139.2641	140.3172	139.2203	140.4496	139.3850	140.6478	**133.8**
C2	140.5440	139.9917	140.5692	139.6770	140.2730	139.6854	140.8393	139.7016	140.7125	139.6834	140.7721	140.5440	139.9916	140.5692	139.6770	140.2730	139.6854	140.8393	139.7016	140.7125	139.6834	140.7721	**132.1**
C3	121.6896	122.3564	123.0312	122.5833	123.4038	122.5622	123.6315	122.5486	123.5686	122.6176	123.7108	121.6896	122.3564	123.0311	122.5833	123.4038	122.5622	123.6315	122.5486	123.5686	122.6176	123.7108	**115.8**
C4	173.3794	174.2348	174.9757	174.6746	175.3987	174.6411	175.9914	174.6147	175.8470	174.7204	176.0960	173.3794	174.2348	174.9756	174.6746	175.3987	174.6411	175.9914	174.6147	175.8470	174.7204	176.0960	**165.8**
C5	119.6442	120.8138	121.5066	121.5143	122.3936	121.4596	122.6609	121.4131	122.5634	121.5816	122.8584	119.6442	120.8140	121.5067	121.5143	122.3937	121.4596	122.6609	121.4131	122.5634	121.5816	122.8584	**115.8**
C6	136.6190	138.0201	139.1415	139.0588	140.5391	138.9844	141.2587	138.9172	141.0233	139.1439	141.5635	136.6190	138.0200	139.1415	139.0588	140.5392	138.9844	141.2587	138.9172	141.0233	139.1439	141.5635	**132.1**
C7	203.4072	209.3010	210.7623	212.2146	213.2021	212.0162	217.9477	211.8286	216.8130	212.4212	219.1293	203.4072	209.3011	210.7622	212.2146	213.2021	212.0162	217.9477	211.8286	216.8130	212.4212	219.1293	**198.9**
C8	61.9542	63.5485	64.3954	64.2641	65.3612	64.2028	65.7924	64.1511	65.6176	64.3389	66.2226	61.9542	63.5486	64.3954	64.2641	65.3612	64.2028	65.7924	64.1511	65.6176	64.3389	66.2226	**69.3**
C9	35.7877	35.3811	35.6369	35.2340	35.6454	35.2369	35.7936	35.2468	35.7234	35.2447	35.8369	35.7877	35.3812	35.6369	35.2340	35.6455	35.2369	35.7936	35.2468	35.7234	35.2447	35.8369	**31.5**
C10	16.7497	17.5868	18.0478	17.9439	18.6854	17.9123	18.5635	17.8885	18.5397	17.9884	18.6445	16.7498	17.5868	18.0478	17.9439	18.6854	17.9123	18.5635	17.8885	18.5397	17.9884	18.6445	**19.9**
C11	15.6901	15.6596	15.8843	15.6650	16.0771	15.6524	15.9933	15.6482	15.9812	15.6918	16.4023	15.6902	15.6596	15.8843	15.6650	16.0772	15.6524	15.9933	15.6482	15.9812	15.6918	16.4023	**14.3**
C1`	50.7374	51.5622	51.9496	52.0003	52.7195	51.9638	52.7186	51.9350	52.6681	52.0495	53.2009	55.1196	56.0449	56.4891	56.5711	57.1984	56.5293	57.4389	56.4952	57.3498	56.6253	57.8474	**50.6**
C2`	23.4218	23.9115	24.3247	24.0780	24.6400	24.0597	24.7117	24.0488	24.6915	24.1098	24.4498	22.2913	22.6693	23.1895	22.7996	23.4794	22.7807	23.3297	22.7700	23.3617	22.8323	22.8485	**23.8**
C3`	22.2912	22.6693	23.1895	22.7996	23.4794	22.7807	23.3297	22.7700	23.3617	22.8323	22.8485	23.4218	23.9115	24.3246	24.0780	24.6400	24.0597	24.7117	24.0488	24.6915	24.1098	24.4498	**23.8**
C4`	55.1195	56.0449	56.4891	56.5711	57.1984	56.5293	57.4389	56.4952	57.3498	56.6253	57.8474	50.7375	51.5622	51.9496	52.0003	52.7196	51.9638	52.7186	51.9350	52.6681	52.0495	53.2009	**50.6**
H2	8.7504	8.5336	8.5336	8.4112	8.3909	8.4199	8.4277	8.4289	8.4206	8.4030	8.3966	8.7504	8.5336	8.5337	8.4112	8.3908	8.4199	8.4277	8.4289	8.4206	8.4030	8.3966	**8.35**
H3	7.3165	7.4747	7.5640	7.4911	7.6085	7.4913	7.6125	7.4919	7.6043	7.4912	7.6167	7.3165	7.4747	7.5640	7.4911	7.6085	7.4913	7.6125	7.4919	7.6043	7.4912	7.6167	**7.06**
H5	7.1178	7.2708	7.3584	7.3474	7.4768	7.3422	7.4985	7.3378	7.4865	7.3529	7.5256	7.1178	7.2708	7.3585	7.3474	7.4768	7.3422	7.4985	7.3378	7.4865	7.3529	7.5256	**7.06**
H6	8.0202	8.1899	8.2795	8.3048	8.4307	8.2981	8.5111	8.2919	8.4906	8.3115	8.5520	8.0202	8.1899	8.2795	8.3048	8.4307	8.2981	8.5111	8.2919	8.4906	8.3115	8.5520	**8.35**
H8	4.4111	4.4204	4.4597	4.4735	4.5499	4.4693	4.6253	4.4657	4.6082	4.4782	4.6702	4.4111	4.4203	4.4597	4.4735	4.5499	4.4693	4.6253	4.4657	4.6082	4.4782	4.6702	**4.88**
H(9A-9B)	1.7754	1.7284	1.7011	1.7283	1.7293	1.7285	1.7393	1.7291	1.7280	1.7285	1.7670	1.7753	1.7284	1.7011	1.7283	1.7293	1.7285	1.7393	1.7291	1.7280	1.7285	1.7670	**2.05**
H(10A-10B)	1.3278	1.1916	1.1442	1.1282	1.0765	1.1321	1.0962	1.1365	1.0963	1.1251	1.0944	1.3278	1.1916	1.1442	1.1282	1.0765	1.1321	1.0962	1.1365	1.0963	1.1251	1.0944	**1.36**
H(11A-11C)	0.7472	0.7318	0.7068	0.7358	0.7093	0.7350	0.7053	0.7349	0.7057	0.7372	0.6895	0.7472	0.7318	0.7068	0.7358	0.7093	0.7350	0.7053	0.7349	0.7057	0.7372	0.6895	**0.77**
H(1`A)	2.6657	2.6307	2.6129	2.6014	2.5600	2.6032	2.5669	2.6055	2.5709	2.6003	2.5489	2.9001	2.8586	2.8607	2.8302	2.7981	2.8312	2.8173	2.8329	2.8204	2.8300	2.7824	**3.03**
H(1`B)	3.0859	3.0897	3.1239	3.1217	3.1803	3.1192	3.1769	3.1173	3.1736	3.1247	3.1811	2.7571	2.6509	2.6319	2.6254	2.6408	2.6256	2.6162	2.6266	2.6154	2.6259	2.6110	**3.23**
H(2`-3`A-2`-3`B)	1.6159	1.6849	1.6504	1.7202	1.6839	1.7178	1.7001	1.7160	1.6946	1.7231	1.7398	1.6159	1.6849	1.6504	1.7202	1.6839	1.7178	1.7001	1.7160	1.6946	1.7231	1.7398	**1.77**
H(4`A)	2.7572	2.6509	2.6319	2.6254	2.6408	2.6256	2.6162	2.6266	2.6154	2.6259	2.6110	3.0859	3.0897	3.1239	3.1217	3.1803	3.1192	3.1769	3.1173	3.1736	3.1247	3.1811	**3.03**
H(4`B)	2.9001	2.8586	2.8607	2.8302	2.7981	2.8312	2.8173	2.8329	2.8204	2.8300	2.7824	2.6657	2.6307	2.6129	2.6014	2.5600	2.6032	2.5669	2.6055	2.5709	2.6003	2.5489	**3.23**
Nuclei	M06-2X											M06-2X										
C1	153.3291	154.7871	155.3185	155.1446	156.8382	155.1472	155.7261	155.1514	155.7127	155.1362	156.0491	153.3291	154.7871	155.3186	155.1447	156.8382	155.1473	155.7261	155.1514	155.7127	155.1362	156.0491	**133.8**
C2	155.0583	154.9839	155.5683	154.8182	155.5016	154.8518	155.9516	154.8863	155.8250	154.7801	155.9906	155.0582	154.9839	155.5684	154.8183	155.5016	154.8520	155.9516	154.8863	155.8250	154.7801	155.9905	**132.1**
C3	135.8412	136.7326	137.3391	136.9751	137.7562	136.9847	138.0048	136.9953	137.9310	136.9592	138.1039	135.8413	136.7326	137.3391	136.9750	137.7562	136.9849	138.0048	136.9953	137.9310	136.9592	138.1038	**115.8**
C4	187.2173	187.9919	188.6609	188.4098	189.0989	188.4045	189.7883	188.4003	189.6232	188.4086	189.9747	187.2174	187.9919	188.6609	188.4097	189.0989	188.4044	189.7883	188.4003	189.6232	188.4086	189.9747	**165.8**
C5	133.6413	135.1246	135.8209	135.8987	136.8542	135.8716	137.1085	135.8456	136.9862	135.9180	137.3251	133.6413	135.1246	135.8207	135.8985	136.8544	135.8714	137.1085	135.8456	136.9862	135.9180	137.3251	**115.8**
C6	151.4165	153.0719	154.3982	154.2636	156.0404	154.2072	156.6989	154.1526	156.4570	154.3108	157.1474	151.4165	153.0719	154.3980	154.2635	156.0404	154.2072	156.6989	154.1526	156.4570	154.3108	157.1476	**132.1**
C7	219.5714	225.6251	226.4951	228.5930	229.0932	228.4336	234.8478	228.2756	233.3454	228.7382	236.1827	219.5713	225.6251	226.4950	228.5930	229.0931	228.4336	234.8478	228.2756	233.3454	228.7382	236.1823	**198.9**
C8	67.3496	68.9257	69.3640	69.5721	70.5321	69.5564	70.9435	69.5415	70.6953	69.5807	71.5060	67.3495	68.9257	69.3641	69.5721	70.5320	69.5563	70.9435	69.5415	70.6953	69.5807	71.5060	**69.3**
C9	36.8567	36.8589	37.0158	36.7999	37.1970	36.8253	37.3284	36.8517	37.2330	36.7693	37.5513	36.8568	36.8589	37.0158	36.7999	37.1970	36.8253	37.3284	36.8517	37.2330	36.7693	37.5513	**31.5**
C10	18.0885	18.5555	18.7874	18.7570	19.2509	18.7656	19.0880	18.7751	19.0752	18.7427	19.1439	18.0887	18.5555	18.7874	18.7570	19.2510	18.7655	19.0880	18.7751	19.0752	18.7427	19.1439	**19.9**
C11	15.0629	15.2089	15.3040	15.2094	15.4713	15.2310	15.4101	15.2538	15.3993	15.1825	15.6383	15.0629	15.2089	15.3040	15.2094	15.4713	15.2311	15.4101	15.2538	15.3993	15.1825	15.6384	**14.3**
C1`	52.8605	53.6361	53.9038	54.0414	54.6565	54.0379	54.5960	54.0357	54.5181	54.0382	54.9503	57.0031	57.9878	58.3074	58.4452	59.0028	58.4380	59.0955	58.4322	59.0095	58.4458	59.3761	**50.6**
C2`	24.6809	25.0293	25.2326	25.2047	25.6210	25.2150	25.5892	25.2263	25.5423	25.1889	25.6187	23.8984	24.0888	24.4330	24.2294	24.7165	24.2408	24.6837	24.2534	24.6853	24.2124	24.7030	**23.8**
C3`	23.8984	24.0888	24.4330	24.2294	24.7165	24.2407	24.6837	24.2534	24.6853	24.2124	24.7030	24.6810	25.0293	25.2326	25.2047	25.6209	25.2149	25.5892	25.2263	25.5423	25.1889	25.6186	**23.8**
C4`	57.0032	57.9878	58.3074	58.4452	59.0027	58.4380	59.0955	58.4322	59.0095	58.4458	59.3761	52.8604	53.6361	53.9037	54.0412	54.6565	54.0378	54.5960	54.0357	54.5181	54.0382	54.9503	**50.6**
H2	9.2435	9.1320	9.1902	9.0953	9.1007	9.0961	9.1720	9.0966	9.1725	9.0947	9.1650	9.2435	9.1320	9.1902	9.0953	9.1007	9.0961	9.1720	9.0966	9.1725	9.0947	9.1650	**8.35**
H3	7.8772	7.9982	8.0934	8.0483	8.1676	8.0444	8.1900	8.0402	8.1807	8.0521	8.2066	7.8772	7.9982	8.0934	8.0483	8.1676	8.0444	8.1900	8.0402	8.1807	8.0521	8.2066	**7.06**
H5	7.6746	7.8772	7.9724	7.9688	8.0991	7.9622	8.1171	7.9553	8.1054	7.9752	8.1429	7.6746	7.8772	7.9724	7.9688	8.0991	7.9622	8.1171	7.9553	8.1054	7.9752	8.1429	**7.06**
H6	8.6459	8.7647	8.8936	8.8676	9.0102	8.8595	9.0759	8.8512	9.0622	8.8755	9.1051	8.6459	8.7647	8.8936	8.8676	9.0102	8.8595	9.0759	8.8512	9.0622	8.8755	9.1051	**8.35**
H8	4.3303	4.3457	4.4379	4.4105	4.4876	4.4042	4.5805	4.3977	4.5668	4.4167	4.5866	4.3303	4.3457	4.4379	4.4105	4.4876	4.4042	4.5805	4.3977	4.5668	4.4167	4.5866	**4.88**
H(9A-9B)	1.6913	1.7175	1.7109	1.7491	1.7610	1.7458	1.7590	1.7421	1.7535	1.7525	1.7975	1.6913	1.7175	1.7109	1.7491	1.7611	1.7458	1.7590	1.7421	1.7535	1.7525	1.7976	**2.05**
H(10A-10B)	1.3094	1.1605	1.1400	1.0918	1.0252	1.0948	1.0487	1.0974	1.0562	1.0891	1.0370	1.3094	1.1605	1.1401	1.0917	1.0252	1.0948	1.0487	1.0974	1.0562	1.0891	1.0370	**1.36**
H(11A-11C)	0.7411	0.7207	0.7099	0.7259	0.6867	0.7241	0.6966	0.7221	0.7011	0.7277	0.6871	0.7412	0.7207	0.7099	0.7259	0.6867	0.7241	0.6966	0.7221	0.7011	0.7277	0.6871	**0.77**
H(1`A)	2.5866	2.5812	2.5720	2.5744	2.5355	2.5741	2.5565	2.5727	2.5557	2.5752	2.5400	2.7747	2.8007	2.7681	2.7901	2.7549	2.7905	2.7525	2.7891	2.7495	2.7905	2.7250	**3.03**
H(1`B)	3.0713	3.0935	3.1264	3.1261	3.1796	3.1201	3.1738	3.1187	3.1697	3.1297	3.1840	2.7188	2.6476	2.5393	2.6074	2.5518	2.6103	2.5494	2.6089	2.5464	2.6068	2.5468	**3.23**
H(2`-3`A-2`-3`B)	1.6590	1.7094	1.6801	1.7477	1.7048	1.7439	1.7265	1.7398	1.7202	1.7515	1.7471	1.6590	1.7094	1.6801	1.7477	1.7048	1.7439	1.7265	1.7398	1.7202	1.7515	1.7471	**1.77**
H(4`A)	2.7188	2.6476	2.5910	2.6074	2.6000	2.6103	2.5494	2.6089	2.5464	2.6068	2.5468	3.0713	3.0935	3.0313	3.1261	3.1762	3.1201	3.1738	3.1187	3.1697	3.1297	3.1840	**3.03**
H(4`B)	2.7747	2.8007	2.7677	2.7901	2.7550	2.7905	2.7525	2.7891	2.7495	2.7905	2.7250	2.5866	2.5812	2.5203	2.5744	2.5589	2.5741	2.5565	2.5727	2.5557	2.5752	2.5400	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. VIII

Nuclei	R											S										Exp. [b]
	mpW1LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.8356	140.7551	141.5393	141.5708	143.3380	141.5390	142.7670	141.5085	142.8018	141.5990	143.1474	139.8356	140.7550	141.5393	141.5707	143.3380	141.5390	142.7670	141.5085	142.8018	141.5990	143.1475	**133.8**
C2	139.8936	139.8117	140.3785	139.6961	140.1507	139.7012	140.6144	139.7078	140.5425	139.6893	140.5949	139.8936	139.8117	140.3787	139.6963	140.1507	139.7013	140.6144	139.7078	140.5425	139.6894	140.5948	**132.1**
C3	121.9367	122.5923	123.1083	122.8622	123.4811	122.8480	123.7561	122.8350	123.6954	122.8735	123.8211	121.9367	122.5922	123.1082	122.8624	123.4811	122.8482	123.7561	122.8350	123.6954	122.8735	123.8210	**115.8**
C4	176.3104	177.0944	177.7085	177.5496	178.2255	177.5218	178.7909	177.4952	178.6500	177.5741	178.8796	176.3104	177.0944	177.7086	177.5495	178.2255	177.5218	178.7909	177.4952	178.6500	177.5740	178.8795	**165.8**
C5	119.9370	121.1966	121.7621	121.8575	122.5921	121.8166	122.7836	121.7768	122.6894	121.8945	122.9039	119.9370	121.1966	121.7622	121.8575	122.5921	121.8164	122.7836	121.7768	122.6894	121.8946	122.9039	**115.8**
C6	136.2352	138.0554	139.1590	139.0014	140.3442	138.9299	140.9774	138.8603	140.7198	139.0675	141.2030	136.2352	138.0555	139.1590	139.0014	140.3442	138.9298	140.9774	138.8603	140.7198	139.0675	141.2031	**132.1**
C7	203.5876	208.4777	209.6892	211.4737	212.2101	211.3031	217.5630	211.1336	216.3437	211.6342	218.7456	203.5876	208.4777	209.6895	211.4737	212.2101	211.3030	217.5630	211.1336	216.3437	211.6341	218.7456	**198.9**
C8	65.8261	66.9441	67.7688	67.5937	68.2546	67.5448	69.0166	67.4979	68.8463	67.6389	69.3302	65.8261	66.9442	67.7688	67.5938	68.2546	67.5448	69.0166	67.4979	68.8463	67.6388	69.3302	**69.3**
C9	38.6093	38.2599	38.5123	37.9672	38.0706	37.9745	38.2488	37.9834	38.2026	37.9582	38.2596	38.6093	38.2599	38.5124	37.9672	38.0706	37.9746	38.2488	37.9834	38.2026	37.9582	38.2596	**31.5**
C10	20.0344	20.4519	20.7617	20.6985	21.1134	20.6777	21.0113	20.6581	20.9981	20.7163	21.1007	20.0344	20.4520	20.7619	20.6985	21.1134	20.6776	21.0113	20.6581	20.9981	20.7164	21.1007	**19.9**
C11	16.2102	16.3479	16.4871	16.4264	16.6030	16.4187	16.5694	16.4126	16.5762	16.4317	16.7050	16.2102	16.3479	16.4872	16.4263	16.6030	16.4187	16.5694	16.4125	16.5762	16.4316	16.7051	**14.3**
C1`	51.9563	52.7773	53.0752	53.3398	53.8163	53.3010	53.8278	53.2634	53.8118	53.3745	54.2584	56.5332	57.4832	57.8466	58.0506	58.5951	58.0156	58.6967	57.9824	58.6302	58.0824	58.9219	**50.6**
C2`	25.9214	26.3457	26.6481	26.5892	26.9854	26.5692	27.0121	26.5510	26.9968	26.6066	26.8527	25.4974	25.6876	25.9879	25.8794	26.4450	25.8655	26.3109	25.8536	26.3122	25.8908	26.1183	**23.8**
C3`	25.4974	25.6876	25.9879	25.8794	26.4450	25.8655	26.3109	25.8536	26.3122	25.8908	26.1184	25.9214	26.3456	26.6482	26.5892	26.9854	26.5691	27.0121	26.5510	26.9968	26.6065	26.8526	**23.8**
C4`	56.5332	57.4831	57.8466	58.0507	58.5951	58.0156	58.6967	57.9824	58.6302	58.0823	58.9220	51.9563	52.7772	53.0753	53.3398	53.8163	53.3010	53.8278	53.2634	53.8118	53.3746	54.2585	**50.6**
H2	8.7102	8.6001	8.6319	8.4981	8.4848	8.5027	8.4902	8.5070	8.4957	8.4936	8.4690	8.7102	8.6001	8.6319	8.4981	8.4848	8.5027	8.4902	8.5070	8.4957	8.4936	8.4690	**8.35**
H3	7.3263	7.4607	7.5494	7.5074	7.6210	7.5055	7.6375	7.5033	7.6313	7.5089	7.6488	7.3263	7.4607	7.5494	7.5073	7.6210	7.5055	7.6375	7.5033	7.6313	7.5089	7.6488	**7.06**
H5	7.1691	7.3525	7.4414	7.4299	7.5506	7.4256	7.5648	7.4211	7.5535	7.4337	7.5817	7.1691	7.3525	7.4414	7.4298	7.5506	7.4256	7.5648	7.4211	7.5535	7.4337	7.5817	**7.06**
H6	7.9988	8.1752	8.2550	8.2640	8.3936	8.2583	8.4294	8.2524	8.4103	8.2692	8.4459	7.9988	8.1752	8.2550	8.2640	8.3936	8.2583	8.4294	8.2524	8.4103	8.2692	8.4459	**8.35**
H8	4.5608	4.6221	4.6358	4.6634	4.7632	4.6610	4.7838	4.6587	4.7653	4.6656	4.7714	4.5608	4.6221	4.6358	4.6634	4.7632	4.6611	4.7838	4.6587	4.7653	4.6656	4.7714	**4.88**
H(9A-9B)	1.6625	1.7071	1.7231	1.7096	1.6856	1.7075	1.6934	1.7051	1.6906	1.7115	1.7113	1.6625	1.7071	1.7231	1.7096	1.6856	1.7075	1.6934	1.7051	1.6906	1.7115	1.7114	**2.05**
H(10A-10B)	1.4121	1.2981	1.2449	1.2382	1.1784	1.2427	1.1905	1.2469	1.1939	1.2339	1.1760	1.4121	1.2981	1.2449	1.2382	1.1784	1.2427	1.1905	1.2469	1.1939	1.2339	1.1760	**1.36**
H(11A-11C)	0.7928	0.7967	0.7702	0.8027	0.7723	0.8024	0.7723	0.8019	0.7730	0.8029	0.7617	0.7928	0.7967	0.7702	0.8027	0.7723	0.8024	0.7723	0.8019	0.7730	0.8028	0.7618	**0.77**
H(1`A)	2.7236	2.7275	2.7055	2.7174	2.6660	2.7185	2.6794	2.7191	2.6803	2.7164	2.6542	2.8554	2.8541	2.8458	2.8386	2.8048	2.8398	2.8166	2.8406	2.8183	2.8374	2.7805	**3.03**
H(1`B)	3.1803	3.2244	3.2675	3.2573	3.3254	3.2550	3.3093	3.2524	3.3051	3.2594	3.3063	2.8521	2.7125	2.7047	2.6810	2.6748	2.6828	2.6568	2.6843	2.6569	2.6793	2.6525	**3.23**
H(2`-3`A-2`-3`B)	1.6666	1.7253	1.6891	1.7717	1.7304	1.7693	1.7496	1.7667	1.7449	1.7739	1.7740	1.6666	1.7253	1.6891	1.7717	1.7304	1.7693	1.7496	1.7667	1.7449	1.7739	1.7739	**1.77**
H(4`A)	2.8521	2.7125	2.7047	2.6810	2.6748	2.6828	2.6568	2.6843	2.6569	2.6794	2.6525	3.1803	3.2244	3.2675	3.2573	3.3254	3.2550	3.3093	3.2524	3.3051	3.2594	3.3063	**3.03**
H(4`B)	2.8554	2.8541	2.8458	2.8386	2.8048	2.8398	2.8166	2.8406	2.8183	2.8374	2.7805	2.7236	2.7275	2.7055	2.7174	2.6660	2.7185	2.6794	2.7191	2.6803	2.7164	2.6542	**3.23**
Nuclei	mpW1PW91																						
C1	136.9559	137.8933	138.5161	138.5364	140.5558	138.4926	140.0136	138.4501	140.0184	138.5751	140.3824	136.9559	137.8933	138.5161	138.5363	140.5558	138.4926	140.0136	138.4501	140.0183	138.5751	140.3824	**133.8**
C2	138.9131	138.8764	139.4426	138.7354	139.3309	138.7450	139.6903	138.7603	139.6319	138.7258	139.6920	138.9131	138.8764	139.4426	138.7355	139.3309	138.7450	139.6903	138.7603	139.6319	138.7259	139.6921	**132.1**
C3	121.0595	121.8043	122.3814	122.0536	122.8153	122.0413	123.1065	122.0342	123.0344	122.0641	123.2061	121.0595	121.8043	122.3814	122.0537	122.8153	122.0413	123.1065	122.0342	123.0344	122.0642	123.2061	**115.8**
C4	173.2952	174.0694	174.6948	174.4526	175.1461	174.4300	175.7536	174.4129	175.6073	174.4733	175.8718	173.2952	174.0694	174.6948	174.4526	175.1461	174.4300	175.7536	174.4129	175.6073	174.4733	175.8718	**165.8**
C5	119.1323	120.4902	121.1083	121.1722	122.0465	121.1316	122.2645	121.0960	122.1539	121.2098	122.4220	119.1323	120.4902	121.1083	121.1721	122.0465	121.1316	122.2645	121.0960	122.1540	121.2096	122.4220	**115.8**
C6	135.1018	136.9403	138.0642	137.8904	139.2324	137.8314	139.8237	137.7800	139.5613	137.9471	140.0936	135.1018	136.9403	138.0642	137.8903	139.2324	137.8314	139.8237	137.7800	139.5613	137.9468	140.0936	**132.1**
C7	201.4508	206.1158	207.1079	208.8566	209.8570	208.6808	215.0117	208.5075	213.7402	209.0216	216.1719	201.4508	206.1157	207.1079	208.8569	209.8570	208.6808	215.0117	208.5075	213.7402	209.0214	216.1719	**198.9**
C8	63.7173	64.9068	65.5328	65.6188	66.5348	65.5678	67.1954	65.5223	66.9610	65.6670	67.6444	63.7173	64.9068	65.5328	65.6188	66.5348	65.5678	67.1954	65.5223	66.9609	65.6670	67.6444	**69.3**
C9	36.5915	36.4355	36.6600	36.2407	36.4857	36.2519	36.5631	36.2705	36.4791	36.2304	36.6567	36.5915	36.4355	36.6600	36.2407	36.4857	36.2519	36.5631	36.2705	36.4791	36.2304	36.6568	**31.5**
C10	18.4168	18.8786	19.1477	19.1084	19.5681	19.0932	19.4539	19.0843	19.4181	19.1227	19.6406	18.4169	18.8786	19.1477	19.1085	19.5681	19.0932	19.4539	19.0843	19.4180	19.1227	19.6406	**19.9**
C11	15.7070	15.8645	15.9583	15.8942	16.1302	15.8921	16.0752	15.8960	16.0731	15.8958	16.2350	15.7070	15.8645	15.9583	15.8942	16.1302	15.8920	16.0752	15.8960	16.0730	15.8958	16.2349	**14.3**
C1`	50.5467	51.3539	51.5885	51.8531	52.3925	51.8221	52.3437	51.7965	52.3054	51.8818	52.8568	54.8323	55.7682	56.1209	56.2585	56.8194	56.2270	56.9768	56.2009	56.9196	56.2876	57.2205	**50.6**
C2`	24.7107	25.0958	25.3710	25.2826	25.7032	25.2695	25.7283	25.2621	25.6958	25.2947	25.5762	24.1643	24.3659	24.6526	24.4783	25.0112	24.4715	24.9328	24.4702	24.9254	24.4839	24.7891	**23.8**
C3`	24.1643	24.3659	24.6526	24.4783	25.0112	24.4715	24.9328	24.4702	24.9254	24.4838	24.7890	24.7107	25.0958	25.3710	25.2826	25.7032	25.2695	25.7283	25.2621	25.6957	25.2946	25.5763	**23.8**
C4`	54.8323	55.7682	56.1209	56.2585	56.8195	56.2270	56.9768	56.2009	56.9196	56.2877	57.2206	50.5467	51.3539	51.5885	51.8531	52.3925	51.8221	52.3437	51.7965	52.3054	51.8818	52.8568	**50.6**
H2	8.7653	8.6546	8.6949	8.5614	8.5274	8.5679	8.5318	8.5749	8.5400	8.5557	8.5160	8.7653	8.6546	8.6949	8.5614	8.5274	8.5679	8.5318	8.57486	8.5400	8.5557	8.5160	**8.35**
H3	7.3564	7.4950	7.5856	7.5399	7.6616	7.5381	7.6806	7.5362	7.6727	7.5419	7.6974	7.3564	7.4950	7.5856	7.5399	7.6616	7.5381	7.6806	7.5362	7.6727	7.5419	7.6974	**7.06**
H5	7.1918	7.3823	7.4740	7.4623	7.5883	7.4580	7.6039	7.4539	7.5917	7.4665	7.6232	7.1918	7.3823	7.4740	7.4623	7.5883	7.4580	7.6039	7.4539	7.5917	7.4665	7.6232	**7.06**
H6	8.0912	8.2617	8.3568	8.3413	8.4516	8.3370	8.4945	8.3330	8.4771	8.3458	8.5141	8.0912	8.2617	8.3568	8.3413	8.4516	8.3370	8.4945	8.3330	8.4771	8.3458	8.5141	**8.35**
H8	4.5583	4.6205	4.6484	4.6484	4.7240	4.6471	4.7702	4.6460	4.7549	4.6499	4.7632	4.5583	4.6205	4.6484	4.6484	4.7240	4.6471	4.7702	4.6460	4.7549	4.6499	4.7632	**4.88**
H(9A-9B)	1.6918	1.7351	1.7416	1.7487	1.7252	1.7479	1.7091	1.7475	1.7044	1.7501	1.7363	1.6918	1.7351	1.7416	1.7487	1.7252	1.7479	1.7091	1.7475	1.7044	1.7501	1.7363	**2.05**
H(10A-10B)	1.3646	1.2488	1.2035	1.1765	1.1081	1.1816	1.1271	1.1867	1.1326	1.1719	1.1140	1.3646	1.2488	1.2035	1.1765	1.1081	1.1816	1.1271	1.1867	1.1326	1.1719	1.1140	**1.36**
H(11A-11C)	0.7361	0.7392	0.7155	0.7396	0.7037	0.7398	0.7066	0.7402	0.7086	0.7396	0.6966	0.7361	0.7392	0.7155	0.7397	0.7037	0.7398	0.7066	0.7402	0.7085	0.7397	0.6966	**0.77**
H(1`A)	2.6642	2.6704	2.6505	2.6544	2.6120	2.6559	2.6257	2.6575	2.6257	2.6533	2.5991	2.7948	2.7932	2.7786	2.7793	2.7486	2.7804	2.7644	2.7817	2.7629	2.7784	2.7336	**3.03**
H(1`B)	3.1541	3.1947	3.2255	3.2216	3.2804	3.2200	3.2629	3.2185	3.2596	3.2236	3.2612	2.8533	2.7136	2.6823	2.6703	2.6865	2.6724	2.6440	2.6747	2.6423	2.6686	2.6336	**3.23**
H(2`-3`A-2`-3`B)	1.6396	1.6975	1.6605	1.7354	1.6969	1.7332	1.7190	1.7311	1.7142	1.7377	1.7463	1.6396	1.6975	1.6605	1.7354	1.6969	1.7332	1.7190	1.7311	1.7142	1.7377	1.7463	**1.77**
H(4`A)	2.8533	2.7136	2.6823	2.6703	2.6865	2.6724	2.6440	2.6747	2.6423	2.6686	2.6336	3.1541	3.1947	3.2255	3.2216	3.2804	3.2200	3.2629	3.2185	3.2596	3.2236	3.2612	**3.03**
H(4`B)	2.7948	2.7932	2.7786	2.7793	2.7486	2.7804	2.7644	2.7817	2.7629	2.7784	2.7336	2.6642	2.6704	2.6505	2.6544	2.6120	2.6559	2.6257	2.6575	2.6257	2.6532	2.5991	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. IX

Nuclei	R											S										Exp. [b]
	O3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	134.6700	136.7350	138.0774	137.7862	139.9680	137.7525	138.6540	137.7169	138.9233	137.8160	138.9525	134.6701	136.7350	138.0774	137.7862	139.9680	137.7525	138.6540	137.7169	138.9233	137.8160	138.9524	**133.8**
C2	134.1521	134.1172	134.7329	134.1503	134.7502	134.1633	135.1355	134.1711	135.0388	134.1313	135.1471	134.1521	134.1172	134.7329	134.1503	134.7503	134.1633	135.1355	134.1711	135.0388	134.1313	135.1470	**132.1**
C3	117.0796	117.7861	118.4184	118.1613	118.8456	118.1571	119.0899	118.1476	119.0204	118.1584	119.1418	117.0795	117.7861	118.4185	118.1613	118.8456	118.1571	119.0899	118.1476	119.0204	118.1584	119.1418	**115.8**
C4	169.5295	170.1231	170.7516	170.4650	171.0573	170.4530	171.6773	170.4354	171.4956	170.4694	171.7619	169.5294	170.1231	170.7516	170.4650	171.0572	170.4530	171.6773	170.4354	171.4956	170.4694	171.7618	**165.8**
C5	115.2924	116.3484	116.9871	116.9459	117.6904	116.9169	117.9563	116.8827	117.8349	116.9666	118.0874	115.2923	116.3484	116.9870	116.9459	117.6904	116.9169	117.9563	116.8827	117.8349	116.9666	118.0873	**115.8**
C6	130.1286	131.5708	132.4547	132.5104	133.6620	132.4536	134.4006	132.3911	134.0803	132.5568	134.6403	130.1286	131.5708	132.4546	132.5104	133.6621	132.4536	134.4006	132.3911	134.0803	132.5568	134.6402	**132.1**
C7	197.0416	202.5614	204.1833	205.5703	206.7569	205.4087	210.8503	205.2457	209.9957	205.7217	211.8476	197.0419	202.5614	204.1833	205.5703	206.7567	205.4087	210.8503	205.2457	209.9957	205.7217	211.8473	**198.9**
C8	64.5007	66.1237	66.7896	66.9482	68.0400	66.9077	68.4198	66.8643	68.3756	66.9825	68.7838	64.5008	66.1237	66.7896	66.9482	68.0399	66.9077	68.4198	66.8643	68.3756	66.9825	68.7837	**69.3**
C9	36.8866	36.4970	36.7329	36.3964	36.6310	36.4109	36.9071	36.4198	36.8496	36.3759	36.9523	36.8866	36.4970	36.7330	36.3964	36.6311	36.4109	36.9071	36.4198	36.8496	36.3760	36.9523	**31.5**
C10	19.5667	20.0008	20.2903	20.3020	20.8140	20.2929	20.7362	20.2786	20.7115	20.3040	20.8623	19.5667	20.0008	20.2903	20.3020	20.8140	20.2929	20.7362	20.2786	20.7115	20.3039	20.8624	**19.9**
C11	16.0407	16.1490	16.3067	16.2326	16.4675	16.2358	16.4305	16.2338	16.4349	16.2231	16.5667	16.0407	16.1490	16.3067	16.2326	16.4676	16.2358	16.4305	16.2338	16.4349	16.2231	16.5666	**14.3**
C1`	50.7757	51.5877	51.9059	52.0796	52.6905	52.0588	52.6700	52.0330	52.6459	52.0927	53.0142	55.2927	56.2797	56.6547	56.8181	57.3377	56.7973	57.3943	56.7718	57.3132	56.8316	57.5927	**50.6**
C2`	25.8874	26.2979	26.5421	26.5335	26.9416	26.5279	26.9525	26.5174	26.9218	26.5325	26.8274	25.6559	25.8485	26.2667	26.0617	26.5537	26.0582	26.3970	26.0502	26.3838	26.0594	26.1411	**23.8**
C3`	25.6559	25.8485	26.2668	26.0617	26.5537	26.0582	26.3970	26.0502	26.3838	26.0594	26.1410	25.8873	26.2979	26.5421	26.5335	26.9417	26.5279	26.9525	26.5174	26.9218	26.5325	26.8275	**23.8**
C4`	55.2927	56.2797	56.6547	56.8181	57.3377	56.7973	57.3943	56.7718	57.3132	56.8316	57.5928	50.7758	51.5877	51.9060	52.0796	52.6904	52.0588	52.6700	52.0330	52.6459	52.0927	53.0141	**50.6**
H2	8.5055	8.3012	8.2945	8.2161	8.1877	8.2208	8.2753	8.2248	8.2525	8.2112	8.2672	8.5055	8.3012	8.2946	8.2161	8.1877	8.2208	8.2753	8.2248	8.2525	8.2112	8.2672	**8.35**
H3	7.2858	7.3932	7.4811	7.4335	7.5463	7.4318	7.5693	7.4296	7.5598	7.4350	7.5821	7.2857	7.3932	7.4811	7.4335	7.5463	7.4318	7.5693	7.4296	7.5598	7.4350	7.5821	**7.06**
H5	7.1355	7.2960	7.3891	7.3704	7.4914	7.3660	7.5096	7.3614	7.4960	7.3743	7.5295	7.1355	7.2960	7.3891	7.3704	7.4914	7.3660	7.5096	7.3614	7.4960	7.3743	7.5295	**7.06**
H6	7.9390	8.0509	8.1185	8.1320	8.2238	8.1268	8.2873	8.1211	8.2535	8.1366	8.3045	7.9390	8.0509	8.1185	8.1320	8.2238	8.1268	8.2873	8.1211	8.2535	8.1366	8.3045	**8.35**
H8	4.7534	4.7762	4.7904	4.8059	4.8401	4.8043	4.8723	4.8022	4.8493	4.8073	4.8600	4.7534	4.7762	4.7904	4.8059	4.8401	4.8043	4.8723	4.8022	4.8493	4.8073	4.8600	**4.88**
H(9A-9B)	1.5857	1.5960	1.5743	1.6144	1.6160	1.6127	1.6478	1.6105	1.6420	1.6158	1.6759	1.5857	1.5960	1.5743	1.6144	1.6160	1.6127	1.6478	1.6105	1.6420	1.6158	1.6759	**2.05**
H(10A-10B)	1.3660	1.2834	1.2609	1.2547	1.1867	1.2579	1.1996	1.2607	1.1992	1.2516	1.1809	1.3660	1.2834	1.2609	1.2547	1.1867	1.2579	1.1996	1.2607	1.1992	1.2516	1.1809	**1.36**
H(11A-11C)	0.7648	0.7704	0.7545	0.7870	0.7544	0.7864	0.7543	0.7855	0.7523	0.7876	0.7412	0.7648	0.7704	0.7545	0.7870	0.7544	0.7864	0.7543	0.7855	0.7523	0.7876	0.7411	**0.77**
H(1`A)	2.7701	2.7625	2.7405	2.7555	2.7038	2.7567	2.7128	2.7576	2.7141	2.7543	2.6909	2.9160	2.9130	2.8950	2.8860	2.8551	2.8877	2.8575	2.8891	2.8620	2.8842	2.8234	**3.03**
H(1`B)	3.2375	3.2724	3.3158	3.3162	3.3800	3.3137	3.3688	3.3111	3.3631	3.3184	3.3660	2.8835	2.7784	2.7910	2.7707	2.7967	2.7708	2.7626	2.7707	2.7732	2.7708	2.7597	**3.23**
H(2`-3`A-2`-3`B)	1.6811	1.7424	1.7163	1.7850	1.7421	1.7829	1.7553	1.7804	1.7499	1.7870	1.7766	1.6811	1.7424	1.7163	1.7850	1.7421	1.7829	1.7553	1.7804	1.7499	1.7870	1.7766	**1.77**
H(4`A)	2.8835	2.7784	2.7910	2.7707	2.7967	2.7708	2.7626	2.7707	2.7732	2.7708	2.7597	3.2376	3.2724	3.3157	3.3162	3.3800	3.3137	3.3688	3.3111	3.3631	3.3184	3.3660	**3.03**
H(4`B)	2.9160	2.9130	2.8950	2.8860	2.8551	2.8877	2.8575	2.8891	2.8620	2.8842	2.8234	2.7701	2.7625	2.7405	2.7555	2.7038	2.7567	2.7128	2.7576	2.7141	2.7543	2.6909	**3.23**
Nuclei	OLYP																						
C1	133.7662	135.8243	136.8482	136.5375	138.7381	136.4802	137.5934	136.4203	137.8888	136.5829	137.8613	133.7663	135.8243	136.8482	136.5375	138.7381	136.4802	137.5934	136.4203	137.8888	136.5830	137.8613	**133.8**
C2	131.6800	131.7598	132.3806	131.7534	132.3384	131.7657	132.7233	131.7722	132.6422	131.7318	132.7671	131.6801	131.7598	132.3808	131.7534	132.3384	131.7657	132.7233	131.7722	132.6422	131.7318	132.7671	**132.1**
C3	115.2861	116.0410	116.6769	116.3352	116.9878	116.3293	117.2608	116.3176	117.1923	116.3311	117.3062	115.2861	116.0410	116.6770	116.3352	116.9878	116.3293	117.2608	116.3176	117.1923	116.3311	117.3062	**115.8**
C4	168.4638	169.0396	169.7744	169.4326	170.0838	169.4209	170.6437	169.4032	170.4653	169.4352	170.7329	168.4638	169.0396	169.7744	169.4326	170.0838	169.4209	170.6437	169.4032	170.4653	169.4351	170.7329	**165.8**
C5	113.4566	114.4501	115.1055	115.0778	115.7698	115.0503	116.0665	115.0167	115.9370	115.0947	116.1973	113.4565	114.4501	115.1053	115.0778	115.7698	115.0503	116.0665	115.0167	115.9370	115.0948	116.1973	**115.8**
C6	127.6564	129.0488	130.0717	130.0799	131.2151	130.0293	131.8524	129.9726	131.5313	130.1199	132.0848	127.6565	129.0488	130.0714	130.0799	131.2151	130.0293	131.8524	129.9726	131.5313	130.1200	132.0848	**132.1**
C7	195.6304	200.9205	202.2732	203.5752	204.9425	203.3942	208.7242	203.2126	207.9733	203.7392	209.6516	195.6304	200.9205	202.2731	203.5752	204.9425	203.3942	208.7242	203.2126	207.9733	203.7392	209.6516	**198.9**
C8	66.0164	67.6742	68.2766	68.4831	69.5230	68.4284	69.9658	68.3702	69.9271	68.5261	70.2727	66.0164	67.6742	68.2768	68.4831	69.5230	68.4284	69.9658	68.3702	69.9271	68.5261	70.2727	**69.3**
C9	37.8775	37.5355	37.8329	37.4817	37.6919	37.4945	37.9963	37.5015	37.9257	37.4599	37.9956	37.8775	37.5355	37.8329	37.4817	37.6919	37.4945	37.9963	37.5015	37.9257	37.4599	37.9956	**31.5**
C10	20.3708	20.8487	21.2009	21.1635	21.6411	21.1551	21.5754	21.1408	21.5473	21.1623	21.6809	20.3708	20.8487	21.2007	21.1635	21.6411	21.1551	21.5754	21.1408	21.5473	21.1623	21.6809	**19.9**
C11	16.1842	16.2669	16.4521	16.3855	16.6001	16.3875	16.5670	16.3839	16.5716	16.3747	16.6889	16.1841	16.2669	16.4521	16.3855	16.6001	16.3875	16.5670	16.3839	16.5716	16.3747	16.6889	**14.3**
C1`	51.7190	52.5287	52.8737	53.0310	53.6180	53.0102	53.6219	52.9837	53.5953	53.0416	53.9470	56.3231	57.2890	57.6654	57.8153	58.3436	57.7917	58.4155	57.7629	58.3216	57.8291	58.6136	**50.6**
C2`	26.4617	26.9073	27.1798	27.1974	27.5680	27.1902	27.5895	27.1773	27.5416	27.1953	27.4841	26.4356	26.6445	27.0375	26.8194	27.3310	26.8124	27.1412	26.8007	27.1395	26.8176	26.8747	**23.8**
C3`	26.4356	26.6445	27.0373	26.8194	27.3310	26.8124	27.1412	26.8007	27.1395	26.8175	26.8747	26.4616	26.9073	27.1798	27.1974	27.5680	27.1902	27.5895	27.1773	27.5416	27.1953	27.4841	**23.8**
C4`	56.3231	57.2890	57.6655	57.8153	58.3436	57.7917	58.4155	57.7629	58.3216	57.8292	58.6136	51.7190	52.5287	52.8739	53.0310	53.6180	53.0102	53.6220	52.9837	53.5953	53.0416	53.9470	**50.6**
H2	8.3122	8.1471	8.1735	8.0875	8.0577	8.0938	8.1401	8.0997	8.1164	8.0809	8.1378	8.3122	8.1471	8.1735	8.0875	8.0577	8.0938	8.1401	8.0997	8.1164	8.0809	8.1378	**8.35**
H3	7.1968	7.3083	7.4006	7.3510	7.4622	7.3492	7.4865	7.3473	7.4763	7.3522	7.4980	7.1968	7.3083	7.4006	7.3510	7.4622	7.3492	7.4865	7.3473	7.4763	7.3522	7.4980	**7.06**
H5	7.0617	7.2114	7.3059	7.2908	7.4116	7.2863	7.4297	7.2817	7.4161	7.2947	7.4486	7.0616	7.2114	7.3058	7.2908	7.4116	7.2863	7.4297	7.2817	7.4161	7.2947	7.4486	**7.06**
H6	7.8271	7.9413	8.0216	8.0276	8.1151	8.0236	8.1721	8.0194	8.1371	8.0310	8.1906	7.8271	7.9413	8.0216	8.0276	8.1151	8.0236	8.1721	8.0194	8.1371	8.0310	8.1906	**8.35**
H8	4.9345	4.9386	4.9511	4.9514	4.9728	4.9514	4.9922	4.9512	4.9740	4.9510	4.9799	4.9345	4.9386	4.9511	4.9514	4.9728	4.9514	4.9922	4.9512	4.9740	4.9510	4.9799	**4.88**
H(9A-9B)	1.6018	1.6344	1.6307	1.6677	1.6629	1.6668	1.6963	1.6656	1.6899	1.6680	1.7229	1.6018	1.6344	1.6307	1.6677	1.6629	1.6668	1.6963	1.6656	1.6899	1.6680	1.7229	**2.05**
H(10A-10B)	1.3968	1.3365	1.3099	1.2954	1.2395	1.2980	1.2503	1.3005	1.2528	1.2925	1.2330	1.3968	1.3365	1.3099	1.2954	1.2395	1.2980	1.2503	1.3005	1.2528	1.2925	1.2330	**1.36**
H(11A-11C)	0.7752	0.7858	0.7691	0.7990	0.7713	0.7981	0.7697	0.7972	0.7690	0.7994	0.7572	0.7752	0.7858	0.7691	0.7990	0.7713	0.7981	0.7697	0.7972	0.7690	0.7994	0.7572	**0.77**
H(1`A)	2.8307	2.8265	2.8045	2.8170	2.7654	2.8180	2.7704	2.8190	2.7715	2.8155	2.7426	2.9862	2.9788	2.9601	2.9549	2.9231	2.9567	2.9221	2.9583	2.9272	2.9528	2.7426	**3.03**
H(1`B)	3.3288	3.3720	3.4187	3.4096	3.4766	3.4072	3.4606	3.4047	3.4562	3.4116	3.4558	2.9692	2.8714	2.8781	2.8638	2.8924	2.8627	2.8599	2.8618	2.8718	2.8645	3.4558	**3.23**
H(2`-3`A-2`-3`B)	1.7212	1.7789	1.7513	1.8155	1.7775	1.8131	1.7899	1.8107	1.7855	1.8174	1.8096	1.7212	1.7789	1.7513	1.8155	1.7775	1.8131	1.7899	1.8107	1.7855	1.8174	1.8096	**1.77**
H(4`A)	2.9691	2.8714	2.8782	2.8638	2.8924	2.8627	2.8599	2.8618	2.8718	2.8645	2.8506	3.3288	3.3720	3.4187	3.4096	3.4766	3.4072	3.4606	3.4047	3.4562	3.4116	2.8506	**3.03**
H(4`B)	2.9861	2.9788	2.9600	2.9549	2.9231	2.9567	2.9221	2.9583	2.9272	2.9528	2.8867	2.8307	2.8265	2.8045	2.8170	2.7654	2.8180	2.7704	2.8190	2.7715	2.8155	2.8867	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. X

Nuclei	R											S										Exp. [b]
	OPBE											OPBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	130.4493	132.8644	133.7230	133.3810	135.5557	133.3573	134.3189	133.3178	134.5747	133.4005	134.7226	130.4493	132.8644	133.7229	133.3810	135.5557	133.3573	134.3189	133.3178	134.5747	133.4005	134.7226	**133.8**
C2	130.3689	130.4777	131.1106	130.4003	131.0794	130.4227	131.4243	130.4267	131.3408	130.3743	131.4713	130.3689	130.4777	131.1104	130.4003	131.0794	130.4227	131.4243	130.4267	131.3408	130.3743	131.4713	**132.1**
C3	114.1253	115.0494	115.6469	115.3003	116.0208	115.3045	116.3076	115.2901	116.2355	115.2913	116.3908	114.1253	115.0494	115.6470	115.3003	116.0208	115.3044	116.3075	115.2901	116.2355	115.2913	116.3908	**115.8**
C4	164.8904	165.5133	166.1484	165.8236	166.4138	165.8225	167.0193	165.8034	166.8477	165.8192	167.1132	164.8904	165.5133	166.1485	165.8236	166.4138	165.8226	167.0193	165.8034	166.8478	165.8192	167.1132	**165.8**
C5	112.4138	113.5251	114.1304	114.1087	114.8563	114.0899	115.1793	114.0531	115.0484	114.1213	115.3343	112.4138	113.5251	114.1305	114.1087	114.8563	114.0899	115.1793	114.0531	115.0483	114.1213	115.3343	**115.8**
C6	126.2446	127.6532	128.5340	128.5693	129.6701	128.5305	130.3399	128.4733	130.0468	128.6008	130.5598	126.2446	127.6532	128.5339	128.5693	129.6701	128.5305	130.3399	128.4733	130.0467	128.6008	130.5598	**132.1**
C7	192.8452	198.2855	199.3972	200.6172	201.8936	200.4792	205.3787	200.3260	204.6650	200.7460	206.4215	192.8452	198.2855	199.3972	200.6172	201.8936	200.4790	205.3787	200.3260	204.6650	200.7460	206.4215	**198.9**
C8	63.3511	65.2455	65.8299	65.9430	67.0082	65.9067	67.4062	65.8548	67.3284	65.9747	67.8269	63.3511	65.2455	65.8299	65.9430	67.0082	65.9067	67.4062	65.8548	67.3284	65.9747	67.8269	**69.3**
C9	35.4839	35.3259	35.4925	35.2408	35.4394	35.2625	35.7811	35.2662	35.6909	35.2151	35.8596	35.4839	35.3259	35.4924	35.2408	35.4394	35.2625	35.7811	35.2662	35.6909	35.2151	35.8596	**31.5**
C10	18.3839	18.9262	19.1709	19.1777	19.5816	19.1792	19.5409	19.1625	19.5080	19.1714	19.7487	18.3839	18.9262	19.1709	19.1777	19.5816	19.1791	19.5409	19.1625	19.5081	19.1714	19.7487	**19.9**
C11	15.5088	15.6615	15.7302	15.6889	15.8422	15.7034	15.8187	15.7002	15.8190	15.6703	15.9747	15.5088	15.6615	15.7301	15.6889	15.8422	15.7035	15.8187	15.7002	15.8190	15.6703	15.9748	**14.3**
C1`	49.8310	50.6853	50.9616	51.0854	51.5959	51.0768	51.5674	51.0503	51.5468	51.0887	51.9458	54.1846	55.2341	55.5306	55.6629	56.1364	55.6521	56.2029	55.6236	56.1348	55.6686	56.4163	**50.6**
C2`	25.0749	25.5194	25.7331	25.6915	26.0326	25.6960	26.0213	25.6827	26.0054	25.6828	25.8849	24.8732	25.1362	25.3971	25.1852	25.6271	25.1955	25.4682	25.1883	25.4683	25.1710	25.1804	**23.8**
C3`	24.8732	25.1363	25.3971	25.1852	25.6271	25.1955	25.4682	25.1883	25.4683	25.1710	25.1805	25.0749	25.5194	25.7331	25.6915	26.0326	25.6959	26.0213	25.6827	26.0054	25.6828	25.8850	**23.8**
C4`	54.1846	55.2340	55.5307	55.6629	56.1364	55.6521	56.2030	55.6236	56.1348	55.6686	56.4160	49.8310	50.6853	50.9616	51.0854	51.5959	51.0769	51.5673	51.0503	51.5468	51.0887	51.9458	**50.6**
H2	8.3740	8.1768	8.2025	8.1261	8.0964	8.1307	8.1856	8.1345	8.1640	8.1207	8.1758	8.3740	8.1768	8.2025	8.1261	8.0964	8.1307	8.1856	8.1345	8.1640	8.1207	8.1758	**8.35**
H3	7.2246	7.3451	7.4322	7.3881	7.4977	7.3867	7.5248	7.3844	7.5145	7.3887	7.5383	7.2246	7.3451	7.4322	7.3881	7.4977	7.3867	7.5247	7.3844	7.5145	7.3887	7.5383	**7.06**
H5	7.0810	7.2395	7.3267	7.3187	7.4394	7.3146	7.4579	7.3098	7.4452	7.3218	7.4772	7.0810	7.2395	7.3267	7.3187	7.4394	7.3146	7.4579	7.3098	7.4452	7.3218	7.4772	**7.06**
H6	7.9066	8.0122	8.0790	8.0965	8.1759	8.0923	8.2338	8.0874	8.2046	8.0995	8.2407	7.9066	8.0122	8.0790	8.0965	8.1759	8.0924	8.2338	8.0874	8.2046	8.0995	8.2407	**8.35**
H8	4.9256	4.9388	4.9338	4.9538	4.9732	4.9534	4.9991	4.9523	4.9798	4.9533	4.9840	4.9256	4.9388	4.9339	4.9538	4.9732	4.9534	4.9991	4.9523	4.9798	4.9533	4.9840	**4.88**
H(9A-9B)	1.6214	1.6370	1.6357	1.6693	1.6561	1.6679	1.6926	1.6659	1.6826	1.6697	1.7222	1.6214	1.6370	1.6357	1.6693	1.6561	1.6680	1.6926	1.6659	1.6826	1.6697	1.7222	**2.05**
H(10A-10B)	1.3274	1.2657	1.2230	1.2199	1.1597	1.2236	1.1691	1.2265	1.1733	1.2157	1.1568	1.3274	1.2657	1.2230	1.2199	1.1597	1.2236	1.1691	1.2265	1.1733	1.2157	1.1568	**1.36**
H(11A-11C)	0.7068	0.7178	0.6922	0.7271	0.6937	0.7269	0.6920	0.7261	0.6924	0.7265	0.6799	0.7068	0.7178	0.6922	0.7271	0.6937	0.7270	0.6920	0.7261	0.6924	0.7265	0.6799	**0.77**
H(1`A)	2.7577	2.7604	2.7294	2.7459	2.6937	2.7476	2.7010	2.7486	2.7028	2.7435	2.6776	2.9072	2.9050	2.8848	2.8821	2.8463	2.8840	2.8482	2.8852	2.8520	2.8795	2.8116	**3.03**
H(1`B)	3.2916	3.3295	3.3588	3.3606	3.4135	3.3589	3.4015	3.3565	3.3967	3.3616	3.3958	2.9565	2.8569	2.8458	2.8304	2.8505	2.8317	2.8185	2.8324	2.8248	2.8286	2.8111	**3.23**
H(2`-3`A-2`-3`B)	1.6772	1.7373	1.7020	1.7688	1.7262	1.7674	1.7389	1.7652	1.7354	1.7696	1.7649	1.6772	1.7373	1.7020	1.7688	1.7262	1.7674	1.7389	1.7652	1.7354	1.7696	1.7649	**1.77**
H(4`A)	2.9565	2.8569	2.8458	2.8304	2.8505	2.8317	2.8185	2.8324	2.8248	2.8286	2.8111	3.2916	3.3294	3.3588	3.3606	3.4135	3.3589	3.4015	3.3565	3.3967	3.3616	3.3958	**3.03**
H(4`B)	2.9072	2.9050	2.8848	2.8821	2.8463	2.8840	2.8482	2.8852	2.8520	2.8795	2.8116	2.7577	2.7604	2.7294	2.7459	2.6937	2.7476	2.7010	2.7486	2.7028	2.7435	2.6776	**3.23**
Nuclei	OPW91											OPW91										
C1	130.7667	133.1792	134.0352	133.7004	135.8728	133.6658	134.6250	133.6167	134.8875	133.7173	135.0268	130.7667	133.1792	134.0351	133.7004	135.8728	133.6658	134.6250	133.6167	134.8875	133.7172	135.0268	**133.8**
C2	130.5896	130.7006	131.3253	130.6292	131.2902	130.6414	131.6411	130.6365	131.5552	130.5989	131.6892	130.5896	130.7006	131.3251	130.6292	131.2902	130.6413	131.6411	130.6365	131.5550	130.5989	131.6891	**132.1**
C3	114.3241	115.2447	115.8366	115.4992	116.2043	115.4934	116.4921	115.4699	116.4192	115.4860	116.5761	114.3241	115.2447	115.8367	115.4992	116.2043	115.4934	116.4921	115.4699	116.4191	115.4861	116.5761	**115.8**
C4	165.2950	165.9218	166.5553	166.2389	166.8184	166.2280	167.4274	166.1994	167.2536	166.2307	167.5234	165.2950	165.9219	166.5553	166.2389	166.8184	166.2280	167.4274	166.1994	167.2535	166.2307	167.5234	**165.8**
C5	112.6079	113.7187	114.3194	114.3065	115.0387	114.2778	115.3624	114.2319	115.2313	114.3152	115.5192	112.6079	113.7188	114.3195	114.3065	115.0387	114.2778	115.3624	114.2319	115.2314	114.3152	115.5192	**115.8**
C6	126.4628	127.8788	128.7584	128.8065	129.8918	128.7573	130.5695	128.6908	130.2737	128.8343	130.7939	126.4628	127.8789	128.7584	128.8065	129.8918	128.7573	130.5695	128.6908	130.2737	128.8343	130.7940	**132.1**
C7	193.2313	198.6873	199.8005	201.0323	202.3062	200.8826	205.8061	200.7188	205.0944	201.1593	206.8474	193.2313	198.6874	199.8004	201.0323	202.3062	200.8826	205.8061	200.7188	205.0944	201.1592	206.8475	**198.9**
C8	63.5767	65.4651	66.0452	66.1615	67.2228	66.1149	67.6145	66.0538	67.5445	66.1896	68.0379	63.5767	65.4651	66.0452	66.1615	67.2228	66.1149	67.6145	66.0538	67.5445	66.1896	68.0379	**69.3**
C9	35.6376	35.4754	35.6401	35.3932	35.5818	35.4050	35.9238	35.3997	35.8366	35.3636	36.0036	35.6376	35.4753	35.6401	35.3932	35.5818	35.4050	35.9238	35.3997	35.8366	35.3636	36.0037	**31.5**
C10	18.5106	19.0562	19.3007	19.3117	19.7102	19.3031	19.6681	19.2774	19.6364	19.3015	19.8723	18.5106	19.0561	19.3007	19.3117	19.7102	19.3031	19.6681	19.2774	19.6363	19.3015	19.8722	**19.9**
C11	15.5472	15.7047	15.7735	15.7387	15.8867	15.7430	15.8623	15.7305	15.8639	15.7162	16.0213	15.5472	15.7047	15.7736	15.7387	15.8867	15.7430	15.8623	15.7305	15.8639	15.7162	16.0213	**14.3**
C1`	49.9712	50.8301	51.1068	51.2369	51.7437	51.2180	51.7174	51.1822	51.6970	51.2363	52.0939	54.3361	55.3900	55.6843	55.8260	56.2909	55.8053	56.3591	55.7678	56.2892	55.8279	56.5750	**50.6**
C2`	25.1936	25.6429	25.8533	25.8205	26.1542	25.8150	26.1443	25.7928	26.1277	25.8077	26.0144	24.9944	25.2626	25.5214	25.3197	25.7547	25.3196	25.5948	25.3033	25.5941	25.3018	25.3107	**23.8**
C3`	24.9944	25.2626	25.5214	25.3197	25.7547	25.3196	25.5948	25.3033	25.5942	25.3018	25.3106	25.1936	25.6429	25.8532	25.8205	26.1542	25.8150	26.1443	25.7928	26.1278	25.8078	26.0143	**23.8**
C4`	54.3361	55.3900	55.6843	55.8260	56.2909	55.8053	56.3591	55.7678	56.2891	55.8280	56.5750	49.9712	50.8300	51.1069	51.2369	51.7437	51.2180	51.7174	51.1822	51.6970	51.2364	52.0939	**50.6**
H2	8.3747	8.1783	8.2038	8.1283	8.0967	8.1324	8.1870	8.1360	8.1645	8.1225	8.1772	8.3747	8.1783	8.2037	8.1283	8.0967	8.1324	8.1870	8.1360	8.1645	8.1225	8.1772	**8.35**
H3	7.2263	7.3462	7.4332	7.3898	7.4982	7.3876	7.5253	7.3852	7.5150	7.3900	7.5388	7.2263	7.3462	7.4332	7.3898	7.4982	7.3876	7.5253	7.3852	7.5150	7.3900	7.5388	**7.06**
H5	7.0832	7.2411	7.3283	7.3208	7.4403	7.3161	7.4590	7.3111	7.4460	7.3236	7.4782	7.0832	7.2411	7.3283	7.3208	7.4403	7.3160	7.4590	7.3111	7.4460	7.3236	7.4782	**7.06**
H6	7.9058	8.0115	8.0785	8.0971	8.1751	8.0923	8.2342	8.0871	8.2041	8.0997	8.2416	7.9058	8.0115	8.0785	8.0971	8.1751	8.0923	8.2342	8.0871	8.2041	8.0998	8.2416	**8.35**
H8	4.9246	4.9379	4.9328	4.9539	4.9719	4.9528	4.9984	4.9516	4.9786	4.9531	4.9834	4.9246	4.9379	4.9328	4.9539	4.9719	4.9528	4.9984	4.9516	4.9786	4.9531	4.9834	**4.88**
H(9A-9B)	1.6183	1.6350	1.6336	1.6680	1.6547	1.6661	1.6913	1.6638	1.6817	1.6682	1.7210	1.6183	1.6350	1.6336	1.6680	1.6547	1.6661	1.6913	1.6638	1.6817	1.6682	1.7210	**2.05**
H(10A-10B)	1.3299	1.2685	1.2258	1.2236	1.1623	1.2266	1.1720	1.2292	1.1758	1.2191	1.1591	1.3299	1.2685	1.2258	1.2236	1.1623	1.2266	1.1720	1.2292	1.1758	1.2191	1.1591	**1.36**
H(11A-11C)	0.7090	0.7203	0.6949	0.7305	0.6965	0.7297	0.6950	0.7286	0.6951	0.7297	0.6829	0.7090	0.7203	0.6949	0.7305	0.6965	0.7297	0.6950	0.7286	0.6951	0.7297	0.6829	**0.77**
H(1`A)	2.7617	2.7640	2.7332	2.7501	2.6971	2.7512	2.7043	2.7520	2.7061	2.7474	2.6810	2.9112	2.9085	2.8882	2.8858	2.8496	2.8871	2.8514	2.8881	2.8553	2.8830	2.8151	**3.03**
H(1`B)	3.2883	3.3267	3.3565	3.3589	3.4115	3.3565	3.3997	3.3539	3.3947	3.3596	3.3940	2.9516	2.8524	2.8425	2.8277	2.8479	2.8281	2.8154	2.8285	2.8224	2.8258	2.8088	**3.23**
H(2`-3`A-2`-3`B)	1.6773	1.7378	1.7028	1.7702	1.7270	1.7681	1.7397	1.7656	1.7359	1.7707	1.7652	1.6773	1.7378	1.7028	1.7702	1.7270	1.7681	1.7397	1.7656	1.7359	1.7708	1.7652	**1.77**
H(4`A)	2.9516	2.8524	2.8425	2.8277	2.8479	2.8282	2.8154	2.8285	2.8224	2.8258	2.8088	3.2883	3.3267	3.3565	3.3589	3.4115	3.3565	3.3997	3.3539	3.3947	3.3596	3.3940	**3.03**
H(4`B)	2.9112	2.9085	2.8882	2.8858	2.8496	2.8870	2.8514	2.8881	2.8553	2.8830	2.8151	2.7617	2.7640	2.7332	2.7501	2.6971	2.7512	2.7043	2.7520	2.7061	2.7474	2.6810	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. XI

Nuclei	R											S										Exp. [b]
	PBE											PBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	135.7538	137.0503	137.5475	137.8060	139.7406	137.7637	139.4272	137.7334	139.3332	137.8648	139.8075	135.7538	137.0503	137.5475	137.8061	139.7406	137.7637	139.4272	137.7334	139.3332	137.8647	139.8074	**133.8**
C2	135.8065	135.8860	136.4810	135.7036	136.4289	135.7123	136.7962	135.7320	136.7400	135.7130	136.8172	135.8066	135.8860	136.4810	135.7036	136.4289	135.7123	136.7962	135.7320	136.7400	135.7130	136.8172	**132.1**
C3	119.3937	120.2555	120.8293	120.4598	121.2955	120.4475	121.6507	120.4456	121.5790	120.4890	121.7777	119.3937	120.2554	120.8293	120.4599	121.2955	120.4475	121.6507	120.4456	121.5790	120.4890	121.7776	**115.8**
C4	174.2136	175.1821	175.8656	175.5336	176.4397	175.5105	176.9941	175.4979	176.8739	175.5729	177.1398	174.2136	175.1821	175.8656	175.5336	176.4397	175.5106	176.9941	175.4979	176.8739	175.5730	177.1398	**165.8**
C5	117.5986	119.0081	119.6203	119.6045	120.5387	119.5663	120.7914	119.5387	120.6893	119.6582	120.9616	117.5986	119.0081	119.6203	119.6045	120.5387	119.5663	120.7914	119.5387	120.6893	119.6582	120.9616	**115.8**
C6	132.3081	134.1508	135.3129	135.0151	136.5859	134.9539	137.0949	134.9038	136.8563	135.0911	137.3931	132.3080	134.1508	135.3129	135.0151	136.5859	134.9538	137.0949	134.9038	136.8563	135.0911	137.3933	**132.1**
C7	201.2795	205.7851	206.7994	208.3176	209.5076	208.1594	213.8421	208.0133	212.7045	208.4866	214.9789	201.2795	205.7848	206.7994	208.3174	209.5076	208.1594	213.8421	208.0133	212.7045	208.4867	214.9789	**198.9**
C8	67.3124	68.7273	69.4684	69.4840	70.5173	69.4274	71.2296	69.3828	70.9057	69.5568	71.6596	67.3124	68.7273	69.4684	69.4840	70.5173	69.4273	71.2296	69.3828	70.9057	69.5569	71.6596	**69.3**
C9	40.1276	40.0069	40.3088	39.7443	40.0956	39.7515	40.2930	39.7702	40.1520	39.7559	40.4120	40.1277	40.0069	40.3088	39.7442	40.0956	39.7514	40.2930	39.7702	40.1520	39.7559	40.4120	**31.5**
C10	20.0763	20.6106	20.9112	20.7941	21.3510	20.7768	21.2710	20.7705	21.2080	20.8283	21.4983	20.0763	20.6106	20.9112	20.7940	21.3510	20.7768	21.2710	20.7707	21.2080	20.8283	21.4983	**19.9**
C11	15.8694	16.1085	16.1979	16.0767	16.3861	16.0740	16.3423	16.0824	16.3286	16.0976	16.5359	15.8693	16.1084	16.1979	16.0766	16.3861	16.0739	16.3423	16.0824	16.3286	16.0976	16.5359	**14.3**
C1`	53.2289	54.1288	54.3704	54.5888	55.2146	54.5567	55.1614	54.5356	55.1128	54.6370	55.7066	57.7454	58.8405	59.1962	59.2838	59.9592	59.2540	60.1471	59.2350	60.1124	59.3302	60.4098	**50.6**
C2`	25.6779	26.2489	26.5423	26.4277	26.9602	26.4116	27.0066	26.4066	26.9614	26.4608	26.9077	25.2774	25.6126	25.8947	25.6955	26.3439	25.6884	26.2808	25.6922	26.2785	25.7195	26.1972	**23.8**
C3`	25.2775	25.6125	25.8947	25.6954	26.3439	25.6885	26.2808	25.6921	26.2785	25.7195	26.1974	25.6779	26.2488	26.5423	26.4277	26.9602	26.4115	27.0066	26.4066	26.9614	26.4608	26.9077	**23.8**
C4`	57.7453	58.8405	59.1962	59.2838	59.9592	59.2540	60.1471	59.2351	60.1124	59.3302	60.4096	53.2289	54.1288	54.3704	54.5888	55.2146	54.5568	55.1614	54.5355	55.1128	54.6370	55.7066	**50.6**
H2	8.5413	8.4249	8.4705	8.3290	8.3128	8.3344	8.3182	8.3402	8.3289	8.3244	8.3070	8.5413	8.4249	8.4705	8.3290	8.3128	8.3344	8.3182	8.3403	8.3289	8.3244	8.3070	**8.35**
H3	7.1939	7.3320	7.4217	7.3724	7.4949	7.3707	7.5141	7.3693	7.5065	7.3747	7.5304	7.1939	7.3320	7.4217	7.3724	7.4949	7.3707	7.5141	7.3693	7.5065	7.3747	7.5304	**7.06**
H5	7.0374	7.2231	7.3131	7.2966	7.4239	7.2926	7.4373	7.2890	7.4263	7.3011	7.4549	7.0374	7.2231	7.3131	7.2966	7.4239	7.2926	7.4373	7.2890	7.4263	7.3011	7.4549	**7.06**
H6	7.9743	8.1212	8.2101	8.1810	8.2933	8.1773	8.3259	8.1741	8.3170	8.1851	8.3441	7.9743	8.1220	8.2101	8.1810	8.2933	8.1773	8.3259	8.1741	8.3170	8.1851	8.3441	**8.35**
H8	4.9863	5.0087	5.0207	5.0083	5.0807	5.0085	5.1095	5.0092	5.1076	5.0089	5.1020	4.9863	5.0087	5.0207	5.0084	5.0807	5.0085	5.1095	5.0092	5.1076	5.0089	5.1020	**4.88**
H(9A-9B)	1.8543	1.8898	1.9093	1.8989	1.8881	1.8970	1.8743	1.8957	1.8641	1.9014	1.9019	1.8543	1.8898	1.9093	1.8989	1.8881	1.8970	1.8743	1.8957	1.8641	1.9014	1.9019	**2.05**
H(10A-10B)	1.4519	1.3468	1.3025	1.2772	1.2192	1.2819	1.2355	1.2870	1.2429	1.2734	1.2243	1.4519	1.3468	1.3025	1.2772	1.2192	1.2819	1.2355	1.2870	1.2429	1.2734	1.2243	**1.36**
H(11A-11C)	0.7585	0.7622	0.7398	0.7594	0.7316	0.7595	0.7316	0.7601	0.7356	0.7599	0.7223	0.7584	0.7622	0.7398	0.7594	0.7316	0.7595	0.7316	0.7601	0.7356	0.7599	0.7223	**0.77**
H(1`A)	2.7941	2.8061	2.7875	2.7895	2.7526	2.7907	2.7598	2.7925	2.7597	2.7890	2.7278	2.9117	2.9223	2.9116	2.9098	2.8864	2.9106	2.8960	2.9121	2.8947	2.9096	2.8590	**3.03**
H(1`B)	3.3775	3.4057	3.4374	3.4252	3.4888	3.4236	3.4656	3.4226	3.4634	3.4274	3.4588	3.0568	2.9041	2.8696	2.8574	2.8623	2.8597	2.8258	2.8626	2.8184	2.8560	2.8095	**3.23**
H(2`-3`A-2`-3`B)	1.7348	1.7907	1.7541	1.8228	1.7870	1.8210	1.8072	1.8196	1.8042	1.8252	1.8373	1.7348	1.7907	1.7541	1.8228	1.7870	1.8210	1.8072	1.8197	1.8042	1.8252	1.8372	**1.77**
H(4`A)	3.0568	2.9041	2.8696	2.8574	2.8623	2.8597	2.8258	2.8627	2.8184	2.8560	2.8095	3.3775	3.4057	3.4374	3.4252	3.4888	3.4236	3.4656	3.4227	3.4634	3.4274	3.4587	**3.03**
H(4`B)	2.9117	2.9223	2.9116	2.9097	2.8864	2.9106	2.8960	2.9121	2.8947	2.9096	2.8590	2.7941	2.8061	2.7875	2.7895	2.7526	2.7907	2.7598	2.7925	2.7597	2.7890	2.7278	**3.23**
Nuclei	PBE0																						
C1	136.4686	137.4247	138.0416	137.8938	140.0424	137.8360	139.5797	137.7866	139.5513	137.9591	139.8415	136.4685	137.4247	138.0416	137.8937	140.0424	137.8360	139.5796	137.7866	139.5513	137.9591	139.8415	**133.8**
C2	138.6351	138.6103	139.1605	138.4797	139.0718	138.4833	139.5175	138.4891	139.3957	138.4794	139.4670	138.6353	138.6103	139.1605	138.4797	139.0718	138.4833	139.5175	138.4891	139.3957	138.4794	139.4670	**132.1**
C3	120.8260	121.5877	122.1674	121.8254	122.5810	121.8075	122.9492	121.7912	122.8216	121.8451	122.9893	120.8261	121.5877	122.1674	121.8254	122.5810	121.8075	122.9492	121.7912	122.8216	121.8451	122.9893	**115.8**
C4	172.9139	173.6981	174.3281	174.0689	174.7360	174.0417	175.4226	174.0161	175.2162	174.0971	175.4854	172.9140	173.6981	174.3280	174.0689	174.7360	174.0417	175.4226	174.0161	175.2162	174.0971	175.4854	**165.8**
C5	118.8731	120.2602	120.8776	120.9475	121.8402	120.8988	122.1400	120.8521	121.9716	120.9970	122.2425	118.8732	120.2602	120.8776	120.9477	121.8402	120.8988	122.1401	120.8521	121.9716	120.9970	122.2426	**115.8**
C6	134.8944	136.7405	137.8709	137.7454	139.0196	137.6852	139.6731	137.6246	139.3535	137.8034	139.9155	134.8944	136.7405	137.8709	137.7454	139.0196	137.6852	139.6731	137.6246	139.3535	137.8034	139.9155	**132.1**
C7	201.1327	205.7535	206.7477	208.2864	209.4138	208.1016	214.5384	207.9254	213.2700	208.4730	215.6100	201.1327	205.7535	206.7477	208.2866	209.4138	208.1016	214.5385	207.9254	213.2700	208.4730	215.6100	**198.9**
C8	63.3643	64.5588	65.1497	65.2013	66.1093	65.1470	66.8326	65.0978	66.5623	65.2595	67.2452	63.3643	64.5588	65.1497	65.2013	66.1093	65.1470	66.8326	65.0978	66.5623	65.2595	67.2452	**69.3**
C9	36.7029	36.5564	36.7690	36.3980	36.5819	36.4075	36.7407	36.4178	36.6034	36.3913	36.8157	36.7029	36.5564	36.7690	36.3981	36.5819	36.4075	36.7408	36.4178	36.6033	36.3913	36.8157	**31.5**
C10	18.3038	18.7809	19.0349	19.0204	19.4473	19.0017	19.4138	18.9846	19.3219	19.0409	19.5600	18.3039	18.7809	19.0349	19.0204	19.4473	19.0017	19.4138	18.9846	19.3219	19.0409	19.5600	**19.9**
C11	15.6012	15.7676	15.8515	15.7904	16.0036	15.7839	16.0273	15.7793	15.9694	15.7998	16.1344	15.6012	15.7676	15.8515	15.7904	16.0036	15.7839	16.0273	15.7793	15.9694	15.7998	16.1344	**14.3**
C1`	50.3555	51.1875	51.3998	51.6650	52.1959	51.6290	52.2187	51.5955	52.1195	51.7027	52.6818	54.6265	55.5628	55.9223	56.0328	56.5940	55.9957	56.8284	55.9612	56.7115	56.0716	57.0056	**50.6**
C2`	24.3377	24.7374	25.0025	24.9136	25.3137	24.8961	25.4208	24.8808	25.3336	24.9338	25.2433	23.7806	24.0065	24.2873	24.1073	24.6266	24.0951	24.6313	24.0848	24.5689	24.1218	24.4625	**23.8**
C3`	23.7805	24.0065	24.2874	24.1073	24.6265	24.0951	24.6313	24.0848	24.5689	24.1218	24.4625	24.3377	24.7374	25.0026	24.9137	25.3137	24.8961	25.4208	24.8808	25.3336	24.9338	25.2433	**23.8**
C4`	54.6265	55.5628	55.9220	56.0328	56.5940	55.9957	56.8284	55.9612	56.7115	56.0716	57.0056	50.3556	51.1875	51.3998	51.6650	52.1959	51.6290	52.2187	51.5955	52.1195	51.7027	52.6818	**50.6**
H2	8.7662	8.6573	8.6954	8.5831	8.5346	8.5899	8.5448	8.5961	8.5475	8.5757	8.5295	8.7662	8.6573	8.6954	8.5831	8.5346	8.5899	8.5448	8.5961	8.5475	8.5757	8.5295	**8.35**
H3	7.3496	7.4870	7.5780	7.5310	7.6523	7.5287	7.6774	7.5264	7.6664	7.5327	7.6913	7.3496	7.4870	7.5780	7.5310	7.6523	7.5287	7.6774	7.5264	7.6664	7.5327	7.6913	**7.06**
H5	7.1827	7.3750	7.4666	7.4573	7.5830	7.4525	7.6019	7.4477	7.5873	7.4615	7.6192	7.1826	7.3750	7.4666	7.4573	7.5830	7.4525	7.6019	7.4477	7.5873	7.4615	7.6193	**7.06**
H6	8.0968	8.2654	8.3625	8.3511	8.4526	8.3470	8.5011	8.3425	8.4796	8.3543	8.5197	8.0968	8.2654	8.3625	8.3511	8.4526	8.3470	8.5011	8.3425	8.4796	8.3543	8.5197	**8.35**
H8	4.5595	4.6199	4.6513	4.6501	4.7223	4.6486	4.7730	4.6468	4.7544	4.6509	4.7634	4.5595	4.6199	4.6513	4.6501	4.7223	4.6486	4.7730	4.6468	4.7544	4.6509	4.7634	**4.88**
H(9A-9B)	1.7092	1.7507	1.7536	1.7754	1.7379	1.7750	1.7243	1.7743	1.7170	1.7752	1.7538	1.7092	1.7507	1.7536	1.7754	1.7379	1.7750	1.7243	1.7743	1.7170	1.7752	1.7538	**2.05**
H(10A-10B)	1.3665	1.2504	1.2064	1.1804	1.1095	1.1851	1.1324	1.1898	1.1348	1.1754	1.1162	1.3665	1.2504	1.2064	1.1804	1.1095	1.1851	1.1324	1.1898	1.1348	1.1754	1.1162	**1.36**
H(11A-11C)	0.7350	0.7375	0.7143	0.7399	0.7000	0.7399	0.7067	0.7399	0.7057	0.7395	0.6936	0.7350	0.7375	0.7144	0.7399	0.7000	0.7399	0.7067	0.7399	0.7057	0.7395	0.6936	**0.77**
H(1`A)	2.6575	2.6629	2.6444	2.6475	2.6041	2.6487	2.6218	2.6498	2.6195	2.6460	2.5912	2.7854	2.7861	2.7694	2.7720	2.7399	2.7726	2.7591	2.7734	2.7558	2.7711	2.7274	**3.03**
H(1`B)	3.1658	3.2038	3.2332	3.2306	3.2859	3.2288	3.2718	3.2269	3.2660	3.2321	3.2667	2.8630	2.7224	2.6881	2.6752	2.6893	2.6767	2.6504	2.6785	2.6477	2.6738	2.6351	**3.23**
H(2`-3`A-2`-3`B)	1.6432	1.7002	1.6634	1.7350	1.6970	1.7325	1.7235	1.7300	1.7158	1.7372	1.7470	1.6432	1.7002	1.6634	1.7350	1.6970	1.7325	1.7235	1.7300	1.7158	1.7372	1.7470	**1.77**
H(4`A)	2.8630	2.7224	2.6881	2.6752	2.6893	2.6767	2.6504	2.6785	2.6477	2.6738	2.6351	3.1658	3.2038	3.2332	3.2306	3.2859	3.2288	3.2718	3.2269	3.2660	3.2321	3.2667	**3.03**
H(4`B)	2.7854	2.7861	2.7694	2.7720	2.7399	2.7726	2.7591	2.7734	2.7558	2.7711	2.7274	2.6575	2.6629	2.6444	2.6475	2.6041	2.6487	2.6218	2.6498	2.6195	2.6460	2.5912	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. XII

Nuclei	R											S										Exp. [b]
	TPSS																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	132.4252	133.2606	134.0626	133.5282	135.4463	133.5171	135.0853	133.5182	134.0244	133.5502	135.4091	132.4252	133.2606	134.0627	133.5282	135.4462	133.5171	135.0853	133.5182	134.6273	133.5502	135.4091	**133.8**
C2	132.8716	132.8075	133.4662	132.7281	133.3610	132.7403	133.7796	132.7642	133.2674	132.7268	133.7640	132.8716	132.8075	133.4663	132.7281	133.3609	132.7403	133.7796	132.7642	133.8789	132.7268	133.7641	**132.1**
C3	116.5341	117.2014	117.8434	117.4791	118.2171	117.4709	118.5555	117.4740	117.9160	117.4971	118.6079	116.5341	117.2014	117.8434	117.4791	118.2170	117.4709	118.5555	117.4740	118.7034	117.4971	118.6079	**115.8**
C4	170.8720	171.6565	172.4080	172.1110	172.9485	172.0898	173.5447	172.0799	172.7403	172.1417	173.6048	170.8720	171.6565	172.4079	172.1110	172.9486	172.0898	173.5447	172.0799	172.8997	172.1417	173.6048	**165.8**
C5	114.7873	116.0079	116.6761	116.6918	117.5648	116.6561	117.8009	116.6318	117.0704	116.7361	117.9140	114.7873	116.0079	116.6761	116.6918	117.5649	116.6561	117.8009	116.6318	117.8675	116.7362	117.9141	**115.8**
C6	129.5145	131.2357	132.3650	132.3133	133.5944	132.2529	134.1706	132.2038	132.7047	132.3812	134.4509	129.5145	131.2357	132.3650	132.3133	133.5945	132.2529	134.1706	132.2038	133.3227	132.3812	134.4509	**132.1**
C7	197.3886	201.4786	202.7123	203.5325	204.4931	203.4121	208.9449	203.3036	204.0889	203.6581	210.1722	197.3885	201.4786	202.7123	203.5325	204.4930	203.4121	208.9449	203.3036	203.8893	203.6581	210.1722	**198.9**
C8	66.1175	67.2102	68.0808	67.7179	68.4103	67.6925	69.1666	67.6788	67.9216	67.7529	69.8127	66.1175	67.2102	68.0807	67.7179	68.4103	67.6925	69.1666	67.6788	69.2817	67.7529	69.8127	**69.3**
C9	38.9328	38.7405	39.1060	38.6825	38.7429	38.6953	39.0004	38.7189	38.8459	38.6805	39.2532	38.9328	38.7405	39.1059	38.6825	38.7429	38.6953	39.0004	38.7189	40.5390	38.6805	39.2532	**31.5**
C10	20.8961	21.2537	21.6284	21.5187	21.9347	21.5080	21.8224	21.5088	21.5669	21.5395	22.0027	20.8961	21.2537	21.6284	21.5187	21.9346	21.5080	21.8224	21.5088	23.4579	21.5396	22.0026	**19.9**
C11	16.7316	16.8366	17.0508	16.9122	17.1364	16.9137	17.1088	16.9269	16.9667	16.9213	17.2672	16.7316	16.8366	17.0508	16.9122	17.1364	16.9137	17.1088	16.9269	18.9104	16.9214	17.2672	**14.3**
C1`	53.0734	53.7846	54.1144	54.2751	54.7525	54.2483	54.7593	54.2333	54.4223	54.3119	55.2518	57.2647	58.1927	58.6434	58.6885	59.3602	58.6623	59.5451	58.6481	60.3187	58.7241	59.6616	**50.6**
C2`	26.3500	26.7405	27.1281	26.9606	27.3558	26.9524	27.4021	26.9558	27.0357	26.9793	27.2559	26.0130	26.2008	26.5733	26.3792	26.9618	26.3743	26.8919	26.3809	28.2935	26.3945	26.7492	**23.8**
C3`	26.0130	26.2008	26.5733	26.3792	26.9619	26.3743	26.8919	26.3809	26.4585	26.3945	26.7491	26.3500	26.7405	27.1281	26.9606	27.3561	26.9524	27.4021	26.9558	28.8641	26.9792	27.2559	**23.8**
C4`	57.2647	58.1927	58.6434	58.6885	59.3602	58.6623	59.5451	58.6481	58.8548	58.7242	59.6616	53.0734	53.7846	54.1144	54.2751	54.7524	54.2483	54.7593	54.2333	55.9370	54.3118	55.2518	**50.6**
H2	8.5444	8.4411	8.4735	8.3949	8.3711	8.3981	8.3698	8.4018	8.2418	8.3922	8.3436	8.5444	8.4411	8.4735	8.3949	8.3711	8.3981	8.3698	8.4018	8.5120	8.3922	8.3436	**8.35**
H3	7.1571	7.2918	7.3886	7.3399	7.4688	7.3375	7.4891	7.3357	7.1714	7.3425	7.5004	7.1571	7.2918	7.3886	7.3399	7.4688	7.3375	7.4891	7.3357	7.4539	7.3425	7.5004	**7.06**
H5	6.9980	7.1862	7.2820	7.2712	7.4032	7.2664	7.4155	7.2622	7.0977	7.2761	7.4309	6.9980	7.1862	7.2820	7.2712	7.4032	7.2664	7.4155	7.2622	7.3809	7.2761	7.4309	**7.06**
H6	7.8769	8.0448	8.1304	8.1465	8.2585	8.1404	8.2937	8.1348	7.9737	8.1527	8.3050	7.8769	8.0448	8.1304	8.1465	8.2585	8.1404	8.2937	8.1348	8.2470	8.1527	8.3050	**8.35**
H8	4.7660	4.8208	4.8400	4.8620	4.9500	4.8596	4.9722	4.8577	4.6835	4.8647	4.9519	4.7661	4.8208	4.8400	4.8620	4.9500	4.8596	4.9722	4.8577	4.9945	4.8647	4.9519	**4.88**
H(9A-9B)	1.7801	1.8251	1.8387	1.8626	1.8155	1.8604	1.8120	1.8588	1.6726	1.8649	1.8574	1.7801	1.8251	1.8387	1.8626	1.8156	1.8604	1.8120	1.8588	2.0180	1.8649	1.8574	**2.05**
H(10A-10B)	1.4435	1.3291	1.2828	1.2725	1.2165	1.2763	1.2267	1.2806	1.0921	1.2692	1.1965	1.4435	1.3291	1.2828	1.2725	1.2165	1.2763	1.2267	1.2806	1.4442	1.2692	1.1965	**1.36**
H(11A-11C)	0.7625	0.7665	0.7452	0.7778	0.7499	0.7771	0.7503	0.7771	0.5866	0.7787	0.7325	0.7625	0.7665	0.7452	0.7778	0.7499	0.7771	0.7503	0.7771	0.9445	0.7787	0.7325	**0.77**
H(1`A)	2.7065	2.7209	2.7113	2.7166	2.6760	2.7172	2.6875	2.7184	2.6931	2.7164	2.6608	2.8208	2.8333	2.8304	2.8224	2.8015	2.8234	2.8121	2.8250	3.0511	2.8218	2.6608	**3.03**
H(1`B)	3.2753	3.3107	3.3498	3.3428	3.4055	3.3408	3.3884	3.3394	3.3693	3.3451	3.3789	3.0362	2.8613	2.8506	2.8046	2.7992	2.8080	2.7659	2.8120	2.9382	2.8017	3.3789	**3.23**
H(2`-3`A-2`-3`B)	1.6803	1.7391	1.7096	1.7781	1.7481	1.7756	1.7695	1.7736	1.5871	1.7810	1.7915	1.6803	1.7391	1.7096	1.7781	1.7481	1.7756	1.7695	1.7736	1.5871	1.7810	1.7915	**1.77**
H(4`A)	3.0362	2.8613	2.8506	2.8046	2.7992	2.8080	2.7659	2.8120	2.9382	2.8018	2.7647	3.2754	3.3107	3.3498	3.3428	3.4055	3.3408	3.3884	3.3394	3.3693	3.3451	2.7648	**3.03**
H(4`B)	2.8208	2.8333	2.8304	2.8224	2.8015	2.8234	2.8121	2.8250	3.0511	2.8218	2.7898	2.7065	2.7209	2.7113	2.7166	2.6760	2.7172	2.6875	2.7184	2.6931	2.7164	2.7898	**3.23**
Nuclei	VSXC																						
C1	132.9799	133.5448	134.3194	133.7889	135.4306	133.7784	134.5787	133.7656	134.8603	133.8001	135.1087	132.9799	133.5448	134.3194	133.7889	135.4306	133.7784	134.5787	133.7656	134.8603	133.8001	135.1087	**133.8**
C2	130.3508	130.4696	131.0673	130.4284	130.9709	130.4361	131.5414	130.4416	131.4163	130.4222	131.6461	130.3508	130.4696	131.0673	130.4284	130.9709	130.4361	131.5414	130.4416	131.4163	130.4222	131.6461	**132.1**
C3	114.7609	115.8434	116.3799	116.2619	116.9330	116.2424	117.2859	116.2202	117.1824	116.2818	117.3883	114.7609	115.8434	116.3799	116.2619	116.9330	116.2424	117.2859	116.2202	117.1824	116.2818	117.3883	**115.8**
C4	168.2029	169.1716	169.8086	169.6749	170.3621	169.6471	170.9472	169.6172	170.7674	169.7030	171.0735	168.2029	169.1716	169.8086	169.6749	170.3621	169.6471	170.9472	169.6172	170.7674	169.7029	171.0735	**165.8**
C5	112.8866	114.3236	114.8634	115.1078	115.8096	115.0619	116.1278	115.0141	115.9813	115.1529	116.2640	112.8866	114.3236	114.8634	115.1078	115.8096	115.0619	116.1278	115.0141	115.9813	115.1530	116.2640	**115.8**
C6	128.8107	130.4481	131.4649	131.4583	132.7728	131.3958	133.3057	131.3316	133.0226	131.5198	133.4595	128.8107	130.4481	131.4649	131.4583	132.7728	131.3958	133.3057	131.3316	133.0226	131.5198	133.4595	**132.1**
C7	193.4717	198.3010	199.5199	200.7253	201.5793	200.5819	205.7683	200.4360	204.9833	200.8623	207.0019	193.4717	198.3010	199.5199	200.7253	201.5793	200.5819	205.7683	200.4360	204.9833	200.8623	207.0019	**198.9**
C8	71.7209	72.5535	73.1801	72.9376	73.8113	72.9181	74.1060	72.8964	74.0842	72.9575	74.6516	71.7209	72.5535	73.1801	72.9376	73.8113	72.9181	74.1060	72.8964	74.0842	72.9574	74.6516	**69.3**
C9	44.3091	44.8449	45.1242	45.1109	45.3318	45.0974	45.8396	45.0821	45.6858	45.1252	45.9770	44.3091	44.8449	45.1242	45.1109	45.3318	45.0974	45.8396	45.0821	45.6858	45.1252	45.9769	**31.5**
C10	25.3631	26.3064	26.4506	26.8102	27.2910	26.7810	27.3351	26.7499	27.2336	26.8398	27.4496	25.3631	26.3064	26.4506	26.8102	27.2910	26.7810	27.3351	26.7499	27.2336	26.8398	27.4496	**19.9**
C11	20.7378	20.7695	20.8784	20.7890	20.9061	20.7909	20.8367	20.7906	20.8679	20.7890	20.9332	20.7378	20.7695	20.8784	20.7890	20.9061	20.7909	20.8367	20.7906	20.8679	20.7890	20.9332	**14.3**
C1`	58.2226	58.8627	59.2141	59.2518	59.7613	59.2296	59.6047	59.2056	59.5721	59.2745	59.7499	61.2855	62.0083	62.3372	62.3910	62.9295	62.3699	62.9168	62.3471	62.8547	62.4125	63.2144	**50.6**
C2`	30.1698	30.5938	30.8097	30.8407	31.1892	30.8292	31.2109	30.8153	31.2002	30.8532	31.3605	28.0487	28.4859	28.7670	28.7405	29.1785	28.7278	29.1540	28.7129	29.1473	28.7542	29.2562	**23.8**
C3`	28.0487	28.4859	28.7670	28.7405	29.1785	28.7278	29.1540	28.7129	29.1473	28.7542	29.2562	30.1698	30.5938	30.8097	30.8407	31.1892	30.8292	31.2109	30.8153	31.2002	30.8532	31.3605	**23.8**
C4`	61.2855	62.0083	62.3372	62.3910	62.9295	62.3699	62.9168	62.3471	62.8547	62.4125	63.2144	58.2226	58.8627	59.2141	59.2518	59.7613	59.2296	59.6047	59.2056	59.5721	59.2745	59.7499	**50.6**
H2	8.5043	8.5259	8.5340	8.5083	8.4923	8.5098	8.5615	8.5113	8.5296	8.5069	8.5306	8.5043	8.5259	8.5340	8.5083	8.4923	8.5098	8.5615	8.5113	8.5296	8.5069	8.5306	**8.35**
H3	7.2041	7.3685	7.4558	7.4223	7.5339	7.4196	7.5584	7.4170	7.5441	7.4248	7.5718	7.2041	7.3685	7.4558	7.4223	7.5339	7.4196	7.5584	7.4170	7.5441	7.4248	7.5718	**7.06**
H5	7.0368	7.2361	7.3195	7.3244	7.4440	7.3193	7.4612	7.3143	7.4505	7.3292	7.4831	7.0368	7.2361	7.3195	7.3244	7.4440	7.3193	7.4612	7.3143	7.4505	7.3292	7.4831	**7.06**
H6	7.9402	8.0804	8.1629	8.1670	8.2799	8.1613	8.3258	8.1558	8.2996	8.1724	8.3474	7.9402	8.0804	8.1629	8.1670	8.2799	8.1613	8.3258	8.1558	8.2996	8.1724	8.3474	**8.35**
H8	4.3488	4.4446	4.4830	4.5059	4.5848	4.5020	4.6379	4.4982	4.6203	4.5097	4.6646	4.3488	4.4446	4.4830	4.5059	4.5848	4.5020	4.6379	4.4982	4.6203	4.5096	4.6646	**4.88**
H(9A-9B)	1.9468	1.9563	1.9635	1.9717	1.9486	1.9705	1.9534	1.9695	1.9460	1.9728	1.9245	1.9468	1.9563	1.9635	1.9717	1.9486	1.9705	1.9534	1.9695	1.9460	1.9728	1.9245	**2.05**
H(10A-10B)	1.6549	1.5515	1.5141	1.4862	1.4021	1.4904	1.3954	1.4949	1.4045	1.4821	1.3472	1.6549	1.5515	1.5141	1.4862	1.4021	1.4904	1.3954	1.4949	1.4045	1.4821	1.3472	**1.36**
H(11A-11C)	1.0078	1.0219	1.0067	1.0310	0.9982	1.0304	1.0023	1.0300	1.0022	1.0315	0.9938	1.0078	1.0219	1.0067	1.0310	0.9982	1.0304	1.0023	1.0300	1.0022	1.0315	0.9938	**0.77**
H(1`A)	2.5129	2.5608	2.5584	2.5744	2.5569	2.5738	2.5791	2.5733	2.5697	2.5749	2.5805	2.9472	2.9433	2.9265	2.9411	2.9221	2.9414	2.9226	2.9418	2.9277	2.9408	2.9271	**3.03**
H(1`B)	3.1586	3.1786	3.2131	3.1874	3.2636	3.1870	3.2590	3.1867	3.2459	3.1878	3.2656	2.8507	2.8087	2.8095	2.8060	2.8161	2.8059	2.8079	2.8060	2.8148	2.8060	2.8195	**3.23**
H(2`-3`A-2`-3`B)	1.9969	2.0391	2.0113	2.0663	2.0287	2.0645	2.0435	2.0630	2.0389	2.0679	2.0571	1.9969	2.0391	2.0113	2.0663	2.0287	2.0645	2.0435	2.0630	2.0389	2.0679	2.0571	**1.77**
H(4`A)	2.8507	2.8087	2.8095	2.8060	2.8161	2.8059	2.8079	2.8060	2.8148	2.8060	2.8195	3.1586	3.1786	3.2131	3.1874	3.2636	3.1870	3.2590	3.1867	3.2459	3.1878	3.2656	**3.03**
H(4`B)	2.9472	2.9433	2.9265	2.9411	2.9221	2.9414	2.9226	2.9418	2.9277	2.9408	2.9271	2.5129	2.5608	2.5584	2.5744	2.5569	2.5738	2.5791	2.5733	2.5697	2.5749	2.5805	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. XIII

Nuclei	R											S										Exp. [b]
	wB97											wB97										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.5194	137.5694	138.0796	137.9903	139.5805	137.9535	139.3576	137.9197	139.4471	138.0303	139.7190	136.5194	137.5694	138.0796	137.9903	139.5805	137.9535	139.3576	137.9197	139.4471	138.0302	139.7190	**133.8**
C2	140.4269	140.3358	140.8691	140.1553	140.7191	140.1691	140.9927	140.1817	140.8869	140.1416	140.9891	140.4269	140.3358	140.8691	140.1553	140.7191	140.1691	140.9927	140.1817	140.8869	140.1415	140.9892	**132.1**
C3	121.5174	122.1379	122.6998	122.3565	123.0564	122.3436	123.3074	122.3300	123.2520	122.3693	123.3970	121.5174	122.1379	122.6998	122.3565	123.0564	122.3434	123.3074	122.3299	123.2520	122.3694	123.3970	**115.8**
C4	174.2894	174.8437	175.4986	175.1890	175.8128	175.1664	176.3604	175.1432	176.2124	175.2102	176.4604	174.2894	174.8437	175.4986	175.1888	175.8128	175.1664	176.3604	175.1432	176.2124	175.2102	176.4604	**165.8**
C5	119.5219	120.7990	121.3961	121.4978	122.3313	121.4508	122.6135	121.4043	122.5189	121.5434	122.7700	119.5219	120.7990	121.3960	121.4976	122.3313	121.4510	122.6135	121.4043	122.5189	121.5434	122.7701	**115.8**
C6	136.6630	138.2616	139.4472	139.3054	140.8374	139.2411	141.0639	139.1751	140.8231	139.3653	141.3891	136.6630	138.2616	139.4472	139.3053	140.8374	139.2411	141.0639	139.1751	140.8231	139.3654	141.3891	**132.1**
C7	201.4834	206.6139	207.4634	209.4417	209.8309	209.2532	215.9182	209.0689	214.6939	209.6265	217.1938	201.4834	206.6139	207.4634	209.4417	209.8309	209.2532	215.9182	209.0689	214.6939	209.6263	217.1939	**198.9**
C8	61.9076	63.1189	63.5285	63.7225	64.5287	63.6812	64.9748	63.6405	64.8162	63.7635	65.4950	61.9077	63.1189	63.5284	63.7226	64.5287	63.6812	64.9748	63.6405	64.8162	63.7633	65.4951	**69.3**
C9	34.9590	34.7431	34.9674	34.6100	34.9988	34.6200	34.7266	34.6286	34.6954	34.5998	34.9146	34.9590	34.7431	34.9674	34.6099	34.9988	34.6200	34.7266	34.6286	34.6954	34.5998	34.9145	**31.5**
C10	18.2182	18.6328	18.8582	18.8774	19.3824	18.8618	19.1645	18.8453	19.1393	18.8923	19.3335	18.2182	18.6328	18.8582	18.8774	19.3824	18.8618	19.1645	18.8453	19.1393	18.8923	19.3335	**19.9**
C11	15.6605	15.7400	15.8627	15.7845	16.0377	15.7803	15.9543	15.7755	15.9469	15.7889	16.0956	15.6605	15.7400	15.8627	15.7845	16.0377	15.7803	15.9543	15.7755	15.9469	15.7890	16.0956	**14.3**
C1`	49.2054	49.9067	50.0783	50.3643	50.9579	50.3319	50.8766	50.2996	50.8098	50.3962	51.3133	52.9405	53.7375	54.0643	54.1917	54.7052	54.1598	54.8156	54.1280	54.7336	54.2229	55.0766	**50.6**
C2`	23.7861	24.0935	24.3287	24.2781	24.6956	24.2639	24.6624	24.2495	24.6296	24.2923	24.6415	23.1695	23.2934	23.6310	23.4056	23.8877	23.3972	23.8486	23.3880	23.8438	23.4142	23.7404	**23.8**
C3`	23.1695	23.2934	23.6310	23.4057	23.8877	23.3971	23.8486	23.3880	23.8438	23.4141	23.7402	23.7861	24.0935	24.3286	24.2780	24.6956	24.2639	24.6624	24.2495	24.6296	24.2923	24.6415	**23.8**
C4`	52.9405	53.7375	54.0643	54.1917	54.7052	54.1598	54.8156	54.1280	54.7336	54.2230	55.0770	49.2054	49.9067	50.0784	50.3643	50.9579	50.3319	50.8766	50.2996	50.8098	50.3961	51.3132	**50.6**
H2	8.8681	8.7541	8.8099	8.6731	8.6884	8.6796	8.6378	8.6854	8.6360	8.6666	8.6181	8.8681	8.7541	8.8099	8.6731	8.6884	8.6796	8.6378	8.6854	8.6360	8.6666	8.6181	**8.35**
H3	7.4384	7.5765	7.6668	7.6169	7.7406	7.6149	7.7561	7.6128	7.7479	7.6187	7.7730	7.4384	7.5765	7.6668	7.6169	7.7406	7.6149	7.7561	7.6128	7.7479	7.6187	7.7730	**7.06**
H5	7.2883	7.4763	7.5666	7.5600	7.6882	7.5550	7.7092	7.5498	7.6977	7.5649	7.7331	7.2883	7.4763	7.5666	7.5600	7.6882	7.5550	7.7092	7.5498	7.6977	7.5649	7.7331	**7.06**
H6	8.1624	8.3146	8.4330	8.4072	8.5462	8.4017	8.5655	8.3959	8.5452	8.4123	8.5874	8.1624	8.3146	8.4330	8.4072	8.5462	8.4017	8.5655	8.3959	8.5452	8.4123	8.5874	**8.35**
H8	4.2134	4.2738	4.3408	4.3252	4.4025	4.3216	4.4817	4.3180	4.4615	4.3285	4.4800	4.2134	4.2738	4.3408	4.3252	4.4025	4.3216	4.4817	4.3180	4.4615	4.3285	4.4800	**4.88**
H(9A-9B)	1.6731	1.7129	1.7065	1.7374	1.7556	1.7364	1.6776	1.7352	1.6726	1.7380	1.7178	1.6731	1.7129	1.7065	1.7374	1.7556	1.7364	1.6776	1.7352	1.6726	1.7381	1.7179	**2.05**
H(10A-10B)	1.3691	1.2281	1.2066	1.1519	1.0911	1.1568	1.1179	1.1616	1.1213	1.1472	1.1010	1.3691	1.2281	1.2066	1.1520	1.0911	1.1568	1.1179	1.1616	1.1213	1.1472	1.1010	**1.36**
H(11A-11C)	0.7709	0.7638	0.7486	0.7647	0.7310	0.7646	0.7311	0.7644	0.7315	0.7648	0.7203	0.7709	0.7638	0.7486	0.7647	0.7310	0.7646	0.7311	0.7644	0.7315	0.7648	0.7203	**0.77**
H(1`A)	2.6214	2.6146	2.6021	2.6010	2.5630	2.6020	2.5787	2.6029	2.5789	2.6000	2.5570	2.7655	2.7690	2.7492	2.7548	2.7238	2.7556	2.7330	2.7563	2.7351	2.7541	2.7077	**3.03**
H(1`B)	3.0521	3.0845	3.1117	3.1168	3.1755	3.1146	3.1592	3.1122	3.1545	3.1191	3.1653	2.7316	2.6336	2.5807	2.5957	2.5927	2.5976	2.5646	2.5995	2.5663	2.5941	2.5585	**3.23**
H(2`-3`A-2`-3`B)	1.6363	1.6962	1.6604	1.7316	1.6915	1.7290	1.7197	1.7265	1.7131	1.7341	1.7428	1.6363	1.6962	1.6603	1.7316	1.6915	1.7290	1.7197	1.7265	1.7131	1.7341	1.7428	**1.77**
H(4`A)	2.7316	2.6336	2.5807	2.5957	2.5927	2.5976	2.5646	2.5995	2.5663	2.5941	2.5585	3.0521	3.0845	3.1117	3.1168	3.1755	3.1146	3.1592	3.1122	3.1545	3.1190	3.1653	**3.03**
H(4`B)	2.7655	2.7690	2.7492	2.7548	2.7238	2.7556	2.7330	2.7563	2.7351	2.7541	2.7077	2.6214	2.6146	2.6020	2.6010	2.5630	2.6020	2.5787	2.6029	2.5789	2.6000	2.5570	**3.23**
Nuclei	wB97X																						
C1	137.9766	139.0348	139.5615	139.7498	141.9038	139.6550	141.1181	139.5647	141.0649	139.8295	141.4398	137.9765	139.0348	139.5616	139.7498	141.9038	139.6550	141.1181	139.5647	141.0649	139.8293	141.4398	**133.8**
C2	140.8355	140.7633	141.2870	140.5879	141.0754	140.6068	141.5044	140.6243	141.3594	140.5719	141.4950	140.8354	140.7633	141.2869	140.5879	141.0754	140.6068	141.5044	140.6242	141.3594	140.5719	141.4950	**132.1**
C3	122.2364	122.8727	123.4342	123.1085	123.8518	123.0954	124.0788	123.0811	123.9538	123.1210	124.1559	122.2364	122.8727	123.4341	123.1085	123.8518	123.0954	124.0788	123.0813	123.9538	123.1209	124.1559	**115.8**
C4	174.9612	175.5579	176.2171	175.8788	176.4658	175.8659	177.0811	175.8512	176.8817	175.8930	177.1775	174.9614	175.5579	176.2170	175.8788	176.4658	175.8659	177.0811	175.8512	176.8817	175.8930	177.1775	**165.8**
C5	120.2272	121.5229	122.1239	122.2792	123.1963	122.2251	123.4025	122.1704	123.2419	122.3290	123.5499	120.2271	121.5229	122.1240	122.2792	123.1963	122.2251	123.4025	122.1702	123.2419	122.3290	123.5500	**115.8**
C6	137.0717	138.7005	139.8784	139.6360	140.9084	139.5986	141.4835	139.5588	141.2029	139.6782	141.7655	137.0718	138.7005	139.8784	139.6360	140.9084	139.5986	141.4835	139.5588	141.2029	139.6783	141.7655	**132.1**
C7	203.1739	208.3154	209.2003	211.3740	212.3025	211.1326	217.7715	210.8968	216.3850	211.5943	218.9603	203.1742	208.3154	209.2004	211.3740	212.3025	211.1326	217.7715	210.8967	216.3850	211.5941	218.9603	**198.9**
C8	63.1864	64.3968	64.8287	65.0941	65.9082	65.0391	66.3729	64.9859	66.1122	65.1463	66.8276	63.1863	64.3968	64.8287	65.0941	65.9082	65.0390	66.3729	64.9859	66.1122	65.1462	66.8276	**69.3**
C9	35.8375	35.5746	35.7926	35.3700	35.5904	35.3964	35.5769	35.4217	35.4781	35.3494	35.7030	35.8375	35.5746	35.7927	35.3700	35.5904	35.3964	35.5769	35.4216	35.4781	35.3496	35.7030	**31.5**
C10	18.3607	18.7927	19.0156	19.0362	19.5064	19.0257	19.3889	19.0143	19.2972	19.0487	19.5359	18.3606	18.7927	19.0155	19.0362	19.5064	19.0257	19.3889	19.0143	19.2972	19.0487	19.5359	**19.9**
C11	15.6750	15.7621	15.8796	15.8054	16.0395	15.8041	16.0035	15.8022	15.9383	15.8082	16.1261	15.6751	15.7621	15.8797	15.8054	16.0396	15.8041	16.0035	15.8022	15.9383	15.8082	16.1261	**14.3**
C1`	49.9646	50.6995	50.8826	51.1794	51.7532	51.1477	51.6978	51.1157	51.5654	51.2108	52.1324	53.9228	54.7550	55.0967	55.2576	55.7916	55.2231	55.9248	55.1882	55.7834	55.2903	56.1503	**50.6**
C2`	24.2807	24.5787	24.8251	24.7702	25.1521	24.7585	25.1748	24.7463	25.0805	24.7824	25.0787	23.6488	23.7758	24.0992	23.8901	24.3927	23.8822	24.3619	23.8736	24.2981	23.8987	24.2530	**23.8**
C3`	23.6488	23.7758	24.0992	23.8902	24.3927	23.8822	24.3619	23.8736	24.2981	23.8987	24.2530	24.2806	24.5787	24.8252	24.7702	25.1521	24.7585	25.1748	24.7462	25.0805	24.7824	25.0787	**23.8**
C4`	53.9229	54.7550	55.0967	55.2576	55.7916	55.2231	55.9248	55.1883	55.7834	55.2904	56.1503	49.9646	50.6995	50.8825	51.1794	51.7532	51.1477	51.6978	51.1159	51.5654	51.2108	52.1324	**50.6**
H2	8.8371	8.7166	8.7711	8.6179	8.5782	8.6296	8.6010	8.6406	8.6048	8.6081	8.5832	8.8371	8.7166	8.7711	8.6179	8.5782	8.6296	8.6010	8.6406	8.6048	8.6081	8.5832	**8.35**
H3	7.4169	7.5537	7.6446	7.5961	7.7176	7.5944	7.7371	7.5927	7.7257	7.5978	7.7513	7.4169	7.5537	7.6446	7.5960	7.7176	7.5944	7.7371	7.5927	7.7257	7.5978	7.7513	**7.06**
H5	7.2613	7.4493	7.5394	7.5408	7.6738	7.5348	7.6911	7.5289	7.6771	7.5463	7.7124	7.2613	7.4493	7.5395	7.5408	7.6738	7.5348	7.6911	7.5289	7.6771	7.5463	7.7124	**7.06**
H6	8.1406	8.2926	8.4087	8.3703	8.4830	8.3681	8.5304	8.3656	8.5119	8.3732	8.5526	8.1406	8.2926	8.4087	8.3703	8.4830	8.3681	8.5304	8.3656	8.5119	8.3732	8.5526	**8.35**
H8	4.3072	4.3630	4.4254	4.4076	4.4891	4.4052	4.5561	4.4026	4.5364	4.4101	4.5532	4.3072	4.3630	4.4254	4.4076	4.4891	4.4052	4.5561	4.4026	4.5364	4.4101	4.5532	**4.88**
H(9A-9B)	1.6674	1.7042	1.7012	1.7158	1.6854	1.7186	1.6644	1.7211	1.6590	1.7142	1.6960	1.6674	1.7042	1.7012	1.7158	1.6854	1.7186	1.6644	1.7211	1.6590	1.7143	1.6960	**2.05**
H(10A-10B)	1.3567	1.2232	1.1944	1.1482	1.0878	1.1535	1.1154	1.1580	1.1170	1.1434	1.0997	1.3566	1.2232	1.1944	1.1482	1.0878	1.1535	1.1154	1.1588	1.1171	1.1434	1.0997	**1.36**
H(11A-11C)	0.7629	0.7583	0.7406	0.7593	0.7211	0.7598	0.7285	0.7603	0.7273	0.7591	0.7172	0.7629	0.7583	0.7406	0.7594	0.7211	0.7598	0.7285	0.7603	0.7273	0.7591	0.7172	**0.77**
H(1`A)	2.6430	2.6373	2.6231	2.6242	2.5827	2.6256	2.5985	2.6269	2.5966	2.6230	2.5733	2.7821	2.7826	2.7613	2.7723	2.7398	2.7728	2.7497	2.7733	2.7474	2.7720	2.7216	**3.03**
H(1`B)	3.0733	3.1032	3.1352	3.1345	3.1889	3.1329	3.1763	3.1312	3.1699	3.1363	3.1779	2.7503	2.6425	2.5949	2.6144	2.6223	2.6149	2.5804	2.6156	2.5770	2.6140	2.5722	**3.23**
H(2`-3`A-2`-3`B)	1.6363	1.6972	1.6607	1.7350	1.6982	1.7323	1.7208	1.7296	1.7115	1.7376	1.7435	1.6363	1.6972	1.6607	1.7350	1.6982	1.7323	1.7208	1.7296	1.7115	1.7376	1.7435	**1.77**
H(4`A)	2.7503	2.6425	2.5949	2.6144	2.6223	2.6149	2.5804	2.6156	2.5770	2.6120	2.5722	3.0733	3.1032	3.1352	3.1345	3.1889	3.1329	3.1763	3.1312	3.1699	3.1363	3.1779	**3.03**
H(4`B)	2.7821	2.7826	2.7613	2.7723	2.7398	2.7728	2.7497	2.7733	2.7474	2.7720	2.7216	2.6430	2.6373	2.6231	2.6242	2.5827	2.6256	2.5985	2.6269	2.5966	2.6230	2.5733	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S4. Cont. XIV

Nuclei	R											S										Exp. [b]
	X3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.6773	140.6339	141.3871	141.3959	143.2104	141.3744	142.6749	141.3492	142.6918	141.4196	143.0874	139.6773	140.6338	141.3870	141.3959	143.2103	141.3743	142.6749	141.3492	142.6917	141.4197	143.0874	**133.8**
C2	139.7585	139.7030	140.2707	139.5959	140.1045	139.6071	140.5552	139.6152	140.4809	139.5891	140.5496	139.7585	139.7031	140.2707	139.5959	140.1045	139.6070	140.5553	139.6152	140.4809	139.5892	140.5496	**132.1**
C3	121.9861	122.6802	123.2021	122.9487	123.6109	122.9409	123.8915	122.9293	123.8260	122.9597	123.9709	121.9861	122.6802	123.2020	122.9487	123.6108	122.9409	123.8915	122.9294	123.8260	122.9598	123.9709	**115.8**
C4	176.3489	177.1519	177.7719	177.5931	178.3081	177.5716	178.8712	177.5469	178.7271	177.6171	178.9724	176.3489	177.1519	177.7719	177.5931	178.3081	177.5717	178.8710	177.5469	178.7272	177.6171	178.9724	**165.8**
C5	120.0117	121.3023	121.8748	121.9683	122.7435	121.9330	122.9374	121.8946	122.8381	122.0053	123.0685	120.0117	121.3021	121.8748	121.9683	122.7435	121.9331	122.9374	121.8946	122.8382	122.0053	123.0685	**115.8**
C6	136.0777	137.9163	139.0245	138.8770	140.2567	138.8111	140.8782	138.7428	140.6178	138.9433	141.1139	136.0777	137.9163	139.0245	138.8770	140.2567	138.8111	140.8781	138.7429	140.6178	138.9433	141.1139	**132.1**
C7	203.8418	208.6857	209.8719	211.5711	212.3697	211.4134	217.6482	211.2522	216.4305	211.7242	218.8619	203.8418	208.6857	209.8719	211.5711	212.3697	211.4134	217.6482	211.2522	216.4305	211.7242	218.8619	**198.9**
C8	66.1642	67.3192	68.1329	67.9557	68.6724	67.9148	69.4452	67.8714	69.2516	67.9988	69.8035	66.1642	67.3193	68.1329	67.9557	68.6724	67.9147	69.4452	67.8713	69.2517	67.9988	69.8035	**69.3**
C9	38.7646	38.4469	38.7057	38.1661	38.2956	38.1796	38.4813	38.1901	38.4199	38.1570	38.5195	38.7646	38.4469	38.7058	38.1661	38.2956	38.1795	38.4814	38.1901	38.4199	38.1570	38.5195	**31.5**
C10	19.9254	20.3688	20.6718	20.6195	21.0584	20.6045	20.9520	20.5865	20.9311	20.6371	21.0703	19.9254	20.3688	20.6717	20.6195	21.0584	20.6046	20.9519	20.5866	20.9311	20.6371	21.0703	**19.9**
C11	16.1032	16.2609	16.3934	16.3309	16.5321	16.3298	16.4931	16.3257	16.4949	16.3356	16.6466	16.1032	16.2610	16.3934	16.3309	16.5321	16.3298	16.4930	16.3257	16.4950	16.3357	16.6466	**14.3**
C1`	52.1349	52.9699	53.2615	53.5201	54.0202	53.4881	54.0262	53.4530	54.0060	53.5539	54.4800	56.6972	57.6795	58.0349	58.2404	58.8200	58.2115	58.9232	58.1797	58.8550	58.2717	59.1638	**50.6**
C2`	25.9378	26.3725	26.6671	26.6054	27.0284	26.5922	27.0481	26.5763	27.0281	26.6219	26.8982	25.4958	25.6991	25.9933	25.8744	26.4624	25.8677	26.3257	25.8582	26.3244	25.8844	26.1388	**23.8**
C3`	25.4958	25.6990	25.9933	25.8744	26.4624	25.8675	26.3257	25.8581	26.3244	25.8845	26.1388	25.9378	26.3725	26.6670	26.6054	27.0284	26.5922	27.0481	26.5763	27.0282	26.6220	26.8982	**23.8**
C4`	56.6972	57.6795	58.0350	58.2404	58.8199	58.2115	58.9232	58.1798	58.8550	58.2717	59.1638	52.1349	52.9698	53.2616	53.5201	54.0201	53.4880	54.0262	53.4530	54.0060	53.5540	54.4800	**50.6**
H2	8.6885	8.5787	8.6123	8.4834	8.4677	8.4876	8.4706	8.4913	8.4769	8.4795	8.4498	8.6885	8.5787	8.6123	8.4834	8.4677	8.4876	8.4706	8.4913	8.4769	8.4795	8.4498	**8.35**
H3	7.3083	7.4443	7.5331	7.4918	7.6070	7.4899	7.6238	7.4873	7.6171	7.4935	7.6369	7.3083	7.4443	7.5331	7.4918	7.6070	7.4898	7.6238	7.4873	7.6171	7.4935	7.6369	**7.06**
H5	7.1554	7.3386	7.4286	7.4154	7.5358	7.4111	7.5494	7.4063	7.5380	7.4194	7.5670	7.1554	7.3386	7.4286	7.4154	7.5358	7.4111	7.5494	7.4063	7.5380	7.4194	7.5670	**7.06**
H6	7.9949	8.1713	8.2504	8.2624	8.3913	8.2566	8.4255	8.2504	8.4072	8.2679	8.4416	7.9949	8.1713	8.2504	8.2624	8.3913	8.2566	8.4255	8.2503	8.4072	8.2679	8.4416	**8.35**
H8	4.6134	4.6719	4.6840	4.7119	4.8091	4.7097	4.8283	4.7071	4.8111	4.7141	4.8165	4.6134	4.6719	4.6840	4.7119	4.8091	4.7097	4.8283	4.7071	4.8111	4.7141	4.8165	**4.88**
H(9A-9B)	1.6826	1.7269	1.7438	1.7330	1.7085	1.7308	1.7151	1.7280	1.7110	1.7352	1.7357	1.6826	1.7269	1.7438	1.7330	1.7085	1.7308	1.7151	1.7280	1.7110	1.7352	1.7357	**2.05**
H(10A-10B)	1.4152	1.3019	1.2490	1.2424	1.1819	1.2468	1.1937	1.2507	1.1977	1.2382	1.1796	1.4152	1.3019	1.2490	1.2424	1.1818	1.2468	1.1937	1.2507	1.1977	1.2382	1.1796	**1.36**
H(11A-11C)	0.7841	0.7886	0.7627	0.7950	0.7650	0.7947	0.7644	0.7939	0.7653	0.7954	0.7547	0.7841	0.7887	0.7627	0.7950	0.7650	0.7947	0.7644	0.7939	0.7654	0.7954	0.7547	**0.77**
H(1`A)	2.7328	2.7377	2.7159	2.7280	2.6777	2.7289	2.6901	2.7294	2.6907	2.7270	2.6660	2.8620	2.8614	2.8530	2.8464	2.8146	2.8476	2.8262	2.8483	2.8270	2.8453	2.7908	**3.03**
H(1`B)	3.1958	3.2381	3.2807	3.2709	3.3390	3.2686	3.3214	3.2659	3.3172	3.2731	3.3189	2.8696	2.7257	2.7170	2.6914	2.6864	2.6934	2.6675	2.6950	2.6661	2.6895	2.6649	**3.23**
H(2`-3`A-2`-3`B)	1.6696	1.7279	1.6920	1.7730	1.7330	1.7707	1.7519	1.7678	1.7473	1.7752	1.7781	1.6696	1.7279	1.6920	1.7730	1.7330	1.7707	1.7519	1.7678	1.7473	1.7752	1.7781	**1.77**
H(4`A)	2.8696	2.7256	2.7171	2.6914	2.6864	2.6934	2.6675	2.6950	2.6661	2.6895	2.6649	3.1958	3.2382	3.2807	3.2709	3.3390	3.2686	3.3214	3.2659	3.3172	3.2731	3.3189	**3.03**
H(4`B)	2.8620	2.8614	2.8530	2.8464	2.8146	2.8476	2.8262	2.8483	2.8270	2.8453	2.7908	2.7328	2.7377	2.7159	2.7280	2.6777	2.7289	2.6901	2.7294	2.6907	2.7270	2.6660	**3.23**

[a] methyl protons shifts are averaged
[b] according to [4]

Table S5. Theoretical chemical shifts (in ppm) of *(R,S)*-4-fluoro-α-pyrrolidinohexanophenone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S										Exp. [b]
	B3LYP											B3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.6461	140.7864	141.4058	141.3136	142.6443	141.2719	143.6401	141.2321	143.8057	141.3540	142.2745	139.6461	140.7864	141.4058	141.3136	142.6441	141.2719	143.6401	141.2321	142.2849	141.3540	142.2745	**132.2**
C2	139.5237	139.5283	140.0799	139.4229	139.8550	139.4233	140.6856	139.4245	140.5631	139.4217	140.3689	139.5237	139.5283	140.0799	139.4229	139.8550	139.4235	140.6856	139.4245	140.3254	139.4215	140.3689	**133.3**
C3	122.0016	122.7109	123.2701	122.8762	123.4842	122.8651	123.8294	122.8532	123.7527	122.8848	123.8436	122.0016	122.7109	123.2701	122.8762	123.4843	122.8651	123.8293	122.8532	123.6960	122.8848	123.8436	**117.6**
C4	176.3776	177.2686	177.9231	177.6172	178.2715	177.5929	178.7148	177.5682	178.5305	177.6383	179.0153	176.3776	177.2686	177.9231	177.6172	178.2715	177.5929	178.7149	177.5682	178.7108	177.6383	179.0153	**168.3**
C5	119.9008	121.1508	121.7637	121.7354	122.5277	121.6950	122.8173	121.6548	122.6947	121.7720	122.9044	119.9008	121.1508	121.7637	121.7355	122.5277	121.6952	122.8174	121.6548	122.6376	121.7721	122.9044	**117.6**
C6	135.7284	137.7097	138.8506	138.7726	140.3125	138.7018	140.2739	138.6307	139.9664	138.8376	141.3542	135.7284	137.7097	138.8506	138.7726	140.3125	138.7019	140.2738	138.6307	140.6449	138.8377	141.3542	**133.3**
C7	203.8433	208.7706	209.8361	211.3608	211.9257	211.1952	218.3779	211.0306	217.2932	211.5170	218.0294	203.8433	208.7706	209.8361	211.3607	211.9257	211.1952	218.3780	211.0306	215.9741	211.5172	218.0294	**195.8**
C8	66.5250	67.8264	68.3186	68.2996	69.3467	68.2734	70.0962	68.2461	69.9127	68.3213	70.3036	66.5250	67.8264	68.3186	68.2996	69.3467	68.2734	70.0962	68.2461	69.8306	68.3213	70.3036	**70.4**
C9	37.2783	36.9954	37.1608	36.7912	37.1386	36.7999	36.9134	36.8081	36.8238	36.7803	37.4426	37.2783	36.9954	37.1608	36.7911	37.1386	36.7999	36.9134	36.8081	37.2550	36.7803	37.4426	**31.1**
C10	29.1554	29.7052	30.2009	29.9688	30.7342	29.9463	30.3781	29.9237	30.3314	29.9886	30.6796	29.1554	29.7052	30.2009	29.9690	30.7343	29.9462	30.3780	29.9236	30.5104	29.9887	30.6796	**26.9**
C11	29.2176	29.3890	29.6800	29.3092	29.7544	29.3137	29.7204	29.3173	29.7037	29.3025	29.8834	29.2176	29.3890	29.6801	29.3092	29.7544	29.3137	29.7204	29.3173	29.7502	29.3025	29.8834	**23.4**
C12	16.6743	16.8847	16.9795	16.9675	17.0657	16.9553	17.1035	16.9436	17.0812	16.9780	17.0345	16.6743	16.8847	16.9795	16.9675	17.0657	16.9553	17.1034	16.9436	17.0289	16.9780	17.0345	**13.8**
C1`	52.3408	53.1867	53.5262	53.7049	54.2316	53.6668	54.3062	53.6291	54.2417	53.7402	54.7652	56.8561	58.0291	58.4014	58.4592	58.9820	58.4317	59.1878	58.4037	59.0555	58.4833	59.3691	**53.3**
C2`	26.1882	26.7217	27.0852	26.8508	27.3658	26.8407	27.3737	26.8301	27.3214	26.8583	27.1841	25.8103	26.0266	26.4225	26.1449	26.6169	26.1303	26.7163	26.1161	26.5729	26.1578	26.3817	**24.2**
C3`	25.8103	26.0266	26.4225	26.1449	26.6168	26.1303	26.7163	26.1161	26.6985	26.1577	26.3817	26.1882	26.7217	27.0852	26.8508	27.3658	26.8408	27.3737	26.8301	27.3873	26.8582	27.1841	**24.1**
C4`	56.8561	58.0291	58.4014	58.4593	58.9820	58.4317	59.1878	58.4037	59.0876	58.4834	59.3691	52.3408	53.1867	53.5262	53.7050	54.2316	53.6670	54.3062	53.6290	54.1753	53.7402	54.7652	**56.3**
H2	8.6809	8.5543	8.6087	8.4781	8.4949	8.4829	8.4082	8.4875	8.3955	8.4732	8.5014	8.6809	8.5543	8.6087	8.4781	8.4949	8.4829	8.4082	8.4875	8.4977	8.4732	8.5014	**8.2**
H3	7.3091	7.4552	7.5406	7.4963	7.6103	7.4942	7.6075	7.4919	7.5968	7.4981	7.6474	7.3091	7.4552	7.5406	7.4963	7.6103	7.4942	7.6075	7.4919	7.6192	7.4981	7.6474	**7.36**
H5	7.1276	7.2806	7.3732	7.3462	7.4808	7.3421	7.5147	7.3379	7.5013	7.3498	7.5128	7.1276	7.2806	7.3732	7.3462	7.4808	7.3421	7.5147	7.3379	7.4705	7.3498	7.5128	**7.36**
H6	7.9680	8.1482	8.2416	8.2410	8.3613	8.2351	8.3599	8.2291	8.3335	8.2462	8.4392	7.9680	8.1482	8.2416	8.2410	8.3613	8.2351	8.3599	8.2291	8.3823	8.2462	8.4392	**8.2**
H8	4.6493	4.7076	4.7462	4.7448	4.7972	4.7412	4.8339	4.7377	4.8186	4.7480	4.8140	4.6493	4.7076	4.7462	4.7448	4.7972	4.7412	4.8339	4.7377	4.8162	4.7480	4.8140	**5.4**
H(9A-9B)	1.7031	1.7451	1.7428	1.7658	1.8039	1.7645	1.6855	1.7631	1.6726	1.7666	1.8372	1.7031	1.7451	1.7428	1.7658	1.8039	1.7645	1.6855	1.7631	1.7829	1.7666	1.8372	**2.08**
H(10A)	1.0022	0.8621	0.8587	0.8274	0.7397	0.8276	0.8447	0.8281	0.8427	0.8272	0.7965	1.0022	0.8621	0.8587	0.8274	0.7397	0.8276	0.8447	0.8281	0.7822	0.8272	0.7965	**1.14**
H(10B)	1.6642	1.5565	1.4947	1.4743	1.3918	1.4794	1.3895	1.4845	1.3962	1.4693	1.3592	1.6642	1.5565	1.4947	1.4743	1.3918	1.4794	1.3895	1.4845	1.3901	1.4693	1.3592	**1.28**
H(11A-11B)	1.0615	1.0779	1.0484	1.0922	1.0551	1.0910	1.0592	1.0898	1.0563	1.0931	1.0432	1.0615	1.0779	1.0484	1.0922	1.0551	1.0910	1.0592	1.0898	1.0490	1.0931	1.0432	**1.28**
H(12A-12C)	0.9351	0.9251	0.9017	0.9172	0.8775	0.9172	0.9015	0.9173	0.9005	0.9171	0.8785	0.9351	0.9251	0.9017	0.9172	0.8775	0.9172	0.9015	0.9173	0.8821	0.9171	0.8785	**0.82**
H(1`A)	2.7510	2.7458	2.7299	2.7316	2.6917	2.7321	2.7055	2.7326	2.7038	2.7310	2.6732	2.8761	2.8891	2.8657	2.8618	2.8352	2.8637	2.8372	2.8655	2.8463	2.8598	2.8089	**3.38**
H(1`B)	3.2052	3.2576	3.2845	3.2906	3.3582	3.2880	3.3290	3.2854	3.3214	3.2928	3.3427	2.8957	2.7389	2.7000	2.7100	2.7063	2.7096	2.6874	2.7096	2.6733	2.7104	2.6644	**3.71**
H(2`A)	1.6352	1.6825	1.6512	1.6984	1.6442	1.6972	1.6749	1.6960	1.6698	1.6994	1.6809	1.5136	1.5612	1.5313	1.5819	1.5258	1.5803	1.5795	1.5786	1.5539	1.5833	1.5775	**2.08**
H(2`B)	1.8433	1.8614	1.8185	1.9039	1.8569	1.8998	1.8670	1.8959	1.8604	1.9077	1.8864	1.6988	1.8177	1.7693	1.8877	1.8415	1.8827	1.8996	1.8777	1.8567	1.8924	1.9131	**2.24**
H(3`A)	1.5136	1.5612	1.5313	1.5819	1.5258	1.5803	1.5795	1.5786	1.5746	1.5833	1.5775	1.6352	1.6825	1.6512	1.6984	1.6442	1.6972	1.6749	1.6960	1.6638	1.6994	1.6809	**2.08**
H(3`B)	1.6988	1.8177	1.7693	1.8877	1.8415	1.8827	1.8996	1.8777	1.8902	1.8924	1.9131	1.8433	1.8614	1.8185	1.9039	1.8569	1.8998	1.8670	1.8959	1.8491	1.9077	1.8864	**2.16**
H(4`A)	2.8957	2.7389	2.7000	2.7100	2.7062	2.7097	2.6874	2.7096	2.6927	2.7104	2.6644	3.2052	3.2576	3.2845	3.2906	3.3582	3.2880	3.3290	3.2854	3.3378	3.2928	3.3427	**3.09**
H(4`B)	2.8761	2.8891	2.8657	2.8618	2.8352	2.8637	2.8372	2.8655	2.8376	2.8598	2.8089	2.7510	2.7458	2.7299	2.7316	2.6917	2.7321	2.7055	2.7326	2.7068	2.7309	2.6732	**3.68**
Nuclei	B3P86											B3P86										
C1	136.9940	137.7944	138.6085	138.2350	139.7431	138.2382	139.0549	138.2181	139.2253	138.2747	139.3602	136.9940	137.7944	138.6085	138.2350	139.7431	138.2382	139.0549	138.2181	139.2253	138.2747	139.3602	**132.2**
C2	138.4918	138.4799	139.0262	138.3378	138.8680	138.3690	139.3660	138.3780	139.3322	138.3524	139.3371	138.4918	138.4799	139.0263	138.3378	138.8680	138.3690	139.3660	138.3780	139.3322	138.3524	139.3370	**133.3**
C3	121.1824	121.9496	122.5869	122.1830	122.8942	122.1927	123.1872	122.1799	123.2106	122.2177	123.2677	121.1824	121.9496	122.5869	122.1830	122.8942	122.1927	123.1872	122.1799	123.2106	122.2176	123.2677	**117.6**
C4	173.8427	174.7165	175.3771	175.1356	175.7951	175.1315	176.4511	175.1055	176.3855	175.1833	176.5856	173.8427	174.7165	175.3770	175.1356	175.7951	175.1316	176.4509	175.1055	176.3855	175.1833	176.5856	**168.3**
C5	119.1719	120.4985	121.1966	121.1547	122.0481	121.1341	122.2667	121.0918	122.2598	121.2183	122.4439	119.1720	120.4985	121.1966	121.1548	122.0481	121.1341	122.2666	121.0918	122.2598	121.2183	122.4440	**117.6**
C6	134.7482	136.6843	137.8759	137.8221	139.4030	137.7676	140.1213	137.6922	139.9543	137.9183	140.4961	134.7482	136.6843	137.8759	137.8222	139.4030	137.7676	140.1212	137.6922	139.9543	137.9184	140.4961	**133.3**
C7	201.9446	206.3100	207.5577	208.7236	209.4429	208.6038	214.1587	208.4609	213.2041	208.8803	215.2563	201.9446	206.3100	207.5577	208.7236	209.4429	208.6038	214.1587	208.4609	213.2041	208.8803	215.2563	**195.8**
C8	64.8267	65.9499	66.7652	66.4439	67.5035	66.4394	68.0435	66.4121	68.0288	66.4911	68.4972	64.8267	65.9499	66.7652	66.4439	67.5035	66.4394	68.0435	66.4121	68.0288	66.4911	68.4972	**70.4**
C9	36.2486	36.0166	36.3080	35.8772	36.2423	35.9043	36.4484	35.9094	36.4633	35.8954	36.5768	36.2486	36.0166	36.3080	35.8771	36.2423	35.9042	36.4484	35.9094	36.4633	35.8953	36.5768	**31.1**
C10	27.9025	28.4047	28.9185	28.7349	29.4674	28.7300	29.2804	28.7039	29.3529	28.7840	29.4513	27.9025	28.4046	28.9185	28.7349	29.4674	28.7300	29.2804	28.7039	29.3529	28.7840	29.4513	**26.9**
C11	27.6635	27.8017	28.0996	27.7450	28.1783	27.7719	28.1762	27.7764	28.2670	27.7630	28.3209	27.6635	27.8016	28.0997	27.7450	28.1783	27.7718	28.1763	27.7764	28.2670	27.7629	28.3209	**23.4**
C12	16.2632	16.4367	16.5321	16.5461	16.6415	16.5582	16.6066	16.5487	16.6923	16.5790	16.6054	16.2632	16.4367	16.5320	16.5462	16.6415	16.5582	16.6066	16.5487	16.6923	16.5790	16.6054	**13.8**
C1`	51.2290	52.0562	52.3501	52.5739	53.1095	52.5603	53.1155	52.5254	53.1243	52.6314	53.6115	55.5727	56.7173	57.1113	57.1649	57.6791	57.1609	57.8424	57.1348	57.8756	57.2124	58.1048	**53.3**
C2`	24.9726	25.3900	25.7808	25.5444	26.0182	25.5568	26.0360	25.5472	26.1322	25.5763	25.8635	24.4400	24.6560	24.9992	24.8082	25.2508	24.8198	25.2291	24.8094	25.3062	24.8411	25.0933	**24.2**
C3`	24.4400	24.6560	24.9990	24.8081	25.2508	24.8198	25.2291	24.8094	25.3062	24.8410	25.0933	24.9726	25.3900	25.7807	25.5444	26.0182	25.5568	26.0361	25.5472	26.1322	25.5763	25.8636	**24.1**
C4`	55.5727	56.7174	57.1114	57.1649	57.6791	57.1610	57.8424	57.1348	57.8756	57.2124	58.1048	51.2290	52.0562	52.3501	52.5740	53.1095	52.5603	53.1154	52.5254	53.1243	52.6314	53.6115	**56.3**
H2	8.7290	8.6450	8.6624	8.5763	8.5750	8.5811	8.6077	8.5843	8.6051	8.5730	8.5861	8.7290	8.6450	8.6624	8.5763	8.5750	8.5811	8.6077	8.5842	8.6051	8.5730	8.5861	**8.2**
H3	7.3236	7.4766	7.5645	7.5245	7.6430	7.5235	7.6668	7.5205	7.6614	7.5267	7.6840	7.3236	7.4766	7.5645	7.5245	7.6430	7.5234	7.6668	7.5205	7.6614	7.5267	7.6839	**7.36**
H5	7.1584	7.3295	7.4289	7.3944	7.5356	7.3914	7.5373	7.3866	7.5325	7.3986	7.5649	7.1584	7.3295	7.4289	7.3944	7.5356	7.3914	7.5373	7.3866	7.5325	7.3985	7.5649	**7.36**
H6	8.0391	8.2172	8.3003	8.3183	8.4387	8.3130	8.5009	8.3060	8.4828	8.3245	8.5279	8.0391	8.2172	8.3003	8.3183	8.4387	8.3130	8.5009	8.3060	8.4828	8.3245	8.5279	**8.2**
H8	4.6504	4.7081	4.7313	4.7587	4.8048	4.7563	4.8490	4.7522	4.8350	4.7621	4.8465	4.6504	4.7081	4.7313	4.7587	4.8048	4.7563	4.8490	4.7522	4.8350	4.7621	4.8465	**5.4**
H(9A-9B)	1.7737	1.8107	1.8173	1.8361	1.8597	1.8350	1.8591	1.8321	1.8559	1.8386	1.8916	1.7737	1.8107	1.8173	1.8361	1.8597	1.8350	1.8591	1.8321	1.8559	1.8386	1.8916	**2.08**
H(10A)	0.9752	0.8444	0.8027	0.7996	0.7098	0.8026	0.7576	0.8038	0.7475	0.7979	0.7640	0.9752	0.8444	0.8027	0.7996	0.7098	0.8026	0.7576	0.8038	0.7475	0.7979	0.7640	**1.14**
H(10B)	1.6857	1.5846	1.5093	1.4961	1.4096	1.5034	1.4026	1.5090	1.4115	1.4903	1.3722	1.6857	1.5846	1.5093	1.4961	1.4096	1.5034	1.4026	1.5090	1.4115	1.4903	1.3722	**1.28**
H(11A-11B)	1.0296	1.0511	1.0141	1.0605	1.0240	1.0614	1.0238	1.0603	1.0254	1.0611	1.0130	1.0296	1.0511	1.0141	1.0605	1.0240	1.0614	1.0238	1.0603	1.0254	1.0611	1.0130	**1.28**
H(12A-12C)	0.8986	0.8890	0.8627	0.8785	0.8412	0.8804	0.8463	0.8804	0.8493	0.8780	0.8425	0.8986	0.8890	0.8627	0.8785	0.8412	0.8804	0.8463	0.8804	0.8493	0.8780	0.8425	**0.82**
H(1`A)	2.7041	2.6985	2.6865	2.6863	2.6464	2.6882	2.6613	2.6883	2.6657	2.6858	2.6366	2.8371	2.8452	2.8347	2.8253	2.7986	2.8283	2.8066	2.8295	2.8150	2.8235	2.7746	**3.38**
H(1`B)	3.2036	3.2482	3.2821	3.2812	3.3423	3.2798	3.3295	3.2766	3.3304	3.2838	3.3300	2.9405	2.7570	2.7404	2.7125	2.7146	2.7151	2.6633	2.7161	2.6706	2.7113	2.6518	**3.71**
H(2`A)	1.6259	1.6711	1.6444	1.6878	1.6399	1.6880	1.6624	1.6865	1.6634	1.6887	1.6744	1.4935	1.5391	1.5121	1.5598	1.5104	1.5599	1.5432	1.5581	1.5414	1.5609	1.5631	**2.08**
H(2`B)	1.8219	1.8427	1.7996	1.8852	1.8441	1.8829	1.8426	1.8789	1.8389	1.8888	1.8732	1.6960	1.8018	1.7559	1.8659	1.8263	1.8630	1.8475	1.8584	1.8422	1.8699	1.9035	**2.24**
H(3`A)	1.4935	1.5391	1.5121	1.5598	1.5104	1.5599	1.5432	1.5581	1.5414	1.5609	1.5631	1.6259	1.6711	1.6444	1.6878	1.6399	1.6880	1.6624	1.6865	1.6634	1.6887	1.6744	**2.08**
H(3`B)	1.6960	1.8018	1.7559	1.8659	1.8263	1.8630	1.8475	1.8584	1.8422	1.8699	1.9035	1.8219	1.8428	1.7996	1.8852	1.8441	1.8829	1.8426	1.8789	1.8389	1.8888	1.8732	**2.16**
H(4`A)	2.9405	2.7570	2.7404	2.7125	2.7146	2.7151	2.6633	2.7161	2.6706	2.7113	2.6518	3.2036	3.2482	3.2821	3.2812	3.3423	3.2797	3.3295	3.2766	3.3304	3.2838	3.3300	**3.09**
H(4`B)	2.8371	2.8452	2.8347	2.8253	2.7986	2.8283	2.8065	2.8295	2.8150	2.8235	2.7746	2.7041	2.6985	2.6865	2.6864	2.6464	2.6882	2.6612	2.6883	2.6657	2.6858	2.6366	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S5. Cont. I

Nuclei	R											S										Exp. [b]
	B3PW91																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.2683	138.3110	139.0251	138.7632	140.5159	138.7452	139.6322	138.7174	139.6500	138.7819	139.7985	137.2684	138.3110	139.0253	138.7632	140.1969	138.7451	139.6321	138.7176	139.6500	138.7819	139.7985	**132.2**
C2	138.6410	138.6605	139.1565	138.5404	139.4008	138.5539	139.5783	138.5587	139.4533	138.5296	139.5357	138.6410	138.6605	139.1563	138.5404	139.0818	138.5541	139.5784	138.5588	139.4534	138.5296	139.5357	**133.3**
C3	121.2594	122.0369	122.5996	122.2518	123.2768	122.2465	123.2362	122.2321	123.1632	122.2587	123.3253	121.2594	122.0369	122.5996	122.2518	122.9578	122.2466	123.2362	122.2321	123.1632	122.2587	123.3253	**117.6**
C4	173.9083	174.7882	175.3849	175.1648	176.1478	175.1468	176.4418	175.1200	176.2919	175.1841	176.5909	173.9084	174.7882	175.3847	175.1648	175.8288	175.1467	176.4417	175.1199	176.2919	175.1841	176.5909	**168.3**
C5	119.2542	120.5663	121.1995	121.2079	122.4095	121.1729	122.3091	121.1291	122.2069	121.2432	122.4865	119.2542	120.5663	121.1995	121.2079	122.0905	121.1728	122.3091	121.1291	122.2069	121.2432	122.4865	**117.6**
C6	134.7732	136.7237	137.8161	137.8284	139.7082	137.7607	140.0363	137.6852	139.7917	137.8952	140.4527	134.7731	136.7237	137.8164	137.8284	139.3892	137.7607	140.0362	137.6852	139.7918	137.8952	140.4527	**133.3**
C7	201.9625	206.6067	207.7419	209.0508	209.9966	208.9099	214.5826	208.7599	213.4600	209.1857	215.5648	201.9625	206.6067	207.7420	209.0508	209.6776	208.9099	214.5827	208.7599	213.4600	209.1857	215.5648	**195.8**
C8	64.7955	66.0465	66.7422	66.5611	67.8989	66.5428	68.2177	66.5141	68.0546	66.5791	68.5848	64.7955	66.0465	66.7421	66.5611	67.5799	66.5427	68.2177	66.5142	68.0547	66.5791	68.5848	**70.4**
C9	35.8212	35.6167	35.7953	35.4785	36.1538	35.4920	36.0457	35.4963	35.9670	35.4673	36.1611	35.8211	35.6167	35.7953	35.4785	35.8348	35.4919	36.0457	35.4963	35.9670	35.4673	36.1611	**31.1**
C10	27.6048	28.1256	28.5599	28.4339	29.4841	28.4158	28.9652	28.3894	28.9490	28.4536	29.1548	27.6048	28.1256	28.5601	28.4339	29.1651	28.4157	28.9652	28.3894	28.9490	28.4536	29.1548	**26.9**
C11	27.6205	27.7953	28.0026	27.7348	28.4759	27.7465	28.1492	27.7489	28.1449	27.7251	28.2980	27.6204	27.7953	28.0026	27.7347	28.1569	27.7465	28.1494	27.7489	28.1449	27.7251	28.2980	**23.4**
C12	16.2867	16.4838	16.5092	16.5803	16.9882	16.5767	16.6234	16.5648	16.6184	16.5862	16.6291	16.2866	16.4838	16.5092	16.5803	16.6692	16.5768	16.6233	16.5649	16.6184	16.5862	16.6291	**13.8**
C1`	51.1535	52.0040	52.2161	52.5029	53.3437	52.4743	53.0216	52.4374	52.9376	52.5328	53.5322	55.5036	56.6599	56.9753	57.0912	57.5895	57.0723	57.7369	57.0442	57.6754	57.1109	57.9949	**53.3**
C2`	25.2271	25.6707	25.9838	25.8063	26.5923	25.8042	26.2842	25.7931	26.2820	25.8101	26.0751	24.7121	24.9298	25.2094	25.0583	25.5027	25.0537	25.4471	25.0406	25.4422	25.0649	25.2887	**24.2**
C3`	24.7122	24.9298	25.2095	25.0584	25.8217	25.0538	25.4471	25.0407	25.4422	25.0649	25.2887	25.2272	25.6707	25.9838	25.8063	26.2733	25.8042	26.2842	25.7932	26.2820	25.8101	26.0751	**24.1**
C4`	55.5037	56.6599	56.9752	57.0912	57.9085	57.0722	57.7369	57.0442	57.6754	57.1109	57.9949	51.1535	52.0040	52.2161	52.5029	53.0247	52.4742	53.0217	52.4375	52.9376	52.5328	53.5322	**56.3**
H2	8.7062	8.5966	8.6228	8.5283	8.5523	8.5326	8.5570	8.5368	8.5576	8.5243	8.5484	8.7062	8.5966	8.6228	8.5283	8.5368	8.5326	8.5570	8.5368	8.5576	8.5243	8.5484	**8.2**
H3	7.3295	7.4785	7.5672	7.5237	7.6568	7.5220	7.6646	7.5199	7.6557	7.5254	7.6799	7.3295	7.4785	7.5672	7.5237	7.6413	7.5220	7.6646	7.5199	7.6557	7.5254	7.6799	**7.36**
H5	7.1489	7.3105	7.4083	7.3811	7.5343	7.3773	7.5250	7.3732	7.5160	7.3848	7.5528	7.1489	7.3105	7.4082	7.3811	7.5188	7.3773	7.5250	7.3732	7.5160	7.3848	7.5528	**7.36**
H6	8.0298	8.2071	8.2903	8.3046	8.4406	8.2988	8.4763	8.2927	8.4580	8.3103	8.5083	8.0298	8.2071	8.2903	8.3046	8.4251	8.2988	8.4763	8.2927	8.4580	8.3103	8.5083	**8.2**
H8	4.6458	4.7027	4.7242	4.7494	4.8097	4.7462	4.8338	4.7427	4.8182	4.7527	4.8284	4.6458	4.7027	4.7242	4.7494	4.7942	4.7462	4.8338	4.7427	4.8182	4.7527	4.8284	**5.4**
H(9A-9B)	1.7271	1.7604	1.7647	1.7862	1.8281	1.7847	1.8116	1.7831	1.8058	1.7877	1.8467	1.7270	1.7604	1.7647	1.7862	1.8126	1.7847	1.8115	1.7831	1.8058	1.7877	1.8467	**2.08**
H(10A)	0.9509	0.8160	0.7754	0.7757	0.7042	0.7773	0.7328	0.7788	0.7236	0.7745	0.7414	0.9509	0.8160	0.7754	0.7757	0.6887	0.7773	0.7328	0.7788	0.7236	0.7745	0.7414	**1.14**
H(10B)	1.6448	1.5409	1.4720	1.4568	1.3876	1.4629	1.3662	1.4686	1.3723	1.4513	1.3371	1.6448	1.5409	1.4720	1.4568	1.3721	1.4629	1.3661	1.4686	1.3723	1.4513	1.3371	**1.28**
H(11A-11B)	1.0151	1.0327	0.9969	1.0448	1.0240	1.0446	1.0073	1.0441	1.0064	1.0451	0.9964	1.0151	1.0327	0.9969	1.0448	1.0085	1.0446	1.0074	1.0441	1.0064	1.0451	0.9964	**1.28**
H(12A-12C)	0.8895	0.8782	0.8516	0.8692	0.8460	0.8701	0.8372	0.8709	0.8369	0.8685	0.8312	0.8895	0.8782	0.8516	0.8692	0.8306	0.8701	0.8372	0.8709	0.8369	0.8685	0.8312	**0.82**
H(1`A)	2.6965	2.6898	2.6781	2.6782	2.6537	2.6793	2.6560	2.6801	2.6567	2.6772	2.6259	2.8310	2.8358	2.8235	2.8145	2.7855	2.8167	2.7978	2.8187	2.8011	2.8123	2.7614	**3.38**
H(1`B)	3.1800	3.2261	3.2593	3.2607	3.3370	3.2586	3.3106	3.2563	3.3077	3.2628	3.3078	2.8932	2.7251	2.7090	2.6878	2.6888	2.6892	2.6489	2.6905	2.6501	2.6868	2.6322	**3.71**
H(2`A)	1.6162	1.6597	1.6325	1.6764	1.6422	1.6759	1.6524	1.6751	1.6488	1.6770	1.6619	1.4873	1.5328	1.5055	1.5538	1.5024	1.5530	1.5382	1.5519	1.5319	1.5547	1.5550	**2.08**
H(2`B)	1.8041	1.8261	1.7829	1.8695	1.8412	1.8663	1.8265	1.8629	1.8198	1.8728	1.8551	1.6820	1.7905	1.7437	1.8569	1.8120	1.8529	1.8384	1.8488	1.8273	1.8608	1.8876	**2.24**
H(3`A)	1.4873	1.5328	1.5055	1.5538	1.5179	1.5530	1.5382	1.5520	1.5319	1.5547	1.5550	1.6162	1.6597	1.6325	1.6764	1.6267	1.6759	1.6524	1.6751	1.6488	1.6770	1.6619	**2.08**
H(3`B)	1.6820	1.7905	1.7437	1.8569	1.8275	1.8530	1.8384	1.8488	1.8273	1.8608	1.8876	1.8041	1.8261	1.7828	1.8695	1.8257	1.8663	1.8265	1.8629	1.8198	1.8728	1.8551	**2.16**
H(4`A)	2.8932	2.7251	2.7090	2.6878	2.7043	2.6892	2.6488	2.6905	2.6501	2.6868	2.6322	3.1800	3.2261	3.2593	3.2607	3.3215	3.2586	3.3107	3.2563	3.3077	3.2628	3.3078	**3.09**
H(4`B)	2.8310	2.8358	2.8235	2.8145	2.8010	2.8168	2.7978	2.8186	2.8010	2.8123	2.7614	2.6964	2.6898	2.6781	2.6782	2.6382	2.6793	2.6560	2.6801	2.6567	2.6772	2.6259	**3.68**
Nuclei	B98																						
C1	138.2717	139.2268	139.9128	139.6404	141.1346	139.6354	140.5187	139.6273	140.5521	139.6471	140.7148	138.2716	139.2268	139.9128	139.6403	141.1346	139.6354	140.5187	139.6273	140.5521	139.6471	140.7148	**132.2**
C2	138.3658	138.4130	138.9400	138.2863	138.8240	138.3104	139.3230	138.3318	139.2146	138.2658	139.2706	138.3659	138.4130	138.9400	138.2864	138.8240	138.3104	139.3230	138.3318	139.2146	138.2658	139.2706	**133.3**
C3	120.9842	121.7099	122.2670	121.9312	122.6018	121.9357	122.8713	121.9373	122.8035	121.9289	122.9366	120.9842	121.7099	122.2670	121.9312	122.6018	121.9357	122.8714	121.9373	122.8035	121.9289	122.9366	**117.6**
C4	173.7110	174.5345	175.1530	174.9251	175.5881	174.9164	176.1881	174.9052	176.0450	174.9356	176.3122	173.7110	174.5345	175.1529	174.9250	175.5881	174.9164	176.1881	174.9052	176.0450	174.9356	176.3121	**168.3**
C5	118.9649	120.2115	120.8309	120.8532	121.6929	120.8287	121.9059	120.8015	121.8085	120.8789	122.0628	118.9649	120.2115	120.8308	120.8531	121.6929	120.8287	121.9058	120.8015	121.8086	120.8789	122.0628	**117.6**
C6	134.7148	136.5886	137.6963	137.6945	139.2264	137.6373	139.8807	137.5782	139.6376	137.7516	140.2548	134.7148	136.5886	137.6962	137.6945	139.2264	137.6373	139.8805	137.5782	139.6376	137.7516	140.2547	**133.3**
C7	200.3965	205.1270	206.2286	207.6183	208.2481	207.4848	213.3382	207.3483	212.1534	207.7463	214.3728	200.3966	205.1270	206.2283	207.6181	208.2481	207.4848	213.3381	207.3483	212.1534	207.7463	214.3729	**195.8**
C8	66.4517	67.6676	68.3328	68.1491	69.2093	68.1435	69.8344	68.1334	69.6562	68.1551	70.2146	66.4518	67.6676	68.3327	68.1492	69.2093	68.1435	69.8344	68.1334	69.6562	68.1551	70.2145	**70.4**
C9	37.0176	36.7658	36.9738	36.6486	37.0069	36.6711	37.2536	36.6906	37.1768	36.6290	37.3166	37.0176	36.7658	36.9738	36.6487	37.0069	36.6711	37.2535	36.6906	37.1768	36.6290	37.3166	**31.1**
C10	29.0963	29.5633	30.0409	29.8649	30.6136	29.8578	30.4248	29.8488	30.4145	29.8742	30.5904	29.0963	29.5633	30.0409	29.8648	30.6136	29.8578	30.4248	29.8488	30.4145	29.8742	30.5904	**26.9**
C11	28.9406	29.0642	29.3038	29.0121	29.4482	29.0334	29.4500	29.0515	29.4499	28.9937	29.5766	28.9406	29.0642	29.3037	29.0122	29.4482	29.0334	29.4499	29.0515	29.4499	28.9937	29.5766	**23.4**
C12	16.8660	17.0178	17.0824	17.1275	17.2327	17.1333	17.1960	17.1370	17.1978	17.1247	17.1872	16.8660	17.0178	17.0824	17.1275	17.2327	17.1333	17.1960	17.1370	17.1978	17.1247	17.1871	**13.8**
C1`	52.4335	53.2373	53.4722	53.7447	54.2542	53.7251	54.2559	53.7037	54.1881	53.7667	54.7388	56.8881	57.9505	58.2822	58.3585	58.8726	58.3505	59.0149	58.3396	58.9555	58.3681	59.2730	**53.3**
C2`	26.4056	26.8263	27.1611	26.9646	27.4451	26.9719	27.4788	26.9766	27.4727	26.9593	27.2819	25.8949	26.0922	26.4234	26.2448	26.6989	26.2484	26.6621	26.2500	26.6634	26.2440	26.4925	**24.2**
C3`	25.8950	26.0922	26.4233	26.2448	26.6989	26.2484	26.6622	26.2500	26.6634	26.2440	26.4925	26.4056	26.8263	27.1611	26.9645	27.4451	26.9719	27.4788	26.9766	27.4727	26.9593	27.2819	**24.1**
C4`	56.8881	57.9505	58.2822	58.3585	58.8726	58.3505	59.0149	58.3396	58.9555	58.3681	59.2731	52.4335	53.2373	53.4723	53.7448	54.2542	53.7251	54.2559	53.7037	54.1881	53.7667	54.7388	**56.3**
H2	8.6982	8.5886	8.6267	8.5270	8.5364	8.5306	8.5595	8.5343	8.5625	8.5239	8.5476	8.6982	8.5886	8.6267	8.5270	8.5364	8.5306	8.5595	8.5343	8.5625	8.5239	8.5476	**8.2**
H3	7.3243	7.4676	7.5579	7.5131	7.6334	7.5110	7.6550	7.5089	7.6467	7.5153	7.6698	7.3243	7.4676	7.5579	7.5131	7.6334	7.5110	7.6550	7.5089	7.6467	7.5153	7.6698	**7.36**
H5	7.1440	7.3083	7.4061	7.3810	7.5164	7.3767	7.5244	7.3726	7.5150	7.3852	7.5500	7.1439	7.3083	7.4061	7.3810	7.5164	7.3767	7.5244	7.3726	7.5150	7.3852	7.5500	**7.36**
H6	7.9991	8.1757	8.2656	8.2788	8.3991	8.2722	8.4528	8.2658	8.4346	8.2852	8.4806	7.9991	8.1757	8.2656	8.2788	8.3991	8.2722	8.4528	8.2658	8.4346	8.2852	8.4806	**8.2**
H8	4.6061	4.6605	4.6938	4.7112	4.7597	4.7072	4.8012	4.7034	4.7869	4.7153	4.7909	4.6061	4.6605	4.6938	4.7112	4.7597	4.7072	4.8012	4.7034	4.7869	4.7153	4.7909	**5.4**
H(9A-9B)	1.7078	1.7440	1.7500	1.7713	1.8003	1.7695	1.8017	1.7677	1.7957	1.7733	1.8332	1.7078	1.7440	1.7500	1.7713	1.8003	1.7695	1.8016	1.7677	1.7957	1.7733	1.8332	**2.08**
H(10A)	1.0100	0.8556	0.8250	0.8148	0.7317	0.8159	0.7784	0.8174	0.7740	0.8141	0.7819	1.0100	0.8556	0.8250	0.8147	0.7317	0.8159	0.7784	0.8174	0.7740	0.8141	0.7819	**1.14**
H(10B)	1.6566	1.5552	1.4953	1.4723	1.3892	1.4780	1.3847	1.4837	1.3917	1.4673	1.3576	1.6566	1.5552	1.4953	1.4723	1.3892	1.4780	1.3847	1.4837	1.3917	1.4673	1.3576	**1.28**
H(11A-11B)	1.0408	1.0554	1.0229	1.0697	1.0330	1.0689	1.0321	1.0683	1.0319	1.0707	1.0208	1.0408	1.0554	1.0229	1.0697	1.0330	1.0689	1.0321	1.0683	1.0319	1.0707	1.0208	**1.28**
H(12A-12C)	0.9137	0.8998	0.8755	0.8914	0.8529	0.8920	0.8600	0.8926	0.8602	0.8913	0.8544	0.9137	0.8998	0.8755	0.8914	0.8529	0.8919	0.8600	0.8926	0.8602	0.8913	0.8544	**0.82**
H(1`A)	2.7147	2.7096	2.6996	2.6998	2.6606	2.7004	2.6788	2.7011	2.6801	2.6994	2.6440	2.8444	2.8541	2.8420	2.8323	2.8064	2.8344	2.8190	2.8364	2.8217	2.8306	2.7831	**3.38**
H(1`B)	3.1966	3.2429	3.2781	3.2791	3.3414	3.2766	3.3292	3.2742	3.3264	3.2818	3.3230	2.8921	2.7320	2.7168	2.7042	2.7055	2.7047	2.6717	2.7055	2.6724	2.7042	2.6580	**3.71**
H(2`A)	1.6333	1.6782	1.6498	1.6962	1.6453	1.6953	1.6711	1.6945	1.6675	1.6974	1.6823	1.5089	1.5555	1.5281	1.5780	1.5262	1.5768	1.5620	1.5757	1.5564	1.5793	1.5795	**2.08**
H(2`B)	1.8213	1.8381	1.7969	1.8847	1.8396	1.8809	1.8420	1.8773	1.8357	1.8888	1.8673	1.7044	1.8128	1.7649	1.8774	1.8326	1.8732	1.8583	1.8691	1.8480	1.8817	1.9094	**2.24**
H(3`A)	1.5089	1.5555	1.5282	1.5780	1.5262	1.5768	1.5620	1.5757	1.5564	1.5793	1.5794	1.6333	1.6782	1.6498	1.6962	1.6453	1.6953	1.6711	1.6945	1.6675	1.6974	1.6823	**2.08**
H(3`B)	1.7044	1.8128	1.7649	1.8774	1.8326	1.8732	1.8583	1.8691	1.8480	1.8817	1.9094	1.8213	1.8381	1.7969	1.8847	1.8396	1.8809	1.8420	1.8773	1.8357	1.8888	1.8674	**2.16**
H(4`A)	2.8922	2.7320	2.7168	2.7042	2.7055	2.7047	2.6717	2.7055	2.6724	2.7042	2.6580	3.1966	3.2429	3.2782	3.2791	3.3414	3.2766	3.3292	3.2742	3.3264	3.2818	3.3229	**3.09**
H(4`B)	2.8445	2.8541	2.8420	2.8323	2.8064	2.8344	2.8190	2.8364	2.8217	2.8306	2.7831	2.7147	2.7096	2.6996	2.6998	2.6606	2.7004	2.6788	2.7011	2.6801	2.6994	2.6440	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S5. Cont. II

Nuclei	R											S										Exp. [b]
	B971											B971										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.8422	138.7483	139.4242	139.1819	140.7120	139.1719	140.0612	139.1604	140.1037	139.1965	140.2855	137.8422	138.7484	139.4242	139.1821	140.7120	139.1719	140.0613	139.1604	140.1037	139.1965	140.2855	**132.2**
C2	138.0799	138.1325	138.6399	138.0013	138.5299	138.0181	139.0158	138.0344	138.9092	137.9914	138.9727	138.0799	138.1323	138.6399	138.0013	138.5299	138.0181	139.0159	138.0344	138.9092	137.9914	138.9727	**133.3**
C3	120.7944	121.5215	122.0745	121.7507	122.4133	121.7473	122.6794	121.7430	122.6120	121.7596	122.7491	120.7944	121.5213	122.0745	121.7507	122.4133	121.7473	122.6794	121.7430	122.6119	121.7596	122.7491	**117.6**
C4	173.5971	174.4353	175.0465	174.8429	175.4966	174.8257	176.0952	174.8081	175.9514	174.8650	176.2233	173.5971	174.4353	175.0464	174.8427	175.4966	174.8257	176.0951	174.8081	175.9514	174.8650	176.2233	**168.3**
C5	118.7655	120.0340	120.6434	120.6887	121.5173	120.6557	121.7292	120.6223	121.6310	120.7260	121.8918	118.7655	120.0341	120.6435	120.6887	121.5173	120.6557	121.7293	120.6223	121.6311	120.7260	121.8918	**117.6**
C6	134.4339	136.3104	137.4295	137.4298	138.9589	137.3639	139.6148	137.2980	139.3694	137.4992	139.9897	134.4339	136.3105	137.4296	137.4299	138.9589	137.3638	139.6149	137.2980	139.3693	137.4992	139.9897	**133.3**
C7	200.2729	204.9044	206.0061	207.3978	208.0832	207.2601	213.0559	207.1201	211.9008	207.5342	214.1161	200.2729	204.9043	206.0060	207.3982	208.0832	207.2600	213.0562	207.1201	211.9008	207.5342	214.1161	**195.8**
C8	66.2684	67.4430	68.1355	67.9281	69.0012	67.9149	69.5789	67.8993	69.4095	67.9447	69.9754	66.2684	67.4428	68.1355	67.9282	69.0012	67.9149	69.5789	67.8993	69.4094	67.9447	69.9754	**70.4**
C9	37.0068	36.7745	37.0004	36.6683	37.0130	36.6820	37.2582	36.6949	37.1794	36.6609	37.3381	37.0068	36.7745	37.0004	36.6683	37.0130	36.6820	37.2583	36.6949	37.1793	36.6609	37.3381	**31.1**
C10	29.1505	29.6168	30.0966	29.9276	30.6566	29.9120	30.4719	29.8963	30.4604	29.9491	30.6448	29.1505	29.6167	30.0966	29.9277	30.6566	29.9120	30.4718	29.8963	30.4603	29.9491	30.6448	**26.9**
C11	28.9245	29.0484	29.2800	29.0001	29.4237	29.0135	29.4199	29.0260	29.4191	28.9929	29.5535	28.9245	29.0484	29.2800	29.0002	29.4237	29.0136	29.4199	29.0260	29.4191	28.9929	29.5535	**23.4**
C12	16.8110	16.9684	17.0237	17.0860	17.1770	17.0840	17.1383	17.0818	17.1401	17.0943	17.1357	16.8110	16.9683	17.0236	17.0860	17.1770	17.0840	17.1384	17.0818	17.1402	17.0943	17.1357	**13.8**
C1`	52.3547	53.1528	53.3732	53.6664	54.1692	53.6388	54.1635	53.6114	54.0937	53.6995	54.6432	56.7953	57.8551	58.1732	58.2702	58.7717	58.2546	58.9084	58.2381	58.8505	58.2908	59.1676	**53.3**
C2`	26.2113	26.6404	26.9708	26.7933	27.2590	26.7924	27.2868	26.7908	27.2809	26.7996	27.1109	25.6996	25.9076	26.2264	26.0756	26.5176	26.0712	26.4850	26.0668	26.4842	26.0859	26.3418	**24.2**
C3`	25.6996	25.9075	26.2264	26.0756	26.5176	26.0712	26.4850	26.0668	26.4841	26.0859	26.3418	26.2113	26.6403	26.9708	26.7933	27.2590	26.7924	27.2869	26.7908	27.2809	26.7996	27.1109	**24.1**
C4`	56.7953	57.8551	58.1732	58.2702	58.7717	58.2546	58.9084	58.2381	58.8505	58.2908	59.1676	52.3547	53.1529	53.3732	53.6663	54.1692	53.6387	54.1636	53.6114	54.0938	53.6995	54.6432	**56.3**
H2	8.6975	8.5947	8.6294	8.5328	8.5358	8.5359	8.5631	8.5391	8.5649	8.5303	8.5487	8.6975	8.5947	8.6294	8.5328	8.5358	8.5359	8.5631	8.5392	8.5649	8.5303	8.5487	**8.2**
H3	7.3205	7.4628	7.5522	7.5095	7.6286	7.5072	7.6504	7.5050	7.6421	7.5121	7.6648	7.3205	7.4628	7.5522	7.5095	7.6286	7.5072	7.6504	7.5050	7.6421	7.5121	7.6648	**7.36**
H5	7.1452	7.3121	7.4102	7.3844	7.5179	7.3799	7.5258	7.3755	7.5164	7.3890	7.5509	7.1452	7.3121	7.4102	7.3844	7.5179	7.3799	7.5258	7.3755	7.5164	7.3890	7.5509	**7.36**
H6	8.0058	8.1773	8.2674	8.2802	8.3987	8.2735	8.4538	8.2669	8.4356	8.2870	8.4802	8.0058	8.1773	8.2674	8.2802	8.3987	8.2735	8.4538	8.2669	8.4356	8.2870	8.4802	**8.2**
H8	4.6088	4.6617	4.6949	4.7134	4.7602	4.7093	4.8019	4.7054	4.7882	4.7177	4.7919	4.6088	4.6617	4.6949	4.7134	4.7602	4.7093	4.8019	4.7054	4.7882	4.7177	4.7919	**5.4**
H(9A-9B)	1.7161	1.7513	1.7594	1.7791	1.8050	1.7769	1.8071	1.7747	1.8006	1.7817	1.8378	1.7161	1.7513	1.7594	1.7791	1.8050	1.7769	1.8071	1.7747	1.8006	1.7817	1.8378	**2.08**
H(10A)	1.0061	0.8545	0.8220	0.8136	0.7285	0.8147	0.7778	0.8160	0.7734	0.8131	0.7805	1.0061	0.8545	0.8220	0.8136	0.7285	0.8147	0.7778	0.8160	0.7734	0.8131	0.7805	**1.14**
H(10B)	1.6552	1.5553	1.4937	1.4723	1.3892	1.4778	1.3845	1.4833	1.3914	1.4676	1.3570	1.6552	1.5553	1.4937	1.4723	1.3892	1.4778	1.3845	1.4833	1.3914	1.4676	1.3570	**1.28**
H(11A-11B)	1.0394	1.0539	1.0204	1.0676	1.0299	1.0668	1.0293	1.0659	1.0291	1.0689	1.0176	1.0394	1.0540	1.0204	1.0676	1.0299	1.0668	1.0293	1.0659	1.0291	1.0689	1.0176	**1.28**
H(12A-12C)	0.9081	0.8931	0.8684	0.8850	0.8458	0.8853	0.8530	0.8857	0.8533	0.8851	0.8480	0.9081	0.8931	0.8684	0.8850	0.8458	0.8853	0.8531	0.8857	0.8533	0.8851	0.8480	**0.82**
H(1`A)	2.7043	2.6996	2.6902	2.6911	2.6510	2.6915	2.6684	2.6920	2.6698	2.6911	2.6344	2.8345	2.8453	2.8343	2.8262	2.8010	2.8280	2.8117	2.8297	2.8145	2.8248	2.7764	**3.38**
H(1`B)	3.1997	3.2445	3.2806	3.2807	3.3411	3.2780	3.3284	3.2754	3.3259	3.2838	3.3220	2.8940	2.7339	2.7203	2.7054	2.7063	2.7059	2.6706	2.7066	2.6719	2.7055	2.6571	**3.71**
H(2`A)	1.6287	1.6741	1.6457	1.6934	1.6426	1.6922	1.6678	1.6912	1.6642	1.6949	1.6794	1.5028	1.5487	1.5215	1.5727	1.5216	1.5713	1.5566	1.5700	1.5510	1.5744	1.5740	**2.08**
H(2`B)	1.8228	1.8394	1.7978	1.8856	1.8402	1.8817	1.8424	1.8780	1.8362	1.8899	1.8679	1.7084	1.8122	1.7635	1.8768	1.8335	1.8725	1.8576	1.8684	1.8477	1.8812	1.9088	**2.24**
H(3`A)	1.5028	1.5487	1.5215	1.5727	1.5216	1.5713	1.5566	1.5700	1.5510	1.5744	1.5740	1.6287	1.6741	1.6458	1.6934	1.6426	1.6922	1.6678	1.6912	1.6642	1.6949	1.6794	**2.08**
H(3`B)	1.7084	1.8122	1.7635	1.8768	1.8335	1.8725	1.8576	1.8684	1.8477	1.8812	1.9088	1.8228	1.8394	1.7978	1.8856	1.8402	1.8817	1.8424	1.8780	1.8362	1.8899	1.8679	**2.16**
H(4`A)	2.8940	2.7339	2.7202	2.7054	2.7063	2.7059	2.6706	2.7066	2.6719	2.7055	2.6571	3.1997	3.2445	3.2806	3.2807	3.3411	3.2780	3.3285	3.2754	3.3259	3.2838	3.3220	**3.09**
H(4`B)	2.8345	2.8453	2.8343	2.8262	2.8010	2.8280	2.8117	2.8297	2.8145	2.8248	2.7764	2.7043	2.6996	2.6902	2.6911	2.6510	2.6915	2.6684	2.6920	2.6698	2.6911	2.6344	**3.68**
Nuclei	B972											B972										
C1	134.6971	135.8753	136.6169	136.6760	139.5533	136.6202	138.6512	136.5674	138.8176	136.7300	138.9783	134.6971	135.8753	136.6169	136.6759	139.5532	136.6203	138.6511	136.5674	138.8176	136.7300	138.9784	**132.2**
C2	136.1423	136.0686	136.6110	136.0524	136.6697	136.0535	137.1061	136.0530	137.0015	136.0477	137.0908	136.1423	136.0686	136.6111	136.0522	136.6695	136.0535	137.1058	136.0530	137.0015	136.0477	137.0908	**133.3**
C3	118.6863	119.3715	119.9318	119.6489	120.3301	119.6370	120.5956	119.6220	120.5384	119.6557	120.6719	118.6863	119.3715	119.9318	119.6490	120.3300	119.6370	120.5956	119.6220	120.5384	119.6557	120.6718	**117.6**
C4	170.5935	171.3556	171.9651	171.7320	172.1420	171.7133	172.7626	171.6911	172.6048	171.7444	172.8736	170.5934	171.3556	171.9650	171.7319	172.1420	171.7133	172.7627	171.6911	172.6048	171.7444	172.8736	**168.3**
C5	116.6790	117.8768	118.5101	118.5696	119.3676	118.5275	119.6225	118.4831	119.5235	118.6058	119.7745	116.6790	117.8768	118.5101	118.5698	119.3676	118.5275	119.6226	118.4831	119.5236	118.6058	119.7746	**117.6**
C6	132.2209	134.0034	135.0675	135.0035	135.8136	134.9461	136.4690	134.8843	136.2020	135.0514	136.7295	132.2209	134.0034	135.0674	135.0036	135.8136	134.9461	136.4689	134.8843	136.2019	135.0514	136.7297	**133.3**
C7	197.8670	202.6198	203.7484	205.3519	207.1219	205.1793	211.9055	205.0088	210.8523	205.5163	213.0007	197.8670	202.6198	203.7482	205.3522	207.1219	205.1793	211.9055	205.0088	210.8523	205.5163	213.0007	**195.8**
C8	63.5056	64.8160	65.4994	65.4760	66.7506	65.4415	67.2458	65.4046	67.0801	65.5049	67.6571	63.5056	64.8160	65.4994	65.4761	66.7505	65.4415	67.2458	65.4046	67.0801	65.5049	67.6571	**70.4**
C9	35.1659	34.9077	35.1070	34.8130	34.8409	34.8226	35.0047	34.8285	34.9106	34.7984	35.0884	35.1659	34.9077	35.1070	34.8131	34.8409	34.8226	35.0047	34.8285	34.9107	34.7984	35.0884	**31.1**
C10	27.4347	27.9105	28.3498	28.2459	28.8451	28.2248	28.6389	28.2010	28.6128	28.2615	28.8073	27.4347	27.9105	28.3499	28.2459	28.8452	28.2247	28.6389	28.2010	28.6128	28.2615	28.8074	**26.9**
C11	27.6676	27.7939	28.0328	27.8076	28.1669	27.8114	28.1400	27.8123	28.1369	27.7989	28.2738	27.6676	27.7939	28.0327	27.8075	28.1669	27.8114	28.1400	27.8123	28.1370	27.7989	28.2739	**23.4**
C12	16.4210	16.5676	16.6312	16.7389	16.8296	16.7272	16.8016	16.7136	16.8013	16.7461	16.8064	16.4210	16.5676	16.6312	16.7389	16.8296	16.7272	16.8016	16.7136	16.8013	16.7461	16.8064	**13.8**
C1`	50.3513	51.1355	51.3757	51.6819	52.1647	51.6473	52.1659	51.6111	52.1124	51.7109	52.6598	54.6831	55.7368	56.0738	56.2267	56.7429	56.2006	56.8535	56.1716	56.7908	56.2470	57.1038	**53.3**
C2`	25.1575	25.5809	25.9072	25.7805	26.1941	25.7710	26.2013	25.7588	26.1797	25.7847	25.9870	24.6675	24.8374	25.1474	25.0423	25.5381	25.0287	25.4907	25.0134	25.4932	25.0513	25.2788	**24.2**
C3`	24.6675	24.8374	25.1475	25.0423	25.5380	25.0287	25.4907	25.0134	25.4932	25.0513	25.2788	25.1574	25.5809	25.9072	25.7806	26.1941	25.7710	26.2013	25.7588	26.1797	25.7847	25.9870	**24.1**
C4`	54.6830	55.7368	56.0739	56.2268	56.7429	56.2006	56.8535	56.1716	56.7908	56.2470	57.1039	50.3513	51.1355	51.3758	51.6818	52.1647	51.6473	52.1659	51.6111	52.1125	51.7109	52.6599	**56.3**
H2	8.7007	8.5592	8.5908	8.4663	8.3592	8.4728	8.4141	8.4787	8.4039	8.4595	8.3953	8.7007	8.5592	8.5908	8.4663	8.3592	8.4728	8.4141	8.4787	8.4039	8.4595	8.3953	**8.2**
H3	7.3297	7.4738	7.5631	7.5139	7.6078	7.5126	7.6304	7.5107	7.6217	7.5149	7.6457	7.3297	7.4738	7.5631	7.5139	7.6078	7.5126	7.6304	7.5107	7.6217	7.5149	7.6457	**7.36**
H5	7.1325	7.2902	7.3841	7.3696	7.5156	7.3646	7.5407	7.3595	7.5307	7.3743	7.5618	7.1325	7.2902	7.3841	7.3696	7.5156	7.3646	7.5407	7.3595	7.5307	7.3743	7.5618	**7.36**
H6	8.0154	8.1828	8.2635	8.2621	8.3160	8.2580	8.3752	8.2534	8.3539	8.2656	8.3870	8.0154	8.1828	8.2635	8.2622	8.3160	8.2580	8.3752	8.2534	8.3539	8.2656	8.3870	**8.2**
H8	4.6168	4.6642	4.6860	4.7066	4.7485	4.7037	4.7874	4.7006	4.7743	4.7091	4.7672	4.6168	4.6642	4.6860	4.7066	4.7485	4.7037	4.7874	4.7006	4.7743	4.7091	4.7672	**5.4**
H(9A-9B)	1.6879	1.7170	1.7219	1.7279	1.6637	1.7278	1.6700	1.7273	1.6567	1.7274	1.7027	1.6879	1.7170	1.7218	1.7279	1.6637	1.7278	1.6700	1.7273	1.6567	1.7274	1.7027	**2.08**
H(10A)	0.9637	0.8246	0.7814	0.7958	0.7462	0.7959	0.7971	0.7962	0.7959	0.7958	0.8043	0.9637	0.8246	0.7814	0.7958	0.7462	0.7959	0.7971	0.7962	0.7959	0.7958	0.8043	**1.14**
H(10B)	1.6217	1.5183	1.4590	1.4425	1.3585	1.4475	1.3581	1.4523	1.3656	1.4377	1.3287	1.6217	1.5183	1.4591	1.4425	1.3585	1.4475	1.3581	1.4523	1.3656	1.4377	1.3287	**1.28**
H(11A-11B)	1.0221	1.0367	1.0037	1.0526	1.0131	1.0518	1.0176	1.0508	1.0171	1.0532	1.0044	1.0221	1.0367	1.0037	1.0526	1.0131	1.0518	1.0176	1.0508	1.0171	1.0532	1.0045	**1.28**
H(12A-12C)	0.9038	0.8919	0.8662	0.8885	0.8592	0.8886	0.8679	0.8886	0.8693	0.8883	0.8616	0.9038	0.8919	0.8662	0.8885	0.8592	0.8886	0.8679	0.8886	0.8693	0.8883	0.8616	**0.82**
H(1`A)	2.6968	2.6878	2.6766	2.6791	2.6372	2.6798	2.6542	2.6802	2.6545	2.6784	2.6219	2.8356	2.8425	2.8290	2.8230	2.7927	2.8246	2.8005	2.8261	2.8024	2.8212	2.7688	**3.38**
H(1`B)	3.1801	3.2276	3.2615	3.2635	3.3127	3.2613	3.3038	3.2588	3.2991	3.2655	3.3001	2.8657	2.7208	2.7098	2.7022	2.7288	2.7020	2.6867	2.7019	2.6919	2.7027	2.6798	**3.71**
H(2`A)	1.6133	1.6575	1.6300	1.6779	1.6287	1.6768	1.6531	1.6756	1.6504	1.6788	1.6625	1.4889	1.5353	1.5078	1.5622	1.5233	1.5606	1.5567	1.5589	1.5539	1.5637	1.5734	**2.08**
H(2`B)	1.7948	1.8147	1.7739	1.8616	1.8208	1.8579	1.8223	1.8542	1.8177	1.8652	1.8493	1.6849	1.7954	1.7490	1.8700	1.8504	1.8649	1.8713	1.8598	1.8649	1.8749	1.9225	**2.24**
H(3`A)	1.4889	1.5353	1.5078	1.5622	1.5233	1.5606	1.5567	1.5589	1.5539	1.5637	1.5734	1.6133	1.6575	1.6300	1.6779	1.6287	1.6768	1.6531	1.6756	1.6504	1.6788	1.6625	**2.08**
H(3`B)	1.6849	1.7954	1.7490	1.8700	1.8504	1.8649	1.8713	1.8598	1.8649	1.8749	1.9225	1.7948	1.8147	1.7739	1.8616	1.8208	1.8579	1.8223	1.8542	1.8177	1.8652	1.8493	**2.16**
H(4`A)	2.8657	2.7208	2.7099	2.7023	2.7288	2.7020	2.6867	2.7019	2.6919	2.7027	2.6798	3.1801	3.2276	3.2614	3.2635	3.3127	3.2613	3.3038	3.2588	3.2992	3.2655	3.3001	**3.09**
H(4`B)	2.8356	2.8425	2.8290	2.8230	2.7927	2.8246	2.8005	2.8261	2.8024	2.8212	2.7688	2.6968	2.6878	2.6766	2.6791	2.6372	2.6798	2.6542	2.6802	2.6545	2.6784	2.6220	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S5. Cont. III

Nuclei	R											S										Exp. [b]
	BHandH											BHandH										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	138.5465	139.0589	140.0282	139.2348	140.8674	139.2148	140.1811	139.2131	140.2774	139.2234	140.5547	138.5464	139.0589	140.0282	139.2348	139.9789	139.2149	140.1811	139.2130	140.2774	139.2234	140.5546	**132.2**
C2	143.5117	143.4353	144.0030	143.2870	143.8194	143.2877	144.2640	143.3068	144.2012	143.2560	144.2993	143.5117	143.4353	144.0030	143.2870	144.0311	143.2877	144.2640	143.3066	144.2012	143.2560	144.2993	**133.3**
C3	123.6216	124.3782	125.0268	124.6233	125.3404	124.6010	125.5677	124.5967	125.5216	124.6141	125.6558	123.6216	124.3782	125.0269	124.6233	125.3674	124.6011	125.5677	124.5967	125.5216	124.6141	125.6558	**117.6**
C4	174.7888	175.5536	176.1854	175.9620	176.5660	175.9263	177.2388	175.9091	177.0774	175.9658	177.3779	174.7888	175.5536	176.1854	175.9620	176.7061	175.9263	177.2388	175.9092	177.0774	175.9658	177.3779	**168.3**
C5	121.5046	122.9341	123.6411	123.6822	124.5984	123.6257	124.8174	123.5876	124.7076	123.7060	124.9940	121.5047	122.9341	123.6411	123.6822	124.4263	123.6257	124.8174	123.5877	124.7076	123.7060	124.9940	**117.6**
C6	139.7122	141.6732	142.8202	142.8468	144.3976	142.7615	145.0656	142.6949	144.7943	142.8980	145.4379	139.7122	141.6732	142.8202	142.8468	143.5909	142.7615	145.0656	142.6950	144.7943	142.8980	145.4378	**133.3**
C7	204.0554	208.3972	209.8032	210.7478	211.4240	210.5925	216.7982	210.4551	215.6159	210.8653	217.9800	204.0553	208.3972	209.8031	210.7478	211.4919	210.5925	216.7982	210.4554	215.6159	210.8653	217.9800	**195.8**
C8	60.0731	61.1362	61.9412	61.6394	62.5544	61.5974	63.2661	61.5739	63.1273	61.6492	63.7607	60.0731	61.1362	61.9412	61.6394	62.3835	61.5974	63.2661	61.5738	63.1273	61.6492	63.7607	**70.4**
C9	34.1020	33.8856	34.1209	33.7869	34.0297	33.7837	34.1234	33.7986	34.0914	33.7597	34.2791	34.1020	33.8856	34.1209	33.7869	34.5310	33.7838	34.1234	33.7987	34.0914	33.7597	34.2791	**31.1**
C10	27.2135	27.7537	28.1167	28.1371	28.8125	28.0995	28.5687	28.0810	28.5478	28.1431	28.8216	27.2135	27.7537	28.1167	28.1371	28.8812	28.0995	28.5687	28.0810	28.5478	28.1431	28.8216	**26.9**
C11	26.1644	26.2342	26.5746	26.1987	26.6023	26.1915	26.5850	26.2026	26.6070	26.1752	26.7570	26.1643	26.2342	26.5745	26.1987	26.9428	26.1914	26.5850	26.2025	26.6070	26.1752	26.7571	**23.4**
C12	15.6496	15.8310	15.8835	15.9590	16.0362	15.9394	15.9509	15.9385	15.9568	15.9476	15.9762	15.6495	15.8311	15.8834	15.9590	16.7031	15.9394	15.9509	15.9385	15.9568	15.9476	15.9762	**13.8**
C1`	48.2959	49.0980	49.4034	49.5638	50.0949	49.5213	50.0509	49.4977	50.0387	49.5750	50.4802	52.2406	53.2551	53.7083	53.7330	54.4771	53.6924	54.4518	53.6704	54.3989	53.7416	54.6924	**53.3**
C2`	21.6367	22.0035	22.3605	22.1802	22.6341	22.1578	22.7044	22.1539	22.7025	22.1716	22.6865	21.0585	21.3095	21.6337	21.4659	22.2100	21.4453	21.8796	21.4431	21.8815	21.4554	21.8474	**24.2**
C3`	21.0585	21.3095	21.6337	21.4659	21.9420	21.4453	21.8796	21.4431	21.8815	21.4554	21.8473	21.6367	22.0035	22.3605	22.1802	22.9243	22.1578	22.7044	22.1539	22.7025	22.1716	22.6865	**24.1**
C4`	52.2406	53.2551	53.7084	53.7330	54.3137	53.6925	54.4518	53.6705	54.3989	53.7416	54.6924	48.2958	49.0980	49.4034	49.5638	50.3079	49.5213	50.0509	49.4977	50.0387	49.5750	50.4801	**56.3**
H2	9.0133	8.9379	8.9431	8.8888	8.8838	8.8928	8.8900	8.8959	8.8935	8.8861	8.8693	9.0133	8.9379	8.9431	8.8888	8.8076	8.8928	8.8900	8.8959	8.8935	8.8861	8.8693	**8.2**
H3	7.4474	7.5927	7.6854	7.6383	7.7626	7.6369	7.7844	7.6346	7.7756	7.6405	7.8000	7.4474	7.5927	7.6854	7.6383	7.5571	7.6369	7.7844	7.6346	7.7756	7.6405	7.8000	**7.36**
H5	7.2803	7.4792	7.5728	7.5667	7.6983	7.5625	7.7142	7.5574	7.7025	7.5718	7.7363	7.2803	7.4792	7.5728	7.5667	7.4855	7.5625	7.7142	7.5574	7.7025	7.5718	7.7363	**7.36**
H6	8.1894	8.3806	8.4651	8.4861	8.6214	8.4803	8.6749	8.4737	8.6488	8.4926	8.7015	8.1894	8.3806	8.4651	8.4861	8.4049	8.4803	8.6749	8.4737	8.6488	8.4926	8.7015	**8.2**
H8	4.2693	4.3483	4.3771	4.4032	4.4839	4.4004	4.5358	4.3968	4.5082	4.4069	4.5389	4.2693	4.3483	4.3771	4.4032	4.3220	4.4004	4.5358	4.3968	4.5082	4.4069	4.5389	**5.4**
H(9A-9B)	1.7884	1.8248	1.8176	1.8632	1.8617	1.8613	1.8484	1.8587	1.8470	1.8660	1.8841	1.7883	1.8248	1.8176	1.8632	1.7820	1.8613	1.8484	1.8587	1.8470	1.8660	1.8841	**2.08**
H(10A)	0.9699	0.8271	0.7545	0.7425	0.6584	0.7484	0.6674	0.7535	0.6673	0.7380	0.6698	0.9699	0.8271	0.7545	0.7425	0.6584	0.7484	0.6674	0.7535	0.6673	0.7380	0.6698	**1.14**
H(10B)	1.6604	1.5673	1.5079	1.4980	1.4014	1.5040	1.3938	1.5089	1.4008	1.4933	1.3675	1.6604	1.5673	1.5080	1.4980	1.4014	1.5040	1.3938	1.5089	1.4008	1.4933	1.3675	**1.28**
H(11A-11B)	0.9886	1.0092	0.9788	1.0287	0.9857	1.0282	0.9820	1.0270	0.9828	1.0301	0.9726	0.9886	1.0092	0.9788	1.0287	0.9474	1.0282	0.9820	1.0270	0.9828	1.0301	0.9726	**1.28**
H(12A-12C)	0.9400	0.9236	0.8941	0.9103	0.8692	0.9121	0.8711	0.9129	0.8722	0.9097	0.8665	0.9400	0.9236	0.8941	0.9103	0.8291	0.9121	0.8711	0.9129	0.8722	0.9097	0.8665	**0.82**
H(1`A)	2.5921	2.5890	2.5638	2.5786	2.5274	2.5803	2.5416	2.5812	2.5420	2.5781	2.5258	2.7460	2.7455	2.7319	2.7273	2.6904	2.7296	2.7107	2.7311	2.7126	2.7260	2.6863	**3.38**
H(1`B)	3.0932	3.1308	3.1577	3.1643	3.2166	3.1627	3.1977	3.1603	3.1933	3.1669	3.2011	2.9077	2.7015	2.6593	2.6386	2.6117	2.6430	2.5508	2.6465	2.5576	2.6356	2.5450	**3.71**
H(2`A)	1.5987	1.6473	1.6123	1.6655	1.6051	1.6653	1.6330	1.6643	1.6301	1.6668	1.6474	1.4624	1.5143	1.4813	1.5342	1.4765	1.5339	1.5179	1.5328	1.5130	1.5355	1.5390	**2.08**
H(2`B)	1.7665	1.7910	1.7431	1.8278	1.7968	1.8259	1.7866	1.8233	1.7805	1.8307	1.8094	1.6896	1.7754	1.7352	1.8298	1.7997	1.8267	1.8301	1.8229	1.8205	1.8338	1.8777	**2.24**
H(3`A)	1.4624	1.5143	1.4813	1.5342	1.4765	1.5339	1.5179	1.5328	1.5130	1.5355	1.5390	1.5987	1.6473	1.6123	1.6655	1.6051	1.6653	1.6330	1.6643	1.6301	1.6668	1.6474	**2.08**
H(3`B)	1.6896	1.7754	1.7352	1.8298	1.7997	1.8267	1.8301	1.8229	1.8205	1.8338	1.8777	1.7665	1.7910	1.7431	1.8278	1.7968	1.8259	1.7866	1.8232	1.7805	1.8307	1.8095	**2.16**
H(4`A)	2.9077	2.7015	2.6593	2.6386	2.6117	2.6430	2.5508	2.6465	2.5576	2.6356	2.5450	3.0932	3.1308	3.1577	3.1643	3.2166	3.1627	3.1977	3.1603	3.1933	3.1669	3.2011	**3.09**
H(4`B)	2.7460	2.7455	2.7320	2.7273	2.6904	2.7296	2.7107	2.7311	2.7126	2.7260	2.6863	2.5921	2.5890	2.5638	2.5786	2.5274	2.5803	2.5416	2.5812	2.5420	2.5781	2.5258	**3.68**
Nuclei	BHandHLYP											BHandHLYP										
C1	139.1706	139.9116	140.6432	140.3296	141.7914	140.3148	140.9419	140.3012	141.1074	140.3424	141.2702	139.1706	139.9116	140.6432	140.3295	141.7914	140.3148	140.9419	140.3012	141.1074	140.3424	141.2702	**132.2**
C2	142.0275	141.9201	142.3974	141.7860	142.2101	141.7956	142.7562	141.8074	142.6462	141.7766	142.7360	142.0275	141.9201	142.3974	141.7860	142.2101	141.7956	142.7562	141.8074	142.6462	141.7767	142.7360	**133.3**
C3	122.5523	123.1684	123.6876	123.3576	123.9512	123.3499	124.1309	123.3441	124.1042	123.3640	124.2025	122.5523	123.1684	123.6877	123.3575	123.9512	123.3499	124.1309	123.3441	124.1042	123.3640	124.2025	**117.6**
C4	174.5864	175.2899	175.8454	175.6713	176.1994	175.6486	176.8750	175.6280	176.7138	175.6927	176.9999	174.5864	175.2899	175.8454	175.6714	176.1994	175.6486	176.8750	175.6280	176.7138	175.6927	176.9999	**168.3**
C5	120.3052	121.5543	122.1308	122.2063	122.9812	122.1668	123.1213	122.1296	123.0494	122.2436	123.2920	120.3052	121.5543	122.1307	122.2064	122.9812	122.1668	123.1213	122.1296	123.0494	122.2436	123.2920	**117.6**
C6	138.0548	139.9133	141.0549	141.0312	142.5246	140.9560	143.2797	140.8840	142.9881	141.1031	143.6154	138.0548	139.9133	141.0548	141.0312	142.5246	140.9560	143.2797	140.8840	142.9881	141.1031	143.6154	**133.3**
C7	202.3068	207.1882	208.3236	209.9129	210.2715	209.7555	215.9054	209.5991	214.6690	210.0607	217.0820	202.3068	207.1882	208.3236	209.9129	210.2715	209.7555	215.9054	209.5991	214.6690	210.0607	217.0820	**195.8**
C8	61.8804	62.9219	63.4905	63.3415	64.2714	63.3206	64.7791	63.3010	64.6980	63.3599	65.1757	61.8804	62.9219	63.4905	63.3415	64.2714	63.3206	64.7791	63.3010	64.6980	63.3599	65.1757	**70.4**
C9	34.1386	33.7725	34.0157	33.6193	33.9168	33.6264	34.0171	33.6361	33.9882	33.6121	34.0669	34.1386	33.7725	34.0157	33.6193	33.9168	33.6264	34.0171	33.6361	33.9882	33.6121	34.0669	**31.1**
C10	27.2497	27.6893	28.1703	28.0164	28.7326	27.9923	28.5308	27.9711	28.5292	28.0393	28.6777	27.2497	27.6893	28.1703	28.0164	28.7326	27.9922	28.5308	27.9711	28.5292	28.0393	28.6777	**26.9**
C11	27.2405	27.3246	27.6178	27.2971	27.7280	27.3011	27.7115	27.3070	27.7273	27.2928	27.8503	27.2405	27.3246	27.6179	27.2972	27.7280	27.3010	27.7115	27.3070	27.7273	27.2928	27.8503	**23.4**
C12	16.4477	16.5986	16.6969	16.7338	16.8490	16.7238	16.7955	16.7165	16.8029	16.7434	16.8068	16.4477	16.5986	16.6969	16.7339	16.8490	16.7239	16.7955	16.7165	16.8029	16.7434	16.8068	**13.8**
C1`	49.0825	49.8396	50.1387	50.3717	50.8895	50.3364	50.8814	50.3041	50.8419	50.4053	51.3647	53.3202	54.3295	54.6354	54.7498	55.2630	54.7265	55.3513	54.7053	55.3102	54.7713	55.6150	**53.3**
C2`	24.4610	24.8112	25.1567	24.9344	25.4163	24.9287	25.4177	24.9250	25.4350	24.9393	25.2394	23.9171	24.0510	24.4256	24.1914	24.6650	24.1829	24.5877	24.1770	24.5932	24.1990	24.4088	**24.2**
C3`	23.9171	24.0510	24.4257	24.1913	24.6650	24.1830	24.5877	24.1770	24.5932	24.1990	24.4088	24.4610	24.8112	25.1568	24.9345	25.4163	24.9287	25.4177	24.9250	25.4350	24.9393	25.2394	**24.1**
C4`	53.3202	54.3295	54.6354	54.7499	55.2630	54.7265	55.3513	54.7053	55.3102	54.7714	55.6150	49.0825	49.8396	50.1387	50.3716	50.8895	50.3365	50.8814	50.3041	50.8419	50.4053	51.3647	**56.3**
H2	8.9174	8.8134	8.8432	8.7435	8.7514	8.7471	8.7822	8.7508	8.7728	8.7400	8.7555	8.9174	8.8134	8.8432	8.7434	8.7514	8.7471	8.7822	8.7508	8.7728	8.7400	8.7555	**8.2**
H3	7.4415	7.5833	7.6682	7.6294	7.7421	7.6275	7.7648	7.6254	7.7556	7.6312	7.7794	7.4415	7.5833	7.6682	7.6294	7.7421	7.6275	7.7648	7.6254	7.7556	7.6312	7.7794	**7.36**
H5	7.2649	7.4404	7.5319	7.5137	7.6436	7.5094	7.6523	7.5050	7.6416	7.5178	7.6758	7.2649	7.4404	7.5319	7.5137	7.6436	7.5094	7.6523	7.5050	7.6416	7.5178	7.6758	**7.36**
H6	8.0825	8.2754	8.3711	8.3872	8.5176	8.3804	8.5843	8.3735	8.5554	8.3937	8.6106	8.0825	8.2754	8.3711	8.3872	8.5176	8.3804	8.5843	8.3735	8.5554	8.3937	8.6106	**8.2**
H8	4.2250	4.3093	4.3596	4.3771	4.4432	4.3727	4.5018	4.3684	4.4740	4.3812	4.4872	4.2250	4.3093	4.3596	4.3771	4.4432	4.3728	4.5018	4.3684	4.4740	4.3812	4.4872	**5.4**
H(9A-9B)	1.5828	1.6221	1.6279	1.6514	1.6739	1.6488	1.6780	1.6462	1.6704	1.6538	1.7051	1.5827	1.6221	1.6279	1.6514	1.6739	1.6488	1.6780	1.6462	1.6704	1.6538	1.7051	**2.08**
H(10A)	0.9846	0.8118	0.7997	0.7653	0.6810	0.7674	0.7233	0.7695	0.7123	0.7634	0.7225	0.9846	0.8118	0.7997	0.7653	0.6810	0.7674	0.7233	0.7695	0.7123	0.7634	0.7225	**1.14**
H(10B)	1.5615	1.4724	1.4065	1.3921	1.3035	1.3980	1.3085	1.4037	1.3114	1.3864	1.2811	1.5615	1.4724	1.4065	1.3921	1.3035	1.3980	1.3085	1.4037	1.3114	1.3864	1.2811	**1.28**
H(11A-11B)	0.9843	1.0042	0.9708	1.0203	0.9796	1.0195	0.9842	1.0186	0.9801	1.0210	0.9727	0.9843	1.0042	0.9708	1.0203	0.9796	1.0195	0.9842	1.0186	0.9801	1.0210	0.9727	**1.28**
H(12A-12C)	0.9401	0.9227	0.8984	0.9153	0.8731	0.9159	0.8823	0.9165	0.8805	0.9146	0.8760	0.9401	0.9227	0.8984	0.9153	0.8731	0.9159	0.8823	0.9165	0.8805	0.9146	0.8760	**0.82**
H(1`A)	2.6097	2.6012	2.5884	2.5909	2.5431	2.5917	2.5662	2.5924	2.5652	2.5900	2.5385	2.7507	2.7499	2.7315	2.7241	2.6891	2.7264	2.7061	2.7286	2.7091	2.7217	2.6739	**3.38**
H(1`B)	3.0196	3.0719	3.1020	3.1129	3.1735	3.1101	3.1671	3.1072	3.1606	3.1156	3.1693	2.7250	2.5707	2.5548	2.5480	2.5462	2.5484	2.5090	2.5489	2.5117	2.5477	2.5052	**3.71**
H(2`A)	1.5817	1.6240	1.5910	1.6417	1.5824	1.6409	1.6104	1.6401	1.6066	1.6424	1.6217	1.4608	1.5084	1.4765	1.5305	1.4719	1.5296	1.5091	1.5286	1.5038	1.5313	1.5265	**2.08**
H(2`B)	1.7190	1.7481	1.7091	1.8017	1.7564	1.7978	1.7602	1.7939	1.7507	1.8056	1.7841	1.5980	1.7096	1.6575	1.7817	1.7361	1.7774	1.7630	1.7731	1.7535	1.7857	1.8122	**2.24**
H(3`A)	1.4608	1.5084	1.4765	1.5305	1.4719	1.5296	1.5091	1.5286	1.5038	1.5313	1.5265	1.5817	1.6240	1.5910	1.6417	1.5824	1.6409	1.6104	1.6401	1.6066	1.6424	1.6217	**2.08**
H(3`B)	1.5980	1.7096	1.6575	1.7817	1.7361	1.7774	1.7630	1.7731	1.7535	1.7857	1.8122	1.7190	1.7481	1.7091	1.8017	1.7564	1.7978	1.7602	1.7939	1.7507	1.8056	1.7841	**2.16**
H(4`A)	2.7250	2.5707	2.5548	2.5480	2.5462	2.5484	2.5090	2.5489	2.5117	2.5477	2.5052	3.0196	3.0719	3.1020	3.1129	3.1735	3.1101	3.1671	3.1072	3.1606	3.1156	3.1693	**3.09**
H(4`B)	2.7507	2.7499	2.7315	2.7241	2.6891	2.7264	2.7061	2.7286	2.7091	2.7217	2.6739	2.6097	2.6012	2.5884	2.5908	2.5431	2.5917	2.5662	2.5924	2.5652	2.5900	2.5385	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S5. Cont. IV

Nuclei	R											S										Exp. [b]
	BLYP											BLYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.5343	140.9652	141.5943	141.7357	144.5172	141.9636	143.4256	141.7300	143.9164	142.1462	143.7361	139.5343	140.9652	141.5943	141.7357	144.5172	141.9636	143.4256	141.7300	143.9164	142.1461	143.7361	**132.2**
C2	137.2556	137.2722	137.8854	137.3003	138.1317	137.5735	138.4112	137.3854	138.4615	137.6688	138.5024	137.2556	137.2722	137.8854	137.3003	138.1317	137.5735	138.4112	137.3854	138.4615	137.6689	138.5024	**133.3**
C3	120.7921	121.4191	121.9349	121.5949	122.2771	121.8658	122.4301	121.6744	122.5403	121.9644	122.5819	120.7921	121.4191	121.9349	121.5949	122.2771	121.8658	122.4301	121.6744	122.5403	121.9643	122.5819	**117.6**
C4	178.0446	178.9278	179.6458	179.2623	179.9892	179.5224	180.4161	179.3202	180.4077	179.6422	180.6443	178.0446	178.9278	179.6458	179.2623	179.9892	179.5224	180.4161	179.3202	180.4077	179.6422	180.6443	**168.3**
C5	118.7346	119.8592	120.4200	120.4485	121.2822	120.6894	121.4129	120.4685	121.4684	120.8468	121.6561	118.7346	119.8592	120.4200	120.4485	121.2822	120.6894	121.4129	120.4685	121.4684	120.8467	121.6561	**117.6**
C6	133.6680	135.5732	136.6203	136.5089	137.5639	136.7306	138.0767	136.4903	137.9461	136.9249	138.5039	133.6680	135.5732	136.6203	136.5089	137.5639	136.7306	138.0767	136.4903	137.9461	136.9250	138.5039	**133.3**
C7	204.1746	208.9870	210.1011	211.5855	213.4733	211.7040	217.6195	211.3603	217.0831	212.0989	218.7030	204.1746	208.9870	210.1011	211.5855	213.4733	211.7040	217.6195	211.3603	217.0831	212.0991	218.7030	**195.8**
C8	70.4591	71.9072	72.3407	72.5539	73.6351	72.8057	73.9567	72.5927	74.1428	72.9387	74.2784	70.4591	71.9072	72.3407	72.5539	73.6351	72.8057	73.9567	72.5927	74.1428	72.9386	74.2784	**70.4**
C9	40.1256	39.7708	39.8045	39.5605	39.5512	39.8527	39.6759	39.6825	39.8226	39.9098	39.7834	40.1256	39.7708	39.8045	39.5605	39.5512	39.8527	39.6759	39.6825	39.8226	39.9098	39.7834	**31.1**
C10	30.9956	31.5038	31.9353	31.7631	32.4330	32.0244	32.0419	31.8239	32.2296	32.1419	32.2060	30.9956	31.5038	31.9353	31.7631	32.4330	32.0244	32.0419	31.8239	32.2296	32.1419	32.2060	**26.9**
C11	31.2026	31.3178	31.5898	31.2585	31.7489	31.5442	31.5381	31.3673	31.7410	31.6138	31.7406	31.2026	31.3178	31.5898	31.2585	31.7489	31.5442	31.5381	31.3673	31.7410	31.6138	31.7406	**23.4**
C12	17.0012	17.1470	17.1923	17.2337	17.4506	17.5040	17.2382	17.3127	17.4172	17.6046	17.3304	17.0012	17.1470	17.1923	17.2337	17.4506	17.5040	17.2382	17.3127	17.4172	17.6045	17.3304	**13.8**
C1`	55.2831	56.0370	56.4053	56.5833	57.2950	56.8244	57.1633	56.6042	57.2744	56.9826	57.7328	59.9830	61.1273	61.5437	61.6339	62.2990	61.8849	62.3006	61.6734	62.3750	62.0222	62.6696	**53.3**
C2`	27.7274	28.2834	28.6122	28.5322	29.0355	28.8001	28.9330	28.6054	29.0959	28.9041	28.8068	27.6644	27.8009	28.1574	27.9578	28.6760	28.2245	28.3891	28.0299	28.5704	28.3322	28.2523	**24.2**
C3`	27.6644	27.8009	28.1574	27.9578	28.6760	28.2246	28.3891	28.0299	28.5704	28.3322	28.2523	27.7274	28.2834	28.6122	28.5322	29.0355	28.8002	28.9330	28.6054	29.0959	28.9042	28.8068	**24.1**
C4`	59.9830	61.1273	61.5437	61.6339	62.2990	61.8849	62.3006	61.6734	62.3750	62.0222	62.6696	55.2831	56.0370	56.4053	56.5833	57.2950	56.8243	57.1633	56.6042	57.2744	56.9825	57.7328	**56.3**
H2	8.4743	8.3172	8.3808	8.2334	8.1741	8.2858	8.4013	8.2457	8.2052	8.2841	8.4152	8.4743	8.3172	8.3808	8.2334	8.1741	8.2858	8.4013	8.2457	8.2052	8.2841	8.4152	**8.2**
H3	7.1772	7.3089	7.3990	7.3393	7.4354	7.3857	7.6265	7.3394	7.4492	7.3955	7.6556	7.1772	7.3089	7.3990	7.3393	7.4354	7.3857	7.6265	7.3394	7.4492	7.3955	7.6556	**7.36**
H5	6.9737	7.1133	7.1996	7.1888	7.3510	7.2313	7.5411	7.1813	7.3621	7.2487	7.5789	6.9737	7.1133	7.1996	7.1888	7.3510	7.2313	7.5411	7.1813	7.3621	7.2487	7.5789	**7.36**
H6	7.8508	8.0008	8.0879	8.0664	8.1493	8.1100	8.3792	8.0612	8.1751	8.1252	8.4240	7.8508	8.0008	8.0879	8.0664	8.1493	8.1100	8.3792	8.0612	8.1751	8.1252	8.4240	**8.2**
H8	4.9846	5.0134	5.0311	5.0158	5.0719	5.0626	5.2534	5.0171	5.0718	5.0716	5.2461	4.9846	5.0134	5.0311	5.0158	5.0719	5.0626	5.2534	5.0171	5.0718	5.0716	5.2461	**5.4**
H(9A-9B)	1.7832	1.8231	1.8147	1.8352	1.7750	1.8823	1.9577	1.8368	1.7845	1.8907	1.9990	1.7832	1.8231	1.8147	1.8352	1.7750	1.8823	1.9577	1.8368	1.7845	1.8908	1.9990	**2.08**
H(10A)	1.0374	0.9218	0.9214	0.8984	0.8849	0.9453	1.0941	0.9001	0.9201	0.9545	1.1206	1.0374	0.9218	0.9214	0.8984	0.8849	0.9453	1.0941	0.9001	0.9201	0.9545	1.1206	**1.14**
H(10B)	1.7538	1.6293	1.5697	1.5413	1.4721	1.5943	1.6301	1.5547	1.4719	1.5913	1.6106	1.7538	1.6293	1.5697	1.5413	1.4721	1.5943	1.6301	1.5547	1.4719	1.5913	1.6106	**1.28**
H(11A-11B)	1.1322	1.1424	1.1178	1.1560	1.1325	1.2024	1.3013	1.1563	1.1316	1.2123	1.3029	1.1322	1.1424	1.1178	1.1560	1.1325	1.2024	1.3013	1.1563	1.1316	1.2123	1.3029	**1.28**
H(12A-12C)	0.9419	0.9312	0.9110	0.9251	0.9070	0.9727	1.0813	0.9279	0.9137	0.9802	1.0909	0.9419	0.9312	0.9110	0.9251	0.9070	0.9727	1.0813	0.9279	0.9137	0.9802	1.0909	**0.82**
H(1`A)	2.8633	2.8501	2.8310	2.8377	2.7979	2.8860	2.9760	2.8418	2.8118	2.8922	2.9544	2.9651	2.9898	2.9671	2.9680	2.9372	3.0180	3.1018	2.9754	2.9444	3.0205	3.0695	**3.38**
H(1`B)	3.3633	3.4089	3.4348	3.4379	3.4925	3.4835	3.6471	3.4365	3.4756	3.4949	3.6586	3.0499	2.8913	2.8353	2.8526	2.8547	2.9002	2.9868	2.8556	2.8331	2.9080	2.9912	**3.71**
H(2`A)	1.6735	1.7250	1.6968	1.7428	1.6993	1.7892	1.8918	1.7431	1.7216	1.7990	1.9188	1.5605	1.6040	1.5772	1.6253	1.5927	1.6713	1.7891	1.6248	1.6193	1.6819	1.8186	**2.08**
H(2`B)	1.9472	1.9524	1.9050	1.9814	1.9489	2.0255	2.1131	1.9774	1.9402	2.0400	2.1618	1.7709	1.8959	1.8552	1.9654	1.9523	2.0081	2.1360	1.9584	1.9618	2.0252	2.1995	**2.24**
H(3`A)	1.5605	1.6040	1.5772	1.6253	1.5927	1.6713	1.7891	1.6248	1.6193	1.6819	1.8186	1.6735	1.7250	1.6968	1.7428	1.6993	1.7892	1.8918	1.7431	1.7216	1.7990	1.9188	**2.08**
H(3`B)	1.7709	1.8959	1.8552	1.9654	1.9523	2.0081	2.1360	1.9584	1.9618	2.0252	2.1995	1.9472	1.9524	1.9050	1.9814	1.9489	2.0255	2.1131	1.9774	1.9402	2.0400	2.1618	**2.16**
H(4`A)	3.0499	2.8913	2.8353	2.8526	2.8547	2.9002	2.9868	2.8556	2.8331	2.9080	2.9912	3.3633	3.4089	3.4348	3.4379	3.4925	3.4835	3.6471	3.4365	3.4756	3.4949	3.6586	**3.09**
H(4`B)	2.9651	2.9898	2.9671	2.9680	2.9372	3.0180	3.1018	2.9754	2.9444	3.0205	3.0695	2.8633	2.8501	2.8310	2.8377	2.7979	2.8860	2.9760	2.8418	2.8118	2.8922	2.9544	**3.68**
Nuclei	BMK											BMK										
C1	154.6743	155.0332	155.8462	155.1583	157.1596	155.1396	156.3883	155.3301	156.3397	155.3339	156.6046	154.6743	155.0332	155.8461	155.1582	157.1596	155.1397	156.3884	155.3301	156.3396	155.3339	156.6046	**132.2**
C2	154.6877	154.7844	155.5459	154.6549	155.3498	154.6489	155.8469	154.8543	155.6657	154.8228	155.7777	154.6877	154.7844	155.5461	154.6548	155.3498	154.6489	155.8467	154.8543	155.6656	154.8230	155.7777	**133.3**
C3	135.9138	136.6373	137.3465	136.8279	137.6933	136.8045	137.9405	136.9917	137.7955	137.0117	137.8683	135.9138	136.6373	137.3465	136.8279	137.6933	136.8046	137.9404	136.9917	137.7954	137.0118	137.8683	**117.6**
C4	189.4877	190.2116	190.9837	190.5712	191.4900	190.5337	192.1186	190.7070	191.8573	190.7682	192.2003	189.4877	190.2116	190.9838	190.5712	191.4900	190.5337	192.1187	190.7070	191.8575	190.7681	192.2003	**168.3**
C5	133.6513	134.9680	135.5869	135.6169	136.6787	135.5615	136.8546	135.7170	136.6382	135.8301	136.9525	133.6513	134.9680	135.5868	135.6171	136.6787	135.5614	136.8546	135.7170	136.6383	135.8300	136.9525	**117.6**
C6	151.3083	153.3283	154.3456	154.4536	156.4249	154.3671	157.0666	154.4912	156.6478	154.6954	157.4119	151.3083	153.3283	154.3454	154.4537	156.4249	154.3671	157.0667	154.4912	156.6476	154.6955	157.4119	**133.3**
C7	218.4275	222.9521	224.3909	225.3913	226.5095	225.2230	232.5082	225.2643	230.9435	225.7107	234.0514	218.4275	222.9521	224.3912	225.3913	226.5095	225.2230	232.5081	225.2643	230.9437	225.7103	234.0514	**195.8**
C8	71.7818	72.7560	73.5185	73.2212	74.7487	73.1831	75.2261	73.3534	74.8979	73.4147	76.0945	71.7818	72.7560	73.5184	73.2212	74.7487	73.1831	75.2261	73.3534	74.8979	73.4148	76.0945	**70.4**
C9	38.9270	38.8753	38.9914	38.7229	39.3377	38.7191	39.5697	38.9259	39.3287	38.8870	39.8348	38.9270	38.8753	38.9914	38.7229	39.3377	38.7192	39.5696	38.9259	39.3287	38.8870	39.8348	**31.1**
C10	31.5063	31.8431	32.2898	32.1042	32.9319	32.0706	32.5932	32.2494	32.5113	32.3000	32.8436	31.5063	31.8431	32.2898	32.1043	32.9319	32.0705	32.5931	32.2494	32.5113	32.3000	32.8436	**26.9**
C11	30.1638	30.0934	30.5280	30.0558	30.6708	30.0424	30.6321	30.2397	30.5415	30.2295	30.7089	30.1638	30.0934	30.5281	30.0558	30.6708	30.0423	30.6321	30.2397	30.5416	30.2295	30.7089	**23.4**
C12	17.9216	17.9663	18.1186	18.0457	18.3196	18.0223	18.2191	18.2104	18.1235	18.2298	18.1813	17.9215	17.9663	18.1186	18.0458	18.3196	18.0222	18.2190	18.2104	18.1236	18.2298	18.1812	**13.8**
C1`	56.2140	56.7042	57.2624	57.3354	57.9775	57.2761	57.8726	57.4271	57.7807	57.5515	57.9072	60.6747	61.2631	61.7498	61.5953	62.2577	61.5585	62.3486	61.7326	62.2082	61.7911	62.6655	**53.3**
C2`	28.1109	28.2884	28.6899	28.4501	29.0183	28.4238	28.9833	28.6085	28.8847	28.6357	28.9334	27.2299	27.4471	27.8451	27.6148	28.2163	27.5901	28.0996	27.7764	28.0059	27.7997	28.0827	**24.2**
C3`	27.2299	27.4471	27.8451	27.6148	28.2163	27.5901	28.0997	27.7764	28.0059	27.7998	28.0827	28.1109	28.2884	28.6900	28.4501	29.0184	28.4240	28.9833	28.6085	28.8847	28.6357	28.9334	**24.1**
C4`	60.6747	61.2631	61.7497	61.5952	62.2576	61.5585	62.3485	61.7326	62.2080	61.7910	62.6655	56.2140	56.7042	57.2624	57.3355	57.9775	57.2760	57.8726	57.4271	57.7808	57.5514	57.9072	**56.3**
H2	8.9918	8.9298	8.9868	8.9078	8.9029	8.9057	8.9653	8.9038	8.9648	8.9005	8.9628	8.9918	8.9298	8.9868	8.9078	8.9029	8.9057	8.9653	8.9038	8.9648	8.9005	8.9628	**8.2**
H3	7.6541	7.7829	7.8752	7.8302	7.9474	7.8246	7.9758	7.8190	7.9680	7.8259	7.9947	7.6541	7.7829	7.8752	7.8302	7.9474	7.8246	7.9758	7.8190	7.9680	7.8259	7.9947	**7.36**
H5	7.4938	7.6754	7.7641	7.7548	7.8712	7.7469	7.8878	7.7390	7.8788	7.7528	7.9076	7.4938	7.6754	7.7641	7.7548	7.8712	7.7469	7.8878	7.7390	7.8788	7.7528	7.9076	**7.36**
H6	8.3432	8.5078	8.6605	8.6235	8.7819	8.6124	8.8278	8.6015	8.8045	8.6250	8.8898	8.3432	8.5078	8.6605	8.6235	8.7819	8.6123	8.8278	8.6015	8.8044	8.6250	8.8898	**8.2**
H8	4.4144	4.4718	4.5598	4.5582	4.6028	4.5477	4.6667	4.5377	4.6543	4.5594	4.6485	4.4144	4.4718	4.5598	4.5582	4.6028	4.5477	4.6667	4.5377	4.6543	4.5594	4.6485	**5.4**
H(9A-9B)	1.6329	1.6976	1.6442	1.7193	1.7410	1.7145	1.7510	1.7099	1.7352	1.7143	1.8258	1.6329	1.6976	1.6442	1.7193	1.7410	1.7145	1.7510	1.7099	1.7352	1.7143	1.8258	**2.08**
H(10A)	1.0054	0.8156	0.8417	0.7556	0.6584	0.7548	0.7160	0.7541	0.7163	0.7469	0.7118	1.0054	0.8156	0.8417	0.7556	0.6584	0.7548	0.7160	0.7541	0.7163	0.7469	0.7118	**1.14**
H(10B)	1.5665	1.5142	1.4152	1.4197	1.3176	1.4233	1.3145	1.4271	1.3225	1.4069	1.3045	1.5665	1.5142	1.4152	1.4197	1.3176	1.4234	1.3145	1.4271	1.3225	1.4069	1.3045	**1.28**
H(11A-11B)	0.9568	0.9779	0.9496	0.9998	0.9492	0.9949	0.9534	0.9903	0.9549	0.9951	0.9505	0.9568	0.9779	0.9497	0.9998	0.9492	0.9949	0.9534	0.9903	0.9550	0.9951	0.9505	**1.28**
H(12A-12C)	0.8618	0.8474	0.8194	0.8457	0.7952	0.8425	0.7967	0.8395	0.8006	0.8395	0.8000	0.8617	0.8474	0.8194	0.8457	0.7952	0.8425	0.7967	0.8395	0.8007	0.8395	0.8000	**0.82**
H(1`A)	2.6238	2.6293	2.5970	2.6303	2.5835	2.6272	2.6067	2.6240	2.6082	2.6234	2.5463	2.7737	2.7853	2.7534	2.7712	2.7426	2.7699	2.7487	2.7683	2.7505	2.7626	2.7334	**3.38**
H(1`B)	3.0937	3.1310	3.1474	3.1725	3.2050	3.1661	3.1984	3.1595	3.1935	3.1689	3.1717	2.7218	2.5991	2.5747	2.5696	2.5484	2.5668	2.5121	2.5643	2.5131	2.5631	2.5093	**3.71**
H(2`A)	1.6066	1.6472	1.6208	1.6740	1.6181	1.6691	1.6399	1.6642	1.6380	1.6690	1.6497	1.4626	1.5173	1.4830	1.5420	1.4897	1.5377	1.5230	1.5334	1.5190	1.5364	1.5474	**2.08**
H(2`B)	1.7500	1.7801	1.7577	1.8454	1.7854	1.8368	1.7922	1.8285	1.7891	1.8442	1.7924	1.6778	1.7533	1.6954	1.8157	1.7687	1.8087	1.7888	1.8016	1.7827	1.8127	1.8332	**2.24**
H(3`A)	1.4626	1.5173	1.4830	1.5420	1.4897	1.5378	1.5230	1.5334	1.5190	1.5365	1.5474	1.6066	1.6472	1.6208	1.6740	1.6181	1.6691	1.6400	1.6642	1.6380	1.6690	1.6497	**2.08**
H(3`B)	1.6778	1.7533	1.6954	1.8157	1.7687	1.8087	1.7888	1.8016	1.7827	1.8127	1.8332	1.7500	1.7801	1.7578	1.8454	1.7854	1.8368	1.7922	1.8285	1.7891	1.8442	1.7924	**2.16**
H(4`A)	2.7218	2.5991	2.5747	2.5696	2.5484	2.5668	2.5120	2.5643	2.5131	2.5631	2.5093	3.0937	3.1310	3.1474	3.1725	3.2050	3.1661	3.1984	3.1595	3.1935	3.1689	3.1717	**3.09**
H(4`B)	2.7737	2.7853	2.7534	2.7712	2.7426	2.7699	2.7487	2.7683	2.7505	2.7626	2.7334	2.6238	2.6293	2.5970	2.6303	2.5835	2.6272	2.6068	2.6240	2.6082	2.6235	2.5463	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S5. Cont. V

Nuclei	R											S										Exp. [b]
	BP86											BP86										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.1088	137.3107	138.0964	137.7831	139.1376	137.7682	138.6145	137.7476	138.6273	137.7918	138.9792	136.1088	137.3107	138.0965	137.7831	139.1376	137.7682	138.6145	137.7476	138.6273	137.7918	138.9792	**132.2**
C2	135.7786	135.9025	136.4035	135.7790	136.2500	135.7953	136.7578	135.8067	136.6297	135.7589	136.8526	135.7786	135.9025	136.4034	135.7790	136.2500	135.7953	136.7578	135.8067	136.6297	135.7589	136.8526	**133.3**
C3	119.6549	120.5419	121.0715	120.7433	121.3759	120.7419	121.7193	120.7350	121.6286	120.7394	121.9674	119.6549	120.5419	121.0715	120.7433	121.3759	120.7419	121.7193	120.7350	121.6286	120.7394	121.9674	**117.6**
C4	174.5771	175.6557	176.2903	176.0366	176.7190	176.0219	177.3180	176.0021	177.1695	176.0455	177.6153	174.5771	175.6557	176.2903	176.0366	176.7190	176.0219	177.3180	176.0021	177.1695	176.0455	177.6153	**168.3**
C5	117.7054	119.0766	119.6753	119.6781	120.4892	119.6486	120.7558	119.6139	120.6434	119.7013	121.0874	117.7054	119.0766	119.6753	119.6781	120.4892	119.6486	120.7558	119.6139	120.6434	119.7013	121.0874	**117.6**
C6	132.2467	134.2864	135.3229	135.3472	136.8781	135.2854	137.5200	135.2189	137.2791	135.4016	138.0862	132.2467	134.2864	135.3229	135.3472	136.8781	135.2854	137.5200	135.2189	137.2791	135.4016	138.0862	**133.3**
C7	201.2567	205.6591	206.8764	207.8846	208.7243	207.7624	212.8796	207.6342	211.9294	207.9947	214.0254	201.2567	205.6591	206.8764	207.8846	208.7243	207.7624	212.8796	207.6342	211.9294	207.9947	214.0254	**195.8**
C8	68.1361	69.5249	70.2639	70.0439	71.1738	70.0330	71.7242	70.0145	71.5644	70.0470	72.2963	68.1361	69.5249	70.2639	70.0439	71.1738	70.0330	71.7242	70.0145	71.5644	70.0470	72.2963	**70.4**
C9	38.8652	38.7336	38.8380	38.5423	38.8956	38.5618	39.1809	38.5758	39.0858	38.5184	39.4764	38.8652	38.7336	38.8380	38.5423	38.8956	38.5619	39.1809	38.5758	39.0858	38.5184	39.4764	**31.1**
C10	29.5240	30.1529	30.5449	30.4255	31.1246	30.4126	30.9274	30.3953	30.9087	30.4332	31.2594	29.5240	30.1529	30.5449	30.4255	31.1246	30.4126	30.9274	30.3953	30.9087	30.4332	31.2594	**26.9**
C11	29.4418	29.6972	29.8600	29.5824	29.9487	29.6022	29.9365	29.6159	29.9309	29.5580	30.2368	29.4418	29.6972	29.8601	29.5824	29.9487	29.6021	29.9365	29.6159	29.9309	29.5580	30.2368	**23.4**
C12	16.5296	16.7824	16.7604	16.8352	16.8320	16.8373	16.8060	16.8346	16.7990	16.8289	16.9542	16.5296	16.7824	16.7604	16.8352	16.8320	16.8373	16.8060	16.8346	16.7990	16.8290	16.9543	**13.8**
C1`	53.7220	54.6467	54.8434	55.1464	55.6019	55.1212	55.6068	55.0916	55.5138	55.1663	56.3013	58.2667	59.6104	59.9327	60.0596	60.4729	60.0450	60.6886	60.0246	60.6186	60.0678	61.1204	**53.3**
C2`	26.2439	26.8649	27.1493	27.0337	27.4594	27.0338	27.4989	27.0283	27.4820	27.0283	27.4483	25.9185	26.2129	26.4676	26.3545	26.7189	26.3512	26.7270	26.3431	26.7097	26.3531	26.7220	**24.2**
C3`	25.9185	26.2129	26.4677	26.3545	26.7189	26.3512	26.7270	26.3431	26.7097	26.3531	26.7220	26.2438	26.8649	27.1491	27.0337	27.4594	27.0338	27.4989	27.0283	27.4820	27.0283	27.4483	**24.1**
C4`	58.2667	59.6104	59.9326	60.0596	60.4729	60.0450	60.6886	60.0246	60.6186	60.0678	61.1203	53.7220	54.6467	54.8434	55.1464	55.6019	55.1212	55.6068	55.0916	55.5138	55.1663	56.3010	**56.3**
H2	8.5202	8.4179	8.4255	8.3541	8.3445	8.3584	8.3760	8.3625	8.3748	8.3498	8.3764	8.5202	8.4179	8.4255	8.3541	8.3445	8.3584	8.3761	8.3625	8.3748	8.3498	8.3764	**8.2**
H3	7.1794	7.3318	7.4109	7.3778	7.4831	7.3764	7.5086	7.3746	7.4988	7.3787	7.5375	7.1794	7.3318	7.4109	7.3778	7.4831	7.3764	7.5086	7.3746	7.4988	7.3787	7.5375	**7.36**
H5	7.0044	7.1582	7.2405	7.2245	7.3556	7.2214	7.3589	7.2179	7.3494	7.2272	7.4008	7.0044	7.1582	7.2405	7.2245	7.3556	7.2214	7.3589	7.2179	7.3494	7.2272	7.4008	**7.36**
H6	7.9135	8.0785	8.1409	8.1670	8.2621	8.1621	8.3188	8.1568	8.3018	8.1713	8.3592	7.9135	8.0785	8.1409	8.1670	8.2621	8.1621	8.3188	8.1568	8.3018	8.1713	8.3592	**8.2**
H8	4.9923	5.0231	5.0204	5.0488	5.0657	5.0471	5.0991	5.0452	5.0903	5.0501	5.0979	4.9923	5.0231	5.0204	5.0488	5.0657	5.0471	5.0991	5.0452	5.0903	5.0501	5.0979	**5.4**
H(9A-9B)	1.8866	1.9233	1.9092	1.9458	1.9709	1.9451	1.9663	1.9441	1.9592	1.9462	2.0157	1.8866	1.9233	1.9092	1.9458	1.9709	1.9451	1.9663	1.9441	1.9592	1.9462	2.0157	**2.08**
H(10A)	1.0160	0.9024	0.8508	0.8713	0.7697	0.8724	0.8288	0.8734	0.8187	0.8670	0.8515	1.0160	0.9024	0.8508	0.8713	0.7697	0.8724	0.8288	0.8734	0.8187	0.8700	0.8515	**1.14**
H(10B)	1.7876	1.6671	1.5902	1.5808	1.4877	1.5871	1.4750	1.5931	1.4819	1.5746	1.4536	1.7876	1.6671	1.5902	1.5808	1.4877	1.5871	1.4750	1.5931	1.4819	1.5746	1.4535	**1.28**
H(11A-11B)	1.1095	1.1243	1.0787	1.1354	1.0880	1.1356	1.0865	1.1355	1.0849	1.1348	1.0877	1.1095	1.1243	1.0788	1.1354	1.0880	1.1356	1.0865	1.1355	1.0849	1.1348	1.0877	**1.28**
H(12A-12C)	0.9116	0.9045	0.8683	0.8963	0.8471	0.8975	0.8543	0.8985	0.8534	0.8948	0.8614	0.9116	0.9045	0.8683	0.8963	0.8471	0.8975	0.8543	0.8985	0.8534	0.8948	0.8614	**0.82**
H(1`A)	2.8037	2.7998	2.7761	2.7875	2.7401	2.7890	2.7544	2.7902	2.7555	2.7857	2.7327	2.9270	2.9443	2.9250	2.9302	2.8972	2.9326	2.9032	2.9346	2.9064	2.9275	2.8769	**3.38**
H(1`B)	3.3751	3.4176	3.4367	3.4453	3.4990	3.4441	3.4838	3.4427	3.4815	3.4461	3.4880	3.1070	2.9109	2.8780	2.8605	2.8494	2.8627	2.8030	2.8649	2.8065	2.8583	2.7978	**3.71**
H(2`A)	1.6748	1.7240	1.6882	1.7424	1.6850	1.7422	1.7086	1.7417	1.7041	1.7422	1.7337	1.5435	1.5855	1.5510	1.6075	1.5463	1.6069	1.5802	1.6060	1.5736	1.6077	1.6113	**2.08**
H(2`B)	1.9335	1.9409	1.8850	1.9746	1.9168	1.9722	1.9183	1.9696	1.9114	1.9768	1.9649	1.7819	1.8931	1.8408	1.9568	1.9001	1.9536	1.9222	1.9501	1.9124	1.9596	1.9912	**2.24**
H(3`A)	1.5435	1.5855	1.5510	1.6075	1.5463	1.6069	1.5802	1.6060	1.5736	1.6077	1.6113	1.6748	1.7240	1.6882	1.7424	1.6850	1.7422	1.7086	1.7417	1.7041	1.7422	1.7337	**2.08**
H(3`B)	1.7819	1.8931	1.8408	1.9568	1.9001	1.9536	1.9222	1.9501	1.9124	1.9596	1.9912	1.9335	1.9409	1.8850	1.9746	1.9168	1.9722	1.9183	1.9696	1.9114	1.9768	1.9649	**2.16**
H(4`A)	3.1070	2.9109	2.8780	2.8605	2.8494	2.8627	2.8030	2.8649	2.8065	2.8583	2.7978	3.3751	3.4176	3.4367	3.4452	3.4990	3.4441	3.4838	3.4427	3.4815	3.4461	3.4880	**3.09**
H(4`B)	2.9270	2.9443	2.9250	2.9302	2.8972	2.9326	2.9032	2.9346	2.9064	2.9275	2.8769	2.8037	2.7998	2.7761	2.7875	2.7401	2.7890	2.7544	2.7902	2.7555	2.7857	2.7327	**3.68**
Nuclei	CAM-B3LYP											CAM-B3LYP										
C1	140.9000	141.8642	142.5134	142.3393	143.9931	142.3245	143.2389	142.3087	143.3053	142.3544	143.4213	140.8999	141.8642	142.5135	142.3392	143.9931	142.3245	143.2389	142.3087	143.3053	142.3544	143.4212	**132.2**
C2	142.3592	142.3291	142.7581	142.1837	142.6753	142.1979	143.2028	142.2124	143.0855	142.1723	143.1775	142.3594	142.3291	142.7582	142.1837	142.6754	142.1979	143.2028	142.2124	143.0855	142.1723	143.1775	**133.3**
C3	123.8875	124.5615	125.0610	124.7361	125.3833	124.7328	125.5918	124.7293	125.5399	124.7413	125.6630	123.8876	124.5615	125.0610	124.7363	125.3832	124.7328	125.5918	124.7293	125.5399	124.7412	125.6631	**117.6**
C4	177.7476	178.5115	179.0552	178.8743	179.4733	178.8556	180.0785	178.8375	179.9280	178.8943	180.2203	177.7477	178.5115	179.0551	178.8744	179.4733	178.8556	180.0785	178.8375	179.9280	178.8944	180.2204	**168.3**
C5	121.8135	123.1003	123.6648	123.7417	124.5660	123.7060	124.7320	123.6710	124.6384	123.7775	124.8939	121.8135	123.1003	123.6648	123.7415	124.5660	123.7060	124.7320	123.6709	124.6384	123.7775	124.8939	**117.6**
C6	138.4687	140.3307	141.5035	141.4320	142.9843	141.3615	143.6195	141.2922	143.3572	141.5021	144.0436	138.4687	140.3307	141.5034	141.4319	142.9843	141.3615	143.6195	141.2922	143.3572	141.5021	144.0435	**133.3**
C7	206.2190	211.2347	212.3397	213.9879	214.6304	213.8311	220.0283	213.6740	218.8123	214.1375	221.0855	206.2190	211.2347	212.3397	213.9878	214.6304	213.8311	220.0283	213.6739	218.8123	214.1374	221.0856	**195.8**
C8	64.6063	65.7712	66.4410	66.2572	67.2927	66.2389	67.9060	66.2194	67.7480	66.2753	68.2828	64.6064	65.7712	66.4410	66.2573	67.2928	66.2389	67.9060	66.2194	67.7480	66.2753	68.2828	**70.4**
C9	35.3917	35.0454	35.2739	34.8733	35.1875	34.8869	35.3176	34.9005	35.2558	34.8622	35.4063	35.3917	35.0454	35.2740	34.8733	35.1874	34.8869	35.3176	34.9006	35.2558	34.8622	35.4064	**31.1**
C10	28.1866	28.6440	29.1029	28.9663	29.6973	28.9451	29.5046	28.9250	29.4847	28.9892	29.6822	28.1867	28.6440	29.1029	28.9664	29.6974	28.9451	29.5046	28.9249	29.4847	28.9892	29.6823	**26.9**
C11	27.8708	27.9976	28.2402	27.9403	28.3933	27.9501	28.3825	27.9597	28.3778	27.9329	28.5418	27.8708	27.9976	28.2403	27.9403	28.3933	27.9501	28.3825	27.9596	28.3778	27.9330	28.5418	**23.4**
C12	16.2567	16.4391	16.4726	16.5524	16.6588	16.5468	16.6036	16.5421	16.5992	16.5601	16.6163	16.2567	16.4391	16.4726	16.5523	16.6589	16.5468	16.6036	16.5420	16.5992	16.5601	16.6163	**13.8**
C1`	50.8435	51.6933	51.8918	52.2148	52.7698	52.1836	52.7649	52.1535	52.6947	52.2469	53.2563	55.1554	56.2469	56.5379	56.6717	57.1952	56.6514	57.3190	56.6314	57.2584	56.6928	57.5773	**53.3**
C2`	25.0342	25.4284	25.7358	25.5492	26.0245	25.5467	26.0407	25.5443	26.0345	25.5535	25.8833	24.4922	24.6878	24.9644	24.8119	25.2810	24.8071	25.1973	24.8028	25.1947	24.8187	25.0647	**24.2**
C3`	24.4923	24.6878	24.9643	24.8118	25.2810	24.8071	25.1973	24.8028	25.1947	24.8188	25.0648	25.0342	25.4285	25.7358	25.5492	26.0245	25.5467	26.0407	25.5444	26.0345	25.5534	25.8833	**24.1**
C4`	55.1553	56.2469	56.5378	56.6715	57.1952	56.6514	57.3190	56.6314	57.2584	56.6927	57.5773	50.8435	51.6933	51.8918	52.2147	52.7697	52.1836	52.7649	52.1534	52.6947	52.2470	53.2562	**56.3**
H2	8.8102	8.6986	8.7289	8.6236	8.6210	8.6275	8.6425	8.6316	8.6418	8.6199	8.6323	8.8102	8.6986	8.7289	8.6236	8.6210	8.6275	8.6425	8.6316	8.6418	8.6199	8.6322	**8.2**
H3	7.4041	7.5438	7.6298	7.5866	7.7036	7.5847	7.7229	7.5828	7.7152	7.5883	7.7368	7.4041	7.5438	7.6298	7.5866	7.7036	7.5847	7.7229	7.5828	7.7152	7.5883	7.7368	**7.36**
H5	7.2406	7.4128	7.5085	7.4855	7.6154	7.4812	7.6240	7.4771	7.6145	7.4895	7.6484	7.2405	7.4128	7.5085	7.4855	7.6154	7.4812	7.6240	7.4771	7.6145	7.4895	7.6484	**7.36**
H6	8.0497	8.2319	8.3255	8.3359	8.4632	8.3292	8.5140	8.3227	8.4924	8.3422	8.5479	8.0497	8.2319	8.3255	8.3359	8.4632	8.3292	8.5140	8.3227	8.4924	8.3422	8.5479	**8.2**
H8	4.4210	4.4951	4.5329	4.5563	4.6154	4.5520	4.6593	4.5478	4.6382	4.5605	4.6576	4.4210	4.4951	4.5329	4.5563	4.6153	4.5520	4.6593	4.5478	4.6382	4.5605	4.6576	**5.4**
H(9A-9B)	1.6746	1.7066	1.7208	1.7333	1.7558	1.7312	1.7557	1.7292	1.7500	1.7352	1.7902	1.6746	1.7066	1.7208	1.7333	1.7558	1.7312	1.7557	1.7292	1.7500	1.7352	1.7902	**2.08**
H(10A)	0.9793	0.8280	0.7905	0.7827	0.6958	0.7844	0.7355	0.7864	0.7297	0.7811	0.7458	0.9793	0.8280	0.7905	0.7827	0.6958	0.7844	0.7355	0.7864	0.7297	0.7811	0.7458	**1.14**
H(10B)	1.6254	1.5324	1.4640	1.4472	1.3642	1.4530	1.3590	1.4589	1.3655	1.4418	1.3321	1.6253	1.5324	1.4640	1.4472	1.3642	1.4530	1.3590	1.4589	1.3655	1.4418	1.3321	**1.28**
H(11A-11B)	1.0293	1.0490	1.0127	1.0612	1.0239	1.0605	1.0223	1.0600	1.0216	1.0618	1.0127	1.0293	1.0490	1.0127	1.0612	1.0239	1.0605	1.0223	1.0600	1.0216	1.0618	1.0127	**1.28**
H(12A-12C)	0.9496	0.9353	0.9077	0.9264	0.8870	0.9270	0.8928	0.9277	0.8929	0.9257	0.8870	0.9496	0.9353	0.9077	0.9264	0.8871	0.9270	0.8928	0.9277	0.8929	0.9257	0.8870	**0.82**
H(1`A)	2.7110	2.7033	2.6912	2.6925	2.6485	2.6932	2.6648	2.6941	2.6655	2.6917	2.6365	2.8448	2.8448	2.8307	2.8212	2.7916	2.8233	2.8027	2.8254	2.8061	2.8191	2.7687	**3.38**
H(1`B)	3.1229	3.1689	3.2079	3.2088	3.2727	3.2060	3.2605	3.2034	3.2561	3.2114	3.2635	2.8211	2.6606	2.6465	2.6360	2.6365	2.6367	2.5996	2.6376	2.6000	2.6354	2.5884	**3.71**
H(2`A)	1.6362	1.6816	1.6509	1.6997	1.6466	1.6989	1.6722	1.6981	1.6689	1.7005	1.6821	1.5140	1.5653	1.5337	1.5881	1.5366	1.5871	1.5718	1.5862	1.5662	1.5891	1.5878	**2.08**
H(2`B)	1.7982	1.8246	1.7824	1.8735	1.8313	1.8698	1.8300	1.8663	1.8234	1.8771	1.8557	1.6828	1.7942	1.7423	1.8642	1.8262	1.8599	1.8521	1.8557	1.8411	1.8683	1.8964	**2.24**
H(3`A)	1.5140	1.5653	1.5337	1.5881	1.5366	1.5871	1.5718	1.5862	1.5662	1.5891	1.5878	1.6362	1.6817	1.6509	1.6997	1.6466	1.6989	1.6722	1.6981	1.6689	1.7004	1.6821	**2.08**
H(3`B)	1.6828	1.7942	1.7423	1.8642	1.8262	1.8599	1.8521	1.8557	1.8411	1.8683	1.8965	1.7982	1.8246	1.7824	1.8735	1.8312	1.8698	1.8300	1.8663	1.8234	1.8771	1.8557	**2.16**
H(4`A)	2.8211	2.6606	2.6465	2.6360	2.6365	2.6367	2.5996	2.6376	2.6000	2.6354	2.5884	3.1229	3.1689	3.2079	3.2088	3.2727	3.2060	3.2605	3.2033	3.2561	3.2114	3.2635	**3.09**
H(4`B)	2.8448	2.8448	2.8307	2.8212	2.7916	2.8233	2.8027	2.8254	2.8061	2.8191	2.7687	2.7110	2.7033	2.6912	2.6925	2.6485	2.6932	2.6648	2.6941	2.6655	2.6917	2.6364	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S5. Cont. VI

Nuclei	R											S										Exp. [b]
	HF											HF										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.4614	137.5594	137.9396	138.2608	141.1588	138.1812	139.8214	138.1121	140.2588	138.3352	140.0156	136.4614	137.5594	137.9396	138.2608	141.1590	138.1812	139.8214	138.1123	140.2588	138.3352	140.0156	**132.2**
C2	144.3880	144.1261	144.6323	143.8817	144.0884	143.9028	144.6434	143.9234	144.4625	143.8613	144.6473	144.3881	144.1261	144.6323	143.8817	144.0886	143.9028	144.6434	143.9233	144.4625	143.8613	144.6474	**133.3**
C3	120.4753	121.0267	121.4081	121.1842	121.9458	121.1734	121.9413	121.1639	121.9814	121.1933	121.9865	120.4753	121.0267	121.4081	121.1842	121.9457	121.1734	121.9413	121.1637	121.9814	121.1933	121.9866	**117.6**
C4	171.1212	171.5718	172.1467	171.7971	172.0666	171.7897	172.8696	171.7808	172.6355	171.8033	173.0028	171.1213	171.5718	172.1467	171.7971	172.0666	171.7897	172.8696	171.7807	172.6354	171.8033	173.0028	**168.3**
C5	117.8593	119.1512	119.5795	119.8198	120.6684	119.7762	120.6727	119.7340	120.6376	119.8599	120.8287	117.8593	119.1512	119.5795	119.8198	120.6682	119.7762	120.6727	119.7339	120.6376	119.8599	120.8287	**117.6**
C6	139.9930	141.4756	142.7481	142.2938	142.9370	142.2616	143.9248	142.2248	143.4971	142.3244	144.2237	139.9930	141.4756	142.7481	142.2938	142.9368	142.2616	143.9248	142.2249	143.4971	142.3244	144.2236	**133.3**
C7	196.4929	202.2641	202.9719	205.5898	206.7292	205.3508	213.4358	205.1213	212.0643	205.8156	214.4845	196.4932	202.2641	202.9719	205.5898	206.7294	205.3508	213.4358	205.1213	212.0643	205.8152	214.4845	**195.8**
C8	55.7610	56.8718	57.1616	57.3487	58.2739	57.3120	58.7513	57.2794	58.6807	57.3824	58.9817	55.7610	56.8718	57.1617	57.3487	58.2738	57.3120	58.7513	57.2794	58.6807	57.3825	58.9816	**70.4**
C9	29.9395	29.4452	29.6637	29.2244	29.3513	29.2420	29.2641	29.2585	29.2555	29.2074	29.2254	29.9396	29.4452	29.6637	29.2244	29.3513	29.2420	29.2641	29.2587	29.2555	29.2074	29.2254	**31.1**
C10	24.5112	24.8855	25.3200	25.1270	25.7191	25.1133	25.5163	25.0997	25.4870	25.1397	25.6454	24.5113	24.8855	25.3200	25.1270	25.7191	25.1133	25.5163	25.0997	25.4869	25.1397	25.6454	**26.9**
C11	24.9934	25.0012	25.2811	24.9675	25.3997	24.9711	25.3586	24.9750	25.3631	24.9631	25.4875	24.9934	25.0012	25.2811	24.9675	25.3997	24.9711	25.3586	24.9751	25.3632	24.9630	25.4875	**23.4**
C12	16.1893	16.3050	16.4087	16.4083	16.5840	16.3998	16.5424	16.3920	16.5403	16.4161	16.5585	16.1893	16.3050	16.4087	16.4083	16.5840	16.3998	16.5424	16.3920	16.5403	16.4161	16.5585	**13.8**
C1`	44.6495	45.3638	45.5995	45.8292	46.3745	45.7972	46.3770	45.7670	46.3398	45.8597	46.7427	48.5492	49.4089	49.6427	49.7948	50.2999	49.7716	50.3741	49.7486	50.3061	49.8158	50.6100	**53.3**
C2`	22.8232	23.0884	23.3924	23.1170	23.5554	23.1184	23.5262	23.1198	23.5079	23.1145	23.3375	22.1997	22.2737	22.6410	22.3541	22.9562	22.3468	22.8286	22.3405	22.8432	22.3604	22.6316	**24.2**
C3`	22.1997	22.2737	22.6410	22.3541	22.9561	22.3468	22.8286	22.3405	22.8431	22.3603	22.6316	22.8232	23.0884	23.3924	23.1170	23.5554	23.1184	23.5262	23.1197	23.5079	23.1145	23.3375	**24.1**
C4`	48.5492	49.4089	49.6427	49.7948	50.3000	49.7716	50.3741	49.7487	50.3060	49.8158	50.6100	44.6494	45.3638	45.5995	45.8291	46.3746	45.7972	46.3770	45.7670	46.3397	45.8597	46.7426	**56.3**
H2	9.0711	8.9082	8.9926	8.7974	8.6994	8.8084	8.7504	8.8181	8.7213	8.7871	8.7457	9.0711	8.9082	8.9926	8.7974	8.6994	8.8084	8.7504	8.8181	8.7212	8.7871	8.7457	**8.2**
H3	7.4358	7.5753	7.6646	7.6196	7.7433	7.6175	7.7557	7.6152	7.7493	7.6217	7.7711	7.4358	7.5753	7.6646	7.6196	7.7433	7.6175	7.7557	7.6152	7.7493	7.6217	7.7711	**7.36**
H5	7.2401	7.4378	7.5258	7.5268	7.6588	7.5216	7.6718	7.5162	7.6614	7.5317	7.6960	7.2401	7.4378	7.5258	7.5268	7.6588	7.5216	7.6718	7.5162	7.6614	7.5317	7.6960	**7.36**
H6	8.0965	8.3044	8.4316	8.4110	8.5225	8.4061	8.5996	8.4004	8.5605	8.4158	8.6363	8.0965	8.3044	8.4316	8.4110	8.5225	8.4061	8.5996	8.4004	8.5606	8.4158	8.6363	**8.2**
H8	3.6381	3.7437	3.8354	3.8239	3.9329	3.8188	4.0011	3.8133	3.9706	3.8288	3.9979	3.6381	3.7437	3.8354	3.8239	3.9329	3.8188	4.0011	3.8133	3.9706	3.8288	3.9979	**5.4**
H(9A-9B)	1.3084	1.3301	1.3445	1.3363	1.2736	1.3379	1.2820	1.3390	1.2675	1.3349	1.3033	1.3084	1.3301	1.3445	1.3363	1.2736	1.3379	1.2820	1.3390	1.2675	1.3349	1.3033	**2.08**
H(10A)	0.9656	0.7280	0.7412	0.6826	0.6635	0.6833	0.6994	0.6843	0.7008	0.6822	0.7041	0.9656	0.7280	0.7412	0.6826	0.6635	0.6833	0.6994	0.6843	0.7008	0.6822	0.7041	**1.14**
H(10B)	1.3770	1.3012	1.2518	1.2206	1.1379	1.2267	1.1517	1.2323	1.1569	1.2149	1.1303	1.3771	1.3012	1.2518	1.2206	1.1379	1.2267	1.1517	1.2323	1.1568	1.2149	1.1303	**1.28**
H(11A-11B)	0.8644	0.8763	0.8546	0.8936	0.8559	0.8927	0.8656	0.8916	0.8636	0.8945	0.8622	0.8644	0.8763	0.8546	0.8936	0.8559	0.8927	0.8656	0.8917	0.8636	0.8944	0.8622	**1.28**
H(12A-12C)	0.9257	0.9009	0.8816	0.8957	0.8713	0.8956	0.8816	0.8955	0.8831	0.8958	0.8787	0.9257	0.9009	0.8817	0.8957	0.8713	0.8956	0.8816	0.8956	0.8831	0.8958	0.8787	**0.82**
H(1`A)	2.3729	2.3640	2.3490	2.3541	2.3106	2.3546	2.3370	2.3550	2.3368	2.3537	2.3150	2.5341	2.5327	2.5042	2.4991	2.4550	2.5016	2.4708	2.5039	2.4741	2.4967	2.4443	**3.38**
H(1`B)	2.7192	2.7822	2.8168	2.8250	2.8747	2.8223	2.8737	2.8195	2.8658	2.8276	2.8825	2.3793	2.2880	2.2538	2.2872	2.3250	2.2852	2.2832	2.2834	2.2964	2.2895	2.2833	**3.71**
H(2`A)	1.4596	1.5065	1.4695	1.5227	1.4643	1.5218	1.4902	1.5207	1.4875	1.5236	1.5015	1.3531	1.4150	1.3758	1.4387	1.3948	1.4370	1.4298	1.4353	1.4285	1.4403	1.4450	**2.08**
H(2`B)	1.5116	1.5543	1.5178	1.6170	1.5855	1.6122	1.5872	1.6073	1.5811	1.6217	1.6111	1.4135	1.5446	1.4828	1.6324	1.6198	1.6256	1.6502	1.6189	1.6431	1.6390	1.6949	**2.24**
H(3`A)	1.3531	1.4150	1.3758	1.4387	1.3948	1.4370	1.4298	1.4352	1.4285	1.4403	1.4450	1.4596	1.5065	1.4695	1.5227	1.4643	1.5218	1.4902	1.5207	1.4875	1.5236	1.5015	**2.08**
H(3`B)	1.4135	1.5446	1.4828	1.6324	1.6198	1.6256	1.6502	1.6189	1.6431	1.6390	1.6949	1.5116	1.5543	1.5178	1.6170	1.5855	1.6122	1.5872	1.6073	1.5811	1.6217	1.6111	**2.16**
H(4`A)	2.3793	2.2880	2.2538	2.2872	2.3250	2.2852	2.2832	2.2834	2.2964	2.2895	2.2833	2.7192	2.7822	2.8168	2.8250	2.8747	2.8223	2.8737	2.8195	2.8658	2.8276	2.8825	**3.09**
H(4`B)	2.5341	2.5327	2.5042	2.4991	2.4550	2.5016	2.4708	2.5039	2.4741	2.4967	2.4443	2.3728	2.3640	2.3490	2.3541	2.3106	2.3546	2.3370	2.3550	2.3368	2.3537	2.3150	**3.68**
Nuclei	LC-BLYP											LC-BLYP										
C1	144.3028	145.1950	146.1042	145.8010	147.4677	145.7589	146.7872	145.7404	146.8037	145.8203	147.0726	144.3028	145.1949	146.1041	145.8010	147.4677	145.7589	146.7872	145.7405	146.8037	145.8203	147.0725	**132.2**
C2	148.6053	148.4336	148.9601	148.2830	148.7557	148.2707	149.2718	148.2857	149.1701	148.2777	149.2677	148.6053	148.4336	148.9602	148.2830	148.7557	148.2707	149.2718	148.2859	149.1701	148.2778	149.2676	**133.3**
C3	128.2541	128.9264	129.5380	129.1390	129.8089	129.1086	129.9774	129.1049	129.9340	129.1500	130.0396	128.2541	128.9264	129.5380	129.1390	129.8089	129.1086	129.9774	129.1048	129.9339	129.1500	130.0397	**117.6**
C4	181.9735	182.5089	183.1029	182.8610	183.3907	182.8163	184.0004	182.7995	183.8613	182.8865	184.1304	181.9735	182.5091	183.1027	182.8610	183.3907	182.8164	184.0004	182.7995	183.8613	182.8865	184.1304	**168.3**
C5	126.1791	127.4745	128.1385	128.2234	129.0703	128.1579	129.2286	128.1194	129.1271	128.2680	129.3934	126.1791	127.4745	128.1384	128.2234	129.0703	128.1579	129.2287	128.1195	129.1270	128.2679	129.3934	**117.6**
C6	144.2567	146.1931	147.4116	147.2757	148.9440	147.1795	149.5452	147.1123	149.2785	147.3512	149.9505	144.2567	146.1930	147.4116	147.2757	148.9440	147.1795	149.5451	147.1124	149.2785	147.3512	149.9505	**133.3**
C7	211.8303	217.0927	218.4451	220.2118	220.7174	220.0151	226.8416	219.8419	225.4392	220.3777	228.0439	211.8303	217.0927	218.4455	220.2118	220.7174	220.0150	226.8416	219.8416	225.4392	220.3777	228.0436	**195.8**
C8	62.4946	63.6122	64.3010	64.2400	65.1246	64.1886	65.9586	64.1624	65.7354	64.2696	66.4491	62.4946	63.6122	64.3010	64.2400	65.1246	64.1886	65.9586	64.1624	65.7354	64.2696	66.4492	**70.4**
C9	33.0906	32.7128	32.9583	32.5697	32.8735	32.5573	33.0162	32.5722	32.9124	32.5640	33.1062	33.0906	32.7128	32.9583	32.5697	32.8734	32.5573	33.0162	32.5722	32.9124	32.5640	33.1062	**31.1**
C10	26.7174	27.0997	27.5416	27.4779	28.1510	27.4294	27.9545	27.4087	27.9216	27.5068	28.1708	26.7174	27.0997	27.5417	27.4779	28.1510	27.4295	27.9545	27.4088	27.9216	27.5068	28.1708	**26.9**
C11	25.6629	25.6738	26.0213	25.6762	26.0987	25.6556	26.0916	25.6622	26.0813	25.6781	26.2660	25.6628	25.6738	26.0212	25.6762	26.0987	25.6557	26.0917	25.6622	26.0813	25.6781	26.2660	**23.4**
C12	15.2825	15.3973	15.4777	15.5469	15.6332	15.5145	15.5678	15.5098	15.5562	15.5604	15.5999	15.2825	15.3974	15.4776	15.5468	15.6333	15.5145	15.5678	15.5098	15.5562	15.5604	15.5999	**13.8**
C1`	48.8633	49.5850	49.8719	50.1266	50.6951	50.0699	50.6789	50.0406	50.6292	50.1636	51.1331	52.7573	53.6750	54.0588	54.1648	54.6804	54.1139	54.7997	54.0904	54.7504	54.1956	55.0687	**53.3**
C2`	23.0097	23.2733	23.5886	23.4460	23.8619	23.4152	23.9107	23.4114	23.8912	23.4575	23.8212	22.3648	22.4849	22.8031	22.6272	23.0962	22.5957	22.9834	22.5919	22.9779	22.6398	22.9003	**24.2**
C3`	22.3648	22.4849	22.8032	22.6272	23.0962	22.5957	22.9834	22.5918	22.9779	22.6398	22.9003	23.0098	23.2733	23.5887	23.4460	23.8619	23.4152	23.9107	23.4114	23.8911	23.4575	23.8213	**24.1**
C4`	52.7572	53.6750	54.0587	54.1648	54.6804	54.1139	54.7997	54.0903	54.7504	54.1956	55.0688	48.8633	49.5850	49.8719	50.1267	50.6951	50.0699	50.6789	50.0406	50.6292	50.1636	51.1331	**56.3**
H2	9.0056	8.8849	8.9030	8.7965	8.7977	8.7995	8.7926	8.8043	8.8043	8.7932	8.7781	9.0056	8.8849	8.9030	8.7965	8.7977	8.7994	8.7926	8.8043	8.8043	8.7932	8.7781	**8.2**
H3	7.5396	7.6763	7.7674	7.7172	7.8365	7.7144	7.8519	7.7131	7.8455	7.7189	7.8671	7.5396	7.6763	7.7674	7.7172	7.8365	7.7144	7.8519	7.7131	7.8455	7.7189	7.8671	**7.36**
H5	7.3877	7.5702	7.6618	7.6532	7.7802	7.6475	7.7925	7.6434	7.7820	7.6575	7.8161	7.3877	7.5702	7.6618	7.6532	7.7802	7.6475	7.7926	7.6434	7.7820	7.6575	7.8161	**7.36**
H6	8.1905	8.3935	8.4921	8.4932	8.6406	8.4854	8.6743	8.4792	8.6601	8.4999	8.7076	8.1905	8.3935	8.4921	8.4932	8.6406	8.4854	8.6743	8.4792	8.6601	8.4999	8.7076	**8.2**
H8	4.2049	4.2951	4.3484	4.3672	4.4527	4.3612	4.4800	4.3569	4.4681	4.3721	4.4886	4.2049	4.2951	4.3484	4.3672	4.4527	4.3612	4.4800	4.3569	4.4681	4.3722	4.4886	**5.4**
H(9A-9B)	1.6602	1.6944	1.6916	1.7190	1.7312	1.7160	1.7354	1.7147	1.7257	1.7209	1.7694	1.6602	1.6944	1.6916	1.7190	1.7312	1.7160	1.7354	1.7147	1.7257	1.7209	1.7694	**2.08**
H(10A)	0.9464	0.7709	0.7337	0.7059	0.6281	0.7076	0.6393	0.7111	0.6461	0.7035	0.6520	0.9464	0.7709	0.7337	0.7059	0.6281	0.7076	0.6393	0.7111	0.6461	0.7035	0.6520	**1.14**
H(10B)	1.5956	1.4998	1.4331	1.4116	1.3290	1.4162	1.3204	1.4225	1.3282	1.4064	1.2946	1.5956	1.4998	1.4331	1.4116	1.3290	1.4162	1.3204	1.4225	1.3282	1.4064	1.2946	**1.28**
H(11A-11B)	0.9922	1.0091	0.9759	1.0198	0.9828	1.0178	0.9739	1.0175	0.9768	1.0208	0.9667	0.9922	1.0091	0.9759	1.0198	0.9828	1.0178	0.9739	1.0175	0.9768	1.0208	0.9667	**1.28**
H(12A-12C)	0.9529	0.9320	0.9064	0.9207	0.8812	0.9204	0.8804	0.9217	0.8832	0.9200	0.8772	0.9529	0.9320	0.9064	0.9207	0.8812	0.9204	0.8803	0.9216	0.8832	0.9200	0.8772	**0.82**
H(1`A)	2.6756	2.6656	2.6476	2.6566	2.6054	2.6565	2.6213	2.6579	2.6203	2.6558	2.6008	2.8095	2.7976	2.7819	2.7777	2.7409	2.7787	2.7655	2.7812	2.7634	2.7757	2.7396	**3.38**
H(1`B)	3.0184	3.0586	3.0951	3.0995	3.1550	3.0957	3.1431	3.0935	3.1381	3.1022	3.1499	2.7332	2.5800	2.5558	2.5523	2.5380	2.5532	2.5182	2.5557	2.5071	2.5505	2.5099	**3.71**
H(2`A)	1.6383	1.6830	1.6519	1.7025	1.6442	1.7006	1.6698	1.7003	1.6669	1.7033	1.6810	1.5189	1.5743	1.5442	1.5997	1.5465	1.5976	1.5824	1.5971	1.5790	1.6007	1.6004	**2.08**
H(2`B)	1.7521	1.7824	1.7443	1.8315	1.7969	1.8269	1.7886	1.8240	1.7826	1.8350	1.8143	1.6609	1.7682	1.7236	1.8425	1.8099	1.8368	1.8308	1.8328	1.8249	1.8469	1.8762	**2.24**
H(3`A)	1.5189	1.5743	1.5442	1.5997	1.5465	1.5976	1.5824	1.5970	1.5790	1.6007	1.6004	1.6383	1.6830	1.6519	1.7025	1.6442	1.7006	1.6698	1.7003	1.6669	1.7033	1.6810	**2.08**
H(3`B)	1.6609	1.7682	1.7236	1.8425	1.8099	1.8368	1.8308	1.8328	1.8249	1.8469	1.8762	1.7521	1.7824	1.7443	1.8315	1.7969	1.8269	1.7886	1.8240	1.7826	1.8350	1.8143	**2.16**
H(4`A)	2.7332	2.5800	2.5558	2.5523	2.5380	2.5532	2.5182	2.5557	2.5071	2.5505	2.5099	3.0184	3.0586	3.0951	3.0995	3.1550	3.0957	3.1431	3.0935	3.1381	3.1022	3.1499	**3.09**
H(4`B)	2.8095	2.7976	2.7819	2.7777	2.7409	2.7787	2.7655	2.7812	2.7634	2.7757	2.7396	2.6756	2.6656	2.6476	2.6566	2.6054	2.6565	2.6213	2.6579	2.6203	2.6558	2.6008	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S5. Cont. VII

Nuclei	R											S										Exp. [b]
	M06																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.6837	138.1845	138.7887	138.8803	142.1616	138.8390	141.0201	138.8028	141.1968	138.9324	141.3525	136.6837	138.1845	138.7887	138.8803	142.1616	138.8390	141.0201	138.8027	141.1968	138.9324	141.3525	**132.2**
C2	139.8288	139.8302	140.5330	139.7616	140.5668	139.7588	141.0927	139.7635	140.9947	139.7793	141.0467	139.8288	139.8302	140.5330	139.7616	140.5668	139.7588	141.0927	139.7635	140.9947	139.7793	141.0466	**133.3**
C3	121.7274	122.3706	123.0781	122.5656	123.3591	122.5459	123.5764	122.5339	123.5302	122.5989	123.6983	121.7273	122.3706	123.0781	122.5656	123.3592	122.5459	123.5764	122.5338	123.5302	122.5989	123.6984	**117.6**
C4	173.6534	174.3654	175.1102	174.6855	175.0219	174.6538	175.6222	174.6298	175.4678	174.7300	175.7595	173.6534	174.3654	175.1102	174.6855	175.0220	174.6538	175.6222	174.6297	175.4678	174.7300	175.7595	**168.3**
C5	119.5548	120.7943	121.4738	121.5477	122.5989	121.4922	122.8231	121.4445	122.7327	121.6146	122.9843	119.5548	120.7943	121.4739	121.5477	122.5989	121.4922	122.8231	121.4445	122.7327	121.6146	122.9844	**117.6**
C6	136.4800	138.1760	139.3711	139.1977	140.2318	139.1198	140.8785	139.0504	140.6173	139.2868	141.1362	136.4800	138.1760	139.3711	139.1977	140.2318	139.1198	140.8785	139.0504	140.6173	139.2868	141.1362	**133.3**
C7	203.9031	208.9344	210.1431	211.5776	213.5179	211.4065	218.3465	211.2396	217.2496	211.7527	219.5336	203.9031	208.9344	210.1431	211.5776	213.5178	211.4065	218.3465	211.2398	217.2496	211.7527	219.5336	**195.8**
C8	62.4081	63.5176	64.2402	64.1969	65.5191	64.1481	66.0334	64.1062	65.8734	64.2578	66.5123	62.4081	63.5176	64.2401	64.1969	65.5191	64.1481	66.0334	64.1062	65.8734	64.2578	66.5124	**70.4**
C9	33.8614	33.5608	34.1825	33.4541	33.5991	33.4442	33.8295	33.4403	33.7236	33.4773	33.9495	33.8614	33.5608	34.1825	33.4541	33.5991	33.4442	33.8295	33.4403	33.7236	33.4773	33.9496	**31.1**
C10	25.9231	26.6415	27.3493	27.1312	28.1401	27.0798	27.8705	27.0349	27.8296	27.1942	28.2499	25.9232	26.6415	27.3493	27.1312	28.1402	27.0798	27.8705	27.0350	27.8296	27.1942	28.2499	**26.9**
C11	26.4897	26.5713	27.0992	26.6108	27.1999	26.5919	27.1386	26.5795	27.1135	26.6426	27.3645	26.4897	26.5713	27.0993	26.6108	27.1998	26.5919	27.1386	26.5795	27.1135	26.6426	27.3645	**23.4**
C12	15.9103	16.1276	16.3119	16.3078	16.6622	16.2818	16.5809	16.2642	16.5652	16.3475	16.6634	15.9104	16.1276	16.3119	16.3078	16.6622	16.2818	16.5809	16.2642	16.5652	16.3475	16.6635	**13.8**
C1`	50.7988	51.7722	52.1796	52.3154	52.9675	52.2717	52.8620	52.2364	52.8195	52.3722	53.3347	55.0385	56.1158	56.5140	56.6961	57.3840	56.6486	57.5406	56.6088	57.4838	56.7556	57.9703	**53.3**
C2`	23.3610	23.8539	24.2807	24.1064	24.6826	24.0798	24.6277	24.0608	24.6002	24.1462	24.5473	22.1499	22.4551	22.8638	22.6320	23.3567	22.6134	23.1653	22.6032	23.1850	22.6645	22.8605	**24.2**
C3`	22.1499	22.4551	22.8637	22.6320	23.3567	22.6134	23.1653	22.6032	23.1850	22.6645	22.8605	23.3610	23.8539	24.2807	24.1064	24.6825	24.0798	24.6277	24.0607	24.6002	24.1462	24.5472	**24.1**
C4`	55.0385	56.1158	56.5140	56.6961	57.3841	56.6486	57.5406	56.6087	57.4838	56.7556	57.9703	50.7988	51.7722	52.1796	52.3154	52.9675	52.2717	52.8620	52.2365	52.8195	52.3722	53.3348	**56.3**
H2	8.7200	8.5356	8.6199	8.4194	8.3302	8.4246	8.3913	8.4306	8.3825	8.4151	8.3799	8.7200	8.5356	8.6199	8.4194	8.3302	8.4246	8.3913	8.4306	8.3825	8.4151	8.3799	**8.2**
H3	7.3688	7.5079	7.6104	7.5243	7.6008	7.5236	7.6221	7.5236	7.6136	7.5255	7.6318	7.3688	7.5079	7.6104	7.5243	7.6008	7.5236	7.6221	7.5236	7.6136	7.5255	7.6319	**7.36**
H5	7.0547	7.2196	7.3131	7.3125	7.4915	7.3067	7.5114	7.3012	7.5006	7.3185	7.5350	7.0547	7.2196	7.3131	7.3125	7.4915	7.3067	7.5114	7.3012	7.5006	7.3185	7.5350	**7.36**
H6	8.0770	8.2186	8.3077	8.3010	8.3629	8.2950	8.4115	8.2895	8.3902	8.3074	8.4458	8.0770	8.2186	8.3077	8.3010	8.3629	8.2950	8.4115	8.2895	8.3902	8.3074	8.4458	**8.2**
H8	4.4275	4.4268	4.4630	4.4703	4.5762	4.4663	4.6245	4.4627	4.6087	4.4746	4.6669	4.4275	4.4268	4.4630	4.4703	4.5762	4.4663	4.6245	4.4627	4.6087	4.4746	4.6669	**5.4**
H(9A-9B)	1.8331	1.7715	1.8082	1.7461	1.6728	1.7461	1.6811	1.7470	1.6718	1.7469	1.7105	1.8331	1.7715	1.8082	1.7461	1.6728	1.7461	1.6811	1.7470	1.6718	1.7469	1.7105	**2.08**
H(10A)	0.7728	0.6586	0.6596	0.6274	0.6472	0.6280	0.6691	0.6289	0.6703	0.6272	0.7166	0.7728	0.6586	0.6596	0.6274	0.6472	0.6280	0.6691	0.6289	0.6678	0.6272	0.7166	**1.14**
H(10B)	1.7663	1.6085	1.5217	1.4729	1.3898	1.4826	1.4047	1.4937	1.4059	1.4648	1.3494	1.7663	1.6085	1.5217	1.4729	1.3897	1.4826	1.4047	1.4937	1.4183	1.4648	1.3494	**1.28**
H(11A-11B)	1.0514	1.0480	1.0176	1.0528	1.0214	1.0520	1.0203	1.0520	1.0195	1.0542	1.0055	1.0514	1.0480	1.0176	1.0528	1.0214	1.0520	1.0203	1.0519	1.0195	1.0542	1.0055	**1.28**
H(12A-12C)	0.9078	0.8833	0.8498	0.8652	0.8460	0.8666	0.8533	0.8688	0.8571	0.8646	0.8353	0.9078	0.8833	0.8498	0.8652	0.8460	0.8666	0.8533	0.8688	0.8571	0.8646	0.8354	**0.82**
H(1`A)	2.6899	2.6721	2.6596	2.6399	2.6025	2.6424	2.6121	2.6455	2.6133	2.6382	2.5768	2.8894	2.8866	2.8724	2.8603	2.8238	2.8625	2.8387	2.8652	2.8412	2.8590	2.8125	**3.38**
H(1`B)	3.1176	3.1382	3.1900	3.1575	3.2127	3.1551	3.2023	3.1532	3.2035	3.1604	3.1870	2.7389	2.6337	2.6366	2.6095	2.6250	2.6103	2.6180	2.6118	2.6158	2.6093	2.6306	**3.71**
H(2`A)	1.5606	1.6136	1.5883	1.6319	1.5867	1.6306	1.6047	1.6300	1.6059	1.6337	1.6278	1.4496	1.4934	1.4610	1.5084	1.4777	1.5076	1.5096	1.5075	1.5081	1.5098	1.5275	**2.08**
H(2`B)	1.7496	1.7708	1.7382	1.8129	1.8060	1.8093	1.8058	1.8063	1.8070	1.8169	1.8371	1.7891	1.8317	1.7800	1.8708	1.8518	1.8678	1.8668	1.8656	1.8648	1.8744	1.9311	**2.24**
H(3`A)	1.4496	1.4934	1.4610	1.5084	1.4777	1.5076	1.5096	1.5075	1.5108	1.5098	1.5275	1.5606	1.6136	1.5883	1.6319	1.5867	1.6306	1.6047	1.6300	1.6007	1.6337	1.6278	**2.08**
H(3`B)	1.7891	1.8317	1.7799	1.8708	1.8518	1.8678	1.8668	1.8656	1.8680	1.8744	1.9311	1.7496	1.7708	1.7382	1.8129	1.8059	1.8093	1.8058	1.8063	1.7990	1.8169	1.8371	**2.16**
H(4`A)	2.7389	2.6337	2.6366	2.6095	2.6225	2.6103	2.6180	2.6118	2.6192	2.6093	2.6306	3.1176	3.1382	3.1900	3.1575	3.2127	3.1551	3.2023	3.1532	3.1996	3.1604	3.1870	**3.09**
H(4`B)	2.8894	2.8866	2.8724	2.8603	2.8238	2.8625	2.8387	2.8652	2.8399	2.8590	2.8125	2.6899	2.6721	2.6596	2.6399	2.6025	2.6424	2.6121	2.6455	2.6150	2.6382	2.5768	**3.68**
Nuclei	M06-2X																						
C1	153.3139	154.1147	155.0923	154.6258	156.4278	154.6074	156.0736	154.5917	155.8323	154.6374	156.7424	153.3140	154.1147	155.0922	154.6258	156.4279	154.6072	156.0736	154.5917	155.8323	154.6374	156.7424	**132.2**
C2	154.9208	154.8472	155.4019	154.6764	155.2728	154.7107	155.7196	154.7454	155.6269	154.6371	155.7829	154.9207	154.8472	155.4018	154.6764	155.2727	154.7105	155.7196	154.7454	155.6269	154.6371	155.7829	**133.3**
C3	136.1763	136.8491	137.4978	137.0428	137.8093	137.0546	138.0584	137.0674	138.0027	137.0251	138.1494	136.1763	136.8491	137.4977	137.0428	137.8093	137.0547	138.0584	137.0674	138.0027	137.0251	138.1494	**117.6**
C4	187.1500	187.9566	188.6296	188.3781	189.0881	188.3727	189.7626	188.3687	189.6217	188.3768	189.9010	187.1498	187.9566	188.6296	188.3781	189.0881	188.3728	189.7626	188.3687	189.6217	188.3768	189.9010	**168.3**
C5	133.6665	135.1820	135.9032	135.9787	136.9449	135.9514	137.1623	135.9252	137.0543	135.9981	137.3183	133.6665	135.1820	135.9032	135.9787	136.9449	135.9515	137.1623	135.9252	137.0543	135.9981	137.3183	**117.6**
C6	151.1929	153.3671	154.5822	154.5301	156.3787	154.4823	156.8323	154.4355	156.6334	154.5694	157.1596	151.1930	153.3671	154.5822	154.5301	156.3788	154.4824	156.8323	154.4355	156.6334	154.5694	157.1596	**133.3**
C7	219.5245	224.8907	226.3983	228.0101	228.7404	227.8294	235.4867	227.6520	233.7316	228.1759	237.1101	219.5241	224.8907	226.3983	228.0101	228.7407	227.8297	235.4867	227.6520	233.7316	228.1759	237.1101	**195.8**
C8	67.2610	68.6483	69.3496	69.3548	70.4448	69.3293	71.3018	69.3060	71.0041	69.3732	72.0281	67.2610	68.6483	69.3496	69.3548	70.4448	69.3292	71.3018	69.3060	71.0041	69.3732	72.0281	**70.4**
C9	35.4642	35.4239	35.5992	35.3385	35.6219	35.3672	35.7953	35.3969	35.7017	35.3048	36.0192	35.4642	35.4239	35.5992	35.3385	35.6220	35.3672	35.7953	35.3969	35.7017	35.3048	36.0192	**31.1**
C10	28.1749	28.5554	28.9127	28.9302	29.6142	28.9248	29.4107	28.9207	29.3703	28.9290	29.6021	28.1749	28.5554	28.9126	28.9302	29.6141	28.9248	29.4107	28.9207	29.3703	28.9290	29.6021	**26.9**
C11	27.0694	27.0411	27.3428	27.0466	27.4659	27.0675	27.4579	27.0895	27.4476	27.0203	27.6157	27.0693	27.0411	27.3428	27.0466	27.4660	27.0676	27.4579	27.0895	27.4476	27.0203	27.6156	**23.4**
C12	15.6785	15.8894	15.9172	16.0069	16.0766	16.0199	16.0059	16.0341	16.0007	15.9879	15.9410	15.6786	15.8894	15.9172	16.0069	16.0767	16.0199	16.0059	16.0341	16.0007	15.9879	15.9410	**13.8**
C1`	52.7471	53.4371	53.7246	53.9470	54.4968	53.9305	54.5272	53.9162	54.4023	53.9572	54.9826	57.2784	58.0992	58.4834	58.4784	59.0562	58.4723	59.1518	58.4681	59.1113	58.4785	59.4310	**53.3**
C2`	24.6913	25.0617	25.3331	25.2432	25.6602	25.2509	25.6528	25.2603	25.6474	25.2298	25.6465	23.7535	24.0580	24.3338	24.2747	24.7880	24.2798	24.7486	24.2866	24.7300	24.2642	24.8143	**24.2**
C3`	23.7535	24.0580	24.3338	24.2747	24.7881	24.2797	24.7486	24.2866	24.7300	24.2642	24.8143	24.6914	25.0617	25.3332	25.2432	25.6603	25.2509	25.6528	25.2603	25.6474	25.2298	25.6465	**24.1**
C4`	57.2790	58.0992	58.4835	58.4784	59.0562	58.4723	59.1518	58.4681	59.1113	58.4785	59.4310	52.7471	53.4371	53.7245	53.9470	54.4969	53.9305	54.5272	53.9162	54.4023	53.9572	54.9826	**56.3**
H2	9.2553	9.1886	9.2043	9.1236	9.1185	9.1277	9.1058	9.1311	9.1346	9.1198	9.0783	9.2553	9.1886	9.2043	9.1236	9.1185	9.1277	9.1058	9.1311	9.1346	9.1198	9.0783	**8.2**
H3	7.8496	7.9991	8.0968	8.0550	8.1780	8.0508	8.2036	8.0462	8.1958	8.0590	8.2179	7.8496	7.9991	8.0968	8.0550	8.1780	8.0508	8.2036	8.0462	8.1958	8.0590	8.2179	**7.36**
H5	7.6700	7.8593	7.9559	7.9464	8.0779	7.9403	8.0866	7.9337	8.0791	7.9524	8.1072	7.6700	7.8593	7.9559	7.9464	8.0779	7.9403	8.0866	7.9337	8.0791	7.9524	8.1072	**7.36**
H6	8.5783	8.7576	8.8602	8.8626	9.0133	8.8546	9.0581	8.8464	9.0490	8.8703	9.0681	8.5783	8.7576	8.8602	8.8626	9.0133	8.8546	9.0581	8.8464	9.0490	8.8703	9.0681	**8.2**
H8	4.2922	4.3772	4.4355	4.4447	4.5306	4.4393	4.5577	4.4336	4.5580	4.4499	4.5479	4.2922	4.3772	4.4355	4.4447	4.5306	4.4393	4.5577	4.4336	4.5580	4.4499	4.5479	**5.4**
H(9A-9B)	1.6952	1.7512	1.7338	1.7870	1.7864	1.7839	1.7723	1.7805	1.7723	1.7901	1.8164	1.6952	1.7512	1.7338	1.7870	1.7864	1.7839	1.7723	1.7805	1.7723	1.7901	1.8164	**2.08**
H(10A)	0.8886	0.7034	0.6742	0.6310	0.5530	0.6339	0.5704	0.6364	0.5766	0.6284	0.6028	0.8886	0.7034	0.6742	0.6310	0.5530	0.6339	0.5704	0.6364	0.5766	0.6284	0.6028	**1.14**
H(10B)	1.5834	1.5136	1.4450	1.4129	1.3259	1.4186	1.3112	1.4240	1.3267	1.4077	1.2702	1.5834	1.5136	1.4449	1.4129	1.3259	1.4186	1.3112	1.4240	1.3267	1.4077	1.2702	**1.28**
H(11A-11B)	0.9471	0.9670	0.9367	0.9816	0.9426	0.9795	0.9338	0.9771	0.9397	0.9837	0.9138	0.9471	0.9670	0.9367	0.9816	0.9426	0.9795	0.9338	0.9771	0.9397	0.9837	0.9138	**1.28**
H(12A-12C)	0.8951	0.8808	0.8572	0.8688	0.8253	0.8683	0.8226	0.8674	0.8290	0.8694	0.8070	0.8951	0.8808	0.8572	0.8688	0.8253	0.8683	0.8226	0.8674	0.8290	0.8694	0.8070	**0.82**
H(1`A)	2.6201	2.6148	2.6019	2.6064	2.5567	2.6061	2.5649	2.6055	2.5694	2.6068	2.5425	2.8027	2.8010	2.7892	2.7839	2.7542	2.7840	2.7717	2.7838	2.7696	2.7840	2.7411	**3.38**
H(1`B)	3.0833	3.1152	3.1403	3.1536	3.1988	3.1498	3.1827	3.1456	3.1831	3.1574	3.1910	2.7295	2.6123	2.5775	2.5866	2.5699	2.5867	2.5575	2.5864	2.5371	2.5867	2.5782	**3.71**
H(2`A)	1.6290	1.6809	1.6547	1.7095	1.6574	1.7067	1.6794	1.7035	1.6774	1.7123	1.6820	1.5087	1.5740	1.5518	1.6067	1.5563	1.6036	1.5922	1.6001	1.5906	1.6099	1.6099	**2.08**
H(2`B)	1.7699	1.7936	1.7566	1.8343	1.7953	1.8301	1.7868	1.8258	1.7846	1.8383	1.8070	1.7124	1.7982	1.7646	1.8623	1.8353	1.8562	1.8634	1.8499	1.8538	1.8684	1.8987	**2.24**
H(3`A)	1.5087	1.5740	1.5519	1.6067	1.5563	1.6035	1.5922	1.6001	1.5906	1.6099	1.6099	1.6290	1.6809	1.6547	1.7095	1.6573	1.7067	1.6794	1.7035	1.6774	1.7123	1.6820	**2.08**
H(3`B)	1.7124	1.7982	1.7646	1.8623	1.8354	1.8562	1.8634	1.8499	1.8538	1.8684	1.8987	1.7699	1.7936	1.7567	1.8343	1.7954	1.8301	1.7868	1.8258	1.7846	1.8383	1.8070	**2.16**
H(4`A)	2.7295	2.6123	2.5775	2.5866	2.5699	2.5867	2.5575	2.5864	2.5371	2.5867	2.5782	3.0833	3.1152	3.1402	3.1536	3.1988	3.1498	3.1827	3.1456	3.1831	3.1574	3.1910	**3.09**
H(4`B)	2.8027	2.8010	2.7892	2.7839	2.7542	2.7840	2.7717	2.7838	2.7696	2.7840	2.7411	2.6201	2.6148	2.6019	2.6064	2.5567	2.6061	2.5649	2.6055	2.5694	2.6068	2.5425	**3.68**

[a] methyl protons shifts are averaged

[b] according to [5]

Table S5. Cont. VIII

Nuclei	R											S										Exp. [b]
	mpW1LYP											mpW1LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.8378	140.8440	141.4180	141.3625	142.7491	141.3294	142.1529	141.2986	142.1820	141.3923	142.2792	139.8378	140.8440	141.4181	141.3622	142.7491	141.3294	142.1530	141.2986	142.1819	141.3923	142.2792	**132.2**
C2	139.8714	139.7984	140.3079	139.7197	140.1190	139.7218	140.6847	139.7258	140.5678	139.7161	140.5968	139.8714	139.7984	140.3079	139.7196	140.1190	139.7218	140.6848	139.7258	140.5678	139.7161	140.5970	**133.3**
C3	122.0463	122.6720	123.2099	122.8903	123.4471	122.8775	123.7073	122.8655	123.6488	122.9006	123.7499	122.0463	122.6720	123.2099	122.8905	123.4470	122.8775	123.7074	122.8655	123.6487	122.9006	123.7498	**117.6**
C4	176.3397	177.1720	177.7901	177.5913	178.1904	177.5635	178.7928	177.5372	178.6520	177.6158	178.9042	176.3397	177.1719	177.7901	177.5914	178.1902	177.5635	178.7927	177.5372	178.6517	177.6158	178.9042	**168.3**
C5	119.8982	121.0713	121.6786	121.7085	122.4580	121.6663	122.6459	121.6259	122.5595	121.7466	122.7780	119.8982	121.0713	121.6786	121.7085	122.4581	121.6663	122.6458	121.6259	122.5594	121.7465	122.7779	**117.6**
C6	136.0966	138.0128	139.1739	139.1635	140.6582	139.0867	141.3023	139.0117	141.0638	139.2346	141.6841	136.0966	138.0128	139.1739	139.1635	140.6585	139.0867	141.3022	139.0117	141.0638	139.2346	141.6841	**133.3**
C7	203.6129	208.5205	209.5677	211.1801	211.7568	211.0176	216.9290	210.8561	215.7371	211.3332	217.9149	203.6129	208.5205	209.5677	211.1801	211.7568	211.0176	216.9290	210.8561	215.7372	211.3332	217.9147	**195.8**
C8	65.8463	67.0437	67.6010	67.5551	68.5804	67.5298	69.1701	67.5042	69.0076	67.5753	69.4725	65.8463	67.0437	67.6010	67.5551	68.5805	67.5298	69.1701	67.5042	69.0077	67.5753	69.4725	**70.4**
C9	37.0169	36.6560	36.8848	36.5180	36.8153	36.5233	37.0170	36.5296	36.9632	36.5106	37.0610	37.0169	36.6560	36.8848	36.5180	36.8153	36.5233	37.0170	36.5296	36.9632	36.5106	37.0610	**31.1**
C10	29.3292	29.7978	30.3192	30.1290	30.8587	30.1027	30.6588	30.0784	30.6559	30.1521	30.7746	29.3292	29.7978	30.3193	30.1290	30.8587	30.1027	30.6588	30.0784	30.6559	30.1521	30.7746	**26.9**
C11	29.4068	29.5120	29.8154	29.4911	29.9151	29.4934	29.9122	29.4963	29.9182	29.4864	30.0182	29.4067	29.5120	29.8153	29.4911	29.9151	29.4934	29.9121	29.4963	29.9182	29.4865	30.0180	**23.4**
C12	16.7769	16.9386	17.0341	17.0893	17.1643	17.0748	17.1257	17.0621	17.1298	17.1017	17.1017	16.7769	16.9387	17.0340	17.0893	17.1642	17.0748	17.1257	17.0621	17.1298	17.1017	17.1017	**13.8**
C1`	51.9766	52.7794	53.1018	53.3629	53.8586	53.3224	53.8640	53.2840	53.8039	53.4001	54.3551	56.5078	57.6071	57.9635	58.0839	58.5838	58.0550	58.7006	58.0272	58.6452	58.1090	58.9220	**53.3**
C2`	25.9559	26.4339	26.8102	26.6257	27.1139	26.6133	27.1490	26.6020	27.1457	26.6349	26.9197	25.5722	25.7544	26.1426	25.9442	26.3949	25.9276	26.3477	25.9127	26.3492	25.9585	26.1388	**24.2**
C3`	25.5722	25.7545	26.1426	25.9444	26.3949	25.9276	26.3478	25.9127	26.3493	25.9585	26.1388	25.9559	26.4339	26.8101	26.6257	27.1139	26.6133	27.1490	26.6020	27.1458	26.6349	26.9196	**24.1**
C4`	56.5078	57.6072	57.9635	58.0838	58.5838	58.0550	58.7006	58.0272	58.6452	58.1090	58.9219	51.9767	52.7795	53.1019	53.3630	53.8586	53.3223	53.8640	53.2840	53.8039	53.4001	54.3551	**56.3**
H2	8.7240	8.6003	8.6562	8.5315	8.5403	8.5359	8.5588	8.5399	8.5634	8.5273	8.5464	8.7240	8.6003	8.6562	8.5315	8.5403	8.5359	8.5588	8.5399	8.5634	8.5273	8.5464	**8.2**
H3	7.3356	7.4800	7.5666	7.5264	7.6381	7.5244	7.6591	7.5221	7.6515	7.5280	7.6715	7.3356	7.4800	7.5666	7.5264	7.6381	7.5244	7.6591	7.5221	7.6515	7.5280	7.6715	**7.36**
H5	7.1538	7.3065	7.4076	7.3765	7.5081	7.3726	7.5127	7.3684	7.5049	7.3800	7.5376	7.1538	7.3065	7.4076	7.3765	7.5081	7.3726	7.5127	7.3684	7.5049	7.3800	7.5376	**7.36**
H6	7.9770	8.1646	8.2590	8.2681	8.3872	8.2620	8.4387	8.2555	8.4208	8.2738	8.4656	7.9770	8.1646	8.2590	8.2681	8.3872	8.2620	8.4387	8.2555	8.4208	8.2738	8.4656	**8.2**
H8	4.5678	4.6311	4.6745	4.6785	4.7338	4.6749	4.7727	4.6711	4.7587	4.6818	4.7496	4.5678	4.6311	4.6745	4.6785	4.7339	4.6749	4.7727	4.6711	4.7588	4.6818	4.7496	**5.4**
H(9A-9B)	1.6834	1.7242	1.7339	1.7539	1.7850	1.7522	1.7829	1.7502	1.7789	1.7553	1.8165	1.6834	1.7242	1.7339	1.7539	1.7850	1.7522	1.7829	1.7502	1.7789	1.7553	1.8165	**2.08**
H(10A)	1.0055	0.8560	0.8506	0.8221	0.7324	0.8230	0.7821	0.8238	0.7767	0.8214	0.7850	1.0055	0.8560	0.8507	0.8221	0.7324	0.8230	0.7820	0.8238	0.7767	0.8214	0.7850	**1.14**
H(10B)	1.6473	1.5445	1.4864	1.4679	1.3838	1.4733	1.3800	1.4783	1.3873	1.4627	1.3500	1.6473	1.5445	1.4864	1.4679	1.3838	1.4733	1.3800	1.4783	1.3873	1.4627	1.3501	**1.28**
H(11A-11B)	1.0567	1.0723	1.0451	1.0911	1.0518	1.0902	1.0512	1.0890	1.0511	1.0918	1.0381	1.0567	1.0723	1.0451	1.0910	1.0518	1.0902	1.0512	1.0890	1.0511	1.0918	1.0380	**1.28**
H(12A-12C)	0.9504	0.9373	0.9166	0.9332	0.8920	0.9336	0.8995	0.9338	0.9000	0.9328	0.8904	0.9504	0.9373	0.9166	0.9332	0.8920	0.9336	0.8995	0.9338	0.9000	0.9328	0.8904	**0.82**
H(1`A)	2.7337	2.7265	2.7160	2.7171	2.6748	2.7178	2.6932	2.7183	2.6947	2.7162	2.6554	2.8635	2.8719	2.8555	2.8496	2.8211	2.8518	2.8323	2.8535	2.8358	2.8473	2.7929	**3.38**
H(1`B)	3.1890	3.2388	3.2723	3.2779	3.3445	3.2754	3.3319	3.2727	3.3288	3.2802	3.3270	2.8791	2.7212	2.6927	2.6981	2.6939	2.6982	2.6620	2.6982	2.6627	2.6981	2.6492	**3.71**
H(2`A)	1.6302	1.6757	1.6471	1.6964	1.6398	1.6955	1.6665	1.6943	1.6635	1.6971	1.6755	1.5104	1.5573	1.5296	1.5826	1.5248	1.5814	1.5608	1.5798	1.5559	1.5836	1.5751	**2.08**
H(2`B)	1.8396	1.8556	1.8161	1.9031	1.8550	1.8993	1.8566	1.8955	1.8505	1.9066	1.8794	1.7018	1.8178	1.7710	1.8908	1.8450	1.8864	1.8696	1.8817	1.8602	1.8949	1.9125	**2.24**
H(3`A)	1.5104	1.5573	1.5296	1.5826	1.5248	1.5814	1.5609	1.5798	1.5559	1.5836	1.5751	1.6302	1.6757	1.6471	1.6964	1.6398	1.6955	1.6665	1.6943	1.6635	1.6971	1.6754	**2.08**
H(3`B)	1.7018	1.8178	1.7710	1.8908	1.8451	1.8864	1.8697	1.8817	1.8602	1.8949	1.9125	1.8396	1.8556	1.8161	1.9030	1.8550	1.8993	1.8566	1.8955	1.8506	1.9066	1.8794	**2.16**
H(4`A)	2.8791	2.7212	2.6928	2.6981	2.6939	2.6982	2.6620	2.6982	2.6627	2.6981	2.6492	3.1890	3.2388	3.2723	3.2779	3.3445	3.2754	3.3319	3.2727	3.3288	3.2802	3.3270	**3.09**
H(4`B)	2.8635	2.8719	2.8555	2.8496	2.8211	2.8518	2.8323	2.8535	2.8358	2.8473	2.7929	2.7337	2.7265	2.7160	2.7171	2.6748	2.7178	2.6932	2.7183	2.6947	2.7162	2.6554	**3.68**
Nuclei	mpW1PW91											mpW1PW91										
C1	136.9119	137.8138	138.5064	138.2193	139.7229	138.2010	139.0452	138.1875	139.1057	138.2354	139.2865	136.9120	137.8138	138.5064	138.2193	139.7229	138.2010	139.0452	138.1875	139.1056	138.2354	139.2865	**132.2**
C2	138.8276	138.8043	139.2973	138.6548	139.2065	138.6657	139.6814	138.6819	139.5637	138.6442	139.6547	138.8278	138.8043	139.2971	138.6548	139.2065	138.6657	139.6814	138.6819	139.5637	138.6442	139.6547	**133.3**
C3	121.1664	121.9017	122.4756	122.1203	122.8340	122.1098	123.0950	122.1047	123.0259	122.1294	123.1776	121.1664	121.9017	122.4756	122.1203	122.8340	122.1098	123.0950	122.1047	123.0259	122.1294	123.1776	**117.6**
C4	173.3303	174.1682	174.7602	174.5577	175.2107	174.5337	175.8375	174.5156	175.6799	174.5797	175.9764	173.3302	174.1682	174.7601	174.5577	175.2107	174.5337	175.8374	174.5156	175.6800	174.5797	175.9764	**168.3**
C5	119.1385	120.4194	121.0633	121.0661	121.9587	121.0256	122.1586	120.9910	122.0561	121.1039	122.3339	119.1384	120.4194	121.0632	121.0661	121.9587	121.0256	122.1586	120.9910	122.0561	121.1039	122.3339	**117.6**
C6	134.9559	136.8628	138.0011	137.9900	139.5612	137.9156	140.2367	137.8478	139.9729	138.0608	140.6233	134.9558	136.8628	138.0011	137.9900	139.5612	137.9156	140.2368	137.8478	139.9729	138.0608	140.6233	**133.3**
C7	201.3961	205.9561	207.0830	208.3989	209.0671	208.2545	213.9532	208.1148	212.8505	208.5345	215.0027	201.3961	205.9561	207.0830	208.3989	209.0671	208.2545	213.9531	208.1148	212.8505	208.5345	215.0027	**195.8**
C8	63.7271	64.9001	65.6204	65.4113	66.4236	65.3869	67.0211	65.3670	66.8807	65.4325	67.4256	63.7271	64.9001	65.6204	65.4113	66.4236	65.3869	67.0211	65.3670	66.8807	65.4325	67.4256	**70.4**
C9	35.2055	34.9743	35.2048	34.8541	35.1994	34.8613	35.3954	34.8739	35.3130	34.8463	35.5099	35.2055	34.9743	35.2048	34.8541	35.1994	34.8613	35.3953	34.8739	35.3130	34.8463	35.5099	**31.1**
C10	27.3826	27.8477	28.3064	28.1713	28.8921	28.1466	28.7034	28.1281	28.6810	28.1948	28.8882	27.3826	27.8477	28.3064	28.1713	28.8921	28.1466	28.7033	28.1281	28.6810	28.1948	28.8882	**26.9**
C11	27.3749	27.5041	27.7467	27.4542	27.8881	27.4594	27.8795	27.4701	27.8744	27.4481	28.0331	27.3749	27.5041	27.7467	27.4542	27.8881	27.4594	27.8795	27.4701	27.8744	27.4481	28.0331	**23.4**
C12	16.2791	16.4535	16.4886	16.5599	16.6580	16.5511	16.6097	16.5484	16.6016	16.5678	16.6160	16.2792	16.4535	16.4886	16.5599	16.6580	16.5511	16.6097	16.5484	16.6016	16.5678	16.6159	**13.8**
C1`	50.5318	51.3520	51.5695	51.8485	52.3867	51.8154	52.3789	51.7886	52.2993	51.8801	52.8661	54.8407	55.9339	56.2529	56.3574	56.8717	56.3332	57.0066	56.3147	56.9463	56.3796	57.2577	**53.3**
C2`	24.7484	25.1441	25.4666	25.2813	25.7455	25.2736	25.7527	25.2717	25.7502	25.2877	25.5751	24.2083	24.4220	24.6984	24.5579	25.0088	24.5487	24.9507	24.5454	24.9402	24.5661	24.8202	**24.2**
C3`	24.2083	24.4220	24.6984	24.5579	25.0088	24.5487	24.9506	24.5454	24.9402	24.5661	24.8202	24.7485	25.1441	25.4666	25.2813	25.7455	25.2736	25.7527	25.2717	25.7502	25.2877	25.5751	**24.1**
C4`	54.8407	55.9339	56.2529	56.3574	56.8717	56.3332	57.0066	56.3147	56.9463	56.3796	57.2577	50.5318	51.3520	51.5695	51.8485	52.3867	51.8154	52.3788	51.7886	52.2993	51.8801	52.8661	**56.3**
H2	8.7635	8.6626	8.6890	8.5947	8.5982	8.5987	8.6271	8.6029	8.6234	8.5912	8.6110	8.7635	8.6626	8.6890	8.5947	8.5982	8.5987	8.6270	8.6029	8.6234	8.5912	8.6110	**8.2**
H3	7.3658	7.5155	7.6032	7.5610	7.6800	7.5592	7.7031	7.5573	7.6942	7.5630	7.7179	7.3658	7.5155	7.6032	7.5610	7.6800	7.5592	7.7031	7.5573	7.6942	7.5630	7.7179	**7.36**
H5	7.1836	7.3496	7.4493	7.4199	7.5570	7.4159	7.5642	7.4120	7.5548	7.4239	7.5904	7.1836	7.3496	7.4493	7.4199	7.5570	7.4159	7.5642	7.4120	7.5548	7.4239	7.5904	**7.36**
H6	8.0628	8.2466	8.3313	8.3493	8.4725	8.3429	8.5300	8.3368	8.5082	8.3556	8.5578	8.0628	8.2466	8.3313	8.3493	8.4725	8.3429	8.5300	8.3368	8.5082	8.3556	8.5578	**8.2**
H8	4.5666	4.6312	4.6552	4.6838	4.7335	4.6802	4.7762	4.6767	4.7569	4.6876	4.7740	4.5667	4.6312	4.6551	4.6838	4.7335	4.6802	4.7761	4.6767	4.7569	4.6876	4.7740	**5.4**
H(9A-9B)	1.7143	1.7479	1.7554	1.7759	1.7961	1.7741	1.7987	1.7723	1.7919	1.7780	1.8300	1.7142	1.7479	1.7554	1.7759	1.7961	1.7741	1.7987	1.7723	1.7919	1.7780	1.8300	**2.08**
H(10A)	0.9433	0.8037	0.7605	0.7576	0.6696	0.7596	0.7118	0.7618	0.7018	0.7561	0.7199	0.9433	0.8037	0.7605	0.7576	0.6696	0.7596	0.7118	0.7618	0.7018	0.7561	0.7199	**1.14**
H(10B)	1.6289	1.5322	1.4591	1.4457	1.3602	1.4519	1.3550	1.4581	1.3605	1.4403	1.3252	1.6289	1.5322	1.4591	1.4457	1.3602	1.4519	1.3550	1.4581	1.3605	1.4403	1.3252	**1.28**
H(11A-11B)	1.0002	1.0196	0.9828	1.0300	0.9938	1.0298	0.9939	1.0296	0.9925	1.0305	0.9821	1.0003	1.0196	0.9828	1.0300	0.9938	1.0298	0.9939	1.0296	0.9925	1.0305	0.9821	**1.28**
H(12A-12C)	0.8944	0.8820	0.8543	0.8714	0.8330	0.8723	0.8394	0.8732	0.8390	0.8708	0.8339	0.8944	0.8820	0.8543	0.8714	0.8330	0.8723	0.8393	0.8732	0.8390	0.8708	0.8339	**0.82**
H(1`A)	2.6698	2.6627	2.6505	2.6511	2.6099	2.6521	2.6276	2.6531	2.6278	2.6505	2.6009	2.8087	2.8120	2.7991	2.7904	2.7608	2.7925	2.7725	2.7948	2.7761	2.7885	2.7396	**3.38**
H(1`B)	3.1591	3.2023	3.2377	3.2375	3.2965	3.2352	3.2866	3.2330	3.2830	3.2401	3.2859	2.8814	2.7114	2.6952	2.6721	2.6718	2.6738	2.6281	2.6757	2.6303	2.6709	2.6132	**3.71**
H(2`A)	1.6097	1.6533	1.6251	1.6698	1.6202	1.6692	1.6456	1.6686	1.6423	1.6707	1.6554	1.4812	1.5282	1.4990	1.5488	1.4982	1.5480	1.5338	1.5472	1.5278	1.5499	1.5511	**2.08**
H(2`B)	1.7940	1.8165	1.7727	1.8597	1.8175	1.8564	1.8170	1.8534	1.8101	1.8632	1.8446	1.6821	1.7880	1.7383	1.8517	1.8105	1.8478	1.8354	1.8441	1.8250	1.8557	1.8844	**2.24**
H(3`A)	1.4812	1.5282	1.4991	1.5488	1.4982	1.5480	1.5338	1.5472	1.5278	1.5499	1.5511	1.6097	1.6533	1.6251	1.6698	1.6202	1.6692	1.6456	1.6686	1.6423	1.6707	1.6554	**2.08**
H(3`B)	1.6821	1.7880	1.7383	1.8517	1.8105	1.8478	1.8354	1.8441	1.8250	1.8557	1.8844	1.7940	1.8165	1.7727	1.8597	1.8175	1.8564	1.8170	1.8534	1.8101	1.8632	1.8446	**2.16**
H(4`A)	2.8814	2.7114	2.6952	2.6721	2.6718	2.6738	2.6281	2.6757	2.6303	2.6709	2.6132	3.1591	3.2023	3.2377	3.2375	3.2965	3.2352	3.2866	3.2330	3.2830	3.2401	3.2859	**3.09**
H(4`B)	2.8087	2.8120	2.7991	2.7904	2.7608	2.7925	2.7725	2.7948	2.7761	2.7885	2.7396	2.6698	2.6627	2.6505	2.6511	2.6099	2.6521	2.6276	2.6531	2.6278	2.6505	2.6009	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S5. Cont. IX

Nuclei	R											S										Exp. [b]
	O3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	134.8316	136.7253	138.2232	137.7522	139.6525	137.7211	138.6578	137.6778	138.8802	137.7701	138.8881	134.8316	136.7253	138.2232	137.7522	139.6525	137.7212	138.6578	137.6778	138.8802	137.7701	138.8880	**132.2**
C2	134.2703	134.3034	134.9028	134.2696	134.8696	134.2834	135.2076	134.2931	135.1090	134.2502	135.1565	134.2703	134.3034	134.9028	134.2695	134.8695	134.2836	135.2076	134.2931	135.1090	134.2502	135.1565	**133.3**
C3	117.1530	117.7967	118.4174	118.0690	118.7418	118.0647	118.9947	118.0553	118.9369	118.0662	119.0549	117.1529	117.7967	118.4174	118.0688	118.7418	118.0647	118.9947	118.0553	118.9369	118.0662	119.0548	**117.6**
C4	169.5381	170.0292	170.6806	170.3884	171.1053	170.3736	171.6575	170.3540	171.5014	170.3967	171.7332	169.5383	170.0292	170.6806	170.3884	171.1053	170.3735	171.6575	170.3540	171.5014	170.3966	171.7334	**168.3**
C5	115.0903	116.2587	116.9125	116.9091	117.6769	116.8807	117.9293	116.8473	117.8196	116.9300	118.0603	115.0903	116.2587	116.9125	116.9091	117.6769	116.8806	117.9293	116.8473	117.8196	116.9299	118.0604	**117.6**
C6	130.2300	131.5111	132.3612	132.3562	133.7414	132.3011	134.3672	132.2439	134.1030	132.4041	134.6024	130.2299	131.5111	132.3612	132.3563	133.7414	132.3011	134.3672	132.2439	134.1030	132.4042	134.6023	**133.3**
C7	197.0256	202.4069	204.2489	205.5483	206.5094	205.3897	210.9074	205.2170	210.0109	205.6862	211.8448	197.0256	202.4069	204.2489	205.5484	206.5094	205.3897	210.9074	205.2170	210.0109	205.6859	211.8450	**195.8**
C8	64.5596	66.2848	66.9158	67.1212	67.8247	67.0947	68.4239	67.0586	68.3028	67.1363	68.7969	64.5596	66.2848	66.9158	67.1213	67.8247	67.0948	68.4239	67.0586	68.3028	67.1362	68.7968	**70.4**
C9	35.5442	35.1982	35.2977	35.1245	35.2805	35.1355	35.5634	35.1421	35.4857	35.1083	35.6327	35.5442	35.1982	35.2977	35.1245	35.2805	35.1354	35.5634	35.1421	35.4857	35.1083	35.6327	**31.1**
C10	27.9914	28.4344	28.8370	28.7329	29.4158	28.7216	29.2733	28.7061	29.2396	28.7375	29.4326	27.9915	28.4344	28.8370	28.7329	29.4156	28.7216	29.2733	28.7061	29.2396	28.7376	29.4325	**26.9**
C11	28.7716	28.8814	29.1958	28.9216	29.3506	28.9307	29.3249	28.9345	29.3252	28.9062	29.4166	28.7716	28.8814	29.1958	28.9217	29.3505	28.9308	29.3249	28.9345	29.3252	28.9062	29.4166	**23.4**
C12	16.6093	16.7634	16.8889	16.9451	17.0851	16.9427	17.0428	16.9355	17.0386	16.9411	17.0277	16.6092	16.7634	16.8889	16.9451	17.0851	16.9427	17.0428	16.9355	17.0386	16.9411	17.0277	**13.8**
C1`	50.8019	51.5543	51.9691	52.1253	52.7447	52.0980	52.7177	52.0662	52.6691	52.1450	53.0975	55.2428	56.2398	56.6369	56.7276	57.3004	56.7088	57.3728	56.6851	57.2958	56.7387	57.5907	**53.3**
C2`	25.9053	26.4060	26.7287	26.6449	27.0942	26.6421	27.1363	26.6341	27.1078	26.6410	26.9388	25.6921	25.8886	26.3279	26.0899	26.6685	26.0890	26.5111	26.0826	26.5199	26.0843	26.2550	**24.2**
C3`	25.6920	25.8886	26.3279	26.0899	26.6685	26.0889	26.5111	26.0826	26.5199	26.0842	26.2549	25.9053	26.4060	26.7287	26.6449	27.0942	26.6421	27.1363	26.6341	27.1078	26.6411	26.9389	**24.1**
C4`	55.2428	56.2398	56.6369	56.7276	57.3004	56.7089	57.3728	56.6851	57.2958	56.7388	57.5907	50.8019	51.5543	51.9691	52.1253	52.7448	52.0981	52.7178	52.0662	52.6691	52.1450	53.0974	**56.3**
H2	8.5172	8.3119	8.3022	8.2114	8.2142	8.2161	8.2765	8.2212	8.2596	8.2074	8.2657	8.5172	8.3119	8.3022	8.2114	8.2142	8.2161	8.2765	8.2212	8.2596	8.2074	8.2656	**8.2**
H3	7.3026	7.4020	7.4910	7.4435	7.5680	7.4415	7.5874	7.4391	7.5799	7.4452	7.5960	7.3026	7.4020	7.4910	7.4435	7.5680	7.4415	7.5874	7.4391	7.5799	7.4452	7.5960	**7.36**
H5	7.0527	7.2542	7.3671	7.3566	7.4848	7.3519	7.5014	7.3466	7.4911	7.3609	7.5199	7.0527	7.2542	7.3671	7.3566	7.4848	7.3518	7.5014	7.3466	7.4911	7.3609	7.5199	**7.36**
H6	7.9525	8.0429	8.1075	8.0893	8.2184	8.0851	8.2708	8.0810	8.2439	8.0936	8.2835	7.9525	8.0429	8.1075	8.0893	8.2184	8.0851	8.2708	8.0810	8.2439	8.0936	8.2835	**8.2**
H8	4.7795	4.7678	4.7948	4.7779	4.8539	4.7763	4.8754	4.7747	4.8616	4.7796	4.8585	4.7795	4.7678	4.7948	4.7779	4.8539	4.7763	4.8754	4.7747	4.8616	4.7796	4.8584	**5.4**
H(9A-9B)	1.6182	1.6249	1.5871	1.6386	1.6272	1.6368	1.6562	1.6349	1.6437	1.6405	1.6970	1.6182	1.6249	1.5871	1.6386	1.6272	1.6368	1.6562	1.6349	1.6437	1.6405	1.6970	**2.08**
H(10A)	0.9587	0.8526	0.8607	0.8353	0.8038	0.8362	0.8278	0.8369	0.8280	0.8343	0.8249	0.9587	0.8526	0.8607	0.8353	0.8038	0.8362	0.8278	0.8369	0.8280	0.8343	0.8249	**1.14**
H(10B)	1.5716	1.4752	1.4290	1.4076	1.3426	1.4126	1.3358	1.4173	1.3447	1.4028	1.3107	1.5716	1.4752	1.4290	1.4076	1.3426	1.4126	1.3358	1.4173	1.3447	1.4028	1.3107	**1.28**
H(11A-11B)	1.0598	1.0760	1.0550	1.0975	1.0725	1.0966	1.0683	1.0953	1.0683	1.0983	1.0500	1.0598	1.0760	1.0550	1.0975	1.0724	1.0966	1.0683	1.0953	1.0683	1.0983	1.0500	**1.28**
H(12A-12C)	0.9311	0.9235	0.9109	0.9235	0.8974	0.9240	0.8992	0.9241	0.9006	0.9229	0.8910	0.9311	0.9235	0.9109	0.9235	0.8974	0.9239	0.8992	0.9241	0.9006	0.9229	0.8910	**0.82**
H(1`A)	2.7818	2.7720	2.7498	2.7606	2.7136	2.7618	2.7281	2.7626	2.7293	2.7594	2.6945	2.9185	2.9246	2.8997	2.8958	2.8542	2.8987	2.8592	2.9012	2.8637	2.8929	2.8314	**3.38**
H(1`B)	3.2477	3.2925	3.3182	3.3299	3.3897	3.3277	3.3821	3.3252	3.3769	3.3319	3.3829	2.9024	2.7877	2.7774	2.7855	2.7869	2.7851	2.7591	2.7844	2.7667	2.7859	2.7593	**3.71**
H(2`A)	1.6302	1.6734	1.6511	1.6905	1.6416	1.6900	1.6653	1.6893	1.6625	1.6908	1.6723	1.5249	1.5696	1.5582	1.5949	1.5522	1.5941	1.5774	1.5929	1.5757	1.5954	1.5892	**2.08**
H(2`B)	1.8442	1.8517	1.8178	1.8948	1.8599	1.8917	1.8559	1.8884	1.8516	1.8978	1.8790	1.7452	1.8526	1.8263	1.9301	1.9019	1.9256	1.9145	1.9206	1.9081	1.9343	1.9549	**2.24**
H(3`A)	1.5249	1.5696	1.5582	1.5949	1.5522	1.5941	1.5774	1.5929	1.5757	1.5954	1.5892	1.6302	1.6734	1.6511	1.6905	1.6416	1.6900	1.6653	1.6893	1.6625	1.6908	1.6724	**2.08**
H(3`B)	1.7452	1.8526	1.8263	1.9302	1.9019	1.9256	1.9144	1.9206	1.9081	1.9343	1.9549	1.8442	1.8517	1.8178	1.8948	1.8599	1.8917	1.8559	1.8884	1.8516	1.8978	1.8790	**2.16**
H(4`A)	2.9024	2.7877	2.7774	2.7855	2.7869	2.7851	2.7591	2.7844	2.7670	2.7859	2.7593	3.2477	3.2925	3.3182	3.3299	3.3897	3.3277	3.3821	3.3252	3.3769	3.3319	3.3829	**3.09**
H(4`B)	2.9185	2.9246	2.8997	2.8958	2.8542	2.8987	2.8592	2.9013	2.8637	2.8929	2.8314	2.7818	2.7720	2.7498	2.7606	2.7136	2.7618	2.7281	2.7626	2.7293	2.7594	2.6945	**3.68**
Nuclei	OLYP																						
C1	133.9821	136.0335	137.1367	136.6843	138.8035	136.6625	137.7402	136.6347	138.0258	136.6956	137.8922	133.9821	136.0335	137.1367	136.6843	138.8035	136.6625	137.7402	136.6347	138.0258	136.6955	137.8922	**132.2**
C2	131.9334	131.9290	132.5576	131.8799	132.4225	131.8897	132.7752	131.8944	132.6437	131.8621	132.7099	131.9334	131.9291	132.5576	131.8799	132.4223	131.8897	132.7752	131.8944	132.6437	131.8621	132.7099	**133.3**
C3	115.3313	115.9906	116.6137	116.2608	116.8575	116.2547	117.1455	116.2428	117.0771	116.2573	117.2258	115.3313	115.9906	116.6137	116.2609	116.8575	116.2547	117.1455	116.2429	117.0771	116.2573	117.2258	**117.6**
C4	168.3478	168.9536	169.7150	169.3969	170.1310	169.3775	170.6738	169.3528	170.4989	169.4065	170.7682	168.3478	168.9536	169.7150	169.3969	170.1309	169.3775	170.6738	169.3529	170.4989	169.4065	170.7682	**168.3**
C5	113.3354	114.4044	115.0462	115.0266	115.7191	114.9969	116.0153	114.9618	115.8944	115.0458	116.1580	113.3354	114.4045	115.0462	115.0266	115.7191	114.9969	116.0153	114.9617	115.8944	115.0458	116.1580	**117.6**
C6	127.6467	128.8978	129.9328	129.9379	131.2665	129.8770	131.8460	129.8113	131.5682	129.9875	132.0896	127.6467	128.8977	129.9328	129.9380	131.2665	129.8770	131.8460	129.8113	131.5682	129.9876	132.0896	**133.3**
C7	195.5731	201.1277	202.5411	203.7564	205.1541	203.6174	209.0255	203.4714	208.3346	203.8785	209.8788	195.5731	201.1277	202.5411	203.7565	205.1539	203.6174	209.0255	203.4717	208.3346	203.8785	209.8788	**195.8**
C8	66.0732	67.9957	68.4903	68.7224	69.6196	68.7003	70.0870	68.6709	70.0972	68.7322	70.3344	66.0732	67.9958	68.4903	68.7226	69.6196	68.7004	70.0870	68.6709	70.0972	68.7322	70.3344	**70.4**
C9	36.5013	36.1561	36.3808	36.1692	36.2657	36.1751	36.6313	36.1753	36.5703	36.1547	36.6703	36.5013	36.1562	36.3808	36.1692	36.2656	36.1751	36.6313	36.1753	36.5703	36.1547	36.6703	**31.1**
C10	28.6233	29.0478	29.5021	29.3898	30.0161	29.3768	29.8944	29.3581	29.8818	29.3929	30.0503	28.6233	29.0477	29.5021	29.3898	30.0160	29.3768	29.8944	29.3580	29.8818	29.3930	30.0503	**26.9**
C11	29.6468	29.7271	30.0848	29.7850	30.1842	29.7907	30.1750	29.7910	30.1811	29.7704	30.2632	29.6468	29.7272	30.0848	29.7849	30.1842	29.7907	30.1749	29.7910	30.1811	29.7704	30.2632	**23.4**
C12	16.7637	16.9097	17.0328	17.0844	17.2029	17.0811	17.1660	17.0727	17.1626	17.0786	17.1506	16.7637	16.9097	17.0328	17.0843	17.2029	17.0811	17.1660	17.0727	17.1626	17.0786	17.1506	**13.8**
C1`	51.7337	52.4858	52.9328	53.0582	53.6707	53.0297	53.6672	52.9964	53.6005	53.0766	54.0194	56.2482	57.2354	57.6350	57.7173	58.2870	57.6968	58.3670	57.6709	58.2796	57.7275	58.6081	**53.3**
C2`	26.4609	26.9933	27.3434	27.2952	27.6992	27.2887	27.7603	27.2761	27.7417	27.2919	27.6012	26.4501	26.6417	27.0756	26.8535	27.4196	26.8487	27.2629	26.8387	27.2654	26.8497	27.0231	**24.2**
C3`	26.4501	26.6418	27.0756	26.8535	27.4195	26.8487	27.2629	26.8388	27.2654	26.8497	27.0231	26.4609	26.9933	27.3434	27.2952	27.6992	27.2887	27.7603	27.2761	27.7417	27.2919	27.6012	**24.1**
C4`	56.2482	57.2355	57.6350	57.7172	58.2870	57.6968	58.3669	57.6709	58.2796	57.7275	58.6081	51.7337	52.4859	52.9328	53.0581	53.6707	53.0297	53.6672	52.9964	53.6005	53.0766	54.0194	**56.3**
H2	8.3249	8.1241	8.1537	8.0646	8.0342	8.0676	8.1182	8.0705	8.0902	8.0614	8.1158	8.3249	8.1241	8.1537	8.0646	8.0341	8.0676	8.1182	8.0705	8.0902	8.0614	8.1158	**8.2**
H3	7.2045	7.3251	7.4204	7.3707	7.4933	7.3687	7.5141	7.3664	7.5040	7.3723	7.5211	7.2045	7.3251	7.4204	7.3707	7.4933	7.3687	7.5141	7.3664	7.5040	7.3723	7.5211	**7.36**
H5	6.9910	7.2033	7.3016	7.2888	7.4115	7.2844	7.4314	7.2798	7.4198	7.2926	7.4471	6.9910	7.2033	7.3016	7.2888	7.4115	7.2844	7.4314	7.2798	7.4198	7.2926	7.4471	**7.36**
H6	7.8487	7.9010	7.9896	7.9745	8.0789	7.9695	8.1350	7.9645	8.1011	7.9789	8.1569	7.8487	7.9010	7.9896	7.9745	8.0789	7.9695	8.1350	7.9645	8.1011	7.9789	8.1569	**8.2**
H8	4.9446	4.9128	4.9412	4.9248	4.9737	4.9235	4.9921	4.9221	4.9774	4.9258	4.9759	4.9446	4.9128	4.9412	4.9248	4.9737	4.9235	4.9921	4.9221	4.9774	4.9258	4.9759	**5.4**
H(9A-9B)	1.6234	1.6455	1.6374	1.6833	1.6640	1.6808	1.6972	1.6781	1.6877	1.6853	1.7322	1.6234	1.6455	1.6374	1.6833	1.6640	1.6808	1.6972	1.6781	1.6877	1.6853	1.7322	**2.08**
H(10A)	0.9953	0.8946	0.8938	0.8729	0.8450	0.8735	0.8734	0.8742	0.8679	0.8721	0.8733	0.9953	0.8946	0.8938	0.8729	0.8450	0.8735	0.8734	0.8742	0.8679	0.8721	0.8733	**1.14**
H(10B)	1.5882	1.4997	1.4577	1.4325	1.3742	1.4374	1.3635	1.4420	1.3716	1.4275	1.3377	1.5882	1.4997	1.4577	1.4325	1.3742	1.4374	1.3635	1.4420	1.3716	1.4275	1.3377	**1.28**
H(11A-11B)	1.1047	1.1212	1.1028	1.1423	1.1197	1.1410	1.1151	1.1396	1.1134	1.1432	1.0967	1.1047	1.1213	1.1028	1.1423	1.1197	1.1410	1.1151	1.1396	1.1134	1.1432	1.0967	**1.28**
H(12A-12C)	0.9447	0.9384	0.9250	0.9365	0.9136	0.9368	0.9157	0.9370	0.9158	0.9358	0.9079	0.9447	0.9384	0.9250	0.9365	0.9136	0.9368	0.9157	0.9370	0.9158	0.9358	0.9079	**0.82**
H(1`A)	2.8493	2.8305	2.8097	2.8183	2.7703	2.8195	2.7798	2.8205	2.7831	2.8167	2.7472	2.9785	2.9775	2.9559	2.9533	2.9142	2.9558	2.9129	2.9582	2.9219	2.9503	2.8855	**3.38**
H(1`B)	3.3360	3.3804	3.4119	3.4210	3.4791	3.4185	3.4699	3.4159	3.4664	3.4229	3.4658	2.9866	2.8809	2.8679	2.8706	2.8859	2.8704	2.8588	2.8703	2.8677	2.8705	2.8536	**3.71**
H(2`A)	1.6502	1.6910	1.6705	1.7077	1.6607	1.7071	1.6856	1.7064	1.6822	1.7079	1.6958	1.5551	1.5955	1.5818	1.6135	1.5777	1.6127	1.6012	1.6118	1.5983	1.6138	1.6130	**2.08**
H(2`B)	1.9000	1.8976	1.8633	1.9323	1.8944	1.9293	1.8932	1.9264	1.8871	1.9348	1.9145	1.7989	1.9092	1.8751	1.9769	1.9570	1.9728	1.9659	1.9687	1.9582	1.9804	2.0063	**2.24**
H(3`A)	1.5551	1.5955	1.5818	1.6135	1.5777	1.6127	1.6012	1.6118	1.5983	1.6138	1.6130	1.6502	1.6910	1.6705	1.7077	1.6607	1.7071	1.6856	1.7064	1.6822	1.7079	1.6958	**2.08**
H(3`B)	1.7989	1.9092	1.8751	1.9769	1.9570	1.9728	1.9659	1.9687	1.9582	1.9804	2.0063	1.9000	1.8976	1.8633	1.9322	1.8944	1.9293	1.8932	1.9264	1.8871	1.9348	1.9145	**2.16**
H(4`A)	2.9866	2.8809	2.8679	2.8706	2.8859	2.8705	2.8588	2.8703	2.8677	2.8705	2.8536	3.3360	3.3804	3.4119	3.4210	3.4791	3.4185	3.4699	3.4159	3.4664	3.4229	3.4658	**3.09**
H(4`B)	2.9785	2.9775	2.9559	2.9533	2.9142	2.9558	2.9129	2.9582	2.9219	2.9503	2.8855	2.8493	2.8305	2.8097	2.8182	2.7703	2.8195	2.7798	2.8205	2.7831	2.8167	2.7472	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S5. Cont. X

Nuclei	R											S										Exp. [b]
	OPBE																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	130.6787	132.6297	133.6336	133.3807	135.3198	133.3723	134.3661	133.3448	134.5349	133.3821	134.5269	130.6787	132.6296	133.6335	133.3807	135.3197	133.3723	134.3660	133.3448	134.5349	133.3821	134.5268	**132.2**
C2	130.5026	130.6500	131.1455	130.5229	131.1203	130.5465	131.4274	130.5522	131.3339	130.4956	131.4311	130.5026	130.6499	131.1455	130.5229	131.1203	130.5465	131.4274	130.5522	131.3339	130.4956	131.4309	**133.3**
C3	114.1774	114.9620	115.5644	115.1917	115.9530	115.1953	116.1865	115.1808	116.1149	115.1830	116.2950	114.1774	114.9619	115.5645	115.1917	115.9531	115.1953	116.1864	115.1808	116.1149	115.1830	116.2949	**117.6**
C4	164.7994	165.4524	166.0718	165.7743	166.4439	165.7692	166.9958	165.7465	166.8494	165.7742	167.1261	164.7994	165.4524	166.0719	165.7743	166.4440	165.7692	166.9958	165.7465	166.8494	165.7742	167.1261	**168.3**
C5	112.2619	113.5119	114.1131	114.0723	114.8593	114.0525	115.1463	114.0152	115.0300	114.0864	115.3281	112.2618	113.5119	114.1130	114.0723	114.8593	114.0525	115.1464	114.0152	115.0300	114.0864	115.3282	**117.6**
C6	126.2248	127.5436	128.4947	128.4132	129.7170	128.3671	130.2985	128.3037	130.0776	128.4529	130.5759	126.2248	127.5437	128.4947	128.4132	129.7170	128.3671	130.2986	128.3037	130.0776	128.4529	130.5758	**133.3**
C7	192.8492	198.0469	199.3180	200.6479	201.7981	200.5296	205.5758	200.3919	204.7558	200.7535	206.3278	192.8491	198.0466	199.3180	200.6479	201.7981	200.5296	205.5759	200.3919	204.7558	200.7535	206.3275	**195.8**
C8	63.5007	65.3509	66.0163	66.0708	67.1112	66.0585	67.5850	66.0270	67.4654	66.0760	67.8053	63.5007	65.3510	66.0163	66.0708	67.1112	66.0585	67.5850	66.0270	67.4654	66.0760	67.8053	**70.4**
C9	34.3082	34.1893	34.3213	34.1125	34.3179	34.1310	34.6281	34.1317	34.5209	34.0902	34.6999	34.3083	34.1893	34.3213	34.1125	34.3179	34.1310	34.6281	34.1317	34.5209	34.0902	34.6998	**31.1**
C10	26.3655	26.8815	27.2838	27.1239	27.8025	27.1222	27.6443	27.1030	27.6205	27.1207	27.8389	26.3655	26.8814	27.2838	27.1239	27.8024	27.1222	27.6443	27.1030	27.6205	27.1207	27.8389	**26.9**
C11	27.3220	27.5273	27.7359	27.4928	27.8362	27.5128	27.8134	27.5147	27.8103	27.4686	27.9319	27.3219	27.5273	27.7360	27.4928	27.8361	27.5128	27.8134	27.5147	27.8103	27.4686	27.9319	**23.4**
C12	16.0776	16.2963	16.3097	16.3835	16.4232	16.3927	16.4102	16.3844	16.4094	16.3702	16.4127	16.0776	16.2963	16.3098	16.3835	16.4232	16.3927	16.4102	16.3844	16.4094	16.3702	16.4127	**13.8**
C1`	49.8315	50.6513	50.9131	51.1124	51.5794	51.0991	51.6068	51.0680	51.5522	51.1202	52.0407	54.1207	55.1917	55.5154	55.5904	56.1099	55.5833	56.1855	55.5579	56.1235	55.5921	56.4254	**53.3**
C2`	25.1000	25.6677	25.9114	25.8276	26.2209	25.8356	26.2347	25.8256	26.2242	25.8151	25.9714	24.9036	25.1884	25.4269	25.2649	25.6750	25.2773	25.5882	25.2721	25.5991	25.2486	25.3040	**24.2**
C3`	24.9037	25.1884	25.4268	25.2649	25.6751	25.2773	25.5881	25.2721	25.5991	25.2486	25.3041	25.1001	25.6677	25.9114	25.8276	26.2210	25.8356	26.2347	25.8256	26.2242	25.8151	25.9714	**24.1**
C4`	54.1207	55.1916	55.5153	55.5904	56.1100	55.5833	56.1855	55.5579	56.1235	55.5921	56.4254	49.8315	50.6514	50.9130	51.1124	51.5794	51.0991	51.6068	51.0680	51.5522	51.1201	52.0406	**56.3**
H2	8.3644	8.1928	8.2044	8.1131	8.0948	8.1166	8.1711	8.1195	8.1553	8.1092	8.1745	8.3644	8.1928	8.2044	8.1131	8.0948	8.1166	8.1711	8.1195	8.1553	8.1092	8.1745	**8.2**
H3	7.2317	7.3506	7.4367	7.3986	7.5153	7.3968	7.5392	7.3943	7.5305	7.3995	7.5502	7.2317	7.3506	7.4367	7.3986	7.5153	7.3968	7.5392	7.3943	7.5305	7.3995	7.5502	**7.36**
H5	7.0085	7.2266	7.3170	7.3144	7.4418	7.3103	7.4561	7.3054	7.4452	7.3175	7.4766	7.0085	7.2266	7.3170	7.3144	7.4418	7.3103	7.4561	7.3054	7.4452	7.3175	7.4766	**7.36**
H6	7.9097	7.9800	8.0576	8.0368	8.1441	8.0322	8.1953	8.0270	8.1733	8.0405	8.2139	7.9097	7.9800	8.0576	8.0368	8.1441	8.0322	8.1953	8.0270	8.1733	8.0405	8.2139	**8.2**
H8	4.9509	4.9173	4.9339	4.9242	4.9761	4.9229	4.9923	4.9211	4.9808	4.9248	4.9868	4.9509	4.9173	4.9339	4.9242	4.9761	4.9229	4.9923	4.9211	4.9808	4.9248	4.9868	**5.4**
H(9A-9B)	1.6537	1.6636	1.6523	1.6862	1.6774	1.6845	1.7050	1.6821	1.6910	1.6872	1.7441	1.6537	1.6636	1.6523	1.6862	1.6774	1.6845	1.7050	1.6821	1.6910	1.6872	1.7441	**2.08**
H(10A)	0.9080	0.8215	0.7760	0.7960	0.7277	0.7977	0.7746	0.7987	0.7708	0.7938	0.7812	0.9080	0.8214	0.7760	0.7960	0.7277	0.7977	0.7746	0.7987	0.7708	0.7938	0.7812	**1.14**
H(10B)	1.5468	1.4570	1.4015	1.3905	1.3184	1.3954	1.3106	1.3997	1.3176	1.3850	1.2885	1.5468	1.4570	1.4015	1.3905	1.3184	1.3954	1.3106	1.3997	1.3176	1.3850	1.2884	**1.28**
H(11A-11B)	1.0380	1.0583	1.0237	1.0740	1.0368	1.0738	1.0344	1.0727	1.0341	1.0737	1.0195	1.0380	1.0583	1.0237	1.0740	1.0368	1.0738	1.0344	1.0727	1.0341	1.0737	1.0195	**1.28**
H(12A-12C)	0.8763	0.8722	0.8453	0.8670	0.8301	0.8680	0.8355	0.8684	0.8363	0.8653	0.8297	0.8763	0.8722	0.8453	0.8670	0.8301	0.8680	0.8355	0.8684	0.8363	0.8653	0.8297	**0.82**
H(1`A)	2.7652	2.7626	2.7400	2.7489	2.7012	2.7503	2.7146	2.7511	2.7162	2.7467	2.6727	2.9190	2.9188	2.8953	2.8880	2.8426	2.8911	2.8529	2.8934	2.8571	2.8843	2.8212	**3.38**
H(1`B)	3.2993	3.3459	3.3765	3.3785	3.4327	3.3769	3.4258	3.3746	3.4221	3.3793	3.4161	2.9751	2.8559	2.8439	2.8403	2.8379	2.8409	2.8138	2.8411	2.8191	2.8390	2.8061	**3.71**
H(2`A)	1.6236	1.6655	1.6386	1.6769	1.6256	1.6769	1.6499	1.6762	1.6468	1.6761	1.6606	1.5167	1.5612	1.5363	1.5781	1.5236	1.5780	1.5576	1.5771	1.5551	1.5774	1.5747	**2.08**
H(2`B)	1.8275	1.8380	1.7934	1.8734	1.8231	1.8710	1.8287	1.8680	1.8227	1.8751	1.8597	1.7579	1.8554	1.8133	1.9228	1.8837	1.9191	1.9005	1.9147	1.8947	1.9257	1.9488	**2.24**
H(3`A)	1.5167	1.5612	1.5363	1.5781	1.5236	1.5780	1.5576	1.5771	1.5551	1.5774	1.5747	1.6236	1.6655	1.6386	1.6769	1.6256	1.6769	1.6499	1.6762	1.6468	1.6761	1.6606	**2.08**
H(3`B)	1.7579	1.8554	1.8133	1.9228	1.8837	1.9191	1.9005	1.9147	1.8947	1.9257	1.9488	1.8275	1.8380	1.7934	1.8734	1.8231	1.8710	1.8287	1.8680	1.8227	1.8751	1.8597	**2.16**
H(4`A)	2.9751	2.8559	2.8439	2.8403	2.8379	2.8409	2.8138	2.8411	2.8191	2.8390	2.8061	3.2993	3.3459	3.3765	3.3785	3.4327	3.3769	3.4258	3.3746	3.4221	3.3793	3.4161	**3.09**
H(4`B)	2.9190	2.9187	2.8953	2.8880	2.8426	2.8911	2.8529	2.8934	2.8571	2.8843	2.8212	2.7652	2.7625	2.7400	2.7489	2.7012	2.7503	2.7146	2.7511	2.7162	2.7467	2.6727	**3.68**
Nuclei	OPW91																						
C1	130.9989	132.9583	133.9539	133.7056	135.6329	133.6877	134.6754	133.6513	134.8514	133.7031	134.8410	130.9989	132.9582	133.9539	133.7056	135.6330	133.6877	134.6754	133.6513	134.8515	133.7031	134.8410	**132.2**
C2	130.7262	130.8703	131.3673	130.7503	131.3340	130.7635	131.6450	130.7599	131.5541	130.7194	131.6496	130.7261	130.8703	131.3673	130.7503	131.3339	130.7635	131.6450	130.7599	131.5542	130.7194	131.6496	**133.3**
C3	114.3764	115.1564	115.7533	115.3897	116.1354	115.3831	116.3698	115.3596	116.2991	115.3771	116.4793	114.3764	115.1565	115.7533	115.3897	116.1354	115.3831	116.3698	115.3596	116.2991	115.3771	116.4793	**117.6**
C4	165.2041	165.8588	166.4788	166.1876	166.8477	166.1725	167.4033	166.1404	167.2572	166.1838	167.5338	165.2041	165.8588	166.4788	166.1876	166.8476	166.1725	167.4033	166.1404	167.2572	166.1838	167.5338	**168.3**
C5	112.4572	113.7054	114.3021	114.2692	115.0406	114.2396	115.3290	114.1931	115.2123	114.2792	115.5116	112.4573	113.7054	114.3021	114.2692	115.0407	114.2396	115.3290	114.1931	115.2123	114.2792	115.5116	**117.6**
C6	126.4459	127.7681	128.7165	128.6476	129.9387	128.5911	130.5278	128.5186	130.3040	128.6837	130.8058	126.4460	127.7681	128.7164	128.6476	129.9387	128.5911	130.5278	128.5186	130.3040	128.6837	130.8058	**133.3**
C7	193.2350	198.4648	199.7275	201.0721	202.2060	200.9435	206.0081	200.7961	205.1882	201.1740	206.7657	193.2352	198.4648	199.7276	201.0721	202.2063	200.9435	206.0081	200.7961	205.1882	201.1740	206.7657	**195.8**
C8	63.7228	65.5786	66.2262	66.3004	67.3297	66.2783	67.7924	66.2379	67.6675	66.3014	68.0264	63.7228	65.5786	66.2262	66.3004	67.3296	66.2783	67.7924	66.2379	67.6675	66.3014	68.0264	**70.4**
C9	34.4593	34.3374	34.4633	34.2679	34.4630	34.2763	34.7706	34.2678	34.6619	34.2417	34.8495	34.4593	34.3374	34.4633	34.2679	34.4630	34.2763	34.7706	34.2678	34.6619	34.2417	34.8495	**31.1**
C10	26.4933	27.0116	27.4118	27.2602	27.9311	27.2485	27.7713	27.2200	27.7463	27.2531	27.9654	26.4932	27.0116	27.4118	27.2602	27.9312	27.2485	27.7713	27.2200	27.7464	27.2531	27.9654	**26.9**
C11	27.4281	27.6358	27.8457	27.6079	27.9463	27.6176	27.9231	27.6102	27.9202	27.5798	28.0426	27.4281	27.6358	27.8457	27.6079	27.9462	27.6176	27.9231	27.6102	27.9203	27.5798	28.0426	**23.4**
C12	16.1147	16.3379	16.3532	16.4317	16.4668	16.4307	16.4541	16.4131	16.4540	16.4146	16.4592	16.1147	16.3380	16.3532	16.4317	16.4669	16.4307	16.4541	16.4131	16.4540	16.4146	16.4592	**13.8**
C1`	49.9744	50.7955	51.0613	51.2629	51.7275	51.2393	51.7560	51.1989	51.7048	51.2672	52.1859	54.2713	55.3450	55.6693	55.7494	56.2629	55.7320	56.3386	55.6974	56.2757	55.7475	56.5821	**53.3**
C2`	25.2138	25.7880	26.0320	25.9569	26.3447	25.9547	26.3594	25.9356	26.3475	25.9405	26.1094	25.0229	25.3126	25.5528	25.3973	25.7998	25.3995	25.7152	25.3852	25.7270	25.3771	25.4366	**24.2**
C3`	25.0230	25.3125	25.5528	25.3973	25.7999	25.3995	25.7152	25.3852	25.7270	25.3771	25.4366	25.2138	25.7880	26.0320	25.9569	26.3447	25.9547	26.3594	25.9356	26.3475	25.9405	26.1094	**24.1**
C4`	54.2713	55.3450	55.6693	55.7494	56.2627	55.7320	56.3386	55.6974	56.2757	55.7475	56.5821	49.9744	50.7955	51.0613	51.2629	51.7274	51.2393	51.7560	51.1989	51.7048	51.2672	52.1859	**56.3**
H2	8.3657	8.1926	8.2058	8.1146	8.0958	8.1174	8.1723	8.1200	8.1563	8.1104	8.1754	8.3657	8.1926	8.2058	8.1146	8.0958	8.1174	8.1723	8.1200	8.1564	8.1104	8.1754	**8.2**
H3	7.2334	7.3518	7.4382	7.4004	7.5160	7.3980	7.5403	7.3952	7.5319	7.4010	7.5508	7.2334	7.3518	7.4382	7.4004	7.5160	7.3980	7.5403	7.3952	7.5319	7.4010	7.5508	**7.36**
H5	7.0105	7.2283	7.3185	7.3163	7.4423	7.3115	7.4569	7.3065	7.4459	7.3190	7.4773	7.0105	7.2283	7.3185	7.3163	7.4423	7.3115	7.4569	7.3065	7.4458	7.3190	7.4773	**7.36**
H6	7.9098	7.9795	8.0579	8.0377	8.1442	8.0324	8.1963	8.0270	8.1738	8.0412	8.2151	7.9098	7.9795	8.0579	8.0377	8.1442	8.0324	8.1963	8.0270	8.1738	8.0412	8.2151	**8.2**
H8	4.9491	4.9159	4.9327	4.9236	4.9747	4.9217	4.9913	4.9198	4.9796	4.9239	4.9859	4.9491	4.9159	4.9327	4.9236	4.9747	4.9217	4.9913	4.9198	4.9796	4.9239	4.9859	**5.4**
H(9A-9B)	1.6497	1.6605	1.6494	1.6849	1.6763	1.6824	1.7032	1.6798	1.6890	1.6857	1.7429	1.6497	1.6605	1.6494	1.6849	1.6763	1.6824	1.7032	1.6798	1.6890	1.6857	1.7429	**2.08**
H(10A)	0.9129	0.8260	0.7820	0.8013	0.7323	0.8023	0.7801	0.8031	0.7773	0.7988	0.7858	0.9129	0.8260	0.7820	0.8013	0.7323	0.8023	0.7801	0.8031	0.7773	0.7988	0.7858	**1.14**
H(10B)	1.5483	1.4585	1.4043	1.3926	1.3200	1.3969	1.3127	1.4010	1.3200	1.3868	1.2904	1.5483	1.4585	1.4043	1.3926	1.3200	1.3969	1.3127	1.4010	1.3200	1.3868	1.2904	**1.28**
H(11A-11B)	1.0395	1.0599	1.0261	1.0765	1.0389	1.0755	1.0369	1.0742	1.0367	1.0758	1.0217	1.0396	1.0599	1.0261	1.0765	1.0389	1.0755	1.0369	1.0742	1.0367	1.0758	1.0217	**1.28**
H(12A-12C)	0.8777	0.8739	0.8474	0.8694	0.8320	0.8698	0.8377	0.8698	0.8386	0.8674	0.8317	0.8777	0.8739	0.8474	0.8694	0.8321	0.8698	0.8377	0.8698	0.8386	0.8674	0.8317	**0.82**
H(1`A)	2.7694	2.7663	2.7435	2.7534	2.7049	2.7542	2.7183	2.7548	2.7196	2.7509	2.6771	2.9218	2.9220	2.8985	2.8920	2.8459	2.8944	2.8559	2.8966	2.8599	2.8879	2.8245	**3.38**
H(1`B)	3.2959	3.3429	3.3734	3.3768	3.4303	3.3745	3.4237	3.3719	3.4196	3.3773	3.4149	2.9704	2.8525	2.8394	2.8380	2.8351	2.8379	2.8108	2.8378	2.8160	2.8365	2.8041	**3.71**
H(2`A)	1.6240	1.6661	1.6394	1.6783	1.6263	1.6776	1.6507	1.6767	1.6476	1.6772	1.6608	1.5177	1.5624	1.5377	1.5798	1.5247	1.5790	1.5586	1.5779	1.5563	1.5788	1.5749	**2.08**
H(2`B)	1.8287	1.8391	1.7947	1.8752	1.8243	1.8721	1.8300	1.8689	1.8242	1.8766	1.8606	1.7568	1.8554	1.8138	1.9233	1.8837	1.9189	1.9008	1.9143	1.8951	1.9259	1.9480	**2.24**
H(3`A)	1.5177	1.5624	1.5377	1.5798	1.5247	1.5790	1.5586	1.5779	1.5563	1.5788	1.5749	1.6240	1.6661	1.6394	1.6783	1.6263	1.6776	1.6507	1.6767	1.6475	1.6772	1.6608	**2.08**
H(3`B)	1.7568	1.8554	1.8138	1.9233	1.8837	1.9189	1.9008	1.9143	1.8951	1.9259	1.9480	1.8287	1.8391	1.7947	1.8752	1.8243	1.8721	1.8300	1.8689	1.8242	1.8766	1.8606	**2.16**
H(4`A)	2.9704	2.8525	2.8394	2.8380	2.8351	2.8379	2.8108	2.8378	2.8160	2.8365	2.8041	3.2959	3.3429	3.3734	3.3768	3.4303	3.3745	3.4237	3.3719	3.4196	3.3773	3.4149	**3.09**
H(4`B)	2.9218	2.9219	2.8985	2.8920	2.8459	2.8944	2.8559	2.8966	2.8599	2.8879	2.8245	2.7694	2.7663	2.7435	2.7534	2.7049	2.7542	2.7183	2.7548	2.7196	2.7509	2.6771	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S5. Cont. XI

Nuclei	R											S										Exp. [b]
	PBE											PBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	135.7483	136.9338	137.8215	137.3803	138.9543	137.3545	138.4508	137.3389	138.4347	137.4219	138.6539	135.7483	136.9338	137.8215	137.3803	138.9543	137.3545	138.4509	137.3389	138.4347	137.4219	138.6539	**132.2**
C2	135.8078	135.8743	136.4215	135.6787	136.3342	135.6882	136.8147	135.7088	136.6975	135.6874	136.7796	135.8078	135.8743	136.4215	135.6787	136.3342	135.6882	136.8147	135.7088	136.6975	135.6874	136.7796	**133.3**
C3	119.5174	120.3563	120.9316	120.5420	121.3293	120.5297	121.6675	120.5282	121.5814	120.5709	121.7766	119.5174	120.3563	120.9316	120.5420	121.3293	120.5297	121.6674	120.5282	121.5814	120.5709	121.7766	**117.6**
C4	174.2361	175.2702	175.9491	175.6389	176.4757	175.6130	177.0574	175.5980	176.9178	175.6810	177.2200	174.2361	175.2703	175.9491	175.6389	176.4758	175.6130	177.0574	175.5980	176.9178	175.6810	177.2200	**168.3**
C5	117.5658	118.8904	119.5358	119.4738	120.4435	119.4339	120.7042	119.4048	120.5965	119.5296	120.8999	117.5658	118.8902	119.5358	119.4738	120.4435	119.4339	120.7041	119.4048	120.5965	119.5296	120.8999	**117.6**
C6	132.1464	134.1194	135.2182	135.1667	136.8848	135.0939	137.4752	135.0329	137.2528	135.2539	137.9118	132.1464	134.1194	135.2182	135.1667	136.8848	135.0939	137.4754	135.0329	137.2528	135.2539	137.9118	**133.3**
C7	201.1356	205.4775	206.7985	207.6645	208.7676	207.5322	212.7870	207.4100	211.8422	207.8073	213.7751	201.1356	205.4775	206.7985	207.6645	208.7676	207.5322	212.7866	207.4100	211.8422	207.8073	213.7751	**195.8**
C8	67.3305	68.6977	69.4799	69.1926	70.5026	69.1716	71.0535	69.1589	70.8716	69.2282	71.4612	67.3305	68.6976	69.4799	69.1926	70.5026	69.1716	71.0534	69.1589	70.8716	69.2282	71.4612	**70.4**
C9	38.5481	38.3924	38.5854	38.2027	38.7100	38.2115	39.0042	38.2308	38.9069	38.2116	39.1515	38.5481	38.3925	38.5854	38.2027	38.7100	38.2115	39.0042	38.2308	38.9069	38.2116	39.1515	**31.1**
C10	29.5828	30.1383	30.5931	30.3952	31.2462	30.3715	31.0588	30.3592	31.0404	30.4359	31.2758	29.5828	30.1382	30.5931	30.3952	31.2462	30.3715	31.0588	30.3592	31.0404	30.4359	31.2759	**26.9**
C11	29.4545	29.6678	29.8873	29.5253	30.0700	29.5343	30.0539	29.5536	30.0482	29.5337	30.2277	29.4545	29.6678	29.8873	29.5253	30.0700	29.5343	30.0540	29.5536	30.0482	29.5337	30.2277	**23.4**
C12	16.4263	16.6550	16.6777	16.6936	16.8479	16.6853	16.8192	16.6882	16.8147	16.7199	16.8332	16.4263	16.6550	16.6777	16.6936	16.8479	16.6853	16.8192	16.6882	16.8147	16.7199	16.8332	**13.8**
C1`	53.1868	54.1192	54.3314	54.5767	55.2085	54.5426	55.1990	54.5200	55.1018	54.6279	55.7537	57.7309	59.0198	59.3593	59.4308	60.0063	59.4053	60.1988	59.3904	60.1340	59.4724	60.4800	**53.3**
C2`	25.7091	26.3084	26.6327	26.4566	27.0413	26.4455	27.0629	26.4450	27.0465	26.4846	26.9107	25.3534	25.6633	25.9658	25.7952	26.3210	25.7806	26.3173	25.7773	26.3051	25.8271	26.2369	**24.2**
C3`	25.3534	25.6633	25.9658	25.7952	26.3211	25.7806	26.3173	25.7773	26.3051	25.8271	26.2369	25.7091	26.3084	26.6327	26.4566	27.0413	26.4455	27.0629	26.4450	27.0465	26.4846	26.9108	**24.1**
C4`	57.7309	59.0198	59.3593	59.4308	60.0063	59.4053	60.1988	59.3904	60.1340	59.4724	60.4800	53.1868	54.1193	54.3314	54.5767	55.2086	54.5426	55.1991	54.5200	55.1018	54.6279	55.7537	**56.3**
H2	8.5422	8.4404	8.4543	8.3726	8.3723	8.3764	8.4041	8.3809	8.4061	8.3697	8.3938	8.5422	8.4404	8.4543	8.3726	8.3723	8.3764	8.4041	8.3809	8.4061	8.3697	8.3938	**8.2**
H3	7.2025	7.3512	7.4409	7.3933	7.5117	7.3913	7.5367	7.3898	7.5283	7.3957	7.5512	7.2025	7.3512	7.4409	7.3933	7.5117	7.3913	7.5367	7.3898	7.5283	7.3957	7.5512	**7.36**
H5	7.0213	7.1777	7.2686	7.2421	7.3835	7.2384	7.3885	7.2352	7.3797	7.2463	7.4165	7.0213	7.1777	7.2686	7.2421	7.3835	7.2384	7.3885	7.2352	7.3797	7.2463	7.4165	**7.36**
H6	7.9455	8.1049	8.1784	8.1913	8.3013	8.1856	8.3527	8.1805	8.3388	8.1973	8.3808	7.9455	8.1050	8.1784	8.1913	8.3014	8.1856	8.3527	8.1805	8.3388	8.1973	8.3808	**8.2**
H8	4.9981	5.0221	5.0362	5.0495	5.0820	5.0469	5.1116	5.0449	5.1050	5.0527	5.1021	4.9981	5.0221	5.0362	5.0495	5.0820	5.0469	5.1116	5.0449	5.1050	5.0527	5.1021	**5.4**
H(9A-9B)	1.8877	1.9213	1.9179	1.9417	1.9768	1.9405	1.9732	1.9398	1.9667	1.9435	2.0076	1.8877	1.9214	1.9179	1.9417	1.9768	1.9405	1.9733	1.9398	1.9667	1.9435	2.0076	**2.08**
H(10A)	0.9903	0.8747	0.8363	0.8393	0.7493	0.8399	0.8067	0.8412	0.7986	0.8395	0.8199	0.9903	0.8747	0.8363	0.8393	0.7493	0.8399	0.8068	0.8413	0.7986	0.8395	0.8199	**1.14**
H(10B)	1.7513	1.6439	1.5780	1.5587	1.4835	1.5641	1.4701	1.5700	1.4779	1.5544	1.4380	1.7513	1.6439	1.5780	1.5587	1.4835	1.5641	1.4701	1.5700	1.4779	1.5544	1.4380	**1.28**
H(11A-11B)	1.1003	1.1160	1.0803	1.1235	1.0909	1.1231	1.0888	1.1233	1.0885	1.1245	1.0766	1.1003	1.1160	1.0803	1.1235	1.0909	1.1231	1.0888	1.1233	1.0885	1.1245	1.0766	**1.28**
H(12A-12C)	0.9133	0.9052	0.8805	0.8941	0.8588	0.8947	0.8663	0.8959	0.8665	0.8942	0.8605	0.9133	0.9052	0.8805	0.8941	0.8588	0.8947	0.8663	0.8959	0.8665	0.8942	0.8605	**0.82**
H(1`A)	2.7998	2.7946	2.7843	2.7819	2.7480	2.7827	2.7606	2.7840	2.7625	2.7819	2.7267	2.9257	2.9415	2.9313	2.9245	2.9038	2.9262	2.9082	2.9283	2.9120	2.9235	2.8692	**3.38**
H(1`B)	3.3750	3.4144	3.4496	3.4414	3.5072	3.4395	3.4925	3.4380	3.4919	3.4439	3.4830	3.0909	2.9057	2.8913	2.8575	2.8578	2.8592	2.8162	2.8617	2.8198	2.8566	2.7942	**3.71**
H(2`A)	1.6652	1.7153	1.6902	1.7321	1.6894	1.7312	1.7138	1.7309	1.7096	1.7335	1.7252	1.5339	1.5767	1.5534	1.5973	1.5509	1.5960	1.5860	1.5953	1.5792	1.5991	1.6048	**2.08**
H(2`B)	1.9457	1.9507	1.9086	1.9809	1.9365	1.9781	1.9392	1.9759	1.9340	1.9845	1.9691	1.8145	1.9190	1.8748	1.9758	1.9350	1.9721	1.9575	1.9689	1.9473	1.9800	2.0114	**2.24**
H(3`A)	1.5339	1.5767	1.5534	1.5973	1.5509	1.5960	1.5860	1.5953	1.5792	1.5991	1.6048	1.6652	1.7153	1.6902	1.7321	1.6894	1.7312	1.7138	1.7309	1.7096	1.7335	1.7252	**2.08**
H(3`B)	1.8145	1.9190	1.8748	1.9758	1.9350	1.9721	1.9575	1.9689	1.9473	1.9800	2.0114	1.9457	1.9507	1.9086	1.9809	1.9365	1.9781	1.9392	1.9759	1.9340	1.9845	1.9691	**2.16**
H(4`A)	3.0909	2.9057	2.8913	2.8575	2.8578	2.8592	2.8162	2.8617	2.8198	2.8566	2.7942	3.3750	3.4144	3.4496	3.4414	3.5072	3.4395	3.4925	3.4380	3.4919	3.4439	3.4830	**3.09**
H(4`B)	2.9257	2.9415	2.9313	2.9245	2.9038	2.9262	2.9082	2.9283	2.9120	2.9235	2.8692	2.7998	2.7946	2.7843	2.7819	2.7480	2.7827	2.7606	2.7840	2.7625	2.7819	2.7267	**3.68**
Nuclei	PBE0											PBE0										
C1	136.4530	137.3089	138.0508	137.7354	139.2688	137.7148	138.6567	137.6949	138.6719	137.7566	138.8652	136.4530	137.3090	138.0509	137.7354	139.2688	137.7148	138.6567	137.6949	138.6719	137.7566	138.8651	**132.2**
C2	138.6013	138.6001	139.0847	138.4264	138.9615	138.4331	139.5038	138.4418	139.3326	138.4230	139.4291	138.6013	138.6001	139.0847	138.4264	138.9613	138.4331	139.5038	138.4418	139.3328	138.4230	139.4292	**133.3**
C3	120.9188	121.6798	122.2526	121.8997	122.5990	121.8840	122.9416	121.8699	122.8160	121.9174	122.9678	120.9188	121.6797	122.2525	121.8997	122.5988	121.8840	122.9416	121.8699	122.8159	121.9174	122.9677	**117.6**
C4	172.9248	173.7704	174.3607	174.1635	174.7944	174.1342	175.5017	174.1070	175.2844	174.1944	175.5847	172.9248	173.7702	174.3606	174.1635	174.7943	174.1342	175.5017	174.1070	175.2844	174.1944	175.5847	**168.3**
C5	118.8873	120.2205	120.8491	120.8784	121.7495	120.8319	122.0378	120.7874	121.8751	120.9256	122.1589	118.8873	120.2204	120.8491	120.8784	121.7495	120.8319	122.0378	120.7874	121.8751	120.9256	122.1590	**117.6**
C6	134.7534	136.6483	137.8002	137.7535	139.3337	137.6742	140.0781	137.5975	139.7552	137.8328	140.4055	134.7534	136.6484	137.8002	137.7535	139.3337	137.6742	140.0781	137.5975	139.7551	137.8328	140.4054	**133.3**
C7	201.0382	205.4916	206.6635	207.9368	208.6564	207.7907	213.5288	207.6448	212.4021	208.0776	214.5410	201.0382	205.4915	206.6632	207.9368	208.6564	207.7907	213.5288	207.6448	212.4025	208.0776	214.5410	**195.8**
C8	63.3741	64.5227	65.2451	65.0149	66.0343	64.9854	66.6890	64.9567	66.5032	65.0447	67.0482	63.3741	64.5227	65.2451	65.0149	66.0342	64.9854	66.6890	64.9567	66.5033	65.0447	67.0483	**70.4**
C9	35.2480	35.0267	35.2621	34.8927	35.2211	34.8944	35.4911	34.8977	35.3528	34.8940	35.5658	35.2480	35.0267	35.2622	34.8927	35.2211	34.8944	35.4911	34.8978	35.3528	34.8940	35.5657	**31.1**
C10	27.5160	27.9999	28.4469	28.3217	29.0203	28.2908	28.9160	28.2627	28.8347	28.3546	29.0522	27.5160	27.9999	28.4468	28.3217	29.0203	28.2908	28.9160	28.2627	28.8348	28.3546	29.0522	**26.9**
C11	27.3762	27.5042	27.7451	27.4397	27.8548	27.4401	27.9245	27.4421	27.8635	27.4419	28.0248	27.3761	27.5043	27.7451	27.4397	27.8548	27.4401	27.9245	27.4422	27.8636	27.4419	28.0247	**23.4**
C12	16.1669	16.3506	16.3714	16.4494	16.5174	16.4361	16.5489	16.4251	16.4828	16.4654	16.4981	16.1668	16.3507	16.3713	16.4494	16.5175	16.4361	16.5489	16.4250	16.4827	16.4654	16.4981	**13.8**
C1`	50.3442	51.1746	51.3791	51.6553	52.1863	51.6178	52.2537	51.5828	52.1219	51.6945	52.6719	54.6441	55.7362	56.0471	56.1526	56.6508	56.1232	56.8627	56.0957	56.7432	56.1835	57.0525	**53.3**
C2`	24.3672	24.7765	25.0807	24.9101	25.3550	24.8969	25.4419	24.8857	25.3814	24.9254	25.2400	23.8126	24.0541	24.3180	24.1905	24.6209	24.1765	24.6494	24.1645	24.5778	24.2070	24.4911	**24.2**
C3`	23.8126	24.0541	24.3180	24.1905	24.6209	24.1765	24.6494	24.1645	24.5779	24.2070	24.4910	24.3672	24.7765	25.0807	24.9101	25.3550	24.8969	25.4419	24.8857	25.3814	24.9254	25.2399	**24.1**
C4`	54.6441	55.7362	56.0470	56.1526	56.6509	56.1232	56.8627	56.0957	56.7433	56.1835	57.0525	50.3442	51.1747	51.3791	51.6553	52.1864	51.6178	52.2537	51.5828	52.1220	51.6945	52.6719	**56.3**
H2	8.7672	8.6747	8.6943	8.6043	8.6001	8.6077	8.6358	8.6113	8.6278	8.6008	8.6154	8.7672	8.6747	8.6943	8.6043	8.6001	8.6077	8.6358	8.6113	8.6278	8.6008	8.6154	**8.2**
H3	7.3555	7.5027	7.5909	7.5485	7.6660	7.5463	7.6937	7.5440	7.6820	7.5502	7.7053	7.3555	7.5027	7.5909	7.5485	7.6660	7.5463	7.6937	7.5440	7.6820	7.5502	7.7053	**7.36**
H5	7.1793	7.3531	7.4495	7.4232	7.5573	7.4188	7.5698	7.4143	7.5575	7.4270	7.5924	7.1793	7.3531	7.4495	7.4232	7.5573	7.4188	7.5698	7.4143	7.5575	7.4270	7.5924	**7.36**
H6	8.0691	8.2434	8.3303	8.3437	8.4667	8.3371	8.5292	8.3305	8.5036	8.3498	8.5531	8.0691	8.2434	8.3303	8.3437	8.4667	8.3371	8.5292	8.3305	8.5036	8.3498	8.5531	**8.2**
H8	4.5650	4.6235	4.6513	4.6787	4.7273	4.6747	4.7749	4.6709	4.7514	4.6822	4.7725	4.5650	4.6235	4.6513	4.6787	4.7273	4.6747	4.7749	4.6708	4.7514	4.6822	4.7725	**5.4**
H(9A-9B)	1.7345	1.7658	1.7709	1.7908	1.8071	1.7885	1.8131	1.7862	1.8041	1.7927	1.8421	1.7345	1.7658	1.7709	1.7908	1.8071	1.7885	1.8131	1.7862	1.8041	1.7927	1.8421	**2.08**
H(10A)	0.9439	0.8046	0.7615	0.7568	0.6649	0.7587	0.9607	0.7606	0.6992	0.7548	0.7188	0.9439	0.8046	0.7615	0.7568	0.6649	0.7587	0.7124	0.7606	0.6992	0.7548	0.7189	**1.14**
H(10B)	1.6350	1.5420	1.4670	1.4541	1.3671	1.4600	1.4933	1.4660	1.3682	1.4482	1.3328	1.6350	1.5420	1.4670	1.4541	1.3671	1.4600	1.3654	1.4660	1.3682	1.4482	1.3327	**1.28**
H(11A-11B)	1.0056	1.0247	0.9871	1.0334	0.9945	1.0329	0.9994	1.0324	0.9951	1.0336	0.9846	1.0056	1.0247	0.9871	1.0334	0.9945	1.0329	0.9994	1.0324	0.9951	1.0336	0.9846	**1.28**
H(12A-12C)	0.8954	0.8818	0.8542	0.8706	0.8300	0.8712	0.8408	0.8719	0.8377	0.8697	0.8328	0.8954	0.8818	0.8542	0.8706	0.8300	0.8712	0.8408	0.8719	0.8377	0.8697	0.8328	**0.82**
H(1`A)	2.6626	2.6552	2.6426	2.6448	2.6013	2.6453	2.8989	2.6459	2.6192	2.6440	2.5936	2.8001	2.8064	2.7926	2.7859	2.7548	2.7878	2.7693	2.7895	2.7706	2.7838	2.7342	**3.38**
H(1`B)	3.1711	3.2099	3.2462	3.2445	3.3001	3.2418	3.6043	3.2391	3.2874	3.2468	3.2911	2.8887	2.7177	2.7028	2.6786	2.6737	2.6802	2.6333	2.6819	2.6335	2.6768	2.6159	**3.71**
H(2`A)	1.6081	1.6522	1.6239	1.6693	1.6181	1.6684	1.8313	1.6674	1.6421	1.6699	1.6551	1.4766	1.5231	1.4941	1.5442	1.4926	1.5431	1.5327	1.5420	1.5241	1.5450	1.5471	**2.08**
H(2`B)	1.8001	1.8195	1.7770	1.8622	1.8181	1.8588	2.0106	1.8554	1.8120	1.8653	1.8463	1.6936	1.7941	1.7444	1.8558	1.8158	1.8518	1.8446	1.8478	1.8316	1.8594	1.8910	**2.24**
H(3`A)	1.4766	1.5231	1.4941	1.5442	1.4926	1.5431	1.7392	1.5419	1.5241	1.5450	1.5471	1.6081	1.6522	1.6239	1.6693	1.6181	1.6684	1.6479	1.6674	1.6421	1.6699	1.6551	**2.08**
H(3`B)	1.6936	1.7941	1.7444	1.8558	1.8158	1.8518	2.0814	1.8478	1.8316	1.8594	1.8910	1.8001	1.8195	1.7770	1.8622	1.8181	1.8588	1.8218	1.8554	1.8120	1.8653	1.8463	**2.16**
H(4`A)	2.8887	2.7177	2.7028	2.6786	2.6737	2.6802	2.9914	2.6818	2.6335	2.6768	2.6159	3.1711	3.2099	3.2462	3.2445	3.3001	3.2418	3.2940	3.2391	3.2874	3.2468	3.2911	**3.09**
H(4`B)	2.8001	2.8064	2.7926	2.7859	2.7548	2.7878	3.0365	2.7895	2.7706	2.7838	2.7342	2.6626	2.6552	2.6426	2.6448	2.6013	2.6453	2.6219	2.6459	2.6192	2.6440	2.5936	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S5. Cont. XII

Nuclei	R											S										Exp. [b]
	TPSS											TPSS										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	132.4356	133.1505	133.9345	133.5892	135.0046	133.5760	134.3940	133.5726	134.0790	133.6107	134.7819	132.4356	133.1505	133.9343	133.5892	135.0046	133.5760	134.3940	133.5726	134.6812	133.6107	134.7819	**132.2**
C2	132.8929	132.8526	133.4725	132.7671	133.3034	132.7794	133.7783	132.8032	133.3065	132.7661	133.7282	132.8929	132.8526	133.4725	132.7671	133.3034	132.7793	133.7783	132.8032	133.9176	132.7661	133.7282	**133.3**
C3	116.6681	117.3246	117.9791	117.5839	118.2462	117.5771	118.5755	117.5815	118.0239	117.6006	118.6358	116.6681	117.3246	117.9791	117.5839	118.2462	117.5771	118.5755	117.5815	118.8101	117.6006	118.6358	**117.6**
C4	170.8911	171.7397	172.4965	172.2075	172.9099	172.1863	173.5612	172.1764	172.8372	172.2385	173.6673	170.8911	171.7397	172.4965	172.2075	172.9099	172.1863	173.5612	172.1764	172.9955	172.2385	173.6673	**168.3**
C5	114.7722	115.9311	116.6167	116.5690	117.3927	116.5353	117.6393	116.5131	116.9513	116.6120	117.7796	114.7722	115.9311	116.6167	116.5690	117.3927	116.5353	117.6393	116.5131	117.7497	116.6120	117.7796	**117.6**
C6	129.3185	131.1397	132.2995	132.2804	133.7885	132.2131	134.5062	132.1577	132.6584	132.3555	134.8302	129.3185	131.1397	132.2995	132.2804	133.7885	132.2131	134.5062	132.1577	133.2770	132.3555	134.8302	**133.3**
C7	197.2729	201.1909	202.3750	203.3951	204.2125	203.2728	208.3467	203.1606	203.9454	203.5200	209.4808	197.2729	201.1909	202.3748	203.3951	204.2125	203.2728	208.3467	203.1606	203.7473	203.5200	209.4808	**195.8**
C8	66.1554	67.2219	67.8668	67.7200	68.8092	67.7027	69.2644	67.6953	67.9382	67.7454	69.7480	66.1554	67.2219	67.8668	67.7200	68.8092	67.7027	69.2644	67.6953	69.2980	67.7454	69.7480	**70.4**
C9	37.7531	37.5421	37.8061	37.4640	37.8295	37.4741	38.1342	37.4954	37.6175	37.4651	38.2427	37.7531	37.5421	37.8059	37.4640	37.8295	37.4740	38.1342	37.4954	39.3246	37.4651	38.2427	**31.1**
C10	29.1817	29.5893	30.1503	29.9117	30.6464	29.8939	30.4886	29.8881	29.9798	29.9393	30.6120	29.1817	29.5893	30.1502	29.9117	30.6464	29.8939	30.4886	29.8881	31.7744	29.9393	30.6120	**26.9**
C11	29.3660	29.4429	29.7794	29.4146	29.8735	29.4257	29.8732	29.4479	29.5378	29.4144	30.0060	29.3660	29.4429	29.7794	29.4146	29.8736	29.4258	29.8732	29.4479	31.3375	29.4144	30.0060	**23.4**
C12	17.2694	17.3881	17.5648	17.5303	17.6714	17.5262	17.6562	17.5339	17.5761	17.5450	17.6292	17.2694	17.3881	17.5648	17.5303	17.6714	17.5262	17.6562	17.5339	19.5128	17.5450	17.6292	**13.8**
C1`	53.0445	53.7558	54.1667	54.3103	54.8418	54.2794	54.8722	54.2605	54.4497	54.3511	55.3404	57.2249	58.3026	58.7280	58.7950	59.3005	58.7753	59.5194	58.7666	60.4363	58.8238	59.7915	**53.3**
C2`	26.3341	26.7286	27.1499	26.9392	27.4229	26.9349	27.4595	26.9415	27.0214	26.9534	27.2605	26.0765	26.1994	26.6761	26.4209	26.8925	26.4135	26.9030	26.4175	28.3298	26.4384	26.7317	**24.2**
C3`	26.0765	26.1994	26.6761	26.4209	26.8925	26.4136	26.9030	26.4175	26.4953	26.4384	26.7317	26.3341	26.7286	27.1499	26.9392	27.4229	26.9349	27.4595	26.9415	28.8499	26.9534	27.2605	**24.1**
C4`	57.2249	58.3026	58.7280	58.7950	59.3005	58.7753	59.5194	58.7666	58.9738	58.8238	59.7915	53.0445	53.7558	54.1668	54.3103	54.8419	54.2794	54.8722	54.2605	55.9640	54.3511	55.3404	**56.3**
H2	8.5524	8.4665	8.5107	8.4102	8.4107	8.4132	8.4523	8.4170	8.2571	8.4079	8.4133	8.5524	8.4665	8.5107	8.4102	8.4107	8.4132	8.4523	8.4170	8.5271	8.4079	8.4133	**8.2**
H3	7.1623	7.3069	7.4039	7.3576	7.4767	7.3553	7.5043	7.3535	7.1893	7.3601	7.5144	7.1623	7.3069	7.4039	7.3576	7.4767	7.3553	7.5043	7.3535	7.4716	7.3601	7.5144	**7.36**
H5	6.9935	7.1616	7.2589	7.2313	7.3713	7.2271	7.3755	7.2236	7.0589	7.2357	7.3952	6.9935	7.1616	7.2589	7.2313	7.3713	7.2271	7.3755	7.2236	7.3426	7.2357	7.3952	**7.36**
H6	7.8543	8.0239	8.1241	8.1246	8.2413	8.1183	8.3087	8.1126	7.9514	8.1310	8.3186	7.8543	8.0239	8.1241	8.1246	8.2413	8.1183	8.3087	8.1126	8.2250	8.1310	8.3186	**8.2**
H8	4.7647	4.8126	4.8538	4.8581	4.9078	4.8551	4.9504	4.8528	4.6786	4.8614	4.9315	4.7647	4.8126	4.8538	4.8581	4.9078	4.8551	4.9504	4.8528	4.9896	4.8614	4.9315	**5.4**
H(9A-9B)	1.8001	1.8427	1.8422	1.8732	1.9021	1.8708	1.9032	1.8691	1.6830	1.8759	1.9251	1.8001	1.8427	1.8422	1.8732	1.9021	1.8708	1.9032	1.8691	2.0283	1.8759	1.9251	**2.08**
H(10A)	1.0002	0.8769	0.8927	0.8464	0.7648	0.8472	0.8274	0.8487	0.6585	0.8461	0.8190	1.0002	0.8769	0.8927	0.8464	0.7648	0.8472	0.8274	0.8487	1.0155	0.8461	0.8190	**1.14**
H(10B)	1.7385	1.6228	1.5525	1.5379	1.4588	1.5440	1.4467	1.5505	1.3631	1.5325	1.4054	1.7385	1.6228	1.5525	1.5379	1.4588	1.5440	1.4467	1.5505	1.9732	1.5325	1.4054	**1.28**
H(11A-11B)	1.0583	1.0759	1.0492	1.0919	1.0592	1.0911	1.0615	1.0909	0.9017	1.0929	1.0424	1.0583	1.0759	1.0492	1.0919	1.0592	1.0911	1.0615	1.0909	1.2559	1.0929	1.0424	**1.28**
H(12A-12C)	0.9078	0.8948	0.8800	0.8900	0.8562	0.8904	0.8645	0.8914	0.7014	0.8900	0.8548	0.9078	0.8948	0.8800	0.8900	0.8562	0.8904	0.8645	0.8914	1.0579	0.8900	0.8548	**0.82**
H(1`A)	2.7122	2.7112	2.7093	2.7074	2.6743	2.7077	2.6920	2.7086	2.5258	2.7075	2.6628	2.8273	2.8487	2.8382	2.8410	2.8258	2.8424	2.8307	2.8444	3.0399	2.8398	2.7945	**3.38**
H(1`B)	3.2745	3.3206	3.3526	3.3541	3.4150	3.3518	3.4072	3.3500	3.1698	3.3568	3.3950	3.0710	2.8744	2.8447	2.8264	2.8319	2.8280	2.7779	2.8303	2.9220	2.8255	2.7603	**3.71**
H(2`A)	1.6509	1.6969	1.6781	1.7203	1.6753	1.7191	1.6999	1.7184	1.5317	1.7219	1.7093	1.5223	1.5627	1.5474	1.5881	1.5405	1.5866	1.5738	1.5858	1.9477	1.5899	1.5867	**2.08**
H(2`B)	1.8625	1.8784	1.8460	1.9212	1.8838	1.9176	1.8876	1.9149	1.7290	1.9252	1.9113	1.7015	1.8125	1.7743	1.8818	1.8445	1.8776	1.8662	1.8740	2.5013	1.8862	1.9287	**2.24**
H(3`A)	1.5223	1.5627	1.5474	1.5881	1.5405	1.5866	1.5738	1.5858	1.3985	1.5899	1.5867	1.6509	1.6969	1.6781	1.7203	1.6753	1.7191	1.6999	1.7184	2.0894	1.7219	1.7093	**2.08**
H(3`B)	1.7015	1.8125	1.7743	1.8818	1.8445	1.8776	1.8662	1.8740	1.6879	1.8862	1.9287	1.8625	1.8784	1.8460	1.9212	1.8838	1.9176	1.8876	1.9149	2.0859	1.9252	1.9113	**2.16**
H(4`A)	3.0710	2.8744	2.8447	2.8264	2.8318	2.8280	2.7779	2.8303	2.6480	2.8255	2.7603	3.2745	3.3206	3.3526	3.3541	3.4150	3.3518	3.4072	3.3500	3.4375	3.3568	3.3950	**3.09**
H(4`B)	2.8273	2.8487	2.8382	2.8410	2.8258	2.8424	2.8307	2.8444	2.6622	2.8398	2.7945	2.7122	2.7112	2.7093	2.7074	2.6743	2.7077	2.6920	2.7086	2.7416	2.7075	2.6628	**3.68**
Nuclei	VSXC											VSXC										
C1	133.6805	134.5405	135.1885	134.8465	136.5075	134.8331	135.4592	134.8176	135.4598	134.8603	135.9108	133.6804	134.5405	135.1885	134.8465	136.5076	134.8331	135.4593	134.8176	135.4596	134.8603	135.9108	**132.2**
C2	130.8568	131.2148	131.6668	131.2177	131.8000	131.2250	132.3394	131.2296	132.2150	131.2117	132.4206	130.8567	131.2148	131.6668	131.2177	131.8000	131.2250	132.3394	131.2296	132.2150	131.2117	132.4206	**133.3**
C3	114.9211	115.9128	116.4365	116.3181	116.9073	116.2991	117.2645	116.2774	117.2025	116.3375	117.3624	114.9211	115.9128	116.4365	116.3181	116.9072	116.2991	117.2645	116.2774	117.2024	116.3375	117.3624	**117.6**
C4	168.3003	169.1032	169.7919	169.5485	170.2398	169.5239	170.8109	169.4971	170.6743	169.5735	170.9192	168.3003	169.1032	169.7919	169.5485	170.2398	169.5239	170.8108	169.4971	170.6743	169.5735	170.9192	**168.3**
C5	112.7729	114.1638	114.7218	114.9628	115.5777	114.9149	115.9637	114.8652	115.8581	115.0102	116.1017	112.7730	114.1638	114.7218	114.9628	115.5778	114.9149	115.9637	114.8652	115.8581	115.0102	116.1017	**117.6**
C6	128.4606	129.9982	131.1249	130.9894	132.3974	130.9269	132.9648	130.8631	132.7529	131.0511	133.1730	128.4606	129.9982	131.1249	130.9894	132.3975	130.9269	132.9647	130.8631	132.7528	131.0511	133.1730	**133.3**
C7	193.6144	198.7380	199.9101	201.2950	202.2459	201.1444	206.3068	200.9911	205.2665	201.4392	207.5617	193.6144	198.7380	199.9101	201.2950	202.2458	201.1444	206.3068	200.9911	205.2666	201.4392	207.5617	**195.8**
C8	71.2958	72.3979	72.9108	72.9017	73.7341	72.8757	74.0459	72.8472	73.8255	72.9277	74.6281	71.2958	72.3979	72.9108	72.9018	73.7341	72.8757	74.0459	72.8472	73.8255	72.9277	74.6281	**70.4**
C9	41.7566	42.2479	42.5811	42.4292	42.7524	42.4240	43.2429	42.4162	43.1046	42.4354	43.3121	41.7566	42.2479	42.5811	42.4293	42.7525	42.4240	43.2429	42.4162	43.1046	42.4354	43.3121	**31.1**
C10	36.4853	37.4189	37.7243	38.0913	38.8133	38.0483	38.7335	38.0038	38.7135	38.1344	39.0207	36.4853	37.4189	37.7243	38.0913	38.8133	38.0483	38.7334	38.0038	38.7134	38.1344	39.0207	**26.9**
C11	35.7245	35.7671	36.0142	35.6725	36.0233	35.6843	35.9517	35.6935	35.9513	35.6625	35.9686	35.7245	35.7671	36.0142	35.6725	36.0233	35.6843	35.9516	35.6935	35.9513	35.6625	35.9686	**23.4**
C12	18.7135	18.9231	19.0967	19.1393	19.3695	19.1260	19.2353	19.1108	19.2302	19.1539	19.2772	18.7135	18.9231	19.0967	19.1393	19.3695	19.1260	19.2353	19.1108	19.2301	19.1539	19.2772	**13.8**
C1`	58.8714	59.4981	59.7451	59.8519	60.3179	59.8335	60.1483	59.8130	60.1663	59.8709	60.3243	60.9536	61.9037	62.1420	62.3605	62.9177	62.3370	62.8341	62.3113	62.7698	62.3842	63.2050	**53.3**
C2`	29.5342	30.0310	30.1911	30.2855	30.6314	30.2737	30.6152	30.2596	30.5864	30.2979	30.6852	28.4893	28.8029	29.0331	29.0094	29.3917	28.9983	29.3626	28.9854	29.3504	29.0216	29.4075	**24.2**
C3`	28.4892	28.8029	29.0331	29.0094	29.3918	28.9983	29.3625	28.9854	29.3504	29.0216	29.4075	29.5341	30.0310	30.1911	30.2855	30.6313	30.2737	30.6153	30.2596	30.5863	30.2979	30.6852	**24.1**
C4`	60.9537	61.9037	62.1420	62.3605	62.9176	62.3370	62.8341	62.3113	62.7699	62.3842	63.2050	58.8714	59.4981	59.7451	59.8519	60.3180	59.8335	60.1482	59.8130	60.1664	59.8710	60.3243	**56.3**
H2	8.5227	8.5081	8.5164	8.4735	8.4550	8.4764	8.5360	8.4794	8.5408	8.4706	8.5151	8.5227	8.5081	8.5164	8.4735	8.4550	8.4764	8.5360	8.4794	8.5408	8.4706	8.5151	**8.2**
H3	7.1829	7.3512	7.4296	7.4126	7.5247	7.4094	7.5501	7.4062	7.5412	7.4155	7.5801	7.1829	7.3512	7.4296	7.4126	7.5247	7.4094	7.5501	7.4062	7.5412	7.4155	7.5801	**7.36**
H5	7.0781	7.2694	7.3540	7.3564	7.4727	7.3513	7.4935	7.3463	7.4820	7.3612	7.5113	7.0781	7.2694	7.3540	7.3564	7.4727	7.3513	7.4935	7.3463	7.4820	7.3612	7.5113	**7.36**
H6	7.8503	8.0072	8.0875	8.1024	8.2216	8.0962	8.2794	8.0902	8.2620	8.1082	8.3027	7.8503	8.0072	8.0875	8.1024	8.2216	8.0962	8.2794	8.0902	8.2620	8.1082	8.3027	**8.2**
H8	4.2573	4.4037	4.4274	4.4919	4.5768	4.4861	4.6320	4.4805	4.6030	4.4974	4.6706	4.2573	4.4037	4.4274	4.4919	4.5768	4.4861	4.6320	4.4805	4.6030	4.4974	4.6706	**5.4**
H(9A-9B)	1.9641	1.9764	1.9714	1.9883	1.9833	1.9875	1.9808	1.9869	1.9785	1.9889	1.9808	1.9641	1.9764	1.9714	1.9883	1.9833	1.9875	1.9808	1.9869	1.9785	1.9889	1.9808	**2.08**
H(10A)	0.9306	0.9326	0.9128	0.9285	0.9053	0.9291	0.8940	0.9297	0.8921	0.9279	0.8858	0.9306	0.9326	0.9128	0.9285	0.9053	0.9291	0.8940	0.9297	0.8921	0.9279	0.8858	**1.14**
H(10B)	2.2764	2.1111	2.0177	1.9949	1.8578	2.0028	1.8386	2.0106	1.8498	1.9873	1.7818	2.2764	2.1111	2.0177	1.9949	1.8578	2.0028	1.8386	2.0106	1.8498	1.9873	1.7818	**1.28**
H(11A-11B)	1.3715	1.3906	1.3742	1.4051	1.3862	1.4042	1.3808	1.4034	1.3793	1.4059	1.3754	1.3715	1.3906	1.3742	1.4051	1.3862	1.4042	1.3808	1.4034	1.3793	1.4059	1.3754	**1.28**
H(12A-12C)	1.0159	1.0221	0.9916	1.0217	0.9772	1.0218	0.9913	1.0219	0.9921	1.0216	0.9943	1.0159	1.0221	0.9916	1.0217	0.9772	1.0218	0.9914	1.0219	0.9921	1.0216	0.9943	**0.82**
H(1`A)	2.5466	2.6087	2.6123	2.6247	2.6165	2.6242	2.6238	2.6237	2.6182	2.6251	2.6253	2.9068	2.9249	2.9160	2.9333	2.9175	2.9330	2.9201	2.9327	2.9165	2.9335	2.9377	**3.38**
H(1`B)	3.2222	3.2385	3.2758	3.2572	3.3242	3.2559	3.3194	3.2547	3.3141	3.2584	3.3295	2.7958	2.7872	2.7812	2.8016	2.8140	2.8006	2.8086	2.7996	2.7986	2.8025	2.8470	**3.71**
H(2`A)	1.9140	1.9742	1.9544	1.9977	1.9460	1.9965	1.9671	1.9954	1.9660	1.9988	1.9528	1.7327	1.8117	1.7846	1.8479	1.7903	1.8458	1.8302	1.8439	1.8243	1.8498	1.8487	**2.08**
H(2`B)	1.9226	1.9364	1.9229	1.9674	1.9573	1.9650	1.9672	1.9627	1.9625	1.9696	1.9907	2.3326	2.3738	2.3431	2.4091	2.3794	2.4065	2.3820	2.4042	2.3779	2.4115	2.4139	**2.24**
H(3`A)	1.7327	1.8117	1.7846	1.8479	1.7903	1.8458	1.8301	1.8439	1.8243	1.8498	1.8487	1.9140	1.9742	1.9544	1.9977	1.9460	1.9965	1.9671	1.9954	1.9660	1.9988	1.9528	**2.08**
H(3`B)	2.3325	2.3738	2.3431	2.4091	2.3793	2.4065	2.3820	2.4042	2.3779	2.4115	2.4139	1.9226	1.9364	1.9229	1.9674	1.9573	1.9650	1.9672	1.9627	1.9625	1.9697	1.9907	**2.16**
H(4`A)	2.7958	2.7872	2.7812	2.8016	2.8140	2.8006	2.8086	2.7996	2.7986	2.8025	2.8470	3.2222	3.2385	3.2758	3.2572	3.3242	3.2559	3.3194	3.2547	3.3141	3.2584	3.3295	**3.09**
H(4`B)	2.9068	2.9249	2.9160	2.9333	2.9174	2.9330	2.9201	2.9327	2.9165	2.9335	2.9377	2.5466	2.6087	2.6123	2.6247	2.6165	2.6242	2.6238	2.6237	2.6182	2.6251	2.6253	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S5. Cont. XIII

Nuclei	R											S										Exp. [b]
	wB97											wB97										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.6036	137.2931	138.0720	137.6679	139.4784	137.6596	138.7685	137.6458	138.8630	137.6709	139.1689	136.6037	137.2932	138.0720	137.6679	139.4785	137.6598	138.7686	137.6458	138.8630	137.6709	139.1689	**132.2**
C2	140.3841	140.2277	140.7307	140.0851	140.5886	140.0918	141.0437	140.0984	140.9507	140.0798	141.0312	140.3840	140.2279	140.7307	140.0850	140.5889	140.0917	141.0438	140.0984	140.9506	140.0796	141.0312	**133.3**
C3	121.6019	122.1976	122.7769	122.3867	123.0830	122.3768	123.2214	122.3659	123.1771	122.3963	123.2651	121.6019	122.1976	122.7769	122.3867	123.0830	122.3768	123.2213	122.3659	123.1771	122.3961	123.2650	**117.6**
C4	174.2312	174.8327	175.4522	175.1881	175.7881	175.1626	176.3324	175.1372	176.1882	175.2135	176.4253	174.2312	174.8326	175.4522	175.1882	175.7881	175.1627	176.3322	175.1372	176.1882	175.2133	176.4254	**168.3**
C5	119.5886	120.8444	121.4620	121.5301	122.3881	121.4874	122.5264	121.4436	122.4326	121.5708	122.6707	119.5886	120.8442	121.4620	121.5301	122.3881	121.4873	122.5263	121.4436	122.4326	121.5708	122.6707	**117.6**
C6	136.6592	138.3616	139.5017	139.3874	140.9361	139.3158	141.4313	139.2458	141.1605	139.4573	141.7769	136.6593	138.3615	139.5017	139.3873	140.9360	139.3158	141.4313	139.2458	141.1605	139.4574	141.7769	**133.3**
C7	201.4930	206.2813	207.4612	209.0200	209.7424	208.8666	215.3336	208.7073	214.1389	209.1604	216.6162	201.4932	206.2813	207.4612	209.0200	209.7424	208.8665	215.3336	208.7073	214.1389	209.1603	216.6162	**195.8**
C8	61.8488	62.9799	63.5330	63.4907	64.4664	63.4706	65.0895	63.4470	64.9281	63.5072	65.6139	61.8488	62.9799	63.5330	63.4908	64.4665	63.4705	65.0895	63.4470	64.9281	63.5073	65.6139	**70.4**
C9	33.4710	33.2416	33.4528	33.1389	33.4830	33.1466	33.5747	33.1536	33.4993	33.1317	33.7715	33.4709	33.2417	33.4528	33.1390	33.4830	33.1467	33.5747	33.1536	33.4993	33.1318	33.7715	**31.1**
C10	27.2566	27.6512	28.0056	27.9994	28.6490	27.9736	28.4332	27.9477	28.3999	28.0248	28.6428	27.2566	27.6512	28.0056	27.9993	28.6490	27.9737	28.4333	27.9477	28.3999	28.0248	28.6428	**26.9**
C11	26.2445	26.3038	26.5962	26.2779	26.6993	26.2792	26.6545	26.2801	26.6480	26.2768	26.8119	26.2446	26.3039	26.5962	26.2778	26.6993	26.2793	26.6544	26.2801	26.6480	26.2768	26.8119	**23.4**
C12	16.0982	16.1941	16.2592	16.3226	16.4257	16.3108	16.3515	16.2989	16.3401	16.3345	16.3725	16.0982	16.1942	16.2592	16.3225	16.4258	16.3108	16.3514	16.2989	16.3401	16.3346	16.3725	**13.8**
C1`	49.2568	49.9126	50.1155	50.3454	50.8618	50.3138	50.7647	50.2823	50.7307	50.3765	51.1612	53.0280	53.8362	54.1787	54.2424	54.7458	54.2152	54.7838	54.1877	54.7368	54.2686	54.9485	**53.3**
C2`	23.8426	24.1307	24.3776	24.2804	24.7127	24.2708	24.6901	24.2604	24.6738	24.2897	24.5996	23.1244	23.2955	23.5764	23.4577	23.9434	23.4448	23.8672	23.4312	23.8527	23.4704	23.8171	**24.2**
C3`	23.1243	23.2956	23.5764	23.4576	23.9434	23.4448	23.8671	23.4312	23.8527	23.4704	23.8171	23.8426	24.1307	24.3776	24.2804	24.7128	24.2708	24.6899	24.2604	24.6738	24.2898	24.5997	**24.1**
C4`	53.0280	53.8363	54.1787	54.2423	54.7459	54.2152	54.7840	54.1877	54.7368	54.2686	54.9485	49.2568	49.9127	50.1155	50.3454	50.8617	50.3139	50.7647	50.2823	50.7307	50.3765	51.1611	**56.3**
H2	8.8611	8.7550	8.7824	8.6884	8.6845	8.6907	8.6892	8.6933	8.6908	8.6868	8.6627	8.8611	8.7551	8.7824	8.6884	8.6845	8.6907	8.6892	8.6933	8.6908	8.6868	8.6628	**8.2**
H3	7.4418	7.5755	7.6657	7.6151	7.7392	7.6130	7.7548	7.6108	7.7474	7.6170	7.7687	7.4418	7.5755	7.6657	7.6151	7.7392	7.6130	7.7548	7.6108	7.7474	7.6170	7.7687	**7.36**
H5	7.2881	7.4745	7.5659	7.5546	7.6853	7.5499	7.6986	7.5450	7.6874	7.5592	7.7204	7.2881	7.4745	7.5659	7.5546	7.6853	7.5499	7.6986	7.5450	7.6874	7.5592	7.7204	**7.36**
H6	8.1472	8.3095	8.4115	8.4085	8.5457	8.4013	8.5816	8.3942	8.5608	8.4158	8.6004	8.1472	8.3095	8.4115	8.4085	8.5457	8.4013	8.5816	8.3942	8.5608	8.4158	8.6004	**8.2**
H8	4.2162	4.2825	4.3391	4.3494	4.4217	4.3438	4.4547	4.3384	4.4370	4.3551	4.4428	4.2162	4.2825	4.3391	4.3494	4.4217	4.3438	4.4547	4.3384	4.4370	4.3551	4.4427	**5.4**
H(9A-9B)	1.6980	1.7347	1.7280	1.7573	1.7680	1.7556	1.7679	1.7541	1.7590	1.7591	1.8079	1.6980	1.7347	1.7280	1.7573	1.7680	1.7556	1.7679	1.7541	1.7590	1.7591	1.8079	**2.08**
H(10A)	1.0016	0.8194	0.8010	0.7626	0.6910	0.7642	0.7142	0.7660	0.7163	0.7614	0.7212	1.0016	0.8194	0.8010	0.7625	0.6910	0.7642	0.7142	0.7660	0.7163	0.7614	0.7213	**1.14**
H(10B)	1.6278	1.5347	1.4753	1.4482	1.3716	1.4533	1.3682	1.4583	1.3751	1.4435	1.3347	1.6278	1.5347	1.4753	1.4482	1.3716	1.4533	1.3682	1.4583	1.3751	1.4435	1.3347	**1.28**
H(11A-11B)	0.9970	1.0164	0.9858	1.0253	0.9913	1.0240	0.9842	1.0229	0.9848	1.0267	0.9701	0.9970	1.0165	0.9858	1.0253	0.9913	1.0240	0.9842	1.0229	0.9848	1.0267	0.9701	**1.28**
H(12A-12C)	0.9260	0.9059	0.8807	0.8925	0.8533	0.8928	0.8544	0.8932	0.8560	0.8923	0.8453	0.9260	0.9059	0.8807	0.8925	0.8533	0.8928	0.8544	0.8932	0.8560	0.8923	0.8453	**0.82**
H(1`A)	2.6270	2.6255	2.6087	2.6149	2.5688	2.6154	2.5814	2.6159	2.5810	2.6146	2.5637	2.7756	2.7821	2.7653	2.7661	2.7415	2.7679	2.7612	2.7694	2.7614	2.7644	2.7326	**3.38**
H(1`B)	3.0717	3.1071	3.1361	3.1419	3.1899	3.1392	3.1745	3.1364	3.1704	3.1448	3.1707	2.7440	2.6065	2.5843	2.5750	2.5724	2.5770	2.5537	2.5787	2.5505	2.5729	2.5550	**3.71**
H(2`A)	1.6256	1.6765	1.6449	1.6937	1.6440	1.6928	1.6664	1.6917	1.6634	1.6947	1.6777	1.4958	1.5538	1.5251	1.5761	1.5317	1.5750	1.5665	1.5737	1.5625	1.5771	1.5832	**2.08**
H(2`B)	1.7472	1.7645	1.7289	1.8078	1.7723	1.8040	1.7693	1.8003	1.7626	1.8116	1.7916	1.6773	1.7645	1.7144	1.8250	1.7982	1.8210	1.8169	1.8169	1.8105	1.8288	1.8581	**2.24**
H(3`A)	1.4957	1.5538	1.5251	1.5761	1.5317	1.5750	1.5665	1.5737	1.5625	1.5771	1.5832	1.6256	1.6765	1.6449	1.6937	1.6440	1.6928	1.6664	1.6917	1.6634	1.6947	1.6777	**2.08**
H(3`B)	1.6772	1.7645	1.7144	1.8250	1.7982	1.8210	1.8169	1.8169	1.8105	1.8288	1.8581	1.7472	1.7645	1.7289	1.8078	1.7723	1.8040	1.7693	1.8003	1.7626	1.8116	1.7916	**2.16**
H(4`A)	2.7440	2.6065	2.5843	2.5750	2.5724	2.5770	2.5537	2.5787	2.5505	2.5729	2.5550	3.0717	3.1071	3.1361	3.1419	3.1899	3.1392	3.1744	3.1364	3.1704	3.1448	3.1707	**3.09**
H(4`B)	2.7756	2.7821	2.7653	2.7661	2.7415	2.7679	2.7612	2.7694	2.7614	2.7644	2.7326	2.6270	2.6255	2.6087	2.6149	2.5688	2.6155	2.5814	2.6159	2.5810	2.6146	2.5637	**3.68**
Nuclei	wB97X																						
C1	138.1726	138.9019	139.6559	139.4374	141.1483	139.4362	140.2893	139.4298	140.5386	139.4351	140.5881	138.1726	138.9020	139.6559	139.4374	141.1483	139.4362	140.2892	139.4298	140.5386	139.4351	140.5881	**132.2**
C2	140.9056	140.7859	141.2893	140.6233	141.1540	140.6326	141.6628	140.6415	141.4810	140.6157	141.6112	140.9055	140.7861	141.2893	140.6233	141.1540	140.6326	141.6628	140.6415	141.4810	140.6157	141.6112	**133.3**
C3	122.3191	122.9195	123.4907	123.1123	123.8008	123.1045	123.9961	123.0956	123.8881	123.1203	124.0304	122.3191	122.9193	123.4908	123.1123	123.8008	123.1045	123.9961	123.0956	123.8881	123.1203	124.0304	**117.6**
C4	174.9105	175.5432	176.1569	175.8933	176.4990	175.8689	177.1226	175.8445	176.8649	175.9183	177.2107	174.9104	175.5433	176.1570	175.8933	176.4990	175.8689	177.1226	175.8446	176.8649	175.9183	177.2107	**168.3**
C5	120.2722	121.5580	122.1552	122.2785	123.1172	122.2378	123.3127	122.1963	123.1518	122.3181	123.4476	120.2722	121.5580	122.1551	122.2785	123.1172	122.2378	123.3127	122.1963	123.1518	122.3181	123.4476	**117.6**
C6	136.9982	138.7129	139.8801	139.7133	141.2649	139.6414	141.8678	139.5704	141.4715	139.7845	142.2578	136.9982	138.7132	139.8800	139.7133	141.2649	139.6414	141.8678	139.5703	141.4715	139.7845	142.2578	**133.3**
C7	203.1280	207.9657	209.1246	210.8225	211.4559	210.6803	216.7975	210.5330	215.8333	210.9532	218.0343	203.1280	207.9653	209.1247	210.8225	211.4559	210.6803	216.7976	210.5330	215.8333	210.9532	218.0343	**195.8**
C8	63.1594	64.2444	64.8483	64.8139	65.7904	64.8024	66.3526	64.7861	66.3173	64.8222	66.9049	63.1594	64.2444	64.8484	64.8139	65.7904	64.8024	66.3525	64.7861	66.3173	64.8222	66.9049	**70.4**
C9	34.2867	33.9981	34.2392	33.8733	34.2116	33.8838	34.2855	33.8926	34.2464	33.8639	34.5266	34.2868	33.9981	34.2391	33.8733	34.2116	33.8838	34.2855	33.8926	34.2464	33.8639	34.5266	**31.1**
C10	27.6239	28.0338	28.4350	28.3754	29.0463	28.3517	28.8760	28.3279	28.7824	28.3996	29.0595	27.6239	28.0339	28.4349	28.3754	29.0463	28.3517	28.8759	28.3278	28.7824	28.3996	29.0595	**26.9**
C11	26.7734	26.8395	27.1217	26.8101	27.2443	26.8150	27.2454	26.8190	27.1824	26.8061	27.3901	26.7733	26.8395	27.1217	26.8101	27.2443	26.8150	27.2453	26.8190	27.1824	26.8061	27.3901	**23.4**
C12	16.1134	16.2233	16.2803	16.3492	16.4455	16.3394	16.4133	16.3295	16.3307	16.3601	16.4150	16.1135	16.2233	16.2803	16.3492	16.4455	16.3394	16.4133	16.3295	16.3307	16.3601	16.4150	**13.8**
C1`	49.9786	50.6789	50.8740	51.1549	51.6976	51.1232	51.6534	51.0913	51.5542	51.1870	52.0498	54.0121	54.8870	55.2128	55.3169	55.7989	55.2921	55.9370	55.2667	55.7988	55.3418	56.0923	**53.3**
C2`	24.3147	24.5823	24.8496	24.7428	25.1842	24.7362	25.2016	24.7285	25.1548	24.7501	25.0887	23.6105	23.7548	24.0311	23.9209	24.4101	23.9100	24.3738	23.8985	24.2790	23.9323	24.2815	**24.2**
C3`	23.6105	23.7548	24.0310	23.9209	24.4101	23.9100	24.3738	23.8985	24.2790	23.9323	24.2815	24.3147	24.5823	24.8496	24.7428	25.1842	24.7362	25.2015	24.7285	25.1548	24.7501	25.0887	**24.1**
C4`	54.0122	54.8869	55.2127	55.3169	55.7989	55.2921	55.9370	55.2667	55.7988	55.3418	56.0923	49.9785	50.6788	50.8741	51.1549	51.6976	51.1232	51.6535	51.0913	51.5542	51.1870	52.0498	**56.3**
H2	8.8389	8.7344	8.7644	8.6467	8.6499	8.6486	8.6801	8.6509	8.6532	8.6456	8.6538	8.8389	8.7344	8.7644	8.6467	8.6499	8.6486	8.6801	8.6509	8.6532	8.6456	8.6538	**8.2**
H3	7.4189	7.5552	7.6448	7.5956	7.7180	7.5936	7.7363	7.5916	7.7258	7.5975	7.7486	7.4189	7.5552	7.6448	7.5956	7.7180	7.5936	7.7363	7.5916	7.7257	7.5975	7.7486	**7.36**
H5	7.2591	7.4494	7.5388	7.5328	7.6613	7.5281	7.6770	7.5234	7.6630	7.5374	7.6981	7.2591	7.4494	7.5388	7.5328	7.6613	7.5281	7.6770	7.5234	7.6630	7.5374	7.6981	**7.36**
H6	8.1258	8.2888	8.3898	8.3787	8.5117	8.3714	8.5602	8.3643	8.5198	8.3862	8.5805	8.1258	8.2888	8.3898	8.3787	8.5117	8.3714	8.5602	8.3643	8.5198	8.3862	8.5805	**8.2**
H8	4.3096	4.3744	4.4229	4.4341	4.4965	4.4284	4.5479	4.4231	4.5054	4.4401	4.5323	4.3096	4.3744	4.4229	4.4341	4.4965	4.4284	4.5479	4.4231	4.5054	4.4401	4.5323	**5.4**
H(9A-9B)	1.6862	1.7156	1.7186	1.7332	1.7474	1.7318	1.7435	1.7303	1.7407	1.7347	1.7933	1.6862	1.7156	1.7186	1.7332	1.7474	1.7318	1.7435	1.7303	1.7407	1.7347	1.7933	**2.08**
H(10A)	0.9741	0.8166	0.7900	0.7615	0.6871	0.7623	0.7271	0.7634	0.7083	0.7612	0.7224	0.9741	0.8166	0.7900	0.7615	0.6871	0.7623	0.7271	0.7634	0.7083	0.7612	0.7224	**1.14**
H(10B)	1.6245	1.5295	1.4648	1.4366	1.3566	1.4418	1.3555	1.4472	1.3556	1.4319	1.3216	1.6245	1.5295	1.4648	1.4366	1.3566	1.4418	1.3555	1.4472	1.3556	1.4319	1.3216	**1.28**
H(11A-11B)	0.9968	1.0179	0.9853	1.0245	0.9912	1.0235	0.9920	1.0226	0.9837	1.0257	0.9745	0.9968	1.0179	0.9853	1.0245	0.9912	1.0235	0.9920	1.0226	0.9837	1.0257	0.9745	**1.28**
H(12A-12C)	0.9175	0.9002	0.8726	0.8866	0.8472	0.8870	0.8543	0.8875	0.8473	0.8864	0.8426	0.9175	0.9002	0.8727	0.8866	0.8472	0.8870	0.8543	0.8875	0.8473	0.8864	0.8426	**0.82**
H(1`A)	2.6470	2.6454	2.6305	2.6365	2.5914	2.6370	2.6054	2.6376	2.6015	2.6363	2.5818	2.7957	2.7944	2.7786	2.7812	2.7529	2.7831	2.7665	2.7849	2.7724	2.7793	2.7420	**3.38**
H(1`B)	3.0808	3.1191	3.1539	3.1560	3.2078	3.1531	3.1986	3.1503	3.1886	3.1590	3.1950	2.7613	2.6199	2.5918	2.5863	2.5940	2.5496	2.5960	2.5607	2.5899	2.5507	3.0809	**3.71**
H(2`A)	1.6199	1.6689	1.6385	1.6874	1.6359	1.6867	1.6587	1.6859	1.6546	1.6884	1.6672	1.4939	1.5491	1.5195	1.5747	1.5281	1.5739	1.5629	1.5729	1.5563	1.5756	1.5757	**2.08**
H(2`B)	1.7534	1.7752	1.7364	1.8180	1.7785	1.8141	1.7797	1.8104	1.7648	1.8221	1.8024	1.6804	1.7692	1.7162	1.8373	1.8050	1.8335	1.8284	1.8297	1.8175	1.8411	1.8621	**2.24**
H(3`A)	1.4939	1.5491	1.5195	1.5747	1.5281	1.5739	1.5629	1.5729	1.5563	1.5756	1.5757	1.6199	1.6689	1.6386	1.6874	1.6359	1.6867	1.6587	1.6859	1.6546	1.6884	1.6672	**2.08**
H(3`B)	1.6805	1.7691	1.7163	1.8373	1.8050	1.8335	1.8283	1.8297	1.8175	1.8411	1.8621	1.7534	1.7752	1.7364	1.8180	1.7785	1.8141	1.7797	1.8104	1.7648	1.8221	1.8024	**2.16**
H(4`A)	2.7613	2.6199	2.6025	2.5918	2.5863	2.5940	2.5496	2.5960	2.5607	2.5899	2.5507	3.0809	3.1191	3.1539	3.1560	3.2078	3.1531	3.1986	3.1503	3.1886	3.1590	3.1950	**3.09**
H(4`B)	2.7957	2.7944	2.7786	2.7812	2.7529	2.7831	2.7665	2.7849	2.7724	2.7793	2.7420	2.6470	2.6454	2.6305	2.6365	2.5914	2.6370	2.6054	2.6376	2.6015	2.6363	2.5818	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S5. Cont. XIV

Nuclei	R											S											Exp. [b]
	X3LYP																						
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.6738	140.7029	141.2879	141.2181	142.6377	141.1931	142.0187	141.1652	142.0627	141.2455	142.1890	139.6738	140.7029	141.2877	141.2181	142.6377	141.1931	142.0187	141.1652	142.0627	141.2455	142.1891	**132.2**
C2	139.7415	139.6983	140.2072	139.6129	140.0578	139.6218	140.6071	139.6280	140.4859	139.6083	140.5357	139.7415	139.6983	140.2071	139.6129	140.0578	139.6218	140.6071	139.6280	140.4859	139.6083	140.5359	**133.3**
C3	122.0899	122.7613	123.3039	122.9822	123.5845	122.9753	123.8523	122.9648	123.7861	122.9920	123.9125	122.0899	122.7613	123.3039	122.9822	123.5845	122.9753	123.8523	122.9648	123.7861	122.9920	123.9125	**117.6**
C4	176.3624	177.2172	177.8363	177.6336	178.2690	177.6121	178.8733	177.5874	178.7243	177.6576	178.9971	176.3624	177.2172	177.8362	177.6336	178.2690	177.6121	178.8733	177.5874	178.7243	177.6576	178.9971	**168.3**
C5	119.9750	121.1943	121.8036	121.8371	122.6276	121.8009	122.8281	121.7616	122.7328	121.8752	122.9752	119.9750	121.1943	121.8037	121.8372	122.6276	121.8009	122.8281	121.7616	122.7328	121.8752	122.9752	**117.6**
C6	135.9479	137.8862	139.0367	139.0291	140.5596	138.9585	141.2161	138.8853	140.9649	139.0998	141.6039	135.9479	137.8862	139.0366	139.0291	140.5596	138.9585	141.2161	138.8853	140.9649	139.0998	141.6039	**133.3**
C7	203.8442	208.6848	209.7423	211.2993	211.9258	211.1467	216.9743	210.9904	215.8222	211.4475	217.9867	203.8442	208.6848	209.7423	211.2993	211.9258	211.1467	216.9743	210.9904	215.8222	211.4475	217.9866	**195.8**
C8	66.1900	67.3996	67.9886	67.9123	68.9737	67.8933	69.5487	67.8696	69.3941	67.9319	69.8838	66.1900	67.3996	67.9886	67.9123	68.9737	67.8933	69.5487	67.8696	69.3941	67.9319	69.8838	**70.4**
C9	37.2125	36.8829	37.1023	36.7383	37.0705	36.7499	37.2814	36.7581	37.2176	36.7305	37.3484	37.2125	36.8829	37.1024	36.7383	37.0705	36.7499	37.2813	36.7581	37.2176	36.7305	37.3483	**31.1**
C10	29.2336	29.7336	30.2430	30.0625	30.8205	30.0426	30.6156	30.0200	30.6061	30.0851	30.7479	29.2336	29.7336	30.2429	30.0624	30.8205	30.0426	30.6156	30.0200	30.6061	30.0851	30.7479	**26.9**
C11	29.2440	29.3726	29.6606	29.3435	29.7886	29.3527	29.7810	29.3582	29.7823	29.3378	29.9009	29.2440	29.3726	29.6607	29.3436	29.7886	29.3527	29.7810	29.3582	29.7823	29.3378	29.9009	**23.4**
C12	16.6790	16.8526	16.9369	16.9924	17.0898	16.9846	17.0466	16.9744	17.0456	17.0037	17.0335	16.6790	16.8526	16.9370	16.9924	17.0898	16.9846	17.0465	16.9744	17.0456	17.0037	17.0336	**13.8**
C1`	52.1500	52.9655	53.2787	53.5431	54.0664	53.5092	54.0666	53.4728	53.9991	53.5797	54.5782	56.6692	57.8046	58.1645	58.2841	58.8069	58.2617	58.9279	58.2356	58.8673	58.3087	59.1667	**53.3**
C2`	25.9688	26.4573	26.8289	26.6445	27.1554	26.6386	27.1840	26.6293	27.1770	26.6532	26.9598	25.5752	25.7645	26.1378	25.9438	26.4160	25.9341	26.3685	25.9216	26.3639	25.9571	26.1690	**24.2**
C3`	25.5752	25.7645	26.1378	25.9439	26.4160	25.9341	26.3685	25.9216	26.3639	25.9571	26.1690	25.9688	26.4573	26.8288	26.6445	27.1554	26.6386	27.1839	26.6293	27.1770	26.6532	26.9597	**24.1**
C4`	56.6692	57.8046	58.1645	58.2842	58.8069	58.2616	58.9278	58.2356	58.8673	58.3087	59.1668	52.1500	52.9655	53.2788	53.5431	54.0664	53.5092	54.0666	53.4728	53.9991	53.5797	54.5781	**56.3**
H2	8.7017	8.5820	8.6334	8.5144	8.5224	8.5185	8.5444	8.5222	8.5458	8.5104	8.5311	8.7017	8.5820	8.6334	8.5144	8.5224	8.5185	8.5444	8.5222	8.5458	8.5104	8.5311	**8.2**
H3	7.3180	7.4626	7.5498	7.5093	7.6221	7.5074	7.6437	7.5048	7.6355	7.5111	7.6574	7.3180	7.4626	7.5498	7.5093	7.6221	7.5074	7.6437	7.5048	7.6355	7.5111	7.6574	**7.36**
H5	7.1388	7.2932	7.3946	7.3636	7.4967	7.3596	7.5018	7.3552	7.4932	7.3672	7.5277	7.1388	7.2932	7.3946	7.3636	7.4967	7.3596	7.5018	7.3552	7.4932	7.3672	7.5277	**7.36**
H6	7.9778	8.1585	8.2522	8.2595	8.3785	8.2534	8.4310	8.2468	8.4121	8.2652	8.4587	7.9778	8.1585	8.2522	8.2595	8.3785	8.2534	8.4310	8.2468	8.4121	8.2652	8.4587	**8.2**
H8	4.6221	4.6810	4.7192	4.7261	4.7782	4.7226	4.8173	4.7187	4.8029	4.7294	4.7963	4.6221	4.6810	4.7192	4.7261	4.7782	4.7226	4.8173	4.7187	4.8029	4.7294	4.7963	**5.4**
H(9A-9B)	1.7073	1.7466	1.7566	1.7758	1.8078	1.7740	1.8065	1.7718	1.8013	1.7774	1.8410	1.7073	1.7466	1.7566	1.7758	1.8078	1.7740	1.8065	1.7718	1.8013	1.7774	1.8410	**2.08**
H(10A)	1.0017	0.8584	0.8480	0.8249	0.7364	0.8258	0.7864	0.8263	0.7798	0.8243	0.7913	1.0017	0.8584	0.8480	0.8249	0.7364	0.8258	0.7864	0.8263	0.7798	0.8243	0.7913	**1.14**
H(10B)	1.6621	1.5559	1.4962	1.4782	1.3946	1.4836	1.3899	1.4885	1.3968	1.4731	1.3608	1.6621	1.5559	1.4962	1.4782	1.3946	1.4836	1.3899	1.4885	1.3968	1.4731	1.3608	**1.28**
H(11A-11B)	1.0602	1.0755	1.0472	1.0937	1.0553	1.0929	1.0546	1.0915	1.0540	1.0945	1.0426	1.0602	1.0755	1.0473	1.0937	1.0553	1.0929	1.0547	1.0915	1.0540	1.0945	1.0426	**1.28**
H(12A-12C)	0.9403	0.9279	0.9065	0.9238	0.8835	0.9241	0.8907	0.9241	0.8907	0.9234	0.8830	0.9403	0.9279	0.9065	0.9238	0.8835	0.9241	0.8906	0.9241	0.8907	0.9234	0.8830	**0.82**
H(1`A)	2.7437	2.7364	2.7259	2.7268	2.6858	2.7276	2.7033	2.7279	2.7047	2.7261	2.6669	2.8709	2.8795	2.8646	2.8584	2.8308	2.8605	2.8410	2.8620	2.8446	2.8562	2.8024	**3.38**
H(1`B)	3.2035	3.2527	3.2856	3.2909	3.3575	3.2884	3.3446	3.2855	3.3413	3.2932	3.3404	2.8974	2.7352	2.7069	2.7090	2.7058	2.7093	2.6710	2.7092	2.6722	2.7090	2.6597	**3.71**
H(2`A)	1.6334	1.6786	1.6508	1.6992	1.6443	1.6983	1.6703	1.6969	1.6671	1.7000	1.6804	1.5112	1.5567	1.5297	1.5819	1.5257	1.5806	1.5610	1.5789	1.5558	1.5830	1.5767	**2.08**
H(2`B)	1.8444	1.8602	1.8198	1.9068	1.8596	1.9031	1.8609	1.8991	1.8545	1.9104	1.8866	1.7037	1.8180	1.7727	1.8911	1.8462	1.8867	1.8698	1.8818	1.8605	1.8953	1.9159	**2.24**
H(3`A)	1.5112	1.5567	1.5297	1.5818	1.5257	1.5806	1.5610	1.5789	1.5558	1.5830	1.5767	1.6334	1.6786	1.6507	1.6992	1.6443	1.6983	1.6703	1.6969	1.6671	1.7000	1.6804	**2.08**
H(3`B)	1.7037	1.8180	1.7727	1.8911	1.8462	1.8867	1.8698	1.8818	1.8605	1.8953	1.9159	1.8444	1.8602	1.8198	1.9068	1.8596	1.9031	1.8609	1.8991	1.8545	1.9104	1.8866	**2.16**
H(4`A)	2.8974	2.7352	2.7069	2.7090	2.7058	2.7093	2.6710	2.7092	2.6722	2.7090	2.6597	3.2035	3.2527	3.2855	3.2909	3.3575	3.2884	3.3446	3.2855	3.3413	3.2932	3.3404	**3.09**
H(4`B)	2.8709	2.8795	2.8646	2.8584	2.8308	2.8605	2.8410	2.8620	2.8446	2.8562	2.8024	2.7437	2.7364	2.7259	2.7268	2.6858	2.7276	2.7033	2.7279	2.7047	2.7261	2.6669	**3.68**

[a] methyl protons shifts are averaged
[b] according to [5]

Table S6. Theoretical chemical shifts (in ppm) of *(R,S)*-4-fluoro-α-pyrrolidinohexanophenone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S										Exp. [b]
	B3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.6461	140.7864	141.4058	141.3136	142.6443	141.2719	143.6401	141.2321	143.8057	141.3540	142.2745	139.6461	140.7864	141.4058	141.3136	142.6441	141.2719	143.6401	141.2321	142.2849	141.3540	142.2745	**132.8**
C2	139.5237	139.5283	140.0799	139.4229	139.8550	139.4233	140.6856	139.4245	140.5631	139.4217	140.3689	139.5237	139.5283	140.0799	139.4229	139.8550	139.4235	140.6856	139.4245	140.3254	139.4215	140.3689	**132.9**
C3	122.0016	122.7109	123.2701	122.8762	123.4842	122.8651	123.8294	122.8532	123.7527	122.8848	123.8436	122.0016	122.7109	123.2701	122.8762	123.4843	122.8651	123.8293	122.8532	123.6960	122.8848	123.8436	**117.2**
C4	176.3776	177.2686	177.9231	177.6172	178.2715	177.5929	178.7148	177.5682	178.5305	177.6383	179.0153	176.3776	177.2686	177.9231	177.6172	178.2715	177.5929	178.7149	177.5682	178.7108	177.6383	179.0153	**167.5**
C5	119.9008	121.1508	121.7637	121.7354	122.5277	121.6950	122.8173	121.6548	122.6947	121.7720	122.9044	119.9008	121.1508	121.7637	121.7355	122.5277	121.6952	122.8174	121.6548	122.6376	121.7721	122.9044	**117.2**
C6	135.7284	137.7097	138.8506	138.7726	140.3125	138.7018	140.2739	138.6307	139.9664	138.8376	141.3542	135.7284	137.7097	138.8506	138.7726	140.3125	138.7019	140.2738	138.6307	140.6449	138.8377	141.3542	**132.9**
C7	203.8433	208.7706	209.8361	211.3608	211.9257	211.1952	218.3779	211.0306	217.2932	211.5170	218.0294	203.8433	208.7706	209.8361	211.3607	211.9257	211.1952	218.3780	211.0306	215.9741	211.5172	218.0294	**195.8**
C8	66.5250	67.8264	68.3186	68.2996	69.3467	68.2734	70.0962	68.2461	69.9127	68.3213	70.3036	66.5250	67.8264	68.3186	68.2996	69.3467	68.2734	70.0962	68.2461	69.8306	68.3213	70.3036	**68.4**
C9	37.2783	36.9954	37.1608	36.7912	37.1386	36.7999	36.9134	36.8081	36.8238	36.7803	37.4426	37.2783	36.9954	37.1608	36.7911	37.1386	36.7999	36.9134	36.8081	37.2550	36.7803	37.4426	**30.5**
C10	29.1554	29.7052	30.2009	29.9688	30.7342	29.9463	30.3781	29.9237	30.3314	29.9886	30.6796	29.1554	29.7052	30.2009	29.9690	30.7343	29.9462	30.3780	29.9236	30.5104	29.9887	30.6796	**27.6**
C11	29.2176	29.3890	29.6800	29.3092	29.7544	29.3137	29.7204	29.3173	29.7037	29.3025	29.8834	29.2176	29.3890	29.6801	29.3092	29.7544	29.3137	29.7204	29.3173	29.7502	29.3025	29.8834	**23.1**
C12	16.6743	16.8847	16.9795	16.9675	17.0657	16.9553	17.1035	16.9436	17.0812	16.9780	17.0345	16.6743	16.8847	16.9795	16.9675	17.0657	16.9553	17.1034	16.9436	17.0289	16.9780	17.0345	**13.8**
C1`	52.3408	53.1867	53.5262	53.7049	54.2316	53.6668	54.3062	53.6291	54.2417	53.7402	54.7652	56.8561	58.0291	58.4014	58.4592	58.9820	58.4317	59.1878	58.4037	59.0555	58.4833	59.3691	**53.5**
C2`	26.1882	26.7217	27.0852	26.8508	27.3658	26.8407	27.3737	26.8301	27.3214	26.8583	27.1841	25.8103	26.0266	26.4225	26.1449	26.6169	26.1303	26.7163	26.1161	26.5729	26.1578	26.3817	**24.5**
C3`	25.8103	26.0266	26.4225	26.1449	26.6168	26.1303	26.7163	26.1161	26.6985	26.1577	26.3817	26.1882	26.7217	27.0852	26.8508	27.3658	26.8408	27.3737	26.8301	27.3873	26.8582	27.1841	**24.3**
C4`	56.8561	58.0291	58.4014	58.4593	58.9820	58.4317	59.1878	58.4037	59.0876	58.4834	59.3691	52.3408	53.1867	53.5262	53.7050	54.2316	53.6668	54.3062	53.6290	54.1753	53.7402	54.7652	**57.5**
H2	8.6809	8.5543	8.6087	8.4781	8.4949	8.4829	8.4082	8.4875	8.3955	8.4732	8.5014	8.6809	8.5543	8.6087	8.4781	8.4949	8.4829	8.4082	8.4875	8.4977	8.4732	8.5014	**8.11**
H3	7.3091	7.4552	7.5406	7.4963	7.6103	7.4942	7.6075	7.4919	7.5968	7.4981	7.6474	7.3091	7.4552	7.5406	7.4963	7.6103	7.4942	7.6075	7.4919	7.6192	7.4981	7.6474	**7.31**
H5	7.1276	7.2806	7.3732	7.3462	7.4808	7.3421	7.5147	7.3379	7.5013	7.3498	7.5128	7.1276	7.2806	7.3732	7.3462	7.4808	7.3421	7.5147	7.3379	7.4705	7.3498	7.5128	**7.31**
H6	7.9680	8.1482	8.2416	8.2410	8.3613	8.2351	8.3599	8.2291	8.3335	8.2462	8.4392	7.9680	8.1482	8.2416	8.2410	8.3613	8.2351	8.3599	8.2291	8.3823	8.2462	8.4392	**8.11**
H8	4.6493	4.7076	4.7462	4.7448	4.7972	4.7412	4.8339	4.7377	4.8186	4.7480	4.8140	4.6493	4.7076	4.7462	4.7448	4.7972	4.7412	4.8339	4.7377	4.8162	4.7480	4.8140	**5.18**
H(9A-9B)	1.7031	1.7451	1.7428	1.7658	1.8039	1.7645	1.6855	1.7631	1.6726	1.7666	1.8372	1.7031	1.7451	1.7428	1.7658	1.8039	1.7645	1.6855	1.7631	1.7829	1.7666	1.8372	**2.05**
H(10A)	1.0022	0.8621	0.8587	0.8274	0.7397	0.8276	0.8447	0.8281	0.8427	0.8272	0.7965	1.0022	0.8621	0.8587	0.8274	0.7397	0.8276	0.8447	0.8281	0.7822	0.8272	0.7965	**1.14**
H(10B)	1.6642	1.5565	1.4947	1.4743	1.3918	1.4794	1.3895	1.4845	1.3962	1.4693	1.3592	1.6642	1.5565	1.4947	1.4743	1.3918	1.4794	1.3895	1.4845	1.3901	1.4693	1.3592	**1.39**
H(11A-11B)	1.0615	1.0779	1.0484	1.0922	1.0551	1.0910	1.0592	1.0898	1.0563	1.0931	1.0432	1.0615	1.0779	1.0484	1.0922	1.0551	1.0910	1.0592	1.0898	1.0490	1.0931	1.0432	**1.22**
H(12A-12C)	0.9351	0.9251	0.9017	0.9172	0.8775	0.9172	0.9015	0.9173	0.9005	0.9171	0.8785	0.9351	0.9251	0.9017	0.9172	0.8775	0.9172	0.9015	0.9173	0.8821	0.9171	0.8785	**0.77**
H(1`A)	2.7510	2.7458	2.7299	2.7316	2.6917	2.7321	2.7055	2.7326	2.7038	2.7310	2.6732	2.8761	2.8891	2.8657	2.8618	2.8352	2.8637	2.8372	2.8655	2.8463	2.8598	2.8089	**3.16**
H(1`B)	3.2052	3.2576	3.2845	3.2906	3.3582	3.2880	3.3290	3.2854	3.3214	3.2928	3.3427	2.8957	2.7389	2.7000	2.7100	2.7063	2.7096	2.6874	2.7096	2.6733	2.7104	2.6644	**3.76**
H(2`A-2`B)	1.7393	1.7720	1.7348	1.8012	1.7505	1.7985	1.7710	1.7960	1.7651	1.8036	1.7836	1.6062	1.6895	1.6503	1.7348	1.6836	1.7315	1.7396	1.7282	1.7053	1.7379	1.7453	**2.13**
H(3`A-3`B)	1.6062	1.6895	1.6503	1.7348	1.6836	1.7315	1.7396	1.7282	1.7324	1.7379	1.7453	1.7393	1.7720	1.7348	1.8012	1.7505	1.7985	1.7710	1.7960	1.7564	1.8036	1.7836	**2.05**
H(4`A)	2.8957	2.7389	2.7000	2.7100	2.7062	2.7097	2.6874	2.7096	2.6927	2.7104	2.6644	3.2052	3.2576	3.2845	3.2906	3.3582	3.2880	3.3290	3.2854	3.3378	3.2928	3.3427	**3.09**
H(4`B)	2.8761	2.8891	2.8657	2.8618	2.8352	2.8637	2.8372	2.8655	2.8376	2.8598	2.8089	2.7510	2.7458	2.7299	2.7316	2.6917	2.7321	2.7055	2.7326	2.7068	2.7309	2.6732	**3.63**
F4	-124.8149	-126.3152	-129.0636	-126.5914	-130.9346	-126.5786	-129.2811	-126.5649	-129.6710	-126.6047	-128.4774	-124.8149	-126.3152	-129.0636	-126.5914	-130.9347	-126.5786	-129.2810	-126.5649	-129.1519	-126.6046	-128.4774	**-104.5**
Nuclei	B3P86																						
C1	136.9940	137.7944	138.6085	138.2350	139.7431	138.2382	139.0549	138.2181	139.2253	138.2747	139.3602	136.9940	137.7944	138.6085	138.2350	139.7431	138.2382	139.0549	138.2181	139.2253	138.2747	139.3602	**132.8**
C2	138.4918	138.4799	139.0262	138.3378	138.8680	138.3690	139.3660	138.3780	139.3322	138.3524	139.3371	138.4918	138.4799	139.0263	138.3378	138.8680	138.3690	139.3660	138.3780	139.3322	138.3524	139.3370	**132.9**
C3	121.1824	121.9496	122.5869	122.1830	122.8942	122.1927	123.1872	122.1799	123.2106	122.2177	123.2677	121.1824	121.9496	122.5869	122.1830	122.8942	122.1927	123.1872	122.1799	123.2106	122.2176	123.2677	**117.2**
C4	173.8427	174.7165	175.3771	175.1356	175.7951	175.1315	176.4511	175.1055	176.3855	175.1833	176.5856	173.8427	174.7165	175.3770	175.1356	175.7951	175.1316	176.4509	175.1055	176.3855	175.1833	176.5856	**167.5**
C5	119.1719	120.4985	121.1966	121.1547	122.0481	121.1341	122.2667	121.0918	122.2598	121.2183	122.4439	119.1720	120.4985	121.1966	121.1548	122.0481	121.1341	122.2666	121.0918	122.2598	121.2183	122.4440	**117.2**
C6	134.7482	136.6843	137.8759	137.8221	139.4030	137.7676	140.1213	137.6922	139.9543	137.9183	140.4961	134.7482	136.6843	137.8759	137.8222	139.4030	137.7676	140.1212	137.6922	139.9543	137.9184	140.4961	**132.9**
C7	201.9446	206.3100	207.5577	208.7236	209.4429	208.6038	214.1587	208.4609	213.2041	208.8803	215.2563	201.9446	206.3100	207.5577	208.7236	209.4429	208.6038	214.1587	208.4609	213.2041	208.8803	215.2563	**195.8**
C8	64.8267	65.9499	66.7652	66.4439	67.5035	66.4394	68.0435	66.4121	68.0288	66.4911	68.4972	64.8267	65.9499	66.7652	66.4439	67.5035	66.4394	68.0435	66.4121	68.0288	66.4911	68.4972	**68.4**
C9	36.2486	36.0166	36.3080	35.8772	36.2423	35.9043	36.4484	35.9094	36.4633	35.8954	36.5768	36.2486	36.0166	36.3080	35.8771	36.2423	35.9042	36.4484	35.9094	36.4633	35.8953	36.5768	**30.5**
C10	27.9025	28.4047	28.9185	28.7349	29.4674	28.7300	29.2804	28.7039	29.3529	28.7840	29.4513	27.9025	28.4046	28.9185	28.7349	29.4674	28.7300	29.2804	28.7039	29.3529	28.7840	29.4513	**27.6**
C11	27.6635	27.8017	28.0996	27.7450	28.1783	27.7719	28.1762	27.7764	28.2670	27.7630	28.3209	27.6635	27.8016	28.0997	27.7450	28.1783	27.7718	28.1763	27.7764	28.2670	27.7629	28.3209	**23.1**
C12	16.2632	16.4367	16.5321	16.5461	16.6415	16.5582	16.6066	16.5487	16.6923	16.5790	16.6054	16.2632	16.4367	16.5320	16.5462	16.6415	16.5582	16.6066	16.5487	16.6923	16.5790	16.6054	**13.8**
C1`	51.2290	52.0562	52.3501	52.5739	53.1095	52.5603	53.1155	52.5254	53.1243	52.6314	53.6115	55.5727	56.7173	57.1113	57.1649	57.6791	57.1609	57.8424	57.1348	57.8756	57.2124	58.1048	**53.5**
C2`	24.9726	25.3900	25.7808	25.5444	26.0182	25.5568	26.0360	25.5472	26.1322	25.5763	25.8635	24.4400	24.6560	24.9992	24.8082	25.2508	24.8198	25.2291	24.8094	25.3062	24.8411	25.0933	**24.5**
C3`	24.4400	24.6560	24.9990	24.8081	25.2508	24.8198	25.2291	24.8094	25.3062	24.8410	25.0933	24.9726	25.3900	25.7807	25.5444	26.0182	25.5568	26.0361	25.5472	26.1322	25.5763	25.8636	**24.3**
C4`	55.5727	56.7174	57.1114	57.1649	57.6791	57.1610	57.8424	57.1348	57.8756	57.2124	58.1048	51.2290	52.0562	52.3501	52.5740	53.1095	52.5603	53.1154	52.5254	53.1243	52.6314	53.6115	**57.5**
H2	8.7290	8.6450	8.6624	8.5763	8.5750	8.5811	8.6077	8.5842	8.6051	8.5730	8.5861	8.7290	8.6450	8.6624	8.5763	8.5750	8.5811	8.6077	8.5842	8.6051	8.5730	8.5861	**8.11**
H3	7.3236	7.4766	7.5645	7.5245	7.6430	7.5235	7.6668	7.5205	7.6614	7.5267	7.6840	7.3236	7.4766	7.5645	7.5245	7.6430	7.5234	7.6668	7.5205	7.6614	7.5267	7.6839	**7.31**
H5	7.1584	7.3295	7.4289	7.3944	7.5356	7.3914	7.5373	7.3866	7.5325	7.3986	7.5649	7.1584	7.3295	7.4289	7.3944	7.5356	7.3914	7.5373	7.3866	7.5325	7.3985	7.5649	**7.31**
H6	8.0391	8.2172	8.3003	8.3183	8.4387	8.3130	8.5009	8.3060	8.4828	8.3245	8.5279	8.0391	8.2172	8.3003	8.3183	8.4387	8.3130	8.5009	8.3060	8.4828	8.3245	8.5279	**8.11**
H8	4.6504	4.7081	4.7313	4.7587	4.8048	4.7563	4.8490	4.7522	4.8350	4.7621	4.8465	4.6504	4.7081	4.7313	4.7587	4.8048	4.7563	4.8490	4.7522	4.8350	4.7621	4.8465	**5.18**
H(9A-9B)	1.7737	1.8107	1.8173	1.8361	1.8597	1.8350	1.8591	1.8321	1.8559	1.8386	1.8916	1.7737	1.8107	1.8173	1.8361	1.8597	1.8350	1.8591	1.8321	1.8559	1.8386	1.8916	**2.05**
H(10A)	0.9752	0.8444	0.8027	0.7996	0.7098	0.8026	0.7576	0.8038	0.7475	0.7979	0.7640	0.9752	0.8444	0.8027	0.7996	0.7098	0.8026	0.7576	0.8038	0.7475	0.7979	0.7640	**1.14**
H(10B)	1.6857	1.5846	1.5093	1.4961	1.4096	1.5034	1.4026	1.5090	1.4115	1.4903	1.3722	1.6857	1.5846	1.5093	1.4961	1.4096	1.5034	1.4026	1.5090	1.4115	1.4903	1.3722	**1.39**
H(11A-11B)	1.0296	1.0511	1.0141	1.0605	1.0240	1.0614	1.0238	1.0603	1.0254	1.0611	1.0130	1.0296	1.0511	1.0141	1.0605	1.0240	1.0614	1.0238	1.0603	1.0254	1.0611	1.0130	**1.22**
H(12A-12C)	0.8986	0.8890	0.8627	0.8785	0.8412	0.8804	0.8463	0.8804	0.8493	0.8780	0.8425	0.8986	0.8890	0.8627	0.8785	0.8412	0.8804	0.8463	0.8804	0.8493	0.8780	0.8425	**0.77**
H(1`A)	2.7041	2.6985	2.6865	2.6863	2.6464	2.6882	2.6613	2.6883	2.6657	2.6858	2.6366	2.8371	2.8452	2.8347	2.8253	2.7986	2.8283	2.8066	2.8295	2.8150	2.8235	2.7746	**3.16**
H(1`B)	3.2036	3.2482	3.2821	3.2812	3.3423	3.2798	3.3295	3.2766	3.3304	3.2838	3.3300	2.9405	2.7570	2.7404	2.7125	2.7146	2.7151	2.6633	2.7161	2.6706	2.7113	2.6518	**3.76**
H(2`A-2`B)	1.7239	1.7569	1.7220	1.7865	1.7420	1.7855	1.7525	1.7827	1.7511	1.7888	1.7738	1.5947	1.6704	1.6340	1.7128	1.6684	1.7115	1.6954	1.7083	1.6918	1.7154	1.7333	**2.13**
H(3`A-3`B)	1.5947	1.6704	1.6340	1.7128	1.6684	1.7115	1.6954	1.7083	1.6918	1.7154	1.7333	1.7239	1.7569	1.7220	1.7865	1.7420	1.7855	1.7525	1.7827	1.7511	1.7888	1.7738	**2.05**
H(4`A)	2.9405	2.7570	2.7404	2.7125	2.7146	2.7151	2.6633	2.7161	2.6706	2.7113	2.6518	3.2036	3.2482	3.2821	3.2812	3.3423	3.2797	3.3295	3.2766	3.3304	3.2838	3.3300	**3.09**
H(4`B)	2.8371	2.8452	2.8347	2.8253	2.7986	2.8283	2.8065	2.8295	2.8150	2.8235	2.7746	2.7041	2.6985	2.6865	2.6864	2.6464	2.6882	2.6612	2.6883	2.6657	2.6858	2.6366	**3.63**
F4	-117.3895	-118.3317	-120.9580	-118.3711	-122.4835	-118.3770	-120.1128	-118.3824	-120.5248	-118.3637	-119.8815	-117.3895	-118.3317	-120.9580	-118.3712	-122.4835	-118.3770	-120.1130	-118.3824	-120.5248	-118.3636	-119.8817	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. I

Nuclei	R											S										Exp. [b]
	B3PW91																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.2683	138.3110	139.0251	138.7632	140.5159	138.7452	139.6322	138.7174	139.6500	138.7819	139.7985	137.2684	138.3110	139.0253	138.7632	140.1969	138.7451	139.6321	138.7176	139.6500	138.7819	139.7985	**132.8**
C2	138.6410	138.6605	139.1565	138.5404	139.4008	138.5539	139.5783	138.5587	139.4533	138.5296	139.5357	138.6410	138.6605	139.1563	138.5404	139.0818	138.5541	139.5784	138.5588	139.4534	138.5296	139.5357	**132.9**
C3	121.2594	122.0369	122.5996	122.2518	123.2768	122.2465	123.2362	122.2321	123.1632	122.2587	123.3253	121.2594	122.0369	122.5996	122.2518	122.9578	122.2466	123.2362	122.2321	123.1632	122.2587	123.3253	**117.2**
C4	173.9083	174.7882	175.3849	175.1648	176.1478	175.1468	176.4418	175.1200	176.2919	175.1841	176.5909	173.9084	174.7882	175.3847	175.1648	175.8288	175.1467	176.4417	175.1199	176.2919	175.1841	176.5909	**167.5**
C5	119.2542	120.5663	121.1995	121.2079	122.4095	121.1729	122.3091	121.1291	122.2069	121.2432	122.4865	119.2542	120.5663	121.1995	121.2079	122.0905	121.1728	122.3091	121.1291	122.2069	121.2432	122.4865	**117.2**
C6	134.7732	136.7237	137.8161	137.8284	139.7082	137.7607	140.0363	137.6852	139.7917	137.8952	140.4527	134.7731	136.7237	137.8164	137.8284	139.3892	137.7607	140.0362	137.6852	139.7918	137.8952	140.4527	**132.9**
C7	201.9625	206.6067	207.7419	209.0508	209.9966	208.9099	214.5826	208.7599	213.4600	209.1857	215.5648	201.9625	206.6067	207.7420	209.0508	209.6776	208.9099	214.5827	208.7599	213.4600	209.1857	215.5648	**195.8**
C8	64.7955	66.0465	66.7422	66.5611	67.8989	66.5428	68.2177	66.5141	68.0546	66.5791	68.5848	64.7955	66.0465	66.7421	66.5611	67.5799	66.5427	68.2177	66.5142	68.0547	66.5791	68.5848	**68.4**
C9	35.8212	35.6167	35.7953	35.4785	36.1538	35.4920	36.0457	35.4963	35.9670	35.4673	36.1611	35.8211	35.6167	35.7953	35.4785	35.8348	35.4919	36.0457	35.4963	35.9670	35.4673	36.1611	**30.5**
C10	27.6048	28.1256	28.5599	28.4339	29.4841	28.4158	28.9652	28.3894	28.9490	28.4536	29.1548	27.6048	28.1256	28.5601	28.4339	29.1651	28.4157	28.9652	28.3894	28.9490	28.4536	29.1548	**27.6**
C11	27.6205	27.7953	28.0026	27.7348	28.4759	27.7465	28.1492	27.7489	28.1449	27.7251	28.2980	27.6204	27.7953	28.0026	27.7347	28.1569	27.7465	28.1494	27.7489	28.1449	27.7251	28.2980	**23.1**
C12	16.2867	16.4838	16.5092	16.5803	16.9882	16.5767	16.6234	16.5648	16.6184	16.5862	16.6291	16.2866	16.4838	16.5092	16.5803	16.6692	16.5768	16.6233	16.5649	16.6184	16.5862	16.6291	**13.8**
C1`	51.1535	52.0040	52.2161	52.5029	53.3437	52.4743	53.0216	52.4374	52.9376	52.5328	53.5322	55.5036	56.6599	56.9753	57.0912	57.5895	57.0723	57.7369	57.0442	57.6754	57.1109	57.9949	**53.5**
C2`	25.2271	25.6707	25.9838	25.8063	26.5923	25.8042	26.2842	25.7931	26.2820	25.8101	26.0751	24.7121	24.9298	25.2094	25.0583	25.5027	25.0537	25.4471	25.0406	25.4422	25.0649	25.2887	**24.5**
C3`	24.7122	24.9298	25.2095	25.0584	25.8217	25.0538	25.4471	25.0407	25.4422	25.0649	25.2887	25.2272	25.6707	25.9838	25.8063	26.2733	25.8042	26.2842	25.7932	26.2820	25.8101	26.0751	**24.3**
C4`	55.5037	56.6599	56.9752	57.0912	57.9085	57.0722	57.7369	57.0442	57.6754	57.1109	57.9949	51.1535	52.0040	52.2161	52.5029	53.0247	52.4742	53.0217	52.4375	52.9376	52.5328	53.5322	**57.5**
H2	8.7062	8.5966	8.6228	8.5283	8.5523	8.5326	8.5570	8.5368	8.5576	8.5243	8.5484	8.7062	8.5966	8.6228	8.5283	8.5368	8.5326	8.5570	8.5368	8.5576	8.5243	8.5484	**8.11**
H3	7.3295	7.4785	7.5672	7.5237	7.6568	7.5220	7.6646	7.5199	7.6557	7.5254	7.6799	7.3295	7.4785	7.5672	7.5237	7.6413	7.5220	7.6646	7.5199	7.6557	7.5254	7.6799	**7.31**
H5	7.1489	7.3105	7.4083	7.3811	7.5343	7.3773	7.5250	7.3732	7.5160	7.3848	7.5528	7.1489	7.3105	7.4082	7.3811	7.5188	7.3773	7.5250	7.3732	7.5160	7.3848	7.5528	**7.31**
H6	8.0298	8.2071	8.2903	8.3046	8.4406	8.2988	8.4763	8.2927	8.4580	8.3103	8.5083	8.0298	8.2071	8.2903	8.3046	8.4251	8.2988	8.4763	8.2927	8.4580	8.3103	8.5083	**8.11**
H8	4.6458	4.7027	4.7242	4.7494	4.8097	4.7462	4.8338	4.7427	4.8182	4.7527	4.8284	4.6458	4.7027	4.7242	4.7494	4.7942	4.7462	4.8338	4.7427	4.8182	4.7527	4.8284	**5.18**
H(9A-9B)	1.7271	1.7604	1.7647	1.7862	1.8281	1.7847	1.8116	1.7831	1.8058	1.7877	1.8467	1.7270	1.7604	1.7647	1.7862	1.8126	1.7847	1.8115	1.7831	1.8058	1.7877	1.8467	**2.05**
H(10A)	0.9509	0.8160	0.7754	0.7757	0.7042	0.7773	0.7328	0.7788	0.7236	0.7745	0.7414	0.9509	0.8160	0.7754	0.7757	0.6887	0.7773	0.7328	0.7788	0.7236	0.7745	0.7414	**1.14**
H(10B)	1.6448	1.5409	1.4720	1.4568	1.3876	1.4629	1.3662	1.4686	1.3723	1.4513	1.3371	1.6448	1.5409	1.4720	1.4568	1.3721	1.4629	1.3661	1.4686	1.3723	1.4513	1.3371	**1.39**
H(11A-11B)	1.0151	1.0327	0.9969	1.0448	1.0240	1.0446	1.0073	1.0441	1.0064	1.0451	0.9964	1.0151	1.0327	0.9969	1.0448	1.0085	1.0446	1.0074	1.0441	1.0064	1.0451	0.9964	**1.22**
H(12A-12C)	0.8895	0.8782	0.8516	0.8692	0.8460	0.8701	0.8372	0.8709	0.8369	0.8685	0.8312	0.8895	0.8782	0.8516	0.8692	0.8306	0.8701	0.8372	0.8709	0.8369	0.8685	0.8312	**0.77**
H(1`A)	2.6965	2.6898	2.6781	2.6782	2.6537	2.6793	2.6560	2.6801	2.6567	2.6772	2.6259	2.8310	2.8358	2.8235	2.8145	2.7855	2.8167	2.7978	2.8187	2.8011	2.8123	2.7614	**3.16**
H(1`B)	3.1800	3.2261	3.2593	3.2607	3.3370	3.2586	3.3106	3.2563	3.3077	3.2628	3.3078	2.8932	2.7251	2.7090	2.6878	2.6888	2.6892	2.6489	2.6905	2.6501	2.6868	2.6322	**3.76**
H(2`A-2`B)	1.7102	1.7429	1.7077	1.7729	1.7417	1.7711	1.7394	1.7690	1.7343	1.7749	1.7585	1.5847	1.6616	1.6246	1.7053	1.6572	1.7029	1.6883	1.7004	1.6796	1.7077	1.7213	**2.13**
H(3`A-3`B)	1.5847	1.6616	1.6246	1.7053	1.6727	1.7030	1.6883	1.7004	1.6796	1.7077	1.7213	1.7102	1.7429	1.7077	1.7729	1.7262	1.7711	1.7394	1.7690	1.7343	1.7749	1.7585	**2.05**
H(4`A)	2.8932	2.7251	2.7090	2.6878	2.7043	2.6892	2.6488	2.6905	2.6501	2.6868	2.6322	3.1800	3.2261	3.2593	3.2607	3.3215	3.2586	3.3107	3.2563	3.3077	3.2628	3.3078	**3.09**
H(4`B)	2.8310	2.8358	2.8235	2.8145	2.8010	2.8168	2.7978	2.8186	2.8010	2.8123	2.7614	2.6964	2.6898	2.6781	2.6782	2.6382	2.6793	2.6560	2.6801	2.6567	2.6772	2.6259	**3.63**
F4	-116.7959	-117.9095	-120.5427	-118.0094	-120.9748	-118.0111	-119.8565	-118.0120	-120.2252	-118.0064	-119.5682	-116.7958	-117.9095	-120.5429	-118.0094	-122.1115	-118.0112	-119.8566	-118.0121	-120.2252	-118.0064	-119.5682	**-104.5**
Nuclei	B98																						
C1	138.2717	139.2268	139.9128	139.6404	141.1346	139.6354	140.5187	139.6273	140.5521	139.6471	140.7148	138.2716	139.2268	139.9128	139.6403	141.1346	139.6354	140.5187	139.6273	140.5521	139.6471	140.7148	**132.8**
C2	138.3658	138.4130	138.9400	138.2863	138.8240	138.3104	139.3230	138.3318	139.2146	138.2658	139.2706	138.3659	138.4130	138.9400	138.2864	138.8240	138.3104	139.3230	138.3318	139.2146	138.2658	139.2706	**132.9**
C3	120.9842	121.7099	122.2670	121.9312	122.6018	121.9357	122.8713	121.9373	122.8035	121.9289	122.9366	120.9842	121.7099	122.2670	121.9312	122.6018	121.9357	122.8714	121.9373	122.8035	121.9289	122.9366	**117.2**
C4	173.7110	174.5345	175.1530	174.9251	175.5881	174.9164	176.1881	174.9052	176.0450	174.9356	176.3122	173.7110	174.5345	175.1529	174.9250	175.5881	174.9164	176.1881	174.9052	176.0450	174.9356	176.3121	**167.5**
C5	118.9649	120.2115	120.8309	120.8532	121.6929	120.8287	121.9059	120.8015	121.8085	120.8789	122.0628	118.9649	120.2115	120.8308	120.8531	121.6929	120.8287	121.9058	120.8015	121.8086	120.8789	122.0628	**117.2**
C6	134.7148	136.5886	137.6963	137.6945	139.2264	137.6373	139.8807	137.5782	139.6376	137.7516	140.2548	134.7148	136.5886	137.6962	137.6945	139.2264	137.6373	139.8805	137.5782	139.6376	137.7516	140.2547	**132.9**
C7	200.3965	205.1270	206.2286	207.6183	208.2481	207.4848	213.3382	207.3483	212.1534	207.7463	214.3728	200.3966	205.1270	206.2283	207.6181	208.2481	207.4848	213.3381	207.3483	212.1534	207.7463	214.3729	**195.8**
C8	66.4517	67.6676	68.3328	68.1491	69.2093	68.1435	69.8344	68.1334	69.6562	68.1551	70.2146	66.4518	67.6676	68.3327	68.1492	69.2093	68.1435	69.8344	68.1334	69.6562	68.1551	70.2145	**68.4**
C9	37.0176	36.7658	36.9738	36.6486	37.0069	36.6711	37.2536	36.6906	37.1768	36.6290	37.3166	37.0176	36.7658	36.9738	36.6487	37.0069	36.6711	37.2535	36.6906	37.1768	36.6290	37.3166	**30.5**
C10	29.0963	29.5633	30.0409	29.8649	30.6136	29.8578	30.4248	29.8488	30.4145	29.8742	30.5904	29.0963	29.5633	30.0409	29.8648	30.6136	29.8578	30.4248	29.8488	30.4145	29.8742	30.5904	**27.6**
C11	28.9406	29.0642	29.3038	29.0121	29.4482	29.0334	29.4500	29.0515	29.4499	28.9937	29.5766	28.9406	29.0642	29.3037	29.0122	29.4482	29.0334	29.4499	29.0515	29.4499	28.9937	29.5766	**23.1**
C12	16.8660	17.0178	17.0824	17.1275	17.2327	17.1333	17.1960	17.1370	17.1978	17.1247	17.1872	16.8660	17.0178	17.0824	17.1275	17.2327	17.1333	17.1960	17.1370	17.1978	17.1247	17.1871	**13.8**
C1`	52.4335	53.2373	53.4722	53.7447	54.2542	53.7251	54.2559	53.7037	54.1881	53.7667	54.7388	56.8881	57.9505	58.2822	58.3585	58.8726	58.3505	59.0149	58.3396	58.9555	58.3681	59.2730	**53.5**
C2`	26.4056	26.8263	27.1611	26.9646	27.4451	26.9719	27.4788	26.9766	27.4727	26.9593	27.2819	25.8949	26.0922	26.4234	26.2448	26.6989	26.2484	26.6621	26.2500	26.6634	26.2440	26.4925	**24.5**
C3`	25.8950	26.0922	26.4233	26.2448	26.6989	26.2484	26.6622	26.2500	26.6634	26.2440	26.4925	26.4056	26.8263	27.1611	26.9645	27.4451	26.9719	27.4788	26.9766	27.4727	26.9593	27.2819	**24.3**
C4`	56.8881	57.9505	58.2822	58.3585	58.8726	58.3505	59.0149	58.3396	58.9555	58.3681	59.2731	52.4335	53.2373	53.4723	53.7448	54.2542	53.7251	54.2559	53.7037	54.1881	53.7667	54.7388	**57.5**
H2	8.6982	8.5886	8.6267	8.5270	8.5364	8.5306	8.5595	8.5343	8.5625	8.5239	8.5476	8.6982	8.5886	8.6267	8.5270	8.5364	8.5306	8.5595	8.5343	8.5625	8.5239	8.5476	**8.11**
H3	7.3243	7.4676	7.5579	7.5131	7.6334	7.5110	7.6550	7.5089	7.6467	7.5153	7.6698	7.3243	7.4676	7.5579	7.5131	7.6334	7.5110	7.6550	7.5089	7.6467	7.5153	7.6698	**7.31**
H5	7.1440	7.3083	7.4061	7.3810	7.5164	7.3767	7.5244	7.3726	7.5150	7.3852	7.5500	7.1439	7.3083	7.4061	7.3810	7.5164	7.3767	7.5244	7.3726	7.5150	7.3852	7.5500	**7.31**
H6	7.9991	8.1757	8.2656	8.2788	8.3991	8.2722	8.4528	8.2658	8.4346	8.2852	8.4806	7.9991	8.1757	8.2656	8.2788	8.3991	8.2722	8.4528	8.2658	8.4346	8.2852	8.4806	**8.11**
H8	4.6061	4.6605	4.6938	4.7112	4.7597	4.7072	4.8012	4.7034	4.7869	4.7153	4.7909	4.6061	4.6605	4.6938	4.7112	4.7597	4.7072	4.8012	4.7034	4.7869	4.7153	4.7909	**5.18**
H(9A-9B)	1.7078	1.7440	1.7500	1.7713	1.8003	1.7695	1.8017	1.7677	1.7957	1.7733	1.8332	1.7078	1.7440	1.7500	1.7713	1.8003	1.7695	1.8016	1.7677	1.7957	1.7733	1.8332	**2.05**
H(10A)	1.0100	0.8556	0.8250	0.8148	0.7317	0.8159	0.7784	0.8174	0.7740	0.8141	0.7819	1.0100	0.8556	0.8250	0.8147	0.7317	0.8159	0.7784	0.8174	0.7740	0.8141	0.7819	**1.14**
H(10B)	1.6566	1.5552	1.4953	1.4723	1.3892	1.4780	1.3847	1.4837	1.3917	1.4673	1.3576	1.6566	1.5552	1.4953	1.4723	1.3892	1.4780	1.3847	1.4837	1.3917	1.4673	1.3576	**1.39**
H(11A-11B)	1.0408	1.0554	1.0229	1.0697	1.0330	1.0689	1.0321	1.0683	1.0319	1.0707	1.0208	1.0408	1.0554	1.0229	1.0697	1.0330	1.0689	1.0321	1.0683	1.0319	1.0707	1.0208	**1.22**
H(12A-12C)	0.9137	0.8998	0.8755	0.8914	0.8528	0.8919	0.8600	0.8926	0.8602	0.8913	0.8544	0.9137	0.8998	0.8755	0.8914	0.8528	0.8919	0.8600	0.8926	0.8602	0.8913	0.8544	**0.77**
H(1`A)	2.7147	2.7096	2.6996	2.6998	2.6606	2.7004	2.6788	2.7011	2.6801	2.6994	2.6440	2.8444	2.8541	2.8420	2.8323	2.8064	2.8344	2.8190	2.8364	2.8217	2.8306	2.7831	**3.16**
H(1`B)	3.1966	3.2429	3.2781	3.2791	3.3414	3.2766	3.3292	3.2742	3.3264	3.2818	3.3230	2.8921	2.7320	2.7168	2.7042	2.7055	2.7047	2.6717	2.7055	2.6724	2.7042	2.6580	**3.76**
H(2`A-2`B)	1.7273	1.7581	1.7234	1.7904	1.7425	1.7881	1.7566	1.7859	1.7516	1.7931	1.7748	1.5089	1.5555	1.5281	1.5780	1.5262	1.5768	1.5620	1.5757	1.5564	1.5793	1.5795	**2.13**
H(3`A-3`B)	1.6066	1.6841	1.6466	1.7277	1.6794	1.7250	1.7102	1.7224	1.7022	1.7305	1.7444	1.6688	1.7455	1.7074	1.7868	1.7390	1.7842	1.7647	1.7818	1.7578	1.7895	1.7959	**2.05**
H(4`A)	2.8922	2.7320	2.7168	2.7042	2.7055	2.7047	2.6717	2.7055	2.6724	2.7042	2.6580	2.5089	2.5405	2.5376	2.5819	2.5905	2.5787	2.5856	2.5757	2.5811	2.5853	2.5952	**3.09**
H(4`B)	2.8444	2.8541	2.8420	2.8323	2.8064	2.8344	2.8190	2.8364	2.8217	2.8306	2.7831	2.7147	2.7096	2.6996	2.6998	2.6606	2.7004	2.6788	2.7011	2.6801	2.6994	2.6440	**3.63**
F4	-119.9176	-121.0442	-123.7574	-121.1149	-125.3354	-121.1187	-123.1429	-121.1210	-123.5029	-121.1108	-122.8648	-119.9177	-121.0442	-123.7575	-121.1149	-125.3354	-121.1187	-123.1431	-121.1210	-123.5029	-121.1108	-122.8649	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. II

Nuclei	R											S										Exp. [b]
	B971											B971										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.8422	138.7483	139.4242	139.1819	140.7120	139.1719	140.0612	139.1604	140.1037	139.1965	140.2855	137.8422	138.7484	139.4242	139.1821	140.7120	139.1719	140.0613	139.1604	140.1037	139.1965	140.2855	**132.8**
C2	138.0799	138.1325	138.6399	138.0013	138.5299	138.0181	139.0158	138.0344	138.9092	137.9914	138.9727	138.0799	138.1323	138.6399	138.0013	138.5299	138.0181	139.0159	138.0344	138.9092	137.9914	138.9727	**132.9**
C3	120.7944	121.5215	122.0745	121.7507	122.4133	121.7473	122.6794	121.7430	122.6120	121.7596	122.7491	120.7944	121.5213	122.0745	121.7507	122.4133	121.7473	122.6794	121.7430	122.6119	121.7596	122.7491	**117.2**
C4	173.5971	174.4353	175.0465	174.8429	175.4966	174.8257	176.0952	174.8081	175.9514	174.8650	176.2233	173.5971	174.4353	175.0464	174.8427	175.4966	174.8257	176.0951	174.8081	175.9514	174.8650	176.2233	**167.5**
C5	118.7655	120.0340	120.6434	120.6887	121.5173	120.6557	121.7292	120.6223	121.6310	120.7260	121.8918	118.7655	120.0341	120.6435	120.6887	121.5173	120.6557	121.7293	120.6223	121.6311	120.7260	121.8918	**117.2**
C6	134.4339	136.3104	137.4295	137.4298	138.9589	137.3639	139.6148	137.2980	139.3694	137.4992	139.9897	134.4339	136.3105	137.4296	137.4299	138.9589	137.3638	139.6149	137.2980	139.3693	137.4992	139.9897	**132.9**
C7	200.2729	204.9044	206.0061	207.3978	208.0832	207.2601	213.0559	207.1201	211.9008	207.5342	214.1161	200.2729	204.9043	206.0060	207.3982	208.0832	207.2600	213.0562	207.1201	211.9008	207.5342	214.1161	**195.8**
C8	66.2684	67.4430	68.1355	67.9281	69.0012	67.9149	69.5789	67.8993	69.4095	67.9447	69.9754	66.2684	67.4428	68.1355	67.9282	69.0012	67.9149	69.5789	67.8993	69.4094	67.9447	69.9754	**68.4**
C9	37.0068	36.7745	37.0004	36.6683	37.0130	36.6820	37.2582	36.6949	37.1794	36.6609	37.3381	37.0068	36.7745	37.0004	36.6683	37.0130	36.6820	37.2583	36.6949	37.1793	36.6609	37.3381	**30.5**
C10	29.1505	29.6168	30.0966	29.9276	30.6566	29.9120	30.4719	29.8963	30.4604	29.9491	30.6448	29.1505	29.6167	30.0966	29.9277	30.6566	29.9120	30.4718	29.8963	30.4603	29.9491	30.6448	**27.6**
C11	28.9245	29.0484	29.2800	29.0001	29.4237	29.0135	29.4199	29.0260	29.4191	28.9929	29.5535	28.9245	29.0484	29.2800	29.0002	29.4237	29.0136	29.4199	29.0260	29.4191	28.9929	29.5535	**23.1**
C12	16.8110	16.9684	17.0237	17.0860	17.1770	17.0840	17.1383	17.0818	17.1401	17.0943	17.1357	16.8110	16.9683	17.0236	17.0860	17.1770	17.0840	17.1384	17.0818	17.1402	17.0943	17.1357	**13.8**
C1`	52.3547	53.1528	53.3732	53.6664	54.1692	53.6388	54.1635	53.6114	54.0937	53.6995	54.6432	56.7953	57.8551	58.1732	58.2702	58.7717	58.2546	58.9084	58.2381	58.8505	58.2908	59.1676	**53.5**
C2`	26.2113	26.6404	26.9708	26.7933	27.2590	26.7924	27.2868	26.7908	27.2809	26.7996	27.1109	25.6996	25.9076	26.2264	26.0756	26.5176	26.0712	26.4850	26.0668	26.4842	26.0859	26.3418	**24.5**
C3`	25.6996	25.9075	26.2264	26.0756	26.5176	26.0712	26.4850	26.0668	26.4841	26.0859	26.3418	26.2113	26.6403	26.9708	26.7933	27.2590	26.7924	27.2869	26.7908	27.2809	26.7996	27.1109	**24.3**
C4`	56.7953	57.8551	58.1732	58.2702	58.7717	58.2546	58.9084	58.2381	58.8505	58.2908	59.1676	52.3547	53.1529	53.3732	53.6663	54.1692	53.6387	54.1636	53.6114	54.0938	53.6995	54.6432	**57.5**
H2	8.6975	8.5947	8.6294	8.5328	8.5358	8.5359	8.5631	8.5392	8.5649	8.5303	8.5487	8.6975	8.5947	8.6294	8.5328	8.5358	8.5359	8.5631	8.5392	8.5649	8.5303	8.5487	**8.11**
H3	7.3205	7.4628	7.5522	7.5095	7.6286	7.5072	7.6504	7.5050	7.6421	7.5121	7.6648	7.3205	7.4628	7.5522	7.5095	7.6286	7.5072	7.6504	7.5050	7.6421	7.5121	7.6648	**7.31**
H5	7.1452	7.3121	7.4102	7.3844	7.5179	7.3799	7.5258	7.3755	7.5164	7.3890	7.5509	7.1452	7.3121	7.4102	7.3844	7.5179	7.3799	7.5258	7.3755	7.5164	7.3890	7.5509	**7.31**
H6	8.0058	8.1773	8.2674	8.2802	8.3987	8.2735	8.4538	8.2669	8.4356	8.2870	8.4802	8.0058	8.1773	8.2674	8.2802	8.3987	8.2735	8.4538	8.2669	8.4356	8.2870	8.4802	**8.11**
H8	4.6088	4.6617	4.6949	4.7134	4.7602	4.7093	4.8019	4.7054	4.7882	4.7177	4.7919	4.6088	4.6617	4.6949	4.7134	4.7602	4.7093	4.8019	4.7054	4.7882	4.7177	4.7919	**5.18**
H(9A-9B)	1.7161	1.7513	1.7594	1.7791	1.8050	1.7769	1.8071	1.7747	1.8006	1.7817	1.8378	1.7161	1.7513	1.7594	1.7791	1.8050	1.7769	1.8071	1.7747	1.8006	1.7817	1.8378	**2.05**
H(10A)	1.0061	0.8545	0.8220	0.8136	0.7285	0.8147	0.7778	0.8160	0.7734	0.8131	0.7805	1.0061	0.8545	0.8220	0.8136	0.7285	0.8147	0.7778	0.8160	0.7734	0.8131	0.7805	**1.14**
H(10B)	1.6552	1.5553	1.4937	1.4723	1.3892	1.4778	1.3845	1.4833	1.3914	1.4676	1.3570	1.6552	1.5553	1.4937	1.4723	1.3892	1.4778	1.3845	1.4833	1.3914	1.4676	1.3570	**1.39**
H(11A-11B)	1.0394	1.0539	1.0204	1.0676	1.0299	1.0668	1.0293	1.0659	1.0291	1.0689	1.0176	1.0394	1.0540	1.0204	1.0676	1.0299	1.0668	1.0293	1.0659	1.0291	1.0689	1.0176	**1.22**
H(12A-12C)	0.9080	0.8931	0.8684	0.8850	0.8458	0.8853	0.8530	0.8857	0.8533	0.8851	0.8480	0.9080	0.8930	0.8684	0.8850	0.8458	0.8853	0.8531	0.8857	0.8533	0.8851	0.8480	**0.77**
H(1`A)	2.7043	2.6996	2.6902	2.6911	2.6510	2.6915	2.6684	2.6920	2.6698	2.6911	2.6344	2.8345	2.8453	2.8343	2.8262	2.8010	2.8280	2.8117	2.8297	2.8145	2.8248	2.7764	**3.16**
H(1`B)	3.1997	3.2445	3.2806	3.2807	3.3411	3.2780	3.3284	3.2754	3.3259	3.2838	3.3220	2.8940	2.7339	2.7203	2.7054	2.7063	2.7059	2.6706	2.7066	2.6719	2.7055	2.6571	**3.76**
H(2`A-2`B)	1.7257	1.7567	1.7217	1.7895	1.7414	1.7870	1.7551	1.7846	1.7502	1.7924	1.7737	1.6056	1.6804	1.6425	1.7247	1.6775	1.7219	1.7071	1.7192	1.6994	1.7278	1.7414	**2.13**
H(3`A-3`B)	1.6056	1.6804	1.6425	1.7247	1.6775	1.7219	1.7071	1.7192	1.6994	1.7278	1.7414	1.7257	1.7567	1.7218	1.7895	1.7414	1.7870	1.7551	1.7846	1.7502	1.7924	1.7737	**2.05**
H(4`A)	2.8940	2.7339	2.7202	2.7054	2.7063	2.7059	2.6706	2.7066	2.6719	2.7055	2.6571	3.1997	3.2445	3.2806	3.2807	3.3411	3.2780	3.3285	3.2754	3.3259	3.2838	3.3220	**3.09**
H(4`B)	2.8345	2.8453	2.8343	2.8262	2.8010	2.8280	2.8117	2.8297	2.8145	2.8248	2.7764	2.7043	2.6996	2.6902	2.6911	2.6510	2.6915	2.6684	2.6920	2.6698	2.6911	2.6344	**3.63**
F4	-120.5398	-121.6484	-124.3709	-121.7179	-125.9690	-121.7225	-123.7522	-121.7262	-124.1160	-121.7121	-123.4809	-120.5398	-121.6485	-124.3711	-121.7180	-125.9690	-121.7225	-123.7523	-121.7262	-124.1161	-121.7121	-123.4809	**-104.5**
Nuclei	B972											B972										
C1	134.6971	135.8753	136.6169	136.6760	139.5533	136.6202	138.6512	136.5674	138.8176	136.7300	138.9783	134.6971	135.8753	136.6169	136.6759	139.5532	136.6203	138.6511	136.5674	138.8176	136.7300	138.9784	**132.8**
C2	136.1423	136.0686	136.6110	136.0524	136.6697	136.0535	137.1061	136.0530	137.0015	136.0477	137.0908	136.1423	136.0686	136.6111	136.0522	136.6695	136.0535	137.1058	136.0530	137.0015	136.0477	137.0908	**132.9**
C3	118.6863	119.3715	119.9318	119.6489	120.3301	119.6370	120.5956	119.6220	120.5384	119.6557	120.6719	118.6863	119.3715	119.9318	119.6490	120.3300	119.6370	120.5956	119.6220	120.5384	119.6557	120.6718	**117.2**
C4	170.5935	171.3556	171.9651	171.7320	172.1420	171.7133	172.7626	171.6911	172.6048	171.7444	172.8736	170.5934	171.3556	171.9650	171.7319	172.1420	171.7133	172.7627	171.6911	172.6048	171.7444	172.8736	**167.5**
C5	116.6790	117.8768	118.5101	118.5696	119.3676	118.5275	119.6225	118.4831	119.5235	118.6058	119.7745	116.6790	117.8768	118.5101	118.5698	119.3676	118.5275	119.6226	118.4831	119.5236	118.6058	119.7746	**117.2**
C6	132.2209	134.0034	135.0675	135.0035	135.8136	134.9461	136.4690	134.8843	136.2020	135.0514	136.7295	132.2209	134.0034	135.0674	135.0036	135.8136	134.9461	136.4689	134.8843	136.2019	135.0514	136.7297	**132.9**
C7	197.8670	202.6198	203.7484	205.3519	207.1219	205.1793	211.9055	205.0088	210.8523	205.5163	213.0007	197.8670	202.6198	203.7482	205.3522	207.1219	205.1793	211.9055	205.0088	210.8523	205.5163	213.0007	**195.8**
C8	63.5056	64.8160	65.4994	65.4760	66.7506	65.4415	67.2458	65.4046	67.0801	65.5049	67.6571	63.5056	64.8160	65.4994	65.4761	66.7505	65.4415	67.2458	65.4046	67.0801	65.5049	67.6571	**68.4**
C9	35.1659	34.9077	35.1070	34.8130	34.8409	34.8226	35.0047	34.8285	34.9106	34.7984	35.0884	35.1659	34.9077	35.1070	34.8131	34.8409	34.8226	35.0047	34.8285	34.9107	34.7984	35.0884	**30.5**
C10	27.4347	27.9105	28.3498	28.2459	28.8451	28.2248	28.6389	28.2010	28.6128	28.2615	28.8073	27.4347	27.9105	28.3499	28.2459	28.8452	28.2247	28.6389	28.2010	28.6128	28.2615	28.8074	**27.6**
C11	27.6676	27.7939	28.0328	27.8076	28.1669	27.8114	28.1400	27.8123	28.1369	27.7989	28.2738	27.6676	27.7939	28.0327	27.8075	28.1669	27.8114	28.1400	27.8123	28.1370	27.7989	28.2739	**23.1**
C12	16.4210	16.5676	16.6312	16.7389	16.8296	16.7272	16.8016	16.7136	16.8013	16.7461	16.8064	16.4210	16.5676	16.6312	16.7389	16.8296	16.7272	16.8016	16.7136	16.8013	16.7461	16.8064	**13.8**
C1`	50.3513	51.1355	51.3757	51.6819	52.1647	51.6473	52.1659	51.6111	52.1124	51.7109	52.6598	54.6831	55.7368	56.0738	56.2267	56.7429	56.2006	56.8535	56.1716	56.7908	56.2470	57.1038	**53.5**
C2`	25.1575	25.5809	25.9072	25.7805	26.1941	25.7710	26.2013	25.7588	26.1797	25.7847	25.9870	24.6675	24.8374	25.1474	25.0423	25.5381	25.0287	25.4907	25.0134	25.4932	25.0513	25.2788	**24.5**
C3`	24.6675	24.8374	25.1475	25.0423	25.5380	25.0287	25.4907	25.0134	25.4932	25.0513	25.2788	25.1574	25.5809	25.9072	25.7806	26.1941	25.7710	26.2013	25.7588	26.1797	25.7847	25.9870	**24.3**
C4`	54.6830	55.7368	56.0739	56.2268	56.7429	56.2006	56.8535	56.1716	56.7908	56.2470	57.1039	50.3513	51.1355	51.3758	51.6818	52.1647	51.6473	52.1659	51.6111	52.1125	51.7109	52.6599	**57.5**
H2	8.7007	8.5592	8.5908	8.4663	8.3592	8.4728	8.4141	8.4787	8.4039	8.4595	8.3953	8.7007	8.5592	8.5908	8.4663	8.3592	8.4728	8.4141	8.4787	8.4039	8.4595	8.3953	**8.11**
H3	7.3297	7.4738	7.5631	7.5139	7.6078	7.5126	7.6304	7.5107	7.6217	7.5149	7.6457	7.3297	7.4738	7.5631	7.5139	7.6078	7.5126	7.6304	7.5107	7.6217	7.5149	7.6457	**7.31**
H5	7.1325	7.2902	7.3841	7.3696	7.5156	7.3646	7.5407	7.3595	7.5307	7.3743	7.5618	7.1325	7.2902	7.3841	7.3696	7.5156	7.3646	7.5407	7.3595	7.5307	7.3743	7.5618	**7.31**
H6	8.0154	8.1828	8.2635	8.2621	8.3160	8.2580	8.3752	8.2534	8.3539	8.2656	8.3870	8.0154	8.1828	8.2635	8.2622	8.3160	8.2580	8.3752	8.2534	8.3539	8.2656	8.3870	**8.11**
H8	4.6168	4.6642	4.6860	4.7066	4.7485	4.7037	4.7874	4.7006	4.7743	4.7091	4.7672	4.6168	4.6642	4.6860	4.7066	4.7485	4.7037	4.7874	4.7006	4.7743	4.7091	4.7672	**5.18**
H(9A-9B)	1.6879	1.7170	1.7219	1.7279	1.6637	1.7278	1.6700	1.7273	1.6567	1.7274	1.7027	1.6879	1.7170	1.7218	1.7279	1.6637	1.7278	1.6700	1.7273	1.6567	1.7274	1.7027	**2.05**
H(10A)	0.9637	0.8246	0.7814	0.7958	0.7462	0.7959	0.7971	0.7962	0.7959	0.7958	0.8043	0.9637	0.8246	0.7814	0.7958	0.7462	0.7959	0.7971	0.7962	0.7959	0.7958	0.8043	**1.14**
H(10B)	1.6217	1.5183	1.4590	1.4425	1.3585	1.4475	1.3581	1.4523	1.3656	1.4377	1.3287	1.6217	1.5183	1.4591	1.4425	1.3585	1.4475	1.3581	1.4523	1.3656	1.4377	1.3287	**1.39**
H(11A-11B)	1.0221	1.0367	1.0037	1.0526	1.0131	1.0518	1.0176	1.0508	1.0171	1.0532	1.0044	1.0221	1.0367	1.0037	1.0526	1.0131	1.0518	1.0176	1.0508	1.0171	1.0532	1.0045	**1.22**
H(12A-12C)	0.9038	0.8919	0.8662	0.8885	0.8592	0.8886	0.8679	0.8886	0.8693	0.8883	0.8616	0.9038	0.8919	0.8662	0.8885	0.8592	0.8886	0.8679	0.8886	0.8693	0.8883	0.8616	**0.77**
H(1`A)	2.6968	2.6878	2.6766	2.6791	2.6372	2.6798	2.6542	2.6802	2.6545	2.6784	2.6219	2.8356	2.8425	2.8290	2.8230	2.7927	2.8246	2.8005	2.8261	2.8024	2.8212	2.7688	**3.16**
H(1`B)	3.1801	3.2276	3.2615	3.2635	3.3127	3.2613	3.3038	3.2588	3.2991	3.2655	3.3001	2.8657	2.7208	2.7098	2.7022	2.7288	2.7020	2.6867	2.7019	2.6919	2.7027	2.6798	**3.76**
H(2`A-2`B)	1.7040	1.7361	1.7020	1.7698	1.7248	1.7673	1.7377	1.7649	1.7341	1.7720	1.7559	1.5869	1.6654	1.6284	1.7161	1.6869	1.7127	1.7140	1.7093	1.7094	1.7193	1.7479	**2.13**
H(3`A-3`B)	1.5869	1.6654	1.6284	1.7161	1.6869	1.7127	1.7140	1.7093	1.7094	1.7193	1.7479	1.7040	1.7361	1.7020	1.7698	1.7248	1.7673	1.7377	1.7649	1.7341	1.7720	1.7559	**2.05**
H(4`A)	2.8657	2.7208	2.7099	2.7023	2.7288	2.7020	2.6867	2.7019	2.6919	2.7027	2.6798	3.1801	3.2276	3.2614	3.2635	3.3127	3.2613	3.3038	3.2588	3.2992	3.2655	3.3001	**3.09**
H(4`B)	2.8356	2.8425	2.8290	2.8230	2.7927	2.8246	2.8005	2.8261	2.8024	2.8212	2.7688	2.6968	2.6878	2.6766	2.6791	2.6372	2.6798	2.6542	2.6802	2.6545	2.6784	2.6220	**3.63**
F4	-114.3977	-115.6364	-118.2166	-115.8900	-120.4650	-115.8748	-118.2436	-115.8631	-118.6277	-115.9061	-118.1036	-114.3977	-115.6364	-118.2168	-115.8901	-120.4650	-115.8748	-118.2438	-115.8631	-118.6278	-115.9061	-118.1037	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. III

Nuclei	R											S										Exp. [b]
	BHandH											BHandH										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	138.5465	139.0589	140.0282	139.2348	140.8674	139.2148	140.1811	139.2131	140.2774	139.2234	140.5547	138.5464	139.0589	140.0282	139.2348	139.9789	139.2149	140.1811	139.2130	140.2774	139.2234	140.5546	**132.8**
C2	143.5117	143.4353	144.0030	143.2870	143.8194	143.2877	144.2640	143.3068	144.2012	143.2560	144.2993	143.5117	143.4353	144.0030	143.2870	144.0311	143.2877	144.2640	143.3066	144.2012	143.2560	144.2993	**132.9**
C3	123.6216	124.3782	125.0268	124.6233	125.3404	124.6010	125.5677	124.5967	125.5216	124.6141	125.6558	123.6216	124.3782	125.0269	124.6233	125.3674	124.6011	125.5677	124.5967	125.5216	124.6141	125.6558	**117.2**
C4	174.7888	175.5536	176.1854	175.9620	176.5660	175.9263	177.2388	175.9091	177.0774	175.9658	177.3779	174.7888	175.5536	176.1854	175.9620	176.7061	175.9263	177.2388	175.9092	177.0774	175.9658	177.3779	**167.5**
C5	121.5046	122.9341	123.6411	123.6822	124.5984	123.6257	124.8174	123.5876	124.7076	123.7060	124.9940	121.5047	122.9341	123.6411	123.6822	124.4263	123.6257	124.8174	123.5877	124.7076	123.7060	124.9940	**117.2**
C6	139.7122	141.6732	142.8202	142.8468	144.3976	142.7615	145.0656	142.6949	144.7943	142.8980	145.4379	139.7122	141.6732	142.8202	142.8468	143.5909	142.7615	145.0656	142.6950	144.7943	142.8980	145.4378	**132.9**
C7	204.0554	208.3972	209.8032	210.7478	211.4240	210.5925	216.7982	210.4551	215.6159	210.8653	217.9800	204.0553	208.3972	209.8031	210.7478	211.4919	210.5925	216.7982	210.4554	215.6159	210.8653	217.9800	**195.8**
C8	60.0731	61.1362	61.9412	61.6394	62.5544	61.5974	63.2661	61.5739	63.1273	61.6492	63.7607	60.0731	61.1362	61.9412	61.6394	62.3835	61.5974	63.2661	61.5738	63.1273	61.6492	63.7607	**68.4**
C9	34.1020	33.8856	34.1209	33.7869	34.0297	33.7837	34.1234	33.7986	34.0914	33.7597	34.2791	34.1020	33.8856	34.1209	33.7869	34.5310	33.7838	34.1234	33.7987	34.0914	33.7597	34.2791	**30.5**
C10	27.2135	27.7537	28.1167	28.1371	28.8125	28.0995	28.5687	28.0810	28.5478	28.1431	28.8216	27.2135	27.7537	28.1167	28.1371	28.8812	28.0995	28.5687	28.0810	28.5478	28.1431	28.8216	**27.6**
C11	26.1644	26.2342	26.5746	26.1987	26.6023	26.1915	26.5850	26.2026	26.6070	26.1752	26.7570	26.1643	26.2342	26.5745	26.1987	26.9428	26.1914	26.5850	26.2025	26.6070	26.1752	26.7571	**23.1**
C12	15.6496	15.8310	15.8835	15.9590	16.0362	15.9394	15.9509	15.9385	15.9568	15.9476	15.9762	15.6495	15.8311	15.8834	15.9590	16.7031	15.9394	15.9509	15.9385	15.9568	15.9476	15.9762	**13.8**
C1`	48.2959	49.0980	49.4034	49.5638	50.0949	49.5213	50.0509	49.4977	50.0387	49.5750	50.4802	52.2406	53.2551	53.7083	53.7330	54.4771	53.6924	54.4518	53.6704	54.3989	53.7416	54.6924	**53.5**
C2`	21.6367	22.0035	22.3605	22.1802	22.6341	22.1578	22.7044	22.1539	22.7025	22.1716	22.6865	21.0585	21.3095	21.6337	21.4659	22.2100	21.4453	21.8796	21.4431	21.8815	21.4554	21.8474	**24.5**
C3`	21.0585	21.3095	21.6337	21.4659	21.9420	21.4453	21.8796	21.4431	21.8815	21.4554	21.8473	21.6367	22.0035	22.3605	22.1802	22.9243	22.1578	22.7044	22.1539	22.7025	22.1716	22.6865	**24.3**
C4`	52.2406	53.2551	53.7084	53.7330	54.3137	53.6925	54.4518	53.6705	54.3989	53.7416	54.6924	48.2958	49.0980	49.4034	49.5638	50.3079	49.5213	50.0509	49.4977	50.0387	49.5750	50.4801	**57.5**
H2	9.0133	8.9379	8.9431	8.8888	8.8838	8.8928	8.8900	8.8959	8.8935	8.8861	8.8693	9.0133	8.9379	8.9431	8.8888	8.8076	8.8928	8.8900	8.8959	8.8935	8.8861	8.8693	**8.11**
H3	7.4474	7.5927	7.6854	7.6383	7.7626	7.6369	7.7844	7.6346	7.7756	7.6405	7.8000	7.4474	7.5927	7.6854	7.6383	7.5571	7.6369	7.7844	7.6346	7.7756	7.6405	7.8000	**7.31**
H5	7.2803	7.4792	7.5728	7.5667	7.6983	7.5625	7.7142	7.5574	7.7025	7.5718	7.7363	7.2803	7.4792	7.5728	7.5667	7.4855	7.5625	7.7142	7.5574	7.7025	7.5718	7.7363	**7.31**
H6	8.1894	8.3806	8.4651	8.4861	8.6214	8.4803	8.6749	8.4737	8.6488	8.4926	8.7015	8.1894	8.3806	8.4651	8.4861	8.4049	8.4803	8.6749	8.4737	8.6488	8.4926	8.7015	**8.11**
H8	4.2693	4.3483	4.3771	4.4032	4.4839	4.4004	4.5358	4.3968	4.5082	4.4069	4.5389	4.2693	4.3483	4.3771	4.4032	4.3220	4.4004	4.5358	4.3968	4.5082	4.4069	4.5389	**5.18**
H(9A-9B)	1.7884	1.8248	1.8176	1.8632	1.8617	1.8613	1.8484	1.8587	1.8470	1.8660	1.8841	1.7883	1.8248	1.8176	1.8632	1.7820	1.8613	1.8484	1.8587	1.8470	1.8660	1.8841	**2.05**
H(10A)	0.9699	0.8271	0.7545	0.7425	0.6584	0.7484	0.6674	0.7535	0.6673	0.7379	0.6698	0.9699	0.8271	0.7545	0.7425	0.6584	0.7484	0.6674	0.7535	0.6673	0.7379	0.6698	**1.14**
H(10B)	1.6604	1.5673	1.5079	1.4980	1.4014	1.5040	1.3938	1.5089	1.4008	1.4933	1.3675	1.6604	1.5673	1.5080	1.4980	1.4014	1.5040	1.3938	1.5089	1.4008	1.4933	1.3675	**1.39**
H(11A-11B)	0.9886	1.0092	0.9788	1.0287	0.9857	1.0282	0.9820	1.0270	0.9828	1.0301	0.9726	0.9886	1.0092	0.9788	1.0287	0.9474	1.0282	0.9820	1.0270	0.9828	1.0301	0.9726	**1.22**
H(12A-12C)	0.9400	0.9236	0.8941	0.9103	0.8692	0.9121	0.8710	0.9129	0.8722	0.9096	0.8665	0.9400	0.9236	0.8941	0.9103	0.8291	0.9121	0.8710	0.9129	0.8722	0.9096	0.8665	**0.77**
H(1`A)	2.5921	2.5890	2.5638	2.5786	2.5274	2.5803	2.5416	2.5812	2.5420	2.5781	2.5258	2.7460	2.7455	2.7319	2.7273	2.6904	2.7296	2.7107	2.7311	2.7126	2.7260	2.6863	**3.16**
H(1`B)	3.0932	3.1308	3.1577	3.1643	3.2166	3.1627	3.1977	3.1603	3.1933	3.1669	3.2011	2.9077	2.7015	2.6593	2.6386	2.6117	2.6430	2.5508	2.6465	2.5576	2.6356	2.5450	**3.76**
H(2`A-2`B)	1.6826	1.7192	1.6777	1.7467	1.7009	1.7456	1.7098	1.7438	1.7053	1.7487	1.7284	1.5760	1.6449	1.6083	1.6820	1.6381	1.6803	1.6740	1.6779	1.6668	1.6846	1.7083	**2.13**
H(3`A-3`B)	1.5760	1.6449	1.6083	1.6820	1.6381	1.6803	1.6740	1.6779	1.6668	1.6846	1.7083	1.6826	1.7192	1.6777	1.7467	1.7009	1.7456	1.7098	1.7438	1.7053	1.7487	1.7284	**2.05**
H(4`A)	2.9077	2.7015	2.6593	2.6386	2.6117	2.6430	2.5508	2.6465	2.5576	2.6356	2.5450	3.0932	3.1308	3.1577	3.1643	3.2166	3.1627	3.1977	3.1603	3.1933	3.1669	3.2011	**3.09**
H(4`B)	2.7460	2.7455	2.7320	2.7273	2.6904	2.7296	2.7107	2.7311	2.7126	2.7260	2.6863	2.5921	2.5890	2.5638	2.5786	2.5274	2.5803	2.5416	2.5812	2.5420	2.5781	2.5258	**3.63**
F4	-105.4115	-106.0759	-108.2201	-105.9738	-109.3505	-105.9854	-107.2526	-105.9960	-107.6314	-105.9624	-107.1068	-105.4115	-106.0759	-108.2201	-105.9738	-106.3105	-105.9854	-107.2526	-105.9960	-107.6314	-105.9624	-107.1068	**-104.5**
Nuclei	BHandHLYP											BHandHLYP										
C1	139.1706	139.9116	140.6432	140.3296	141.7914	140.3148	140.9419	140.3012	141.1074	140.3424	141.2702	139.1706	139.9116	140.6432	140.3295	141.7914	140.3148	140.9419	140.3012	141.1074	140.3424	141.2702	**132.8**
C2	142.0275	141.9201	142.3974	141.7860	142.2101	141.7956	142.7562	141.8074	142.6462	141.7766	142.7360	142.0275	141.9201	142.3974	141.7860	142.2101	141.7956	142.7562	141.8074	142.6462	141.7767	142.7360	**132.9**
C3	122.5523	123.1684	123.6876	123.3576	123.9512	123.3499	124.1309	123.3441	124.1042	123.3640	124.2025	122.5523	123.1684	123.6877	123.3575	123.9512	123.3499	124.1309	123.3441	124.1042	123.3640	124.2025	**117.2**
C4	174.5864	175.2899	175.8454	175.6713	176.1994	175.6486	176.8750	175.6280	176.7138	175.6927	176.9999	174.5864	175.2899	175.8454	175.6714	176.1994	175.6486	176.8750	175.6280	176.7138	175.6927	176.9999	**167.5**
C5	120.3052	121.5543	122.1308	122.2063	122.9812	122.1668	123.1213	122.1296	123.0494	122.2436	123.2920	120.3052	121.5543	122.1307	122.2064	122.9812	122.1668	123.1213	122.1296	123.0494	122.2436	123.2920	**117.2**
C6	138.0548	139.9133	141.0549	141.0312	142.5246	140.9560	143.2797	140.8840	142.9881	141.1031	143.6154	138.0548	139.9133	141.0548	141.0312	142.5246	140.9560	143.2797	140.8840	142.9881	141.1031	143.6154	**132.9**
C7	202.3068	207.1882	208.3236	209.9129	210.2715	209.7555	215.9054	209.5991	214.6690	210.0607	217.0820	202.3068	207.1882	208.3236	209.9129	210.2715	209.7555	215.9054	209.5991	214.6690	210.0607	217.0820	**195.8**
C8	61.8804	62.9219	63.4905	63.3415	64.2714	63.3206	64.7791	63.3010	64.6980	63.3599	65.1757	61.8804	62.9219	63.4905	63.3415	64.2714	63.3206	64.7791	63.3010	64.6980	63.3599	65.1757	**68.4**
C9	34.1386	33.7725	34.0157	33.6193	33.9168	33.6264	34.0171	33.6361	33.9882	33.6121	34.0669	34.1386	33.7725	34.0157	33.6193	33.9168	33.6264	34.0171	33.6361	33.9882	33.6121	34.0669	**30.5**
C10	27.2497	27.6893	28.1703	28.0164	28.7326	27.9923	28.5308	27.9711	28.5292	28.0393	28.6777	27.2497	27.6893	28.1703	28.0164	28.7326	27.9922	28.5308	27.9711	28.5292	28.0393	28.6777	**27.6**
C11	27.2405	27.3246	27.6178	27.2971	27.7280	27.3011	27.7115	27.3070	27.7273	27.2928	27.8503	27.2405	27.3246	27.6179	27.2972	27.7280	27.3010	27.7115	27.3070	27.7273	27.2928	27.8503	**23.1**
C12	16.4477	16.5986	16.6969	16.7338	16.8490	16.7238	16.7955	16.7165	16.8029	16.7434	16.8068	16.4477	16.5986	16.6969	16.7339	16.8490	16.7239	16.7955	16.7165	16.8029	16.7434	16.8068	**13.8**
C1`	49.0825	49.8396	50.1387	50.3717	50.8895	50.3364	50.8814	50.3041	50.8419	50.4053	51.3647	53.3202	54.3295	54.6354	54.7498	55.2630	54.7265	55.3513	54.7053	55.3102	54.7713	55.6150	**53.5**
C2`	24.4610	24.8112	25.1567	24.9344	25.4163	24.9287	25.4177	24.9250	25.4350	24.9393	25.2394	23.9171	24.0510	24.4256	24.1914	24.6650	24.1829	24.5877	24.1770	24.5932	24.1990	24.4088	**24.5**
C3`	23.9171	24.0510	24.4257	24.1913	24.6650	24.1830	24.5877	24.1770	24.5932	24.1990	24.4088	24.4610	24.8112	25.1568	24.9345	25.4163	24.9287	25.4177	24.9250	25.4350	24.9393	25.2394	**24.3**
C4`	53.3202	54.3295	54.6354	54.7499	55.2630	54.7265	55.3513	54.7053	55.3102	54.7714	55.6150	49.0825	49.8396	50.1387	50.3716	50.8895	50.3365	50.8814	50.3041	50.8419	50.4053	51.3647	**57.5**
H2	8.9174	8.8134	8.8432	8.7435	8.7514	8.7471	8.7822	8.7508	8.7728	8.7400	8.7555	8.9174	8.8134	8.8432	8.7434	8.7514	8.7471	8.7822	8.7508	8.7728	8.7400	8.7555	**8.11**
H3	7.4415	7.5833	7.6682	7.6294	7.7421	7.6275	7.7648	7.6254	7.7556	7.6312	7.7794	7.4415	7.5833	7.6682	7.6294	7.7421	7.6275	7.7648	7.6254	7.7556	7.6312	7.7794	**7.31**
H5	7.2649	7.4404	7.5319	7.5137	7.6436	7.5094	7.6523	7.5050	7.6416	7.5178	7.6758	7.2649	7.4404	7.5319	7.5137	7.6436	7.5094	7.6523	7.5050	7.6416	7.5178	7.6758	**7.31**
H6	8.0825	8.2754	8.3711	8.3872	8.5176	8.3804	8.5843	8.3735	8.5554	8.3937	8.6106	8.0825	8.2754	8.3711	8.3872	8.5176	8.3804	8.5843	8.3735	8.5554	8.3937	8.6106	**8.11**
H8	4.2250	4.3093	4.3596	4.3771	4.4432	4.3727	4.5018	4.3684	4.4740	4.3812	4.4872	4.2250	4.3093	4.3596	4.3771	4.4432	4.3728	4.5018	4.3684	4.4740	4.3812	4.4872	**5.18**
H(9A-9B)	1.5827	1.6221	1.6279	1.6514	1.6739	1.6488	1.6780	1.6462	1.6704	1.6538	1.7051	1.5827	1.6221	1.6279	1.6514	1.6739	1.6488	1.6780	1.6462	1.6704	1.6538	1.7051	**2.05**
H(10A)	0.9846	0.8118	0.7997	0.7653	0.6810	0.7674	0.7233	0.7695	0.7123	0.7634	0.7225	0.9846	0.8118	0.7997	0.7653	0.6810	0.7674	0.7233	0.7695	0.7123	0.7634	0.7225	**1.14**
H(10B)	1.5615	1.4724	1.4065	1.3921	1.3035	1.3980	1.3085	1.4037	1.3114	1.3864	1.2811	1.5615	1.4724	1.4065	1.3921	1.3035	1.3980	1.3085	1.4037	1.3114	1.3864	1.2811	**1.39**
H(11A-11B)	0.9843	1.0042	0.9708	1.0203	0.9796	1.0195	0.9842	1.0186	0.9801	1.0210	0.9727	0.9843	1.0042	0.9708	1.0203	0.9796	1.0195	0.9842	1.0186	0.9801	1.0210	0.9727	**1.22**
H(12A-12C)	0.9401	0.9227	0.8984	0.9153	0.8731	0.9159	0.8823	0.9165	0.8805	0.9146	0.8760	0.9401	0.9227	0.8984	0.9153	0.8731	0.9159	0.8823	0.9165	0.8805	0.9146	0.8760	**0.77**
H(1`A)	2.6097	2.6012	2.5884	2.5909	2.5431	2.5917	2.5662	2.5924	2.5652	2.5900	2.5385	2.7507	2.7499	2.7315	2.7241	2.6891	2.7264	2.7061	2.7286	2.7091	2.7217	2.6739	**3.16**
H(1`B)	3.0196	3.0719	3.1020	3.1129	3.1735	3.1101	3.1671	3.1072	3.1606	3.1156	3.1693	2.7250	2.5707	2.5548	2.5489	2.5462	2.5484	2.5090	2.5489	2.5117	2.5477	2.5052	**3.76**
H(2`A-2`B)	1.6503	1.6861	1.6501	1.7217	1.6694	1.7194	1.6853	1.7170	1.6787	1.7240	1.7029	1.5294	1.6090	1.5670	1.6561	1.6040	1.6535	1.6361	1.6508	1.6287	1.6585	1.6693	**2.13**
H(3`A-3`B)	1.5294	1.6090	1.5670	1.6561	1.6040	1.6535	1.6361	1.6508	1.6287	1.6585	1.6693	1.6503	1.6861	1.6501	1.7217	1.6694	1.7194	1.6853	1.7170	1.6787	1.7240	1.7029	**2.05**
H(4`A)	2.7250	2.5707	2.5548	2.5480	2.5462	2.5484	2.5090	2.5489	2.5117	2.5477	2.5052	3.0196	3.0719	3.1020	3.1129	3.1735	3.1101	3.1671	3.1072	3.1606	3.1156	3.1693	**3.09**
H(4`B)	2.7507	2.7499	2.7315	2.7241	2.6891	2.7264	2.7061	2.7286	2.7091	2.7217	2.6739	2.6097	2.6012	2.5884	2.5908	2.5431	2.5917	2.5662	2.5924	2.5652	2.5900	2.5385	**3.63**
F4	-109.0357	-110.2556	-112.5349	-110.4787	-114.0316	-110.4726	-112.0026	-110.4662	-112.3770	-110.4837	-111.8763	-109.0357	-110.2556	-112.5350	-110.4787	-114.0316	-110.4726	-112.0026	-110.4662	-112.3770	-110.4836	-111.8763	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. IV

Nuclei	R											S										Exp. [b]
	BLYP											BLYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.5343	140.9652	141.5943	141.7357	144.5172	141.9636	143.4256	141.7300	143.9164	142.1462	143.7361	139.5343	140.9652	141.5943	141.7357	144.5172	141.9636	143.4256	141.7300	143.9164	142.1461	143.7361	**132.8**
C2	137.2556	137.2722	137.8854	137.3003	138.1317	137.5735	138.4112	137.3854	138.4615	137.6688	138.5024	137.2556	137.2722	137.8854	137.3003	138.1317	137.5735	138.4112	137.3854	138.4615	137.6689	138.5024	**132.9**
C3	120.7921	121.4191	121.9349	121.5949	122.2771	121.8658	122.4301	121.6744	122.5403	121.9644	122.5819	120.7921	121.4191	121.9349	121.5949	122.2771	121.8658	122.4301	121.6744	122.5403	121.9643	122.5819	**117.2**
C4	178.0446	178.9278	179.6458	179.2623	179.9892	179.5224	180.4161	179.3202	180.4077	179.6422	180.6443	178.0446	178.9278	179.6458	179.2623	179.9892	179.5224	180.4161	179.3202	180.4077	179.6422	180.6443	**167.5**
C5	118.7346	119.8592	120.4200	120.4485	121.2822	120.6894	121.4129	120.4685	121.4684	120.8468	121.6561	118.7346	119.8592	120.4200	120.4485	121.2822	120.6894	121.4129	120.4685	121.4684	120.8467	121.6561	**117.2**
C6	133.6680	135.5732	136.6203	136.5089	137.5639	136.7306	138.0767	136.4903	137.9461	136.9249	138.5039	133.6680	135.5732	136.6203	136.5089	137.5639	136.7306	138.0767	136.4903	137.9461	136.9250	138.5039	**132.9**
C7	204.1746	208.9870	210.1011	211.5855	213.4733	211.7040	217.6195	211.3603	217.0831	212.0989	218.7030	204.1746	208.9870	210.1011	211.5855	213.4733	211.7040	217.6195	211.3603	217.0831	212.0991	218.7030	**195.8**
C8	70.4591	71.9072	72.3407	72.5539	73.6351	72.8057	73.9567	72.5927	74.1428	72.9387	74.2784	70.4591	71.9072	72.3407	72.5539	73.6351	72.8057	73.9567	72.5927	74.1428	72.9386	74.2784	**68.4**
C9	40.1256	39.7708	39.8045	39.5605	39.5512	39.8527	39.6759	39.6825	39.8226	39.9098	39.7834	40.1256	39.7708	39.8045	39.5605	39.5512	39.8527	39.6759	39.6825	39.8226	39.9098	39.7834	**30.5**
C10	30.9956	31.5038	31.9353	31.7631	32.4330	32.0244	32.0419	31.8239	32.2296	32.1419	32.2060	30.9956	31.5038	31.9353	31.7631	32.4330	32.0244	32.0419	31.8239	32.2296	32.1419	32.2060	**27.6**
C11	31.2026	31.3178	31.5898	31.2585	31.7489	31.5442	31.5381	31.3673	31.7410	31.6138	31.7406	31.2026	31.3178	31.5898	31.2585	31.7489	31.5442	31.5381	31.3673	31.7410	31.6138	31.7406	**23.1**
C12	17.0012	17.1470	17.1923	17.2337	17.4506	17.5040	17.2382	17.3127	17.4172	17.6046	17.3304	17.0012	17.1470	17.1923	17.2337	17.4506	17.5040	17.2382	17.3127	17.4172	17.6045	17.3304	**13.8**
C1`	55.2831	56.0370	56.4053	56.5833	57.2950	56.8244	57.1633	56.6042	57.2744	56.9826	57.7328	59.9830	61.1273	61.5437	61.6339	62.2990	61.8849	62.3006	61.6734	62.3750	62.0222	62.6696	**53.5**
C2`	27.7274	28.2834	28.6122	28.5322	29.0355	28.8001	28.9330	28.6054	29.0959	28.9041	28.8068	27.6644	27.8009	28.1574	27.9578	28.6760	28.2245	28.3891	28.0299	28.5704	28.3322	28.2523	**24.5**
C3`	27.6644	27.8009	28.1574	27.9578	28.6760	28.2246	28.3891	28.0299	28.5704	28.3322	28.2523	27.7274	28.2834	28.6122	28.5322	29.0355	28.8002	28.9330	28.6054	29.0959	28.9042	28.8068	**24.3**
C4`	59.9830	61.1273	61.5437	61.6339	62.2990	61.8849	62.3006	61.6734	62.3750	62.0222	62.6696	55.2831	56.0370	56.4053	56.5833	57.2950	56.8243	57.1633	56.6042	57.2744	56.9825	57.7328	**57.5**
H2	8.4743	8.3172	8.3808	8.2334	8.1741	8.2858	8.4013	8.2457	8.2052	8.2841	8.4152	8.4743	8.3172	8.3808	8.2334	8.1741	8.2858	8.4013	8.2457	8.2052	8.2841	8.4152	**8.11**
H3	7.1772	7.3089	7.3990	7.3393	7.4354	7.3857	7.6265	7.3394	7.4492	7.3955	7.6556	7.1772	7.3089	7.3990	7.3393	7.4354	7.3857	7.6265	7.3394	7.4492	7.3955	7.6556	**7.31**
H5	6.9737	7.1133	7.1996	7.1888	7.3510	7.2313	7.5411	7.1813	7.3621	7.2487	7.5789	6.9737	7.1133	7.1996	7.1888	7.3510	7.2313	7.5411	7.1813	7.3621	7.2487	7.5789	**7.31**
H6	7.8508	8.0008	8.0879	8.0664	8.1493	8.1100	8.3792	8.0612	8.1751	8.1252	8.4240	7.8508	8.0008	8.0879	8.0664	8.1493	8.1100	8.3792	8.0612	8.1751	8.1252	8.4240	**8.11**
H8	4.9846	5.0134	5.0311	5.0158	5.0719	5.0626	5.2534	5.0171	5.0718	5.0716	5.2461	4.9846	5.0134	5.0311	5.0158	5.0719	5.0626	5.2534	5.0171	5.0718	5.0716	5.2461	**5.18**
H(9A-9B)	1.7832	1.8231	1.8147	1.8352	1.7750	1.8823	1.9577	1.8368	1.7845	1.8907	1.9990	1.7832	1.8231	1.8147	1.8352	1.7750	1.8823	1.9577	1.8368	1.7845	1.8908	1.9990	**2.05**
H(10A)	1.0374	0.9218	0.9214	0.8984	0.8849	0.9453	1.0941	0.9001	0.9201	0.9545	1.1206	1.0374	0.9218	0.9214	0.8984	0.8849	0.9453	1.0941	0.9001	0.9201	0.9545	1.1206	**1.14**
H(10B)	1.7538	1.6293	1.5697	1.5413	1.4721	1.5943	1.6301	1.5547	1.4719	1.5913	1.6106	1.7538	1.6293	1.5697	1.5413	1.4721	1.5943	1.6301	1.5547	1.4719	1.5913	1.6106	**1.39**
H(11A-11B)	1.1322	1.1424	1.1178	1.1560	1.1325	1.2024	1.3013	1.1563	1.1316	1.2123	1.3029	1.1322	1.1424	1.1178	1.1560	1.1325	1.2024	1.3013	1.1563	1.1316	1.2123	1.3029	**1.22**
H(12A-12C)	0.9419	0.9312	0.9110	0.9251	0.9070	0.9727	1.0813	0.9279	0.9137	0.9802	1.0909	0.9419	0.9312	0.9110	0.9251	0.9070	0.9727	1.0813	0.9279	0.9137	0.9802	1.0909	**0.77**
H(1`A)	2.8633	2.8501	2.8310	2.8377	2.7979	2.8860	2.9760	2.8418	2.8118	2.8922	2.9544	2.9651	2.9898	2.9671	2.9680	2.9372	3.0180	3.1018	2.9754	2.9444	3.0205	3.0695	**3.16**
H(1`B)	3.3633	3.4089	3.4348	3.4379	3.4925	3.4835	3.6471	3.4365	3.4756	3.4949	3.6586	3.0499	2.8913	2.8353	2.8526	2.8547	2.9002	2.9868	2.8556	2.8331	2.9080	2.9912	**3.76**
H(2`A-2`B)	1.8103	1.8387	1.8009	1.8621	1.8241	1.9073	2.0025	1.8602	1.8309	1.9195	2.0403	1.6657	1.7499	1.7162	1.7953	1.7725	1.8397	1.9626	1.7916	1.7906	1.8535	2.0090	**2.13**
H(3`A-3`B)	1.6657	1.7499	1.7162	1.7953	1.7725	1.8397	1.9626	1.7916	1.7906	1.8535	2.0090	1.8103	1.8387	1.8009	1.8621	1.8241	1.9073	2.0025	1.8602	1.8309	1.9195	2.0403	**2.05**
H(4`A)	3.0499	2.8913	2.8353	2.8526	2.8547	2.9002	2.9868	2.8556	2.8331	2.9080	2.9912	3.3633	3.4089	3.4348	3.4379	3.4925	3.4835	3.6471	3.4365	3.4756	3.4949	3.6586	**3.09**
H(4`B)	2.9651	2.9898	2.9671	2.9680	2.9372	3.0180	3.1018	2.9754	2.9444	3.0205	3.0695	2.8633	2.8501	2.8310	2.8377	2.7979	2.8860	2.9760	2.8418	2.8118	2.8922	2.9544	**3.63**
F4	-142.5703	-144.4267	-147.7209	-144.8583	-150.4862	-144.6289	-146.8437	-144.8151	-148.3973	-144.8127	-147.0218	-142.5703	-144.4267	-147.7209	-144.8583	-150.4862	-144.6289	-146.8437	-144.8151	-148.3973	-144.8126	-147.0218	**-104.5**
Nuclei	BMK											BMK											
C1	154.6743	155.0332	155.8462	155.1583	157.1596	155.1396	156.3883	155.3301	156.3397	155.3339	156.6046	154.6743	155.0332	155.8461	155.1582	157.1596	155.1397	156.3884	155.3301	156.3396	155.3339	156.6046	**132.8**
C2	154.6877	154.7844	155.5459	154.6549	155.3498	154.6489	155.8469	154.8543	155.6657	154.8228	155.7777	154.6877	154.7844	155.5461	154.6548	155.3498	154.6489	155.8467	154.8543	155.6656	154.8230	155.7777	**132.9**
C3	135.9138	136.6373	137.3465	136.8279	137.6933	136.8045	137.9405	136.9917	137.7955	137.0117	137.8683	135.9138	136.6373	137.3465	136.8279	137.6933	136.8046	137.9404	136.9917	137.7954	137.0118	137.8683	**117.2**
C4	189.4877	190.2116	190.9837	190.5712	191.4900	190.5337	192.1186	190.7070	191.8573	190.7682	192.2003	189.4877	190.2116	190.9838	190.5712	191.4900	190.5337	192.1187	190.7070	191.8575	190.7681	192.2003	**167.5**
C5	133.6513	134.9680	135.5869	135.6169	136.6787	135.5615	136.8546	135.7170	136.6382	135.8301	136.9525	133.6513	134.9680	135.5868	135.6171	136.6787	135.5614	136.8546	135.7170	136.6383	135.8300	136.9525	**117.2**
C6	151.3083	153.3283	154.3456	154.4536	156.4249	154.3671	157.0666	154.4912	156.6478	154.6954	157.4119	151.3083	153.3283	154.3454	154.4537	156.4249	154.3671	157.0667	154.4912	156.6476	154.6955	157.4119	**132.9**
C7	218.4275	222.9521	224.3909	225.3913	226.5095	225.2230	232.5082	225.2643	230.9435	225.7107	234.0514	218.4275	222.9521	224.3912	225.3913	226.5095	225.2230	232.5081	225.2643	230.9437	225.7103	234.0514	**195.8**
C8	71.7818	72.7560	73.5185	73.2212	74.7487	73.1831	75.2261	73.3534	74.8979	73.4147	76.0945	71.7818	72.7560	73.5184	73.2212	74.7487	73.1831	75.2261	73.3534	74.8979	73.4148	76.0945	**68.4**
C9	38.9270	38.8753	38.9914	38.7229	39.3377	38.7191	39.5697	38.9259	39.3287	38.8870	39.8348	38.9270	38.8753	38.9914	38.7229	39.3377	38.7192	39.5696	38.9259	39.3287	38.8870	39.8348	**30.5**
C10	31.5063	31.8431	32.2898	32.1042	32.9319	32.0706	32.5932	32.2494	32.5113	32.3000	32.8436	31.5063	31.8431	32.2898	32.1043	32.9319	32.0705	32.5931	32.2494	32.5113	32.3000	32.8436	**27.6**
C11	30.1638	30.0934	30.5280	30.0558	30.6708	30.0424	30.6321	30.2397	30.5415	30.2295	30.7089	30.1638	30.0934	30.5281	30.0558	30.6708	30.0423	30.6321	30.2397	30.5416	30.2295	30.7089	**23.1**
C12	17.9216	17.9663	18.1186	18.0457	18.3196	18.0223	18.2191	18.2104	18.1235	18.2298	18.1813	17.9215	17.9663	18.1186	18.0458	18.3196	18.0222	18.2190	18.2104	18.1236	18.2298	18.1812	**13.8**
C1`	56.2140	56.7042	57.2624	57.3354	57.9775	57.2761	57.8726	57.4271	57.7807	57.5515	57.9072	60.6747	61.2631	61.7498	61.5953	62.2577	61.5585	62.3486	61.7326	62.2082	61.7911	62.6655	**53.5**
C2`	28.1109	28.2884	28.6899	28.4501	29.0183	28.4238	28.9833	28.6085	28.8847	28.6357	28.9334	27.2299	27.4471	27.8451	27.6148	28.2163	27.5901	28.0996	27.7764	28.0059	27.7997	28.0827	**24.5**
C3`	27.2299	27.4471	27.8451	27.6148	28.2163	27.5901	28.0997	27.7764	28.0059	27.7998	28.0827	28.1109	28.2884	28.6900	28.4501	29.0184	28.4240	28.9833	28.6085	28.8847	28.6357	28.9334	**24.3**
C4`	60.6747	61.2631	61.7497	61.5952	62.2576	61.5585	62.3485	61.7326	62.2080	61.7910	62.6655	56.2140	56.7042	57.2624	57.3355	57.9775	57.2760	57.8726	57.4271	57.7808	57.5514	57.9072	**57.5**
H2	8.9918	8.9298	8.9868	8.9078	8.9029	8.9057	8.9653	8.9038	8.9648	8.9005	8.9628	8.9918	8.9298	8.9868	8.9078	8.9029	8.9057	8.9653	8.9038	8.9648	8.9005	8.9628	**8.11**
H3	7.6541	7.7829	7.8752	7.8302	7.9474	7.8246	7.9758	7.8190	7.9680	7.8259	7.9947	7.6541	7.7829	7.8752	7.8302	7.9474	7.8246	7.9758	7.8190	7.9680	7.8259	7.9947	**7.31**
H5	7.4938	7.6754	7.7641	7.7548	7.8712	7.7469	7.8878	7.7390	7.8788	7.7528	7.9076	7.4938	7.6754	7.7641	7.7548	7.8712	7.7469	7.8878	7.7390	7.8788	7.7528	7.9076	**7.31**
H6	8.3432	8.5078	8.6605	8.6235	8.7819	8.6124	8.8278	8.6015	8.8045	8.6250	8.8898	8.3432	8.5078	8.6605	8.6235	8.7819	8.6123	8.8278	8.6015	8.8044	8.6250	8.8898	**8.11**
H8	4.4144	4.4718	4.5598	4.5582	4.6028	4.5477	4.6667	4.5377	4.6543	4.5594	4.6485	4.4144	4.4718	4.5598	4.5582	4.6028	4.5477	4.6667	4.5377	4.6543	4.5594	4.6485	**5.18**
H(9A-9B)	1.6329	1.6976	1.6442	1.7193	1.7410	1.7145	1.7510	1.7099	1.7352	1.7143	1.8258	1.6329	1.6976	1.6442	1.7193	1.7410	1.7145	1.7510	1.7099	1.7352	1.7143	1.8258	**2.05**
H(10A)	1.0054	0.8156	0.8417	0.7556	0.6584	0.7548	0.7160	0.7541	0.7163	0.7469	0.7118	1.0054	0.8156	0.8417	0.7556	0.6584	0.7548	0.7160	0.7541	0.7163	0.7469	0.7118	**1.14**
H(10B)	1.5665	1.5142	1.4152	1.4197	1.3176	1.4233	1.3145	1.4271	1.3225	1.4069	1.3045	1.5665	1.5142	1.4152	1.4197	1.3176	1.4234	1.3145	1.4271	1.3225	1.4069	1.3045	**1.39**
H(11A-11B)	0.9568	0.9779	0.9496	0.9998	0.9492	0.9949	0.9534	0.9903	0.9549	0.9951	0.9505	0.9568	0.9779	0.9497	0.9998	0.9492	0.9949	0.9534	0.9903	0.9550	0.9951	0.9505	**1.22**
H(12A-12C)	0.8618	0.8474	0.8194	0.8457	0.7952	0.8425	0.7967	0.8395	0.8006	0.8395	0.8000	0.8617	0.8474	0.8194	0.8457	0.7952	0.8425	0.7967	0.8395	0.8007	0.8395	0.8000	**0.77**
H(1`A)	2.6238	2.6293	2.5970	2.6303	2.5835	2.6272	2.6067	2.6240	2.6082	2.6234	2.5463	2.7737	2.7853	2.7534	2.7712	2.7426	2.7699	2.7487	2.7683	2.7505	2.7626	2.7334	**3.16**
H(1`B)	3.0937	3.1310	3.1474	3.1725	3.2050	3.1661	3.1984	3.1595	3.1935	3.1689	3.1717	2.7218	2.5991	2.5747	2.5696	2.5484	2.5668	2.5121	2.5643	2.5131	2.5631	2.5093	**3.76**
H(2`A-2`B)	1.6783	1.7136	1.6893	1.7597	1.7017	1.7529	1.7160	1.7464	1.7135	1.7566	1.7210	1.4626	1.5173	1.4830	1.5420	1.4897	1.5377	1.5230	1.5334	1.5190	1.5364	1.5474	**2.13**
H(3`A-3`B)	1.5702	1.6353	1.5892	1.6789	1.6292	1.6732	1.6559	1.6675	1.6508	1.6746	1.6903	1.6422	1.7002	1.6581	1.7449	1.6934	1.7389	1.7144	1.7329	1.7103	1.7409	1.7414	**2.05**
H(4`A)	2.7218	2.5991	2.5747	2.5696	2.5484	2.5668	2.5120	2.5643	2.5131	2.5631	2.5093	2.4219	2.4555	2.4526	2.5090	2.4952	2.5014	2.4953	2.4940	2.4913	2.5066	2.4820	**3.09**
H(4`B)	2.7737	2.7853	2.7534	2.7712	2.7426	2.7699	2.7487	2.7683	2.7505	2.7626	2.7334	2.6238	2.6293	2.5970	2.6303	2.5835	2.6272	2.6068	2.6240	2.6082	2.6235	2.5463	**3.63**
F4	-118.0260	-119.1096	-121.7794	-119.1175	-123.2437	-119.1250	-121.0201	-119.1311	-121.3999	-119.1100	-120.7181	-118.0260	-119.1096	-121.7793	-119.1175	-123.2437	-119.1250	-121.0200	-119.1311	-121.3999	-119.1101	-120.7181	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. V

Nuclei	R											S										Exp. [b]
	BP86											BP86										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.1088	137.3107	138.0964	137.7831	139.1376	137.7682	138.6145	137.7476	138.6273	137.7918	138.9792	136.1088	137.3107	138.0965	137.7831	139.1376	137.7682	138.6145	137.7476	138.6273	137.7918	138.9792	**132.8**
C2	135.7786	135.9025	136.4035	135.7790	136.2500	135.7953	136.7578	135.8067	136.6297	135.7589	136.8526	135.7786	135.9025	136.4034	135.7790	136.2500	135.7953	136.7578	135.8067	136.6297	135.7589	136.8526	**132.9**
C3	119.6549	120.5419	121.0715	120.7433	121.3759	120.7419	121.7193	120.7350	121.6286	120.7394	121.9674	119.6549	120.5419	121.0715	120.7433	121.3759	120.7419	121.7193	120.7350	121.6286	120.7394	121.9674	**117.2**
C4	174.5771	175.6557	176.2903	176.0366	176.7190	176.0219	177.3180	176.0021	177.1695	176.0455	177.6153	174.5771	175.6557	176.2903	176.0366	176.7190	176.0219	177.3180	176.0021	177.1695	176.0455	177.6153	**167.5**
C5	117.7054	119.0766	119.6753	119.6781	120.4892	119.6486	120.7558	119.6139	120.6434	119.7013	121.0874	117.7054	119.0766	119.6753	119.6781	120.4892	119.6486	120.7558	119.6139	120.6434	119.7013	121.0874	**117.2**
C6	132.2467	134.2864	135.3229	135.3472	136.8781	135.2854	137.5200	135.2189	137.2791	135.4016	138.0862	132.2467	134.2864	135.3229	135.3472	136.8781	135.2854	137.5200	135.2189	137.2791	135.4016	138.0862	**132.9**
C7	201.2567	205.6591	206.8764	207.8846	208.7243	207.7624	212.8796	207.6342	211.9294	207.9947	214.0254	201.2567	205.6591	206.8764	207.8846	208.7243	207.7624	212.8796	207.6342	211.9294	207.9947	214.0254	**195.8**
C8	68.1361	69.5249	70.2639	70.0439	71.1738	70.0330	71.7242	70.0145	71.5644	70.0470	72.2963	68.1361	69.5249	70.2639	70.0439	71.1738	70.0330	71.7242	70.0145	71.5644	70.0470	72.2963	**68.4**
C9	38.8652	38.7336	38.8380	38.5423	38.8956	38.5618	39.1809	38.5758	39.0858	38.5184	39.4764	38.8652	38.7336	38.8380	38.5423	38.8956	38.5619	39.1809	38.5758	39.0858	38.5184	39.4764	**30.5**
C10	29.5240	30.1529	30.5449	30.4255	31.1246	30.4126	30.9274	30.3953	30.9087	30.4332	31.2594	29.5240	30.1529	30.5449	30.4255	31.1246	30.4126	30.9274	30.3953	30.9087	30.4332	31.2594	**27.6**
C11	29.4418	29.6972	29.8600	29.5824	29.9487	29.6022	29.9365	29.6159	29.9309	29.5580	30.2368	29.4418	29.6972	29.8601	29.5824	29.9487	29.6021	29.9365	29.6159	29.9309	29.5580	30.2368	**23.1**
C12	16.5296	16.7824	16.7604	16.8352	16.8320	16.8373	16.8060	16.8346	16.7990	16.8289	16.9542	16.5296	16.7824	16.7604	16.8352	16.8320	16.8373	16.8060	16.8346	16.7990	16.8290	16.9543	**13.8**
C1`	53.7220	54.6467	54.8434	55.1464	55.6019	55.1212	55.6068	55.0916	55.5138	55.1663	56.3013	58.2667	59.6104	59.9327	60.0596	60.4729	60.0450	60.6886	60.0246	60.6186	60.0678	61.1204	**53.5**
C2`	26.2439	26.8649	27.1493	27.0337	27.4594	27.0338	27.4989	27.0283	27.4820	27.0283	27.4483	25.9185	26.2129	26.4676	26.3545	26.7189	26.3512	26.7270	26.3431	26.7097	26.3531	26.7220	**24.5**
C3`	25.9185	26.2129	26.4677	26.3545	26.7189	26.3512	26.7270	26.3431	26.7097	26.3531	26.7220	26.2439	26.8649	27.1491	27.0337	27.4594	27.0338	27.4989	27.0283	27.4820	27.0283	27.4483	**24.3**
C4`	58.2667	59.6104	59.9326	60.0596	60.4729	60.0450	60.6886	60.0246	60.6186	60.0678	61.1203	53.7220	54.6467	54.8434	55.1464	55.6019	55.1212	55.6068	55.0916	55.5138	55.1663	56.3012	**57.5**
H2	8.5202	8.4179	8.4255	8.3541	8.3445	8.3584	8.3761	8.3625	8.3748	8.3498	8.3764	8.5202	8.4179	8.4255	8.3541	8.3445	8.3584	8.3761	8.3625	8.3748	8.3498	8.3764	**8.11**
H3	7.1794	7.3318	7.4109	7.3778	7.4831	7.3764	7.5086	7.3746	7.4988	7.3787	7.5375	7.1794	7.3318	7.4109	7.3778	7.4831	7.3764	7.5086	7.3746	7.4988	7.3787	7.5375	**7.31**
H5	7.0044	7.1582	7.2405	7.2245	7.3556	7.2214	7.3589	7.2179	7.3494	7.2272	7.4008	7.0044	7.1582	7.2405	7.2245	7.3556	7.2214	7.3589	7.2179	7.3494	7.2272	7.4008	**7.31**
H6	7.9135	8.0785	8.1409	8.1670	8.2621	8.1621	8.3188	8.1568	8.3018	8.1713	8.3592	7.9135	8.0785	8.1409	8.1670	8.2621	8.1621	8.3188	8.1568	8.3018	8.1713	8.3592	**8.11**
H8	4.9923	5.0231	5.0204	5.0488	5.0657	5.0471	5.0991	5.0452	5.0903	5.0501	5.0979	4.9923	5.0231	5.0204	5.0488	5.0657	5.0471	5.0991	5.0452	5.0903	5.0501	5.0979	**5.18**
H(9A-9B)	1.8866	1.9233	1.9092	1.9458	1.9709	1.9451	1.9663	1.9441	1.9592	1.9462	2.0157	1.8866	1.9233	1.9092	1.9458	1.9709	1.9451	1.9663	1.9441	1.9592	1.9462	2.0157	**2.05**
H(10A)	1.0160	0.9024	0.8508	0.8713	0.7697	0.8724	0.8287	0.8734	0.8187	0.8700	0.8515	1.0160	0.9024	0.8508	0.8713	0.7697	0.8724	0.8287	0.8734	0.8187	0.8700	0.8515	**1.14**
H(10B)	1.7876	1.6671	1.5902	1.5808	1.4877	1.5871	1.4750	1.5931	1.4819	1.5746	1.4536	1.7876	1.6671	1.5902	1.5808	1.4877	1.5871	1.4750	1.5931	1.4819	1.5746	1.4535	**1.39**
H(11A-11B)	1.1095	1.1243	1.0787	1.1354	1.0880	1.1356	1.0865	1.1355	1.0849	1.1348	1.0877	1.1095	1.1243	1.0788	1.1354	1.0880	1.1356	1.0865	1.1355	1.0849	1.1348	1.0877	**1.22**
H(12A-12C)	0.9116	0.9045	0.8683	0.8963	0.8471	0.8975	0.8543	0.8985	0.8534	0.8948	0.8614	0.9116	0.9045	0.8683	0.8963	0.8471	0.8975	0.8543	0.8985	0.8534	0.8948	0.8614	**0.77**
H(1`A)	2.8037	2.7998	2.7761	2.7875	2.7401	2.7890	2.7544	2.7902	2.7555	2.7857	2.7327	2.9270	2.9443	2.9250	2.9302	2.8972	2.9326	2.9032	2.9346	2.9064	2.9275	2.8769	**3.16**
H(1`B)	3.3751	3.4176	3.4367	3.4453	3.4990	3.4441	3.4838	3.4427	3.4815	3.4461	3.4880	3.1070	2.9109	2.8780	2.8605	2.8494	2.8627	2.8030	2.8649	2.8065	2.8583	2.7978	**3.76**
H(2`A-2`B)	1.8041	1.8324	1.7866	1.8585	1.8009	1.8572	1.8134	1.8556	1.8078	1.8595	1.8493	1.6627	1.7393	1.6959	1.7821	1.7232	1.7802	1.7512	1.7780	1.7430	1.7836	1.8013	**2.13**
H(3`A-3`B)	1.6627	1.7393	1.6959	1.7821	1.7232	1.7802	1.7512	1.7780	1.7430	1.7836	1.8013	1.8041	1.8324	1.7866	1.8585	1.8009	1.8572	1.8134	1.8556	1.8078	1.8595	1.8493	**2.05**
H(4`A)	3.1070	2.9109	2.8780	2.8605	2.8494	2.8627	2.8030	2.8649	2.8065	2.8583	2.7978	3.3751	3.4176	3.4367	3.4453	3.4990	3.4441	3.4838	3.4427	3.4815	3.4461	3.4880	**3.09**
H(4`B)	2.9270	2.9443	2.9250	2.9302	2.8972	2.9326	2.9032	2.9346	2.9064	2.9275	2.8769	2.8037	2.7998	2.7761	2.7875	2.7401	2.7890	2.7544	2.7902	2.7555	2.7857	2.7327	**3.63**
F4	-133.7224	-134.7487	-137.9211	-134.7351	-139.6524	-134.7459	-136.9829	-134.7552	-137.4182	-134.7242	-136.5988	-133.7224	-134.7487	-137.9211	-134.7351	-139.6524	-134.7459	-136.9829	-134.7552	-137.4182	-134.7242	-136.5988	**-104.5**
Nuclei	CAM-B3LYP											CAM-B3LYP										
C1	140.9000	141.8642	142.5134	142.3393	143.9931	142.3245	143.2389	142.3087	143.3053	142.3544	143.4213	140.8999	141.8642	142.5135	142.3392	143.9931	142.3245	143.2389	142.3087	143.3053	142.3544	143.4212	**132.8**
C2	142.3592	142.3291	142.7581	142.1837	142.6753	142.1979	143.2028	142.2124	143.0855	142.1723	143.1775	142.3594	142.3291	142.7582	142.1837	142.6754	142.1979	143.2028	142.2124	143.0855	142.1723	143.1775	**132.9**
C3	123.8875	124.5615	125.0610	124.7361	125.3833	124.7328	125.5918	124.7293	125.5399	124.7413	125.6630	123.8876	124.5615	125.0610	124.7363	125.3832	124.7328	125.5918	124.7293	125.5399	124.7412	125.6631	**117.2**
C4	177.7476	178.5115	179.0552	178.8743	179.4733	178.8556	180.0785	178.8375	179.9280	178.8943	180.2203	177.7477	178.5115	179.0551	178.8744	179.4733	178.8556	180.0785	178.8375	179.9280	178.8944	180.2204	**167.5**
C5	121.8135	123.1003	123.6648	123.7417	124.5660	123.7060	124.7320	123.6710	124.6384	123.7775	124.8939	121.8135	123.1003	123.6648	123.7415	124.5660	123.7060	124.7320	123.6709	124.6384	123.7775	124.8939	**117.2**
C6	138.4687	140.3307	141.5035	141.4320	142.9843	141.3615	143.6195	141.2922	143.3572	141.5021	144.0436	138.4687	140.3307	141.5034	141.4319	142.9843	141.3615	143.6195	141.2922	143.3572	141.5021	144.0435	**132.9**
C7	206.2190	211.2347	212.3397	213.9879	214.6304	213.8311	220.0283	213.6740	218.8123	214.1375	221.0855	206.2190	211.2347	212.3397	213.9878	214.6304	213.8311	220.0283	213.6739	218.8123	214.1374	221.0856	**195.8**
C8	64.6063	65.7712	66.4410	66.2572	67.2927	66.2389	67.9060	66.2194	67.7480	66.2753	68.2828	64.6064	65.7712	66.4410	66.2573	67.2928	66.2389	67.9060	66.2194	67.7480	66.2753	68.2828	**68.4**
C9	35.3917	35.0454	35.2739	34.8733	35.1875	34.8869	35.3176	34.9005	35.2558	34.8622	35.4063	35.3917	35.0454	35.2740	34.8733	35.1874	34.8869	35.3176	34.9006	35.2558	34.8622	35.4064	**30.5**
C10	28.1866	28.6440	29.1029	28.9663	29.6973	28.9451	29.5046	28.9250	29.4847	28.9892	29.6822	28.1867	28.6440	29.1029	28.9664	29.6974	28.9451	29.5046	28.9249	29.4847	28.9892	29.6823	**27.6**
C11	27.8708	27.9976	28.2402	27.9403	28.3933	27.9501	28.3825	27.9597	28.3778	27.9329	28.5418	27.8708	27.9976	28.2403	27.9403	28.3933	27.9501	28.3825	27.9596	28.3778	27.9330	28.5418	**23.1**
C12	16.2567	16.4391	16.4726	16.5524	16.6588	16.5468	16.6036	16.5421	16.5992	16.5601	16.6163	16.2567	16.4391	16.4726	16.5523	16.6589	16.5468	16.6036	16.5420	16.5992	16.5601	16.6163	**13.8**
C1`	50.8435	51.6933	51.8918	52.2148	52.7698	52.1836	52.7649	52.1535	52.6947	52.2469	53.2563	55.1554	56.2469	56.5379	56.6717	57.1952	56.6514	57.3190	56.6314	57.2584	56.6928	57.5773	**53.5**
C2`	25.0342	25.4284	25.7358	25.5492	26.0245	25.5467	26.0407	25.5443	26.0345	25.5535	25.8833	24.4922	24.6878	24.9644	24.8119	25.2810	24.8071	25.1973	24.8028	25.1947	24.8187	25.0647	**24.5**
C3`	24.4923	24.6878	24.9643	24.8118	25.2810	24.8071	25.1973	24.8028	25.1947	24.8188	25.0648	25.0342	25.4285	25.7358	25.5492	26.0245	25.5467	26.0407	25.5444	26.0345	25.5534	25.8833	**24.3**
C4`	55.1553	56.2469	56.5378	56.6716	57.1952	56.6514	57.3190	56.6314	57.2584	56.6927	57.5773	50.8435	51.6933	51.8918	52.2147	52.7697	52.1836	52.7649	52.1534	52.6947	52.2470	53.2562	**57.5**
H2	8.8102	8.6986	8.7289	8.6236	8.6210	8.6275	8.6425	8.6316	8.6418	8.6199	8.6323	8.8102	8.6986	8.7289	8.6236	8.6210	8.6275	8.6425	8.6316	8.6418	8.6199	8.6322	**8.11**
H3	7.4041	7.5438	7.6298	7.5866	7.7036	7.5847	7.7229	7.5828	7.7152	7.5883	7.7368	7.4041	7.5438	7.6298	7.5866	7.7036	7.5847	7.7229	7.5828	7.7152	7.5883	7.7368	**7.31**
H5	7.2406	7.4128	7.5085	7.4855	7.6154	7.4812	7.6240	7.4771	7.6145	7.4895	7.6484	7.2405	7.4128	7.5085	7.4855	7.6154	7.4812	7.6240	7.4771	7.6145	7.4895	7.6484	**7.31**
H6	8.0497	8.2319	8.3255	8.3359	8.4632	8.3292	8.5140	8.3227	8.4924	8.3422	8.5479	8.0497	8.2319	8.3255	8.3359	8.4632	8.3292	8.5140	8.3227	8.4924	8.3422	8.5479	**8.11**
H8	4.4210	4.4951	4.5329	4.5563	4.6154	4.5520	4.6593	4.5478	4.6382	4.5605	4.6576	4.4210	4.4951	4.5329	4.5563	4.6153	4.5520	4.6593	4.5478	4.6382	4.5605	4.6576	**5.18**
H(9A-9B)	1.6746	1.7066	1.7208	1.7333	1.7558	1.7312	1.7557	1.7292	1.7500	1.7352	1.7902	1.6746	1.7066	1.7208	1.7333	1.7558	1.7312	1.7557	1.7292	1.7500	1.7352	1.7902	**2.05**
H(10A)	0.9793	0.8280	0.7905	0.7827	0.6958	0.7844	0.7355	0.7864	0.7297	0.7811	0.7458	0.9793	0.8280	0.7905	0.7827	0.6958	0.7844	0.7355	0.7864	0.7297	0.7811	0.7458	**1.14**
H(10B)	1.6254	1.5324	1.4640	1.4472	1.3642	1.4530	1.3590	1.4589	1.3655	1.4418	1.3321	1.6253	1.5324	1.4640	1.4472	1.3642	1.4530	1.3590	1.4589	1.3655	1.4418	1.3321	**1.39**
H(11A-11B)	1.0293	1.0490	1.0127	1.0612	1.0239	1.0605	1.0223	1.0600	1.0216	1.0618	1.0127	1.0293	1.0490	1.0127	1.0612	1.0239	1.0605	1.0223	1.0600	1.0216	1.0618	1.0127	**1.22**
H(12A-12C)	0.9496	0.9353	0.9077	0.9264	0.8870	0.9270	0.8927	0.9277	0.8929	0.9257	0.8870	0.9496	0.9353	0.9077	0.9264	0.8871	0.9270	0.8927	0.9277	0.8929	0.9257	0.8870	**0.77**
H(1`A)	2.7110	2.7033	2.6912	2.6925	2.6485	2.6932	2.6648	2.6941	2.6655	2.6917	2.6365	2.8448	2.8448	2.8307	2.8212	2.7916	2.8233	2.8027	2.8254	2.8061	2.8191	2.7687	**3.16**
H(1`B)	3.1229	3.1689	3.2079	3.2088	3.2727	3.2060	3.2605	3.2034	3.2561	3.2114	3.2635	2.8211	2.6606	2.6465	2.6360	2.6365	2.6367	2.6027	2.6376	2.6000	2.6354	2.5884	**3.76**
H(2`A-2`B)	1.7172	1.7531	1.7166	1.7866	1.7389	1.7843	1.7511	1.7822	1.7461	1.7888	1.7689	1.5984	1.6798	1.6380	1.7262	1.6814	1.7235	1.7120	1.7209	1.7036	1.7287	1.7421	**2.13**
H(3`A-3`B)	1.5984	1.6798	1.6380	1.7262	1.6814	1.7235	1.7120	1.7209	1.7036	1.7287	1.7422	1.7172	1.7532	1.7166	1.7866	1.7389	1.7843	1.7511	1.7822	1.7461	1.7887	1.7689	**2.05**
H(4`A)	2.8211	2.6606	2.6465	2.6360	2.6365	2.6367	2.5996	2.6376	2.6000	2.6354	2.5884	3.1229	3.1689	3.2079	3.2088	3.2727	3.2060	3.2605	3.2033	3.2561	3.2114	3.2635	**3.09**
H(4`B)	2.8448	2.8448	2.8307	2.8212	2.7916	2.8233	2.8027	2.8254	2.8061	2.8191	2.7687	2.7110	2.7033	2.6912	2.6925	2.6485	2.6932	2.6648	2.6941	2.6655	2.6917	2.6364	**3.63**
F4	-115.7732	-117.3132	-119.8083	-117.6410	-121.5488	-117.6299	-119.5812	-117.6175	-119.8864	-117.6514	-119.3760	-115.7731	-117.3132	-119.8084	-117.6410	-121.5487	-117.6299	-119.5812	-117.6176	-119.8864	-117.6513	-119.3760	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. VI

Nuclei	R											S										Exp. [b]
	HF											HF										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.4614	137.5594	137.9396	138.2608	141.1588	138.1812	139.8214	138.1121	140.2588	138.3352	140.0156	136.4614	137.5594	137.9396	138.2608	141.1590	138.1812	139.8214	138.1123	140.2588	138.3352	140.0156	**132.8**
C2	144.3880	144.1261	144.6323	143.8817	144.0884	143.9028	144.6434	143.9234	144.4625	143.8613	144.6473	144.3881	144.1261	144.6323	143.8817	144.0886	143.9028	144.6434	143.9233	144.4625	143.8613	144.6474	**132.9**
C3	120.4753	121.0267	121.4081	121.1842	121.9458	121.1734	121.9413	121.1639	121.9814	121.1933	121.9865	120.4753	121.0267	121.4081	121.1842	121.9457	121.1734	121.9413	121.1637	121.9814	121.1933	121.9866	**117.2**
C4	171.1212	171.5718	172.1467	171.7971	172.0666	171.7897	172.8696	171.7808	172.6355	171.8033	173.0028	171.1213	171.5718	172.1467	171.7971	172.0666	171.7897	172.8696	171.7807	172.6354	171.8033	173.0028	**167.5**
C5	117.8593	119.1512	119.5795	119.8198	120.6684	119.7762	120.6727	119.7340	120.6376	119.8599	120.8287	117.8593	119.1512	119.5795	119.8198	120.6682	119.7762	120.6727	119.7339	120.6376	119.8599	120.8287	**117.2**
C6	139.9930	141.4756	142.7481	142.2938	142.9370	142.2616	143.9248	142.2248	143.4971	142.3244	144.2237	139.9930	141.4756	142.7481	142.2938	142.9368	142.2616	143.9248	142.2249	143.4971	142.3244	144.2236	**132.9**
C7	196.4929	202.2641	202.9719	205.5898	206.7292	205.3508	213.4358	205.1213	212.0643	205.8156	214.4845	196.4932	202.2641	202.9719	205.5898	206.7294	205.3508	213.4358	205.1213	212.0643	205.8152	214.4845	**195.8**
C8	55.7610	56.8718	57.1616	57.3487	58.2739	57.3120	58.7513	57.2794	58.6807	57.3824	58.9817	55.7610	56.8718	57.1617	57.3487	58.2738	57.3120	58.7513	57.2794	58.6807	57.3825	58.9816	**68.4**
C9	29.9395	29.4452	29.6637	29.2244	29.3513	29.2420	29.2641	29.2585	29.2555	29.2074	29.2254	29.9396	29.4452	29.6637	29.2244	29.3513	29.2420	29.2641	29.2587	29.2555	29.2074	29.2254	**30.5**
C10	24.5112	24.8855	25.3200	25.1270	25.7191	25.1133	25.5163	25.0997	25.4870	25.1397	25.6454	24.5113	24.8855	25.3200	25.1270	25.7191	25.1133	25.5163	25.0997	25.4869	25.1397	25.6454	**27.6**
C11	24.9934	25.0012	25.2811	24.9675	25.3997	24.9711	25.3586	24.9750	25.3631	24.9631	25.4875	24.9934	25.0012	25.2811	24.9675	25.3997	24.9711	25.3586	24.9751	25.3632	24.9630	25.4875	**23.1**
C12	16.1893	16.3050	16.4087	16.4083	16.5840	16.3998	16.5424	16.3920	16.5403	16.4161	16.5585	16.1893	16.3050	16.4087	16.4083	16.5840	16.3998	16.5424	16.3920	16.5403	16.4161	16.5585	**13.8**
C1`	44.6495	45.3638	45.5995	45.8292	46.3745	45.7972	46.3770	45.7670	46.3398	45.8597	46.7427	48.5492	49.4089	49.6427	49.7948	50.2999	49.7716	50.3741	49.7486	50.3061	49.8158	50.6100	**53.5**
C2`	22.8232	23.0884	23.3924	23.1170	23.5554	23.1184	23.5262	23.1198	23.5079	23.1145	23.3375	22.1997	22.2737	22.6410	22.3541	22.9562	22.3468	22.8286	22.3405	22.8432	22.3604	22.6316	**24.5**
C3`	22.1997	22.2737	22.6410	22.3541	22.9561	22.3468	22.8286	22.3405	22.8431	22.3603	22.6316	22.8232	23.0884	23.3924	23.1170	23.5554	23.1184	23.5262	23.1197	23.5079	23.1145	23.3375	**24.3**
C4`	48.5492	49.4089	49.6427	49.7948	50.3000	49.7716	50.3741	49.7487	50.3060	49.8158	50.6100	44.6494	45.3638	45.5995	45.8291	46.3746	45.7972	46.3770	45.7670	46.3397	45.8597	46.7426	**57.5**
H2	9.0711	8.9082	8.9926	8.7974	8.6994	8.8084	8.7504	8.8181	8.7213	8.7871	8.7457	9.0711	8.9082	8.9926	8.7974	8.6994	8.8084	8.7504	8.8181	8.7212	8.7871	8.7457	**8.11**
H3	7.4358	7.5753	7.6646	7.6196	7.7433	7.6175	7.7557	7.6152	7.7493	7.6217	7.7711	7.4358	7.5753	7.6646	7.6196	7.7433	7.6175	7.7557	7.6152	7.7493	7.6217	7.7711	**7.31**
H5	7.2401	7.4378	7.5258	7.5268	7.6588	7.5216	7.6718	7.5162	7.6614	7.5317	7.6960	7.2401	7.4378	7.5258	7.5268	7.6588	7.5216	7.6718	7.5162	7.6614	7.5317	7.6960	**7.31**
H6	8.0965	8.3044	8.4316	8.4110	8.5225	8.4061	8.5996	8.4004	8.5605	8.4158	8.6363	8.0965	8.3044	8.4316	8.4110	8.5225	8.4061	8.5996	8.4004	8.5606	8.4158	8.6363	**8.11**
H8	3.6381	3.7437	3.8354	3.8239	3.9329	3.8188	4.0011	3.8133	3.9706	3.8288	3.9979	3.6381	3.7437	3.8354	3.8239	3.9329	3.8188	4.0011	3.8133	3.9706	3.8288	3.9979	**5.18**
H(9A-9B)	1.3084	1.3301	1.3445	1.3363	1.2736	1.3379	1.2820	1.3390	1.2675	1.3349	1.3033	1.3084	1.3301	1.3445	1.3363	1.2736	1.3379	1.2820	1.3390	1.2675	1.3349	1.3033	**2.05**
H(10A)	0.9656	0.7280	0.7412	0.6826	0.6635	0.6833	0.6994	0.6843	0.7008	0.6822	0.7041	0.9656	0.7280	0.7412	0.6826	0.6635	0.6833	0.6994	0.6843	0.7008	0.6822	0.7041	**1.14**
H(10B)	1.3770	1.3012	1.2518	1.2206	1.1379	1.2267	1.1517	1.2323	1.1569	1.2149	1.1303	1.3771	1.3012	1.2518	1.2206	1.1379	1.2267	1.1517	1.2323	1.1568	1.2149	1.1303	**1.39**
H(11A-11B)	0.8644	0.8763	0.8546	0.8936	0.8559	0.8927	0.8656	0.8916	0.8636	0.8945	0.8622	0.8644	0.8763	0.8546	0.8936	0.8559	0.8927	0.8656	0.8917	0.8636	0.8944	0.8622	**1.22**
H(12A-12C)	0.9257	0.9009	0.8816	0.8957	0.8713	0.8956	0.8816	0.8955	0.8831	0.8958	0.8787	0.9257	0.9009	0.8817	0.8957	0.8713	0.8956	0.8816	0.8955	0.8831	0.8958	0.8787	**0.77**
H(1`A)	2.3729	2.3640	2.3490	2.3541	2.3106	2.3546	2.3370	2.3550	2.3368	2.3537	2.3150	2.5341	2.5327	2.5042	2.4991	2.4550	2.5016	2.4708	2.5039	2.4741	2.4967	2.4443	**3.16**
H(1`B)	2.7192	2.7822	2.8168	2.8250	2.8747	2.8223	2.8737	2.8195	2.8658	2.8276	2.8825	2.3793	2.2880	2.2538	2.2872	2.3250	2.2852	2.2832	2.2834	2.2964	2.2895	2.2833	**3.76**
H(2`A-2`B)	1.4856	1.5304	1.4937	1.5699	1.5249	1.5670	1.5387	1.5640	1.5343	1.5727	1.5563	1.3833	1.4798	1.4293	1.5356	1.5073	1.5313	1.5400	1.5271	1.5358	1.5397	1.5700	**2.13**
H(3`A-3`B)	1.3833	1.4798	1.4293	1.5356	1.5073	1.5313	1.5400	1.5270	1.5358	1.5397	1.5700	1.4856	1.5304	1.4937	1.5699	1.5249	1.5670	1.5387	1.5640	1.5343	1.5727	1.5563	**2.05**
H(4`A)	2.3793	2.2880	2.2538	2.2872	2.3250	2.2852	2.2832	2.2834	2.2964	2.2895	2.2833	2.7192	2.7822	2.8168	2.8250	2.8747	2.8223	2.8737	2.8195	2.8658	2.8276	2.8825	**3.09**
H(4`B)	2.5341	2.5327	2.5042	2.4991	2.4550	2.5016	2.4708	2.5039	2.4741	2.4967	2.4443	2.3728	2.3640	2.3490	2.3541	2.3106	2.3546	2.3370	2.3550	2.3368	2.3537	2.3150	**3.63**
F4	-92.4769	-93.7757	-95.4120	-94.1485	-97.5580	-94.1133	-95.6118	-94.0822	-96.0599	-94.1816	-95.4835	-92.4768	-93.7757	-95.4120	-94.1485	-97.5580	-94.1133	-95.6118	-94.0823	-96.0600	-94.1816	-95.4835	**-104.5**
Nuclei	**LC-BLYP**																						
C1	144.3028	145.1950	146.1042	145.8010	147.4677	145.7589	146.7872	145.7404	146.8037	145.8203	147.0726	144.3028	145.1949	146.1041	145.8010	147.4677	145.7589	146.7872	145.7405	146.8037	145.8203	147.0725	**132.8**
C2	148.6053	148.4336	148.9601	148.2830	148.7557	148.2707	149.2718	148.2857	149.1701	148.2777	149.2677	148.6053	148.4336	148.9602	148.2830	148.7557	148.2707	149.2718	148.2859	149.1701	148.2778	149.2676	**132.9**
C3	128.2541	128.9264	129.5380	129.1390	129.8089	129.1086	129.9774	129.1049	129.9340	129.1500	130.0396	128.2541	128.9264	129.5380	129.1390	129.8089	129.1086	129.9774	129.1048	129.9339	129.1500	130.0397	**117.2**
C4	181.9735	182.5089	183.1029	182.8610	183.3907	182.8163	184.0004	182.7995	183.8613	182.8865	184.1304	181.9735	182.5091	183.1027	182.8610	183.3907	182.8164	184.0004	182.7995	183.8613	182.8865	184.1304	**167.5**
C5	126.1791	127.4745	128.1385	128.2234	129.0703	128.1579	129.2286	128.1194	129.1271	128.2680	129.3934	126.1791	127.4745	128.1384	128.2234	129.0703	128.1579	129.2287	128.1195	129.1270	128.2679	129.3934	**117.2**
C6	144.2567	146.1931	147.4116	147.2757	148.9440	147.1795	149.5452	147.1123	149.2785	147.3512	149.9505	144.2567	146.1930	147.4116	147.2757	148.9440	147.1795	149.5451	147.1124	149.2785	147.3512	149.9505	**132.9**
C7	211.8303	217.0927	218.4451	220.2118	220.7174	220.0151	226.8416	219.8419	225.4392	220.3777	228.0439	211.8303	217.0927	218.4455	220.2118	220.7174	220.0150	226.8416	219.8416	225.4392	220.3777	228.0436	**195.8**
C8	62.4946	63.6122	64.3010	64.2400	65.1246	64.1886	65.9586	64.1624	65.7354	64.2696	66.4491	62.4946	63.6122	64.3010	64.2400	65.1246	64.1886	65.9586	64.1624	65.7354	64.2696	66.4492	**68.4**
C9	33.0906	32.7128	32.9583	32.5697	32.8735	32.5573	33.0162	32.5722	32.9124	32.5640	33.1062	33.0906	32.7128	32.9583	32.5697	32.8734	32.5573	33.0162	32.5722	32.9124	32.5640	33.1062	**30.5**
C10	26.7174	27.0997	27.5416	27.4779	28.1510	27.4294	27.9545	27.4087	27.9216	27.5068	28.1708	26.7174	27.0997	27.5417	27.4779	28.1510	27.4295	27.9545	27.4088	27.9216	27.5068	28.1708	**27.6**
C11	25.6629	25.6738	26.0213	25.6762	26.0987	25.6556	26.0916	25.6622	26.0813	25.6781	26.2660	25.6628	25.6738	26.0212	25.6762	26.0987	25.6557	26.0917	25.6622	26.0813	25.6781	26.2660	**23.1**
C12	15.2825	15.3973	15.4777	15.5469	15.6332	15.5145	15.5678	15.5098	15.5562	15.5604	15.5999	15.2825	15.3974	15.4776	15.5468	15.6333	15.5145	15.5678	15.5098	15.5562	15.5604	15.5999	**13.8**
C1`	48.8633	49.5850	49.8719	50.1266	50.6951	50.0699	50.6789	50.0406	50.6292	50.1636	51.1331	52.7573	53.6750	54.0588	54.1648	54.6804	54.1139	54.7997	54.0904	54.7504	54.1956	55.0687	**53.5**
C2`	23.0097	23.2733	23.5886	23.4460	23.8619	23.4152	23.9107	23.4114	23.8912	23.4575	23.8212	22.3648	22.4849	22.8031	22.6272	23.0962	22.5957	22.9834	22.5919	22.9779	22.6398	22.9003	**24.5**
C3`	22.3648	22.4849	22.8032	22.6272	23.0962	22.5957	22.9834	22.5918	22.9779	22.6398	22.9003	23.0098	23.2733	23.5887	23.4460	23.8619	23.4152	23.9107	23.4114	23.8911	23.4575	23.8213	**24.3**
C4`	52.7572	53.6750	54.0587	54.1648	54.6804	54.1139	54.7997	54.0903	54.7504	54.1956	55.0688	48.8633	49.5850	49.8719	50.1267	50.6951	50.0699	50.6789	50.0406	50.6292	50.1636	51.1331	**57.5**
H2	9.0056	8.8849	8.9030	8.7965	8.7977	8.7995	8.7926	8.8043	8.8043	8.7932	8.7781	9.0056	8.8849	8.9030	8.7965	8.7977	8.7994	8.7926	8.8043	8.8043	8.7932	8.7781	**8.11**
H3	7.5396	7.6763	7.7674	7.7172	7.8365	7.7144	7.8519	7.7131	7.8455	7.7189	7.8671	7.5396	7.6763	7.7674	7.7172	7.8365	7.7144	7.8519	7.7131	7.8455	7.7189	7.8671	**7.31**
H5	7.3877	7.5702	7.6618	7.6532	7.7802	7.6475	7.7925	7.6434	7.7820	7.6575	7.8161	7.3877	7.5702	7.6618	7.6532	7.7802	7.6475	7.7926	7.6434	7.7820	7.6575	7.8161	**7.31**
H6	8.1905	8.3935	8.4921	8.4932	8.6406	8.4854	8.6743	8.4792	8.6601	8.4999	8.7076	8.1905	8.3935	8.4921	8.4932	8.6406	8.4854	8.6743	8.4792	8.6601	8.4999	8.7076	**8.11**
H8	4.2049	4.2951	4.3484	4.3672	4.4527	4.3612	4.4800	4.3569	4.4681	4.3721	4.4886	4.2049	4.2951	4.3484	4.3672	4.4527	4.3612	4.4800	4.3569	4.4681	4.3722	4.4886	**5.18**
H(9A-9B)	1.6602	1.6944	1.6916	1.7190	1.7312	1.7160	1.7354	1.7147	1.7257	1.7209	1.7694	1.6602	1.6944	1.6916	1.7190	1.7312	1.7160	1.7354	1.7147	1.7257	1.7209	1.7694	**2.05**
H(10A)	0.9464	0.7709	0.7337	0.7059	0.6281	0.7076	0.6393	0.7111	0.6461	0.7035	0.6520	0.9464	0.7709	0.7337	0.7059	0.6281	0.7076	0.6393	0.7111	0.6461	0.7035	0.6520	**1.14**
H(10B)	1.5956	1.4998	1.4331	1.4116	1.3290	1.4162	1.3204	1.4225	1.3282	1.4064	1.2946	1.5956	1.4998	1.4331	1.4116	1.3290	1.4162	1.3204	1.4225	1.3282	1.4064	1.2946	**1.39**
H(11A-11B)	0.9922	1.0091	0.9759	1.0198	0.9828	1.0178	0.9739	1.0175	0.9768	1.0208	0.9667	0.9922	1.0091	0.9759	1.0198	0.9828	1.0178	0.9739	1.0175	0.9768	1.0208	0.9667	**1.22**
H(12A-12C)	0.9529	0.9320	0.9064	0.9207	0.8812	0.9204	0.8804	0.9217	0.8832	0.9200	0.8772	0.9529	0.9320	0.9064	0.9207	0.8812	0.9204	0.8803	0.9216	0.8832	0.9200	0.8772	**0.77**
H(1`A)	2.6756	2.6656	2.6476	2.6566	2.6054	2.6565	2.6213	2.6579	2.6203	2.6558	2.6008	2.8095	2.7976	2.7819	2.7777	2.7409	2.7787	2.7655	2.7812	2.7634	2.7757	2.7396	**3.16**
H(1`B)	3.0184	3.0586	3.0951	3.0995	3.1550	3.0957	3.1431	3.0935	3.1381	3.1022	3.1499	2.7332	2.5800	2.5558	2.5523	2.5380	2.5532	2.5182	2.5557	2.5071	2.5505	2.5099	**3.76**
H(2`A-2`B)	1.6952	1.7327	1.6981	1.7670	1.7206	1.7638	1.7292	1.7622	1.7248	1.7691	1.7476	1.5899	1.6712	1.6339	1.7211	1.6782	1.7172	1.7066	1.7150	1.7020	1.7238	1.7383	**2.13**
H(3`A-3`B)	1.5899	1.6712	1.6339	1.7211	1.6782	1.7172	1.7066	1.7149	1.7020	1.7238	1.7383	1.6952	1.7327	1.6981	1.7670	1.7206	1.7638	1.7292	1.7622	1.7248	1.7691	1.7476	**2.05**
H(4`A)	2.7332	2.5800	2.5558	2.5523	2.5380	2.5532	2.5182	2.5557	2.5071	2.5505	2.5099	3.0184	3.0586	3.0951	3.0995	3.1550	3.0957	3.1431	3.0935	3.1381	3.1022	3.1499	**3.09**
H(4`B)	2.8095	2.7976	2.7819	2.7777	2.7409	2.7787	2.7655	2.7812	2.7634	2.7757	2.7396	2.6756	2.6656	2.6476	2.6566	2.6054	2.6565	2.6213	2.6579	2.6203	2.6558	2.6008	**3.63**
F4	-102.7646	-104.5332	-106.7278	-104.9953	-108.4054	-104.9782	-106.6670	-104.9590	-106.8896	-105.0099	-106.5740	-102.7646	-104.5332	-106.7278	-104.9953	-108.4055	-104.9782	-106.6671	-104.9589	-106.8897	-105.0099	-106.5740	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. VII

Nuclei	R											S										Exp. [b]
	M06											M06										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.6837	138.1845	138.7887	138.8803	142.1616	138.8390	141.0201	138.8028	141.1968	138.9324	141.3525	136.6837	138.1845	138.7887	138.8803	142.1616	138.8390	141.0201	138.8027	141.1968	138.9324	141.3525	**132.8**
C2	139.8288	139.8302	140.5330	139.7616	140.5668	139.7588	141.0927	139.7635	140.9947	139.7793	141.0467	139.8288	139.8302	140.5330	139.7616	140.5668	139.7588	141.0927	139.7635	140.9947	139.7793	141.0466	**132.9**
C3	121.7274	122.3706	123.0781	122.5656	123.3591	122.5459	123.5764	122.5339	123.5302	122.5989	123.6983	121.7273	122.3706	123.0781	122.5656	123.3592	122.5459	123.5764	122.5338	123.5302	122.5989	123.6984	**117.2**
C4	173.6534	174.3654	175.1102	174.6855	175.0219	174.6538	175.6222	174.6298	175.4678	174.7300	175.7595	173.6534	174.3654	175.1102	174.6855	175.0220	174.6538	175.6222	174.6297	175.4678	174.7300	175.7595	**167.5**
C5	119.5548	120.7943	121.4738	121.5477	122.5989	121.4922	122.8231	121.4445	122.7327	121.6146	122.9843	119.5548	120.7943	121.4739	121.5477	122.5989	121.4922	122.8231	121.4445	122.7327	121.6146	122.9844	**117.2**
C6	136.4800	138.1760	139.3711	139.1977	140.2318	139.1198	140.8785	139.0504	140.6173	139.2868	141.1362	136.4800	138.1760	139.3711	139.1977	140.2318	139.1198	140.8785	139.0504	140.6173	139.2868	141.1362	**132.9**
C7	203.9031	208.9344	210.1431	211.5776	213.5179	211.4065	218.3465	211.2396	217.2496	211.7527	219.5336	203.9031	208.9344	210.1431	211.5776	213.5178	211.4065	218.3465	211.2398	217.2496	211.7527	219.5336	**195.8**
C8	62.4081	63.5176	64.2402	64.1969	65.5191	64.1481	66.0334	64.1062	65.8734	64.2578	66.5123	62.4081	63.5176	64.2401	64.1969	65.5191	64.1481	66.0334	64.1062	65.8734	64.2578	66.5124	**68.4**
C9	33.8614	33.5608	34.1825	33.4541	33.5991	33.4442	33.8295	33.4403	33.7236	33.4773	33.9495	33.8614	33.5608	34.1825	33.4541	33.5991	33.4442	33.8295	33.4403	33.7236	33.4773	33.9496	**30.5**
C10	25.9231	26.6415	27.3493	27.1312	28.1401	27.0798	27.8705	27.0349	27.8296	27.1942	28.2499	25.9232	26.6415	27.3493	27.1312	28.1402	27.0798	27.8705	27.0350	27.8296	27.1942	28.2499	**27.6**
C11	26.4897	26.5713	27.0992	26.6108	27.1999	26.5919	27.1386	26.5795	27.1135	26.6426	27.3645	26.4897	26.5713	27.0993	26.6108	27.1998	26.5919	27.1386	26.5795	27.1135	26.6426	27.3645	**23.1**
C12	15.9103	16.1276	16.3119	16.3078	16.6622	16.2818	16.5809	16.2642	16.5652	16.3475	16.6634	15.9104	16.1276	16.3119	16.3078	16.6622	16.2818	16.5809	16.2642	16.5652	16.3475	16.6635	**13.8**
C1`	50.7988	51.7722	52.1796	52.3154	52.9675	52.2717	52.8620	52.2364	52.8195	52.3722	53.3347	55.0385	56.1158	56.5140	56.6961	57.3840	56.6486	57.5406	56.6088	57.4838	56.7556	57.9703	**53.5**
C2`	23.3610	23.8539	24.2807	24.1064	24.6826	24.0798	24.6277	24.0608	24.6002	24.1462	24.5473	22.1499	22.4551	22.8638	22.6320	23.3567	22.6134	23.1653	22.6032	23.1850	22.6645	22.8605	**24.5**
C3`	22.1499	22.4551	22.8637	22.6320	23.3567	22.6134	23.1653	22.6032	23.1850	22.6645	22.8605	23.3610	23.8539	24.2807	24.1064	24.6825	24.0798	24.6277	24.0607	24.6002	24.1462	24.5472	**24.3**
C4`	55.0385	56.1158	56.5140	56.6961	57.3841	56.6486	57.5406	56.6087	57.4838	56.7556	57.9703	50.7988	51.7722	52.1796	52.3154	52.9675	52.2717	52.8620	52.2365	52.8195	52.3722	53.3348	**57.5**
H2	8.7200	8.5356	8.6199	8.4194	8.3302	8.4246	8.3913	8.4306	8.3825	8.4151	8.3799	8.7200	8.5356	8.6199	8.4194	8.3302	8.4246	8.3913	8.4306	8.3825	8.4151	8.3799	**8.11**
H3	7.3688	7.5079	7.6104	7.5243	7.6008	7.5236	7.6221	7.5236	7.6136	7.5255	7.6318	7.3688	7.5079	7.6104	7.5243	7.6008	7.5236	7.6221	7.5236	7.6136	7.5255	7.6319	**7.31**
H5	7.0547	7.2196	7.3131	7.3125	7.4915	7.3067	7.5114	7.3012	7.5006	7.3185	7.5350	7.0547	7.2196	7.3131	7.3125	7.4915	7.3067	7.5114	7.3012	7.5006	7.3185	7.5350	**7.31**
H6	8.0770	8.2186	8.3077	8.3010	8.3629	8.2950	8.4115	8.2895	8.3902	8.3074	8.4458	8.0770	8.2186	8.3077	8.3010	8.3629	8.2950	8.4115	8.2895	8.3902	8.3074	8.4458	**8.11**
H8	4.4275	4.4268	4.4630	4.4703	4.5762	4.4663	4.6245	4.4627	4.6087	4.4746	4.6669	4.4275	4.4268	4.4630	4.4703	4.5762	4.4663	4.6245	4.4627	4.6087	4.4746	4.6669	**5.18**
H(9A-9B)	1.8331	1.7715	1.8082	1.7461	1.6728	1.7461	1.6811	1.7470	1.6718	1.7469	1.7105	1.8331	1.7715	1.8082	1.7461	1.6728	1.7461	1.6811	1.7470	1.6718	1.7469	1.7105	**2.05**
H(10A)	0.7728	0.6586	0.6596	0.6274	0.6472	0.6280	0.6691	0.6289	0.6703	0.6272	0.7166	0.7728	0.6586	0.6596	0.6274	0.6472	0.6280	0.6691	0.6289	0.6678	0.6272	0.7166	**1.14**
H(10B)	1.7663	1.6085	1.5217	1.4729	1.3898	1.4826	1.4047	1.4937	1.4059	1.4648	1.3494	1.7663	1.6085	1.5217	1.4729	1.3897	1.4826	1.4047	1.4937	1.4183	1.4648	1.3494	**1.39**
H(11A-11B)	1.0514	1.0480	1.0176	1.0528	1.0214	1.0520	1.0203	1.0520	1.0195	1.0542	1.0055	1.0514	1.0480	1.0176	1.0528	1.0214	1.0520	1.0203	1.0519	1.0195	1.0542	1.0055	**1.22**
H(12A-12C)	0.9078	0.8833	0.8498	0.8652	0.8460	0.8666	0.8533	0.8688	0.8571	0.8646	0.8353	0.9078	0.8833	0.8498	0.8652	0.8460	0.8666	0.8533	0.8688	0.8571	0.8646	0.8354	**0.77**
H(1`A)	2.6899	2.6721	2.6596	2.6399	2.6025	2.6424	2.6121	2.6455	2.6133	2.6382	2.5768	2.8894	2.8866	2.8724	2.8603	2.8238	2.8625	2.8387	2.8652	2.8412	2.8590	2.8125	**3.16**
H(1`B)	3.1176	3.1382	3.1900	3.1575	3.2127	3.1551	3.2023	3.1532	3.2035	3.1604	3.1870	2.7389	2.6337	2.6366	2.6095	2.6225	2.6103	2.6180	2.6118	2.6158	2.6093	2.6306	**3.76**
H(2`A-2`B)	1.6551	1.6922	1.6633	1.7224	1.6963	1.7200	1.7052	1.7181	1.7064	1.7253	1.7325	1.6193	1.6626	1.6205	1.6896	1.6647	1.6882	1.6865	1.6864	1.6921	1.7293		**2.13**
H(3`A-3`B)	1.6193	1.6626	1.6205	1.6896	1.6647	1.6877	1.6882	1.6865	1.6894	1.6921	1.7293	1.6551	1.6922	1.6633	1.7224	1.6963	1.7200	1.7052	1.7181	1.6998	1.7253	1.7325	**2.05**
H(4`A)	2.7389	2.6337	2.6366	2.6095	2.6225	2.6103	2.6180	2.6118	2.6192	2.6093	2.6306	3.1176	3.1382	3.1900	3.1575	3.2127	3.1551	3.2023	3.1532	3.1996	3.1604	3.1870	**3.09**
H(4`B)	2.8894	2.8866	2.8724	2.8603	2.8238	2.8625	2.8387	2.8652	2.8399	2.8590	2.8125	2.6899	2.6721	2.6596	2.6399	2.6025	2.6424	2.6121	2.6455	2.6150	2.6382	2.5768	**3.63**
F4	-117.6983	-119.2994	-121.3029	-118.9567	-123.8039	-118.9528	-121.7203	-118.9471	-122.0604	-118.9592	-121.5181	-117.6983	-119.2994	-121.3029	-118.9567	-123.8038	-118.9528	-121.7203	-118.9472	-122.0604	-118.9592	-121.5182	**-104.5**
Nuclei	M06-2X											M06-2X										
C1	153.3139	154.1147	155.0923	154.6258	156.4278	154.6074	156.0736	154.5917	155.8323	154.6374	156.7424	153.3140	154.1147	155.0922	154.6258	156.4279	154.6072	156.0736	154.5917	155.8323	154.6374	156.7424	**132.8**
C2	154.9208	154.8472	155.4019	154.6764	155.2728	154.7107	155.7196	154.7454	155.6269	154.6371	155.7829	154.9207	154.8472	155.4018	154.6764	155.2727	154.7105	155.7196	154.7454	155.6269	154.6371	155.7829	**132.9**
C3	136.1763	136.8491	137.4978	137.0428	137.8093	137.0546	138.0584	137.0674	138.0027	137.0251	138.1494	136.1763	136.8491	137.4977	137.0428	137.8093	137.0547	138.0584	137.0674	138.0027	137.0251	138.1494	**117.2**
C4	187.1500	187.9566	188.6296	188.3781	189.0881	188.3727	189.7626	188.3687	189.6217	188.3768	189.9010	187.1498	187.9566	188.6296	188.3781	189.0881	188.3728	189.7626	188.3687	189.6217	188.3768	189.9010	**167.5**
C5	133.6665	135.1820	135.9032	135.9787	136.9449	135.9514	137.1623	135.9252	137.0543	135.9981	137.3183	133.6665	135.1820	135.9032	135.9787	136.9449	135.9515	137.1623	135.9252	137.0543	135.9981	137.3183	**117.2**
C6	151.1929	153.3671	154.5822	154.5301	156.3787	154.4823	156.8323	154.4355	156.6334	154.5694	157.1596	151.1930	153.3671	154.5822	154.5301	156.3788	154.4824	156.8323	154.4355	156.6334	154.5694	157.1596	**132.9**
C7	219.5245	224.8907	226.3983	228.0101	228.7404	227.8294	235.4867	227.6520	233.7316	228.1759	237.1101	219.5241	224.8907	226.3983	228.0101	228.7407	227.8297	235.4867	227.6520	233.7316	228.1759	237.1101	**195.8**
C8	67.2610	68.6483	69.3496	69.3548	70.4448	69.3293	71.3018	69.3060	71.0041	69.3732	72.0281	67.2610	68.6483	69.3496	69.3548	70.4448	69.3292	71.3018	69.3060	71.0041	69.3732	72.0281	**68.4**
C9	35.4642	35.4239	35.5992	35.3385	35.6219	35.3672	35.7953	35.3969	35.7017	35.3048	36.0192	35.4642	35.4239	35.5992	35.3385	35.6220	35.3672	35.7953	35.3969	35.7017	35.3048	36.0192	**30.5**
C10	28.1749	28.5554	28.9127	28.9302	29.6142	28.9248	29.4107	28.9207	29.3703	28.9290	29.6021	28.1749	28.5554	28.9126	28.9302	29.6141	28.9248	29.4107	28.9207	29.3703	28.9290	29.6021	**27.6**
C11	27.0694	27.0411	27.3428	27.0466	27.4659	27.0675	27.4579	27.0895	27.4476	27.0203	27.6157	27.0693	27.0411	27.3428	27.0466	27.4660	27.0676	27.4579	27.0895	27.4476	27.0203	27.6156	**23.1**
C12	15.6785	15.8894	15.9172	16.0069	16.0766	16.0199	16.0059	16.0341	16.0007	15.9879	15.9410	15.6786	15.8894	15.9172	16.0069	16.0767	16.0199	16.0059	16.0341	16.0007	15.9879	15.9410	**13.8**
C1`	52.7471	53.4371	53.7246	53.9470	54.4968	53.9305	54.5272	53.9162	54.4023	53.9572	54.9826	57.2784	58.0992	58.4834	58.4784	59.0562	58.4723	59.1518	58.4681	59.1113	58.4785	59.4310	**53.5**
C2`	24.6913	25.0617	25.3331	25.2432	25.6602	25.2509	25.6528	25.2603	25.6474	25.2298	25.6465	23.7535	24.0580	24.3338	24.2747	24.7880	24.2798	24.7486	24.2866	24.7300	24.2642	24.8143	**24.5**
C3`	23.7535	24.0580	24.3338	24.2747	24.7881	24.2797	24.7486	24.2866	24.7300	24.2642	24.8143	24.6914	25.0617	25.3332	25.2432	25.6603	25.2509	25.6528	25.2603	25.6474	25.2298	25.6465	**24.3**
C4`	57.2784	58.0992	58.4835	58.4784	59.0562	58.4723	59.1518	58.4681	59.1113	58.4785	59.4310	52.7471	53.4371	53.7245	53.9470	54.4969	53.9305	54.5272	53.9162	54.4023	53.9572	54.9826	**57.5**
H2	9.2553	9.1886	9.2043	9.1236	9.1185	9.1277	9.1058	9.1311	9.1346	9.1198	9.0783	9.2553	9.1886	9.2043	9.1236	9.1185	9.1277	9.1058	9.1311	9.1346	9.1198	9.0783	**8.11**
H3	7.8496	7.9991	8.0968	8.0550	8.1780	8.0508	8.2036	8.0462	8.1958	8.0590	8.2179	7.8496	7.9991	8.0968	8.0550	8.1780	8.0508	8.2036	8.0462	8.1958	8.0590	8.2179	**7.31**
H5	7.6700	7.8593	7.9559	7.9464	8.0779	7.9403	8.0866	7.9337	8.0791	7.9524	8.1072	7.6700	7.8593	7.9559	7.9464	8.0779	7.9403	8.0866	7.9337	8.0791	7.9524	8.1072	**7.31**
H6	8.5783	8.7576	8.8602	8.8626	9.0133	8.8546	9.0581	8.8464	9.0490	8.8703	9.0681	8.5783	8.7576	8.8602	8.8626	9.0133	8.8546	9.0581	8.8464	9.0490	8.8703	9.0681	**8.11**
H8	4.2922	4.3772	4.4355	4.4447	4.5306	4.4393	4.5577	4.4336	4.5580	4.4499	4.5479	4.2922	4.3772	4.4355	4.4447	4.5306	4.4393	4.5577	4.4336	4.5580	4.4499	4.5479	**5.18**
H(9A-9B)	1.6952	1.7512	1.7338	1.7870	1.7864	1.7839	1.7723	1.7805	1.7723	1.7901	1.8164	1.6952	1.7512	1.7338	1.7870	1.7864	1.7839	1.7723	1.7805	1.7723	1.7901	1.8164	**2.05**
H(10A)	0.8886	0.7034	0.6742	0.6310	0.5530	0.6339	0.5704	0.6364	0.5766	0.6284	0.6028	0.8886	0.7034	0.6742	0.6310	0.5530	0.6339	0.5704	0.6364	0.5766	0.6284	0.6028	**1.14**
H(10B)	1.5834	1.5136	1.4450	1.4129	1.3259	1.4186	1.3112	1.4240	1.3267	1.4077	1.2702	1.5834	1.5136	1.4449	1.4129	1.3259	1.4186	1.3112	1.4240	1.3267	1.4077	1.2702	**1.39**
H(11A-11B)	0.9471	0.9670	0.9367	0.9816	0.9426	0.9795	0.9338	0.9771	0.9397	0.9837	0.9138	0.9471	0.9670	0.9367	0.9816	0.9426	0.9795	0.9338	0.9771	0.9397	0.9837	0.9138	**1.22**
H(12A-12C)	0.8951	0.8808	0.8572	0.8688	0.8253	0.8683	0.8226	0.8674	0.8290	0.8694	0.8069	0.8951	0.8808	0.8572	0.8688	0.8253	0.8683	0.8226	0.8674	0.8290	0.8694	0.8069	**0.77**
H(1`A)	2.6201	2.6148	2.6019	2.6064	2.5567	2.6061	2.5649	2.6055	2.5694	2.6068	2.5425	2.8027	2.8010	2.7892	2.7839	2.7542	2.7840	2.7717	2.7838	2.7696	2.7840	2.7411	**3.16**
H(1`B)	3.0833	3.1152	3.1403	3.1536	3.1988	3.1498	3.1827	3.1456	3.1831	3.1574	3.1910	2.7295	2.6123	2.5775	2.5866	2.5699	2.5867	2.5575	2.5864	2.5371	2.5867	2.5782	**3.76**
H(2`A-2`B)	1.6995	1.7373	1.7056	1.7719	1.7264	1.7684	1.7331	1.7647	1.7310	1.7753	1.7445	1.6106	1.6861	1.6582	1.7345	1.6958	1.7299	1.7278	1.7250	1.7222	1.7391	1.7543	**2.13**
H(3`A-3`B)	1.6106	1.6861	1.6582	1.7345	1.6959	1.7299	1.7278	1.7250	1.7222	1.7391	1.7543	1.6995	1.7373	1.7057	1.7719	1.7264	1.7684	1.7331	1.7647	1.7310	1.7753	1.7445	**2.05**
H(4`A)	2.7295	2.6123	2.5775	2.5866	2.5699	2.5867	2.5575	2.5864	2.5371	2.5867	2.5782	3.0833	3.1152	3.1402	3.1536	3.1988	3.1498	3.1827	3.1456	3.1831	3.1574	3.1910	**3.09**
H(4`B)	2.8027	2.8010	2.7892	2.7839	2.7542	2.7840	2.7717	2.7838	2.7696	2.7840	2.7411	2.6201	2.6148	2.6019	2.6064	2.5567	2.6061	2.5649	2.6055	2.5694	2.6068	2.5425	**3.63**
F4	-114.4379	-115.5001	-117.9210	-115.5535	-119.2724	-115.5557	-117.3185	-115.5562	-117.5468	-115.5516	-117.2639	-114.4381	-115.5001	-117.9210	-115.5535	-119.2724	-115.5556	-117.3185	-115.5562	-117.5468	-115.5516	-117.2639	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. VIII

Nuclei	R											S										Exp. [b]
	mpW1LYP											mpW1LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.8378	140.8440	141.4180	141.3625	142.7491	141.3294	142.1529	141.2986	142.1820	141.3923	142.2792	139.8378	140.8440	141.4181	141.3622	142.7491	141.3294	142.1530	141.2986	142.1819	141.3923	142.2792	**132.8**
C2	139.8714	139.7984	140.3079	139.7197	140.1190	139.7218	140.6847	139.7258	140.5678	139.7161	140.5968	139.8714	139.7984	140.3079	139.7196	140.1190	139.7218	140.6848	139.7258	140.5678	139.7161	140.5970	**132.9**
C3	122.0463	122.6720	123.2099	122.8903	123.4471	122.8775	123.7073	122.8655	123.6488	122.9006	123.7499	122.0463	122.6720	123.2099	122.8905	123.4470	122.8775	123.7074	122.8655	123.6487	122.9006	123.7498	**117.2**
C4	176.3397	177.1720	177.7901	177.5913	178.1904	177.5635	178.7928	177.5372	178.6520	177.6158	178.9042	176.3397	177.1719	177.7901	177.5914	178.1902	177.5635	178.7927	177.5372	178.6517	177.6158	178.9042	**167.5**
C5	119.8982	121.0713	121.6786	121.7085	122.4580	121.6663	122.6459	121.6259	122.5595	121.7466	122.7780	119.8982	121.0713	121.6786	121.7085	122.4581	121.6663	122.6458	121.6259	122.5594	121.7465	122.7779	**117.2**
C6	136.0966	138.0128	139.1739	139.1635	140.6582	139.0867	141.3023	139.0117	141.0638	139.2346	141.6841	136.0966	138.0128	139.1739	139.1635	140.6585	139.0867	141.3022	139.0117	141.0638	139.2346	141.6841	**132.9**
C7	203.6129	208.5205	209.5677	211.1801	211.7568	211.0176	216.9290	210.8561	215.7371	211.3332	217.9149	203.6129	208.5205	209.5677	211.1801	211.7568	211.0176	216.9290	210.8561	215.7372	211.3332	217.9147	**195.8**
C8	65.8463	67.0437	67.6010	67.5551	68.5804	67.5298	69.1701	67.5042	69.0076	67.5753	69.4725	65.8463	67.0437	67.6010	67.5551	68.5805	67.5298	69.1701	67.5042	69.0077	67.5753	69.4725	**68.4**
C9	37.0169	36.6560	36.8848	36.5180	36.8153	36.5233	37.0170	36.5296	36.9632	36.5106	37.0610	37.0169	36.6560	36.8848	36.5180	36.8153	36.5233	37.0170	36.5296	36.9632	36.5106	37.0610	**30.5**
C10	29.3292	29.7978	30.3192	30.1290	30.8587	30.1027	30.6588	30.0784	30.6559	30.1521	30.7746	29.3292	29.7978	30.3193	30.1290	30.8587	30.1027	30.6588	30.0784	30.6559	30.1521	30.7746	**27.6**
C11	29.4068	29.5120	29.8154	29.4911	29.9151	29.4934	29.9122	29.4963	29.9182	29.4864	30.0182	29.4067	29.5120	29.8153	29.4911	29.9151	29.4934	29.9121	29.4963	29.9182	29.4865	30.0180	**23.1**
C12	16.7769	16.9386	17.0341	17.0893	17.1643	17.0748	17.1257	17.0621	17.1298	17.1017	17.1017	16.7769	16.9387	17.0340	17.0893	17.1642	17.0748	17.1257	17.0621	17.1298	17.1017	17.1017	**13.8**
C1`	51.9766	52.7794	53.1018	53.3629	53.8586	53.3224	53.8640	53.2840	53.8039	53.4001	54.3551	56.5078	57.6071	57.9635	58.0839	58.5838	58.0550	58.7006	58.0272	58.6452	58.1090	58.9220	**53.5**
C2`	25.9559	26.4339	26.8102	26.6257	27.1139	26.6133	27.1490	26.6020	27.1457	26.6349	26.9197	25.5722	25.7544	26.1426	25.9442	26.3949	25.9276	26.3477	25.9127	26.3492	25.9585	26.1388	**24.5**
C3`	25.5722	25.7545	26.1426	25.9444	26.3949	25.9276	26.3478	25.9127	26.3493	25.9585	26.1388	25.9559	26.4339	26.8101	26.6257	27.1139	26.6133	27.1490	26.6020	27.1458	26.6349	26.9196	**24.3**
C4`	56.5078	57.6072	57.9635	58.0838	58.5838	58.0550	58.7006	58.0272	58.6452	58.1090	58.9219	51.9767	52.7795	53.1019	53.3630	53.8586	53.3223	53.8640	53.2840	53.8039	53.4001	54.3551	**57.5**
H2	8.7240	8.6003	8.6562	8.5315	8.5403	8.5359	8.5588	8.5399	8.5634	8.5273	8.5464	8.7240	8.6003	8.6562	8.5315	8.5403	8.5359	8.5588	8.5399	8.5634	8.5273	8.5464	**8.11**
H3	7.3356	7.4800	7.5666	7.5264	7.6381	7.5244	7.6591	7.5221	7.6515	7.5280	7.6715	7.3356	7.4800	7.5666	7.5264	7.6381	7.5244	7.6591	7.5221	7.6515	7.5280	7.6715	**7.31**
H5	7.1538	7.3065	7.4076	7.3765	7.5081	7.3726	7.5127	7.3684	7.5049	7.3800	7.5376	7.1538	7.3065	7.4076	7.3765	7.5081	7.3726	7.5127	7.3684	7.5049	7.3800	7.5376	**7.31**
H6	7.9770	8.1646	8.2590	8.2681	8.3872	8.2620	8.4387	8.2555	8.4208	8.2738	8.4656	7.9770	8.1646	8.2590	8.2681	8.3872	8.2620	8.4387	8.2555	8.4208	8.2738	8.4656	**8.11**
H8	4.5678	4.6311	4.6745	4.6785	4.7338	4.6749	4.7727	4.6711	4.7587	4.6818	4.7496	4.5678	4.6311	4.6745	4.6785	4.7339	4.6749	4.7727	4.6711	4.7588	4.6818	4.7496	**5.18**
H(9A-9B)	1.6834	1.7242	1.7339	1.7539	1.7850	1.7522	1.7829	1.7502	1.7789	1.7553	1.8165	1.6834	1.7242	1.7339	1.7539	1.7850	1.7522	1.7829	1.7502	1.7789	1.7553	1.8165	**2.05**
H(10A)	1.0055	0.8560	0.8506	0.8221	0.7324	0.8230	0.7821	0.8238	0.7767	0.8214	0.7850	1.0055	0.8560	0.8507	0.8221	0.7324	0.8230	0.7820	0.8238	0.7767	0.8214	0.7850	**1.14**
H(10B)	1.6473	1.5445	1.4864	1.4679	1.3838	1.4733	1.3800	1.4783	1.3873	1.4627	1.3500	1.6473	1.5445	1.4864	1.4679	1.3838	1.4733	1.3800	1.4783	1.3873	1.4627	1.3501	**1.39**
H(11A-11B)	1.0567	1.0723	1.0451	1.0911	1.0518	1.0902	1.0512	1.0890	1.0511	1.0918	1.0381	1.0567	1.0723	1.0451	1.0910	1.0518	1.0902	1.0512	1.0890	1.0511	1.0918	1.0380	**1.22**
H(12A-12C)	0.9504	0.9373	0.9166	0.9332	0.8920	0.9336	0.8995	0.9338	0.9000	0.9328	0.8904	0.9504	0.9373	0.9166	0.9332	0.8920	0.9336	0.8995	0.9338	0.9000	0.9328	0.8904	**0.77**
H(1`A)	2.7337	2.7265	2.7160	2.7171	2.6748	2.7178	2.6932	2.7183	2.6947	2.7162	2.6554	2.8635	2.8719	2.8555	2.8496	2.8211	2.8518	2.8323	2.8535	2.8358	2.8473	2.7929	**3.16**
H(1`B)	3.1890	3.2388	3.2723	3.2779	3.3445	3.2754	3.3319	3.2727	3.3288	3.2802	3.3270	2.8791	2.7212	2.6927	2.6981	2.6939	2.6982	2.6620	2.6982	2.6627	2.6981	2.6492	**3.76**
H(2`A-2`B)	1.7349	1.7657	1.7316	1.7997	1.7474	1.7974	1.7616	1.7949	1.7570	1.8019	1.7774	1.6061	1.6876	1.6503	1.7367	1.6849	1.7339	1.7152	1.7308	1.7080	1.7393	1.7438	**2.13**
H(3`A-3`B)	1.6061	1.6876	1.6503	1.7367	1.6850	1.7339	1.7153	1.7308	1.7080	1.7393	1.7438	1.7349	1.7657	1.7316	1.7997	1.7474	1.7974	1.7616	1.7949	1.7570	1.8019	1.7774	**2.05**
H(4`A)	2.8791	2.7212	2.6928	2.6981	2.6939	2.6982	2.6620	2.6982	2.6627	2.6981	2.6492	3.1890	3.2388	3.2723	3.2779	3.3445	3.2754	3.3319	3.2727	3.3288	3.2802	3.3270	**3.09**
H(4`B)	2.8635	2.8719	2.8555	2.8496	2.8211	2.8518	2.8323	2.8535	2.8358	2.8473	2.7929	2.7337	2.7265	2.7160	2.7171	2.6748	2.7178	2.6932	2.7183	2.6947	2.7162	2.6554	**3.63**
F4	-123.6800	-125.1567	-127.8792	-125.4417	-129.7061	-125.4315	-127.5801	-125.4197	-127.9117	-125.4509	-127.3327	-123.6800	-125.1568	-127.8792	-125.4416	-129.7063	-125.4315	-127.5801	-125.4197	-127.9118	-125.4509	-127.3325	**-104.5**
Nuclei	mpW1PW91											mpW1PW91										
C1	136.9119	137.8138	138.5064	138.2193	139.7229	138.2010	139.0452	138.1875	139.1057	138.2354	139.2865	136.9120	137.8138	138.5064	138.2193	139.7229	138.2010	139.0452	138.1875	139.1056	138.2354	139.2865	**132.8**
C2	138.8276	138.8043	139.2973	138.6548	139.2065	138.6657	139.6814	138.6819	139.5637	138.6442	139.6547	138.8278	138.8043	139.2971	138.6548	139.2065	138.6657	139.6814	138.6819	139.5637	138.6442	139.6547	**132.9**
C3	121.1664	121.9017	122.4756	122.1203	122.8340	122.1098	123.0950	122.1047	123.0259	122.1294	123.1776	121.1664	121.9017	122.4756	122.1203	122.8340	122.1098	123.0950	122.1047	123.0259	122.1294	123.1776	**117.2**
C4	173.3303	174.1682	174.7602	174.5577	175.2107	174.5337	175.8375	174.5156	175.6799	174.5797	175.9764	173.3302	174.1682	174.7601	174.5577	175.2107	174.5337	175.8374	174.5156	175.6800	174.5797	175.9764	**167.5**
C5	119.1385	120.4194	121.0633	121.0661	121.9587	121.0256	122.1586	120.9910	122.0561	121.1039	122.3339	119.1384	120.4194	121.0632	121.0661	121.9587	121.0256	122.1586	120.9910	122.0561	121.1039	122.3339	**117.2**
C6	134.9559	136.8628	138.0011	137.9900	139.5612	137.9156	140.2367	137.8478	139.9729	138.0608	140.6233	134.9558	136.8628	138.0011	137.9900	139.5612	137.9156	140.2368	137.8478	139.9729	138.0608	140.6233	**132.9**
C7	201.3961	205.9561	207.0830	208.3989	209.0671	208.2545	213.9532	208.1148	212.8505	208.5345	215.0027	201.3961	205.9561	207.0830	208.3989	209.0671	208.2545	213.9531	208.1148	212.8505	208.5345	215.0027	**195.8**
C8	63.7271	64.9001	65.6204	65.4113	66.4236	65.3869	67.0211	65.3670	66.8807	65.4325	67.4256	63.7271	64.9001	65.6204	65.4113	66.4236	65.3869	67.0211	65.3670	66.8807	65.4325	67.4256	**68.4**
C9	35.2055	34.9743	35.2048	34.8541	35.1994	34.8613	35.3954	34.8739	35.3130	34.8463	35.5099	35.2055	34.9743	35.2048	34.8541	35.1994	34.8613	35.3953	34.8739	35.3130	34.8463	35.5099	**30.5**
C10	27.3826	27.8477	28.3064	28.1713	28.8921	28.1466	28.7034	28.1281	28.6810	28.1948	28.8882	27.3826	27.8477	28.3064	28.1713	28.8921	28.1466	28.7033	28.1281	28.6810	28.1948	28.8882	**27.6**
C11	27.3749	27.5041	27.7467	27.4542	27.8881	27.4594	27.8795	27.4701	27.8744	27.4481	28.0331	27.3749	27.5041	27.7467	27.4542	27.8881	27.4594	27.8795	27.4701	27.8744	27.4481	28.0331	**23.1**
C12	16.2791	16.4535	16.4886	16.5599	16.6580	16.5511	16.6097	16.5484	16.6016	16.5678	16.6160	16.2792	16.4535	16.4886	16.5599	16.6580	16.5511	16.6097	16.5484	16.6016	16.5678	16.6159	**13.8**
C1`	50.5318	51.3520	51.5695	51.8485	52.3867	51.8154	52.3789	51.7886	52.2993	51.8801	52.8661	54.8407	55.9339	56.2529	56.3574	56.8717	56.3332	57.0066	56.3147	56.9463	56.3796	57.2577	**53.5**
C2`	24.7484	25.1441	25.4666	25.2813	25.7455	25.2736	25.7527	25.2717	25.7502	25.2877	25.5751	24.2083	24.4220	24.6984	24.5579	25.0088	24.5487	24.9507	24.5454	24.9402	24.5661	24.8202	**24.5**
C3`	24.2083	24.4220	24.6984	24.5579	25.0088	24.5487	24.9506	24.5454	24.9402	24.5661	24.8202	24.7485	25.1441	25.4666	25.2813	25.7455	25.2736	25.7527	25.2717	25.7502	25.2877	25.5751	**24.3**
C4`	54.8407	55.9339	56.2529	56.3574	56.8717	56.3332	57.0066	56.3147	56.9463	56.3796	57.2577	50.5318	51.3520	51.5695	51.8485	52.3867	51.8154	52.3788	51.7886	52.2993	51.8801	52.8661	**57.5**
H2	8.7635	8.6626	8.6890	8.5947	8.5982	8.5987	8.6271	8.6029	8.6234	8.5912	8.6110	8.7635	8.6626	8.6890	8.5947	8.5982	8.5987	8.6270	8.6029	8.6234	8.5912	8.6110	**8.11**
H3	7.3658	7.5155	7.6032	7.5610	7.6800	7.5592	7.7031	7.5573	7.6942	7.5630	7.7179	7.3658	7.5155	7.6032	7.5610	7.6800	7.5592	7.7031	7.5573	7.6942	7.5630	7.7179	**7.31**
H5	7.1836	7.3496	7.4493	7.4199	7.5570	7.4159	7.5642	7.4120	7.5548	7.4239	7.5904	7.1836	7.3496	7.4493	7.4199	7.5570	7.4159	7.5642	7.4120	7.5548	7.4239	7.5904	**7.31**
H6	8.0628	8.2466	8.3313	8.3493	8.4725	8.3429	8.5300	8.3368	8.5082	8.3556	8.5578	8.0628	8.2466	8.3313	8.3493	8.4725	8.3429	8.5300	8.3368	8.5082	8.3556	8.5578	**8.11**
H8	4.5666	4.6312	4.6552	4.6838	4.7335	4.6802	4.7762	4.6767	4.7569	4.6876	4.7740	4.5667	4.6312	4.6551	4.6838	4.7335	4.6802	4.7761	4.6767	4.7569	4.6876	4.7740	**5.18**
H(9A-9B)	1.7143	1.7479	1.7554	1.7759	1.7961	1.7741	1.7987	1.7723	1.7919	1.7780	1.8300	1.7142	1.7479	1.7554	1.7759	1.7961	1.7741	1.7987	1.7723	1.7919	1.7780	1.8300	**2.05**
H(10A)	0.9433	0.8037	0.7605	0.7576	0.6696	0.7596	0.7118	0.7618	0.7018	0.7561	0.7199	0.9433	0.8037	0.7605	0.7576	0.6696	0.7596	0.7118	0.7618	0.7018	0.7561	0.7199	**1.14**
H(10B)	1.6289	1.5322	1.4591	1.4457	1.3602	1.4519	1.3550	1.4581	1.3605	1.4403	1.3252	1.6289	1.5322	1.4591	1.4457	1.3602	1.4519	1.3550	1.4581	1.3605	1.4403	1.3252	**1.39**
H(11A-11B)	1.0002	1.0196	0.9828	1.0300	0.9938	1.0298	0.9939	1.0296	0.9925	1.0305	0.9821	1.0003	1.0196	0.9828	1.0300	0.9938	1.0298	0.9939	1.0296	0.9925	1.0305	0.9821	**1.22**
H(12A-12C)	0.8944	0.8820	0.8543	0.8714	0.8330	0.8723	0.8394	0.8732	0.8390	0.8708	0.8339	0.8944	0.8820	0.8543	0.8714	0.8330	0.8723	0.8393	0.8732	0.8390	0.8708	0.8339	**0.77**
H(1`A)	2.6698	2.6627	2.6505	2.6511	2.6099	2.6521	2.6276	2.6531	2.6278	2.6505	2.6009	2.8087	2.8120	2.7991	2.7904	2.7608	2.7925	2.7725	2.7948	2.7761	2.7885	2.7396	**3.16**
H(1`B)	3.1591	3.2023	3.2377	3.2375	3.2965	3.2352	3.2866	3.2330	3.2830	3.2401	3.2859	2.8814	2.7114	2.6952	2.6721	2.6718	2.6738	2.6281	2.6757	2.6303	2.6709	2.6132	**3.76**
H(2`A-2`B)	1.7019	1.7349	1.6989	1.7648	1.7189	1.7628	1.7313	1.7610	1.7262	1.7670	1.7500	1.5817	1.6581	1.6186	1.7003	1.6544	1.6979	1.6846	1.6956	1.6764	1.7028	1.7178	**2.13**
H(3`A-3`B)	1.5817	1.6581	1.6187	1.7003	1.6544	1.6979	1.6846	1.6956	1.6764	1.7028	1.7178	1.7019	1.7349	1.6989	1.7648	1.7189	1.7628	1.7313	1.7610	1.7262	1.7670	1.7500	**2.05**
H(4`A)	2.8814	2.7114	2.6952	2.6721	2.6718	2.6738	2.6281	2.6757	2.6303	2.6709	2.6132	3.1591	3.2023	3.2377	3.2375	3.2965	3.2352	3.2866	3.2330	3.2830	3.2401	3.2859	**3.09**
H(4`B)	2.8087	2.8120	2.7991	2.7904	2.7608	2.7925	2.7725	2.7948	2.7761	2.7885	2.7396	2.6698	2.6627	2.6505	2.6511	2.6099	2.6521	2.6276	2.6531	2.6278	2.6505	2.6009	**3.63**
F4	-113.6339	-114.6702	-117.2070	-114.7395	-118.7138	-114.7443	-116.4756	-114.7472	-116.8590	-114.7353	-116.2551	-113.6339	-114.6702	-117.2070	-114.7395	-118.7138	-114.7443	-116.4758	-114.7472	-116.8590	-114.7353	-116.2551	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. IX

Nuclei	R											S										Exp. [b]
	O3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	134.8316	136.7253	138.2232	137.7522	139.6525	137.7211	138.6578	137.6778	138.8802	137.7701	138.8881	134.8316	136.7253	138.2232	137.7522	139.6525	137.7212	138.6578	137.6778	138.8802	137.7701	138.8880	**132.8**
C2	134.2703	134.3034	134.9028	134.2696	134.8696	134.2834	135.2076	134.2931	135.1090	134.2502	135.1565	134.2703	134.3034	134.9028	134.2695	134.8695	134.2836	135.2076	134.2931	135.1090	134.2502	135.1565	**132.9**
C3	117.1530	117.7967	118.4174	118.0690	118.7418	118.0647	118.9947	118.0553	118.9369	118.0662	119.0549	117.1529	117.7967	118.4174	118.0688	118.7418	118.0647	118.9947	118.0553	118.9369	118.0662	119.0548	**117.2**
C4	169.5381	170.0292	170.6806	170.3884	171.1053	170.3736	171.6575	170.3540	171.5014	170.3967	171.7332	169.5383	170.0292	170.6806	170.3884	171.1053	170.3735	171.6575	170.3540	171.5014	170.3966	171.7334	**167.5**
C5	115.0903	116.2587	116.9125	116.9091	117.6769	116.8807	117.9293	116.8473	117.8196	116.9300	118.0603	115.0903	116.2587	116.9125	116.9091	117.6769	116.8806	117.9293	116.8473	117.8196	116.9299	118.0604	**117.2**
C6	130.2300	131.5111	132.3612	132.3562	133.7414	132.3011	134.3672	132.2439	134.1030	132.4041	134.6024	130.2299	131.5111	132.3612	132.3563	133.7414	132.3011	134.3672	132.2439	134.1030	132.4042	134.6023	**132.9**
C7	197.0256	202.4069	204.2489	205.5483	206.5094	205.3897	210.9074	205.2170	210.0109	205.6862	211.8448	197.0256	202.4069	204.2489	205.5484	206.5094	205.3897	210.9074	205.2170	210.0109	205.6859	211.8450	**195.8**
C8	64.5596	66.2848	66.9158	67.1212	67.8247	67.0947	68.4239	67.0586	68.3028	67.1363	68.7969	64.5596	66.2848	66.9158	67.1213	67.8247	67.0948	68.4239	67.0586	68.3028	67.1362	68.7968	**68.4**
C9	35.5442	35.1982	35.2977	35.1245	35.2805	35.1355	35.5634	35.1421	35.4857	35.1083	35.6327	35.5442	35.1982	35.2977	35.1245	35.2805	35.1354	35.5634	35.1421	35.4857	35.1083	35.6327	**30.5**
C10	27.9914	28.4344	28.8370	28.7329	29.4158	28.7216	29.2733	28.7061	29.2396	28.7375	29.4326	27.9915	28.4344	28.8370	28.7329	29.4156	28.7216	29.2733	28.7061	29.2396	28.7376	29.4325	**27.6**
C11	28.7716	28.8814	29.1958	28.9216	29.3506	28.9307	29.3249	28.9345	29.3252	28.9062	29.4166	28.7716	28.8814	29.1958	28.9217	29.3505	28.9308	29.3249	28.9345	29.3252	28.9062	29.4166	**23.1**
C12	16.6093	16.7634	16.8889	16.9451	17.0851	16.9427	17.0428	16.9355	17.0386	16.9411	17.0277	16.6092	16.7634	16.8889	16.9451	17.0851	16.9427	17.0428	16.9355	17.0386	16.9411	17.0277	**13.8**
C1`	50.8019	51.5543	51.9691	52.1253	52.7447	52.0980	52.7177	52.0662	52.6691	52.1450	53.0975	55.2428	56.2398	56.6369	56.7276	57.3004	56.7088	57.3728	56.6851	57.2958	56.7387	57.5907	**53.5**
C2`	25.9053	26.4060	26.7287	26.6449	27.0942	26.6421	27.1363	26.6341	27.1078	26.6410	26.9388	25.6921	25.8886	26.3279	26.0899	26.6685	26.0890	26.5111	26.0826	26.5199	26.0843	26.2550	**24.5**
C3`	25.6920	25.8886	26.3279	26.0899	26.6685	26.0889	26.5111	26.0826	26.5199	26.0842	26.2549	25.9053	26.4060	26.7287	26.6449	27.0942	26.6421	27.1363	26.6341	27.1078	26.6411	26.9389	**24.3**
C4`	55.2428	56.2398	56.6369	56.7276	57.3004	56.7089	57.3728	56.6851	57.2958	56.7388	57.5907	50.8019	51.5543	51.9691	52.1253	52.7448	52.0981	52.7178	52.0662	52.6691	52.1450	53.0974	**57.5**
H2	8.5172	8.3119	8.3022	8.2114	8.2142	8.2161	8.2765	8.2212	8.2596	8.2074	8.2657	8.5172	8.3119	8.3022	8.2114	8.2142	8.2161	8.2765	8.2212	8.2596	8.2074	8.2656	**8.11**
H3	7.3026	7.4020	7.4910	7.4435	7.5680	7.4415	7.5874	7.4391	7.5799	7.4452	7.5960	7.3026	7.4020	7.4910	7.4435	7.5680	7.4415	7.5874	7.4391	7.5799	7.4452	7.5960	**7.31**
H5	7.0527	7.2542	7.3671	7.3566	7.4848	7.3519	7.5014	7.3466	7.4911	7.3609	7.5199	7.0527	7.2542	7.3671	7.3566	7.4848	7.3518	7.5014	7.3466	7.4911	7.3609	7.5199	**7.31**
H6	7.9525	8.0429	8.1075	8.0893	8.2184	8.0851	8.2708	8.0810	8.2439	8.0936	8.2835	7.9525	8.0429	8.1075	8.0893	8.2184	8.0851	8.2708	8.0810	8.2439	8.0936	8.2835	**8.11**
H8	4.7795	4.7678	4.7948	4.7779	4.8539	4.7763	4.8754	4.7747	4.8616	4.7796	4.8585	4.7795	4.7678	4.7948	4.7779	4.8539	4.7763	4.8754	4.7747	4.8616	4.7796	4.8584	**5.18**
H(9A-9B)	1.6182	1.6249	1.5871	1.6386	1.6272	1.6368	1.6562	1.6349	1.6437	1.6405	1.6970	1.6182	1.6249	1.5871	1.6386	1.6272	1.6368	1.6562	1.6349	1.6437	1.6405	1.6970	**2.05**
H(10A)	0.9587	0.8526	0.8607	0.8353	0.8038	0.8362	0.8278	0.8369	0.8280	0.8343	0.8249	0.9587	0.8526	0.8607	0.8353	0.8038	0.8362	0.8278	0.8369	0.8280	0.8343	0.8249	**1.14**
H(10B)	1.5716	1.4752	1.4290	1.4076	1.3426	1.4126	1.3358	1.4173	1.3447	1.4028	1.3107	1.5716	1.4752	1.4290	1.4076	1.3426	1.4126	1.3358	1.4173	1.3447	1.4028	1.3107	**1.39**
H(11A-11B)	1.0598	1.0760	1.0550	1.0975	1.0725	1.0966	1.0683	1.0953	1.0683	1.0983	1.0500	1.0598	1.0760	1.0550	1.0975	1.0724	1.0966	1.0683	1.0953	1.0683	1.0983	1.0500	**1.22**
H(12A-12C)	0.9311	0.9235	0.9109	0.9235	0.8974	0.9240	0.8992	0.9241	0.9006	0.9229	0.8910	0.9311	0.9235	0.9109	0.9235	0.8974	0.9239	0.8992	0.9241	0.9006	0.9229	0.8910	**0.77**
H(1`A)	2.7818	2.7720	2.7498	2.7606	2.7136	2.7618	2.7281	2.7626	2.7293	2.7594	2.6945	2.9185	2.9246	2.8997	2.8958	2.8542	2.8987	2.8592	2.9012	2.8637	2.8929	2.8314	**3.16**
H(1`B)	3.2477	3.2925	3.3182	3.3299	3.3897	3.3277	3.3821	3.3252	3.3769	3.3319	3.3829	2.9024	2.7877	2.7774	2.7855	2.7869	2.7851	2.7591	2.7844	2.7670	2.7859	2.7593	**3.76**
H(2`A-2`B)	1.7372	1.7625	1.7344	1.7927	1.7507	1.7909	1.7606	1.7888	1.7570	1.7943	1.7756	1.6350	1.7111	1.6922	1.7625	1.7270	1.7599	1.7459	1.7567	1.7419	1.7649	1.7720	**2.13**
H(3`A-3`B)	1.6350	1.7111	1.6922	1.7626	1.7270	1.7599	1.7459	1.7567	1.7419	1.7649	1.7720	1.7372	1.7625	1.7344	1.7927	1.7507	1.7909	1.7606	1.7888	1.7570	1.7943	1.7757	**2.05**
H(4`A)	2.9024	2.7877	2.7774	2.7855	2.7869	2.7851	2.7591	2.7844	2.7670	2.7859	2.7593	3.2477	3.2925	3.3182	3.3299	3.3897	3.3277	3.3821	3.3252	3.3769	3.3319	3.3829	**3.09**
H(4`B)	2.9185	2.9246	2.8997	2.8958	2.8542	2.8987	2.8592	2.9012	2.8637	2.8929	2.8314	2.7818	2.7720	2.7498	2.7606	2.7136	2.7618	2.7281	2.7626	2.7293	2.7594	2.6945	**3.63**
F4	-119.1850	-121.2457	-124.2185	-121.8398	-126.1256	-121.8215	-123.9355	-121.7987	-124.3373	-121.8539	-123.7649	-119.1848	-121.2457	-124.2185	-121.8396	-126.1256	-121.8216	-123.9355	-121.7987	-124.3373	-121.8539	-123.7646	**-104.5**
Nuclei	OLYP																						
C1	133.9821	136.0335	137.1367	136.6843	138.8035	136.6625	137.7402	136.6347	138.0258	136.6956	137.8922	133.9821	136.0335	137.1367	136.6843	138.8035	136.6625	137.7402	136.6347	138.0258	136.6955	137.8922	**132.8**
C2	131.9334	131.9290	132.5576	131.8799	132.4225	131.8897	132.7752	131.8944	132.6437	131.8621	132.7099	131.9334	131.9291	132.5576	131.8799	132.4223	131.8897	132.7752	131.8944	132.6437	131.8621	132.7099	**132.9**
C3	115.3313	115.9906	116.6137	116.2608	116.8575	116.2547	117.1455	116.2428	117.0771	116.2573	117.2258	115.3313	115.9906	116.6137	116.2609	116.8575	116.2547	117.1455	116.2429	117.0771	116.2573	117.2258	**117.2**
C4	168.3478	168.9536	169.7150	169.3969	170.1310	169.3775	170.6738	169.3528	170.4989	169.4065	170.7682	168.3478	168.9536	169.7150	169.3969	170.1309	169.3775	170.6738	169.3529	170.4989	169.4065	170.7682	**167.5**
C5	113.3354	114.4044	115.0462	115.0266	115.7191	114.9969	116.0153	114.9618	115.8944	115.0458	116.1580	113.3354	114.4045	115.0462	115.0266	115.7191	114.9969	116.0153	114.9617	115.8944	115.0458	116.1580	**117.2**
C6	127.6467	128.8978	129.9328	129.9379	131.2665	129.8770	131.8460	129.8113	131.5682	129.9875	132.0896	127.6467	128.8977	129.9328	129.9380	131.2665	129.8770	131.8460	129.8113	131.5682	129.9876	132.0896	**132.9**
C7	195.5731	201.1277	202.5411	203.7564	205.1541	203.6174	209.0255	203.4714	208.3346	203.8785	209.8788	195.5731	201.1277	202.5411	203.7565	205.1539	203.6174	209.0255	203.4717	208.3346	203.8785	209.8788	**195.8**
C8	66.0732	67.9957	68.4903	68.7224	69.6196	68.7003	70.0870	68.6709	70.0972	68.7322	70.3344	66.0732	67.9958	68.4903	68.7226	69.6196	68.7004	70.0870	68.6709	70.0972	68.7322	70.3344	**68.4**
C9	36.5013	36.1561	36.3808	36.1692	36.2657	36.1751	36.6313	36.1753	36.5703	36.1547	36.6703	36.5013	36.1562	36.3808	36.1692	36.2656	36.1751	36.6313	36.1753	36.5703	36.1547	36.6703	**30.5**
C10	28.6233	29.0478	29.5021	29.3898	30.0161	29.3768	29.8944	29.3581	29.8818	29.3929	30.0503	28.6233	29.0477	29.5021	29.3898	30.0160	29.3768	29.8944	29.3580	29.8818	29.3929	30.0503	**27.6**
C11	29.6468	29.7271	30.0848	29.7850	30.1842	29.7907	30.1750	29.7910	30.1811	29.7704	30.2632	29.6468	29.7272	30.0848	29.7849	30.1842	29.7907	30.1749	29.7910	30.1811	29.7704	30.2632	**23.1**
C12	16.7637	16.9097	17.0328	17.0844	17.2029	17.0811	17.1660	17.0727	17.1626	17.0786	17.1506	16.7637	16.9097	17.0328	17.0843	17.2029	17.0811	17.1660	17.0727	17.1626	17.0786	17.1506	**13.8**
C1`	51.7337	52.4858	52.9328	53.0582	53.6707	53.0297	53.6672	52.9964	53.6005	53.0766	54.0194	56.2482	57.2354	57.6350	57.7173	58.2870	57.6968	58.3670	57.6709	58.2796	57.7275	58.6081	**53.5**
C2`	26.4609	26.9933	27.3434	27.2952	27.6992	27.2887	27.7603	27.2761	27.7417	27.2919	27.6012	26.4501	26.6417	27.0756	26.8535	27.4196	26.8487	27.2629	26.8387	27.2654	26.8497	27.0231	**24.5**
C3`	26.4501	26.6418	27.0756	26.8535	27.4195	26.8487	27.2629	26.8388	27.2654	26.8497	27.0231	26.4609	26.9933	27.3434	27.2952	27.6992	27.2887	27.7603	27.2761	27.7417	27.2919	27.6012	**24.3**
C4`	56.2482	57.2355	57.6350	57.7172	58.2870	57.6968	58.3669	57.6709	58.2796	57.7275	58.6081	51.7337	52.4859	52.9328	53.0581	53.6707	53.0297	53.6672	52.9964	53.6005	53.0766	54.0194	**57.5**
H2	8.3249	8.1241	8.1537	8.0646	8.0342	8.0676	8.1182	8.0705	8.0902	8.0614	8.1158	8.3249	8.1241	8.1537	8.0646	8.0341	8.0676	8.1182	8.0705	8.0902	8.0614	8.1158	**8.11**
H3	7.2045	7.3251	7.4204	7.3707	7.4933	7.3687	7.5141	7.3664	7.5040	7.3723	7.5211	7.2045	7.3251	7.4204	7.3707	7.4933	7.3687	7.5141	7.3664	7.5040	7.3723	7.5211	**7.31**
H5	6.9910	7.2033	7.3016	7.2888	7.4115	7.2844	7.4314	7.2798	7.4198	7.2926	7.4471	6.9910	7.2033	7.3016	7.2888	7.4115	7.2844	7.4314	7.2798	7.4198	7.2926	7.4471	**7.31**
H6	7.8487	7.9010	7.9896	7.9745	8.0789	7.9695	8.1350	7.9645	8.1011	7.9789	8.1569	7.8487	7.9010	7.9896	7.9745	8.0789	7.9695	8.1350	7.9645	8.1011	7.9789	8.1569	**8.11**
H8	4.9446	4.9128	4.9412	4.9248	4.9737	4.9235	4.9921	4.9221	4.9774	4.9258	4.9759	4.9446	4.9128	4.9412	4.9248	4.9737	4.9235	4.9921	4.9221	4.9774	4.9258	4.9759	**5.18**
H(9A-9B)	1.6234	1.6455	1.6374	1.6833	1.6640	1.6808	1.6972	1.6781	1.6877	1.6853	1.7322	1.6234	1.6455	1.6374	1.6833	1.6640	1.6808	1.6972	1.6781	1.6877	1.6853	1.7322	**2.05**
H(10A)	0.9953	0.8946	0.8938	0.8729	0.8450	0.8735	0.8733	0.8742	0.8679	0.8721	0.8733	0.9953	0.8946	0.8938	0.8729	0.8450	0.8735	0.8733	0.8742	0.8679	0.8721	0.8733	**1.14**
H(10B)	1.5882	1.4997	1.4577	1.4325	1.3742	1.4374	1.3635	1.4420	1.3716	1.4275	1.3377	1.5882	1.4997	1.4577	1.4325	1.3742	1.4374	1.3635	1.4420	1.3716	1.4275	1.3377	**1.39**
H(11A-11B)	1.1047	1.1212	1.1028	1.1423	1.1197	1.1410	1.1151	1.1396	1.1134	1.1432	1.0967	1.1047	1.1213	1.1028	1.1423	1.1197	1.1410	1.1151	1.1396	1.1134	1.1432	1.0967	**1.22**
H(12A-12C)	0.9447	0.9384	0.9250	0.9365	0.9136	0.9368	0.9156	0.9370	0.9158	0.9358	0.9079	0.9447	0.9384	0.9250	0.9365	0.9136	0.9368	0.9156	0.9370	0.9158	0.9358	0.9079	**0.77**
H(1`A)	2.8493	2.8305	2.8097	2.8183	2.7703	2.8195	2.7798	2.8205	2.7831	2.8167	2.7472	2.9785	2.9775	2.9559	2.9533	2.9142	2.9558	2.9129	2.9582	2.9219	2.9503	2.8855	**3.16**
H(1`B)	3.3360	3.3804	3.4119	3.4210	3.4791	3.4185	3.4699	3.4159	3.4664	3.4229	3.4658	2.9866	2.8809	2.8679	2.8706	2.8859	2.8704	2.8588	2.8703	2.8677	2.8705	2.8536	**3.76**
H(2`A-2`B)	1.7751	1.7943	1.7669	1.8200	1.7776	1.8182	1.7894	1.8164	1.7847	1.8214	1.8051	1.6770	1.7523	1.7284	1.7952	1.7674	1.7928	1.7835	1.7902	1.7783	1.7971	1.8096	**2.13**
H(3`A-3`B)	1.6770	1.7523	1.7284	1.7952	1.7674	1.7928	1.7835	1.7902	1.7783	1.7971	1.8096	1.7751	1.7943	1.7669	1.8200	1.7776	1.8182	1.7894	1.8164	1.7847	1.8214	1.8051	**2.05**
H(4`A)	2.9866	2.8809	2.8679	2.8706	2.8859	2.8705	2.8588	2.8703	2.8677	2.8705	2.8536	3.3360	3.3804	3.4119	3.4210	3.4791	3.4185	3.4699	3.4159	3.4664	3.4229	3.4658	**3.09**
H(4`B)	2.9785	2.9775	2.9559	2.9533	2.9142	2.9558	2.9129	2.9582	2.9219	2.9503	2.8855	2.8493	2.8305	2.8097	2.8182	2.7703	2.8195	2.7798	2.8205	2.7831	2.8167	2.7472	**3.63**
F4	-126.8941	-129.2746	-132.2452	-129.6606	-134.4154	-129.6500	-132.0547	-129.6387	-132.5484	-129.6690	-131.7814	-126.8941	-129.2745	-132.2452	-129.6605	-134.4155	-129.6500	-132.0547	-129.6385	-132.5484	-129.6690	-131.7814	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. X

Nuclei	R											S										Exp. [b]
	OPBE											OPBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	130.6787	132.6297	133.6336	133.3807	135.3198	133.3723	134.3661	133.3448	134.5349	133.3821	134.5269	130.6787	132.6296	133.6335	133.3807	135.3197	133.3723	134.3660	133.3448	134.5349	133.3821	134.5268	**132.8**
C2	130.5026	130.6500	131.1455	130.5229	131.1203	130.5465	131.4274	130.5522	131.3339	130.4956	131.4311	130.5026	130.6499	131.1455	130.5229	131.1203	130.5465	131.4274	130.5522	131.3339	130.4956	131.4309	**132.9**
C3	114.1774	114.9620	115.5644	115.1917	115.9530	115.1953	116.1865	115.1808	116.1149	115.1830	116.2950	114.1774	114.9619	115.5645	115.1917	115.9531	115.1953	116.1864	115.1808	116.1149	115.1830	116.2949	**117.2**
C4	164.7994	165.4524	166.0718	165.7743	166.4439	165.7692	166.9958	165.7465	166.8494	165.7742	167.1261	164.7994	165.4524	166.0719	165.7743	166.4440	165.7692	166.9958	165.7465	166.8494	165.7742	167.1261	**167.5**
C5	112.2619	113.5119	114.1131	114.0723	114.8593	114.0525	115.1463	114.0152	115.0300	114.0864	115.3281	112.2618	113.5119	114.1130	114.0723	114.8593	114.0525	115.1464	114.0152	115.0300	114.0864	115.3282	**117.2**
C6	126.2248	127.5436	128.4947	128.4132	129.7170	128.3671	130.2985	128.3037	130.0776	128.4529	130.5759	126.2248	127.5437	128.4947	128.4132	129.7170	128.3671	130.2986	128.3037	130.0776	128.4529	130.5758	**132.9**
C7	192.8492	198.0469	199.3180	200.6479	201.7981	200.5296	205.5758	200.3919	204.7558	200.7535	206.3278	192.8491	198.0466	199.3180	200.6479	201.7981	200.5296	205.5759	200.3919	204.7558	200.7535	206.3275	**195.8**
C8	63.5007	65.3509	66.0163	66.0708	67.1112	66.0585	67.5850	66.0270	67.4654	66.0760	67.8053	63.5007	65.3510	66.0163	66.0708	67.1112	66.0585	67.5850	66.0270	67.4654	66.0760	67.8053	**68.4**
C9	34.3082	34.1893	34.3213	34.1125	34.3179	34.1310	34.6281	34.1317	34.5209	34.0902	34.6999	34.3083	34.1893	34.3213	34.1125	34.3179	34.1310	34.6281	34.1317	34.5209	34.0902	34.6998	**30.5**
C10	26.3655	26.8815	27.2838	27.1239	27.8025	27.1222	27.6443	27.1030	27.6205	27.1207	27.8389	26.3655	26.8814	27.2838	27.1239	27.8024	27.1222	27.6443	27.1030	27.6205	27.1207	27.8389	**27.6**
C11	27.3220	27.5273	27.7359	27.4928	27.8362	27.5128	27.8134	27.5147	27.8103	27.4686	27.9319	27.3219	27.5273	27.7360	27.4928	27.8361	27.5128	27.8134	27.5147	27.8103	27.4686	27.9319	**23.1**
C12	16.0776	16.2963	16.3097	16.3835	16.4232	16.3927	16.4102	16.3844	16.4094	16.3702	16.4127	16.0776	16.2963	16.3098	16.3835	16.4232	16.3927	16.4102	16.3844	16.4094	16.3702	16.4127	**13.8**
C1`	49.8315	50.6513	50.9131	51.1124	51.5794	51.0991	51.6068	51.0680	51.5522	51.1202	52.0407	54.1207	55.1917	55.5154	55.5904	56.1099	55.5833	56.1855	55.5579	56.1235	55.5921	56.4254	**53.5**
C2`	25.1000	25.6677	25.9114	25.8276	26.2209	25.8356	26.2347	25.8256	26.2242	25.8151	25.9714	24.9036	25.1884	25.4269	25.2649	25.6750	25.2773	25.5882	25.2721	25.5991	25.2486	25.3040	**24.5**
C3`	24.9037	25.1884	25.4268	25.2649	25.6751	25.2773	25.5881	25.2721	25.5991	25.2486	25.3041	25.1001	25.6677	25.9114	25.8276	26.2210	25.8356	26.2347	25.8256	26.2242	25.8151	25.9714	**24.3**
C4`	54.1207	55.1916	55.5153	55.5904	56.1100	55.5833	56.1855	55.5579	56.1235	55.5921	56.4254	49.8315	50.6514	50.9130	51.1124	51.5794	51.0991	51.6068	51.0680	51.5522	51.1201	52.0406	**57.5**
H2	8.3644	8.1928	8.2044	8.1131	8.0948	8.1166	8.1711	8.1195	8.1553	8.1092	8.1745	8.3644	8.1928	8.2044	8.1131	8.0948	8.1166	8.1711	8.1195	8.1553	8.1092	8.1745	**8.11**
H3	7.2317	7.3506	7.4367	7.3986	7.5153	7.3968	7.5392	7.3943	7.5305	7.3995	7.5502	7.2317	7.3506	7.4367	7.3986	7.5153	7.3968	7.5392	7.3943	7.5305	7.3995	7.5502	**7.31**
H5	7.0085	7.2266	7.3170	7.3144	7.4418	7.3103	7.4561	7.3054	7.4452	7.3175	7.4766	7.0085	7.2266	7.3170	7.3144	7.4418	7.3103	7.4561	7.3054	7.4452	7.3175	7.4766	**7.31**
H6	7.9097	7.9800	8.0576	8.0368	8.1441	8.0322	8.1953	8.0270	8.1733	8.0405	8.2139	7.9097	7.9800	8.0576	8.0368	8.1441	8.0322	8.1953	8.0270	8.1733	8.0405	8.2139	**8.11**
H8	4.9509	4.9173	4.9339	4.9242	4.9761	4.9229	4.9923	4.9211	4.9808	4.9248	4.9868	4.9509	4.9173	4.9339	4.9242	4.9761	4.9229	4.9923	4.9211	4.9808	4.9248	4.9868	**5.18**
H(9A-9B)	1.6537	1.6636	1.6523	1.6862	1.6774	1.6845	1.7050	1.6821	1.6910	1.6872	1.7441	1.6537	1.6636	1.6523	1.6862	1.6774	1.6845	1.7050	1.6821	1.6910	1.6872	1.7441	**2.05**
H(10A)	0.9080	0.8215	0.7760	0.7960	0.7277	0.7977	0.7746	0.7987	0.7708	0.7938	0.7812	0.9080	0.8214	0.7760	0.7960	0.7277	0.7977	0.7746	0.7987	0.7708	0.7938	0.7812	**1.14**
H(10B)	1.5468	1.4570	1.4015	1.3905	1.3184	1.3954	1.3106	1.3997	1.3176	1.3850	1.2885	1.5468	1.4570	1.4015	1.3905	1.3184	1.3954	1.3106	1.3997	1.3176	1.3850	1.2884	**1.39**
H(11A-11B)	1.0380	1.0583	1.0237	1.0740	1.0368	1.0738	1.0344	1.0727	1.0341	1.0737	1.0195	1.0380	1.0583	1.0237	1.0740	1.0368	1.0738	1.0344	1.0727	1.0341	1.0737	1.0195	**1.22**
H(12A-12C)	0.8763	0.8722	0.8453	0.8670	0.8301	0.8680	0.8355	0.8684	0.8363	0.8653	0.8297	0.8763	0.8722	0.8453	0.8670	0.8301	0.8680	0.8355	0.8684	0.8363	0.8653	0.8297	**0.77**
H(1`A)	2.7652	2.7626	2.7400	2.7489	2.7012	2.7503	2.7146	2.7511	2.7162	2.7467	2.6727	2.9190	2.9188	2.8953	2.8880	2.8426	2.8911	2.8529	2.8934	2.8571	2.8843	2.8212	**3.16**
H(1`B)	3.2993	3.3459	3.3765	3.3785	3.4327	3.3769	3.4258	3.3746	3.4221	3.3793	3.4161	2.9751	2.8559	2.8439	2.8403	2.8379	2.8409	2.8138	2.8411	2.8191	2.8390	2.8061	**3.76**
H(2`A-2`B)	1.7256	1.7518	1.7160	1.7751	1.7243	1.7740	1.7393	1.7721	1.7348	1.7756	1.7601	1.6373	1.7083	1.6748	1.7504	1.7036	1.7486	1.7291	1.7459	1.7249	1.7515	1.7617	**2.13**
H(3`A-3`B)	1.6373	1.7083	1.6748	1.7504	1.7036	1.7486	1.7291	1.7459	1.7249	1.7515	1.7617	1.7256	1.7518	1.7160	1.7751	1.7243	1.7740	1.7393	1.7721	1.7348	1.7756	1.7601	**2.05**
H(4`A)	2.9751	2.8559	2.8439	2.8403	2.8379	2.8409	2.8138	2.8411	2.8191	2.8390	2.8061	3.2993	3.3459	3.3765	3.3785	3.4327	3.3769	3.4258	3.3746	3.4221	3.3793	3.4161	**3.09**
H(4`B)	2.9190	2.9187	2.8953	2.8880	2.8426	2.8911	2.8529	2.8934	2.8571	2.8843	2.8212	2.7652	2.7625	2.7400	2.7489	2.7012	2.7503	2.7146	2.7511	2.7162	2.7467	2.6727	**3.63**
F4	-115.7719	-117.4650	-120.2202	-117.7317	-122.1750	-117.7322	-119.6997	-117.7324	-120.1322	-117.7293	-119.3803	-115.7717	-117.4650	-120.2200	-117.7317	-122.1749	-117.7322	-119.6998	-117.7324	-120.1322	-117.7293	-119.3804	**-104.5**
Nuclei	OPW91											OPW91										
C1	130.9989	132.9583	133.9539	133.7056	135.6329	133.6877	134.6754	133.6513	134.8514	133.7031	134.8410	130.9989	132.9582	133.9539	133.7056	135.6330	133.6877	134.6754	133.6513	134.8515	133.7031	134.8410	**132.8**
C2	130.7262	130.8703	131.3673	130.7503	131.3340	130.7635	131.6450	130.7599	131.5541	130.7194	131.6496	130.7261	130.8703	131.3673	130.7503	131.3339	130.7635	131.6450	130.7599	131.5542	130.7194	131.6496	**132.9**
C3	114.3764	115.1564	115.7533	115.3897	116.1354	115.3831	116.3698	115.3596	116.2991	115.3771	116.4793	114.3764	115.1565	115.7533	115.3897	116.1354	115.3831	116.3698	115.3596	116.2991	115.3771	116.4793	**117.2**
C4	165.2041	165.8588	166.4788	166.1876	166.8477	166.1725	167.4033	166.1404	167.2572	166.1838	167.5338	165.2041	165.8588	166.4788	166.1876	166.8476	166.1725	167.4033	166.1404	167.2572	166.1838	167.5338	**167.5**
C5	112.4572	113.7054	114.3021	114.2692	115.0406	114.2396	115.3290	114.1931	115.2123	114.2792	115.5116	112.4573	113.7054	114.3021	114.2692	115.0407	114.2396	115.3290	114.1931	115.2123	114.2792	115.5116	**117.2**
C6	126.4459	127.7681	128.7165	128.6476	129.9387	128.5911	130.5278	128.5186	130.3040	128.6837	130.8058	126.4460	127.7681	128.7164	128.6476	129.9387	128.5911	130.5278	128.5186	130.3040	128.6837	130.8058	**132.9**
C7	193.2350	198.4648	199.7275	201.0721	202.2060	200.9435	206.0081	200.7961	205.1882	201.1740	206.7657	193.2352	198.4648	199.7276	201.0721	202.2063	200.9435	206.0081	200.7961	205.1882	201.1740	206.7657	**195.8**
C8	63.7228	65.5786	66.2262	66.3004	67.3297	66.2783	67.7924	66.2379	67.6675	66.3014	68.0264	63.7228	65.5786	66.2262	66.3004	67.3296	66.2783	67.7924	66.2379	67.6675	66.3014	68.0264	**68.4**
C9	34.4593	34.3374	34.4633	34.2679	34.4630	34.2763	34.7706	34.2678	34.6619	34.2417	34.8495	34.4593	34.3374	34.4633	34.2679	34.4630	34.2763	34.7706	34.2678	34.6619	34.2417	34.8495	**30.5**
C10	26.4933	27.0116	27.4118	27.2602	27.9311	27.2485	27.7713	27.2200	27.7463	27.2531	27.9654	26.4932	27.0116	27.4118	27.2602	27.9312	27.2485	27.7713	27.2200	27.7464	27.2531	27.9654	**27.6**
C11	27.4281	27.6358	27.8457	27.6079	27.9463	27.6176	27.9231	27.6102	27.9202	27.5798	28.0426	27.4281	27.6358	27.8457	27.6079	27.9462	27.6176	27.9231	27.6102	27.9203	27.5798	28.0426	**23.1**
C12	16.1147	16.3379	16.3532	16.4317	16.4668	16.4307	16.4541	16.4131	16.4540	16.4146	16.4592	16.1147	16.3380	16.3532	16.4317	16.4669	16.4307	16.4541	16.4131	16.4540	16.4146	16.4592	**13.8**
C1`	49.9744	50.7955	51.0613	51.2629	51.7275	51.2393	51.7560	51.1989	51.7048	51.2672	52.1859	54.2713	55.3450	55.6693	55.7494	56.2629	55.7320	56.3386	55.6974	56.2757	55.7475	56.5821	**53.5**
C2`	25.2138	25.7880	26.0320	25.9569	26.3447	25.9547	26.3594	25.9356	26.3475	25.9405	26.1094	25.0229	25.3126	25.5528	25.3973	25.7998	25.3995	25.7152	25.3852	25.7270	25.3771	25.4366	**24.5**
C3`	25.0230	25.3125	25.5528	25.3973	25.7999	25.3995	25.7152	25.3852	25.7270	25.3771	25.4366	25.2138	25.7880	26.0320	25.9569	26.3447	25.9547	26.3594	25.9356	26.3475	25.9405	26.1094	**24.3**
C4`	54.2713	55.3450	55.6693	55.7494	56.2627	55.7320	56.3386	55.6974	56.2757	55.7475	56.5821	49.9744	50.7955	51.0613	51.2629	51.7274	51.2393	51.7560	51.1989	51.7048	51.2672	52.1859	**57.5**
H2	8.3657	8.1926	8.2058	8.1146	8.0958	8.1174	8.1723	8.1200	8.1563	8.1104	8.1754	8.3657	8.1926	8.2058	8.1146	8.0958	8.1174	8.1723	8.1200	8.1564	8.1104	8.1754	**8.11**
H3	7.2334	7.3518	7.4382	7.4004	7.5160	7.3980	7.5403	7.3952	7.5319	7.4010	7.5508	7.2334	7.3518	7.4382	7.4004	7.5160	7.3980	7.5403	7.3952	7.5319	7.4010	7.5508	**7.31**
H5	7.0105	7.2283	7.3185	7.3163	7.4423	7.3115	7.4569	7.3065	7.4459	7.3190	7.4773	7.0105	7.2283	7.3185	7.3163	7.4423	7.3115	7.4569	7.3065	7.4458	7.3190	7.4773	**7.31**
H6	7.9098	7.9795	8.0579	8.0377	8.1442	8.0324	8.1963	8.0270	8.1738	8.0412	8.2151	7.9098	7.9795	8.0579	8.0377	8.1442	8.0324	8.1963	8.0270	8.1738	8.0412	8.2151	**8.11**
H8	4.9491	4.9159	4.9327	4.9236	4.9747	4.9217	4.9913	4.9198	4.9796	4.9239	4.9859	4.9491	4.9159	4.9327	4.9236	4.9747	4.9217	4.9913	4.9198	4.9796	4.9239	4.9859	**5.18**
H(9A-9B)	1.6497	1.6605	1.6494	1.6849	1.6763	1.6824	1.7032	1.6798	1.6890	1.6857	1.7429	1.6497	1.6605	1.6494	1.6849	1.6763	1.6824	1.7032	1.6798	1.6890	1.6857	1.7429	**2.05**
H(10A)	0.9129	0.8260	0.7820	0.8013	0.7323	0.8023	0.7801	0.8031	0.7773	0.7988	0.7858	0.9129	0.8260	0.7820	0.8013	0.7323	0.8023	0.7801	0.8031	0.7773	0.7988	0.7858	**1.14**
H(10B)	1.5483	1.4585	1.4043	1.3926	1.3200	1.3969	1.3127	1.4010	1.3200	1.3868	1.2904	1.5483	1.4585	1.4043	1.3926	1.3200	1.3969	1.3127	1.4010	1.3200	1.3868	1.2904	**1.39**
H(11A-11B)	1.0395	1.0599	1.0261	1.0765	1.0389	1.0755	1.0369	1.0742	1.0367	1.0758	1.0217	1.0396	1.0599	1.0261	1.0765	1.0389	1.0755	1.0369	1.0742	1.0367	1.0758	1.0217	**1.22**
H(12A-12C)	0.8777	0.8739	0.8474	0.8694	0.8320	0.8698	0.8377	0.8698	0.8386	0.8674	0.8317	0.8777	0.8739	0.8474	0.8694	0.8321	0.8698	0.8377	0.8698	0.8386	0.8674	0.8317	**0.77**
H(1`A)	2.7694	2.7663	2.7435	2.7534	2.7049	2.7542	2.7183	2.7548	2.7196	2.7509	2.6771	2.9218	2.9220	2.8985	2.8920	2.8459	2.8944	2.8559	2.8966	2.8599	2.8879	2.8245	**3.16**
H(1`B)	3.2959	3.3429	3.3734	3.3768	3.4303	3.3745	3.4237	3.3719	3.4196	3.3773	3.4149	2.9704	2.8525	2.8394	2.8380	2.8351	2.8379	2.8108	2.8378	2.8160	2.8365	2.8041	**3.76**
H(2`A-2`B)	1.7263	1.7526	1.7171	1.7767	1.7253	1.7749	1.7403	1.7728	1.7359	1.7769	1.7607	1.6372	1.7089	1.6758	1.7515	1.7042	1.7490	1.7297	1.7461	1.7257	1.7524	1.7615	**2.13**
H(3`A-3`B)	1.6372	1.7089	1.6758	1.7515	1.7042	1.7490	1.7297	1.7461	1.7257	1.7524	1.7615	1.7263	1.7526	1.7171	1.7767	1.7253	1.7749	1.7403	1.7728	1.7359	1.7769	1.7607	**2.05**
H(4`A)	2.9704	2.8525	2.8394	2.8380	2.8351	2.8379	2.8108	2.8378	2.8160	2.8365	2.8041	3.2959	3.3429	3.3734	3.3768	3.4303	3.3745	3.4237	3.3719	3.4196	3.3773	3.4149	**3.09**
H(4`B)	2.9218	2.9219	2.8985	2.8920	2.8459	2.8944	2.8559	2.8966	2.8599	2.8879	2.8245	2.7694	2.7663	2.7435	2.7534	2.7049	2.7542	2.7183	2.7548	2.7196	2.7509	2.6771	**3.63**
F4	-116.3894	-118.1382	-120.9029	-118.4211	-122.8862	-118.4208	-120.4042	-118.4200	-120.8382	-118.4199	-120.0932	-116.3894	-118.1382	-120.9028	-118.4211	-122.8863	-118.4208	-120.4042	-118.4200	-120.8382	-118.4199	-120.0932	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. XI

Nuclei	R											S										Exp. [b]
	PBE											PBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	135.7483	136.9338	137.8215	137.3803	138.9543	137.3545	138.4508	137.3389	138.4347	137.4219	138.6539	135.7483	136.9338	137.8215	137.3803	138.9543	137.3545	138.4509	137.3389	138.4347	137.4219	138.6539	**132.8**
C2	135.8078	135.8743	136.4215	135.6787	136.3342	135.6882	136.8147	135.7088	136.6975	135.6874	136.7796	135.8078	135.8743	136.4215	135.6787	136.3342	135.6882	136.8147	135.7088	136.6975	135.6874	136.7796	**132.9**
C3	119.5174	120.3563	120.9316	120.5420	121.3293	120.5297	121.6675	120.5282	121.5814	120.5709	121.7766	119.5174	120.3563	120.9316	120.5420	121.3293	120.5297	121.6674	120.5282	121.5814	120.5709	121.7766	**117.2**
C4	174.2361	175.2702	175.9491	175.6389	176.4757	175.6130	177.0574	175.5980	176.9178	175.6810	177.2200	174.2361	175.2703	175.9491	175.6389	176.4758	175.6130	177.0574	175.5980	176.9178	175.6810	177.2200	**167.5**
C5	117.5658	118.8904	119.5358	119.4738	120.4435	119.4339	120.7042	119.4048	120.5965	119.5296	120.8999	117.5658	118.8902	119.5358	119.4738	120.4435	119.4339	120.7041	119.4048	120.5965	119.5296	120.8999	**117.2**
C6	132.1464	134.1194	135.2182	135.1667	136.8848	135.0939	137.4752	135.0329	137.2528	135.2539	137.9118	132.1464	134.1194	135.2182	135.1667	136.8848	135.0939	137.4754	135.0329	137.2528	135.2539	137.9118	**132.9**
C7	201.1356	205.4775	206.7985	207.6645	208.7676	207.5322	212.7870	207.4100	211.8422	207.8073	213.7751	201.1356	205.4775	206.7985	207.6645	208.7676	207.5322	212.7866	207.4100	211.8422	207.8073	213.7751	**195.8**
C8	67.3305	68.6977	69.4799	69.1926	70.5026	69.1716	71.0535	69.1589	70.8716	69.2282	71.4612	67.3305	68.6976	69.4799	69.1926	70.5026	69.1716	71.0534	69.1589	70.8716	69.2282	71.4612	**68.4**
C9	38.5481	38.3924	38.5854	38.2027	38.7100	38.2115	39.0042	38.2308	38.9069	38.2116	39.1515	38.5481	38.3925	38.5854	38.2027	38.7100	38.2115	39.0042	38.2308	38.9069	38.2116	39.1515	**30.5**
C10	29.5828	30.1383	30.5931	30.3952	31.2462	30.3715	31.0588	30.3592	31.0404	30.4359	31.2758	29.5828	30.1382	30.5931	30.3952	31.2462	30.3715	31.0588	30.3592	31.0404	30.4359	31.2759	**27.6**
C11	29.4545	29.6678	29.8873	29.5253	30.0700	29.5343	30.0539	29.5536	30.0482	29.5337	30.2277	29.4545	29.6678	29.8873	29.5253	30.0700	29.5343	30.0540	29.5536	30.0482	29.5337	30.2277	**23.1**
C12	16.4263	16.6550	16.6777	16.6936	16.8479	16.6853	16.8192	16.6882	16.8147	16.7199	16.8332	16.4263	16.6550	16.6777	16.6936	16.8479	16.6853	16.8192	16.6882	16.8147	16.7199	16.8332	**13.8**
C1`	53.1868	54.1192	54.3314	54.5767	55.2085	54.5426	55.1990	54.5200	55.1018	54.6279	55.7537	57.7309	59.0198	59.3593	59.4308	60.0063	59.4053	60.1988	59.3904	60.1340	59.4724	60.4800	**53.5**
C2`	25.7091	26.3084	26.6327	26.4566	27.0413	26.4455	27.0629	26.4450	27.0465	26.4846	26.9107	25.3534	25.6633	25.9658	25.7952	26.3210	25.7806	26.3173	25.7773	26.3051	25.8271	26.2369	**24.5**
C3`	25.3534	25.6633	25.9658	25.7952	26.3211	25.7806	26.3173	25.7773	26.3051	25.8271	26.2369	25.7091	26.3084	26.6327	26.4566	27.0413	26.4455	27.0629	26.4450	27.0465	26.4846	26.9108	**24.3**
C4`	57.7309	59.0198	59.3593	59.4308	60.0063	59.4053	60.1988	59.3904	60.1340	59.4724	60.4800	53.1868	54.1193	54.3314	54.5767	55.2086	54.5426	55.1991	54.5200	55.1018	54.6279	55.7537	**57.5**
H2	8.5422	8.4404	8.4543	8.3726	8.3723	8.3764	8.4041	8.3809	8.4061	8.3697	8.3938	8.5422	8.4404	8.4543	8.3726	8.3723	8.3764	8.4041	8.3809	8.4061	8.3697	8.3938	**8.11**
H3	7.2025	7.3512	7.4409	7.3933	7.5117	7.3913	7.5367	7.3898	7.5283	7.3957	7.5512	7.2025	7.3512	7.4409	7.3933	7.5117	7.3913	7.5367	7.3898	7.5283	7.3957	7.5512	**7.31**
H5	7.0213	7.1777	7.2686	7.2421	7.3835	7.2384	7.3885	7.2352	7.3797	7.2463	7.4165	7.0213	7.1777	7.2686	7.2421	7.3835	7.2384	7.3885	7.2352	7.3797	7.2463	7.4165	**7.31**
H6	7.9455	8.1049	8.1784	8.1913	8.3013	8.1856	8.3527	8.1805	8.3388	8.1973	8.3808	7.9455	8.1050	8.1784	8.1913	8.3014	8.1856	8.3527	8.1805	8.3388	8.1973	8.3808	**8.11**
H8	4.9981	5.0221	5.0362	5.0495	5.0820	5.0469	5.1116	5.0449	5.1050	5.0527	5.1021	4.9981	5.0221	5.0362	5.0495	5.0820	5.0469	5.1116	5.0449	5.1050	5.0527	5.1021	**5.18**
H(9A-9B)	1.8877	1.9213	1.9179	1.9417	1.9768	1.9405	1.9732	1.9398	1.9667	1.9435	2.0076	1.8877	1.9214	1.9179	1.9417	1.9768	1.9405	1.9733	1.9398	1.9667	1.9435	2.0076	**2.05**
H(10A)	0.9903	0.8747	0.8363	0.8393	0.7493	0.8399	0.8067	0.8412	0.7986	0.8395	0.8199	0.9903	0.8747	0.8363	0.8393	0.7493	0.8399	0.8068	0.8413	0.7986	0.8395	0.8199	**1.14**
H(10B)	1.7513	1.6439	1.5780	1.5587	1.4835	1.5641	1.4701	1.5700	1.4779	1.5544	1.4380	1.7513	1.6439	1.5780	1.5587	1.4835	1.5641	1.4701	1.5700	1.4779	1.5544	1.4380	**1.39**
H(11A-11B)	1.1003	1.1160	1.0803	1.1235	1.0909	1.1231	1.0888	1.1233	1.0885	1.1245	1.0766	1.1003	1.1160	1.0803	1.1235	1.0909	1.1231	1.0888	1.1233	1.0885	1.1245	1.0766	**1.22**
H(12A-12C)	0.9133	0.9052	0.8805	0.8941	0.8588	0.8947	0.8663	0.8959	0.8665	0.8942	0.8605	0.9133	0.9052	0.8805	0.8941	0.8588	0.8947	0.8663	0.8959	0.8665	0.8942	0.8605	**0.77**
H(1`A)	2.7998	2.7946	2.7843	2.7819	2.7480	2.7827	2.7606	2.7840	2.7625	2.7819	2.7267	2.9257	2.9415	2.9313	2.9245	2.9038	2.9262	2.9082	2.9283	2.9120	2.9235	2.8692	**3.16**
H(1`B)	3.3750	3.4144	3.4496	3.4414	3.5072	3.4395	3.4925	3.4380	3.4919	3.4439	3.4830	3.0909	2.9057	2.8913	2.8575	2.8578	2.8592	2.8162	2.8617	2.8198	2.8566	2.7942	**3.76**
H(2`A-2`B)	1.8055	1.8330	1.7994	1.8565	1.8130	1.8547	1.8265	1.8534	1.8218	1.8590	1.8472	1.6742	1.7478	1.7141	1.7866	1.7430	1.7841	1.7717	1.7821	1.7633	1.7896	1.8081	**2.13**
H(3`A-3`B)	1.6742	1.7478	1.7141	1.7866	1.7430	1.7841	1.7717	1.7821	1.7633	1.7896	1.8081	1.8055	1.8330	1.7994	1.8565	1.8130	1.8547	1.8265	1.8534	1.8218	1.8590	1.8472	**2.05**
H(4`A)	3.0909	2.9057	2.8913	2.8575	2.8578	2.8592	2.8162	2.8617	2.8198	2.8566	2.7942	3.3750	3.4144	3.4496	3.4414	3.5072	3.4395	3.4925	3.4380	3.4919	3.4439	3.4830	**3.09**
H(4`B)	2.9257	2.9415	2.9313	2.9245	2.9038	2.9262	2.9082	2.9283	2.9120	2.9235	2.8692	2.7998	2.7946	2.7843	2.7819	2.7480	2.7827	2.7606	2.7840	2.7625	2.7819	2.7267	**3.63**
F4	-131.3443	-132.3866	-135.5345	-132.3677	-137.2648	-132.3799	-134.6625	-132.3899	-135.0650	-132.3559	-134.2918	-131.3443	-132.3863	-135.5345	-132.3677	-137.2648	-132.3799	-134.6625	-132.3899	-135.0650	-132.3559	-134.2918	**-104.5**
Nuclei	PBE0																						
C1	136.4530	137.3089	138.0508	137.7354	139.2688	137.7148	138.6567	137.6949	138.6719	137.7566	138.8652	136.4530	137.3090	138.0509	137.7354	139.2688	137.7148	138.6567	137.6949	138.6719	137.7566	138.8651	**132.8**
C2	138.6013	138.6001	139.0847	138.4264	138.9615	138.4331	139.5038	138.4418	139.3326	138.4230	139.4291	138.6013	138.6001	139.0847	138.4264	138.9613	138.4331	139.5038	138.4418	139.3328	138.4230	139.4292	**132.9**
C3	120.9188	121.6798	122.2526	121.8997	122.5990	121.8840	122.9416	121.8699	122.8160	121.9174	122.9678	120.9188	121.6797	122.2525	121.8997	122.5988	121.8840	122.9416	121.8699	122.8159	121.9174	122.9677	**117.2**
C4	172.9248	173.7704	174.3607	174.1635	174.7944	174.1342	175.5017	174.1070	175.2844	174.1944	175.5847	172.9248	173.7702	174.3606	174.1635	174.7943	174.1342	175.5017	174.1070	175.2844	174.1944	175.5847	**167.5**
C5	118.8873	120.2205	120.8491	120.8784	121.7495	120.8319	122.0378	120.7874	121.8751	120.9256	122.1589	118.8873	120.2204	120.8491	120.8784	121.7495	120.8319	122.0378	120.7874	121.8751	120.9256	122.1590	**117.2**
C6	134.7534	136.6483	137.8002	137.7535	139.3337	137.6742	140.0781	137.5975	139.7552	137.8328	140.4055	134.7534	136.6484	137.8002	137.7535	139.3337	137.6742	140.0781	137.5975	139.7551	137.8328	140.4054	**132.9**
C7	201.0382	205.4916	206.6635	207.9368	208.6564	207.7907	213.5288	207.6448	212.4021	208.0776	214.5410	201.0382	205.4915	206.6632	207.9368	208.6564	207.7907	213.5288	207.6448	212.4025	208.0776	214.5410	**195.8**
C8	63.3741	64.5227	65.2451	65.0149	66.0343	64.9854	66.6890	64.9567	66.5032	65.0447	67.0482	63.3741	64.5227	65.2451	65.0149	66.0342	64.9854	66.6890	64.9567	66.5033	65.0447	67.0483	**68.4**
C9	35.2480	35.0267	35.2621	34.8927	35.2211	34.8944	35.4911	34.8977	35.3528	34.8940	35.5658	35.2480	35.0267	35.2622	34.8927	35.2211	34.8944	35.4911	34.8978	35.3528	34.8940	35.5657	**30.5**
C10	27.5160	27.9999	28.4469	28.3217	29.0203	28.2908	28.9160	28.2627	28.8347	28.3546	29.0522	27.5160	27.9999	28.4468	28.3217	29.0203	28.2908	28.9160	28.2627	28.8348	28.3546	29.0522	**27.6**
C11	27.3762	27.5042	27.7451	27.4397	27.8548	27.4401	27.9245	27.4421	27.8635	27.4419	28.0248	27.3761	27.5043	27.7451	27.4397	27.8548	27.4401	27.9245	27.4422	27.8636	27.4419	28.0247	**23.1**
C12	16.1669	16.3506	16.3714	16.4494	16.5174	16.4361	16.5489	16.4251	16.4828	16.4654	16.4981	16.1668	16.3507	16.3713	16.4494	16.5175	16.4361	16.5489	16.4250	16.4827	16.4654	16.4981	**13.8**
C1`	50.3442	51.1746	51.3791	51.6553	52.1863	51.6178	52.2537	51.5828	52.1219	51.6945	52.6719	54.6441	55.7362	56.0471	56.1526	56.6508	56.1232	56.8627	56.0957	56.7432	56.1835	57.0525	**53.5**
C2`	24.3672	24.7765	25.0807	24.9101	25.3550	24.8969	25.4419	24.8857	25.3814	24.9254	25.2400	23.8126	24.0541	24.3180	24.1905	24.6209	24.1765	24.6494	24.1645	24.5778	24.2070	24.4911	**24.5**
C3`	23.8126	24.0541	24.3180	24.1905	24.6209	24.1765	24.6494	24.1645	24.5779	24.2070	24.4910	24.3672	24.7765	25.0807	24.9101	25.3550	24.8969	25.4419	24.8857	25.3814	24.9254	25.2399	**24.3**
C4`	54.6441	55.7362	56.0470	56.1526	56.6509	56.1232	56.8627	56.0957	56.7433	56.1835	57.0525	50.3442	51.1747	51.3791	51.6553	52.1864	51.6178	52.2537	51.5828	52.1220	51.6945	52.6719	**57.5**
H2	8.7672	8.6747	8.6943	8.6043	8.6001	8.6077	8.6358	8.6113	8.6278	8.6008	8.6154	8.7672	8.6747	8.6943	8.6043	8.6001	8.6077	8.6358	8.6113	8.6278	8.6008	8.6154	**8.11**
H3	7.3555	7.5027	7.5909	7.5485	7.6660	7.5463	7.6937	7.5440	7.6820	7.5502	7.7053	7.3555	7.5027	7.5909	7.5485	7.6660	7.5463	7.6937	7.5440	7.6820	7.5502	7.7053	**7.31**
H5	7.1793	7.3531	7.4495	7.4232	7.5573	7.4188	7.5698	7.4143	7.5575	7.4270	7.5924	7.1793	7.3531	7.4495	7.4232	7.5573	7.4188	7.5698	7.4143	7.5575	7.4270	7.5924	**7.31**
H6	8.0691	8.2434	8.3303	8.3437	8.4667	8.3371	8.5292	8.3305	8.5036	8.3498	8.5531	8.0691	8.2434	8.3303	8.3437	8.4667	8.3371	8.5292	8.3305	8.5036	8.3498	8.5531	**8.11**
H8	4.5650	4.6235	4.6513	4.6787	4.7273	4.6747	4.7749	4.6709	4.7514	4.6822	4.7725	4.5650	4.6235	4.6513	4.6787	4.7273	4.6747	4.7749	4.6708	4.7514	4.6822	4.7725	**5.18**
H(9A-9B)	1.7345	1.7658	1.7709	1.7908	1.8071	1.7885	1.8131	1.7862	1.8041	1.7927	1.8421	1.7345	1.7658	1.7709	1.7908	1.8071	1.7885	1.8131	1.7862	1.8041	1.7927	1.8421	**2.05**
H(10A)	0.9439	0.8046	0.7615	0.7568	0.6649	0.7587	0.9607	0.7606	0.6992	0.7548	0.7188	0.9439	0.8046	0.7615	0.7568	0.6649	0.7587	0.7124	0.7606	0.6992	0.7548	0.7189	**1.14**
H(10B)	1.6350	1.5420	1.4670	1.4541	1.3671	1.4600	1.4933	1.4660	1.3682	1.4482	1.3328	1.6350	1.5420	1.4670	1.4541	1.3671	1.4600	1.3654	1.4660	1.3682	1.4482	1.3327	**1.39**
H(11A-11B)	1.0056	1.0247	0.9871	1.0334	0.9945	1.0329	0.9994	1.0324	0.9951	1.0336	0.9846	1.0056	1.0247	0.9871	1.0334	0.9945	1.0329	0.9994	1.0324	0.9951	1.0336	0.9846	**1.22**
H(12A-12C)	0.8954	0.8818	0.8542	0.8706	0.8300	0.8712	0.8408	0.8719	0.8377	0.8697	0.8328	0.8954	0.8818	0.8542	0.8706	0.8300	0.8712	0.8408	0.8719	0.8377	0.8697	0.8328	**0.77**
H(1`A)	2.6626	2.6552	2.6426	2.6448	2.6013	2.6453	2.8989	2.6459	2.6192	2.6440	2.5936	2.8001	2.8064	2.7926	2.7859	2.7548	2.7878	2.7693	2.7895	2.7706	2.7838	2.7342	**3.16**
H(1`B)	3.1711	3.2099	3.2462	3.2445	3.3001	3.2418	3.6043	3.2391	3.2874	3.2468	3.2911	2.8887	2.7177	2.7028	2.6786	2.6737	2.6335	2.6819	2.6335	2.6768	2.6159	**3.76**
H(2`A-2`B)	1.7041	1.7358	1.7004	1.7657	1.7181	1.7636	1.9209	1.7614	1.7270	1.7676	1.7507	1.5851	1.6586	1.6192	1.7000	1.6542	1.6974	1.6886	1.6949	1.6778	1.7022	1.7191	**2.13**
H(3`A-3`B)	1.5851	1.6586	1.6192	1.7000	1.6542	1.6974	1.9103	1.6948	1.6778	1.7022	1.7191	1.7041	1.7358	1.7004	1.7657	1.7181	1.7636	1.7348	1.7614	1.7270	1.7676	1.7507	**2.05**
H(4`A)	2.8887	2.7177	2.7028	2.6786	2.6737	2.6802	2.9914	2.6818	2.6335	2.6768	2.6159	3.1711	3.2099	3.2462	3.2445	3.3001	3.2418	3.2940	3.2391	3.2874	3.2468	3.2911	**3.09**
H(4`B)	2.8001	2.8064	2.7926	2.7859	2.7548	2.7878	3.0365	2.7895	2.7706	2.7838	2.7342	2.6626	2.6552	2.6426	2.6448	2.6013	2.6453	2.6219	2.6459	2.6192	2.6440	2.5936	**3.63**
F4	-113.6775	-114.6292	-117.1471	-114.6715	-118.6310	-114.6782	-116.3951	-114.6840	-116.7842	-114.6635	-116.1705	-113.6775	-114.6293	-117.1472	-114.6715	-118.6310	-114.6782	-116.3951	-114.6840	-116.7840	-114.6635	-116.1704	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. XII

Nuclei	R											S										Exp. [b]
	TPSS																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	132.4356	133.1505	133.9345	133.5892	135.0046	133.5760	134.3940	133.5726	134.0790	133.6107	134.7819	132.4356	133.1505	133.9343	133.5892	135.0046	133.5760	134.3940	133.5726	134.6812	133.6107	134.7819	**132.8**
C2	132.8929	132.8526	133.4725	132.7671	133.3034	132.7794	133.7783	132.8032	133.3065	132.7661	133.7282	132.8929	132.8526	133.4725	132.7671	133.3034	132.7793	133.7783	132.8032	133.9176	132.7661	133.7282	**132.9**
C3	116.6681	117.3246	117.9791	117.5839	118.2462	117.5771	118.5755	117.5815	118.0239	117.6006	118.6358	116.6681	117.3246	117.9791	117.5839	118.2462	117.5771	118.5755	117.5815	118.8101	117.6006	118.6358	**117.2**
C4	170.8911	171.7397	172.4965	172.2075	172.9099	172.1863	173.5612	172.1764	172.8372	172.2385	173.6673	170.8911	171.7397	172.4965	172.2075	172.9099	172.1863	173.5612	172.1764	172.9955	172.2385	173.6673	**167.5**
C5	114.7722	115.9311	116.6167	116.5690	117.3927	116.5353	117.6393	116.5131	116.9513	116.6120	117.7796	114.7722	115.9311	116.6167	116.5690	117.3927	116.5353	117.6393	116.5131	117.7497	116.6120	117.7796	**117.2**
C6	129.3185	131.1397	132.2995	132.2804	133.7885	132.2131	134.5062	132.1577	132.6584	132.3555	134.8302	129.3185	131.1397	132.2995	132.2804	133.7885	132.2131	134.5062	132.1577	133.2770	132.3555	134.8302	**132.9**
C7	197.2729	201.1909	202.3750	203.3951	204.2125	203.2728	208.3467	203.1606	203.9454	203.5200	209.4808	197.2729	201.1909	202.3748	203.3951	204.2125	203.2728	208.3467	203.1606	203.7473	203.5200	209.4808	**195.8**
C8	66.1554	67.2219	67.8668	67.7200	68.8092	67.7027	69.2644	67.6953	67.9382	67.7454	69.7480	66.1554	67.2219	67.8668	67.7200	68.8092	67.7027	69.2644	67.6953	69.2980	67.7454	69.7480	**68.4**
C9	37.7531	37.5421	37.8061	37.4640	37.8295	37.4741	38.1342	37.4954	37.6175	37.4651	38.2427	37.7531	37.5421	37.8059	37.4640	37.8295	37.4740	38.1342	37.4954	39.3246	37.4651	38.2427	**30.5**
C10	29.1817	29.5893	30.1503	29.9117	30.6464	29.8939	30.4886	29.8881	29.9798	29.9393	30.6120	29.1817	29.5893	30.1502	29.9117	30.6464	29.8939	30.4886	29.8881	31.7744	29.9393	30.6120	**27.6**
C11	29.3660	29.4429	29.7794	29.4146	29.8735	29.4257	29.8732	29.4479	29.5378	29.4144	30.0060	29.3660	29.4429	29.7794	29.4146	29.8736	29.4258	29.8732	29.4479	31.3375	29.4144	30.0060	**23.1**
C12	17.2694	17.3881	17.5648	17.5303	17.6714	17.5262	17.6562	17.5339	17.5761	17.5450	17.6292	17.2694	17.3881	17.5648	17.5303	17.6714	17.5262	17.6562	17.5339	19.5128	17.5450	17.6292	**13.8**
C1`	53.0445	53.7558	54.1667	54.3103	54.8418	54.2794	54.8722	54.2605	54.4497	54.3511	55.3404	57.2249	58.3026	58.7280	58.7950	59.3005	58.7753	59.5194	58.7666	60.4363	58.8238	59.7915	**53.5**
C2`	26.3341	26.7286	27.1499	26.9392	27.4229	26.9349	27.4595	26.9415	27.0214	26.9534	27.2605	26.0765	26.1994	26.6761	26.4209	26.8925	26.4135	26.9030	26.4175	28.3298	26.4384	26.7317	**24.5**
C3`	26.0765	26.1994	26.6761	26.4209	26.8925	26.4136	26.9030	26.4175	26.4953	26.4384	26.7317	26.3341	26.7286	27.1499	26.9392	27.4229	26.9349	27.4595	26.9415	28.8499	26.9534	27.2605	**24.3**
C4`	57.2249	58.3026	58.7280	58.7950	59.3005	58.7753	59.5194	58.7666	58.9738	58.8238	59.7915	53.0445	53.7558	54.1668	54.3103	54.8419	54.2794	54.8722	54.2605	55.9640	54.3511	55.3404	**57.5**
H2	8.5524	8.4665	8.5107	8.4102	8.4107	8.4132	8.4523	8.4170	8.2571	8.4079	8.4133	8.5524	8.4665	8.5107	8.4102	8.4107	8.4132	8.4523	8.4170	8.5271	8.4079	8.4133	**8.11**
H3	7.1623	7.3069	7.4039	7.3576	7.4767	7.3553	7.5043	7.3535	7.1893	7.3601	7.5144	7.1623	7.3069	7.4039	7.3576	7.4767	7.3553	7.5043	7.3535	7.4716	7.3601	7.5144	**7.31**
H5	6.9935	7.1616	7.2589	7.2313	7.3713	7.2271	7.3755	7.2236	7.0589	7.2357	7.3952	6.9935	7.1616	7.2589	7.2313	7.3713	7.2271	7.3755	7.2236	7.3426	7.2357	7.3952	**7.31**
H6	7.8543	8.0239	8.1241	8.1246	8.2413	8.1183	8.3087	8.1126	7.9514	8.1310	8.3186	7.8543	8.0239	8.1241	8.1246	8.2413	8.1183	8.3087	8.1126	8.2250	8.1310	8.3186	**8.11**
H8	4.7647	4.8126	4.8538	4.8581	4.9078	4.8551	4.9504	4.8528	4.6786	4.8614	4.9315	4.7647	4.8126	4.8538	4.8581	4.9078	4.8551	4.9504	4.8528	4.9896	4.8614	4.9315	**5.18**
H(9A-9B)	1.8001	1.8427	1.8422	1.8732	1.9021	1.8708	1.9032	1.8691	1.6830	1.8759	1.9251	1.8001	1.8427	1.8422	1.8732	1.9021	1.8708	1.9032	1.8691	2.0283	1.8759	1.9251	**2.05**
H(10A)	1.0002	0.8769	0.8927	0.8464	0.7648	0.8472	0.8274	0.8487	0.6585	0.8461	0.8190	1.0002	0.8769	0.8927	0.8464	0.7648	0.8472	0.8274	0.8487	1.0155	0.8461	0.8190	**1.14**
H(10B)	1.7385	1.6228	1.5525	1.5379	1.4588	1.5440	1.4467	1.5505	1.3631	1.5325	1.4054	1.7385	1.6228	1.5525	1.5379	1.4588	1.5440	1.4467	1.5505	1.9732	1.5325	1.4054	**1.39**
H(11A-11B)	1.0583	1.0759	1.0492	1.0919	1.0592	1.0911	1.0615	1.0909	0.9017	1.0929	1.0424	1.0583	1.0759	1.0492	1.0919	1.0592	1.0911	1.0615	1.0909	1.2559	1.0929	1.0424	**1.22**
H(12A-12C)	0.9078	0.8948	0.8800	0.8900	0.8562	0.8904	0.8645	0.8914	0.7014	0.8900	0.8548	0.9078	0.8948	0.8800	0.8900	0.8562	0.8904	0.8645	0.8914	1.0579	0.8900	0.8548	**0.77**
H(1`A)	2.7122	2.7112	2.7093	2.7074	2.6743	2.7077	2.6920	2.7086	2.5258	2.7075	2.6628	2.8273	2.8487	2.8382	2.8410	2.8258	2.8424	2.8307	2.8444	3.0399	2.8398	2.7945	**3.16**
H(1`B)	3.2745	3.3206	3.3526	3.3541	3.4150	3.3518	3.4072	3.3500	3.1698	3.3568	3.3950	3.0710	2.8744	2.8447	2.8264	2.8319	2.8280	2.7779	2.8303	2.9220	2.8255	2.7603	**3.76**
H(2`A-2`B)	1.7567	1.7877	1.7621	1.8208	1.7796	1.8184	1.7937	1.8167	1.6303	1.8235	1.8103	1.6119	1.6876	1.6609	1.7350	1.6925	1.7321	1.7200	1.7299	2.2245	1.7380	1.7577	**2.13**
H(3`A-3`B)	1.6119	1.6876	1.6609	1.7350	1.6925	1.7321	1.7200	1.7299	1.5432	1.7380	1.7577	1.7567	1.7877	1.7621	1.8208	1.7796	1.8184	1.7937	1.8167	2.0876	1.8235	1.8103	**2.05**
H(4`A)	3.0710	2.8744	2.8447	2.8264	2.8318	2.8280	2.7779	2.8303	2.6480	2.8255	2.7603	3.2745	3.3206	3.3526	3.3541	3.4150	3.3518	3.4072	3.3500	3.4375	3.3568	3.3950	**3.09**
H(4`B)	2.8273	2.8487	2.8382	2.8410	2.8258	2.8424	2.8307	2.8444	2.6622	2.8398	2.7945	2.7122	2.7112	2.7093	2.7074	2.6743	2.7077	2.6920	2.7086	2.7416	2.7075	2.6628	**3.63**
F4	-124.9440	-126.1785	-129.1128	-126.2557	-130.9715	-126.2608	-128.2470	-126.2651	-127.7783	-126.2491	-128.0382	-124.9440	-126.1785	-129.1129	-126.2557	-130.9715	-126.2608	-128.2470	-126.2651	-124.7287	-126.2491	-128.0382	**-104.5**
Nuclei	VSXC																						
C1	133.6805	134.5405	135.1885	134.8465	136.5075	134.8331	135.4592	134.8176	135.4598	134.8603	135.9108	133.6804	134.5405	135.1885	134.8465	136.5076	134.8331	135.4593	134.8176	135.4596	134.8603	135.9108	**132.8**
C2	130.8568	131.2148	131.6668	131.2177	131.8000	131.2250	132.3394	131.2296	132.2150	131.2117	132.4206	130.8567	131.2148	131.6668	131.2177	131.8000	131.2250	132.3394	131.2296	132.2150	131.2117	132.4206	**132.9**
C3	114.9211	115.9128	116.4365	116.3181	116.9073	116.2991	117.2645	116.2774	117.2025	116.3375	117.3624	114.9211	115.9128	116.4365	116.3181	116.9072	116.2991	117.2645	116.2774	117.2024	116.3375	117.3624	**117.2**
C4	168.3003	169.1032	169.7919	169.5485	170.2398	169.5239	170.8109	169.4971	170.6743	169.5735	170.9192	168.3003	169.1032	169.7919	169.5485	170.2398	169.5239	170.8108	169.4971	170.6743	169.5735	170.9192	**167.5**
C5	112.7729	114.1638	114.7218	114.9628	115.5777	114.9149	115.9637	114.8652	115.8581	115.0102	116.1017	112.7730	114.1638	114.7218	114.9628	115.5778	114.9149	115.9637	114.8652	115.8581	115.0102	116.1017	**117.2**
C6	128.4606	129.9982	131.1249	130.9894	132.3974	130.9269	132.9648	130.8631	132.7529	131.0511	133.1730	128.4606	129.9982	131.1249	130.9894	132.3975	130.9269	132.9647	130.8631	132.7528	131.0511	133.1730	**132.9**
C7	193.6144	198.7380	199.9101	201.2950	202.2459	201.1444	206.3068	200.9911	205.2665	201.4392	207.5617	193.6144	198.7380	199.9101	201.2950	202.2458	201.1444	206.3068	200.9911	205.2666	201.4392	207.5617	**195.8**
C8	71.2958	72.3979	72.9108	72.9017	73.7341	72.8757	74.0459	72.8472	73.8255	72.9277	74.6281	71.2958	72.3979	72.9108	72.9018	73.7341	72.8757	74.0459	72.8472	73.8255	72.9277	74.6281	**68.4**
C9	41.7566	42.2479	42.5811	42.4292	42.7524	42.4240	43.2429	42.4162	43.1046	42.4354	43.3121	41.7566	42.2479	42.5811	42.4293	42.7525	42.4240	43.2429	42.4162	43.1046	42.4354	43.3121	**30.5**
C10	36.4853	37.4189	37.7243	38.0913	38.8133	38.0483	38.7335	38.0038	38.7135	38.1344	39.0207	36.4853	37.4189	37.7243	38.0913	38.8133	38.0483	38.7334	38.0038	38.7134	38.1344	39.0207	**27.6**
C11	35.7245	35.7671	36.0142	35.6725	36.0233	35.6843	35.9517	35.6935	35.9513	35.6625	35.9686	35.7245	35.7671	36.0142	35.6725	36.0233	35.6843	35.9516	35.6935	35.9513	35.6625	35.9686	**23.1**
C12	18.7135	18.9231	19.0967	19.1393	19.3695	19.1260	19.2353	19.1108	19.2302	19.1539	19.2772	18.7135	18.9231	19.0967	19.1393	19.3695	19.1260	19.2353	19.1108	19.2301	19.1539	19.2772	**13.8**
C1`	58.8714	59.4981	59.7451	59.8519	60.3179	59.8335	60.1483	59.8130	60.1663	59.8709	60.3243	60.9536	61.9037	62.1420	62.3605	62.9177	62.3370	62.8341	62.3113	62.7698	62.3842	63.2050	**53.5**
C2`	29.5342	30.0310	30.1911	30.2855	30.6314	30.2737	30.6152	30.2596	30.5864	30.2979	30.6852	28.4893	28.8029	29.0331	29.0094	29.3917	28.9983	29.3626	28.9854	29.3504	29.0216	29.4075	**24.5**
C3`	28.4892	28.8029	29.0331	29.0094	29.3918	28.9983	29.3625	28.9854	29.3504	29.0216	29.4075	29.5341	30.0310	30.1911	30.2855	30.6313	30.2737	30.6153	30.2596	30.5863	30.2979	30.6852	**24.3**
C4`	60.9537	61.9037	62.1420	62.3605	62.9176	62.3370	62.8341	62.3113	62.7699	62.3842	63.2050	58.8714	59.4981	59.7451	59.8519	60.3180	59.8335	60.1482	59.8130	60.1664	59.8710	60.3243	**57.5**
H2	8.5227	8.5081	8.5164	8.4735	8.4550	8.4764	8.5360	8.4794	8.5408	8.4706	8.5151	8.5227	8.5081	8.5164	8.4735	8.4550	8.4764	8.5360	8.4794	8.5408	8.4706	8.5151	**8.11**
H3	7.1829	7.3512	7.4296	7.4126	7.5247	7.4094	7.5501	7.4062	7.5412	7.4155	7.5801	7.1829	7.3512	7.4296	7.4126	7.5247	7.4094	7.5501	7.4062	7.5412	7.4155	7.5801	**7.31**
H5	7.0781	7.2694	7.3540	7.3564	7.4727	7.3513	7.4935	7.3463	7.4820	7.3612	7.5113	7.0781	7.2694	7.3540	7.3564	7.4727	7.3513	7.4935	7.3463	7.4820	7.3612	7.5113	**7.31**
H6	7.8503	8.0072	8.0875	8.1024	8.2216	8.0962	8.2794	8.0902	8.2620	8.1082	8.3027	7.8503	8.0072	8.0875	8.1024	8.2216	8.0962	8.2794	8.0902	8.2620	8.1082	8.3027	**8.11**
H8	4.2573	4.4037	4.4274	4.4919	4.5768	4.4861	4.6320	4.4805	4.6030	4.4974	4.6706	4.2573	4.4037	4.4274	4.4919	4.5768	4.4861	4.6320	4.4805	4.6030	4.4974	4.6706	**5.18**
H(9A-9B)	1.9641	1.9764	1.9714	1.9883	1.9833	1.9875	1.9808	1.9869	1.9785	1.9889	1.9808	1.9641	1.9764	1.9714	1.9883	1.9833	1.9875	1.9808	1.9869	1.9785	1.9889	1.9808	**2.05**
H(10A)	0.9306	0.9326	0.9128	0.9285	0.9053	0.9291	0.8940	0.9297	0.8921	0.9279	0.8858	0.9306	0.9326	0.9128	0.9285	0.9053	0.9291	0.8940	0.9297	0.8921	0.9279	0.8858	**1.14**
H(10B)	2.2764	2.1111	2.0177	1.9949	1.8578	2.0028	1.8386	2.0106	1.8498	1.9873	1.7818	2.2764	2.1111	2.0177	1.9949	1.8578	2.0028	1.8386	2.0106	1.8498	1.9873	1.7818	**1.39**
H(11A-11B)	1.3715	1.3906	1.3742	1.4051	1.3862	1.4042	1.3808	1.4034	1.3793	1.4059	1.3754	1.3715	1.3906	1.3742	1.4051	1.3862	1.4042	1.3808	1.4034	1.3793	1.4059	1.3754	**1.22**
H(12A-12C)	1.0159	1.0221	0.9916	1.0217	0.9772	1.0218	0.9913	1.0219	0.9921	1.0216	0.9943	1.0159	1.0221	0.9916	1.0217	0.9772	1.0218	0.9914	1.0219	0.9921	1.0216	0.9943	**0.77**
H(1`A)	2.5466	2.6087	2.6123	2.6247	2.6165	2.6242	2.6238	2.6237	2.6182	2.6251	2.6253	2.9068	2.9249	2.9160	2.9333	2.9175	2.9330	2.9201	2.9327	2.9165	2.9335	2.9377	**3.16**
H(1`B)	3.2222	3.2385	3.2758	3.2572	3.3242	3.2559	3.3194	3.2547	3.3141	3.2584	3.3295	2.7958	2.7872	2.7812	2.8016	2.8140	2.8006	2.8086	2.7996	2.7986	2.8025	2.8470	**3.76**
H(2`A-2`B)	1.9183	1.9553	1.9386	1.9826	1.9516	1.9807	1.9672	1.9790	1.9642	1.9842	1.9718	2.0326	2.0928	2.0638	2.1285	2.0848	2.1261	2.1061	2.1240	2.1011	2.1307	2.1313	**2.13**
H(3`A-3`B)	2.0326	2.0928	2.0638	2.1285	2.0848	2.1261	2.1061	2.1240	2.1011	2.1307	2.1313	1.9183	1.9553	1.9386	1.9826	1.9516	1.9807	1.9672	1.9790	1.9642	1.9843	1.9718	**2.05**
H(4`A)	2.7958	2.7872	2.7812	2.8016	2.8140	2.8006	2.8086	2.7996	2.7986	2.8025	2.8470	3.2222	3.2385	3.2758	3.2572	3.3242	3.2559	3.3194	3.2547	3.3141	3.2584	3.3295	**3.09**
H(4`B)	2.9068	2.9249	2.9160	2.9333	2.9174	2.9330	2.9201	2.9327	2.9165	2.9335	2.9377	2.5466	2.6087	2.6123	2.6247	2.6165	2.6242	2.6238	2.6237	2.6182	2.6251	2.6253	**3.63**
F4	-126.7028	-127.8970	-130.8935	-127.7985	-132.7002	-127.8157	-129.8887	-127.8226	-130.2655	-127.7806	-129.6275	-126.7030	-127.8970	-130.8935	-127.7985	-132.7001	-127.8157	-129.8888	-127.8226	-130.2654	-127.7806	-129.6275	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. XIII

Nuclei	R											S										Exp. [b]
	wB97											wB97										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.6036	137.2931	138.0720	137.6679	139.4784	137.6596	138.7685	137.6458	138.8630	137.6709	139.1689	136.6037	137.2932	138.0720	137.6679	139.4785	137.6598	138.7686	137.6458	138.8630	137.6709	139.1689	**132.8**
C2	140.3841	140.2277	140.7307	140.0851	140.5886	140.0918	141.0437	140.0984	140.9507	140.0798	141.0312	140.3840	140.2279	140.7307	140.0850	140.5889	140.0917	141.0438	140.0984	140.9506	140.0796	141.0312	**132.9**
C3	121.6019	122.1976	122.7769	122.3867	123.0830	122.3768	123.2214	122.3659	123.1771	122.3963	123.2651	121.6019	122.1976	122.7769	122.3867	123.0830	122.3768	123.2213	122.3659	123.1771	122.3961	123.2650	**117.2**
C4	174.2312	174.8327	175.4522	175.1881	175.7881	175.1626	176.3324	175.1372	176.1882	175.2135	176.4253	174.2312	174.8326	175.4522	175.1882	175.7881	175.1627	176.3322	175.1372	176.1882	175.2133	176.4254	**167.5**
C5	119.5886	120.8444	121.4620	121.5301	122.3881	121.4874	122.5264	121.4436	122.4326	121.5708	122.6707	119.5886	120.8442	121.4620	121.5301	122.3881	121.4873	122.5263	121.4436	122.4326	121.5708	122.6707	**117.2**
C6	136.6592	138.3616	139.5017	139.3874	140.9361	139.3158	141.4313	139.2458	141.1605	139.4573	141.7769	136.6593	138.3615	139.5017	139.3873	140.9360	139.3158	141.4313	139.2458	141.1605	139.4574	141.7769	**132.9**
C7	201.4930	206.2813	207.4612	209.0200	209.7424	208.8666	215.3336	208.7073	214.1389	209.1604	216.6162	201.4932	206.2813	207.4612	209.0200	209.7424	208.8665	215.3336	208.7073	214.1389	209.1603	216.6162	**195.8**
C8	61.8488	62.9799	63.5330	63.4907	64.4664	63.4706	65.0895	63.4470	64.9281	63.5072	65.6139	61.8488	62.9799	63.5330	63.4908	64.4665	63.4705	65.0895	63.4470	64.9281	63.5073	65.6139	**68.4**
C9	33.4710	33.2416	33.4528	33.1389	33.4830	33.1466	33.5747	33.1536	33.4993	33.1317	33.7715	33.4709	33.2417	33.4528	33.1390	33.4830	33.1467	33.5747	33.1536	33.4993	33.1318	33.7715	**30.5**
C10	27.2566	27.6512	28.0056	27.9994	28.6490	27.9736	28.4332	27.9477	28.3999	28.0248	28.6428	27.2566	27.6512	28.0056	27.9993	28.6490	27.9737	28.4333	27.9477	28.3999	28.0248	28.6428	**27.6**
C11	26.2445	26.3038	26.5962	26.2779	26.6993	26.2792	26.6545	26.2801	26.6480	26.2768	26.8119	26.2446	26.3039	26.5962	26.2778	26.6993	26.2793	26.6544	26.2801	26.6480	26.2768	26.8119	**23.1**
C12	16.0982	16.1941	16.2592	16.3226	16.4257	16.3108	16.3515	16.2989	16.3401	16.3345	16.3725	16.0982	16.1942	16.2592	16.3225	16.4258	16.3108	16.3514	16.2989	16.3401	16.3346	16.3725	**13.8**
C1`	49.2568	49.9126	50.1155	50.3454	50.8618	50.3138	50.7647	50.2823	50.7307	50.3765	51.1612	53.0280	53.8362	54.1787	54.2424	54.7458	54.2152	54.7838	54.1877	54.7368	54.2686	54.9485	**53.5**
C2`	23.8426	24.1307	24.3776	24.2804	24.7127	24.2708	24.6901	24.2604	24.6738	24.2897	24.5996	23.1244	23.2955	23.5764	23.4577	23.9434	23.4448	23.8672	23.4312	23.8527	23.4704	23.8171	**24.5**
C3`	23.1243	23.2956	23.5764	23.4576	23.9434	23.4448	23.8671	23.4312	23.8527	23.4704	23.8171	23.8426	24.1307	24.3776	24.2804	24.7128	24.2708	24.6899	24.2604	24.6738	24.2898	24.5997	**24.3**
C4`	53.0280	53.8363	54.1787	54.2423	54.7459	54.2152	54.7840	54.1877	54.7368	54.2686	54.9485	49.2568	49.9127	50.1155	50.3454	50.8617	50.3139	50.7647	50.2823	50.7307	50.3765	51.1611	**57.5**
H2	8.8611	8.7550	8.7824	8.6884	8.6845	8.6907	8.6892	8.6933	8.6908	8.6868	8.6627	8.8611	8.7551	8.7824	8.6884	8.6845	8.6907	8.6892	8.6933	8.6908	8.6868	8.6628	**8.11**
H3	7.4418	7.5755	7.6657	7.6151	7.7392	7.6130	7.7548	7.6108	7.7474	7.6170	7.7687	7.4418	7.5755	7.6657	7.6151	7.7392	7.6130	7.7548	7.6108	7.7474	7.6170	7.7687	**7.31**
H5	7.2881	7.4745	7.5659	7.5546	7.6853	7.5499	7.6986	7.5450	7.6874	7.5592	7.7204	7.2881	7.4745	7.5659	7.5546	7.6853	7.5499	7.6986	7.5450	7.6874	7.5592	7.7204	**7.31**
H6	8.1472	8.3095	8.4115	8.4085	8.5457	8.4013	8.5816	8.3942	8.5608	8.4158	8.6004	8.1472	8.3095	8.4115	8.4085	8.5457	8.4013	8.5816	8.3942	8.5608	8.4158	8.6004	**8.11**
H8	4.2162	4.2825	4.3391	4.3494	4.4217	4.3438	4.4547	4.3384	4.4370	4.3551	4.4428	4.2162	4.2825	4.3391	4.3494	4.4217	4.3438	4.4547	4.3384	4.4370	4.3551	4.4427	**5.18**
H(9A-9B)	1.6980	1.7347	1.7280	1.7573	1.7680	1.7556	1.7679	1.7541	1.7590	1.7591	1.8079	1.6980	1.7347	1.7280	1.7573	1.7680	1.7556	1.7679	1.7541	1.7590	1.7591	1.8079	**2.05**
H(10A)	1.0016	0.8194	0.8010	0.7626	0.6910	0.7642	0.7142	0.7660	0.7163	0.7614	0.7212	1.0016	0.8194	0.8010	0.7625	0.6910	0.7642	0.7142	0.7660	0.7163	0.7614	0.7213	**1.14**
H(10B)	1.6278	1.5347	1.4753	1.4482	1.3716	1.4533	1.3682	1.4583	1.3751	1.4435	1.3347	1.6278	1.5347	1.4753	1.4482	1.3716	1.4533	1.3682	1.4583	1.3751	1.4435	1.3347	**1.39**
H(11A-11B)	0.9970	1.0164	0.9858	1.0253	0.9913	1.0240	0.9842	1.0229	0.9848	1.0267	0.9701	0.9970	1.0165	0.9858	1.0253	0.9913	1.0240	0.9842	1.0229	0.9848	1.0267	0.9701	**1.22**
H(12A-12C)	0.9260	0.9059	0.8807	0.8925	0.8533	0.8928	0.8544	0.8932	0.8560	0.8923	0.8453	0.9260	0.9059	0.8807	0.8925	0.8533	0.8928	0.8544	0.8932	0.8560	0.8923	0.8453	**0.77**
H(1`A)	2.6270	2.6255	2.6087	2.6149	2.5688	2.6154	2.5814	2.6159	2.5810	2.6146	2.5637	2.7756	2.7821	2.7653	2.7661	2.7415	2.7679	2.7612	2.7694	2.7614	2.7644	2.7326	**3.16**
H(1`B)	3.0717	3.1071	3.1361	3.1419	3.1899	3.1392	3.1745	3.1364	3.1704	3.1448	3.1707	2.7440	2.6065	2.5843	2.5750	2.5724	2.5770	2.5537	2.5787	2.5505	2.5729	2.5550	**3.76**
H(2`A-2`B)	1.6864	1.7205	1.6869	1.7508	1.7082	1.7484	1.7178	1.7460	1.7130	1.7532	1.7346	1.5865	1.6591	1.6198	1.7006	1.6650	1.6980	1.6917	1.6953	1.6865	1.7030	1.7206	**2.13**
H(3`A-3`B)	1.5864	1.6591	1.6198	1.7006	1.6650	1.6980	1.6917	1.6953	1.6865	1.7030	1.7206	1.6864	1.7205	1.6869	1.7508	1.7082	1.7484	1.7178	1.7460	1.7130	1.7532	1.7346	**2.05**
H(4`A)	2.7440	2.6065	2.5843	2.5750	2.5724	2.5770	2.5537	2.5787	2.5505	2.5729	2.5550	3.0717	3.1071	3.1361	3.1419	3.1899	3.1392	3.1744	3.1364	3.1704	3.1448	3.1707	**3.09**
H(4`B)	2.7756	2.7821	2.7653	2.7661	2.7415	2.7679	2.7612	2.7694	2.7614	2.7644	2.7326	2.6270	2.6255	2.6087	2.6149	2.5688	2.6155	2.5814	2.6159	2.5810	2.6146	2.5637	**3.63**
F4	-108.0081	-109.6688	-111.9384	-110.0751	-113.6828	-110.0627	-111.9416	-110.0477	-112.1966	-110.0845	-111.9270	-108.0083	-109.6688	-111.9384	-110.0751	-113.6827	-110.0627	-111.9418	-110.0477	-112.1966	-110.0845	-111.9269	**-104.5**
Nuclei	wB97X																						
C1	138.1726	138.9019	139.6559	139.4374	141.1483	139.4362	140.2893	139.4298	140.5386	139.4351	140.5881	138.1726	138.9020	139.6559	139.4374	141.1483	139.4362	140.2892	139.4298	140.5386	139.4351	140.5881	**132.8**
C2	140.9056	140.7859	141.2893	140.6233	141.1540	140.6326	141.6628	140.6415	141.4810	140.6157	141.6112	140.9055	140.7861	141.2893	140.6233	141.1540	140.6326	141.6628	140.6415	141.4810	140.6157	141.6112	**132.9**
C3	122.3191	122.9195	123.4907	123.1123	123.8008	123.1045	123.9961	123.0956	123.8881	123.1203	124.0304	122.3191	122.9193	123.4908	123.1123	123.8008	123.1045	123.9961	123.0956	123.8881	123.1203	124.0304	**117.2**
C4	174.9105	175.5432	176.1569	175.8933	176.4990	175.8689	177.1226	175.8445	176.8649	175.9183	177.2107	174.9104	175.5433	176.1570	175.8933	176.4990	175.8689	177.1226	175.8446	176.8649	175.9183	177.2107	**167.5**
C5	120.2722	121.5580	122.1552	122.2785	123.1172	122.2378	123.3127	122.1963	123.1518	122.3181	123.4476	120.2722	121.5580	122.1551	122.2785	123.1172	122.2378	123.3127	122.1963	123.1518	122.3181	123.4476	**117.2**
C6	136.9982	138.7129	139.8801	139.7133	141.2649	139.6414	141.8678	139.5704	141.4715	139.7845	142.2578	136.9982	138.7132	139.8800	139.7133	141.2649	139.6414	141.8678	139.5703	141.4715	139.7845	142.2578	**132.9**
C7	203.1280	207.9657	209.1246	210.8225	211.4559	210.6803	216.7975	210.5330	215.8333	210.9532	218.0343	203.1280	207.9653	209.1247	210.8225	211.4559	210.6803	216.7976	210.5330	215.8333	210.9532	218.0343	**195.8**
C8	63.1594	64.2444	64.8483	64.8139	65.7904	64.8024	66.3526	64.7861	66.3173	64.8222	66.9049	63.1594	64.2444	64.8484	64.8139	65.7904	64.8024	66.3525	64.7861	66.3173	64.8222	66.9049	**68.4**
C9	34.2867	33.9981	34.2392	33.8733	34.2116	33.8838	34.2855	33.8926	34.2464	33.8639	34.5266	34.2868	33.9981	34.2391	33.8733	34.2116	33.8838	34.2855	33.8926	34.2464	33.8639	34.5266	**30.5**
C10	27.6239	28.0338	28.4350	28.3754	29.0463	28.3517	28.8760	28.3279	28.7824	28.3996	29.0595	27.6239	28.0339	28.4349	28.3754	29.0463	28.3517	28.8759	28.3278	28.7824	28.3996	29.0595	**27.6**
C11	26.7734	26.8395	27.1217	26.8101	27.2443	26.8150	27.2454	26.8190	27.1824	26.8061	27.3901	26.7733	26.8395	27.1217	26.8101	27.2443	26.8150	27.2453	26.8190	27.1824	26.8061	27.3901	**23.1**
C12	16.1134	16.2233	16.2803	16.3492	16.4455	16.3394	16.4133	16.3295	16.3307	16.3601	16.4150	16.1135	16.2233	16.2803	16.3492	16.4455	16.3394	16.4133	16.3295	16.3307	16.3601	16.4150	**13.8**
C1`	49.9786	50.6789	50.8740	51.1549	51.6976	51.1232	51.6534	51.0913	51.5542	51.1870	52.0498	54.0121	54.8870	55.2128	55.3169	55.7989	55.2921	55.9370	55.2667	55.7988	55.3418	56.0923	**53.5**
C2`	24.3147	24.5823	24.8496	24.7428	25.1842	24.7362	25.2016	24.7285	25.1548	24.7501	25.0887	23.6105	23.7548	24.0311	23.9209	24.4101	23.9100	24.3738	23.8985	24.2790	23.9323	24.2815	**24.5**
C3`	23.6105	23.7548	24.0310	23.9209	24.4101	23.9100	24.3738	23.8985	24.2790	23.9323	24.2815	24.3147	24.5823	24.8496	24.7428	25.1842	24.7362	25.2015	24.7285	25.1548	24.7501	25.0887	**24.3**
C4`	54.0122	54.8869	55.2127	55.3169	55.7989	55.2921	55.9370	55.2667	55.7988	55.3418	56.0923	49.9785	50.6788	50.8741	51.1549	51.6976	51.1232	51.6535	51.0913	51.5542	51.1870	52.0498	**57.5**
H2	8.8389	8.7344	8.7644	8.6467	8.6499	8.6486	8.6801	8.6509	8.6532	8.6456	8.6538	8.8389	8.7344	8.7644	8.6467	8.6499	8.6486	8.6801	8.6509	8.6532	8.6456	8.6538	**8.11**
H3	7.4189	7.5552	7.6448	7.5956	7.7180	7.5936	7.7363	7.5916	7.7258	7.5975	7.7486	7.4189	7.5552	7.6448	7.5956	7.7180	7.5936	7.7363	7.5916	7.7257	7.5975	7.7486	**7.31**
H5	7.2591	7.4494	7.5388	7.5328	7.6613	7.5281	7.6770	7.5234	7.6630	7.5374	7.6981	7.2591	7.4494	7.5388	7.5328	7.6613	7.5281	7.6770	7.5234	7.6630	7.5374	7.6981	**7.31**
H6	8.1258	8.2888	8.3898	8.3787	8.5117	8.3714	8.5602	8.3643	8.5198	8.3862	8.5805	8.1258	8.2888	8.3898	8.3787	8.5117	8.3714	8.5602	8.3643	8.5198	8.3862	8.5805	**8.11**
H8	4.3096	4.3744	4.4229	4.4341	4.4965	4.4284	4.5479	4.4231	4.5054	4.4401	4.5323	4.3096	4.3744	4.4229	4.4341	4.4965	4.4284	4.5479	4.4231	4.5054	4.4401	4.5323	**5.18**
H(9A-9B)	1.6862	1.7156	1.7186	1.7332	1.7474	1.7318	1.7435	1.7303	1.7407	1.7347	1.7933	1.6862	1.7156	1.7186	1.7332	1.7474	1.7318	1.7435	1.7303	1.7407	1.7347	1.7933	**2.05**
H(10A)	0.9741	0.8166	0.7900	0.7615	0.6871	0.7623	0.7271	0.7634	0.7083	0.7612	0.7224	0.9741	0.8166	0.7900	0.7615	0.6871	0.7623	0.7271	0.7634	0.7083	0.7612	0.7224	**1.14**
H(10B)	1.6245	1.5295	1.4648	1.4366	1.3566	1.4418	1.3555	1.4472	1.3556	1.4319	1.3216	1.6245	1.5295	1.4648	1.4366	1.3566	1.4418	1.3555	1.4472	1.3556	1.4319	1.3216	**1.39**
H(11A-11B)	0.9968	1.0179	0.9853	1.0245	0.9912	1.0235	0.9920	1.0226	0.9837	1.0257	0.9745	0.9968	1.0179	0.9853	1.0245	0.9912	1.0235	0.9920	1.0226	0.9837	1.0257	0.9745	**1.22**
H(12A-12C)	0.9175	0.9002	0.8726	0.8866	0.8472	0.8870	0.8543	0.8875	0.8473	0.8864	0.8426	0.9175	0.9002	0.8727	0.8866	0.8472	0.8870	0.8543	0.8875	0.8473	0.8864	0.8426	**0.77**
H(1`A)	2.6470	2.6454	2.6305	2.6365	2.5914	2.6370	2.6054	2.6376	2.6015	2.6363	2.5818	2.7957	2.7944	2.7786	2.7812	2.7529	2.7831	2.7665	2.7849	2.7724	2.7793	2.7420	**3.16**
H(1`B)	3.0808	3.1191	3.1539	3.1560	3.2078	3.1531	3.1986	3.1503	3.1886	3.1590	3.1950	2.7613	2.6199	2.6024	2.5918	2.5863	2.5940	2.5496	2.5960	2.5607	2.5899	2.5507	**3.76**
H(2`A-2`B)	1.6866	1.7220	1.6875	1.7527	1.7072	1.7504	1.7192	1.7481	1.7097	1.7552	1.7348	1.5871	1.6591	1.6179	1.7060	1.6665	1.7037	1.6956	1.7013	1.6869	1.7083	1.7189	**2.13**
H(3`A-3`B)	1.5872	1.6591	1.6179	1.7060	1.6665	1.7037	1.6956	1.7013	1.6869	1.7083	1.7189	1.6866	1.7220	1.6875	1.7527	1.7072	1.7504	1.7192	1.7481	1.7097	1.7552	1.7348	**2.05**
H(4`A)	2.7613	2.6199	2.6025	2.5918	2.5863	2.5940	2.5496	2.5960	2.5607	2.5899	2.5507	3.0809	3.1191	3.1539	3.1560	3.2078	3.1531	3.1986	3.1503	3.1886	3.1590	3.1950	**3.09**
H(4`B)	2.7957	2.7944	2.7786	2.7812	2.7529	2.7831	2.7665	2.7849	2.7724	2.7793	2.7420	2.6470	2.6454	2.6305	2.6365	2.5914	2.6370	2.6054	2.6376	2.6015	2.6363	2.5818	**3.63**
F4	-110.3425	-111.8026	-114.1109	-112.1812	-115.8382	-112.1764	-113.9559	-112.1690	-114.3523	-112.1830	-113.9045	-110.3428	-111.8023	-114.1108	-112.1812	-115.8382	-112.1764	-113.9558	-112.1689	-114.3524	-112.1830	-113.9045	**-104.5**

[a] methyl protons shifts are averaged

[b] according to [6]

Table S6. Cont. XIV

Nuclei	R											S										Exp. [b]
	X3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.6738	140.7029	141.2879	141.2181	142.6377	141.1931	142.0187	141.1652	142.0627	141.2455	142.1890	139.6738	140.7029	141.2877	141.2181	142.6377	141.1931	142.0187	141.1652	142.0627	141.2455	142.1891	**132.8**
C2	139.7415	139.6983	140.2072	139.6129	140.0578	139.6218	140.6071	139.6280	140.4859	139.6083	140.5357	139.7415	139.6983	140.2071	139.6129	140.0578	139.6218	140.6071	139.6280	140.4859	139.6083	140.5359	**132.9**
C3	122.0899	122.7613	123.3039	122.9822	123.5845	122.9753	123.8523	122.9648	123.7861	122.9920	123.9125	122.0899	122.7613	123.3039	122.9822	123.5845	122.9753	123.8523	122.9648	123.7861	122.9920	123.9125	**117.2**
C4	176.3624	177.2172	177.8363	177.6336	178.2690	177.6121	178.8733	177.5874	178.7243	177.6576	178.9971	176.3624	177.2172	177.8362	177.6336	178.2690	177.6121	178.8733	177.5874	178.7243	177.6576	178.9971	**167.5**
C5	119.9750	121.1943	121.8036	121.8371	122.6276	121.8009	122.8281	121.7616	122.7328	121.8752	122.9752	119.9750	121.1943	121.8037	121.8372	122.6276	121.8009	122.8281	121.7616	122.7328	121.8752	122.9752	**117.2**
C6	135.9479	137.8862	139.0367	139.0291	140.5596	138.9585	141.2161	138.8853	140.9649	139.0998	141.6039	135.9479	137.8862	139.0366	139.0291	140.5596	138.9585	141.2161	138.8853	140.9649	139.0998	141.6039	**132.9**
C7	203.8442	208.6848	209.7423	211.2993	211.9258	211.1467	216.9743	210.9904	215.8222	211.4475	217.9867	203.8442	208.6848	209.7423	211.2993	211.9258	211.1467	216.9743	210.9904	215.8222	211.4475	217.9866	**195.8**
C8	66.1900	67.3996	67.9886	67.9123	68.9737	67.8933	69.5487	67.8696	69.3941	67.9319	69.8838	66.1900	67.3996	67.9886	67.9123	68.9737	67.8933	69.5487	67.8696	69.3941	67.9319	69.8838	**68.4**
C9	37.2125	36.8829	37.1023	36.7383	37.0705	36.7499	37.2814	36.7581	37.2176	36.7305	37.3484	37.2125	36.8829	37.1024	36.7383	37.0705	36.7499	37.2813	36.7581	37.2176	36.7305	37.3483	**30.5**
C10	29.2336	29.7336	30.2430	30.0625	30.8205	30.0426	30.6156	30.0200	30.6061	30.0851	30.7479	29.2336	29.7336	30.2429	30.0624	30.8205	30.0426	30.6156	30.0200	30.6061	30.0851	30.7479	**27.6**
C11	29.2440	29.3726	29.6606	29.3435	29.7886	29.3527	29.7810	29.3582	29.7823	29.3378	29.9009	29.2440	29.3726	29.6607	29.3436	29.7886	29.3527	29.7810	29.3582	29.7823	29.3378	29.9009	**23.1**
C12	16.6790	16.8526	16.9369	16.9924	17.0898	16.9846	17.0466	16.9744	17.0456	17.0037	17.0335	16.6790	16.8526	16.9370	16.9924	17.0898	16.9846	17.0465	16.9744	17.0456	17.0037	17.0336	**13.8**
C1`	52.1500	52.9655	53.2787	53.5431	54.0664	53.5092	54.0666	53.4728	53.9991	53.5797	54.5782	56.6692	57.8046	58.1645	58.2841	58.8069	58.2617	58.9279	58.2356	58.8673	58.3087	59.1667	**53.5**
C2`	25.9688	26.4573	26.8289	26.6445	27.1554	26.6386	27.1840	26.6293	27.1770	26.6532	26.9598	25.5752	25.7645	26.1378	25.9438	26.4160	25.9341	26.3685	25.9216	26.3639	25.9571	26.1690	**24.5**
C3`	25.5752	25.7645	26.1378	25.9439	26.4160	25.9341	26.3685	25.9216	26.3639	25.9571	26.1690	25.9688	26.4573	26.8288	26.6445	27.1554	26.6386	27.1839	26.6293	27.1770	26.6532	26.9597	**24.3**
C4`	56.6692	57.8046	58.1645	58.2842	58.8069	58.2616	58.9278	58.2356	58.8673	58.3087	59.1668	52.1500	52.9655	53.2788	53.5431	54.0664	53.5092	54.0666	53.4728	53.9991	53.5797	54.5781	**57.5**
H2	8.7017	8.5820	8.6334	8.5144	8.5224	8.5185	8.5444	8.5222	8.5458	8.5104	8.5311	8.7017	8.5820	8.6334	8.5144	8.5224	8.5185	8.5444	8.5222	8.5458	8.5104	8.5311	**8.11**
H3	7.3180	7.4626	7.5498	7.5093	7.6221	7.5074	7.6437	7.5048	7.6355	7.5111	7.6574	7.3180	7.4626	7.5498	7.5093	7.6221	7.5074	7.6437	7.5048	7.6355	7.5111	7.6574	**7.31**
H5	7.1388	7.2932	7.3946	7.3636	7.4967	7.3596	7.5018	7.3552	7.4932	7.3672	7.5277	7.1388	7.2932	7.3946	7.3636	7.4967	7.3596	7.5018	7.3552	7.4932	7.3672	7.5277	**7.31**
H6	7.9778	8.1585	8.2522	8.2595	8.3785	8.2534	8.4310	8.2468	8.4121	8.2652	8.4587	7.9778	8.1585	8.2522	8.2595	8.3785	8.2534	8.4310	8.2468	8.4121	8.2652	8.4587	**8.11**
H8	4.6221	4.6810	4.7192	4.7261	4.7782	4.7226	4.8173	4.7187	4.8029	4.7294	4.7963	4.6221	4.6810	4.7192	4.7261	4.7782	4.7226	4.8173	4.7187	4.8029	4.7294	4.7963	**5.18**
H(9A-9B)	1.7073	1.7466	1.7566	1.7758	1.8078	1.7740	1.8065	1.7718	1.8013	1.7774	1.8410	1.7073	1.7466	1.7566	1.7758	1.8078	1.7740	1.8065	1.7718	1.8013	1.7774	1.8410	**2.05**
H(10A)	1.0017	0.8584	0.8480	0.8249	0.7364	0.8258	0.7864	0.8263	0.7798	0.8243	0.7913	1.0017	0.8584	0.8480	0.8249	0.7364	0.8258	0.7864	0.8263	0.7798	0.8243	0.7913	**1.14**
H(10B)	1.6621	1.5559	1.4962	1.4782	1.3946	1.4836	1.3899	1.4885	1.3968	1.4731	1.3608	1.6621	1.5559	1.4962	1.4782	1.3946	1.4836	1.3899	1.4885	1.3968	1.4731	1.3608	**1.39**
H(11A-11B)	1.0602	1.0755	1.0472	1.0937	1.0553	1.0929	1.0546	1.0915	1.0540	1.0945	1.0426	1.0602	1.0755	1.0473	1.0937	1.0553	1.0929	1.0547	1.0915	1.0540	1.0945	1.0426	**1.22**
H(12A-12C)	0.9403	0.9279	0.9065	0.9238	0.8835	0.9241	0.8907	0.9241	0.8907	0.9234	0.8830	0.9403	0.9279	0.9065	0.9238	0.8835	0.9241	0.8906	0.9241	0.8907	0.9234	0.8830	**0.77**
H(1`A)	2.7437	2.7364	2.7259	2.7268	2.6858	2.7276	2.7033	2.7279	2.7047	2.7261	2.6669	2.8709	2.8795	2.8646	2.8584	2.8308	2.8605	2.8410	2.8620	2.8446	2.8562	2.8024	**3.16**
H(1`B)	3.2035	3.2527	3.2856	3.2909	3.3575	3.2884	3.3446	3.2855	3.3413	3.2932	3.3404	2.8974	2.7352	2.7069	2.7090	2.7058	2.7093	2.6710	2.7092	2.6722	2.7090	2.6597	**3.76**
H(2`A-2`B)	1.7389	1.7694	1.7353	1.8030	1.7519	1.8007	1.7656	1.7980	1.7608	1.8052	1.7835	1.6075	1.6874	1.6512	1.7365	1.6859	1.7336	1.7154	1.7303	1.7082	1.7392	1.7463	**2.13**
H(3`A-3`B)	1.6075	1.6874	1.6512	1.7364	1.6859	1.7336	1.7154	1.7303	1.7082	1.7392	1.7463	1.7389	1.7694	1.7352	1.8030	1.7519	1.8007	1.7656	1.7980	1.7608	1.8052	1.7835	**2.05**
H(4`A)	2.8974	2.7352	2.7069	2.7090	2.7058	2.7093	2.6710	2.7092	2.6722	2.7090	2.6597	3.2035	3.2527	3.2855	3.2909	3.3575	3.2884	3.3446	3.2855	3.3413	3.2932	3.3404	**3.09**
H(4`B)	2.8709	2.8795	2.8646	2.8584	2.8308	2.8605	2.8410	2.8620	2.8446	2.8562	2.8024	2.7437	2.7364	2.7259	2.7268	2.6858	2.7276	2.7033	2.7279	2.7047	2.7261	2.6669	**3.63**
F4	-124.1700	-125.6079	-128.3558	-125.8662	-130.1796	-125.8578	-127.9823	-125.8489	-128.3359	-125.8737	-127.7278	-124.1700	-125.6079	-128.3558	-125.8663	-130.1796	-125.8578	-127.9823	-125.8489	-128.3359	-125.8737	-127.7277	**-104.5**

[a] methyl protons shifts are averaged
[b] according to [6]

Table S7. Theoretical chemical shifts (in ppm) of *(R,S)*-4-fluoro-α-pyrrolidinononanophenone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S										Exp. [b]
	B3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
H2	8.6693	8.5547	8.5907	8.4593	8.4987	8.4663	8.4890	8.4733	8.4013	8.4526	8.5172	8.6693	8.5547	8.5907	8.4593	8.4987	8.4663	8.4074	8.4733	8.4013	8.4526	8.5172	**8.07**
H3	7.3116	7.4512	7.5342	7.4886	7.6059	7.4867	7.5964	7.4848	7.5971	7.4902	7.6449	7.3116	7.4512	7.5342	7.4886	7.6059	7.4867	7.6071	7.4848	7.5971	7.4902	7.6449	**7.24**
H5	7.1309	7.3065	7.3948	7.3863	7.5022	7.3812	7.5008	7.3761	7.5337	7.3907	7.5420	7.1309	7.3065	7.3948	7.3863	7.5022	7.3812	7.5468	7.3761	7.5337	7.3907	7.5420	**7.24**
H6	7.9655	8.1627	8.2357	8.2433	8.3768	8.2391	8.3986	8.2347	8.3278	8.2472	8.4483	7.9655	8.1627	8.2357	8.2433	8.3768	8.2391	8.3515	8.2347	8.3278	8.2472	8.4483	**8.07**
H8	4.6433	4.7289	4.7500	4.7575	4.8095	4.7566	4.9005	4.7554	4.8158	4.7579	4.8360	4.6433	4.7289	4.7500	4.7575	4.8095	4.7566	4.8330	4.7554	4.8157	4.7579	4.8360	**5.24**
H(9A-9B)	1.7222	1.7545	1.7554	1.7680	1.8251	1.7663	1.7917	1.7651	1.6955	1.7701	1.8393	1.7222	1.7545	1.7554	1.7680	1.8251	1.7663	1.7066	1.7651	1.6955	1.7701	1.8393	**2.135**
H(10A-10B)	1.3431	1.2354	1.1938	1.1670	1.0950	1.1714	1.1011	1.1757	1.1250	1.1626	1.1135	1.3432	1.2354	1.1938	1.1670	1.0950	1.1714	1.1248	1.1757	1.1250	1.1626	1.1135	**1.275**
H(11A-11B)	0.9890	1.0109	0.9726	1.0284	0.9917	1.0266	0.9794	1.0250	0.9728	1.0300	0.9829	0.9890	1.0109	0.9726	1.0284	0.9917	1.0266	0.9762	1.0250	0.9728	1.0300	0.9829	**1.28**
H(12A-12B)	1.2375	1.2278	1.1976	1.2122	1.1670	1.2130	1.1658	1.2138	1.1829	1.2111	1.1744	1.2375	1.2278	1.1976	1.2122	1.1670	1.2130	1.1840	1.2138	1.1829	1.2111	1.1744	**1.285**
H(13A-13B)	1.1508	1.1568	1.1229	1.1633	1.1273	1.1624	1.1149	1.1615	1.1200	1.1641	1.1228	1.1508	1.1568	1.1229	1.1634	1.1273	1.1624	1.1226	1.1615	1.1200	1.1641	1.1228	**1.29**
H(14A-14B)	1.3097	1.3103	1.2856	1.3059	1.2726	1.3059	1.2612	1.3059	1.2795	1.3057	1.2750	1.3097	1.3103	1.2856	1.3059	1.2726	1.3059	1.2813	1.3059	1.2795	1.3057	1.2750	**1.295**
H(15A-15C)	0.9551	0.9535	0.9276	0.9506	0.9207	0.9505	0.8987	0.9503	0.9200	0.9505	0.9190	0.9551	0.9535	0.9276	0.9506	0.9207	0.9505	0.9219	0.9503	0.9200	0.9505	0.9190	**0.82**
H(1`A)	2.7487	2.7479	2.7208	2.7338	2.6854	2.7347	2.7043	2.7354	2.6956	2.7328	2.6736	2.8743	2.8645	2.8562	2.8422	2.8141	2.8430	2.8174	2.8438	2.8192	2.8414	2.7793	**3.82**
H(1`B)	3.2194	3.2608	3.2819	3.2881	3.3399	3.2861	3.3328	3.2841	3.3184	3.2898	3.3406	2.8699	2.7074	2.6744	2.6831	2.6934	2.6832	2.6813	2.6834	2.6802	2.6831	2.6443	**3.78**
H(2`A-2`B)	1.7379	1.7827	1.7394	1.8102	1.7582	1.8082	1.7578	1.8062	1.7637	1.8118	1.7850	1.5835	1.6758	1.6369	1.7260	1.6678	1.7224	1.7153	1.7187	1.7075	1.7292	1.7255	**2.26**
H(3`A-3`B)	1.5835	1.6758	1.6369	1.7260	1.6678	1.7224	1.6799	1.7187	1.7075	1.7292	1.7255	1.7380	1.7827	1.7394	1.8102	1.7582	1.8082	1.7705	1.8062	1.7637	1.8118	1.7850	**2.01**
H(4`A)	2.8699	2.7074	2.6744	2.6831	2.6934	2.6832	2.6795	2.6834	2.6802	2.6831	2.6443	3.2194	3.2608	3.2819	3.2881	3.3399	3.2861	3.3253	3.2841	3.3184	3.2898	3.3406	**3.68**
H(4`B)	2.8743	2.8645	2.8562	2.8422	2.8141	2.8430	2.8187	2.8438	2.8192	2.8414	2.7793	2.7486	2.7479	2.7208	2.7338	2.6854	2.7347	2.6976	2.7354	2.6956	2.7328	2.6736	**2.88**
Nuclei	B3P86																						
H2	8.7403	8.6754	8.6602	8.5732	8.5747	8.5834	8.5932	8.5916	8.6190	8.5641	8.5845	8.7403	8.6754	8.6602	8.5732	8.5747	8.5834	8.6167	8.5916	8.6190	8.5641	8.5845	**8.07**
H3	7.3317	7.4774	7.5723	7.5245	7.6458	7.5238	7.6354	7.5211	7.6610	7.5262	7.6837	7.3317	7.4774	7.5723	7.5245	7.6458	7.5238	7.6654	7.5211	7.6610	7.5262	7.6837	**7.24**
H5	7.1472	7.3358	7.4228	7.4044	7.5340	7.4017	7.5241	7.3971	7.5461	7.4081	7.5714	7.1472	7.3358	7.4228	7.4044	7.5340	7.4017	7.5542	7.3971	7.5461	7.4081	7.5714	**7.24**
H6	8.0225	8.2297	8.2939	8.3160	8.4305	8.3123	8.4715	8.3064	8.4849	8.3201	8.5353	8.0225	8.2297	8.2939	8.3160	8.4304	8.3123	8.5049	8.3064	8.4849	8.3201	8.5353	**8.07**
H8	4.6484	4.7296	4.7658	4.7652	4.8174	4.7659	4.9040	4.7639	4.8681	4.7649	4.8720	4.6484	4.7296	4.7658	4.7652	4.8174	4.7659	4.8794	4.7639	4.8681	4.7649	4.8720	**5.24**
H(9A-9B)	1.7933	1.8417	1.8102	1.8531	1.8752	1.8523	1.8728	1.8504	1.8610	1.8559	1.8873	1.7933	1.8416	1.8102	1.8531	1.8752	1.8523	1.8659	1.8504	1.8610	1.8559	1.8873	**2.135**
H(10A-10B)	1.3555	1.2402	1.2054	1.1692	1.1077	1.1752	1.1032	1.1792	1.1267	1.1648	1.1100	1.3555	1.2402	1.2054	1.1691	1.1077	1.1752	1.1197	1.1792	1.1267	1.1648	1.1100	**1.275**
H(11A-11B)	0.9713	0.9976	0.9548	1.0141	0.9765	1.0138	0.9661	1.0118	0.9711	1.0157	0.9646	0.9713	0.9976	0.9548	1.0141	0.9765	1.0138	0.9683	1.0118	0.9711	1.0157	0.9646	**1.28**
H(12A-12B)	1.2227	1.2083	1.1845	1.1914	1.1539	1.1939	1.1453	1.1944	1.1635	1.1903	1.1572	1.2227	1.2083	1.1845	1.1914	1.1539	1.1939	1.1583	1.1944	1.1634	1.1903	1.1572	**1.285**
H(13A-13B)	1.1281	1.1319	1.1013	1.1382	1.1048	1.1388	1.0891	1.1376	1.1018	1.1391	1.0987	1.1281	1.1319	1.1013	1.1383	1.1048	1.1388	1.0979	1.1376	1.1018	1.1391	1.0987	**1.29**
H(14A-14B)	1.2803	1.2766	1.2573	1.2717	1.2431	1.2733	1.2266	1.2729	1.2484	1.2716	1.2438	1.2803	1.2766	1.2573	1.2717	1.2431	1.2733	1.2440	1.2729	1.2485	1.2716	1.2438	**1.295**
H(15A-15C)	0.9213	0.9193	0.8972	0.9160	0.8890	0.9174	0.8642	0.9170	0.8914	0.9159	0.8861	0.9213	0.9193	0.8972	0.9160	0.8890	0.9174	0.8868	0.9170	0.8914	0.9159	0.8861	**0.82**
H(1`A)	2.7048	2.7089	2.6899	2.6926	2.6501	2.6953	2.6647	2.6961	2.6668	2.6911	2.6359	2.8302	2.8173	2.8105	2.8030	2.7716	2.8046	2.7750	2.8046	2.7819	2.8030	2.7462	**3.82**
H(1`B)	3.2227	3.2611	3.2768	3.2837	3.3293	3.2835	3.3203	3.2815	3.3230	3.2850	3.3277	2.9188	2.7123	2.7132	2.6794	2.7077	2.6795	2.6380	2.6787	2.6483	2.6817	2.6399	**3.78**
H(2`A-2`B)	1.7225	1.7609	1.7300	1.7869	1.7457	1.7864	1.7378	1.7839	1.7560	1.7888	1.7760	1.5695	1.6493	1.6195	1.6967	1.6507	1.6949	1.6753	1.6911	1.6739	1.6995	1.7185	**2.26**
H(3`A-3`B)	1.5695	1.6493	1.6195	1.6967	1.6507	1.6949	1.6528	1.6912	1.6739	1.6995	1.7185	1.7225	1.7609	1.7300	1.7869	1.7457	1.7864	1.7566	1.7840	1.7560	1.7888	1.7760	**2.01**
H(4`A)	2.9188	2.7123	2.7132	2.6794	2.7077	2.6795	2.6746	2.6787	2.6483	2.6817	2.6399	3.2227	3.2610	3.2768	3.2837	3.3293	3.2835	3.3234	3.2815	3.3230	3.2850	3.3277	**3.68**
H(4`B)	2.8302	2.8172	2.8105	2.8030	2.7716	2.8046	2.7840	2.8045	2.7819	2.8030	2.7462	2.7048	2.7089	2.6899	2.6926	2.6500	2.6953	2.6621	2.6961	2.6668	2.6911	2.6359	**2.88**
Nuclei	B3PW91																						
H2	8.7093	8.5947	8.6296	8.5029	8.5475	8.5105	8.5319	8.5174	8.5774	8.4956	8.5148	8.7093	8.5947	8.6296	8.5029	8.5320	8.5105	8.5584	8.5174	8.5774	8.4956	8.5148	**8.07**
H3	7.3315	7.4773	7.5665	7.5151	7.6534	7.5140	7.6281	7.5125	7.6516	7.5163	7.6727	7.3315	7.4773	7.5665	7.5151	7.6379	7.5140	7.6590	7.5125	7.6516	7.5163	7.6727	**7.24**
H5	7.1504	7.3277	7.4240	7.4068	7.5461	7.4027	7.5275	7.3983	7.5420	7.4106	7.5642	7.1504	7.3277	7.4240	7.4068	7.5306	7.4027	7.5506	7.3983	7.5420	7.4106	7.5642	**7.24**
H6	8.0045	8.2018	8.2745	8.3017	8.4629	8.2970	8.4558	8.2917	8.4654	8.3057	8.5091	8.0045	8.2018	8.2745	8.3017	8.4474	8.2970	8.4871	8.2917	8.4653	8.3058	8.5091	**8.07**
H8	4.6390	4.7201	4.7465	4.7519	4.8277	4.7516	4.8910	4.7506	4.8440	4.7519	4.8363	4.6390	4.7201	4.7465	4.7519	4.8122	4.7516	4.8522	4.7506	4.8440	4.7519	4.8363	**5.24**
H(9A-9B)	1.7418	1.7634	1.7672	1.7873	1.8487	1.7851	1.8084	1.7830	1.8158	1.7900	1.8213	1.7418	1.7633	1.7672	1.7873	1.8332	1.7851	1.8183	1.7830	1.8158	1.7900	1.8213	**2.135**
H(10A-10B)	1.3208	1.2036	1.1695	1.1336	1.0802	1.1386	1.0704	1.1433	1.0892	1.1290	1.0672	1.3208	1.2036	1.1695	1.1336	1.0647	1.1386	1.0819	1.1433	1.0892	1.1290	1.0672	**1.275**
H(11A-11B)	0.9479	0.9654	0.9293	0.9852	0.9675	0.9840	0.9384	0.9827	0.9432	0.9866	0.9301	0.9479	0.9654	0.9293	0.9852	0.9520	0.9841	0.9404	0.9827	0.9432	0.9867	0.9301	**1.28**
H(12A-12B)	1.1983	1.1829	1.1570	1.1665	1.1403	1.1681	1.1216	1.1695	1.1340	1.1651	1.1269	1.1983	1.1829	1.1570	1.1665	1.1248	1.1681	1.1311	1.1695	1.1340	1.1651	1.1269	**1.285**
H(13A-13B)	1.1073	1.1086	1.0783	1.1155	1.0979	1.1154	1.0676	1.1149	1.0768	1.1160	1.0721	1.1073	1.1086	1.0783	1.1155	1.0824	1.1154	1.0752	1.1149	1.0768	1.1160	1.0721	**1.29**
H(14A-14B)	1.2651	1.2621	1.2399	1.2576	1.2412	1.2584	1.2136	1.2588	1.2297	1.2570	1.2259	1.2651	1.2621	1.2399	1.2576	1.2257	1.2584	1.2288	1.2588	1.2297	1.2570	1.2259	**1.295**
H(15A-15C)	0.9104	0.9067	0.8840	0.9044	0.8911	0.9050	0.8538	0.9053	0.8766	0.9040	0.8719	0.9104	0.9067	0.8839	0.9044	0.8756	0.9050	0.8753	0.9053	0.8766	0.9040	0.8719	**0.82**
H(1`A)	2.6998	2.6997	2.6782	2.6831	2.6510	2.6848	2.6566	2.6863	2.6540	2.6815	2.6212	2.8232	2.8093	2.8031	2.7940	2.7612	2.7951	2.7703	2.7959	2.7696	2.7934	2.7387	**3.82**
H(1`B)	3.1960	3.2324	3.2531	3.2600	3.3199	3.2586	3.3003	3.2569	3.2992	3.2615	3.3021	2.8718	2.6962	2.6803	2.6637	2.6791	2.6640	2.6301	2.6646	2.6271	2.6643	2.6335	**3.78**
H(2`A-2`B)	1.7098	1.7508	1.7149	1.7758	1.7511	1.7746	1.7272	1.7731	1.7400	1.7772	1.7605	1.5602	1.6462	1.6068	1.6919	1.6423	1.6895	1.6688	1.6869	1.6602	1.6943	1.7139	**2.26**
H(3`A-3`B)	1.5602	1.6462	1.6068	1.6919	1.6578	1.6895	1.6488	1.6869	1.6602	1.6943	1.7139	1.7098	1.7508	1.7149	1.7758	1.7356	1.7746	1.7441	1.7731	1.7400	1.7772	1.7605	**2.01**
H(4`A)	2.8718	2.6962	2.6803	2.6637	2.6946	2.6640	2.6598	2.6646	2.6270	2.6643	2.6335	3.1960	3.2324	3.2531	3.2600	3.3044	3.2586	3.3037	3.2569	3.2992	3.2615	3.3021	**3.68**
H(4`B)	2.8232	2.8093	2.8031	2.7941	2.7767	2.7951	2.7747	2.7959	2.7696	2.7933	2.7386	2.6998	2.6997	2.6781	2.6831	2.6355	2.6848	2.6530	2.6863	2.6540	2.6815	2.6212	**2.88**
Nuclei	B98																						
H2	8.6854	8.5945	8.6132	8.5090	8.5292	8.5158	8.5704	8.5223	8.4385	8.5022	8.5395	8.6854	8.5945	8.6132	8.5090	8.5292	8.5158	8.4417	8.5223	8.4385	8.5022	8.5395	**8.07**
H3	7.3204	7.4616	7.5520	7.5049	7.6257	7.5030	7.6469	7.5011	7.6254	7.5068	7.6634	7.3204	7.4616	7.5520	7.5049	7.6257	7.5030	7.6334	7.5012	7.6254	7.5068	7.6634	**7.24**
H5	7.1529	7.3313	7.4256	7.4141	7.5381	7.4094	7.5577	7.4048	7.5623	7.4187	7.5722	7.1529	7.3313	7.4256	7.4141	7.5380	7.4094	7.5729	7.4048	7.5623	7.4187	7.5722	**7.24**
H6	8.0107	8.2017	8.2813	8.2935	8.4286	8.2885	8.4883	8.2834	8.3708	8.2982	8.5149	8.0107	8.2017	8.2813	8.2935	8.4286	8.2885	8.3904	8.2834	8.3708	8.2982	8.5149	**8.07**
H8	4.6099	4.6916	4.7237	4.7319	4.7887	4.7305	4.8405	4.7288	4.7931	4.7332	4.8346	4.6099	4.6916	4.7237	4.7319	4.7887	4.7305	4.8066	4.7288	4.7931	4.7332	4.8346	**5.24**
H(9A-9B)	1.7236	1.7570	1.7496	1.7733	1.8072	1.7717	1.8083	1.7702	1.6894	1.7754	1.8246	1.7235	1.7570	1.7496	1.7733	1.8072	1.7717	1.6990	1.7702	1.6894	1.7754	1.8246	**2.135**
H(10A-10B)	1.3506	1.2333	1.1950	1.1590	1.0899	1.1643	1.1084	1.1696	1.1203	1.1541	1.0977	1.3506	1.2333	1.1950	1.1590	1.0899	1.1643	1.1168	1.1696	1.1203	1.1541	1.0977	**1.275**
H(11A-11B)	0.9772	0.9946	0.9578	1.0135	0.9777	1.0120	0.9737	1.0106	0.9615	1.0154	0.9684	0.9772	0.9946	0.9578	1.0135	0.9777	1.0120	0.9620	1.0106	0.9615	1.0154	0.9684	**1.28**
H(12A-12B)	1.2204	1.2038	1.1781	1.1869	1.1455	1.1883	1.1542	1.1897	1.1659	1.1859	1.1526	1.2204	1.2038	1.1781	1.1869	1.1455	1.1883	1.1643	1.1897	1.1659	1.1859	1.1526	**1.285**
H(13A-13B)	1.1314	1.1330	1.1028	1.1401	1.1049	1.1396	1.1025	1.1392	1.1022	1.1409	1.1015	1.1314	1.1330	1.1028	1.1401	1.1049	1.1396	1.1020	1.1392	1.1022	1.1409	1.1015	**1.29**
H(14A-14B)	1.2851	1.2810	1.2600	1.2762	1.2448	1.2767	1.2490	1.2773	1.2562	1.2761	1.2466	1.2851	1.2810	1.2600	1.2762	1.2448	1.2767	1.2552	1.2773	1.2562	1.2761	1.2466	**1.295**
H(15A-15C)	0.9303	0.9255	0.9035	0.9235	0.8946	0.9237	0.8955	0.9240	0.8985	0.9235	0.8925	0.9303	0.9255	0.9035	0.9235	0.8946	0.9237	0.8977	0.9240	0.8985	0.9235	0.8925	**0.82**
H(1`A)	2.7132	2.7100	2.6906	2.6975	2.6553	2.6984	2.6699	2.6994	2.6714	2.6969	2.6463	2.8410	2.8275	2.8256	2.8114	2.7814	2.8123	2.7707	2.7860	2.7915	2.8110	2.7560	**3.82**
H(1`B)	3.2060	3.2428	3.2681	3.2664	3.3137	3.2654	3.3135	3.2644	3.3034	3.2675	3.3177	2.8666	2.6969	2.6851	2.6720	2.6908	2.6721	2.6390	2.6728	2.6821	2.6728	2.6373	**3.78**
H(2`A-2`B)	1.7256	1.7702	1.7345	1.8002	1.7523	1.7985	1.7678	1.7969	1.7606	1.8020	1.7847	1.5864	1.6710	1.6361	1.7198	1.6689	1.7167	1.6943	1.7138	1.7091	1.7230	1.7300	**2.26**
H(3`A-3`B)	1.5864	1.6710	1.6361	1.7198	1.6689	1.7167	1.6943	1.7138	1.7091	1.7230	1.7300	1.7256	1.7702	1.7345	1.8002	1.7523	1.7985	1.7646	1.7969	1.7606	1.8020	1.7847	**2.01**
H(4`A)	2.8666	2.6969	2.6851	2.6720	2.6908	2.6721	2.6390	2.6728	2.6821	2.6728	2.6373	3.2059	3.2428	3.2681	3.2664	3.3137	3.2654	3.3075	3.2644	3.3034	3.2675	3.3177	**3.68**
H(4`B)	2.8410	2.8275	2.8256	2.8114	2.7814	2.8123	2.7860	2.8133	2.7915	2.8110	2.7560	2.7132	2.7100	2.6906	2.6975	2.6553	2.6984	2.6707	2.6994	2.6714	2.6969	2.6463	**2.88**

[a] methyl protons shifts are averaged
[b] according to [7]

Table S7. Cont. I

Nuclei	R											S										Exp. [b]
	B971																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
H2	8.6852	8.6078	8.6116	8.5185	8.5287	8.5250	8.5705	8.5310	8.4361	8.5120	8.5410	8.6852	8.6078	8.6116	8.5185	8.5287	8.5249	8.4392	8.5310	8.4361	8.5120	8.5410	**8.07**
H3	7.3178	7.4574	7.5488	7.5026	7.6222	7.5005	7.6432	7.4984	7.6220	7.5049	7.6593	7.3178	7.4574	7.5488	7.5026	7.6222	7.5005	7.6300	7.4984	7.6220	7.5049	7.6592	**7.24**
H5	7.1534	7.3313	7.4252	7.4137	7.5380	7.4088	7.5567	7.4040	7.5597	7.4186	7.5715	7.1534	7.3313	7.4252	7.4137	7.5380	7.4088	7.5700	7.4040	7.5596	7.4186	7.5715	**7.24**
H6	8.0174	8.2095	8.2837	8.2988	8.4300	8.2934	8.4882	8.2879	8.3690	8.3040	8.5132	8.0174	8.2095	8.2837	8.2988	8.4300	8.2934	8.3881	8.2879	8.3690	8.3040	8.5132	**8.07**
H8	4.6121	4.6898	4.7260	4.7349	4.7908	4.7330	4.8426	4.7309	4.7969	4.7365	4.8374	4.6121	4.6898	4.7260	4.7348	4.7908	4.7330	4.8099	4.7309	4.7969	4.7365	4.8374	**5.24**
H(9A-9B)	1.7314	1.7750	1.7545	1.7849	1.8122	1.7829	1.8125	1.7811	1.6934	1.7874	1.8300	1.7314	1.7749	1.7545	1.7849	1.8122	1.7829	1.7029	1.7810	1.6934	1.7874	1.8300	**2.135**
H(10A-10B)	1.3490	1.2309	1.1938	1.1592	1.0905	1.1643	1.1088	1.1692	1.1193	1.1548	1.0994	1.3490	1.2309	1.1938	1.1592	1.0905	1.1643	1.1157	1.1692	1.1193	1.1548	1.0994	**1.275**
H(11A-11B)	0.9780	0.9957	0.9567	1.0136	0.9764	1.0118	0.9721	1.0102	0.9587	1.0158	0.9673	0.9780	0.9957	0.9567	1.0136	0.9764	1.0118	0.9591	1.0102	0.9587	1.0158	0.9673	**1.28**
H(12A-12B)	1.2202	1.2018	1.1771	1.1860	1.1448	1.1873	1.1531	1.1885	1.1645	1.1853	1.1521	1.2202	1.2018	1.1771	1.1860	1.1448	1.1873	1.1628	1.1884	1.1645	1.1853	1.1521	**1.285**
H(13A-13B)	1.1304	1.1311	1.1014	1.1391	1.1035	1.1384	1.1009	1.1377	1.1004	1.1403	1.1002	1.1304	1.1311	1.1014	1.1391	1.1035	1.1384	1.1001	1.1377	1.1004	1.1403	1.1002	**1.29**
H(14A-14B)	1.2837	1.2785	1.2584	1.2749	1.2432	1.2752	1.2473	1.2755	1.2542	1.2751	1.2449	1.2837	1.2785	1.2584	1.2749	1.2432	1.2752	1.2532	1.2755	1.2542	1.2751	1.2449	**1.295**
H(15A-15C)	0.9254	0.9202	0.8986	0.9191	0.8896	0.9191	0.8904	0.9191	0.8932	0.9195	0.8876	0.9254	0.9201	0.8986	0.9191	0.8897	0.9191	0.8924	0.9191	0.8932	0.9195	0.8876	**0.82**
H(1`A)	2.7029	2.6995	2.6816	2.6881	2.6466	2.6887	2.6597	2.6895	2.6602	2.6879	2.6349	2.8303	2.8189	2.8165	2.8046	2.7740	2.8052	2.7827	2.8060	2.7852	2.8045	2.7485	**3.82**
H(1`B)	3.2102	3.2465	3.2707	3.2695	3.3157	3.2684	3.3141	3.2672	3.3043	3.2708	3.3175	2.8720	2.6942	2.6887	2.6702	2.6903	2.6701	2.6811	2.6706	2.6831	2.6714	2.6365	**3.78**
H(2`A-2`B)	1.7231	1.7664	1.7330	1.7983	1.7513	1.7964	1.7661	1.7945	1.7583	1.8005	1.7830	1.5856	1.6670	1.6352	1.7174	1.6677	1.7143	1.7136	1.7112	1.7089	1.7208	1.7283	**2.26**
H(3`A-3`B)	1.5856	1.6670	1.6352	1.7174	1.6677	1.7142	1.6930	1.7112	1.7089	1.7208	1.7284	1.7231	1.7664	1.7330	1.7983	1.7513	1.7964	1.7622	1.7945	1.7583	1.8005	1.7830	**2.01**
H(4`A)	2.8720	2.6942	2.6887	2.6702	2.6903	2.6701	2.6378	2.6706	2.6831	2.6714	2.6365	3.2102	3.2465	3.2707	3.2695	3.3157	3.2684	3.3082	3.2672	3.3044	3.2708	3.3175	**3.68**
H(4`B)	2.8303	2.8189	2.8165	2.8046	2.7740	2.8052	2.7782	2.8060	2.7852	2.8045	2.7485	2.7029	2.6995	2.6816	2.6881	2.6466	2.6887	2.6594	2.6895	2.6602	2.6879	2.6349	**2.88**
Nuclei	B972																						
H2	8.6887	8.5379	8.6200	8.4376	8.4966	8.4437	8.4298	8.4495	8.4265	8.4315	8.4204	8.6887	8.5379	8.6200	8.4376	8.4966	8.4437	8.4298	8.4495	8.4265	8.4315	8.4204	**8.07**
H3	7.3253	7.4602	7.5558	7.4952	7.6251	7.4934	7.6266	7.4914	7.6190	7.4968	7.6412	7.3253	7.4602	7.5558	7.4952	7.6251	7.4934	7.6266	7.4914	7.6190	7.4968	7.6412	**7.24**
H5	7.1513	7.3315	7.4222	7.4177	7.5230	7.4129	7.5667	7.4078	7.5559	7.4221	7.5806	7.1513	7.3315	7.4222	7.4177	7.5230	7.4129	7.5667	7.4078	7.5559	7.4221	7.5806	**7.24**
H6	7.9809	8.1701	8.2489	8.2449	8.3897	8.2407	8.3824	8.2361	8.3607	8.2487	8.4095	7.9809	8.1701	8.2489	8.2450	8.3897	8.2407	8.3824	8.2361	8.3607	8.2487	8.4095	**8.07**
H8	4.6069	4.6785	4.7065	4.7030	4.7545	4.7017	4.7979	4.7001	4.7822	4.7040	4.7920	4.6069	4.6785	4.7065	4.7030	4.7545	4.7017	4.7979	4.7001	4.7822	4.7040	4.7920	**5.24**
H(9A-9B)	1.6994	1.7027	1.7372	1.7113	1.7930	1.7092	1.6834	1.7072	1.6746	1.7135	1.7038	1.6994	1.7027	1.7372	1.7113	1.7930	1.7092	1.6834	1.7072	1.6747	1.7135	1.7038	**2.135**
H(10A-10B)	1.3142	1.1970	1.1667	1.1347	1.0648	1.1386	1.0894	1.1424	1.0928	1.1307	1.0889	1.3142	1.1970	1.1667	1.1347	1.0648	1.1386	1.0893	1.1424	1.0928	1.1307	1.0889	**1.275**
H(11A-11B)	0.9493	0.9627	0.9332	0.9844	0.9480	0.9826	0.9388	0.9807	0.9380	0.9858	0.9390	0.9493	0.9627	0.9332	0.9844	0.9480	0.9826	0.9388	0.9807	0.9379	0.9858	0.9390	**1.28**
H(12A-12B)	1.2000	1.1847	1.1585	1.1744	1.1254	1.1752	1.1453	1.1759	1.1469	1.1733	1.1476	1.2000	1.1847	1.1585	1.1744	1.1254	1.1752	1.1453	1.1759	1.1469	1.1733	1.1476	**1.285**
H(13A-13B)	1.1099	1.1101	1.0815	1.1208	1.0830	1.1199	1.0827	1.1189	1.0826	1.1215	1.0851	1.1099	1.1101	1.0815	1.1208	1.0830	1.1199	1.0827	1.1189	1.0826	1.1215	1.0851	**1.29**
H(14A-14B)	1.2721	1.2702	1.2473	1.2704	1.2335	1.2705	1.2438	1.2704	1.2446	1.2701	1.2432	1.2721	1.2702	1.2473	1.2704	1.2335	1.2705	1.2438	1.2704	1.2446	1.2701	1.2432	**1.295**
H(15A-15C)	0.9220	0.9174	0.8953	0.9192	0.8872	0.9192	0.8901	0.9189	0.8906	0.9192	0.8892	0.9220	0.9174	0.8953	0.9192	0.8872	0.9192	0.8901	0.9189	0.8906	0.9192	0.8891	**0.82**
H(1`A)	2.7009	2.6940	2.6729	2.6791	2.6330	2.6803	2.6446	2.6813	2.6445	2.6778	2.6161	2.8292	2.8167	2.8096	2.8028	2.7727	2.8036	2.7761	2.8042	2.7785	2.8020	2.7405	**3.82**
H(1`B)	3.1955	3.2319	3.2600	3.2641	3.3159	3.2618	3.3000	3.2593	3.2953	3.2662	3.3005	2.8475	2.7035	2.6734	2.6832	2.6943	2.6837	2.6698	2.6843	2.6719	2.6831	2.6607	**3.78**
H(2`A-2`B)	1.7038	1.7444	1.7062	1.7718	1.7225	1.7700	1.7382	1.7682	1.7341	1.7733	1.7555	1.5630	1.6516	1.6076	1.7033	1.6425	1.7002	1.6903	1.6969	1.6850	1.7061	1.7309	**2.26**
H(3`A-3`B)	1.5630	1.6516	1.6076	1.7033	1.6425	1.7002	1.6903	1.6969	1.6850	1.7061	1.7309	1.7038	1.7444	1.7062	1.7718	1.7225	1.7700	1.7382	1.7682	1.7341	1.7733	1.7555	**2.01**
H(4`A)	2.8475	2.7035	2.6734	2.6832	2.6943	2.6837	2.6698	2.6843	2.6719	2.6831	2.6607	3.1955	3.2319	3.2600	3.2641	3.3159	3.2618	3.3000	3.2593	3.2953	3.2662	3.3005	**3.68**
H(4`B)	2.8292	2.8167	2.8096	2.8028	2.7727	2.8036	2.7761	2.8042	2.7785	2.8020	2.7405	2.7009	2.6940	2.6728	2.6791	2.6330	2.6803	2.6446	2.6813	2.6445	2.6778	2.6162	**2.88**
Nuclei	BHandH																						
H2	9.0170	8.9051	8.9385	8.8508	8.8461	8.8543	8.8769	8.8573	8.8930	8.8488	8.8828	9.0170	8.9051	8.9385	8.8508	8.7696	8.8543	8.8976	8.8573	8.8930	8.8488	8.8828	**8.07**
H3	7.4567	7.6000	7.6942	7.6445	7.7691	7.6431	7.7516	7.6408	7.7802	7.6469	7.8030	7.4567	7.6000	7.6942	7.6445	7.5633	7.6431	7.7884	7.6408	7.7802	7.6469	7.8030	**7.24**
H5	7.2801	7.4726	7.5649	7.5606	7.6921	7.5563	7.6814	7.5511	7.6974	7.5657	7.7331	7.2801	7.4726	7.5649	7.5606	7.4794	7.5563	7.7096	7.5511	7.6974	7.5657	7.7331	**7.24**
H6	8.1878	8.3660	8.4746	8.4772	8.6311	8.4704	8.6569	8.4630	8.6783	8.4848	8.7278	8.1878	8.3660	8.4746	8.4772	8.3960	8.4704	8.7047	8.4630	8.6783	8.4848	8.7278	**8.07**
H8	4.2844	4.3094	4.4069	4.3786	4.4963	4.3734	4.5524	4.3679	4.5574	4.3849	4.5830	4.2844	4.3094	4.4069	4.3786	4.2974	4.3734	4.5805	4.3679	4.5574	4.3849	4.5830	**5.24**
H(9A-9B)	1.8028	1.8603	1.8244	1.8782	1.8611	1.8781	1.8839	1.8773	1.8377	1.8792	1.8759	1.8029	1.8603	1.8244	1.8782	1.7969	1.8781	1.8434	1.8773	1.8377	1.8792	1.8760	**2.135**
H(10A-10B)	1.3477	1.2142	1.1778	1.1397	1.0616	1.1450	1.0642	1.1496	1.0823	1.1357	1.0635	1.3477	1.2142	1.1778	1.1397	1.0585	1.1450	1.0794	1.1496	1.0823	1.1358	1.0635	**1.275**
H(11A-11B)	0.9522	0.9783	0.9304	0.9933	0.9406	0.9931	0.9365	0.9921	0.9372	0.9946	0.9392	0.9522	0.9783	0.9304	0.9933	0.9120	0.9931	0.9391	0.9921	0.9372	0.9946	0.9392	**1.28**
H(12A-12B)	1.2257	1.2025	1.1740	1.1807	1.1354	1.1830	1.1278	1.1844	1.1448	1.1795	1.1429	1.2257	1.2025	1.1741	1.1807	1.0995	1.1830	1.1440	1.1844	1.1447	1.1795	1.1429	**1.285**
H(13A-13B)	1.1158	1.1190	1.0803	1.1239	1.0799	1.1243	1.0676	1.1239	1.0772	1.1246	1.0790	1.1158	1.1190	1.0803	1.1239	1.0427	1.1243	1.0777	1.1239	1.0772	1.1246	1.0790	**1.29**
H(14A-14B)	1.2680	1.2599	1.2323	1.2505	1.2138	1.2520	1.1977	1.2526	1.2177	1.2501	1.2159	1.2680	1.2599	1.2323	1.2505	1.1693	1.2519	1.2172	1.2526	1.2177	1.2501	1.2159	**1.295**
H(15A-15C)	0.9621	0.9564	0.9305	0.9540	0.9210	0.9549	0.8964	0.9550	0.9221	0.9541	0.9207	0.9621	0.9564	0.9305	0.9540	0.8727	0.9549	0.9215	0.9549	0.9221	0.9541	0.9207	**0.82**
H(1`A)	2.5936	2.5836	2.5694	2.5710	2.5281	2.5725	2.5421	2.5732	2.5456	2.5706	2.5204	2.7283	2.7398	2.7023	2.7213	2.6711	2.7239	2.6817	2.7256	2.6846	2.7197	2.6522	**3.82**
H(1`B)	3.1160	3.1325	3.1676	3.1602	3.2130	3.1587	3.1941	3.1566	3.2046	3.1629	3.2121	2.8959	2.7170	2.6626	2.6386	2.6231	2.6444	2.5402	2.6492	2.5510	2.6340	2.5341	**3.78**
H(2`A-2`B)	1.6779	1.7129	1.6806	1.7437	1.7028	1.7423	1.6923	1.7402	1.7106	1.7461	1.7347	1.5667	1.6372	1.5957	1.6777	1.5965	1.6759	1.6604	1.6734	1.6540	1.6804	1.6970	**2.26**
H(3`A-3`B)	1.5667	1.6372	1.5957	1.6777	1.6303	1.6759	1.6296	1.6734	1.6540	1.6804	1.6970	1.6779	1.7129	1.6806	1.7437	1.6625	1.7424	1.7155	1.7402	1.7106	1.7461	1.7347	**2.01**
H(4`A)	2.8959	2.7170	2.6626	2.6386	2.6231	2.6444	2.5946	2.6493	2.5510	2.6340	2.5342	3.1160	3.1325	3.1676	3.1602	3.2130	3.1587	3.2089	3.1566	3.2046	3.1628	3.2121	**3.68**
H(4`B)	2.7283	2.7398	2.7023	2.7213	2.6711	2.7240	2.6935	2.7256	2.6846	2.7197	2.6522	2.5936	2.5836	2.5694	2.5710	2.5281	2.5725	2.5454	2.5733	2.5455	2.5706	2.5204	**2.88**
Nuclei	BHandHLYP																						
H2	8.9150	8.8436	8.8258	8.7456	8.7390	8.7530	8.7662	8.7602	8.7959	8.7381	8.7752	8.9150	8.8436	8.8258	8.7456	8.7390	8.7530	8.8002	8.7602	8.7959	8.7381	8.7752	**8.07**
H3	7.4400	7.5788	7.6683	7.6260	7.7400	7.6241	7.7309	7.6220	7.7510	7.6277	7.7763	7.4400	7.5788	7.6683	7.6260	7.7400	7.6241	7.7597	7.6220	7.7510	7.6277	7.7763	**7.24**
H5	7.2661	7.4512	7.5377	7.5306	7.6504	7.5264	7.6464	7.5219	7.6606	7.5345	7.6916	7.2661	7.4512	7.5377	7.5306	7.6504	7.5264	7.6732	7.5219	7.6606	7.5345	7.6916	**7.24**
H6	8.0607	8.2729	8.3529	8.3735	8.5027	8.3677	8.5458	8.3617	8.5589	8.3786	8.6143	8.0607	8.2729	8.3529	8.3735	8.5027	8.3677	8.5866	8.3617	8.5589	8.3786	8.6143	**8.07**
H8	4.2225	4.3192	4.3753	4.3833	4.4522	4.3806	4.5570	4.3775	4.5065	4.3854	4.5171	4.2225	4.3192	4.3754	4.3833	4.4522	4.3806	4.5259	4.3775	4.5065	4.3854	4.5170	**5.24**
H(9A-9B)	1.5911	1.6478	1.6127	1.6576	1.6756	1.6552	1.6784	1.6532	1.6700	1.6602	1.7027	1.5911	1.6478	1.6127	1.6576	1.6756	1.6552	1.6822	1.6532	1.6700	1.6602	1.7027	**2.135**
H(10A-10B)	1.2887	1.1642	1.1247	1.0942	1.0167	1.0997	1.0229	1.1049	1.0456	1.0889	1.0320	1.2887	1.1642	1.1247	1.0942	1.0167	1.0997	1.0434	1.1049	1.0456	1.0889	1.0320	**1.275**
H(11A-11B)	0.9093	0.9316	0.8869	0.9506	0.9053	0.9493	0.9009	0.9479	0.9065	0.9520	0.9055	0.9093	0.9316	0.8869	0.9507	0.9053	0.9493	0.9096	0.9479	0.9066	0.9520	0.9055	**1.28**
H(12A-12B)	1.1678	1.1474	1.1206	1.1333	1.0872	1.1348	1.0861	1.1360	1.0992	1.1318	1.0967	1.1678	1.1474	1.1206	1.1333	1.0872	1.1348	1.0989	1.1360	1.0992	1.1318	1.0967	**1.285**
H(13A-13B)	1.0767	1.0777	1.0456	1.0881	1.0488	1.0876	1.0391	1.0869	1.0482	1.0887	1.0495	1.0767	1.0777	1.0456	1.0881	1.0488	1.0876	1.0496	1.0869	1.0482	1.0887	1.0495	**1.29**
H(14A-14B)	1.2389	1.2324	1.2099	1.2306	1.1956	1.2311	1.1853	1.2314	1.2013	1.2301	1.2004	1.2389	1.2324	1.2099	1.2306	1.1956	1.2311	1.2017	1.2314	1.2013	1.2301	1.2004	**1.295**
H(15A-15C)	0.9538	0.9474	0.9238	0.9484	0.9161	0.9486	0.8962	0.9486	0.9188	0.9482	0.9174	0.9538	0.9474	0.9238	0.9484	0.9161	0.9486	0.9192	0.9486	0.9188	0.9482	0.9174	**0.82**
H(1`A)	2.6102	2.6077	2.5823	2.5955	2.5429	2.5968	2.5666	2.5980	2.5639	2.5941	2.5424	2.7444	2.7240	2.7194	2.7068	2.6699	2.7075	2.6791	2.7081	2.6814	2.7064	2.6529	**3.82**
H(1`B)	3.0301	3.0830	3.1019	3.1164	3.1619	3.1144	3.1614	3.1122	3.1587	3.1183	3.1711	2.7085	2.5378	2.5326	2.5189	2.5482	2.5181	2.4839	2.5178	2.4875	2.5204	2.4861	**3.78**
H(2`A-2`B)	1.6501	1.6897	1.6532	1.7229	1.6721	1.7212	1.6718	1.7192	1.6829	1.7246	1.7050	1.5130	1.5887	1.5598	1.6429	1.5910	1.6399	1.6176	1.6365	1.6114	1.6458	1.6490	**2.26**
H(3`A-3`B)	1.5130	1.5887	1.5598	1.6430	1.5910	1.6399	1.5978	1.6365	1.6114	1.6458	1.6490	1.6501	1.6897	1.6532	1.7229	1.6721	1.7212	1.6886	1.7192	1.6829	1.7246	1.7050	**2.01**
H(4`A)	2.7085	2.5378	2.5326	2.5189	2.5482	2.5181	2.5197	2.5178	2.4875	2.5204	2.4861	3.0301	3.0830	3.1019	3.1164	3.1619	3.1144	3.1648	3.1122	3.1587	3.1183	3.1711	**3.68**
H(4`B)	2.7444	2.7240	2.7194	2.7068	2.6699	2.7075	2.6844	2.7081	2.6814	2.7064	2.6529	2.6102	2.6076	2.5823	2.5955	2.5429	2.5968	2.5652	2.5980	2.5639	2.5941	2.5424	**2.88**

[a] methyl protons shifts are averaged
[b] according to [7]

Table S7. Cont. II

Nuclei	R											S										Exp. [b]
	BLYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
H2	8.4535	8.3099	8.3833	8.2361	8.2020	8.2891	8.4374	8.2494	8.2316	8.2857	8.4096	8.4535	8.3099	8.3833	8.2361	8.2020	8.2891	8.4070	8.2494	8.2316	8.2857	8.4096	**8.07**
H3	7.1756	7.3027	7.3883	7.3357	7.4452	7.3817	7.6153	7.3351	7.4602	7.3923	7.6595	7.1756	7.3027	7.3883	7.3357	7.4452	7.3817	7.6349	7.3351	7.4602	7.3923	7.6595	**7.24**
H5	6.9972	7.1760	7.2493	7.2583	7.3909	7.3008	7.5465	7.2508	7.3965	7.3183	7.5953	6.9972	7.1760	7.2493	7.2583	7.3909	7.3008	7.5751	7.2508	7.3965	7.3183	7.5954	**7.24**
H6	7.8298	7.9878	8.0732	8.0594	8.1592	8.1031	8.3714	8.0542	8.1777	8.1180	8.4080	7.8298	7.9878	8.0732	8.0594	8.1592	8.1031	8.3682	8.0542	8.1777	8.1180	8.4081	**8.07**
H8	4.9684	5.0143	5.0187	5.0206	5.0867	5.0682	5.3137	5.0231	5.0770	5.0754	5.2626	4.9684	5.0143	5.0187	5.0206	5.0867	5.0682	5.2614	5.0231	5.0770	5.0754	5.2626	**5.24**
H(9A-9B)	1.8142	1.8165	1.8632	1.8292	1.7940	1.8756	2.0185	1.8296	1.8152	1.8854	2.0229	1.8142	1.8165	1.8632	1.8292	1.7940	1.8756	1.9886	1.8296	1.8152	1.8854	2.0229	**2.135**
H(10A-10B)	1.4126	1.3080	1.2577	1.2451	1.1827	1.2967	1.3551	1.2558	1.2017	1.2962	1.3775	1.4126	1.3080	1.2577	1.2451	1.1827	1.2967	1.3678	1.2558	1.2017	1.2962	1.3775	**1.275**
H(11A-11B)	1.0598	1.0728	1.0408	1.0906	1.0452	1.1365	1.2140	1.0900	1.0463	1.1474	1.2261	1.0598	1.0728	1.0408	1.0906	1.0452	1.1365	1.2142	1.0900	1.0463	1.1474	1.2261	**1.28**
H(12A-12B)	1.2980	1.2896	1.2562	1.2758	1.2410	1.3241	1.4039	1.2800	1.2496	1.3302	1.4297	1.2980	1.2896	1.2562	1.2758	1.2410	1.3241	1.4158	1.2800	1.2496	1.3302	1.4297	**1.285**
H(13A-13B)	1.2137	1.2165	1.1832	1.2230	1.1880	1.2697	1.3480	1.2240	1.1882	1.2789	1.3694	1.2137	1.2165	1.1832	1.2230	1.1880	1.2697	1.3555	1.2240	1.1882	1.2789	1.3694	**1.29**
H(14A-14B)	1.3717	1.3721	1.3463	1.3683	1.3423	1.4160	1.4972	1.3710	1.3470	1.4233	1.5254	1.3717	1.3721	1.3463	1.3683	1.3423	1.4159	1.5136	1.3710	1.3470	1.4233	1.5254	**1.295**
H(15A-15C)	0.9642	0.9602	0.9334	0.9573	0.9316	1.0048	1.0783	0.9598	0.9326	1.0123	1.1103	0.9642	0.9602	0.9334	0.9573	0.9316	1.0048	1.0994	0.9598	0.9326	1.0123	1.1103	**0.82**
H(1`A)	2.8596	2.8522	2.8271	2.8391	2.7974	2.8874	2.9814	2.8432	2.8051	2.8934	2.9497	2.9705	2.9701	2.9630	2.9434	2.9187	2.9927	3.0862	2.9494	2.9252	2.9970	3.0573	**3.82**
H(1`B)	3.3821	3.4122	3.4355	3.4344	3.4933	3.4804	3.6513	3.4337	3.4718	3.4910	3.6540	3.0238	2.8539	2.8033	2.8196	2.8379	2.8683	2.9769	2.8245	2.8108	2.8738	2.9857	**3.78**
H(2`A-2`B)	1.8078	1.8484	1.8015	1.8724	1.8323	1.9184	1.9918	1.8717	1.8358	1.9291	2.0394	1.6432	1.7393	1.6954	1.7862	1.7519	1.8303	1.9442	1.7821	1.7725	1.8446	1.9937	**2.26**
H(3`A-3`B)	1.6432	1.7393	1.6954	1.7861	1.7519	1.8303	1.9131	1.7821	1.7725	1.8446	1.9937	1.8078	1.8484	1.8015	1.8724	1.8323	1.9184	2.0079	1.8717	1.8358	1.9291	2.0395	**2.01**
H(4`A)	3.0238	2.8539	2.8033	2.8196	2.8379	2.8683	2.9907	2.8245	2.8108	2.8738	2.9858	3.3821	3.4122	3.4355	3.4344	3.4933	3.4804	3.6433	3.4337	3.4718	3.4910	3.6540	**3.68**
H(4`B)	2.9705	2.9701	2.9630	2.9435	2.9187	2.9927	3.0900	2.9494	2.9252	2.9970	3.0574	2.8596	2.8522	2.8271	2.8391	2.7974	2.8874	2.9712	2.8432	2.8051	2.8934	2.9497	**2.88**
Nuclei	BMK																						
H2	9.0627	9.0228	9.0111	8.9585	8.9678	8.9579	9.0493	8.9569	9.0453	8.9490	9.0386	9.0627	9.0228	9.0111	8.9585	8.9678	8.9579	9.0493	8.9569	9.0453	8.9490	9.0386	**8.07**
H3	7.6124	7.7732	7.8608	7.8262	7.9489	7.8202	7.9736	7.8141	7.9661	7.8224	7.9999	7.6124	7.7732	7.8608	7.8262	7.9489	7.8202	7.9736	7.8141	7.9661	7.8224	7.9999	**7.24**
H5	7.4921	7.6732	7.7490	7.7424	7.8695	7.7345	7.8914	7.7266	7.8802	7.7405	7.9089	7.4921	7.6732	7.7490	7.7424	7.8695	7.7345	7.8914	7.7266	7.8802	7.7404	7.9089	**7.24**
H6	8.4292	8.6281	8.6811	8.7248	8.8657	8.7127	8.8858	8.7014	8.8628	8.7280	8.9015	8.4292	8.6281	8.6811	8.7248	8.8657	8.7127	8.8858	8.7014	8.8628	8.7280	8.9015	**8.07**
H8	4.4581	4.4657	4.5471	4.5017	4.6695	4.4909	4.6627	4.4817	4.6492	4.5054	4.6577	4.4581	4.4656	4.5471	4.5017	4.6695	4.4909	4.6627	4.4817	4.6492	4.5053	4.6577	**5.24**
H(9A-9B)	1.6621	1.7742	1.6807	1.8006	1.7342	1.7978	1.8198	1.7935	1.8050	1.7906	1.8791	1.6621	1.7742	1.6807	1.8006	1.7342	1.7978	1.8197	1.7935	1.8050	1.7906	1.8791	**2.135**
H(10A-10B)	1.3436	1.1984	1.1153	1.0959	0.9961	1.0999	1.0490	1.1030	1.0512	1.0811	1.0583	1.3436	1.1984	1.1153	1.0960	0.9961	1.0999	1.0490	1.1030	1.0512	1.0811	1.0583	**1.275**
H(11A-11B)	0.9400	0.9525	0.8875	0.9640	0.9155	0.9584	0.9126	0.9532	0.9126	0.9605	0.9106	0.9401	0.9525	0.8875	0.9640	0.9155	0.9584	0.9126	0.9532	0.9126	0.9605	0.9106	**1.28**
H(12A-12B)	1.1929	1.1688	1.1216	1.1452	1.0958	1.1429	1.1039	1.1407	1.1066	1.1380	1.1009	1.1929	1.1688	1.1216	1.1452	1.0958	1.1429	1.1039	1.1407	1.1066	1.1380	1.1009	**1.285**
H(13A-13B)	1.0816	1.0826	1.0376	1.0872	1.0427	1.0832	1.0447	1.0792	1.0457	1.0815	1.0483	1.0816	1.0826	1.0376	1.0872	1.0427	1.0832	1.0447	1.0792	1.0457	1.0815	1.0483	**1.29**
H(14A-14B)	1.2204	1.2100	1.1762	1.2020	1.1608	1.1992	1.1674	1.1963	1.1693	1.1951	1.1682	1.2203	1.2100	1.1762	1.2020	1.1608	1.1992	1.1674	1.1963	1.1693	1.1951	1.1682	**1.295**
H(15A-15C)	0.8777	0.8689	0.8386	0.8681	0.8316	0.8648	0.8349	0.8615	0.8364	0.8616	0.8381	0.8777	0.8689	0.8386	0.8681	0.8316	0.8648	0.8349	0.8615	0.8364	0.8616	0.8381	**0.82**
H(1`A)	2.6154	2.6064	2.5872	2.5983	2.5634	2.5944	2.5546	2.5910	2.5576	2.5932	2.5132	2.7379	2.7451	2.7372	2.7380	2.6936	2.7367	2.6943	2.7353	2.7007	2.7299	2.6676	**3.82**
H(1`B)	3.0946	3.1480	3.1367	3.1610	3.1704	3.1595	3.1981	3.1566	3.1951	3.1504	3.1955	2.6890	2.4769	2.5208	2.4811	2.5279	2.4758	2.4416	2.4716	2.4507	2.4785	2.4512	**3.78**
H(2`A-2`B)	1.6966	1.7123	1.6876	1.7418	1.7076	1.7356	1.6990	1.7297	1.6977	1.7389	1.7027	1.5428	1.6152	1.5833	1.6615	1.6157	1.6550	1.6272	1.6489	1.6240	1.6588	1.6562	**2.26**
H(3`A-3`B)	1.5428	1.6152	1.5833	1.6615	1.6157	1.6550	1.6271	1.6489	1.6240	1.6588	1.6562	1.6966	1.7123	1.6876	1.7418	1.7076	1.7356	1.6990	1.7297	1.6977	1.7389	1.7027	**2.01**
H(4`A)	2.6890	2.4769	2.5208	2.4811	2.5279	2.4758	2.4416	2.4716	2.4507	2.4785	2.4512	3.0946	3.1480	3.1367	3.1610	3.1704	3.1595	3.1981	3.1566	3.1951	3.1504	3.1955	**3.68**
H(4`B)	2.7379	2.7451	2.7372	2.7380	2.6936	2.7367	2.6943	2.7353	2.7007	2.7299	2.6676	2.6154	2.6064	2.5872	2.5983	2.5634	2.5944	2.5546	2.5910	2.5576	2.5932	2.5132	**2.88**
Nuclei	BP86																						
H2	8.5211	8.4160	8.4356	8.3431	8.3460	8.3496	8.3612	8.3555	8.3850	8.3361	8.3758	8.5211	8.4160	8.4356	8.3431	8.3460	8.3496	8.3734	8.3555	8.3850	8.3361	8.3758	**8.07**
H3	7.1929	7.3340	7.4134	7.3753	7.4851	7.3743	7.4787	7.3728	7.4971	7.3760	7.5362	7.1929	7.3340	7.4134	7.3753	7.4852	7.3743	7.5058	7.3728	7.4971	7.3760	7.5362	**7.24**
H5	6.9950	7.1707	7.2555	7.2507	7.3666	7.2469	7.3611	7.2428	7.3740	7.2538	7.4177	6.9950	7.1707	7.2555	7.2506	7.3666	7.2469	7.3841	7.2428	7.3740	7.2538	7.4177	**7.24**
H6	7.9235	8.1146	8.1659	8.1933	8.2926	8.1904	8.3271	8.1868	8.3382	8.1953	8.4034	7.9235	8.1146	8.1659	8.1933	8.2926	8.1904	8.3574	8.1868	8.3382	8.1953	8.4034	**8.07**
H8	4.9854	5.0537	5.0470	5.0682	5.0819	5.0697	5.1716	5.0705	5.1218	5.0659	5.1501	4.9854	5.0537	5.0470	5.0682	5.0819	5.0697	5.1324	5.0705	5.1218	5.0659	5.1501	**5.24**
H(9A-9B)	1.9156	1.9378	1.9296	1.9623	1.9953	1.9602	1.9733	1.9582	1.9753	1.9643	2.0210	1.9156	1.9379	1.9296	1.9623	1.9953	1.9602	1.9806	1.9582	1.9753	1.9643	2.0210	**2.135**
H(10A-10B)	1.4202	1.3133	1.2640	1.2494	1.1743	1.2545	1.1770	1.2593	1.1895	1.2443	1.1977	1.4202	1.3133	1.2640	1.2494	1.1743	1.2545	1.1859	1.2593	1.1895	1.2443	1.1977	**1.275**
H(11A-11B)	1.0518	1.0710	1.0227	1.0903	1.0424	1.0895	1.0327	1.0885	1.0341	1.0908	1.0471	1.0518	1.0710	1.0227	1.0903	1.0424	1.0895	1.0334	1.0885	1.0341	1.0909	1.0471	**1.28**
H(12A-12B)	1.2900	1.2812	1.2428	1.2659	1.2133	1.2680	1.2104	1.2696	1.2207	1.2636	1.2340	1.2900	1.2812	1.2428	1.2659	1.2133	1.2680	1.2193	1.2696	1.2207	1.2636	1.2340	**1.285**
H(13A-13B)	1.2001	1.2041	1.1613	1.2108	1.1644	1.2110	1.1522	1.2109	1.1590	1.2103	1.1737	1.2001	1.2041	1.1613	1.2108	1.1644	1.2110	1.1587	1.2109	1.1590	1.2103	1.1737	**1.29**
H(14A-14B)	1.3511	1.3509	1.3184	1.3462	1.3041	1.3474	1.2915	1.3483	1.3071	1.3447	1.3190	1.3511	1.3509	1.3184	1.3462	1.3041	1.3474	1.3069	1.3483	1.3071	1.3447	1.3190	**1.295**
H(15A-15C)	0.9368	0.9356	0.9010	0.9325	0.8926	0.9336	0.8710	0.9343	0.8923	0.9312	0.9037	0.9368	0.9356	0.9010	0.9325	0.8926	0.9336	0.8919	0.9343	0.8923	0.9312	0.9037	**0.82**
H(1`A)	2.8051	2.8086	2.7800	2.7948	2.7420	2.7967	2.7582	2.7983	2.7511	2.7925	2.7334	2.9245	2.9231	2.9062	2.9072	2.8712	2.9089	2.8718	2.9104	2.8727	2.9053	2.8464	**3.82**
H(1`B)	3.3976	3.4262	3.4319	3.4461	3.4796	3.4459	3.4732	3.4453	3.4677	3.4459	3.4874	3.0775	2.8757	2.8390	2.8259	2.8309	2.8282	2.7764	2.8308	2.7751	2.8240	2.7809	**3.78**
H(2`A-2`B)	1.8009	1.8424	1.7943	1.8664	1.8096	1.8657	1.8055	1.8648	1.8178	1.8667	1.8549	1.6352	1.7278	1.6788	1.7716	1.7091	1.7698	1.7378	1.7676	1.7302	1.7728	1.7894	**2.26**
H(3`A-3`B)	1.6352	1.7278	1.6788	1.7716	1.7091	1.7698	1.7168	1.7676	1.7302	1.7728	1.7895	1.8009	1.8424	1.7943	1.8664	1.8096	1.8657	1.8232	1.8648	1.8178	1.8667	1.8549	**2.01**
H(4`A)	3.0775	2.8757	2.8390	2.8259	2.8309	2.8282	2.8063	2.8307	2.7751	2.8240	2.7810	3.3976	3.4262	3.4319	3.4461	3.4796	3.4459	3.4727	3.4452	3.4677	3.4459	3.4873	**3.68**
H(4`B)	2.9245	2.9231	2.9062	2.9072	2.8712	2.9089	2.8772	2.9103	2.8727	2.9053	2.8464	2.8051	2.8086	2.7800	2.7948	2.7420	2.7967	2.7504	2.7982	2.7511	2.7925	2.7334	**2.88**
Nuclei	CAM-B3LYP																						
H2	8.8137	8.7427	8.7185	8.6046	8.6226	8.6133	8.6259	8.6217	8.6669	8.5956	8.5831	8.8137	8.7427	8.7185	8.6046	8.6226	8.6133	8.6539	8.6217	8.6669	8.5956	8.5831	**8.07**
H3	7.4056	7.5424	7.6331	7.5855	7.7038	7.5840	7.6921	7.5824	7.7150	7.5868	7.7349	7.4056	7.5424	7.6331	7.5855	7.7038	7.5839	7.7225	7.5824	7.7150	7.5868	7.7349	**7.24**
H5	7.2427	7.4267	7.5144	7.4995	7.6257	7.4954	7.6153	7.4914	7.6329	7.5033	7.6554	7.2427	7.4267	7.5144	7.4995	7.6258	7.4954	7.6417	7.4914	7.6329	7.5033	7.6554	**7.24**
H6	8.0301	8.2398	8.3133	8.3260	8.4567	8.3209	8.4890	8.3154	8.5026	8.3304	8.5351	8.0301	8.2398	8.3133	8.3260	8.4568	8.3209	8.5206	8.3154	8.5026	8.3304	8.5351	**8.07**
H8	4.4185	4.5093	4.5609	4.5563	4.6265	4.5552	4.7167	4.5537	4.6736	4.5567	4.6645	4.4185	4.5093	4.5609	4.5563	4.6265	4.5552	4.6844	4.5537	4.6736	4.5567	4.6645	**5.24**
H(9A-9B)	1.6860	1.7382	1.7028	1.7332	1.7652	1.7310	1.7525	1.7292	1.7521	1.7356	1.7549	1.6860	1.7382	1.7028	1.7332	1.7651	1.7310	1.7567	1.7292	1.7521	1.7356	1.7549	**2.135**
H(10A-10B)	1.3235	1.2065	1.1686	1.1281	1.0653	1.1334	1.0616	1.1388	1.0865	1.1229	1.0600	1.3235	1.2065	1.1686	1.1281	1.0653	1.1334	1.0797	1.1388	1.0865	1.1229	1.0600	**1.275**
H(11A-11B)	0.9652	0.9883	0.9435	0.9989	0.9632	0.9975	0.9493	0.9964	0.9570	1.0001	0.9406	0.9652	0.9883	0.9436	0.9989	0.9632	0.9975	0.9549	0.9964	0.9570	1.0001	0.9406	**1.28**
H(12A-12B)	1.2202	1.2025	1.1771	1.1852	1.1451	1.1867	1.1385	1.1882	1.1533	1.1837	1.1452	1.2202	1.2024	1.1771	1.1853	1.1451	1.1867	1.1507	1.1882	1.1533	1.1837	1.1452	**1.285**
H(13A-13B)	1.1315	1.1337	1.1023	1.1400	1.1063	1.1394	1.0915	1.1391	1.1023	1.1404	1.0967	1.1315	1.1337	1.1023	1.1400	1.1063	1.1394	1.1010	1.1391	1.1023	1.1404	1.0967	**1.29**
H(14A-14B)	1.2864	1.2817	1.2602	1.2787	1.2470	1.2792	1.2339	1.2797	1.2508	1.2782	1.2469	1.2864	1.2817	1.2602	1.2787	1.2470	1.2792	1.2499	1.2797	1.2508	1.2782	1.2469	**1.295**
H(15A-15C)	0.9690	0.9644	0.9415	0.9633	0.9347	0.9635	0.9118	0.9638	0.9354	0.9630	0.9308	0.9690	0.9644	0.9414	0.9633	0.9347	0.9635	0.9344	0.9638	0.9354	0.9630	0.9308	**0.82**
H(1`A)	2.7122	2.7112	2.6890	2.6973	2.6501	2.6987	2.6685	2.7002	2.6667	2.6957	2.6354	2.8374	2.8193	2.8158	2.8689	2.7726	2.8086	2.7811	2.8094	2.7817	2.8077	2.6354	**3.82**
H(1`B)	3.1354	3.1829	3.2019	3.2098	3.2596	3.2081	3.2536	3.2065	3.2535	3.2113	3.2592	2.8053	2.6264	2.6258	2.6789	2.6368	2.6172	2.5885	2.6172	2.5863	2.6193	3.2592	**3.78**
H(2`A-2`B)	1.7172	1.7561	1.7220	1.7856	1.7408	1.7840	1.7358	1.7825	1.7498	1.7871	1.7711	1.5823	1.6597	1.6318	1.7170	1.6665	1.7139	1.6941	1.7110	1.6865	1.7198	1.7378	**2.26**
H(3`A-3`B)	1.5823	1.6597	1.6318	1.7170	1.6666	1.7139	1.6727	1.7110	1.6865	1.7198	1.7378	1.7172	1.7561	1.7220	1.7856	1.7408	1.7840	1.7541	1.7825	1.7498	1.7871	1.7711	**2.01**
H(4`A)	2.8053	2.6264	2.6258	2.6178	2.6368	2.6172	2.6177	2.6172	2.5863	2.6193	2.6007	3.1354	3.1829	3.2018	3.2549	3.2596	3.2081	3.2581	3.2065	3.2535	3.2113	2.6007	**3.68**
H(4`B)	2.8374	2.8193	2.8158	2.8081	2.7726	2.8086	2.7865	2.8094	2.7817	2.8077	2.7551	2.7122	2.7112	2.6890	2.7421	2.6501	2.6987	2.6658	2.7002	2.6667	2.6957	2.7551	**2.88**

[a] methyl protons shifts are averaged
[b] according to [7]

Table S7. Cont. III

Nuclei	R											S										Exp. [b]
	HF																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
H2	9.0669	8.9556	8.9901	8.7631	8.7246	8.7728	8.7533	8.7820	8.7511	8.7528	8.7429	9.0669	8.9556	8.9901	8.7631	8.7246	8.7728	8.7533	8.7820	8.7511	8.7528	8.7430	**8.07**
H3	7.4294	7.5691	7.6582	7.6152	7.7384	7.6132	7.7511	7.6108	7.7442	7.6172	7.7667	7.4294	7.5691	7.6582	7.6152	7.7384	7.6132	7.7511	7.6108	7.7442	7.6172	7.7667	**7.24**
H5	7.2468	7.4436	7.5321	7.5293	7.6578	7.5244	7.6694	7.5193	7.6586	7.5340	7.6936	7.2468	7.4436	7.5321	7.5293	7.6578	7.5244	7.6694	7.5193	7.6586	7.5340	7.6936	**7.24**
H6	8.0744	8.3036	8.4070	8.3982	8.5365	8.3926	8.5911	8.3866	8.5665	8.4031	8.6246	8.0744	8.3036	8.4070	8.3982	8.5365	8.3926	8.5911	8.3866	8.5665	8.4031	8.6246	**8.07**
H8	3.6336	3.7565	3.8251	3.8267	3.9402	3.8226	3.9863	3.8182	3.9645	3.8305	3.9882	3.6336	3.7565	3.8251	3.8267	3.9402	3.8226	3.9863	3.8182	3.9645	3.8305	3.9882	**5.24**
H(9A-9B)	1.3084	1.3386	1.3327	1.3126	1.2781	1.3118	1.3017	1.3109	1.2912	1.3131	1.3209	1.3084	1.3386	1.3327	1.3126	1.2781	1.3118	1.3017	1.3109	1.2912	1.3131	1.3209	**2.135**
H(10A-10B)	1.1757	1.0355	1.0026	0.9528	0.8871	0.9579	0.8942	0.9628	0.8992	0.9481	0.8886	1.1757	1.0355	1.0026	0.9528	0.8871	0.9579	0.8942	0.9628	0.8992	0.9481	0.8886	**1.275**
H(11A-11B)	0.7727	0.7822	0.7491	0.7923	0.7424	0.7906	0.7424	0.7890	0.7420	0.7939	0.7448	0.7727	0.7822	0.7491	0.7923	0.7424	0.7906	0.7424	0.7890	0.7420	0.7939	0.7449	**1.28**
H(12A-12B)	1.0258	1.0005	0.9756	0.9869	0.9484	0.9879	0.9519	0.9888	0.9539	0.9861	0.9534	1.0258	1.0005	0.9756	0.9870	0.9484	0.9879	0.9518	0.9888	0.9539	0.9861	0.9534	**1.285**
H(13A-13B)	0.9397	0.9382	0.9089	0.9459	0.9080	0.9451	0.9055	0.9442	0.9057	0.9467	0.9091	0.9397	0.9381	0.9089	0.9459	0.9080	0.9451	0.9055	0.9442	0.9057	0.9467	0.9091	**1.29**
H(14A-14B)	1.1123	1.1065	1.0835	1.1061	1.0752	1.1063	1.0765	1.1063	1.0774	1.1060	1.0771	1.1123	1.1065	1.0835	1.1061	1.0752	1.1063	1.0765	1.1063	1.0774	1.1060	1.0771	**1.295**
H(15A-15C)	0.9246	0.9168	0.8945	0.9193	0.8903	0.9192	0.8899	0.9188	0.8904	0.9196	0.8908	0.9246	0.9168	0.8945	0.9193	0.8903	0.9192	0.8899	0.9188	0.8904	0.9196	0.8908	**0.82**
H(1`A)	2.3785	2.3730	2.3471	2.3565	2.3023	2.3578	2.3282	2.3589	2.3267	2.3554	2.3100	2.5255	2.5057	2.4921	2.4867	3.2393	2.4877	2.4710	2.4886	2.4713	2.4859	2.4432	**3.82**
H(1`B)	2.7269	2.7948	2.8266	2.8273	2.8806	2.8249	2.8793	2.8224	2.8729	2.8295	2.8867	2.3711	2.2566	2.2390	2.2718	3.1035	2.2707	2.2847	2.2697	2.2843	2.2734	2.2859	**3.78**
H(2`A-2`B)	1.4839	1.5326	1.4910	1.5677	1.5188	1.5657	1.5290	1.5636	1.5244	1.5697	1.5471	1.3771	1.4631	1.4254	1.5342	1.4936	1.5302	1.5186	1.5261	1.5127	1.5383	1.5479	**2.26**
H(3`A-3`B)	1.3771	1.4631	1.4254	1.5342	1.4936	1.5302	1.5186	1.5261	1.5127	1.5383	1.5479	1.4839	1.5326	1.4910	1.5677	1.5188	1.5658	1.5289	1.5636	1.5244	1.5697	1.5471	**2.01**
H(4`A)	2.3711	2.2566	2.2390	2.2718	2.3030	2.2707	2.2847	2.2697	2.2843	2.2734	2.2859	2.7269	2.7948	2.8267	2.8273	3.7263	2.8249	2.8793	2.8224	2.8729	2.8295	2.8867	**3.68**
H(4`B)	2.5255	2.5057	2.4920	2.4867	2.4422	2.4877	2.4710	2.4886	2.4713	2.4858	2.4432	2.3785	2.3730	2.3471	2.3565	3.1168	2.3579	2.3282	2.3589	2.3267	2.3554	2.3100	**2.88**
Nuclei	**LC-BLYP**																						
H2	9.0090	8.9172	8.8774	8.7674	8.7637	8.7674	8.7446	8.8105	8.7309	8.7642	8.7211	9.0090	8.9172	8.8774	8.7674	8.7637	8.7672	8.7446	8.8105	8.7309	8.7642	8.7211	**8.07**
H3	7.5442	7.6758	7.7680	7.7162	7.8367	7.7133	7.8535	7.7128	7.8459	7.7180	7.8685	7.5442	7.6758	7.7680	7.7163	7.8367	7.7133	7.8535	7.7128	7.8459	7.7180	7.8685	**7.24**
H5	7.3920	7.5824	7.6728	7.6621	7.7888	7.6563	7.7984	7.6543	7.7872	7.6664	7.8208	7.3920	7.5824	7.6728	7.6621	7.7888	7.6563	7.7984	7.6544	7.7872	7.6664	7.8208	**7.24**
H6	8.1874	8.3994	8.4752	8.4661	8.6185	8.4552	8.6584	8.4705	8.6298	8.4737	8.6873	8.1875	8.3993	8.4752	8.4660	8.6185	8.4552	8.6583	8.4705	8.6298	8.4737	8.6873	**8.07**
H8	4.2077	4.3175	4.3817	4.3246	4.4577	4.3126	4.5153	4.3399	4.4897	4.3333	4.5219	4.2077	4.3175	4.3817	4.3246	4.4577	4.3125	4.5153	4.3399	4.4897	4.3333	4.5219	**5.24**
H(9A-9B)	1.6659	1.6997	1.6590	1.7261	1.7126	1.7266	1.6785	1.7206	1.6702	1.7247	1.7099	1.6659	1.6997	1.6590	1.7261	1.7126	1.7266	1.6785	1.7206	1.6702	1.7247	1.7099	**2.135**
H(10A-10B)	1.2866	1.1578	1.1207	1.0620	1.0043	1.0654	1.0050	1.0764	1.0076	1.0578	0.9989	1.2865	1.1578	1.1206	1.0620	1.0043	1.0654	1.0050	1.0764	1.0076	1.0578	0.9989	**1.275**
H(11A-11B)	0.9378	0.9566	0.9095	0.9662	0.9234	0.9644	0.9016	0.9649	0.8999	0.9668	0.9023	0.9378	0.9566	0.9095	0.9661	0.9234	0.9644	0.9016	0.9649	0.8999	0.9668	0.9023	**1.28**
H(12A-12B)	1.1999	1.1746	1.1506	1.1485	1.1119	1.1487	1.1132	1.1527	1.1141	1.1474	1.1144	1.1999	1.1746	1.1506	1.1486	1.1119	1.1487	1.1132	1.1527	1.1141	1.1475	1.1144	**1.285**
H(13A-13B)	1.1103	1.1093	1.0778	1.1134	1.0777	1.1121	1.0675	1.1125	1.0671	1.1137	1.0699	1.1103	1.1093	1.0778	1.1134	1.0777	1.1121	1.0674	1.1125	1.0670	1.1137	1.0699	**1.29**
H(14A-14B)	1.2590	1.2495	1.2279	1.2428	1.2107	1.2423	1.2123	1.2434	1.2129	1.2423	1.2128	1.2590	1.2494	1.2279	1.2428	1.2108	1.2422	1.2123	1.2434	1.2129	1.2423	1.2128	**1.295**
H(15A-15C)	0.9733	0.9650	0.9432	0.9632	0.9343	0.9622	0.9324	0.9634	0.9327	0.9632	0.9327	0.9732	0.9650	0.9432	0.9632	0.9344	0.9622	0.9324	0.9633	0.9327	0.9631	0.9327	**0.82**
H(1`A)	2.6766	2.6717	2.6489	2.6511	2.6063	2.6507	2.6202	2.6556	2.6204	2.5622	2.5969	2.7970	2.7801	2.7657	2.7792	2.7297	2.7811	2.7498	2.7746	2.7535	2.7768	2.7222	**3.82**
H(1`B)	3.0280	3.0713	3.0899	3.0911	3.1423	3.0863	3.1407	3.0926	3.1345	2.7776	3.1488	2.7236	2.5359	2.5536	2.5538	2.5546	2.5606	2.5267	2.5313	2.5351	2.5491	2.5240	**3.78**
H(2`A-2`B)	1.6938	1.7312	1.7027	1.7597	1.7219	1.7563	1.7326	1.7563	1.7275	1.7620	1.7524	1.5820	1.6600	1.6326	1.7150	1.6703	1.7107	1.7064	1.7072	1.7008	1.7182	1.7430	**2.26**
H(3`A-3`B)	1.5820	1.6600	1.6326	1.7150	1.6703	1.7107	1.7064	1.7072	1.7008	1.7182	1.7430	1.6938	1.7312	1.7027	1.7597	1.7219	1.7563	1.7326	1.7564	1.7275	1.7620	1.7524	**2.01**
H(4`A)	2.7236	2.5359	2.5536	2.5538	2.5545	2.5606	2.5267	2.5313	2.5351	2.5491	2.5240	3.0280	3.0713	3.0899	3.0911	3.1423	3.0863	3.1408	3.0926	3.1345	3.0942	3.1488	**3.68**
H(4`B)	2.7970	2.7801	2.7657	2.7792	2.7297	2.7811	2.7498	2.7746	2.7535	2.7768	2.7222	2.6766	2.6717	2.6489	2.6511	2.6063	2.6507	2.6202	2.6557	2.6204	2.6502	2.5969	**2.88**
Nuclei	**M06**																						
H2	8.7928	8.4981	8.5707	8.4194	8.4125	8.4243	8.4639	8.4296	8.4620	8.4154	8.4538	8.7928	8.4981	8.5707	8.4194	8.4125	8.4243	8.4635	8.4296	8.4620	8.4154	8.4538	**8.07**
H3	7.3654	7.4406	7.5625	7.4698	7.5889	7.4682	7.5910	7.4671	7.6073	7.4719	7.6465	7.3654	7.4406	7.5625	7.4698	7.5889	7.4682	7.6142	7.4671	7.6073	7.4719	7.6465	**7.24**
H5	6.9860	7.2831	7.3165	7.3832	7.5260	7.3775	7.5112	7.3723	7.5229	7.3890	7.5911	6.9860	7.2831	7.3165	7.3832	7.5260	7.3775	7.5414	7.3723	7.5229	7.3890	7.5911	**7.24**
H6	7.9129	8.1474	8.1943	8.2181	8.3472	8.2135	8.3817	8.2095	8.3682	8.2229	8.4170	7.9129	8.1474	8.1943	8.2181	8.3472	8.2135	8.3910	8.2095	8.3682	8.2229	8.4170	**8.07**
H8	4.3875	4.4787	4.4779	4.5111	4.5782	4.5089	4.6607	4.5071	4.5985	4.5136	4.6913	4.3875	4.4787	4.4779	4.5111	4.5782	4.5089	4.6204	4.5071	4.5985	4.5136	4.6913	**5.24**
H(9A-9B)	1.8387	1.7688	1.7995	1.7696	1.7495	1.7683	1.7853	1.7676	1.7550	1.7717	1.7108	1.8387	1.7688	1.7995	1.7696	1.7495	1.7683	1.7507	1.7676	1.7550	1.7717	1.7108	**2.135**
H(10A-10B)	1.3386	1.1655	1.1535	1.1144	1.0456	1.1173	1.0660	1.1207	1.0603	1.1123	1.0297	1.3386	1.1655	1.1536	1.1144	1.0456	1.1173	1.0537	1.1207	1.0603	1.1123	1.0297	**1.275**
H(11A-11B)	1.0466	1.0091	1.0034	1.0230	0.9823	1.0215	0.9775	1.0205	0.9836	1.0252	0.9346	1.0466	1.0091	1.0034	1.0230	0.9823	1.0215	0.9812	1.0205	0.9836	1.0252	0.9347	**1.28**
H(12A-12B)	1.1887	1.1855	1.1623	1.1773	1.1430	1.1778	1.1367	1.1787	1.1489	1.1775	1.1440	1.1887	1.1855	1.1624	1.1773	1.1430	1.1778	1.1482	1.1788	1.1489	1.1775	1.1440	**1.285**
H(13A-13B)	1.1510	1.1397	1.1200	1.1472	1.1089	1.1463	1.1035	1.1460	1.1090	1.1486	1.1008	1.1510	1.1397	1.1200	1.1472	1.1089	1.1463	1.1080	1.1460	1.1090	1.1486	1.1008	**1.29**
H(14A-14B)	1.2292	1.2248	1.2093	1.2150	1.1934	1.2154	1.1749	1.2163	1.1967	1.2152	1.1959	1.2293	1.2248	1.2093	1.2150	1.1934	1.2154	1.1954	1.2163	1.1967	1.2152	1.1959	**1.295**
H(15A-15C)	0.9148	0.9145	0.8994	0.9138	0.8937	0.9135	0.8693	0.9136	0.8957	0.9148	0.9001	0.9148	0.9145	0.8994	0.9138	0.8937	0.9135	0.8952	0.9136	0.8957	0.9148	0.9001	**0.82**
H(1`A)	2.7167	2.6896	2.6661	2.6699	2.6343	2.6711	2.6475	2.6729	2.6449	2.6692	2.6479	2.8881	2.8154	2.8217	2.7853	2.7501	2.7870	2.7779	2.7894	2.7801	2.7842	2.7525	**3.82**
H(1`B)	3.0905	3.1403	3.1518	3.1683	3.2274	3.1658	3.2112	3.1639	3.2028	3.1712	3.2009	2.7251	2.6174	2.6394	2.6205	2.6119	2.6193	2.6250	2.6188	2.6288	2.6225	2.5793	**3.78**
H(2`A-2`B)	1.6210	1.7047	1.6519	1.7362	1.7015	1.7338	1.6961	1.7321	1.7050	1.7389	1.7622	1.5772	1.6691	1.6316	1.6941	1.6542	1.6924	1.6693	1.6912	1.6642	1.6962	1.7078	**2.26**
H(3`A-3`B)	1.5772	1.6691	1.6316	1.6941	1.6543	1.6924	1.6532	1.6912	1.6642	1.6962	1.7078	1.6210	1.7047	1.6519	1.7361	1.7015	1.7338	1.7111	1.7321	1.7050	1.7389	1.7622	**2.01**
H(4`A)	2.7251	2.6174	2.6394	2.6205	2.6119	2.6193	2.6270	2.6188	2.6288	2.6225	2.5793	3.0905	3.1403	3.1518	3.1683	3.2274	3.1658	3.2059	3.1639	3.2028	3.1712	3.2009	**3.68**
H(4`B)	2.8881	2.8154	2.8217	2.7853	2.7501	2.7870	2.7642	2.7894	2.7801	2.7842	2.7525	2.7167	2.6896	2.6661	2.6699	2.6343	2.6711	2.6457	2.6729	2.6449	2.6692	2.6479	**2.88**
Nuclei	**M06-2X**																						
H2	9.2688	9.2022	9.2172	9.0689	9.1055	9.0698	9.1149	9.0705	9.0488	9.0684	9.0786	9.2688	9.2022	9.2172	9.0689	9.1055	9.0698	9.0583	9.0705	9.0488	9.0684	9.0786	**8.07**
H3	7.8638	7.9995	8.0888	8.0689	8.1821	8.0652	8.1797	8.0611	8.1877	8.0725	8.2067	7.8638	7.9995	8.0888	8.0689	8.1821	8.0652	8.1961	8.0611	8.1877	8.0725	8.2067	**7.24**
H5	7.6717	7.8528	7.9530	7.9157	8.0613	7.9095	8.0370	7.9030	8.0561	7.9216	8.0935	7.6717	7.8528	7.9530	7.9157	8.0613	7.9095	8.0681	7.9030	8.0561	7.9216	8.0935	**7.24**
H6	8.6124	8.8188	8.8989	8.8904	9.0545	8.8808	9.0649	8.8712	9.0535	8.9000	9.1025	8.6124	8.8188	8.8989	8.8904	9.0545	8.8808	9.0792	8.8712	9.0535	8.9000	9.1025	**8.07**
H8	4.3271	4.4158	4.4543	4.4033	4.5256	4.3941	4.5771	4.3853	4.6108	4.4129	4.6134	4.3271	4.4158	4.4543	4.4032	4.5256	4.3941	4.6342	4.3853	4.6108	4.4129	4.6134	**5.24**
H(9A-9B)	1.6984	1.7184	1.7356	1.7776	1.7778	1.7746	1.7854	1.7711	1.6992	1.7805	1.7994	1.6984	1.7184	1.7356	1.7776	1.7778	1.7746	1.7084	1.7711	1.6992	1.7805	1.7994	**2.135**
H(10A-10B)	1.2515	1.1192	1.0834	1.0230	0.9580	1.0266	0.9551	1.0298	0.9629	1.0198	0.9420	1.2515	1.1192	1.0834	1.0230	0.9580	1.0266	0.9586	1.0298	0.9629	1.0198	0.9420	**1.275**
H(11A-11B)	0.8898	0.9068	0.8693	0.9307	0.8776	0.9276	0.8778	0.9243	0.8547	0.9338	0.8533	0.8898	0.9068	0.8693	0.9307	0.8776	0.9276	0.8549	0.9243	0.8547	0.9338	0.8533	**1.28**
H(12A-12B)	1.1622	1.1268	1.1062	1.0940	1.0555	1.0940	1.0457	1.0936	1.0687	1.0943	1.0549	1.1622	1.1268	1.1062	1.0940	1.0555	1.0940	1.0672	1.0936	1.0687	1.0943	1.0549	**1.285**
H(13A-13B)	1.0631	1.0675	1.0305	1.0758	1.0370	1.0739	1.0244	1.0716	1.0312	1.0779	1.0207	1.0630	1.0675	1.0305	1.0759	1.0370	1.0739	1.0302	1.0716	1.0312	1.0779	1.0207	**1.29**
H(14A-14B)	1.2185	1.2100	1.1842	1.2033	1.1719	1.2026	1.1560	1.2015	1.1776	1.2042	1.1658	1.2185	1.2100	1.1843	1.2033	1.1719	1.2026	1.1761	1.2015	1.1776	1.2042	1.1658	**1.295**
H(15A-15C)	0.9426	0.9362	0.9102	0.9177	0.9033	0.9167	0.8643	0.9154	0.9057	0.9188	0.8933	0.9426	0.9362	0.9102	0.9177	0.9033	0.9167	0.9047	0.9154	0.9057	0.9188	0.8933	**0.82**
H(1`A)	2.6291	2.6208	2.6156	2.5808	2.5564	2.5793	2.5634	2.5779	2.5812	2.5823	2.5617	2.7832	2.7594	2.7291	2.7620	2.7345	2.7649	2.7321	2.7635	2.7351	2.7609	2.7081	**3.82**
H(1`B)	3.0890	3.1187	3.1545	3.1443	3.2041	3.1365	3.1858	3.1351	3.1888	3.1488	3.2018	2.7102	2.5544	2.5468	2.5983	2.5686	2.6036	2.5662	2.6022	2.5716	2.5960	2.5628	**3.78**
H(2`A-2`B)	1.6998	1.7388	1.7080	1.7684	1.7294	1.7646	1.7227	1.7607	1.7393	1.7722	1.7567	1.5990	1.6808	1.6378	1.7377	1.6807	1.7331	1.7376	1.7283	1.7313	1.7423	1.7569	**2.26**
H(3`A-3`B)	1.5990	1.6808	1.6378	1.7377	1.6807	1.7331	1.6948	1.7283	1.7313	1.7423	1.7569	1.6998	1.7388	1.7080	1.7684	1.7294	1.7646	1.7446	1.7607	1.7393	1.7722	1.7567	**2.01**
H(4`A)	2.7102	2.5544	2.5752	2.5983	2.5739	2.6036	2.5693	2.6022	2.5716	2.5960	2.5628	3.0890	3.1187	3.0592	3.1443	3.1979	3.1365	3.1955	3.1351	3.1888	3.1488	3.2018	**3.68**
H(4`B)	2.7832	2.7595	2.7552	2.7620	2.7174	2.7649	2.7380	2.7635	2.7351	2.7609	2.7081	2.6291	2.6208	2.5735	2.5808	2.5846	2.5793	2.5822	2.5779	2.5812	2.5823	2.5617	**2.88**

[a] methyl protons shifts are averaged
[b] according to [7]

Table S7. Cont. IV

Nuclei	R											S										Exp. [b]
	mpW1LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
H2	8.7132	8.6044	8.6317	8.5148	8.5386	8.5221	8.5395	8.5286	8.4416	8.5072	8.5605	8.7132	8.6044	8.6317	8.5148	8.5386	8.5221	8.4445	8.5286	8.4416	8.5072	8.5605	**8.07**
H3	7.3358	7.4726	7.5601	7.5162	7.6306	7.5144	7.6218	7.5123	7.6266	7.5176	7.6660	7.3358	7.4726	7.5601	7.5161	7.6306	7.5144	7.6335	7.5123	7.6266	7.5176	7.6660	**7.24**
H5	7.1570	7.3289	7.4220	7.4117	7.5266	7.4072	7.5253	7.4023	7.5671	7.4158	7.5630	7.1570	7.3289	7.4220	7.4117	7.5266	7.4072	7.5769	7.4023	7.5671	7.4159	7.5630	**7.24**
H6	7.9788	8.1794	8.2570	8.2701	8.4015	8.2657	8.4281	8.2607	8.3427	8.2738	8.4692	7.9787	8.1794	8.2570	8.2701	8.4015	8.2657	8.3636	8.2607	8.3427	8.2738	8.4692	**8.07**
H8	4.5689	4.6562	4.6892	4.6947	4.7499	4.6938	4.8442	4.6923	4.7552	4.6950	4.7758	4.5689	4.6562	4.6892	4.6947	4.7499	4.6938	4.7696	4.6923	4.7552	4.6950	4.7758	**5.24**
H(9A-9B)	1.7079	1.7412	1.7392	1.7633	1.8086	1.7615	1.7837	1.7596	1.6745	1.7651	1.8186	1.7079	1.7412	1.7392	1.7633	1.8086	1.7615	1.6829	1.7596	1.6745	1.7651	1.8186	**2.135**
H(10A-10B)	1.3383	1.2285	1.1912	1.1619	1.0885	1.1669	1.0951	1.1716	1.1228	1.1570	1.1058	1.3383	1.2285	1.1912	1.1619	1.0885	1.1669	1.1194	1.1716	1.1228	1.1570	1.1058	**1.275**
H(11A-11B)	0.9852	1.0054	0.9704	1.0267	0.9875	1.0254	0.9768	1.0238	0.9713	1.0280	0.9766	0.9852	1.0054	0.9704	1.0267	0.9875	1.0254	0.9717	1.0238	0.9713	1.0280	0.9766	**1.28**
H(12A-12B)	1.2362	1.2234	1.1981	1.2108	1.1649	1.2122	1.1641	1.2132	1.1858	1.2095	1.1704	1.2362	1.2234	1.1982	1.2108	1.1649	1.2122	1.1840	1.2132	1.1858	1.2095	1.1704	**1.285**
H(13A-13B)	1.1485	1.1528	1.1235	1.1639	1.1264	1.1632	1.1153	1.1624	1.1235	1.1644	1.1201	1.1485	1.1528	1.1235	1.1639	1.1264	1.1632	1.1231	1.1624	1.1235	1.1644	1.1201	**1.29**
H(14A-14B)	1.3106	1.3088	1.2887	1.3083	1.2741	1.3088	1.2634	1.3089	1.2855	1.3079	1.2742	1.3106	1.3088	1.2887	1.3084	1.2741	1.3088	1.2843	1.3089	1.2855	1.3079	1.2742	**1.295**
H(15A-15C)	0.9698	0.9659	0.9445	0.9673	0.9358	0.9675	0.9150	0.9674	0.9396	0.9671	0.9320	0.9698	0.9659	0.9445	0.9673	0.9358	0.9675	0.9386	0.9674	0.9396	0.9671	0.9321	**0.82**
H(1`A)	2.7315	2.7295	2.7063	2.7196	2.6695	2.7208	2.6895	2.7216	2.6841	2.7183	2.6574	2.8607	2.8475	2.8460	2.8321	2.8015	2.8329	2.8065	2.8335	2.8107	2.8314	2.7667	**3.82**
H(1`B)	3.2045	3.2461	3.2724	3.2786	3.3290	3.2769	3.3237	3.2749	3.3102	3.2800	3.3283	2.8543	2.6888	2.6649	2.6700	2.6829	2.6701	2.6742	2.6703	2.6760	2.6703	2.6307	**3.78**
H(2`A-2`B)	1.7343	1.7767	1.7381	1.8083	1.7550	1.8067	1.7555	1.8048	1.7653	1.8097	1.7796	1.5860	1.6743	1.6419	1.7285	1.6712	1.7252	1.7197	1.7218	1.7151	1.7316	1.7246	**2.26**
H(3`A-3`B)	1.5860	1.6743	1.6419	1.7285	1.6712	1.7252	1.6822	1.7218	1.7151	1.7315	1.7246	1.7343	1.7767	1.7381	1.8083	1.7550	1.8067	1.7692	1.8048	1.7653	1.8097	1.7796	**2.01**
H(4`A)	2.8543	2.6888	2.6649	2.6700	2.6829	2.6701	2.6676	2.6703	2.6760	2.6703	2.6307	3.2045	3.2461	3.2724	3.2786	3.3290	3.2769	3.3142	3.2749	3.3101	3.2801	3.3283	**3.68**
H(4`B)	2.8607	2.8475	2.8460	2.8321	2.8015	2.8329	2.8082	2.8335	2.8107	2.8314	2.7667	2.7315	2.7295	2.7063	2.7196	2.6695	2.7208	2.6832	2.7216	2.6841	2.7183	2.6574	**2.88**
Nuclei	mpW1PW91																						
H2	8.7696	8.7001	8.6845	8.5654	8.5923	8.5734	8.5921	8.5809	8.6337	8.5576	8.5671	8.7696	8.7001	8.6845	8.5654	8.5923	8.5734	8.6194	8.5809	8.6337	8.5576	8.5671	**8.07**
H3	7.3657	7.5081	7.6005	7.5492	7.6728	7.5478	7.6614	7.5465	7.6850	7.5506	7.7083	7.3657	7.5081	7.6005	7.5492	7.6728	7.5478	7.6927	7.5465	7.6850	7.5506	7.7083	**7.24**
H5	7.1837	7.3637	7.4562	7.4371	7.5635	7.4329	7.5576	7.4287	7.5737	7.4412	7.5970	7.1837	7.3637	7.4562	7.4371	7.5635	7.4329	7.5827	7.4287	7.5737	7.4412	7.5970	**7.24**
H6	8.0406	8.2555	8.3153	8.3466	8.4607	8.3417	8.5044	8.3364	8.5126	8.3508	8.5559	8.0406	8.2555	8.3153	8.3466	8.4607	8.3417	8.5364	8.3364	8.5126	8.3508	8.5559	**8.07**
H8	4.5694	4.6538	4.6890	4.6897	4.7465	4.6894	4.8344	4.6888	4.7931	4.6894	4.7815	4.5694	4.6538	4.6890	4.6897	4.7465	4.6894	4.8037	4.6888	4.7931	4.6894	4.7815	**5.24**
H(9A-9B)	1.7346	1.7854	1.7537	1.7828	1.8157	1.7805	1.8030	1.7786	1.8015	1.7856	1.8016	1.7346	1.7854	1.7537	1.7828	1.8157	1.7805	1.8054	1.7786	1.8015	1.7856	1.8016	**2.135**
H(10A-10B)	1.3123	1.1970	1.1608	1.1205	1.0617	1.1256	1.0567	1.1307	1.0785	1.1161	1.0500	1.3123	1.1970	1.1608	1.1205	1.0617	1.1256	1.0712	1.1307	1.0785	1.1161	1.0500	**1.275**
H(11A-11B)	0.9365	0.9609	0.9176	0.9720	0.9379	0.9708	0.9250	0.9696	0.9306	0.9736	0.9133	0.9365	0.9609	0.9175	0.9720	0.9379	0.9708	0.9279	0.9696	0.9306	0.9736	0.9133	**1.28**
H(12A-12B)	1.1889	1.1716	1.1470	1.1534	1.1151	1.1551	1.1081	1.1567	1.1229	1.1521	1.1141	1.1889	1.1716	1.1470	1.1534	1.1151	1.1550	1.1200	1.1567	1.1229	1.1521	1.1142	**1.285**
H(13A-13B)	1.0963	1.0988	1.0675	1.1038	1.0704	1.1035	1.0557	1.1033	1.0659	1.1045	1.0598	1.0963	1.0988	1.0675	1.1038	1.0704	1.1035	1.0644	1.1033	1.0659	1.1045	1.0598	**1.29**
H(14A-14B)	1.2564	1.2514	1.2304	1.2465	1.2160	1.2472	1.2022	1.2480	1.2196	1.2462	1.2150	1.2564	1.2514	1.2304	1.2465	1.2160	1.2472	1.2186	1.2480	1.2196	1.2462	1.2150	**1.295**
H(15A-15C)	0.9153	0.9114	0.8884	0.9082	0.8801	0.9087	0.8573	0.9092	0.8808	0.9079	0.8754	0.9153	0.9114	0.8884	0.9082	0.8801	0.9087	0.8796	0.9092	0.8807	0.9079	0.8754	**0.82**
H(1`A)	2.6736	2.6743	2.6528	2.6560	2.6120	2.6579	2.6291	2.6598	2.6283	2.6543	2.5953	2.7998	2.7854	2.7780	2.7732	2.7382	2.7741	2.7484	2.7752	2.7481	2.7729	2.7184	**3.82**
H(1`B)	3.1778	3.2179	3.2347	3.2407	3.2872	3.2394	3.2798	3.2381	3.2798	3.2421	3.2811	2.8613	2.6680	2.6711	2.6489	2.6689	2.6487	2.6742	2.6528	2.6582	2.6543	2.6182	**3.78**
H(2`A-2`B)	1.7019	1.7403	1.7077	1.7675	1.7244	1.7661	1.7193	1.7648	1.7333	1.7692	1.7523	1.5594	1.6374	1.6057	1.6902	1.6381	1.6877	1.6683	1.6853	1.6601	1.6928	1.7143	**2.26**
H(3`A-3`B)	1.5594	1.6374	1.6056	1.6902	1.6381	1.6877	1.6470	1.6853	1.6601	1.6928	1.7143	1.7019	1.7403	1.7077	1.7675	1.7244	1.7661	1.7374	1.7648	1.7333	1.7692	1.7523	**2.01**
H(4`A)	2.8613	2.6680	2.6711	2.6489	2.6689	2.6487	2.6448	2.6493	2.6123	2.6503	2.6182	3.1778	3.2180	3.2347	3.2407	3.2872	3.2394	3.2840	3.2381	3.2797	3.2421	3.2811	**3.68**
H(4`B)	2.7998	2.7854	2.7779	2.7732	2.7382	2.7741	2.7542	2.7752	2.7481	2.7729	2.7184	2.6736	2.6743	2.6528	2.6560	2.6120	2.6579	2.6273	2.6598	2.6283	2.6543	2.5953	**2.88**
Nuclei	O3LYP																						
H2	8.5108	8.3361	8.3595	8.2440	8.2909	8.2584	8.3327	8.2630	8.3236	8.2348	8.3200	8.5108	8.3361	8.3595	8.2440	8.2909	8.2584	8.3327	8.2631	8.3236	8.2348	8.3200	**8.07**
H3	7.2901	7.3999	7.4958	7.4500	7.5610	7.4478	7.5814	7.4413	7.5741	7.4515	7.5921	7.2901	7.3998	7.4958	7.4500	7.5610	7.4478	7.5814	7.4413	7.5741	7.4515	7.5921	**7.24**
H5	7.1348	7.3190	7.4090	7.3885	7.5118	7.3860	7.5264	7.3846	7.5163	7.3911	7.5353	7.1348	7.3190	7.4090	7.3885	7.5118	7.3860	7.5265	7.3847	7.5163	7.3911	7.5353	**7.24**
H6	7.8977	8.0346	8.1139	8.1024	8.2544	8.1012	8.2954	8.1047	8.2732	8.1051	8.3171	7.8977	8.0346	8.1139	8.1024	8.2544	8.1012	8.2954	8.1046	8.2732	8.1051	8.3171	**8.07**
H8	4.7575	4.7780	4.7992	4.7896	4.8754	4.7911	4.8898	4.7935	4.8736	4.7890	4.8741	4.7575	4.7780	4.7992	4.7896	4.8754	4.7911	4.8898	4.7935	4.8736	4.7890	4.8741	**5.24**
H(9A-9B)	1.6371	1.6211	1.6327	1.6403	1.6588	1.6418	1.6900	1.6455	1.6821	1.6412	1.7050	1.6370	1.6211	1.6327	1.6403	1.6588	1.6418	1.6900	1.6455	1.6821	1.6412	1.7050	**2.135**
H(10A-10B)	1.2764	1.1837	1.1462	1.1350	1.0686	1.1374	1.0851	1.1414	1.0873	1.1317	1.0870	1.2764	1.1838	1.1462	1.1350	1.0686	1.1374	1.0851	1.1415	1.0873	1.1317	1.0870	**1.275**
H(11A-11B)	0.9651	0.9764	0.9462	1.0039	0.9600	1.0018	0.9590	0.9989	0.9581	1.0054	0.9580	0.9651	0.9764	0.9462	1.0038	0.9600	1.0018	0.9590	0.9990	0.9581	1.0054	0.9580	**1.28**
H(12A-12B)	1.2153	1.2073	1.1814	1.2043	1.1587	1.2042	1.1633	1.2026	1.1645	1.2036	1.1663	1.2153	1.2073	1.1814	1.2043	1.1587	1.2042	1.1633	1.2027	1.1645	1.2036	1.1663	**1.285**
H(13A-13B)	1.1340	1.1352	1.1076	1.1511	1.1115	1.1500	1.1096	1.1472	1.1095	1.1517	1.1112	1.1340	1.1352	1.1076	1.1511	1.1115	1.1500	1.1096	1.1472	1.1095	1.1517	1.1112	**1.29**
H(14A-14B)	1.3176	1.3196	1.2996	1.3233	1.2898	1.3230	1.2919	1.3219	1.2925	1.3230	1.2913	1.3176	1.3196	1.2996	1.3233	1.2898	1.3230	1.2919	1.3219	1.2925	1.3230	1.2913	**1.295**
H(15A-15C)	0.9493	0.9446	0.9232	0.9489	0.9186	0.9487	0.9178	0.9476	0.9181	0.9487	0.9157	0.9493	0.9447	0.9232	0.9489	0.9186	0.9487	0.9178	0.9476	0.9181	0.9487	0.9157	**0.82**
H(1`A)	2.7774	2.7637	2.7396	2.7555	2.7041	2.7568	2.7147	2.7547	2.7154	2.7544	2.6826	2.9128	2.8942	2.8872	2.8696	2.8347	2.8723	2.8401	2.8738	2.8441	2.8669	2.8018	**3.82**
H(1`B)	3.2635	3.2960	3.3296	3.3276	3.3894	3.3259	3.3790	3.3257	3.3746	3.3294	3.3772	2.8798	2.7677	2.7543	2.7567	2.7532	2.7561	2.7362	2.7551	2.7389	2.7567	2.7349	**3.78**
H(2`A-2`B)	1.7323	1.7680	1.7331	1.7990	1.7516	1.7980	1.7625	1.7931	1.7583	1.8000	1.7794	1.6117	1.6893	1.6613	1.7464	1.6931	1.7421	1.7145	1.7328	1.7097	1.7496	1.7527	**2.26**
H(3`A-3`B)	1.6117	1.6893	1.6613	1.7464	1.6931	1.7421	1.7145	1.7328	1.7097	1.7496	1.7527	1.7323	1.7680	1.7331	1.7990	1.7516	1.7980	1.7625	1.7932	1.7583	1.8000	1.7794	**2.01**
H(4`A)	2.8798	2.7677	2.7543	2.7567	2.7532	2.7561	2.7362	2.7548	2.7389	2.7567	2.7349	3.2635	3.2960	3.3296	3.3276	3.3894	3.3259	3.3790	3.3256	3.3746	3.3294	3.3771	**3.68**
H(4`B)	2.9128	2.8942	2.8872	2.8696	2.8347	2.8723	2.8401	2.8743	2.8441	2.8669	2.8018	2.7774	2.7637	2.7396	2.7555	2.7041	2.7568	2.7147	2.7550	2.7154	2.7544	2.6826	**2.88**
Nuclei	OLYP																						
H2	8.3248	8.1648	8.2538	8.0803	8.0015	8.0861	8.1354	8.0916	8.0872	8.0741	8.2124	8.3247	8.1648	8.2538	8.0803	8.0015	8.0861	8.0988	8.0916	8.0872	8.0741	8.2124	**8.07**
H3	7.2142	7.3287	7.4254	7.3644	7.4628	7.3630	7.4767	7.3615	7.4811	7.3651	7.5155	7.2142	7.3287	7.4254	7.3644	7.4628	7.3630	7.4870	7.3615	7.4811	7.3651	7.5155	**7.24**
H5	7.0994	7.2395	7.3358	7.3006	7.4044	7.2973	7.4189	7.2939	7.4181	7.3033	7.4518	7.0995	7.2395	7.3358	7.3006	7.4044	7.2973	7.4298	7.2939	7.4181	7.3033	7.4518	**7.24**
H6	7.7912	7.9146	8.0145	7.9898	8.0895	7.9855	8.1272	7.9810	8.1012	7.9933	8.2037	7.7912	7.9146	8.0145	7.9898	8.0895	7.9855	8.1269	7.9810	8.1012	7.9933	8.2037	**8.07**
H8	4.9255	4.9263	4.9478	4.9302	4.9556	4.9304	5.0427	4.9304	4.9578	4.9293	5.0069	4.9256	4.9263	4.9478	4.9302	4.9556	4.9304	4.9756	4.9304	4.9578	4.9293	5.0069	**5.24**
H(9A-9B)	1.6378	1.6482	1.6929	1.6836	1.6528	1.6811	1.7021	1.6786	1.6857	1.6856	1.7602	1.6378	1.6482	1.6929	1.6836	1.6528	1.6811	1.6907	1.6786	1.6857	1.6856	1.7602	**2.135**
H(10A-10B)	1.2986	1.2200	1.1776	1.1729	1.1263	1.1764	1.1192	1.1797	1.1387	1.1691	1.1219	1.2986	1.2200	1.1776	1.1729	1.1263	1.1764	1.1374	1.1797	1.1387	1.1691	1.1219	**1.275**
H(11A-11B)	0.9956	1.0127	0.9857	1.0388	1.0080	1.0371	0.9919	1.0354	1.0026	1.0400	0.9927	0.9956	1.0127	0.9857	1.0388	1.0080	1.0371	1.0022	1.0354	1.0026	1.0400	0.9927	**1.28**
H(12A-12B)	1.2490	1.2466	1.2155	1.2396	1.2113	1.2406	1.1975	1.2413	1.2137	1.2384	1.1999	1.2490	1.2466	1.2155	1.2396	1.2113	1.2406	1.2127	1.2413	1.2137	1.2384	1.1999	**1.285**
H(13A-13B)	1.1676	1.1730	1.1449	1.1854	1.1577	1.1848	1.1407	1.1840	1.1534	1.1857	1.1449	1.1676	1.1730	1.1449	1.1854	1.1577	1.1848	1.1531	1.1840	1.1534	1.1857	1.1449	**1.29**
H(14A-14B)	1.3596	1.3646	1.3413	1.3660	1.3422	1.3663	1.3251	1.3664	1.3428	1.3653	1.3324	1.3596	1.3646	1.3413	1.3660	1.3422	1.3663	1.3422	1.3664	1.3428	1.3653	1.3324	**1.295**
H(15A-15C)	0.9612	0.9582	0.9357	0.9607	0.9364	0.9607	0.9121	0.9607	0.9353	0.9601	0.9259	0.9612	0.9582	0.9357	0.9607	0.9364	0.9607	0.9351	0.9607	0.9353	0.9601	0.9259	**0.82**
H(1`A)	2.8378	2.8260	2.8047	2.8160	2.7664	2.8169	2.7846	2.8177	2.7763	2.8147	2.7410	2.9774	2.9588	2.9520	2.9351	2.9032	2.9372	2.9052	2.9391	2.9044	2.9324	2.8589	**3.82**
H(1`B)	3.3555	3.3841	3.4251	3.4191	3.4774	3.4169	3.4686	3.4147	3.4614	3.4207	3.4677	2.9631	2.8588	2.8417	2.8491	2.8809	2.8491	2.8573	2.8492	2.8578	2.8488	2.8263	**3.78**
H(2`A-2`B)	1.7671	1.8012	1.7690	1.8260	1.7833	1.8247	1.7762	1.8233	1.7903	1.8269	1.8151	1.6586	1.7375	1.7010	1.7856	1.7718	1.7826	1.7804	1.7795	1.7751	1.7880	1.7849	**2.26**
H(3`A-3`B)	1.6586	1.7375	1.7010	1.7856	1.7718	1.7826	1.7419	1.7795	1.7751	1.7880	1.7849	1.7671	1.8012	1.7690	1.8260	1.7833	1.8247	1.7950	1.8233	1.7903	1.8269	1.8151	**2.01**
H(4`A)	2.9631	2.8588	2.8417	2.8491	2.8809	2.8491	2.8573	2.8492	2.8578	2.8488	2.8263	3.3555	3.3841	3.4251	3.4191	3.4774	3.4169	3.4642	3.4147	3.4614	3.4207	2.8263	**3.68**
H(4`B)	2.9774	2.9588	2.9520	2.9351	2.9032	2.9372	2.9052	2.9391	2.9044	2.9324	2.8589	2.8378	2.8260	2.8047	2.8160	2.7664	2.8169	2.7745	2.8177	2.7762	2.8147	2.8589	**2.88**

[a] methyl protons shifts are averaged

[b] according to [7]

Table S7. Cont. V

Nuclei	R											S										Exp. [b]
	OPBE																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
H2	8.3493	8.2392	8.2718	8.1296	8.2064	8.1369	8.1837	8.1437	8.2434	8.1222	8.2247	8.3493	8.2392	8.2718	8.1296	8.2064	8.1369	8.2501	8.1437	8.2434	8.1221	8.2247	**8.07**
H3	7.2200	7.3458	7.4385	7.3939	7.5142	7.3929	7.5066	7.3911	7.5205	7.3941	7.5396	7.2200	7.3458	7.4385	7.3939	7.5142	7.3929	7.5275	7.3911	7.5205	7.3941	7.5396	**7.24**
H5	7.0981	7.2640	7.3492	7.3273	7.4517	7.3243	7.4461	7.3206	7.4585	7.3294	7.4808	7.0981	7.2640	7.3492	7.3273	7.4517	7.3243	7.4685	7.3206	7.4585	7.3294	7.4808	**7.24**
H6	7.8722	8.0145	8.0860	8.0625	8.2039	8.0600	8.1936	8.0566	8.2311	8.0641	8.2568	7.8722	8.0145	8.0860	8.0625	8.2039	8.0599	8.2512	8.0566	8.2311	8.0641	8.2568	**8.07**
H8	4.9240	4.9392	4.9500	4.9341	5.0091	4.9354	5.0372	4.9359	5.0098	4.9321	5.0098	4.9240	4.9392	4.9500	4.9341	5.0091	4.9354	5.0241	4.9359	5.0097	4.9321	5.0098	**5.24**
H(9A-9B)	1.6489	1.6720	1.6887	1.6820	1.6995	1.6801	1.6958	1.6778	1.7303	1.6833	1.7437	1.6489	1.6720	1.6887	1.6820	1.6995	1.6801	1.7362	1.6778	1.7303	1.6833	1.7437	**2.135**
H(10A-10B)	1.2436	1.1591	1.1199	1.1143	1.0434	1.1182	1.0550	1.1212	1.0658	1.1099	1.0670	1.2436	1.1591	1.1199	1.1143	1.0434	1.1182	1.0628	1.1212	1.0658	1.1098	1.0670	**1.275**
H(11A-11B)	0.9363	0.9558	0.9228	0.9816	0.9369	0.9805	0.9297	0.9787	0.9321	0.9819	0.9300	0.9363	0.9558	0.9228	0.9816	0.9369	0.9805	0.9322	0.9787	0.9321	0.9819	0.9300	**1.28**
H(12A-12B)	1.1882	1.1824	1.1506	1.1782	1.1284	1.1796	1.1296	1.1801	1.1335	1.1761	1.1363	1.1882	1.1823	1.1506	1.1782	1.1284	1.1796	1.1322	1.1801	1.1335	1.1761	1.1363	**1.285**
H(13A-13B)	1.1023	1.1082	1.0754	1.1204	1.0779	1.1204	1.0684	1.1196	1.0740	1.1198	1.0746	1.1023	1.1082	1.0754	1.1204	1.0779	1.1204	1.0738	1.1196	1.0740	1.1198	1.0746	**1.29**
H(14A-14B)	1.2966	1.2986	1.2725	1.2993	1.2608	1.3001	1.2515	1.3001	1.2628	1.2977	1.2615	1.2966	1.2986	1.2725	1.2993	1.2608	1.3001	1.2621	1.3001	1.2628	1.2977	1.2615	**1.295**
H(15A-15C)	0.8937	0.8918	0.8646	0.8928	0.8584	0.8935	0.8385	0.8934	0.8568	0.8914	0.8546	0.8937	0.8918	0.8646	0.8928	0.8585	0.8935	0.8564	0.8934	0.8568	0.8914	0.8546	**0.82**
H(1`A)	2.7613	2.7514	2.7263	2.7415	2.6913	2.7426	2.7077	2.7431	2.6992	2.7396	2.6618	2.9015	2.8885	2.8777	2.8595	2.8206	2.8623	2.8281	2.8642	2.8304	2.8561	2.7954	**3.82**
H(1`B)	3.3195	3.3467	3.3748	3.3738	3.4263	3.3724	3.4124	3.3702	3.4131	3.3745	3.4125	2.9527	2.8309	2.8138	2.8147	2.8015	2.8153	2.7845	2.8154	2.7866	2.8135	2.7913	**3.78**
H(2`A-2`B)	1.7220	1.7581	1.7210	1.7831	1.7379	1.7824	1.7296	1.7809	1.7436	1.7831	1.7663	1.6145	1.6835	1.6484	1.7372	1.6799	1.7345	1.6995	1.7310	1.6937	1.7390	1.7470	**2.26**
H(3`A-3`B)	1.6145	1.6835	1.6484	1.7372	1.6799	1.7345	1.6902	1.7310	1.6937	1.7390	1.7470	1.7220	1.7581	1.7210	1.7831	1.7379	1.7824	1.7469	1.7809	1.7436	1.7831	1.7663	**2.01**
H(4`A)	2.9527	2.8309	2.8138	2.8147	2.8015	2.8153	2.8102	2.8154	2.7866	2.8135	2.7913	3.3195	3.3467	3.3748	3.3738	3.4263	3.3724	3.4169	3.3702	3.4130	3.3745	3.4125	**3.68**
H(4`B)	2.9015	2.8885	2.8777	2.8595	2.8206	2.8623	2.8268	2.8642	2.8304	2.8561	2.7954	2.7613	2.7514	2.7263	2.7414	2.6913	2.7426	2.6981	2.7431	2.6992	2.7396	2.6618	**2.88**
Nuclei	OPW91																						
H2	8.3512	8.2401	8.2730	8.1313	8.0596	8.1378	8.1844	8.1442	8.2442	8.1235	8.2281	8.3512	8.2401	8.2730	8.1313	8.0596	8.1378	8.2518	8.1442	8.2442	8.1235	8.2281	**8.07**
H3	7.2224	7.3473	7.4399	7.3959	7.4884	7.3942	7.5076	7.3922	7.5214	7.3958	7.5404	7.2224	7.3473	7.4399	7.3959	7.4883	7.3942	7.5285	7.3922	7.5214	7.3958	7.5404	**7.24**
H5	7.1011	7.2662	7.3514	7.3297	7.4376	7.3260	7.4475	7.3221	7.4602	7.3314	7.4821	7.1011	7.2662	7.3514	7.3297	7.4377	7.3260	7.4703	7.3221	7.4602	7.3314	7.4821	**7.24**
H6	7.8704	8.0137	8.0851	8.0634	8.1417	8.0600	8.1939	8.0564	8.2309	8.0647	8.2591	7.8704	8.0137	8.0851	8.0634	8.1417	8.0600	8.2515	8.0564	8.2309	8.0647	8.2592	**8.07**
H8	4.9226	4.9378	4.9488	4.9339	4.9572	4.9344	5.0369	4.9346	5.0088	4.9316	5.0093	4.9226	4.9378	4.9488	4.9339	4.9572	4.9344	5.0235	4.9346	5.0088	4.9316	5.0093	**5.24**
H(9A-9B)	1.6463	1.6700	1.6867	1.6811	1.6483	1.6785	1.6945	1.6758	1.7291	1.6821	1.7437	1.6463	1.6700	1.6867	1.6811	1.6484	1.6785	1.7353	1.6758	1.7291	1.6821	1.7437	**2.135**
H(10A-10B)	1.2459	1.1611	1.1220	1.1172	1.0498	1.1204	1.0574	1.1233	1.0679	1.1124	1.0693	1.2459	1.1611	1.1220	1.1172	1.0498	1.1204	1.0651	1.1232	1.0679	1.1124	1.0693	**1.275**
H(11A-11B)	0.9378	0.9575	0.9248	0.9841	0.9384	0.9824	0.9318	0.9804	0.9342	0.9842	0.9326	0.9378	0.9575	0.9248	0.9841	0.9384	0.9824	0.9344	0.9804	0.9342	0.9842	0.9326	**1.28**
H(12A-12B)	1.1896	1.1838	1.1522	1.1805	1.1400	1.1812	1.1315	1.1815	1.1352	1.1782	1.1380	1.1896	1.1838	1.1522	1.1805	1.1400	1.1812	1.1339	1.1815	1.1352	1.1782	1.1380	**1.285**
H(13A-13B)	1.1039	1.1099	1.0773	1.1230	1.0830	1.1223	1.0707	1.1213	1.0761	1.1222	1.0769	1.1039	1.1099	1.0773	1.1231	1.0830	1.1223	1.0760	1.1213	1.0761	1.1222	1.0769	**1.29**
H(14A-14B)	1.2971	1.2993	1.2734	1.3008	1.2681	1.3010	1.2527	1.3008	1.2638	1.2990	1.2626	1.2971	1.2993	1.2734	1.3008	1.2681	1.3009	1.2632	1.3008	1.2638	1.2990	1.2626	**1.295**
H(15A-15C)	0.8951	0.8933	0.8664	0.8951	0.8635	0.8952	0.8404	0.8948	0.8586	0.8935	0.8565	0.8951	0.8933	0.8664	0.8951	0.8635	0.8951	0.8584	0.8948	0.8586	0.8935	0.8565	**0.82**
H(1`A)	2.7654	2.7551	2.7299	2.7457	2.6947	2.7462	2.7115	2.7466	2.7028	2.7435	2.6658	2.9049	2.8918	2.8810	2.8636	2.8325	2.8657	2.8312	2.8674	2.8336	2.8598	2.7980	**3.82**
H(1`B)	3.3164	3.3442	3.3724	3.3721	3.4175	3.3700	3.4105	3.3676	3.4109	3.3725	3.4107	2.9478	2.8271	2.8104	2.8121	2.8346	2.8120	2.7814	2.8119	2.7837	2.8106	2.7879	**3.78**
H(2`A-2`B)	1.7220	1.7583	1.7215	1.7843	1.7323	1.7828	1.7304	1.7811	1.7441	1.7841	1.7672	1.6145	1.6839	1.6490	1.7384	1.7103	1.7351	1.6998	1.7315	1.6941	1.7399	1.7461	**2.26**
H(3`A-3`B)	1.6145	1.6839	1.6490	1.7384	1.7103	1.7351	1.6909	1.7314	1.6941	1.7399	1.7461	1.7220	1.7583	1.7215	1.7843	1.7323	1.7828	1.7476	1.7811	1.7441	1.7841	1.7672	**2.01**
H(4`A)	2.9478	2.8271	2.8104	2.8121	2.8346	2.8120	2.8076	2.8119	2.7837	2.8106	2.7879	3.3164	3.3442	3.3724	3.3721	3.4174	3.3700	3.4148	3.3676	3.4109	3.3725	3.4107	**3.68**
H(4`B)	2.9049	2.8918	2.8810	2.8636	2.8325	2.8657	2.8303	2.8674	2.8336	2.8598	2.7980	2.7654	2.7551	2.7299	2.7457	2.6947	2.7462	2.7018	2.7466	2.7028	2.7435	2.6658	**2.88**
Nuclei	PBE																						
H2	8.5376	8.4278	8.4550	8.3490	8.3529	8.3550	8.3808	8.3612	8.3954	8.3435	8.3588	8.5376	8.4278	8.4550	8.3490	8.3529	8.3550	8.3913	8.3612	8.3954	8.3435	8.3588	**8.07**
H3	7.2081	7.3473	7.4380	7.3857	7.5089	7.3840	7.5023	7.3828	7.5222	7.3879	7.5433	7.2081	7.3473	7.4380	7.3857	7.5089	7.3840	7.5303	7.3828	7.5222	7.3879	7.5433	**7.24**
H5	7.0242	7.1954	7.2915	7.2732	7.3971	7.2688	7.3961	7.2649	7.4067	7.2779	7.4283	7.0242	7.1954	7.2915	7.2732	7.3971	7.2688	7.4167	7.2649	7.4067	7.2779	7.4283	**7.24**
H6	7.9566	8.1463	8.2083	8.2153	8.3301	8.2122	8.3630	8.2091	8.3747	8.2185	8.3849	7.9566	8.1464	8.2083	8.2153	8.3301	8.2122	8.3930	8.2091	8.3747	8.2186	8.3849	**8.07**
H8	4.9984	5.0614	5.0715	5.0695	5.1008	5.0707	5.1869	5.0719	5.1406	5.0683	5.1182	4.9984	5.0614	5.0715	5.0695	5.1008	5.0707	5.1510	5.0719	5.1406	5.0683	5.1182	**5.24**
H(9A-9B)	1.9217	1.9412	1.9445	1.9561	2.0018	1.9536	1.9803	1.9521	1.9828	1.9596	1.9803	1.9217	1.9412	1.9445	1.9561	2.0018	1.9536	1.9857	1.9521	1.9828	1.9596	1.9803	**2.135**
H(10A-10B)	1.3972	1.2918	1.2578	1.2275	1.1703	1.2317	1.1719	1.2364	1.1848	1.2242	1.1751	1.3972	1.2918	1.2578	1.2275	1.1703	1.2317	1.1808	1.2364	1.1848	1.2242	1.1751	**1.275**
H(11A-11B)	1.0474	1.0631	1.0274	1.0788	1.0455	1.0774	1.0352	1.0766	1.0367	1.0809	1.0228	1.0474	1.0631	1.0274	1.0788	1.0455	1.0774	1.0356	1.0766	1.0367	1.0809	1.0227	**1.28**
H(12A-12B)	1.2874	1.2759	1.2506	1.2583	1.2203	1.2597	1.2171	1.2617	1.2287	1.2576	1.2244	1.2874	1.2759	1.2506	1.2583	1.2203	1.2597	1.2270	1.2617	1.2287	1.2576	1.2244	**1.285**
H(13A-13B)	1.1952	1.1986	1.1680	1.2031	1.1707	1.2026	1.1589	1.2028	1.1666	1.2042	1.1611	1.1952	1.1987	1.1680	1.2031	1.1707	1.2026	1.1659	1.2028	1.1666	1.2042	1.1611	**1.29**
H(14A-14B)	1.3524	1.3519	1.3307	1.3450	1.3166	1.3456	1.3046	1.3466	1.3208	1.3451	1.3164	1.3524	1.3519	1.3307	1.3450	1.3166	1.3456	1.3200	1.3466	1.3208	1.3451	1.3164	**1.295**
H(15A-15C)	0.9401	0.9382	0.9153	0.9328	0.9065	0.9333	0.8855	0.9342	0.9075	0.9331	0.9028	0.9401	0.9382	0.9153	0.9328	0.9065	0.9333	0.9067	0.9342	0.9075	0.9331	0.9028	**0.82**
H(1`A)	2.8023	2.8053	2.7873	2.7873	2.7471	2.7887	2.7633	2.7907	2.7585	2.7866	2.7199	2.9200	2.9195	2.9111	2.9036	2.8805	2.9046	2.8809	2.9061	2.8833	2.9034	2.8420	**3.82**
H(1`B)	3.4002	3.4272	3.4462	3.4428	3.4914	3.4419	3.4838	3.4415	3.4808	3.4441	3.4777	3.0638	2.8750	2.8551	2.8274	2.8470	2.8285	2.7937	2.8307	2.7956	2.8277	2.7952	**3.78**
H(2`A-2`B)	1.8038	1.8449	1.8095	1.8654	1.8238	1.8642	1.8189	1.8635	1.8337	1.8673	1.8500	1.6481	1.7395	1.7013	1.7787	1.7332	1.7766	1.7612	1.7748	1.7551	1.7814	1.8066	**2.26**
H(3`A-3`B)	1.6481	1.7395	1.7013	1.7787	1.7332	1.7766	1.7379	1.7748	1.7551	1.7814	1.8066	1.8038	1.8449	1.8095	1.8654	1.8238	1.8642	1.8380	1.8635	1.8337	1.8673	1.8500	**2.01**
H(4`A)	3.0638	2.8750	2.8551	2.8274	2.8470	2.8285	2.8221	2.8307	2.7956	2.8277	2.7952	3.4002	3.4272	3.4462	3.4428	3.4914	3.4419	3.4848	3.4415	3.4808	3.4441	3.4777	**3.68**
H(4`B)	2.9200	2.9195	2.9111	2.9036	2.8805	2.9046	2.8870	2.9061	2.8833	2.9034	2.8420	2.8023	2.8053	2.7873	2.7873	2.7471	2.7887	2.7570	2.7907	2.7585	2.7866	2.7199	**2.88**
Nuclei	PBE0																						
H2	8.7681	8.6983	8.6797	8.5826	8.5885	8.5922	8.6077	8.6023	8.6333	8.5729	8.5672	8.7681	8.6983	8.6797	8.5826	8.5885	8.5922	8.6260	8.6023	8.6333	8.5729	8.5672	**8.07**
H3	7.3567	7.4986	7.5920	7.5425	7.6631	7.5408	7.6566	7.5389	7.6771	7.5437	7.7002	7.3567	7.4986	7.5920	7.5425	7.6631	7.5408	7.6879	7.5389	7.6771	7.5437	7.7002	**7.24**
H5	7.1816	7.3657	7.4557	7.4371	7.5642	7.4329	7.5602	7.4286	7.5753	7.4408	7.5952	7.1816	7.3657	7.4557	7.4371	7.5642	7.4328	7.5874	7.4286	7.5753	7.4408	7.5952	**7.24**
H6	8.0476	8.2582	8.3194	8.3440	8.4588	8.3395	8.5044	8.3347	8.5103	8.3473	8.5492	8.0476	8.2582	8.3194	8.3440	8.4588	8.3395	8.5351	8.3347	8.5103	8.3473	8.5492	**8.07**
H8	4.5684	4.6522	4.6899	4.6823	4.7431	4.6823	4.8286	4.6816	4.7923	4.6811	4.7822	4.5684	4.6522	4.6899	4.6823	4.7431	4.6823	4.8062	4.6816	4.7923	4.6811	4.7822	**5.24**
H(9A-9B)	1.7516	1.7990	1.7632	1.8043	1.8225	1.8030	1.8243	1.8028	1.8084	1.8062	1.8103	1.7516	1.7990	1.7632	1.8043	1.8225	1.8030	1.8158	1.8028	1.8084	1.8062	1.8103	**2.135**
H(10A-10B)	1.3175	1.2021	1.1663	1.1256	1.0654	1.1304	1.0642	1.1353	1.0841	1.1208	1.0561	1.3175	1.2021	1.1663	1.1256	1.0654	1.1305	1.0803	1.1353	1.0841	1.1208	1.0561	**1.275**
H(11A-11B)	0.9459	0.9690	0.9245	0.9804	0.9421	0.9792	0.9349	0.9781	0.9366	0.9815	0.9191	0.9459	0.9690	0.9246	0.9804	0.9421	0.9792	0.9372	0.9781	0.9366	0.9815	0.9191	**1.28**
H(12A-12B)	1.1988	1.1808	1.1562	1.1611	1.1218	1.1625	1.1180	1.1638	1.1316	1.1595	1.1225	1.1988	1.1808	1.1562	1.1611	1.1218	1.1625	1.1317	1.1637	1.1316	1.1595	1.1225	**1.285**
H(13A-13B)	1.1041	1.1059	1.0743	1.1103	1.0748	1.1097	1.0643	1.1092	1.0723	1.1107	1.0659	1.1041	1.1059	1.0743	1.1103	1.0748	1.1098	1.0737	1.1092	1.0723	1.1107	1.0659	**1.29**
H(14A-14B)	1.2633	1.2579	1.2366	1.2520	1.2200	1.2523	1.2099	1.2526	1.2256	1.2514	1.2206	1.2633	1.2579	1.2366	1.2520	1.2200	1.2523	1.2273	1.2526	1.2256	1.2514	1.2206	**1.295**
H(15A-15C)	0.9168	0.9124	0.8892	0.9087	0.8787	0.9089	0.8602	0.9091	0.8814	0.9083	0.8759	0.9168	0.9124	0.8892	0.9087	0.8787	0.9089	0.8830	0.9092	0.8814	0.9083	0.8759	**0.82**
H(1`A)	2.6659	2.6665	2.6456	2.6482	2.6026	2.6500	2.6231	2.6515	2.6203	2.6461	2.5870	2.7915	2.7807	2.7695	2.7694	2.7313	2.7697	2.7252	2.7528	2.7127	2.7689	2.7127	**3.82**
H(1`B)	3.1885	3.2257	3.2425	3.2467	3.2909	3.2455	3.2870	3.2442	3.2848	3.2474	3.2855	2.8709	2.6728	2.6797	2.6514	2.6707	2.6500	2.6189	2.6492	2.6167	2.6535	2.6221	**3.78**
H(2`A-2`B)	1.7045	1.7405	1.7093	1.7670	1.7237	1.7651	1.7212	1.7633	1.7342	1.7684	1.7528	1.5640	1.6413	1.6095	1.6899	1.6396	1.6869	1.6731	1.6836	1.6628	1.6924	1.7181	**2.26**
H(3`A-3`B)	1.5640	1.6412	1.6095	1.6899	1.6396	1.6869	1.6494	1.6836	1.6628	1.6924	1.7181	1.7045	1.7405	1.7093	1.7670	1.7237	1.7651	1.7412	1.7633	1.7342	1.7685	1.7528	**2.01**
H(4`A)	2.8709	2.6728	2.6797	2.6514	2.6707	2.6500	2.6493	2.6492	2.6167	2.6535	2.6221	3.1885	3.2257	3.2425	3.2467	3.2909	3.2454	3.2915	3.2442	3.2848	3.2474	3.2855	**3.68**
H(4`B)	2.7915	2.7807	2.7695	2.7694	2.7313	2.7697	2.7528	2.7702	2.7423	2.7689	2.7127	2.6659	2.6665	2.6456	2.6482	2.6026	2.6499	2.6220	2.6516	2.6203	2.6461	2.5870	**2.88**

[a] methyl protons shifts are averaged
[b] according to [7]

Table S7. Cont. VI

Nuclei	R											S										Exp. [b]
	TPSS																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
H2	8.5344	8.4605	8.4553	8.3885	8.3733	8.3942	8.4120	8.4002	8.2402	8.3828	8.3958	8.5344	8.4604	8.4553	8.3885	8.3733	8.3942	8.4231	8.4002	8.5104	8.3828	8.3958	**8.07**
H3	7.1653	7.3018	7.4016	7.3518	7.4739	7.3496	7.4691	7.3478	7.1836	7.3542	7.5105	7.1653	7.3018	7.4016	7.3518	7.4739	7.3496	7.4970	7.3478	7.4659	7.3542	7.5105	**7.24**
H5	6.9980	7.1744	7.2660	7.2508	7.3782	7.2462	7.3768	7.2421	7.0775	7.2556	7.4107	6.9980	7.1744	7.2660	7.2508	7.3782	7.2462	7.4001	7.2421	7.3610	7.2556	7.4107	**7.24**
H6	7.8602	8.0740	8.1335	8.1578	8.2718	8.1533	8.3177	8.1492	7.9882	8.1617	8.3602	7.8602	8.0740	8.1335	8.1578	8.2718	8.1533	8.3430	8.1492	8.2613	8.1617	8.3602	**8.07**
H8	4.7765	4.8553	4.8874	4.8990	4.9457	4.8983	5.0348	4.8975	4.7235	4.8988	4.9980	4.7765	4.8553	4.8874	4.8990	4.9457	4.8983	5.0032	4.8975	5.0340	4.8989	4.9980	**5.24**
H(9A-9B)	1.8183	1.8707	1.8513	1.8946	1.9166	1.8918	1.9239	1.8901	1.7040	1.8982	1.9375	1.8183	1.8707	1.8513	1.8946	1.9166	1.8918	1.9151	1.8901	2.0491	1.8982	1.9375	**2.135**
H(10A-10B)	1.3748	1.2619	1.2343	1.2042	1.1424	1.2083	1.1457	1.2131	1.0243	1.2006	1.1477	1.3748	1.2618	1.2343	1.2042	1.1424	1.2083	1.1568	1.2131	1.3772	1.2006	1.1477	**1.275**
H(11A-11B)	0.9969	1.0174	0.9836	1.0416	1.0066	1.0396	1.0017	1.0383	0.8488	1.0443	1.0000	0.9969	1.0173	0.9836	1.0416	1.0066	1.0396	1.0040	1.0383	1.2037	1.0443	1.0000	**1.28**
H(12A-12B)	1.2302	1.2141	1.1970	1.2044	1.1681	1.2053	1.1655	1.2069	1.0181	1.2037	1.1736	1.2302	1.2141	1.1970	1.2044	1.1681	1.2053	1.1769	1.2069	1.3711	1.2037	1.1736	**1.285**
H(13A-13B)	1.1404	1.1423	1.1191	1.1555	1.1238	1.1545	1.1137	1.1542	0.9652	1.1569	1.1193	1.1404	1.1423	1.1191	1.1555	1.1238	1.1545	1.1219	1.1542	1.3187	1.1569	1.1193	**1.29**
H(14A-14B)	1.2898	1.2864	1.2731	1.2876	1.2611	1.2878	1.2496	1.2885	1.1000	1.2878	1.2596	1.2898	1.2865	1.2731	1.2876	1.2611	1.2878	1.2652	1.2885	1.4520	1.2878	1.2596	**1.295**
H(15A-15C)	0.9257	0.9212	0.9047	0.9235	0.8975	0.9236	0.8774	0.9242	0.7342	0.9238	0.8927	0.9257	0.9212	0.9047	0.9235	0.8975	0.9236	0.8986	0.9242	1.0904	0.9238	0.8927	**0.82**
H(1`A)	2.7127	2.7178	2.7102	2.7102	2.6750	2.7111	2.6914	2.7125	2.6337	2.7096	2.6589	2.8260	2.8289	2.8263	2.8210	2.8000	2.8216	2.8003	2.8229	3.0758	2.8209	2.6589	**3.82**
H(1`B)	3.2909	3.3309	3.3545	3.3572	3.4044	3.3561	3.4007	3.3553	3.5656	3.3583	3.3932	3.0450	2.8239	2.8203	2.7747	2.8087	2.7755	2.7363	2.7776	2.7646	2.7759	3.3932	**3.78**
H(2`A-2`B)	1.7502	1.7958	1.7709	1.8300	1.7917	1.8280	1.7869	1.8265	1.6402	1.8324	1.8112	1.5908	1.6769	1.6541	1.7289	1.6875	1.7261	1.7151	1.7238	1.8840	1.7317	1.7516	**2.26**
H(3`A-3`B)	1.5908	1.6769	1.6541	1.7289	1.6875	1.7261	1.6900	1.7238	1.5370	1.7317	1.7516	1.7502	1.7959	1.7709	1.8300	1.7916	1.8280	1.8040	1.8265	1.9860	1.8324	1.8112	**2.01**
H(4`A)	3.0450	2.8239	2.8203	2.7747	2.8087	2.7755	2.7742	2.7776	2.7646	2.7758	2.7312	3.2909	3.3309	3.3545	3.3572	3.4044	3.3561	3.3969	3.3553	3.5656	3.3583	2.7312	**3.68**
H(4`B)	2.8260	2.8289	2.8263	2.8210	2.8000	2.8216	2.8091	2.8229	3.0758	2.8209	2.7679	2.7127	2.7178	2.7102	2.7102	2.6750	2.7111	2.6868	2.7125	2.6337	2.7096	2.7679	**2.88**
Nuclei	VSXC																						
H2	8.3988	8.3636	8.3860	8.3429	8.3459	8.3453	8.3826	8.3479	8.3995	8.3406	8.3943	8.3988	8.3636	8.3860	8.3429	8.3459	8.3453	8.4051	8.3479	8.3995	8.3406	8.3943	**8.07**
H3	7.2438	7.3807	7.4860	7.4142	7.5275	7.4117	7.5214	7.4094	7.5472	7.4165	7.5710	7.2437	7.3807	7.4860	7.4142	7.5275	7.4117	7.5553	7.4094	7.5472	7.4165	7.5710	**7.24**
H5	7.0522	7.2438	7.3088	7.3334	7.4452	7.3283	7.4462	7.3233	7.4560	7.3381	7.4816	7.0522	7.2438	7.3088	7.3334	7.4452	7.3283	7.4663	7.3233	7.4560	7.3381	7.4816	**7.24**
H6	8.0720	8.1953	8.2679	8.2596	8.3808	8.2563	8.4200	8.2532	8.3883	8.2629	8.4136	8.0720	8.1953	8.2679	8.2596	8.3808	8.2563	8.4001	8.2532	8.3883	8.2629	8.4136	**8.07**
H8	4.4372	4.5131	4.5324	4.5732	4.6373	4.5701	4.7152	4.5671	4.6645	4.5760	4.7037	4.4372	4.5131	4.5324	4.5732	4.6373	4.5701	4.6832	4.5671	4.6645	4.5760	4.7037	**5.24**
H(9A-9B)	2.0361	2.0457	2.1007	2.0505	2.0349	2.0484	2.0533	2.0466	2.0673	2.0528	2.0674	2.0361	2.0457	2.1007	2.0505	2.0349	2.0484	2.0773	2.0466	2.0673	2.0528	2.0674	**2.135**
H(10A-10B)	1.7784	1.6868	1.6612	1.6079	1.5394	1.6121	1.5186	1.6165	1.5390	1.6038	1.4950	1.7784	1.6868	1.6612	1.6079	1.5394	1.6121	1.5240	1.6165	1.5390	1.6038	1.4950	**1.275**
H(11A-11B)	1.4970	1.5023	1.4845	1.4801	1.4645	1.4815	1.4369	1.4830	1.4439	1.4788	1.4318	1.4970	1.5022	1.4845	1.4801	1.4645	1.4815	1.4325	1.4830	1.4439	1.4788	1.4318	**1.28**
H(12A-12B)	1.4833	1.4795	1.4536	1.4763	1.4203	1.4762	1.4270	1.4764	1.4444	1.4763	1.4483	1.4833	1.4795	1.4536	1.4763	1.4203	1.4762	1.4518	1.4764	1.4444	1.4763	1.4483	**1.285**
H(13A-13B)	1.4353	1.4394	1.4135	1.4443	1.4036	1.4436	1.3921	1.4432	1.4036	1.4448	1.4057	1.4353	1.4394	1.4135	1.4443	1.4036	1.4436	1.4042	1.4432	1.4036	1.4448	1.4057	**1.29**
H(14A-14B)	1.4717	1.4714	1.4430	1.4674	1.4283	1.4676	1.4186	1.4679	1.4322	1.4671	1.4322	1.4717	1.4713	1.4430	1.4674	1.4283	1.4676	1.4324	1.4680	1.4322	1.4671	1.4322	**1.295**
H(15A-15C)	1.0851	1.0821	1.0599	1.0800	1.0488	1.0800	1.0268	1.0802	1.0499	1.0799	1.0500	1.0851	1.0821	1.0599	1.0800	1.0488	1.0800	1.0487	1.0802	1.0499	1.0799	1.0500	**0.82**
H(1`A)	2.4739	2.5242	2.5459	2.5195	2.5150	2.5193	2.5065	2.5193	2.5103	2.5197	2.5107	2.9591	2.9754	2.9681	2.9692	2.9491	2.9699	2.9467	2.9707	2.9524	2.9686	2.9616	**3.82**
H(1`B)	3.3549	3.3780	3.4140	3.3893	3.4396	3.3883	3.4303	3.3875	3.4422	3.3902	3.4489	2.7107	2.6435	2.6243	2.6511	2.6400	2.6503	2.6487	2.6497	2.6412	2.6518	2.6682	**3.78**
H(2`A-2`B)	1.9376	1.9694	1.9490	1.9633	1.9355	1.9631	1.9217	1.9632	1.9355	1.9635	1.9424	2.0155	2.0509	2.0052	2.1050	2.0552	2.1022	2.0689	2.0994	2.0642	2.1076	2.0886	**2.26**
H(3`A-3`B)	2.0155	2.0509	2.0052	2.1050	2.0552	2.1022	2.0601	2.0994	2.0642	2.1076	2.0886	1.9376	1.9694	1.9490	1.9633	1.9355	1.9631	1.9323	1.9632	1.9355	1.9635	1.9424	**2.01**
H(4`A)	2.7107	2.6435	2.6243	2.6511	2.6400	2.6503	2.6260	2.6497	2.6412	2.6518	2.6682	3.3549	3.3780	3.4140	3.3893	3.4396	3.3883	3.4427	3.3875	3.4422	3.3902	3.4489	**3.68**
H(4`B)	2.9591	2.9754	2.9681	2.9692	2.9491	2.9699	2.9544	2.9707	2.9524	2.9686	2.9616	2.4739	2.5242	2.5459	2.5195	2.5150	2.5193	2.5061	2.5193	2.5103	2.5197	2.5107	**2.88**
Nuclei	wB97																						
H2	8.8640	8.7938	8.7724	8.6950	8.6604	8.7064	8.7098	8.7158	8.6221	8.6822	8.6045	8.8640	8.7938	8.7724	8.6950	8.6604	8.7064	8.6297	8.7158	8.6221	8.6822	8.6045	**8.07**
H3	7.4417	7.5762	7.6681	7.6190	7.7439	7.6167	7.7286	7.6142	7.7489	7.6212	7.7739	7.4416	7.5762	7.6681	7.6190	7.7439	7.6167	7.7566	7.6142	7.7489	7.6212	7.7739	**7.24**
H5	7.2983	7.4946	7.5901	7.5772	7.7114	7.5718	7.6975	7.5663	7.7118	7.5824	7.7409	7.2983	7.4946	7.5901	7.5772	7.7114	7.5718	7.7227	7.5663	7.7117	7.5824	7.7409	**7.24**
H6	8.1494	8.3316	8.3946	8.4104	8.5338	8.4085	8.5645	8.4056	8.5406	8.4113	8.5970	8.1494	8.3316	8.3946	8.4104	8.5337	8.4085	8.5654	8.4056	8.5406	8.4113	8.5970	**8.07**
H8	4.2038	4.2950	4.3535	4.3298	4.4371	4.3286	4.4900	4.3268	4.4695	4.3305	4.5006	4.2038	4.2949	4.3535	4.3298	4.4371	4.3286	4.4908	4.3268	4.4695	4.3305	4.5006	**5.24**
H(9A-9B)	1.7093	1.7342	1.6955	1.7645	1.7470	1.7629	1.7759	1.7612	1.6995	1.7657	1.7494	1.7093	1.7342	1.6955	1.7645	1.7470	1.7629	1.7066	1.7612	1.6995	1.7657	1.7493	**2.135**
H(10A-10B)	1.3372	1.2063	1.1725	1.1059	1.0455	1.1122	1.0403	1.1182	1.0640	1.0998	1.0543	1.3372	1.2064	1.1725	1.1059	1.0455	1.1123	1.0605	1.1182	1.0640	1.0998	1.0543	**1.275**
H(11A-11B)	0.9598	0.9683	0.9240	0.9796	0.9393	0.9787	0.9300	0.9778	0.9124	0.9805	0.9139	0.9598	0.9683	0.9240	0.9796	0.9393	0.9787	0.9137	0.9778	0.9124	0.9805	0.9139	**1.28**
H(12A-12B)	1.2118	1.1858	1.1641	1.1590	1.1261	1.1607	1.1137	1.1623	1.1290	1.1575	1.1259	1.2118	1.1858	1.1641	1.1590	1.1261	1.1606	1.1277	1.1623	1.1290	1.1575	1.1259	**1.285**
H(13A-13B)	1.1189	1.1154	1.0843	1.1183	1.0864	1.1178	1.0705	1.1174	1.0744	1.1187	1.0755	1.1189	1.1154	1.0843	1.1182	1.0864	1.1178	1.0748	1.1174	1.0745	1.1187	1.0755	**1.29**
H(14A-14B)	1.2522	1.2402	1.2213	1.2310	1.2052	1.2315	1.1878	1.2320	1.2067	1.2306	1.2060	1.2522	1.2402	1.2213	1.2310	1.2052	1.2315	1.2064	1.2319	1.2067	1.2306	1.2059	**1.295**
H(15A-15C)	0.9462	0.9415	0.9170	0.9372	0.9108	0.9373	0.8882	0.9374	0.9079	0.9371	0.9053	0.9462	0.9415	0.9170	0.9371	0.9108	0.9373	0.9078	0.9375	0.9079	0.9371	0.9053	**0.82**
H(1`A)	2.6200	2.6194	2.5974	2.6038	2.5658	2.6048	2.5825	2.6057	2.5759	2.6028	2.5496	2.7670	2.7640	2.7475	2.7515	2.7169	2.7516	2.7449	2.7518	2.7464	2.7518	2.7175	**3.82**
H(1`B)	3.0872	3.1201	3.1388	3.1409	3.1867	3.1396	3.1822	3.1380	3.1747	3.1420	3.1805	2.7305	2.5597	2.5819	2.5594	2.5927	2.5558	2.5743	2.5533	2.5790	2.5641	2.5750	**3.78**
H(2`A-2`B)	1.6835	1.7199	1.6886	1.7501	1.7148	1.7478	1.7063	1.7457	1.7198	1.7522	1.7457	1.5756	1.6498	1.6199	1.6950	1.6556	1.6915	1.6897	1.6881	1.6839	1.6986	1.7204	**2.26**
H(3`A-3`B)	1.5756	1.6498	1.6199	1.6950	1.6556	1.6915	1.6564	1.6881	1.6839	1.6986	1.7204	1.6835	1.7199	1.6886	1.7501	1.7147	1.7478	1.7253	1.7457	1.7198	1.7522	1.7456	**2.01**
H(4`A)	2.7305	2.5597	2.5819	2.5594	2.5927	2.5558	2.5617	2.5533	2.5790	2.5641	2.5750	3.0872	3.1200	3.1388	3.1409	3.1867	3.1396	3.1795	3.1380	3.1747	3.1420	3.1805	**3.68**
H(4`B)	2.7670	2.7640	2.7475	2.7515	2.7169	2.7516	2.7351	2.7518	2.7464	2.7518	2.7175	2.6199	2.6194	2.5974	2.6037	2.5658	2.6048	2.5766	2.6057	2.5759	2.6028	2.5496	**2.88**
Nuclei	wB97X																						
H2	8.8359	8.7674	8.7372	8.6493	8.6282	8.6649	8.6656	8.6764	8.5997	8.6342	8.5816	8.8359	8.7675	8.7372	8.6493	8.6282	8.6649	8.6122	8.6764	8.5996	8.6342	8.5816	**8.07**
H3	7.4161	7.5506	7.6418	7.5968	7.7182	7.5947	7.7064	7.5923	7.7239	7.5987	7.7502	7.4161	7.5506	7.6419	7.5968	7.7182	7.5947	7.7346	7.5923	7.7239	7.5987	7.7502	**7.24**
H5	7.2774	7.4724	7.5691	7.5618	7.6917	7.5567	7.6810	7.5516	7.6895	7.5665	7.7159	7.2774	7.4724	7.5691	7.5618	7.6917	7.5567	7.7033	7.5516	7.6895	7.5665	7.7159	**7.24**
H6	8.1156	8.3072	8.3717	8.3609	8.4893	8.3624	8.5165	8.3623	8.5000	8.3606	8.5574	8.1156	8.3072	8.3717	8.3609	8.4893	8.3625	8.5277	8.3623	8.5000	8.3605	8.5574	**8.07**
H8	4.3016	4.3950	4.4437	4.4142	4.5020	4.4138	4.5734	4.4135	4.5351	4.4150	4.5618	4.3016	4.3950	4.4437	4.4142	4.5020	4.4138	4.5588	4.4135	4.5351	4.4150	4.5618	**5.24**
H(9A-9B)	1.6953	1.7237	1.6844	1.7316	1.7266	1.7350	1.7408	1.7361	1.6842	1.7290	1.7289	1.6953	1.7237	1.6844	1.7316	1.7266	1.7350	1.6945	1.7361	1.6842	1.7290	1.7289	**2.135**
H(10A-10B)	1.3226	1.1982	1.1647	1.1086	1.0488	1.1151	1.0445	1.1214	1.0566	1.1029	1.0469	1.3226	1.1982	1.1647	1.1086	1.0488	1.1151	1.0563	1.1214	1.0566	1.1029	1.0469	**1.275**
H(11A-11B)	0.9574	0.9695	0.9246	0.9722	0.9341	0.9726	0.9218	0.9727	0.9126	0.9724	0.9161	0.9574	0.9695	0.9246	0.9722	0.9341	0.9726	0.9172	0.9727	0.9126	0.9724	0.9161	**1.28**
H(12A-12B)	1.2030	1.1788	1.1568	1.1540	1.1191	1.1557	1.1084	1.1574	1.1218	1.1528	1.1226	1.2031	1.1789	1.1568	1.1540	1.1191	1.1557	1.1236	1.1574	1.1218	1.1528	1.1226	**1.285**
H(13A-13B)	1.1145	1.1132	1.0807	1.1146	1.0810	1.1145	1.0664	1.1144	1.0700	1.1150	1.0716	1.1145	1.1132	1.0807	1.1146	1.0810	1.1145	1.0733	1.1144	1.0700	1.1150	1.0716	**1.29**
H(14A-14B)	1.2493	1.2390	1.2197	1.2311	1.2031	1.2315	1.1873	1.2320	1.2047	1.2309	1.2053	1.2493	1.2390	1.2197	1.2311	1.2031	1.2315	1.2072	1.2321	1.2047	1.2309	1.2052	**1.295**
H(15A-15C)	0.9401	0.9367	0.9111	0.9336	0.9049	0.9338	0.8836	0.9341	0.9011	0.9335	0.8986	0.9402	0.9367	0.9111	0.9336	0.9049	0.9338	0.9037	0.9341	0.9011	0.9335	0.8986	**0.82**
H(1`A)	2.6475	2.6473	2.6235	2.6282	2.5867	2.6300	2.6039	2.6317	2.6000	2.6268	2.5774	2.7857	2.7730	2.7577	2.7669	2.7299	2.7665	2.7549	2.7666	2.7542	2.7672	2.7273	**3.82**
H(1`B)	3.0968	3.1328	3.1511	3.1509	3.1938	3.1507	3.1906	3.1501	3.1857	3.1513	3.1923	2.7492	2.5754	2.5888	2.5733	2.6017	2.5684	2.5796	2.5654	2.5823	2.5780	2.5774	**3.78**
H(2`A-2`B)	1.6843	1.7247	1.6922	1.7506	1.7118	1.7491	1.7042	1.7476	1.7178	1.7524	1.7451	1.5751	1.6502	1.6210	1.6570	1.6965	1.6917	1.6929	1.6836	1.7045	1.7192	**2.26**
H(3`A-3`B)	1.5751	1.6502	1.6210	1.7006	1.6570	1.6965	1.6602	1.6929	1.6836	1.7045	1.7192	1.6842	1.7247	1.6922	1.7506	1.7118	1.7491	1.7259	1.7476	1.7178	1.7524	1.7451	**2.01**
H(4`A)	2.7492	2.5754	2.5888	2.5733	2.6017	2.5684	2.5750	2.5654	2.5823	2.5780	2.5774	3.0968	3.1328	3.1511	3.1509	3.1938	3.1507	3.1933	3.1501	3.1857	3.1513	3.1923	**3.68**
H(4`B)	2.7857	2.7730	2.7578	2.7669	2.7299	2.7666	2.7491	2.7666	2.7543	2.7672	2.7273	2.6475	2.6472	2.6235	2.6282	2.5868	2.6300	2.6032	2.6317	2.6000	2.6268	2.5774	**2.88**

[a] methyl protons shifts are averaged
[b] according to [7]

Table S7. Cont. VII

Nuclei	R											S											Exp. [b]
	X3LYP																						
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
H2	8.6923	8.5851	8.6120	8.4998	8.5204	8.5067	8.5248	8.5126	8.4234	8.4928	8.5420	8.6923	8.5851	8.6120	8.4998	8.5204	8.5067	8.4265	8.5126	8.4234	8.4928	8.5420	**8.07**
H3	7.3199	7.4577	7.5459	7.5018	7.6170	7.5000	7.6088	7.4977	7.6123	7.5034	7.6546	7.3199	7.4577	7.5459	7.5018	7.6170	7.5000	7.6198	7.4977	7.6124	7.5034	7.6546	**7.24**
H5	7.1428	7.3159	7.4091	7.3975	7.5161	7.3930	7.5127	7.3880	7.5496	7.4016	7.5534	7.1428	7.3159	7.4091	7.3975	7.5161	7.3930	7.5599	7.3880	7.5496	7.4016	7.5534	**7.24**
H6	7.9762	8.1754	8.2527	8.2676	8.3950	8.2630	8.4240	8.2577	8.3426	8.2715	8.4642	7.9762	8.1754	8.2527	8.2676	8.3950	8.2630	8.3637	8.2577	8.3426	8.2715	8.4642	**8.07**
H8	4.6192	4.7050	4.7349	4.7424	4.7934	4.7415	4.8878	4.7398	4.8024	4.7427	4.8221	4.6192	4.7050	4.7349	4.7424	4.7934	4.7415	4.8169	4.7398	4.8024	4.7427	4.8221	**5.24**
H(9A-9B)	1.7276	1.7609	1.7597	1.7860	1.8299	1.7838	1.8069	1.7813	1.6968	1.7884	1.8419	1.7276	1.7609	1.7597	1.7860	1.8299	1.7838	1.7055	1.7813	1.6968	1.7884	1.8419	**2.135**
H(10A-10B)	1.3436	1.2341	1.1966	1.1686	1.0964	1.1736	1.1028	1.1778	1.1301	1.1640	1.1146	1.3436	1.2341	1.1966	1.1686	1.0964	1.1736	1.1270	1.1778	1.1301	1.1640	1.1146	**1.275**
H(11A-11B)	0.9902	1.0107	0.9751	1.0328	0.9936	1.0313	0.9836	1.0294	0.9776	1.0343	0.9838	0.9902	1.0107	0.9751	1.0328	0.9936	1.0313	0.9783	1.0294	0.9776	1.0343	0.9838	**1.28**
H(12A-12B)	1.2402	1.2279	1.2024	1.2155	1.1705	1.2167	1.1693	1.2175	1.1906	1.2142	1.1771	1.2402	1.2279	1.2024	1.2155	1.1705	1.2167	1.1890	1.2175	1.1906	1.2142	1.1771	**1.285**
H(13A-13B)	1.1521	1.1562	1.1267	1.1672	1.1302	1.1666	1.1189	1.1655	1.1267	1.1678	1.1249	1.1521	1.1563	1.1267	1.1672	1.1302	1.1666	1.1266	1.1655	1.1267	1.1678	1.1249	**1.29**
H(14A-14B)	1.3115	1.3097	1.2896	1.3093	1.2758	1.3097	1.2648	1.3095	1.2866	1.3090	1.2770	1.3115	1.3097	1.2896	1.3093	1.2758	1.3097	1.2858	1.3095	1.2867	1.3090	1.2770	**1.295**
H(15A-15C)	0.9605	0.9568	0.9354	0.9584	0.9276	0.9585	0.9066	0.9582	0.9308	0.9582	0.9248	0.9605	0.9568	0.9355	0.9584	0.9276	0.9585	0.9300	0.9582	0.9308	0.9582	0.9248	**0.82**
H(1`A)	2.7415	2.7395	2.7170	2.7296	2.6807	2.7308	2.7002	2.7314	2.6945	2.7285	2.6685	2.8686	2.8553	2.8539	2.8395	2.8103	2.8403	2.8152	2.8407	2.8191	2.8389	2.7756	**3.82**
H(1`B)	3.2180	3.2580	3.2831	3.2902	3.3399	3.2885	3.3345	3.2863	3.3214	3.2918	3.3402	2.8731	2.7021	2.6790	2.6801	2.6954	2.6804	2.6835	2.6806	2.6852	2.6804	2.6419	**3.78**
H(2`A-2`B)	1.7378	1.7799	1.7420	1.8113	1.7596	1.8096	1.7593	1.8075	1.7689	1.8129	1.7855	1.5853	1.6737	1.6412	1.7272	1.6716	1.7240	1.7208	1.7203	1.7158	1.7302	1.7275	**2.26**
H(3`A-3`B)	1.5853	1.6737	1.6412	1.7272	1.6716	1.7240	1.6816	1.7203	1.7158	1.7302	1.7275	1.7378	1.7799	1.7420	1.8113	1.7596	1.8096	1.7730	1.8075	1.7689	1.8129	1.7855	**2.01**
H(4`A)	2.8731	2.7021	2.6790	2.6801	2.6954	2.6804	2.6773	2.6806	2.6852	2.6804	2.6419	3.2180	3.2580	3.2831	3.2902	3.3399	3.2885	3.3258	3.2863	3.3214	3.2918	3.3402	**3.68**
H(4`B)	2.8686	2.8553	2.8539	2.8395	2.8103	2.8403	2.8165	2.8407	2.8191	2.8389	2.7755	2.7415	2.7395	2.7170	2.7296	2.6807	2.7308	2.6939	2.7314	2.6946	2.7285	2.6685	**2.88**

[a] methyl protons shifts are averaged

[b] according to [7]

Table S8. Theoretical chemical shifts (in ppm) of *(R,S)*-3,5-difluoromethcathinone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S										Exp. [b]
	B3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	146.4677	146.9292	148.0988	147.6979	148.4736	147.6833	147.7806	147.6707	148.2614	147.7123	147.9596	145.1719	145.8243	146.9929	146.9594	148.1381	146.9613	148.5756	146.9602	148.3632	146.9530	148.5403	**136.1**
C2	118.2357	118.4415	119.2285	118.4740	119.0625	118.4789	119.5910	118.4837	119.5263	118.4676	119.6157	117.9173	118.1733	118.8888	118.3268	118.9778	118.3295	119.6312	118.3314	119.4749	118.3219	119.6136	**112.1**
C3	173.8901	174.1596	174.6988	174.1841	174.9250	174.1785	174.8915	174.1727	174.8780	174.1880	174.9444	173.8909	174.1647	174.7247	174.2315	174.9695	174.2248	174.9659	174.2180	174.9403	174.2361	175.0141	**162.6**
C4	113.3666	114.9502	115.5066	115.4999	116.1902	115.4557	117.1667	115.4109	116.8136	115.5401	117.3254	113.7037	115.0369	115.5638	115.3656	116.0247	115.3261	116.5833	115.2867	116.4317	115.4020	116.7917	**110.1**
C5	173.0985	173.7005	174.3084	173.9312	174.8307	173.9123	174.7786	173.8929	174.7050	173.9472	174.8439	173.3682	173.8541	174.3768	173.9601	174.7817	173.9440	174.6338	173.9278	174.6196	173.9740	174.7006	**162.5**
C6	116.2639	118.0937	119.0762	118.7843	120.6195	118.7221	121.0739	118.6593	120.7098	118.8407	121.3768	116.6165	118.6555	119.8320	119.3449	121.1227	119.2776	121.1635	119.2116	121.0566	119.4084	121.5448	**112.1**
C7	203.0400	208.1918	209.9625	211.4121	211.6927	211.2368	216.6248	211.0647	215.8909	211.5796	217.4578	207.8788	211.9529	213.2793	214.1274	214.9452	214.0189	220.0550	213.9076	218.8762	214.2254	220.4478	**194.5**
C8	65.7863	66.8618	67.6156	67.4306	68.1115	67.4068	68.7102	67.3819	68.6981	67.4507	69.4071	60.2985	61.8411	62.7739	63.1168	63.8414	63.0696	64.7521	63.0220	64.4420	63.1596	64.9809	**58.4**
C9	22.7168	22.9952	23.0739	23.0415	23.4528	23.0238	23.5512	23.0064	23.4437	23.0574	23.6823	19.3599	19.6571	19.9384	19.8480	20.1286	19.8299	20.1631	19.8126	20.0976	19.8645	20.5201	**15**
C8`	36.4011	37.2578	37.5459	37.6238	37.9821	37.6012	38.1346	37.5775	38.0714	37.6428	38.5413	31.9457	32.4408	32.5072	32.3536	32.6983	32.3345	32.7300	32.3154	32.7241	32.3704	32.8014	**30.6**
H2	7.9509	7.9079	7.9469	7.7980	7.9264	7.8011	7.9600	7.8041	7.9178	7.7946	7.9552	8.0159	7.9363	7.9537	7.7952	7.8738	7.7959	7.8128	7.7969	7.8288	7.7946	7.8284	**7.77**
H4	7.0566	7.2663	7.3996	7.3392	7.5222	7.3346	7.5629	7.3300	7.5412	7.3433	7.5859	7.0719	7.2685	7.3989	7.3290	7.5116	7.3250	7.5370	7.3209	7.5223	7.3326	7.5607	**7.71**
H6	7.4558	7.6869	7.7969	7.7595	7.9898	7.7522	8.0226	7.7448	7.9800	7.7662	8.0546	7.2829	7.4978	7.6339	7.5509	7.7952	7.5444	7.7655	7.5381	7.7586	7.5568	7.8162	**7.77**
H8	4.2675	4.3715	4.3854	4.4256	4.5217	4.4195	4.5442	4.4136	4.5179	4.4315	4.5673	4.3981	4.5613	4.6292	4.6357	4.7688	4.6310	4.7873	4.6263	4.7701	4.6399	4.8193	**5.21**
H(9A-9C)	1.3037	1.3032	1.2744	1.2674	1.2627	1.2682	1.2876	1.2688	1.2697	1.2664	1.3035	1.3822	1.4261	1.4103	1.4292	1.4110	1.4265	1.4041	1.4238	1.4015	1.4318	1.4343	**1.43**
H(8`A-8`C)	2.5005	2.4483	2.4213	2.4402	2.3951	2.4411	2.3865	2.4421	2.3958	2.4391	2.3719	2.9283	2.8026	2.7259	2.6969	2.6502	2.6998	2.5619	2.7027	2.5795	2.6942	2.5324	**2.58**
Nuclei	B3P86																						
C1	144.1660	144.4797	145.4429	144.8774	146.0553	144.8655	145.5049	144.8368	146.1053	144.9425	145.6123	143.1406	143.5737	144.8111	144.6471	145.7610	144.6639	145.8547	144.6578	145.8265	144.6747	145.9738	**136.1**
C2	117.1888	117.2869	118.0833	117.2508	117.9809	117.2729	118.5007	117.2740	118.5577	117.2762	118.5105	116.9546	117.1028	117.8952	117.2670	117.9437	117.2929	118.4927	117.2964	118.4581	117.2862	118.5197	**112.1**
C3	171.4614	171.7172	172.3130	171.7935	172.5569	171.8106	172.5150	171.8057	172.6070	171.8208	172.5919	171.4545	171.6953	172.3058	171.7939	172.5506	171.8099	172.5417	171.8041	172.6302	171.8227	172.6086	**162.6**
C4	112.6935	114.2631	114.9216	114.9543	115.6565	114.9348	116.6256	114.8930	116.3813	115.0160	116.8114	112.9577	114.3484	114.9712	114.7667	115.5303	114.7487	116.1670	114.7089	116.0943	114.8276	116.3590	**110.1**
C5	170.6396	171.2286	171.8606	171.5322	172.4184	171.5341	172.3812	171.5142	172.4223	171.5746	172.4697	170.8641	171.3394	171.9146	171.4849	172.3365	171.4886	172.1824	171.4706	172.2769	171.5255	172.2618	**162.5**
C6	115.1391	116.9725	118.0918	117.7875	119.5088	117.7611	119.8391	117.7107	119.6009	117.8524	120.2013	115.4610	117.4757	118.6570	118.2342	120.1056	118.1968	120.3513	118.1375	120.3252	118.3135	120.6914	**112.1**
C7	201.2424	205.9139	207.3479	208.5755	209.2297	208.4230	214.1956	208.2553	213.6177	208.7764	214.8811	205.4731	209.3552	210.7967	211.5125	212.2399	211.4135	216.8930	211.2924	215.8719	211.6489	217.3854	**194.5**
C8	64.2040	65.3664	66.1786	65.8597	66.6954	65.8541	67.1728	65.8252	67.2596	65.9068	67.9407	58.8166	60.1415	61.0329	61.3340	62.1120	61.3184	62.9127	61.2806	62.7586	61.3920	63.2267	**58.4**
C9	22.5143	22.8390	23.0810	22.9979	23.3784	23.0117	23.3286	23.0021	23.3230	23.0258	23.5336	19.2207	19.5615	19.8115	19.8253	20.1843	19.8395	20.2690	19.8308	20.3207	19.8571	20.6964	**15**
C8`	35.7833	36.5853	36.8683	36.9408	37.3138	36.9391	37.5076	36.9156	37.5815	36.9872	37.9639	31.1841	31.6716	31.7883	31.6040	31.9477	31.6036	32.0120	31.5817	32.0897	31.6487	32.0763	**30.6**
H2	7.9786	7.9412	7.9991	7.8711	7.9591	7.8776	7.9830	7.8818	7.9472	7.8653	7.9834	8.0190	7.9594	7.9790	7.8261	7.9101	7.8289	7.8714	7.8300	7.8893	7.8247	7.8757	**7.77**
H4	7.0496	7.2640	7.4025	7.3415	7.5279	7.3384	7.5689	7.3335	7.5532	7.3456	7.5929	7.0605	7.2639	7.4003	7.3291	7.5160	7.3262	7.5433	7.3215	7.5335	7.3329	7.5672	**7.71**
H6	7.4934	7.7155	7.8209	7.7953	8.0030	7.7918	8.0369	7.7864	8.0008	7.7997	8.0728	7.3080	7.5286	7.6680	7.5849	7.8409	7.5797	7.8294	7.5726	7.8251	7.5912	7.8753	**7.77**
H8	4.2911	4.3817	4.3832	4.4432	4.5173	4.4400	4.5561	4.4353	4.5396	4.4479	4.5755	4.4482	4.6057	4.6829	4.6830	4.8179	4.6795	4.8361	4.6742	4.8242	4.6875	4.8679	**5.21**
H(9A-9C)	1.3189	1.3286	1.3159	1.3066	1.2900	1.3098	1.2964	1.3108	1.2843	1.3042	1.3215	1.3944	1.4437	1.4215	1.4457	1.4327	1.4453	1.4410	1.4433	1.4431	1.4472	1.4705	**1.43**
H(8`A-8`C)	2.4791	2.4261	2.4038	2.4104	2.3732	2.4125	2.3542	2.4127	2.3706	2.4097	2.3422	2.8724	2.7513	2.6774	2.6438	2.6000	2.6476	2.5044	2.6496	2.5301	2.6416	2.4762	**2.58**
Nuclei	B3PW91																						
C1	144.4592	145.2078	145.9935	145.7239	147.0015	145.7191	145.9285	145.7072	146.3789	145.7326	146.3444	143.3662	143.8506	145.0132	145.0815	146.1621	145.0843	146.8130	145.0770	146.6448	145.0799	146.7877	**136.1**
C2	117.3307	117.5489	118.2475	117.5206	118.5354	117.5346	118.6517	117.5398	118.6043	117.5093	118.6949	117.0832	117.2591	117.9688	117.4343	118.1073	117.4441	118.6963	117.4446	118.5750	117.4271	118.7057	**112.1**
C3	171.5132	171.7956	172.3082	171.8477	172.9313	171.8494	172.5768	171.8421	172.5747	171.8482	172.6619	171.5364	171.8090	172.3416	171.9001	172.6567	171.9014	172.6539	171.8939	172.6430	171.9009	172.7272	**162.6**
C4	112.7108	114.2346	114.8779	114.8862	115.9273	114.8488	116.5867	114.8024	116.2602	114.9234	116.6946	112.9678	114.3785	114.9162	114.7374	115.5101	114.7065	115.9680	114.6669	115.8284	114.7684	116.2085	**110.1**
C5	170.7078	171.2992	171.8919	171.5720	172.7862	171.5603	172.4196	171.5395	172.3632	171.5850	172.4914	170.9345	171.4513	171.9527	171.5863	172.4462	171.5778	172.2691	171.5608	172.2700	171.5962	172.3650	**162.5**
C6	115.0871	116.8012	117.8678	117.5993	119.6959	117.5463	119.8014	117.4838	119.4710	117.6512	120.0586	115.4555	117.4808	118.5970	118.1662	119.9965	118.1103	119.9481	118.0458	119.8519	118.2219	120.3434	**112.1**
C7	201.4194	206.5504	208.0253	209.5367	210.1574	209.3785	214.7275	209.2146	213.9946	209.6915	215.6703	205.5779	209.6147	210.9505	211.8651	212.6209	211.7645	217.8155	211.6534	216.6474	211.9608	218.2041	**194.5**
C8	63.9919	65.2281	65.7920	65.7140	66.8128	65.6970	66.9647	65.6706	66.9471	65.7314	67.7902	58.7798	60.1105	60.9641	61.4005	62.0754	61.3592	63.0761	61.3092	62.7828	61.4417	63.3176	**58.4**
C9	22.2342	22.5003	22.5539	22.5857	23.3101	22.5760	23.0658	22.5577	22.9749	22.5973	23.2204	18.9613	19.2770	19.4721	19.5102	19.7921	19.4993	19.7986	19.4797	19.7485	19.5228	20.1855	**15**
C8`	35.7629	36.6018	36.8457	36.9870	37.6410	36.9718	37.4614	36.9478	37.4343	37.0029	37.8867	31.2201	31.7770	31.8162	31.6900	32.0674	31.6802	32.0347	31.6617	32.0352	31.7016	32.1307	**30.6**
H2	7.9465	7.8719	7.9441	7.7902	7.9161	7.7938	7.9414	7.7970	7.9062	7.7867	7.9115	7.9918	7.9331	7.9518	7.7857	7.8746	7.7877	7.7926	7.7895	7.8085	7.7840	7.8089	**7.77**
H4	7.0444	7.2542	7.3936	7.3330	7.5309	7.3290	7.5605	7.3247	7.5413	7.3370	7.5799	7.0574	7.2582	7.3929	7.3231	7.5082	7.3196	7.5345	7.3159	7.5214	7.3264	7.5573	**7.71**
H6	7.4717	7.6694	7.8034	7.7640	7.9880	7.7574	8.0207	7.7505	7.9831	7.7703	8.0372	7.2894	7.5101	7.6493	7.5623	7.8144	7.5567	7.7733	7.5508	7.7681	7.5679	7.8238	**7.77**
H8	4.2708	4.3565	4.3850	4.4296	4.5207	4.4242	4.5487	4.4186	4.5249	4.4352	4.5617	4.4224	4.5811	4.6535	4.6574	4.7923	4.6535	4.8078	4.6492	4.7939	4.6612	4.8399	**5.21**
H(9A-9C)	1.2804	1.2719	1.2534	1.2437	1.2527	1.2451	1.2572	1.2462	1.2421	1.2423	1.2686	1.3599	1.4063	1.3877	1.4070	1.3888	1.4051	1.3782	1.4029	1.3767	1.4091	1.4090	**1.43**
H(8`A-8`C)	2.4504	2.4051	2.3680	2.3871	2.3633	2.3888	2.3347	2.3902	2.3449	2.3856	2.3256	2.8413	2.7264	2.6509	2.6181	2.5764	2.6219	2.4793	2.6255	2.4999	2.6147	2.4510	**2.58**
Nuclei	B98																						
C1	145.2431	145.5980	146.7950	146.3977	147.2239	146.4086	146.5088	146.4181	147.0144	146.3917	146.6730	144.1542	144.6542	145.8254	145.8226	146.9890	145.8402	147.4686	145.8538	147.3092	145.8062	147.4307	**136.1**
C2	116.9915	117.1179	117.9091	117.1859	117.8073	117.2097	118.2952	117.2307	118.2607	117.1658	118.3202	116.7168	116.8872	117.5941	117.0412	117.7268	117.0618	118.3354	117.0796	118.2141	117.0232	118.3310	**112.1**
C3	171.3612	171.6009	172.1331	171.6672	172.4253	171.6789	172.3790	171.6878	172.3846	171.6586	172.4389	171.3851	171.6106	172.1649	171.7162	172.4760	171.7272	172.4651	171.7354	172.4603	171.7082	172.5217	**162.6**
C4	112.4441	113.9792	114.5487	114.5843	115.3250	114.5562	116.2656	114.5254	115.9370	114.6128	116.4350	112.6999	114.0387	114.5880	114.4269	115.1536	114.4048	115.6603	114.3803	115.5245	114.4504	115.8801	**110.1**
C5	170.6107	171.1556	171.7356	171.4091	172.3104	171.4076	172.2359	171.4036	172.1912	171.4127	172.3156	170.8199	171.2728	171.7973	171.4455	172.2870	171.4471	172.1421	171.4462	172.1445	171.4464	172.2188	**162.5**
C6	115.1035	116.8800	117.8041	117.5537	119.3779	117.5086	119.7883	117.4605	119.4619	117.5980	120.1077	115.4563	117.3985	118.5192	118.0815	119.8712	118.0331	119.8560	117.9829	119.7633	118.1306	120.2467	**112.1**
C7	199.6940	204.6260	206.4252	207.8938	208.1597	207.7477	213.1306	207.6003	212.4048	208.0376	213.9202	203.9754	208.0267	209.4013	210.3396	211.1517	210.2463	216.3829	210.1489	215.2059	210.4288	216.7846	**194.5**
C8	65.6127	66.6919	67.4152	67.2716	67.9782	67.2638	68.5429	67.2525	68.5500	67.2808	69.2417	60.4790	61.8152	62.6691	63.0463	63.7590	63.0172	64.6701	62.9853	64.3898	63.0757	64.8913	**58.4**
C9	22.9777	23.2841	23.3017	23.3293	23.7525	23.3292	23.8171	23.3269	23.7341	23.3316	23.9675	19.7846	20.0685	20.2914	20.2802	20.5401	20.2810	20.5315	20.2795	20.4854	20.2816	20.8848	**15**
C8`	36.5987	37.3601	37.6605	37.7622	38.1220	37.7564	38.2519	37.7478	38.2238	37.7697	38.6612	32.0510	32.4888	32.5522	32.4601	32.8095	32.4597	32.8534	32.4570	32.8663	32.4630	32.9323	**30.6**
H2	7.9554	7.9125	7.9530	7.8065	7.9316	7.8092	7.9690	7.8119	7.9301	7.8040	7.9629	8.0028	7.9321	7.9532	7.7901	7.8731	7.7915	7.8110	7.7931	7.8271	7.7892	7.8264	**7.77**
H4	7.0511	7.2646	7.4038	7.3423	7.5295	7.3379	7.5718	7.3335	7.5526	7.3467	7.5935	7.0634	7.2646	7.4028	7.3312	7.5185	7.3274	7.5453	7.3236	7.5327	7.3351	7.5674	**7.71**
H6	7.4491	7.6755	7.7918	7.7533	7.9836	7.7462	8.0188	7.7392	7.9806	7.7603	8.0497	7.2724	7.4928	7.6349	7.5483	7.7990	7.5422	7.7725	7.5363	7.7658	7.5544	7.8214	**7.77**
H8	4.2495	4.3497	4.3666	4.4112	4.5056	4.4055	4.5336	4.4001	4.5108	4.4172	4.5540	4.3937	4.5607	4.6374	4.6394	4.7756	4.6351	4.7917	4.6308	4.7776	4.6438	4.8206	**5.21**
H(9A-9C)	1.3064	1.3078	1.2759	1.2671	1.2609	1.2678	1.2863	1.2685	1.2718	1.2665	1.3019	1.3874	1.4304	1.4109	1.4276	1.4088	1.4253	1.3976	1.4230	1.3968	1.4303	1.4263	**1.43**
H(8`A-8`C)	2.4759	2.4262	2.4014	2.4176	2.3734	2.4189	2.3654	2.4204	2.3768	2.4165	2.3488	2.8759	2.7574	2.6855	2.6540	2.6107	2.6571	2.5201	2.6605	2.5391	2.6513	2.4889	**2.58**

[a] methyl protons shifts are averaged

[b] according to [8]

Table S8. Cont. I

Nuclei	R											S										Exp. [b]
	B971											B971										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	144.7908	145.1093	146.3417	145.9190	146.7460	145.9246	146.1038	145.9281	146.5947	145.9188	146.2517	143.7231	144.2297	145.3982	145.3717	146.5184	145.3816	146.9613	145.3899	146.6704	145.3670	146.9021	**136.1**
C2	116.7182	116.8200	117.6086	116.8908	117.4976	116.9070	117.9891	116.9219	117.9558	116.8814	118.0112	116.4392	116.6069	117.2999	116.7533	117.4193	116.7665	118.0110	116.7787	117.8707	116.7465	118.0089	**112.1**
C3	171.2626	171.5182	172.0500	171.5966	172.3488	171.6000	172.3020	171.6029	172.3033	171.5993	172.3670	171.2881	171.5208	172.0750	171.6321	172.3860	171.6350	172.3728	171.6373	172.3660	171.6354	172.4332	**162.6**
C4	112.2224	113.7518	114.3155	114.3799	115.1007	114.3436	116.0188	114.3069	115.6983	114.4203	116.1951	112.4728	113.8137	114.3596	114.2176	114.9344	114.1873	115.4543	114.1563	115.3506	114.2526	115.6843	**110.1**
C5	170.4955	171.0524	171.6296	171.3271	172.2176	171.3169	172.1396	171.3062	172.0959	171.3428	172.2276	170.6965	171.1633	171.6896	171.3509	172.1897	171.3436	172.0494	171.3361	172.0515	171.3639	172.1303	**162.5**
C6	114.8922	116.6615	117.5659	117.3309	119.1494	117.2771	119.5178	117.2234	119.2033	117.3882	119.8532	115.2149	117.1499	118.2656	117.8768	119.6626	117.8203	119.6607	117.7636	119.6298	117.9365	120.0793	**112.1**
C7	199.5894	204.4154	206.2513	207.6529	207.9480	207.5030	212.8864	207.3513	212.1825	207.8003	213.6578	203.8543	207.8620	209.2559	210.1489	210.9593	210.0463	216.1016	209.9424	214.8453	210.2518	216.4761	**194.5**
C8	65.5762	66.6481	67.3645	67.1942	67.9166	67.1783	68.4640	67.1609	68.4666	67.2145	69.1705	60.4393	61.7639	62.5905	62.9625	63.6824	62.9274	64.5187	62.8912	64.2085	63.0012	64.7482	**58.4**
C9	22.9853	23.2974	23.3010	23.3515	23.7733	23.3449	23.8047	23.3383	23.7195	23.3645	23.9697	19.8190	20.1285	20.3131	20.3366	20.5942	20.3311	20.5734	20.3247	20.5386	20.3479	20.9544	**15**
C8`	36.6012	37.3492	37.6400	37.7561	38.0902	37.7416	38.2237	37.7265	38.1980	37.7754	38.6405	31.9953	32.4301	32.4867	32.3980	32.7264	32.3887	32.7809	32.3794	32.8055	32.4132	32.8620	**30.6**
H2	7.9539	7.9146	7.9531	7.8123	7.9347	7.8145	7.9671	7.8168	7.9300	7.8107	7.9621	7.9991	7.9313	7.9504	7.7906	7.8731	7.7917	7.8134	7.7931	7.8414	7.7901	7.8310	**7.77**
H4	7.0456	7.2571	7.3968	7.3361	7.5220	7.3315	7.5629	7.3269	7.5442	7.3407	7.5844	7.0581	7.2584	7.3958	7.3249	7.5109	7.3209	7.5379	7.3169	7.5260	7.3291	7.5599	**7.71**
H6	7.4531	7.6745	7.7878	7.7523	7.9803	7.7450	8.0129	7.7380	7.9760	7.7596	8.0444	7.2715	7.4906	7.6316	7.5491	7.8001	7.5425	7.7770	7.5361	7.7763	7.5558	7.8280	**7.77**
H8	4.2479	4.3439	4.3620	4.4093	4.5006	4.4038	4.5285	4.3985	4.5075	4.4150	4.5475	4.3980	4.5632	4.6392	4.6411	4.7758	4.6366	4.7954	4.6321	4.7814	4.6459	4.8239	**5.21**
H(9A-9C)	1.3073	1.3119	1.2785	1.2700	1.2649	1.2704	1.2855	1.2709	1.2716	1.2701	1.3028	1.3907	1.4321	1.4117	1.4321	1.4137	1.4296	1.4018	1.4272	1.4073	1.4349	1.4330	**1.43**
H(8`A-8`C)	2.4734	2.4226	2.3973	2.4131	2.3686	2.4142	2.3595	2.4154	2.3710	2.4124	2.3429	2.8697	2.7511	2.6789	2.6470	2.6044	2.6497	2.5157	2.6526	2.5369	2.6450	2.4840	**2.58**
Nuclei	B972											B972											
C1	141.8439	142.8654	143.1956	143.0833	144.1751	143.0638	143.9325	143.0439	143.6594	143.1008	144.1551	140.6755	141.1808	142.3711	142.5940	143.5923	142.5645	144.3190	142.5363	144.7296	142.6256	144.3994	**136.1**
C2	114.9470	115.1874	115.8039	115.1402	115.8049	115.1464	116.2043	115.1500	116.1383	115.1305	116.2403	114.6936	114.8345	115.5573	115.0816	115.7095	115.0796	116.2393	115.0757	116.1568	115.0802	116.2656	**112.1**
C3	168.2354	168.4487	168.9790	168.5864	169.2875	168.5793	169.2747	168.5699	169.2536	168.5889	169.3570	168.2697	168.4906	169.0340	168.6546	169.3476	168.6474	169.3309	168.6378	169.3265	168.6576	169.4098	**162.6**
C4	110.2761	111.6462	112.3831	112.4020	113.0320	112.3592	113.7895	112.3135	113.6999	112.4377	113.9584	110.5291	111.8474	112.3834	112.2213	112.9342	112.1896	113.3018	112.1543	112.9880	112.2447	113.5098	**110.1**
C5	167.4761	167.9585	168.5759	168.2716	169.1049	168.2552	168.9765	168.2362	168.9946	168.2821	169.0703	167.7028	168.1692	168.6883	168.3809	169.1709	168.3660	168.9739	168.3480	168.9279	168.3903	169.0750	**162.5**
C6	112.6701	114.1657	115.3979	115.1558	116.7553	115.0985	116.9985	115.0384	116.9119	115.2047	117.2955	113.0675	114.9703	116.0492	115.6347	117.3656	115.5827	117.2613	115.5267	116.9661	115.6770	117.5938	**112.1**
C7	197.4999	202.8944	203.8939	205.5273	205.9613	205.3584	211.1350	205.1890	209.8629	205.6872	211.9595	201.4696	205.4837	206.8409	207.8610	208.5232	207.7389	213.6605	207.6153	212.8596	207.9752	214.1411	**194.5**
C8	62.7349	63.9221	64.3656	64.4061	65.1057	64.3834	65.8092	64.3576	65.5035	64.4226	66.4974	57.7428	58.9731	59.8460	60.3582	60.9534	60.3032	62.0355	60.2478	62.0271	60.4098	62.2889	**58.4**
C9	21.9310	22.0409	22.2645	22.3171	22.6537	22.2988	22.6494	22.2782	22.6406	22.3302	22.8106	18.7661	18.9404	19.1733	19.2028	19.4546	19.1883	19.4725	19.1717	19.4320	19.2125	19.8083	**15**
C8`	35.5496	36.3363	36.5462	36.7280	37.0369	36.7090	37.1429	36.6870	37.1188	36.7414	37.5449	31.1103	31.6217	31.6970	31.6065	31.9556	31.5929	31.8398	31.5762	31.7355	31.6135	31.9205	**30.6**
H2	7.9209	7.8097	7.9281	7.7663	7.8571	7.7699	7.8452	7.7730	7.8812	7.7626	7.8379	7.9746	7.9072	7.9237	7.7502	7.8423	7.7540	7.7507	7.7572	7.7175	7.7457	7.7588	**7.77**
H4	7.0439	7.2494	7.3897	7.3322	7.5095	7.3276	7.5474	7.3228	7.5364	7.3363	7.5692	7.0587	7.2567	7.3900	7.3226	7.5036	7.3188	7.5267	7.3147	7.5080	7.3260	7.5491	**7.71**
H6	7.4491	7.6326	7.7901	7.7452	7.9493	7.7385	7.9561	7.7316	7.9657	7.7513	7.9864	7.2702	7.4888	7.6217	7.5390	7.7831	7.5341	7.7375	7.5287	7.7044	7.5432	7.7808	**7.77**
H8	4.2386	4.3183	4.3640	4.4014	4.4813	4.3949	4.4923	4.3885	4.4986	4.4076	4.5152	4.3860	4.5444	4.6100	4.6159	4.7492	4.6117	4.7586	4.6071	4.7357	4.6198	4.7886	**5.21**
H(9A-9C)	1.2591	1.2359	1.2374	1.2289	1.2091	1.2300	1.2221	1.2309	1.2235	1.2276	1.2364	1.3458	1.3850	1.3673	1.3874	1.3669	1.3857	1.3581	1.3839	1.3441	1.3886	1.3823	**1.43**
H(8`A-8`C)	2.4434	2.4060	2.3644	2.3902	2.3509	2.3910	2.3540	2.3916	2.3470	2.3894	2.3383	2.8346	2.7236	2.6516	2.6205	2.5775	2.6242	2.4780	2.6276	2.4784	2.6165	2.4472	**2.58**
Nuclei	BHandH											BHandH											
C1	146.7064	146.8721	147.2928	146.8977	148.0630	146.8813	146.9542	146.8840	147.0552	146.8842	147.1233	145.9642	146.2100	147.4073	146.9364	147.6805	146.9319	147.9625	146.9439	148.1084	146.9088	148.1326	**136.1**
C2	119.9100	119.9902	120.6706	119.8826	120.6318	119.8801	121.0134	119.8961	120.9247	119.8547	121.0659	119.6804	119.8548	120.6824	119.9626	120.7067	119.9596	121.2208	119.9742	121.1200	119.9351	121.2628	**112.1**
C3	172.2567	172.3929	172.8671	172.4554	173.0529	172.4410	173.0058	172.4449	173.0124	172.4392	173.0805	172.2586	172.3753	172.9182	172.4783	173.2224	172.4641	173.0850	172.4684	173.1016	172.4615	173.1634	**162.6**
C4	114.9759	116.6253	117.4413	117.4281	118.1524	117.3708	119.2122	117.3318	118.9792	117.4522	119.4304	115.1761	116.7063	117.4027	117.2929	118.0370	117.2369	118.7856	117.1995	118.5670	117.3164	118.9966	**110.1**
C5	171.2234	171.7595	172.3061	172.0950	172.7920	172.0630	172.7565	172.0494	172.7490	172.0957	172.8671	171.3805	171.8197	172.3516	172.0549	172.7990	172.0260	172.6367	172.0159	172.6366	172.0526	172.7433	**162.5**
C6	118.0817	120.0847	121.5048	121.0732	122.9831	121.0051	123.5080	120.9549	123.3004	121.1074	123.8619	118.3488	120.5725	121.7374	121.5071	122.2512	121.4335	123.7351	121.3783	123.5374	121.5472	124.0530	**112.1**
C7	202.7549	207.4807	208.5761	209.8995	210.5153	209.7392	215.1259	209.5972	214.0518	210.0219	215.9636	206.9694	210.8941	212.5542	213.0323	213.7764	212.8968	218.5207	212.7790	217.5757	213.1303	219.1415	**194.5**
C8	60.4789	61.6908	62.3385	62.1804	63.0803	62.1429	63.5213	62.1233	63.3957	62.1857	64.2664	54.6338	55.8086	56.5061	56.6895	57.4336	56.6501	58.0980	56.6282	57.9527	56.6959	58.4204	**58.4**
C9	22.0369	22.3206	22.6715	22.5066	23.0416	22.4845	22.9913	22.4810	22.9733	22.4980	23.1296	18.6708	18.9972	19.1888	19.2223	19.9664	19.2063	19.6216	19.2083	19.5967	19.2076	20.0390	**15**
C8`	33.6317	34.3952	34.6480	34.8072	35.1457	34.7713	35.3476	34.7537	35.3224	34.8108	35.8572	28.4775	29.0384	29.2076	29.1366	29.8807	29.0972	29.5714	29.0769	29.5099	29.1448	29.6949	**30.6**
H2	8.2482	8.1975	8.2915	8.1550	8.2278	8.1590	8.2797	8.1621	8.2848	8.1522	8.2777	8.2682	8.2009	8.2173	8.0945	8.0133	8.0967	8.1337	8.0983	8.1284	8.0935	8.1332	**7.77**
H4	7.1939	7.4165	7.5628	7.5004	7.6920	7.4966	7.7381	7.4920	7.7211	7.5049	7.7628	7.2009	7.4137	7.5595	7.4886	7.4074	7.4851	7.7155	7.4806	7.7001	7.4930	7.7396	**7.71**
H6	7.6590	7.8848	8.0543	7.9916	8.2135	7.9862	8.2796	7.9800	8.2645	7.9977	8.3180	7.4772	7.7169	7.8518	7.7932	7.7120	7.7870	8.0555	7.7800	8.0344	7.8002	8.0990	**7.77**
H8	4.0534	4.1514	4.1898	4.2256	4.2878	4.2212	4.3484	4.2162	4.3361	4.2309	4.3713	4.3154	4.4796	4.5678	4.5630	4.4818	4.5586	4.7339	4.5534	4.7180	4.5683	4.7644	**5.21**
H(9A-9C)	1.3835	1.3943	1.3965	1.3879	1.3775	1.3896	1.4024	1.3904	1.4000	1.3873	1.4191	1.4655	1.5053	1.4605	1.5036	1.4224	1.5031	1.4851	1.5017	1.4773	1.5052	1.5066	**1.43**
H(8`A-8`C)	2.5330	2.4697	2.4177	2.4412	2.4156	2.4434	2.3734	2.4449	2.3715	2.4401	2.3582	2.8714	2.7371	2.6691	2.6377	2.5565	2.6409	2.4994	2.6433	2.5150	2.6360	2.4756	**2.58**
Nuclei	BHandHLYP											BHandHLYP											
C1	147.0971	147.2298	147.5497	147.9509	148.7783	147.9374	147.8318	147.6746	148.4558	147.9583	147.9533	146.0335	146.3909	147.4660	147.4217	148.4707	147.4315	148.7285	147.4424	148.5924	147.4106	148.7594	**136.1**
C2	119.5227	119.6680	120.3645	119.7178	120.3946	119.7218	120.8936	119.6850	120.8465	119.7126	120.9314	119.2874	119.5095	120.2517	119.6599	120.3547	119.6635	120.8804	119.6691	120.7781	119.6560	120.9149	**112.1**
C3	172.0357	172.0965	172.5046	172.1449	172.7200	172.1441	172.6262	172.1415	172.6767	172.1453	172.6940	172.0160	172.0722	172.5389	172.1617	172.7395	172.1606	172.7333	172.1617	172.7419	172.1625	172.7915	**162.6**
C4	114.2460	115.7960	116.5442	116.4361	117.1432	116.3942	118.1497	116.3910	117.7942	116.4760	118.3346	114.5222	115.8680	116.4472	116.2796	117.0009	116.2395	117.5558	116.2020	117.4273	116.3174	117.7716	**110.1**
C5	171.1374	171.5666	172.0569	171.8620	172.5659	171.8447	172.4706	171.8198	172.4596	171.8780	172.5571	171.2862	171.6155	172.0672	171.7872	172.4725	171.7739	172.3182	171.7633	172.3367	171.7998	172.4002	**162.5**
C6	117.3272	119.2703	120.5898	119.9846	121.8171	119.9249	122.2865	119.9810	121.9118	120.0429	122.6318	117.6757	119.7621	120.9231	120.5248	122.3432	120.4555	122.3658	120.3887	122.2931	120.5904	122.7478	**112.1**
C7	201.0448	206.1473	207.1844	209.5334	209.7078	209.3518	215.1195	208.8831	214.3153	209.7002	215.9252	205.5713	209.7144	211.0502	212.0244	212.6582	211.9099	218.2110	211.7969	216.9179	212.1326	218.7267	**194.5**
C8	61.2366	62.2261	62.8487	62.7281	63.4265	62.7023	63.8920	62.6593	63.9175	62.7503	64.5689	56.0892	57.3845	58.1792	58.5311	59.1898	58.4930	59.9860	58.4565	59.7307	58.5660	60.2602	**58.4**
C9	21.8618	22.0458	22.3029	22.0300	22.4413	22.0232	22.3578	22.0945	22.3095	22.0386	22.5029	18.6877	18.7881	18.9723	18.9484	19.1985	18.9403	19.1018	18.9340	19.0958	18.9554	19.4121	**15**
C8`	34.6600	35.4024	35.6884	35.8401	36.1743	35.8143	36.3317	35.7719	36.3122	35.8629	36.7499	30.4097	30.8430	30.9567	30.8479	31.2009	30.8274	31.2358	30.8099	31.2481	30.8677	31.3427	**30.6**
H2	8.1616	8.1166	8.2260	8.0090	8.1249	8.0131	8.1718	8.0399	8.1232	8.0055	8.1680	8.2094	8.1272	8.1512	7.9911	8.0749	7.9919	8.0109	7.9928	8.0299	7.9904	8.0210	**7.77**
H4	7.2191	7.4319	7.5736	7.5113	7.6944	7.5070	7.7432	7.5029	7.7211	7.5152	7.7653	7.2298	7.4303	7.5656	7.4969	7.6803	7.4930	7.7122	7.4889	7.6979	7.5005	7.7347	**7.71**
H6	7.5433	7.7826	7.9395	7.8725	8.0978	7.8654	8.1474	7.8646	8.1024	7.8793	8.1810	7.4025	7.6306	7.7763	7.6978	7.9515	7.6910	7.9310	7.6841	7.9240	7.7044	7.9778	**7.77**
H8	3.9839	4.1060	4.1399	4.1860	4.2819	4.1802	4.3259	4.1728	4.2989	4.1917	4.3440	4.1684	4.3384	4.4123	4.4170	4.5523	4.4122	4.5784	4.4074	4.5609	4.4215	4.6056	**5.21**
H(9A-9C)	1.2824	1.2858	1.2917	1.2441	1.2347	1.2456	1.2585	1.2613	1.2390	1.2430	1.2754	1.3564	1.3944	1.3718	1.3949	1.3723	1.3927	1.3657	1.3903	1.3658	1.3970	1.3897	**1.43**
H(8`A-8`C)	2.4352	2.3896	2.3432	2.3810	2.3361	2.3820	2.3282	2.3819	2.3409	2.3800	2.3164	2.8350	2.7097	2.6385	2.6113	2.5658	2.6140	2.4840	2.6167	2.5034	2.6089	2.4560	**2.58**

[a] methyl protons shifts are averaged

[b] according to [8]

Table S8. Cont. II

Nuclei	R											S										Exp. [b]
	BLYP											BLYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	145.7481	146.8706	147.3418	147.0888	147.9633	147.3352	147.2820	147.1276	147.7789	147.4947	147.5994	144.0788	144.8979	146.2644	146.1471	147.7877	146.4160	147.8386	146.2215	147.8771	146.5178	147.9227	**136.1**
C2	116.4574	116.7505	117.2905	116.6437	117.2313	116.9289	117.5743	116.7529	117.7128	117.0012	117.7019	115.9818	116.2054	116.9121	116.4173	117.1907	116.6996	117.6546	116.5197	117.7062	116.7762	117.7244	**112.1**
C3	175.3583	175.6542	176.2566	175.7443	176.7032	176.0181	176.4713	175.8298	176.6457	176.1111	176.6223	175.3884	175.7148	176.3291	175.8216	176.7719	176.0936	176.5261	175.9035	176.7097	176.1904	176.6780	**162.6**
C4	112.0104	113.3624	113.9696	114.0411	114.7335	114.2805	115.4764	114.0571	115.3784	114.4393	115.7255	112.4719	113.6058	114.0369	113.9156	114.5243	114.1606	114.9126	113.9436	114.9654	114.3100	115.2086	**110.1**
C5	174.6266	175.2069	175.9037	175.4811	176.6205	175.7455	176.3533	175.5468	176.4868	175.8551	176.5106	175.0554	175.5021	176.0823	175.6082	176.6294	175.8717	176.2473	175.6732	176.4509	175.9849	176.4108	**162.5**
C6	114.7550	116.2176	117.3879	117.1399	119.0051	117.3672	119.2124	117.1298	119.1127	117.5462	119.6123	115.1558	117.0394	118.0233	117.7093	119.3599	117.9323	119.3263	117.6933	119.3849	118.1247	119.7777	**112.1**
C7	203.7110	209.1298	210.3612	211.7992	212.3368	211.8863	216.6956	211.5228	216.1393	212.3623	217.6394	209.0453	212.6434	214.2845	214.7480	216.1069	214.9130	220.3152	214.6147	219.5577	215.2168	220.7642	**194.5**
C8	69.7611	71.0057	71.5907	71.4206	72.2656	71.6796	72.6969	71.4758	72.8563	71.8008	73.5243	63.7226	65.7810	66.6301	67.1532	68.0268	67.3851	68.7420	67.1549	68.6250	67.5601	69.0623	**58.4**
C9	23.5482	23.7279	23.9360	23.9672	24.4435	24.2302	24.4467	24.0298	24.5339	24.3418	24.6971	20.0053	20.5233	20.7078	20.7866	21.0712	21.0526	21.0558	20.8572	21.1539	21.1613	21.5792	**15**
C8`	38.1020	38.9152	39.1223	39.2641	39.7206	39.5239	39.6339	39.3218	39.7846	39.6453	40.1395	33.5181	33.8937	33.9448	33.8367	34.2271	34.0980	34.0487	33.8976	34.2564	34.2155	34.1800	**30.6**
H2	7.7531	7.6581	7.7617	7.6106	7.7383	7.6627	7.9305	7.6216	7.7414	7.6604	7.9364	7.8508	7.7603	7.7641	7.6200	7.6750	7.6694	7.8109	7.6264	7.6568	7.6735	7.8356	**7.77**
H4	6.9112	7.1081	7.2442	7.1837	7.3660	7.2268	7.5731	7.1774	7.3888	7.2431	7.6067	6.9350	7.1191	7.2495	7.1764	7.3586	7.2202	7.5510	7.1714	7.3725	7.2351	7.5854	**7.71**
H6	7.3448	7.5275	7.6783	7.6355	7.8663	7.6765	8.0600	7.6248	7.8603	7.6967	8.1010	7.1617	7.3501	7.4740	7.3959	7.6214	7.4379	7.7712	7.3873	7.5975	7.4563	7.8297	**7.77**
H8	4.4798	4.5331	4.5649	4.5980	4.6856	4.6398	4.8698	4.5893	4.6804	4.6591	4.9043	4.5619	4.7117	4.7798	4.7860	4.9186	4.8294	5.1022	4.7801	4.9212	4.8452	5.1465	**5.21**
H(9A-9C)	1.3278	1.3077	1.3070	1.2962	1.2951	1.3455	1.4884	1.3018	1.3117	1.3491	1.5150	1.4064	1.4581	1.4321	1.4644	1.4361	1.5100	1.6147	1.4633	1.4427	1.5213	1.6575	**1.43**
H(8`A-8`C)	2.5630	2.5162	2.4786	2.4920	2.4524	2.5408	2.6127	2.4971	2.4539	2.5459	2.6061	3.0206	2.8759	2.8075	2.7694	2.7262	2.8200	2.8068	2.7782	2.6641	2.8216	2.7859	**2.58**
Nuclei	BMK											BMK										
C1	162.7315	162.6727	163.4322	162.8365	164.3766	162.8053	163.3756	162.9856	163.0232	163.0268	163.6289	161.8248	162.1219	163.4819	163.3052	164.6111	163.2831	164.5881	163.4722	164.3198	163.4875	164.6967	**136.1**
C2	130.9957	130.8889	131.6701	130.6982	131.6464	130.6949	132.0539	130.9028	131.8371	130.8633	132.0636	130.8393	130.6982	131.4966	130.6425	131.5797	130.6357	132.1162	130.8401	131.8633	130.8104	132.0880	**112.1**
C3	187.2124	187.2749	187.9692	187.2900	188.2319	187.2740	188.1455	187.4691	188.0715	187.4668	188.1443	187.2458	187.2726	187.8942	187.2019	188.1463	187.1854	188.0705	187.3805	187.9725	187.3790	188.1003	**162.6**
C4	126.1275	127.6104	128.4605	128.2640	129.1944	128.2109	130.1213	128.3686	129.8697	128.4757	130.2526	126.3061	127.5785	128.2780	127.9476	128.9377	127.8961	129.5448	128.0559	129.3015	128.1578	129.6499	**110.1**
C5	186.2743	186.7477	187.4664	186.9863	188.0708	186.9555	187.9481	187.1363	187.8597	187.1772	188.0091	186.2210	186.5854	187.2395	186.8041	187.7969	186.7739	187.6214	186.9550	187.5197	186.9945	187.6170	**162.5**
C6	129.0780	131.0787	132.3496	131.9671	133.9931	131.8970	134.3492	132.0379	134.0524	132.1953	134.6750	129.2190	131.2344	132.7079	132.1544	134.3901	132.0817	134.6006	132.2204	134.4055	132.3848	134.8976	**112.1**
C7	216.7020	221.9096	223.5339	224.8278	225.7871	224.6304	231.3580	224.6448	229.8414	225.1759	232.3444	221.0110	225.6175	227.2602	228.3265	229.1189	228.1640	234.7506	228.2115	233.2768	228.6421	235.1988	**194.5**
C8	71.1897	72.2890	72.9929	72.8023	73.8837	72.7579	74.3671	72.9259	74.0597	73.0068	75.0631	65.2505	66.5369	67.7039	67.9007	68.8828	67.8484	69.7076	68.0074	69.3153	68.1119	70.0736	**58.4**
C9	25.2414	25.5009	25.8219	25.6540	26.2407	25.6246	26.2211	25.8058	26.0413	25.8433	26.3165	21.9800	21.9981	22.5167	22.3986	22.9018	22.3830	22.7306	22.5785	22.7129	22.5750	23.2128	**15**
C8`	38.8135	39.5255	39.7964	39.9061	40.4240	39.8777	40.5014	40.0610	40.3642	40.0952	40.9021	33.6850	34.1404	34.3964	34.3149	34.7561	34.2765	34.7112	34.4489	34.6334	34.5129	34.8165	**30.6**
H2	8.2738	8.2592	8.3378	8.2067	8.2816	8.2073	8.3336	8.2078	8.3546	8.1967	8.3272	8.3152	8.2376	8.2501	8.1116	8.1851	8.1102	8.1497	8.1088	8.1712	8.1032	8.1653	**7.77**
H4	7.3357	7.5509	7.6898	7.6330	7.8183	7.6254	7.8583	7.6178	7.8443	7.6305	7.8840	7.3302	7.5358	7.6733	7.6128	7.7954	7.6054	7.8212	7.5980	7.8111	7.6102	7.8394	**7.71**
H6	7.7226	7.9733	8.1216	8.0758	8.3049	8.0671	8.3433	8.0584	8.3341	8.0746	8.3824	7.5361	7.7448	7.9351	7.8786	8.1407	7.8688	8.1259	7.8589	8.1358	7.8784	8.1323	**7.77**
H8	4.1465	4.2490	4.3025	4.3121	4.4089	4.3042	4.4414	4.2963	4.4517	4.3100	4.4603	4.3736	4.5403	4.6411	4.6470	4.7854	4.6391	4.7838	4.6312	4.7905	4.6450	4.7720	**5.21**
H(9A-9C)	1.2990	1.3318	1.3084	1.3230	1.2855	1.3203	1.3117	1.3177	1.3166	1.3161	1.3255	1.3588	1.3981	1.3775	1.4016	1.3840	1.3974	1.4004	1.3933	1.4002	1.3961	1.4166	**1.43**
H(8`A-8`C)	2.4247	2.3701	2.3247	2.3683	2.3202	2.3649	2.3052	2.3616	2.2913	2.3620	2.2928	2.7914	2.6684	2.5947	2.5685	2.5254	2.5674	2.4314	2.5663	2.4700	2.5602	2.3779	**2.58**
Nuclei	BP86											BP86										
C1	142.7538	143.4513	144.5775	144.1907	145.0356	144.1952	144.5412	144.1946	144.9194	144.1825	144.8732	141.4617	142.1656	143.3316	143.3152	144.4516	143.3270	144.8687	143.3320	144.4752	143.2976	144.9621	**136.1**
C2	114.9274	115.1445	115.8552	115.1479	115.6876	115.1686	116.1738	115.1842	116.1359	115.1227	116.3537	114.5927	114.8280	115.4815	114.9951	115.5581	115.0133	116.2025	115.0258	116.0166	114.9724	116.3334	**112.1**
C3	172.0493	172.5220	173.0745	172.5605	173.3928	172.5656	173.3561	172.5656	173.3351	172.5504	173.5903	172.0582	172.5221	173.0948	172.5909	173.4087	172.5955	173.3829	172.5948	173.3705	172.5815	173.6099	**162.6**
C4	110.9860	112.6318	113.1453	113.2279	113.8562	113.1935	114.7930	113.1540	114.4847	113.2553	115.1289	111.3231	112.7636	113.2292	113.0964	113.7399	113.0694	114.3116	113.0376	114.2126	113.1172	114.7015	**110.1**
C5	171.2599	172.0320	172.6542	172.2838	173.2497	172.2751	173.2009	172.2610	173.1351	172.2874	173.4429	171.5908	172.2342	172.7533	172.3093	173.2108	172.3048	173.0358	172.2953	173.0464	172.3088	173.2758	**162.5**
C6	113.1764	114.9405	115.8289	115.5842	117.3085	115.5368	117.6679	115.4840	117.3720	115.6244	118.1684	113.5099	115.5241	116.6130	116.2054	117.9367	116.1546	118.0325	116.0990	118.0123	116.2490	118.6108	**112.1**
C7	200.8740	205.6351	207.3718	208.5818	208.9794	208.4408	213.3927	208.2958	212.7636	208.7118	214.2723	205.4772	209.2841	210.5621	211.2242	212.0901	211.1381	216.5337	211.0452	215.3777	211.3010	216.9615	**194.5**
C8	67.7193	68.9807	69.6770	69.4781	70.2197	69.4688	70.7818	69.4533	70.7615	69.4808	71.7372	62.1228	63.6359	64.5221	64.9077	65.6311	64.8730	66.4515	64.8324	66.1235	64.9349	66.8802	**58.4**
C9	23.2849	23.7487	23.7013	23.7870	24.1448	23.7815	24.2820	23.7712	24.1688	23.7878	24.6409	19.9380	20.4850	20.7072	20.7855	21.0266	20.7754	21.1255	20.7599	21.0785	20.7900	21.8011	**15**
C8`	37.3382	38.2084	38.4190	38.5638	38.8090	38.5521	38.9623	38.5346	38.9321	38.5694	39.5682	32.5225	33.0970	33.0398	32.9133	33.1895	32.9082	33.2254	32.8983	33.2582	32.9138	33.4315	**30.6**
H2	7.7724	7.7317	7.7645	7.6369	7.7426	7.6403	7.7694	7.6433	7.7390	7.6332	7.7790	7.8354	7.7769	7.7834	7.6413	7.7099	7.6432	7.6606	7.6450	7.6943	7.6393	7.6912	**7.77**
H4	6.8897	7.1017	7.2283	7.1789	7.3524	7.1752	7.3924	7.1712	7.3734	7.1819	7.4276	6.9069	7.1061	7.2290	7.1689	7.3440	7.1659	7.3699	7.1625	7.3576	7.1714	7.4058	**7.71**
H6	7.3735	7.5819	7.6754	7.6507	7.8531	7.6444	7.8854	7.6378	7.8495	7.6563	7.9286	7.1622	7.3706	7.4969	7.4202	7.6575	7.4148	7.6321	7.4092	7.6377	7.4250	7.7005	**7.77**
H8	4.5068	4.5848	4.5783	4.6315	4.6945	4.6277	4.7184	4.6238	4.6969	4.6350	4.7524	4.6215	4.7696	4.8319	4.8493	4.9678	4.8460	4.9887	4.8425	4.9722	4.8520	5.0351	**5.21**
H(9A-9C)	1.3547	1.3540	1.3166	1.3196	1.3050	1.3212	1.3244	1.3224	1.3114	1.3176	1.3578	1.4375	1.4867	1.4630	1.4945	1.4687	1.4928	1.4670	1.4910	1.4739	1.4957	1.5196	**1.43**
H(8`A-8`C)	2.5474	2.4876	2.4474	2.4694	2.4179	2.4719	2.4031	2.4741	2.4129	2.4668	2.3990	2.9606	2.8361	2.7475	2.7252	2.6672	2.7293	2.5745	2.7333	2.5980	2.7211	2.5556	**2.58**
Nuclei	CAM-B3LYP											CAM-B3LYP										
C1	148.4624	148.6841	149.5577	149.3093	150.3034	149.2366	149.5630	149.1940	150.1230	149.4908	149.7081	147.3433	147.7962	148.9027	148.9377	149.9895	148.9426	150.6402	148.9472	150.3560	148.9346	150.6085	**136.1**
C2	120.3697	120.5288	121.2664	120.5450	121.2654	120.5429	121.7675	120.5459	121.7171	120.5678	121.7990	120.0897	120.3536	121.0773	120.5409	121.2386	120.5481	121.8243	120.5558	121.6912	120.5360	121.8482	**112.1**
C3	175.3492	175.4926	175.9358	175.5369	176.1861	175.5384	176.1153	175.5405	176.1333	175.5379	176.1841	175.3442	175.4726	175.9346	175.5461	176.1974	175.5484	176.2002	175.5514	176.1881	175.5461	176.2573	**162.6**
C4	115.1853	116.7203	117.3027	117.3420	118.0574	117.3114	118.9781	117.2787	118.6454	117.3619	119.1496	115.4504	116.8025	117.3467	117.1829	117.9449	117.1505	118.3719	117.1183	118.2754	117.2157	118.6005	**110.1**
C5	174.4445	174.9458	175.4191	175.2281	176.0054	175.2117	175.9367	175.1974	175.9002	175.2501	176.0203	174.6122	175.0145	175.4513	175.1606	175.9162	175.1514	175.7560	175.1425	175.7605	175.1717	175.8379	**162.5**
C6	118.2349	120.2035	121.2809	120.9421	122.7939	120.9171	123.1401	120.8794	122.7903	120.9217	123.4948	118.5853	120.7015	121.8580	121.4563	123.3720	121.3956	123.2336	121.3353	123.1908	121.5160	123.6524	**112.1**
C7	204.9813	210.0516	211.5270	213.2288	213.7015	212.9808	218.9767	212.7744	218.2644	213.6165	219.7880	209.5376	213.7156	215.0999	216.0406	216.7885	215.9258	222.3449	215.8104	221.0486	216.1513	222.7788	**194.5**
C8	64.0306	65.1714	65.8913	65.6727	66.4716	65.6559	66.9160	65.6362	66.9212	65.6891	67.6537	58.5409	59.9286	60.7324	61.1462	61.8646	61.1083	62.7669	61.0705	62.4393	61.1839	63.0463	**58.4**
C9	22.0699	22.3268	22.4756	22.3917	22.7878	22.4051	22.6785	22.4083	22.6005	22.3384	22.8481	19.0012	19.1778	19.3019	19.3324	19.6057	19.3296	19.4870	19.3270	19.4631	19.3369	19.8518	**15**
C8`	35.4169	36.2356	36.4687	36.6181	36.9937	36.5948	37.1573	36.5744	37.1322	36.6513	37.6150	30.8785	31.3840	31.4431	31.3509	31.7242	31.3347	31.7233	31.3192	31.7367	31.3691	31.8575	**30.6**
H2	8.0798	8.0390	8.0961	7.9447	8.0515	7.9541	8.0852	7.9610	8.0417	7.9264	8.0787	8.1333	8.0587	8.0806	7.9149	8.0062	7.9164	7.9131	7.9182	7.9416	7.9134	7.9290	**7.77**
H4	7.1631	7.3729	7.5130	7.4499	7.6374	7.4457	7.6793	7.4416	7.6601	7.4539	7.7001	7.1734	7.3716	7.5092	7.4358	7.6246	7.4321	7.6486	7.4284	7.6373	7.4393	7.6708	**7.71**
H6	7.5236	7.7575	7.8789	7.8388	8.0671	7.8338	8.1068	7.8287	8.0661	7.8423	8.1386	7.3719	7.5974	7.7446	7.6580	7.9202	7.6515	7.8749	7.6451	7.8763	7.6641	7.9251	**7.77**
H8	4.1228	4.2306	4.2498	4.3082	4.4012	4.3011	4.4473	4.2954	4.4231	4.3181	4.4637	4.3004	4.4681	4.5457	4.5464	4.6862	4.5418	4.7032	4.5373	4.6904	4.5507	4.7319	**5.21**
H(9A-9C)	1.3143	1.3232	1.3076	1.2895	1.2794	1.2947	1.2903	1.2979	1.2735	1.2776	1.3088	1.3899	1.4312	1.4104	1.4309	1.4163	1.4289	1.3952	1.4270	1.3990	1.4327	1.4240	**1.43**
H(8`A-8`C)	2.5060	2.4548	2.4325	2.4448	2.4053	2.4460	2.3904	2.4471	2.4032	2.4427	2.3783	2.8981	2.7725	2.6987	2.6658	2.6251	2.6687	2.5302	2.6719	2.5552	2.6629	2.5016	**2.58**

[a] methyl protons shifts are averaged

[b] according to [8]

Table S8. Cont. III

Nuclei	R											S										Exp. [b]
	HF											HF										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	147.7121	148.1462	148.1492	149.1412	149.0104	149.0759	149.1926	148.9499	149.6027	149.1850	149.3437	146.2560	146.4572	148.9780	149.1791	150.1652	149.1278	149.7021	149.0849	150.0837	149.2368	149.9227	**136.1**
C2	118.3809	118.6300	119.3684	118.5413	119.3777	118.5527	119.7793	118.5693	119.6702	118.5314	119.8114	118.2524	118.5590	119.3010	118.4610	119.3758	118.4680	119.7023	118.4743	119.5755	118.4525	119.7337	**112.1**
C3	168.2802	168.1502	168.3945	168.1534	168.4870	168.1530	168.4813	168.1468	168.5414	168.1515	168.5428	168.1871	168.0226	168.5400	168.2712	168.6623	168.2682	168.5933	168.2665	168.6476	168.2748	168.6620	**162.6**
C4	112.6244	114.0962	114.9583	114.5391	115.5871	114.5192	116.2181	114.5177	115.8932	114.5620	116.3700	112.9802	114.3797	114.5193	114.1872	114.9663	114.1677	115.5798	114.1457	115.2770	114.2015	115.7131	**110.1**
C5	167.2757	167.5153	167.8482	167.7332	168.2463	167.7202	168.1164	167.7050	168.1379	167.7436	168.2049	167.2550	167.4221	167.8461	167.6776	168.1690	167.6656	167.9812	167.6546	168.0061	167.6890	168.0711	**162.5**
C6	115.6813	117.5848	118.9797	118.2479	120.4077	118.2059	120.3553	118.1894	120.0329	118.2948	120.6350	116.2984	118.4587	118.7549	118.2796	120.0365	118.2485	120.2939	118.2135	119.9941	118.3031	120.5345	**112.1**
C7	195.0864	201.1974	202.1057	205.1486	204.3050	204.9023	211.8991	204.6015	210.6015	205.3645	212.8018	199.0531	203.6043	205.9457	207.2282	207.6496	207.0438	213.5072	206.8640	212.2390	207.4078	214.2805	**194.5**
C8	55.1031	56.1200	56.4604	56.7648	57.0692	56.7164	57.8833	56.6498	57.7961	56.8040	58.4563	50.5284	51.7328	52.8831	53.2938	53.8474	53.2468	54.6595	53.2029	54.5809	53.3414	54.9739	**58.4**
C9	20.2409	20.1666	20.3679	20.1759	20.6108	20.1760	20.3164	20.1834	20.3224	20.1785	20.3997	17.4792	17.3170	17.3609	17.2432	17.5132	17.2524	17.4287	17.2617	17.4510	17.2335	17.6278	**15**
C8`	32.6404	33.3530	33.5761	33.6875	34.0417	33.6635	34.1472	33.6358	34.1005	33.7070	34.5026	28.8853	29.2953	29.2756	29.2181	29.5394	29.2016	29.5492	29.1854	29.4937	29.2326	29.6273	**30.6**
H2	8.1484	8.0454	8.1890	7.9006	8.1149	7.9103	8.0336	7.9258	8.0133	7.8932	8.0280	8.2369	8.1426	8.0199	7.8305	7.9414	7.8371	7.9338	7.8428	7.9118	7.8235	7.9287	**7.77**
H4	7.2655	7.4862	7.6373	7.5616	7.7619	7.5579	7.7990	7.5545	7.7775	7.5652	7.8213	7.2777	7.4892	7.6158	7.5371	7.7287	7.5336	7.7595	7.5297	7.7393	7.5404	7.7810	**7.71**
H6	7.4308	7.6757	7.8611	7.7642	8.0522	7.7593	8.0401	7.7569	8.0074	7.7697	8.0738	7.3542	7.6087	7.6943	7.6137	7.8665	7.6093	7.8640	7.6044	7.8341	7.6174	7.8978	**7.77**
H8	3.5241	3.6685	3.7491	3.7576	3.9052	3.7528	3.9202	3.7502	3.8944	3.7630	3.9383	3.7343	3.9245	3.9760	3.9636	4.1151	3.9591	4.1356	3.9542	4.1100	3.9676	4.1523	**5.21**
H(9A-9C)	1.1624	1.1432	1.1461	1.1019	1.1090	1.1042	1.0923	1.1080	1.0841	1.1003	1.1037	1.2474	1.2758	1.1946	1.2212	1.1918	1.2213	1.2139	1.2210	1.2036	1.2209	1.2251	**1.43**
H(8`A-8`C)	2.2753	2.2539	2.2078	2.2558	2.1999	2.2553	2.2229	2.2539	2.2248	2.2562	2.2153	2.6485	2.5366	2.4501	2.4179	2.3834	2.4206	2.3149	2.4231	2.3181	2.4152	2.2848	**2.58**
Nuclei	LC-BLYP																						
C1	153.0659	152.9932	153.9478	153.2994	154.4610	153.2671	153.6006	153.2592	154.4471	153.3100	153.6985	152.0909	152.3376	153.5064	153.5214	154.4478	153.4803	155.3938	153.4680	154.4876	153.5446	155.3545	**136.1**
C2	125.1117	125.2547	126.1171	125.2424	126.0930	125.2238	126.5824	125.2320	126.5273	125.2427	126.6298	124.8423	125.1096	125.9858	125.3336	126.1148	125.3094	126.6441	125.3129	126.5069	125.3393	126.6964	**112.1**
C3	179.4625	179.3659	179.8001	179.3978	179.9041	179.3751	179.8505	179.3795	179.8994	179.4019	179.9048	179.4596	179.3560	179.8147	179.4436	179.9341	179.4199	180.0140	179.4236	179.9283	179.4489	180.0556	**162.6**
C4	119.5922	121.1275	121.8706	121.8511	122.6302	121.7861	123.5400	121.7485	123.1661	121.8957	123.7389	119.7976	121.1785	121.8792	121.6443	122.5102	121.5858	122.8575	121.5539	122.8882	121.6819	123.0895	**110.1**
C5	178.4282	178.7477	179.2235	179.0477	179.6740	179.0069	179.6143	178.9933	179.6084	179.0693	179.6988	178.5367	178.7820	179.2208	178.9749	179.5914	178.9375	179.4631	178.9275	179.4263	178.9932	179.5311	**162.5**
C6	122.6656	124.8212	126.0160	125.7973	127.6946	125.7145	128.0371	125.6606	127.5187	125.8591	128.4352	123.0495	125.2950	126.5670	126.1254	128.2068	126.0458	127.9644	125.9928	128.2584	126.1828	128.4251	**112.1**
C7	210.1898	215.3210	216.9461	218.2917	218.9503	218.0958	224.3773	217.9244	223.8948	218.4584	225.2030	214.4768	218.7950	220.4137	221.4119	222.1020	221.2386	228.1827	221.0926	226.1958	221.5591	228.6369	**194.5**
C8	61.8392	63.0647	63.7969	63.6198	64.5104	63.5665	64.9590	63.5405	64.8427	63.6531	65.6885	56.1591	57.4696	58.2939	58.6291	59.3491	58.5642	60.3658	58.5274	59.9644	58.6739	60.7091	**58.4**
C9	21.0891	21.2058	21.4708	21.4307	21.8569	21.3946	21.6607	21.3855	21.4620	21.4473	21.8487	18.2806	18.3535	18.4911	18.4804	18.7770	18.4595	18.6189	18.4658	18.7216	18.4825	19.0174	**15**
C8`	33.5289	34.3585	34.6715	34.7962	35.2003	34.7498	35.3864	34.7313	35.3205	34.8234	35.8886	28.9379	29.4680	29.6380	29.5517	29.9040	29.5046	29.8876	29.4849	29.9104	29.5789	30.0694	**30.6**
H2	8.2569	8.2183	8.2766	8.1508	8.2350	8.1534	8.2673	8.1580	8.2074	8.1476	8.2684	8.2975	8.2232	8.2466	8.0788	8.1757	8.0813	8.0491	8.0853	8.1311	8.0754	8.0660	**7.77**
H4	7.3112	7.5223	7.6691	7.6022	7.7950	7.5970	7.8358	7.5933	7.8167	7.6061	7.8596	7.3178	7.5189	7.6634	7.5867	7.7812	7.5819	7.8014	7.5785	7.7933	7.5903	7.8256	**7.71**
H6	7.6561	7.9003	8.0344	8.0002	8.2277	7.9930	8.2620	7.9876	8.2108	8.0061	8.3036	7.5204	7.7594	7.9103	7.8231	8.0993	7.8161	8.0347	7.8106	8.0708	7.8287	8.0877	**7.77**
H8	3.9976	4.1071	4.1478	4.1990	4.2868	4.1918	4.3340	4.1861	4.3243	4.2049	4.3563	4.2244	4.3979	4.4877	4.4818	4.6295	4.4756	4.6345	4.4709	4.6231	4.4866	4.6627	**5.21**
H(9A-9C)	1.3288	1.3469	1.3244	1.3317	1.3134	1.3316	1.3208	1.3332	1.2881	1.3309	1.3443	1.4005	1.4383	1.4092	1.4335	1.4191	1.4317	1.3878	1.4315	1.4220	1.4340	1.4200	**1.43**
H(8`A-8`C)	2.4935	2.4373	2.4110	2.4286	2.3914	2.4284	2.3746	2.4297	2.3874	2.4278	2.3644	2.8450	2.7166	2.6464	2.6119	2.5768	2.6138	2.4655	2.6173	2.4997	2.6090	2.4403	**2.58**
Nuclei	M06																						
C1	143.6087	143.8341	144.1560	144.1466	145.4179	144.0943	144.6247	144.0567	145.2393	144.2187	144.7782	142.5659	142.8141	144.0659	144.3025	145.2584	144.2758	146.2582	144.2587	146.0881	144.3454	146.1763	**136.1**
C2	117.4969	117.6906	118.4694	117.6902	118.5084	117.6767	119.0643	117.6730	119.0111	117.7191	119.0861	117.3658	117.4199	118.3149	117.9277	118.6176	117.9154	119.5130	117.9116	119.3533	117.9549	119.4995	**112.1**
C3	171.0655	171.1576	171.6496	171.2572	172.0725	171.2405	171.9445	171.2313	172.0207	171.2873	172.0360	171.0875	171.2518	171.8988	171.4330	172.2147	171.4186	172.2217	171.4124	172.2255	171.4612	172.2612	**162.6**
C4	112.9084	114.5496	115.4222	115.3123	116.1173	115.2612	117.1351	115.2171	116.7511	115.3749	117.3127	112.9794	114.3851	115.0462	114.7549	115.6813	114.7084	116.0940	114.6689	115.9579	114.8129	116.3443	**110.1**
C5	170.4005	170.8302	171.5303	171.1355	172.0720	171.1040	172.0447	171.0813	171.9917	171.1814	172.0878	170.6007	170.8887	171.4197	170.9603	171.8434	170.9364	171.6630	170.9201	171.6715	170.9975	171.7353	**162.5**
C6	115.4653	117.3110	118.7542	118.2416	120.0756	118.1830	120.5423	118.1300	120.1478	118.3092	120.8598	116.0240	118.1108	119.3577	118.7529	120.8129	118.6840	120.6537	118.6219	120.5518	118.8320	121.0971	**112.1**
C7	201.9616	206.6108	207.7146	209.1984	209.8619	209.0015	214.6669	208.8227	214.1517	209.4126	215.4547	206.3552	210.2643	211.5991	212.2398	212.9368	212.1160	218.1946	211.9993	217.0620	212.3726	218.5362	**194.5**
C8	61.6157	62.7862	63.4448	63.1823	64.2103	63.1600	64.6298	63.1425	64.5045	63.2151	65.3923	54.7279	55.9736	56.9908	57.5120	58.3429	57.4505	59.2905	57.3979	58.9831	57.5862	59.6495	**58.4**
C9	22.0089	22.3738	22.7469	22.5355	23.0391	22.5242	23.0830	22.5175	22.8484	22.5571	23.1318	19.0663	19.1434	19.4193	19.5446	20.0187	19.5245	19.7995	19.5119	19.7729	19.5782	20.3394	**15**
C8`	36.6161	37.4384	37.6918	37.9406	38.3867	37.8952	38.6169	37.8602	38.6376	38.0014	39.1063	31.7384	32.2819	32.4719	32.2631	32.7052	32.2332	32.9206	32.2113	32.8556	32.3066	33.0530	**30.6**
H2	7.9698	7.9068	8.0191	7.8235	7.9100	7.8307	7.9337	7.8378	7.8931	7.8167	7.9258	8.0414	7.9552	8.0009	7.8337	7.9444	7.8368	7.8456	7.8403	7.8625	7.8311	7.8545	**7.77**
H4	6.9321	7.1543	7.3096	7.2320	7.4279	7.2277	7.4765	7.2239	7.4533	7.2368	7.4990	6.8809	7.0866	7.2281	7.1530	7.3512	7.1488	7.3800	7.1451	7.3652	7.1575	7.4064	**7.71**
H6	7.4835	7.7066	7.8772	7.8004	8.0089	7.7948	8.0705	7.7901	8.0210	7.8066	8.0863	7.3031	7.5132	7.6395	7.4952	7.7803	7.4896	7.6863	7.4846	7.6846	7.5008	7.7551	**7.77**
H8	4.2773	4.3549	4.3740	4.4090	4.4769	4.4049	4.5198	4.4017	4.4988	4.4137	4.5316	4.3646	4.5231	4.5871	4.5656	4.7090	4.5613	4.6783	4.5576	4.6733	4.5702	4.7342	**5.21**
H(9A-9C)	1.3212	1.3089	1.3280	1.2793	1.2697	1.2828	1.2807	1.2863	1.2576	1.2759	1.2984	1.3636	1.4097	1.3879	1.3910	1.3879	1.3895	1.3416	1.3885	1.3449	1.3929	1.3814	**1.43**
H(8`A-8`C)	2.4391	2.4091	2.3648	2.3976	2.3659	2.3979	2.3504	2.3988	2.3614	2.3977	2.3353	2.8564	2.7442	2.6579	2.5989	2.5664	2.6026	2.4555	2.6069	2.4814	2.5958	2.4296	**2.58**
Nuclei	M06-2X																						
C1	160.6475	160.9144	161.4815	161.0437	162.3465	161.0480	161.3271	161.0554	161.2325	161.0351	161.6236	160.0712	160.3972	161.6524	161.6045	162.7588	161.6050	162.9854	161.6083	162.7446	161.5997	163.2824	**136.1**
C2	130.9181	130.9182	131.5635	130.7532	131.4908	130.7852	131.8866	130.8187	131.7769	130.7164	131.9578	130.9607	130.9962	131.7658	131.0960	131.8330	131.1223	132.3766	131.1498	132.2266	131.0652	132.4467	**112.1**
C3	184.9329	185.0581	185.5654	185.0935	185.7983	185.1120	185.7543	185.1319	185.7356	185.0696	185.8423	184.9790	185.0980	185.6365	185.1575	185.8625	185.1752	185.8343	185.1940	185.8270	185.1345	185.9251	**162.6**
C4	125.6445	127.2128	127.9809	127.9383	128.7259	127.9178	129.7092	127.8979	129.5080	127.9512	129.9048	125.6848	127.1393	127.7953	127.6456	128.4840	127.6290	129.1001	127.6132	128.9477	127.6544	129.2943	**110.1**
C5	183.7556	184.2929	184.8831	184.6107	185.4542	184.6110	185.4231	184.6127	185.3957	184.6043	185.5193	183.8092	184.3112	184.8262	184.4932	185.3302	184.4954	185.1394	184.4991	185.1480	184.4848	185.2539	**162.5**
C6	129.0692	131.0857	132.4045	132.0845	134.0470	132.0477	134.4655	132.0110	134.2846	132.1126	134.8331	129.3298	131.4863	132.7479	132.3374	134.4293	132.3041	134.6571	132.2714	134.5460	132.3614	134.9566	**112.1**
C7	217.9685	223.3424	224.6748	226.1066	226.8183	225.9537	232.2546	225.8038	230.9246	226.2471	233.3156	221.9367	226.6882	228.3374	229.4086	230.1664	229.2713	235.8710	229.1354	234.4798	229.5329	236.7275	**194.5**
C8	66.7616	68.0409	68.6275	68.5924	69.5352	68.5805	69.9392	68.5696	69.7162	68.5968	70.7665	60.9624	62.2785	63.1475	63.4975	64.3331	63.4745	65.2376	63.4535	64.9234	63.5138	65.6052	**58.4**
C9	22.7521	23.1173	23.3932	23.4185	23.9222	23.4153	23.9593	23.4145	23.8682	23.4162	24.1436	19.9903	20.1564	20.3508	20.4075	20.7366	20.4268	20.7761	20.4472	20.7172	20.3830	21.1365	**15**
C8`	36.0489	36.6336	36.8478	36.9812	37.3318	36.9812	37.4719	36.9822	37.4087	36.9742	37.9825	30.6120	31.2137	31.4167	31.4523	31.7885	31.4526	31.8112	31.4542	31.7986	31.4457	32.0585	**30.6**
H2	8.5068	8.4519	8.5399	8.4036	8.4745	8.4062	8.5326	8.4083	8.5494	8.4011	8.5167	8.5232	8.4741	8.5005	8.3533	8.4358	8.3551	8.3895	8.3565	8.4116	8.3516	8.3854	**7.77**
H4	7.4581	7.6639	7.8093	7.7447	7.9311	7.7390	7.9740	7.7330	7.9597	7.7502	7.9947	7.4492	7.6452	7.7866	7.7203	7.9047	7.7148	7.9364	7.7089	7.9219	7.7256	7.9562	**7.71**
H6	8.0004	8.2271	8.3948	8.3308	8.5611	8.3239	8.6143	8.3166	8.6101	8.3374	8.6392	7.8271	8.0529	8.1960	8.1185	8.3804	8.1113	8.3619	8.1036	8.3608	8.1254	8.3921	**7.77**
H8	4.1763	4.2775	4.3389	4.3510	4.4417	4.3446	4.4925	4.3380	4.4918	4.3573	4.4967	4.4074	4.5573	4.6485	4.6471	4.7853	4.6404	4.7794	4.6334	4.7762	4.6535	4.7970	**5.21**
H(9A-9C)	1.3553	1.3677	1.3612	1.3661	1.3464	1.3655	1.3698	1.3645	1.3722	1.3666	1.3833	1.4090	1.4501	1.4248	1.4498	1.4343	1.4476	1.4389	1.4449	1.4425	1.4520	1.4478	**1.43**
H(8`A-8`C)	2.4514	2.4056	2.3644	2.3975	2.3613	2.3963	2.3388	2.3949	2.3302	2.3989	2.3264	2.7544	2.6581	2.5921	2.5605	2.5220	2.5613	2.4334	2.5618	2.4571	2.5598	2.3975	**2.58**

[a] methyl protons shifts are averaged

[b] according to [8]

Table S8. Cont. IV

Nuclei	R											S									Exp. [b]
	mpW1LYP																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	146.6954	147.0297	148.2564	147.8907	148.6400	147.8778	147.9006	147.8678	148.4150	147.9029	148.0401	145.3975	145.9526	147.0982	147.1090	148.2406	147.1142	148.6029	147.1179	148.3530	147.0991	148.5512	**136.1**
C2	118.3114	118.4569	119.2628	118.5775	119.1262	118.5797	119.6482	118.5838	119.6100	118.5732	119.6569	118.0065	118.2052	118.9127	118.4124	119.0242	118.4141	119.6563	118.4164	119.5123	118.4082	119.6296	**112.1**
C3	173.8150	174.0060	174.5295	174.0927	174.7686	174.0856	174.6998	174.0799	174.7223	174.0975	174.7407	173.8076	174.0114	174.5579	174.1436	174.8245	174.1355	174.7995	174.1288	174.8010	174.1493	174.8317	**162.6**
C4	113.3275	114.8491	115.4058	115.4788	116.1242	115.4321	117.0762	115.3865	116.7496	115.5212	117.2251	113.6575	114.9373	115.4666	115.3459	115.9657	115.3033	116.5200	115.2623	116.4116	115.3849	116.7151	**110.1**
C5	173.0482	173.5647	174.1519	173.8579	174.6917	173.8369	174.6095	173.8172	174.5693	173.8756	174.6638	173.3048	173.7268	174.2432	173.9135	174.6800	173.8957	174.5185	173.8795	174.5322	173.9285	174.5686	**162.5**
C6	116.4785	118.2937	119.2255	118.9964	120.8217	118.9309	121.2423	118.8665	120.9070	119.0559	121.5448	116.7801	118.7954	119.9818	119.5693	121.3296	119.4964	121.3555	119.4261	121.3103	119.6378	121.7355	**112.1**
C7	202.6954	207.7338	209.6104	211.1097	211.3784	210.9360	216.3296	210.7657	215.6070	211.2754	217.1413	207.6460	211.6587	212.9987	213.8871	214.6863	213.7779	219.7701	213.6685	218.5665	213.9862	220.1650	**194.5**
C8	65.3085	66.3279	67.0698	66.9121	67.5805	66.8855	68.1375	66.8589	68.1550	66.9344	68.8103	59.9284	61.3760	62.2698	62.6392	63.3412	62.5920	64.1517	62.5455	63.8601	62.6809	64.3777	**58.4**
C9	22.7183	22.9747	22.9907	23.0217	23.4088	23.0033	23.4478	22.9868	23.3719	23.0377	23.5694	19.3696	19.5970	19.8456	19.8268	20.0576	19.8078	20.0460	19.7902	20.0217	19.8429	20.3845	**15**
C8`	36.2154	36.9814	37.3077	37.4364	37.7591	37.4100	37.8959	37.3843	37.8664	37.4585	38.2890	31.7290	32.1618	32.2327	32.1434	32.4620	32.1208	32.4852	32.1003	32.5146	32.1636	32.5516	**30.6**
H2	7.9970	7.9549	7.9939	7.8470	7.9734	7.8502	8.0094	7.8530	7.9702	7.8437	8.0023	8.0627	7.9784	8.0021	7.8446	7.9222	7.8453	7.8654	7.8459	7.8909	7.8442	7.8776	**7.77**
H4	7.0944	7.3016	7.4406	7.3797	7.5621	7.3755	7.6039	7.3709	7.5853	7.3836	7.6231	7.1094	7.3039	7.4400	7.3700	7.5518	7.3663	7.5797	7.3622	7.5681	7.3734	7.5992	**7.71**
H6	7.4794	7.7086	7.8257	7.7887	8.0197	7.7816	8.0548	7.7742	8.0150	7.7954	8.0834	7.3093	7.5248	7.6697	7.5860	7.8327	7.5796	7.8067	7.5729	7.8065	7.5921	7.8541	**7.77**
H8	4.2159	4.3197	4.3397	4.3826	4.4807	4.3770	4.5051	4.3714	4.4817	4.3881	4.5231	4.3616	4.5250	4.5988	4.6027	4.7354	4.5982	4.7549	4.5934	4.7415	4.6069	4.7822	**5.21**
H(9A-9C)	1.3129	1.3128	1.2823	1.2746	1.2695	1.2755	1.2944	1.2760	1.2797	1.2735	1.3073	1.3946	1.4360	1.4230	1.4411	1.4216	1.4385	1.4142	1.4357	1.4183	1.4436	1.4403	**1.43**
H(8`A-8`C)	2.5118	2.4603	2.4356	2.4540	2.4078	2.4553	2.3995	2.4562	2.4124	2.4528	2.3810	2.9355	2.8059	2.7355	2.7062	2.6583	2.7091	2.5732	2.7120	2.5952	2.7034	2.5396	**2.58**
Nuclei	mpW1PW91																						
C1	144.2225	144.6598	145.7040	145.3799	146.2379	145.3716	145.5329	145.3679	146.0569	145.3858	145.7331	143.1728	143.5731	144.7415	144.7586	145.7980	144.7551	146.4282	144.7571	146.1584	144.7610	146.3758	**136.1**
C2	117.2526	117.3898	118.1545	117.4212	118.0982	117.4293	118.5695	117.4425	118.5255	117.4126	118.5909	117.0273	117.1670	117.8923	117.3338	118.0065	117.3382	118.5880	117.3481	118.4544	117.3290	118.5954	**112.1**
C3	170.9185	171.1504	171.6651	171.2107	171.9534	171.2079	171.9032	171.2107	171.9086	171.2129	171.9840	170.9451	171.1682	171.7046	171.2683	172.0025	171.2643	172.0079	171.2663	171.9935	171.2712	172.0717	**162.6**
C4	112.5855	114.1255	114.7398	114.7594	115.5112	114.7164	116.4703	114.6788	116.1288	114.7997	116.6327	112.8243	114.2167	114.7815	114.6091	115.3972	114.5723	115.8720	114.5411	115.7564	114.6430	116.1076	**110.1**
C5	170.1326	170.6821	171.2539	170.9502	171.8287	170.9328	171.7689	170.9210	171.7130	170.9659	171.8579	170.3544	170.8292	171.3428	170.9936	171.8314	170.9794	171.6724	170.9707	171.6763	171.0067	171.7541	**162.5**
C6	115.0757	116.8642	117.8399	117.5632	119.4041	117.5045	119.7868	117.4528	119.4366	117.6183	120.1171	115.4038	117.4235	118.5471	118.1370	120.0137	118.0767	119.9540	118.0217	119.8987	118.1937	120.3774	**112.1**
C7	200.7895	205.6480	207.3324	208.7822	209.0294	208.6217	213.9502	208.4636	213.2810	208.9327	214.7277	204.8778	208.8681	210.2474	211.1288	211.8437	211.0165	217.0660	210.9092	215.8143	211.2338	217.4156	**194.5**
C8	63.1000	64.2403	64.8967	64.7653	65.5504	64.7429	66.0201	64.7247	66.0144	64.7852	66.7798	58.0020	59.2660	60.0876	60.4729	61.1841	60.4308	62.0933	60.3940	61.7725	60.5122	62.3622	**58.4**
C9	22.1261	22.4109	22.4089	22.4368	22.8830	22.4248	22.8945	22.4206	22.8007	22.4484	23.0762	18.8754	19.1563	19.3318	19.3779	19.6906	19.3670	19.6451	19.3613	19.6060	19.3874	20.0629	**15**
C8`	35.4186	36.2057	36.4938	36.6074	36.9572	36.5854	37.0943	36.5678	37.0740	36.6266	37.5278	30.8382	31.3589	31.4328	31.3034	31.6769	31.2857	31.6655	31.2743	31.6728	31.3199	31.7523	**30.6**
H2	7.9984	7.9462	7.9926	7.8437	7.9619	7.8472	7.9988	7.8508	7.9566	7.8408	7.9884	8.0381	7.9804	7.9995	7.8367	7.9277	7.8386	7.8462	7.8407	7.8716	7.8351	7.8636	**7.77**
H4	7.0832	7.2948	7.4334	7.3724	7.5572	7.3683	7.6011	7.3642	7.5818	7.3766	7.6225	7.0956	7.2971	7.4332	7.3637	7.5496	7.3601	7.5778	7.3566	7.5651	7.3673	7.6001	**7.71**
H6	7.5080	7.7233	7.8376	7.7993	8.0168	7.7927	8.0585	7.7861	8.0187	7.8060	8.0873	7.3277	7.5509	7.6920	7.6059	7.8635	7.5999	7.8225	7.5941	7.8231	7.6118	7.8746	**7.77**
H8	4.2244	4.3218	4.3363	4.3859	4.4639	4.3805	4.5066	4.3754	4.4841	4.3914	4.5242	4.3982	4.5566	4.6310	4.6308	4.7673	4.6266	4.7817	4.6225	4.7690	4.6350	4.8120	**5.21**
H(9A-9C)	1.2876	1.2869	1.2584	1.2481	1.2462	1.2494	1.2633	1.2508	1.2451	1.2472	1.2817	1.3692	1.4158	1.3930	1.4134	1.3981	1.4117	1.3832	1.4100	1.3862	1.4152	1.4170	**1.43**
H(8`A-8`C)	2.4511	2.4020	2.3692	2.3869	2.3468	2.3885	2.3327	2.3902	2.3449	2.3856	2.3205	2.8305	2.7152	2.6404	2.6069	2.5659	2.6103	2.4699	2.6139	2.4942	2.6039	2.4399	**2.58**
Nuclei	O3LYP																						
C1	141.3626	142.5917	143.4253	143.2785	144.7702	143.2292	143.9688	143.1840	144.3758	143.3425	144.1238	139.5491	141.4273	142.7236	142.9561	144.1120	142.9115	144.0561	142.8662	144.3164	142.9969	144.2411	**136.1**
C2	113.3703	113.4602	114.1215	113.4378	114.1196	113.4506	114.4476	113.4585	114.4048	113.4207	114.4618	112.9638	113.3134	114.0646	113.4415	114.1732	113.4479	114.5354	113.4494	114.4548	113.4293	114.5486	**112.1**
C3	167.2430	167.5085	168.1326	167.6741	168.4865	167.6758	168.4599	167.6720	168.4406	167.6643	168.5310	167.3751	167.6171	168.2128	167.7928	168.5569	167.7911	168.5084	167.7847	168.4988	167.7878	168.5684	**162.6**
C4	108.3682	109.6094	110.1761	110.2097	110.7348	110.1846	111.5917	110.1542	111.3103	110.2257	111.7229	108.7484	109.6303	110.1384	109.8983	110.5667	109.8821	111.0426	109.8595	110.7912	109.9051	111.1742	**110.1**
C5	166.5608	166.8955	167.5845	167.1445	168.0148	167.1419	167.9649	167.1328	167.9086	167.1370	168.0393	166.9785	167.3075	167.9004	167.4880	168.3477	167.4816	168.1602	167.4698	168.1189	167.4871	168.2288	**162.5**
C6	110.7147	112.1256	113.2291	113.0516	114.4820	113.0033	114.8817	112.9494	114.6110	113.0893	115.1454	111.3304	112.8001	113.7613	113.3356	114.9980	113.3060	115.1716	113.2692	114.9381	113.3550	115.4111	**112.1**
C7	197.1096	202.9227	204.0759	205.9307	206.6632	205.7257	211.1972	205.5335	210.6445	206.1620	211.8380	201.1308	205.4540	207.2431	208.2396	209.0233	208.0862	213.3073	207.9318	212.4937	208.3824	213.8264	**194.5**
C8	63.4071	64.6633	65.4427	65.3447	66.1262	65.3194	66.6835	65.2877	66.6497	65.3608	67.3719	58.3781	60.5921	61.4222	61.9639	62.6179	61.9184	63.5423	61.8694	63.4816	62.0026	63.8364	**58.4**
C9	21.6163	21.8223	22.0722	22.1483	22.4499	22.1292	22.5737	22.1078	22.4968	22.1649	22.6690	18.2684	18.4982	18.6825	18.6658	18.9344	18.6724	19.0724	18.6734	19.0207	18.6526	19.3603	**15**
C8`	35.8449	36.6061	36.8159	37.0179	37.3811	37.0044	37.4439	36.9872	37.4422	37.0283	37.8042	31.3601	31.6168	31.8255	31.7541	32.1167	31.7420	32.0608	31.7245	32.0052	31.7589	32.0695	**30.6**
H2	7.7654	7.6576	7.7241	7.5827	7.6548	7.5893	7.7013	7.5949	7.6739	7.5741	7.6983	7.8819	7.6803	7.7054	7.5307	7.6316	7.5358	7.6236	7.5402	7.6028	7.5253	7.6210	**7.77**
H4	6.9999	7.2006	7.3323	7.2754	7.4478	7.2716	7.4875	7.2675	7.4708	7.2788	7.5074	7.0293	7.2055	7.3385	7.2666	7.4450	7.2634	7.4681	7.2597	7.4517	7.2695	7.4881	**7.71**
H6	7.3873	7.5699	7.6916	7.6502	7.8505	7.6454	7.8778	7.6403	7.8485	7.6547	7.9048	7.2170	7.3700	7.4951	7.4119	7.6454	7.4082	7.6324	7.4040	7.6060	7.4150	7.6663	**7.77**
H8	4.3029	4.3767	4.3942	4.4296	4.5168	4.4250	4.5324	4.4205	4.5098	4.4343	4.5527	4.4484	4.5879	4.6569	4.6523	4.7905	4.6483	4.8028	4.6440	4.7818	4.6558	4.8290	**5.21**
H(9A-9C)	1.2073	1.1916	1.1914	1.1840	1.1583	1.1856	1.1894	1.1866	1.1765	1.1814	1.2046	1.3141	1.3340	1.3130	1.3401	1.3206	1.3398	1.3446	1.3391	1.3349	1.3401	1.3621	**1.43**
H(8`A-8`C)	2.4839	2.4429	2.4280	2.4396	2.4097	2.4402	2.4035	2.4405	2.4078	2.4390	2.3838	2.8879	2.7280	2.6798	2.6412	2.6063	2.6447	2.5273	2.6477	2.5313	2.6379	2.4875	**2.58**
Nuclei	OLYP																						
C1	139.9317	141.4893	141.9757	142.3264	144.1779	141.9699	143.5152	141.8960	143.4707	142.3356	143.5090	137.8422	139.8035	140.8771	141.3357	142.4088	141.2953	142.5404	141.2530	142.6580	141.3692	142.7229	**136.1**
C2	111.2607	111.3302	111.9291	111.3563	112.0438	111.3476	112.3810	111.3472	112.3202	111.3404	112.3789	110.8998	111.2102	111.9201	111.3416	112.0082	111.3460	112.3951	111.3452	112.3215	111.3287	112.4020	**112.1**
C3	166.1497	166.4561	167.1627	166.6043	167.4439	166.6241	167.4295	166.6204	167.4082	166.5963	167.5092	166.3507	166.6408	167.2835	166.8169	167.6269	166.8143	167.5598	166.8059	167.5509	166.8102	167.6178	**162.6**
C4	106.4331	107.5541	108.2744	108.1019	108.4532	108.1704	109.1728	108.1487	109.0950	108.1216	109.3670	106.9212	107.6884	108.1950	107.8978	108.5118	107.8833	108.9122	107.8620	108.7216	107.9008	109.0409	**110.1**
C5	165.4456	165.7469	166.5158	166.0783	166.9903	166.0754	166.9235	166.0589	166.9417	166.0844	166.9844	166.0689	166.3827	167.0307	166.5237	167.4338	166.5176	167.2233	166.5056	167.1985	166.5198	167.2896	**162.5**
C6	108.5633	109.9551	111.0626	110.9096	112.1659	110.9017	112.4208	110.8482	112.3470	110.9540	112.7072	109.3378	110.6674	111.7118	111.1800	112.8401	111.1455	112.9211	111.1038	112.7493	111.2019	113.1364	**112.1**
C7	196.1447	202.1235	203.2664	205.4845	206.6248	204.8831	210.6583	204.6537	209.9919	205.6478	211.1253	200.0067	204.2912	205.6616	206.9151	207.4985	206.7907	211.6259	206.6619	210.8097	207.0263	212.1594	**194.5**
C8	64.6454	66.0080	66.4984	66.7441	67.6551	66.5864	68.4561	66.5415	68.1288	66.7621	69.0325	59.2123	61.7856	62.8049	63.3246	64.0800	63.2618	65.0788	63.1959	64.9446	63.3777	65.3227	**58.4**
C9	21.7818	22.1684	22.4047	22.4255	22.6858	22.4461	22.8620	22.4340	22.8390	22.4269	23.0031	18.2976	18.6452	18.9362	18.8551	19.1674	18.8500	19.3449	18.8395	19.2711	18.8509	19.6177	**15**
C8`	36.4717	37.2166	37.5427	37.7192	38.0812	37.6914	38.0701	37.6695	38.1060	37.7376	38.4066	32.0326	32.2148	32.4179	32.3497	32.6591	32.3414	32.5761	32.3270	32.5628	32.3478	32.5677	**30.6**
H2	7.5999	7.4786	7.5958	7.3931	7.4452	7.4296	7.4930	7.4377	7.4967	7.3894	7.5064	7.7420	7.5478	7.6011	7.4092	7.5167	7.4133	7.5020	7.4171	7.4929	7.4045	7.4989	**7.77**
H4	6.9196	7.1122	7.2510	7.1848	7.3514	7.1837	7.3835	7.1800	7.3757	7.1881	7.4054	6.9544	7.1227	7.2540	7.1796	7.3553	7.1765	7.3758	7.1732	7.3616	7.1820	7.3947	**7.71**
H6	7.3116	7.4687	7.6349	7.5494	7.7186	7.5623	7.7153	7.5591	7.7268	7.5546	7.7549	7.1445	7.2752	7.4043	7.3090	7.5407	7.3055	7.5166	7.3016	7.4983	7.3117	7.5496	**7.77**
H8	4.4155	4.4608	4.4984	4.5091	4.5700	4.5087	4.5678	4.5049	4.5728	4.5124	4.5944	4.5330	4.6738	4.7440	4.7345	4.8709	4.7309	4.8761	4.7270	4.8588	4.7374	4.9028	**5.21**
H(9A-9C)	1.2034	1.1869	1.1887	1.1784	1.1488	1.1851	1.1898	1.1861	1.1785	1.1773	1.2046	1.3048	1.3421	1.3385	1.3528	1.3432	1.3515	1.3635	1.3501	1.3565	1.3535	1.3790	**1.43**
H(8`A-8`C)	2.5203	2.4877	2.4625	2.4859	2.4600	2.4826	2.4515	2.4824	2.4579	2.4854	2.4231	2.9420	2.7818	2.7233	2.6889	2.6446	2.6935	2.5668	2.6978	2.5744	2.6840	2.5264	**2.58**

[a] methyl protons shifts are averaged
[b] according to [8]

Table S8. Cont. V

Nuclei	R												S										Exp. [b]
	OPBE												OPBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.1812	138.8723	139.1163	139.4007	141.3382	139.3392	140.7373	139.2702	140.7294	139.4461	140.7684	135.6936	137.9869	138.2517	138.8857	140.7933	138.7908	140.2411	138.6942	140.0456	138.9967	140.3037	**136.1**
C2	109.8919	110.0173	110.5680	109.9350	110.6768	109.9539	110.9628	109.9563	110.9088	109.9135	110.9840	109.7048	110.0227	110.6205	109.9990	110.7310	110.0165	111.0026	110.0158	110.9537	109.9766	111.0267	**112.1**
C3	162.7071	163.0900	163.7248	163.1824	163.9798	163.1966	163.9918	163.1921	163.9661	163.1640	164.1116	162.8916	163.2572	163.8507	163.3748	164.1396	163.3860	164.1179	163.3786	164.1185	163.3582	164.2212	**162.6**
C4	105.4060	106.6202	107.3523	107.1368	107.5273	107.1357	108.2322	107.1143	108.1145	107.1363	108.4534	105.7018	106.5047	107.2449	106.8213	107.1853	106.8426	107.8126	106.8384	107.7685	106.7844	108.0344	**110.1**
C5	161.9164	162.3320	163.0243	162.5860	163.4548	162.5877	163.4218	162.5718	163.4143	162.5808	163.5195	162.4480	162.8275	163.5172	162.9936	163.7483	163.0087	163.6737	163.0030	163.6944	162.9696	163.7994	**162.5**
C6	106.9347	108.4280	109.4508	109.2584	110.4890	109.2292	110.7407	109.1815	110.6431	109.2853	111.0318	107.5274	108.8555	110.0114	109.3994	110.7165	109.4062	111.0252	109.3887	110.9879	109.3779	111.3368	**112.1**
C7	193.8597	199.7724	200.5894	202.4636	203.6628	202.2557	207.7374	202.0459	206.9446	202.6493	208.1667	197.0287	201.4856	202.6204	203.8990	204.9440	203.7358	208.7355	203.5619	207.7152	204.0614	209.1422	**194.5**
C8	62.0499	63.5352	63.8315	64.1699	65.0526	64.1327	65.8606	64.0792	65.5834	64.1917	66.5203	57.5673	59.9740	60.1727	60.9227	61.9934	60.8433	62.6928	60.7594	62.3345	61.0141	62.9129	**58.4**
C9	21.0213	21.4673	21.6288	21.6535	21.9018	21.6620	22.0532	21.6529	22.0202	21.6449	22.2126	17.7135	18.1133	18.1861	18.1690	18.4254	18.1815	18.6235	18.1769	18.5344	18.1540	18.9474	**15**
C8`	35.4110	36.2146	36.4350	36.5937	36.9190	36.5825	36.8950	36.5544	36.9150	36.5974	37.2735	30.7794	30.9977	31.3304	31.1931	31.3099	31.2089	31.3431	31.2022	31.4174	31.1660	31.3730	**30.6**
H2	7.5766	7.4529	7.5784	7.3907	7.4291	7.3995	7.4747	7.4067	7.4740	7.3824	7.4893	7.6608	7.4523	7.5762	7.3715	7.4058	7.3820	7.4462	7.3903	7.4647	7.3585	7.4563	**7.77**
H4	6.9048	7.1049	7.2391	7.1769	7.3396	7.1740	7.3728	7.1703	7.3619	7.1790	7.3974	6.9316	7.1080	7.2431	7.1705	7.3316	7.1686	7.3613	7.1657	7.3523	7.1710	7.3852	**7.71**
H6	7.3078	7.4687	7.6341	7.5464	7.7024	7.5450	7.6982	7.5424	7.7009	7.5477	7.7400	7.1032	7.2382	7.4012	7.2978	7.4777	7.2985	7.4906	7.2974	7.4933	7.2947	7.5355	**7.77**
H8	4.4207	4.4774	4.5101	4.5129	4.5671	4.5118	4.5675	4.5102	4.5668	4.5146	4.5972	4.5673	4.6985	4.7702	4.7580	4.8639	4.7571	4.8853	4.7547	4.8808	4.7571	4.9206	**5.21**
H(9A-9C)	1.1579	1.1423	1.1394	1.1402	1.1007	1.1419	1.1426	1.1425	1.1316	1.1379	1.1616	1.2676	1.2969	1.2853	1.3068	1.2710	1.3074	1.3042	1.3072	1.3029	1.3053	1.3266	**1.43**
H(8`A-8`C)	2.4393	2.4071	2.3704	2.3982	2.3658	2.3985	2.3593	2.3985	2.3633	2.3972	2.3334	2.7958	2.6308	2.6094	2.5655	2.4923	2.5721	2.4383	2.5771	2.4578	2.5571	2.4038	**2.58**
Nuclei	OPW91																						
C1	137.4649	139.1592	139.4169	139.6610	141.6192	139.5905	141.0231	139.5198	141.0076	139.7106	141.0485	135.9557	138.2763	138.5406	139.1355	141.0648	139.0425	140.4970	138.9459	140.3175	139.2166	140.5653	**136.1**
C2	110.1375	110.2661	110.8141	110.1874	110.9185	110.1968	111.2077	110.1903	111.1546	110.1619	111.2312	109.9425	110.2676	110.8643	110.2492	110.9718	110.2566	111.2474	110.2466	111.1970	110.2234	111.2745	**112.1**
C3	163.0964	163.4809	164.1118	163.5792	164.3651	163.5832	164.3755	163.5690	164.3505	163.5567	164.4971	163.2811	163.6458	164.2359	163.7698	164.5237	163.7705	164.5015	163.7535	164.5018	163.7505	164.6057	**162.6**
C4	105.6185	106.8346	107.5563	107.3683	107.7346	107.3572	108.4397	107.3242	108.3272	107.3613	108.6653	105.9244	106.7214	107.4557	107.0607	107.3992	107.0668	108.0369	107.0497	107.9846	107.0309	108.2592	**110.1**
C5	162.3102	162.7241	163.4119	162.9843	163.8421	162.9762	163.8068	162.9507	163.8018	162.9744	163.9064	162.8434	163.2203	163.9061	163.3985	164.1385	163.4014	164.0653	163.3852	164.0839	163.3751	164.1918	**162.5**
C6	107.1867	108.6822	109.7033	109.5296	110.7452	109.4903	110.9969	109.4319	110.9022	109.5506	111.2930	107.7879	109.1154	110.2699	109.6850	110.9795	109.6769	111.2976	109.6464	111.2534	109.6699	111.6092	**112.1**
C7	194.1982	200.1322	200.9603	202.8148	204.0355	202.5992	208.1332	202.3891	207.3379	203.0053	208.5588	197.4052	201.8757	203.0092	204.2746	205.3210	204.1075	209.1191	203.9293	208.1088	204.4200	209.5337	**194.5**
C8	62.2341	63.7170	64.0244	64.3411	65.2301	64.2932	66.0436	64.2338	65.7594	64.3640	66.7003	57.7227	60.1597	60.3639	61.0879	62.1725	61.0070	62.8615	60.9199	62.5151	61.1566	63.0850	**58.4**
C9	21.0828	21.5343	21.6908	21.7299	21.9658	21.7286	22.1168	21.7091	22.0865	21.7154	22.2778	17.7891	18.1949	18.2691	18.2576	18.5064	18.2600	18.7061	18.2461	18.6163	18.2380	19.0298	**15**
C8`	35.4773	36.2829	36.5031	36.6722	36.9885	36.6515	36.9687	36.6153	36.9900	36.6728	37.3482	30.8712	31.0887	31.4196	31.3002	31.4020	31.3026	31.4406	31.2844	31.5120	31.2757	31.4754	**30.6**
H2	7.5829	7.4592	7.5830	7.4002	7.4347	7.4084	7.4796	7.4147	7.4797	7.3908	7.4947	7.6697	7.4578	7.5813	7.3815	7.4120	7.3902	7.4536	7.3975	7.4706	7.3705	7.4633	**7.77**
H4	6.9089	7.1088	7.2427	7.1818	7.3430	7.1783	7.3763	7.1742	7.3656	7.1835	7.4008	6.9362	7.1118	7.2468	7.1755	7.3350	7.1728	7.3654	7.1695	7.3559	7.1762	7.3889	**7.71**
H6	7.3110	7.4719	7.6361	7.5537	7.7066	7.5516	7.7021	7.5483	7.7059	7.5541	7.7441	7.1085	7.2422	7.4048	7.3053	7.4824	7.3046	7.4965	7.3027	7.4979	7.3035	7.5410	**7.77**
H8	4.4204	4.4775	4.5098	4.5151	4.5678	4.5134	4.5680	4.5114	4.5679	4.5160	4.5975	4.5628	4.6945	4.7660	4.7566	4.8607	4.7544	4.8833	4.7514	4.8776	4.7562	4.9181	**5.21**
H(9A-9C)	1.1599	1.1444	1.1417	1.1432	1.1027	1.1441	1.1446	1.1444	1.1334	1.1406	1.1635	1.2686	1.2979	1.2867	1.3091	1.2728	1.3090	1.3062	1.3084	1.3045	1.3076	1.3284	**1.43**
H(8`A-8`C)	2.4408	2.4087	2.3725	2.4002	2.3676	2.3999	2.3614	2.3997	2.3653	2.3990	2.3356	2.8007	2.6350	2.6134	2.5722	2.4972	2.5776	2.4439	2.5820	2.4625	2.5648	2.4093	**2.58**
Nuclei	PBE																						
C1	142.3264	142.9692	144.1140	143.6534	144.6389	143.5845	144.3049	143.5172	144.6953	143.6967	144.4630	140.9980	141.6745	142.9296	142.8397	144.0948	142.8359	144.5159	142.8421	144.1071	142.8602	144.4215	**136.1**
C2	114.6465	114.8007	115.5427	114.7739	115.4551	114.7664	115.9778	114.7677	115.9491	114.7876	116.0037	114.3100	114.4990	115.1982	114.6369	115.3349	114.6447	115.9596	114.6625	115.7841	114.6471	115.9521	**112.1**
C3	171.7230	172.1720	172.7788	172.2080	173.1901	172.2058	173.1540	172.2141	173.1313	172.2296	173.2513	171.7500	172.1886	172.8133	172.2495	173.2218	172.2434	173.2035	172.2478	173.1868	172.2732	173.2844	**162.6**
C4	110.6135	112.2095	112.7580	112.7919	113.5797	112.7526	114.4831	112.7264	114.1839	112.8507	114.6795	110.9480	112.3532	112.8695	112.6836	113.4832	112.6466	114.0561	112.6206	113.9495	112.7363	114.2975	**110.1**
C5	170.9566	171.6896	172.3417	171.9184	173.0405	171.9015	172.9803	171.8955	172.9167	171.9540	173.0912	171.2912	171.9293	172.5189	172.0257	173.0859	172.0095	172.9227	172.0045	172.9243	172.0590	173.0127	**162.5**
C6	112.9770	114.7134	115.6669	115.3335	117.2369	115.3017	117.5110	115.2840	117.2177	115.3969	117.8935	113.2854	115.2657	116.3852	115.9336	117.8610	115.8750	117.9666	115.8270	117.9573	116.0070	118.4525	**112.1**
C7	200.8509	205.4530	207.1570	208.2153	208.8747	207.9959	213.2527	207.7855	212.6962	208.3981	213.9443	205.5002	209.2264	210.6267	211.1437	212.1756	211.0402	216.4495	210.9467	215.2852	211.2597	216.6164	**194.5**
C8	67.1268	68.3681	69.1368	68.8469	69.7914	68.8299	70.3156	68.8198	70.2917	68.8812	71.1404	61.6919	63.1272	64.0110	64.2948	65.2230	64.2534	65.9732	64.2220	65.7025	64.3512	66.3289	**58.4**
C9	23.1425	23.6066	23.6477	23.6635	24.1923	23.6677	24.2576	23.6820	24.1399	23.6884	24.5020	19.8413	20.3637	20.5834	20.6126	21.0496	20.5977	21.1236	20.5930	21.1134	20.6442	21.7535	**15**
C8`	36.9383	37.7451	37.9826	38.0604	38.4970	38.0341	38.6438	38.0196	38.6344	38.1013	39.1128	31.9936	32.5377	32.5508	32.3542	32.7959	32.3362	32.8235	32.3296	32.8398	32.3895	32.8605	**30.6**
H2	7.7868	7.7481	7.7927	7.6571	7.7742	7.6648	7.7943	7.6738	7.7638	7.6537	7.7916	7.8541	7.7964	7.8112	7.6571	7.7401	7.6587	7.6940	7.6609	7.7282	7.6562	7.7124	**7.77**
H4	6.8986	7.1083	7.2450	7.1820	7.3688	7.1778	7.4079	7.1742	7.3902	7.1866	7.4289	6.9185	7.1160	7.2504	7.1780	7.3648	7.1744	7.3924	7.1712	7.3796	7.1820	7.4126	**7.71**
H6	7.4038	7.6094	7.7089	7.6683	7.8894	7.6634	7.9151	7.6602	7.8817	7.6749	7.9457	7.1780	7.3881	7.5272	7.4387	7.6931	7.4327	7.6723	7.4272	7.6774	7.4451	7.7276	**7.77**
H8	4.4981	4.5739	4.5775	4.6157	4.6915	4.6104	4.7198	4.6062	4.7001	4.6208	4.7375	4.6331	4.7814	4.8582	4.8598	4.9935	4.8557	5.0146	4.8522	4.9971	4.8642	5.0431	**5.21**
H(9A-9C)	1.3572	1.3602	1.3373	1.3264	1.3268	1.3308	1.3382	1.3360	1.3247	1.3249	1.3608	1.4537	1.5017	1.4843	1.5026	1.4938	1.5009	1.4929	1.4996	1.5029	1.5049	1.5373	**1.43**
H(8`A-8`C)	2.5581	2.4988	2.4735	2.4798	2.4405	2.4818	2.4244	2.4838	2.4349	2.4785	2.4056	2.9585	2.8351	2.7604	2.7228	2.6787	2.7261	2.5878	2.7299	2.6101	2.7205	2.5499	**2.58**
Nuclei	PBE0																						
C1	143.7461	144.0537	144.9521	144.4974	145.5986	144.4554	145.1130	144.4229	145.5819	144.5521	145.1926	142.7533	143.1733	144.3512	144.3031	145.3449	144.2894	145.8180	144.2776	145.4321	144.3186	145.7442	**136.1**
C2	116.8542	116.9461	117.6760	116.9089	117.6070	116.9051	118.1795	116.9043	118.0904	116.9176	118.1421	116.6200	116.7717	117.4939	116.9207	117.5687	116.9203	118.1939	116.9217	117.9969	116.9242	118.1537	**112.1**
C3	170.5711	170.8237	171.3384	170.8919	171.6113	170.8833	171.6526	170.8766	171.5934	170.9029	171.6736	170.5958	170.8311	171.3650	170.9264	171.6399	170.9171	171.7266	170.9096	171.6474	170.9382	171.7307	**162.6**
C4	112.2591	113.8270	114.4269	114.4955	115.1959	114.4510	116.2103	114.4078	115.8161	114.5397	116.3379	112.4907	113.8980	114.4624	114.3076	115.0705	114.2658	115.6922	114.2254	115.5153	114.3503	115.8544	**110.1**
C5	169.7460	170.3268	170.8778	170.6171	171.4603	170.5937	171.4896	170.5723	171.3802	170.6425	171.5286	169.9477	170.4466	170.9573	170.6144	171.4293	170.5933	171.3601	170.5739	171.2951	170.6379	171.3812	**162.5**
C6	114.7836	116.6396	117.6901	117.4177	119.1506	117.3682	119.5336	117.3176	119.1379	117.4626	119.8318	115.1057	117.1331	118.2471	117.8622	119.7407	117.8009	119.8831	117.7415	119.8177	117.9233	120.2527	**112.1**
C7	200.4246	205.1043	206.5017	207.8220	208.4140	207.6373	213.4387	207.4637	212.7269	208.0149	214.1148	204.5369	208.4835	209.8905	210.7092	211.4193	210.5820	216.4328	210.4558	215.0489	210.8322	216.7267	**194.5**
C8	63.0036	64.1501	64.8786	64.6307	65.4465	64.6012	65.9772	64.5720	65.9054	64.6600	66.6666	57.7852	59.0529	59.8501	60.1927	60.9323	60.1504	61.8163	60.1099	61.4928	60.2359	62.0696	**58.4**
C9	22.1140	22.4409	22.6095	22.5719	22.9486	22.5614	22.9482	22.5508	22.7920	22.5812	23.0886	18.8504	19.1591	19.3141	19.3668	19.6962	19.3562	19.7491	19.3475	19.7050	19.3798	20.1570	**15**
C8`	35.3215	36.1066	36.3265	36.4449	36.7998	36.4180	37.0460	36.3936	36.9698	36.4744	37.4328	30.5943	31.1062	31.1761	31.0537	31.3870	31.0284	31.4879	31.0054	31.4180	31.0811	31.4971	**30.6**
H2	8.0001	7.9597	8.0168	7.8853	7.9746	7.8909	8.0071	7.8959	7.9631	7.8786	8.0008	8.0375	7.9791	7.9965	7.8393	7.9246	7.8413	7.8671	7.8434	7.8949	7.8370	7.8783	**7.77**
H4	7.0682	7.2802	7.4180	7.3579	7.5417	7.3536	7.5886	7.3492	7.5665	7.3616	7.6076	7.0802	7.2817	7.4180	7.3486	7.5328	7.3446	7.5662	7.3406	7.5500	7.3520	7.5849	**7.71**
H6	7.5106	7.7314	7.8402	7.8086	8.0186	7.8040	8.0571	7.7992	8.0142	7.8124	8.0884	7.3219	7.5445	7.6856	7.6025	7.8594	7.5963	7.8387	7.5900	7.8383	7.6082	7.8863	**7.77**
H8	4.2176	4.3106	4.3166	4.3741	4.4479	4.3693	4.4955	4.3648	4.4723	4.3787	4.5115	4.4008	4.5577	4.6351	4.6346	4.7687	4.6299	4.7928	4.6251	4.7730	4.6388	4.8164	**5.21**
H(9A-9C)	1.2972	1.3059	1.2906	1.2811	1.2640	1.2834	1.2767	1.2852	1.2565	1.2777	1.2948	1.3816	1.4270	1.4015	1.4245	1.4088	1.4232	1.4084	1.4219	1.4146	1.4256	1.4404	**1.43**
H(8`A-8`C)	2.4583	2.4055	2.3811	2.3913	2.3498	2.3921	2.3382	2.3930	2.3480	2.3902	2.3206	2.8339	2.7160	2.6412	2.6083	2.5641	2.6110	2.4752	2.6138	2.4949	2.6055	2.4399	**2.58**

[a] methyl protons shifts are averaged

[b] according to [8]

Table S8. Cont. VI

Nuclei	R											S										Exp. [b]
	TPSS																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.0320	139.1927	139.8805	139.6963	140.8651	139.6715	140.4903	139.6590	140.1897	139.7346	140.5585	137.8969	138.3691	139.6062	139.3674	140.5425	139.3728	140.3747	139.3877	140.4527	139.3712	140.4449	**136.1**
C2	112.6267	112.6374	113.3677	112.6440	113.3116	112.6494	113.8609	112.6669	113.0897	112.6505	113.8475	112.3073	112.4047	113.1583	112.5649	113.1915	112.5767	113.7134	112.5991	113.8650	112.5637	113.7020	**112.1**
C3	168.1648	168.4103	169.0601	168.5412	169.3567	168.5411	169.3212	168.5523	169.1986	168.5515	169.3772	168.2185	168.4575	169.1344	168.5952	169.4188	168.5935	169.3950	168.6030	169.4489	168.6074	169.4494	**162.6**
C4	108.6424	110.0741	110.8358	110.7551	111.4035	110.7224	112.3338	110.7010	111.1159	110.7968	112.5058	108.9467	110.1588	110.7639	110.5940	111.2688	110.5601	111.9747	110.5379	111.8193	110.6371	112.1574	**110.1**
C5	167.4574	167.9837	168.7324	168.2968	169.2479	168.2844	169.1829	168.2835	168.9287	168.3189	169.2587	167.7620	168.2007	168.8555	168.3932	169.3017	168.3806	169.1518	168.3796	169.2272	168.4164	169.2226	**162.5**
C6	110.8894	112.5810	113.7273	113.3672	114.9798	113.3251	115.2832	113.2936	113.7189	113.4157	115.6298	111.0950	112.9078	114.0786	113.7000	115.4240	113.6475	115.8192	113.6066	114.8650	113.7609	116.1284	**112.1**
C7	196.8898	201.0326	202.3886	203.5739	204.3978	203.4243	208.8853	203.2879	204.0732	203.7317	209.5248	201.1453	204.6201	206.0260	206.5468	207.4085	206.4406	211.3099	206.3453	206.9081	206.6577	211.7826	**194.5**
C8	65.6505	66.7365	67.3988	67.2040	68.0191	67.1783	68.5460	67.1629	67.4037	67.2378	69.2740	60.9437	62.2356	63.1513	63.3814	64.1964	63.3533	64.9001	63.3354	64.9708	63.4172	65.1130	**58.4**
C9	23.7373	24.0413	24.3455	24.2739	24.6158	24.2687	24.6603	24.2744	24.3436	24.2875	24.8535	20.5507	20.9426	21.2845	21.2925	21.6427	21.2874	21.9056	21.2934	23.2441	21.3074	22.3209	**15**
C8`	37.3639	38.0816	38.4074	38.4438	38.8144	38.4249	39.0149	38.4179	38.5437	38.4734	39.4169	33.0644	33.3942	33.5030	33.3087	33.6361	33.2916	33.6935	33.2868	35.1476	33.3365	33.7248	**30.6**
H2	7.8252	7.7977	7.8940	7.7309	7.8235	7.7355	7.8412	7.7406	7.5780	7.7267	7.8368	7.8721	7.8044	7.8260	7.6834	7.7618	7.6844	7.7525	7.6862	7.8018	7.6831	7.7531	**7.77**
H4	6.9040	7.1119	7.2605	7.1929	7.3821	7.1886	7.4232	7.1849	7.0200	7.1973	7.4416	6.9252	7.1216	7.2632	7.1918	7.3797	7.1876	7.4108	7.1841	7.3034	7.1961	7.4288	**7.71**
H6	7.3174	7.5411	7.6864	7.6209	7.8341	7.6166	7.8578	7.6129	7.4497	7.6254	7.8906	7.1229	7.3367	7.4845	7.4089	7.6600	7.4021	7.6705	7.3959	7.5136	7.4159	7.7128	**7.77**
H8	4.3763	4.4463	4.4832	4.5118	4.5949	4.5086	4.6190	4.5061	4.3305	4.5155	4.6337	4.4877	4.6419	4.7253	4.7309	4.8643	4.7260	4.8878	4.7218	4.8596	4.7359	4.9156	**5.21**
H(9A-9C)	1.3498	1.3703	1.3660	1.3492	1.3314	1.3504	1.3433	1.3521	1.1638	1.3480	1.3628	1.4356	1.4849	1.4734	1.4977	1.4863	1.4959	1.5128	1.4947	1.6566	1.4998	1.5367	**1.43**
H(8`A-8`C)	2.5139	2.4524	2.4122	2.4440	2.4057	2.4445	2.3918	2.4455	2.2616	2.4439	2.3718	2.9239	2.7964	2.7296	2.6961	2.6526	2.6981	2.5640	2.7009	2.8538	2.6948	2.5317	**2.58**
Nuclei	VSXC																						
C1	136.4899	136.5707	137.2694	136.5436	137.6629	136.5500	137.1133	136.5540	137.1949	136.5390	137.2307	136.4584	136.7193	137.6773	137.6452	139.2991	137.6318	138.6256	137.6170	138.6294	137.6600	138.7786	**136.1**
C2	110.7860	110.9165	111.4359	110.8176	111.3120	110.8320	111.8107	110.8430	111.7327	110.8046	111.8623	110.2901	110.5045	111.0804	110.3228	110.8104	110.3311	111.2166	110.3371	111.1379	110.3161	111.2502	**112.1**
C3	165.9127	166.2688	166.8285	166.4713	167.2394	166.4599	167.1798	166.4472	167.1710	166.4841	167.2522	166.6137	166.9403	167.5028	167.1734	167.9889	167.1650	167.9516	167.1544	167.9288	167.1828	168.0245	**162.6**
C4	106.3237	107.9853	108.6190	108.8608	109.5102	108.8097	110.4017	108.7567	110.1607	108.9109	110.6389	106.3246	107.8270	108.4136	108.4550	108.9912	108.4154	109.8011	108.3733	109.5933	108.4938	110.0055	**110.1**
C5	165.2128	165.8995	166.5559	166.3090	167.2505	166.2853	167.1638	166.2598	167.1371	166.3333	167.2734	165.8733	166.4278	167.0232	166.8227	167.6567	166.8064	167.5709	166.7880	167.5430	166.8397	167.6586	**162.5**
C6	110.4069	112.1813	113.2342	113.1372	114.7166	113.0823	115.1142	113.0250	114.8896	113.1903	115.4863	110.1809	112.0242	113.1047	112.9314	114.4672	112.8798	114.8442	112.8259	114.6752	112.9818	115.1008	**112.1**
C7	191.1783	195.0592	196.3405	197.0699	198.0032	196.9526	201.5361	196.8329	200.7591	197.1822	202.2738	192.7128	196.2309	197.5011	198.0639	199.4455	197.9479	202.8024	197.8297	201.9453	198.1760	203.5027	**194.5**
C8	71.4856	72.2249	72.7672	72.5613	73.2980	72.5432	73.5879	72.5231	73.5167	72.5800	74.1214	63.5660	64.6615	65.3151	65.6520	66.7735	65.6137	66.9966	65.5735	66.8262	65.6903	67.4190	**58.4**
C9	27.3817	28.2799	28.6395	28.9932	29.5289	28.9381	29.6567	28.8839	29.5426	29.0505	29.7187	27.8953	27.9558	28.0274	28.5419	28.7874	28.5400	28.6536	28.5364	28.6330	28.5454	28.8949	**15**
C8`	40.5326	40.9917	41.0961	41.2845	41.4705	41.2682	41.5452	41.2499	41.5351	41.3016	41.9592	35.6840	36.4721	36.4542	36.8912	37.2295	36.8664	37.3102	36.8396	37.2360	36.9162	37.6915	**30.6**
H2	7.9505	7.9214	7.9800	7.8838	7.9436	7.8869	7.9781	7.8900	7.9781	7.8806	7.9767	7.9894	7.9329	7.9810	7.8988	7.8971	7.9024	7.9258	7.9060	7.9343	7.8953	7.9209	**7.77**
H4	6.9210	7.1330	7.2738	7.2145	7.4005	7.2102	7.4386	7.2058	7.4219	7.2185	7.4660	6.9619	7.1593	7.2992	7.2489	7.4289	7.2448	7.4639	7.2407	7.4473	7.2527	7.4842	**7.71**
H6	7.4961	7.6999	7.8382	7.8141	8.0312	7.8064	8.0578	7.7989	8.0390	7.8216	8.0949	7.1529	7.3593	7.4825	7.3795	7.6045	7.3738	7.6326	7.3680	7.6129	7.3849	7.6674	**7.77**
H8	4.2838	4.3651	4.3977	4.4448	4.5240	4.4385	4.5551	4.4325	4.5353	4.4511	4.5771	4.5819	4.7449	4.8133	4.7860	4.9358	4.7803	4.9634	4.7747	4.9426	4.7914	4.9967	**5.21**
H(9A-9C)	1.5988	1.6163	1.6026	1.6251	1.6006	1.6243	1.6225	1.6237	1.6177	1.6260	1.6324	1.8175	1.8343	1.8045	1.7137	1.6896	1.7132	1.7080	1.7128	1.7028	1.7142	1.7182	**1.43**
H(8`A-8`C)	2.6256	2.5899	2.5626	2.5759	2.5414	2.5766	2.5379	2.5776	2.5393	2.5752	2.5209	2.8621	2.7762	2.7019	2.6401	2.5700	2.6422	2.5503	2.6445	2.5608	2.6381	2.5171	**2.58**
Nuclei	wB97																						
C1	145.0826	144.9223	145.9029	145.0505	146.2222	145.0328	145.3538	145.0135	145.8907	145.0655	145.4755	144.2803	144.4261	145.5347	145.5296	146.4749	145.5118	146.6544	145.4943	146.3506	145.5484	146.8025	**136.1**
C2	118.1726	118.2742	119.0406	118.2213	119.0099	118.2243	119.4293	118.2267	119.3604	118.2189	119.4690	117.9485	118.1550	118.9170	118.2967	119.0518	118.2952	119.4923	118.2931	119.3739	118.2986	119.5328	**112.1**
C3	172.0070	171.9914	172.4482	172.0128	172.6148	172.0097	172.5295	172.0060	172.5450	172.0161	172.5793	172.0384	171.9949	172.4605	172.0596	172.6431	172.0558	172.6090	172.0517	172.5861	172.0637	172.6669	**162.6**
C4	113.2888	114.7490	115.4215	115.4241	116.2153	115.3840	117.0173	115.3432	116.7046	115.4627	117.1969	113.4176	114.7417	115.3931	115.1702	116.0260	115.1343	116.4766	115.0972	116.3765	115.2043	116.6526	**110.1**
C5	171.0046	171.3571	171.8358	171.6189	172.3403	171.5997	172.2476	171.5803	172.2210	171.6378	172.3346	171.0775	171.3627	171.8136	171.5531	172.2290	171.5365	172.0609	171.5193	172.0466	171.5695	172.1434	**162.5**
C6	115.9785	117.9769	119.0565	118.9213	120.7117	118.8665	121.0521	118.8112	120.6774	118.9744	121.3902	116.3838	118.4291	119.6122	119.1708	121.1674	119.1165	121.2452	119.0611	121.2338	119.2221	121.5429	**112.1**
C7	200.1093	204.7281	206.3248	207.3562	208.0548	207.1858	212.9349	207.0137	212.2226	207.5165	213.7911	203.5137	207.6133	209.1336	210.1467	210.7829	210.0042	215.8404	209.8607	214.5107	210.2822	216.5410	**194.5**
C8	61.6202	62.5762	63.2299	63.0115	63.8145	62.9864	64.2175	62.9609	64.1337	63.0364	64.8408	56.2260	57.3419	58.1165	58.4065	59.1322	58.3670	59.8998	58.3272	59.6263	58.4454	60.1581	**58.4**
C9	21.6048	21.7553	21.9731	21.9694	22.3893	21.9515	22.2642	21.9325	22.1502	21.9863	22.3841	19.2381	19.2990	19.4243	19.3675	19.7073	19.3674	19.6431	19.3663	19.6338	19.3674	19.9386	**15**
C8`	35.0716	35.7062	35.9678	36.0640	36.4100	36.0444	36.5589	36.0243	36.4966	36.0835	36.9939	30.3904	30.8863	31.0502	30.9975	31.3322	30.9739	31.2648	30.9497	31.2906	31.0203	31.4255	**30.6**
H2	8.1073	8.0899	8.1395	8.0383	8.1248	8.0423	8.1608	8.0464	8.1212	8.0347	8.1593	8.1326	8.0849	8.1020	7.9343	8.0324	7.9375	7.9647	7.9404	7.9979	7.9313	7.9669	**7.77**
H4	7.1872	7.3977	7.5404	7.4745	7.6675	7.4702	7.7068	7.4658	7.6881	7.4785	7.7293	7.1904	7.3904	7.5305	7.4542	7.6469	7.4504	7.6702	7.4464	7.6582	7.4579	7.6921	**7.71**
H6	7.5486	7.7850	7.9139	7.8803	8.1113	7.8749	8.1459	7.8695	8.1044	7.8855	8.1828	7.4139	7.6493	7.7974	7.7138	7.9807	7.7080	7.9500	7.7020	7.9567	7.7192	7.9905	**7.77**
H8	3.9702	4.0846	4.1184	4.1610	4.2571	4.1551	4.2909	4.1492	4.2740	4.1667	4.3126	4.1904	4.3475	4.4334	4.4273	4.5640	4.4225	4.5663	4.4175	4.5563	4.4318	4.5933	**5.21**
H(9A-9C)	1.3175	1.3402	1.3126	1.3274	1.3084	1.3286	1.3219	1.3300	1.3042	1.3263	1.3411	1.3947	1.4344	1.4039	1.4225	1.4124	1.4219	1.4134	1.4212	1.4202	1.4231	1.4308	**1.43**
H(8`A-8`C)	2.4496	2.4001	2.3793	2.3914	2.3555	2.3914	2.3419	2.3914	2.3537	2.3913	2.3288	2.7846	2.6734	2.6007	2.5656	2.5306	2.5682	2.4343	2.5709	2.4590	2.5630	2.4091	**2.58**
Nuclei	wB97X																						
C1	146.1533	146.0408	147.0630	146.3235	147.4985	146.3094	146.7087	146.2899	147.4259	146.3337	146.7758	145.2819	145.4934	146.6234	146.6407	147.5883	146.6277	148.5151	146.6145	147.5264	146.6549	148.3190	**136.1**
C2	118.8280	118.9086	119.6873	118.8638	119.6383	118.8692	120.1058	118.8732	119.9772	118.8594	120.1250	118.5660	118.7553	119.5141	118.8998	119.6210	118.9016	120.1059	118.9027	119.9349	118.8994	120.1334	**112.1**
C3	172.7139	172.7559	173.2264	172.8015	173.4277	172.7999	173.3966	172.7976	173.3654	172.8038	173.4317	172.7736	172.7904	173.2737	172.8788	173.4875	172.8770	173.5371	172.8747	173.4168	172.8819	173.5665	**162.6**
C4	113.7735	115.2536	115.8992	115.9264	116.6794	115.8879	117.5491	115.8493	117.1411	115.9643	117.7262	113.9279	115.2663	115.8959	115.7017	116.5290	115.6675	116.8714	115.6320	116.8556	115.7349	117.1119	**110.1**
C5	171.7216	172.1256	172.6258	172.4202	173.1643	172.4021	173.1174	172.3834	173.0385	172.4384	173.1939	171.8205	172.1586	172.6298	172.3663	173.0788	172.3517	172.9999	172.3363	172.8833	172.3814	173.0482	**162.5**
C6	116.5474	118.5245	119.5713	119.4110	121.1714	119.3587	121.5130	119.3074	120.9845	119.4636	121.8886	116.9492	118.9693	120.1294	119.7106	121.6734	119.6566	121.3860	119.6015	121.6875	119.7628	121.8870	**112.1**
C7	201.8675	206.5338	208.1370	209.3110	209.9762	209.1429	215.0236	208.9703	214.5731	209.4676	215.7754	205.5387	209.6469	211.1262	212.1533	212.7801	212.0169	218.6313	211.8787	216.5475	212.2840	218.9106	**194.5**
C8	62.6875	63.6992	64.3519	64.1313	64.9471	64.1039	65.3578	64.0753	65.2340	64.1577	66.0205	57.2642	58.4161	59.2042	59.5452	60.2474	59.5068	61.1728	59.4682	60.7630	59.5834	61.4158	**58.4**
C9	21.8596	22.0221	22.2439	22.2484	22.6326	22.2383	22.5022	22.2274	22.2411	22.2596	22.6780	19.3448	19.3922	19.5193	19.5010	19.8116	19.5023	19.6051	19.5028	19.7154	19.5009	20.0120	**15**
C8`	35.3135	36.0071	36.2338	36.3520	36.7174	36.3308	36.8859	36.3086	36.7846	36.3729	37.3249	30.6160	31.0923	31.2302	31.1627	31.5000	31.1419	31.4760	31.1203	31.4397	31.1835	31.5930	**30.6**
H2	8.0877	8.0686	8.1159	8.0053	8.0919	8.0093	8.1262	8.0138	8.0641	8.0019	8.1269	8.1197	8.0643	8.0830	7.9130	8.0118	7.9160	7.8863	7.9189	7.9697	7.9102	7.9141	**7.77**
H4	7.1555	7.3665	7.5075	7.4458	7.6352	7.4416	7.6762	7.4374	7.6552	7.4498	7.6974	7.1630	7.3625	7.5012	7.4292	7.6189	7.4255	7.6413	7.4216	7.6291	7.4329	7.6628	**7.71**
H6	7.5293	7.7636	7.8866	7.8553	8.0797	7.8498	8.1141	7.8445	8.0651	7.8609	8.1517	7.3888	7.6136	7.7621	7.6811	7.9460	7.6753	7.8840	7.6694	7.9178	7.6868	7.9366	**7.77**
H8	4.0316	4.1351	4.1676	4.2171	4.3034	4.2119	4.3468	4.2067	4.3449	4.2222	4.3621	4.2337	4.3870	4.4706	4.4696	4.6064	4.4651	4.6162	4.4604	4.5973	4.4741	4.6360	**5.21**
H(9A-9C)	1.3041	1.3261	1.2975	1.3075	1.2880	1.3088	1.2990	1.3102	1.2636	1.3066	1.3214	1.3829	1.4235	1.3954	1.4156	1.4040	1.4147	1.3676	1.4140	1.4060	1.4164	1.4032	**1.43**
H(8`A-8`C)	2.4586	2.4067	2.3861	2.4003	2.3618	2.4010	2.3484	2.4015	2.3566	2.3997	2.3332	2.8075	2.6909	2.6191	2.5864	2.5511	2.5893	2.4477	2.5920	2.4749	2.5837	2.4178	**2.58**

[a] methyl protons shifts are averaged

[b] according to [8]

Table S8. Cont. VII

Nuclei	R											S										Exp. [b]
	X3LYP											X3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	146.5131	146.8886	148.1114	147.7279	148.5350	147.7222	147.8140	147.7144	148.3180	147.7403	147.9695	145.2469	145.8238	146.9766	146.9756	148.1417	146.9865	148.4999	146.9916	148.2323	146.9661	148.4624	**136.1**
C2	118.2943	118.4446	119.2449	118.5465	119.1345	118.5562	119.6437	118.5626	119.6028	118.5413	119.6659	117.9804	118.1916	118.8999	118.3918	119.0352	118.4002	119.6544	118.4049	119.5052	118.3866	119.6400	**112.1**
C3	173.8687	174.0969	174.6254	174.1783	174.9047	174.1774	174.8405	174.1732	174.8510	174.1828	174.8963	173.8692	174.0976	174.6471	174.2208	174.9462	174.2190	174.9203	174.2140	174.9156	174.2260	174.9690	**162.6**
C4	113.4075	114.9495	115.5069	115.5806	116.2576	115.5400	117.2070	115.4961	116.8765	115.6221	117.3707	113.7360	115.0424	115.5709	115.4450	116.1044	115.4087	116.6601	115.3698	116.5481	115.4831	116.8709	**110.1**
C5	173.0715	173.6274	174.2204	173.9225	174.7983	173.9075	174.7187	173.8893	174.6709	173.9401	174.7883	173.3300	173.7791	174.2988	173.9554	174.7688	173.9436	174.6024	173.9292	174.6114	173.9703	174.6701	**162.5**
C6	116.3968	118.2160	119.1487	118.9222	120.7628	118.8635	121.1769	118.8015	120.8400	118.9807	121.4949	116.7224	118.7434	119.9230	119.5108	121.3023	119.4453	121.3395	119.3777	121.2933	119.5777	121.7341	**112.1**
C7	202.9876	208.0050	209.8673	211.3345	211.6414	211.1695	216.5488	211.0033	215.8373	211.4987	217.3552	207.8705	211.8760	213.2107	214.0825	214.9054	213.9813	219.9420	213.8748	218.7319	214.1806	220.3322	**194.5**
C8	65.5754	66.6287	67.3695	67.2047	67.9103	67.1847	68.4674	67.1606	68.4791	67.2266	69.1711	60.1100	61.5763	62.4770	62.8571	63.5886	62.8163	64.4103	62.7715	64.1073	62.8984	64.6548	**58.4**
C9	22.7411	23.0238	23.0347	23.0706	23.4886	23.0585	23.5335	23.0440	23.4491	23.0858	23.6756	19.3798	19.6455	19.8964	19.8878	20.1551	19.8747	20.1559	19.8583	20.1226	19.9038	20.5216	**15**
C8`	36.2822	37.0691	37.3895	37.5204	37.8660	37.5004	38.0025	37.4765	37.9679	37.5421	38.4156	31.7762	32.2300	32.2895	32.1927	32.5392	32.1770	32.5622	32.1588	32.5884	32.2120	32.6385	**30.6**
H2	7.9718	7.9297	7.9690	7.8247	7.9488	7.8278	7.9838	7.8303	7.9445	7.8215	7.9780	8.0353	7.9546	7.9777	7.8211	7.8992	7.8218	7.8426	7.8222	7.8688	7.8207	7.8562	**7.77**
H4	7.0673	7.2752	7.4142	7.3538	7.5367	7.3495	7.5783	7.3447	7.5593	7.3578	7.5988	7.0821	7.2773	7.4133	7.3435	7.5260	7.3397	7.5537	7.3354	7.5418	7.3470	7.5748	**7.71**
H6	7.4687	7.6954	7.8099	7.7748	8.0026	7.7677	8.0371	7.7601	7.9973	7.7814	8.0669	7.2926	7.5069	7.6512	7.5681	7.8151	7.5616	7.7900	7.5548	7.7900	7.5743	7.8393	**7.77**
H8	4.2514	4.3527	4.3701	4.4145	4.5091	4.4091	4.5334	4.4033	4.5102	4.4200	4.5527	4.3907	4.5522	4.6269	4.6326	4.7652	4.6282	4.7866	4.6232	4.7722	4.6368	4.8159	**5.21**
H(9A-9C)	1.3127	1.3128	1.2832	1.2763	1.2711	1.2771	1.2954	1.2773	1.2805	1.2753	1.3103	1.3927	1.4352	1.4227	1.4420	1.4235	1.4394	1.4173	1.4363	1.4214	1.4445	1.4458	**1.43**
H(8`A-8`C)	2.5092	2.4567	2.4317	2.4494	2.4045	2.4506	2.3955	2.4513	2.4080	2.4482	2.3785	2.9338	2.8045	2.7332	2.7037	2.6564	2.7067	2.5696	2.7094	2.5917	2.7010	2.5374	**2.58**

[a] methyl protons shifts are averaged

[b] according to [8]

Table S9. Theoretical chemical shifts (in ppm) of *(R,S)*-flephedrone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S										Exp. [b]
	B3LYP											B3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.3516	139.8992	140.9781	140.1863	142.0735	140.1611	141.5120	140.1358	141.5012	140.2082	141.7819	137.8738	139.3186	139.9816	139.9577	141.5554	139.9093	141.4183	139.8637	141.2810	140.0057	141.4292	**129**
C2	139.7181	139.6929	140.2565	139.4633	139.9708	139.4799	140.4199	139.4943	140.2834	139.4440	140.3925	139.0099	139.2247	139.7699	139.1806	139.8028	139.1780	140.3740	139.1755	140.2362	139.1821	140.3704	**132**
C3	121.9147	122.6511	123.2036	122.8744	123.4797	122.8576	123.7880	122.8405	123.7263	122.8887	123.8478	122.0546	122.6999	123.1853	122.8846	123.4913	122.8701	123.7328	122.8554	123.6526	122.8966	123.7867	**116**
C4	176.1996	177.1548	177.8016	177.6113	178.2556	177.5774	178.9142	177.5440	178.7922	177.6426	179.0429	176.5723	177.1853	177.8667	177.4190	178.1469	177.4023	178.5696	177.3850	178.4546	177.4322	178.7245	**167**
C5	119.7381	121.1100	121.7159	121.7876	122.5392	121.7417	122.8148	121.6959	122.7064	121.8299	122.9605	119.9339	121.1749	121.7562	121.7216	122.4902	121.6855	122.6663	121.6489	122.5622	121.7540	122.7986	**116**
C6	135.8982	137.9272	138.9534	138.9372	140.4067	138.8712	141.0202	138.8048	140.7434	138.9983	141.3636	136.2778	138.3528	139.6434	139.3323	140.9568	139.2716	141.4709	139.2095	141.2669	139.3872	141.8771	**132**
C7	202.8768	208.0691	209.7045	210.9565	211.8939	210.7561	217.3250	210.5621	216.3636	211.1520	218.3042	208.1087	212.3579	213.4837	214.5278	215.3474	214.3946	220.1153	214.2618	218.9963	214.6532	220.5944	**196**
C8	65.2601	66.4393	67.0844	66.6651	67.6873	66.6448	68.1168	66.6260	67.8105	66.6832	68.8556	59.4742	61.6544	62.2820	62.6180	63.4923	62.5505	64.2487	62.4848	63.9791	62.6825	64.4890	**60**
C9	22.9937	23.3369	23.4371	23.5103	23.7870	23.5040	23.8454	23.4947	23.7278	23.5117	23.9610	19.5432	20.0549	20.2357	20.2537	20.4684	20.2366	20.6702	20.2197	20.5736	20.2683	21.0311	**15**
C8`	36.5076	37.3387	37.5483	37.6307	37.9535	37.5944	38.1848	37.5637	38.1616	37.6692	38.6153	32.1915	32.3577	32.6229	32.4742	32.7092	32.4611	32.8316	32.4474	32.8288	32.4845	32.9175	**31**
H2	8.6288	8.5708	8.5739	8.5193	8.4862	8.5229	8.5099	8.5264	8.5151	8.5156	8.4958	8.6701	8.4976	8.5384	8.4115	8.4156	8.4168	8.3988	8.4218	8.4120	8.4060	8.4143	**8.07**
H3	7.3119	7.4474	7.5313	7.4874	7.6000	7.4852	7.6152	7.4829	7.6051	7.4891	7.6305	7.2978	7.4323	7.5140	7.4748	7.5907	7.4723	7.6048	7.4697	7.5943	7.4770	7.6211	**7.31**
H5	7.1614	7.3510	7.4352	7.4344	7.5536	7.4291	7.5704	7.4238	7.5589	7.4393	7.5939	7.1540	7.3281	7.4120	7.4019	7.5234	7.3974	7.5322	7.3928	7.5197	7.4059	7.5549	**7.31**
H6	8.0695	8.2736	8.3471	8.3829	8.4942	8.3751	8.5470	8.3677	8.5388	8.3904	8.5777	7.8720	8.0370	8.1480	8.1191	8.2781	8.1143	8.2908	8.1093	8.2781	8.1233	8.3419	**8.07**
H8	4.3623	4.4552	4.4783	4.5600	4.6044	4.5533	4.6526	4.5464	4.6504	4.5660	4.6741	4.4999	4.6578	4.7050	4.7188	4.8309	4.7153	4.8477	4.7118	4.8326	4.7217	4.8820	**5.09**
H(9A-9C)	1.3154	1.3242	1.3019	1.3025	1.2691	1.3041	1.2806	1.3055	1.2685	1.3007	1.2933	1.3888	1.4276	1.4302	1.4455	1.4215	1.4441	1.4397	1.4427	1.4360	1.4466	1.4683	**1.6**
H(8`A-8`C)	2.5071	2.4491	2.4216	2.4281	2.4102	2.4290	2.3990	2.4298	2.3931	2.4269	2.3861	2.9770	2.8044	2.7564	2.7204	2.6721	2.7257	2.5872	2.7307	2.6042	2.7151	2.5595	**2.81**
F4	-124.5867	-125.7404	-128.6276	-125.7622	-130.2938	-125.7680	-128.0611	-125.7715	-128.3171	-125.7554	-127.8310	-124.2856	-126.1284	-128.8884	-126.5189	-130.7445	-126.4983	-129.0169	-126.4776	-129.2395	-126.5402	-128.6511	**-102.1**
Nuclei	B3P86											B3P86										
C1	136.8453	137.2808	138.3582	137.5043	139.4519	137.5074	138.8537	137.4898	139.1351	137.5460	139.1283	135.6233	136.9063	137.5597	137.4853	138.9540	137.4549	138.8749	137.4076	138.7415	137.5634	138.9677	**129**
C2	138.7919	138.7416	139.3998	138.5747	139.1636	138.6075	139.5971	138.6182	139.5645	138.5873	139.5816	138.1598	138.3322	138.9376	138.3113	138.9809	138.3306	139.5077	138.3287	139.4734	138.3375	139.5260	**132**
C3	121.1158	121.8832	122.5099	122.1552	122.8745	122.1613	123.1693	122.1453	123.2080	122.1932	123.2475	121.2077	121.9036	122.4956	122.1573	122.8618	122.1638	123.0956	122.1483	123.1217	122.1950	123.1750	**116**
C4	173.6985	174.6092	175.2829	175.0662	175.7535	175.0598	176.4063	175.0315	176.3576	175.1159	176.5491	173.9907	174.6001	175.3439	174.8861	175.6462	174.8935	176.0480	174.8781	176.0672	174.9218	176.2106	**167**
C5	118.9511	120.3570	121.0389	121.0865	121.9545	121.0629	122.2291	121.0175	122.2236	121.1526	122.3983	119.0968	120.3750	121.0516	121.0069	121.8780	120.9911	122.0417	120.9530	122.0531	121.0653	122.1965	**116**
C6	134.9391	136.9571	138.0470	138.0317	139.4694	137.9871	140.0383	137.9202	139.8454	138.1179	140.4254	135.2870	137.3568	138.6630	138.3561	140.0839	138.3212	140.5742	138.2627	140.5163	138.4312	140.9668	**132**
C7	200.9937	205.8309	207.3690	208.3757	209.4937	208.2408	214.5962	208.0849	213.8337	208.5478	215.4998	205.5040	209.6504	210.9178	211.8502	212.6202	211.7370	217.2310	211.6033	216.1910	212.0035	217.7281	**196**
C8	63.6796	64.8464	65.6285	65.2068	66.1771	65.2071	66.5812	65.1854	66.4957	65.2505	67.3827	58.1084	59.9428	60.4781	60.8007	61.6333	60.7568	62.3872	60.6942	62.1777	60.8896	62.6693	**60**
C9	22.8065	23.0897	23.3077	23.3623	23.6359	23.3647	23.6593	23.3452	23.6707	23.4035	23.8216	19.4663	20.0187	20.1559	20.2089	20.4941	20.2153	20.6857	20.2003	20.7001	20.2472	21.1119	**15**
C8`	35.9286	36.7158	37.0084	37.0027	37.3475	37.0082	37.5596	36.9918	37.6189	37.0414	38.0311	31.3622	31.5731	31.9325	31.7646	32.0364	31.7748	32.1533	31.7622	32.2999	31.7969	32.2578	**31**
H2	8.6937	8.6392	8.6481	8.5947	8.5586	8.5992	8.5883	8.6018	8.5814	8.5915	8.5744	8.7028	8.5480	8.5959	8.4713	8.4868	8.4787	8.4611	8.4838	8.4913	8.4649	8.4716	**8.07**
H3	7.3323	7.4749	7.5633	7.5186	7.6361	7.5176	7.6523	7.5147	7.6476	7.5207	7.6690	7.3188	7.4600	7.5477	7.5057	7.6274	7.5044	7.6414	7.5013	7.6367	7.5080	7.6590	**7.31**
H5	7.1767	7.3724	7.4616	7.4573	7.5836	7.4536	7.6013	7.4480	7.5944	7.4620	7.6265	7.1655	7.3489	7.4382	7.4270	7.5553	7.4237	7.5640	7.4186	7.5573	7.4312	7.5880	**7.31**
H6	8.1523	8.3571	8.4270	8.4597	8.5681	8.4550	8.6211	8.4484	8.6073	8.4654	8.6536	7.9340	8.1076	8.2276	8.1948	8.3652	8.1917	8.3755	8.1865	8.3750	8.1986	8.4257	**8.07**
H8	4.3930	4.4836	4.4927	4.5762	4.6265	4.5711	4.6819	4.5642	4.6796	4.5824	4.7038	4.5540	4.6976	4.7569	4.7623	4.8783	4.7605	4.8928	4.7566	4.8883	4.7650	4.9288	**5.09**
H(9A-9C)	1.3335	1.3438	1.3286	1.3321	1.2867	1.3343	1.2965	1.3346	1.2886	1.3313	1.3143	1.4092	1.4428	1.4421	1.4554	1.4353	1.4561	1.4505	1.4549	1.4566	1.4559	1.4796	**1.6**
H(8`A-8`C)	2.4876	2.4212	2.3951	2.4005	2.3811	2.4023	2.3602	2.4024	2.3671	2.4001	2.3503	2.9176	2.7485	2.7146	2.6728	2.6287	2.6800	2.5349	2.6851	2.5651	2.6670	2.5072	**2.81**
F4	-117.1651	-117.8836	-120.5922	-117.7226	-121.9927	-117.7352	-119.6541	-117.7485	-120.0548	-117.7094	-119.4165	-117.0081	-118.3431	-120.8782	-118.5063	-122.4355	-118.4942	-120.6607	-118.4844	-120.8650	-118.5187	-120.3178	**-102.1**
Nuclei	B3PW91											B3PW91										
C1	137.0994	137.5782	138.7234	137.8703	140.2084	137.8485	139.3905	137.8187	139.3095	137.8939	139.6388	135.8270	137.2800	137.7781	137.8580	139.3488	137.8089	139.3951	137.7573	139.1374	137.9141	139.4828	**129**
C2	138.8604	138.8385	139.3967	138.6503	139.5459	138.6706	139.6266	138.6815	139.5161	138.6320	139.6248	138.2843	138.4871	139.0226	138.4452	139.1209	138.4505	139.6147	138.4477	139.5068	138.4432	139.6376	**132**
C3	121.2185	122.0069	122.5742	122.2708	123.2963	122.2610	123.2495	122.2421	123.2072	122.2821	123.3409	121.3071	122.0247	122.5329	122.2639	122.9651	122.2553	123.1906	122.2380	123.1214	122.2739	123.2752	**116**
C4	173.7409	174.6858	175.2871	175.1369	176.1105	175.1138	176.3924	175.0819	176.3209	175.1612	176.5562	174.0199	174.6397	175.3121	174.9084	175.6627	174.9018	176.0329	174.8849	175.9623	174.9153	176.2007	**167**
C5	119.0599	120.4861	121.1030	121.2065	122.3683	121.1668	122.2995	121.1183	122.2138	121.2461	122.4777	119.2098	120.5084	121.1087	121.1148	121.9791	121.0849	122.1342	121.0458	122.0478	121.1449	122.2957	**116**
C6	134.8881	136.9286	137.8816	137.9622	139.7104	137.9061	139.9572	137.8415	139.7281	138.0174	140.3326	135.2770	137.3211	138.5843	138.3076	139.9907	138.2583	140.3962	138.1982	140.2701	138.3538	140.7941	**132**
C7	201.1247	206.1066	207.7353	208.8082	210.2420	208.6327	215.1374	208.4510	214.2009	208.9795	216.0833	205.6165	209.9651	211.0502	212.1644	212.9527	212.0348	217.7726	211.8977	216.5723	212.2928	218.2699	**196**
C8	63.4567	64.6178	65.2257	64.9342	66.2583	64.9202	66.4879	64.8987	66.1020	64.9510	67.2318	58.0320	59.9926	60.4452	60.8767	61.6836	60.8128	62.5182	60.7445	62.2018	60.9444	62.8000	**60**
C9	22.5160	22.8553	22.9353	23.0789	23.6687	23.0753	23.3953	23.0617	23.2786	23.0832	23.5418	19.1832	19.7035	19.7883	19.8973	20.1279	19.8867	20.3038	19.8683	20.2280	19.9102	20.7016	**15**
C8`	35.8834	36.7085	36.8598	36.9828	37.6339	36.9657	37.5129	36.9420	37.5231	37.0038	37.9753	31.4292	31.6510	31.9335	31.8297	32.1026	31.8260	32.1558	31.8123	32.2185	31.8333	32.2536	**31**
H2	8.6633	8.6108	8.6056	8.5605	8.5329	8.5652	8.5339	8.5693	8.5526	8.5562	8.5242	8.6835	8.5130	8.5718	8.4375	8.4524	8.4445	8.4188	8.4505	8.4482	8.4303	8.4283	**8.07**
H3	7.3301	7.4703	7.5577	7.5143	7.6458	7.5126	7.6483	7.5105	7.6406	7.5160	7.6634	7.3189	7.4577	7.5443	7.5040	7.6238	7.5020	7.6404	7.4996	7.6317	7.5060	7.6558	**7.31**
H5	7.1771	7.3713	7.4596	7.4576	7.5958	7.4530	7.5980	7.4480	7.5902	7.4622	7.6214	7.1690	7.3494	7.4382	7.4277	7.5538	7.4237	7.5651	7.4194	7.5542	7.4316	7.5870	**7.31**
H6	8.1341	8.3392	8.4057	8.4426	8.5635	8.4366	8.5897	8.4305	8.5951	8.4485	8.6240	7.9194	8.0892	8.2103	8.1769	8.3421	8.1732	8.3457	8.1688	8.3441	8.1801	8.3934	**8.07**
H8	4.3741	4.4705	4.4922	4.5694	4.6265	4.5633	4.6458	4.5568	4.6625	4.5752	4.6720	4.5270	4.6702	4.7258	4.7346	4.8501	4.7322	4.8642	4.7292	4.8566	4.7367	4.8976	**5.09**
H(9A-9C)	1.2980	1.3052	1.2789	1.2881	1.2601	1.2903	1.2615	1.2922	1.2492	1.2862	1.2747	1.3734	1.4034	1.4070	1.4206	1.3953	1.4203	1.4103	1.4196	1.4138	1.4210	1.4367	**1.6**
H(8`A-8`C)	2.4555	2.3914	2.3685	2.3743	2.3708	2.3754	2.3485	2.3764	2.3407	2.3732	2.3328	2.8889	2.7195	2.6844	2.6446	2.6004	2.6510	2.5113	2.6569	2.5341	2.6383	2.4811	**2.81**
F4	-116.5680	-117.3601	-120.1088	-117.2553	-120.4514	-117.2656	-119.3899	-117.2753	-119.5897	-117.2446	-119.1158	-116.3972	-117.8565	-120.3794	-118.0672	-122.0110	-118.0509	-120.3403	-118.0375	-120.5104	-118.0852	-119.9935	**-102.1**
Nuclei	B98											B98										
C1	137.8984	138.3641	139.2698	138.5615	140.4825	138.5589	139.6880	138.5551	139.9714	138.5675	140.0693	136.6672	137.9623	138.5980	138.5797	140.1392	138.5482	140.0261	138.5178	139.8988	138.6168	140.0992	**129**
C2	138.5254	138.4721	139.0519	138.3240	138.8948	138.3503	139.3548	138.3736	139.2402	138.3008	139.3473	137.9447	138.0861	138.6429	138.0628	138.7300	138.0773	139.2568	138.0902	139.1509	138.0518	139.2683	**132**
C3	120.9751	121.6883	122.2401	121.9412	122.6168	121.9423	122.8875	121.9406	122.8295	121.9422	122.9429	121.0500	121.6961	122.2005	121.9352	122.6051	121.9366	122.8272	121.9354	122.7659	121.9361	122.8940	**116**
C4	173.5548	174.4326	175.0664	174.8850	175.5697	174.8724	176.2406	174.8571	176.0696	174.8994	176.3345	173.8262	174.4272	175.1004	174.7024	175.4540	174.7034	175.8475	174.7008	175.7561	174.7028	176.0007	**167**
C5	118.7946	120.1408	120.7556	120.8501	121.6768	120.8218	121.9460	120.7906	121.8434	120.8797	122.0849	118.9548	120.1808	120.7785	120.7832	121.6150	120.7632	121.7668	120.7403	121.6817	120.8040	121.9090	**116**
C6	134.9458	136.9033	137.9770	137.9779	139.4196	137.9297	140.0378	137.8779	139.7250	138.0256	140.3768	135.2851	137.2480	138.5012	138.2327	139.8890	138.1917	140.3423	138.1470	140.1749	138.2722	140.7184	**132**
C7	199.5271	204.5615	206.0295	207.1995	208.2386	207.0479	213.5136	206.8943	212.6014	207.3482	214.4291	204.1599	208.4637	209.6427	210.7144	211.5176	210.5930	216.3722	210.4697	215.2290	210.8323	216.8957	**196**
C8	65.0962	66.2575	66.8997	66.5776	67.5549	66.5763	67.8574	66.5723	67.7776	66.5806	68.7079	59.7427	61.6256	62.1747	62.5454	63.3980	62.4979	64.1348	62.4503	63.8905	62.5954	64.3856	**60**
C9	23.2897	23.5779	23.6929	23.8388	24.0941	23.8397	24.1215	23.8371	24.0489	23.8399	24.2881	20.0303	20.4587	20.5633	20.6605	20.8945	20.6623	21.0556	20.6621	20.9805	20.6615	21.4185	**15**
C8`	36.7092	37.4629	37.6740	37.7309	38.1053	37.7287	38.3351	37.7243	38.2965	37.7357	38.7417	32.2204	32.4032	32.6737	32.5780	32.8420	32.5807	32.9732	32.5806	33.0077	32.5770	33.0565	**31**
H2	8.6652	8.6018	8.6259	8.5647	8.5366	8.5677	8.5885	8.5705	8.5669	8.5621	8.5601	8.6821	8.5181	8.5678	8.4391	8.4515	8.4446	8.4365	8.4498	8.4543	8.4338	8.4469	**8.07**
H3	7.3240	7.4617	7.5525	7.5069	7.6251	7.5048	7.6424	7.5026	7.6335	7.5092	7.6562	7.3088	7.4478	7.5364	7.4945	7.6157	7.4921	7.6318	7.4897	7.6238	7.4970	7.6471	**7.31**
H5	7.1716	7.3643	7.4556	7.4510	7.5764	7.4460	7.5983	7.4411	7.5859	7.4560	7.6179	7.1649	7.3464	7.4371	7.4256	7.5523	7.4212	7.5629	7.4169	7.5523	7.4299	7.5837	**7.31**
H6	8.0929	8.2967	8.3821	8.4075	8.5267	8.4008	8.6016	8.3943	8.5719	8.4141	8.6200	7.8961	8.0681	8.1863	8.1586	8.3256	8.1538	8.3364	8.1488	8.3271	8.1631	8.3835	**8.07**
H8	4.3470	4.4366	4.4606	4.5354	4.5891	4.5287	4.6555	4.5220	4.6334	4.5423	4.6625	4.4951	4.6493	4.7037	4.7151	4.8293	4.7118	4.8454	4.7085	4.8323	4.7182	4.8756	**5.09**
H(9A-9C)	1.3189	1.3268	1.3143	1.3162	1.2740	1.3175	1.2894	1.3187	1.2788	1.3151	1.3029	1.3937	1.4261	1.4275	1.4419	1.4166	1.4413	1.4301	1.4407	1.4303	1.4425	1.4532	**1.6**
H(8`A-8`C)	2.4802	2.4260	2.3972	2.4073	2.3842	2.4082	2.3651	2.4093	2.3720	2.4067	2.3565	2.9208	2.7533	2.7171	2.6803	2.6349	2.6856	2.5498	2.6907	2.5670	2.6754	2.5194	**2.81**
F4	-119.6030	-120.4442	-123.1898	-120.3267	-124.6696	-120.3380	-122.3243	-120.3491	-122.7908	-120.3158	-122.1756	-119.4577	-120.8773	-123.5272	-121.1015	-125.1436	-121.0896	-123.4668	-121.0780	-123.6940	-121.1150	-123.1078	**-102.1**

[a] methyl protons shifts are averaged
[b] according to [9]

Table S9. Cont. I

Nuclei	R											S										Exp. [b]
	B971											B971										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.5124	137.9668	138.8036	138.1617	140.0037	138.1528	139.1730	138.1442	139.5653	138.1768	139.6476	136.2962	137.5659	138.2070	138.1911	139.7146	138.1505	139.5849	138.1134	139.4699	138.2405	139.6733	**129**
C2	138.2273	138.1790	138.7520	138.0411	138.6151	138.0588	139.0874	138.0759	138.9703	138.0298	139.0743	137.6507	137.7943	138.3494	137.7788	138.4352	137.7852	138.9549	137.7921	138.8493	137.7793	138.9688	**132**
C3	120.7723	121.4948	122.0366	121.7575	122.4239	121.7508	122.6953	121.7432	122.6290	121.7695	122.7532	120.8439	121.4989	122.0013	121.7481	122.4060	121.7414	122.6248	121.7343	122.5637	121.7602	122.6979	**116**
C4	173.4520	174.3378	174.9730	174.7959	175.4831	174.7758	176.1541	174.7552	175.9535	174.8209	176.2409	173.7091	174.3304	175.0011	174.6204	175.3683	174.6132	175.7597	174.6046	175.6659	174.6323	175.9170	**167**
C5	118.5912	119.9438	120.5513	120.6619	121.4796	120.6255	121.7575	120.5889	121.6419	120.7023	121.8945	118.7577	119.9871	120.5816	120.5974	121.4204	120.5694	121.5676	120.5405	121.4822	120.6294	121.7173	**116**
C6	134.7050	136.6708	137.7813	137.7564	139.2253	137.6992	139.8111	137.6410	139.4847	137.8168	140.1424	135.0285	137.0109	138.2571	138.0065	139.6769	137.9579	140.1333	137.9074	139.9591	138.0571	140.5087	**132**
C7	199.4123	204.3866	205.8037	206.9774	207.9980	206.8235	213.1394	206.6697	212.2541	207.1300	214.1117	204.0187	208.2806	209.4897	210.5322	211.3305	210.4028	216.0716	210.2738	214.9613	210.6620	216.6144	**196**
C8	65.0628	66.2181	66.8745	66.5493	67.4912	66.5398	67.7569	66.5294	67.7680	66.5644	68.6439	59.7053	61.5405	62.0853	62.4460	63.2954	62.3913	63.9952	62.3385	63.7609	62.5067	64.2505	**60**
C9	23.2952	23.5805	23.7317	23.8547	24.1127	23.8461	24.1179	23.8365	24.0691	23.8689	24.2944	20.0444	20.4947	20.5876	20.7006	20.9390	20.6951	21.1020	20.6896	21.0266	20.7123	21.4780	**15**
C8`	36.7170	37.4689	37.6835	37.7337	38.0702	37.7257	38.3145	37.7173	38.2603	37.7475	38.7194	32.1504	32.3460	32.6128	32.5305	32.7822	32.5259	32.9103	32.5202	32.9431	32.5401	32.9962	**31**
H2	8.6629	8.6020	8.6311	8.5654	8.5437	8.5681	8.6026	8.5708	8.5678	8.5633	8.5647	8.6781	8.5197	8.5677	8.4422	8.4548	8.4475	8.4418	8.4527	8.4583	8.4370	8.4509	**8.07**
H3	7.3215	7.4590	7.5493	7.5044	7.6225	7.5021	7.6392	7.4997	7.6299	7.5070	7.6527	7.3076	7.4456	7.5341	7.4931	7.6131	7.4905	7.6286	7.4879	7.6208	7.4959	7.6437	**7.31**
H5	7.1696	7.3613	7.4527	7.4481	7.5728	7.4430	7.5957	7.4379	7.5815	7.4533	7.6142	7.1650	7.3449	7.4351	7.4237	7.5495	7.4192	7.5594	7.4147	7.5489	7.4283	7.5805	**7.31**
H6	8.0974	8.2998	8.3897	8.4087	8.5283	8.4021	8.6053	8.3956	8.5653	8.4153	8.6195	7.8972	8.0707	8.1892	8.1631	8.3306	8.1581	8.3421	8.1530	8.3320	8.1679	8.3885	**8.07**
H8	4.3445	4.4318	4.4558	4.5292	4.5852	4.5223	4.6544	4.5157	4.6229	4.5361	4.6585	4.4978	4.6489	4.7036	4.7168	4.8297	4.7133	4.8452	4.7097	4.8315	4.7203	4.8758	**5.09**
H(9A-9C)	1.3191	1.3280	1.3197	1.3196	1.2780	1.3205	1.2937	1.3214	1.2832	1.3191	1.3053	1.3960	1.4276	1.4283	1.4433	1.4195	1.4425	1.4331	1.4418	1.4326	1.4442	1.4560	**1.6**
H(8`A-8`C)	2.4778	2.4208	2.3902	2.4035	2.3793	2.4041	2.3533	2.4048	2.3662	2.4033	2.3481	2.9110	2.7452	2.7096	2.6744	2.6284	2.6794	2.5438	2.6843	2.5610	2.6698	2.5128	**2.81**
F4	-120.2351	-121.0807	-123.8156	-120.9622	-125.2909	-120.9730	-122.9021	-120.9844	-123.4531	-120.9506	-122.8061	-120.1050	-121.5166	-124.1797	-121.7361	-125.7875	-121.7233	-124.0920	-121.7123	-124.3270	-121.7490	-123.7384	**-102.1**
Nuclei	B972											B972											
C1	134.4302	134.9580	135.9573	135.2517	137.1882	135.2339	136.9092	135.2172	137.2291	135.2642	136.9986	133.0960	134.5569	135.0556	135.2214	136.6788	135.1632	136.7562	135.1090	136.5422	135.2805	136.8545	**129**
C2	136.2385	136.1466	136.7094	135.9825	136.5017	135.9974	136.8781	136.0094	136.7762	135.9648	136.9004	135.6839	135.8309	136.3876	135.8469	136.4661	135.8466	136.9148	135.8443	136.8312	135.8431	136.9435	**132**
C3	118.6420	119.3619	119.9304	119.6913	120.3271	119.6734	120.6091	119.6533	120.5621	119.7042	120.6885	118.7138	119.3622	119.8746	119.6667	120.3028	119.6505	120.5119	119.6318	120.4478	119.6777	120.5982	**116**
C4	170.4080	171.2888	171.9012	171.8240	172.3935	171.7908	172.9800	171.7559	172.8201	171.8517	173.1417	170.6771	171.2152	171.8947	171.5417	172.2306	171.5278	172.5783	171.5099	172.5046	171.5489	172.7454	**167**
C5	116.5455	117.8870	118.4963	118.6438	119.4131	118.5990	119.6446	118.5521	119.5386	118.6819	119.8150	116.6811	117.8807	118.4867	118.5356	119.3203	118.4989	119.4656	118.4592	119.3807	118.5657	119.6278	**116**
C6	132.2984	134.1683	135.1909	135.2810	136.6319	135.2152	137.0709	135.1451	136.7199	135.3380	137.5017	132.7192	134.6132	135.8785	135.6223	137.1863	135.5695	137.5344	135.5120	137.4030	135.6656	137.9182	**132**
C7	197.1472	202.1820	203.6394	205.0747	205.9500	204.8855	211.4809	204.7016	210.7109	205.2515	212.1626	201.5167	205.7889	206.8296	208.0334	208.7686	207.8942	213.5796	207.7543	212.4081	208.1644	214.0847	**196**
C8	62.2129	63.1640	63.7653	63.5253	64.4519	63.5132	65.0374	63.4956	64.9409	63.5298	65.7131	56.9800	58.9172	59.3838	59.8622	60.6095	59.7928	61.4484	59.7250	61.1550	59.9290	61.7202	**60**
C9	22.2017	22.5014	22.6308	22.6974	22.9802	22.6894	22.9728	22.6772	22.8720	22.7010	23.1432	18.9615	19.3718	19.4861	19.6193	19.7902	19.6032	19.9459	19.5854	19.8717	19.6315	20.3049	**15**
C8`	35.6349	36.3454	36.5312	36.8429	37.0375	36.8098	37.2438	36.7749	37.2215	36.8693	37.6484	31.3495	31.4924	31.7924	31.7285	31.9630	31.7188	31.9659	31.7053	32.0216	31.7314	32.0500	**31**
H2	8.6537	8.5910	8.6014	8.5457	8.5058	8.5490	8.4992	8.5518	8.4749	8.5424	8.5039	8.6825	8.4992	8.5620	8.4234	8.4354	8.4301	8.3959	8.4360	8.4226	8.4161	8.4046	**8.07**
H3	7.3227	7.4597	7.5484	7.5068	7.6209	7.5045	7.6375	7.5020	7.6284	7.5088	7.6533	7.3120	7.4483	7.5346	7.4976	7.6140	7.4951	7.6296	7.4923	7.6214	7.4999	7.6455	**7.31**
H5	7.1739	7.3666	7.4552	7.4573	7.5754	7.4520	7.5903	7.4465	7.5774	7.4620	7.6138	7.1665	7.3420	7.4301	7.4225	7.5446	7.4180	7.5559	7.4132	7.5449	7.4267	7.5779	**7.31**
H6	8.1158	8.3161	8.3945	8.4358	8.5373	8.4282	8.5663	8.4204	8.5382	8.4429	8.6045	7.9070	8.0727	8.1924	8.1605	8.3194	8.1565	8.3186	8.1518	8.3151	8.1637	8.3642	**8.07**
H8	4.3399	4.4508	4.4730	4.5472	4.5919	4.5405	4.6226	4.5339	4.6079	4.5536	4.6488	4.4883	4.6298	4.6848	4.6954	4.8083	4.6924	4.8202	4.6889	4.8127	4.6977	4.8518	**5.09**
H(9A-9C)	1.2779	1.2737	1.2581	1.2603	1.2187	1.2618	1.2249	1.2628	1.2101	1.2586	1.2452	1.3585	1.3871	1.3915	1.4080	1.3784	1.4071	1.3926	1.4058	1.3948	1.4087	1.4173	**1.6**
H(8`A-8`C)	2.4444	2.3879	2.3637	2.3740	2.3543	2.3748	2.3536	2.3753	2.3559	2.3732	2.3366	2.8829	2.7146	2.6793	2.6431	2.5976	2.6486	2.5129	2.6536	2.5335	2.6373	2.4818	**2.81**
F4	-114.1394	-114.9916	-117.6165	-114.8823	-119.1303	-114.8982	-117.0933	-114.9144	-117.5459	-114.8661	-116.7899	-113.9897	-115.4937	-117.9379	-115.7417	-119.5861	-115.7233	-118.0262	-115.7090	-118.1925	-115.7622	-117.6994	**-102.1**
Nuclei	BHandH											BHandH											
C1	138.2231	138.5552	139.4722	138.6613	140.1957	138.6447	139.2014	138.6466	139.2910	138.6472	139.3414	137.3260	138.1227	139.0514	138.6686	139.4127	138.6143	139.9113	138.5817	139.6959	138.6934	140.0677	**129**
C2	143.5201	143.3955	144.0049	143.2268	143.8191	143.2277	144.3374	143.2468	144.2139	143.1959	144.3719	143.1561	143.1628	143.7749	143.0888	143.8329	143.0819	144.2258	143.0940	144.0867	143.0659	144.2500	**132**
C3	123.7766	124.4896	125.0912	124.7508	125.4195	124.7262	125.6101	124.7198	125.5593	124.7437	125.6833	123.8317	124.5005	125.1213	124.7551	125.4992	124.7302	125.6175	124.7238	125.5792	124.7487	125.7026	**116**
C4	174.6910	175.5022	176.1372	175.9474	176.5413	175.9096	177.2138	175.8903	177.0668	175.9534	177.3817	174.9086	175.5511	176.2159	175.8630	176.6071	175.8357	176.9768	175.8261	176.9107	175.8585	177.1498	**167**
C5	121.3254	122.7876	123.4824	123.5575	124.4251	123.5004	124.6212	123.4617	124.5293	123.5816	124.7930	121.4351	122.8143	123.5066	123.5206	124.2647	123.4688	124.5249	123.4348	124.4609	123.5397	124.7001	**116**
C6	139.9383	142.0591	143.3061	143.2147	144.9304	143.1340	145.6585	143.0715	145.4144	143.2611	146.1074	140.2023	142.4966	143.7026	143.6179	144.3620	143.5430	145.9734	143.4853	145.7743	143.6576	146.3435	**132**
C7	202.9300	207.7859	209.1882	210.2924	210.9441	210.1306	215.8168	209.9874	214.6983	210.4156	216.6335	207.3621	211.4788	213.0278	213.6769	214.4210	213.5328	219.1023	213.4077	218.0494	213.7841	219.7557	**196**
C8	59.9494	61.2143	61.9067	61.6436	62.6312	61.6098	63.0978	61.5942	62.9356	61.6453	63.8442	54.0631	55.4214	55.9382	56.1974	56.9415	56.1327	57.6583	56.0882	57.3239	56.2306	57.9608	**60**
C9	22.4684	22.7173	23.0362	22.9961	23.4920	22.9658	23.4131	22.9537	23.4079	22.9951	23.6098	19.0747	19.5603	19.6330	19.8271	20.5712	19.7976	20.2453	19.7870	20.1575	19.8256	20.6529	**15**
C8`	33.7500	34.5612	34.8118	34.8998	35.2711	34.8687	35.5037	34.8562	35.4510	34.8996	35.9918	28.6454	29.0946	29.4036	29.3316	30.0757	29.3102	29.7782	29.3056	29.7931	29.3204	29.9429	**31**
H2	8.9875	8.9200	8.9348	8.8802	8.8770	8.8834	8.9222	8.8858	8.9249	8.8781	8.9222	8.9840	8.8580	8.8706	8.7732	8.6920	8.7803	8.7507	8.7862	8.7811	8.7672	8.7533	**8.07**
H3	7.4553	7.5997	7.6892	7.6466	7.7674	7.6451	7.7842	7.6427	7.7763	7.6491	7.8000	7.4516	7.5922	7.6830	7.6387	7.5575	7.6372	7.7745	7.6347	7.7677	7.6412	7.7910	**7.31**
H5	7.3003	7.5022	7.5933	7.5917	7.7206	7.5873	7.7378	7.5822	7.7268	7.5967	7.7629	7.2950	7.4886	7.5794	7.5727	7.4915	7.5687	7.7122	7.5639	7.7021	7.5774	7.7361	**7.31**
H6	8.3317	8.5445	8.6361	8.6585	8.7941	8.6524	8.8645	8.6454	8.8495	8.6654	8.9071	8.1293	8.3337	8.4417	8.4287	8.3475	8.4246	8.6263	8.4194	8.6221	8.4334	8.6718	**8.07**
H8	4.1505	4.2528	4.2749	4.3463	4.3866	4.3407	4.4438	4.3343	4.4339	4.3528	4.4693	4.4049	4.5696	4.6414	4.6481	4.5669	4.6447	4.7936	4.6404	4.7922	4.6522	4.8291	**5.09**
H(9A-9C)	1.3947	1.4083	1.3944	1.4043	1.3835	1.4056	1.4087	1.4060	1.4066	1.4041	1.4308	1.4777	1.5048	1.4783	1.5114	1.4301	1.5120	1.4963	1.5117	1.4978	1.5117	1.5179	**1.6**
H(8`A-8`C)	2.5482	2.4741	2.4402	2.4443	2.4243	2.4467	2.3801	2.4483	2.3790	2.4430	2.3667	2.9170	2.7545	2.7130	2.6709	2.5897	2.6772	2.5211	2.6825	2.5633	2.6659	2.4973	**2.81**
F4	-105.2660	-105.8310	-107.9761	-105.6345	-109.0248	-105.6521	-106.8723	-105.6688	-107.2259	-105.6171	-106.6144	-105.1037	-106.0291	-108.1331	-106.1131	-106.4498	-106.1094	-107.7443	-106.1061	-107.9144	-106.1172	-107.4800	**-102.1**
Nuclei	BHandHLYP											BHandHLYP											
C1	138.8640	139.2644	139.9330	139.4014	141.4115	139.3890	140.3239	139.3799	140.8073	139.4140	140.7808	137.7359	138.7863	139.5663	139.4872	141.0279	139.4436	140.6370	139.4057	140.4914	139.5319	140.6845	**129**
C2	142.1451	142.0033	142.5518	141.8479	142.3133	141.8593	142.8334	141.8728	142.6946	141.8367	142.8238	141.6846	141.6776	142.2130	141.6154	142.1662	141.6189	142.6674	141.6254	142.5678	141.6119	142.7010	**132**
C3	122.5311	123.1246	123.6134	123.3344	123.9644	123.3231	124.1502	123.3143	124.1344	123.3446	124.2197	122.6170	123.1643	123.6329	123.3811	123.9687	123.3691	124.1171	123.3594	124.0780	123.3922	124.1810	**116**
C4	174.4859	175.2386	175.8387	175.6759	176.2231	175.6490	176.9757	175.6248	176.7716	175.7009	177.0601	174.7783	175.2638	175.8588	175.5025	176.1211	175.4893	176.5698	175.4775	176.5010	175.5141	176.7410	**167**
C5	120.1712	121.4535	122.0189	122.1435	122.9398	122.1013	123.1049	122.0616	123.0479	122.1835	123.2751	120.2936	121.5123	122.0694	122.1337	122.8970	122.0972	123.0006	122.0628	122.9395	122.1680	123.1441	**116**
C6	138.1510	140.1493	141.3422	141.2896	142.5504	141.2223	143.2999	141.1564	142.9195	141.3529	143.5841	138.4674	140.5298	141.7475	141.5098	143.1000	141.4526	143.6578	141.3968	143.5207	141.5620	144.0715	**132**
C7	201.2543	206.5546	207.7752	209.3182	210.2498	209.1454	216.0604	208.9760	215.0849	209.4828	217.0651	206.1611	210.4578	211.6283	212.8433	213.4066	212.7018	218.6263	212.5625	217.3826	212.9773	219.2046	**196**
C8	60.7965	61.8811	62.5000	62.2233	63.0588	62.2069	63.2656	62.1924	63.2636	62.2383	64.1041	55.4804	57.1821	57.8021	58.1054	58.8956	58.0473	59.5516	57.9937	59.2868	58.1628	59.8130	**60**
C9	22.2333	22.3886	22.6124	22.6282	22.8233	22.6139	22.7047	22.6016	22.6825	22.6409	22.8547	18.9648	19.2708	19.4004	19.4144	19.6557	19.4060	19.6995	19.4005	19.6674	19.4225	20.0180	**15**
C8`	34.7377	35.5130	35.7819	35.8289	36.1801	35.8108	36.3989	35.7951	36.3597	35.8459	36.8091	30.5960	30.8142	31.0655	30.9812	31.2247	30.9680	31.3407	30.9569	31.3887	30.9927	31.4699	**31**
H2	8.8761	8.8039	8.8520	8.7659	8.7241	8.7690	8.7906	8.7718	8.7505	8.7629	8.7519	8.8981	8.7359	8.7665	8.6405	8.6466	8.6464	8.6344	8.6519	8.6571	8.6345	8.6458	**8.07**
H3	7.4433	7.5783	7.6654	7.6233	7.7361	7.6213	7.7566	7.6190	7.7465	7.6252	7.7698	7.4323	7.5668	7.6511	7.6133	7.7280	7.6111	7.7441	7.6087	7.7353	7.6153	7.7592	**7.31**
H5	7.2878	7.4785	7.5663	7.5650	7.6852	7.5602	7.7061	7.5552	7.6928	7.5695	7.7273	7.2798	7.4603	7.5446	7.5400	7.6603	7.5356	7.6720	7.5311	7.6611	7.5440	7.6938	**7.31**
H6	8.1765	8.3928	8.4992	8.5149	8.6356	8.5078	8.7226	8.5005	8.6822	8.5217	8.7376	8.0113	8.2014	8.3159	8.2915	8.4587	8.2866	8.4826	8.2813	8.4746	8.2959	8.5310	**8.07**
H8	4.0776	4.1885	4.2247	4.3024	4.3719	4.2945	4.4593	4.2868	4.4300	4.3099	4.4624	4.2587	4.4280	4.4860	4.5022	4.6169	4.4983	4.6464	4.4943	4.6344	4.5056	4.6772	**5.09**
H(9A-9C)	1.2993	1.3062	1.3063	1.3002	1.2417	1.3014	1.2609	1.3023	1.2448	1.2990	1.2689	1.3682	1.3960	1.3920	1.4076	1.3798	1.4070	1.4019	1.4061	1.4026	1.4081	1.4244	**1.6**
H(8`A-8`C)	2.4396	2.3870	2.3452	2.3723	2.3466	2.3731	2.3248	2.3737	2.3360	2.3717	2.3239	2.8786	2.7124	2.6679	2.6359	2.5874	2.6411	2.5108	2.6458	2.5345	2.6307	2.4845	**2.81**
F4	-108.7738	-109.8192	-112.0485	-109.8454	-113.5515	-109.8482	-111.3452	-109.8508	-111.8572	-109.8427	-111.3217	-108.4921	-110.0709	-112.3417	-110.4795	-113.9112	-110.4590	-112.3617	-110.4396	-112.5235	-110.5005	-112.0844	**-102.1**

[a] methyl protons shifts are averaged
[b] according to [9]

Table S9. Cont. II

Nuclei	R											S										Exp. [b]
	BLYP											BLYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.2740	140.0627	140.7302	140.3557	142.0482	140.6261	141.6136	140.4250	141.4809	140.7208	141.8598	138.3037	138.8878	139.5939	139.5904	141.4131	139.8236	141.0985	139.5956	141.3416	139.9982	141.2014	**129**
C2	137.3888	137.3557	137.9052	137.1077	137.7439	137.4006	137.9857	137.2334	138.0955	137.4576	138.0801	136.8040	136.8446	137.3898	136.8417	137.6112	137.1207	137.9926	136.9376	138.0835	137.2041	138.0703	**132**
C3	120.6544	121.3842	121.8707	121.6716	122.2855	121.9330	122.4590	121.7316	122.5866	122.0499	122.6336	119.6392	121.4514	121.9240	121.6569	122.3097	121.9238	122.3772	121.7284	122.4989	122.0306	122.5353	**116**
C4	177.6519	178.7185	179.3932	179.3068	180.0988	179.5462	180.5234	179.3230	180.6223	179.7057	180.7915	178.1086	178.8813	179.6485	179.1527	180.0400	179.4160	180.2300	179.2172	180.2861	179.5290	180.4844	**167**
C5	118.5470	119.8601	120.3998	120.5456	121.3222	120.7815	121.4404	120.5550	121.5434	120.9483	121.6902	118.6599	120.0133	120.5942	120.5540	121.3508	120.8003	121.3513	120.5845	121.4329	120.9468	121.5891	**116**
C6	133.7911	135.6052	136.7931	136.6678	138.3637	136.8753	138.6685	136.6243	138.6992	137.1000	139.1691	138.8182	136.2738	137.4058	137.2526	138.9036	137.4733	139.2393	137.2316	139.1572	137.6692	139.7543	**132**
C7	203.2767	208.6048	209.8305	211.6985	212.3595	211.7964	217.3300	211.4147	216.3806	212.2229	218.3121	205.2971	212.7975	214.3032	214.9277	216.0897	215.0775	220.0988	214.7652	219.4181	215.4121	220.5992	**196**
C8	69.1241	70.1253	70.7992	70.3573	71.5764	70.6395	71.9231	70.4601	71.8008	70.7169	72.6971	68.1488	65.4631	65.8331	66.4810	67.5528	66.6957	68.0924	66.4492	68.1157	66.9054	68.4506	**60**
C9	23.7215	24.0520	24.2062	24.1836	24.6500	24.4455	24.6108	24.2503	24.7226	24.5640	24.8492	16.4537	20.8061	20.7678	21.0333	21.2955	21.2977	21.4360	21.1003	21.5017	21.4093	21.9663	**15**
C8`	38.2242	38.9477	39.0730	39.4073	39.6721	39.6658	39.7283	39.4601	39.9360	39.7878	40.2492	32.8912	33.8280	34.1359	33.9651	34.2232	34.2348	34.1613	34.0423	34.3099	34.3359	34.3012	**31**
H2	8.3954	8.3311	8.3657	8.2850	8.2783	8.3345	8.4554	8.2924	8.3194	8.3386	8.4701	8.3743	8.3060	8.3480	8.2230	8.2163	8.2757	8.3816	8.2357	8.2114	8.2732	8.4083	**8.07**
H3	7.1679	7.2953	7.3831	7.3318	7.4491	7.3773	7.6306	7.3305	7.4581	7.3888	7.6578	7.0966	7.2855	7.3681	7.3259	7.4422	7.3712	7.6247	7.3239	7.4500	7.3832	7.6520	**7.31**
H5	7.0230	7.2052	7.2897	7.2883	7.4065	7.3310	7.5902	7.2811	7.4161	7.3480	7.6256	6.9899	7.1903	7.2755	7.2597	7.3808	7.3031	7.5580	7.2540	7.3806	7.3187	7.5918	**7.31**
H6	7.9452	8.1295	8.2114	8.2406	8.3476	8.2808	8.5506	8.2286	8.3909	8.3029	8.6025	8.9754	7.8764	7.9806	7.9535	8.0977	7.9966	8.2837	7.9470	8.0952	8.0128	8.3454	**8.07**
H8	4.5730	4.6582	4.6658	4.7406	4.7734	4.7808	4.9699	4.7284	4.7971	4.8027	5.0172	4.4807	4.8131	4.8614	4.8724	4.9776	4.9165	5.1608	4.8680	4.9755	4.9306	5.2060	**5.09**
H(9A-9C)	1.3344	1.3224	1.3240	1.2985	1.2925	1.3477	1.4693	1.3049	1.3035	1.3524	1.4944	1.2856	1.4612	1.4487	1.4808	1.4580	1.5270	1.6506	1.4807	1.4754	1.5371	1.6944	**1.6**
H(8`A-8`C)	2.5702	2.5055	2.4761	2.4845	2.4652	2.5330	2.6299	2.4890	2.4571	2.5387	2.6207	2.5654	2.8839	2.8478	2.7998	2.7482	2.8522	2.8332	2.8121	2.6782	2.8501	2.8119	**2.81**
F4	-142.4546	-143.7783	-147.0938	-143.7711	-149.1057	-143.5779	-145.7067	-143.7967	-146.8744	-143.6896	-145.8209	-141.1875	-144.2745	-147.5672	-144.6769	-149.7768	-144.4505	-146.7327	-144.6396	-148.1049	-144.6295	-146.7999	**-102.1**
Nuclei	BMK											BMK										
C1	154.5489	154.7956	155.8147	155.0346	156.7869	155.0048	155.7582	155.1850	155.9437	155.2232	155.7278	153.3708	154.7062	155.5737	155.3493	157.1804	155.2822	157.0114	155.4300	156.7717	155.5792	157.0888	**129**
C2	155.5489	155.3349	156.1444	155.0820	155.8798	155.0811	156.4462	155.2910	156.2529	155.2438	156.4023	154.7572	154.6732	155.3927	154.5734	155.4851	154.5591	155.9928	154.7574	155.7913	154.7494	155.9653	**132**
C3	135.9186	136.5742	137.2866	136.7717	137.6790	136.7457	137.8453	136.9307	137.6978	136.9577	137.8467	136.0540	136.5812	137.2516	136.7609	137.6638	136.7339	137.8432	136.9186	137.6908	136.9479	137.8865	**116**
C4	189.4005	190.1835	191.0076	190.6219	191.5290	190.5810	192.1342	190.7513	191.8731	190.8217	192.2418	189.7985	190.2293	191.0560	190.4438	191.4104	190.4180	191.7002	190.6026	191.5626	190.6291	191.8308	**167**
C5	133.4295	134.7613	135.4788	135.4278	136.5512	135.3675	136.6886	135.5196	136.4925	135.6472	136.8148	133.4535	134.7683	135.5390	135.3777	136.4835	135.3275	136.5822	135.4877	136.3606	135.5868	136.7328	**116**
C6	151.4094	153.6757	155.2637	155.0157	156.8896	154.9195	157.7543	155.0316	157.2746	155.2662	158.1427	152.1159	153.9639	155.4209	155.0094	157.0550	154.9327	157.4837	155.0660	157.2182	155.2429	157.8187	**132**
C7	216.9478	222.5474	224.1482	225.4916	226.2743	225.2972	232.0453	225.3132	230.7791	225.8361	232.8163	221.5389	226.5692	228.0915	229.2000	230.0942	229.0219	235.6763	229.0559	234.3215	229.5316	236.4133	**196**
C8	70.5725	71.6400	72.4428	72.1543	73.3210	72.1213	73.7576	72.2984	73.5299	72.3466	74.4771	64.4902	66.3795	67.0821	67.2150	68.2924	67.1424	69.1388	67.2827	68.7153	67.4478	69.3740	**60**
C9	25.4816	25.8566	26.3477	26.2252	26.6325	26.1938	26.7756	26.3697	26.5780	26.4143	26.8310	22.1260	22.5585	22.7087	22.6468	23.0607	22.6251	23.2222	22.8150	23.0572	22.8297	23.5137	**15**
C8`	38.7886	39.4905	39.7965	39.7916	40.2856	39.7653	40.4650	39.9500	40.3114	39.9781	40.8997	33.9443	34.1818	34.5674	34.3474	34.7515	34.3245	34.7335	34.5118	34.8069	34.5294	34.8356	**31**
H2	9.0522	9.0233	9.0737	8.9738	8.9666	8.9734	9.0551	8.9730	9.0302	8.9645	9.0669	9.0430	8.8827	8.9188	8.8117	8.8174	8.8133	8.8099	8.8146	8.8396	8.8005	8.8138	**8.07**
H3	7.6503	7.8088	7.9094	7.8680	7.9716	7.8622	8.0008	7.8561	7.9908	7.8636	8.0111	7.6582	7.8152	7.8999	7.8689	7.9851	7.8629	7.9933	7.8568	7.9965	7.8650	8.0096	**7.31**
H5	7.5098	7.7043	7.7841	7.7896	7.9181	7.7809	7.9299	7.7723	7.9192	7.7883	7.9561	7.4861	7.6973	7.7852	7.7793	7.9021	7.7717	7.9135	7.7640	7.8990	7.7768	7.9393	**7.31**
H6	8.4072	8.6270	8.7828	8.7961	8.9052	8.7837	9.0195	8.7706	8.9763	8.7979	9.0628	8.3050	8.4960	8.6092	8.6017	8.7715	8.5925	8.7332	8.5831	8.7698	8.6007	8.7910	**8.07**
H8	4.2317	4.3488	4.4104	4.4856	4.5292	4.4731	4.5903	4.4604	4.5756	4.4876	4.6005	4.4400	4.6482	4.6995	4.7284	4.8382	4.7206	4.8188	4.7127	4.8373	4.7262	4.8615	**5.09**
H(9A-9C)	1.3048	1.3335	1.3264	1.3372	1.2998	1.3347	1.3417	1.3320	1.3281	1.3300	1.3703	1.3776	1.3895	1.3774	1.4034	1.3701	1.3999	1.3895	1.3963	1.3784	1.3971	1.4125	**1.6**
H(8`A-8`C)	2.4334	2.3750	2.3238	2.3567	2.3235	2.3539	2.2956	2.3513	2.3080	2.3498	2.2771	2.8035	2.6688	2.6299	2.6096	2.5602	2.6105	2.4481	2.6113	2.4916	2.5990	2.4288	**2.81**
F4	-117.8305	-118.8370	-121.4737	-118.7660	-122.8911	-118.7769	-120.6770	-118.7873	-121.0954	-118.7564	-120.3901	-117.3179	-118.7955	-121.4641	-119.0073	-122.9757	-118.9968	-121.4127	-118.9864	-121.5751	-119.0189	-121.0973	**-102.1**
Nuclei	BP86											BP86										
C1	135.9939	136.6320	137.6362	136.9544	138.7298	136.9390	138.2948	136.9186	138.3141	136.9642	138.7051	134.4352	135.9816	136.4890	136.5815	138.0085	136.5423	138.0378	136.5022	137.9223	136.6187	138.2985	**129**
C2	136.0461	136.1412	136.6915	135.9389	136.4876	135.9629	136.9072	135.9812	136.7985	135.9104	137.0603	135.2799	135.6510	136.1578	135.6672	136.3174	135.6758	136.8585	135.6802	136.7480	135.6552	137.0159	**132**
C3	119.5556	120.4857	121.0080	120.7308	121.3490	120.7247	121.6928	120.7132	121.6404	120.7314	121.9360	119.6977	120.5178	120.9979	120.7317	121.3594	120.7284	121.6195	120.7195	121.5439	120.7299	121.8637	**116**
C4	174.3602	175.5049	176.1304	175.8536	176.5630	175.8334	177.1710	175.8083	177.0813	175.8678	177.4848	174.7072	175.5024	176.1986	175.7445	176.5291	175.7420	176.8841	175.7330	176.7851	175.7408	177.2044	**167**
C5	117.4531	118.9871	119.5529	119.6506	120.4030	119.6163	120.7206	119.5768	120.6236	119.6782	121.0496	117.6959	119.0396	119.6143	119.6262	120.4183	119.6030	120.5906	119.5742	120.4936	119.6424	120.9111	**116**
C6	132.4823	134.5222	135.5397	135.4991	136.9975	135.4473	137.5315	135.3905	137.2521	135.5440	138.0880	132.8422	134.9807	136.2191	135.9532	137.6251	135.9065	138.0996	135.8536	137.8931	135.9910	138.6398	**132**
C7	200.3568	205.1844	206.6915	207.6362	208.7456	207.4854	213.3518	207.3301	212.6663	207.7757	214.3906	205.2587	209.2590	210.3906	211.2385	212.1476	211.1283	216.2414	211.0136	215.3050	211.3390	216.8705	**196**
C8	67.0914	68.3350	69.0224	68.6336	69.6697	68.6283	70.1232	68.6177	69.8169	68.6343	71.1003	61.2199	63.3467	63.8475	64.2565	65.1036	64.1999	65.8529	64.1410	65.6179	64.3090	66.2851	**60**
C9	23.4788	23.9387	24.0159	24.1770	24.4194	24.1716	24.5594	24.1605	24.4086	24.1770	24.8922	20.0447	20.8111	20.8964	21.0566	21.2467	21.0482	21.5506	21.0352	21.4325	21.0604	22.1852	**15**
C8`	37.5056	38.3780	38.4809	38.5899	38.8300	38.5853	39.0439	38.5763	39.0514	38.5903	39.6736	32.7385	32.9732	33.1909	33.0751	33.2543	33.0771	33.3634	33.0731	33.3752	33.0673	33.5888	**31**
H2	8.4690	8.4251	8.4168	8.3721	8.3303	8.3765	8.3610	8.3805	8.3653	8.3675	8.3657	8.5023	8.3508	8.3888	8.2771	8.2780	8.2836	8.2597	8.2894	8.2717	8.2701	8.2813	**8.07**
H3	7.1833	7.3254	7.4023	7.3644	7.4695	7.3630	7.4872	7.3613	7.4789	7.3653	7.5157	7.1759	7.3137	7.3896	7.3551	7.4646	7.3535	7.4797	7.3516	7.4705	7.3561	7.5088	**7.31**
H5	7.0316	7.2248	7.3017	7.3045	7.4170	7.3004	7.4360	7.2960	7.4267	7.3081	7.4730	7.0289	7.2047	7.2838	7.2819	7.3979	7.2785	7.4064	7.2747	7.3955	7.2847	7.4416	**7.31**
H6	8.0317	8.2270	8.2775	8.3141	8.4038	8.3094	8.4531	8.3044	8.4474	8.3183	8.4976	7.7817	7.9419	8.0474	8.0258	8.1760	8.0224	8.1879	8.0185	8.1750	8.0284	8.2496	**8.07**
H8	4.6085	4.6845	4.6748	4.7603	4.7803	4.7553	4.8233	4.7502	4.8256	4.7646	4.8587	4.7327	4.8659	4.9018	4.9243	5.0225	4.9224	5.0356	4.9199	5.0205	4.9256	5.0853	**5.09**
H(9A-9C)	1.3656	1.3684	1.3441	1.3548	1.3143	1.3570	1.3284	1.3589	1.3132	1.3524	1.3589	1.4453	1.4875	1.4805	1.5086	1.4790	1.5084	1.4981	1.5079	1.4947	1.5083	1.5410	**1.6**
H(8`A-8`C)	2.5546	2.4795	2.4461	2.4610	2.4324	2.4627	2.4144	2.4642	2.4411	2.4590	2.4105	3.0093	2.8351	2.7840	2.7540	2.6945	2.7609	2.6012	2.7671	2.6178	2.7468	2.5828	**2.81**
F4	-133.5336	-134.1591	-137.3936	-133.9827	-139.0671	-134.0019	-136.4323	-134.0203	-136.7655	-133.9638	-136.0779	-133.3260	-134.6989	-137.7252	-134.9784	-139.6686	-134.9729	-137.5976	-134.9689	-137.9175	-134.9853	-137.1579	**-102.1**
Nuclei	CAM-B3LYP											CAM-B3LYP										
C1	140.5940	141.0501	141.9502	141.2482	143.3376	141.2328	142.6219	141.2195	142.7966	141.2664	142.8916	139.3811	140.7764	141.3414	141.3955	142.9372	141.3447	142.8551	141.3003	142.5657	141.4530	142.9212	**129**
C2	142.4322	142.3676	142.8920	142.2031	142.7302	142.2185	143.2393	142.2342	143.1183	142.1902	143.2313	141.9632	142.0722	142.5741	142.0137	142.6143	142.0196	143.1220	142.0264	143.0134	142.0107	143.1501	**132**
C3	123.8770	124.5297	125.0152	124.7351	125.3944	124.7281	125.5969	124.7212	125.5656	124.7437	125.6728	123.9590	124.5672	125.0168	124.7695	125.4058	124.7619	125.5862	124.7548	125.5220	124.7791	125.6510	**116**
C4	177.6432	178.4616	179.0236	178.8866	179.5004	178.8652	180.0958	178.8438	179.9671	178.9091	180.2452	177.9270	178.4619	179.0815	178.7166	179.4216	178.7091	179.7910	178.7009	179.7287	178.7245	179.9540	**167**
C5	121.6531	122.9882	123.5423	123.6761	124.5002	123.6378	124.6833	123.5998	124.6086	123.7146	124.8524	121.7948	123.0474	123.5984	123.6473	124.4684	123.6163	124.5780	123.5853	124.4990	123.6786	124.7226	**116**
C6	138.6325	140.6802	141.7768	141.7799	143.1835	141.7181	143.7450	141.6562	143.4517	141.8399	144.1171	138.9686	141.0487	142.3055	142.0534	143.7538	142.0017	144.1534	141.9484	144.0548	142.1023	144.5739	**132**
C7	205.1841	210.4669	211.8770	213.2659	214.3729	213.0946	219.8334	212.9249	218.8841	213.4315	220.8758	210.1044	214.5528	215.7343	216.9360	217.6675	216.7972	222.7736	216.6596	221.5003	217.0720	223.3268	**196**
C8	63.5728	64.7701	65.4574	65.1172	66.1087	65.1025	66.5638	65.0883	66.3449	65.1333	67.2834	57.9234	59.8230	60.3104	60.7065	61.5242	60.6433	62.2922	60.5845	61.9726	60.7729	62.5903	**60**
C9	22.4381	22.6575	22.8386	22.9008	23.1565	22.8881	23.1031	22.8752	23.0434	22.9144	23.2395	19.2771	19.6649	19.7105	19.7757	20.0125	19.7699	20.0783	19.7654	20.0320	19.7840	20.4496	**15**
C8`	35.5076	36.3386	36.5579	36.6501	37.0360	36.6375	37.2208	36.6255	37.1657	36.6643	37.6889	31.0486	31.2767	31.5537	31.4840	31.7595	31.4764	31.8336	31.4681	31.8936	31.4915	31.9753	**31**
H2	8.7689	8.7049	8.7244	8.6617	8.6168	8.6654	8.6438	8.6690	8.6389	8.6580	8.6285	8.7980	8.6167	8.6695	8.5340	8.5473	8.5409	8.5118	8.5472	8.5462	8.5267	8.5219	**8.07**
H3	7.4063	7.5412	7.6281	7.5846	7.6999	7.5826	7.7160	7.5807	7.7091	7.5865	7.7301	7.3996	7.5311	7.6171	7.5747	7.6929	7.5726	7.7060	7.5705	7.6986	7.5766	7.7206	**7.31**
H5	7.2620	7.4507	7.5382	7.5345	7.6567	7.5299	7.6715	7.5253	7.6620	7.5389	7.6941	7.2579	7.4349	7.5221	7.5119	7.6365	7.5077	7.6445	7.5036	7.6350	7.5158	7.6658	**7.31**
H6	8.1470	8.3590	8.4476	8.4737	8.5894	8.4673	8.6366	8.4608	8.6223	8.4796	8.6702	7.9705	8.1468	8.2705	8.2373	8.4092	8.2331	8.4121	8.2286	8.4132	8.2409	8.4600	**8.07**
H8	4.2201	4.3249	4.3484	4.4341	4.4931	4.4267	4.5388	4.4195	4.5400	4.4412	4.5650	4.3966	4.5587	4.6191	4.6315	4.7523	4.6282	4.7687	4.6248	4.7611	4.6343	4.8001	**5.09**
H(9A-9C)	1.3297	1.3390	1.3314	1.3291	1.2821	1.3304	1.2971	1.3316	1.2847	1.3277	1.3077	1.4016	1.4258	1.4289	1.4408	1.4198	1.4402	1.4318	1.4396	1.4375	1.4411	1.4563	**1.6**
H(8`A-8`C)	2.5132	2.4524	2.4238	2.4345	2.4170	2.4350	2.4044	2.4357	2.4044	2.4340	2.3914	2.9425	2.7653	2.7314	2.6913	2.6489	2.6974	2.5595	2.7032	2.5861	2.6851	2.5306	**2.81**
F4	-115.5485	-116.8719	-119.4187	-116.9933	-121.0302	-116.9892	-119.0882	-116.9849	-119.3688	-116.9983	-118.9035	-115.2826	-117.1929	-119.6136	-117.6345	-121.3475	-117.6057	-119.9108	-117.5789	-120.0081	-117.6651	-119.6376	**-102.1**

[a] methyl protons shifts are averaged
[b] according to [9]

Table S9. Cont. III

Nuclei	R											S										Exp. [b]
	HF											HF										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.0859	136.4286	136.9983	136.5642	138.6394	136.5601	136.8559	136.5607	137.5918	136.5707	137.8340	135.1106	136.0099	136.9165	136.8715	138.6196	136.8298	138.1526	136.7906	138.0357	136.9136	138.1693	**129**
C2	144.2959	144.1109	144.6184	143.9366	144.2969	143.9493	145.0625	143.9624	144.8336	143.9247	144.9263	144.1862	143.9606	144.4423	143.6963	144.1843	143.7105	144.6238	143.7251	144.5752	143.6812	144.6859	**132**
C3	120.5425	120.9815	121.3393	121.0997	121.6987	121.0951	121.5914	121.0919	121.6723	121.1042	121.7618	120.5755	121.0153	121.3955	121.1911	121.7425	121.1823	121.7739	121.1741	121.7432	121.1992	121.8101	**116**
C4	171.0685	171.6891	172.2443	172.0947	172.4686	172.0696	173.4111	172.0452	173.0954	172.1179	173.3624	171.3313	171.6695	172.1524	171.7723	172.2704	171.7643	172.7640	171.7564	172.6801	171.7787	172.9382	**167**
C5	117.7778	118.9699	119.4399	119.5840	120.3789	119.5486	120.2895	119.5143	120.3140	119.6174	120.5553	117.8113	119.0523	119.5559	119.6851	120.4237	119.6494	120.4603	119.6142	120.3849	119.7186	120.5859	**116**
C6	139.8710	141.8434	143.0414	142.9329	144.0689	142.8614	145.3610	142.7878	144.7144	142.9974	145.2266	140.2153	142.1535	143.2403	142.9363	144.2865	142.8868	144.8278	142.8360	144.6896	142.9813	145.2440	**132**
C7	195.4655	201.2748	202.3678	204.5817	204.9342	204.3815	211.4166	204.1898	210.2401	204.7750	212.8652	200.3146	204.7891	205.8595	207.3684	207.7885	207.2162	214.0876	207.0655	212.5722	207.5129	214.7501	**196**
C8	54.6914	55.6162	56.0452	55.7978	56.6132	55.7884	56.8235	55.7770	56.8761	55.8047	57.6680	49.9453	51.5670	52.1910	52.5059	53.2429	52.4542	53.9705	52.4041	53.6974	52.5554	54.1978	**60**
C9	20.7069	20.7584	20.8662	20.7421	21.0481	20.7452	20.9072	20.7468	20.8745	20.7388	20.9507	17.7976	17.8056	17.9115	17.8577	18.0665	17.8560	17.9858	17.8550	17.9557	17.8592	18.1883	**15**
C8`	32.6429	33.3486	33.5660	33.7469	34.0103	33.7215	34.1987	33.6970	34.1551	33.7689	34.5312	29.0930	29.3330	29.5248	29.4519	29.7044	29.4395	29.7559	29.4273	29.7928	29.4622	29.8640	**31**
H2	9.0358	8.9576	9.0240	8.9122	8.8795	8.9150	8.9903	8.9172	8.9268	8.9093	8.8935	9.0687	8.8942	8.9168	8.7657	8.7690	8.7719	8.7430	8.7777	8.7685	8.7596	8.7567	**8.07**
H3	7.4286	7.5694	7.6559	7.6163	7.7372	7.6140	7.7469	7.6115	7.7419	7.6185	7.7658	7.4270	7.5652	7.6521	7.6122	7.7319	7.6098	7.7417	7.6072	7.7343	7.6145	7.7576	**7.31**
H5	7.2620	7.4585	7.5485	7.5471	7.6720	7.5420	7.6831	7.5367	7.6720	7.5520	7.7063	7.2588	7.4515	7.5381	7.5363	7.6607	7.5316	7.6678	7.5266	7.6572	7.5408	7.6908	**7.31**
H6	8.1772	8.4177	8.5445	8.5717	8.7053	8.5623	8.8158	8.5526	8.7578	8.5806	8.8070	8.0620	8.2816	8.3955	8.3692	8.5389	8.3639	8.5572	8.3581	8.5485	8.3743	8.6055	**8.07**
H8	3.6262	3.7734	3.8337	3.9160	4.0002	3.9073	4.0866	3.8987	4.0448	3.9245	4.0816	3.7998	3.9985	4.0614	4.0795	4.2064	4.0749	4.2416	4.0700	4.2283	4.0838	4.2685	**5.09**
H(9A-9C)	1.2094	1.2101	1.2114	1.1856	1.1335	1.1867	1.1817	1.1873	1.1548	1.1845	1.1607	1.2797	1.2815	1.2708	1.2849	1.2453	1.2842	1.2618	1.2832	1.2631	1.2857	1.2803	**1.6**
H(8`A-8`C)	2.2583	2.2315	2.1858	2.2178	2.1970	2.2185	2.1768	2.2190	2.1940	2.2172	2.1932	2.6962	2.5446	2.4939	2.4664	2.4243	2.4706	2.3592	2.4746	2.3767	2.4625	2.3361	**2.81**
F4	-92.2012	-93.1244	-94.8492	-93.1160	-96.2760	-93.1234	-93.9449	-93.1302	-94.6053	-93.1088	-94.2664	-91.8275	-93.2856	-95.1728	-93.8334	-96.7123	-93.8098	-95.3711	-93.7864	-95.5009	-93.8563	-95.1316	**-102.1**
Nuclei	**LC-BLYP**																						
C1	143.9454	144.3001	145.4097	144.5079	146.3392	144.4682	145.1219	144.4578	146.1915	144.5303	146.2836	142.9429	144.2114	144.8868	144.9354	146.3990	144.8458	146.3781	144.7913	145.9849	145.0111	146.5188	**129**
C2	148.5022	148.3123	148.9120	148.1799	148.7307	148.1681	149.3075	148.1834	149.1118	148.1736	149.2571	148.2367	148.1595	148.7302	148.0898	148.6521	148.0728	149.1473	148.0835	149.0482	148.0884	149.1787	**132**
C3	128.3981	128.9432	129.5272	129.1700	129.8249	129.1365	129.9435	129.1302	129.9864	129.1845	130.1049	128.4577	128.9850	129.5383	129.2181	129.8639	129.1821	130.0193	129.1738	129.9481	129.2354	130.0806	**116**
C4	181.8964	182.5361	183.1128	182.9647	183.4846	182.9173	184.1724	182.8968	183.9350	182.9925	184.2385	182.1104	182.5115	183.1648	182.7723	183.4027	182.7394	183.7928	182.7322	183.7403	182.7849	183.9455	**167**
C5	126.0329	127.3491	128.0096	128.0921	128.9347	128.0253	129.0515	127.9857	129.0367	128.1384	129.2952	126.1441	127.4212	128.0695	128.1002	128.9526	128.0385	129.0416	128.0038	128.9555	128.1414	129.1882	**116**
C6	144.4457	146.5586	147.7101	147.7244	149.3132	147.6325	150.0897	147.5676	149.3684	147.7936	150.0269	144.7647	146.8890	148.2216	147.9599	149.7654	147.8834	150.1624	147.8313	150.0717	148.0120	150.5715	**132**
C7	210.7961	216.2518	217.8303	219.2261	219.8730	219.0191	225.3038	218.8395	225.0653	219.4065	227.1999	215.4470	220.1457	221.5590	222.7455	223.3196	222.5572	228.8329	222.3988	227.4675	222.9103	229.4875	**196**
C8	61.3984	62.6319	63.4214	63.1097	64.1261	63.0645	64.5480	63.0462	64.4091	63.1347	65.2976	55.6431	57.3143	57.8214	58.2576	59.0058	58.1666	59.8648	58.1066	59.4794	58.3300	60.2244	**60**
C9	21.5377	21.6825	21.9377	21.8979	22.3180	21.8578	22.1872	21.8462	22.0012	21.9197	22.1735	18.6324	18.8728	18.9378	19.0093	19.2711	18.9777	19.3164	18.9740	19.2407	19.0228	19.6888	**15**
C8`	33.6021	34.3992	34.7145	34.8359	35.1835	34.7918	35.4065	34.7739	35.3393	34.8597	35.8933	29.0895	29.3897	29.7641	29.6827	29.9584	29.6509	30.0425	29.6443	30.1159	29.6934	30.2365	**31**
H2	8.9711	8.8976	8.9038	8.8550	8.8357	8.8575	8.9003	8.8613	8.8099	8.8515	8.8027	8.9912	8.8085	8.8563	8.7154	8.7346	8.7227	8.6856	8.7307	8.7297	8.7068	8.6896	**8.07**
H3	7.5427	7.6754	7.7638	7.7201	7.8369	7.7170	7.8517	7.7154	7.8451	7.7221	7.8687	7.5437	7.6708	7.7599	7.7138	7.8323	7.7108	7.8425	7.7093	7.8366	7.7157	7.8586	**7.31**
H5	7.4058	7.5954	7.6843	7.6812	7.8049	7.6755	7.8189	7.6712	7.8049	7.6857	7.8395	7.4060	7.5871	7.6767	7.6670	7.7928	7.6617	7.7982	7.6579	7.7897	7.6710	7.8216	**7.31**
H6	8.3027	8.5213	8.6081	8.6422	8.7669	8.6342	8.8393	8.6277	8.7770	8.6487	8.8307	8.1441	8.3320	8.4605	8.4236	8.6087	8.4188	8.6040	8.4150	8.6111	8.4268	8.6501	**8.07**
H8	4.0994	4.2241	4.2473	4.3375	4.3854	4.3282	4.4499	4.3208	4.4440	4.3453	4.4811	4.3161	4.4914	4.5661	4.5712	4.6984	4.5663	4.7098	4.5628	4.7083	4.5747	4.7424	**5.09**
H(9A-9C)	1.3477	1.3582	1.3449	1.3500	1.3227	1.3501	1.3530	1.3517	1.2974	1.3487	1.3187	1.4131	1.4278	1.4251	1.4407	1.4202	1.4395	1.4310	1.4398	1.4374	1.4406	1.4542	**1.6**
H(8`A-8`C)	2.5010	2.4391	2.4146	2.4167	2.4026	2.4164	2.3702	2.4179	2.3908	2.4162	2.3818	2.8887	2.7145	2.6860	2.6365	2.5978	2.6411	2.5031	2.6470	2.5362	2.6309	2.4788	**2.81**
F4	-102.5915	-104.1036	-106.3783	-104.3438	-107.8530	-104.3346	-105.8842	-104.3254	-106.4778	-104.3524	-106.0793	-102.3680	-104.3796	-106.4884	-104.9374	-108.1733	-104.9008	-106.9030	-104.8663	-106.9326	-104.9747	-106.7271	**-102.1**
Nuclei	**M06**																						
C1	135.4072	135.7741	137.0115	135.8816	138.0210	135.8649	136.8091	135.8563	137.3380	135.9123	137.0556	134.1674	135.5202	136.1558	136.2300	137.8135	136.1538	137.9154	136.0917	137.5984	136.3238	137.9805	**129**
C2	140.6153	140.3648	140.9748	140.1830	140.7472	140.1863	141.1872	140.1968	141.0177	140.1945	141.1811	139.8441	139.8784	140.4612	139.8960	140.5961	139.8814	141.2124	139.8755	141.0600	139.9255	141.2192	**132**
C3	121.6176	122.2938	122.9735	122.5729	123.4101	122.5477	123.6473	122.5304	123.5932	122.6111	123.7286	121.6738	122.2553	122.8671	122.5213	123.3123	122.4950	123.5158	122.4767	123.4472	122.5609	123.5784	**116**
C4	173.1165	173.9963	174.7342	174.4927	175.3210	174.4521	176.0927	174.4196	175.9087	174.5457	176.2448	173.8447	174.2720	175.0646	174.5038	175.3524	174.4860	175.6260	174.4744	175.6126	174.5338	175.7886	**167**
C5	119.7718	121.0559	121.7752	121.7509	122.7315	121.6989	122.7996	121.6545	122.7382	121.8148	122.9828	119.7041	120.9774	121.6509	121.6232	122.5692	121.5755	122.6711	121.5353	122.6020	121.6826	122.8037	**116**
C6	136.8085	138.7038	139.7562	139.8590	141.2826	139.7763	142.3109	139.7016	141.8293	139.9522	142.5930	137.1469	139.1678	140.5409	140.2006	141.9881	140.1354	142.4239	140.0763	142.2946	140.2746	142.8394	**132**
C7	201.8270	206.8005	208.5395	209.3151	210.6085	209.1531	215.3851	208.9988	214.6233	209.4836	216.2344	206.3715	210.6515	211.8254	212.8411	213.6353	212.6921	218.3336	212.5525	217.1976	212.9995	218.7520	**196**
C8	60.7304	61.8816	62.6495	62.3326	63.4023	62.2980	63.5929	62.2707	63.6589	62.3799	64.4145	54.1844	55.7499	56.3619	56.6790	57.5433	56.6009	58.4113	56.5332	58.0797	56.7709	58.7141	**60**
C9	22.1450	22.4238	22.6903	22.7400	23.1676	22.7095	23.3573	22.6872	23.2995	22.7835	23.4614	19.4572	19.6907	19.8485	19.8638	20.2293	19.8402	20.3336	19.8248	20.2582	19.9018	20.8431	**15**
C8`	36.9348	37.6867	37.9199	37.9636	38.3405	37.9372	38.4473	37.9185	38.4095	38.0033	38.9535	31.7679	31.9520	32.3660	32.1758	32.5544	32.1571	32.7194	32.1443	32.7693	32.2063	32.7972	**31**
H2	8.7387	8.6519	8.6561	8.6165	8.5956	8.6186	8.6674	8.6211	8.6218	8.6152	8.6525	8.7596	8.5499	8.5974	8.4553	8.4747	8.4624	8.4395	8.4698	8.4663	8.4487	8.4486	**8.07**
H3	7.3369	7.4633	7.5604	7.5046	7.6321	7.5024	7.6528	7.5006	7.6377	7.5073	7.6581	7.2874	7.4302	7.5150	7.4793	7.6060	7.4760	7.6356	7.4734	7.6197	7.4830	7.6504	**7.31**
H5	7.1579	7.3516	7.4440	7.4353	7.5710	7.4303	7.5755	7.4258	7.5657	7.4405	7.6026	7.1555	7.3358	7.4320	7.4048	7.5377	7.4011	7.5349	7.3979	7.5315	7.4086	7.5553	**7.31**
H6	8.2198	8.4571	8.5350	8.5706	8.6748	8.5635	8.7980	8.5570	8.7357	8.5779	8.8111	7.9934	8.1490	8.2703	8.2290	8.4027	8.2251	8.4051	8.2215	8.4052	8.2330	8.4572	**8.07**
H8	4.3442	4.4692	4.4989	4.5607	4.6243	4.5542	4.7164	4.5485	4.6836	4.5675	4.7345	4.4477	4.6028	4.6519	4.6647	4.7811	4.6617	4.7907	4.6590	4.7893	4.6679	4.8239	**5.09**
H(9A-9C)	1.3018	1.3045	1.2808	1.2978	1.2531	1.2981	1.2815	1.2991	1.2659	1.2981	1.2924	1.3858	1.4182	1.4256	1.4306	1.4133	1.4304	1.4165	1.4305	1.4256	1.4312	1.4437	**1.6**
H(8`A-8`C)	2.4763	2.4121	2.3914	2.3956	2.3829	2.3959	2.3669	2.3969	2.3791	2.3959	2.3540	2.9033	2.7432	2.7104	2.6626	2.6248	2.6682	2.5329	2.6741	2.5623	2.6576	2.5047	**2.81**
F4	-117.9861	-119.2076	-121.2891	-118.5282	-122.5446	-118.5433	-120.1915	-118.5580	-120.6873	-118.5136	-119.9422	-117.1236	-118.6403	-120.5867	-118.2581	-122.0157	-118.2436	-120.5752	-118.2316	-120.6654	-118.2748	-120.2123	**-102.1**
Nuclei	**M06-2X**																						
C1	153.0917	153.5294	154.5657	153.6798	155.3824	153.6910	154.3824	153.7038	154.6410	153.6636	154.5610	152.3025	153.6253	154.2248	154.4172	155.8548	154.3561	155.9192	154.3050	155.6636	154.4801	156.1304	**129**
C2	155.1746	155.0543	155.6859	154.8589	155.5556	154.8934	156.0475	154.9292	155.9461	154.8195	156.0984	154.7655	154.7734	155.3565	154.6837	155.4125	154.7088	155.8874	154.7355	155.7791	154.6544	155.9277	**132**
C3	136.1590	136.8604	137.4721	137.0980	137.8395	137.1065	138.0767	137.1160	138.0006	137.0834	138.1754	136.1934	136.8293	137.4400	137.0599	137.8148	137.0677	137.9965	137.0767	137.9426	137.0459	138.0999	**116**
C4	186.9866	187.8245	188.4710	188.2660	188.9823	188.2597	189.6225	188.2546	189.4454	188.2657	189.8145	187.4071	187.9865	188.7105	188.2373	189.0085	188.2488	189.3855	188.2602	189.3135	188.2178	189.5659	**167**
C5	133.5146	135.0251	135.7169	135.8167	136.7899	135.7892	136.9947	135.7628	136.8748	135.8366	137.2061	133.4360	134.8666	135.5636	135.5696	136.5427	135.5491	136.6670	135.5297	136.5791	135.5821	136.8705	**116**
C6	151.2911	153.5510	154.7995	154.7508	156.6302	154.6981	157.2971	154.6466	156.9660	154.7945	157.7502	151.6315	153.9149	155.3078	154.9928	157.0373	154.9595	157.4443	154.9245	157.2709	155.0146	157.8386	**132**
C7	218.4206	224.0871	225.6863	227.0228	227.7392	226.8634	233.4654	226.7049	232.2929	227.1679	234.4902	222.3731	227.5635	229.0579	230.3177	230.9202	230.1563	236.7866	230.0003	235.3937	230.4701	237.6501	**196**
C8	66.1021	67.3894	68.1145	67.8657	68.9271	67.8608	69.3536	67.8567	69.2455	67.8636	70.1061	60.3620	62.0622	62.4883	63.0156	63.8536	62.9637	64.7319	62.9168	64.3967	63.0637	65.0835	**60**
C9	23.2058	23.4985	23.7070	23.7340	24.1504	23.7389	24.1959	23.7459	24.1017	23.7236	24.3456	20.3942	20.6118	20.6433	20.7319	21.0349	20.7420	21.1263	20.7541	21.0549	20.7172	21.5210	**15**
C8`	36.0510	36.7555	36.9669	37.1150	37.4247	37.1125	37.6459	37.1106	37.5970	37.1109	38.1632	30.7152	31.1896	31.5368	31.3585	31.6695	31.3831	31.7058	31.4062	31.7955	31.3257	31.8659	**31**
H2	9.2412	9.1940	9.2146	9.1667	9.1653	9.1672	9.2317	9.1673	9.2138	9.1663	9.2327	9.2302	9.0921	9.1468	9.0068	9.0354	9.0138	9.0044	9.0198	9.0317	8.9993	9.0042	**8.07**
H3	7.8930	8.0315	8.1240	8.0797	8.2018	8.0760	8.2142	8.0720	8.2077	8.0833	8.2275	7.8444	7.9817	8.0724	8.0317	8.1517	8.0277	8.1674	8.0235	8.1599	8.0355	8.1819	**7.31**
H5	7.7188	7.9115	8.0040	8.0015	8.1305	7.9950	8.1471	7.9882	8.1342	8.0078	8.1715	7.7205	7.8974	7.9934	7.9760	8.1058	7.9705	8.1095	7.9646	8.1016	7.9813	8.1306	**7.31**
H6	8.7195	8.9331	9.0357	9.0522	9.2020	9.0436	9.2622	9.0346	9.2341	9.0605	9.2978	8.5491	8.7357	8.8647	8.8195	9.0069	8.8151	9.0001	8.8099	9.0002	8.8232	9.0400	**8.07**
H8	4.2292	4.3451	4.3884	4.4506	4.5168	4.4418	4.5788	4.4328	4.5575	4.4593	4.6093	4.4880	4.6312	4.7027	4.6959	4.8114	4.6915	4.8114	4.6865	4.8097	4.7000	4.8405	**5.09**
H(9A-9C)	1.3567	1.3681	1.3531	1.3672	1.3372	1.3663	1.3712	1.3650	1.3600	1.3682	1.3871	1.4261	1.4313	1.4276	1.4367	1.4173	1.4356	1.4268	1.4342	1.4284	1.4376	1.4441	**1.6**
H(8`A-8`C)	2.4619	2.4039	2.3762	2.3853	2.3641	2.3849	2.3357	2.3842	2.3446	2.3860	2.3207	2.7873	2.6416	2.6191	2.5775	2.5343	2.5805	2.4563	2.5830	2.4800	2.5745	2.4273	**2.81**
F4	-114.4865	-115.5461	-118.0466	-115.5383	-119.2719	-115.5463	-117.2772	-115.5522	-117.6551	-115.5307	-117.0120	-114.0898	-115.5429	-117.8876	-115.8591	-119.4131	-115.8335	-118.0296	-115.8097	-118.1523	-115.8875	-117.7694	**-102.1**

[a] methyl protons shifts are averaged
[b] according to [9]

Table S9. Cont. IV

Nuclei	R											S										Exp. [b]
	mpW1LYP											mpW1LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.4828	139.9525	140.8951	140.2162	142.1269	140.1880	141.3847	140.1639	141.5911	140.2438	141.6737	138.0239	139.3201	140.0314	140.0519	141.6015	140.0019	141.3526	139.9557	141.2617	140.1006	141.3699	**129**
C2	140.0654	139.9633	140.5214	139.8120	140.2594	139.8221	140.7067	139.8327	140.5833	139.8000	140.6754	139.3485	139.4849	140.0212	139.4970	140.0614	139.4929	140.6129	139.4906	140.4986	139.4995	140.6006	**132**
C3	121.9628	122.6121	123.1375	122.8712	123.4386	122.8537	123.7099	122.8374	123.6709	122.8862	123.7449	122.0772	122.6487	123.1165	122.8876	123.4426	122.8714	123.6473	122.8567	123.5970	122.9013	123.6861	**116**
C4	176.1473	177.0246	177.6646	177.5228	178.1467	177.4890	178.8123	177.4567	178.6743	177.5533	178.9071	176.5361	177.1020	177.7627	177.3919	178.0767	177.3729	178.4887	177.3548	178.3978	177.4074	178.6295	**167**
C5	119.7588	121.0521	121.6454	121.7767	122.5021	121.7290	122.7447	121.6831	122.6591	121.8202	122.8719	119.9121	121.1021	121.6630	121.7119	122.4355	121.6731	122.5793	121.6353	122.5049	121.7464	122.6956	**116**
C6	136.3411	138.3279	139.4122	139.4387	140.8254	139.3726	141.4341	139.3066	141.1391	139.4983	141.7648	136.6810	138.7304	140.0172	139.7711	141.3801	139.7081	141.9011	139.6456	141.7184	139.8277	142.2839	**132**
C7	202.6211	207.7782	209.3145	210.5766	211.6308	210.3901	217.0461	210.2089	216.1478	210.7558	217.9713	207.9684	212.1537	213.3072	214.4009	215.1623	214.2635	219.8843	214.1282	218.8057	214.5296	220.3958	**196**
C8	64.8087	65.9413	66.6307	66.2710	67.2010	66.2555	67.4970	66.2398	67.3414	66.2823	68.2675	59.1606	61.1502	61.8125	62.1638	63.0102	62.0972	63.6763	62.0334	63.4471	62.2269	63.9055	**60**
C9	23.0194	23.2782	23.4066	23.5626	23.7640	23.5450	23.7639	23.5280	23.6835	23.5763	23.8872	19.5716	19.9981	20.1757	20.2377	20.4306	20.2213	20.5847	20.2064	20.5225	20.2514	20.9210	**15**
C8`	36.3159	37.0893	37.3474	37.4110	37.7421	37.3893	37.9553	37.3691	37.9323	37.4299	38.3577	31.9503	32.0958	32.3503	32.2714	32.4808	32.2555	32.5948	32.2408	32.6120	32.2842	32.6749	**31**
H2	8.6760	8.6134	8.6345	8.5731	8.5352	8.5769	8.5767	8.5801	8.5650	8.5692	8.5537	8.7155	8.5439	8.5843	8.4575	8.4611	8.4631	8.4509	8.4681	8.4656	8.4518	8.4608	**8.07**
H3	7.3397	7.4720	7.5610	7.5164	7.6269	7.5145	7.6429	7.5123	7.6350	7.5181	7.6539	7.3222	7.4540	7.5397	7.5009	7.6151	7.4987	7.6299	7.4961	7.6226	7.5029	7.6422	**7.31**
H5	7.1905	7.3768	7.4660	7.4635	7.5825	7.4586	7.6016	7.4535	7.5914	7.4679	7.6207	7.1791	7.3532	7.4411	7.4319	7.5518	7.4276	7.5619	7.4231	7.5524	7.4357	7.5804	**7.31**
H6	8.0834	8.2895	8.3770	8.4032	8.5186	8.3966	8.5837	8.3898	8.5634	8.4092	8.6049	7.8914	8.0614	8.1768	8.1478	8.3090	8.1432	8.3269	8.1382	8.3161	8.1519	8.3729	**8.07**
H8	4.3063	4.3981	4.4252	4.5055	4.5605	4.4978	4.6229	4.4902	4.6105	4.5128	4.6327	4.4564	4.6192	4.6720	4.6856	4.7973	4.6823	4.8170	4.6786	4.8046	4.6884	4.8463	**5.09**
H(9A-9C)	1.3216	1.3308	1.3202	1.3215	1.2774	1.3232	1.2903	1.3245	1.2801	1.3196	1.3009	1.4008	1.4361	1.4422	1.4560	1.4325	1.4551	1.4529	1.4538	1.4517	1.4567	1.4756	**1.6**
H(8`A-8`C)	2.5203	2.4606	2.4330	2.4451	2.4238	2.4459	2.4070	2.4465	2.4101	2.4443	2.3934	2.9829	2.8104	2.7656	2.7300	2.6802	2.7354	2.5986	2.7403	2.6192	2.7247	2.5674	**2.81**
F4	-123.5335	-124.7384	-127.5322	-124.8079	-129.1894	-124.8085	-126.9584	-124.8080	-127.3233	-124.8073	-126.7826	-123.2212	-124.9948	-127.7245	-125.4158	-129.5143	-125.3951	-127.8153	-125.3738	-128.0377	-125.4361	-127.4735	**-102.1**
Nuclei	mpW1PW91											mpW1PW91											
C1	136.7091	137.1261	138.2904	137.3527	139.3925	137.3342	138.8484	137.3222	138.8794	137.3708	139.0868	135.4965	136.8443	137.3776	137.4319	138.8932	137.3747	138.9047	137.3297	138.6184	137.4927	138.9966	**129**
C2	139.0510	138.9813	139.5567	138.8023	139.3841	138.8154	139.7972	138.8338	139.6690	138.7889	139.7849	138.4920	138.6376	139.1844	138.5926	139.2587	138.5931	139.7425	138.5998	139.6330	138.5920	139.7648	**132**
C3	121.1434	121.8839	122.4572	122.1398	122.8577	122.1259	123.1111	122.1175	123.0669	122.1523	123.1972	121.1969	121.8835	122.4042	122.1282	122.8348	122.1142	123.0503	122.1059	122.9791	122.1411	123.1290	**116**
C4	173.1450	174.0361	174.6361	174.4798	175.1382	174.4530	175.7414	174.4320	175.6481	174.5044	175.9056	173.4356	174.0253	174.6981	174.2966	175.0454	174.2852	175.4189	174.2781	175.3524	174.3057	175.5825	**167**
C5	118.9666	120.3546	120.9855	121.0745	121.9413	121.0305	122.1805	120.9922	122.0946	121.1155	122.3576	119.0635	120.3480	120.9568	120.9724	121.8462	120.9359	121.9978	120.9051	121.9093	121.0057	122.1526	**116**
C6	135.1188	137.1393	138.1020	138.2106	139.6150	138.1465	140.1616	138.0877	139.9062	138.2707	140.5379	135.4925	137.5198	138.7879	138.5089	140.2202	138.4556	140.6265	138.4058	140.5120	138.5558	141.0214	**132**
C7	200.5499	205.4732	207.1087	208.0696	209.2352	207.9079	214.4321	207.7523	213.5361	208.2238	215.3863	204.9687	209.2878	210.4288	211.5065	212.2688	211.3693	217.0803	211.2400	215.8598	211.6406	217.5855	**196**
C8	62.5871	63.7277	64.3921	64.0779	65.0594	64.0579	65.5692	64.0437	65.2428	64.0959	66.2934	57.3088	59.1083	59.5712	59.9715	60.7733	59.9036	61.5602	59.8450	61.2368	60.0391	61.8431	**60**
C9	22.4303	22.7074	22.8165	22.9714	23.2346	22.9561	23.2515	22.9463	23.1372	22.9849	23.3928	19.1269	19.5971	19.6794	19.7761	20.0297	19.7623	20.1776	19.7543	20.1086	19.7888	20.5773	**15**
C8`	35.5389	36.3291	36.5286	36.6000	36.9580	36.5839	37.1500	36.5735	37.1332	36.6149	37.6110	31.0253	31.2540	31.5589	31.4502	31.7343	31.4412	31.7914	31.4363	31.8597	31.4556	31.8914	**31**
H2	8.7270	8.6729	8.6666	8.6268	8.5829	8.6306	8.6029	8.6343	8.6110	8.6233	8.5930	8.7399	8.5718	8.6280	8.4933	8.5106	8.5006	8.4771	8.5073	8.5099	8.4860	8.4856	**8.07**
H3	7.3666	7.5071	7.5941	7.5506	7.6672	7.5488	7.6842	7.5469	7.6761	7.5526	7.6994	7.3521	7.4918	7.5782	7.5379	7.6587	7.5357	7.6748	7.5336	7.6662	7.5401	7.6902	**7.31**
H5	7.2156	7.4099	7.4980	7.4952	7.6199	7.4906	7.6379	7.4860	7.6293	7.4999	7.6618	7.2035	7.3869	7.4755	7.4658	7.5930	7.4616	7.6047	7.4575	7.5936	7.4700	7.6265	**7.31**
H6	8.1720	8.3810	8.4466	8.4858	8.5927	8.4800	8.6356	8.4742	8.6335	8.4916	8.6714	7.9622	8.1369	8.2584	8.2244	8.3946	8.2208	8.3985	8.2168	8.3988	8.2277	8.4460	**8.07**
H8	4.3244	4.4232	4.4417	4.5212	4.5686	4.5149	4.6073	4.5088	4.6209	4.5275	4.6357	4.4958	4.6417	4.6998	4.6708	4.8233	4.7033	4.8370	4.7007	4.8311	4.7081	4.8693	**5.09**
H(9A-9C)	1.3031	1.3123	1.2861	1.3005	1.2512	1.3018	1.2673	1.3032	1.2532	1.2994	1.2798	1.3839	1.4107	1.4119	1.4245	1.4007	1.4244	1.4147	1.4241	1.4196	1.4248	1.4408	**1.6**
H(8`A-8`C)	2.4582	2.3926	2.3693	2.3752	2.3559	2.3760	2.3459	2.3770	2.3405	2.3747	2.3305	2.8765	2.7109	2.6756	2.6345	2.5913	2.6410	2.5022	2.6472	2.5276	2.6285	2.4719	**2.81**
F4	-113.4956	-114.2818	-116.9359	-114.1722	-118.3272	-114.1834	-116.1885	-114.1934	-116.4533	-114.1628	-115.9268	-113.3010	-114.6367	-117.0827	-114.8267	-118.6086	-114.8120	-116.9763	-114.7988	-117.1332	-114.8441	-116.6468	**-102.1**
Nuclei	O3LYP											O3LYP											
C1	133.9706	135.2869	135.1280	135.8992	137.5413	135.8935	136.8634	135.8840	136.9936	135.9000	136.9568	131.9841	134.0269	134.9667	134.8776	136.4625	134.8098	136.5165	134.7451	136.4801	134.9454	136.6774	**129**
C2	134.2294	134.0386	134.6059	134.0020	134.6215	134.0143	135.0928	134.0931	135.0297	133.9844	135.0347	133.6011	133.8315	134.4861	133.8598	134.5658	133.8686	134.9908	133.8725	134.9155	133.8449	134.9967	**132**
C3	117.1429	117.8472	118.4244	118.1586	118.8498	118.1512	119.1048	118.1420	119.0383	118.1592	119.1705	117.2423	117.8329	118.4008	118.1462	118.7940	118.1374	118.9776	118.1236	118.9199	118.1480	119.0503	**116**
C4	169.3331	170.2178	170.9930	170.6800	171.4504	170.6575	171.9898	170.6246	171.8402	170.6953	172.1262	169.6935	170.1374	170.8394	170.4612	171.2113	170.4568	171.5048	170.4458	171.4066	170.4567	171.6400	**167**
C5	115.1244	116.3261	117.0316	116.9791	117.7550	116.9488	117.9702	116.9062	117.8594	117.0010	118.1340	115.2829	116.3481	116.9834	116.9736	117.7506	116.9474	117.8633	116.9154	117.7787	116.9914	118.0028	**116**
C6	130.1343	131.8403	133.2468	132.9143	134.4244	132.8471	134.9826	132.7768	134.7083	132.9717	135.3818	130.8195	132.4740	133.5676	133.4119	134.9398	133.3757	135.3121	133.3309	135.1128	133.4364	135.6140	**132**
C7	196.4324	202.4039	202.9208	205.2799	206.3184	205.1284	211.0569	204.9884	210.1352	205.4208	211.6531	200.9322	205.3707	206.9113	207.7346	208.6887	207.5898	212.9882	207.4429	212.0350	207.8698	213.5094	**196**
C8	62.7269	63.8638	64.1933	64.6392	65.2111	64.6247	65.7186	64.6144	65.5898	64.6448	66.4308	57.3727	59.9629	60.5156	61.0054	61.8178	60.9369	62.7983	60.8688	62.5812	61.0698	63.0624	**60**
C9	21.9077	22.1497	22.4381	22.4448	22.6922	22.4333	22.8050	22.4257	22.7348	22.4497	22.9545	18.3907	18.7982	18.9135	19.0083	19.2082	19.0039	19.4486	18.9953	19.3637	19.0069	19.7532	**15**
C8`	35.8615	36.6415	36.9984	37.0897	37.4384	37.0783	37.5559	37.0769	37.5415	37.0931	37.8889	31.6791	31.7885	32.1081	32.0205	32.3175	32.0201	32.2296	32.0132	32.2550	32.0126	32.2365	**31**
H2	8.5171	8.3815	8.5110	8.3059	8.3131	8.3086	8.3569	8.3167	8.3480	8.3030	8.3618	8.6115	8.3742	8.4056	8.2874	8.3033	8.2956	8.2770	8.3028	8.2844	8.2784	8.2790	**8.07**
H3	7.2896	7.4098	7.5061	7.4543	7.5768	7.4521	7.6030	7.4468	7.5953	7.4562	7.6133	7.2766	7.4071	7.4943	7.4552	7.5707	7.4530	7.5845	7.4505	7.5766	7.4572	7.5999	**7.31**
H5	7.1552	7.3290	7.4298	7.3986	7.5094	7.3950	7.5202	7.3889	7.5085	7.4017	7.5463	7.1395	7.3009	7.3898	7.3774	7.4980	7.3735	7.5074	7.3692	7.4968	7.3810	7.5278	**7.31**
H6	8.0527	8.2175	8.3672	8.3017	8.4640	8.2946	8.5029	8.2853	8.4809	8.3083	8.5390	7.8574	7.9837	8.0812	8.0642	8.2140	8.0612	8.2127	8.0575	8.2001	8.0664	8.2508	**8.07**
H8	4.4166	4.5098	4.5410	4.5642	4.6714	4.5583	4.6852	4.5532	4.6658	4.5699	4.7170	4.5458	4.6793	4.7411	4.7470	4.8642	4.7444	4.8665	4.7410	4.8556	4.7490	4.8955	**5.09**
H(9A-9C)	1.2321	1.2056	1.2312	1.2013	1.1647	1.2018	1.1980	1.2027	1.1895	1.2008	1.2166	1.3321	1.3605	1.3485	1.3797	1.3521	1.3795	1.3771	1.3787	1.3725	1.3796	1.3957	**1.6**
H(8`A-8`C)	2.4772	2.4452	2.4019	2.4401	2.4019	2.4414	2.3990	2.4451	2.4021	2.4388	2.3752	2.9410	2.7694	2.7347	2.6983	2.6563	2.7041	2.5681	2.7092	2.5820	2.6922	2.5313	**2.81**
F4	-118.7922	-120.1360	-122.4287	-120.4098	-124.6326	-120.4123	-122.4604	-120.5582	-122.8366	-120.4073	-122.1699	-118.5618	-120.4429	-123.1971	-120.8378	-124.9656	-120.8070	-123.4420	-120.7796	-123.6814	-120.8716	-123.1412	**-102.1**
Nuclei	OLYP											OLYP											
C1	132.8188	134.1516	135.6656	135.1449	137.5235	135.1515	135.6652	135.1532	135.8434	135.1337	135.7556	130.8981	132.7261	133.7888	133.6768	135.1782	133.6081	135.1883	133.5382	135.1931	133.7379	135.3980	**129**
C2	131.6623	131.6975	132.2794	131.7465	132.3472	131.7531	132.6913	131.7546	132.6220	131.7302	132.7039	131.2536	131.3661	132.0518	131.4162	132.0990	131.4235	132.5894	131.4250	132.5059	131.4005	132.5752	**132**
C3	115.3417	116.0422	116.6555	116.3161	116.9608	116.3056	117.2576	116.2899	117.1915	116.3169	117.3369	114.4114	116.0541	116.6230	116.3750	116.9979	116.3650	117.1604	116.3492	117.1047	116.3752	117.2329	**116**
C4	168.2126	169.2294	169.9205	169.5710	170.1814	169.5487	170.9191	169.5215	170.7744	169.5840	171.0771	168.4577	169.1151	169.8267	169.4427	170.2413	169.4360	170.4899	169.4224	170.3927	169.4386	170.6134	**167**
C5	113.3427	114.4633	115.0535	115.0655	115.7600	115.0339	116.1215	114.9960	116.0017	115.0864	116.2699	113.4100	114.5734	115.1849	115.1704	115.9016	115.1450	116.0297	115.1131	115.9473	115.1848	116.1602	**116**
C6	127.6886	129.4580	130.3992	130.3959	131.5991	130.3259	132.5021	130.2522	132.2325	130.4552	132.8719	132.4882	129.9940	131.1063	130.8821	132.4316	130.8446	132.8458	130.8002	132.6433	130.9066	133.1053	**132**
C7	195.3251	201.0301	202.9899	204.5243	206.1991	204.3850	209.0998	204.2443	208.2692	204.6535	209.6663	194.9333	204.0205	205.4470	206.3531	207.3591	206.2114	211.0678	206.0639	210.2799	206.4776	211.6073	**196**
C8	63.8385	65.2339	66.0677	65.6811	66.8369	65.6883	66.9203	65.6854	66.8721	65.6665	67.5606	62.8816	61.2250	62.0414	62.3546	63.1411	62.2822	64.2114	62.2081	64.0080	62.4201	64.4616	**60**
C9	22.0417	22.3211	22.5251	22.7061	22.8886	22.6962	23.1868	22.6811	23.0909	22.7070	23.3016	15.7972	18.8615	19.1193	19.1190	19.3070	19.1099	19.6432	19.0962	19.5371	19.1202	19.9486	**15**
C8`	36.5297	37.3375	37.5614	37.8176	38.0745	37.8036	38.1673	37.7827	38.1190	37.8211	38.5013	31.4966	32.4077	32.6511	32.6378	32.9272	32.6373	32.7834	32.6299	32.8079	32.6276	32.7561	**31**
H2	8.3522	8.2235	8.1969	8.1272	8.0714	8.1268	8.2234	8.1264	8.2066	8.1267	8.2299	8.4369	8.2352	8.2566	8.1468	8.1702	8.1543	8.1611	8.1613	8.1618	8.1388	8.1574	**8.07**
H3	7.2072	7.3275	7.4178	7.4008	7.5127	7.3974	7.5330	7.3939	7.5211	7.4035	7.5445	7.1593	7.3325	7.4196	7.3792	7.4934	7.3770	7.5033	7.3746	7.4956	7.3809	7.5175	**7.31**
H5	7.0851	7.2353	7.3143	7.2988	7.4157	7.2941	7.4375	7.2893	7.4251	7.3029	7.4576	7.0403	7.2266	7.3145	7.2993	7.4188	7.2955	7.4288	7.2915	7.4188	7.3025	7.4474	**7.31**
H6	7.9775	8.1327	8.1956	8.2132	8.2977	8.2041	8.4009	8.1954	8.3698	8.2217	8.4374	8.7484	7.8865	7.9743	7.9576	8.1089	7.9547	8.1075	7.9514	8.0939	7.9595	8.1417	**8.07**
H8	4.5323	4.5911	4.6096	4.6267	4.6824	4.6200	4.7353	4.6144	4.7106	4.6332	4.7707	4.4883	4.7554	4.8166	4.8221	4.9436	4.8190	4.9419	4.8155	4.9305	4.8243	4.9712	**5.09**
H(9A-9C)	1.2237	1.2082	1.1959	1.1823	1.1420	1.1826	1.2055	1.1826	1.1992	1.1815	1.2218	1.2466	1.3653	1.3601	1.3854	1.3618	1.3848	1.3978	1.3840	1.3909	1.3856	1.4134	**1.6**
H(8`A-8`C)	2.5179	2.4873	2.4697	2.4886	2.4649	2.4895	2.4510	2.4902	2.4526	2.4873	2.4211	2.3523	2.8150	2.7687	2.7435	2.7024	2.7489	2.6101	2.7538	2.6211	2.7376	2.5695	**2.81**
F4	-126.2399	-127.8764	-131.1829	-128.1328	-133.2759	-128.1639	-130.3061	-128.1920	-130.7905	-128.1043	-129.9584	-125.1106	-127.9468	-131.0095	-128.4021	-132.8593	-128.3693	-131.3222	-128.3392	-131.5975	-128.4363	-131.0041	**-102.1**

[a] methyl protons shifts are averaged
[b] according to [9]

Table S9. Cont. V

Nuclei	R											S										Exp. [b]
	OPBE											OPBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	129.7640	131.1387	132.6552	132.1246	134.4950	132.1378	132.7494	132.1341	132.8307	132.0968	132.7529	127.9531	129.7572	131.3960	130.9073	132.9633	130.8138	132.2249	130.6965	132.6314	130.9636	132.5011	**129**
C2	130.3586	130.4886	130.9968	130.4429	131.0543	130.4635	131.3872	130.4661	131.3319	130.3820	131.3838	129.9865	130.2359	130.9157	130.1823	130.9380	130.1990	131.3075	130.1994	131.2030	130.1628	131.3207	**132**
C3	114.2213	115.0550	115.6259	115.3016	116.0144	115.3021	116.3293	115.2846	116.2561	115.3063	116.4542	114.3041	115.0698	115.5900	115.3365	116.0072	115.3394	116.2309	115.3240	116.1537	115.3295	116.3409	**116**
C4	164.6226	165.6789	166.2199	165.9412	166.5402	165.9340	167.2498	165.9090	167.1104	166.0101	167.4931	164.9027	165.5555	166.0292	165.7368	166.3569	165.7530	166.8192	165.7519	166.6262	165.7218	166.9648	**167**
C5	112.2687	113.5344	114.0760	114.0744	114.8381	114.0527	115.1922	114.0131	115.0739	114.1130	115.4008	112.4202	113.6143	114.1128	114.1369	114.8497	114.1271	115.0869	114.0994	114.9493	114.1433	115.2524	**116**
C6	126.1608	127.9997	128.8093	128.8180	129.9411	128.7696	130.8401	128.7038	130.6005	128.8489	131.2575	126.8203	128.5704	129.4079	129.2674	130.6027	129.2570	131.2141	129.2292	130.8690	129.2803	131.4889	**132**
C7	192.8626	198.3520	200.1588	201.6561	203.2107	201.5462	206.1754	201.4188	205.3233	201.7358	206.5747	196.3497	200.6868	202.1872	203.0429	204.1492	202.9127	207.7285	202.7568	207.1557	203.1474	208.2542	**196**
C8	61.2284	62.7133	63.5636	63.1881	64.3519	63.1850	64.4468	63.1637	64.3074	63.1720	65.1108	56.6311	58.7512	59.9248	59.9517	61.0884	59.8539	61.5973	59.7391	61.6414	60.0230	61.9029	**60**
C9	21.2805	21.6678	21.7922	21.9610	22.1440	21.9624	22.3933	21.9464	22.3075	21.9463	22.5303	17.8291	18.2838	18.5005	18.5007	18.7647	18.4933	18.9349	18.4692	18.8763	18.4996	19.2950	**15**
C8`	35.4845	36.3569	36.4549	36.7323	36.9249	36.7278	37.0000	36.7052	36.9687	36.7163	37.3820	31.0988	31.3654	31.3318	31.4174	31.5251	31.4408	31.6115	31.4469	31.5375	31.3965	31.5941	**31**
H2	8.3870	8.2642	8.2215	8.1564	8.0952	8.1575	8.2408	8.1577	8.2328	8.1562	8.2594	8.4575	8.2769	8.2227	8.1564	8.1258	8.1678	8.1855	8.1792	8.1490	8.1477	8.1810	**8.07**
H3	7.2282	7.3602	7.4433	7.4277	7.5438	7.4252	7.5609	7.4218	7.5508	7.4327	7.5779	7.2304	7.3678	7.4497	7.4149	7.5264	7.4130	7.5438	7.4104	7.5341	7.4158	7.5608	**7.31**
H5	7.1021	7.2653	7.3426	7.3260	7.4471	7.3219	7.4668	7.3170	7.4549	7.3330	7.4935	7.0869	7.2574	7.3371	7.3302	7.4448	7.3268	7.4602	7.3227	7.4473	7.3327	7.4817	**7.31**
H6	8.0380	8.1929	8.2297	8.2560	8.3210	8.2498	8.4322	8.2430	8.4104	8.2608	8.4821	7.8021	7.9511	7.9981	8.0067	8.1209	8.0068	8.1616	8.0062	8.1245	8.0072	8.1968	**8.07**
H8	4.5419	4.6115	4.6071	4.6376	4.6660	4.6345	4.7386	4.6308	4.7174	4.6371	4.7816	4.6657	4.7892	4.8168	4.8395	4.9337	4.8401	4.9559	4.8394	4.9298	4.8389	4.9886	**5.09**
H(9A-9C)	1.1827	1.1710	1.1506	1.1424	1.0922	1.1427	1.1573	1.1423	1.1499	1.1403	1.1786	1.2938	1.3294	1.3061	1.3393	1.2986	1.3395	1.3428	1.3392	1.3289	1.3389	1.3621	**1.6**
H(8`A-8`C)	2.4371	2.4087	2.3861	2.4045	2.3742	2.4058	2.3612	2.4063	2.3625	2.4000	2.3311	2.8529	2.7064	2.6163	2.6177	2.5447	2.6266	2.4933	2.6347	2.4903	2.6099	2.4549	**2.81**
F4	-115.1642	-116.2433	-119.3426	-116.3765	-121.1136	-116.4067	-118.1552	-116.4377	-118.5815	-116.2483	-117.6067	-115.0982	-116.3610	-119.4888	-116.7532	-121.2078	-116.7051	-119.0436	-116.6554	-119.6253	-116.7819	-118.7471	**-102.1**
Nuclei	OPW91											OPW91										
C1	130.0734	131.4711	132.9769	132.4406	134.8087	132.4451	133.0129	132.4321	133.1402	132.4191	133.0519	128.2394	130.0724	131.7005	131.1724	133.2463	131.0761	132.5216	130.9590	132.9078	131.2337	132.7953	**129**
C2	130.5806	130.7074	131.2089	130.6288	131.2637	130.6390	131.5719	130.6356	131.5478	130.6007	131.6048	130.1962	130.4533	131.1259	130.4042	131.1441	130.4116	131.5201	130.4034	131.4168	130.3802	131.5359	**132**
C3	114.4183	115.2508	115.8151	115.5092	116.1968	115.4994	116.5211	115.4732	116.4393	115.4999	116.6391	114.5029	115.2650	115.7792	115.5361	116.1909	115.5285	116.4136	115.5035	116.3378	115.5247	116.5251	**116**
C4	165.0246	166.0821	166.6217	166.4195	166.9443	166.4003	167.7080	166.3664	167.5188	166.4192	167.9027	165.3169	165.9654	166.4385	166.1639	166.7698	166.1681	167.2288	166.1553	167.0408	166.1434	167.3773	**167**
C5	112.4634	113.7286	114.2665	114.2944	115.0217	114.2618	115.3914	114.2128	115.2585	114.3067	115.5871	112.6210	113.8117	114.3056	114.3432	115.0398	114.3225	115.2744	114.2843	115.1397	114.3450	115.4419	**116**
C6	126.3826	128.2204	129.0301	129.0438	130.1652	128.9844	131.0735	128.9103	130.8310	129.0819	131.4938	127.0499	128.7969	129.6351	129.5203	130.8358	129.4965	131.4451	129.4563	131.1082	129.5270	131.7238	**132**
C7	193.2195	198.7503	200.5473	202.0469	203.6032	201.9273	206.5400	201.7965	205.7249	202.1429	206.9853	196.7445	201.1005	202.5918	203.4416	204.5479	203.3022	208.1416	203.1393	207.5501	203.5465	208.6706	**196**
C8	61.4164	62.9130	63.7519	63.3730	64.5345	63.3605	64.5943	63.3262	64.4929	63.3665	65.2823	56.7828	58.9381	60.1067	60.1087	61.2534	60.0077	61.7812	59.8918	61.8124	60.1818	62.0859	**60**
C9	21.3412	21.7318	21.8564	22.0225	22.2056	22.0139	22.4453	21.9905	22.3695	22.0127	22.5934	17.9020	18.3623	18.5810	18.5780	18.8386	18.5624	19.0151	18.5310	18.9558	18.5743	19.3737	**15**
C8`	35.5474	36.4260	36.5197	36.7969	36.9960	36.7816	37.0617	36.7522	37.0400	36.7928	37.4582	31.1915	31.4588	31.4241	31.5288	31.6223	31.5399	31.7046	31.5341	31.6351	31.5020	31.6928	**31**
H2	8.3887	8.2639	8.2222	8.1590	8.0961	8.1592	8.2467	8.1596	8.2338	8.1570	8.2615	8.4616	8.2780	8.2245	8.1636	8.1292	8.1736	8.1874	8.1840	8.1527	8.1537	8.1831	**8.07**
H3	7.2300	7.3612	7.4442	7.4326	7.5443	7.4293	7.5651	7.4261	7.5509	7.4339	7.5785	7.2318	7.3686	7.4505	7.4163	7.5267	7.4137	7.5442	7.4109	7.5345	7.4169	7.5610	**7.31**
H5	7.1042	7.2672	7.3446	7.3319	7.4481	7.3269	7.4705	7.3219	7.4560	7.3348	7.4945	7.0894	7.2592	7.3388	7.3327	7.4461	7.3286	7.4614	7.3242	7.4485	7.3348	7.4827	**7.31**
H6	8.0365	8.1901	8.2278	8.2553	8.3202	8.2483	8.4351	8.2419	8.4096	8.2601	8.4824	7.8035	7.9505	7.9980	8.0099	8.1218	8.0088	8.1616	8.0074	8.1258	8.0096	8.1969	**8.07**
H8	4.5413	4.6099	4.6067	4.6350	4.6660	4.6313	4.7388	4.6276	4.7179	4.6370	4.7820	4.6622	4.7853	4.8138	4.8390	4.9316	4.8382	4.9531	4.8368	4.9279	4.8379	4.9856	**5.09**
H(9A-9C)	1.1844	1.1724	1.1522	1.1437	1.0939	1.1434	1.1586	1.1424	1.1520	1.1425	1.1806	1.2943	1.3301	1.3074	1.3418	1.3002	1.3413	1.3445	1.3406	1.3308	1.3411	1.3636	**1.6**
H(8`A-8`C)	2.4383	2.4106	2.3882	2.4045	2.3762	2.4051	2.3601	2.4055	2.3644	2.4024	2.3329	2.8575	2.7104	2.6209	2.6250	2.5505	2.6328	2.4979	2.6400	2.4956	2.6165	2.4597	**2.81**
F4	-115.7848	-116.9206	-120.0301	-116.9646	-121.8199	-116.9928	-118.7228	-117.0127	-119.2902	-116.9380	-118.3062	-115.7012	-117.0262	-120.1651	-117.4050	-121.8965	-117.3613	-119.7414	-117.3169	-120.3065	-117.4400	-119.4445	**-102.1**
Nuclei	PBE											PBE										
C1	135.5369	136.0918	137.1653	136.3677	138.3715	136.3432	137.9723	136.3302	138.0000	136.4097	138.2666	133.9549	135.5103	136.0530	136.0986	137.6401	136.0426	137.7558	136.0033	137.5912	136.1760	137.8979	**129**
C2	135.9657	136.0179	136.6216	135.7847	136.4967	135.7983	136.9066	135.8222	136.8094	135.7890	136.9073	135.2241	135.5670	136.1193	135.5057	136.3042	135.5028	136.8654	135.5121	136.7580	135.5269	136.8854	**132**
C3	119.4465	120.3299	120.8882	120.5608	121.3376	120.5455	121.6570	120.5407	121.5966	120.5927	121.7624	119.5345	120.3283	120.8574	120.5295	121.3174	120.5157	121.5667	120.5123	121.4938	120.5600	121.6702	**116**
C4	173.9823	175.0866	175.7504	175.5136	176.3815	175.4853	176.9469	175.4679	176.8322	175.5580	177.1272	174.3115	175.1027	175.8451	175.3569	176.3062	175.3425	176.6457	175.3376	176.5574	175.3868	176.8245	**167**
C5	117.3377	118.8348	119.4453	119.5117	120.4263	119.4676	120.7320	119.4345	120.6335	119.5712	120.9231	117.5420	118.8521	119.4821	119.4030	120.3643	119.3686	120.5554	119.3443	120.4643	119.4527	120.7344	**116**
C6	132.4775	134.5082	135.5902	135.4775	137.1352	135.4145	137.6377	135.3620	137.3771	135.5552	138.0465	132.8577	134.9572	136.2454	135.8915	137.7657	135.8360	138.2041	135.7900	138.0185	135.9600	138.5976	**132**
C7	200.2846	204.9361	206.5139	207.3187	208.7358	207.1695	213.0970	207.0319	212.3370	207.4784	214.0538	205.2335	209.1883	210.4404	211.1454	212.2526	211.0237	216.2129	210.9132	215.2932	211.2804	216.6930	**196**
C8	66.5088	67.7352	68.5365	68.0186	69.2245	67.9992	69.7030	67.9905	69.4643	68.0544	70.5121	60.8379	62.8084	63.3380	63.6487	64.6563	63.5816	65.3895	63.5289	65.1438	63.7343	65.6928	**60**
C9	23.3476	23.7914	23.9606	24.0315	24.4395	24.0128	24.5728	24.0048	24.4653	24.0668	24.7581	19.9739	20.6830	20.7908	20.8644	21.2357	20.8478	21.5194	20.8429	21.4105	20.8983	22.0261	**15**
C8`	37.1172	37.9328	38.1214	38.1135	38.5395	38.1010	38.7049	38.0990	38.6815	38.1431	39.1975	32.1770	32.4188	32.7113	32.5246	32.8859	32.5166	32.9628	32.5184	32.9920	32.5484	33.0440	**31**
H2	8.4940	8.4541	8.4552	8.4051	8.3713	8.4089	8.3990	8.4131	8.4018	8.4020	8.3885	8.5295	8.3765	8.4273	8.2992	8.3159	8.3056	8.2934	8.3120	8.3107	8.2932	8.2994	**8.07**
H3	7.2033	7.3447	7.4313	7.3857	7.5032	7.3838	7.5208	7.3823	7.5132	7.3881	7.5355	7.1915	7.3278	7.4143	7.3701	7.4921	7.3680	7.5036	7.3664	7.4955	7.3727	7.5186	**7.31**
H5	7.0554	7.2476	7.3344	7.3285	7.4528	7.3239	7.4719	7.3198	7.4630	7.3335	7.4950	7.0514	7.2254	7.3152	7.2983	7.4275	7.2942	7.4386	7.2906	7.4284	7.3027	7.4597	**7.31**
H6	8.0650	8.2613	8.3213	8.3484	8.4499	8.3435	8.4938	8.3391	8.4841	8.3536	8.5258	7.8075	7.9693	8.0875	8.0493	8.2174	8.0456	8.2265	8.0420	8.2172	8.0532	8.2729	**8.07**
H8	4.5942	4.6682	4.6640	4.7434	4.7783	4.7384	4.8154	4.7339	4.8140	4.7488	4.8411	4.7365	4.8721	4.9225	4.9285	5.0427	4.9260	5.0540	4.9238	5.0416	4.9312	5.0891	**5.09**
H(9A-9C)	1.3652	1.3737	1.3620	1.3582	1.3268	1.3594	1.3445	1.3610	1.3344	1.3577	1.3585	1.4620	1.4973	1.5000	1.5101	1.4967	1.5097	1.5158	1.5096	1.5145	1.5110	1.5442	**1.6**
H(8`A-8`C)	2.5658	2.4898	2.4677	2.4656	2.4518	2.4665	2.4330	2.4680	2.4322	2.4654	2.4135	3.0023	2.8324	2.7952	2.7516	2.7069	2.7580	2.6127	2.7646	2.6329	2.7457	2.5792	**2.81**
F4	-131.1424	-131.7563	-134.9700	-131.5194	-136.5599	-131.5379	-134.0199	-131.5553	-134.3640	-131.5024	-133.6741	-130.9917	-132.3049	-135.2933	-132.4127	-137.0364	-132.4049	-135.1822	-132.3985	-135.4687	-132.4236	-134.7644	**-102.1**
Nuclei	PBE0											PBE0										
C1	136.2247	136.6526	137.6494	136.8626	138.8179	136.8401	138.3389	136.8206	138.4202	136.8878	138.5165	135.0705	136.3670	136.9426	136.9688	138.3856	136.9063	138.4604	136.8512	138.1253	137.0380	138.5078	**129**
C2	138.7455	138.6972	139.2899	138.5224	139.1126	138.5294	139.6279	138.5381	139.4524	138.5187	139.5604	138.2240	138.3806	138.9274	138.3295	138.9750	138.3256	139.5396	138.3238	139.3720	138.3367	139.5045	**132**
C3	120.8925	121.6540	122.2093	121.9097	122.6105	121.8907	122.9447	121.8736	122.8377	121.9304	122.9696	120.9444	121.6525	122.1782	121.8956	122.5853	121.8764	122.8788	121.8592	122.7522	121.9168	122.9010	**116**
C4	172.7695	173.6677	174.2592	174.1060	174.7504	174.0748	175.4368	174.0455	175.2494	174.1384	175.5356	173.0167	173.6449	174.3079	173.9164	174.6482	173.8991	175.1081	173.8827	174.9805	173.9346	175.2141	**167**
C5	118.6951	120.1057	120.7177	120.8251	121.6797	120.7761	122.0034	120.7290	121.8560	120.8746	122.1212	118.8136	120.1112	120.7251	120.7385	121.6008	120.6967	121.8294	120.6564	121.6863	120.7809	121.9289	**116**
C6	134.9467	136.9717	138.0243	138.0376	139.4645	137.9675	140.0789	137.8990	139.7408	138.1064	140.4199	135.3034	137.3666	138.6127	138.3429	140.0727	138.2853	140.5728	138.2274	140.3897	138.3981	140.9095	**132**
C7	200.1830	205.0445	206.4951	207.5876	208.7013	207.4269	213.8365	207.2685	212.8952	207.7437	214.6933	204.6033	208.8622	210.0809	211.0822	211.8366	210.9380	216.6033	210.7982	215.3664	211.2259	217.0626	**196**
C8	62.4961	63.6480	64.3663	63.9871	64.9554	63.9622	65.4882	63.9393	65.2096	64.0139	66.1783	57.1221	58.8511	59.3074	59.6939	60.4822	59.6234	61.3132	59.5575	60.9413	59.7669	61.5421	**60**
C9	22.4232	22.7099	22.8836	22.9713	23.2313	22.9485	23.3154	22.9273	23.1815	22.9957	23.4231	19.1174	19.6122	19.6632	19.7712	20.0251	19.7540	20.2525	19.7389	20.1245	19.7907	20.6140	**15**
C8`	35.4509	36.2307	36.4509	36.4979	36.8360	36.4785	37.0927	36.4609	36.9944	36.5195	37.4940	30.7624	31.0177	31.3187	31.2114	31.4738	31.1980	31.6175	31.1846	31.6291	31.2246	31.6596	**31**
H2	8.7291	8.6745	8.6839	8.6307	8.5912	8.6340	8.6207	8.6372	8.6136	8.6271	8.6069	8.7394	8.5811	8.6311	8.4997	8.5161	8.5067	8.4889	8.5132	8.5182	8.4920	8.4934	**8.07**
H3	7.3570	7.4984	7.5860	7.5429	7.6585	7.5407	7.6805	7.5383	7.6697	7.5447	7.6928	7.3444	7.4827	7.5699	7.5283	7.6473	7.5259	7.6672	7.5234	7.6563	7.5302	7.6796	**7.31**
H5	7.2043	7.3984	7.4865	7.4833	7.6061	7.4784	7.6287	7.4735	7.6162	7.4877	7.6494	7.1957	7.3777	7.4663	7.4563	7.5822	7.4518	7.5978	7.4472	7.5841	7.4603	7.6170	**7.31**
H6	8.1786	8.3833	8.4552	8.4878	8.5945	8.4818	8.6451	8.4757	8.6289	8.4931	8.6774	7.9635	8.1395	8.2598	8.2257	8.3971	8.2217	8.4076	8.2174	8.4040	8.2288	8.4520	**8.07**
H8	4.3167	4.4108	4.4199	4.5072	4.5534	4.5008	4.6039	4.4943	4.6020	4.5131	4.6265	4.4991	4.6448	4.7045	4.7095	4.8253	4.7065	4.8443	4.7033	4.8349	4.7119	4.8737	**5.09**
H(9A-9C)	1.3125	1.3212	1.3067	1.3099	1.2608	1.3109	1.2798	1.3118	1.2649	1.3088	1.2919	1.3963	1.4224	1.4195	1.4330	1.4094	1.4328	1.4284	1.4324	1.4298	1.4329	1.4515	**1.6**
H(8`A-8`C)	2.4651	2.3989	2.3727	2.3791	2.3574	2.3796	2.3472	2.3802	2.3450	2.3785	2.3301	2.8767	2.7128	2.6773	2.6349	2.5897	2.6409	2.5049	2.6468	2.5284	2.6289	2.4711	**2.81**
F4	-113.4353	-114.1433	-116.7497	-113.9892	-118.1064	-114.0013	-115.9498	-114.0142	-116.2896	-113.9770	-115.6973	-113.3277	-114.5966	-117.0322	-114.7673	-118.5219	-114.7530	-116.8851	-114.7415	-117.0489	-114.7824	-116.5622	**-102.1**

[a] methyl protons shifts are averaged
[b] according to [9]

Table S9. Cont. VI

Nuclei	R											S										Exp. [b]
	TPSS																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	132.3080	132.7323	133.5947	132.9917	134.6209	132.9794	133.9174	132.9795	133.4835	133.0145	134.1627	130.9473	132.0464	132.8321	132.7165	134.1527	132.6760	133.8514	132.6492	133.7648	132.7685	133.9904	**129**
C2	133.0997	133.0157	133.6822	132.9050	133.5045	132.9199	133.9437	132.9461	133.4500	132.9010	133.9167	132.3746	132.5433	133.1843	132.5871	133.2524	132.5896	133.7520	132.6038	133.7197	132.5960	133.7438	**132**
C3	116.6148	117.2984	117.9237	117.5959	118.2555	117.5862	118.5980	117.5876	118.0301	117.6152	118.6571	116.6745	117.2824	117.8745	117.5564	118.2099	117.5476	118.4658	117.5497	118.7785	117.5754	118.5352	**116**
C4	170.6841	171.5811	172.3374	172.0858	172.8432	172.0623	173.5294	172.0498	172.7101	172.1186	173.6596	170.9980	171.6247	172.4068	171.9513	172.7573	171.9401	173.2076	171.9397	172.7606	171.9719	173.3439	**167**
C5	114.5838	115.8370	116.5194	116.5569	117.3608	116.5197	117.6964	116.4938	116.9319	116.6029	117.8309	114.7542	115.8493	116.5202	116.4562	117.2683	116.4268	117.4654	116.4086	117.6460	116.4943	117.6013	**116**
C6	129.6014	131.4435	132.6218	132.4972	133.9868	132.4389	134.5452	132.3920	132.8937	132.5630	134.9193	129.9037	131.8399	133.1059	132.8246	134.4809	132.7742	135.0675	132.7346	133.8495	132.8818	135.3960	**132**
C7	196.4615	200.8812	202.3135	203.2587	204.2943	203.1209	208.8163	202.9947	203.7788	203.4005	209.6447	201.0290	204.6160	205.9348	206.6362	207.5175	206.5206	211.4415	206.4167	206.9790	206.7570	211.9588	**196**
C8	65.1158	66.2120	66.9967	66.5823	67.5160	66.5694	67.7566	66.5676	66.8060	66.6049	68.5367	60.1278	61.8831	62.5632	62.8019	63.6923	62.7474	64.2607	62.7059	64.3460	62.8662	64.4976	**60**
C9	23.9382	24.2126	24.5053	24.5049	24.8006	24.4912	24.8817	24.4888	24.5589	24.5284	25.0320	20.6506	21.2665	21.4915	21.5390	21.8543	21.5290	22.1455	21.5306	23.4796	21.5593	22.5571	**15**
C8`	37.5256	38.2274	38.5539	38.5318	38.8578	38.5228	39.1217	38.5251	38.6513	38.5508	39.5382	33.2385	33.3352	33.6679	33.4955	33.7511	33.4908	33.9306	33.4973	35.3565	33.5099	33.9584	**31**
H2	8.5053	8.4506	8.4858	8.4146	8.4078	8.4174	8.4634	8.4207	8.2608	8.4123	8.4454	8.5333	8.3896	8.4302	8.3110	8.3267	8.3165	8.3314	8.3222	8.4330	8.3060	8.3282	**8.07**
H3	7.1662	7.3060	7.4014	7.3539	7.4751	7.3516	7.4934	7.3498	7.1856	7.3564	7.5050	7.1476	7.2856	7.3782	7.3357	7.4586	7.3331	7.4748	7.3311	7.4493	7.3384	7.4865	**7.31**
H5	7.0222	7.2106	7.3064	7.2978	7.4257	7.2928	7.4508	7.2885	7.1240	7.3028	7.4683	7.0178	7.1891	7.2832	7.2681	7.3973	7.2637	7.4087	7.2598	7.3786	7.2727	7.4263	**7.31**
H6	7.9512	8.1457	8.2359	8.2495	8.3724	8.2435	8.4400	8.2381	8.0774	8.2555	8.4692	7.7288	7.9081	8.0237	7.9982	8.1671	7.9933	8.1988	7.9889	8.1022	8.0030	8.2393	**8.07**
H8	4.4709	4.5419	4.5602	4.6283	4.6855	4.6222	4.7477	4.6168	4.4417	4.6345	4.7669	4.5859	4.7329	4.7881	4.8006	4.9128	4.7971	4.9372	4.7941	4.9314	4.8041	4.9650	**5.09**
H(9A-9C)	1.3567	1.3679	1.3676	1.3629	1.3311	1.3636	1.3485	1.3649	1.1767	1.3626	1.3622	1.4392	1.4842	1.4875	1.5034	1.4900	1.5025	1.5193	1.5021	1.6640	1.5046	1.5408	**1.6**
H(8`A-8`C)	2.5215	2.4527	2.4256	2.4341	2.4118	2.4348	2.3810	2.4361	2.2522	2.4338	2.3643	2.9653	2.7995	2.7626	2.7257	2.6817	2.7310	2.6015	2.7368	2.8894	2.7208	2.5649	**2.81**
F4	-124.7102	-125.6695	-128.6489	-125.5433	-130.3088	-125.5555	-127.4659	-125.5685	-127.0790	-125.5312	-127.1658	-124.6252	-126.1659	-129.1136	-126.4163	-130.9115	-126.4042	-128.7170	-126.3932	-124.8559	-126.4283	-128.3327	**-102.1**
Nuclei	VSXC																						
C1	130.0829	130.4045	131.1400	130.4934	131.6615	130.4929	131.1365	130.4902	131.2057	130.4951	131.2579	129.9454	130.6445	131.8488	131.2031	132.5520	131.1505	132.4267	131.1004	132.2788	131.2589	132.5715	**129**
C2	131.4719	131.5765	132.0332	131.5476	131.9755	131.5536	132.4149	131.5574	132.3103	131.5434	132.5007	131.5035	131.5629	132.0835	131.4748	131.9974	131.4854	132.4275	131.4940	132.3584	131.4659	132.4408	**132**
C3	115.0253	115.9281	116.4781	116.3182	116.9617	116.2986	117.2532	116.2767	117.1666	116.3381	117.3602	115.1018	115.8625	116.3437	116.1552	116.7869	116.1441	116.9700	116.1304	116.9294	116.1665	117.0707	**116**
C4	168.4085	169.4140	170.1094	169.9432	170.7388	169.9139	171.2602	169.8824	171.1101	169.9727	171.4432	168.2644	169.1345	169.7602	169.5550	170.3438	169.5352	170.7332	169.5129	170.6261	169.5745	170.8988	**167**
C5	112.9381	114.3706	114.9696	115.1434	115.9400	115.0989	116.2089	115.0522	116.0882	115.1874	116.3893	112.8384	114.1341	114.6817	114.8040	115.5837	114.7687	115.7340	114.7306	115.6555	114.8386	115.8930	**116**
C6	129.7735	131.5896	132.6289	132.6050	134.1264	132.5458	134.6888	132.4845	134.4417	132.6624	135.0466	129.7921	131.8114	132.8618	132.8875	134.4094	132.8259	134.9250	132.7615	134.6909	132.9470	135.2245	**132**
C7	190.4964	194.5948	195.8890	196.6716	197.5040	196.5484	201.3041	196.4236	200.4899	196.7897	202.0685	192.4201	196.4292	197.9570	198.6054	199.5513	198.4654	203.3086	198.3255	202.3644	198.7417	203.9258	**196**
C8	71.0293	71.8644	72.4464	72.1610	72.9614	72.1470	73.3160	72.1307	73.2068	72.1762	73.9137	63.2954	64.4627	65.0975	65.1337	65.9999	65.0894	66.5041	65.0447	66.3060	65.1788	66.9366	**60**
C9	27.6811	28.6013	28.9238	29.2582	29.7109	29.2182	30.0806	29.1763	29.9393	29.2980	30.1347	28.6031	28.7198	28.7057	28.8776	29.0104	28.8658	28.9877	28.8527	28.9354	28.8913	29.2920	**15**
C8`	40.4536	40.9423	41.0239	41.1700	41.3482	41.1601	41.3711	41.1480	41.3482	41.1808	41.7912	35.6942	36.3333	36.3426	36.5410	36.8365	36.5434	36.8289	36.5411	36.8765	36.5384	37.0830	**31**
H2	8.7013	8.6318	8.6383	8.5965	8.5956	8.5987	8.6008	8.6009	8.6015	8.5945	8.6002	8.6698	8.5714	8.5462	8.4980	8.4914	8.5044	8.4746	8.5105	8.4951	8.4915	8.4705	**8.07**
H3	7.2076	7.3421	7.4286	7.3891	7.5038	7.3867	7.5214	7.3843	7.5128	7.3914	7.5352	7.2377	7.3761	7.4621	7.4257	7.5415	7.4230	7.5574	7.4205	7.5480	7.4281	7.5730	**7.31**
H5	7.1085	7.2957	7.3836	7.3798	7.5056	7.3750	7.5203	7.3702	7.5095	7.3844	7.5443	7.1230	7.2984	7.3840	7.3775	7.4993	7.3729	7.5080	7.3684	7.4968	7.3817	7.5256	**7.31**
H6	8.1799	8.3473	8.4451	8.4415	8.5921	8.4354	8.6432	8.4296	8.6230	8.4472	8.6738	7.8041	7.9933	8.0857	8.0898	8.2480	8.0846	8.2771	8.0794	8.2615	8.0945	8.3072	**8.07**
H8	4.3876	4.4583	4.4912	4.5227	4.5993	4.5183	4.6338	4.5141	4.6138	4.5269	4.6595	4.6175	4.7683	4.8270	4.8563	4.9599	4.8507	5.0035	4.8453	4.9843	4.8616	5.0218	**5.09**
H(9A-9C)	1.5961	1.6138	1.6048	1.6171	1.6025	1.6170	1.6242	1.6171	1.6201	1.6172	1.6378	1.7731	1.7717	1.7506	1.7772	1.7569	1.7769	1.7723	1.7766	1.7683	1.7776	1.7889	**1.6**
H(8`A-8`C)	2.6858	2.6354	2.6002	2.6143	2.5757	2.6156	2.5544	2.6170	2.5572	2.6129	2.5289	2.8671	2.7641	2.7059	2.7132	2.6678	2.7172	2.6228	2.7210	2.6423	2.7093	2.5927	**2.81**
F4	-125.4361	-126.1598	-129.1323	-125.9174	-130.4800	-125.9405	-127.8419	-125.9540	-128.3085	-125.8941	-127.4076	-125.7847	-126.8972	-129.9759	-126.9215	-131.4340	-126.9246	-129.2349	-126.9188	-129.5967	-126.9184	-128.8423	**-102.1**
Nuclei	wB97																						
C1	136.3743	136.5643	137.5508	136.6805	138.3186	136.6682	137.1758	136.6563	137.6400	136.6935	137.3306	135.5496	136.5810	137.2430	137.2393	138.6376	137.1701	138.5360	137.1091	138.2897	137.3170	138.7211	**129**
C2	140.2891	140.1704	140.7301	140.0418	140.6111	140.0495	141.1373	140.0566	141.0098	140.0348	141.1780	140.0931	140.0448	140.6006	139.9574	140.5644	139.9621	140.9964	139.9662	140.9089	139.9528	141.0199	**132**
C3	121.6439	122.2148	122.7714	122.4318	123.1041	122.4188	123.2000	122.4051	123.1728	122.4445	123.2668	121.6716	122.2096	122.7417	122.4350	123.1020	122.4187	123.2279	122.4023	123.1663	122.4515	123.2949	**116**
C4	174.2577	174.9242	175.5185	175.3214	175.9512	175.2956	176.5447	175.2691	176.3511	175.3461	176.6908	174.3838	174.8494	175.5012	175.0939	175.7994	175.0823	176.1349	175.0683	176.0692	175.1036	176.2686	**167**
C5	119.4831	120.7345	121.3443	121.4210	122.2577	121.3777	122.3482	121.3337	122.2709	121.4624	122.5094	119.5892	120.7784	121.3962	121.3974	122.2486	121.3581	122.3057	121.3179	122.2298	121.4354	122.4485	**116**
C6	136.8221	138.8055	139.9029	139.8974	141.4938	139.8285	142.2089	139.7589	141.7730	139.9631	142.5634	137.0806	139.0577	140.2748	140.0174	141.7669	139.9692	142.1277	139.9168	141.9973	140.0596	142.4749	**132**
C7	200.5554	205.5196	206.9736	208.1930	208.8203	208.0253	213.7590	207.8570	212.9387	208.3529	214.6659	204.2854	208.7429	210.1036	211.2165	211.7853	211.0496	216.9049	210.8871	215.6715	211.3809	217.6015	**196**
C8	61.2286	62.1722	62.8269	62.5542	63.4515	62.5338	63.8040	62.5119	63.7336	62.5735	64.4107	55.7397	57.1823	57.6139	58.0157	58.7514	57.9530	59.4666	57.8934	59.1612	58.0807	59.7826	**60**
C9	22.0700	22.2380	22.4228	22.4373	22.8248	22.4194	22.7743	22.4016	22.6602	22.4557	22.8715	19.5465	19.7727	19.7821	19.8738	20.1420	19.8648	20.1501	19.8559	20.0913	19.8837	20.5181	**15**
C8`	35.1652	35.7649	35.9908	36.0743	36.3679	36.0567	36.5472	36.0377	36.5002	36.0907	36.9598	30.5263	30.8779	31.2072	31.0800	31.3808	31.0803	31.3789	31.0759	31.4642	31.0751	31.4895	**31**
H2	8.8384	8.7915	8.8061	8.7534	8.7565	8.7561	8.8198	8.7586	8.7788	8.7508	8.8177	8.844383	8.699283	8.746017	8.604942	8.634042	8.613558	8.589467	8.621308	8.622242	8.595417	8.591583	**8.07**
H3	7.4415	7.5770	7.6646	7.6196	7.7405	7.6173	7.7555	7.6149	7.7454	7.6217	7.7699	7.4525	7.5863	7.6739	7.6277	7.7500	7.6258	7.7576	7.6236	7.7514	7.6295	7.7730	**7.31**
H5	7.3028	7.4922	7.5805	7.5754	7.7036	7.5705	7.7161	7.5655	7.7041	7.5800	7.7398	7.3123	7.4932	7.5821	7.5675	7.6967	7.5632	7.7017	7.5588	7.6926	7.5714	7.7244	**7.31**
H6	8.2363	8.4473	8.5401	8.5626	8.6990	8.5558	8.7730	8.5487	8.7240	8.5691	8.8069	8.0771	8.2684	8.3886	8.3453	8.5299	8.3432	8.5210	8.3402	8.5241	8.3465	8.5617	**8.07**
H8	4.0794	4.2013	4.2289	4.3015	4.3612	4.2941	4.4167	4.2867	4.3964	4.3088	4.4426	4.2843	4.4417	4.5098	4.5068	4.6254	4.5039	4.6339	4.5005	4.6294	4.5091	4.6610	**5.09**
H(9A-9C)	1.3373	1.3502	1.3355	1.3434	1.3206	1.3441	1.3538	1.3446	1.3316	1.3428	1.3678	1.4052	1.4218	1.4124	1.4283	1.4126	1.4285	1.4264	1.4284	1.4276	1.4279	1.4449	**1.6**
H(8`A-8`C)	2.4600	2.4029	2.3721	2.3774	2.3594	2.3781	2.3295	2.3790	2.3441	2.3770	2.3180	2.8246	2.6620	2.6344	2.5859	2.5485	2.5907	2.4603	2.5952	2.4869	2.5812	2.4374	**2.81**
F4	-107.7949	-109.3040	-111.6571	-109.5462	-113.1227	-109.5381	-111.1741	-109.5298	-111.6029	-109.5542	-110.9940	-107.6757	-109.6708	-111.8955	-110.2470	-113.6052	-110.2079	-112.3236	-110.1720	-112.3996	-110.2883	-112.1601	**-102.1**
Nuclei	wB97X																						
C1	137.8029	138.0540	139.0211	138.1992	139.8961	138.1870	138.7316	138.1755	139.5920	138.2141	139.6814	136.9016	138.0110	138.6568	138.6712	140.0912	138.6060	140.0704	138.5482	139.7173	138.7443	140.1871	**129**
C2	140.7055	140.6032	141.1665	140.4847	141.0596	140.4945	141.6070	140.5037	141.4061	140.4762	141.5856	140.5526	140.5103	141.0764	140.4186	141.0232	140.4259	141.4852	140.4318	141.3445	140.4125	141.4959	**132**
C3	122.3475	122.9417	123.4842	123.1709	123.8319	123.1596	123.9911	123.1475	123.9336	123.1825	124.0993	122.3753	122.9427	123.4616	123.1718	123.8332	123.1584	124.0179	123.1444	123.8893	123.1862	124.0701	**116**
C4	174.9165	175.6237	176.2197	176.0405	176.6624	176.0165	177.3046	175.9916	177.0258	176.0640	177.3657	175.0408	175.5562	176.2009	175.8192	176.5285	175.8083	176.9078	175.7954	176.7811	175.8288	177.0410	**167**
C5	120.1726	121.4443	122.0434	122.1523	122.9687	122.1105	123.1411	122.0679	123.0163	122.1931	123.3151	120.2954	121.5031	122.1147	122.1275	122.9742	122.0916	123.0943	122.0548	122.9461	122.1629	123.2277	**116**
C6	137.1768	139.1619	140.2691	140.2457	141.8067	140.1813	142.5581	140.1156	141.8911	140.3073	142.5689	137.4753	139.4432	140.6731	140.4268	142.1500	140.3797	142.5033	140.3282	142.3574	140.4684	142.8687	**132**
C7	202.1768	207.1982	208.6196	209.9149	210.5679	209.7483	215.5392	209.5818	215.1279	210.0748	217.1331	206.1849	210.6989	211.9868	213.1284	213.7439	212.9665	218.9548	212.8080	217.5873	213.2885	219.5702	**196**
C8	62.2638	63.2785	63.9563	63.6403	64.5673	63.6254	64.9558	63.6092	64.7914	63.6554	65.6105	56.7269	58.2485	58.7010	59.1431	59.8693	59.0782	60.6326	59.0159	60.2657	59.2102	60.9139	**60**
C9	22.2545	22.4780	22.6788	22.6724	23.0493	22.6560	23.0235	22.6394	22.7994	22.6898	23.0038	19.5952	19.8548	19.8730	19.9815	20.2271	19.9737	20.2590	19.9655	20.1660	19.9902	20.6043	**15**
C8`	35.4261	36.0803	36.3153	36.4017	36.7065	36.3882	36.9314	36.3733	36.7947	36.4152	37.3166	30.7265	31.0292	31.3557	31.2646	31.5524	31.2617	31.6100	31.2549	31.6389	31.2646	31.7241	**31**
H2	8.8045	8.7552	8.7713	8.7178	8.7132	8.7209	8.7796	8.7237	8.6982	8.7149	8.6978	8.8202	8.6677	8.7159	8.5736	8.5991	8.5821	8.5540	8.5897	8.5893	8.5645	8.5574	**8.07**
H3	7.4131	7.5511	7.6385	7.5956	7.7147	7.5935	7.7298	7.5914	7.7207	7.5978	7.7443	7.4226	7.5575	7.6444	7.6018	7.7223	7.5997	7.7328	7.5974	7.7240	7.6039	7.7460	**7.31**
H5	7.2774	7.4679	7.5557	7.5537	7.6786	7.5490	7.6961	7.5442	7.6777	7.5583	7.7129	7.2894	7.4695	7.5577	7.5457	7.6732	7.5418	7.6791	7.5378	7.6674	7.5496	7.7001	**7.31**
H6	8.2021	8.4135	8.5069	8.5295	8.6573	8.5233	8.7307	8.5170	8.6684	8.5355	8.7254	8.0367	8.2260	8.3460	8.3104	8.4911	8.3074	8.4771	8.3036	8.4843	8.3126	8.5189	**8.07**
H8	4.1390	4.2501	4.2742	4.3513	4.4040	4.3440	4.4602	4.3368	4.4505	4.3585	4.4898	4.3255	4.4860	4.5491	4.5527	4.6724	4.5495	4.6828	4.5459	4.6757	4.5555	4.7093	**5.09**
H(9A-9C)	1.3232	1.3360	1.3236	1.3281	1.3024	1.3291	1.3388	1.3299	1.2880	1.3271	1.3094	1.3934	1.4128	1.4075	1.4242	1.4050	1.4244	1.4147	1.4244	1.4169	1.4237	1.4340	**1.6**
H(8`A-8`C)	2.4671	2.4104	2.3794	2.3869	2.3692	2.3875	2.3398	2.3882	2.3568	2.3865	2.3429	2.8470	2.6868	2.6544	2.6087	2.5717	2.6137	2.4834	2.6186	2.5074	2.6037	2.4553	**2.81**
F4	-110.1038	-111.3687	-113.7560	-111.4876	-115.1632	-111.4851	-113.1412	-111.4826	-113.7242	-111.4904	-113.2461	-110.0121	-111.7897	-114.0512	-112.2600	-115.6866	-112.2271	-114.3918	-112.1969	-114.4583	-112.2953	-114.1696	**-102.1**

[a] methyl protons shifts are averaged
[b] according to [9]

Table S9. Cont. VII

Nuclei	R											S										Exp. [b]
	X3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.3564	139.8444	140.8482	140.1134	142.0566	140.0909	141.3658	140.0679	141.5227	140.1411	141.6467	137.9117	139.2562	139.9366	139.9579	141.5273	139.9149	141.3110	139.8710	141.2013	140.0058	141.3487	**129**
C2	139.9182	139.8474	140.4108	139.6953	140.1921	139.7116	140.6326	139.7238	140.5055	139.6831	140.6144	139.2169	139.3848	139.9238	139.3913	140.0004	139.3937	140.5425	139.3932	140.4245	139.3932	140.5430	**132**
C3	122.0092	122.6988	123.2345	122.9633	123.5748	122.9518	123.8529	122.9370	123.8097	122.9783	123.9078	122.1353	122.7433	123.2197	122.9818	123.5816	122.9719	123.7914	122.9587	123.7342	122.9949	123.8481	**116**
C4	176.1825	177.0882	177.7250	177.5818	178.2391	177.5544	178.8901	177.5242	178.7610	177.6114	179.0087	176.5499	177.1393	177.8065	177.4289	178.1522	177.4164	178.5567	177.4002	178.4628	177.4439	178.7115	**167**
C5	119.8141	121.1439	121.7439	121.8710	122.6356	121.8294	122.8875	121.7849	122.7972	121.9143	123.0321	119.9992	121.2093	121.7793	121.8153	122.5836	121.7831	122.7292	121.7474	122.6490	121.8494	122.8641	**116**
C6	136.1581	138.1629	139.2158	139.2637	140.6897	139.2042	141.2883	139.1404	140.9981	139.3229	141.6419	136.5146	138.5767	139.8645	139.6151	141.2627	139.5588	141.7748	139.4982	141.5895	139.6709	142.1688	**132**
C7	202.8571	207.9768	209.5518	210.7426	211.8371	210.5640	217.1792	210.3863	216.3022	210.9197	218.1127	208.1208	212.3136	213.4589	214.5395	215.3412	214.4092	220.0232	214.2763	218.9420	214.6672	220.5368	**196**
C8	65.0592	66.2153	66.9018	66.5407	67.5099	66.5316	67.8451	66.5179	67.6413	66.5516	68.6175	59.3212	61.3577	61.9949	62.3629	63.2348	62.3022	63.9246	62.2400	63.6812	62.4263	64.1714	**60**
C9	23.0316	23.3183	23.4327	23.5997	23.8343	23.5889	23.8506	23.5740	23.7548	23.6127	23.9870	19.5775	20.0461	20.2181	20.2904	20.5151	20.2799	20.6827	20.2663	20.6108	20.3042	21.0438	**15**
C8`	36.3944	37.1898	37.4326	37.5008	37.8523	37.4859	38.0604	37.4681	38.0401	37.5189	38.4847	31.9991	32.1508	32.4082	32.3228	32.5612	32.3139	32.6685	32.3014	32.6855	32.3346	32.7610	**31**
H2	8.6524	8.5918	8.6063	8.5511	8.5135	8.5549	8.5499	8.5579	8.5426	8.5473	8.5316	8.6901	8.5204	8.5632	8.4372	8.4423	8.4428	8.4297	8.4475	8.4451	8.4317	8.4405	**8.07**
H3	7.3213	7.4551	7.5439	7.5005	7.6121	7.4985	7.6290	7.4960	7.6209	7.5023	7.6416	7.3067	7.4391	7.5255	7.4863	7.6016	7.4841	7.6164	7.4812	7.6087	7.4884	7.6303	**7.31**
H5	7.1716	7.3592	7.4485	7.4464	7.5662	7.4416	7.5856	7.4362	7.5755	7.4510	7.6064	7.1634	7.3365	7.4251	7.4152	7.5364	7.4110	7.5463	7.4062	7.5365	7.4192	7.5665	**7.31**
H6	8.0809	8.2845	8.3663	8.3962	8.5098	8.3898	8.5716	8.3828	8.5557	8.4024	8.5971	7.8813	8.0490	8.1656	8.1364	8.2978	8.1318	8.3147	8.1265	8.3041	8.1406	8.3622	**8.07**
H8	4.3443	4.4331	4.4575	4.5383	4.5907	4.5308	4.6494	4.5230	4.6418	4.5456	4.6641	4.4903	4.6483	4.7010	4.7147	4.8269	4.7114	4.8459	4.7075	4.8333	4.7177	4.8776	**5.09**
H(9A-9C)	1.3227	1.3314	1.3179	1.3217	1.2790	1.3235	1.2915	1.3245	1.2806	1.3199	1.3039	1.3991	1.4351	1.4417	1.4560	1.4332	1.4550	1.4533	1.4534	1.4521	1.4569	1.4778	**1.6**
H(8`A-8`C)	2.5170	2.4557	2.4302	2.4400	2.4194	2.4409	2.4037	2.4412	2.4048	2.4393	2.3899	2.9813	2.8071	2.7639	2.7278	2.6788	2.7332	2.5951	2.7379	2.6158	2.7225	2.5651	**2.81**
F4	-123.9446	-125.0794	-127.9228	-125.1110	-129.5643	-125.1134	-127.2940	-125.1155	-127.6376	-125.1089	-127.0904	-123.6606	-125.4316	-128.1731	-125.8293	-129.9814	-125.8093	-128.2500	-125.7897	-128.4739	-125.8494	-127.9006	**-102.1**

[a] methyl protons shifts are averaged

[b] according to [9]

Table S10. Theoretical chemical shifts (in ppm) of *(R,S)*-flephedrone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S										Exp. [b]
	B3LYP											B3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.3516	139.8992	140.9781	140.1863	142.0735	140.1611	141.5120	140.1358	141.5012	140.2082	141.7819	137.8738	139.3186	139.9816	139.9577	141.5554	139.9093	141.4183	139.8637	141.2810	140.0057	141.4292	**130.99**
C2	139.7181	139.6929	140.2565	139.4633	139.9708	139.4799	140.4199	139.4943	140.2834	139.4440	140.3925	139.0099	139.2247	139.7699	139.1806	139.8028	139.1780	140.3740	139.1755	140.2362	139.1821	140.3704	**133.34**
C3	121.9147	122.6511	123.2036	122.8744	123.4797	122.8576	123.7880	122.8405	123.7263	122.8887	123.8478	122.0546	122.6999	123.1853	122.8846	123.4913	122.8701	123.7328	122.8554	123.6526	122.8966	123.7867	**117.55**
C4	176.1996	177.1548	177.8016	177.6113	178.2556	177.5774	178.9142	177.5440	178.7922	177.6426	179.0429	176.5723	177.1853	177.8667	177.4190	178.1469	177.4023	178.5696	177.3850	178.4546	177.4322	178.7245	**168.13**
C5	119.7381	121.1100	121.7159	121.7876	122.5392	121.7417	122.8148	121.6959	122.7064	121.8299	122.9605	119.9339	121.1749	121.7562	121.7216	122.4902	121.6855	122.6663	121.6489	122.5622	121.7540	122.7986	**117.55**
C6	135.8982	137.9272	138.9534	138.9372	140.4067	138.8712	141.0202	138.8048	140.7434	138.9983	141.3636	136.2778	138.3528	139.6434	139.3323	140.9568	139.2716	141.4709	139.2095	141.2669	139.3872	141.8771	**133.34**
C7	202.8768	208.0691	209.7045	210.9565	211.8939	210.7561	217.3250	210.5621	216.3636	211.1520	218.3042	208.1087	212.3579	213.4837	214.5278	215.3474	214.3946	220.1153	214.2618	218.9963	214.6532	220.5944	**195.87**
C8	65.2601	66.4393	67.0844	66.6651	67.6873	66.6448	68.1168	66.6260	67.8105	66.6832	68.8556	59.4742	61.6544	62.2820	62.6180	63.4923	62.5505	64.2487	62.4848	63.9791	62.6825	64.4890	**60.75**
C9	22.9937	23.3369	23.4371	23.5103	23.7870	23.5040	23.8454	23.4947	23.7278	23.5117	23.9610	19.5432	20.0549	20.2357	20.2537	20.4684	20.2366	20.6702	20.2197	20.5736	20.2683	21.0311	**16.39**
C8`	36.5076	37.3387	37.5483	37.6307	37.9535	37.5944	38.1848	37.5637	38.1616	37.6692	38.6153	32.1915	32.3577	32.6229	32.4742	32.7092	32.4611	32.8316	32.4474	32.8288	32.4845	32.9175	**32**
H2	8.6288	8.5708	8.5739	8.5193	8.4862	8.5229	8.5099	8.5264	8.5151	8.5156	8.4958	8.6701	8.4976	8.5384	8.4115	8.4156	8.4168	8.3988	8.4218	8.4120	8.4060	8.4143	**7.971**
H3	7.3119	7.4474	7.5313	7.4874	7.6000	7.4852	7.6152	7.4829	7.6051	7.4891	7.6305	7.2978	7.4323	7.5140	7.4748	7.5907	7.4723	7.6048	7.4697	7.5943	7.4770	7.6211	**7.22**
H5	7.1614	7.3510	7.4352	7.4344	7.5536	7.4291	7.5704	7.4238	7.5589	7.4393	7.5939	7.1540	7.3281	7.4120	7.4019	7.5234	7.3974	7.5322	7.3928	7.5197	7.4059	7.5549	**7.22**
H6	8.0695	8.2736	8.3471	8.3829	8.4942	8.3751	8.5470	8.3677	8.5388	8.3904	8.5777	7.8720	8.0370	8.1480	8.1191	8.2781	8.1143	8.2908	8.1093	8.2781	8.1233	8.3419	**7.971**
H8	4.3623	4.4552	4.4783	4.5600	4.6044	4.5533	4.6526	4.5464	4.6504	4.5660	4.6741	4.4999	4.6578	4.7050	4.7188	4.8309	4.7153	4.8477	4.7118	4.8326	4.7217	4.8820	**5.2**
H(9A-9C)	1.3154	1.3242	1.3019	1.3025	1.2691	1.3041	1.2806	1.3055	1.2685	1.3007	1.2933	1.3888	1.4276	1.4302	1.4455	1.4215	1.4441	1.4397	1.4427	1.4360	1.4466	1.4683	**1.611**
H(8`A-8`C)	2.5071	2.4491	2.4216	2.4281	2.4102	2.4290	2.3990	2.4298	2.3931	2.4269	2.3861	2.9770	2.8044	2.7564	2.7204	2.6721	2.7257	2.5872	2.7307	2.6042	2.7151	2.5595	**2.82**
Nuclei	B3P86											B3P86										
C1	136.8453	137.2808	138.3582	137.5043	139.4519	137.5074	138.8537	137.4898	139.1351	137.5460	139.1283	135.6233	136.9063	137.5597	137.4853	138.9540	137.4549	138.8749	137.4076	138.7415	137.5634	138.9677	**130.99**
C2	138.7919	138.7416	139.3998	138.5747	139.1636	138.6075	139.5971	138.6182	139.5645	138.5873	139.5816	138.1598	138.3322	138.9376	138.3113	138.9809	138.3306	139.5077	138.3287	139.4734	138.3375	139.5260	**133.34**
C3	121.1158	121.8832	122.5099	122.1552	122.8745	122.1613	123.1693	122.1453	123.2080	122.1932	123.2475	121.2077	121.9036	122.4956	122.1573	122.8618	122.1638	123.0956	122.1483	123.1217	122.1950	123.1750	**117.55**
C4	173.6985	174.6092	175.2829	175.0662	175.7535	175.0598	176.4063	175.0315	176.3576	175.1159	176.5491	173.9907	174.6001	175.3439	174.8861	175.6462	174.8935	176.0480	174.8781	176.0672	174.9218	176.2106	**168.13**
C5	118.9511	120.3570	121.0389	121.0865	121.9545	121.0629	122.2291	121.0175	122.2236	121.1526	122.3983	119.0968	120.3750	121.0516	121.0069	121.8780	120.9911	122.0417	120.9530	122.0531	121.0653	122.1965	**117.55**
C6	134.9391	136.9571	138.0470	138.0317	139.4694	137.9871	140.0383	137.9202	139.8454	138.1179	140.4254	135.2870	137.3568	138.6630	138.3561	140.0839	138.3212	140.5742	138.2627	140.5163	138.4312	140.9668	**133.34**
C7	200.9937	205.8309	207.3690	208.3757	209.4937	208.2408	214.5962	208.0849	213.8337	208.5478	215.4998	205.5040	209.6504	210.9178	211.8502	212.6202	211.7370	217.2310	211.6033	216.1910	212.0035	217.7281	**195.87**
C8	63.6796	64.8464	65.6285	65.2068	66.1771	65.2071	66.5812	65.1854	66.4957	65.2505	67.3827	58.1084	59.9428	60.4781	60.8007	61.6333	60.7568	62.3872	60.6942	62.1777	60.8896	62.6693	**60.75**
C9	22.8065	23.0897	23.3077	23.3623	23.6359	23.3647	23.6593	23.3452	23.6707	23.4035	23.8216	19.4663	20.0187	20.1559	20.2089	20.4941	20.2153	20.6857	20.2003	20.7001	20.2472	21.1119	**16.39**
C8`	35.9286	36.7158	37.0084	37.0027	37.3475	37.0082	37.5596	36.9918	37.6189	37.0414	38.0311	31.3622	31.5731	31.9325	31.7646	32.0364	31.7748	32.1533	31.7622	32.2999	31.7969	32.2578	**32**
H2	8.6937	8.6392	8.6481	8.5947	8.5586	8.5992	8.5883	8.6018	8.5814	8.5915	8.5744	8.7028	8.5480	8.5959	8.4713	8.4868	8.4787	8.4611	8.4838	8.4913	8.4649	8.4716	**7.971**
H3	7.3323	7.4749	7.5633	7.5186	7.6361	7.5176	7.6523	7.5147	7.6476	7.5207	7.6690	7.3188	7.4600	7.5477	7.5057	7.6274	7.5044	7.6414	7.5013	7.6367	7.5080	7.6590	**7.22**
H5	7.1767	7.3724	7.4616	7.4573	7.5836	7.4536	7.6013	7.4480	7.5944	7.4620	7.6265	7.1655	7.3489	7.4382	7.4270	7.5553	7.4237	7.5640	7.4186	7.5573	7.4312	7.5880	**7.22**
H6	8.1523	8.3571	8.4270	8.4597	8.5681	8.4550	8.6211	8.4484	8.6073	8.4654	8.6536	7.9340	8.1076	8.2276	8.1948	8.3652	8.1917	8.3755	8.1865	8.3750	8.1986	8.4257	**7.971**
H8	4.3930	4.4836	4.4927	4.5762	4.6265	4.5711	4.6819	4.5642	4.6796	4.5824	4.7038	4.5540	4.6976	4.7569	4.7623	4.8783	4.7605	4.8928	4.7566	4.8883	4.7650	4.9288	**5.2**
H(9A-9C)	1.3335	1.3438	1.3286	1.3321	1.2867	1.3343	1.2965	1.3346	1.2886	1.3313	1.3143	1.4092	1.4428	1.4421	1.4554	1.4353	1.4561	1.4505	1.4549	1.4566	1.4559	1.4796	**1.611**
H(8`A-8`C)	2.4876	2.4212	2.3951	2.4005	2.3811	2.4023	2.3602	2.4024	2.3671	2.4001	2.3503	2.9176	2.7485	2.7146	2.6728	2.6287	2.6800	2.5349	2.6851	2.5651	2.6670	2.5072	**2.82**
Nuclei	B3PW91											B3PW91										
C1	137.0994	137.5782	138.7234	137.8703	140.2084	137.8485	139.3905	137.8187	139.3095	137.8939	139.6388	135.8270	137.2800	137.7781	137.8580	139.3488	137.8089	139.3951	137.7573	139.1374	137.9141	139.4828	**130.99**
C2	138.8604	138.8385	139.3967	138.6503	139.5459	138.6706	139.6266	138.6815	139.5161	138.6320	139.6248	138.2843	138.4871	139.0226	138.4452	139.1209	138.4505	139.6147	138.4477	139.5068	138.4432	139.6376	**133.34**
C3	121.2185	122.0069	122.5742	122.2708	123.2963	122.2610	123.2495	122.2421	123.2072	122.2821	123.3409	121.3071	122.0247	122.5329	122.2639	122.9651	122.2553	123.1906	122.2380	123.1214	122.2739	123.2752	**117.55**
C4	173.7409	174.6858	175.2871	175.1369	176.1105	175.1138	176.3924	175.0819	176.3209	175.1612	176.5562	174.0199	174.6397	175.3121	174.9084	175.6627	174.9018	176.0329	174.8849	175.9623	174.9153	176.2007	**168.13**
C5	119.0599	120.4861	121.1030	121.2065	122.3683	121.1668	122.2995	121.1183	122.2138	121.2461	122.4777	119.2098	120.5084	121.1087	121.1148	121.9791	121.0849	122.1342	121.0458	122.0478	121.1449	122.2957	**117.55**
C6	134.8881	136.9286	137.8816	137.9622	139.7104	137.9061	139.9572	137.8415	139.7281	138.0174	140.3326	135.2770	137.3211	138.5843	138.3076	139.9907	138.2583	140.3962	138.1982	140.2701	138.3538	140.7941	**133.34**
C7	201.1247	206.1066	207.7353	208.8082	210.2420	208.6327	215.1374	208.4510	214.2009	208.9795	216.0833	205.6165	209.9651	211.0502	212.1644	212.9527	212.0348	217.7726	211.8977	216.5723	212.2928	218.2699	**195.87**
C8	63.4567	64.6178	65.2257	64.9342	66.2583	64.9202	66.4879	64.8987	66.1020	64.9510	67.2318	58.0320	59.9926	60.4452	60.8767	61.6836	60.8128	62.5182	60.7445	62.2018	60.9444	62.8000	**60.75**
C9	22.5160	22.8553	22.9353	23.0789	23.6687	23.0753	23.3953	23.0617	23.2786	23.0832	23.5418	19.1832	19.7035	19.7883	19.8973	20.1279	19.8867	20.3038	19.8683	20.2280	19.9102	20.7016	**16.39**
C8`	35.8834	36.7085	36.8598	36.9828	37.6339	36.9657	37.5129	36.9420	37.5231	37.0038	37.9753	31.4292	31.6510	31.9335	31.8297	32.1026	31.8260	32.1558	31.8123	32.2185	31.8333	32.2536	**32**
H2	8.6633	8.6108	8.6056	8.5605	8.5329	8.5652	8.5339	8.5693	8.5526	8.5562	8.5242	8.6835	8.5130	8.5718	8.4375	8.4524	8.4445	8.4188	8.4505	8.4482	8.4303	8.4283	**7.971**
H3	7.3301	7.4703	7.5577	7.5143	7.6458	7.5126	7.6483	7.5105	7.6406	7.5160	7.6634	7.3189	7.4577	7.5443	7.5040	7.6238	7.5020	7.6404	7.4996	7.6317	7.5060	7.6558	**7.22**
H5	7.1771	7.3713	7.4596	7.4576	7.5958	7.4530	7.5980	7.4480	7.5902	7.4622	7.6214	7.1690	7.3494	7.4382	7.4277	7.5538	7.4237	7.5651	7.4194	7.5542	7.4316	7.5870	**7.22**
H6	8.1341	8.3392	8.4057	8.4426	8.5635	8.4366	8.5897	8.4305	8.5951	8.4485	8.6240	7.9194	8.0892	8.2103	8.1769	8.3421	8.1732	8.3457	8.1688	8.3441	8.1801	8.3934	**7.971**
H8	4.3741	4.4705	4.4922	4.5694	4.6265	4.5633	4.6458	4.5568	4.6625	4.5752	4.6720	4.5270	4.6702	4.7258	4.7346	4.8501	4.7322	4.8642	4.7292	4.8566	4.7367	4.8976	**5.2**
H(9A-9C)	1.2980	1.3052	1.2789	1.2881	1.2601	1.2903	1.2615	1.2922	1.2492	1.2862	1.2747	1.3734	1.4034	1.4070	1.4206	1.3953	1.4203	1.4103	1.4196	1.4138	1.4210	1.4367	**1.611**
H(8`A-8`C)	2.4555	2.3914	2.3685	2.3743	2.3708	2.3754	2.3485	2.3764	2.3407	2.3732	2.3328	2.8889	2.7195	2.6844	2.6446	2.6004	2.6510	2.5113	2.6569	2.5341	2.6383	2.4811	**2.82**
Nuclei	B98											B98										
C1	137.8984	138.3641	139.2698	138.5615	140.4825	138.5589	139.6880	138.5551	139.9714	138.5675	140.0693	136.6672	137.9623	138.5980	138.5797	140.1392	138.5482	140.0261	138.5178	139.8988	138.6168	140.0992	**130.99**
C2	138.5254	138.4721	139.0519	138.3240	138.8948	138.3503	139.3548	138.3736	139.2402	138.3008	139.3473	137.9447	138.0861	138.6429	138.0628	138.7300	138.0773	139.2568	138.0902	139.1509	138.0518	139.2683	**133.34**
C3	120.9751	121.6883	122.2401	121.9412	122.6168	121.9423	122.8875	121.9406	122.8295	121.9422	122.9429	121.0500	121.6961	122.2005	121.9352	122.6051	121.9366	122.8272	121.9354	122.7659	121.9361	122.8940	**117.55**
C4	173.5548	174.4326	175.0664	174.8850	175.5697	174.8724	176.2406	174.8571	176.0696	174.8994	176.3345	173.8262	174.4272	175.1004	174.7024	175.4540	174.7034	175.8475	174.7008	175.7561	174.7028	176.0007	**168.13**
C5	118.7946	120.1408	120.7556	120.8501	121.6768	120.8218	121.9460	120.7906	121.8434	120.8797	122.0849	118.9548	120.1808	120.7785	120.7832	121.6150	120.7632	121.7668	120.7403	121.6817	120.8040	121.9090	**117.55**
C6	134.9458	136.9033	137.9770	137.9779	139.4196	137.9297	140.0378	137.8779	139.7250	138.0256	140.3768	135.2851	137.2480	138.5012	138.2327	139.8890	138.1917	140.3423	138.1470	140.1749	138.2722	140.7184	**133.34**
C7	199.5271	204.5615	206.0295	207.1995	208.2386	207.0479	213.5136	206.8943	212.6014	207.3482	214.4291	204.1599	208.4637	209.6427	210.7144	211.5176	210.5930	216.3722	210.4697	215.2290	210.8323	216.8957	**195.87**
C8	65.0962	66.2575	66.8997	66.5776	67.5549	66.5763	67.8574	66.5723	67.7776	66.5806	68.7079	59.7427	61.6256	62.1747	62.5454	63.3980	62.4979	64.1348	62.4503	63.8905	62.5954	64.3856	**60.75**
C9	23.2897	23.5779	23.6929	23.8388	24.0941	23.8397	24.1215	23.8371	24.0489	23.8399	24.2881	20.0303	20.4587	20.5633	20.6605	20.8945	20.6623	21.0556	20.6621	20.9805	20.6615	21.4185	**16.39**
C8`	36.7092	37.4629	37.6740	37.7309	38.1053	37.7287	38.3351	37.7243	38.2965	37.7357	38.7417	32.2204	32.4032	32.6737	32.5780	32.8420	32.5807	32.9732	32.5806	33.0077	32.5770	33.0565	**32**
H2	8.6652	8.6018	8.6259	8.5647	8.5366	8.5677	8.5885	8.5705	8.5669	8.5621	8.5601	8.6821	8.5181	8.5678	8.4391	8.4515	8.4446	8.4365	8.4498	8.4543	8.4338	8.4469	**7.971**
H3	7.3240	7.4617	7.5525	7.5069	7.6251	7.5048	7.6424	7.5026	7.6335	7.5092	7.6562	7.3088	7.4478	7.5364	7.4945	7.6157	7.4921	7.6318	7.4897	7.6238	7.4970	7.6471	**7.22**
H5	7.1716	7.3643	7.4556	7.4510	7.5764	7.4460	7.5983	7.4411	7.5859	7.4560	7.6179	7.1649	7.3464	7.4371	7.4256	7.5523	7.4212	7.5629	7.4169	7.5523	7.4299	7.5837	**7.22**
H6	8.0929	8.2967	8.3821	8.4075	8.5267	8.4008	8.6016	8.3943	8.5719	8.4141	8.6200	7.8961	8.0681	8.1863	8.1586	8.3256	8.1538	8.3364	8.1488	8.3271	8.1631	8.3835	**7.971**
H8	4.3470	4.4366	4.4606	4.5354	4.5891	4.5287	4.6555	4.5220	4.6334	4.5423	4.6625	4.4951	4.6493	4.7037	4.7151	4.8293	4.7118	4.8454	4.7085	4.8323	4.7182	4.8756	**5.2**
H(9A-9C)	1.3189	1.3268	1.3143	1.3162	1.2740	1.3175	1.2894	1.3187	1.2788	1.3151	1.3029	1.3937	1.4261	1.4275	1.4419	1.4166	1.4413	1.4301	1.4407	1.4303	1.4425	1.4532	**1.611**
H(8`A-8`C)	2.4802	2.4260	2.3972	2.4073	2.3842	2.4082	2.3651	2.4093	2.3720	2.4067	2.3565	2.9208	2.7533	2.7171	2.6803	2.6349	2.6856	2.5498	2.6907	2.5670	2.6754	2.5194	**2.82**

[a] methyl protons shifts are averaged
[b] according to [10]

Table S10. Cont. I

Nuclei	R												S										Exp. [b]
	B971												B971										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.5124	137.9668	138.8036	138.1617	140.0037	138.1528	139.1730	138.1442	139.5653	138.1768	139.6476	136.2962	137.5659	138.2070	138.1911	139.7146	138.1505	139.5849	138.1134	139.4699	138.2405	139.6733	**130.99**
C2	138.2273	138.1790	138.7520	138.0411	138.6151	138.0588	139.0874	138.0759	138.9703	138.0298	139.0743	137.6507	137.7943	138.3494	137.7788	138.4352	137.7852	138.9549	137.7921	138.8493	137.7793	138.9688	**133.34**
C3	120.7723	121.4948	122.0366	121.7575	122.4239	121.7508	122.6953	121.7432	122.6290	121.7695	122.7532	120.8439	121.4989	122.0013	121.7481	122.4060	121.7414	122.6248	121.7343	122.5637	121.7602	122.6979	**117.55**
C4	173.4520	174.3378	174.9730	174.7959	175.4831	174.7758	176.1541	174.7552	175.9535	174.8209	176.2409	173.7091	174.3304	175.0011	174.6204	175.3683	174.6132	175.7597	174.6046	175.6659	174.6323	175.9170	**168.13**
C5	118.5912	119.9438	120.5513	120.6619	121.4796	120.6255	121.7575	120.5889	121.6419	120.7023	121.8945	118.7577	119.9871	120.5816	120.5974	121.4204	120.5694	121.5676	120.5405	121.4822	120.6294	121.7173	**117.55**
C6	134.7050	136.6708	137.7813	137.7564	139.2253	137.6992	139.8111	137.6410	139.4847	137.8168	140.1424	135.0285	137.0109	138.2571	138.0065	139.6769	137.9579	140.1333	137.9074	139.9591	138.0571	140.5087	**133.34**
C7	199.4123	204.3866	205.8037	206.9774	207.9980	206.8235	213.1394	206.6697	212.2541	207.1300	214.1117	204.0187	208.2806	209.4897	210.5322	211.3305	210.4028	216.0716	210.2738	214.9613	210.6620	216.6144	**195.87**
C8	65.0628	66.2181	66.8745	66.5493	67.4912	66.5398	67.7569	66.5294	67.7680	66.5644	68.6439	59.7053	61.5405	62.0853	62.4460	63.2954	62.3913	63.9952	62.3385	63.7609	62.5067	64.2505	**60.75**
C9	23.2952	23.5805	23.7317	23.8547	24.1127	23.8461	24.1179	23.8365	24.0691	23.8689	24.2944	20.0444	20.4947	20.5876	20.7006	20.9390	20.6951	21.1020	20.6896	21.0266	20.7123	21.4780	**16.39**
C8`	36.7170	37.4689	37.6835	37.7337	38.0702	37.7257	38.3145	37.7173	38.2603	37.7475	38.7194	32.1504	32.3460	32.6128	32.5305	32.7822	32.5259	32.9103	32.5202	32.9431	32.5401	32.9962	**32**
H2	8.6629	8.6020	8.6311	8.5654	8.5437	8.5681	8.6026	8.5708	8.5678	8.5633	8.5647	8.6781	8.5197	8.5677	8.4422	8.4548	8.4475	8.4418	8.4527	8.4583	8.4370	8.4509	**7.971**
H3	7.3215	7.4590	7.5493	7.5044	7.6225	7.5021	7.6392	7.4997	7.6299	7.5070	7.6527	7.3076	7.4456	7.5341	7.4931	7.6131	7.4905	7.6286	7.4879	7.6208	7.4959	7.6437	**7.22**
H5	7.1696	7.3613	7.4527	7.4481	7.5728	7.4430	7.5957	7.4379	7.5815	7.4533	7.6142	7.1650	7.3449	7.4351	7.4237	7.5495	7.4192	7.5594	7.4147	7.5489	7.4283	7.5805	**7.22**
H6	8.0974	8.2998	8.3897	8.4087	8.5283	8.4021	8.6053	8.3956	8.5653	8.4153	8.6195	7.8972	8.0707	8.1892	8.1631	8.3306	8.1581	8.3421	8.1530	8.3320	8.1679	8.3885	**7.971**
H8	4.3445	4.4318	4.4558	4.5292	4.5852	4.5223	4.6544	4.5157	4.6229	4.5361	4.6585	4.4978	4.6489	4.7036	4.7168	4.8297	4.7133	4.8452	4.7097	4.8315	4.7203	4.8758	**5.2**
H(9A-9C)	1.3191	1.3280	1.3197	1.3196	1.2780	1.3205	1.2937	1.3214	1.2832	1.3191	1.3053	1.3960	1.4276	1.4283	1.4433	1.4195	1.4425	1.4331	1.4418	1.4326	1.4442	1.4560	**1.611**
H(8`A-8`C)	2.4778	2.4208	2.3902	2.4035	2.3793	2.4041	2.3533	2.4048	2.3662	2.4033	2.3481	2.9110	2.7452	2.7096	2.6744	2.6284	2.6794	2.5438	2.6843	2.5610	2.6698	2.5128	**2.82**
Nuclei	B972											B972											
C1	134.4302	134.9580	135.9573	135.2517	137.1882	135.2339	136.9092	135.2172	137.2291	135.2642	136.9986	133.0960	134.5569	135.0556	135.2214	136.6788	135.1632	136.7562	135.1090	136.5422	135.2805	136.8545	**130.99**
C2	136.2385	136.1466	136.7094	135.9825	136.5017	135.9974	136.8781	136.0094	136.7762	135.9648	136.9004	135.6839	135.8309	136.3876	135.8469	136.4661	135.8466	136.9148	135.8443	136.8312	135.8431	136.9435	**133.34**
C3	118.6420	119.3619	119.9304	119.6913	120.3271	119.6734	120.6091	119.6533	120.5621	119.7042	120.6885	118.7138	119.3622	119.8746	119.6667	120.3028	119.6505	120.5119	119.6318	120.4478	119.6777	120.5982	**117.55**
C4	170.4080	171.2888	171.9012	171.8240	172.3935	171.7908	172.9800	171.7559	172.8201	171.8517	173.1417	170.6771	171.2152	171.8947	171.5417	172.2306	171.5278	172.5783	171.5099	172.5046	171.5489	172.7454	**168.13**
C5	116.5455	117.8870	118.4963	118.6438	119.4131	118.5990	119.6446	118.5521	119.5386	118.6819	119.8150	116.6811	117.8807	118.4867	118.5356	119.3203	118.4989	119.4656	118.4592	119.3807	118.5657	119.6278	**117.55**
C6	132.2984	134.1683	135.1909	135.2810	136.6319	135.2152	137.0709	135.1451	136.7199	135.3380	137.5017	132.7192	134.6132	135.8785	135.6223	137.1863	135.5695	137.5344	135.5120	137.4030	135.6656	137.9182	**133.34**
C7	197.1472	202.1820	203.6394	205.0747	205.9500	204.8855	211.4809	204.7016	210.7109	205.2515	212.1626	201.5167	205.7889	206.8296	208.0334	208.7686	207.8942	213.5796	207.7543	212.4081	208.1644	214.0847	**195.87**
C8	62.2129	63.1640	63.7653	63.5253	64.4519	63.5132	65.0374	63.4956	64.9409	63.5298	65.7131	56.9800	58.9172	59.3838	59.8622	60.6095	59.7928	61.4484	59.7250	61.1550	59.9290	61.7202	**60.75**
C9	22.2017	22.5014	22.6308	22.6974	22.9802	22.6894	22.9728	22.6772	22.8720	22.7010	23.1432	18.9615	19.3718	19.4861	19.6193	19.7902	19.6032	19.9459	19.5854	19.8717	19.6315	20.3049	**16.39**
C8`	35.6349	36.3454	36.5312	36.8429	37.0375	36.8098	37.2438	36.7749	37.2215	36.8693	37.6484	31.3495	31.4924	31.7924	31.7285	31.9630	31.7188	31.9659	31.7053	32.0216	31.7314	32.0500	**32**
H2	8.6537	8.5910	8.6014	8.5457	8.5058	8.5490	8.4992	8.5518	8.4749	8.5424	8.5039	8.6825	8.4992	8.5620	8.4234	8.4354	8.4301	8.3959	8.4360	8.4226	8.4161	8.4046	**7.971**
H3	7.3227	7.4597	7.5484	7.5068	7.6209	7.5045	7.6375	7.5020	7.6284	7.5088	7.6533	7.3120	7.4483	7.5346	7.4976	7.6140	7.4951	7.6296	7.4923	7.6214	7.4999	7.6455	**7.22**
H5	7.1739	7.3666	7.4552	7.4573	7.5754	7.4520	7.5903	7.4465	7.5774	7.4620	7.6138	7.1665	7.3420	7.4301	7.4225	7.5446	7.4180	7.5559	7.4132	7.5449	7.4267	7.5779	**7.22**
H6	8.1158	8.3161	8.3945	8.4358	8.5373	8.4282	8.5663	8.4204	8.5382	8.4429	8.6045	7.9070	8.0727	8.1924	8.1605	8.3194	8.1565	8.3186	8.1518	8.3151	8.1637	8.3642	**7.971**
H8	4.3399	4.4508	4.4730	4.5472	4.5919	4.5405	4.6226	4.5339	4.6079	4.5536	4.6488	4.4883	4.6298	4.6848	4.6954	4.8083	4.6924	4.8202	4.6889	4.8127	4.6977	4.8518	**5.2**
H(9A-9C)	1.2779	1.2737	1.2581	1.2603	1.2187	1.2618	1.2249	1.2628	1.2101	1.2586	1.2452	1.3585	1.3871	1.3915	1.4080	1.3784	1.4071	1.3926	1.4058	1.3948	1.4087	1.4173	**1.611**
H(8`A-8`C)	2.4444	2.3879	2.3637	2.3740	2.3543	2.3748	2.3536	2.3753	2.3559	2.3732	2.3366	2.8829	2.7146	2.6793	2.6431	2.5976	2.6486	2.5129	2.6536	2.5335	2.6373	2.4818	**2.82**
Nuclei	BHandH											BHandH											
C1	138.2231	138.5552	139.4722	138.6613	140.1957	138.6447	139.2014	138.6466	139.2910	138.6472	139.3414	137.3260	138.1227	139.0514	138.6686	139.4127	138.6143	139.9113	138.5817	139.6959	138.6934	140.0677	**130.99**
C2	143.5201	143.3955	144.0049	143.2268	143.8191	143.2277	144.3374	143.2468	144.2139	143.1959	144.3719	143.1561	143.1628	143.7749	143.0888	143.8329	143.0819	144.2258	143.0940	144.0867	143.0659	144.2500	**133.34**
C3	123.7766	124.4896	125.0912	124.7508	125.4195	124.7262	125.6101	124.7198	125.5593	124.7437	125.6833	123.8317	124.5005	125.1213	124.7551	125.4992	124.7302	125.6175	124.7238	125.5792	124.7487	125.7026	**117.55**
C4	174.6910	175.5022	176.1372	175.9474	176.5413	175.9096	177.2138	175.8903	177.0668	175.9534	177.3817	174.9086	175.5511	176.2159	175.8630	176.6071	175.8357	176.9768	175.8261	176.9107	175.8585	177.1498	**168.13**
C5	121.3254	122.7876	123.4824	123.5575	124.4251	123.5004	124.6212	123.4617	124.5293	123.5816	124.7930	121.4351	122.8143	123.5066	123.5206	124.2647	123.4688	124.5249	123.4348	124.4609	123.5397	124.7001	**117.55**
C6	139.9383	142.0591	143.3061	143.2147	144.9304	143.1340	145.6585	143.0715	145.4144	143.2611	146.1074	140.2023	142.4966	143.7026	143.6179	144.3620	143.5430	145.9734	143.4853	145.7743	143.6576	146.3435	**133.34**
C7	202.9300	207.7859	209.1882	210.2924	210.9441	210.1306	215.8168	209.9874	214.6983	210.4156	216.6335	207.3621	211.4788	213.0278	213.6769	214.4210	213.5328	219.1023	213.4077	218.0494	213.7841	219.7557	**195.87**
C8	59.9494	61.2143	61.9067	61.6436	62.6312	61.6098	63.0978	61.5942	62.9356	61.6453	63.8442	54.0631	55.4214	55.9382	56.1974	56.9415	56.1327	57.6583	56.0882	57.3239	56.2306	57.9608	**60.75**
C9	22.4684	22.7173	23.0362	22.9961	23.4920	22.9658	23.4131	22.9537	23.4079	22.9951	23.6098	19.0747	19.5603	19.6330	19.8271	20.5712	19.7976	20.2453	19.7870	20.1575	19.8256	20.6529	**16.39**
C8`	33.7500	34.5612	34.8118	34.8998	35.2711	34.8687	35.5037	34.8562	35.4510	34.8996	35.9918	28.6454	29.0946	29.4036	29.3316	30.0757	29.3102	29.7782	29.3056	29.7931	29.3204	29.9429	**32**
H2	8.9875	8.9200	8.9348	8.8802	8.8770	8.8834	8.9222	8.8858	8.9249	8.8781	8.9222	8.9840	8.8580	8.8706	8.7732	8.6920	8.7803	8.7507	8.7862	8.7811	8.7672	8.7533	**7.971**
H3	7.4553	7.5997	7.6892	7.6466	7.7674	7.6451	7.7842	7.6427	7.7763	7.6491	7.8000	7.4516	7.5922	7.6830	7.6387	7.5575	7.6372	7.7745	7.6347	7.7677	7.6412	7.7910	**7.22**
H5	7.3003	7.5022	7.5933	7.5917	7.7206	7.5873	7.7378	7.5822	7.7268	7.5967	7.7629	7.2950	7.4886	7.5794	7.5727	7.4915	7.5687	7.7122	7.5639	7.7021	7.5774	7.7361	**7.22**
H6	8.3317	8.5445	8.6361	8.6585	8.7941	8.6524	8.8645	8.6454	8.8495	8.6654	8.9071	8.1293	8.3337	8.4417	8.4287	8.3475	8.4246	8.6263	8.4194	8.6221	8.4334	8.6718	**7.971**
H8	4.1505	4.2528	4.2749	4.3463	4.3866	4.3407	4.4438	4.3343	4.4339	4.3528	4.4603	4.4049	4.5696	4.6414	4.6481	4.5669	4.6447	4.7936	4.6404	4.7922	4.6522	4.8291	**5.2**
H(9A-9C)	1.3947	1.4083	1.3944	1.4043	1.3835	1.4056	1.4087	1.4060	1.4066	1.4041	1.4308	1.4777	1.5048	1.4783	1.5114	1.4301	1.5120	1.4963	1.5117	1.4978	1.5117	1.5179	**1.611**
H(8`A-8`C)	2.5482	2.4741	2.4402	2.4443	2.4243	2.4467	2.3801	2.4483	2.3790	2.4430	2.3667	2.9170	2.7545	2.7130	2.6709	2.5897	2.6772	2.5211	2.6825	2.5633	2.6659	2.4973	**2.82**
Nuclei	BHandHLYP											BHandHLYP											
C1	138.8640	139.2644	139.9330	139.4014	141.4115	139.3890	140.3239	139.3799	140.8073	139.4140	140.7808	137.7359	138.7863	139.5663	139.4872	141.0279	139.4436	140.6370	139.4057	140.4914	139.5319	140.6845	**130.99**
C2	142.1451	142.0033	142.5518	141.8479	142.3133	141.8593	142.8334	141.8728	142.6946	141.8367	142.8238	141.6846	141.6776	142.2130	141.6154	142.1662	141.6189	142.6674	141.6254	142.5678	141.6119	142.7010	**133.34**
C3	122.5311	123.1246	123.6134	123.3344	123.9644	123.3231	124.1502	123.3143	124.1344	123.3446	124.2197	122.6170	123.1643	123.6329	123.3811	123.9687	123.3691	124.1171	123.3594	124.0780	123.3922	124.1810	**117.55**
C4	174.4859	175.2386	175.8387	175.6759	176.2231	175.6490	176.9757	175.6248	176.7716	175.7009	177.0601	174.7783	175.2638	175.8588	175.5025	176.1211	175.4893	176.5698	175.4775	176.5010	175.5141	176.7410	**168.13**
C5	120.1712	121.4535	122.0189	122.1435	122.9398	122.1013	123.1049	122.0616	123.0479	122.1835	123.2751	120.2936	121.5123	122.0694	122.1337	122.8970	122.0972	123.0006	122.0628	122.9395	122.1680	123.1441	**117.55**
C6	138.1510	140.1493	141.3422	141.2896	142.5504	141.2223	143.2999	141.1564	142.9195	141.3529	143.5841	138.4674	140.5298	141.7475	141.5098	143.1000	141.4526	143.6578	141.3968	143.5207	141.5620	144.0715	**133.34**
C7	201.2543	206.5546	207.7752	209.3182	210.2498	209.1454	216.0604	208.9760	215.0849	209.4828	217.0651	206.1611	210.4578	211.6283	212.8433	213.4066	212.7018	218.6263	212.5625	217.3826	212.9773	219.2046	**195.87**
C8	60.7965	61.8811	62.5000	62.2233	63.0588	62.2069	63.2656	62.1924	63.2636	62.2383	64.1041	55.4804	57.1821	57.8021	58.1054	58.8956	58.0473	59.5516	57.9937	59.2868	58.1628	59.8130	**60.75**
C9	22.2333	22.3886	22.6124	22.6282	22.8233	22.6139	22.7047	22.6016	22.6825	22.6409	22.8547	18.9648	19.2708	19.4004	19.4144	19.6557	19.4060	19.6995	19.4005	19.6674	19.4225	20.0180	**16.39**
C8`	34.7377	35.5130	35.7819	35.8289	36.1801	35.8108	36.3989	35.7951	36.3597	35.8459	36.8091	30.5960	30.8142	31.0655	30.9812	31.2247	30.9680	31.3407	30.9569	31.3887	30.9927	31.4699	**32**
H2	8.8761	8.8039	8.8520	8.7659	8.7241	8.7690	8.7906	8.7718	8.7505	8.7629	8.7519	8.8981	8.7359	8.7665	8.6405	8.6466	8.6464	8.6344	8.6519	8.6571	8.6345	8.6458	**7.971**
H3	7.4433	7.5783	7.6654	7.6233	7.7361	7.6213	7.7566	7.6190	7.7465	7.6252	7.7698	7.4323	7.5668	7.6511	7.6133	7.7280	7.6111	7.7441	7.6087	7.7353	7.6153	7.7592	**7.22**
H5	7.2878	7.4785	7.5663	7.5650	7.6852	7.5602	7.7061	7.5552	7.6928	7.5695	7.7273	7.2798	7.4603	7.5446	7.5400	7.6603	7.5356	7.6720	7.5311	7.6611	7.5440	7.6938	**7.22**
H6	8.1765	8.3928	8.4992	8.5149	8.6356	8.5078	8.7226	8.5005	8.6822	8.5217	8.7376	8.0113	8.2014	8.3159	8.2915	8.4587	8.2866	8.4826	8.2813	8.4746	8.2959	8.5310	**7.971**
H8	4.0776	4.1885	4.2247	4.3024	4.3719	4.2945	4.4593	4.2868	4.4300	4.3099	4.4624	4.2587	4.4280	4.4860	4.5022	4.6169	4.4983	4.6464	4.4943	4.6344	4.5056	4.6772	**5.2**
H(9A-9C)	1.2993	1.3062	1.3063	1.3002	1.2417	1.3014	1.2609	1.3023	1.2448	1.2990	1.2689	1.3682	1.3960	1.3920	1.4076	1.3798	1.4070	1.4019	1.4061	1.4026	1.4081	1.4244	**1.611**
H(8`A-8`C)	2.4396	2.3870	2.3452	2.3723	2.3466	2.3731	2.3248	2.3737	2.3360	2.3717	2.3239	2.8786	2.7124	2.6679	2.6359	2.5874	2.6411	2.5108	2.6458	2.5345	2.6307	2.4845	**2.82**

[a] methyl protons shifts are averaged
[b] according to [10]

Table S10. Cont. II

Nuclei	R											S										Exp. [b]
	BLYP											BLYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.2740	140.0627	140.7302	140.3557	142.0482	140.6261	141.6136	140.4250	141.4809	140.7208	141.8598	138.3037	138.8878	139.5939	139.5904	141.4131	139.8236	141.0985	139.5956	141.3416	139.9982	141.2014	**130.99**
C2	137.3888	137.3557	137.9052	137.1077	137.7439	137.4006	137.9857	137.2334	138.0955	137.4576	138.0801	136.8040	136.8446	137.3898	136.8417	137.6112	137.1207	137.9926	136.9376	138.0835	137.2041	138.0703	**133.34**
C3	120.6544	121.3842	121.8707	121.6716	122.2855	121.9330	122.4590	121.7316	122.5866	122.0499	122.6336	119.6392	121.4514	121.9240	121.6569	122.3097	121.9238	122.3772	121.7284	122.4989	122.0306	122.5353	**117.55**
C4	177.6519	178.7185	179.3932	179.3068	180.0988	179.5462	180.5234	179.3230	180.6223	179.7057	180.7915	178.1086	178.8813	179.6485	179.1527	180.0400	179.4160	180.2300	179.2172	180.2861	179.5290	180.4844	**168.13**
C5	118.5470	119.8601	120.3998	120.5456	121.3222	120.7815	121.4404	120.5550	121.5434	120.9483	121.6902	118.6599	120.0133	120.5942	120.5540	121.3508	120.8003	121.3513	120.5845	121.4329	120.9468	121.5891	**117.55**
C6	133.7911	135.6052	136.7931	136.6678	138.3637	136.8753	138.6685	136.6243	138.6992	137.1000	139.1691	138.8182	136.2738	137.4058	137.2526	138.9036	137.4733	139.2393	137.2316	139.1572	137.6692	139.7543	**133.34**
C7	203.2767	208.6048	209.8305	211.6985	212.3595	211.7964	217.3300	211.4147	216.3806	212.2229	218.3121	205.2971	212.7975	214.3032	214.9277	216.0897	215.0775	220.0988	214.7652	219.4181	215.4121	220.5992	**195.87**
C8	69.1241	70.1253	70.7992	70.3573	71.5764	70.6395	71.9231	70.4601	71.8008	70.7169	72.6971	68.1488	65.4631	65.8331	66.4810	67.5528	66.6957	68.0924	66.4492	68.1157	66.9054	68.4506	**60.75**
C9	23.7215	24.0520	24.2062	24.1836	24.6500	24.4455	24.6108	24.2503	24.7226	24.5640	24.8492	16.4537	20.8061	20.7678	21.0333	21.2955	21.2977	21.4360	21.1003	21.5017	21.4093	21.9663	**16.39**
C8`	38.2242	38.9477	39.0730	39.4073	39.6721	39.6658	39.7283	39.4601	39.9360	39.7878	40.2492	32.8912	33.8280	34.1359	33.9651	34.2232	34.2348	34.1613	34.0423	34.3099	34.3359	34.3012	**32**
H2	8.3954	8.3311	8.3657	8.2850	8.2783	8.3345	8.4554	8.2924	8.3194	8.3386	8.4701	8.3743	8.3060	8.3480	8.2230	8.2163	8.2757	8.3816	8.2357	8.2114	8.2732	8.4083	**7.971**
H3	7.1679	7.2953	7.3831	7.3318	7.4491	7.3773	7.6306	7.3305	7.4581	7.3888	7.6578	7.0966	7.2855	7.3681	7.3259	7.4422	7.3712	7.6247	7.3239	7.4500	7.3832	7.6520	**7.22**
H5	7.0230	7.2052	7.2897	7.2883	7.4065	7.3310	7.5902	7.2811	7.4161	7.3480	7.6256	6.9899	7.1903	7.2755	7.2597	7.3808	7.3031	7.5580	7.2540	7.3806	7.3187	7.5918	**7.22**
H6	7.9452	8.1295	8.2114	8.2406	8.3476	8.2808	8.5506	8.2286	8.3909	8.3029	8.6025	8.9754	7.8764	7.9806	7.9535	8.0977	7.9966	8.2837	7.9470	8.0952	8.0128	8.3454	**7.971**
H8	4.5730	4.6582	4.6658	4.7406	4.7734	4.7808	4.9699	4.7284	4.7971	4.8027	5.0172	4.4807	4.8131	4.8614	4.8724	4.9776	4.9165	5.1608	4.8680	4.9755	4.9306	5.2060	**5.2**
H(9A-9C)	1.3344	1.3224	1.3240	1.2985	1.2925	1.3477	1.4693	1.3049	1.3035	1.3524	1.4944	1.2856	1.4612	1.4487	1.4808	1.4580	1.5270	1.6506	1.4807	1.4754	1.5371	1.6944	**1.611**
H(8`A-8`C)	2.5702	2.5055	2.4761	2.4845	2.4652	2.5330	2.6299	2.4890	2.4571	2.5387	2.6207	2.5654	2.8839	2.8478	2.7998	2.7482	2.8522	2.8332	2.8121	2.6782	2.8501	2.8119	**2.82**
Nuclei	BMK											BMK											
C1	154.5489	154.7956	155.8147	155.0346	156.7869	155.0048	155.7582	155.1850	155.9437	155.2232	155.7278	153.3708	154.7062	155.5737	155.3493	157.1804	155.2822	157.0114	155.4300	156.7717	155.5792	157.0888	**130.99**
C2	155.5489	155.3349	156.1444	155.0820	155.8798	155.0811	156.4462	155.2910	156.2529	155.2438	156.4023	154.7572	154.6732	155.3927	154.5734	155.4851	154.5591	155.9928	154.7574	155.7913	154.7494	155.9653	**133.34**
C3	135.9186	136.5742	137.2866	136.7717	137.6790	136.7457	137.8453	136.9307	137.6978	136.9577	137.8467	136.0540	136.5812	137.2516	136.7609	137.6638	136.7339	137.8432	136.9186	137.6908	136.9479	137.8865	**117.55**
C4	189.4005	190.1835	191.0076	190.6219	191.5290	190.5810	192.1342	190.7513	191.8731	190.8217	192.2418	189.7985	190.2293	191.0560	190.4438	191.4104	190.4180	191.7002	190.6026	191.5626	190.6291	191.8308	**168.13**
C5	133.4295	134.7613	135.4788	135.4278	136.5512	135.3675	136.6886	135.5196	136.4925	135.6472	136.8148	133.4535	134.7683	135.5390	135.3777	136.4835	135.3275	136.5822	135.4877	136.3606	135.5868	136.7328	**117.55**
C6	151.4094	153.6757	155.2637	155.0157	156.8896	154.9195	157.7543	155.0316	157.2746	155.2662	158.1427	152.1159	153.9639	155.4209	155.0094	157.0550	154.9327	157.4837	155.0660	157.2182	155.2429	157.8187	**133.34**
C7	216.9478	222.5474	224.1482	225.4916	226.2743	225.2972	232.0453	225.3132	230.7791	225.8361	232.8163	221.5389	226.5692	228.0915	229.2000	230.0942	229.0219	235.6763	229.0559	234.3215	229.5316	236.4133	**195.87**
C8	70.5725	71.6400	72.4428	72.1543	73.3210	72.1213	73.7576	72.2984	73.5299	72.3466	74.4771	64.4902	66.3795	67.0821	67.2150	68.2924	67.1424	69.1388	67.2827	68.7153	67.4478	69.3740	**60.75**
C9	25.4816	25.8566	26.3477	26.2252	26.6325	26.1938	26.7756	26.3697	26.5780	26.4143	26.8310	22.1260	22.5585	22.7087	22.6468	23.0607	22.6251	23.2222	22.8150	23.0572	22.8297	23.5137	**16.39**
C8`	38.7886	39.4905	39.7965	39.7916	40.2856	39.7653	40.4650	39.9500	40.3114	39.9781	40.8997	33.9443	34.1818	34.5674	34.3474	34.7515	34.3245	34.7335	34.5118	34.8069	34.5294	34.8356	**32**
H2	9.0522	9.0233	9.0737	8.9738	8.9666	8.9734	9.0551	8.9730	9.0302	8.9645	9.0669	9.0430	8.8827	8.9188	8.8117	8.8174	8.8133	8.8099	8.8146	8.8396	8.8005	8.8138	**7.971**
H3	7.6503	7.8088	7.9094	7.8680	7.9716	7.8622	8.0008	7.8561	7.9908	7.8636	8.0111	7.6582	7.8152	7.8999	7.8689	7.9851	7.8629	7.9933	7.8568	7.9965	7.8650	8.0096	**7.22**
H5	7.5098	7.7043	7.7841	7.7896	7.9181	7.7809	7.9299	7.7723	7.9192	7.7883	7.9561	7.4861	7.6973	7.7852	7.7793	7.9021	7.7717	7.9135	7.7640	7.8990	7.7768	7.9393	**7.22**
H6	8.4072	8.6270	8.7828	8.7961	8.9052	8.7837	9.0195	8.7706	8.9763	8.7979	9.0628	8.3050	8.4960	8.6092	8.6017	8.7715	8.5925	8.7332	8.5831	8.7698	8.6007	8.7910	**7.971**
H8	4.2317	4.3488	4.4104	4.4856	4.5292	4.4731	4.5903	4.4604	4.5756	4.4876	4.6005	4.4400	4.6482	4.6995	4.7284	4.8382	4.7206	4.8188	4.7127	4.8373	4.7262	4.8615	**5.2**
H(9A-9C)	1.3048	1.3335	1.3264	1.3372	1.2998	1.3347	1.3417	1.3320	1.3281	1.3300	1.3703	1.3776	1.3895	1.3774	1.4034	1.3701	1.3999	1.3895	1.3963	1.3784	1.3971	1.4125	**1.611**
H(8`A-8`C)	2.4334	2.3750	2.3238	2.3567	2.3235	2.3539	2.2956	2.3513	2.3080	2.3498	2.2771	2.8035	2.6688	2.6299	2.6096	2.5602	2.6105	2.4481	2.6113	2.4916	2.5990	2.4288	**2.82**
Nuclei	BP86											BP86											
C1	135.9939	136.6320	137.6362	136.9544	138.7298	136.9390	138.2948	136.9186	138.3141	136.9642	138.7051	134.4352	135.9816	136.4890	136.5815	138.0085	136.5423	138.0378	136.5022	137.9223	136.6187	138.2985	**130.99**
C2	136.0461	136.1412	136.6915	135.9389	136.4876	135.9629	136.9072	135.9812	136.7985	135.9104	137.0603	135.2799	135.6510	136.1578	135.6672	136.3174	135.6758	136.8585	135.6802	136.7480	135.6552	137.0159	**133.34**
C3	119.5556	120.4857	121.0080	120.7308	121.3490	120.7247	121.6928	120.7132	121.6404	120.7314	121.9360	119.6977	120.5178	120.9979	120.7317	121.3594	120.7284	121.6195	120.7195	121.5439	120.7299	121.8637	**117.55**
C4	174.3602	175.5049	176.1304	175.8536	176.5630	175.8334	177.1710	175.8083	177.0813	175.8678	177.4848	174.7072	175.5024	176.1986	175.7445	176.5291	175.7420	176.8841	175.7330	176.7851	175.7408	177.2044	**168.13**
C5	117.4531	118.9871	119.5529	119.6506	120.4030	119.6163	120.7206	119.5768	120.6236	119.6782	121.0496	117.6959	119.0396	119.6143	119.6262	120.4183	119.6030	120.5906	119.5742	120.4936	119.6424	120.9111	**117.55**
C6	132.4823	134.5222	135.5397	135.4991	136.9975	135.4473	137.5315	135.3905	137.2521	135.5440	138.0880	132.8422	134.9807	136.2191	135.9532	137.6251	135.9065	138.0996	135.8536	137.8931	135.9910	138.6398	**133.34**
C7	200.3568	205.1844	206.6915	207.6362	208.7456	207.4854	213.3518	207.3301	212.6663	207.7757	214.3906	205.2587	209.2590	210.3906	211.2385	212.1476	211.1283	216.2414	211.0136	215.3050	211.3390	216.8705	**195.87**
C8	67.0914	68.3350	69.0224	68.6336	69.6697	68.6283	70.1232	68.6177	69.8169	68.6343	71.1003	61.2199	63.3467	63.8475	64.2565	65.1036	64.1999	65.8529	64.1410	65.6179	64.3090	66.2851	**60.75**
C9	23.4788	23.9387	24.0159	24.1770	24.4194	24.1716	24.5594	24.1605	24.4086	24.1770	24.8922	20.0447	20.8111	20.8964	21.0566	21.2467	21.0482	21.5506	21.0352	21.4325	21.0604	22.1852	**16.39**
C8`	37.5056	38.3780	38.4809	38.5899	38.8300	38.5853	39.0439	38.5763	39.0514	38.5903	39.6736	32.7385	32.9732	33.1909	33.0751	33.2543	33.0771	33.3634	33.0731	33.3752	33.0673	33.5888	**32**
H2	8.4690	8.4251	8.4168	8.3721	8.3303	8.3765	8.3610	8.3805	8.3653	8.3675	8.3657	8.5023	8.3508	8.3888	8.2771	8.2780	8.2836	8.2597	8.2894	8.2717	8.2701	8.2813	**7.971**
H3	7.1833	7.3254	7.4023	7.3644	7.4695	7.3630	7.4872	7.3613	7.4789	7.3653	7.5157	7.1759	7.3137	7.3896	7.3551	7.4646	7.3535	7.4797	7.3516	7.4705	7.3561	7.5088	**7.22**
H5	7.0316	7.2248	7.3017	7.3045	7.4170	7.3004	7.4360	7.2960	7.4267	7.3081	7.4730	7.0289	7.2047	7.2838	7.2819	7.3979	7.2785	7.4064	7.2747	7.3955	7.2847	7.4416	**7.22**
H6	8.0317	8.2270	8.2775	8.3141	8.4038	8.3094	8.4531	8.3044	8.4474	8.3183	8.4976	7.7817	7.9419	8.0474	8.0258	8.1760	8.0224	8.1879	8.0185	8.1750	8.0284	8.2496	**7.971**
H8	4.6085	4.6845	4.6748	4.7603	4.7803	4.7553	4.8233	4.7502	4.8256	4.7646	4.8587	4.7327	4.8659	4.9018	4.9243	5.0225	4.9224	5.0356	4.9199	5.0205	4.9256	5.0853	**5.2**
H(9A-9C)	1.3656	1.3684	1.3441	1.3548	1.3143	1.3570	1.3284	1.3589	1.3132	1.3524	1.3589	1.4453	1.4875	1.4805	1.5086	1.4790	1.5084	1.4981	1.5079	1.4947	1.5083	1.5410	**1.611**
H(8`A-8`C)	2.5546	2.4795	2.4461	2.4610	2.4324	2.4627	2.4144	2.4642	2.4111	2.4590	2.4105	3.0093	2.8351	2.7840	2.7540	2.6945	2.7609	2.6012	2.7671	2.6178	2.7468	2.5828	**2.82**
Nuclei	CAM-B3LYP											CAM-B3LYP											
C1	140.5940	141.0501	141.9502	141.2482	143.3376	141.2328	142.6219	141.2195	142.7966	141.2664	142.8916	139.3811	140.7764	141.3414	141.3955	142.9372	141.3447	142.8551	141.3003	142.5657	141.4530	142.9212	**130.99**
C2	142.4322	142.3676	142.8920	142.2031	142.7302	142.2185	143.2393	142.2342	143.1183	142.1902	143.2313	141.9632	142.0722	142.5741	142.0137	142.6143	142.0196	143.1220	142.0264	143.0134	142.0107	143.1501	**133.34**
C3	123.8770	124.5297	125.0152	124.7351	125.3944	124.7281	125.5969	124.7212	125.5656	124.7437	125.6728	123.9590	124.5672	125.0168	124.7695	125.4058	124.7619	125.5862	124.7548	125.5220	124.7791	125.6510	**117.55**
C4	177.6432	178.4616	179.0236	178.8866	179.5004	178.8652	180.0958	178.8438	179.9671	178.9091	180.2452	177.9270	178.4619	179.0815	178.7166	179.4216	178.7091	179.7910	178.7009	179.7287	178.7245	179.9540	**168.13**
C5	121.6531	122.9882	123.5423	123.6761	124.5002	123.6378	124.6833	123.5998	124.6086	123.7146	124.8524	121.7948	123.0474	123.5984	123.6473	124.4684	123.6163	124.5780	123.5853	124.4990	123.6786	124.7226	**117.55**
C6	138.6325	140.6802	141.7768	141.7799	143.1835	141.7181	143.7450	141.6562	143.4517	141.8399	144.1171	138.9686	141.0487	142.3055	142.0534	143.7538	142.0017	144.1534	141.9484	144.0548	142.1023	144.5739	**133.34**
C7	205.1841	210.4669	211.8770	213.2659	214.3729	213.0946	219.8334	212.9249	218.8841	213.4315	220.8758	210.1044	214.5528	215.7343	216.9360	217.6675	216.7972	222.7736	216.6596	221.5003	217.0720	223.3268	**195.87**
C8	63.5728	64.7701	65.4574	65.1172	66.1087	65.1025	66.5638	65.0883	66.3449	65.1333	67.2834	57.9234	59.8230	60.3104	60.7065	61.5242	60.6433	62.2922	60.5845	61.9726	60.7729	62.5903	**60.75**
C9	22.4381	22.6575	22.8386	22.9008	23.1565	22.8881	23.1031	22.8752	23.0434	22.9144	23.2395	19.2771	19.6649	19.7105	19.7757	20.0125	19.7699	20.0783	19.7654	20.0320	19.7840	20.4496	**16.39**
C8`	35.5076	36.3386	36.5579	36.6501	37.0360	36.6375	37.2208	36.6255	37.1657	36.6643	37.6889	31.0486	31.2767	31.5537	31.4840	31.7595	31.4764	31.8336	31.4681	31.8936	31.4915	31.9753	**32**
H2	8.7689	8.7049	8.7244	8.6617	8.6168	8.6654	8.6438	8.6690	8.6389	8.6580	8.6285	8.7980	8.6167	8.6695	8.5340	8.5473	8.5409	8.5118	8.5472	8.5462	8.5267	8.5219	**7.971**
H3	7.4063	7.5412	7.6281	7.5846	7.6999	7.5826	7.7160	7.5807	7.7091	7.5865	7.7301	7.3996	7.5311	7.6171	7.5747	7.6929	7.5726	7.7060	7.5705	7.6986	7.5766	7.7206	**7.22**
H5	7.2620	7.4507	7.5382	7.5345	7.6567	7.5299	7.6715	7.5253	7.6620	7.5389	7.6941	7.2579	7.4349	7.5221	7.5119	7.6365	7.5077	7.6445	7.5036	7.6350	7.5158	7.6658	**7.22**
H6	8.1470	8.3590	8.4476	8.4737	8.5894	8.4673	8.6366	8.4608	8.6223	8.4796	8.6702	7.9705	8.1468	8.2705	8.2373	8.4092	8.2331	8.4121	8.2286	8.4132	8.2409	8.4600	**7.971**
H8	4.2201	4.3249	4.3484	4.4341	4.4931	4.4267	4.5388	4.4195	4.5400	4.4412	4.5650	4.3966	4.5587	4.6191	4.6315	4.7523	4.6282	4.7687	4.6248	4.7611	4.6343	4.8001	**5.2**
H(9A-9C)	1.3297	1.3390	1.3314	1.3291	1.2821	1.3304	1.2971	1.3316	1.2847	1.3277	1.3077	1.4016	1.4258	1.4289	1.4408	1.4198	1.4402	1.4318	1.4396	1.4375	1.4411	1.4563	**1.611**
H(8`A-8`C)	2.5132	2.4524	2.4238	2.4345	2.4170	2.4350	2.4044	2.4357	2.4044	2.4340	2.3914	2.9425	2.7653	2.7314	2.6913	2.6489	2.6974	2.5595	2.7032	2.5861	2.6851	2.5306	**2.82**

[a] methyl protons shifts are averaged
[b] according to [10]

Table S10. Cont. III

Nuclei	R											S										Exp. [b]
	HF											HF										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.0859	136.4286	136.9983	136.5642	138.6394	136.5601	136.8559	136.5607	137.5918	136.5707	137.8340	135.1106	136.0099	136.9165	136.8715	138.6196	136.8298	138.1526	136.7906	138.0357	136.9136	138.1693	**130.99**
C2	144.2959	144.1109	144.6184	143.9366	144.2969	143.9493	145.0625	143.9624	144.8336	143.9247	144.9263	144.1862	143.9606	144.4423	143.6963	144.1843	143.7105	144.6238	143.7251	144.5752	143.6812	144.6859	**133.34**
C3	120.5425	120.9815	121.3393	121.0997	121.6987	121.0951	121.5914	121.0919	121.6723	121.1042	121.7618	120.5755	121.0153	121.3955	121.1911	121.7425	121.1823	121.7739	121.1741	121.7432	121.1992	121.8101	**117.55**
C4	171.0685	171.6891	172.2443	172.0947	172.4686	172.0696	173.4111	172.0452	173.0954	172.1179	173.3624	171.3313	171.6695	172.1524	171.7723	172.2704	171.7643	172.7640	171.7564	172.6801	171.7787	172.9382	**168.13**
C5	117.7778	118.9699	119.4399	119.5840	120.3789	119.5486	120.2895	119.5143	120.3140	119.6174	120.5553	117.8113	119.0523	119.5559	119.6851	120.4237	119.6494	120.4603	119.6142	120.3849	119.7186	120.5859	**117.55**
C6	139.8710	141.8434	143.0414	142.9329	144.0689	142.8614	145.3610	142.7878	144.7144	142.9974	145.2266	140.2153	142.1535	143.2403	142.9363	144.2865	142.8868	144.8278	142.8360	144.6896	142.9813	145.2440	**133.34**
C7	195.4655	201.2748	202.3678	204.5817	204.9342	204.3815	211.4166	204.1898	210.2401	204.7750	212.8652	200.3146	204.7891	205.8595	207.3684	207.7885	207.2162	214.0876	207.0655	212.5722	207.5129	214.7501	**195.87**
C8	54.6914	55.6162	56.0452	55.7978	56.6132	55.7884	56.8235	55.7770	56.8761	55.8047	57.6680	49.9453	51.5670	52.1910	52.5059	53.2429	52.4542	53.9705	52.4041	53.6974	52.5554	54.1978	**60.75**
C9	20.7069	20.7584	20.8662	20.7421	21.0481	20.7452	20.9072	20.7468	20.8745	20.7388	20.9507	17.7976	17.8056	17.9115	17.8577	18.0665	17.8560	17.9858	17.8550	17.9557	17.8592	18.1883	**16.39**
C8`	32.6429	33.3486	33.5660	33.7469	34.0103	33.7215	34.1987	33.6970	34.1551	33.7689	34.5312	29.0930	29.3330	29.5248	29.4519	29.7044	29.4395	29.7559	29.4273	29.7928	29.4622	29.8640	**32**
H2	9.0358	8.9576	9.0240	8.9122	8.8795	8.9150	8.9903	8.9172	8.9268	8.9093	8.8935	9.0687	8.8942	8.9168	8.7657	8.7690	8.7719	8.7430	8.7777	8.7685	8.7596	8.7567	**7.971**
H3	7.4286	7.5694	7.6559	7.6163	7.7372	7.6140	7.7469	7.6115	7.7419	7.6185	7.7658	7.4270	7.5652	7.6521	7.6122	7.7319	7.6098	7.7417	7.6072	7.7343	7.6145	7.7576	**7.22**
H5	7.2620	7.4585	7.5485	7.5471	7.6720	7.5420	7.6831	7.5367	7.6720	7.5520	7.7063	7.2588	7.4515	7.5381	7.5363	7.6607	7.5316	7.6678	7.5266	7.6572	7.5408	7.6908	**7.22**
H6	8.1772	8.4177	8.5445	8.5717	8.7053	8.5623	8.8158	8.5526	8.7578	8.5806	8.8070	8.0620	8.2816	8.3955	8.3692	8.5389	8.3639	8.5572	8.3581	8.5485	8.3743	8.6055	**7.971**
H8	3.6262	3.7734	3.8337	3.9160	4.0002	3.9073	4.0866	3.8987	4.0448	3.9245	4.0816	3.7998	3.9985	4.0614	4.0795	4.2064	4.0749	4.2416	4.0700	4.2283	4.0838	4.2685	**5.2**
H(9A-9C)	1.2094	1.2101	1.2114	1.1856	1.1335	1.1867	1.1817	1.1873	1.1548	1.1845	1.1607	1.2797	1.2815	1.2708	1.2849	1.2453	1.2842	1.2618	1.2832	1.2631	1.2857	1.2803	**1.611**
H(8`A-8`C)	2.2583	2.2315	2.1858	2.2178	2.1970	2.2185	2.1768	2.2190	2.1940	2.2172	2.1932	2.6962	2.5446	2.4939	2.4664	2.4243	2.4706	2.3592	2.4746	2.3767	2.4625	2.3361	**2.82**
Nuclei	LC-BLYP																						
C1	143.9454	144.3001	145.4097	144.5079	146.3392	144.4682	145.1219	144.4578	146.1915	144.5303	146.2836	142.9429	144.2114	144.8868	144.9354	146.3990	144.8458	146.3781	144.7913	145.9849	145.0111	146.5188	**130.99**
C2	148.5022	148.3123	148.9120	148.1799	148.7307	148.1681	149.3075	148.1834	149.1118	148.1736	149.2571	148.2367	148.1595	148.7302	148.0898	148.6521	148.0728	149.1473	148.0835	149.0482	148.0884	149.1787	**133.34**
C3	128.3981	128.9432	129.5272	129.1700	129.8249	129.1365	129.9435	129.1302	129.9864	129.1845	130.1049	128.4577	128.9850	129.5383	129.2181	129.8639	129.1821	130.0193	129.1738	129.9481	129.2354	130.0806	**117.55**
C4	181.8964	182.5361	183.1128	182.9647	183.4846	182.9173	184.1724	182.8968	183.9350	182.9925	184.2385	182.1104	182.5115	183.1648	182.7723	183.4027	182.7394	183.7928	182.7322	183.7403	182.7849	183.9455	**168.13**
C5	126.0329	127.3491	128.0096	128.0921	128.9347	128.0253	129.0515	127.9857	129.0367	128.1384	129.2952	126.1441	127.4212	128.0695	128.1002	128.9526	128.0385	129.0416	128.0038	128.9555	128.1414	129.1882	**117.55**
C6	144.4457	146.5586	147.7101	147.7244	149.3132	147.6325	150.0897	147.5676	149.3684	147.7936	150.0269	144.7647	146.8890	148.2216	147.9599	149.7654	147.8834	150.1624	147.8313	150.0717	148.0120	150.5715	**133.34**
C7	210.7961	216.2518	217.8303	219.2261	219.8730	219.0191	225.3038	218.8395	225.0653	219.4065	227.1999	215.4470	220.1457	221.5590	222.7455	223.3196	222.5572	228.8329	222.3988	227.4675	222.9103	229.4875	**195.87**
C8	61.3984	62.6319	63.4214	63.1097	64.1261	63.0645	64.5480	63.0462	64.4091	63.1347	65.2976	55.6431	57.3143	57.8214	58.2576	59.0058	58.1666	59.8648	58.1066	59.4794	58.3300	60.2244	**60.75**
C9	21.5377	21.6825	21.9377	21.8979	22.3180	21.8578	22.1872	21.8462	22.0012	21.9197	22.1735	18.6324	18.8728	18.9378	19.0093	19.2711	18.9777	19.3164	18.9740	19.2407	19.0228	19.6888	**16.39**
C8`	33.6021	34.3992	34.7145	34.8359	35.1835	34.7918	35.4065	34.7739	35.3393	34.8597	35.8933	29.0895	29.3897	29.7641	29.6827	29.9584	29.6509	30.0425	29.6443	30.1159	29.6934	30.2365	**32**
H2	8.9711	8.8976	8.9038	8.8550	8.8357	8.8575	8.9003	8.8613	8.8099	8.8515	8.8027	8.9912	8.8085	8.8563	8.7154	8.7346	8.7227	8.6856	8.7307	8.7297	8.7068	8.6896	**7.971**
H3	7.5427	7.6754	7.7638	7.7201	7.8369	7.7170	7.8517	7.7154	7.8451	7.7221	7.8687	7.5437	7.6708	7.7599	7.7138	7.8323	7.7108	7.8425	7.7093	7.8366	7.7157	7.8586	**7.22**
H5	7.4058	7.5954	7.6843	7.6812	7.8049	7.6755	7.8189	7.6712	7.8049	7.6857	7.8395	7.4060	7.5871	7.6767	7.6670	7.7928	7.6617	7.7982	7.6579	7.7897	7.6710	7.8216	**7.22**
H6	8.3027	8.5213	8.6081	8.6422	8.7669	8.6342	8.8393	8.6277	8.7770	8.6487	8.8307	8.1441	8.3320	8.4605	8.4236	8.6087	8.4188	8.6040	8.4150	8.6111	8.4268	8.6501	**7.971**
H8	4.0994	4.2241	4.2473	4.3375	4.3854	4.3282	4.4499	4.3208	4.4440	4.3453	4.4811	4.3161	4.4914	4.5661	4.5712	4.6984	4.5663	4.7098	4.5628	4.7083	4.5747	4.7424	**5.2**
H(9A-9C)	1.3477	1.3582	1.3449	1.3500	1.3227	1.3501	1.3530	1.3517	1.2974	1.3487	1.3187	1.4131	1.4278	1.4251	1.4407	1.4202	1.4395	1.4310	1.4398	1.4374	1.4406	1.4542	**1.611**
H(8`A-8`C)	2.5010	2.4391	2.4146	2.4167	2.4026	2.4164	2.3702	2.4179	2.3908	2.4162	2.3818	2.8887	2.7145	2.6860	2.6365	2.5978	2.6411	2.5031	2.6470	2.5362	2.6309	2.4788	**2.82**
Nuclei	M06																						
C1	135.4072	135.7741	137.0115	135.8816	138.0210	135.8649	136.8091	135.8563	137.3380	135.9123	137.0556	134.1674	135.5202	136.1558	136.2300	137.8135	136.1538	137.9154	136.0917	137.5984	136.3238	137.9805	**130.99**
C2	140.6153	140.3648	140.9748	140.1830	140.7472	140.1863	141.1872	140.1968	141.0177	140.1945	141.1811	139.8441	139.8784	140.4612	139.8960	140.5961	139.8814	141.2124	139.8755	141.0600	139.9255	141.2192	**133.34**
C3	121.6176	122.2938	122.9735	122.5729	123.4101	122.5477	123.6473	122.5304	123.5932	122.6111	123.7286	121.6738	122.2553	122.8671	122.5213	123.3123	122.4950	123.5158	122.4767	123.4472	122.5609	123.5784	**117.55**
C4	173.1165	173.9963	174.7342	174.4927	175.3210	174.4521	176.0927	174.4196	175.9087	174.5457	176.2448	173.8447	174.2720	175.0646	174.5038	175.3524	174.4860	175.6260	174.4744	175.6126	174.5338	175.7886	**168.13**
C5	119.7718	121.0559	121.7752	121.7509	122.7315	121.6989	122.7996	121.6545	122.7382	121.8148	122.9828	119.7041	120.9774	121.6509	121.6232	122.5692	121.5755	122.6711	121.5353	122.6020	121.6826	122.8037	**117.55**
C6	136.8085	138.7038	139.7562	139.8590	141.2826	139.7763	142.3109	139.7016	141.8293	139.9522	142.5930	137.1469	139.1678	140.5409	140.2006	141.9881	140.1354	142.4239	140.0763	142.2946	140.2746	142.8394	**133.34**
C7	201.8270	206.8005	208.5395	209.3151	210.6085	209.1531	215.3851	208.9988	214.6233	209.4836	216.2344	206.3715	210.6515	211.8254	212.8411	213.6353	212.6921	218.3336	212.5525	217.1976	212.9995	218.7520	**195.87**
C8	60.7304	61.8816	62.6495	62.3326	63.4023	62.2980	63.5929	62.2707	63.6589	62.3799	64.4145	54.1844	55.7499	56.3619	56.6790	57.5433	56.6009	58.4113	56.5332	58.0797	56.7709	58.7141	**60.75**
C9	22.1450	22.4238	22.6903	22.7400	23.1676	22.7095	23.3573	22.6872	23.2995	22.7835	23.4614	19.4572	19.6907	19.8485	19.8638	20.2293	19.8402	20.3336	19.8248	20.2582	19.9018	20.8431	**16.39**
C8`	36.9348	37.6867	37.9199	37.9636	38.3405	37.9372	38.4473	37.9185	38.4095	38.0033	38.9535	31.7679	31.9520	32.3660	32.1758	32.5544	32.1571	32.7194	32.1443	32.7693	32.2063	32.7972	**32**
H2	8.7387	8.6519	8.6561	8.6165	8.5956	8.6186	8.6674	8.6211	8.6218	8.6152	8.6525	8.7596	8.5499	8.5974	8.4553	8.4747	8.4624	8.4395	8.4698	8.4663	8.4486	8.4486	**7.971**
H3	7.3369	7.4633	7.5604	7.5046	7.6321	7.5024	7.6528	7.5006	7.6377	7.5073	7.6581	7.2874	7.4302	7.5150	7.4793	7.6060	7.4760	7.6356	7.4734	7.6197	7.4830	7.6504	**7.22**
H5	7.1579	7.3516	7.4440	7.4353	7.5710	7.4303	7.5755	7.4258	7.5657	7.4405	7.6026	7.1555	7.3358	7.4320	7.4048	7.5377	7.4011	7.5349	7.3979	7.5315	7.4086	7.5553	**7.22**
H6	8.2198	8.4571	8.5350	8.5706	8.6748	8.5635	8.7980	8.5570	8.7357	8.5779	8.8111	7.9934	8.1490	8.2703	8.2290	8.4027	8.2251	8.4051	8.2215	8.4052	8.2330	8.4572	**7.971**
H8	4.3442	4.4692	4.4989	4.5607	4.6243	4.5542	4.7164	4.5485	4.6836	4.5675	4.7345	4.4477	4.6028	4.6519	4.6647	4.7811	4.6617	4.7907	4.6590	4.7893	4.6679	4.8239	**5.2**
H(9A-9C)	1.3018	1.3045	1.2808	1.2978	1.2531	1.2981	1.2815	1.2991	1.2659	1.2981	1.2924	1.3858	1.4182	1.4256	1.4306	1.4133	1.4304	1.4165	1.4305	1.4256	1.4312	1.4437	**1.611**
H(8`A-8`C)	2.4763	2.4121	2.3914	2.3956	2.3829	2.3959	2.3669	2.3969	2.3791	2.3959	2.3540	2.9033	2.7432	2.7104	2.6626	2.6248	2.6682	2.5329	2.6741	2.5623	2.6576	2.5047	**2.82**
Nuclei	M06-2X																						
C1	153.0917	153.5294	154.5657	153.6798	155.3824	153.6910	154.3824	153.7038	154.6410	153.6636	154.5610	152.3025	153.6253	154.2248	154.4172	155.8548	154.3561	155.9192	154.3050	155.6636	154.4801	156.1304	**130.99**
C2	155.1746	155.0543	155.6859	154.8589	155.5556	154.8934	156.0475	154.9292	155.9461	154.8195	156.0984	154.7655	154.7734	155.3565	154.6837	155.4125	154.7088	155.8874	154.7355	155.7791	154.6544	155.9277	**133.34**
C3	136.1590	136.8604	137.4721	137.0980	137.8395	137.1065	138.0767	137.1160	138.0006	137.0834	138.1754	136.1934	136.8293	137.4400	137.0599	137.8148	137.0677	137.9965	137.0767	137.9426	137.0459	138.0999	**117.55**
C4	186.9866	187.8245	188.4710	188.2660	188.9823	188.2597	189.6225	188.2546	189.4454	188.2657	189.8145	187.4071	187.9865	188.7105	188.2373	189.0085	188.2488	189.3855	188.2602	189.3135	188.2178	189.5659	**168.13**
C5	133.5146	135.0251	135.7169	135.8167	136.7899	135.7892	136.9947	135.7628	136.8748	135.8366	137.2061	133.4360	134.8666	135.5636	135.5696	136.5427	135.5491	136.6670	135.5297	136.5791	135.5821	136.8705	**117.55**
C6	151.2911	153.5510	154.7995	154.7508	156.6302	154.6981	157.2971	154.6466	156.9660	154.7945	157.7502	151.6315	153.9149	155.3078	154.9928	157.0373	154.9595	157.4443	154.9245	157.2709	155.0146	157.8386	**133.34**
C7	218.4206	224.0871	225.6863	227.0228	227.7392	226.8634	233.4654	226.7049	232.2929	227.1679	234.4902	222.3731	227.5635	229.0579	230.3177	230.9202	230.1563	236.7866	230.0003	235.3937	230.4701	237.6501	**195.87**
C8	66.1021	67.3894	68.1145	67.8657	68.9271	67.8608	69.3536	67.8567	69.2455	67.8636	70.1061	60.3620	62.0622	62.4883	63.0156	63.8536	62.9637	64.7319	62.9168	64.3967	63.0637	65.0835	**60.75**
C9	23.2058	23.4985	23.7070	23.7340	24.1504	23.7389	24.1959	23.7459	24.1017	23.7236	24.3456	20.3942	20.6118	20.6433	20.7319	21.0349	20.7420	21.1263	20.7541	21.0549	20.7172	21.5210	**16.39**
C8`	36.0510	36.7555	36.9669	37.1150	37.4247	37.1125	37.6459	37.1106	37.5970	37.1109	38.1632	30.7152	31.1896	31.5368	31.3585	31.6695	31.3831	31.7058	31.4062	31.7955	31.3257	31.8659	**32**
H2	9.2412	9.1940	9.2146	9.1667	9.1653	9.1672	9.2317	9.1673	9.2138	9.1663	9.2327	9.2302	9.0921	9.1468	9.0068	9.0354	9.0138	9.0044	9.0198	9.0317	8.9993	9.0042	**7.971**
H3	7.8930	8.0315	8.1240	8.0797	8.2018	8.0760	8.2142	8.0720	8.2077	8.0833	8.2275	7.8444	7.9817	8.0724	8.0317	8.1517	8.0277	8.1674	8.0235	8.1599	8.0355	8.1819	**7.22**
H5	7.7188	7.9115	8.0040	8.0015	8.1305	7.9950	8.1471	7.9882	8.1342	8.0078	8.1715	7.7205	7.8974	7.9934	7.9760	8.1058	7.9705	8.1095	7.9646	8.1016	7.9813	8.1306	**7.22**
H6	8.7195	8.9331	9.0357	9.0522	9.2020	9.0436	9.2622	9.0346	9.2341	9.0605	9.2978	8.5491	8.7357	8.8647	8.8195	9.0069	8.8151	9.0001	8.8099	9.0002	8.8232	9.0400	**7.971**
H8	4.2292	4.3451	4.3884	4.4506	4.5168	4.4418	4.5788	4.4328	4.5575	4.4593	4.6093	4.4880	4.6312	4.7027	4.6959	4.8114	4.6915	4.8114	4.6865	4.8097	4.7000	4.8405	**5.2**
H(9A-9C)	1.3567	1.3681	1.3531	1.3672	1.3372	1.3663	1.3712	1.3650	1.3600	1.3682	1.3871	1.4261	1.4313	1.4276	1.4367	1.4173	1.4356	1.4268	1.4342	1.4284	1.4376	1.4441	**1.611**
H(8`A-8`C)	2.4619	2.4039	2.3762	2.3853	2.3641	2.3849	2.3357	2.3842	2.3446	2.3860	2.3207	2.7873	2.6416	2.6191	2.5775	2.5343	2.5805	2.4563	2.5830	2.4800	2.5745	2.4273	**2.82**

[a] methyl protons shifts are averaged
[b] according to [10]

Table S10. Cont. IV

Nuclei	R											S										Exp. [b]
	mpW1LYP											mpW1LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.4828	139.9525	140.8951	140.2162	142.1269	140.1880	141.3847	140.1639	141.5911	140.2438	141.6737	138.0239	139.3201	140.0314	140.0519	141.6015	140.0019	141.3526	139.9557	141.2617	140.1006	141.3699	**130.99**
C2	140.0654	139.9633	140.5214	139.8120	140.2594	139.8221	140.7067	139.8327	140.5833	139.8000	140.6754	139.3485	139.4849	140.0212	139.4970	140.0614	139.4929	140.6129	139.4906	140.4986	139.4995	140.6006	**133.34**
C3	121.9628	122.6121	123.1375	122.8712	123.4386	122.8537	123.7099	122.8374	123.6709	122.8862	123.7449	122.0772	122.6487	123.1165	122.8876	123.4426	122.8714	123.6473	122.8567	123.5970	122.9013	123.6861	**117.55**
C4	176.1473	177.0246	177.6646	177.5228	178.1467	177.4890	178.8123	177.4567	178.6743	177.5533	178.9071	176.5361	177.1020	177.7627	177.3919	178.0767	177.3729	178.4887	177.3548	178.3978	177.4074	178.6295	**168.13**
C5	119.7588	121.0521	121.6454	121.7767	122.5021	121.7290	122.7447	121.6831	122.6591	121.8202	122.8719	119.9121	121.1021	121.6630	121.7119	122.4355	121.6731	122.5793	121.6353	122.5049	121.7464	122.6956	**117.55**
C6	136.3411	138.3279	139.4122	139.4387	140.8254	139.3726	141.4341	139.3066	141.1391	139.4983	141.7648	136.6810	138.7304	140.0172	139.7711	141.3801	139.7081	141.9011	139.6456	141.7184	139.8277	142.2839	**133.34**
C7	202.6211	207.7782	209.3145	210.5766	211.6308	210.3901	217.0461	210.2089	216.1478	210.7558	217.9713	207.9684	212.1537	213.3072	214.4009	215.1623	214.2635	219.8843	214.1282	218.8057	214.5296	220.3958	**195.87**
C8	64.8087	65.9413	66.6307	66.2710	67.2010	66.2555	67.4970	66.2398	67.3414	66.2823	68.2675	59.1606	61.1502	61.8125	62.1638	63.0102	62.0972	63.6763	62.0334	63.4471	62.2269	63.9055	**60.75**
C9	23.0194	23.2782	23.4066	23.5626	23.7640	23.5450	23.7639	23.5280	23.6835	23.5763	23.8872	19.5716	19.9981	20.1757	20.2377	20.4306	20.2213	20.5847	20.2064	20.5225	20.2514	20.9210	**16.39**
C8`	36.3159	37.0893	37.3474	37.4110	37.7421	37.3893	37.9553	37.3691	37.9323	37.4299	38.3577	31.9503	32.0958	32.3503	32.2714	32.4808	32.2555	32.5948	32.2408	32.6120	32.2842	32.6749	**32**
H2	8.6760	8.6134	8.6345	8.5731	8.5352	8.5769	8.5767	8.5801	8.5650	8.5692	8.5537	8.7155	8.5439	8.5843	8.4575	8.4611	8.4631	8.4509	8.4681	8.4656	8.4518	8.4608	**7.971**
H3	7.3397	7.4720	7.5610	7.5164	7.6269	7.5145	7.6429	7.5123	7.6350	7.5181	7.6539	7.3222	7.4540	7.5397	7.5009	7.6151	7.4987	7.6299	7.4961	7.6226	7.5029	7.6422	**7.22**
H5	7.1905	7.3768	7.4660	7.4635	7.5825	7.4586	7.6016	7.4535	7.5914	7.4679	7.6207	7.1791	7.3532	7.4411	7.4319	7.5518	7.4276	7.5619	7.4231	7.5524	7.4357	7.5804	**7.22**
H6	8.0834	8.2895	8.3770	8.4032	8.5186	8.3966	8.5837	8.3898	8.5634	8.4092	8.6049	7.8914	8.0614	8.1768	8.1478	8.3090	8.1432	8.3269	8.1382	8.3161	8.1519	8.3729	**7.971**
H8	4.3063	4.3981	4.4252	4.5055	4.5605	4.4978	4.6229	4.4902	4.6105	4.5128	4.6327	4.4564	4.6192	4.6720	4.6856	4.7973	4.6823	4.8170	4.6786	4.8046	4.6884	4.8463	**5.2**
H(9A-9C)	1.3216	1.3308	1.3202	1.3215	1.2774	1.3232	1.2903	1.3245	1.2801	1.3196	1.3009	1.4008	1.4361	1.4422	1.4560	1.4325	1.4551	1.4529	1.4538	1.4517	1.4567	1.4756	**1.611**
H(8`A-8`C)	2.5203	2.4606	2.4330	2.4451	2.4238	2.4459	2.4070	2.4465	2.4101	2.4443	2.3934	2.9829	2.8104	2.7656	2.7300	2.6802	2.7354	2.5986	2.7403	2.6192	2.7247	2.5674	**2.82**
Nuclei	mpW1PW91											mpW1PW91										
C1	136.7091	137.1261	138.2904	137.3527	139.3925	137.3342	138.8484	137.3222	138.8794	137.3708	139.0868	135.4965	136.8443	137.3776	137.4319	138.8932	137.3747	138.9047	137.3297	138.6184	137.4927	138.9966	**130.99**
C2	139.0510	138.9813	139.5567	138.8023	139.3841	138.8154	139.7972	138.8338	139.6690	138.7889	139.7849	138.4920	138.6376	139.1844	138.5926	139.2587	138.5931	139.7425	138.5998	139.6330	138.5920	139.7648	**133.34**
C3	121.1434	121.8839	122.4572	122.1398	122.8577	122.1259	123.1111	122.1175	123.0669	122.1523	123.1972	121.1969	121.8835	122.4042	122.1282	122.8348	122.1142	123.0503	122.1059	122.9791	122.1411	123.1290	**117.55**
C4	173.1450	174.0361	174.6361	174.4798	175.1382	174.4530	175.7414	174.4320	175.6481	174.5044	175.9056	173.4356	174.0253	174.6981	174.2966	175.0454	174.2852	175.4189	174.2781	175.3524	174.3057	175.5825	**168.13**
C5	118.9666	120.3546	120.9855	121.0745	121.9413	121.0305	122.1805	120.9922	122.0946	121.1155	122.3576	119.0635	120.3480	120.9568	120.9724	121.8462	120.9359	121.9978	120.9051	121.9093	121.0057	122.1526	**117.55**
C6	135.1188	137.1393	138.1020	138.2106	139.6150	138.1465	140.1616	138.0877	139.9062	138.2707	140.5379	135.4925	137.5198	138.7879	138.5089	140.2202	138.4556	140.6265	138.4058	140.5120	138.5558	141.0214	**133.34**
C7	200.5499	205.4732	207.1087	208.0696	209.2352	207.9079	214.4321	207.7523	213.5361	208.2238	215.3863	204.9687	209.2878	210.4288	211.5065	212.2688	211.3693	217.0803	211.2400	215.8598	211.6406	217.5855	**195.87**
C8	62.5871	63.7277	64.3921	64.0779	65.0594	64.0579	65.5692	64.0437	65.2428	64.0959	66.2934	57.3088	59.1083	59.5712	59.9715	60.7733	59.9036	61.5602	59.8450	61.2368	60.0391	61.8431	**60.75**
C9	22.4303	22.7074	22.8165	22.9714	23.2346	22.9561	23.2515	22.9463	23.1372	22.9849	23.3928	19.1269	19.5971	19.6794	19.7761	20.0297	19.7623	20.1776	19.7543	20.1086	19.7888	20.5773	**16.39**
C8`	35.5389	36.3291	36.5286	36.6000	36.9580	36.5839	37.1500	36.5735	37.1332	36.6149	37.6110	31.0253	31.2540	31.5589	31.4502	31.7343	31.4412	31.7914	31.4363	31.8597	31.4556	31.8914	**32**
H2	8.7270	8.6729	8.6666	8.6268	8.5829	8.6306	8.6029	8.6343	8.6110	8.6233	8.5930	8.7399	8.5718	8.6280	8.4933	8.5106	8.5006	8.4771	8.5073	8.5099	8.4860	8.4856	**7.971**
H3	7.3666	7.5071	7.5941	7.5506	7.6672	7.5488	7.6842	7.5469	7.6761	7.5526	7.6994	7.3521	7.4918	7.5782	7.5379	7.6587	7.5357	7.6748	7.5336	7.6662	7.5401	7.6902	**7.22**
H5	7.2156	7.4099	7.4980	7.4952	7.6199	7.4906	7.6379	7.4860	7.6293	7.4999	7.6618	7.2035	7.3869	7.4755	7.4658	7.5930	7.4616	7.6047	7.4575	7.5936	7.4700	7.6265	**7.22**
H6	8.1720	8.3810	8.4466	8.4858	8.5927	8.4800	8.6356	8.4742	8.6335	8.4916	8.6714	7.9622	8.1369	8.2584	8.2244	8.3946	8.2208	8.3985	8.2168	8.3988	8.2277	8.4460	**7.971**
H8	4.3244	4.4232	4.4417	4.5212	4.5686	4.5149	4.6073	4.5088	4.6209	4.5275	4.6357	4.4958	4.6417	4.6998	4.7058	4.8233	4.7033	4.8370	4.7007	4.8311	4.7081	4.8693	**5.2**
H(9A-9C)	1.3031	1.3123	1.2861	1.3005	1.2512	1.3018	1.2673	1.3032	1.2532	1.2994	1.2798	1.3839	1.4107	1.4119	1.4245	1.4007	1.4244	1.4147	1.4241	1.4196	1.4248	1.4408	**1.611**
H(8`A-8`C)	2.4582	2.3926	2.3693	2.3752	2.3559	2.3760	2.3459	2.3770	2.3405	2.3747	2.3305	2.8765	2.7109	2.6756	2.6345	2.5913	2.6410	2.5022	2.6472	2.5276	2.6285	2.4719	**2.82**
Nuclei	O3LYP											O3LYP										
C1	133.9706	135.2869	135.1280	135.8992	137.5413	135.8935	136.8634	135.8840	136.9936	135.9000	136.9568	131.9841	134.0269	134.9667	134.8776	136.4625	134.8098	136.5165	134.7451	136.4801	134.9454	136.6774	**130.99**
C2	134.2294	134.0386	134.6059	134.0020	134.6215	134.0143	135.0928	134.0931	135.0297	133.9844	135.0347	133.6011	133.8315	134.4861	133.8598	134.5658	133.8686	134.9908	133.8725	134.9155	133.8449	134.9967	**133.34**
C3	117.1429	117.8472	118.4244	118.1586	118.8498	118.1512	119.1048	118.1420	119.0383	118.1592	119.1705	117.2423	117.8329	118.4008	118.1462	118.7940	118.1374	118.9776	118.1236	118.9199	118.1480	119.0503	**117.55**
C4	169.3331	170.2178	170.9930	170.6800	171.4504	170.6575	171.9898	170.6246	171.8402	170.6953	172.1262	169.6935	170.1374	170.8394	170.4612	171.2113	170.4568	171.5048	170.4458	171.4066	170.4567	171.6400	**168.13**
C5	115.1244	116.3261	117.0316	116.9791	117.7550	116.9488	117.9702	116.9062	117.8594	117.0010	118.1340	115.2829	116.3481	116.9834	116.9736	117.7506	116.9474	117.8633	116.9154	117.7787	116.9914	118.0028	**117.55**
C6	130.1343	131.8403	133.2468	132.9143	134.4244	132.8471	134.9826	132.7768	134.7083	132.9717	135.3818	130.8195	132.4740	133.5676	133.4119	134.9398	133.3757	135.3121	133.3309	135.1128	133.4364	135.6140	**133.34**
C7	196.4324	202.4039	202.9208	205.2799	206.3184	205.1284	211.0569	204.9884	210.1352	205.4208	211.6531	200.9322	205.3707	206.9113	207.7346	208.6887	207.5898	212.9882	207.4429	212.0350	207.8698	213.5094	**195.87**
C8	62.7269	63.8638	64.1933	64.6392	65.2111	64.6247	65.7186	64.6144	65.5898	64.6448	66.4308	57.3727	59.9629	60.5156	61.0054	61.8178	60.9369	62.7983	60.8688	62.5812	61.0698	63.0624	**60.75**
C9	21.9077	22.1497	22.4381	22.4448	22.6922	22.4333	22.8050	22.4257	22.7348	22.4497	22.9545	18.3907	18.7982	18.9135	19.0083	19.2082	19.0039	19.4486	18.9953	19.3637	19.0069	19.7532	**16.39**
C8`	35.8615	36.6415	36.9984	37.0897	37.4384	37.0783	37.5559	37.0769	37.5415	37.0931	37.8889	31.6791	31.7885	32.1081	32.0205	32.3175	32.0201	32.2296	32.0132	32.2550	32.0126	32.2365	**32**
H2	8.5171	8.3815	8.5110	8.3059	8.3131	8.3086	8.3569	8.3167	8.3480	8.3030	8.3618	8.6115	8.3742	8.4056	8.2874	8.3033	8.2956	8.2770	8.3028	8.2844	8.2784	8.2790	**7.971**
H3	7.2896	7.4098	7.5061	7.4543	7.5768	7.4521	7.6030	7.4468	7.5953	7.4562	7.6133	7.2766	7.4071	7.4943	7.4552	7.5707	7.4530	7.5845	7.4505	7.5766	7.4572	7.5999	**7.22**
H5	7.1552	7.3290	7.4298	7.3986	7.5094	7.3950	7.5202	7.3889	7.5085	7.4017	7.5463	7.1395	7.3009	7.3898	7.3774	7.4980	7.3735	7.5074	7.3692	7.4968	7.3810	7.5278	**7.22**
H6	8.0527	8.2175	8.3672	8.3017	8.4640	8.2946	8.5029	8.2853	8.4809	8.3083	8.5390	7.8574	7.9837	8.0812	8.0642	8.2140	8.0612	8.2127	8.0575	8.2001	8.0664	8.2508	**7.971**
H8	4.4166	4.5098	4.5410	4.5642	4.6714	4.5583	4.6852	4.5532	4.6658	4.5699	4.7170	4.5458	4.6793	4.7411	4.7470	4.8642	4.7444	4.8665	4.7410	4.8556	4.7490	4.8955	**5.2**
H(9A-9C)	1.2321	1.2056	1.2312	1.2013	1.1647	1.2018	1.1980	1.2027	1.1895	1.2008	1.2166	1.3321	1.3605	1.3485	1.3797	1.3521	1.3795	1.3771	1.3787	1.3725	1.3796	1.3957	**1.611**
H(8`A-8`C)	2.4772	2.4452	2.4019	2.4401	2.4019	2.4414	2.3990	2.4451	2.4021	2.4388	2.3752	2.9410	2.7694	2.7347	2.6983	2.6563	2.7041	2.5681	2.7092	2.5820	2.6922	2.5313	**2.82**
Nuclei	OLYP											OLYP										
C1	132.8188	134.1516	135.6656	135.1449	137.5235	135.1515	135.6652	135.1532	135.8434	135.1337	135.7556	130.8981	132.7261	133.7888	133.6768	135.1782	133.6081	135.1883	133.5382	135.1931	133.7379	135.3980	**130.99**
C2	131.6623	131.6975	132.2794	131.7465	132.3472	131.7531	132.6913	131.7546	132.6220	131.7302	132.7039	131.2536	131.3661	132.0518	131.4162	132.0990	131.4235	132.5894	131.4250	132.5059	131.4005	132.5752	**133.34**
C3	115.3417	116.0422	116.6555	116.3161	116.9608	116.3056	117.2576	116.2899	117.1915	116.3169	117.3369	114.4114	116.0541	116.6230	116.3750	116.9979	116.3650	117.1604	116.3492	117.1047	116.3752	117.2329	**117.55**
C4	168.2126	169.2294	169.9205	169.5710	170.1814	169.5487	170.9191	169.5215	170.7744	169.5840	171.0771	168.4577	169.1151	169.8267	169.4427	170.2413	169.4360	170.4899	169.4224	170.3927	169.4386	170.6134	**168.13**
C5	113.3427	114.4633	115.0535	115.0655	115.7600	115.0339	116.1215	114.9960	116.0017	115.0864	116.2699	113.4100	114.5734	115.1849	115.1704	115.9016	115.1450	116.0297	115.1131	115.9473	115.1848	116.1602	**117.55**
C6	127.6886	129.4580	130.3992	130.3959	131.5991	130.3259	132.5021	130.2522	132.2325	130.4552	132.8719	132.4882	129.9940	131.1063	130.8821	132.4316	130.8446	132.8458	130.8002	132.6433	130.9066	133.1053	**133.34**
C7	195.3251	201.0301	202.9899	204.5243	206.1991	204.3850	209.0998	204.2443	208.2692	204.6535	209.6663	194.9333	204.0205	205.4470	206.3531	207.3591	206.2114	211.0678	206.0639	210.2799	206.4776	211.6073	**195.87**
C8	63.8385	65.2339	66.0677	65.6811	66.8369	65.6883	66.9203	65.6854	66.8721	65.6665	67.5606	62.8816	61.2250	62.0414	62.3546	63.1411	62.2822	64.2114	62.2081	64.0080	62.4201	64.4616	**60.75**
C9	22.0417	22.3211	22.5251	22.7061	22.8886	22.6962	23.1868	22.6811	23.0909	22.7070	23.3016	15.7972	18.8615	19.1193	19.1190	19.3070	19.1099	19.6432	19.0962	19.5371	19.1202	19.9486	**16.39**
C8`	36.5297	37.3375	37.5614	37.8176	38.0745	37.8036	38.1673	37.7827	38.1190	37.8211	38.5013	31.4966	32.4077	32.6511	32.6378	32.9272	32.6373	32.7834	32.6299	32.8079	32.6276	32.7561	**32**
H2	8.3522	8.2235	8.1969	8.1272	8.0714	8.1268	8.2234	8.1264	8.2066	8.1267	8.2299	8.4369	8.2352	8.2566	8.1468	8.1702	8.1543	8.1611	8.1613	8.1618	8.1388	8.1574	**7.971**
H3	7.2072	7.3275	7.4178	7.4008	7.5127	7.3974	7.5330	7.3939	7.5211	7.4035	7.5445	7.1593	7.3325	7.4196	7.3792	7.4934	7.3770	7.5033	7.3746	7.4956	7.3809	7.5175	**7.22**
H5	7.0851	7.2353	7.3143	7.2988	7.4157	7.2941	7.4375	7.2893	7.4251	7.3029	7.4576	7.0403	7.2266	7.3145	7.2993	7.4188	7.2955	7.4288	7.2915	7.4188	7.3025	7.4474	**7.22**
H6	7.9775	8.1327	8.1956	8.2132	8.2977	8.2041	8.4009	8.1954	8.3698	8.2217	8.4374	8.7484	7.8865	7.9743	7.9576	8.1089	7.9547	8.1075	7.9514	8.0939	7.9595	8.1417	**7.971**
H8	4.5323	4.5911	4.6096	4.6267	4.6824	4.6200	4.7353	4.6144	4.7106	4.6332	4.7707	4.4883	4.7554	4.8166	4.8221	4.9436	4.8190	4.9419	4.8155	4.9305	4.8243	4.9712	**5.2**
H(9A-9C)	1.2237	1.2082	1.1959	1.1823	1.1420	1.1826	1.2055	1.1826	1.1992	1.1815	1.2218	1.2466	1.3653	1.3601	1.3854	1.3618	1.3848	1.3978	1.3840	1.3909	1.3856	1.4134	**1.611**
H(8`A-8`C)	2.5179	2.4873	2.4697	2.4886	2.4649	2.4895	2.4510	2.4902	2.4526	2.4873	2.4211	2.3523	2.8150	2.7687	2.7435	2.7024	2.7489	2.6101	2.7538	2.6211	2.7376	2.5695	**2.82**

[a] methyl protons shifts are averaged
[b] according to [10]

Table S10. Cont. V

Nuclei	R											S										Exp. [b]
	OPBE											OPBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	129.7640	131.1387	132.6552	132.1246	134.4950	132.1378	132.7494	132.1341	132.8307	132.0968	132.7529	127.9531	129.7572	131.3960	130.9073	132.9633	130.8138	132.2249	130.6965	132.6314	130.9636	132.5011	**130.99**
C2	130.3586	130.4886	130.9968	130.4429	131.0543	130.4635	131.3872	130.4661	131.3319	130.3820	131.3838	129.9865	130.2359	130.9157	130.1823	130.9380	130.1990	131.3075	130.1994	131.2030	130.1628	131.3207	**133.34**
C3	114.2213	115.0550	115.6259	115.3016	116.0144	115.3021	116.3293	115.2846	116.2561	115.3063	116.4542	114.3041	115.0698	115.5900	115.3365	116.0072	115.3394	116.2309	115.3240	116.1537	115.3295	116.3409	**117.55**
C4	164.6226	165.6789	166.2199	165.9412	166.5402	165.9340	167.2498	165.9090	167.1104	166.0101	167.4931	164.9027	165.5555	166.0292	165.7368	166.3569	165.7530	166.8192	165.7519	166.6262	165.7218	166.9648	**168.13**
C5	112.2687	113.5344	114.0760	114.0744	114.8381	114.0527	115.1922	114.0131	115.0739	114.1130	115.4008	112.4202	113.6143	114.1128	114.1369	114.8497	114.1271	115.0869	114.0994	114.9493	114.1433	115.2524	**117.55**
C6	126.1608	127.9997	128.8093	128.8180	129.9411	128.7696	130.8401	128.7038	130.6005	128.8489	131.2575	126.8203	128.5704	129.4079	129.2674	130.6027	129.2570	131.2141	129.2292	130.8690	129.2803	131.4889	**133.34**
C7	192.8626	198.3520	200.1588	201.6561	203.2107	201.5462	206.1754	201.4188	205.3233	201.7358	206.5747	196.3497	200.6868	202.1872	203.0429	204.1492	202.9127	207.7285	202.7568	207.1557	203.1474	208.2542	**195.87**
C8	61.2284	62.7133	63.5636	63.1881	64.3519	63.1850	64.4468	63.1637	64.3074	63.1720	65.1108	56.6311	58.7512	59.9248	59.9517	61.0884	59.8539	61.5973	59.7391	61.6414	60.0230	61.9029	**60.75**
C9	21.2805	21.6678	21.7922	21.9610	22.1440	21.9624	22.3933	21.9464	22.3075	21.9463	22.5303	17.8291	18.2838	18.5005	18.5007	18.7647	18.4933	18.9349	18.4692	18.8763	18.4996	19.2950	**16.39**
C8`	35.4845	36.3569	36.4549	36.7323	36.9249	36.7278	37.0000	36.7052	36.9687	36.7163	37.3820	31.0988	31.3654	31.3318	31.4174	31.5251	31.4408	31.6115	31.4469	31.5375	31.3965	31.5941	**32**
H2	8.3870	8.2642	8.2215	8.1564	8.0952	8.1575	8.2408	8.1577	8.2328	8.1562	8.2594	8.4575	8.2769	8.2227	8.1564	8.1258	8.1678	8.1855	8.1792	8.1490	8.1477	8.1810	**7.971**
H3	7.2282	7.3602	7.4433	7.4277	7.5438	7.4252	7.5609	7.4218	7.5508	7.4327	7.5779	7.2304	7.3678	7.4497	7.4149	7.5264	7.4130	7.5438	7.4104	7.5341	7.4158	7.5608	**7.22**
H5	7.1021	7.2653	7.3426	7.3260	7.4471	7.3219	7.4668	7.3170	7.4549	7.3330	7.4935	7.0869	7.2574	7.3371	7.3302	7.4448	7.3268	7.4602	7.3227	7.4473	7.3327	7.4817	**7.22**
H6	8.0380	8.1929	8.2297	8.2560	8.3210	8.2498	8.4322	8.2430	8.4104	8.2608	8.4821	7.8021	7.9511	7.9981	8.0067	8.1209	8.0068	8.1616	8.0062	8.1245	8.0072	8.1968	**7.971**
H8	4.5419	4.6115	4.6071	4.6376	4.6660	4.6345	4.7386	4.6308	4.7174	4.6371	4.7816	4.6657	4.7892	4.8168	4.8395	4.9337	4.8401	4.9559	4.8394	4.9298	4.8389	4.9886	**5.2**
H(9A-9C)	1.1827	1.1710	1.1506	1.1424	1.0922	1.1427	1.1573	1.1423	1.1499	1.1403	1.1786	1.2938	1.3294	1.3061	1.3393	1.2986	1.3395	1.3428	1.3392	1.3289	1.3389	1.3621	**1.611**
H(8`A-8`C)	2.4371	2.4087	2.3861	2.4045	2.3742	2.4058	2.3612	2.4063	2.3625	2.4000	2.3311	2.8529	2.7064	2.6163	2.6177	2.5447	2.6266	2.4933	2.6347	2.4903	2.6099	2.4549	**2.82**
Nuclei	OPW91											OPW91										
C1	130.0734	131.4711	132.9769	132.4406	134.8087	132.4451	133.0129	132.4321	133.1402	132.4191	133.0519	128.2394	130.0724	131.7005	131.1724	133.2463	131.0761	132.5216	130.9590	132.9078	131.2337	132.7953	**130.99**
C2	130.5806	130.7074	131.2089	130.6288	131.2637	130.6390	131.5719	130.6356	131.5478	130.6007	131.6048	130.1962	130.4533	131.1259	130.4042	131.1441	130.4116	131.5201	130.4034	131.4168	130.3802	131.5359	**133.34**
C3	114.4183	115.2508	115.8151	115.5092	116.1968	115.4994	116.5211	115.4732	116.4393	115.4999	116.6391	114.5029	115.2650	115.7792	115.5361	116.1909	115.5285	116.4136	115.5035	116.3378	115.5247	116.5251	**117.55**
C4	165.0246	166.0821	166.6217	166.4195	166.9443	166.4003	167.7080	166.3664	167.5188	166.4192	167.9027	165.3169	165.9654	166.4385	166.1639	166.7698	166.1681	167.2288	166.1553	167.0408	166.1434	167.3773	**168.13**
C5	112.4634	113.7286	114.2665	114.2944	115.0217	114.2618	115.3914	114.2128	115.2585	114.3067	115.5871	112.6210	113.8117	114.3056	114.3432	115.0398	114.3225	115.2744	114.2843	115.1397	114.3450	115.4419	**117.55**
C6	126.3826	128.2204	129.0301	129.0438	130.1652	128.9844	131.0735	128.9103	130.8310	129.0819	131.4938	127.0499	128.7969	129.6351	129.5203	130.8358	129.4965	131.4451	129.4563	131.1082	129.5270	131.7238	**133.34**
C7	193.2195	198.7503	200.5473	202.0469	203.6032	201.9273	206.5400	201.7965	205.7249	202.1429	206.9853	196.7445	201.1005	202.5918	203.4416	204.5479	203.3022	208.1416	203.1393	207.5501	203.5465	208.6706	**195.87**
C8	61.4164	62.9130	63.7519	63.3730	64.5345	63.3605	64.5943	63.3262	64.4929	63.3665	65.2823	56.7828	58.9381	60.1067	60.1087	61.2534	60.0077	61.7812	59.8918	61.8124	60.1818	62.0859	**60.75**
C9	21.3412	21.7318	21.8564	22.0225	22.2056	22.0139	22.4453	21.9905	22.3695	22.0127	22.5934	17.9020	18.3623	18.5810	18.5780	18.8386	18.5624	19.0151	18.5310	18.9558	18.5743	19.3737	**16.39**
C8`	35.5474	36.4260	36.5197	36.7969	36.9960	36.7816	37.0617	36.7522	37.0400	36.7928	37.4582	31.1915	31.4588	31.4241	31.5288	31.6223	31.5399	31.7046	31.5341	31.6351	31.5020	31.6928	**32**
H2	8.3887	8.2639	8.2222	8.1590	8.0961	8.1592	8.2467	8.1596	8.2338	8.1570	8.2615	8.4616	8.2780	8.2245	8.1636	8.1292	8.1736	8.1874	8.1840	8.1527	8.1537	8.1831	**7.971**
H3	7.2300	7.3612	7.4442	7.4326	7.5443	7.4293	7.5651	7.4261	7.5509	7.4339	7.5785	7.2318	7.3686	7.4505	7.4163	7.5267	7.4137	7.5442	7.4109	7.5345	7.4169	7.5610	**7.22**
H5	7.1042	7.2672	7.3446	7.3319	7.4481	7.3269	7.4705	7.3219	7.4560	7.3348	7.4945	7.0894	7.2592	7.3388	7.3327	7.4461	7.3286	7.4614	7.3242	7.4485	7.3348	7.4827	**7.22**
H6	8.0365	8.1901	8.2278	8.2553	8.3202	8.2483	8.4351	8.2419	8.4096	8.2601	8.4824	7.8035	7.9505	7.9980	8.0099	8.1218	8.0088	8.1616	8.0074	8.1258	8.0096	8.1969	**7.971**
H8	4.5413	4.6099	4.6067	4.6350	4.6660	4.6313	4.7388	4.6276	4.7179	4.6370	4.7820	4.6622	4.7853	4.8138	4.8390	4.9316	4.8382	4.9531	4.8368	4.9279	4.8379	4.9856	**5.2**
H(9A-9C)	1.1844	1.1724	1.1522	1.1437	1.0939	1.1434	1.1586	1.1424	1.1520	1.1425	1.1806	1.2943	1.3301	1.3074	1.3418	1.3002	1.3413	1.3445	1.3406	1.3308	1.3411	1.3636	**1.611**
H(8`A-8`C)	2.4383	2.4106	2.3882	2.4045	2.3762	2.4051	2.3601	2.4055	2.3644	2.4024	2.3329	2.8575	2.7104	2.6209	2.6250	2.5505	2.6328	2.4979	2.6400	2.4956	2.6165	2.4597	**2.82**
Nuclei	PBE											PBE										
C1	135.5369	136.0918	137.1653	136.3677	138.3715	136.3432	137.9723	136.3302	138.0000	136.4097	138.2666	133.9549	135.5103	136.0530	136.0986	137.6401	136.0426	137.7558	136.0033	137.5912	136.1760	137.8979	**130.99**
C2	135.9657	136.0179	136.6216	135.7847	136.4967	135.7983	136.9066	135.8222	136.8094	135.7890	136.9073	135.2241	135.5670	136.1193	135.5057	136.3042	135.5028	136.8654	135.5121	136.7580	135.5269	136.8854	**133.34**
C3	119.4465	120.3299	120.8882	120.5608	121.3376	120.5455	121.6570	120.5407	121.5966	120.5927	121.7624	119.5345	120.3283	120.8574	120.5295	121.3174	120.5157	121.5667	120.5123	121.4938	120.5600	121.6702	**117.55**
C4	173.9823	175.0866	175.7504	175.5136	176.3815	175.4853	176.9469	175.4679	176.8322	175.5580	177.1272	174.3115	175.1027	175.8451	175.3569	176.3062	175.3425	176.6457	175.3376	176.5574	175.3868	176.8245	**168.13**
C5	117.3377	118.8348	119.4453	119.5117	120.4263	119.4676	120.7320	119.4345	120.6335	119.5712	120.9231	117.5420	118.8521	119.4821	119.4030	120.3643	119.3686	120.5554	119.3443	120.4643	119.4527	120.7344	**117.55**
C6	132.4775	134.5082	135.5902	135.4775	137.1352	135.4145	137.6377	135.3620	137.3771	135.5552	138.0465	132.8577	134.9572	136.2454	135.8915	137.7657	135.8360	138.2041	135.7900	138.0185	135.9600	138.5976	**133.34**
C7	200.2846	204.9361	206.5139	207.3187	208.7358	207.1695	213.0970	207.0319	212.3370	207.4784	214.0538	205.2335	209.1883	210.4404	211.1454	212.2526	211.0237	216.2129	210.9132	215.2932	211.2804	216.6930	**195.87**
C8	66.5088	67.7352	68.5365	68.0186	69.2245	67.9992	69.7030	67.9905	69.4643	68.0544	70.5121	60.8379	62.8084	63.3380	63.6487	64.6563	63.5816	65.3895	63.5289	65.1438	63.7343	65.6928	**60.75**
C9	23.3476	23.7914	23.9606	24.0315	24.4395	24.0128	24.5728	24.0048	24.4653	24.0668	24.7581	19.9739	20.6830	20.7908	20.8644	21.2357	20.8478	21.5194	20.8429	21.4105	20.8983	22.0261	**16.39**
C8`	37.1172	37.9328	38.1214	38.1135	38.5395	38.1010	38.7049	38.0990	38.6815	38.1431	39.1975	32.1770	32.4188	32.7113	32.5246	32.8859	32.5166	32.9628	32.5184	32.9920	32.5484	33.0440	**32**
H2	8.4940	8.4541	8.4552	8.4051	8.3713	8.4089	8.3990	8.4131	8.4018	8.4020	8.3885	8.5295	8.3765	8.4273	8.2992	8.3159	8.3056	8.2934	8.3120	8.3107	8.2932	8.2994	**7.971**
H3	7.2033	7.3447	7.4313	7.3857	7.5032	7.3838	7.5208	7.3823	7.5132	7.3881	7.5355	7.1915	7.3278	7.4143	7.3701	7.4921	7.3680	7.5036	7.3664	7.4955	7.3727	7.5186	**7.22**
H5	7.0554	7.2476	7.3344	7.3285	7.4528	7.3239	7.4719	7.3198	7.4630	7.3335	7.4950	7.0514	7.2254	7.3152	7.2983	7.4275	7.2942	7.4386	7.2906	7.4284	7.3027	7.4597	**7.22**
H6	8.0650	8.2613	8.3213	8.3484	8.4499	8.3435	8.4938	8.3391	8.4841	8.3536	8.5258	7.8075	7.9693	8.0875	8.0493	8.2174	8.0456	8.2265	8.0420	8.2172	8.0532	8.2729	**7.971**
H8	4.5942	4.6682	4.6640	4.7434	4.7783	4.7384	4.8154	4.7339	4.8140	4.7488	4.8411	4.7365	4.8721	4.9225	4.9285	5.0427	4.9260	5.0540	4.9238	5.0416	4.9312	5.0891	**5.2**
H(9A-9C)	1.3652	1.3737	1.3620	1.3582	1.3268	1.3594	1.3445	1.3610	1.3344	1.3577	1.3585	1.4620	1.4973	1.5000	1.5101	1.4967	1.5097	1.5158	1.5096	1.5145	1.5110	1.5442	**1.611**
H(8`A-8`C)	2.5658	2.4898	2.4677	2.4656	2.4518	2.4665	2.4330	2.4680	2.4322	2.4654	2.4135	3.0023	2.8324	2.7952	2.7516	2.7069	2.7580	2.6137	2.7646	2.6329	2.7457	2.5792	**2.82**
Nuclei	PBE0											PBE0										
C1	136.2247	136.6526	137.6494	136.8626	138.8179	136.8401	138.3389	136.8206	138.4202	136.8878	138.5165	135.0705	136.3670	136.9426	136.9688	138.3856	136.9063	138.4604	136.8512	138.1253	137.0380	138.5078	**130.99**
C2	138.7455	138.6972	139.2899	138.5224	139.1126	138.5294	139.6279	138.5381	139.4524	138.5187	139.5604	138.2240	138.3806	138.9274	138.3295	138.9750	138.3256	139.5396	138.3238	139.3720	138.3367	139.5045	**133.34**
C3	120.8925	121.6540	122.2093	121.9097	122.6105	121.8907	122.9447	121.8736	122.8377	121.9304	122.9696	120.9444	121.6525	122.1782	121.8956	122.5853	121.8764	122.8788	121.8592	122.7522	121.9168	122.9010	**117.55**
C4	172.7695	173.6677	174.2592	174.1060	174.7504	174.0748	175.4368	174.0455	175.2494	174.1384	175.5356	173.0167	173.6449	174.3079	173.9164	174.6482	173.8991	175.1081	173.8827	174.9805	173.9346	175.2141	**168.13**
C5	118.6951	120.1057	120.7177	120.8251	121.6797	120.7761	122.0034	120.7290	121.8560	120.8746	122.1212	118.8136	120.1112	120.7251	120.7385	121.6008	120.6967	121.8294	120.6564	121.6863	120.7809	121.9289	**117.55**
C6	134.9467	136.9717	138.0243	138.0376	139.4645	137.9675	140.0789	137.8990	139.7408	138.1064	140.4199	135.3034	137.3666	138.6127	138.3429	140.0727	138.2853	140.5728	138.2274	140.3897	138.3981	140.9095	**133.34**
C7	200.1830	205.0445	206.4951	207.5876	208.7013	207.4269	213.8365	207.2685	212.8952	207.7437	214.6933	204.6033	208.8622	210.0809	211.0822	211.8366	210.9380	216.6033	210.7982	215.3664	211.2259	217.0626	**195.87**
C8	62.4961	63.6480	64.3663	63.9871	64.9554	63.9622	65.4882	63.9393	65.2096	64.0139	66.1783	57.1221	58.8511	59.3074	59.6939	60.4822	59.6234	61.3132	59.5575	60.9413	59.7669	61.5421	**60.75**
C9	22.4232	22.7099	22.8836	22.9713	23.2313	22.9485	23.3154	22.9273	23.1815	22.9957	23.4231	19.1174	19.6122	19.6632	19.7712	20.0251	19.7540	20.2525	19.7389	20.1245	19.7907	20.6140	**16.39**
C8`	35.4509	36.2307	36.4509	36.4979	36.8360	36.4785	37.0927	36.4609	36.9944	36.5195	37.4940	30.7624	31.0177	31.3187	31.2114	31.4738	31.1980	31.6175	31.1846	31.6291	31.2246	31.6596	**32**
H2	8.7291	8.6745	8.6839	8.6307	8.5912	8.6340	8.6207	8.6372	8.6136	8.6271	8.6069	8.7394	8.5811	8.6311	8.4997	8.5161	8.5067	8.4889	8.5132	8.5182	8.4920	8.4934	**7.971**
H3	7.3570	7.4984	7.5860	7.5429	7.6585	7.5407	7.6805	7.5383	7.6697	7.5447	7.6928	7.3444	7.4827	7.5699	7.5283	7.6473	7.5259	7.6672	7.5234	7.6563	7.5302	7.6796	**7.22**
H5	7.2043	7.3984	7.4865	7.4833	7.6061	7.4784	7.6287	7.4735	7.6162	7.4877	7.6494	7.1957	7.3777	7.4663	7.4563	7.5822	7.4518	7.5978	7.4472	7.5841	7.4603	7.6170	**7.22**
H6	8.1786	8.3833	8.4552	8.4878	8.5945	8.4818	8.6451	8.4757	8.6289	8.4931	8.6774	7.9635	8.1395	8.2598	8.2257	8.3971	8.2217	8.4076	8.2174	8.4040	8.2288	8.4520	**7.971**
H8	4.3167	4.4108	4.4199	4.5072	4.5534	4.5008	4.6039	4.4943	4.6020	4.5131	4.6265	4.4991	4.6448	4.7045	4.7095	4.8253	4.7065	4.8443	4.7033	4.8349	4.7119	4.8737	**5.2**
H(9A-9C)	1.3125	1.3212	1.3067	1.3099	1.2608	1.3109	1.2798	1.3118	1.2649	1.3088	1.2919	1.3963	1.4224	1.4195	1.4330	1.4094	1.4328	1.4284	1.4324	1.4298	1.4329	1.4515	**1.611**
H(8`A-8`C)	2.4651	2.3989	2.3727	2.3791	2.3574	2.3796	2.3472	2.3802	2.3450	2.3785	2.3301	2.8767	2.7128	2.6773	2.6349	2.5897	2.6409	2.5049	2.6468	2.5284	2.6289	2.4711	**2.82**

[a] methyl protons shifts are averaged
[b] according to [10]

Table S10. Cont. VI

Nuclei	R											S										Exp. [b]
	TPSS																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	132.3080	132.7323	133.5947	132.9917	134.6209	132.9794	133.9174	132.9795	133.4835	133.0145	134.1627	130.9473	132.0464	132.8321	132.7165	134.1527	132.6760	133.8514	132.6492	133.7648	132.7685	133.9904	**130.99**
C2	133.0997	133.0157	133.6822	132.9050	133.5045	132.9199	133.9437	132.9461	133.4500	132.9010	133.9167	132.3746	132.5433	133.1843	132.5871	133.2524	132.5896	133.7520	132.6038	133.7197	132.5960	133.7438	**133.34**
C3	116.6148	117.2984	117.9237	117.5959	118.2555	117.5862	118.5980	117.5876	118.0301	117.6152	118.6571	116.6745	117.2824	117.8745	117.5564	118.2099	117.5476	118.4658	117.5497	118.7785	117.5754	118.5352	**117.55**
C4	170.6841	171.5811	172.3374	172.0858	172.8432	172.0623	173.5294	172.0498	172.7101	172.1186	173.6596	170.9980	171.6247	172.4068	171.9513	172.7573	171.9401	173.2076	171.9397	172.7606	171.9719	173.3439	**168.13**
C5	114.5838	115.8370	116.5194	116.5569	117.3608	116.5197	117.6964	116.4938	116.9319	116.6029	117.8309	114.7542	115.8493	116.5202	116.4562	117.2683	116.4268	117.4654	116.4086	117.6460	116.4943	117.6013	**117.55**
C6	129.6014	131.4435	132.6218	132.4972	133.9868	132.4389	134.5452	132.3920	132.8937	132.5630	134.9193	129.9037	131.8399	133.1059	132.8246	134.4809	132.7742	135.0675	132.7346	133.8495	132.8818	135.3960	**133.34**
C7	196.4615	200.8812	202.3135	203.2587	204.2943	203.1209	208.8163	202.9947	203.7788	203.4005	209.6447	201.0290	204.6160	205.9348	206.6362	207.5175	206.5206	211.4415	206.4167	206.9790	206.7570	211.9588	**195.87**
C8	65.1158	66.2120	66.9967	66.5823	67.5160	66.5694	67.7566	66.5676	66.8060	66.6049	68.5367	60.1278	61.8831	62.5632	62.8019	63.6923	62.7474	64.2607	62.7059	64.3460	62.8662	64.4976	**60.75**
C9	23.9382	24.2126	24.5053	24.5049	24.8006	24.4912	24.8817	24.4888	24.5589	24.5284	25.0320	20.6506	21.2665	21.4915	21.5390	21.8543	21.5290	22.1455	21.5306	23.4796	21.5593	22.5571	**16.39**
C8`	37.5256	38.2274	38.5539	38.5318	38.8578	38.5228	39.1217	38.5251	38.6513	38.5508	39.5382	33.2385	33.3352	33.6679	33.4955	33.7511	33.4908	33.9306	33.4973	35.3565	33.5099	33.9584	**32**
H2	8.5053	8.4506	8.4858	8.4146	8.4078	8.4174	8.4634	8.4207	8.2608	8.4123	8.4454	8.5333	8.3896	8.4302	8.3110	8.3267	8.3165	8.3314	8.3222	8.4330	8.3060	8.3282	**7.971**
H3	7.1662	7.3060	7.4014	7.3539	7.4751	7.3516	7.4934	7.3498	7.1856	7.3564	7.5050	7.1476	7.2856	7.3782	7.3357	7.4586	7.3331	7.4748	7.3311	7.4493	7.3384	7.4865	**7.22**
H5	7.0222	7.2106	7.3064	7.2978	7.4257	7.2928	7.4508	7.2885	7.1240	7.3028	7.4683	7.0178	7.1891	7.2832	7.2681	7.3973	7.2637	7.4087	7.2598	7.3786	7.2727	7.4263	**7.22**
H6	7.9512	8.1457	8.2359	8.2495	8.3724	8.2435	8.4400	8.2381	8.0774	8.2555	8.4692	7.7288	7.9081	8.0237	7.9982	8.1671	7.9933	8.1988	7.9889	8.1022	8.0030	8.2393	**7.971**
H8	4.4709	4.5419	4.5602	4.6283	4.6855	4.6222	4.7477	4.6168	4.4417	4.6345	4.7669	4.5859	4.7329	4.7881	4.8006	4.9128	4.7971	4.9372	4.7941	4.9314	4.8041	4.9650	**5.2**
H(9A-9C)	1.3567	1.3679	1.3676	1.3629	1.3311	1.3636	1.3485	1.3649	1.1767	1.3626	1.3622	1.4392	1.4842	1.4875	1.5034	1.4900	1.5025	1.5193	1.5021	1.6640	1.5046	1.5408	**1.611**
H(8`A-8`C)	2.5215	2.4527	2.4256	2.4341	2.4118	2.4348	2.3810	2.4361	2.2522	2.4338	2.3643	2.9653	2.7995	2.7626	2.7257	2.6817	2.7310	2.6015	2.7368	2.8894	2.7208	2.5649	**2.82**
Nuclei	VSXC																						
C1	130.0829	130.4045	131.1400	130.4934	131.6615	130.4929	131.1365	130.4902	131.2057	130.4951	131.2579	129.9454	130.6445	131.8488	131.2031	132.5520	131.1505	132.4267	131.1004	132.2788	131.2589	132.5715	**130.99**
C2	131.4719	131.5765	132.0332	131.5476	131.9755	131.5536	132.4149	131.5574	132.3103	131.5434	132.5007	131.5035	131.5629	132.0835	131.4748	131.9974	131.4854	132.4275	131.4940	132.3584	131.4659	132.4408	**133.34**
C3	115.0253	115.9281	116.4781	116.3182	116.9617	116.2986	117.2532	116.2767	117.1666	116.3381	117.3602	115.1018	115.8625	116.3437	116.1552	116.7869	116.1441	116.9700	116.1304	116.9294	116.1665	117.0707	**117.55**
C4	168.4085	169.4140	170.1094	169.9432	170.7388	169.9139	171.2602	169.8824	171.1101	169.9727	171.4432	168.2644	169.1345	169.7602	169.5550	170.3438	169.5352	170.7332	169.5129	170.6261	169.5745	170.8988	**168.13**
C5	112.9381	114.3706	114.9696	115.1434	115.9400	115.0989	116.2089	115.0522	116.0882	115.1874	116.3893	112.8384	114.1341	114.6817	114.8040	115.5837	114.7687	115.7340	114.7306	115.6555	114.8386	115.8930	**117.55**
C6	129.7735	131.5896	132.6289	132.6050	134.1264	132.5458	134.6888	132.4845	134.4417	132.6624	135.0466	129.7921	131.8114	132.8618	132.8875	134.4094	132.8259	134.9250	132.7615	134.6909	132.9470	135.2245	**133.34**
C7	190.4964	194.5948	195.8890	196.6716	197.5040	196.5484	201.3041	196.4236	200.4899	196.7897	202.0685	192.4201	196.4292	197.9570	198.6054	199.5513	198.4654	203.3086	198.3255	202.3644	198.7417	203.9258	**195.87**
C8	71.0293	71.8644	72.4464	72.1610	72.9614	72.1470	73.3160	72.1307	73.2068	72.1762	73.9137	63.2954	64.4627	65.0975	65.1337	65.9999	65.0894	66.5041	65.0447	66.3060	65.1788	66.9366	**60.75**
C9	27.6811	28.6013	28.9238	29.2582	29.7109	29.2182	30.0806	29.1763	29.9393	29.2980	30.1347	28.6031	28.7198	28.7057	28.8776	29.0104	28.8658	28.9877	28.8527	28.9354	28.8913	29.2920	**16.39**
C8`	40.4536	40.9423	41.0239	41.1700	41.3482	41.1601	41.3711	41.1480	41.3482	41.1808	41.7912	35.6942	36.3333	36.3426	36.5410	36.8365	36.5434	36.8289	36.5411	36.8765	36.5384	37.0830	**32**
H2	8.7013	8.6318	8.6383	8.5965	8.5956	8.5987	8.6008	8.6009	8.6015	8.5945	8.6002	8.6698	8.5714	8.5462	8.4980	8.4914	8.5044	8.4746	8.5105	8.4951	8.4915	8.4705	**7.971**
H3	7.2076	7.3421	7.4286	7.3891	7.5038	7.3867	7.5214	7.3843	7.5128	7.3914	7.5352	7.2377	7.3761	7.4621	7.4257	7.5415	7.4230	7.5574	7.4205	7.5480	7.4281	7.5730	**7.22**
H5	7.1085	7.2957	7.3836	7.3798	7.5056	7.3750	7.5203	7.3702	7.5095	7.3844	7.5443	7.1230	7.2984	7.3840	7.3775	7.4993	7.3729	7.5080	7.3684	7.4968	7.3817	7.5256	**7.22**
H6	8.1799	8.3473	8.4451	8.4415	8.5921	8.4354	8.6432	8.4296	8.6230	8.4472	8.6738	7.8041	7.9933	8.0857	8.0898	8.2480	8.0846	8.2771	8.0794	8.2615	8.0945	8.3072	**7.971**
H8	4.3876	4.4583	4.4912	4.5227	4.5993	4.5183	4.6338	4.5141	4.6138	4.5269	4.6595	4.6175	4.7683	4.8270	4.8563	4.9599	4.8507	5.0035	4.8453	4.9843	4.8616	5.0218	**5.2**
H(9A-9C)	1.5961	1.6138	1.6048	1.6171	1.6025	1.6170	1.6242	1.6171	1.6201	1.6172	1.6378	1.7731	1.7717	1.7506	1.7772	1.7569	1.7769	1.7723	1.7766	1.7683	1.7776	1.7889	**1.611**
H(8`A-8`C)	2.6858	2.6354	2.6002	2.6143	2.5757	2.6156	2.5544	2.6170	2.5572	2.6129	2.5289	2.8671	2.7641	2.7059	2.7132	2.6678	2.7172	2.6228	2.7210	2.6423	2.7093	2.5927	**2.82**
Nuclei	wB97																						
C1	136.3743	136.5643	137.5508	136.6805	138.3186	136.6682	137.1758	136.6563	137.6400	136.6935	137.3306	135.5496	136.5810	137.2430	137.2393	138.6376	137.1701	138.5360	137.1091	138.2897	137.3170	138.7211	**130.99**
C2	140.2891	140.1704	140.7301	140.0418	140.6111	140.0495	141.1373	140.0566	141.0098	140.0348	141.1780	140.0931	140.0448	140.6006	139.9574	140.5644	139.9621	140.9964	139.9662	140.9089	139.9528	141.0199	**133.34**
C3	121.6439	122.2148	122.7714	122.4318	123.1041	122.4188	123.2000	122.4051	123.1728	122.4445	123.2668	121.6716	122.2096	122.7417	122.4350	123.1020	122.4187	123.2279	122.4023	123.1663	122.4515	123.2949	**117.55**
C4	174.2577	174.9242	175.5185	175.3214	175.9512	175.2956	176.5447	175.2691	176.3511	175.3461	176.6908	174.3838	174.8494	175.5012	175.0939	175.7994	175.0823	176.1349	175.0683	176.0692	175.1036	176.2686	**168.13**
C5	119.4831	120.7345	121.3443	121.4210	122.2577	121.3777	122.3482	121.3337	122.2709	121.4624	122.5094	119.5892	120.7784	121.3962	121.3974	122.2486	121.3581	122.3057	121.3179	122.2298	121.4354	122.4485	**117.55**
C6	136.8221	138.8055	139.9029	139.8974	141.4938	139.8285	142.2089	139.7589	141.7730	139.9631	142.5634	137.0806	139.0577	140.2748	140.0174	141.7669	139.9692	142.1277	139.9168	141.9973	140.0596	142.4749	**133.34**
C7	200.5554	205.5196	206.9736	208.1930	208.8203	208.0253	213.7590	207.8570	212.9387	208.3529	214.6659	204.2854	208.7429	210.1036	211.2165	211.7853	211.0496	216.9049	210.8871	215.6715	211.3809	217.6015	**195.87**
C8	61.2286	62.1722	62.8269	62.5542	63.4515	62.5338	63.8040	62.5119	63.7336	62.5735	64.4107	55.7397	57.1823	57.6139	58.0157	58.7514	57.9530	59.4666	57.8934	59.1612	58.0807	59.7826	**60.75**
C9	22.0700	22.2380	22.4228	22.4373	22.8248	22.4194	22.7743	22.4016	22.6602	22.4557	22.8715	19.5465	19.7727	19.7821	19.8738	20.1420	19.8648	20.1501	19.8559	20.0913	19.8837	20.5181	**16.39**
C8`	35.1652	35.7649	35.9908	36.0743	36.3679	36.0567	36.5472	36.0377	36.5002	36.0907	36.9598	30.5263	30.8779	31.2072	31.0800	31.3808	31.0803	31.3789	31.0759	31.4642	31.0751	31.4895	**32**
H2	8.8384	8.7915	8.8061	8.7534	8.7565	8.7561	8.8198	8.7586	8.7788	8.7508	8.8177	8.8444	8.6993	8.7460	8.6049	8.6340	8.6136	8.5895	8.6213	8.6222	8.5954	8.5916	**7.971**
H3	7.4415	7.5770	7.6646	7.6196	7.7405	7.6173	7.7555	7.6149	7.7454	7.6217	7.7699	7.4525	7.5863	7.6739	7.6277	7.7500	7.6258	7.7576	7.6236	7.7514	7.6295	7.7730	**7.22**
H5	7.3028	7.4922	7.5805	7.5754	7.7036	7.5705	7.7161	7.5655	7.7041	7.5800	7.7398	7.3123	7.4932	7.5821	7.5675	7.6967	7.5632	7.7017	7.5588	7.6926	7.5714	7.7244	**7.22**
H6	8.2363	8.4473	8.5401	8.5626	8.6990	8.5558	8.7730	8.5487	8.7240	8.5691	8.8069	8.0771	8.2684	8.3886	8.3453	8.5299	8.3432	8.5210	8.3402	8.5241	8.3465	8.5617	**7.971**
H8	4.0794	4.2013	4.2289	4.3015	4.3612	4.2941	4.4167	4.2867	4.3964	4.3088	4.4426	4.2843	4.4417	4.5098	4.5068	4.6254	4.5039	4.6339	4.5005	4.6294	4.5091	4.6610	**5.2**
H(9A-9C)	1.3373	1.3502	1.3355	1.3434	1.3206	1.3441	1.3538	1.3446	1.3316	1.3428	1.3678	1.4052	1.4218	1.4124	1.4283	1.4126	1.4285	1.4264	1.4284	1.4276	1.4279	1.4449	**1.611**
H(8`A-8`C)	2.4600	2.4029	2.3721	2.3774	2.3594	2.3781	2.3295	2.3790	2.3441	2.3770	2.3180	2.8246	2.6620	2.6344	2.5859	2.5485	2.5907	2.4603	2.5952	2.4869	2.5812	2.4374	**2.82**
Nuclei	wB97Z																						
C1	137.8029	138.0540	139.0211	138.1992	139.8961	138.1870	138.7316	138.1755	139.5920	138.2141	139.6814	136.9016	138.0110	138.6568	138.6712	140.0912	138.6060	140.0704	138.5482	139.7173	138.7443	140.1871	**130.99**
C2	140.7055	140.6032	141.1665	140.4847	141.0596	140.4945	141.6070	140.5037	141.4061	140.4762	141.5856	140.5526	140.5103	141.0764	140.4186	141.0232	140.4259	141.4852	140.4318	141.3445	140.4125	141.4959	**133.34**
C3	122.3475	122.9417	123.4842	123.1709	123.8319	123.1596	123.9911	123.1475	123.9336	123.1825	124.0993	122.3753	122.9427	123.4616	123.1718	123.8332	123.1584	124.0179	123.1444	123.8893	123.1862	124.0701	**117.55**
C4	174.9165	175.6237	176.2197	176.0405	176.6624	176.0165	177.3046	175.9916	177.0258	176.0640	177.3657	175.0408	175.5562	176.2009	175.8192	176.5285	175.8083	176.9078	175.7954	176.7811	175.8288	177.0410	**168.13**
C5	120.1726	121.4443	122.0434	122.1523	122.9687	122.1105	123.1411	122.0679	123.0163	122.1931	123.3151	120.2954	121.5031	122.1147	122.1275	122.9742	122.0916	123.0943	122.0548	122.9461	122.1629	123.2277	**117.55**
C6	137.1768	139.1619	140.2691	140.2457	141.8067	140.1813	142.5581	140.1156	141.8911	140.3073	142.5689	137.4753	139.4432	140.6731	140.4268	142.1500	140.3797	142.5033	140.3282	142.3574	140.4684	142.8687	**133.34**
C7	202.1768	207.1982	208.6196	209.9149	210.5679	209.7483	215.5392	209.5818	215.1279	210.0748	217.1331	206.1849	210.6989	211.9868	213.1284	213.7439	212.9665	218.9548	212.8080	217.5873	213.2885	219.5702	**195.87**
C8	62.2638	63.2785	63.9563	63.6403	64.5673	63.6254	64.9558	63.6092	64.7914	63.6554	65.6105	56.7269	58.2485	58.7010	59.1431	59.8693	59.0782	60.6326	59.0159	60.2657	59.2102	60.9139	**60.75**
C9	22.2545	22.4780	22.6788	22.6724	23.0493	22.6560	23.0235	22.6394	22.7994	22.6898	23.0038	19.5952	19.8548	19.8730	19.9815	20.2271	19.9737	20.2590	19.9655	20.1660	19.9902	20.6043	**16.39**
C8`	35.4261	36.0803	36.3153	36.4017	36.7065	36.3882	36.9314	36.3733	36.7947	36.4152	37.3166	30.7265	31.0292	31.3557	31.2646	31.5524	31.2617	31.6100	31.2549	31.6389	31.2646	31.7241	**32**
H2	8.8045	8.7552	8.7713	8.7178	8.7132	8.7209	8.7796	8.7237	8.6982	8.7149	8.6978	8.8202	8.6677	8.7159	8.5736	8.5991	8.5821	8.5540	8.5897	8.5893	8.5645	8.5574	**7.971**
H3	7.4131	7.5511	7.6385	7.5956	7.7147	7.5935	7.7298	7.5914	7.7207	7.5978	7.7443	7.4226	7.5575	7.6444	7.6018	7.7223	7.5997	7.7328	7.5974	7.7240	7.6039	7.7460	**7.22**
H5	7.2774	7.4679	7.5557	7.5537	7.6786	7.5490	7.6961	7.5442	7.6777	7.5583	7.7129	7.2894	7.4695	7.5577	7.5457	7.6732	7.5418	7.6791	7.5378	7.6674	7.5496	7.7001	**7.22**
H6	8.2021	8.4135	8.5069	8.5295	8.6573	8.5233	8.7307	8.5170	8.6684	8.5355	8.7254	8.0367	8.2260	8.3460	8.3104	8.4911	8.3074	8.4771	8.3036	8.4843	8.3126	8.5189	**7.971**
H8	4.1390	4.2501	4.2742	4.3513	4.4040	4.3440	4.4602	4.3368	4.4505	4.3585	4.4898	4.3255	4.4860	4.5491	4.5527	4.6724	4.5495	4.6828	4.5459	4.6757	4.5555	4.7093	**5.2**
H(9A-9C)	1.3232	1.3360	1.3236	1.3281	1.3024	1.3291	1.3388	1.3299	1.2880	1.3271	1.3094	1.3934	1.4128	1.4075	1.4242	1.4050	1.4244	1.4147	1.4244	1.4169	1.4237	1.4340	**1.611**
H(8`A-8`C)	2.4671	2.4104	2.3794	2.3869	2.3692	2.3875	2.3398	2.3882	2.3568	2.3865	2.3429	2.8470	2.6868	2.6544	2.6087	2.5717	2.6137	2.4834	2.6186	2.5074	2.6037	2.4553	**2.82**

[a] methyl protons shifts are averaged

[b] according to [10]

Table S10. Cont. VII

Nuclei	R											S											Exp. [b]
	X3LYP											X3LYP											
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.3564	139.8444	140.8482	140.1134	142.0566	140.0909	141.3658	140.0679	141.5227	140.1411	141.6467	137.9117	139.2562	139.9366	139.9579	141.5273	139.9149	141.3110	139.8710	141.2013	140.0058	141.3487	**130.99**
C2	139.9182	139.8474	140.4108	139.6953	140.1921	139.7116	140.6326	139.7238	140.5055	139.6831	140.6144	139.2169	139.3848	139.9238	139.3913	140.0004	139.3937	140.5425	139.3932	140.4245	139.3932	140.5430	**133.34**
C3	122.0092	122.6988	123.2345	122.9633	123.5748	122.9518	123.8529	122.9370	123.8097	122.9783	123.9078	122.1353	122.7433	123.2197	122.9818	123.5816	122.9719	123.7914	122.9587	123.7342	122.9949	123.8481	**117.55**
C4	176.1825	177.0882	177.7250	177.5818	178.2391	177.5544	178.8901	177.5242	178.7610	177.6114	179.0087	176.5499	177.1393	177.8065	177.4289	178.1522	177.4164	178.5567	177.4002	178.4628	177.4439	178.7115	**168.13**
C5	119.8141	121.1439	121.7439	121.8710	122.6356	121.8294	122.8875	121.7849	122.7972	121.9143	123.0321	119.9992	121.2093	121.7793	121.8153	122.5836	121.7831	122.7292	121.7474	122.6490	121.8494	122.8641	**117.55**
C6	136.1581	138.1629	139.2158	139.2637	140.6897	139.2042	141.2883	139.1404	140.9981	139.3229	141.6419	136.5146	138.5767	139.8645	139.6151	141.2627	139.5588	141.7748	139.4982	141.5895	139.6709	142.1688	**133.34**
C7	202.8571	207.9768	209.5518	210.7426	211.8371	210.5640	217.1792	210.3863	216.3022	210.9197	218.1127	208.1208	212.3136	213.4589	214.5395	215.3412	214.4092	220.0232	214.2763	218.9420	214.6672	220.5368	**195.87**
C8	65.0592	66.2153	66.9018	66.5407	67.5099	66.5316	67.8451	66.5179	67.6413	66.5516	68.6175	59.3212	61.3577	61.9949	62.3629	63.2348	62.3022	63.9246	62.2400	63.6812	62.4263	64.1714	**60.75**
C9	23.0316	23.3183	23.4327	23.5997	23.8343	23.5889	23.8506	23.5740	23.7548	23.6127	23.9870	19.5775	20.0461	20.2181	20.2904	20.5151	20.2799	20.6827	20.2663	20.6108	20.3042	21.0438	**16.39**
C8`	36.3944	37.1898	37.4326	37.5008	37.8523	37.4859	38.0604	37.4681	38.0401	37.5189	38.4847	31.9991	32.1508	32.4082	32.3228	32.5612	32.3139	32.6685	32.3014	32.6855	32.3346	32.7610	**32**
H2	8.6524	8.5918	8.6063	8.5511	8.5135	8.5549	8.5499	8.5579	8.5426	8.5473	8.5316	8.6901	8.5204	8.5632	8.4372	8.4423	8.4428	8.4297	8.4475	8.4451	8.4317	8.4405	**7.971**
H3	7.3213	7.4551	7.5439	7.5005	7.6121	7.4985	7.6290	7.4960	7.6209	7.5023	7.6416	7.3067	7.4391	7.5255	7.4863	7.6016	7.4841	7.6164	7.4812	7.6087	7.4884	7.6303	**7.22**
H5	7.1716	7.3592	7.4485	7.4464	7.5662	7.4416	7.5856	7.4362	7.5755	7.4510	7.6064	7.1634	7.3365	7.4251	7.4152	7.5364	7.4110	7.5463	7.4062	7.5365	7.4192	7.5665	**7.22**
H6	8.0809	8.2845	8.3663	8.3962	8.5098	8.3898	8.5716	8.3828	8.5557	8.4024	8.5971	7.8813	8.0490	8.1656	8.1364	8.2978	8.1318	8.3147	8.1265	8.3041	8.1406	8.3622	**7.971**
H8	4.3443	4.4331	4.4575	4.5383	4.5907	4.5308	4.6494	4.5230	4.6418	4.5456	4.6641	4.4903	4.6483	4.7010	4.7147	4.8269	4.7114	4.8459	4.7075	4.8333	4.7177	4.8776	**5.2**
H(9A-9C)	1.3227	1.3314	1.3179	1.3217	1.2790	1.3235	1.2915	1.3245	1.2806	1.3199	1.3039	1.3991	1.4351	1.4417	1.4560	1.4332	1.4550	1.4533	1.4534	1.4521	1.4569	1.4778	**1.611**
H(8`A-8`C)	2.5170	2.4557	2.4302	2.4400	2.4194	2.4409	2.4037	2.4412	2.4048	2.4393	2.3899	2.9813	2.8071	2.7639	2.7278	2.6788	2.7332	2.5951	2.7379	2.6158	2.7225	2.5651	**2.82**

[a] methyl protons shifts are averaged
[b] according to [10]

Table S11. Theoretical chemical shifts (in ppm) of *(R,S)*-flephedrone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S										Exp. [b]
	B3LYP											B3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.3516	139.8992	140.9781	140.1863	142.0735	140.1611	141.5120	140.1358	141.5012	140.2082	141.7819	137.8738	139.3186	139.9816	139.9577	141.5554	139.9093	141.4183	139.8637	141.2810	140.0057	141.4292	**129.02**
C2	139.7181	139.6929	140.2565	139.4633	139.9708	139.4799	140.4199	139.4943	140.2834	139.4440	140.3925	139.0099	139.2247	139.7699	139.1806	139.8028	139.1780	140.3740	139.1755	140.2362	139.1821	140.3704	**132.19**
C3	121.9147	122.6511	123.2036	122.8744	123.4797	122.8576	123.7880	122.8405	123.7263	122.8887	123.8478	122.0546	122.6999	123.1853	122.8846	123.4913	122.8701	123.7328	122.8554	123.6526	122.8966	123.7867	**116.16**
C4	176.1996	177.1548	177.8016	177.6113	178.2556	177.5774	178.9142	177.5440	178.7922	177.6426	179.0429	176.5723	177.1853	177.8667	177.4190	178.1469	177.4023	178.5696	177.3850	178.4546	177.4322	178.7245	**166.89**
C5	119.7381	121.1100	121.7159	121.7876	122.5392	121.7417	122.8148	121.6959	122.7064	121.8299	122.9605	119.9339	121.1749	121.7562	121.7216	122.4902	121.6855	122.6663	121.6489	122.5622	121.7540	122.7986	**116.16**
C6	135.8982	137.9272	138.9534	138.9372	140.4067	138.8712	141.0202	138.8048	140.7434	138.9983	141.3636	136.2778	138.3528	139.6434	139.3323	140.9568	139.2716	141.4709	139.2095	141.2669	139.3872	141.8771	**132.19**
C7	202.8768	208.0691	209.7045	210.9565	211.8939	210.7561	217.3250	210.5621	216.3636	211.1520	218.3042	208.1087	212.3579	213.4837	214.5278	215.3474	214.3946	220.1153	214.2618	218.9963	214.6532	220.5944	**196.22**
C8	65.2601	66.4393	67.0844	66.6651	67.6873	66.6448	68.1168	66.6260	67.8105	66.6832	68.8556	59.4742	61.6544	62.2820	62.6180	63.4923	62.5505	64.2487	62.4848	63.9791	62.6825	64.4890	**59.75**
C9	22.9937	23.3369	23.4371	23.5103	23.7870	23.5040	23.8454	23.4947	23.7278	23.5117	23.9610	19.5432	20.0549	20.2357	20.2537	20.4684	20.2366	20.6702	20.2197	20.5736	20.2683	21.0311	**15.44**
C8`	36.5076	37.3387	37.5483	37.6307	37.9535	37.5944	38.1848	37.5637	38.1616	37.6692	38.6153	32.1915	32.3577	32.6229	32.4742	32.7092	32.4611	32.8316	32.4474	32.8288	32.4845	32.9175	**31.11**
H2	8.6288	8.5708	8.5739	8.5193	8.4862	8.5229	8.5099	8.5264	8.5151	8.5156	8.4958	8.6701	8.4976	8.5384	8.4115	8.4156	8.4168	8.3988	8.4218	8.4120	8.4060	8.4143	**7.97**
H3	7.3119	7.4474	7.5313	7.4874	7.6000	7.4852	7.6152	7.4829	7.6051	7.4891	7.6305	7.2978	7.4323	7.5140	7.4748	7.5907	7.4723	7.6048	7.4697	7.5943	7.4770	7.6211	**7.22**
H5	7.1614	7.3510	7.4352	7.4344	7.5536	7.4291	7.5704	7.4238	7.5589	7.4393	7.5939	7.1540	7.3281	7.4120	7.4019	7.5234	7.3974	7.5322	7.3928	7.5197	7.4059	7.5549	**7.22**
H6	8.0695	8.2736	8.3471	8.3829	8.4942	8.3751	8.5470	8.3677	8.5388	8.3904	8.5777	7.8720	8.0370	8.1480	8.1191	8.2781	8.2113	8.2908	8.1093	8.2781	8.1233	8.3419	**7.97**
H8	4.3623	4.4552	4.4783	4.5600	4.6044	4.5533	4.6526	4.5464	4.6504	4.5660	4.6741	4.4999	4.6578	4.7050	4.7188	4.8309	4.7153	4.8477	4.7118	4.8326	4.7217	4.8820	**4.99**
H(9A-9C)	1.3154	1.3242	1.3019	1.3025	1.2691	1.3041	1.2806	1.3055	1.2685	1.3007	1.2933	1.3888	1.4276	1.4302	1.4455	1.4215	1.4441	1.4397	1.4302	1.4465	1.4466	1.4683	**1.51**
H(8`A-8`C)	2.5071	2.4491	2.4216	2.4281	2.4102	2.4290	2.3990	2.4298	2.3931	2.4269	2.3861	2.9770	2.8044	2.7564	2.7204	2.6721	2.7257	2.5872	2.7307	2.6042	2.7151	2.5595	**2.71**
Nuclei	B3P86											B3P86										
C1	136.8453	137.2808	138.3582	137.5043	139.4519	137.5074	138.8537	137.4898	139.1351	137.5460	139.1283	135.6233	136.9063	137.5597	137.4853	138.9540	137.4549	138.8749	137.4076	138.7415	137.5634	138.9677	**129.02**
C2	138.7919	138.7416	139.3998	138.5747	139.1636	138.6075	139.5971	138.6182	139.5645	138.5873	139.5816	138.1598	138.3322	138.9376	138.3113	138.9809	138.3306	139.5077	138.3287	139.4734	138.3375	139.5260	**132.19**
C3	121.1158	121.8832	122.5099	122.1552	122.8745	122.1613	123.1693	122.1453	123.2080	122.1932	123.2475	121.2077	121.9036	122.4956	122.1573	122.8618	122.1638	123.0956	122.1483	123.1217	122.1950	123.1750	**116.16**
C4	173.6985	174.6092	175.2829	175.0662	175.7535	175.0598	176.4063	175.0315	176.3576	175.1159	176.5491	173.9907	174.6001	175.3439	174.8861	175.6462	174.8935	176.0480	174.8781	176.0672	174.9218	176.2106	**166.89**
C5	118.9511	120.3570	121.0389	121.0865	121.9545	121.0629	122.2291	121.0175	122.2236	121.1526	122.3983	119.0968	120.3750	121.0516	121.0069	121.8780	120.9911	122.0417	120.9530	122.0531	121.0653	122.1965	**116.16**
C6	134.9391	136.9571	138.0470	138.0317	139.4694	137.9871	140.0383	137.9202	139.8454	138.1179	140.4254	135.2870	137.3568	138.6630	138.3561	140.0839	138.3212	140.5742	138.2627	140.5163	138.4312	140.9668	**132.19**
C7	200.9937	205.8309	207.3690	208.3757	209.4937	208.2408	214.5962	208.0849	213.8337	208.5478	215.4998	205.5040	209.6504	210.9178	211.8502	212.6202	211.7370	217.2310	211.6033	216.1910	212.0035	217.7281	**196.22**
C8	63.6796	64.8464	65.6285	65.2068	66.1771	65.2071	66.5812	65.1854	66.4957	65.2505	67.3827	58.1084	59.9428	60.4781	60.8007	61.6333	60.7568	62.3872	60.6942	62.1777	60.8896	62.6693	**59.75**
C9	22.8065	23.0897	23.3077	23.3623	23.6359	23.3647	23.6593	23.3452	23.6707	23.4035	23.8216	19.4663	20.0187	20.1559	20.2089	20.4941	20.2153	20.6857	20.2003	20.7001	20.2472	21.1119	**15.44**
C8`	35.9286	36.7158	37.0084	37.0027	37.3475	37.0082	37.5596	36.9918	37.6189	37.0414	38.0311	31.3622	31.5731	31.9325	31.7646	32.0364	31.7748	32.1533	31.7622	32.2999	31.7969	32.2578	**31.11**
H2	8.6937	8.6392	8.6481	8.5947	8.5586	8.5992	8.5883	8.6018	8.5814	8.5915	8.5744	8.7028	8.5480	8.5959	8.4713	8.4868	8.4787	8.4611	8.4838	8.4913	8.4649	8.4716	**7.97**
H3	7.3323	7.4749	7.5633	7.5186	7.6361	7.5176	7.6523	7.5147	7.6476	7.5207	7.6690	7.3188	7.4600	7.5477	7.5057	7.6274	7.5044	7.6414	7.5013	7.6367	7.5080	7.6590	**7.22**
H5	7.1767	7.3724	7.4616	7.4573	7.5836	7.4536	7.6013	7.4480	7.5944	7.4620	7.6265	7.1655	7.3489	7.4382	7.4270	7.5553	7.4237	7.5640	7.4186	7.5573	7.4312	7.5880	**7.22**
H6	8.1523	8.3571	8.4270	8.4597	8.5681	8.4550	8.6211	8.4484	8.6073	8.4654	8.6536	7.9340	8.1076	8.2276	8.1948	8.3652	8.1917	8.3755	8.1865	8.3750	8.1986	8.4257	**7.97**
H8	4.3930	4.4836	4.4927	4.5762	4.6265	4.5711	4.6819	4.5642	4.6796	4.5824	4.7038	4.5540	4.6976	4.7569	4.7623	4.8783	4.7605	4.8928	4.7566	4.8883	4.7650	4.9288	**4.99**
H(9A-9C)	1.3335	1.3438	1.3286	1.3321	1.2867	1.3343	1.2965	1.3346	1.2886	1.3313	1.3143	1.4092	1.4428	1.4421	1.4554	1.4353	1.4561	1.4505	1.4549	1.4566	1.4559	1.4796	**1.51**
H(8`A-8`C)	2.4876	2.4212	2.3951	2.4005	2.3811	2.4023	2.3602	2.4024	2.3671	2.4001	2.3503	2.9176	2.7485	2.7146	2.6728	2.6287	2.6800	2.5349	2.6851	2.5651	2.6670	2.5072	**2.71**
Nuclei	B3PW91											B3PW91										
C1	137.0994	137.5782	138.7234	137.8703	140.2084	137.8485	139.3905	137.8187	139.3095	137.8939	139.6388	135.8270	137.2800	137.7781	137.8580	139.3488	137.8089	139.3951	137.7573	139.1374	137.9141	139.4828	**129.02**
C2	138.8604	138.8385	139.3967	138.6503	139.5459	138.6706	139.6266	138.6815	139.5161	138.6320	139.6248	138.2843	138.4871	139.0226	138.4452	139.1209	138.4505	139.6147	138.4477	139.5068	138.4432	139.6376	**132.19**
C3	121.2185	122.0069	122.5742	122.2708	123.2963	122.2610	123.2495	122.2421	123.2072	122.2821	123.3409	121.3071	122.0247	122.5329	122.2639	122.9651	122.2553	123.1906	122.2380	123.1214	122.2739	123.2752	**116.16**
C4	173.7409	174.6858	175.2871	175.1369	176.1105	175.1138	176.3924	175.0819	176.3209	175.1612	176.5562	174.0199	174.6397	175.3121	174.9084	175.6627	174.9018	176.0329	174.8849	175.9623	174.9153	176.2007	**166.89**
C5	119.0599	120.4861	121.1030	121.2065	122.3683	121.1668	122.2995	121.1183	122.2138	121.2461	122.4777	119.2098	120.5084	121.1087	121.1148	121.9791	121.0849	122.1342	121.0458	122.0478	121.1449	122.2957	**116.16**
C6	134.8881	136.9286	137.8816	137.9622	139.7104	137.9061	139.9572	137.8415	139.7281	138.0174	140.3326	135.2770	137.3211	138.5843	138.3076	139.9907	138.2583	140.3962	138.1982	140.2701	138.3538	140.7941	**132.19**
C7	201.1247	206.1066	207.7353	208.8082	210.2420	208.6327	215.1374	208.4510	214.2009	208.9795	216.0833	205.6165	209.9651	211.0502	212.1644	212.9527	212.0348	217.7726	211.8977	216.5723	212.2928	218.2699	**196.22**
C8	63.4567	64.6178	65.2257	64.9342	66.2583	64.9202	66.4879	64.8987	66.1020	64.9510	67.2318	58.0320	59.9926	60.4452	60.8767	61.6836	60.8128	62.5182	60.7445	62.2018	60.9444	62.8000	**59.75**
C9	22.5160	22.8553	22.9353	23.0789	23.6687	23.0753	23.3953	23.0617	23.2786	23.0832	23.5418	19.1832	19.7035	19.7883	19.8973	20.1279	19.8867	20.3038	19.8683	20.2280	19.9102	20.7016	**15.44**
C8`	35.8834	36.7085	36.8598	36.9828	37.6339	36.9657	37.5129	36.9420	37.5231	37.0038	37.9753	31.4292	31.6510	31.9335	31.8297	32.1026	31.8260	32.1558	31.8123	32.2185	31.8333	32.2536	**31.11**
H2	8.6633	8.6108	8.6056	8.5605	8.5329	8.5652	8.5339	8.5693	8.5526	8.5562	8.5242	8.6835	8.5130	8.5718	8.4375	8.4524	8.4445	8.4188	8.4505	8.4482	8.4303	8.4283	**7.97**
H3	7.3301	7.4703	7.5577	7.5143	7.6458	7.5126	7.6483	7.5105	7.6406	7.5160	7.6634	7.3189	7.4577	7.5443	7.5040	7.6238	7.5020	7.6404	7.4996	7.6317	7.5060	7.6558	**7.22**
H5	7.1771	7.3713	7.4596	7.4576	7.5958	7.4530	7.5980	7.4480	7.5902	7.4622	7.6214	7.1690	7.3494	7.4382	7.4277	7.5538	7.4237	7.5651	7.4194	7.5542	7.4316	7.5870	**7.22**
H6	8.1341	8.3392	8.4057	8.4426	8.5635	8.4366	8.5897	8.4305	8.5951	8.4485	8.6240	7.9194	8.0892	8.2103	8.1769	8.3421	8.1732	8.3457	8.1688	8.3441	8.1801	8.3934	**7.97**
H8	4.3741	4.4705	4.4922	4.5694	4.6265	4.5633	4.6458	4.5568	4.6625	4.5752	4.6720	4.5270	4.6702	4.7258	4.7346	4.8501	4.7322	4.8642	4.7292	4.8566	4.7367	4.8976	**4.99**
H(9A-9C)	1.2980	1.3052	1.2789	1.2881	1.2601	1.2903	1.2615	1.2922	1.2492	1.2862	1.2747	1.3734	1.4034	1.4070	1.4206	1.3953	1.4203	1.4103	1.4196	1.4138	1.4210	1.4367	**1.51**
H(8`A-8`C)	2.4555	2.3914	2.3685	2.3743	2.3708	2.3754	2.3485	2.3764	2.3407	2.3732	2.3328	2.8889	2.7195	2.6844	2.6446	2.6004	2.6510	2.5113	2.6569	2.5341	2.6383	2.4811	**2.71**
Nuclei	B98											B98										
C1	137.8984	138.3641	139.2698	138.5615	140.4825	138.5589	139.6880	138.5551	139.9714	138.5675	140.0693	136.6672	137.9623	138.5980	138.5797	140.1392	138.5482	140.0261	138.5178	139.8988	138.6168	140.0992	**129.02**
C2	138.5254	138.4721	139.0519	138.3240	138.8948	138.3503	139.3548	138.3736	139.2402	138.3008	139.3473	137.9447	138.0861	138.6429	138.0628	138.7300	138.0773	139.2568	138.0902	139.1509	138.0518	139.2683	**132.19**
C3	120.9751	121.6883	122.2401	121.9412	122.6168	121.9423	122.8875	121.9406	122.8295	121.9422	122.9429	121.0500	121.6961	122.2005	121.9352	122.6051	121.9366	122.8272	121.9354	122.7659	121.9361	122.8940	**116.16**
C4	173.5548	174.4326	175.0664	174.8850	175.5697	174.8724	176.2406	174.8571	176.0696	174.8994	176.3345	173.8262	174.4272	175.1004	174.7024	175.4540	174.7034	175.8475	174.7008	175.7561	174.7028	176.0007	**166.89**
C5	118.7946	120.1408	120.7556	120.8501	121.6768	120.8218	121.9460	120.7906	121.8434	120.8797	122.0849	118.9548	120.1808	120.7785	120.7832	121.6150	120.7632	121.7668	120.7403	121.6817	120.8040	121.9090	**116.16**
C6	134.9458	136.9033	137.9770	137.9779	139.4196	137.9297	140.0378	137.8779	139.7250	138.0256	140.3768	135.2851	137.2480	138.5012	138.2327	139.8890	138.1917	140.3423	138.1470	140.1749	138.2722	140.7184	**132.19**
C7	199.5271	204.5615	206.0295	207.1995	208.2386	207.0479	213.5136	206.8943	212.6014	207.3482	214.4291	204.1599	208.4637	209.6427	210.7144	211.5176	210.5930	216.3722	210.4697	215.2290	210.8323	216.8957	**196.22**
C8	65.0962	66.2575	66.8997	66.5776	67.5549	66.5763	67.8574	66.5723	67.7776	66.5806	68.7079	59.7427	61.6256	62.1747	62.5454	63.3980	62.4979	64.1348	62.4503	63.8905	62.5954	64.3856	**59.75**
C9	23.2897	23.5779	23.6929	23.8388	24.0941	23.8397	24.1215	23.8371	24.0489	23.8399	24.2881	20.0303	20.4587	20.5633	20.6605	20.8945	20.6623	21.0556	20.6621	20.9805	20.6615	21.4185	**15.44**
C8`	36.7092	37.4629	37.6740	37.7309	38.1053	37.7287	38.3351	37.7243	38.2965	37.7357	38.7417	32.2204	32.4032	32.6737	32.5780	32.8420	32.5807	32.9732	32.5806	33.0077	32.5770	33.0565	**31.11**
H2	8.6652	8.6018	8.6259	8.5647	8.5366	8.5677	8.5885	8.5705	8.5669	8.5621	8.5601	8.6821	8.5181	8.5678	8.4391	8.4515	8.4446	8.4365	8.4498	8.4543	8.4338	8.4469	**7.97**
H3	7.3240	7.4617	7.5525	7.5069	7.6251	7.5048	7.6424	7.5026	7.6335	7.5092	7.6562	7.3088	7.4478	7.5364	7.4945	7.6157	7.4921	7.6318	7.4897	7.6238	7.4970	7.6471	**7.22**
H5	7.1716	7.3643	7.4556	7.4510	7.5764	7.4460	7.5983	7.4411	7.5859	7.4560	7.6179	7.1649	7.3464	7.4371	7.4256	7.5523	7.4212	7.5629	7.4169	7.5523	7.4299	7.5837	**7.22**
H6	8.0929	8.2967	8.3821	8.4075	8.5267	8.4008	8.6016	8.3943	8.5719	8.4141	8.6200	7.8961	8.0681	8.1863	8.1586	8.3256	8.1538	8.3364	8.1488	8.3271	8.1631	8.3835	**7.97**
H8	4.3470	4.4366	4.4606	4.5354	4.5891	4.5287	4.6555	4.5220	4.6334	4.5423	4.6625	4.4951	4.6493	4.7037	4.7151	4.8293	4.7118	4.8454	4.7085	4.8323	4.7182	4.8756	**4.99**
H(9A-9C)	1.3189	1.3268	1.3143	1.3162	1.2740	1.3175	1.2894	1.3187	1.2788	1.3151	1.3029	1.3937	1.4261	1.4275	1.4419	1.4166	1.4413	1.4301	1.4407	1.4303	1.4425	1.4532	**1.51**
H(8`A-8`C)	2.4802	2.4260	2.3972	2.4073	2.3842	2.4082	2.3651	2.4093	2.3720	2.4067	2.3565	2.9208	2.7533	2.7171	2.6803	2.6349	2.6856	2.5498	2.6907	2.5670	2.6754	2.5194	**2.71**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S11. Cont. I

Nuclei	R											S										Exp. [b]
	B971											B971										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.5124	137.9668	138.8036	138.1617	140.0037	138.1528	139.1730	138.1442	139.5653	138.1768	139.6476	136.2962	137.5659	138.2070	138.1911	139.7146	138.1505	139.5849	138.1134	139.4699	138.2405	139.6733	**129.02**
C2	138.2273	138.1790	138.7520	138.0411	138.6151	138.0588	139.0874	138.0759	138.9703	138.0298	139.0743	137.6507	137.7943	138.3494	137.7788	138.4352	137.7852	138.9549	137.7921	138.8493	137.7793	138.9688	**132.19**
C3	120.7723	121.4948	122.0366	121.7575	122.4239	121.7508	122.6953	121.7432	122.6290	121.7695	122.7532	120.8439	121.4989	122.0013	121.7481	122.4060	121.7414	122.6248	121.7343	122.5637	121.7602	122.6979	**116.16**
C4	173.4520	174.3378	174.9730	174.7959	175.4831	174.7758	176.1541	174.7552	175.9535	174.8209	176.2409	173.7091	174.3304	175.0011	174.6204	175.3683	174.6132	175.7597	174.6046	175.6659	174.6323	175.9170	**166.89**
C5	118.5912	119.9438	120.5513	120.6619	121.4796	120.6255	121.7575	120.5889	121.6419	120.7023	121.8945	118.7577	119.9871	120.5816	120.5974	121.4204	120.5694	121.5676	120.5405	121.4822	120.6294	121.7173	**116.16**
C6	134.7050	136.6708	137.7813	137.7564	139.2253	137.6992	139.8111	137.6410	139.4847	137.8168	140.1424	135.0285	137.0109	138.2571	138.0065	139.6769	137.9579	140.1333	137.9074	139.9591	138.0571	140.5087	**132.19**
C7	199.4123	204.3866	205.8037	206.9774	207.9980	206.8235	213.1394	206.6697	212.2541	207.1300	214.1117	204.0187	208.2806	209.4897	210.5322	211.3305	210.4028	216.0716	210.2738	214.9613	210.6620	216.6144	**196.22**
C8	65.0628	66.2181	66.8745	66.5493	67.4912	66.5398	67.7569	66.5294	67.7680	66.5644	68.6439	59.7053	61.5405	62.0853	62.4460	63.2954	62.3913	63.9952	62.3385	63.7609	62.5067	64.2505	**59.75**
C9	23.2952	23.5805	23.7317	23.8547	24.1127	23.8461	24.1179	23.8365	24.0691	23.8689	24.2944	20.0444	20.4947	20.5876	20.7006	20.9390	20.6951	21.1020	20.6896	21.0266	20.7123	21.4780	**15.44**
C8`	36.7170	37.4689	37.6835	37.7337	38.0702	37.7257	38.3145	37.7173	38.2603	37.7475	38.7194	32.1504	32.3460	32.6128	32.5305	32.7822	32.5259	32.9103	32.5202	32.9431	32.5401	32.9962	**31.11**
H2	8.6629	8.6020	8.6311	8.5654	8.5437	8.5681	8.6026	8.5708	8.5678	8.5633	8.5647	8.6781	8.5197	8.5677	8.4422	8.4548	8.4475	8.4418	8.4527	8.4583	8.4370	8.4509	**7.97**
H3	7.3215	7.4590	7.5493	7.5044	7.6225	7.5021	7.6392	7.4997	7.6299	7.5070	7.6527	7.3076	7.4456	7.5341	7.4931	7.6131	7.4905	7.6286	7.4879	7.6208	7.4959	7.6437	**7.22**
H5	7.1696	7.3613	7.4527	7.4481	7.5728	7.4430	7.5957	7.4379	7.5815	7.4533	7.6142	7.1650	7.3449	7.4351	7.4237	7.5495	7.4192	7.5594	7.4147	7.5489	7.4283	7.5805	**7.22**
H6	8.0974	8.2998	8.3897	8.4087	8.5283	8.4021	8.6053	8.3956	8.5653	8.4153	8.6195	7.8972	8.0707	8.1892	8.1631	8.3306	8.1581	8.3421	8.1530	8.3320	8.1679	8.3885	**7.97**
H8	4.3445	4.4318	4.4558	4.5292	4.5852	4.5223	4.6544	4.5157	4.6229	4.5361	4.6585	4.4978	4.6489	4.7036	4.7168	4.8297	4.7133	4.8452	4.7097	4.8315	4.7203	4.8758	**4.99**
H(9A-9C)	1.3191	1.3280	1.3197	1.3196	1.2780	1.3205	1.2937	1.3214	1.2832	1.3191	1.3053	1.3960	1.4276	1.4283	1.4433	1.4195	1.4425	1.4331	1.4418	1.4326	1.4442	1.4560	**1.51**
H(8`A-8`C)	2.4778	2.4208	2.3902	2.4035	2.3793	2.4041	2.3533	2.4048	2.3662	2.4033	2.3481	2.9110	2.7452	2.7096	2.6744	2.6284	2.6794	2.5438	2.6843	2.5610	2.6698	2.5128	**2.71**
Nuclei	**B972**											**B972**										
C1	134.4302	134.9580	135.9573	135.2517	137.1882	135.2339	136.9092	135.2172	137.2291	135.2642	136.9986	133.0960	134.5569	135.0556	135.2214	136.6788	135.1632	136.7562	135.1090	136.5422	135.2805	136.8545	**129.02**
C2	136.2385	136.1466	136.7094	135.9825	136.5017	135.9974	136.8781	136.0094	136.7762	135.9648	136.9004	135.6839	135.8309	136.3876	135.8469	136.4661	135.8466	136.9148	135.8443	136.8312	135.8431	136.9435	**132.19**
C3	118.6420	119.3619	119.9304	119.6913	120.3271	119.6734	120.6091	119.6533	120.5621	119.7042	120.6885	118.7138	119.3622	119.8746	119.6667	120.3028	119.6505	120.5119	119.6318	120.4478	119.6777	120.5982	**116.16**
C4	170.4080	171.2888	171.9012	171.8240	172.3935	171.7908	172.9800	171.7559	172.8201	171.8517	173.1417	170.6771	171.2152	171.8947	171.5417	172.2306	171.5278	172.5783	171.5099	172.5046	171.5489	172.7454	**166.89**
C5	116.5455	117.8870	118.4963	118.6438	119.4131	118.5990	119.6446	118.5521	119.5386	118.6819	119.8150	116.6811	117.8807	118.4867	118.5356	119.3203	118.4989	119.4656	118.4592	119.3807	118.5657	119.6278	**116.16**
C6	132.2984	134.1683	135.1909	135.2810	136.6319	135.2152	137.0709	135.1451	136.7199	135.3380	137.5017	132.7192	134.6132	135.8785	135.6223	137.1863	135.5695	137.5344	135.5120	137.4030	135.6656	137.9182	**132.19**
C7	197.1472	202.1820	203.6394	205.0747	205.9500	204.8855	211.4809	204.7016	210.7109	205.2515	212.1626	201.5167	205.7889	206.8296	208.0334	208.7686	207.8942	213.5796	207.7543	212.4081	208.1644	214.0847	**196.22**
C8	62.2129	63.1640	63.7653	63.5253	64.4519	63.5132	65.0374	63.4956	64.9409	63.5298	65.7131	56.9800	58.9172	59.3838	59.8622	60.6095	59.7928	61.4484	59.7250	61.1550	59.9290	61.7202	**59.75**
C9	22.2017	22.5014	22.6308	22.6974	22.9802	22.6894	22.9728	22.6772	22.8720	22.7010	23.1432	18.9615	19.3718	19.4861	19.6193	19.7902	19.6032	19.9459	19.5854	19.8717	19.6315	20.3049	**15.44**
C8`	35.6349	36.3454	36.5312	36.8429	37.0375	36.8098	37.2438	36.7749	37.2215	36.8693	37.6484	31.3495	31.4924	31.7924	31.7285	31.9630	31.7188	31.9659	31.7053	32.0216	31.7314	32.0500	**31.11**
H2	8.6537	8.5910	8.6014	8.5457	8.5058	8.5490	8.4992	8.5518	8.4749	8.5424	8.5039	8.6825	8.4992	8.5620	8.4234	8.4354	8.4301	8.3959	8.4360	8.4226	8.4161	8.4046	**7.97**
H3	7.3227	7.4597	7.5484	7.5068	7.6209	7.5045	7.6375	7.5020	7.6284	7.5088	7.6533	7.3120	7.4483	7.5346	7.4976	7.6140	7.4951	7.6296	7.4923	7.6214	7.4999	7.6455	**7.22**
H5	7.1739	7.3666	7.4552	7.4573	7.5754	7.4520	7.5903	7.4465	7.5774	7.4620	7.6138	7.1665	7.3420	7.4301	7.4225	7.5446	7.4180	7.5559	7.4132	7.5449	7.4267	7.5779	**7.22**
H6	8.1158	8.3161	8.3945	8.4358	8.5373	8.4282	8.5663	8.4204	8.5382	8.4429	8.6045	7.9070	8.0727	8.1924	8.1605	8.3194	8.1565	8.3186	8.1518	8.3151	8.1637	8.3642	**7.97**
H8	4.3399	4.4508	4.4730	4.5472	4.5919	4.5405	4.6226	4.5339	4.6079	4.5536	4.6488	4.4883	4.6298	4.6848	4.6954	4.8083	4.6924	4.8202	4.6889	4.8127	4.6977	4.8518	**4.99**
H(9A-9C)	1.2779	1.2737	1.2581	1.2603	1.2187	1.2618	1.2249	1.2628	1.2101	1.2586	1.2452	1.3585	1.3871	1.3915	1.4080	1.3784	1.4071	1.3926	1.4058	1.3948	1.4087	1.4173	**1.51**
H(8`A-8`C)	2.4444	2.3879	2.3637	2.3740	2.3543	2.3748	2.3536	2.3753	2.3559	2.3732	2.3366	2.8829	2.7146	2.6793	2.6431	2.5976	2.6486	2.5129	2.6536	2.5335	2.6373	2.4818	**2.71**
Nuclei	**BHandH**											**BHandH**										
C1	138.2231	138.5552	139.4722	138.6613	140.1957	138.6447	139.2014	138.6466	139.2910	138.6472	139.3414	137.3260	138.1227	139.0514	138.6686	139.4127	138.6143	139.9113	138.5817	139.6959	138.6934	140.0677	**129.02**
C2	143.5201	143.3955	144.0049	143.2268	143.8191	143.2277	144.3374	143.2468	144.2139	143.1959	144.3719	143.1561	143.1628	143.7749	143.0888	143.8329	143.0819	144.2258	143.0940	144.0867	143.0659	144.2500	**132.19**
C3	123.7766	124.4896	125.0912	124.7508	125.4195	124.7262	125.6101	124.7198	125.5593	124.7437	125.6833	123.8317	124.5005	125.1213	124.7551	125.4992	124.7302	125.6175	124.7238	125.5792	124.7487	125.7026	**116.16**
C4	174.6910	175.5022	176.1372	175.9474	176.5413	175.9096	177.2138	175.8903	177.0668	175.9534	177.3817	174.9086	175.5511	176.2159	175.8630	176.6071	175.8357	176.9768	175.8261	176.9107	175.8585	177.1498	**166.89**
C5	121.3254	122.7876	123.4824	123.5575	124.4251	123.5004	124.6212	123.4617	124.5293	123.5816	124.7930	121.4351	122.8143	123.5066	123.5206	124.2647	123.4688	124.5249	123.4348	124.4609	123.5397	124.7001	**116.16**
C6	139.9383	142.0591	143.3061	143.2147	144.9304	143.1340	145.6585	143.0715	145.4144	143.2611	146.1074	140.2023	142.4966	143.7026	143.6179	144.3620	143.5430	145.9734	143.4853	145.7743	143.6576	146.3435	**132.19**
C7	202.9300	207.7859	209.1882	210.2924	210.9441	210.1306	215.8168	209.9874	214.6983	210.4156	216.6335	207.3621	211.4788	213.0278	213.6769	214.4210	213.5328	219.1023	213.4077	218.0494	213.7841	219.7557	**196.22**
C8	59.9494	61.2143	61.9067	61.6436	62.6312	61.6098	63.0978	61.5942	62.9356	61.6453	63.8442	54.0631	55.4214	55.9382	56.1974	56.9415	56.1327	57.6583	56.0882	57.3239	56.2306	57.9608	**59.75**
C9	22.4684	22.7173	23.0362	22.9961	23.4920	22.9658	23.4131	22.9537	23.4079	22.9951	23.6098	19.0747	19.5603	19.6330	19.8271	20.5712	19.7976	20.2453	19.7870	20.1575	19.8256	20.6529	**15.44**
C8`	33.7500	34.5612	34.8118	34.8998	35.2711	34.8687	35.5037	34.8562	35.4510	34.8996	35.9918	28.6454	29.0946	29.4036	29.3316	30.0757	29.3102	29.7782	29.3056	29.7931	29.3204	29.9429	**31.11**
H2	8.9875	8.9200	8.9348	8.8802	8.8770	8.8834	8.9222	8.8858	8.9249	8.8781	8.9222	8.9840	8.8580	8.8706	8.7732	8.6920	8.7803	8.7507	8.7862	8.7811	8.7672	8.7533	**7.97**
H3	7.4553	7.5997	7.6892	7.6466	7.7674	7.6451	7.7842	7.6427	7.7763	7.6491	7.8000	7.4516	7.5922	7.6830	7.6387	7.5575	7.6372	7.7745	7.6347	7.7677	7.6412	7.7910	**7.22**
H5	7.3003	7.5022	7.5933	7.5917	7.7206	7.5873	7.7378	7.5822	7.7268	7.5967	7.7629	7.2950	7.4886	7.5794	7.5727	7.4915	7.5687	7.7122	7.5639	7.7021	7.5774	7.7361	**7.22**
H6	8.3317	8.5445	8.6361	8.6585	8.7941	8.6524	8.8645	8.6454	8.8495	8.6654	8.9071	8.1293	8.3337	8.4417	8.4287	8.3475	8.4246	8.6263	8.4194	8.6221	8.4334	8.6718	**7.97**
H8	4.1505	4.2528	4.2749	4.3463	4.3866	4.3407	4.4438	4.3343	4.3739	4.3528	4.4693	4.4049	4.5696	4.6414	4.6481	4.5669	4.6447	4.7936	4.6404	4.7922	4.6522	4.8291	**4.99**
H(9A-9C)	1.3947	1.4083	1.3944	1.4043	1.3835	1.4056	1.4087	1.4060	1.4066	1.4041	1.4308	1.4777	1.5048	1.4783	1.5114	1.4301	1.5120	1.4963	1.5117	1.4978	1.5117	1.5179	**1.51**
H(8`A-8`C)	2.5482	2.4741	2.4402	2.4443	2.4243	2.4467	2.3801	2.4483	2.3790	2.4430	2.3667	2.9170	2.7545	2.7130	2.6709	2.5897	2.6772	2.5211	2.6825	2.5633	2.6659	2.4973	**2.71**
Nuclei	**BHandHLYP**											**BHandHLYP**										
C1	138.8640	139.2644	139.9330	139.4014	141.4115	139.3890	140.3239	139.3799	140.8073	139.4140	140.7808	137.7359	138.7863	139.5663	139.4872	141.0279	139.4436	140.6370	139.4057	140.4914	139.5319	140.6845	**129.02**
C2	142.1451	142.0033	142.5518	141.8479	142.3133	141.8593	142.8334	141.8728	142.6946	141.8367	142.8238	141.6846	141.6776	142.2130	141.6154	142.1662	141.6189	142.6674	141.6254	142.5678	141.6119	142.7010	**132.19**
C3	122.5311	123.1246	123.6134	123.3344	123.9644	123.3231	124.1502	123.3143	124.1344	123.3446	124.2197	122.6170	123.1643	123.6329	123.3811	123.9687	123.3691	124.1171	123.3594	124.0780	123.3922	124.1810	**116.16**
C4	174.4859	175.2386	175.8387	175.6759	176.2231	175.6490	176.9757	175.6248	176.7716	175.7009	177.0601	174.7783	175.2638	175.8588	175.5025	176.1211	175.4893	176.5698	175.4775	176.5010	175.5141	176.7410	**166.89**
C5	120.1712	121.4535	122.0189	122.1435	122.9398	122.1013	123.1049	122.0616	123.0479	122.1835	123.2751	120.2936	121.5123	122.0694	122.1337	122.8970	122.0972	123.0006	122.0628	122.9395	122.1680	123.1441	**116.16**
C6	138.1510	140.1493	141.3422	141.2896	142.5504	141.2223	143.2999	141.1564	142.9195	141.3529	143.5841	138.4674	140.5298	141.7475	141.5098	143.1000	141.4526	143.6578	141.3968	143.5207	141.5620	144.0715	**132.19**
C7	201.2543	206.5546	207.7752	209.3182	210.2498	209.1454	216.0604	208.9760	215.0849	209.4828	217.0651	206.1611	210.4578	211.6283	212.8433	213.4066	212.7018	218.6263	212.5625	217.3826	212.9773	219.2046	**196.22**
C8	60.7965	61.8811	62.5000	62.2233	63.0588	62.2069	63.2656	62.1924	63.2636	62.2383	64.1041	55.4804	57.1821	57.8021	58.1054	58.8956	58.0473	59.5516	57.9937	59.2868	58.1628	59.8130	**59.75**
C9	22.2333	22.3886	22.6124	22.6282	22.8233	22.6139	22.7047	22.6016	22.6825	22.6409	22.8547	18.9648	19.2708	19.4004	19.4144	19.6557	19.4060	19.6995	19.4005	19.6674	19.4225	20.0180	**15.44**
C8`	34.7377	35.5130	35.7819	35.8289	36.1801	35.8108	36.3989	35.7951	36.3597	35.8459	36.8091	30.5960	30.8142	31.0655	30.9812	31.2247	30.9680	31.3407	30.9569	31.3887	30.9927	31.4699	**31.11**
H2	8.8761	8.8039	8.8520	8.7659	8.7241	8.7690	8.7906	8.7718	8.7505	8.7629	8.7519	8.8981	8.7359	8.7665	8.6405	8.6466	8.6464	8.6344	8.6519	8.6571	8.6345	8.6458	**7.97**
H3	7.4433	7.5783	7.6654	7.6233	7.7361	7.6213	7.7566	7.6190	7.7465	7.6252	7.7698	7.4323	7.5668	7.6511	7.6133	7.7280	7.6111	7.7441	7.6087	7.7353	7.6153	7.7592	**7.22**
H5	7.2878	7.4785	7.5663	7.5650	7.6852	7.5602	7.7061	7.5552	7.6928	7.5695	7.7273	7.2798	7.4603	7.5446	7.5400	7.6603	7.5356	7.6720	7.5311	7.6611	7.5440	7.6938	**7.22**
H6	8.1765	8.3928	8.4992	8.5149	8.6356	8.5078	8.7226	8.5005	8.6822	8.5217	8.7376	8.0113	8.2014	8.3159	8.2915	8.4587	8.2866	8.4826	8.2813	8.4746	8.2959	8.5310	**7.97**
H8	4.0776	4.1885	4.2247	4.3024	4.3719	4.2945	4.4593	4.2868	4.4300	4.3099	4.4624	4.2587	4.4280	4.4860	4.5022	4.6169	4.4983	4.6464	4.4943	4.6344	4.5056	4.6772	**4.99**
H(9A-9C)	1.2993	1.3062	1.3063	1.3002	1.2417	1.3014	1.2609	1.3023	1.2448	1.2990	1.2689	1.3682	1.3960	1.3920	1.4076	1.3798	1.4070	1.4019	1.4061	1.4026	1.4081	1.4244	**1.51**
H(8`A-8`C)	2.4396	2.3870	2.3452	2.3723	2.3466	2.3731	2.3248	2.3737	2.3360	2.3717	2.3239	2.8786	2.7124	2.6679	2.6359	2.5874	2.6411	2.5108	2.6458	2.5345	2.6307	2.4845	**2.71**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S11. Cont. II

Nuclei	R											S										Exp. [b]
	BLYP											BLYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.2740	140.0627	140.7302	140.3557	142.0482	140.6261	141.6136	140.4250	141.4809	140.7208	141.8598	138.3037	138.8878	139.5939	139.5904	141.4131	139.8236	141.0985	139.5956	141.3416	139.9982	141.2014	**129.02**
C2	137.3888	137.3557	137.9052	137.1077	137.7439	137.4006	137.9857	137.2334	138.0955	137.4576	138.0801	136.8040	136.8446	137.3898	136.8417	137.6112	137.1207	137.9926	136.9376	138.0835	137.2041	138.0703	**132.19**
C3	120.6544	121.3842	121.8707	121.6716	122.2855	121.9330	122.4590	121.7316	122.5866	122.0499	122.6336	119.6392	121.4514	121.9240	121.6569	122.3097	121.9238	122.3772	121.7284	122.4989	122.0306	122.5353	**116.16**
C4	177.6519	178.7185	179.3932	179.3068	180.0988	179.5462	180.5234	179.3230	180.6223	179.7057	180.7915	178.1086	178.8813	179.6485	179.1527	180.0400	179.4160	180.2300	179.2172	180.2861	179.5290	180.4844	**166.89**
C5	118.5470	119.8601	120.3998	120.5456	121.3222	120.7815	121.4404	120.5550	121.5434	120.9483	121.6902	118.6599	120.0133	120.5942	120.5540	121.3508	120.8003	121.3513	120.5845	121.4329	120.9468	121.5891	**116.16**
C6	133.7911	135.6052	136.7931	136.6678	138.3637	136.8753	138.6685	136.6243	138.6992	137.1000	139.1691	138.8182	136.2738	137.4058	137.2526	138.9036	137.4733	139.2393	137.2316	139.1572	137.6692	139.7543	**132.19**
C7	203.2767	208.6048	209.8305	211.6985	212.3595	211.7964	217.3300	211.4147	216.3806	212.2229	218.3121	205.2971	212.7975	214.3032	214.9277	216.0897	215.0775	220.0988	214.7652	219.4181	215.4121	220.5992	**196.22**
C8	69.1241	70.1253	70.7992	70.3573	71.5764	70.6395	71.9231	70.4601	71.8008	70.7169	72.6971	68.1488	65.4631	65.8331	66.4810	67.5528	66.6957	68.0924	66.4492	68.1157	66.9054	68.4506	**59.75**
C9	23.7215	24.0520	24.2062	24.1836	24.6500	24.4455	24.6108	24.2503	24.7226	24.5640	24.8492	16.4537	20.8061	20.7678	21.0333	21.2955	21.2977	21.4360	21.1003	21.5017	21.4093	21.9663	**15.44**
C8`	38.2242	38.9477	39.0730	39.4073	39.6721	39.6658	39.7283	39.4601	39.9360	39.7878	40.2492	32.8912	33.8280	34.1359	33.9651	34.2232	34.2348	34.1613	34.0423	34.3099	34.3359	34.3012	**31.11**
H2	8.3954	8.3311	8.3657	8.2850	8.2783	8.3345	8.4554	8.2924	8.3194	8.3386	8.4701	8.3743	8.3060	8.3480	8.2230	8.2163	8.2757	8.3816	8.2357	8.2114	8.2732	8.4083	**7.97**
H3	7.1679	7.2953	7.3831	7.3318	7.4491	7.3773	7.6306	7.3305	7.4581	7.3888	7.6578	7.0966	7.2855	7.3681	7.3259	7.4422	7.3712	7.6247	7.3239	7.4500	7.3832	7.6520	**7.22**
H5	7.0230	7.2052	7.2897	7.2883	7.4065	7.3310	7.5902	7.2811	7.4161	7.3480	7.6256	6.9899	7.1903	7.2755	7.2597	7.3808	7.3031	7.5580	7.2540	7.3806	7.3187	7.5918	**7.22**
H6	7.9452	8.1295	8.2114	8.2406	8.3476	8.2808	8.5506	8.2286	8.3909	8.3029	8.6025	8.9754	7.8764	7.9806	7.9535	8.0977	7.9966	8.2837	7.9470	8.0952	8.0128	8.3454	**7.97**
H8	4.5730	4.6582	4.6658	4.7406	4.7734	4.7808	4.9699	4.7284	4.7971	4.8027	5.0172	4.4807	4.8131	4.8614	4.8724	4.9776	4.9165	5.1608	4.8680	4.9755	4.9306	5.2060	**4.99**
H(9A-9C)	1.3344	1.3224	1.3240	1.2985	1.2925	1.3477	1.4693	1.3049	1.3035	1.3524	1.4944	1.2856	1.4612	1.4487	1.4808	1.4580	1.5270	1.6506	1.4807	1.4754	1.5371	1.6944	**1.51**
H(8`A-8`C)	2.5702	2.5055	2.4761	2.4845	2.4652	2.5330	2.6299	2.4890	2.4571	2.5387	2.6207	2.5654	2.8839	2.8478	2.7998	2.7482	2.8522	2.8332	2.8121	2.6782	2.8501	2.8119	**2.71**
Nuclei	BMK											BMK										
C1	154.5489	154.7956	155.8147	155.0346	156.7869	155.0048	155.7582	155.1850	155.9437	155.2232	155.7278	153.3708	154.7062	155.5737	155.3493	157.1804	155.2822	157.0114	155.4300	156.7717	155.5792	157.0888	**129.02**
C2	155.5489	155.3349	156.1444	155.0820	155.8798	155.0811	156.4462	155.2910	156.2529	155.2438	156.4023	154.7572	154.6732	155.3927	154.5734	155.4851	154.5591	155.9928	154.7574	155.7913	154.7494	155.9653	**132.19**
C3	135.9186	136.5742	137.2866	136.7717	137.6790	136.7457	137.8453	136.9307	137.6978	136.9577	137.8467	136.0540	136.5812	137.2516	136.7609	137.6638	136.7339	137.8432	136.9186	137.6908	136.9479	137.8865	**116.16**
C4	189.4005	190.1835	191.0076	190.6219	191.5290	190.5810	192.1342	190.7513	191.8731	190.8217	192.2418	189.7985	190.2293	191.0560	190.4438	191.4104	190.4180	191.7002	190.6026	191.5626	190.6291	191.8308	**166.89**
C5	133.4295	134.7613	135.4788	135.4278	136.5512	135.3675	136.6886	135.5196	136.4925	135.6472	136.8148	133.4535	134.7683	135.5390	135.3777	136.4835	135.3275	136.5822	135.4877	136.3606	135.5868	136.7328	**116.16**
C6	151.4094	153.6757	155.2637	155.0157	156.8896	154.9195	157.7543	155.0316	157.2746	155.2662	158.1427	152.1159	153.9639	155.4209	155.0094	157.0550	154.9327	157.4837	155.0660	157.2182	155.2429	157.8187	**132.19**
C7	216.9478	222.5474	224.1482	225.4916	226.2743	225.2972	232.0453	225.3132	230.7791	225.8361	232.8163	221.5389	226.5692	228.0915	229.2000	230.0942	229.0219	235.6763	229.0559	234.3215	229.5316	236.4133	**196.22**
C8	70.5725	71.6400	72.4428	72.1543	73.3210	72.1213	73.7576	72.2984	73.5299	72.3466	74.4771	64.4902	66.3795	67.0821	67.2150	68.2924	67.1424	69.1388	67.2827	68.7153	67.4478	69.3740	**59.75**
C9	25.4816	25.8566	26.3477	26.2252	26.6325	26.1938	26.7756	26.3697	26.5780	26.4143	26.8310	22.1260	22.5585	22.7087	22.6468	23.0607	22.6251	23.2222	22.8150	23.0572	22.8297	23.5137	**15.44**
C8`	38.7886	39.4905	39.7965	39.7916	40.2856	39.7653	40.4650	39.9500	40.3114	39.9781	40.8997	33.9443	34.1818	34.5674	34.3474	34.7515	34.3245	34.7335	34.5118	34.8069	34.5294	34.8356	**31.11**
H2	9.0522	9.0233	9.0737	8.9738	8.9666	8.9734	9.0551	8.9730	9.0302	8.9645	9.0669	9.0430	8.8827	8.9188	8.8117	8.8174	8.8133	8.8099	8.8146	8.8396	8.8005	8.8138	**7.97**
H3	7.6503	7.8088	7.9094	7.8680	7.9716	7.8622	8.0008	7.8561	7.9908	7.8636	8.0111	7.6582	7.8152	7.8999	7.8689	7.9851	7.8629	7.9933	7.8568	7.9965	7.8650	8.0096	**7.22**
H5	7.5098	7.7043	7.7841	7.7896	7.9181	7.7809	7.9299	7.7723	7.9192	7.7883	7.9561	7.4861	7.6973	7.7852	7.7793	7.9021	7.7717	7.9135	7.7640	7.8990	7.7768	7.9393	**7.22**
H6	8.4072	8.6270	8.7828	8.7961	8.9052	8.7837	9.0195	8.7706	8.9763	8.7979	9.0628	8.3050	8.4960	8.6092	8.6017	8.7715	8.5925	8.7332	8.5831	8.7698	8.6007	8.7910	**7.97**
H8	4.2317	4.3488	4.4104	4.4856	4.5292	4.4731	4.5903	4.4604	4.5756	4.4876	4.6005	4.4400	4.6482	4.6995	4.7284	4.8382	4.7206	4.8188	4.7127	4.8373	4.7262	4.8615	**4.99**
H(9A-9C)	1.3048	1.3335	1.3264	1.3372	1.2998	1.3347	1.3417	1.3320	1.3281	1.3300	1.3703	1.3776	1.3895	1.3774	1.4034	1.3701	1.3999	1.3895	1.3963	1.3784	1.3971	1.4125	**1.51**
H(8`A-8`C)	2.4334	2.3750	2.3238	2.3567	2.3235	2.3539	2.2956	2.3513	2.3080	2.3498	2.2771	2.8035	2.6688	2.6299	2.6096	2.5602	2.6105	2.4481	2.6113	2.4916	2.5990	2.4288	**2.71**
Nuclei	BP86											BP86										
C1	135.9939	136.6320	137.6362	136.9544	138.7298	136.9390	138.2948	136.9186	138.3141	136.9642	138.7051	134.4352	135.9816	136.4890	136.5815	138.0085	136.5423	138.0378	136.5022	137.9223	136.6187	138.2985	**129.02**
C2	136.0461	136.1412	136.6915	135.9389	136.4876	135.9629	136.9072	135.9812	136.7985	135.9104	137.0603	135.2799	135.6510	136.1578	135.6672	136.3174	135.6758	136.8585	135.6802	136.7480	135.6552	137.0159	**132.19**
C3	119.5556	120.4857	121.0080	120.7308	121.3490	120.7247	121.6928	120.7132	121.6404	120.7314	121.9360	119.6977	120.5178	120.9979	120.7317	121.3594	120.7284	121.6195	120.7195	121.5439	120.7299	121.8637	**116.16**
C4	174.3602	175.5049	176.1304	175.8536	176.5630	175.8334	177.1710	175.8083	177.0813	175.8678	177.4848	174.7072	175.5024	176.1986	175.7445	176.5291	175.7420	176.8841	175.7330	176.7851	175.7408	177.2044	**166.89**
C5	117.4531	118.9871	119.5529	119.6506	120.4030	119.6163	120.7206	119.5768	120.6236	119.6782	121.0496	117.6959	119.0396	119.6143	119.6262	120.4183	119.6030	120.5906	119.5742	120.4936	119.6424	120.9111	**116.16**
C6	132.4823	134.5222	135.5397	135.4991	136.9975	135.4473	137.5315	135.3905	137.2521	135.5440	138.0880	132.8422	134.9807	136.2191	135.9532	137.6251	135.9065	138.0996	135.8536	137.8931	135.9910	138.6398	**132.19**
C7	200.3568	205.1844	206.6915	207.6362	208.7456	207.4854	213.3518	207.3301	212.6663	207.7757	214.3906	205.2587	209.2590	210.3906	211.2385	212.1476	211.1283	216.2414	211.0136	215.3050	211.3390	216.8705	**196.22**
C8	67.0914	68.3350	69.0224	68.6336	69.6697	68.6283	70.1232	68.6177	69.8169	68.6343	71.1003	61.2199	63.3467	63.8475	64.2565	65.1036	64.1999	65.8529	64.1410	65.6179	64.3090	66.2851	**59.75**
C9	23.4788	23.9387	24.0159	24.1770	24.4194	24.1716	24.5594	24.1605	24.4086	24.1770	24.8922	20.0447	20.8111	20.8964	21.0566	21.2467	21.0482	21.5506	21.0352	21.4325	21.0604	22.1852	**15.44**
C8`	37.5056	38.3780	38.4809	38.5899	38.8300	38.5853	39.0439	38.5763	39.0514	38.5903	39.6736	32.7385	32.9732	33.1909	33.0751	33.2543	33.0771	33.3634	33.0731	33.3752	33.0673	33.5888	**31.11**
H2	8.4690	8.4251	8.4168	8.3721	8.3303	8.3765	8.3610	8.3805	8.3653	8.3675	8.3657	8.5023	8.3508	8.3888	8.2771	8.2780	8.2836	8.2597	8.2894	8.2717	8.2701	8.2813	**7.97**
H3	7.1833	7.3254	7.4023	7.3644	7.4695	7.3630	7.4872	7.3613	7.4789	7.3653	7.5157	7.1759	7.3137	7.3896	7.3551	7.4646	7.3535	7.4797	7.3516	7.4705	7.3561	7.5088	**7.22**
H5	7.0316	7.2248	7.3017	7.3045	7.4170	7.3004	7.4360	7.2960	7.4267	7.3081	7.4730	7.0289	7.2047	7.2838	7.2819	7.3979	7.2785	7.4064	7.2747	7.3955	7.2847	7.4416	**7.22**
H6	8.0317	8.2270	8.2775	8.3141	8.4038	8.3094	8.4531	8.3044	8.4474	8.3183	8.4976	7.7817	7.9419	8.0474	8.0258	8.1760	8.0224	8.1879	8.0185	8.1750	8.0284	8.2496	**7.97**
H8	4.6085	4.6845	4.6748	4.7603	4.7803	4.7553	4.8233	4.7502	4.8256	4.7646	4.8587	4.7327	4.8659	4.9018	4.9243	5.0225	4.9224	5.0356	4.9199	5.0205	4.9256	5.0853	**4.99**
H(9A-9C)	1.3656	1.3684	1.3441	1.3548	1.3143	1.3570	1.3284	1.3589	1.3132	1.3524	1.3589	1.4453	1.4875	1.4805	1.5086	1.4790	1.5084	1.4981	1.5079	1.4947	1.5083	1.5410	**1.51**
H(8`A-8`C)	2.5546	2.4795	2.4461	2.4610	2.4324	2.4627	2.4144	2.4642	2.4111	2.4590	2.4105	3.0093	2.8351	2.7840	2.6945	2.7609	2.6012	2.7671	2.6178	2.7468	2.5828		**2.71**
Nuclei	CAM-B3LYP											CAM-B3LYP										
C1	140.5940	141.0501	141.9502	141.2482	143.3376	141.2328	142.6219	141.2195	142.7966	141.2664	142.8916	139.3811	140.7764	141.3414	141.3955	142.9372	141.3447	142.8551	141.3003	142.5657	141.4530	142.9212	**129.02**
C2	142.4322	142.3676	142.8920	142.2031	142.7302	142.2185	143.2393	142.2342	143.1183	142.1902	143.2313	141.9632	142.0722	142.5741	142.0137	142.6143	142.0196	143.1220	142.0264	143.0134	142.0107	143.1501	**132.19**
C3	123.8770	124.5297	125.0152	124.7351	125.3944	124.7281	125.5969	124.7212	125.5656	124.7437	125.6728	123.9590	124.5672	125.0168	124.7695	125.4058	124.7619	125.5862	124.7548	125.5220	124.7791	125.6510	**116.16**
C4	177.6432	178.4616	179.0236	178.8866	179.5004	178.8652	180.0958	178.8438	179.9671	178.9091	180.2452	177.9270	178.4619	179.0815	178.7166	179.4216	178.7091	179.7910	178.7009	179.7287	178.7245	179.9540	**166.89**
C5	121.6531	122.9882	123.5423	123.6761	124.5002	123.6378	124.6833	123.5998	124.6086	123.7146	124.8524	121.7948	123.0474	123.5984	123.6473	124.4684	123.6163	124.5780	123.5853	124.4990	123.6786	124.7226	**116.16**
C6	138.6325	140.6802	141.7768	141.7799	143.1835	141.7181	143.7450	141.6562	143.4517	141.8399	144.1171	138.9686	141.0487	142.3055	142.0534	143.7538	142.0017	144.1534	141.9484	144.0548	142.1023	144.5739	**132.19**
C7	205.1841	210.4669	211.8770	213.2659	214.3729	213.0946	219.8334	212.9249	218.8841	213.4315	220.8758	210.1044	214.5528	215.7343	216.9360	217.6675	216.7972	222.7736	216.6596	221.5003	217.0720	223.3268	**196.22**
C8	63.5728	64.7701	65.4574	65.1172	66.1087	65.1025	66.5638	65.0883	66.3449	65.1333	67.2834	57.9234	59.8230	60.3104	60.7065	61.5242	60.6433	62.2922	60.5845	61.9726	60.7729	62.5903	**59.75**
C9	22.4381	22.6575	22.8386	22.9008	23.1565	22.8881	23.1031	22.8752	23.0434	22.9144	23.2395	19.2771	19.6649	19.7105	19.7757	20.0125	19.7699	20.0783	19.7654	20.0320	19.7840	20.4496	**15.44**
C8`	35.5076	36.3386	36.5579	36.6501	37.0360	36.6375	37.2208	36.6255	37.1657	36.6643	37.6889	31.0486	31.2767	31.5537	31.4840	31.7595	31.4764	31.8336	31.4681	31.8936	31.4915	31.9753	**31.11**
H2	8.7689	8.7049	8.7244	8.6617	8.6168	8.6654	8.6438	8.6690	8.6389	8.6580	8.6285	8.7980	8.6167	8.6695	8.5340	8.5473	8.5409	8.5118	8.5472	8.5462	8.5267	8.5219	**7.97**
H3	7.4063	7.5412	7.6281	7.5846	7.6999	7.5826	7.6716	7.5807	7.7091	7.5865	7.7301	7.3996	7.5311	7.6171	7.5747	7.6929	7.5726	7.7060	7.5705	7.6986	7.5766	7.7206	**7.22**
H5	7.2620	7.4507	7.5382	7.5345	7.6567	7.5299	7.6715	7.5253	7.6620	7.5389	7.6941	7.2579	7.4349	7.5221	7.5119	7.6365	7.5077	7.6445	7.5036	7.6350	7.5158	7.6658	**7.22**
H6	8.1470	8.3590	8.4476	8.4737	8.5894	8.4673	8.6366	8.4608	8.6223	8.4796	8.6702	7.9705	8.1468	8.2705	8.2373	8.4092	8.2331	8.4121	8.2286	8.4132	8.2409	8.4600	**7.97**
H8	4.2201	4.3249	4.3484	4.4341	4.4931	4.4267	4.5388	4.4195	4.5400	4.4412	4.5650	4.3966	4.5587	4.6191	4.6315	4.7523	4.6282	4.7687	4.6248	4.7611	4.6343	4.8001	**4.99**
H(9A-9C)	1.3297	1.3390	1.3314	1.3291	1.2821	1.3304	1.2971	1.3316	1.2847	1.3277	1.3077	1.4016	1.4258	1.4289	1.4408	1.4198	1.4402	1.4318	1.4396	1.4375	1.4411	1.4563	**1.51**
H(8`A-8`C)	2.5132	2.4524	2.4238	2.4345	2.4170	2.4350	2.4044	2.4357	2.4044	2.4340	2.3914	2.9425	2.7653	2.7314	2.6913	2.6489	2.6974	2.5595	2.7032	2.5861	2.6851	2.5306	**2.71**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S11. Cont. III

Nuclei	R											S										Exp. [b]
	HF																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.0859	136.4286	136.9983	136.5642	138.6394	136.5601	136.8559	136.5607	137.5918	136.5707	137.8340	135.1106	136.0099	136.9165	136.8715	138.6196	136.8298	138.1526	136.7906	138.0357	136.9136	138.1693	**129.02**
C2	144.2959	144.1109	144.6184	143.9366	144.2969	143.9493	145.0625	143.9624	144.8336	143.9247	144.9263	144.1862	143.9606	144.4423	143.6963	144.1843	143.7105	144.6238	143.7251	144.5752	143.6812	144.6859	**132.19**
C3	120.5425	120.9815	121.3393	121.0997	121.6987	121.0951	121.5914	121.0919	121.6723	121.1042	121.7618	120.5755	121.0153	121.3955	121.1911	121.7425	121.1823	121.7739	121.1741	121.7432	121.1992	121.8101	**116.16**
C4	171.0685	171.6891	172.2443	172.0947	172.4686	172.0696	173.4111	172.0452	173.0954	172.1179	173.3624	171.3313	171.6695	172.1524	171.7723	172.2704	171.7643	172.7640	171.7564	172.6801	171.7787	172.9382	**166.89**
C5	117.7778	118.9699	119.4399	119.5840	120.3789	119.5486	120.2895	119.5143	120.3140	119.6174	120.5553	117.8113	119.0523	119.5559	119.6851	120.4237	119.6494	120.4603	119.6142	120.3849	119.7186	120.5859	**116.16**
C6	139.8710	141.8434	143.0414	142.9329	144.0689	142.8614	145.3610	142.7878	144.7144	142.9974	145.2266	140.2153	142.1535	143.2403	142.9363	144.2865	142.8868	144.8278	142.8360	144.6896	142.9813	145.2440	**132.19**
C7	195.4655	201.2748	202.3678	204.5817	204.9342	204.3815	211.4166	204.1898	210.2401	204.7750	212.8652	200.3146	204.7891	205.8595	207.3684	207.7885	207.2162	214.0876	207.0655	212.5722	207.5129	214.7501	**196.22**
C8	54.6914	55.6162	56.0452	55.7978	56.6132	55.7884	56.8235	55.7770	56.8761	55.8047	57.6680	49.9453	51.5670	52.1910	52.5059	53.2429	52.4542	53.9705	52.4041	53.6974	52.5554	54.1978	**59.75**
C9	20.7069	20.7584	20.8662	20.7421	21.0481	20.7452	20.9072	20.7468	20.8745	20.7388	20.9507	17.7976	17.8056	17.9115	17.8577	18.0665	17.8560	17.9858	17.8550	17.9557	17.8592	18.1883	**15.44**
C8`	32.6429	33.3486	33.5660	33.7469	34.0103	33.7215	34.1987	33.6970	34.1551	33.7689	34.5312	29.0930	29.3330	29.5248	29.4519	29.7044	29.4395	29.7559	29.4273	29.7928	29.4622	29.8640	**31.11**
H2	9.0358	8.9576	9.0240	8.9122	8.8795	8.9150	8.9903	8.9172	8.9268	8.9093	8.8935	9.0687	8.8942	8.9168	8.7657	8.7690	8.7719	8.7430	8.7777	8.7685	8.7596	8.7567	**7.97**
H3	7.4286	7.5694	7.6559	7.6163	7.7372	7.6140	7.7469	7.6115	7.7419	7.6185	7.7658	7.4270	7.5652	7.6521	7.6122	7.7319	7.6098	7.7417	7.6072	7.7343	7.6145	7.7576	**7.22**
H5	7.2620	7.4585	7.5485	7.5471	7.6720	7.5420	7.6831	7.5367	7.6720	7.5520	7.7063	7.2588	7.4515	7.5381	7.5363	7.6607	7.5316	7.6678	7.5266	7.6572	7.5408	7.6908	**7.22**
H6	8.1772	8.4177	8.5445	8.5717	8.7053	8.5623	8.8158	8.5526	8.7578	8.5806	8.8070	8.0620	8.2816	8.3955	8.3692	8.5389	8.3639	8.5572	8.3581	8.5485	8.3743	8.6055	**7.97**
H8	3.6262	3.7734	3.8337	3.9160	4.0002	3.9073	4.0866	3.8987	4.0448	3.9245	4.0816	3.7998	3.9985	4.0614	4.0795	4.2064	4.0749	4.2416	4.0700	4.2283	4.0838	4.2685	**4.99**
H(9A-9C)	1.2094	1.2101	1.2114	1.1856	1.1335	1.1867	1.1817	1.1873	1.1548	1.1845	1.1607	1.2797	1.2815	1.2708	1.2849	1.2453	1.2842	1.2618	1.2832	1.2631	1.2857	1.2803	**1.51**
H(8`A-8`C)	2.2583	2.2315	2.1858	2.2178	2.1970	2.2185	2.1768	2.2190	2.1940	2.2172	2.1932	2.6962	2.5446	2.4939	2.4664	2.4243	2.4706	2.3592	2.4746	2.3767	2.4625	2.3361	**2.71**
Nuclei	**LC-BLYP**																						
C1	143.9454	144.3001	145.4097	144.5079	146.3392	144.4682	145.1219	144.4578	146.1915	144.5303	146.2836	142.9429	144.2114	144.8868	144.9354	146.3990	144.8458	146.3781	144.7913	145.9849	145.0111	146.5188	**129.02**
C2	148.5022	148.3123	148.9120	148.1799	148.7307	148.1681	149.3075	148.1834	149.1118	148.1736	149.2571	148.2367	148.1595	148.7302	148.0898	148.6521	148.0728	149.1473	148.0835	149.0482	148.0884	149.1787	**132.19**
C3	128.3981	128.9432	129.5272	129.1700	129.8249	129.1365	129.9435	129.1302	129.9864	129.1845	130.1049	128.4577	128.9850	129.5383	129.2181	129.8639	129.1821	130.0193	129.1738	129.9481	129.2354	130.0806	**116.16**
C4	181.8964	182.5361	183.1128	182.9647	183.4846	182.9173	184.1724	182.8968	183.9350	182.9925	184.2385	182.1104	182.5115	183.1648	182.7723	183.4027	182.7394	183.7928	182.7322	183.7403	182.7849	183.9455	**166.89**
C5	126.0329	127.3491	128.0096	128.0921	128.9347	128.0253	129.0515	127.9857	129.0367	128.1384	129.2952	126.1441	127.4212	128.0695	128.1002	128.9526	128.0385	129.0416	128.0038	128.9555	128.1414	129.1882	**116.16**
C6	144.4457	146.5586	147.7101	147.7244	149.3132	147.6325	150.0897	147.5676	149.3684	147.7936	150.0269	144.7647	146.8890	148.2216	147.9599	149.7654	147.8834	150.1624	147.8313	150.0717	148.0120	150.5715	**132.19**
C7	210.7961	216.2518	217.8303	219.2261	219.8730	219.0191	225.3038	218.8395	225.0653	219.4065	227.1999	215.4470	220.1457	221.5590	222.7455	223.3196	222.5572	228.8329	222.3988	227.4675	222.9103	229.4875	**196.22**
C8	61.3984	62.6319	63.4214	63.1097	64.1261	63.0645	64.5480	63.0462	64.4091	63.1347	65.2976	55.6431	57.3143	57.8214	58.2576	59.0058	58.1666	59.8648	58.1066	59.4794	58.3300	60.2244	**59.75**
C9	21.5377	21.6825	21.9377	21.8979	22.3180	21.8578	22.1872	21.8462	22.0012	21.9197	22.1735	18.6324	18.8728	18.9378	19.0093	19.2711	18.9777	19.3164	18.9740	19.2407	19.0228	19.6888	**15.44**
C8`	33.6021	34.3992	34.7145	34.8359	35.1835	34.7918	35.4065	34.7739	35.3393	34.8597	35.8933	29.0895	29.3897	29.7641	29.6827	29.9584	29.6509	30.0425	29.6443	30.1159	29.6934	30.2365	**31.11**
H2	8.9711	8.8976	8.9038	8.8550	8.8357	8.8575	8.9003	8.8613	8.8099	8.8515	8.8027	8.9912	8.8085	8.8563	8.7154	8.7346	8.7227	8.6856	8.7307	8.7297	8.7068	8.6896	**7.97**
H3	7.5427	7.6754	7.7638	7.7201	7.8369	7.7170	7.8517	7.7154	7.8451	7.7221	7.8687	7.5437	7.6708	7.7599	7.7138	7.8323	7.7108	7.8425	7.7093	7.8366	7.7157	7.8586	**7.22**
H5	7.4058	7.5954	7.6843	7.6812	7.8049	7.6755	7.8189	7.6712	7.8049	7.6857	7.8395	7.4060	7.5871	7.6767	7.6670	7.7928	7.6617	7.7982	7.6579	7.7897	7.6710	7.8216	**7.22**
H6	8.3027	8.5213	8.6081	8.6422	8.7669	8.6342	8.8393	8.6277	8.7770	8.6487	8.8307	8.1441	8.3320	8.4605	8.4236	8.6087	8.4188	8.6040	8.4150	8.6111	8.4268	8.6501	**7.97**
H8	4.0994	4.2241	4.2473	4.3375	4.3854	4.3282	4.4499	4.3208	4.4440	4.3453	4.4811	4.3161	4.4914	4.5661	4.5712	4.6984	4.5663	4.7098	4.5628	4.7083	4.5747	4.7424	**4.99**
H(9A-9C)	1.3477	1.3582	1.3449	1.3500	1.3227	1.3501	1.3530	1.3517	1.2974	1.3487	1.3187	1.4131	1.4278	1.4251	1.4407	1.4202	1.4395	1.4310	1.4398	1.4374	1.4406	1.4542	**1.51**
H(8`A-8`C)	2.5010	2.4391	2.4146	2.4167	2.4026	2.4164	2.3702	2.4179	2.3908	2.4162	2.3818	2.8887	2.7145	2.6860	2.6365	2.5978	2.6411	2.5031	2.6470	2.5362	2.6309	2.4788	**2.71**
Nuclei	**M06**																						
C1	135.4072	135.7741	137.0115	135.8816	138.0210	135.8649	136.8091	135.8563	137.3380	135.9123	137.0556	134.1674	135.5202	136.1558	136.2300	137.8135	136.1538	137.9154	136.0917	137.5984	136.3238	137.9805	**129.02**
C2	140.6153	140.3648	140.9748	140.1830	140.7472	140.1863	141.1872	140.1968	141.0177	140.1945	141.1811	139.8441	139.8784	140.4612	139.8960	140.5961	139.8814	141.2124	139.8755	141.0600	139.9255	141.2192	**132.19**
C3	121.6176	122.2938	122.9735	122.5729	123.4101	122.5477	123.6473	122.5304	123.5932	122.6111	123.7286	121.6738	122.2553	122.8671	122.5213	123.3123	122.4950	123.5158	122.4767	123.4472	122.5609	123.5784	**116.16**
C4	173.1165	173.9963	174.7342	174.4927	175.3210	174.4521	176.0927	174.4196	175.9087	174.5457	176.2448	173.8447	174.2720	175.0646	174.5038	175.3524	174.4860	175.6260	174.4744	175.6126	174.5338	175.7886	**166.89**
C5	119.7718	121.0559	121.7752	121.7509	122.7315	121.6989	122.7996	121.6545	122.7382	121.8148	122.9828	119.7041	120.9774	121.6509	121.6232	122.5692	121.5755	122.6711	121.5353	122.6020	121.6826	122.8037	**116.16**
C6	136.8085	138.7038	139.7562	139.8590	141.2826	139.7763	142.3109	139.7016	141.8293	139.9522	142.5930	137.1469	139.1678	140.5409	140.2006	141.9881	140.1354	142.4239	140.0763	142.2946	140.2746	142.8394	**132.19**
C7	201.8270	206.8005	208.5395	209.3151	210.6085	209.1531	215.3851	208.9988	214.6233	209.4836	216.2344	206.3715	210.6515	211.8254	212.8411	213.6353	212.6921	218.3336	212.5525	217.1976	212.9995	218.7520	**196.22**
C8	60.7304	61.8816	62.6495	62.3326	63.4023	62.2980	63.5929	62.2707	63.6589	62.3799	64.4145	54.1844	55.7499	56.3619	56.6790	57.5433	56.6009	58.4113	56.5332	58.0797	56.7709	58.7141	**59.75**
C9	22.1450	22.4238	22.6903	22.7400	23.1676	22.7095	23.3573	22.6872	23.2995	22.7835	23.4614	19.4572	19.6907	19.8485	19.8638	20.2293	19.8402	20.3336	19.8248	20.2582	19.9018	20.8431	**15.44**
C8`	36.9348	37.6867	37.9199	37.9636	38.3405	37.9372	38.4473	37.9185	38.4095	38.0033	38.9535	31.7679	31.9520	32.3660	32.1758	32.5544	32.1571	32.7194	32.1443	32.7693	32.2063	32.7972	**31.11**
H2	8.7387	8.6519	8.6561	8.6165	8.5956	8.6186	8.6674	8.6211	8.6218	8.6152	8.6525	8.7596	8.5499	8.5974	8.4553	8.4747	8.4624	8.4395	8.4698	8.4663	8.4487	8.4486	**7.97**
H3	7.3369	7.4633	7.5604	7.5046	7.6321	7.5024	7.6528	7.5006	7.6377	7.5073	7.6581	7.2874	7.4302	7.5150	7.4793	7.6060	7.4760	7.6356	7.4734	7.6197	7.4830	7.6504	**7.22**
H5	7.1579	7.3516	7.4440	7.4353	7.5710	7.4303	7.5755	7.4258	7.5657	7.4405	7.6026	7.1555	7.3358	7.4320	7.4048	7.5377	7.4011	7.5349	7.3979	7.5315	7.4086	7.5553	**7.22**
H6	8.2198	8.4571	8.5350	8.5706	8.6748	8.5635	8.7980	8.5570	8.7357	8.5779	8.8111	7.9934	8.1490	8.2703	8.2290	8.4027	8.2251	8.4051	8.2215	8.4052	8.2330	8.4572	**7.97**
H8	4.3442	4.4692	4.4989	4.5607	4.6243	4.5542	4.7164	4.5485	4.6836	4.5675	4.7345	4.4477	4.6028	4.6519	4.6647	4.7811	4.6617	4.7907	4.6590	4.7893	4.6679	4.8239	**4.99**
H(9A-9C)	1.3018	1.3045	1.2808	1.2978	1.2531	1.2981	1.2815	1.2991	1.2659	1.2981	1.2924	1.3858	1.4182	1.4256	1.4306	1.4133	1.4304	1.4165	1.4305	1.4256	1.4312	1.4437	**1.51**
H(8`A-8`C)	2.4763	2.4121	2.3914	2.3956	2.3829	2.3959	2.3669	2.3969	2.3791	2.3959	2.3540	2.9033	2.7432	2.7104	2.6648	2.6248	2.6682	2.5329	2.6741	2.5623	2.6576	2.5047	**2.71**
Nuclei	**M06-2X**																						
C1	153.0917	153.5294	154.5657	153.6798	155.3824	153.6910	154.3824	153.7038	154.6410	153.6636	154.5610	152.3025	153.6253	154.2248	154.4172	155.8548	154.3561	155.9192	154.3050	155.6636	154.4801	156.1304	**129.02**
C2	155.1746	155.0543	155.6859	154.8589	155.5556	154.8934	156.0475	154.9292	155.9461	154.8195	156.0984	154.7655	154.7734	155.3565	154.6837	155.4125	154.7088	155.8874	154.7355	155.7791	154.6544	155.9277	**132.19**
C3	136.1590	136.8604	137.4721	137.0980	137.8395	137.1065	138.0767	137.1160	138.0006	137.0834	138.1754	136.1934	136.8293	137.4400	137.0599	137.8148	137.0677	137.9965	137.0767	137.9426	137.0459	138.0999	**116.16**
C4	186.9866	187.8245	188.4710	188.2660	188.9823	188.2597	189.6225	188.2546	189.4454	188.2657	189.8145	187.4071	187.9865	188.7105	188.2373	189.0085	188.2488	189.3855	188.2602	189.3135	188.2178	189.5659	**166.89**
C5	133.5146	135.0251	135.7169	135.8167	136.7899	135.7892	136.9947	135.7628	136.8748	135.8366	137.2061	133.4360	134.8666	135.5636	135.5696	136.5427	135.5491	136.6670	135.5297	136.5791	135.5821	136.8705	**116.16**
C6	151.2911	153.5510	154.7995	154.7508	156.6302	154.6981	157.2971	154.6466	156.9660	154.7945	157.7502	151.6315	153.9149	155.3078	154.9928	157.0373	154.9595	157.4443	154.9245	157.2709	155.0146	157.8386	**132.19**
C7	218.4206	224.0871	225.6863	227.0228	227.7392	226.8634	233.4654	226.7049	232.2929	227.1679	234.4902	222.3731	227.5635	229.0579	230.3177	230.9202	230.1563	236.7866	230.0003	235.3937	230.4701	237.6501	**196.22**
C8	66.1021	67.3894	68.1145	67.8657	68.9271	67.8608	69.3536	67.8567	69.2455	67.8636	70.1061	60.3620	62.0622	62.4883	63.0156	63.8536	62.9637	64.7319	62.9168	64.3967	63.0637	65.0835	**59.75**
C9	23.2058	23.4985	23.7070	23.7340	24.1504	23.7389	24.1959	23.7459	24.1017	23.7236	24.3456	20.3942	20.6118	20.6433	20.7319	21.0349	20.7420	21.1263	20.7541	21.0549	20.7172	21.5210	**15.44**
C8`	36.0510	36.7555	36.9669	37.1150	37.4247	37.1125	37.6459	37.1106	37.5970	37.1109	38.1632	30.7152	31.1896	31.5368	31.3585	31.6695	31.3831	31.7058	31.4062	31.7955	31.3257	31.8659	**31.11**
H2	9.2412	9.1940	9.2146	9.1667	9.1653	9.1672	9.2317	9.1673	9.2138	9.1663	9.2327	9.2302	9.0921	9.1468	9.0068	9.0354	9.0138	9.0044	9.0198	9.0317	8.9993	9.0042	**7.97**
H3	7.8930	8.0315	8.1240	8.0797	8.2018	8.0760	8.2142	8.0720	8.2077	8.0833	8.2275	7.8444	7.9817	8.0724	8.0317	8.1517	8.0277	8.1674	8.0235	8.1599	8.0355	8.1819	**7.22**
H5	7.7188	7.9115	8.0040	8.0015	8.1305	7.9950	8.1471	7.9882	8.1342	8.0078	8.1715	7.7205	7.8974	7.9934	7.9760	8.1058	7.9705	8.1095	7.9646	8.1016	7.9813	8.1306	**7.22**
H6	8.7195	8.9331	9.0357	9.0522	9.2020	9.0436	9.2622	9.0346	9.2341	9.0605	9.2978	8.5491	8.7357	8.8647	8.8195	9.0069	8.8151	9.0001	8.8099	9.0002	8.8232	9.0400	**7.97**
H8	4.2292	4.3451	4.3884	4.4506	4.5168	4.4418	4.5788	4.4328	4.5575	4.4593	4.6093	4.4880	4.6312	4.7027	4.6959	4.8114	4.6915	4.8114	4.6865	4.8097	4.7000	4.8405	**4.99**
H(9A-9C)	1.3567	1.3681	1.3531	1.3672	1.3372	1.3663	1.3712	1.3650	1.3600	1.3682	1.3871	1.4261	1.4313	1.4276	1.4367	1.4173	1.4356	1.4268	1.4342	1.4284	1.4376	1.4441	**1.51**
H(8`A-8`C)	2.4619	2.4039	2.3762	2.3853	2.3641	2.3849	2.3357	2.3842	2.3446	2.3860	2.3207	2.7873	2.6416	2.6191	2.5775	2.5343	2.5805	2.4563	2.5830	2.4800	2.5745	2.4273	**2.71**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S11. Cont. IV

Nuclei	R											S										Exp. [b]
	mpW1LYP											mpW1LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.4828	139.9525	140.8951	140.2162	142.1269	140.1880	141.3847	140.1639	141.5911	140.2438	141.6737	138.0239	139.3201	140.0314	140.0519	141.6015	140.0019	141.3526	139.9557	141.2617	140.1006	141.3699	**129.02**
C2	140.0654	139.9633	140.5214	139.8120	140.2594	139.8221	140.7067	139.8327	140.5833	139.8000	140.6754	139.3485	139.4849	140.0212	139.4970	140.0614	139.4929	140.6129	139.4906	140.4986	139.4995	140.6006	**132.19**
C3	121.9628	122.6121	123.1375	122.8712	123.4386	122.8537	123.7099	122.8374	123.6709	122.8862	123.7449	122.0772	122.6487	123.1165	122.8876	123.4426	122.8714	123.6473	122.8567	123.5970	122.9013	123.6861	**116.16**
C4	176.1473	177.0246	177.6646	177.5228	178.1467	177.4890	178.8123	177.4567	178.6743	177.5533	178.9071	176.5361	177.1020	177.7627	177.3919	178.0767	177.3729	178.4887	177.3548	178.3978	177.4074	178.6295	**166.89**
C5	119.7588	121.0521	121.6454	121.7767	122.5021	121.7290	122.7447	121.6831	122.6591	121.8202	122.8719	119.9121	121.1021	121.6630	121.7119	122.4355	121.6731	122.5793	121.6353	122.5049	121.7464	122.6956	**116.16**
C6	136.3411	138.3279	139.4122	139.4387	140.8254	139.3726	141.4341	139.3066	141.1391	139.4983	141.7648	136.6810	138.7304	140.0172	139.7711	141.3801	139.7081	141.9011	139.6456	141.7184	139.8277	142.2839	**132.19**
C7	202.6211	207.7782	209.3145	210.5766	211.6308	210.3901	217.0461	210.2089	216.1478	210.7558	217.9713	207.9684	212.1537	213.3072	214.4009	215.1623	214.2635	219.8843	214.1282	218.8057	214.5296	220.3958	**196.22**
C8	64.8087	65.9413	66.6307	66.2710	67.2010	66.2555	67.4970	66.2398	67.3414	66.2823	68.2675	59.1606	61.1502	61.8125	62.1638	63.0102	62.0972	63.6763	62.0334	63.4471	62.2269	63.9055	**59.75**
C9	23.0194	23.2782	23.4066	23.5626	23.7640	23.5450	23.7639	23.5280	23.6835	23.5763	23.8872	19.5716	19.9981	20.1757	20.2377	20.4306	20.2213	20.5847	20.2064	20.5225	20.2514	20.9210	**15.44**
C8`	36.3159	37.0893	37.3474	37.4110	37.7421	37.3893	37.9553	37.3691	37.9323	37.4299	38.3577	31.9503	32.0958	32.3503	32.2714	32.4808	32.2555	32.5948	32.2408	32.6120	32.2842	32.6749	**31.11**
H2	8.6760	8.6134	8.6345	8.5731	8.5352	8.5769	8.5767	8.5801	8.5650	8.5692	8.5537	8.7155	8.5439	8.5843	8.4575	8.4611	8.4631	8.4509	8.4681	8.4656	8.4518	8.4608	**7.97**
H3	7.3397	7.4720	7.5610	7.5164	7.6269	7.5145	7.6429	7.5123	7.6350	7.5181	7.6539	7.3222	7.4540	7.5397	7.5009	7.6151	7.4987	7.6299	7.4961	7.6226	7.5029	7.6422	**7.22**
H5	7.1905	7.3768	7.4660	7.4635	7.5825	7.4586	7.6016	7.4535	7.5914	7.4679	7.6207	7.1791	7.3532	7.4411	7.4319	7.5518	7.4276	7.5619	7.4231	7.5524	7.4357	7.5804	**7.22**
H6	8.0834	8.2895	8.3770	8.4032	8.5186	8.3966	8.5837	8.3898	8.5634	8.4092	8.6049	7.8914	8.0614	8.1768	8.1478	8.3090	8.1432	8.3269	8.1382	8.3161	8.1519	8.3729	**7.97**
H8	4.3063	4.3981	4.4252	4.5055	4.5605	4.4978	4.6229	4.4902	4.6105	4.5128	4.6327	4.4564	4.6192	4.6720	4.6856	4.7973	4.6823	4.8170	4.6786	4.8046	4.6884	4.8463	**4.99**
H(9A-9C)	1.3216	1.3308	1.3202	1.3215	1.2774	1.3232	1.2903	1.3245	1.2801	1.3196	1.3009	1.4008	1.4361	1.4422	1.4560	1.4325	1.4551	1.4529	1.4538	1.4517	1.4567	1.4756	**1.51**
H(8`A-8`C)	2.5203	2.4606	2.4330	2.4451	2.4238	2.4459	2.4070	2.4465	2.4101	2.4443	2.3934	2.9829	2.8104	2.7656	2.7300	2.6802	2.7354	2.5986	2.7403	2.6192	2.7247	2.5674	**2.71**
Nuclei	mpW1PW91											mpW1PW91										
C1	136.7091	137.1261	138.2904	137.3527	139.3925	137.3342	138.8484	137.3222	138.8794	137.3708	139.0868	135.4965	136.8443	137.3776	137.4319	138.8932	137.3747	138.9047	137.3297	138.6184	137.4927	138.9966	**129.02**
C2	139.0510	138.9813	139.5567	138.8023	139.3841	138.8154	139.7972	138.8338	139.6690	138.7889	139.7849	138.4920	138.6376	139.1844	138.5926	139.2587	138.5931	139.7425	138.5998	139.6330	138.5920	139.7648	**132.19**
C3	121.1434	121.8839	122.4572	122.1398	122.8577	122.1259	123.1111	122.1175	123.0669	122.1523	123.1972	121.1969	121.8835	122.4042	122.1282	122.8348	122.1142	123.0503	122.1059	122.9791	122.1411	123.1290	**116.16**
C4	173.1450	174.0361	174.6361	174.4798	175.1382	174.4530	175.7414	174.4320	175.6481	174.5044	175.9056	173.4356	174.0253	174.6981	174.2966	175.0454	174.2852	175.4189	174.2781	175.3524	174.3057	175.5825	**166.89**
C5	118.9666	120.3546	120.9855	121.0745	121.9413	121.0305	122.1805	120.9922	122.0946	121.1155	122.3576	119.0635	120.3480	120.9568	120.9724	121.8462	120.9359	121.9978	120.9051	121.9093	121.0057	122.1526	**116.16**
C6	135.1188	137.1393	138.1020	138.2106	139.6150	138.1465	140.1616	138.0877	139.9062	138.2707	140.5379	135.4925	137.5198	138.7879	138.5089	140.2202	138.4556	140.6265	138.4058	140.5120	138.5558	141.0214	**132.19**
C7	200.5499	205.4732	207.1087	208.0696	209.2352	207.9079	214.4321	207.7523	213.5361	208.2238	215.3863	204.9687	209.2878	210.4288	211.5065	212.2688	211.3693	217.0803	211.2400	215.8598	211.6406	217.5855	**196.22**
C8	62.5871	63.7277	64.3921	64.0779	65.0594	64.0579	65.5692	64.0437	65.2428	64.0959	66.2934	57.3088	59.1083	59.5712	59.9715	60.7733	59.9036	61.5602	59.8450	61.2368	60.0391	61.8431	**59.75**
C9	22.4303	22.7074	22.8165	22.9714	23.2346	22.9561	23.2515	22.9463	23.1372	22.9849	23.3928	19.1269	19.5971	19.6794	19.7761	20.0297	19.7623	20.1776	19.7543	20.1086	19.7888	20.5773	**15.44**
C8`	35.5389	36.3291	36.5286	36.6000	36.9580	36.5839	37.1500	36.5735	37.1332	36.6149	37.6110	31.0253	31.2540	31.5589	31.4502	31.7343	31.4412	31.7914	31.4363	31.8597	31.4556	31.8914	**31.11**
H2	8.7270	8.6729	8.6666	8.6268	8.5829	8.6306	8.6029	8.6343	8.6110	8.6233	8.5930	8.7399	8.5718	8.6280	8.4933	8.5106	8.5006	8.4771	8.5073	8.5099	8.4860	8.4856	**7.97**
H3	7.3666	7.5071	7.5941	7.5506	7.6672	7.5488	7.6842	7.5469	7.6761	7.5526	7.6994	7.3521	7.4918	7.5782	7.5379	7.6587	7.5357	7.6748	7.5336	7.6662	7.5401	7.6902	**7.22**
H5	7.2156	7.4099	7.4980	7.4952	7.6199	7.4906	7.6379	7.4860	7.6293	7.4999	7.6618	7.2035	7.3869	7.4755	7.4658	7.5930	7.4616	7.6047	7.4575	7.5936	7.4700	7.6265	**7.22**
H6	8.1720	8.3810	8.4466	8.4858	8.5927	8.4800	8.6356	8.4742	8.6335	8.4916	8.6714	7.9622	8.1369	8.2584	8.2244	8.3946	8.2208	8.3985	8.2168	8.3988	8.2277	8.4460	**7.97**
H8	4.3244	4.4232	4.4417	4.5212	4.5686	4.5149	4.6073	4.5088	4.6209	4.5275	4.6357	4.4958	4.6417	4.6998	4.7058	4.8233	4.7033	4.8370	4.7007	4.8311	4.7081	4.8693	**4.99**
H(9A-9C)	1.3031	1.3123	1.2861	1.3005	1.2512	1.3018	1.2673	1.3032	1.2532	1.2994	1.2798	1.3839	1.4107	1.4119	1.4245	1.4007	1.4244	1.4147	1.4241	1.4196	1.4248	1.4408	**1.51**
H(8`A-8`C)	2.4582	2.3926	2.3693	2.3752	2.3559	2.3760	2.3459	2.3770	2.3405	2.3747	2.3305	2.8765	2.7109	2.6756	2.6345	2.5913	2.6410	2.5022	2.6472	2.5276	2.6285	2.4719	**2.71**
Nuclei	O3LYP											O3LYP										
C1	133.9706	135.2869	135.1280	135.8992	137.5413	135.8935	136.8634	135.8840	136.9936	135.9000	136.9568	131.9841	134.0269	134.9667	134.8776	136.4625	134.8098	136.5165	134.7451	136.4801	134.9454	136.6774	**129.02**
C2	134.2294	134.0386	134.6059	134.0020	134.6215	134.0143	135.0928	134.0931	135.0297	133.9844	135.0347	133.6011	133.8315	134.4861	133.8598	134.5658	133.8686	134.9908	133.8725	134.9155	133.8449	134.9967	**132.19**
C3	117.1429	117.8472	118.4244	118.1586	118.8498	118.1512	119.1048	118.1420	119.0383	118.1592	119.1705	117.2423	117.8329	118.4008	118.1462	118.7940	118.1374	118.9776	118.1236	118.9199	118.1480	119.0503	**116.16**
C4	169.3331	170.2178	170.9930	170.6800	171.4504	170.6575	171.9898	170.6246	171.8402	170.6953	172.1262	169.6935	170.1374	170.8394	170.4612	171.2113	170.4568	171.5048	170.4458	171.4066	170.4567	171.6400	**166.89**
C5	115.1244	116.3261	117.0316	116.9791	117.7550	116.9488	117.9702	116.9062	117.8594	117.0010	118.1340	115.2829	116.3481	116.9834	116.9736	117.7506	116.9474	117.8633	116.9154	117.7787	116.9914	118.0028	**116.16**
C6	130.1343	131.8403	133.2468	132.9143	134.4244	132.8471	134.9826	132.7768	134.7083	132.9717	135.3818	130.8195	132.4740	133.5676	133.4119	134.9398	133.3757	135.3121	133.3309	135.1128	133.4364	135.6140	**132.19**
C7	196.4324	202.4039	202.9208	205.2799	206.3184	205.1284	211.0569	204.9884	210.1352	205.4208	211.6531	200.9322	205.3707	206.9113	207.7346	208.6887	207.5898	212.9882	207.4429	212.0350	207.8698	213.5094	**196.22**
C8	62.7269	63.8638	64.1933	64.6392	65.2111	64.6247	65.7186	64.6144	65.5898	64.6448	66.4308	57.3727	59.9629	60.5156	61.0054	61.8178	60.9369	62.7983	60.8688	62.5812	61.0698	63.0624	**59.75**
C9	21.9077	22.1497	22.4381	22.4448	22.6922	22.4333	22.8050	22.4257	22.7348	22.4497	22.9545	18.3907	18.7982	18.9135	19.0083	19.2082	19.0039	19.4486	18.9953	19.3637	19.0069	19.7532	**15.44**
C8`	35.8615	36.6415	36.9984	37.0897	37.4384	37.0783	37.5559	37.0769	37.5415	37.0931	37.8889	31.6791	31.7885	32.1081	32.0205	32.3175	32.0201	32.2296	32.0132	32.2550	32.0126	32.2365	**31.11**
H2	8.5171	8.3815	8.5110	8.3059	8.3131	8.3086	8.3569	8.3167	8.3480	8.3030	8.3618	8.6115	8.3742	8.4056	8.2874	8.3033	8.2956	8.2770	8.3028	8.2844	8.2784	8.2790	**7.97**
H3	7.2896	7.4098	7.5061	7.4543	7.5768	7.4521	7.6030	7.4468	7.5953	7.4562	7.6133	7.2766	7.4071	7.4943	7.4552	7.5707	7.4530	7.5845	7.4505	7.5766	7.4572	7.5999	**7.22**
H5	7.1552	7.3290	7.4298	7.3986	7.5094	7.3950	7.5202	7.3889	7.5085	7.4017	7.5463	7.1395	7.3009	7.3898	7.3774	7.4980	7.3735	7.5074	7.3692	7.4968	7.3810	7.5278	**7.22**
H6	8.0527	8.2175	8.3672	8.3017	8.4640	8.2946	8.5029	8.2853	8.4809	8.3083	8.5390	7.8574	7.9837	8.0812	8.0642	8.2140	8.0612	8.2127	8.0575	8.2001	8.0664	8.2508	**7.97**
H8	4.4166	4.5098	4.5410	4.5642	4.6714	4.5583	4.6852	4.5532	4.6658	4.5699	4.7170	4.5458	4.6793	4.7411	4.7470	4.8642	4.7444	4.8665	4.7410	4.8556	4.7490	4.8955	**4.99**
H(9A-9C)	1.2321	1.2056	1.2312	1.2013	1.1647	1.2018	1.1980	1.2027	1.1895	1.2008	1.2166	1.3321	1.3605	1.3485	1.3797	1.3521	1.3795	1.3771	1.3787	1.3725	1.3796	1.3957	**1.51**
H(8`A-8`C)	2.4772	2.4452	2.4019	2.4401	2.4019	2.4414	2.3990	2.4451	2.4021	2.4388	2.3752	2.9410	2.7694	2.7347	2.6983	2.6563	2.7041	2.5681	2.7092	2.5820	2.6922	2.5313	**2.71**
Nuclei	OLYP											OLYP										
C1	132.8188	134.1516	135.6656	135.1449	137.5235	135.1515	135.6652	135.1532	135.8434	135.1337	135.7556	130.8981	132.7261	133.7888	133.6768	135.1782	133.6081	135.1883	133.5382	135.1931	133.7379	135.3980	**129.02**
C2	131.6623	131.6975	132.2794	131.7465	132.3472	131.7531	132.6913	131.7546	132.6220	131.7302	132.7039	131.2536	131.3661	132.0518	131.4162	132.0990	131.4235	132.5894	131.4250	132.5059	131.4005	132.5752	**132.19**
C3	115.3417	116.0422	116.6555	116.3161	116.9608	116.3056	117.2576	116.2899	117.1915	116.3169	117.3369	114.4114	116.0541	116.6230	116.3750	116.9979	116.3650	117.1604	116.3492	117.1047	116.3752	117.2329	**116.16**
C4	168.2126	169.2294	169.9205	169.5710	170.1814	169.5487	170.9191	169.5215	170.7744	169.5840	171.0771	168.4577	169.1151	169.8267	169.4427	170.2413	169.4360	170.4899	169.4224	170.3927	169.4386	170.6134	**166.89**
C5	113.3427	114.4633	115.0535	115.0655	115.7600	115.0339	116.1215	114.9960	116.0017	115.0864	116.2699	113.4100	114.5734	115.1849	115.1704	115.9016	115.1450	116.0297	115.1131	115.9473	115.1848	116.1602	**116.16**
C6	127.6886	129.4580	130.3992	130.3959	131.5991	130.3259	132.5021	130.2522	132.2325	130.4552	132.8719	132.4882	129.9940	131.1063	130.8821	132.4316	130.8446	132.8458	130.8002	132.6433	130.9066	133.1053	**132.19**
C7	195.3251	201.0301	202.9899	204.5243	206.1991	204.3850	209.0998	204.2443	208.2692	204.6535	209.6663	194.9333	204.0205	205.4470	206.3531	207.3591	206.2114	211.0678	206.0639	210.2799	206.4776	211.6073	**196.22**
C8	63.8385	65.2339	66.0677	65.6811	66.8369	65.6883	66.9203	65.6854	66.8721	65.6665	67.5606	62.8816	61.2250	62.0414	62.3546	63.1411	62.2822	64.2114	62.2081	64.0080	62.4201	64.4616	**59.75**
C9	22.0417	22.3211	22.5251	22.7061	22.8886	22.6962	23.1868	22.6811	23.0909	22.7070	23.3016	15.7972	18.8615	19.1193	19.1190	19.3070	19.1099	19.6432	19.0962	19.5371	19.1202	19.9486	**15.44**
C8`	36.5297	37.3375	37.5614	37.8176	38.0745	37.8036	38.1673	37.7827	38.1190	37.8211	38.5013	31.4966	32.4077	32.6511	32.6378	32.9272	32.6373	32.7834	32.6299	32.8079	32.6276	32.7561	**31.11**
H2	8.3522	8.2235	8.1969	8.1272	8.0714	8.1268	8.2234	8.1264	8.2066	8.1267	8.2299	8.4369	8.2352	8.2566	8.1468	8.1702	8.1543	8.1611	8.1613	8.1618	8.1388	8.1574	**7.97**
H3	7.2072	7.3275	7.4178	7.4008	7.5127	7.3974	7.5330	7.3939	7.5211	7.4035	7.5445	7.1593	7.3325	7.4196	7.3792	7.4934	7.3770	7.5033	7.3746	7.4956	7.3809	7.5175	**7.22**
H5	7.0851	7.2353	7.3143	7.2988	7.4157	7.2941	7.4375	7.2893	7.4251	7.3029	7.4576	7.0403	7.2266	7.3145	7.2993	7.4188	7.2955	7.4288	7.2915	7.4188	7.3025	7.4474	**7.22**
H6	7.9775	8.1327	8.1956	8.2132	8.2977	8.2041	8.4009	8.1954	8.3698	8.2217	8.4374	8.7484	7.8865	7.9743	7.9576	8.1089	7.9547	8.1075	7.9514	8.0939	7.9595	8.1417	**7.97**
H8	4.5323	4.5911	4.6096	4.6267	4.6824	4.6200	4.7353	4.6144	4.7106	4.6332	4.7707	4.4883	4.7554	4.8166	4.8221	4.9436	4.8190	4.9419	4.8155	4.9305	4.8243	4.9712	**4.99**
H(9A-9C)	1.2237	1.2082	1.1959	1.1823	1.1420	1.1826	1.2055	1.1826	1.1992	1.1815	1.2218	1.2466	1.3653	1.3601	1.3854	1.3618	1.3848	1.3978	1.3840	1.3909	1.3856	1.4134	**1.51**
H(8`A-8`C)	2.5179	2.4873	2.4697	2.4886	2.4649	2.4895	2.4510	2.4902	2.4526	2.4873	2.4211	2.3523	2.8150	2.7687	2.7435	2.7024	2.7489	2.6101	2.7538	2.6211	2.7376	2.5695	**2.71**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S11. Cont. V

Nuclei	R											S										Exp. [b]
	OPBE																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	129.7640	131.1387	132.6552	132.1246	134.4950	132.1378	132.7494	132.1341	132.8307	132.0968	132.7529	127.9531	129.7572	131.3960	130.9073	132.9633	130.8138	132.2249	130.6965	132.6314	130.9636	132.5011	**129.02**
C2	130.3586	130.4886	130.9968	130.4429	131.0543	130.4635	131.3872	130.4661	131.3319	130.3820	131.3838	129.9865	130.2359	130.9157	130.1823	130.9380	130.1990	131.3075	130.1994	131.2030	130.1628	131.3207	**132.19**
C3	114.2213	115.0550	115.6259	115.3016	116.0144	115.3021	116.3293	115.2846	116.2561	115.3063	116.4542	114.3041	115.0698	115.5900	115.3365	116.0072	115.3394	116.2309	115.3240	116.1537	115.3295	116.3409	**116.16**
C4	164.6226	165.6789	166.2199	165.9412	166.5402	165.9340	167.2498	165.9090	167.1104	166.0101	167.4931	164.9027	165.5555	166.0292	165.7368	166.3569	165.7530	166.8192	165.7519	166.6262	165.7218	166.9648	**166.89**
C5	112.2687	113.5344	114.0760	114.0744	114.8381	114.0527	115.1922	114.0131	115.0739	114.1130	115.4008	112.4202	113.6143	114.1128	114.1369	114.8497	114.1271	115.0869	114.0994	114.9493	114.1433	115.2524	**116.16**
C6	126.1608	127.9997	128.8093	128.8180	129.9411	128.7696	130.8401	128.7038	130.6005	128.8489	131.2575	126.8203	128.5704	129.4079	129.2674	130.6027	129.2570	131.2141	129.2292	130.8690	129.2803	131.4889	**132.19**
C7	192.8626	198.3520	200.1588	201.6561	203.2107	201.5462	206.1754	201.4188	205.3233	201.7358	206.5747	196.3497	200.6868	202.1872	203.0429	204.1492	202.9127	207.7285	202.7568	207.1557	203.1474	208.2542	**196.22**
C8	61.2284	62.7133	63.5636	63.1881	64.3519	63.1850	64.4468	63.1637	64.3074	63.1720	65.1108	56.6311	58.7512	59.9248	59.9517	61.0884	59.8539	61.5973	59.7391	61.6414	60.0230	61.9029	**59.75**
C9	21.2805	21.6678	21.7922	21.9610	22.1440	21.9624	22.3933	21.9464	22.3075	21.9463	22.5303	17.8291	18.2838	18.5005	18.5007	18.7647	18.4933	18.9349	18.4692	18.8763	18.4996	19.2950	**15.44**
C8`	35.4845	36.3569	36.4549	36.7323	36.9249	36.7278	37.0000	36.7052	36.9687	36.7163	37.3820	31.0988	31.3654	31.3318	31.4174	31.5251	31.4408	31.6115	31.4469	31.5375	31.3965	31.5941	**31.11**
H2	8.3870	8.2642	8.2215	8.1564	8.0952	8.1575	8.2408	8.1577	8.2328	8.1562	8.2594	8.4575	8.2769	8.2227	8.1564	8.1258	8.1678	8.1855	8.1792	8.1490	8.1477	8.1810	**7.97**
H3	7.2282	7.3602	7.4433	7.4277	7.5438	7.4252	7.5609	7.4218	7.5508	7.4327	7.5779	7.2304	7.3678	7.4497	7.4149	7.5264	7.4130	7.5438	7.4104	7.5341	7.4158	7.5608	**7.22**
H5	7.1021	7.2653	7.3426	7.3260	7.4471	7.3219	7.4668	7.3170	7.4549	7.3330	7.4935	7.0869	7.2574	7.3371	7.3302	7.4448	7.3268	7.4602	7.3227	7.4473	7.3327	7.4817	**7.22**
H6	8.0380	8.1929	8.2297	8.2560	8.3210	8.2498	8.4322	8.2430	8.4104	8.2608	8.4821	7.8021	7.9511	7.9981	8.0067	8.1209	8.0068	8.1616	8.0062	8.1245	8.0072	8.1968	**7.97**
H8	4.5419	4.6115	4.6071	4.6376	4.6660	4.6345	4.7386	4.6308	4.7174	4.6371	4.7816	4.6657	4.7892	4.8168	4.8395	4.9337	4.8401	4.9559	4.8394	4.9298	4.8389	4.9886	**4.99**
H(9A-9C)	1.1827	1.1710	1.1506	1.1424	1.0922	1.1427	1.1573	1.1423	1.1499	1.1403	1.1786	1.2938	1.3294	1.3061	1.3393	1.2986	1.3395	1.3428	1.3392	1.3289	1.3389	1.3621	**1.51**
H(8`A-8`C)	2.4371	2.4087	2.3861	2.4045	2.3742	2.4058	2.3612	2.4063	2.3625	2.4000	2.3311	2.8529	2.7064	2.6163	2.6177	2.5447	2.6266	2.4933	2.6347	2.4903	2.6099	2.4549	**2.71**
Nuclei	OPW91																						
C1	130.0734	131.4711	132.9769	132.4406	134.8087	132.4451	133.0129	132.4321	133.1402	132.4191	133.0519	128.2394	130.0724	131.7005	131.1724	133.2463	131.0761	132.5216	130.9590	132.9078	131.2337	132.7953	**129.02**
C2	130.5806	130.7074	131.2089	130.6288	131.2637	130.6390	131.5719	130.6356	131.5478	130.6007	131.6048	130.1962	130.4533	131.1259	130.4042	131.1441	130.4116	131.5201	130.4034	131.4168	130.3802	131.5359	**132.19**
C3	114.4183	115.2508	115.8151	115.5092	116.1968	115.4994	116.5211	115.4732	116.4393	115.4999	116.6391	114.5029	115.2650	115.7792	115.5361	116.1909	115.5285	116.4136	115.5035	116.3378	115.5247	116.5251	**116.16**
C4	165.0246	166.0821	166.6217	166.4195	166.9443	166.4003	167.7080	166.3664	167.5188	166.4192	167.9027	165.3169	165.9654	166.4385	166.1639	166.7698	166.1681	167.2288	166.1553	167.0408	166.1434	167.3773	**166.89**
C5	112.4634	113.7286	114.2665	114.2944	115.0217	114.2618	115.3914	114.2128	115.2585	114.3067	115.5871	112.6210	113.8117	114.3056	114.3432	115.0398	114.3225	115.2744	114.2843	115.1397	114.3450	115.4419	**116.16**
C6	126.3826	128.2204	129.0301	129.0438	130.1652	128.9844	131.0735	128.9103	130.8310	129.0819	131.4938	127.0499	128.7969	129.6351	129.5203	130.8358	129.4965	131.4451	129.4563	131.1082	129.5270	131.7238	**132.19**
C7	193.2195	198.7503	200.5473	202.0469	203.6032	201.9273	206.5400	201.7965	205.7249	202.1429	206.9853	196.7445	201.1005	202.5918	203.4416	204.5479	203.3022	208.1416	203.1393	207.5501	203.5465	208.6706	**196.22**
C8	61.4164	62.9130	63.7519	63.3730	64.5345	63.3605	64.5943	63.3262	64.4929	63.3665	65.2823	56.7828	58.9381	60.1067	60.1087	61.2534	60.0077	61.7812	59.8918	61.8124	60.1818	62.0859	**59.75**
C9	21.3412	21.7318	21.8564	22.0225	22.2056	22.0139	22.4453	21.9905	22.3695	22.0127	22.5934	17.9020	18.3623	18.5810	18.5780	18.8386	18.5624	19.0151	18.5310	18.9558	18.5743	19.3737	**15.44**
C8`	35.5474	36.4260	36.5197	36.7969	36.9960	36.7816	37.0617	36.7522	37.0400	36.7928	37.4582	31.1915	31.4588	31.4241	31.5288	31.6223	31.5399	31.7046	31.5341	31.6351	31.5020	31.6928	**31.11**
H2	8.3887	8.2639	8.2222	8.1590	8.0961	8.1592	8.2467	8.1596	8.2338	8.1570	8.2615	8.4616	8.2780	8.2245	8.1636	8.1292	8.1736	8.1874	8.1840	8.1527	8.1537	8.1831	**7.97**
H3	7.2300	7.3612	7.4442	7.4326	7.5443	7.4293	7.5651	7.4261	7.5509	7.4339	7.5785	7.2318	7.3686	7.4505	7.4163	7.5267	7.4137	7.5442	7.4109	7.5345	7.4169	7.5610	**7.22**
H5	7.1042	7.2672	7.3446	7.3319	7.4481	7.3269	7.4705	7.3219	7.4560	7.3348	7.4945	7.0894	7.2592	7.3388	7.3327	7.4461	7.3286	7.4614	7.3242	7.4485	7.3348	7.4827	**7.22**
H6	8.0365	8.1901	8.2278	8.2553	8.3202	8.2483	8.4351	8.2419	8.4096	8.2601	8.4824	7.8035	7.9505	7.9980	8.0099	8.1218	8.0088	8.1616	8.0074	8.1258	8.0096	8.1969	**7.97**
H8	4.5413	4.6099	4.6067	4.6350	4.6660	4.6313	4.7388	4.6276	4.7179	4.6370	4.7820	4.6622	4.7853	4.8138	4.8390	4.9316	4.8382	4.9531	4.8368	4.9279	4.8379	4.9856	**4.99**
H(9A-9C)	1.1844	1.1724	1.1522	1.1437	1.0939	1.1434	1.1586	1.1424	1.1520	1.1425	1.1806	1.2943	1.3301	1.3074	1.3418	1.3002	1.3413	1.3445	1.3406	1.3308	1.3411	1.3636	**1.51**
H(8`A-8`C)	2.4383	2.4106	2.3882	2.4045	2.3762	2.4051	2.3601	2.4055	2.3644	2.4024	2.3329	2.8575	2.7104	2.6209	2.6250	2.5505	2.6328	2.4979	2.6400	2.4956	2.6165	2.4597	**2.71**
Nuclei	PBE																						
C1	135.5369	136.0918	137.1653	136.3677	138.3715	136.3432	137.9723	136.3302	138.0000	136.4097	138.2666	133.9549	135.5103	136.0530	136.0986	137.6401	136.0426	137.7558	136.0033	137.5912	136.1760	137.8979	**129.02**
C2	135.9657	136.0179	136.6216	135.7847	136.4967	135.7983	136.9066	135.8222	136.8094	135.7890	136.9073	135.2241	135.5670	136.1193	135.5057	136.3042	135.5028	136.8654	135.5121	136.7580	135.5269	136.8854	**132.19**
C3	119.4465	120.3299	120.8882	120.5608	121.3376	120.5455	121.6570	120.5407	121.5966	120.5927	121.7624	119.5345	120.3283	120.8574	120.5295	121.3174	120.5157	121.5667	120.5123	121.4938	120.5600	121.6702	**116.16**
C4	173.9823	175.0866	175.7504	175.5136	176.3815	175.4853	176.9469	175.4679	176.8322	175.5580	177.1272	174.3115	175.1027	175.8451	175.3569	176.3062	175.3425	176.6457	175.3376	176.5574	175.3868	176.8245	**166.89**
C5	117.3377	118.8348	119.4453	119.5117	120.4263	119.4676	120.7320	119.4345	120.6335	119.5712	120.9231	117.5420	118.8521	119.4821	119.4030	120.3643	119.3686	120.5554	119.3443	120.4643	119.4527	120.7344	**116.16**
C6	132.4775	134.5082	135.5902	135.4775	137.1352	135.4145	137.6377	135.3620	137.3771	135.5552	138.0465	132.8577	134.9572	136.2454	135.8915	137.7657	135.8360	138.2041	135.7900	138.0185	135.9600	138.5976	**132.19**
C7	200.2846	204.9361	206.5139	207.3187	208.7358	207.1695	213.0970	207.0319	212.3370	207.4784	214.0538	205.2335	209.1883	210.4404	211.1454	212.2526	211.0237	216.2129	210.9132	215.2932	211.2804	216.6930	**196.22**
C8	66.5088	67.7352	68.5365	68.0186	69.2245	67.9992	69.7030	67.9905	69.4643	68.0544	70.5121	60.8379	62.8084	63.3380	63.6487	64.6563	63.5816	65.3895	63.5289	65.1438	63.7343	65.6928	**59.75**
C9	23.3476	23.7914	23.9606	24.0315	24.4395	24.0128	24.5728	24.0048	24.4653	24.0668	24.7581	19.9739	20.6830	20.7908	20.8644	21.2357	20.8478	21.5194	20.8429	21.4105	20.8983	22.0261	**15.44**
C8`	37.1172	37.9328	38.1214	38.1135	38.5395	38.1010	38.7049	38.0990	38.6815	38.1431	39.1975	32.1770	32.4188	32.7113	32.5246	32.8859	32.5166	32.9628	32.5184	32.9920	32.5484	33.0440	**31.11**
H2	8.4940	8.4541	8.4552	8.4051	8.3713	8.4089	8.3990	8.4131	8.4018	8.4020	8.3885	8.5295	8.3765	8.4273	8.2992	8.3159	8.3056	8.2934	8.3120	8.3107	8.2932	8.2994	**7.97**
H3	7.2033	7.3447	7.4313	7.3857	7.5032	7.3838	7.5208	7.3823	7.5132	7.3881	7.5355	7.1915	7.3278	7.4143	7.3701	7.4921	7.3680	7.5036	7.3664	7.4955	7.3727	7.5186	**7.22**
H5	7.0554	7.2476	7.3344	7.3285	7.4528	7.3239	7.4719	7.3198	7.4630	7.3335	7.4950	7.0514	7.2254	7.3152	7.2983	7.4275	7.2942	7.4386	7.2906	7.4284	7.3027	7.4597	**7.22**
H6	8.0650	8.2613	8.3213	8.3484	8.4499	8.3435	8.4938	8.3391	8.4841	8.3536	8.5258	7.8075	7.9693	8.0875	8.0493	8.2174	8.0456	8.2265	8.0420	8.2172	8.0532	8.2729	**7.97**
H8	4.5942	4.6682	4.6640	4.7434	4.7783	4.7384	4.8154	4.7339	4.8140	4.7488	4.8411	4.7365	4.8721	4.9225	4.9285	5.0427	4.9260	5.0540	4.9238	5.0416	4.9312	5.0891	**4.99**
H(9A-9C)	1.3652	1.3737	1.3620	1.3582	1.3268	1.3594	1.3445	1.3610	1.3344	1.3577	1.3585	1.4620	1.4973	1.5000	1.5101	1.4967	1.5097	1.5158	1.5096	1.5145	1.5110	1.5442	**1.51**
H(8`A-8`C)	2.5658	2.4898	2.4677	2.4656	2.4518	2.4665	2.4330	2.4680	2.4322	2.4654	2.4135	3.0023	2.8324	2.7952	2.7516	2.7069	2.7580	2.6137	2.7646	2.6329	2.7457	2.5792	**2.71**
Nuclei	PBE0																						
C1	136.2247	136.6526	137.6494	136.8626	138.8179	136.8401	138.3389	136.8206	138.4202	136.8878	138.5165	135.0705	136.3670	136.9426	136.9688	138.3856	136.9063	138.4604	136.8512	138.1253	137.0380	138.5078	**129.02**
C2	138.7455	138.6972	139.2899	138.5224	139.1126	138.5294	139.6279	138.5381	139.4524	138.5187	139.5604	138.2240	138.3806	138.9274	138.3295	138.9750	138.3256	139.5396	138.3238	139.3720	138.3367	139.5045	**132.19**
C3	120.8925	121.6540	122.2093	121.9097	122.6105	121.8907	122.9447	121.8736	122.8377	121.9304	122.9696	120.9444	121.6525	122.1782	121.8956	122.5853	121.8764	122.8788	121.8592	122.7522	121.9012	122.9010	**116.16**
C4	172.7695	173.6677	174.2592	174.1060	174.7504	174.0748	175.4368	174.0455	175.2494	174.1384	175.5356	173.0167	173.6449	174.3079	173.9164	174.6482	173.8991	175.1081	173.8827	174.9805	173.9346	175.2141	**166.89**
C5	118.6951	120.1057	120.7177	120.8251	121.6797	120.7761	122.0034	120.7290	121.8560	120.8746	122.1212	118.8136	120.1112	120.7251	120.7385	121.6008	120.6967	121.8294	120.6564	121.6863	120.7809	121.9289	**116.16**
C6	134.9467	136.9717	138.0243	138.0376	139.4645	137.9675	140.0789	137.8990	139.7408	138.1064	140.4199	135.3034	137.3666	138.6127	138.3429	140.0727	138.2853	140.5728	138.2274	140.3897	138.3981	140.9095	**132.19**
C7	200.1830	205.0445	206.4951	207.5876	208.7013	207.4269	213.8365	207.2685	212.8952	207.7437	214.6933	204.6033	208.8622	210.0809	211.0822	211.8366	210.9380	216.6033	210.7982	215.3664	211.2259	217.0626	**196.22**
C8	62.4961	63.6480	64.3663	63.9871	64.9554	63.9622	65.4882	63.9393	65.2096	64.0139	66.1783	57.1221	58.8511	59.3074	59.6939	60.4822	59.6234	61.3132	59.5575	60.9413	59.7669	61.5421	**59.75**
C9	22.4232	22.7099	22.8836	22.9713	23.2313	22.9485	23.3154	22.9273	23.1815	22.9957	23.4231	19.1174	19.6122	19.6632	19.7712	20.0251	19.7540	20.2525	19.7389	20.1245	19.7907	20.6140	**15.44**
C8`	35.4509	36.2307	36.4509	36.4979	36.8360	36.4785	37.0927	36.4609	36.9944	36.5195	37.4940	30.7624	31.0177	31.3187	31.2114	31.4738	31.1980	31.6175	31.5195	31.1846	31.6291	31.2246	31.6596	**31.11**
H2	8.7291	8.6745	8.6839	8.6307	8.5912	8.6340	8.6207	8.6372	8.6136	8.6271	8.6069	8.7394	8.5811	8.6311	8.4997	8.5161	8.5067	8.4889	8.5132	8.5182	8.4920	8.4934	**7.97**
H3	7.3570	7.4984	7.5860	7.5429	7.6585	7.5407	7.6805	7.5383	7.6697	7.5447	7.6928	7.3444	7.4827	7.5699	7.5283	7.6473	7.5259	7.6672	7.5234	7.6563	7.5302	7.6796	**7.22**
H5	7.2043	7.3984	7.4865	7.4833	7.6061	7.4784	7.6287	7.4735	7.6162	7.4877	7.6494	7.1957	7.3777	7.4663	7.4563	7.5822	7.4518	7.5978	7.4472	7.5841	7.4603	7.6170	**7.22**
H6	8.1786	8.3833	8.4552	8.4878	8.5945	8.4818	8.6451	8.4757	8.6289	8.4931	8.6774	7.9635	8.1395	8.2598	8.2257	8.3971	8.2217	8.4076	8.2174	8.4040	8.2288	8.4520	**7.97**
H8	4.3167	4.4108	4.4199	4.5072	4.5534	4.5008	4.6039	4.4943	4.6020	4.5131	4.6265	4.4991	4.6448	4.7045	4.7095	4.8253	4.7065	4.8443	4.7033	4.8349	4.7119	4.8737	**4.99**
H(9A-9C)	1.3125	1.3212	1.3067	1.3099	1.2608	1.3109	1.2798	1.3118	1.2649	1.3088	1.2919	1.3963	1.4224	1.4195	1.4330	1.4094	1.4328	1.4284	1.4324	1.4298	1.4329	1.4515	**1.51**
H(8`A-8`C)	2.4651	2.3989	2.3727	2.3791	2.3574	2.3796	2.3472	2.3802	2.3450	2.3785	2.3301	2.8767	2.7128	2.6773	2.6349	2.5897	2.6409	2.5049	2.6468	2.5284	2.6289	2.4711	**2.71**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S11. Cont. VI

Nuclei	R											S										Exp. [b]
	TPSS																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	132.3080	132.7323	133.5947	132.9917	134.6209	132.9794	133.9174	132.9795	133.4835	133.0145	134.1627	130.9473	132.0464	132.8321	132.7165	134.1527	132.6760	133.8514	132.6492	133.7648	132.7685	133.9904	**129.02**
C2	133.0997	133.0157	133.6822	132.9050	133.5045	132.9199	133.9437	132.9461	133.4500	132.9010	133.9167	132.3746	132.5433	133.1843	132.5871	133.2524	132.5896	133.7520	132.6038	133.7197	132.5960	133.7438	**132.19**
C3	116.6148	117.2984	117.9237	117.5959	118.2555	117.5862	118.5980	117.5876	118.0301	117.6152	118.6571	116.6745	117.2824	117.8745	117.5564	118.2099	117.5476	118.4658	117.5497	118.7785	117.5754	118.5352	**116.16**
C4	170.6841	171.5811	172.3374	172.0858	172.8432	172.0623	173.5294	172.0498	172.7101	172.1186	173.6596	170.9980	171.6247	172.4068	171.9513	172.7573	171.9401	173.2076	171.9397	172.7606	171.9719	173.3439	**166.89**
C5	114.5838	115.8370	116.5194	116.5569	117.3608	116.5197	117.6964	116.4938	116.9319	116.6029	117.8309	114.7542	115.8493	116.5202	116.4562	117.2683	116.4268	117.4654	116.4086	117.6460	116.4943	117.6013	**116.16**
C6	129.6014	131.4435	132.6218	132.4972	133.9868	132.4389	134.5452	132.3920	132.8937	132.5630	134.9193	129.9037	131.8399	133.1059	132.8246	134.4809	132.7742	135.0675	132.7346	133.8495	132.8818	135.3960	**132.19**
C7	196.4615	200.8812	202.3135	203.2587	204.2943	203.1209	208.8163	202.9947	203.7788	203.4005	209.6447	201.0290	204.6160	205.9348	206.6362	207.5175	206.5206	211.4415	206.4167	206.9790	206.7570	211.9588	**196.22**
C8	65.1158	66.2120	66.9967	66.5823	67.5160	66.5694	67.7566	66.5676	66.8060	66.6049	68.5367	60.1278	61.8831	62.5632	62.8019	63.6923	62.7474	64.2607	62.7059	64.3460	62.8662	64.4976	**59.75**
C9	23.9382	24.2126	24.5053	24.5049	24.8006	24.4912	24.8817	24.4888	24.5589	24.5284	25.0320	20.6506	21.2665	21.4915	21.5390	21.8543	21.5290	22.1455	21.5306	23.4796	21.5593	22.5571	**15.44**
C8`	37.5256	38.2274	38.5539	38.5318	38.8578	38.5228	39.1217	38.5251	38.6513	38.5508	39.5382	33.2385	33.3352	33.6679	33.4955	33.7511	33.4908	33.9306	33.4973	35.3565	33.5099	33.9584	**31.11**
H2	8.5053	8.4506	8.4858	8.4146	8.4078	8.4174	8.4634	8.4207	8.2608	8.4123	8.4454	8.5333	8.3896	8.4302	8.3110	8.3267	8.3165	8.3314	8.3222	8.4330	8.3060	8.3282	**7.97**
H3	7.1662	7.3060	7.4014	7.3539	7.4751	7.3516	7.4934	7.3498	7.1856	7.3564	7.5050	7.1476	7.2856	7.3782	7.3357	7.4586	7.3331	7.4748	7.3311	7.4493	7.3384	7.4865	**7.22**
H5	7.0222	7.2106	7.3064	7.2978	7.4257	7.2928	7.4508	7.2885	7.1240	7.3028	7.4683	7.0178	7.1891	7.2832	7.2681	7.3973	7.2637	7.4087	7.2598	7.3786	7.2727	7.4263	**7.22**
H6	7.9512	8.1457	8.2359	8.2495	8.3724	8.2435	8.4400	8.2381	8.0774	8.2555	8.4692	7.7288	7.9081	8.0237	7.9982	8.1671	7.9933	8.1988	7.9889	8.1022	8.0030	8.2393	**7.97**
H8	4.4709	4.5419	4.5602	4.6283	4.6855	4.6222	4.7477	4.6168	4.4417	4.6345	4.7669	4.5859	4.7329	4.7881	4.8006	4.9128	4.7971	4.9372	4.7941	4.9314	4.8041	4.9650	**4.99**
H(9A-9C)	1.3567	1.3679	1.3676	1.3629	1.3311	1.3636	1.3485	1.3649	1.1767	1.3626	1.3622	1.4392	1.4842	1.4857	1.5034	1.4900	1.5025	1.5193	1.5021	1.6640	1.5046	1.5408	**1.51**
H(8`A-8`C)	2.5215	2.4527	2.4256	2.4341	2.4118	2.4348	2.3810	2.4361	2.2522	2.4338	2.3643	2.9653	2.7995	2.7626	2.7257	2.6817	2.7310	2.6015	2.7368	2.8894	2.7208	2.5649	**2.71**
Nuclei	VSXC																					
C1	130.0829	130.4045	131.1400	130.4934	131.6615	130.4929	131.1365	130.4902	131.2057	130.4951	131.2579	129.9454	130.6445	131.8488	131.2031	132.5520	131.1505	132.4267	131.1004	132.2788	131.2589	132.5715	**129.02**
C2	131.4719	131.5765	132.0332	131.5476	131.9755	131.5536	132.4149	131.5574	132.3103	131.5434	132.5007	131.5035	131.5629	132.0835	131.4748	131.9974	131.4854	132.4275	131.4940	132.3584	131.4659	132.4408	**132.19**
C3	115.0253	115.9281	116.4781	116.3182	116.9617	116.2986	117.2532	116.2767	117.1666	116.3381	117.3602	115.1018	115.8625	116.3437	116.1552	116.7869	116.1441	116.9700	116.1304	116.9294	116.1665	117.0707	**116.16**
C4	168.4085	169.4140	170.1094	169.9432	170.7388	169.9139	171.2602	169.8824	171.1101	169.9727	171.4432	168.2644	169.1345	169.7602	169.5550	170.3438	169.5352	170.7332	169.5129	170.6261	169.5745	170.8988	**166.89**
C5	112.9381	114.3706	114.9696	115.1434	115.9400	115.0989	116.2089	115.0522	116.0882	115.1874	116.3893	112.8384	114.1341	114.6817	114.8040	115.5837	114.7687	115.7340	114.7306	115.6555	114.8386	115.8930	**116.16**
C6	129.7735	131.5896	132.6289	132.6050	134.1264	132.5458	134.6888	132.4845	134.4417	132.6624	135.0466	129.7921	131.8114	132.8618	132.8875	134.4094	132.8259	134.9250	132.7615	134.6909	132.9470	135.2245	**132.19**
C7	190.4964	194.5948	195.8890	196.6716	197.5040	196.5484	201.3041	196.4236	200.4899	196.7897	202.0685	192.4201	196.4292	197.9570	198.6054	199.5513	198.4654	203.3086	198.3255	202.3644	198.7417	203.9258	**196.22**
C8	71.0293	71.8644	72.4464	72.1610	72.9614	72.1470	73.3160	72.1307	73.2068	72.1762	73.9137	63.2954	64.4627	65.0975	65.1337	65.9999	65.0894	66.5041	65.0447	66.3060	65.1788	66.9366	**59.75**
C9	27.6811	28.6013	28.9238	29.2582	29.7109	29.2182	30.0806	29.1763	29.9393	29.2980	30.1347	28.6031	28.7198	28.7057	28.8776	29.0104	28.8658	28.9877	28.8527	28.9354	28.8913	29.2920	**15.44**
C8`	40.4536	40.9423	41.0239	41.1700	41.3482	41.1601	41.3711	41.1480	41.3482	41.1808	41.7912	35.6942	36.3333	36.3426	36.5410	36.8365	36.5434	36.8289	36.5411	36.8765	36.5384	37.0830	**31.11**
H2	8.7013	8.6318	8.6383	8.5965	8.5956	8.5987	8.6008	8.6009	8.6015	8.5945	8.6002	8.6698	8.5714	8.5462	8.4980	8.4914	8.5044	8.4746	8.5105	8.4951	8.4915	8.4705	**7.97**
H3	7.2076	7.3421	7.4286	7.3891	7.5038	7.3867	7.5214	7.3843	7.5128	7.3914	7.5352	7.2377	7.3761	7.4621	7.4257	7.5415	7.4230	7.5574	7.4205	7.5480	7.4281	7.5730	**7.22**
H5	7.1085	7.2957	7.3836	7.3798	7.5056	7.3750	7.5203	7.3702	7.5095	7.3844	7.5443	7.1230	7.2984	7.3840	7.3775	7.4993	7.3729	7.5080	7.3684	7.4968	7.3817	7.5256	**7.22**
H6	8.1799	8.3473	8.4451	8.4415	8.5921	8.4354	8.6432	8.4296	8.6230	8.4472	8.6738	7.8041	7.9933	8.0857	8.0898	8.2480	8.0846	8.2771	8.0794	8.2615	8.0945	8.3072	**7.97**
H8	4.3876	4.4583	4.4912	4.5227	4.5993	4.5183	4.6338	4.5141	4.6138	4.5269	4.6595	4.6175	4.7683	4.8270	4.8563	4.9599	4.8507	5.0035	4.8453	4.9843	4.8616	5.0218	**4.99**
H(9A-9C)	1.5961	1.6138	1.6048	1.6171	1.6025	1.6170	1.6242	1.6171	1.6201	1.6172	1.6378	1.7731	1.7717	1.7506	1.7772	1.7569	1.7769	1.7723	1.7766	1.7683	1.7776	1.7889	**1.51**
H(8`A-8`C)	2.6858	2.6354	2.6002	2.6143	2.5757	2.6156	2.5544	2.6170	2.5572	2.6129	2.5289	2.8671	2.7641	2.7059	2.7132	2.6678	2.7172	2.6228	2.7210	2.6423	2.7093	2.5927	**2.71**
Nuclei	wB97																					
C1	136.3743	136.5643	137.5508	136.6805	138.3186	136.6682	137.1758	136.6563	137.6400	136.6935	137.3306	135.5496	136.5810	137.2430	137.2393	138.6376	137.1701	138.5360	137.1091	138.2897	137.3170	138.7211	**129.02**
C2	140.2891	140.1704	140.7301	140.0418	140.6111	140.0495	141.1373	140.0566	141.0098	140.0348	141.1780	140.0931	140.0448	140.6006	139.9574	140.5644	139.9621	140.9964	139.9662	140.9089	139.9528	141.0199	**132.19**
C3	121.6439	122.2148	122.7714	122.4318	123.1041	122.4188	123.2000	122.4051	123.1728	122.4445	123.2668	121.6716	122.2096	122.7417	122.4350	123.1020	122.4187	123.2279	122.4023	123.1663	122.4515	123.2949	**116.16**
C4	174.2577	174.9242	175.5185	175.3214	175.9512	175.2956	176.5447	175.2691	176.3511	175.3461	176.6908	174.3838	174.8494	175.5012	175.0939	175.7994	175.0823	176.1349	175.0683	176.0692	175.1036	176.2686	**166.89**
C5	119.4831	120.7345	121.3443	121.4210	122.2577	121.3777	122.3482	121.3337	122.2709	121.4624	122.5094	119.5892	120.7784	121.3962	121.3974	122.2486	121.3581	122.3057	121.3179	122.2298	121.4354	122.4485	**116.16**
C6	136.8221	138.8055	139.9029	139.8974	141.4938	139.8285	142.2089	139.7589	141.7730	139.9631	142.5634	137.0806	139.0577	140.2748	140.0174	141.7669	139.9692	142.1277	139.9168	141.9973	140.0596	142.4749	**132.19**
C7	200.5554	205.5196	206.9736	208.1930	208.8203	208.0253	213.7590	207.8570	212.9387	208.3529	214.6659	204.2854	208.7429	210.1036	211.2165	211.7853	211.0496	216.9049	210.8871	215.6715	211.3809	217.6015	**196.22**
C8	61.2286	62.1722	62.8269	62.5542	63.4515	62.5338	63.8040	62.5119	63.7336	62.5735	64.4107	55.7397	57.1823	57.6139	58.0157	58.7514	57.9530	59.4666	57.8934	59.1612	58.0807	59.7826	**59.75**
C9	22.0700	22.2380	22.4228	22.4373	22.8248	22.4194	22.7743	22.4016	22.6602	22.4557	22.8715	19.5465	19.7727	19.7821	19.8738	20.1420	19.8648	20.1501	19.8559	20.0913	19.8837	20.5181	**15.44**
C8`	35.1652	35.7649	35.9908	36.0743	36.3679	36.0567	36.5472	36.0377	36.5002	36.0907	36.9598	30.5263	30.8779	31.2072	31.0800	31.3808	31.0803	31.3789	31.0759	31.4642	31.0751	31.4895	**31.11**
H2	8.8384	8.7915	8.8061	8.7534	8.7565	8.7561	8.8198	8.7586	8.7788	8.7508	8.8177	8.8444	8.6993	8.7460	8.6049	8.6340	8.6136	8.5895	8.6213	8.6222	8.5954	8.5916	**7.97**
H3	7.4415	7.5770	7.6646	7.6196	7.7405	7.6173	7.7555	7.6149	7.7454	7.6217	7.7699	7.4525	7.5863	7.6739	7.6277	7.7500	7.6258	7.7576	7.6236	7.7514	7.6295	7.7730	**7.22**
H5	7.3028	7.4922	7.5805	7.5754	7.7036	7.5705	7.7161	7.5655	7.7041	7.5800	7.7398	7.3123	7.4932	7.5821	7.5675	7.6967	7.5632	7.7017	7.5588	7.6926	7.5714	7.7244	**7.22**
H6	8.2363	8.4473	8.5401	8.5626	8.6990	8.5558	8.7730	8.5487	8.7240	8.5691	8.8069	8.0771	8.2684	8.3886	8.3453	8.5299	8.3432	8.5210	8.3402	8.5241	8.3465	8.5617	**7.97**
H8	4.0794	4.2013	4.2289	4.3015	4.3612	4.2941	4.4167	4.2867	4.3964	4.3088	4.4426	4.2843	4.4417	4.5098	4.5068	4.6254	4.5039	4.6339	4.5005	4.6294	4.5091	4.6610	**4.99**
H(9A-9C)	1.3373	1.3502	1.3355	1.3434	1.3206	1.3441	1.3538	1.3446	1.3316	1.3428	1.3678	1.4052	1.4218	1.4124	1.4283	1.4126	1.4285	1.4264	1.4284	1.4276	1.4279	1.4449	**1.51**
H(8`A-8`C)	2.4600	2.4029	2.3721	2.3774	2.3594	2.3781	2.3295	2.3790	2.3441	2.3770	2.3180	2.8246	2.6620	2.6344	2.5859	2.5485	2.5907	2.4603	2.5952	2.4869	2.5812	2.4374	**2.71**
Nuclei	wB97X																					
C1	137.8029	138.0540	139.0211	138.1992	139.8961	138.1870	138.7316	138.1755	139.5920	138.2141	139.6814	136.9016	138.0110	138.6568	138.6712	140.0912	138.6060	140.0704	138.5482	139.7173	138.7443	140.1871	**129.02**
C2	140.7055	140.6032	141.1665	140.4847	141.0596	140.4945	141.6070	140.5037	141.4061	140.4762	141.5856	140.5526	140.5103	141.0764	140.4186	141.0232	140.4259	141.4852	140.4318	141.3445	140.4125	141.4959	**132.19**
C3	122.3475	122.9417	123.4842	123.1709	123.8319	123.1596	123.9911	123.1475	123.9336	123.1825	124.0993	122.3753	122.9427	123.4616	123.1718	123.8332	123.1584	124.0179	123.1444	123.8893	123.1862	124.0701	**116.16**
C4	174.9165	175.6237	176.2197	176.0405	176.6624	176.0165	177.3046	175.9916	177.0258	176.0640	177.3657	175.0408	175.5562	176.2009	175.8192	176.5285	175.8083	176.9078	175.7954	176.7811	175.8288	177.0410	**166.89**
C5	120.1726	121.4443	122.0434	122.1523	122.9687	122.1105	123.1411	122.0679	123.0163	122.1931	123.3151	120.2954	121.5031	122.1147	122.1275	122.9742	122.0916	123.0943	122.0548	122.9461	122.1629	123.2277	**116.16**
C6	137.1768	139.1619	140.2691	140.2457	141.8067	140.1813	142.5581	140.1156	141.8911	140.3073	142.5689	137.4753	139.4432	140.6731	140.4268	142.1500	140.3797	142.5033	140.3282	142.3574	140.4684	142.8687	**132.19**
C7	202.1768	207.1982	208.6196	209.9149	210.5679	209.7483	215.5392	209.5818	215.1279	210.0748	217.1331	206.1849	210.6989	211.9868	213.1284	213.7439	212.9665	218.9548	212.8080	217.5873	213.2885	219.5702	**196.22**
C8	62.2638	63.2785	63.9563	63.6403	64.5673	63.6254	64.9558	63.6092	64.7914	63.6554	65.6105	56.7269	58.2485	58.7010	59.1431	59.8693	59.0782	60.6326	59.0159	60.2657	59.2102	60.9139	**59.75**
C9	22.2545	22.4780	22.6788	22.6724	23.0493	22.6560	23.0235	22.6394	22.7994	22.6898	23.0038	19.5952	19.8548	19.8730	19.9815	20.2271	19.9737	20.2590	19.9655	20.1660	19.9902	20.6043	**15.44**
C8`	35.4261	36.0803	36.3153	36.4017	36.7065	36.3882	36.9314	36.3733	36.7947	36.4152	37.3166	30.7265	31.0292	31.3557	31.2646	31.5524	31.2617	31.6100	31.2549	31.6389	31.2646	31.7241	**31.11**
H2	8.8045	8.7552	8.7713	8.7178	8.7132	8.7209	8.7796	8.7237	8.6982	8.7149	8.6978	8.8202	8.6677	8.7159	8.5736	8.5991	8.5821	8.5540	8.5897	8.5893	8.5645	8.5574	**7.97**
H3	7.4131	7.5511	7.6385	7.5956	7.7147	7.5935	7.7298	7.5914	7.7207	7.5978	7.7443	7.4226	7.5575	7.6444	7.6018	7.7223	7.5997	7.7328	7.5974	7.7240	7.6039	7.7460	**7.22**
H5	7.2774	7.4679	7.5557	7.5537	7.6786	7.5490	7.6961	7.5442	7.6777	7.5583	7.7129	7.2894	7.4695	7.5577	7.5457	7.6732	7.5418	7.6791	7.5378	7.6674	7.5496	7.7001	**7.22**
H6	8.2021	8.4135	8.5069	8.5295	8.6573	8.5233	8.7307	8.5170	8.6684	8.5355	8.7254	8.0367	8.2260	8.3460	8.3104	8.4911	8.3074	8.4771	8.3036	8.4843	8.3126	8.5189	**7.97**
H8	4.1390	4.2501	4.2742	4.3513	4.4040	4.3440	4.4602	4.3368	4.4505	4.3585	4.4898	4.3255	4.4860	4.5491	4.5527	4.6724	4.5495	4.6828	4.5459	4.6757	4.5555	4.7093	**4.99**
H(9A-9C)	1.3232	1.3360	1.3236	1.3281	1.3024	1.3291	1.3388	1.3299	1.2880	1.3271	1.3094	1.3934	1.4128	1.4075	1.4242	1.4050	1.4244	1.4147	1.4244	1.4169	1.4237	1.4340	**1.51**
H(8`A-8`C)	2.4671	2.4104	2.3794	2.3869	2.3692	2.3875	2.3398	2.3882	2.3568	2.3865	2.3429	2.8470	2.6868	2.6544	2.6087	2.5717	2.6137	2.4834	2.6186	2.5074	2.6037	2.4553	**2.71**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S11. Cont. VII

Nuclei	R											S										Exp. [b]
	X3LYP											X3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.3564	139.8444	140.8482	140.1134	142.0566	140.0909	141.3658	140.0679	141.5227	140.1411	141.6467	137.9117	139.2562	139.9366	139.9579	141.5273	139.9149	141.3110	139.8710	141.2013	140.0058	141.3487	**129.02**
C2	139.9182	139.8474	140.4108	139.6953	140.1921	139.7116	140.6326	139.7238	140.5055	139.6831	140.6144	139.2169	139.3848	139.9238	139.3913	140.0004	139.3937	140.5425	139.3932	140.4245	139.3932	140.5430	**132.19**
C3	122.0092	122.6988	123.2345	122.9633	123.5748	122.9518	123.8529	122.9370	123.8097	122.9783	123.9078	122.1353	122.7433	123.2197	122.9818	123.5816	122.9719	123.7914	122.9587	123.7342	122.9949	123.8481	**116.16**
C4	176.1825	177.0882	177.7250	177.5818	178.2391	177.5544	178.8901	177.5242	178.7610	177.6114	179.0087	176.5499	177.1393	177.8065	177.4289	178.1522	177.4164	178.5567	177.4002	178.4628	177.4439	178.7115	**166.89**
C5	119.8141	121.1439	121.7439	121.8710	122.6356	121.8294	122.8875	121.7849	122.7972	121.9143	123.0321	119.9992	121.2093	121.7793	121.8153	122.5836	121.7831	122.7292	121.7474	122.6490	121.8494	122.8641	**116.16**
C6	136.1581	138.1629	139.2158	139.2637	140.6897	139.2042	141.2883	139.1404	140.9981	139.3229	141.6419	136.5146	138.5767	139.8645	139.6151	141.2627	139.5588	141.7748	139.4982	141.5895	139.6709	142.1688	**132.19**
C7	202.8571	207.9768	209.5518	210.7426	211.8371	210.5640	217.1792	210.3863	216.3022	210.9197	218.1127	208.1208	212.3136	213.4589	214.5395	215.3412	214.4092	220.0232	214.2763	218.9420	214.6672	220.5368	**196.22**
C8	65.0592	66.2153	66.9018	66.5407	67.5099	66.5316	67.8451	66.5179	67.6413	66.5516	68.6175	59.3212	61.3577	61.9949	62.3629	63.2348	62.3022	63.9246	62.2400	63.6812	62.4263	64.1714	**59.75**
C9	23.0316	23.3183	23.4327	23.5997	23.8343	23.5889	23.8506	23.5740	23.7548	23.6127	23.9870	19.5775	20.0461	20.2181	20.2904	20.5151	20.2799	20.6827	20.2663	20.6108	20.3042	21.0438	**15.44**
C8`	36.3944	37.1898	37.4326	37.5008	37.8523	37.4859	38.0604	37.4681	38.0401	37.5189	38.4847	31.9991	32.1508	32.4082	32.3228	32.5612	32.3139	32.6685	32.3014	32.6855	32.3346	32.7610	**31.11**
H2	8.6524	8.5918	8.6063	8.5511	8.5135	8.5549	8.5499	8.5579	8.5426	8.5473	8.5316	8.6901	8.5204	8.5632	8.4372	8.4423	8.4428	8.4297	8.4475	8.4451	8.4317	8.4405	**7.97**
H3	7.3213	7.4551	7.5439	7.5005	7.6121	7.4985	7.6290	7.4960	7.6209	7.5023	7.6416	7.3067	7.4391	7.5255	7.4863	7.6016	7.4841	7.6164	7.4812	7.6087	7.4884	7.6303	**7.22**
H5	7.1716	7.3592	7.4485	7.4464	7.5662	7.4416	7.5856	7.4362	7.5755	7.4510	7.6064	7.1634	7.3365	7.4251	7.4152	7.5364	7.4110	7.5463	7.4062	7.5365	7.4192	7.5665	**7.22**
H6	8.0809	8.2845	8.3663	8.3962	8.5098	8.3898	8.5716	8.3828	8.5557	8.4024	8.5971	7.8813	8.0490	8.1656	8.1364	8.2978	8.1318	8.3147	8.1265	8.3041	8.1406	8.3622	**7.97**
H8	4.3443	4.4331	4.4575	4.5383	4.5907	4.5308	4.6494	4.5230	4.6418	4.5456	4.6641	4.4903	4.6483	4.7010	4.7147	4.8269	4.7114	4.8459	4.7075	4.8333	4.7177	4.8776	**4.99**
H(9A-9C)	1.3227	1.3314	1.3179	1.3217	1.2790	1.3235	1.2915	1.3245	1.2806	1.3199	1.3039	1.3991	1.4351	1.4417	1.4560	1.4332	1.4550	1.4533	1.4534	1.4521	1.4569	1.4778	**1.51**
H(8`A-8`C)	2.5170	2.4557	2.4302	2.4400	2.4194	2.4409	2.4037	2.4412	2.4048	2.4393	2.3899	2.9813	2.8071	2.7639	2.7278	2.6788	2.7332	2.5951	2.7379	2.6158	2.7225	2.5651	**2.71**

[a] methyl protons shifts are averaged
[b] according to [3]

Table S12. Theoretical chemical shifts (in ppm) of *(R,S)*-4-fluoro-3-methyl-α-pyrrolidinopentiophenone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S										Exp. [b]
	B3LYP											B3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.3755	140.0427	142.7648	140.5668	143.1256	140.4942	142.1439	140.4324	142.3391	140.6510	142.5183	139.3757	140.0427	142.7649	140.5666	143.1255	140.4942	142.1439	140.4324	142.3392	140.6510	142.5183	**131.615**
C2	140.4036	140.2933	140.1983	140.0339	140.5590	140.0477	140.9647	140.0620	140.8421	140.0201	140.9432	140.4037	140.2932	140.1983	140.0341	140.5590	140.0477	140.9647	140.0620	140.8422	140.0202	140.9432	**133.405**
C3	133.9440	135.1377	136.1303	135.4566	136.4910	135.4358	136.8612	135.4144	136.7649	135.4750	137.0063	133.9439	135.1376	136.1302	135.4566	136.4910	135.4358	136.8612	135.4144	136.7650	135.4748	137.0063	**126.19**
C4	175.0792	176.1018	176.8933	176.6232	177.2539	176.5809	177.9822	176.5396	177.7833	176.6634	178.0779	175.0792	176.1018	176.8932	176.6231	177.2540	176.5809	177.9822	176.5396	177.7832	176.6633	178.0779	**165.04**
C5	119.1645	120.4066	121.4952	121.0395	121.8558	120.9904	122.1814	120.9432	122.0557	121.0871	122.3008	119.1644	120.4066	121.4953	121.0394	121.8560	120.9904	122.1814	120.9433	122.0557	121.0871	122.3008	**116.425**
C6	133.2854	134.9765	136.3836	135.8189	136.7443	135.7750	137.5550	135.7275	137.2382	135.8526	137.8211	133.2853	134.9766	136.3837	135.8189	136.7443	135.7750	137.5550	135.7275	137.2381	135.8527	137.8211	**129.92**
C7	204.0478	208.6264	212.4871	211.3148	212.8480	211.1090	217.7068	210.9135	216.7338	211.5241	218.9014	204.0478	208.6263	212.4873	211.3149	212.8477	211.1090	217.7068	210.9135	216.7338	211.5244	218.9014	**195.9**
C8	66.3870	67.4898	68.8273	68.0355	69.1880	67.9921	69.6095	67.9500	69.5372	68.0774	70.0273	66.3870	67.4897	68.8273	68.0357	69.1880	67.9921	69.6095	67.9500	69.5372	68.0774	70.0273	**67.6**
C9	38.8637	38.5069	38.1349	38.2985	38.4957	38.3121	38.6517	38.3239	38.5708	38.2809	38.7252	38.8637	38.5069	38.1349	38.2985	38.4955	38.3121	38.6517	38.3239	38.5708	38.2809	38.7252	**32.2**
C10	19.9220	20.4111	20.7730	20.6425	21.1338	20.6258	21.0400	20.6084	21.0077	20.6555	21.1435	19.9221	20.4111	20.7731	20.6426	21.1338	20.6258	21.0400	20.6083	21.0077	20.6555	21.1435	**23.4**
C11	16.1211	16.2907	16.1611	16.3120	16.5218	16.3082	16.4855	16.3038	16.4696	16.3129	16.6485	16.1210	16.2907	16.1610	16.3119	16.5218	16.3082	16.4855	16.3038	16.4696	16.3128	16.6486	**17.9**
C1`	52.3772	53.2656	53.9433	53.7458	54.3041	53.7148	54.2632	53.6829	54.2101	53.7723	54.6892	56.8929	58.0272	58.6062	58.4745	58.9669	58.4411	59.1773	58.4080	59.0987	58.5051	59.4059	**52.4**
C2`	26.1369	26.6323	26.8080	26.7823	27.1686	26.7692	27.2343	26.7556	27.2235	26.7928	27.1286	25.8015	25.9684	26.3079	26.0974	26.6686	26.0796	26.6164	26.0632	26.5864	26.1146	26.3895	**14.5**
C3`	25.8015	25.9683	26.3079	26.0972	26.6686	26.0796	26.6164	26.0632	26.5864	26.1146	26.3895	26.1368	26.6323	26.8080	26.7823	27.1686	26.7692	27.2343	26.7556	27.2235	26.7929	27.1286	**14.2**
C4`	56.8929	58.0273	58.6064	58.4745	58.9669	58.4411	59.1773	58.4080	59.0986	58.5051	59.4058	52.3772	53.2656	53.9433	53.7457	54.3041	53.7148	54.2632	53.6828	54.2101	53.7722	54.6892	**53.9**
H2	8.5043	8.4250	8.3022	8.3514	8.2863	8.3583	8.3299	8.3645	8.3140	8.3433	8.3138	8.5043	8.4250	8.3022	8.3514	8.2863	8.3583	8.3299	8.3645	8.3140	8.3433	8.3138	**8.13**
H5	7.0921	7.2500	7.4512	7.3157	7.4353	7.3115	7.4552	7.3074	7.4420	7.3196	7.4769	7.0921	7.2501	7.4512	7.3157	7.4353	7.3115	7.4552	7.3074	7.4420	7.3196	7.4769	**8.03**
H6	7.7808	7.9632	8.1461	8.0508	8.1302	8.0461	8.1971	8.0410	8.1685	8.0546	8.2240	7.7808	7.9632	8.1461	8.0509	8.1302	8.0461	8.1971	8.0410	8.1685	8.0546	8.2240	**7.4**
H(3``A-3``C)	2.3644	2.4096	2.4611	2.4225	2.4452	2.4212	2.4528	2.4200	2.4474	2.4236	2.4601	2.3644	2.4096	2.4611	2.4225	2.4452	2.4212	2.4528	2.4200	2.4474	2.4236	2.4601	**2.32**
H8	4.6160	4.6788	4.7835	4.7191	4.7676	4.7163	4.8213	4.7133	4.7986	4.7215	4.8118	4.6160	4.6788	4.7835	4.7191	4.7676	4.7163	4.8213	4.7133	4.7986	4.7215	4.8118	**5.64**
H(9A-9B)	1.6648	1.7163	1.7262	1.7361	1.7103	1.7367	1.7043	1.7364	1.6942	1.7345	1.7317	1.6648	1.7163	1.7262	1.7362	1.7103	1.7367	1.7043	1.7364	1.6942	1.7345	1.7317	**1.92**
H(10A)	1.0804	0.9756	0.8678	0.9260	0.8519	0.9290	0.9026	0.9321	0.8926	0.9229	0.9126	1.0804	0.9756	0.8678	0.9260	0.8519	0.9290	0.9026	0.9321	0.8926	0.9229	0.9126	**1.26**
H(10B)	1.7462	1.6391	1.5015	1.5641	1.4856	1.5682	1.4844	1.5724	1.4863	1.5600	1.4513	1.7462	1.6391	1.5015	1.5641	1.4856	1.5682	1.4844	1.5724	1.4863	1.5600	1.4513	**1.07**
H(11A-11C)	0.7741	0.7878	0.7686	0.7923	0.7528	0.7917	0.7585	0.7911	0.7541	0.7926	0.7490	0.7741	0.7878	0.7686	0.7923	0.7527	0.7917	0.7585	0.7911	0.7541	0.7926	0.7490	**0.78**
H(1`A)	2.7322	2.7249	2.6772	2.7097	2.6613	2.7105	2.6677	2.7112	2.6676	2.7087	2.6527	2.8527	2.8515	2.8315	2.8353	2.8156	2.8358	2.8203	2.8364	2.8237	2.8348	2.7952	**3.47**
H(1`B)	3.1916	3.2330	3.3417	3.2639	3.3258	3.2618	3.3041	3.2595	3.2957	3.2655	3.3097	2.8692	2.7005	2.7317	2.6722	2.7158	2.6720	2.6616	2.6722	2.6626	2.6726	2.6622	**3.63**
H(4`A)	2.8692	2.7005	2.7317	2.6722	2.7158	2.6720	2.6616	2.6722	2.6626	2.6726	2.6622	3.1916	3.2330	3.3417	3.2639	3.3258	3.2618	3.3041	3.2595	3.2957	3.2655	3.3097	**3.07**
H(4`B)	2.8526	2.8515	2.8315	2.8353	2.8156	2.8358	2.8203	2.8364	2.8237	2.8348	2.7952	2.7322	2.7249	2.6772	2.7097	2.6613	2.7105	2.6677	2.7112	2.6676	2.7087	2.6527	**3.25**
Nuclei	B3P86											B3P86										
C1	136.8295	137.4209	138.1401	137.8085	139.4870	137.7905	138.6374	137.7537	138.7146	137.8735	138.9687	136.8295	137.4209	138.1401	137.8085	139.4870	137.7903	138.6373	137.7538	138.7146	137.8734	138.9687	**131.615**
C2	139.6013	139.4796	139.9370	139.2408	139.8134	139.2819	140.0902	139.3003	140.1047	139.2447	140.0817	139.6012	139.4796	139.9370	139.2408	139.8134	139.2819	140.0904	139.3004	140.1047	139.2445	140.0817	**133.405**
C3	132.0870	133.3567	134.3510	133.7464	134.8443	133.7466	135.1908	133.7244	135.1953	133.7900	135.3475	132.0869	133.3568	134.3511	133.7464	134.8443	133.7465	135.1909	133.7244	135.1953	133.7900	135.3475	**126.19**
C4	172.5187	173.4314	174.1336	173.9211	174.5502	173.9074	175.3563	173.8729	175.2591	173.9788	175.5104	172.5188	173.4315	174.1336	173.9211	174.5501	173.9074	175.3563	173.8730	175.2590	173.9789	175.5104	**165.04**
C5	118.3657	119.6147	120.2815	120.2784	121.1201	120.2564	121.4226	120.2131	121.3943	120.3438	121.5872	118.3656	119.6147	120.2814	120.2784	121.1201	120.2565	121.4227	120.2131	121.3943	120.3438	121.5872	**116.425**
C6	132.3825	134.0649	135.1198	135.0139	136.3572	134.9801	137.0877	134.9234	136.9696	135.0884	137.4042	132.3824	134.0649	135.1197	135.0139	136.3572	134.9801	137.0878	134.9233	136.9696	135.0884	137.4042	**129.92**
C7	202.1737	206.4036	207.4086	208.8194	209.5878	208.6743	214.2270	208.5108	213.1729	209.0057	215.3496	202.1736	206.4036	207.4086	208.8194	209.5878	208.6745	214.2273	208.5110	213.1729	209.0055	215.3496	**195.9**
C8	64.6997	65.8115	66.2596	66.3673	67.3068	66.3501	67.7370	66.3121	67.6435	66.4284	68.1601	64.6995	65.8115	66.2596	66.3673	67.3068	66.3502	67.7370	66.3121	67.6435	66.4284	68.1601	**67.6**
C9	37.7290	37.4811	37.7349	37.3766	37.7863	37.4041	37.8947	37.4097	37.9104	37.3942	38.0409	37.7290	37.4811	37.7348	37.3766	37.7864	37.4041	37.8947	37.4098	37.9104	37.3942	38.0409	**32.2**
C10	18.6596	19.1347	19.4324	19.4345	19.9540	19.4372	19.8043	19.4179	19.8809	19.4755	19.9523	18.6596	19.1347	19.4324	19.4345	19.9539	19.4371	19.8043	19.4178	19.8809	19.4755	19.9523	**23.4**
C11	15.7178	15.8557	16.0180	15.9133	16.1369	15.9305	16.0762	15.9255	16.1701	15.9408	16.2599	15.7178	15.8557	16.0180	15.9133	16.1368	15.9304	16.0762	15.9255	16.1701	15.9408	16.2599	**17.9**
C1`	51.2961	52.1242	52.3788	52.6108	53.1461	52.6025	53.0963	52.5718	53.1618	52.6620	53.5407	55.5635	56.6358	57.0546	57.0874	57.5827	57.0806	57.8202	57.0522	57.8535	57.1376	58.0713	**52.4**
C2`	24.9356	25.3534	25.6763	25.5182	25.9499	25.5290	25.9593	25.5180	26.0584	25.5516	25.8309	24.4380	24.5916	25.0348	24.7215	25.2332	24.7318	25.1479	24.7206	25.2377	24.7560	24.9572	**14.5**
C3`	24.4379	24.5916	25.0349	24.7215	25.2332	24.7319	25.1479	24.7206	25.2377	24.7561	24.9571	24.9356	25.3534	25.6764	25.5182	25.9499	25.5291	25.9593	25.5179	26.0584	25.5516	25.8309	**14.2**
C4`	55.5634	56.6358	57.0546	57.0874	57.5828	57.0807	57.8202	57.0522	57.8535	57.1376	58.0713	51.2960	52.1242	52.3787	52.6108	53.1461	52.6024	53.0962	52.5719	53.1618	52.6620	53.5407	**53.9**
H2	8.5589	8.4844	8.5153	8.4223	8.4239	8.4288	8.4540	8.4331	8.4632	8.4171	8.4418	8.5589	8.4844	8.5153	8.4223	8.4239	8.4288	8.4540	8.4331	8.4632	8.4171	8.4418	**8.13**
H5	7.1119	7.2807	7.3752	7.3491	7.4737	7.3466	7.4871	7.3421	7.4823	7.3527	7.5085	7.1119	7.2807	7.3752	7.3491	7.4738	7.3466	7.4871	7.3421	7.4823	7.3527	7.5085	**8.03**
H6	7.8606	8.0344	8.1337	8.1253	8.2514	8.1211	8.3216	8.1150	8.3099	8.1305	8.3473	7.8606	8.0344	8.1337	8.1253	8.2514	8.1211	8.3216	8.1149	8.3099	8.1305	8.3473	**7.4**
H(3``A-3``C)	2.3528	2.3991	2.4152	2.4110	2.4349	2.4115	2.4414	2.4102	2.4420	2.4118	2.4506	2.3528	2.3991	2.4152	2.4110	2.4349	2.4115	2.4415	2.4102	2.4420	2.4118	2.4506	**2.32**
H8	4.6145	4.6807	4.7497	4.7251	4.7937	4.7231	4.8542	4.7194	4.8422	4.7282	4.8541	4.6145	4.6807	4.7497	4.7251	4.7937	4.7231	4.8543	4.7194	4.8422	4.7282	4.8541	**5.64**
H(9A-9B)	1.7347	1.7800	1.7641	1.8098	1.8250	1.8097	1.8119	1.8075	1.8121	1.8112	1.8427	1.7347	1.7799	1.7641	1.8098	1.8250	1.8097	1.8119	1.8075	1.8121	1.8112	1.8427	**1.92**
H(10A)	1.0371	0.9309	0.9356	0.8799	0.8098	0.8846	0.8521	0.8874	0.8556	0.8765	0.8620	1.0371	0.9308	0.9356	0.8799	0.8098	0.8846	0.8521	0.8874	0.8556	0.8765	0.8620	**1.26**
H(10B)	1.7619	1.6513	1.5951	1.5752	1.4998	1.5809	1.4980	1.5848	1.5093	1.5711	1.4652	1.7619	1.6513	1.5951	1.5752	1.4998	1.5809	1.4980	1.5848	1.5093	1.5711	1.4652	**1.07**
H(11A-11C)	0.7378	0.7516	0.7360	0.7562	0.7247	0.7571	0.7305	0.7562	0.7358	0.7566	0.7228	0.7378	0.7517	0.7360	0.7562	0.7247	0.7570	0.7305	0.7562	0.7358	0.7566	0.7228	**0.78**
H(1`A)	2.6871	2.6842	2.6690	2.6754	2.6359	2.6771	2.6413	2.6769	2.6461	2.6750	2.6265	2.8044	2.8092	2.7946	2.7927	2.7700	2.7948	2.7756	2.7951	2.7802	2.7920	2.7503	**3.47**
H(1`B)	3.1964	3.2353	3.2638	3.2658	3.3315	3.2649	3.3071	3.2621	3.3065	3.2680	3.3120	2.9088	2.7204	2.6825	2.6841	2.6992	2.6860	2.6352	2.6862	2.6315	2.6838	2.6379	**3.63**
H(4`A)	2.9088	2.7204	2.6825	2.6841	2.6992	2.6860	2.6352	2.6862	2.6315	2.6838	2.6379	3.1964	3.2353	3.2638	3.2658	3.3316	3.2649	3.3071	3.2621	3.3065	3.2680	3.3120	**3.07**
H(4`B)	2.8044	2.8092	2.7946	2.7927	2.7700	2.7948	2.7756	2.7951	2.7802	2.7920	2.7503	2.6871	2.6842	2.6690	2.6754	2.6359	2.6770	2.6413	2.6769	2.6461	2.6750	2.6265	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. I

Nuclei	R											S										Exp. [b]
	B3PW91											B3PW91										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.0403	137.7221	138.3072	138.2788	140.9199	138.2202	139.8997	138.1604	140.0100	138.3475	140.3049	137.0402	137.7220	138.3071	138.2786	140.6011	138.2202	139.8996	138.1604	140.0101	138.3475	140.3050	**131.615**
C2	139.7092	139.6170	140.0050	139.3682	140.2496	139.3928	140.2496	139.4080	140.1605	139.3461	140.2213	139.7090	139.6170	140.0049	139.3681	139.9306	139.3928	140.2497	139.4080	140.1606	139.3461	140.2214	**133.405**
C3	132.1402	133.4300	134.3487	133.8139	135.2383	133.7985	135.2880	133.7742	135.2004	133.8304	135.4588	132.1401	133.4300	134.3486	133.8140	134.9193	133.7985	135.2878	133.7742	135.2003	133.8304	135.4587	**126.19**
C4	172.6321	173.5898	174.2255	174.0868	175.0779	174.0584	175.4870	174.0212	175.3174	174.1168	175.5947	172.6321	173.5898	174.2255	174.0869	174.7589	174.0584	175.4870	174.0212	175.3174	174.1168	175.5946	**165.04**
C5	118.5053	119.7733	120.3612	120.4279	121.6393	120.3901	121.6485	120.3440	121.5329	120.4669	121.7955	118.5053	119.7734	120.3612	120.4278	121.3203	120.3901	121.6487	120.3440	121.5330	120.4669	121.7954	**116.425**
C6	132.3426	134.0470	135.0527	134.9248	136.2711	134.8833	136.5931	134.8310	136.3313	134.9622	136.8953	132.3425	134.0471	135.0527	134.9248	135.9521	134.8833	136.5932	134.8310	136.3313	134.9622	136.8954	**129.92**
C7	202.1763	206.5424	207.4324	209.1500	210.7982	208.9626	215.3942	208.7747	214.3674	209.3414	216.6349	202.1763	206.5427	207.4323	209.1498	210.4790	208.9626	215.3942	208.7747	214.3675	209.3414	216.6349	**195.9**
C8	64.6471	65.8094	66.1215	66.4144	67.8268	66.3722	67.9977	66.3240	67.8865	66.4604	68.5238	64.6471	65.8094	66.1214	66.4144	67.5078	66.3722	67.9978	66.3240	67.8864	66.4604	68.5238	**67.6**
C9	37.2320	37.0096	37.2074	36.8817	37.4464	36.8940	37.1930	36.8976	37.1256	36.8715	37.3336	37.2320	37.0096	37.2074	36.8818	37.1274	36.8940	37.1930	36.8976	37.1255	36.8715	37.3336	**32.2**
C10	18.6232	19.1379	19.3618	19.4063	20.1898	19.3958	19.7341	19.3763	19.7148	19.4177	19.9053	18.6232	19.1379	19.3618	19.4063	19.8708	19.3958	19.7341	19.3763	19.7147	19.4177	19.9053	**23.4**
C11	15.7464	15.9094	15.9924	15.9450	16.4560	15.9486	16.0764	15.9430	16.0768	15.9432	16.2582	15.7464	15.9095	15.9924	15.9450	16.1371	15.9486	16.0764	15.9430	16.0768	15.9432	16.2582	**17.9**
C1`	51.2166	52.0914	52.2518	52.5475	53.4078	52.5272	53.0134	52.4976	52.9857	52.5681	53.4769	55.5120	56.6077	56.9334	57.0536	57.5727	57.0315	57.7811	57.0008	57.7207	57.0768	58.0230	**52.4**
C2`	25.1812	25.6166	25.8406	25.7624	26.4873	25.7589	26.1784	25.7463	26.1896	25.7675	26.0594	24.7226	24.8846	25.2413	25.0099	25.5695	25.0044	25.5095	24.9903	25.5050	25.0177	25.2750	**14.5**
C3`	24.7226	24.8847	25.2412	25.0100	25.8886	25.0044	25.5095	24.9903	25.5050	25.0177	25.2750	25.1813	25.6166	25.8406	25.7625	26.1683	25.7589	26.1784	25.7463	26.1898	25.7675	26.0594	**14.2**
C4`	55.5120	56.6077	56.9334	57.0535	57.8918	57.0315	57.7811	57.0008	57.7207	57.0768	58.0229	51.2165	52.0915	52.2518	52.5475	53.0889	52.5272	53.0134	52.4976	52.9856	52.5681	53.4769	**53.9**
H2	8.5362	8.4551	8.4943	8.3800	8.3471	8.3877	8.3598	8.3944	8.3538	8.3719	8.3397	8.5362	8.4551	8.4943	8.3800	8.3316	8.3877	8.3598	8.3944	8.3538	8.3719	8.3397	**8.13**
H5	7.1068	7.2706	7.3648	7.3399	7.4780	7.3363	7.4860	7.3324	7.4744	7.3434	7.5067	7.1068	7.2707	7.3649	7.3399	7.4625	7.3363	7.4860	7.3324	7.4744	7.3434	7.5067	**8.03**
H6	7.8438	8.0201	8.1233	8.1067	8.2119	8.1028	8.2536	8.0982	8.2316	8.1102	8.2766	7.8438	8.0201	8.1233	8.1067	8.1964	8.1028	8.2536	8.0982	8.2316	8.1102	8.2766	**7.4**
H(3``A-3``C)	2.3434	2.3898	2.4059	2.4044	2.4441	2.4039	2.4399	2.4033	2.4369	2.4051	2.4461	2.3434	2.3899	2.4058	2.4044	2.4286	2.4039	2.4399	2.4033	2.4369	2.4051	2.4461	**2.32**
H8	4.6079	4.6693	4.7385	4.7110	4.7783	4.7091	4.8234	4.7066	4.8017	4.7128	4.8142	4.6079	4.6693	4.7385	4.7110	4.7628	4.7091	4.8234	4.7066	4.8017	4.7128	4.8142	**5.64**
H(9A-9B)	1.6892	1.7347	1.7214	1.7568	1.7451	1.7568	1.7107	1.7563	1.7050	1.7565	1.7395	1.6892	1.7347	1.7214	1.7568	1.7296	1.7568	1.7106	1.7563	1.7050	1.7565	1.7395	**1.92**
H(10A)	1.0241	0.9190	0.9195	0.8653	0.8106	0.8700	0.8492	0.8742	0.8418	0.8607	0.8539	1.0241	0.9190	0.9195	0.8653	0.7951	0.8700	0.8492	0.8742	0.8418	0.8607	0.8539	**1.26**
H(10B)	1.7216	1.6103	1.5615	1.5381	1.4733	1.5427	1.4533	1.5471	1.4588	1.5337	1.4193	1.7216	1.6104	1.5615	1.5381	1.4578	1.5427	1.4533	1.5471	1.4588	1.5337	1.4192	**1.07**
H(11A-11C)	0.7285	0.7397	0.7250	0.7442	0.7211	0.7444	0.7124	0.7444	0.7117	0.7441	0.6997	0.7285	0.7398	0.7250	0.7442	0.7057	0.7444	0.7124	0.7444	0.7117	0.7441	0.6997	**0.78**
H(1`A)	2.6823	2.6742	2.6584	2.6636	2.6340	2.6648	2.6258	2.6656	2.6272	2.6626	2.6099	2.8004	2.8017	2.7829	2.7872	2.7675	2.7883	2.7780	2.7892	2.7820	2.7864	2.7514	**3.47**
H(1`B)	3.1722	3.2108	3.2404	3.2414	3.3115	3.2398	3.2744	3.2379	3.2690	3.2430	3.2771	2.8663	2.6883	2.6542	2.6604	2.6903	2.6606	2.6394	2.6608	2.6378	2.6609	2.6369	**3.63**
H(4`A)	2.8663	2.6883	2.6542	2.6604	2.7058	2.6606	2.6394	2.6608	2.6378	2.6609	2.6369	3.1722	3.2108	3.2404	3.2414	3.2960	3.2398	3.2744	3.2379	3.2690	3.2430	3.2771	**3.07**
H(4`B)	2.8004	2.8017	2.7829	2.7872	2.7830	2.7883	2.7780	2.7892	2.7820	2.7864	2.7514	2.6823	2.6743	2.6584	2.6636	2.6185	2.6648	2.6258	2.6656	2.6272	2.6626	2.6099	**3.25**
Nuclei	B98											B98										
C1	137.9211	138.5798	139.2734	139.0736	141.4106	139.0383	140.6735	139.0051	140.8533	139.1162	141.0483	137.9211	138.5798	139.2734	139.0737	141.4108	139.0385	140.6735	139.0050	140.8533	139.1163	141.0483	**131.615**
C2	139.2758	139.1442	139.5291	138.9343	139.4902	138.9655	139.8079	138.9935	139.7159	138.9066	139.7756	139.2757	139.1443	139.5292	138.9344	139.4900	138.9655	139.8081	138.9935	139.7159	138.9066	139.7756	**133.405**
C3	132.6234	133.8277	134.7505	134.1920	135.2659	134.1883	135.6179	134.1818	135.5434	134.1975	135.7735	132.6234	133.8278	134.7505	134.1920	135.2657	134.1882	135.6180	134.1817	135.5435	134.1976	135.7735	**126.19**
C4	172.4828	173.3581	174.0426	173.8295	174.4933	173.8134	175.2262	173.7952	175.0530	173.8476	175.3221	172.4828	173.3579	174.0425	173.8295	174.4931	173.8133	175.2260	173.7951	175.0529	173.8475	175.3221	**165.04**
C5	118.2957	119.4783	120.0595	120.1013	120.9583	120.0766	121.2853	120.0500	121.1785	120.1276	121.4198	118.2957	119.4782	120.0595	120.1012	120.9582	120.0766	121.2852	120.0499	121.1785	120.1275	121.4198	**116.425**
C6	132.3682	134.0113	134.9610	134.9078	135.8816	134.8731	136.5314	134.8346	136.2545	134.9403	136.8059	132.3682	134.0113	134.9610	134.9078	135.8817	134.8731	136.5314	134.8345	136.2547	134.9403	136.8059	**129.92**
C7	200.6081	205.1118	206.1644	207.7224	209.0355	207.5537	214.1409	207.3876	213.1374	207.8924	215.3578	200.6081	205.1118	206.1644	207.7224	209.0354	207.5537	214.1409	207.3873	213.1373	207.8924	215.3578	**195.9**
C8	66.2711	67.3951	67.7401	67.9768	69.0758	67.9487	69.5517	67.9200	69.4808	68.0081	70.0175	66.2711	67.3952	67.7401	67.9768	69.0758	67.9488	69.5517	67.9200	69.4808	68.0081	70.0175	**67.6**
C9	38.5312	38.2384	38.4596	38.0938	38.3588	38.1174	38.4289	38.1386	38.3707	38.0734	38.5097	38.5312	38.2383	38.4596	38.0937	38.3587	38.1173	38.4288	38.1387	38.3706	38.0734	38.5097	**32.2**
C10	20.0430	20.4824	20.7437	20.7413	21.2037	20.7418	21.0840	20.7396	21.0723	20.7427	21.1981	20.0429	20.4824	20.7437	20.7413	21.2037	20.7418	21.0840	20.7396	21.0723	20.7428	21.1981	**23.4**
C11	16.3459	16.4532	16.5836	16.5049	16.7119	16.5173	16.6578	16.5269	16.6626	16.4951	16.8257	16.3459	16.4531	16.5836	16.5048	16.7119	16.5173	16.6578	16.5269	16.6627	16.4951	16.8257	**17.9**
C1`	52.4759	53.3041	53.5114	53.7966	54.3257	53.7837	54.2702	53.7677	54.2452	53.8101	54.7016	56.9251	57.9074	58.3002	58.3531	58.8738	58.3399	59.0782	58.3243	59.0187	58.3682	59.2848	**52.4**
C2`	26.3508	26.7353	27.0204	26.9044	27.3140	26.9079	27.3476	26.9089	27.3567	26.9035	27.2354	25.8887	26.0193	26.3702	26.1745	26.7324	26.1785	26.6952	26.1802	26.6902	26.1735	26.4841	**14.5**
C3`	25.8887	26.0193	26.3702	26.1745	26.7324	26.1785	26.6952	26.1802	26.6902	26.1734	26.4841	26.3510	26.7354	27.0204	26.9045	27.3140	26.9079	27.3475	26.9089	27.3567	26.9035	27.2354	**14.2**
C4`	56.9250	57.9073	58.3002	58.3531	58.8739	58.3399	59.0782	58.3242	59.0187	58.3682	59.2848	52.4759	53.3041	53.5114	53.7966	54.3257	53.7837	54.2702	53.7676	54.2452	53.8102	54.7016	**53.9**
H2	8.5336	8.4544	8.4877	8.3889	8.3455	8.3947	8.3689	8.4003	8.3585	8.3830	8.3487	8.5336	8.4544	8.4877	8.3889	8.3455	8.3947	8.3689	8.4003	8.3585	8.3830	8.3487	**8.13**
H5	7.1008	7.2669	7.3604	7.3367	7.4582	7.3328	7.4812	7.3290	7.4700	7.3407	7.5015	7.1008	7.2669	7.3604	7.3367	7.4582	7.3328	7.4812	7.3290	7.4700	7.3406	7.5015	**8.03**
H6	7.8185	7.9981	8.1054	8.0877	8.1781	8.0828	8.2390	8.0779	8.2142	8.0923	8.2641	7.8185	7.9981	8.1054	8.0877	8.1781	8.0829	8.2390	8.0779	8.2142	8.0923	8.2641	**7.4**
H(3``A-3``C)	2.3614	2.4093	2.4266	2.4231	2.4481	2.4224	2.4577	2.4218	2.4550	2.4242	2.4625	2.3614	2.4093	2.4266	2.4231	2.4481	2.4224	2.4577	2.4218	2.4550	2.4242	2.4625	**2.32**
H8	4.5750	4.6359	4.7129	4.6777	4.7297	4.6751	4.7972	4.6725	4.7740	4.6803	4.7838	4.5750	4.6359	4.7129	4.6777	4.7297	4.6751	4.7973	4.6725	4.7740	4.6803	4.7838	**5.64**
H(9A-9B)	1.6832	1.7296	1.7179	1.7516	1.7261	1.7509	1.7072	1.7501	1.7003	1.7522	1.7302	1.6832	1.7296	1.7179	1.7515	1.7261	1.7508	1.7072	1.7501	1.7003	1.7522	1.7302	**1.92**
H(10A)	1.0852	0.9633	0.9711	0.9093	0.8364	0.9135	0.8883	0.9176	0.8808	0.9054	0.8920	1.0852	0.9633	0.9711	0.9093	0.8364	0.9135	0.8883	0.9176	0.8808	0.9054	0.8920	**1.26**
H(10B)	1.7310	1.6250	1.5780	1.5509	1.4743	1.5554	1.4716	1.5599	1.4769	1.5471	1.4367	1.7310	1.6250	1.5780	1.5509	1.4743	1.5554	1.4716	1.5599	1.4769	1.5471	1.4367	**1.07**
H(11A-11C)	0.7552	0.7650	0.7507	0.7698	0.7308	0.7695	0.7370	0.7693	0.7356	0.7702	0.7241	0.7552	0.7650	0.7507	0.7697	0.7308	0.7695	0.7369	0.7693	0.7356	0.7702	0.7241	**0.78**
H(1`A)	2.7001	2.6901	2.6759	2.6808	2.6348	2.6814	2.6447	2.6822	2.6467	2.6803	2.6314	2.8208	2.8186	2.8016	2.8037	2.7834	2.8045	2.7945	2.8055	2.7997	2.8032	2.7681	**3.47**
H(1`B)	3.1860	3.2218	3.2579	3.2526	3.3082	3.2505	3.2906	3.2485	3.2844	3.2547	3.2913	2.8627	2.7059	2.6760	2.6765	2.7080	2.6772	2.6656	2.6781	2.6671	2.6764	2.6609	**3.63**
H(4`A)	2.8627	2.7059	2.6708	2.6765	2.7080	2.6772	2.6656	2.6781	2.6671	2.6764	2.6609	3.1860	3.2218	3.2579	3.2526	3.3082	3.2505	3.2906	3.2485	3.2844	3.2547	3.2913	**3.07**
H(4`B)	2.8208	2.8185	2.8016	2.8037	2.7834	2.8045	2.7945	2.8055	2.7997	2.8031	2.7681	2.7001	2.6901	2.6760	2.6808	2.6348	2.6814	2.6447	2.6822	2.6467	2.6803	2.6314	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. II

Nuclei	R											S										Exp. [b]
	B971											B971										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.5023	138.1554	138.8248	138.6517	140.5655	138.6077	140.2965	138.5669	140.4574	138.7038	140.6705	137.5023	138.1554	138.8249	138.6515	140.5654	138.6077	140.2965	138.5670	140.4576	138.7038	140.6704	**131.615**
C2	138.9808	138.8679	139.2516	138.6718	139.2349	138.6951	139.5148	138.7171	139.4247	138.6555	139.4835	138.9808	138.8679	139.2516	138.6718	139.2348	138.6951	139.5148	138.7171	139.4247	138.6555	139.4835	**133.405**
C3	132.3901	133.6047	134.5247	133.9773	135.0276	133.9658	135.3912	133.9534	135.3152	133.9941	135.5527	132.3901	133.6047	134.5247	133.9773	135.0276	133.9658	135.3912	133.9534	135.3151	133.9939	135.5527	**126.19**
C4	172.3979	173.2721	173.9443	173.7416	174.3753	173.7181	175.1405	173.6944	174.9699	173.7699	175.2418	172.3979	173.2721	173.9442	173.7416	174.3753	173.7180	175.1405	173.6944	174.9698	173.7698	175.2418	**165.04**
C5	118.0738	119.2602	119.8390	119.8882	120.6908	119.8562	121.0571	119.8240	120.9493	119.9247	121.1962	118.0738	119.2602	119.8389	119.8881	120.6908	119.8562	121.0571	119.8240	120.9493	119.9248	121.1962	**116.425**
C6	132.1219	133.7655	134.7170	134.6759	135.8521	134.6335	136.2608	134.5895	135.9936	134.7208	136.5477	132.1219	133.7655	134.7170	134.6759	135.8522	134.6336	136.2608	134.5895	135.9936	134.7210	136.5478	**129.92**
C7	200.5079	204.9371	205.9614	207.5218	208.4653	207.3457	213.9130	207.1744	212.9147	207.6995	215.1477	200.5079	204.9371	205.9615	207.5217	208.4653	207.3461	213.9130	207.1744	212.9147	207.6995	215.1476	**195.9**
C8	66.1003	67.2120	67.5690	67.7979	68.7688	67.7621	69.3420	67.7277	69.2645	67.8399	69.8154	66.1003	67.2120	67.5691	67.7979	68.7688	67.7621	69.3420	67.7277	69.2644	67.8400	69.8153	**67.6**
C9	38.5329	38.2732	38.5047	38.1445	38.4938	38.1598	38.4546	38.1749	38.3961	38.1364	38.5557	38.5328	38.2733	38.5048	38.1445	38.4939	38.1597	38.4546	38.1749	38.3961	38.1365	38.5558	**32.2**
C10	20.0511	20.4991	20.7580	20.7694	21.2305	20.7620	21.0941	20.7539	21.0801	20.7823	21.2157	20.0511	20.4990	20.7580	20.7694	21.2305	20.7620	21.0941	20.7539	21.0802	20.7823	21.2157	**23.4**
C11	16.2983	16.4105	16.5318	16.4740	16.6754	16.4782	16.6076	16.4817	16.6117	16.4758	16.7834	16.2983	16.4105	16.5318	16.4740	16.6755	16.4782	16.6076	16.4817	16.6116	16.4758	16.7834	**17.9**
C1`	52.4017	53.2148	53.4250	53.7169	54.2285	53.6959	54.1637	53.6737	54.1399	53.7420	54.6001	56.8263	57.7875	58.1812	58.2424	58.7303	58.2211	58.9632	58.1995	58.9039	58.2685	59.1712	**52.4**
C2`	26.1737	26.5501	26.8443	26.7385	27.1369	26.7335	27.1666	26.7281	27.1757	26.7492	27.0687	25.6913	25.8433	26.1892	26.0034	26.5164	25.9995	26.5178	25.9954	26.5127	26.0129	26.3215	**14.5**
C3`	25.6914	25.8433	26.1893	26.0034	26.5164	25.9996	26.5178	25.9954	26.5127	26.0128	26.3215	26.1737	26.5501	26.8443	26.7386	27.1370	26.7336	27.1667	26.7281	27.1757	26.7493	27.0687	**14.2**
C4`	56.8263	57.7875	58.1812	58.2423	58.7302	58.2211	58.9632	58.1996	58.9040	58.2683	59.1711	52.4017	53.2148	53.4251	53.7169	54.2285	53.6959	54.1637	53.6737	54.1399	53.7420	54.6001	**53.9**
H2	8.5316	8.4545	8.4879	8.3916	8.3798	8.3972	8.3696	8.4025	8.3605	8.3863	8.3500	8.5316	8.4545	8.4879	8.3916	8.3798	8.3972	8.3696	8.4025	8.3605	8.3863	8.3500	**8.13**
H5	7.1010	7.2667	7.3608	7.3363	7.4552	7.3324	7.4770	7.3285	7.4659	7.3404	7.4972	7.1010	7.2667	7.3608	7.3363	7.4552	7.3324	7.4770	7.3285	7.4659	7.3405	7.4972	**8.03**
H6	7.8264	8.0008	8.1059	8.0899	8.1973	8.0850	8.2380	8.0800	8.2146	8.0947	8.2627	7.8264	8.0008	8.1059	8.0899	8.1973	8.0850	8.2380	8.0800	8.2146	8.0948	8.2627	**7.4**
H(3``A-3``C)	2.3544	2.4012	2.4186	2.4152	2.4382	2.4143	2.4507	2.4135	2.4482	2.4165	2.4557	2.3544	2.4012	2.4186	2.4152	2.4382	2.4143	2.4507	2.4135	2.4481	2.4165	2.4557	**2.32**
H8	4.5787	4.6379	4.7146	4.6802	4.7383	4.6775	4.7988	4.6748	4.7764	4.6831	4.7847	4.5787	4.6379	4.7146	4.6802	4.7383	4.6775	4.7988	4.6748	4.7765	4.6831	4.7847	**5.64**
H(9A-9B)	1.6909	1.7338	1.7235	1.7575	1.7577	1.7566	1.7090	1.7555	1.7025	1.7588	1.7330	1.6909	1.7338	1.7235	1.7575	1.7578	1.7566	1.7090	1.7555	1.7025	1.7588	1.7330	**1.92**
H(10A)	1.0781	0.9592	0.9693	0.9078	0.8335	0.9117	0.8879	0.9156	0.8806	0.9042	0.8908	1.0781	0.9592	0.9693	0.9078	0.8335	0.9117	0.8879	0.9156	0.8806	0.9042	0.8909	**1.26**
H(10B)	1.7292	1.6230	1.5745	1.5490	1.4774	1.5533	1.4692	1.5576	1.4747	1.5455	1.4352	1.7292	1.6230	1.5745	1.5491	1.4774	1.5533	1.4692	1.5576	1.4748	1.5455	1.4353	**1.07**
H(11A-11C)	0.7494	0.7582	0.7437	0.7634	0.7279	0.7630	0.7298	0.7627	0.7288	0.7642	0.7171	0.7493	0.7582	0.7437	0.7634	0.7279	0.7630	0.7298	0.7627	0.7288	0.7642	0.7171	**0.78**
H(1`A)	2.6897	2.6816	2.6674	2.6745	2.6310	2.6748	2.6369	2.6753	2.6388	2.6745	2.6229	2.8111	2.8097	2.7940	2.7964	2.7732	2.7970	2.7869	2.7977	2.7919	2.7962	2.7601	**3.47**
H(1`B)	3.1902	3.2235	3.2584	3.2548	3.3141	3.2526	3.2902	3.2504	3.2844	3.2574	3.2904	2.8604	2.7056	2.6677	2.6758	2.6986	2.6761	2.6646	2.6768	2.6656	2.6761	2.6602	**3.63**
H(4`A)	2.8604	2.7056	2.6677	2.6758	2.6986	2.6761	2.6646	2.6768	2.6656	2.6761	2.6602	3.1902	3.2235	3.2584	3.2548	3.3141	3.2526	3.2903	3.2504	3.2844	3.2574	3.2904	**3.07**
H(4`B)	2.8111	2.8097	2.7940	2.7964	2.7733	2.7969	2.7869	2.7977	2.7919	2.7962	2.7601	2.6897	2.6816	2.6674	2.6745	2.6310	2.6749	2.6369	2.6753	2.6388	2.6745	2.6229	**3.25**
Nuclei	B972											B972										
C1	134.4281	135.1489	136.2116	136.2220	138.2141	136.1461	137.2162	136.0737	137.3801	136.2992	137.6722	134.4282	135.1488	136.2117	136.2220	138.2141	136.1461	137.2156	136.0736	137.3801	136.2993	137.6721	**131.615**
C2	137.0114	136.8759	137.3370	136.7029	137.2107	136.7149	137.5467	136.7241	137.4567	136.6860	137.5214	137.0114	136.8759	137.3372	136.7027	137.2107	136.7149	137.5468	136.7240	137.4567	136.6860	137.5214	**133.405**
C3	129.4761	130.6751	131.5774	131.1349	132.1706	131.1126	132.4963	131.0875	132.4150	131.1517	132.6733	129.4761	130.6751	131.5774	131.1350	132.1706	131.1126	132.4964	131.0874	132.4150	131.1518	132.6733	**126.19**
C4	169.3810	170.2839	170.9947	170.8307	171.3548	170.8062	172.0589	170.7779	171.8857	170.8484	172.1553	169.3810	170.2839	170.9946	170.8307	171.3548	170.8061	172.0590	170.7779	171.8857	170.8483	172.1552	**165.04**
C5	116.0208	117.1948	117.8247	117.9435	118.7106	117.8975	119.0111	117.8494	118.9013	117.9834	119.1617	116.0208	117.1948	117.8246	117.9434	118.7106	117.8975	119.0111	117.8494	118.9013	117.9834	119.1616	**116.425**
C6	129.7820	131.3511	132.1260	132.1091	133.1708	132.0629	133.9092	132.0131	133.6344	132.1456	134.1640	129.7819	131.3510	132.1261	132.1089	133.1708	132.0630	133.9095	132.0132	133.6344	132.1457	134.1639	**129.92**
C7	198.0969	202.4565	203.7760	205.5634	206.5521	205.3566	211.1615	205.1545	210.1947	205.7663	212.3969	198.0969	202.4566	203.7761	205.5632	206.5521	205.3566	211.1613	205.1545	210.1947	205.7664	212.3969	**195.9**
C8	63.3683	64.4415	64.9688	65.2435	66.2201	65.1775	66.6094	65.1144	66.5334	65.3088	67.0683	63.3683	64.4415	64.9688	65.2434	66.2201	65.1775	66.6089	65.1143	66.5334	65.3089	67.0683	**67.6**
C9	36.5430	36.2532	36.3741	36.1334	36.3972	36.1377	36.5148	36.1404	36.4525	36.1251	36.6258	36.5431	36.2532	36.3743	36.1333	36.3972	36.1378	36.5150	36.1405	36.4526	36.1252	36.6259	**32.2**
C10	18.7723	19.2439	19.4839	19.5650	20.0350	19.5449	19.9146	19.5224	19.8995	19.5801	20.0596	18.7724	19.2440	19.4840	19.5651	20.0350	19.5448	19.9146	19.5224	19.8995	19.5801	20.0597	**23.4**
C11	15.9213	16.0316	16.1329	16.1175	16.3056	16.1137	16.2484	16.1075	16.2495	16.1171	16.4222	15.9213	16.0316	16.1330	16.1176	16.3056	16.1137	16.2483	16.1075	16.2495	16.1170	16.4222	**17.9**
C1`	50.3924	51.2113	51.4065	51.7029	52.2259	51.6755	52.1413	51.6456	52.1125	51.7240	52.5743	54.6976	55.6987	56.0698	56.2264	56.6664	56.1964	56.8386	56.1643	56.7820	56.2507	57.0758	**52.4**
C2`	25.1067	25.4933	25.7434	25.7066	26.0791	25.6942	26.0912	25.6794	26.1035	25.7142	25.9753	24.6934	24.8150	25.2349	25.0281	25.5090	25.0192	25.4248	25.0071	25.4154	25.0316	25.2151	**14.5**
C3`	24.6934	24.8149	25.2350	25.0281	25.5090	25.0191	25.4253	25.0071	25.4154	25.0316	25.2150	25.1067	25.4933	25.7435	25.7066	26.0791	25.6942	26.0912	25.6794	26.1035	25.7142	25.9753	**14.2**
C4`	54.6976	55.6988	56.0698	56.2264	56.6664	56.1965	56.8384	56.1644	56.7820	56.2506	57.0758	50.3924	51.2113	51.4066	51.7028	52.2259	51.6755	52.1407	51.6457	52.1125	51.7239	52.5743	**53.9**
H2	8.5259	8.4359	8.4464	8.3267	8.2997	8.3351	8.3490	8.3425	8.3390	8.3176	8.3254	8.5259	8.4359	8.4464	8.3267	8.2997	8.3351	8.3490	8.3425	8.3390	8.3176	8.3253	**8.13**
H5	7.0970	7.2557	7.3422	7.3329	7.4529	7.3280	7.4745	7.3230	7.4633	7.3374	7.4960	7.0970	7.2557	7.3422	7.3329	7.4529	7.3280	7.4745	7.3230	7.4633	7.3374	7.4960	**8.03**
H6	7.8288	7.9988	8.0753	8.0672	8.1633	8.0638	8.2300	8.0599	8.2054	8.0700	8.2511	7.8288	7.9988	8.0753	8.0672	8.1633	8.0638	8.2300	8.0599	8.2054	8.0700	8.2511	**7.4**
H(3``A-3``C)	2.3521	2.3995	2.4188	2.4205	2.4384	2.4196	2.4486	2.4184	2.4454	2.4212	2.4549	2.3521	2.3995	2.4188	2.4205	2.4384	2.4196	2.4486	2.4184	2.4454	2.4212	2.4549	**2.32**
H8	4.5842	4.6361	4.6887	4.6705	4.7264	4.6688	4.7847	4.6667	4.7629	4.6718	4.7760	4.5842	4.6361	4.6887	4.6705	4.7264	4.6688	4.7847	4.6667	4.7629	4.6718	4.7760	**5.64**
H(9A-9B)	1.6515	1.6921	1.6557	1.6940	1.6871	1.6931	1.6861	1.6920	1.6797	1.6946	1.7088	1.6515	1.6921	1.6557	1.6940	1.6871	1.6931	1.6861	1.6921	1.6797	1.6946	1.7088	**1.92**
H(10A)	1.0437	0.9397	0.9161	0.8857	0.8210	0.8903	0.8712	0.8943	0.8635	0.8810	0.8808	1.0437	0.9397	0.9161	0.8857	0.8210	0.8903	0.8712	0.8943	0.8635	0.8810	0.8808	**1.26**
H(10B)	1.7027	1.5952	1.5541	1.5289	1.4487	1.5333	1.4496	1.5372	1.4540	1.5245	1.4176	1.7027	1.5952	1.5541	1.5289	1.4487	1.5332	1.4496	1.5372	1.4540	1.5245	1.4176	**1.07**
H(11A-11C)	0.7425	0.7519	0.7330	0.7583	0.7190	0.7580	0.7275	0.7574	0.7261	0.7584	0.7156	0.7425	0.7519	0.7330	0.7583	0.7190	0.7580	0.7275	0.7575	0.7261	0.7584	0.7156	**0.78**
H(1`A)	2.6841	2.6726	2.6522	2.6602	2.6150	2.6610	2.6233	2.6616	2.6251	2.6593	2.6057	2.8082	2.8081	2.7978	2.8011	2.7744	2.8016	2.7817	2.8019	2.7866	2.8006	2.7566	**3.47**
H(1`B)	3.1705	3.2089	3.2370	3.2399	3.2976	3.2376	3.2792	3.2351	3.2739	3.2421	3.2814	2.8427	2.6855	2.6639	2.6745	2.7047	2.6736	2.6513	2.6730	2.6523	2.6758	2.6524	**3.63**
H(4`A)	2.8427	2.6855	2.6639	2.6745	2.7047	2.6736	2.6513	2.6730	2.6523	2.6758	2.6524	3.1705	3.2089	3.2370	3.2400	3.2976	3.2376	3.2792	3.2351	3.2739	3.2421	3.2814	**3.07**
H(4`B)	2.8082	2.8081	2.7978	2.8011	2.7744	2.8016	2.7818	2.8019	2.7866	2.8005	2.7566	2.6841	2.6726	2.6522	2.6602	2.6150	2.6610	2.6233	2.6616	2.6251	2.6593	2.6057	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. III

Nuclei	R											S										Exp. [b]
	BHandH											BHandH										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	138.5231	139.0089	140.0484	139.2169	140.8206	139.2009	140.0353	139.2020	139.8269	139.2012	140.3005	138.5231	139.0089	140.0483	139.2169	139.9610	139.2009	140.0352	139.2020	139.8269	139.2013	140.3005	**131.615**
C2	143.6560	143.4520	144.0173	143.2363	143.7038	143.2417	144.0998	143.2650	144.0438	143.2009	144.0901	143.6561	143.4520	144.0173	143.2363	143.9804	143.2416	144.0998	143.2650	144.0437	143.2008	144.0902	**133.405**
C3	133.9273	135.1849	136.1533	135.5744	136.6556	135.5459	136.9059	135.5348	136.8238	135.5710	137.0520	133.9274	135.1849	136.1534	135.5744	136.3185	135.5457	136.9059	135.5348	136.8240	135.5709	137.0520	**126.19**
C4	172.9977	173.8020	174.3871	174.2354	174.7534	174.1977	175.4712	174.1786	175.3400	174.2414	175.5908	172.9977	173.8020	174.3872	174.2354	174.9795	174.1976	175.4712	174.1786	175.3401	174.2414	175.5907	**165.04**
C5	120.8195	122.1800	122.8532	122.8946	123.7688	122.8410	123.9883	122.8058	123.8658	122.9153	124.1428	120.8194	122.1800	122.8534	122.8946	123.6387	122.8411	123.9885	122.8058	123.8658	122.9153	124.1427	**116.425**
C6	136.8177	138.5905	139.5296	139.6440	141.0709	139.5616	141.8010	139.4990	141.6438	139.6930	142.2005	136.8176	138.5905	139.5296	139.6440	140.3881	139.5618	141.8010	139.4990	141.6438	139.6931	142.2006	**129.92**
C7	204.3560	208.8294	210.2410	211.2214	211.8276	211.0726	217.1203	210.9402	215.5238	211.3317	218.2226	204.3564	208.8294	210.2410	211.2214	211.9655	211.0722	217.1203	210.9402	215.5237	211.3320	218.2225	**195.9**
C8	59.9710	61.1513	61.9676	61.6176	62.4581	61.5856	63.0398	61.5711	62.7043	61.6170	63.4925	59.9711	61.1513	61.9677	61.6176	62.3617	61.5857	63.0397	61.5711	62.7043	61.6169	63.4926	**67.6**
C9	36.1990	35.9426	36.1735	35.7678	36.1538	35.7674	36.1778	35.7852	36.0766	35.7381	36.4154	36.1990	35.9426	36.1735	35.7678	36.5119	35.7674	36.1778	35.7852	36.0766	35.7381	36.4154	**32.2**
C10	16.4266	16.8265	17.2160	17.1627	17.6889	17.1304	17.5426	17.1165	17.5312	17.1634	17.7174	16.4266	16.8265	17.2160	17.1627	17.9068	17.1305	17.5426	17.1165	17.5311	17.1634	17.7174	**23.4**
C11	15.0818	15.1659	15.3458	15.2140	15.4221	15.2011	15.3850	15.2065	15.3937	15.1963	15.5738	15.0817	15.1659	15.3459	15.2140	15.9581	15.2012	15.3851	15.2065	15.3936	15.1963	15.5738	**17.9**
C1`	48.3052	49.0773	49.4876	49.5717	50.1422	49.5314	50.1232	49.5097	50.0703	49.5798	50.5682	52.1378	53.1666	53.5836	53.6420	54.3861	53.6044	54.3440	53.5850	54.2807	53.6476	54.6197	**52.4**
C2`	21.6445	22.0099	22.4106	22.1936	22.6486	22.1737	22.6993	22.1721	22.6448	22.1821	22.7065	21.0580	21.2399	21.5903	21.4125	22.1566	21.3904	21.8122	21.3868	21.8273	21.4037	21.7538	**14.5**
C3`	21.0579	21.2399	21.5903	21.4125	21.8971	21.3904	21.8122	21.3868	21.8273	21.4038	21.7539	21.6445	22.0099	22.4107	22.1936	22.9377	22.1737	22.6993	22.1721	22.6447	22.1821	22.7065	**14.2**
C4`	52.1378	53.1666	53.5836	53.6420	54.1928	53.6044	54.3439	53.5850	54.2807	53.6475	54.6198	48.3052	49.0773	49.4875	49.5717	50.3158	49.5315	50.1232	49.5097	50.0703	49.5798	50.5682	**53.9**
H2	8.8186	8.7294	8.7294	8.6790	8.6755	8.6823	8.6918	8.6850	8.7274	8.6770	8.6792	8.8186	8.7294	8.7294	8.6790	8.5978	8.6823	8.6918	8.6850	8.7274	8.6770	8.6792	**8.13**
H5	7.2358	7.4200	7.5085	7.5012	7.6284	7.4972	7.6456	7.4925	7.6367	7.5059	7.6679	7.2358	7.4200	7.5085	7.5012	7.4200	7.4972	7.6456	7.4925	7.6367	7.5059	7.6679	**8.03**
H6	8.0025	8.1826	8.2567	8.2840	8.4233	8.2779	8.4869	8.2710	8.4820	8.2910	8.5171	8.0025	8.1826	8.2567	8.2840	8.2028	8.2779	8.4869	8.2710	8.4820	8.2910	8.5171	**7.4**
H(3``A-3``C)	2.4320	2.4746	2.4883	2.4853	2.5047	2.4856	2.5112	2.4851	2.5092	2.4859	2.5191	2.4321	2.4746	2.4884	2.4853	2.4040	2.4856	2.5112	2.4851	2.5092	2.4859	2.5191	**2.32**
H8	4.2562	4.3350	4.3421	4.4012	4.4805	4.3969	4.5478	4.3919	4.5369	4.4065	4.5641	4.2562	4.3350	4.3421	4.4012	4.3200	4.3969	4.5478	4.3919	4.5370	4.4065	4.5641	**5.64**
H(9A-9B)	1.7454	1.7813	1.7762	1.8032	1.8093	1.8023	1.7945	1.8006	1.7948	1.8051	1.8317	1.7454	1.7813	1.7762	1.8032	1.7220	1.8023	1.7945	1.8006	1.7948	1.8051	1.8317	**1.92**
H(10A)	1.0219	0.8509	0.8037	0.7929	0.7154	0.7965	0.7431	0.7994	0.7742	0.7906	0.7455	1.0219	0.8510	0.8037	0.7929	0.7154	0.7965	0.7430	0.7994	0.7742	0.7906	0.7455	**1.26**
H(10B)	1.7102	1.6304	1.5538	1.5563	1.4590	1.5615	1.4536	1.5659	1.4657	1.5525	1.4241	1.7102	1.6304	1.5538	1.5563	1.4590	1.5615	1.4536	1.5659	1.4656	1.5525	1.4240	**1.07**
H(11A-11C)	0.7561	0.7663	0.7315	0.7725	0.7301	0.7727	0.7313	0.7721	0.7436	0.7735	0.7260	0.7561	0.7663	0.7315	0.7725	0.6913	0.7727	0.7314	0.7721	0.7436	0.7735	0.7260	**0.78**
H(1`A)	2.5684	2.5623	2.5390	2.5523	2.5016	2.5538	2.5187	2.5545	2.5185	2.5519	2.5002	2.7069	2.7131	2.7033	2.6971	2.6610	2.6993	2.6771	2.7006	2.6693	2.6960	2.6545	**3.47**
H(1`B)	3.0770	3.1058	3.1306	3.1328	3.1871	3.1315	3.1710	3.1295	3.1713	3.1351	3.1756	2.8942	2.6788	2.6485	2.6088	2.5995	2.6132	2.5398	2.6167	2.5165	2.6058	2.5311	**3.63**
H(4`A)	2.8942	2.6788	2.6485	2.6088	2.5995	2.6132	2.5398	2.6167	2.5165	2.6058	2.5311	3.0770	3.1058	3.1306	3.1328	3.1871	3.1315	3.1710	3.1295	3.1713	3.1351	3.1756	**3.07**
H(4`B)	2.7069	2.7131	2.7033	2.6971	2.6610	2.6993	2.6771	2.7006	2.6693	2.6960	2.6545	2.5684	2.5623	2.5390	2.5523	2.5016	2.5538	2.5187	2.5545	2.5185	2.5518	2.5002	**3.25**
Nuclei	BHandHLYP											BHandHLYP										
C1	139.0935	139.5781	140.2537	139.8902	141.6619	139.8596	140.5194	139.8339	140.8006	139.9233	141.8788	139.0935	139.5781	140.2537	139.8902	141.6619	139.8595	140.5194	139.8338	140.8006	139.9233	141.8788	**131.615**
C2	142.3563	142.1689	142.5366	141.9714	142.4129	141.9866	142.7982	142.0039	142.7184	141.9560	142.7515	142.3564	142.1690	142.5366	141.9714	142.4129	141.9866	142.7982	142.0039	142.7184	141.9560	142.7517	**133.405**
C3	133.7017	134.7422	135.6058	135.0545	136.0378	135.0384	136.2323	135.0246	136.1984	135.0696	136.4859	133.7017	134.7423	135.6058	135.0546	136.0378	135.0386	136.2323	135.0246	136.1984	135.0696	136.4860	**126.19**
C4	173.0336	173.8142	174.4035	174.2646	174.7558	174.2348	175.5620	174.2081	175.3775	174.2931	175.6506	173.0337	173.8141	174.4035	174.2646	174.7558	174.2350	175.5620	174.2081	175.3775	174.2931	175.6505	**165.04**
C5	119.8627	121.0296	121.6010	121.6710	122.4508	121.6300	122.6183	121.5918	122.5543	121.7103	122.9242	119.8627	121.0295	121.6010	121.6708	122.4508	121.6299	122.6183	121.5918	122.5543	121.7103	122.9240	**116.425**
C6	135.3208	137.0210	138.0159	138.0138	139.1592	137.9580	140.0664	137.9030	139.7228	138.0642	139.7503	135.3208	137.0209	138.0159	138.0137	139.1592	137.9579	140.0664	137.9030	139.7228	138.0642	139.7503	**129.92**
C7	202.5936	207.3125	208.3313	209.9802	210.5430	209.8023	216.0223	209.6303	214.9167	210.1534	218.2154	202.5939	207.3124	208.3313	209.9806	210.5430	209.8024	216.0223	209.6303	214.9168	210.1534	218.2153	**195.9**
C8	61.7523	62.7483	63.0651	63.2236	64.0215	63.1928	64.3600	63.1649	64.3666	63.2529	65.0687	61.7523	62.7483	63.0651	63.2235	64.0215	63.1927	64.3600	63.1649	64.3665	63.2529	65.0687	**67.6**
C9	35.6300	35.2316	35.4893	35.0833	35.4232	35.0938	35.4144	35.1066	35.4013	35.0723	35.2899	35.6300	35.2317	35.4893	35.0833	35.4233	35.0939	35.4144	35.1066	35.4013	35.0723	35.2900	**32.2**
C10	18.2448	18.6433	18.9476	18.9323	19.4227	18.9152	19.2756	18.9001	19.2814	18.9479	19.3552	18.2448	18.6433	18.9476	18.9324	19.4228	18.9151	19.2756	18.9001	19.2814	18.9479	19.3552	**23.4**
C11	15.9367	16.0201	16.1876	16.0982	16.3194	16.0935	16.2590	16.0911	16.2725	16.1022	16.3945	15.9366	16.0201	16.1876	16.0982	16.3194	16.0935	16.2590	16.0911	16.2725	16.1022	16.3945	**17.9**
C1`	49.1257	49.9121	50.1571	50.4178	50.9480	50.3871	50.8730	50.3583	50.8725	50.4463	51.3085	53.3300	54.2956	54.6152	54.7513	55.2096	54.7231	55.3704	54.6972	55.3230	54.7782	55.6537	**52.4**
C2`	24.4387	24.7726	25.0457	24.9270	25.3437	24.9175	25.3375	24.9105	25.3733	24.9356	25.2057	23.9114	23.9971	24.3946	24.1330	24.6541	24.1226	24.5293	24.1152	24.5516	24.1429	24.4128	**14.5**
C3`	23.9114	23.9971	24.3946	24.1330	24.6541	24.1226	24.5293	24.1152	24.5516	24.1429	24.4128	24.4386	24.7726	25.0457	24.9271	25.3437	24.9175	25.3375	24.9105	25.3732	24.9356	25.2058	**14.2**
C4`	53.3300	54.2956	54.6152	54.7513	55.2096	54.7231	55.3704	54.6972	55.3230	54.7782	55.6536	49.1256	49.9120	50.1571	50.4177	50.9480	50.3871	50.8730	50.3583	50.8726	50.4463	51.3085	**53.9**
H2	8.7296	8.6465	8.6812	8.5873	8.5827	8.5924	8.6264	8.5972	8.6101	8.5820	8.5233	8.7296	8.6465	8.6812	8.5873	8.5827	8.5924	8.6264	8.5972	8.6101	8.5820	8.5233	**8.13**
H5	7.2306	7.3990	7.4904	7.4721	7.5889	7.4682	7.6079	7.4642	7.5955	7.4757	7.6302	7.2306	7.3990	7.4904	7.4721	7.5889	7.4682	7.6079	7.4642	7.5955	7.4757	7.6302	**8.03**
H6	7.8857	8.0768	8.1789	8.1841	8.3094	8.1779	8.3948	8.1715	8.3600	8.1899	8.3735	7.8857	8.0768	8.1789	8.1841	8.3094	8.1779	8.3948	8.1715	8.3600	8.1899	8.3735	**7.4**
H(3``A-3``C)	2.4202	2.4603	2.4730	2.4732	2.4898	2.4727	2.4996	2.4721	2.4965	2.4736	2.5089	2.4202	2.4602	2.4730	2.4732	2.4898	2.4727	2.4996	2.4721	2.4964	2.4736	2.5089	**2.32**
H8	4.1992	4.2886	4.3623	4.3556	4.4381	4.3512	4.5126	4.3468	4.4802	4.3597	4.4840	4.1992	4.2886	4.3623	4.3556	4.4381	4.3512	4.5126	4.3468	4.4802	4.3597	4.4840	**5.64**
H(9A-9B)	1.5520	1.5987	1.5909	1.6324	1.6380	1.6311	1.6370	1.6294	1.6279	1.6334	1.5981	1.5520	1.5987	1.5909	1.6324	1.6380	1.6311	1.6370	1.6294	1.6279	1.6334	1.5982	**1.92**
H(10A)	1.0619	0.9158	0.9261	0.8642	0.7859	0.8678	0.8336	0.8711	0.8214	0.8608	0.8369	1.0619	0.9158	0.9261	0.8642	0.7859	0.8677	0.8336	0.8711	0.8214	0.8608	0.8369	**1.26**
H(10B)	1.6379	1.5445	1.4942	1.4735	1.3984	1.4781	1.4094	1.4826	1.4104	1.4692	1.3665	1.6379	1.5446	1.4942	1.4735	1.3984	1.4781	1.4094	1.4826	1.4104	1.4692	1.3665	**1.07**
H(11A-11C)	0.7728	0.7821	0.7651	0.7906	0.7526	0.7902	0.7666	0.7897	0.7611	0.7909	0.7450	0.7728	0.7821	0.7651	0.7906	0.7526	0.7902	0.7666	0.7897	0.7611	0.7909	0.7450	**0.78**
H(1`A)	2.5918	2.5834	2.5679	2.5764	2.5262	2.5770	2.5437	2.5775	2.5431	2.5758	2.5237	2.7263	2.7196	2.6936	2.6997	2.6675	2.7012	2.6769	2.7025	2.6838	2.6984	2.6637	**3.47**
H(1`B)	3.0055	3.0567	3.0846	3.0964	3.1566	3.0940	3.1482	3.0914	3.1395	3.0987	3.1421	2.7070	2.5447	2.5125	2.5163	2.5371	2.5171	2.4767	2.5179	2.4831	2.5158	2.5100	**3.63**
H(4`A)	2.7070	2.5447	2.5125	2.5163	2.5371	2.5171	2.4767	2.5179	2.4831	2.5158	2.5100	3.0055	3.0567	3.0846	3.0964	3.1566	3.0940	3.1482	3.0914	3.1395	3.0987	3.1421	**3.07**
H(4`B)	2.7263	2.7196	2.6936	2.6998	2.6675	2.7012	2.6769	2.7025	2.6838	2.6984	2.6637	2.5918	2.5834	2.5679	2.5764	2.5262	2.5770	2.5437	2.5775	2.5431	2.5758	2.5237	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. IV

Nuclei	R											S										Exp. [b]
	BLYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.1023	139.8307	140.7373	140.7483	142.9806	140.9580	141.8737	140.7116	142.2899	141.1834	142.3558	139.1023	139.8307	140.7373	140.7483	142.9805	140.9580	141.8737	140.7116	142.2899	141.1834	142.3558	**131.615**
C2	138.3075	138.1046	138.6118	137.9924	138.6335	138.2746	138.8389	138.0957	138.9199	138.3526	138.9335	138.3075	138.1046	138.6118	137.9924	138.6336	138.2746	138.8389	138.0957	138.9198	138.3526	138.9335	**133.405**
C3	133.6207	134.8133	135.6698	135.1959	136.2533	135.4544	136.4909	135.2509	136.5884	135.5774	136.7451	133.6207	134.8133	135.6698	135.1959	136.2533	135.4544	136.4909	135.2509	136.5885	135.5774	136.7451	**126.19**
C4	177.0599	178.2527	178.9276	178.7632	179.5034	179.0167	179.9651	178.8071	179.9764	179.1485	180.1703	177.0599	178.2527	178.9276	178.7632	179.5034	179.0167	179.9651	178.8071	179.9765	179.1485	180.1703	**165.04**
C5	117.8710	119.0826	119.6048	119.7418	120.4829	119.9793	120.6509	119.7551	120.7215	120.1438	120.8583	117.8710	119.0826	119.6048	119.7418	120.4829	119.9793	120.6510	119.7551	120.7215	120.1438	120.8583	**116.425**
C6	131.3114	132.8151	133.6851	133.6401	134.8688	133.8647	135.4234	133.6268	135.3290	134.0528	135.8245	131.3114	132.8151	133.6851	133.6401	134.8688	133.8647	135.4234	133.6268	135.3290	134.0528	135.8245	**129.92**
C7	204.2394	208.5677	209.9137	211.3715	212.8671	211.4664	216.9166	211.1043	216.3391	211.9138	218.1791	204.2394	208.5677	209.9138	211.3715	212.8672	211.4664	216.9167	211.1043	216.3392	211.9138	218.1791	**195.9**
C8	70.2995	71.2192	71.9656	71.9524	73.3942	72.1812	73.6457	71.9488	73.7815	72.3627	74.1224	70.2995	71.2192	71.9655	71.9524	73.3941	72.1812	73.6457	71.9488	73.7815	72.3627	74.1224	**67.6**
C9	41.8145	41.2997	41.5414	41.0759	41.4499	41.3675	41.5417	41.1963	41.6358	41.4252	41.7008	41.8145	41.2997	41.5414	41.0759	41.4499	41.3675	41.5417	41.1963	41.6358	41.4252	41.7008	**32.2**
C10	21.7311	22.1582	22.4351	22.3999	23.0339	22.6624	22.7506	22.4627	22.9244	22.7768	22.9351	21.7311	22.1582	22.4351	22.3999	23.0339	22.6624	22.7506	22.4627	22.9244	22.7768	22.9351	**23.4**
C11	16.4195	16.5063	16.6282	16.5371	16.8576	16.8136	16.6301	16.6280	16.8180	16.9014	16.8962	16.4195	16.5063	16.6282	16.5371	16.8575	16.8136	16.6301	16.6280	16.8180	16.9014	16.8962	**17.9**
C1`	55.3279	56.0908	56.3397	56.5755	57.2738	56.8226	57.0693	56.6074	57.2059	56.9677	57.5947	60.0410	61.2268	61.5342	61.7120	62.2350	61.9623	62.2824	61.7507	62.3998	62.1014	62.6294	**52.4**
C2`	27.6834	28.1709	28.3699	28.3979	28.8588	28.6638	28.7555	28.4673	28.9424	28.7714	28.7790	27.5948	27.8034	28.0882	27.9527	28.5247	28.2184	28.2541	28.0231	28.4320	28.3288	28.1366	**14.5**
C3`	27.5948	27.8034	28.0882	27.9527	28.5247	28.2184	28.2542	28.0231	28.4322	28.3288	28.1366	27.6834	28.1709	28.3699	28.3978	28.8587	28.6638	28.7554	28.4673	28.9424	28.7714	28.7790	**14.2**
C4`	60.0410	61.2268	61.5342	61.7120	62.2350	61.9623	62.2824	61.7507	62.3997	62.1014	62.6294	55.3279	56.0908	56.3397	56.5755	57.2738	56.8226	57.0694	56.6074	57.2060	56.9677	57.5947	**53.9**
H2	8.3058	8.2281	8.2401	8.1366	8.1018	8.1909	8.3154	8.1521	8.1326	8.1848	8.3136	8.3058	8.2281	8.2401	8.1366	8.1018	8.1909	8.3154	8.1521	8.1326	8.1848	8.3136	**8.13**
H5	6.9499	7.0955	7.1758	7.1650	7.2815	7.2079	7.4693	7.1584	7.2922	7.2246	7.5014	6.9499	7.0955	7.1758	7.1650	7.2815	7.2079	7.4693	7.1584	7.2922	7.2246	7.5014	**8.03**
H6	7.6665	7.8440	7.9011	7.9016	7.9802	7.9460	8.2096	7.8977	8.0180	7.9595	8.2500	7.6665	7.8440	7.9011	7.9016	7.9802	7.9460	8.2096	7.8977	8.0180	7.9595	8.2500	**7.4**
H(3``A-3``C)	2.3207	2.3668	2.3823	2.3807	2.4030	2.4276	2.5792	2.3819	2.4090	2.4364	2.5972	2.3207	2.3668	2.3823	2.3807	2.4030	2.4276	2.5792	2.3819	2.4090	2.4364	2.5972	**2.32**
H8	4.9473	4.9949	5.0049	5.0048	5.0360	5.0513	5.2383	5.0054	5.0590	5.0611	5.2389	4.9473	4.9949	5.0049	5.0048	5.0360	5.0513	5.2383	5.0054	5.0590	5.0611	5.2389	**5.64**
H(9A-9B)	1.7415	1.7722	1.7758	1.7885	1.8089	1.8350	1.9786	1.7887	1.8016	1.8442	2.0160	1.7415	1.7722	1.7758	1.7885	1.8089	1.8350	1.9786	1.7887	1.8016	1.8442	2.0160	**1.92**
H(10A)	1.1227	1.0569	1.0061	1.0073	0.9252	1.0574	1.1442	1.0151	0.9716	1.0602	1.1702	1.1227	1.0569	1.0061	1.0073	0.9252	1.0574	1.1442	1.0151	0.9715	1.0602	1.1702	**1.26**
H(10B)	1.8379	1.7168	1.6704	1.6399	1.5669	1.6918	1.7280	1.6512	1.5671	1.6908	1.7041	1.8379	1.7168	1.6704	1.6399	1.5669	1.6918	1.7280	1.6512	1.5671	1.6908	1.7041	**1.07**
H(11A-11C)	0.7854	0.7956	0.7708	0.7998	0.7647	0.8468	0.9361	0.8013	0.7678	0.8555	0.9392	0.7854	0.7956	0.7708	0.7998	0.7647	0.8468	0.9361	0.8013	0.7678	0.8555	0.9392	**0.78**
H(1`A)	2.8373	2.8287	2.8039	2.8107	2.7636	2.8595	2.9351	2.8157	2.7713	2.8646	2.9267	2.9507	2.9504	2.9346	2.9383	2.9253	2.9865	3.0934	2.9421	2.9337	2.9929	3.0779	**3.47**
H(1`B)	3.3462	3.3752	3.4165	3.3990	3.4767	3.4445	3.6175	3.3975	3.4452	3.4561	3.6333	3.0201	2.8340	2.8312	2.8107	2.8476	2.8583	2.9695	2.8138	2.8063	2.8661	2.9770	**3.63**
H(4`A)	3.0201	2.8340	2.8312	2.8107	2.8476	2.8583	2.9695	2.8138	2.8063	2.8661	2.9770	3.3462	3.3752	3.4165	3.3990	3.4767	3.4445	3.6175	3.3975	3.4452	3.4561	3.6333	**3.07**
H(4`B)	2.9507	2.9504	2.9346	2.9383	2.9253	2.9865	3.0934	2.9421	2.9337	2.9929	3.0779	2.8373	2.8287	2.8039	2.8107	2.7636	2.8595	2.9351	2.8157	2.7713	2.8646	2.9267	**3.25**
Nuclei	BMK																						
C1	154.5953	155.0700	155.8393	155.2298	157.2579	155.2045	156.2680	155.3907	156.1737	155.4160	156.4508	154.5954	155.0700	155.8393	155.2298	157.2579	155.2045	156.2681	155.3907	156.1735	155.4158	156.4507	**131.615**
C2	156.2832	155.7767	156.4349	155.4521	156.1769	155.4582	156.4567	155.6756	156.3051	155.6074	156.4481	156.2832	155.7768	156.4349	155.4521	156.1769	155.4582	156.4566	155.6754	156.3051	155.6075	156.4481	**133.405**
C3	148.5728	149.6892	150.7410	149.9666	151.2428	149.9389	151.4493	150.1218	151.2931	150.1539	151.5252	148.5729	149.6892	150.7410	149.9666	151.2428	149.9389	151.4492	150.1218	151.2931	150.1539	151.5254	**126.19**
C4	188.0443	188.7213	189.5032	189.1026	189.9730	189.0631	190.6451	189.2349	190.3564	189.3020	190.7229	188.0442	188.7214	189.5032	189.1026	189.9730	189.0631	190.6451	189.2350	190.3564	189.3021	190.7229	**165.04**
C5	132.7638	134.0032	134.7389	134.6531	135.7470	134.5975	135.9333	134.7532	135.7072	134.8674	136.0266	132.7638	134.0032	134.7389	134.6530	135.7470	134.5975	135.9333	134.7534	135.7072	134.8674	136.0266	**116.425**
C6	148.7418	150.5055	151.8640	151.5792	153.1718	151.4945	153.8956	151.6212	153.6229	151.8216	154.2581	148.7418	150.5055	151.8640	151.5792	153.1718	151.4945	153.8954	151.6211	153.6231	151.8215	154.2580	**129.92**
C7	218.4913	223.2471	224.4007	226.0069	226.9150	225.8185	232.9452	225.8419	231.3494	226.3487	234.0987	218.4914	223.2472	224.4007	226.0069	226.9150	225.8185	232.9453	225.8419	231.3490	226.3484	234.0986	**195.9**
C8	71.7640	72.8963	73.4172	73.4380	74.5797	73.3922	75.0619	73.5574	74.7021	73.6429	75.4106	71.7641	72.8963	73.4172	73.4380	74.5797	73.3922	75.0620	73.5575	74.7020	73.6430	75.4106	**67.6**
C9	40.3663	40.4399	40.6858	40.4164	41.1542	40.4043	41.1181	40.6033	40.9415	40.5893	41.3374	40.3664	40.4399	40.6857	40.4163	41.1542	40.4043	41.1181	40.6033	40.9416	40.5892	41.3374	**32.2**
C10	21.4559	21.8392	22.1200	22.0395	22.7228	22.0118	22.5067	22.1955	22.4010	22.2274	22.5108	21.4558	21.8393	22.1199	22.0395	22.7228	22.0118	22.5067	22.1954	22.4010	22.2275	22.5108	**23.4**
C11	17.3136	17.2802	17.5523	17.3092	17.6787	17.2897	17.5890	17.4818	17.5016	17.4897	17.7787	17.3136	17.2802	17.5523	17.3092	17.6787	17.2897	17.5890	17.4818	17.5018	17.4897	17.7787	**17.9**
C1`	56.3986	56.7890	57.3295	57.1702	57.7680	57.1275	57.7895	57.2969	57.6895	57.3725	58.0585	60.5768	61.0850	61.4703	61.4511	62.1299	61.4130	62.2472	61.5861	62.0826	61.6490	62.4507	**52.4**
C2`	27.8518	27.9355	28.2439	28.1074	28.7043	28.0813	28.6897	28.2665	28.5560	28.2938	28.6605	27.3065	27.4390	27.9737	27.4414	28.0369	27.4217	27.9671	27.6137	27.8963	27.6218	27.7496	**14.5**
C3`	27.3064	27.4391	27.9737	27.4414	28.0369	27.4217	27.9671	27.6138	27.8962	27.6218	27.7495	27.8516	27.9354	28.2439	28.1074	28.7043	28.0813	28.6897	28.2666	28.5559	28.2938	28.6605	**14.2**
C4`	60.5769	61.0850	61.4702	61.4511	62.1299	61.4130	62.2472	61.5860	62.0826	61.6489	62.4508	56.3986	56.7891	57.3294	57.1702	57.7680	57.1275	57.7895	57.2967	57.6896	57.3725	58.0586	**53.9**
H2	8.9131	8.8096	8.8517	8.7629	8.7532	8.7626	8.7834	8.7623	8.7889	8.7536	8.7896	8.9131	8.8096	8.8517	8.7629	8.7532	8.7626	8.7834	8.7622	8.7889	8.7536	8.7896	**8.13**
H5	7.4079	7.5890	7.6719	7.6719	7.7898	7.6640	7.8055	7.6560	7.7981	7.6698	7.8294	7.4079	7.5890	7.6718	7.6719	7.7898	7.6640	7.8055	7.6560	7.7981	7.6698	7.8294	**8.03**
H6	8.1831	8.3821	8.4746	8.5002	8.6259	8.4896	8.6994	8.4791	8.6792	8.5007	8.7274	8.1831	8.3821	8.4746	8.5002	8.6259	8.4896	8.6994	8.4791	8.6792	8.5007	8.7274	**7.4**
H(3``A-3``C)	2.3407	2.3986	2.4141	2.4216	2.4430	2.4172	2.4541	2.4128	2.4498	2.4163	2.4685	2.3407	2.3986	2.4141	2.4216	2.4430	2.4172	2.4541	2.4128	2.4498	2.4163	2.4685	**2.32**
H8	4.3983	4.4643	4.4754	4.5266	4.5805	4.5191	4.6391	4.5116	4.6226	4.5243	4.6404	4.3983	4.4643	4.4754	4.5266	4.5805	4.5191	4.6391	4.5116	4.6226	4.5243	4.6404	**5.64**
H(9A-9B)	1.5996	1.6604	1.6389	1.7168	1.7305	1.7102	1.7139	1.7036	1.7088	1.7136	1.7736	1.5996	1.6604	1.6389	1.7168	1.7305	1.7102	1.7139	1.7036	1.7088	1.7136	1.7735	**1.92**
H(10A)	1.0656	0.8935	0.9246	0.8365	0.7703	0.8363	0.8082	0.8361	0.8162	0.8272	0.8214	1.0656	0.8935	0.9246	0.8365	0.7703	0.8363	0.8082	0.8362	0.8162	0.8272	0.8215	**1.26**
H(10B)	1.6499	1.5451	1.4844	1.4770	1.3963	1.4783	1.3907	1.4796	1.3998	1.4661	1.3625	1.6499	1.5451	1.4844	1.4770	1.3963	1.4783	1.3907	1.4796	1.3998	1.4661	1.3624	**1.07**
H(11A-11C)	0.6958	0.6946	0.6838	0.7097	0.6666	0.7054	0.6721	0.7012	0.6762	0.7043	0.6737	0.6957	0.6946	0.6838	0.7097	0.6666	0.7054	0.6722	0.7012	0.6762	0.7043	0.6737	**0.78**
H(1`A)	2.6172	2.6232	2.6134	2.6228	2.5732	2.6197	2.5923	2.6167	2.5919	2.6162	2.5730	2.7391	2.7609	2.7194	2.7526	2.7093	2.7504	2.7260	2.7482	2.7287	2.7451	2.6960	**3.47**
H(1`B)	3.0581	3.0696	3.0873	3.1209	3.1634	3.1143	3.1589	3.1077	3.1538	3.1178	3.1781	2.7381	2.6001	2.5522	2.5588	2.5539	2.5574	2.5085	2.5561	2.5046	2.5506	2.4950	**3.63**
H(4`A)	2.7381	2.6001	2.5522	2.5588	2.5539	2.5574	2.5085	2.5561	2.5046	2.5506	2.4950	3.0582	3.0696	3.0873	3.1209	3.1634	3.1143	3.1589	3.1077	3.1538	3.1178	3.1781	**3.07**
H(4`B)	2.7391	2.7609	2.7194	2.7526	2.7093	2.7504	2.7259	2.7482	2.7287	2.7451	2.6960	2.6172	2.6232	2.6134	2.6228	2.5732	2.6197	2.5923	2.6166	2.5919	2.6162	2.5730	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. V

Nuclei	R											S										Exp. [b]
	BP86																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	135.8495	136.6689	137.3066	137.1648	138.8647	137.1188	138.8268	137.0731	138.9655	137.2099	139.3922	135.8495	136.6688	137.3066	137.1648	138.8647	137.1188	138.8267	137.0731	138.9655	137.2099	139.3922	**131.615**
C2	137.1580	137.1273	137.4634	136.8237	137.3944	136.8545	137.6705	136.8798	137.5720	136.7892	137.8095	137.1580	137.1274	137.4634	136.8237	137.3944	136.8545	137.6706	136.8798	137.5720	136.7892	137.8095	**133.405**
C3	131.2546	132.7135	133.6445	133.1012	134.1399	133.0900	134.5922	133.0730	134.4864	133.1064	134.9261	131.2546	132.7136	133.6445	133.1012	134.1399	133.0900	134.5921	133.0730	134.4864	133.1064	134.9261	**126.19**
C4	173.5094	174.6598	175.4049	175.1708	175.8332	175.1449	176.6466	175.1141	176.4759	175.1906	176.9237	173.5094	174.6599	175.4049	175.1708	175.8332	175.1449	176.6466	175.1141	176.4760	175.1906	176.9237	**165.04**
C5	116.7347	118.0887	118.6556	118.7192	119.4601	118.6869	119.9173	118.6498	119.7898	118.7453	120.2057	116.7347	118.0886	118.6556	118.7192	119.4601	118.6869	119.9174	118.6498	119.7899	118.7453	120.2057	**116.425**
C6	130.0241	131.6968	132.6228	132.5377	133.8109	132.4973	134.1749	132.4511	133.9164	132.5700	134.6480	130.0241	131.6967	132.6228	132.5377	133.8109	132.4973	134.1752	132.4511	133.9164	132.5700	134.6480	**129.92**
C7	201.3531	205.4954	206.4738	207.8151	208.8001	207.6547	213.4912	207.4954	212.6871	207.9694	214.8552	201.3531	205.4954	206.4738	207.8151	208.8001	207.6547	213.4915	207.4954	212.6872	207.9694	214.8552	**195.9**
C8	67.9572	69.2530	69.5507	69.8540	70.8565	69.8146	71.4310	69.7729	71.3366	69.8900	72.1225	67.9572	69.2531	69.5508	69.8540	70.8565	69.8146	71.4310	69.7729	71.3366	69.8900	72.1225	**67.6**
C9	40.4637	40.2504	40.3612	40.0966	40.4368	40.1125	40.3996	40.1237	40.3132	40.0774	40.7261	40.4637	40.2504	40.3612	40.0966	40.4368	40.1125	40.3994	40.1237	40.3132	40.0774	40.7261	**32.2**
C10	20.2223	20.8053	20.9872	21.0456	21.4920	21.0383	21.3175	21.0264	21.2974	21.0476	21.6503	20.2223	20.8052	20.9872	21.0456	21.4920	21.0383	21.3175	21.0264	21.2975	21.0476	21.6503	**23.4**
C11	15.9623	16.2096	16.2346	16.2095	16.3481	16.2179	16.2556	16.2213	16.2579	16.1965	16.6174	15.9623	16.2096	16.2346	16.2095	16.3481	16.2179	16.2555	16.2213	16.2579	16.1965	16.6174	**17.9**
C1`	53.7829	54.7406	54.8451	55.1919	55.6558	55.1740	55.5814	55.1504	55.5503	55.2035	56.2153	58.2864	59.5681	59.9372	60.0034	60.3997	59.9861	60.7371	59.9633	60.6626	60.0145	61.1344	**52.4**
C2`	26.1951	26.8168	26.9812	26.9805	27.3139	26.9785	27.3480	26.9714	27.3473	26.9775	27.4367	25.9009	26.1838	26.5226	26.2878	26.7346	26.2875	26.7740	26.2823	26.7608	26.2833	26.6926	**14.5**
C3`	25.9009	26.1839	26.5227	26.2878	26.7346	26.2875	26.7741	26.2823	26.7609	26.2833	26.6926	26.1951	26.8168	26.9812	26.9805	27.3139	26.9785	27.3480	26.9714	27.3473	26.9775	27.4367	**14.2**
C4`	58.2864	59.5681	59.9371	60.0034	60.3997	59.9861	60.7371	59.9633	60.6626	60.0145	61.1344	53.7829	54.7406	54.8451	55.1919	55.6558	55.1740	55.5815	55.1504	55.5504	55.2035	56.2153	**53.9**
H2	8.3612	8.2860	8.3027	8.2214	8.2039	8.2281	8.1941	8.2340	8.1837	8.2142	8.1912	8.3612	8.2860	8.3027	8.2214	8.2039	8.2281	8.1941	8.2340	8.1837	8.2142	8.1912	**8.13**
H5	6.9613	7.1202	7.1998	7.1871	7.2969	7.1841	7.3205	7.1807	7.3088	7.1896	7.3540	6.9613	7.1202	7.1998	7.1871	7.2969	7.1841	7.3205	7.1807	7.3088	7.1896	7.3540	**8.03**
H6	7.7401	7.9051	7.9937	7.9859	8.0781	7.9824	8.1108	7.9784	8.0894	7.9886	8.1475	7.7401	7.9051	7.9937	7.9859	8.0781	7.9824	8.1108	7.9784	8.0893	7.9886	8.1475	**7.4**
H(3``A-3``C)	2.3125	2.3615	2.3688	2.3760	2.3904	2.3760	2.4024	2.3756	2.3987	2.3757	2.4220	2.3125	2.3615	2.3688	2.3760	2.3904	2.3760	2.4024	2.3756	2.3987	2.3757	2.4220	**2.32**
H8	4.9453	4.9831	5.0348	5.0075	5.0434	5.0070	5.0842	5.0061	5.0681	5.0074	5.0885	4.9453	4.9831	5.0348	5.0075	5.0434	5.0070	5.0842	5.0061	5.0681	5.0074	5.0885	**5.64**
H(9A-9B)	1.8372	1.8848	1.8480	1.9112	1.9166	1.9107	1.8542	1.9097	1.8466	1.9112	1.8997	1.8372	1.8848	1.8480	1.9112	1.9166	1.9107	1.8541	1.9097	1.8466	1.9112	1.8997	**1.92**
H(10A)	1.0845	1.0051	0.9907	0.9589	0.8776	0.9636	0.9342	0.9678	0.9268	0.9539	0.9592	1.0845	1.0051	0.9907	0.9589	0.8776	0.9636	0.9342	0.9678	0.9268	0.9539	0.9592	**1.26**
H(10B)	1.8693	1.7419	1.6809	1.6674	1.5836	1.6725	1.5678	1.6773	1.5735	1.6621	1.5408	1.8693	1.7419	1.6809	1.6674	1.5836	1.6725	1.5678	1.6773	1.5735	1.6621	1.5408	**1.07**
H(11A-11C)	0.7551	0.7684	0.7423	0.7735	0.7313	0.7740	0.7311	0.7743	0.7294	0.7727	0.7325	0.7551	0.7684	0.7423	0.7735	0.7313	0.7740	0.7311	0.7743	0.7294	0.7727	0.7325	**0.78**
H(1`A)	2.7902	2.7841	2.7553	2.7729	2.7233	2.7744	2.7188	2.7756	2.7209	2.7711	2.7166	2.8954	2.9111	2.8842	2.8996	2.8701	2.9010	2.8800	2.9021	2.8845	2.8980	2.8623	**3.47**
H(1`B)	3.3691	3.3961	3.4194	3.4227	3.4818	3.4216	3.4434	3.4202	3.4380	3.4234	3.4565	3.0749	2.8672	2.8241	2.8261	2.8371	2.8276	2.7866	2.8292	2.7876	2.8247	2.7945	**3.63**
H(4`A)	3.0749	2.8672	2.8241	2.8261	2.8371	2.8276	2.7866	2.8292	2.7876	2.8247	2.7945	3.3691	3.3961	3.4194	3.4227	3.4818	3.4216	3.4434	3.4202	3.4380	3.4234	3.4565	**3.07**
H(4`B)	2.8954	2.9111	2.8842	2.8996	2.8701	2.9010	2.8800	2.9021	2.8845	2.8980	2.8623	2.7902	2.7841	2.7553	2.7729	2.7233	2.7744	2.7188	2.7756	2.7209	2.7711	2.7166	**3.25**
Nuclei	CAM-B3LYP																						
C1	140.7673	141.4022	142.0344	141.9590	143.7829	141.8996	143.7179	141.8445	143.7932	142.0224	144.0912	140.7674	141.4023	142.0344	141.9591	143.7829	141.8996	143.7178	141.8445	143.7932	142.0223	144.0913	**131.615**
C2	142.8778	142.7805	143.1265	142.5784	143.0953	142.5986	143.4370	142.6183	143.3496	142.5609	143.4037	142.8778	142.7805	143.1265	142.5783	143.0953	142.5986	143.4371	142.6184	143.3496	142.5609	143.4036	**133.405**
C3	135.1922	136.3104	137.1668	136.6368	137.6759	136.6225	137.9967	136.6084	137.9332	136.6522	138.1491	135.1922	136.3103	137.1669	136.6367	137.6759	136.6225	137.9966	136.6085	137.9332	136.6522	138.1491	**126.19**
C4	176.1497	176.9796	177.5684	177.4121	177.9814	177.3875	178.6692	177.3634	178.5164	177.4375	178.7643	176.1496	176.9797	177.5685	177.4121	177.9815	177.3875	178.6692	177.3635	178.5164	177.4373	178.7645	**165.04**
C5	121.2550	122.4661	123.0200	123.1070	123.9183	123.0684	124.2249	123.0309	124.1273	123.1459	124.3710	121.2549	122.4660	123.0198	123.1070	123.9182	123.0684	124.2250	123.0308	124.1273	123.1459	124.3710	**116.425**
C6	135.7553	137.4800	138.4589	138.3653	139.6274	138.3258	139.8853	138.2856	139.6373	138.4039	140.1915	135.7552	137.4800	138.4589	138.3654	139.6275	138.3258	139.8854	138.2856	139.6374	138.4040	140.1916	**129.92**
C7	206.5296	211.2980	212.2868	214.1749	214.8891	213.9691	221.0968	213.7692	219.8941	214.3769	222.3800	206.5296	211.2982	212.2872	214.1747	214.8887	213.9691	221.0969	213.7691	219.8940	214.3768	222.3801	**195.9**
C8	64.4903	65.5933	65.9290	66.1598	67.0446	66.1216	67.7350	66.0854	67.5907	66.1999	68.2492	64.4903	65.5934	65.9290	66.1599	67.0447	66.1216	67.7350	66.0853	67.5907	66.1999	68.2491	**67.6**
C9	37.0107	36.6612	36.8601	36.4685	36.8137	36.4856	36.6654	36.5036	36.6098	36.4544	36.7796	37.0107	36.6613	36.8602	36.4684	36.8136	36.4856	36.6655	36.5034	36.6098	36.4544	36.7796	**32.2**
C10	18.6342	19.0887	19.3201	19.3569	19.8512	19.3462	19.6814	19.3357	19.6574	19.3687	19.8232	18.6342	19.0887	19.3202	19.3569	19.8512	19.3462	19.6814	19.3357	19.6575	19.3687	19.8231	**23.4**
C11	15.7228	15.8573	15.9562	15.9062	16.1315	15.9080	16.0611	15.9099	16.0546	15.9063	16.2365	15.7228	15.8573	15.9562	15.9063	16.1316	15.9080	16.0611	15.9098	16.0547	15.9063	16.2366	**17.9**
C1`	50.9019	51.7724	51.9853	52.2605	52.8135	52.2380	52.7664	52.2151	52.7311	52.2831	53.2215	55.1542	56.1982	56.4964	56.6552	57.1631	56.6311	57.3428	56.6073	57.2882	56.6802	57.6062	**52.4**
C2`	25.0134	25.3949	25.6401	25.5375	25.9761	25.5336	25.9790	25.5299	25.9871	25.5431	25.8650	24.4930	24.6381	24.9909	24.7688	25.3057	24.7623	25.2718	24.7562	25.2731	24.7772	25.0593	**14.5**
C3`	24.4930	24.6382	24.9909	24.7688	25.3058	24.7623	25.2717	24.7562	25.2731	24.7773	25.0592	25.0134	25.3948	25.6401	25.5376	25.9760	25.5336	25.9789	25.5300	25.9870	25.5432	25.8650	**14.2**
C4`	55.1542	56.1982	56.4963	56.6552	57.1631	56.6311	57.3430	56.6074	57.2881	56.6802	57.6063	50.9020	51.7725	51.9853	52.2605	52.8135	52.2380	52.7664	52.2150	52.7311	52.2830	53.2215	**53.9**
H2	8.6290	8.5436	8.5812	8.4642	8.4628	8.4720	8.4221	8.4795	8.4223	8.4563	8.4006	8.6289	8.5436	8.5812	8.4642	8.4628	8.4720	8.4221	8.4795	8.4223	8.4563	8.4006	**8.13**
H5	7.2013	7.3670	7.4587	7.4362	7.5563	7.4325	7.5731	7.4289	7.5625	7.4397	7.5936	7.2013	7.3670	7.4587	7.4362	7.5563	7.4325	7.5731	7.4289	7.5625	7.4397	7.5936	**8.03**
H6	7.8575	8.0381	8.1443	8.1298	8.2551	8.1251	8.2805	8.1205	8.2606	8.1341	8.3042	7.8575	8.0381	8.1443	8.1298	8.2551	8.1251	8.2805	8.1205	8.2606	8.1342	8.3042	**7.4**
H(3``A-3``C)	2.3848	2.4269	2.4415	2.4403	2.4617	2.4396	2.4708	2.4390	2.4686	2.4410	2.4765	2.3848	2.4269	2.4415	2.4404	2.4617	2.4396	2.4708	2.4390	2.4686	2.4409	2.4765	**2.32**
H8	4.3943	4.4695	4.5467	4.5250	4.6080	4.5214	4.6578	4.5180	4.6362	4.5284	4.6464	4.3943	4.4695	4.5467	4.5250	4.6079	4.5214	4.6578	4.5179	4.6362	4.5284	4.6464	**5.64**
H(9A-9B)	1.6413	1.6850	1.6756	1.7081	1.7169	1.7079	1.6565	1.7079	1.6509	1.7079	1.6853	1.6413	1.6850	1.6756	1.7081	1.7169	1.7079	1.6565	1.7078	1.6509	1.7079	1.6853	**1.92**
H(10A)	1.0475	0.9231	0.9283	0.8699	0.8001	0.8740	0.8544	0.8780	0.8489	0.8657	0.8533	1.0475	0.9231	0.9283	0.9814	0.8001	0.8740	0.8544	0.8781	0.8490	0.8657	0.8533	**1.26**
H(10B)	1.6969	1.5965	1.5475	1.5235	1.4519	1.5279	1.4416	1.5325	1.4479	1.5193	1.4118	1.6969	1.5965	1.5475	1.6006	1.4519	1.5279	1.4416	1.5325	1.4479	1.5193	1.4118	**1.07**
H(11A-11C)	0.7816	0.7916	0.7753	0.7965	0.7637	0.7964	0.7619	0.7964	0.7624	0.7966	0.7501	0.7816	0.7916	0.7753	0.7965	0.7637	0.7964	0.7619	0.7964	0.7624	0.7966	0.7501	**0.78**
H(1`A)	2.6925	2.6852	2.6697	2.6786	2.6330	2.6792	2.6420	2.6798	2.6428	2.6780	2.6235	2.8184	2.8149	2.7940	2.8471	2.7730	2.7999	2.7883	2.8009	2.7915	2.7980	2.6235	**3.47**
H(1`B)	3.1130	3.1575	3.1861	3.1924	3.2560	3.1902	3.2309	3.1881	3.2249	3.1944	3.2361	2.8046	2.6373	2.5959	2.6490	2.6281	2.6158	2.6015	2.6156	2.5956	2.6169	3.2361	**3.63**
H(4`A)	2.8046	2.6373	2.5959	2.6163	2.6281	2.6158	2.6015	2.6156	2.5956	2.6170	2.6006	3.1130	3.1576	3.1860	3.2391	3.2560	3.1902	3.2309	3.1881	3.2249	3.1944	2.6006	**3.07**
H(4`B)	2.8183	2.8149	2.7940	2.7989	2.7730	2.7999	2.7883	2.8009	2.7915	2.7980	2.7605	2.6925	2.6852	2.6697	2.7228	2.6330	2.6792	2.6419	2.6798	2.6428	2.6780	2.7605	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. VI

Nuclei	R											S										Exp. [b]
	HF											HF										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.7700	137.4506	138.5121	138.3885	140.2679	138.3305	138.9667	138.2848	139.3491	138.4603	139.4218	136.7699	137.4506	138.5121	138.3877	140.2679	138.3303	138.9666	138.2848	139.3492	138.4603	139.4218	**131.615**
C2	143.5411	143.2428	143.6356	142.9366	143.2603	142.9589	143.7604	142.9792	143.6162	142.9118	143.7036	143.5409	143.2428	143.6356	142.9368	143.2603	142.9589	143.7601	142.9792	143.6164	142.9115	143.7036	**133.405**
C3	131.0776	132.0180	132.8003	132.3447	133.3025	132.3299	133.2728	132.3173	133.3095	132.3610	133.4360	131.0776	132.0180	132.8003	132.3446	133.3025	132.3299	133.2727	132.3173	133.3094	132.3610	133.4360	**126.19**
C4	169.3417	169.9108	170.3885	170.1367	170.4612	170.1240	171.2854	170.1102	171.0491	170.1454	171.3430	169.3418	169.9108	170.3885	170.1367	170.4612	170.1239	171.2854	170.1102	171.0490	170.1458	171.3430	**165.04**
C5	118.0916	119.2727	119.8232	119.9283	120.7251	119.8894	120.7243	119.8523	120.7011	119.9662	120.8996	118.0915	119.2727	119.8232	119.9282	120.7251	119.8894	120.7243	119.8522	120.7010	119.9664	120.8996	**116.425**
C6	136.5481	138.0556	138.7096	138.6500	139.6108	138.6082	140.6638	138.5609	140.2241	138.6798	140.7970	136.5481	138.0555	138.7096	138.6504	139.6108	138.6082	140.6638	138.5609	140.2242	138.6797	140.7970	**129.92**
C7	196.8686	202.2947	203.6023	205.8404	206.0147	205.6200	212.7906	205.4118	211.4247	206.0655	214.1018	196.8685	202.2947	203.6023	205.8398	206.0147	205.6197	212.7908	205.4118	211.4242	206.0652	214.1018	**195.9**
C8	55.6369	56.6278	56.9786	57.2050	57.9480	57.1651	58.5084	57.1281	58.4969	57.2477	58.8852	55.6369	56.6278	56.9786	57.2053	57.9480	57.1650	58.5085	57.1281	58.4969	57.2476	58.8852	**67.6**
C9	31.1525	30.6520	30.7940	30.3781	30.6671	30.3933	30.6402	30.4071	30.6304	30.3613	30.6525	31.1525	30.6520	30.7940	30.3784	30.6671	30.3933	30.6401	30.4072	30.6304	30.3614	30.6525	**32.2**
C10	16.6895	17.0661	17.3193	17.2668	17.7688	17.2555	17.6589	17.2435	17.6444	17.2758	17.7397	16.6895	17.0662	17.3193	17.2670	17.7688	17.2554	17.6588	17.2435	17.6444	17.2759	17.7397	**23.4**
C11	15.7952	15.8252	15.9804	15.8538	16.0978	15.8522	16.0508	15.8509	16.0503	15.8545	16.1727	15.7951	15.8252	15.9804	15.8538	16.0978	15.8522	16.0508	15.8510	16.0503	15.8544	16.1727	**17.9**
C1`	44.7153	45.4285	45.6742	45.8487	46.3788	45.8246	46.3455	45.8008	46.3209	45.8705	46.7024	48.5690	49.4218	49.7058	49.8232	50.2869	49.7992	50.3683	49.7759	50.3294	49.8459	50.6024	**52.4**
C2`	22.8507	23.0851	23.3369	23.1460	23.5864	23.1416	23.5884	23.1375	23.6079	23.1492	23.4291	22.2077	22.2518	22.6057	22.3581	22.8846	22.3510	22.7464	22.3449	22.7511	22.3652	22.5856	**14.5**
C3`	22.2078	22.2518	22.6057	22.3583	22.8846	22.3510	22.7464	22.3450	22.7511	22.3652	22.5856	22.8507	23.0851	23.3369	23.1461	23.5864	23.1416	23.5885	23.1375	23.6079	23.1492	23.4291	**14.2**
C4`	48.5690	49.4218	49.7058	49.8232	50.2869	49.7992	50.3682	49.7759	50.3294	49.8458	50.6024	44.7153	45.4285	45.6742	45.8486	46.3788	45.8245	46.3456	45.8007	46.3209	45.8704	46.7024	**53.9**
H2	8.8665	8.7438	8.7622	8.6084	8.6166	8.6170	8.6556	8.6241	8.6319	8.5985	8.6261	8.8665	8.7438	8.7622	8.6085	8.6166	8.6170	8.6556	8.6241	8.6319	8.5985	8.6261	**8.13**
H5	7.2274	7.4088	7.4982	7.4886	7.6148	7.4840	7.6279	7.4792	7.6176	7.4930	7.6509	7.2274	7.4088	7.4982	7.4886	7.6148	7.4840	7.6279	7.4792	7.6176	7.4931	7.6509	**8.03**
H6	7.8778	8.0900	8.1831	8.1892	8.3218	8.1830	8.4016	8.1763	8.3605	8.1946	8.4236	7.8778	8.0900	8.1831	8.1892	8.3218	8.1830	8.4016	8.1763	8.3605	8.1946	8.4236	**7.4**
H(3``A-3``C)	2.4305	2.4725	2.4854	2.4847	2.4997	2.4841	2.5061	2.4834	2.5036	2.4852	2.5132	2.4305	2.4725	2.4854	2.4847	2.4997	2.4841	2.5061	2.4834	2.5036	2.4852	2.5132	**2.32**
H8	3.6213	3.7331	3.8135	3.8152	3.9205	3.8098	3.9903	3.8042	3.9529	3.8202	3.9867	3.6212	3.7331	3.8135	3.8152	3.9205	3.8098	3.9903	3.8042	3.9529	3.8202	3.9867	**5.64**
H(9A-9B)	1.2882	1.3245	1.2983	1.3195	1.3168	1.3196	1.3306	1.3186	1.3195	1.3186	1.3429	1.2882	1.3245	1.2983	1.3196	1.3168	1.3195	1.3306	1.3186	1.3195	1.3186	1.3429	**1.92**
H(10A)	1.0531	0.8619	0.8575	0.8056	0.7347	0.8089	0.7622	0.8123	0.7522	0.8027	0.7649	1.0531	0.8619	0.8575	0.8055	1.2668	0.8089	0.7622	0.8123	0.7522	0.8027	0.7649	**1.26**
H(10B)	1.4564	1.3727	1.3350	1.3045	1.2270	1.3085	1.2390	1.3123	1.2393	1.3007	1.2161	1.4564	1.3727	1.3350	1.3045	1.9186	1.3085	1.2389	1.3122	1.2393	1.3007	1.2161	**1.07**
H(11A-11C)	0.7568	0.7585	0.7391	0.7662	0.7252	0.7653	0.7329	0.7643	0.7291	0.7671	0.7249	0.7567	0.7585	0.7391	0.7661	0.7252	0.7653	0.7329	0.7644	0.7291	0.7671	0.7249	**0.78**
H(1`A)	2.3616	2.3539	2.3340	2.3444	2.2877	2.3452	2.3152	2.3457	2.3144	2.3438	2.2992	2.5162	2.5090	2.4837	2.4846	3.2397	2.4863	2.4642	2.4879	2.4710	2.4830	2.4445	**3.47**
H(1`B)	2.7076	2.7712	2.8004	2.8146	2.8730	2.8118	2.8748	2.8087	2.8650	2.8173	2.8833	2.3779	2.2663	2.2499	2.2622	3.0948	2.2620	2.2553	2.2620	2.2619	2.2629	2.2660	**3.63**
H(4`A)	2.3779	2.2664	2.2499	2.2621	2.2901	2.2620	2.2553	2.2620	2.2619	2.2629	2.2660	2.7076	2.7712	2.8004	2.8146	3.7227	2.8118	2.8748	2.8086	2.8650	2.8173	2.8833	**3.07**
H(4`B)	2.5162	2.5090	2.4837	2.4846	2.4435	2.4864	2.4642	2.4880	2.4709	2.4830	2.4445	2.3616	2.3539	2.3340	2.3444	3.0997	2.3452	2.3153	2.3457	2.3144	2.3438	2.2992	**3.25**
Nuclei	LC-BLYP											LC-BLYP										
C1	144.3471	145.1746	146.1271	145.5455	147.4054	145.4985	147.8195	145.4808	146.3253	145.5740	148.0885	144.3471	145.1746	146.1271	145.5454	147.4054	145.4987	147.8195	145.4806	146.3253	145.5741	148.0885	**131.615**
C2	148.4754	148.2648	148.7467	148.0884	148.5602	148.0797	148.8570	148.0984	148.8914	148.0786	148.8342	148.4754	148.2648	148.7467	148.0883	148.5603	148.0798	148.8570	148.0985	148.8911	148.0786	148.8343	**133.405**
C3	138.7252	139.7530	140.6841	140.0785	141.1387	140.0411	141.4830	140.0306	141.2436	140.0964	141.6279	138.7252	139.7530	140.6843	140.0785	141.1388	140.0410	141.4830	140.0306	141.2435	140.0965	141.6281	**126.19**
C4	179.9222	180.5387	181.1389	180.9357	181.4004	180.8895	181.9408	180.8705	181.9657	180.9623	182.0533	179.9221	180.5386	181.1390	180.9356	181.4002	180.8894	181.9409	180.8706	181.9659	180.9623	182.0532	**165.04**
C5	125.8235	127.0707	127.7455	127.7575	128.6337	127.6939	128.9163	127.6577	128.6770	127.8007	129.0752	125.8235	127.0706	127.7455	127.7575	128.6337	127.6938	128.9164	127.6577	128.6771	127.8006	129.0751	**116.425**
C6	141.1115	142.7647	143.7145	143.8647	145.1527	143.7761	145.1332	143.7143	145.7000	143.9307	145.4752	141.1115	142.7647	143.7146	143.8647	145.1528	143.7762	145.1332	143.7143	145.6999	143.9306	145.4753	**129.92**
C7	212.2284	217.5525	218.8102	220.4161	221.0428	220.2164	228.4143	220.0453	225.3084	220.5896	229.5681	212.2284	217.5525	218.8102	220.4161	221.0427	220.2163	228.4143	220.0453	225.3083	220.5899	229.5681	**195.9**
C8	62.4068	63.5784	64.2070	64.1330	65.0092	64.0796	66.0646	64.0535	65.2574	64.1666	66.4450	62.4068	63.5784	64.2070	64.1329	65.0092	64.0796	66.0645	64.0535	65.2575	64.1666	66.4450	**67.6**
C9	34.8248	34.4400	34.6162	34.2810	34.5810	34.2731	34.3774	34.2918	34.5123	34.2704	34.4894	34.8248	34.4401	34.6163	34.2810	34.5810	34.2731	34.3775	34.2917	34.5123	34.2703	34.4893	**32.2**
C10	16.5280	16.8981	17.1967	17.2082	17.6860	17.1681	17.5187	17.1551	17.5105	17.2288	17.6525	16.5280	16.8981	17.1967	17.2082	17.6861	17.1681	17.5186	17.1550	17.5104	17.2288	17.6526	**23.4**
C11	14.7564	14.8096	14.9731	14.8900	15.0938	14.8638	15.0275	14.8647	15.0419	14.8976	15.2119	14.7564	14.8096	14.9731	14.8900	15.0938	14.8638	15.0275	14.8647	15.0420	14.8977	15.2118	**17.9**
C1`	48.8671	49.6225	49.9314	50.1222	50.6946	50.0688	50.7020	50.0428	50.6232	50.1557	51.1340	52.7212	53.6567	54.0446	54.1546	54.7052	54.1021	54.8613	54.0773	54.7563	54.1872	55.1516	**52.4**
C2`	23.0397	23.2914	23.6281	23.4380	23.8793	23.4085	23.9010	23.4061	23.8641	23.4488	23.7717	22.3704	22.4556	22.8366	22.5886	23.0727	22.5583	23.0331	22.5554	22.9648	22.6002	22.8703	**14.5**
C3`	22.3704	22.4557	22.8366	22.5886	23.0728	22.5583	23.0331	22.5555	22.9647	22.6002	22.8704	23.0397	23.2915	23.6282	23.4380	23.8794	23.4084	23.9009	23.4060	23.8640	23.4487	23.7717	**14.2**
C4`	52.7212	53.6566	54.0446	54.1546	54.7052	54.1021	54.8615	54.0774	54.7564	54.1873	55.1517	48.8671	49.6225	49.9314	50.1223	50.6945	50.0688	50.7021	50.0428	50.6233	50.1558	51.1340	**53.9**
H2	8.8092	8.6826	8.7074	8.6206	8.6143	8.6238	8.5161	8.6285	8.6608	8.6164	8.5091	8.8092	8.6826	8.7074	8.6206	8.6144	8.6238	8.5161	8.6285	8.6608	8.6164	8.5091	**8.13**
H5	7.3575	7.5268	7.6168	7.6041	7.7270	7.5988	7.7339	7.5950	7.7325	7.6081	7.7567	7.3575	7.5268	7.6168	7.6041	7.7270	7.5988	7.7339	7.5950	7.7325	7.6081	7.7567	**8.03**
H6	7.9955	8.1707	8.2717	8.2788	8.4132	8.2711	8.4015	8.2651	8.4670	8.2851	8.4323	7.9955	8.1707	8.2717	8.2788	8.4132	8.2711	8.4015	8.2651	8.4670	8.2851	8.4323	**7.4**
H(3``A-3``C)	2.4131	2.4510	2.4662	2.4646	2.4843	2.4630	2.4929	2.4630	2.4900	2.4651	2.5009	2.4131	2.4510	2.4662	2.4646	2.4843	2.4630	2.4929	2.4629	2.4900	2.4651	2.5009	**2.32**
H8	4.1886	4.2740	4.3471	4.3522	4.4413	4.3456	4.4823	4.3408	4.4969	4.3576	4.4948	4.1886	4.2740	4.3471	4.3522	4.4413	4.3456	4.4823	4.3408	4.4969	4.3576	4.4948	**5.64**
H(9A-9B)	1.6303	1.6632	1.6493	1.6916	1.6941	1.6894	1.6166	1.6887	1.6858	1.6926	1.6481	1.6303	1.6632	1.6493	1.6917	1.6941	1.6894	1.6166	1.6887	1.6858	1.6926	1.6480	**1.92**
H(10A)	0.9991	0.8346	0.8200	0.7845	0.7143	0.7862	0.7437	0.7896	0.7638	0.7819	0.7575	0.9991	0.8346	0.8200	0.7845	0.7143	0.7863	0.7437	0.7896	0.7638	0.7819	0.7575	**1.26**
H(10B)	1.6465	1.5484	1.4942	1.4756	1.3942	1.4794	1.3841	1.4847	1.4039	1.4711	1.3599	1.6465	1.5484	1.4942	1.4756	1.3942	1.4794	1.3841	1.4847	1.4039	1.4711	1.3599	**1.07**
H(11A-11C)	0.7782	0.7796	0.7577	0.7883	0.7502	0.7868	0.7401	0.7869	0.7596	0.7888	0.7348	0.7782	0.7796	0.7577	0.7884	0.7502	0.7868	0.7402	0.7869	0.7596	0.7888	0.7348	**0.78**
H(1`A)	2.6544	2.6487	2.6305	2.6418	2.5896	2.6417	2.6032	2.6431	2.6064	2.6410	2.5862	2.7818	2.7823	2.7668	2.7622	2.7279	2.7629	2.7539	2.7652	2.7342	2.7605	2.7249	**3.47**
H(1`B)	3.0063	3.0474	3.0782	3.0838	3.1401	3.0804	3.1156	3.0786	3.1249	3.0860	3.1249	2.7260	2.5820	2.5307	2.5386	2.5326	2.5402	2.5235	2.5434	2.4737	2.5362	2.5222	**3.63**
H(4`A)	2.7260	2.5820	2.5307	2.5386	2.5326	2.5402	2.5235	2.5434	2.4736	2.5362	2.5222	3.0063	3.0474	3.0782	3.0838	3.1401	3.0804	3.1157	3.0786	3.1250	3.0860	3.1249	**3.07**
H(4`B)	2.7818	2.7823	2.7668	2.7622	2.7279	2.7629	2.7539	2.7652	2.7342	2.7606	2.7249	2.6543	2.6487	2.6305	2.6419	2.5896	2.6417	2.6032	2.6431	2.6064	2.6410	2.5862	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. VII

Nuclei	R											S										Exp. [b]
	M06											M06										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.0654	138.4516	140.2395	139.3236	141.3503	139.2467	140.1123	139.1720	140.4485	139.4069	140.3634	137.0654	138.4516	140.2398	139.3235	141.3504	139.2467	140.1121	139.1721	140.4484	139.4069	140.3634	**131.615**
C2	141.0015	140.3104	140.8587	140.0820	140.7204	140.0833	141.1742	140.0927	141.0845	140.0951	141.1353	141.0016	140.3104	140.8587	140.0820	140.7204	140.0832	141.1741	140.0926	141.0844	140.0952	141.1353	**133.405**
C3	130.9031	132.0791	133.0375	132.4179	133.6008	132.3928	133.8570	132.3762	133.7813	132.4567	134.0117	130.9030	132.0792	133.0375	132.4179	133.6008	132.3928	133.8570	132.3761	133.7814	132.4567	134.0117	**126.19**
C4	171.8317	173.1475	173.7103	173.3977	174.0439	173.3927	174.6046	173.3944	174.4353	173.4163	174.6999	171.8316	173.1473	173.7102	173.3977	174.0439	173.3927	174.6047	173.3946	174.4353	173.4162	174.6999	**165.04**
C5	119.3016	120.8022	121.4723	121.4782	122.3461	121.4305	122.5495	121.3899	122.4467	121.5376	122.6841	119.3016	120.8022	121.4723	121.4782	122.3461	121.4305	122.5494	121.3900	122.4466	121.5376	122.6841	**116.425**
C6	133.8836	134.9666	135.5843	135.7167	136.9736	135.6628	137.7766	135.6201	137.3978	135.7850	138.0348	133.8836	134.9667	135.5844	135.7167	136.9736	135.6628	137.7764	135.6201	137.3978	135.7851	138.0348	**129.92**
C7	204.0628	209.7572	211.7199	212.7334	213.5690	212.5343	218.3399	212.3391	217.4244	212.9344	219.4025	204.0628	209.7574	211.7199	212.7333	213.5689	212.5343	218.3399	212.3391	217.4244	212.9344	219.4025	**195.9**
C8	61.9162	63.3412	64.4897	64.1687	65.1960	64.1061	65.7786	64.0496	65.7619	64.2417	66.3624	61.9162	63.3412	64.4897	64.1686	65.1960	64.1061	65.7787	64.0496	65.7618	64.2418	66.3624	**67.6**
C9	35.6222	35.2871	35.5108	35.0907	35.4757	35.1023	35.6010	35.1220	35.5344	35.0941	35.6326	35.6222	35.2872	35.5107	35.0907	35.4756	35.1023	35.6010	35.1220	35.5343	35.0942	35.6326	**32.2**
C10	16.7083	17.5813	18.1514	18.0859	18.8059	18.0490	18.6582	18.0189	18.6456	18.1346	18.8069	16.7083	17.5813	18.1514	18.0859	18.8057	18.0491	18.6582	18.0190	18.6456	18.1347	18.8069	**23.4**
C11	15.7148	15.7061	15.9629	15.7600	16.1540	15.7418	16.0965	15.7320	16.1293	15.7928	16.4520	15.7148	15.7062	15.9629	15.7600	16.1539	15.7418	16.0965	15.7321	16.1294	15.7928	16.4520	**17.9**
C1`	50.9543	51.6493	52.0331	52.0880	52.7707	52.0474	52.7164	52.0150	52.7142	52.1411	53.1882	55.2346	56.1683	56.6054	56.7013	57.3066	56.6585	57.4892	56.6233	57.4017	56.7561	57.8339	**52.4**
C2`	23.7434	24.1299	24.4939	24.2390	24.8309	24.2235	24.8726	24.2161	24.8491	24.2685	24.8089	22.3749	22.6194	23.0874	22.7231	23.4548	22.7089	23.3382	22.7025	23.3656	22.7512	22.9773	**14.5**
C3`	22.3749	22.6195	23.0875	22.7231	23.4548	22.7090	23.3382	22.7026	23.3655	22.7512	22.9773	23.7432	24.1299	24.4938	24.2390	24.8309	24.2236	24.8725	24.2161	24.8491	24.2684	24.8089	**14.2**
C4`	55.2346	56.1682	56.6053	56.7013	57.3067	56.6585	57.4893	56.6234	57.4017	56.7562	57.8339	50.9543	51.6491	52.0331	52.0880	52.7707	52.0474	52.7165	52.0149	52.7142	52.1412	53.1882	**53.9**
H2	8.4710	8.3003	8.2646	8.2010	8.2098	8.2085	8.2547	8.2168	8.2356	8.1948	8.2447	8.4710	8.3004	8.2646	8.2011	8.2098	8.2085	8.2547	8.2168	8.2356	8.1948	8.2447	**8.13**
H5	7.0190	7.2548	7.3533	7.3406	7.4661	7.3364	7.4790	7.3327	7.4666	7.3450	7.5012	7.0190	7.2548	7.3533	7.3406	7.4661	7.3364	7.4790	7.3327	7.4666	7.3449	7.5012	**8.03**
H6	7.8965	8.0718	8.0862	8.1049	8.2127	8.1041	8.2688	8.1044	8.2319	8.1066	8.3138	7.8965	8.0718	8.0862	8.1049	8.2127	8.1041	8.2687	8.1044	8.2319	8.1066	8.3138	**7.4**
H(3``A-3``C)	2.4118	2.5040	2.5244	2.5148	2.5391	2.5145	2.5449	2.5147	2.5432	2.5156	2.5449	2.4118	2.5040	2.5244	2.5148	2.5391	2.5145	2.5449	2.5147	2.5432	2.5156	2.5449	**2.32**
H8	4.3790	4.4188	4.4309	4.4650	4.5350	4.4607	4.5910	4.4573	4.5556	4.4698	4.6395	4.3790	4.4188	4.4309	4.4650	4.5350	4.4607	4.5910	4.4573	4.5556	4.4698	4.6395	**5.64**
H(9A-9B)	1.7493	1.7094	1.6776	1.7022	1.7023	1.7034	1.7160	1.7054	1.7097	1.7018	1.7519	1.7493	1.7094	1.6776	1.7022	1.7023	1.7034	1.7160	1.7054	1.7097	1.7018	1.7519	**1.92**
H(10A)	0.8741	0.7912	0.7792	0.7652	0.7380	0.7659	0.7503	0.7671	0.7494	0.7652	0.7732	0.8741	0.7912	0.7792	0.7653	0.7380	0.7659	0.7503	0.7671	0.7494	0.7652	0.7732	**1.26**
H(10B)	1.7340	1.5759	1.5334	1.4945	1.4180	1.4990	1.4175	1.5041	1.4261	1.4907	1.3680	1.7340	1.5759	1.5334	1.4945	1.4180	1.4990	1.4175	1.5041	1.4261	1.4908	1.3680	**1.07**
H(11A-11C)	0.7419	0.7472	0.7182	0.7425	0.7135	0.7428	0.7109	0.7437	0.7109	0.7428	0.6819	0.7419	0.7472	0.7182	0.7425	0.7135	0.7428	0.7109	0.7437	0.7109	0.7427	0.6819	**0.78**
H(1`A)	2.6595	2.6310	2.6033	2.6005	2.5642	2.6018	2.5733	2.6038	2.5724	2.6000	2.5569	2.8983	2.8520	2.8409	2.8186	2.7856	2.8201	2.8149	2.8222	2.8185	2.8178	2.7893	**3.47**
H(1`B)	3.1047	3.0988	3.1243	3.1274	3.1824	3.1247	3.1714	3.1227	3.1622	3.1307	3.1733	2.8031	2.6561	2.6455	2.6169	2.6287	2.6187	2.5969	2.6211	2.6037	2.6161	2.5760	**3.63**
H(4`A)	2.8031	2.6561	2.6455	2.6169	2.6287	2.6187	2.5969	2.6211	2.6037	2.6161	2.5760	3.1047	3.0988	3.1243	3.1274	3.1824	3.1247	3.1714	3.1227	3.1622	3.1307	3.1733	**3.07**
H(4`B)	2.8983	2.8520	2.8409	2.8186	2.7856	2.8201	2.8149	2.8223	2.8185	2.8177	2.7893	2.6595	2.6310	2.6034	2.6005	2.5642	2.6018	2.5734	2.6038	2.5724	2.6000	2.5569	**3.25**
Nuclei	M06-2X											M06-2X										
C1	153.2701	154.2918	155.2203	154.6145	156.2513	154.6227	155.5608	154.6307	156.0977	154.5977	155.9505	153.2701	154.2918	155.2203	154.6145	156.2513	154.6227	155.5608	154.6306	156.0977	154.5977	155.9504	**131.615**
C2	155.6852	155.6175	156.2016	155.3655	155.9885	155.4052	156.2748	155.4457	156.2335	155.3216	156.2383	155.6852	155.6175	156.2016	155.3655	155.9886	155.4052	156.2748	155.4455	156.2335	155.3216	156.2383	**133.405**
C3	147.8397	149.1050	150.0569	149.4466	150.5836	149.4522	150.8370	149.4581	150.7565	149.4347	150.9812	147.8397	149.1049	150.0569	149.4466	150.5836	149.4521	150.8369	149.4580	150.7565	149.4347	150.9812	**126.19**
C4	185.6334	186.4291	187.0524	186.8793	187.5227	186.8717	188.3306	186.8654	188.1116	186.8804	188.5326	185.6334	186.4290	187.0524	186.8793	187.5226	186.8717	188.3306	186.8653	188.1116	186.8805	188.5326	**165.04**
C5	132.4865	133.9357	134.6020	134.6717	135.6116	134.6477	135.8981	134.6250	135.7901	134.6877	136.1072	132.4864	133.9358	134.6020	134.6717	135.6117	134.6478	135.8981	134.6251	135.7901	134.6877	136.1071	**116.425**
C6	148.6156	150.3509	151.3580	151.4476	153.0243	151.3974	153.5483	151.3494	153.0819	151.4894	153.8860	148.6156	150.3508	151.3580	151.4476	153.0243	151.3975	153.5483	151.3493	153.0819	151.4894	153.8862	**129.92**
C7	219.8759	225.6379	226.9337	228.5720	228.9333	228.4221	235.4422	228.2707	234.5748	228.7048	236.8006	219.8759	225.6379	226.9337	228.5720	228.9333	228.4221	235.4422	228.2707	234.5748	228.7048	236.8005	**195.9**
C8	67.2387	68.8031	69.4851	69.4405	70.2220	69.4312	70.9265	69.4210	71.1182	69.4408	71.3988	67.2387	68.8031	69.4851	69.4405	70.2220	69.4313	70.9265	69.4210	71.1183	69.4408	71.3988	**67.6**
C9	36.9696	36.9458	37.1478	36.9032	37.2728	36.9277	37.3983	36.9530	37.3539	36.8736	37.5866	36.9696	36.9457	37.1478	36.9032	37.2728	36.9277	37.3983	36.9531	37.3539	36.8736	37.5866	**32.2**
C10	18.1477	18.5362	18.8172	18.7811	19.2816	18.7856	19.1087	18.7916	19.0516	18.7711	19.0875	18.1476	18.5362	18.8172	18.7811	19.2816	18.7856	19.1087	18.7915	19.0516	18.7711	19.0875	**23.4**
C11	15.1800	15.2020	15.3180	15.1823	15.3831	15.2037	15.2840	15.2266	15.3231	15.1556	15.5654	15.1800	15.2020	15.3180	15.1823	15.3831	15.2038	15.2840	15.2266	15.3231	15.1556	15.5654	**17.9**
C1`	52.8402	53.4905	53.7693	53.9360	54.5072	53.9285	54.4838	53.9223	54.4927	53.9368	54.9763	56.9817	57.9829	58.3494	58.4105	58.9562	58.4068	59.0951	58.4043	59.0618	58.4073	59.3981	**52.4**
C2`	24.7714	25.1364	25.3996	25.3126	25.7001	25.3263	25.7565	25.3403	25.8918	25.2925	25.6859	23.8439	24.0932	24.3628	24.2469	24.7248	24.2570	24.6742	24.2688	24.6511	24.2309	24.6514	**14.5**
C3`	23.8439	24.0932	24.3628	24.2468	24.7246	24.2570	24.6742	24.2687	24.6511	24.2311	24.6514	24.7714	25.1365	25.3996	25.3125	25.7002	25.3263	25.7565	25.3403	25.8918	25.2925	25.6859	**14.2**
C4`	56.9817	57.9830	58.3494	58.4105	58.9562	58.4069	59.0950	58.4043	59.0618	58.4073	59.3982	52.8402	53.4904	53.7693	53.9360	54.5072	53.9285	54.4838	53.9222	54.4927	53.9369	54.9763	**53.9**
H2	9.0581	8.9654	8.9916	8.9196	8.9408	8.9206	8.9529	8.9215	8.9111	8.9190	8.9394	9.0581	8.9654	8.9916	8.9196	8.9408	8.9206	8.9529	8.9215	8.9111	8.9190	8.9394	**8.13**
H5	7.6107	7.7856	7.8778	7.8682	7.9943	7.8622	8.0101	7.8558	7.9976	7.8740	8.0314	7.6107	7.7856	7.8778	7.8682	7.9943	7.8622	8.0101	7.8558	7.9976	7.8740	8.0314	**8.03**
H6	8.3971	8.5484	8.6390	8.6544	8.7977	8.6460	8.8607	8.6375	8.8110	8.6625	8.8901	8.3971	8.5484	8.6390	8.6544	8.7977	8.6460	8.8607	8.6375	8.8110	8.6625	8.8901	**7.4**
H(3``A-3``C)	2.4798	2.5017	2.5211	2.5122	2.5364	2.5104	2.5411	2.5083	2.5389	2.5141	2.5505	2.4798	2.5017	2.5211	2.5122	2.5365	2.5104	2.5410	2.5082	2.5389	2.5141	2.5505	**2.32**
H8	4.3193	4.3616	4.4037	4.4282	4.5269	4.4214	4.5863	4.4145	4.5260	4.4352	4.6028	4.3193	4.3616	4.4037	4.4282	4.5269	4.4214	4.5863	4.4145	4.5260	4.4352	4.6028	**5.64**
H(9A-9B)	1.6803	1.6995	1.6943	1.7378	1.7405	1.7341	1.7320	1.7300	1.7301	1.7416	1.7687	1.6803	1.6995	1.6943	1.7378	1.7405	1.7341	1.7320	1.7300	1.7301	1.7416	1.7687	**1.92**
H(10A)	0.9398	0.7567	0.7382	0.7032	0.6622	0.7068	0.6864	0.7054	0.6630	0.7024	0.7059	0.9398	0.7567	0.6866	0.7032	0.6888	0.7068	0.6864	0.7054	0.6630	0.7024	0.7059	**1.26**
H(10B)	1.6488	1.5352	1.4812	1.4564	1.3725	1.4644	1.3706	1.4630	1.3623	1.4534	1.3464	1.6488	1.5352	1.4408	1.4564	1.3730	1.4644	1.3706	1.4630	1.3623	1.4534	1.3464	**1.07**
H(11A-11C)	0.7277	0.7091	0.6856	0.7150	0.6795	0.7131	0.6779	0.7109	0.6680	0.7171	0.6711	0.7277	0.7091	0.6856	0.7150	0.6795	0.7131	0.6779	0.7110	0.6680	0.7171	0.6711	**0.78**
H(1`A)	2.5821	2.5881	2.5775	2.5884	2.5466	2.5871	2.5703	2.5857	2.5747	2.5896	2.5519	2.7647	2.8026	2.7483	2.7947	2.7758	2.7958	2.7734	2.7944	2.7988	2.7946	2.7450	**3.47**
H(1`B)	3.0495	3.0681	3.1025	3.1065	3.1673	3.0992	3.1581	3.0978	3.1500	3.1107	3.1804	2.7129	2.5976	2.5529	2.5617	2.5202	2.5641	2.5178	2.5627	2.5406	2.5613	2.5144	**3.63**
H(4`A)	2.7129	2.5976	2.5701	2.5617	2.5561	2.5641	2.5178	2.5627	2.5406	2.5613	2.5144	3.0495	3.0681	3.0317	3.1065	3.1605	3.0992	3.1581	3.0978	3.1500	3.1107	3.1804	**3.07**
H(4`B)	2.7647	2.8026	2.7881	2.7947	2.7514	2.7958	2.7734	2.7944	2.7989	2.7946	2.7450	2.5821	2.5881	2.5108	2.5884	2.5727	2.5871	2.5703	2.5857	2.5747	2.5896	2.5519	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. VIII

Nuclei	R											S										Exp. [b]
	mpW1LYP											mpW1LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.5814	140.1751	140.9777	140.6894	143.2752	140.6339	142.2699	140.5868	142.4938	140.7481	142.6277	139.5814	140.1751	140.9777	140.6894	143.2752	140.6339	142.2698	140.5868	142.4939	140.7481	142.6277	**131.615**
C2	140.6100	140.4399	140.7913	140.2286	140.6777	140.2422	141.0622	140.2566	140.9689	140.2140	141.0227	140.6098	140.4399	140.7913	140.2286	140.6779	140.2422	141.0622	140.2566	140.9689	140.2139	141.0227	**133.405**
C3	134.1464	135.2290	136.1264	135.5715	136.5570	135.5515	136.8796	135.5326	136.8156	135.5884	137.0117	134.1461	135.2290	136.1264	135.5715	136.5569	135.5515	136.8796	135.5326	136.8156	135.5884	137.0118	**126.19**
C4	174.9125	175.8657	176.6014	176.4549	177.0773	176.4119	177.7718	176.3716	177.6013	176.4949	177.8533	174.9125	175.8657	176.6014	176.4549	177.0775	176.4119	177.7718	176.3716	177.6012	176.4949	177.8532	**165.04**
C5	119.2010	120.3495	120.9195	121.0114	121.7973	120.9653	122.0837	120.9217	121.9890	121.0543	122.1934	119.2010	120.3495	120.9195	121.0114	121.7973	120.9653	122.0837	120.9217	121.9889	121.0542	122.1935	**116.425**
C6	133.6017	135.2712	136.2078	136.2118	137.0592	136.1573	137.8393	136.1018	137.5482	136.2586	138.0932	133.6016	135.2712	136.2078	136.2118	137.0591	136.1573	137.8392	136.1018	137.5482	136.2585	138.0934	**129.92**
C7	203.8368	208.4344	209.6616	211.1899	212.7198	210.9948	217.6963	210.8083	216.7168	211.3808	218.8838	203.8365	208.4344	209.6616	211.1899	212.7194	210.9948	217.6963	210.8083	216.7168	211.3810	218.8840	**195.9**
C8	65.7144	66.7517	67.0420	67.3286	68.4046	67.2862	68.8000	67.2464	68.7584	67.3685	69.1910	65.7143	66.7517	67.0420	67.3286	68.4046	67.2862	68.8000	67.2464	68.7584	67.3684	69.1910	**67.6**
C9	38.6903	38.2641	38.4588	38.1116	38.2426	38.1202	38.3578	38.1294	38.3106	38.1003	38.4110	38.6902	38.2641	38.4588	38.1116	38.2425	38.1202	38.3578	38.1294	38.3107	38.1004	38.4110	**32.2**
C10	19.9646	20.3826	20.6745	20.6752	21.1266	20.6555	21.0109	20.6369	21.0055	20.6915	21.0948	19.9646	20.3826	20.6745	20.6752	21.1266	20.6555	21.0109	20.6369	21.0055	20.6914	21.0948	**23.4**
C11	16.2356	16.3458	16.5064	16.4356	16.6122	16.4286	16.5569	16.4228	16.5670	16.4400	16.7073	16.2356	16.3458	16.5063	16.4356	16.6123	16.4286	16.5569	16.4228	16.5670	16.4400	16.7074	**17.9**
C1`	52.0088	52.8564	53.0822	53.4081	53.9346	53.3740	53.8687	53.3408	53.8452	53.4378	54.2795	56.5396	57.5874	57.9602	58.0930	58.5770	58.0584	58.7417	58.0257	58.6925	58.1243	58.9582	**52.4**
C2`	25.8957	26.3447	26.5842	26.5645	26.9311	26.5482	26.9756	26.5335	26.9902	26.5778	26.8635	25.5661	25.6938	26.1283	25.8900	26.4535	25.8720	26.3801	25.8561	26.3761	25.9062	26.1494	**14.5**
C3`	25.5661	25.6938	26.1283	25.8900	26.4535	25.8720	26.3800	25.8561	26.3761	25.9061	26.1494	25.8957	26.3447	26.5841	26.5645	26.9311	26.5482	26.9756	26.5335	26.9902	26.5778	26.8635	**14.2**
C4`	56.5395	57.5874	57.9603	58.0930	58.5769	58.0584	58.7418	58.0257	58.6926	58.1243	58.9584	52.0087	52.8564	53.0821	53.4081	53.9347	53.3740	53.8687	53.3408	53.8452	53.4378	54.2795	**53.9**
H2	8.5453	8.4648	8.4937	8.4003	8.3306	8.4062	8.3740	8.4113	8.3614	8.3939	8.3539	8.5453	8.4648	8.4937	8.4003	8.3306	8.4062	8.3740	8.4113	8.3614	8.3939	8.3539	**8.13**
H5	7.1145	7.2719	7.3612	7.3423	7.4603	7.3384	7.4815	7.3342	7.4711	7.3459	7.4995	7.1145	7.2719	7.3612	7.3423	7.4603	7.3384	7.4815	7.3342	7.4711	7.3459	7.4995	**8.03**
H6	7.7941	7.9721	8.0730	8.0664	8.1444	8.0614	8.2114	8.0559	8.1854	8.0707	8.2343	7.7941	7.9721	8.0730	8.0664	8.1444	8.0614	8.2114	8.0559	8.1854	8.0707	8.2343	**7.4**
H(3``A-3``C)	2.3861	2.4282	2.4451	2.4435	2.4632	2.4428	2.4717	2.4419	2.4693	2.4441	2.4747	2.3861	2.4282	2.4451	2.4435	2.4631	2.4428	2.4717	2.4419	2.4693	2.4441	2.4747	**2.32**
H8	4.5405	4.6030	4.6753	4.6513	4.7031	4.6484	4.7590	4.6450	4.7379	4.6538	4.7451	4.5404	4.6030	4.6753	4.6513	4.7031	4.6484	4.7590	4.6450	4.7379	4.6538	4.7451	**5.64**
H(9A-9B)	1.6505	1.6989	1.6808	1.7247	1.6890	1.7245	1.6835	1.7235	1.6770	1.7245	1.7065	1.6505	1.6989	1.6808	1.7247	1.6890	1.7245	1.6835	1.7235	1.6770	1.7245	1.7065	**1.92**
H(10A)	1.0855	0.9687	0.9729	0.9227	0.8473	0.9263	0.8999	0.9295	0.8925	0.9192	0.9047	1.0855	0.9687	0.9729	0.9227	0.8473	0.9263	0.8999	0.9295	0.8925	0.9192	0.9047	**1.26**
H(10B)	1.7318	1.6280	1.5872	1.5585	1.4795	1.5628	1.4809	1.5668	1.4854	1.5543	1.4454	1.7318	1.6280	1.5872	1.5585	1.4795	1.5628	1.4809	1.5668	1.4854	1.5543	1.4454	**1.07**
H(11A-11C)	0.7863	0.7963	0.7825	0.8052	0.7636	0.8049	0.7711	0.8042	0.7695	0.8055	0.7578	0.7863	0.7963	0.7825	0.8052	0.7636	0.8049	0.7711	0.8042	0.7695	0.8055	0.7578	**0.78**
H(1`A)	2.7162	2.7062	2.6903	2.6973	2.6464	2.6982	2.6556	2.6987	2.6583	2.6964	2.6372	2.8399	2.8370	2.8159	2.8246	2.8038	2.8255	2.8101	2.8262	2.8166	2.8236	2.7809	**3.47**
H(1`B)	3.1751	3.2169	3.2545	3.2533	3.3124	3.2512	3.2939	3.2488	3.2882	3.2551	3.2961	2.8533	2.6856	2.6641	2.6621	2.7031	2.6625	2.6526	2.6629	2.6567	2.6620	2.6500	**3.63**
H(4`A)	2.8533	2.6856	2.6641	2.6621	2.7031	2.6625	2.6526	2.6629	2.6567	2.6619	2.6500	3.1751	3.2169	3.2545	3.2533	3.3124	3.2512	3.2939	3.2488	3.2882	3.2550	3.2962	**3.07**
H(4`B)	2.8399	2.8370	2.8159	2.8246	2.8038	2.8255	2.8101	2.8262	2.8166	2.8236	2.7809	2.7162	2.7062	2.6903	2.6973	2.6464	2.6982	2.6556	2.6987	2.6583	2.6964	2.6372	**3.25**
Nuclei	mpW1PW91											mpW1PW91											
C1	136.6939	137.3276	137.9762	137.8634	139.5017	137.8071	139.5506	137.7608	138.6614	137.9208	139.9257	136.6939	137.3276	137.9762	137.8634	139.5017	137.8071	139.5508	137.7608	138.6614	137.9208	139.9256	**131.615**
C2	139.7884	139.6733	140.0697	139.4195	140.0010	139.4408	140.2455	139.4672	140.2182	139.3977	140.2078	139.7884	139.6734	140.0697	139.4195	140.0010	139.4408	140.2455	139.4673	140.2182	139.3977	140.2078	**133.405**
C3	131.9261	133.1562	134.0791	133.5280	134.6189	133.5084	134.9850	133.4943	134.8363	133.5456	135.1528	131.9261	133.1562	134.0791	133.5280	134.6189	133.5084	134.9849	133.4943	134.8365	133.5456	135.1528	**126.19**
C4	171.9409	172.8370	173.4594	173.3402	173.9484	173.3046	174.7576	173.2751	174.5278	173.3737	174.8649	171.9409	172.8371	173.4594	173.3402	173.9484	173.3046	174.7575	173.2751	174.5279	173.3737	174.8650	**165.04**
C5	118.4212	119.6411	120.2487	120.2781	121.1201	120.2373	121.4977	120.2027	121.2636	120.3167	121.6446	118.4211	119.6411	120.2488	120.2781	121.1200	120.2373	121.4976	120.2027	121.2635	120.3167	121.6447	**116.425**
C6	132.4768	134.1867	135.1767	135.1048	136.4472	135.0544	136.7242	135.0087	136.9411	135.1509	137.0395	132.4768	134.1868	135.1767	135.1048	136.4472	135.0544	136.7243	135.0087	136.9409	135.1509	137.0394	**129.92**
C7	201.6360	205.9828	206.9194	208.5946	209.2684	208.4081	214.9780	208.2323	212.9177	208.7757	216.2004	201.6360	205.9825	206.9195	208.5946	209.2683	208.4081	214.9778	208.2322	212.9177	208.7757	216.2007	**195.9**
C8	63.6022	64.7282	65.1276	65.3172	66.2170	65.2750	66.9036	65.2400	66.5231	65.3582	67.4149	63.6022	64.7283	65.1276	65.3172	66.2170	65.2750	66.9035	65.2399	66.5232	65.3582	67.4149	**67.6**
C9	36.6617	36.4371	36.6363	36.3113	36.6987	36.3199	36.5807	36.3343	36.7354	36.3024	36.7199	36.6617	36.4372	36.6363	36.3113	36.6987	36.3198	36.5807	36.3343	36.7354	36.3024	36.7200	**32.2**
C10	18.3302	18.8139	19.0513	19.0869	19.5919	19.0721	19.4035	19.0627	19.4369	19.1000	19.5724	18.3302	18.8139	19.0512	19.0869	19.5918	19.0721	19.4035	19.0626	19.4368	19.1000	19.5724	**23.4**
C11	15.7468	15.8768	15.9750	15.9232	16.1381	15.9211	16.0623	15.9245	16.0769	15.9241	16.2395	15.7468	15.8768	15.9750	15.9232	16.1381	15.9211	16.0622	15.9245	16.0769	15.9241	16.2394	**17.9**
C1`	50.6020	51.4331	51.6436	51.8910	52.4300	51.8659	52.3758	51.8458	52.3430	51.9139	52.8324	54.8332	55.8629	56.2050	56.3078	56.8174	56.2802	57.0452	56.2586	56.9406	56.3333	57.2896	**52.4**
C2`	24.7040	25.0991	25.3658	25.2486	25.6805	25.2403	25.6737	25.2375	25.6946	25.2555	25.5575	24.2157	24.3640	24.7322	24.5023	25.0103	24.4911	25.0153	24.4858	24.9091	24.5124	24.7926	**14.5**
C3`	24.2156	24.3640	24.7323	24.5023	25.0103	24.4911	25.0152	24.4858	24.9091	24.5124	24.7926	24.7040	25.0991	25.3658	25.2486	25.6805	25.2403	25.6737	25.2376	25.6946	25.2555	25.5575	**14.2**
C4`	54.8331	55.8629	56.2050	56.3078	56.8174	56.2802	57.0453	56.2587	56.9406	56.3333	57.2897	50.6021	51.4331	51.6435	51.8910	52.4299	51.8659	52.3758	51.8458	52.3429	51.9139	52.8324	**53.9**
H2	8.5913	8.5113	8.5471	8.4368	8.4432	8.4438	8.4110	8.4505	8.4815	8.4300	8.3923	8.5913	8.5113	8.5471	8.4368	8.4432	8.4438	8.4109	8.4505	8.4815	8.4300	8.3923	**8.13**
H5	7.1374	7.3037	7.3973	7.3727	7.4968	7.3691	7.5201	7.3655	7.5046	7.3765	7.5417	7.1374	7.3037	7.3973	7.3727	7.4968	7.3691	7.5201	7.3655	7.5046	7.3765	7.5417	**8.03**
H6	7.8828	8.0560	8.1592	8.1417	8.2688	8.1374	8.2840	8.1330	8.3175	8.1459	8.3083	7.8828	8.0560	8.1592	8.1417	8.2688	8.1374	8.2840	8.1331	8.3175	8.1459	8.3083	**7.4**
H(3``A-3``C)	2.3608	2.4068	2.4222	2.4197	2.4418	2.4192	2.4532	2.4188	2.4477	2.4203	2.4590	2.3608	2.4068	2.4222	2.4197	2.4418	2.4192	2.4532	2.4188	2.4477	2.4203	2.4590	**2.32**
H8	4.5358	4.6003	4.6682	4.6448	4.7161	4.6421	4.7598	4.6396	4.7558	4.6474	4.7517	4.5358	4.6003	4.6682	4.6448	4.7161	4.6421	4.7598	4.6396	4.7558	4.6474	4.7517	**5.64**
H(9A-9B)	1.6837	1.7267	1.7130	1.7470	1.7593	1.7471	1.6905	1.7470	1.7486	1.7469	1.7202	1.6837	1.7267	1.7130	1.7470	1.7594	1.7471	1.6906	1.7470	1.7485	1.7469	1.7202	**1.92**
H(10A)	1.0162	0.9022	0.8993	0.8458	0.7767	0.8502	0.8292	0.8546	0.8167	0.8417	0.8316	1.0162	0.9022	0.8993	0.8458	0.7766	0.8502	0.8292	0.8546	0.8167	0.8417	0.8316	**1.26**
H(10B)	1.7063	1.5987	1.5480	1.5258	1.4525	1.5304	1.4408	1.5350	1.4574	1.5217	1.4087	1.7063	1.5987	1.5480	1.5258	1.4525	1.5304	1.4408	1.5350	1.4574	1.5217	1.4087	**1.07**
H(11A-11C)	0.7308	0.7402	0.7238	0.7432	0.7107	0.7433	0.7101	0.7435	0.7175	0.7433	0.6979	0.7308	0.7402	0.7238	0.7432	0.7107	0.7433	0.7101	0.7435	0.7175	0.7433	0.6979	**0.78**
H(1`A)	2.6561	2.6496	2.6336	2.6398	2.5970	2.6408	2.6030	2.6418	2.6086	2.6391	2.5871	2.7779	2.7789	2.7625	2.7647	2.7386	2.7657	2.7581	2.7668	2.7498	2.7640	2.7318	**3.47**
H(1`B)	3.1516	3.1916	3.2180	3.2216	3.2831	3.2199	3.2523	3.2183	3.2602	3.2235	3.2571	2.8531	2.6777	2.6350	2.6494	2.6574	2.6497	2.6262	2.6505	2.5969	2.6495	2.6225	**3.63**
H(4`A)	2.8531	2.6777	2.6350	2.6494	2.6574	2.6497	2.6262	2.6505	2.5969	2.6495	2.6225	3.1516	3.1916	3.2180	3.2216	3.2831	3.2199	3.2524	3.2183	3.2602	3.2235	3.2571	**3.07**
H(4`B)	2.7779	2.7789	2.7625	2.7647	2.7386	2.7657	2.7581	2.7668	2.7498	2.7640	2.7318	2.6561	2.6496	2.6336	2.6398	2.5970	2.6408	2.6030	2.6418	2.6086	2.6391	2.5870	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. IX

Nuclei	R											S										Exp. [b]
	O3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	134.4305	136.0139	137.9574	137.1814	139.5771	137.1179	138.4207	137.0526	138.7558	137.2392	138.7828	134.4307	136.0139	137.9574	137.1814	139.5771	137.1179	138.4208	137.0526	138.7558	137.2392	138.7828	**131.615**
C2	135.1040	135.0620	135.7541	135.0220	135.7085	135.0380	136.0387	135.0487	135.8986	134.9998	135.9981	135.1041	135.0620	135.7541	135.0220	135.7085	135.0380	136.0387	135.0487	135.8985	134.9998	135.9981	**133.405**
C3	128.1027	129.4127	130.3350	129.8526	130.8538	129.8424	131.1689	129.8261	131.0709	129.8552	131.3013	128.1026	129.4127	130.3349	129.8526	130.8538	129.8424	131.1687	129.8261	131.0708	129.8552	131.3013	**126.19**
C4	168.6663	169.3575	169.7684	169.5991	170.0928	169.5950	170.7061	169.5852	170.5278	169.5957	170.7645	168.6663	169.3575	169.7683	169.5991	170.0928	169.5950	170.7061	169.5852	170.5278	169.5957	170.7645	**165.04**
C5	114.5502	115.7242	116.2170	116.2527	116.8387	116.2344	117.1374	116.2103	117.0089	116.2626	117.2369	114.5502	115.7242	116.2170	116.2527	116.8387	116.2344	117.1374	116.2103	117.0087	116.2626	117.2369	**116.425**
C6	127.5968	128.8400	129.5626	129.8281	130.8978	129.7743	131.5685	129.7154	131.3073	129.8721	131.7886	127.5969	128.8400	129.5627	129.8281	130.8978	129.7743	131.5686	129.7154	131.3074	129.8721	131.7886	**129.92**
C7	197.3149	202.3848	204.5863	205.5630	206.9613	205.3692	211.2504	205.1748	210.5828	205.7455	212.3456	197.3149	202.3848	204.5862	205.5630	206.9613	205.3692	211.2505	205.1748	210.5828	205.7455	212.3456	**195.9**
C8	64.3639	65.7214	66.8563	66.7463	67.8531	66.6788	68.2920	66.6103	68.3035	66.8083	68.6082	64.3639	65.7214	66.8563	66.7463	67.8531	66.6788	68.2920	66.6103	68.3034	66.8083	68.6082	**67.6**
C9	36.9425	36.6165	36.7516	36.5067	36.6592	36.5226	36.9282	36.5337	36.8474	36.4852	36.9229	36.9425	36.6165	36.7517	36.5067	36.6592	36.5228	36.9282	36.5337	36.8475	36.4852	36.9229	**32.2**
C10	19.4987	19.9738	20.3140	20.3197	20.8098	20.3079	20.7221	20.2909	20.6949	20.3242	20.7827	19.4988	19.9738	20.3139	20.3197	20.8097	20.3079	20.7222	20.2909	20.6950	20.3242	20.7827	**23.4**
C11	16.0561	16.1417	16.3097	16.2617	16.4860	16.2635	16.4415	16.2606	16.4421	16.2538	16.5680	16.0561	16.1417	16.3097	16.2617	16.4860	16.2635	16.4417	16.2606	16.4421	16.2538	16.5680	**17.9**
C1`	50.8183	51.5522	51.9154	52.1010	52.6666	52.0772	52.6347	52.0482	52.5901	52.1169	53.0371	55.3148	56.2422	56.7045	56.8054	57.3623	56.7815	57.4538	56.7522	57.3887	56.8214	57.6664	**52.4**
C2`	25.9067	26.2739	26.5823	26.5115	26.8869	26.5055	26.9100	26.4945	26.9113	26.5109	26.7430	25.7740	25.9669	26.3359	26.0920	26.6513	26.0951	26.4600	26.0938	26.4697	26.0827	26.2127	**14.5**
C3`	25.7740	25.9669	26.3358	26.0920	26.6513	26.0951	26.4599	26.0938	26.4696	26.0827	26.2127	25.9067	26.2739	26.5823	26.5115	26.8869	26.5056	26.9100	26.4945	26.9113	26.5109	26.7430	**14.2**
C4`	55.3148	56.2422	56.7045	56.8054	57.3623	56.7815	57.4539	56.7522	57.3887	56.8214	57.6664	50.8183	51.5522	51.9154	52.1010	52.6666	52.0772	52.6348	52.0482	52.5902	52.1169	53.0371	**53.9**
H2	8.3569	8.1900	8.1234	8.0662	8.0208	8.0749	8.0938	8.0830	8.0613	8.0573	8.0811	8.3569	8.1900	8.1234	8.0662	8.0208	8.0749	8.0938	8.0830	8.0613	8.0573	8.0811	**8.13**
H5	7.0545	7.2194	7.2975	7.2865	7.3946	7.2832	7.4164	7.2794	7.4046	7.2895	7.4330	7.0545	7.2194	7.2975	7.2865	7.3946	7.2832	7.4165	7.2794	7.4045	7.2895	7.4330	**8.03**
H6	7.7520	7.8578	7.8909	7.9209	8.0020	7.9176	8.0547	7.9139	8.0266	7.9236	8.0727	7.7520	7.8578	7.8909	7.9209	8.0020	7.9176	8.0547	7.9139	8.0266	7.9236	8.0727	**7.4**
H(3``A-3``C)	2.3520	2.3915	2.4027	2.4013	2.4183	2.4012	2.4275	2.4007	2.4234	2.4012	2.4319	2.3521	2.3915	2.4027	2.4013	2.4183	2.4012	2.4275	2.4007	2.4234	2.4012	2.4319	**2.32**
H8	4.7384	4.7673	4.7634	4.7784	4.8071	4.7783	4.8337	4.7779	4.8158	4.7783	4.8145	4.7384	4.7673	4.7634	4.7784	4.8071	4.7784	4.8337	4.7779	4.8158	4.7783	4.8145	**5.64**
H(9A-9B)	1.5682	1.5951	1.5689	1.6249	1.6058	1.6230	1.6378	1.6207	1.6226	1.6266	1.6569	1.5681	1.5951	1.5689	1.6249	1.6058	1.6230	1.6378	1.6207	1.6227	1.6266	1.6569	**1.92**
H(10A)	1.0566	0.9964	0.9826	0.9640	0.9298	0.9674	0.9602	0.9705	0.9581	0.9605	0.9652	1.0566	0.9964	0.9825	0.9640	0.9298	0.9674	0.9602	0.9705	0.9581	0.9605	0.9652	**1.26**
H(10B)	1.6642	1.5683	1.5303	1.5138	1.4464	1.5180	1.4472	1.5218	1.4534	1.5096	1.4200	1.6642	1.5683	1.5303	1.5138	1.4464	1.5180	1.4472	1.5218	1.4534	1.5096	1.4200	**1.07**
H(11A-11C)	0.7585	0.7698	0.7538	0.7850	0.7581	0.7846	0.7601	0.7838	0.7600	0.7853	0.7493	0.7585	0.7698	0.7538	0.7850	0.7581	0.7846	0.7601	0.7838	0.7600	0.7853	0.7493	**0.78**
H(1`A)	2.7600	2.7462	2.7246	2.7326	2.6846	2.7339	2.6932	2.7349	2.6962	2.7312	2.6672	2.8987	2.8955	2.8865	2.8784	2.8448	2.8798	2.8458	2.8810	2.8530	2.8770	2.8209	**3.47**
H(1`B)	3.2315	3.2637	3.2930	3.2992	3.3560	3.2968	3.3425	3.2941	3.3370	3.3014	3.3398	2.8789	2.7804	2.7781	2.7692	2.7903	2.7691	2.7649	2.7690	2.7713	2.7695	2.7604	**3.63**
H(4`A)	2.8789	2.7804	2.7781	2.7692	2.7903	2.7691	2.7649	2.7690	2.7713	2.7695	2.7604	3.2314	3.2637	3.2929	3.2992	3.3560	3.2968	3.3425	3.2941	3.3370	3.3014	3.3398	**3.07**
H(4`B)	2.8987	2.8955	2.8865	2.8784	2.8448	2.8798	2.8458	2.8810	2.8530	2.8770	2.8209	2.7601	2.7462	2.7246	2.7326	2.6846	2.7339	2.6932	2.7349	2.6963	2.7312	2.6672	**3.25**
Nuclei	OLYP																						
C1	133.4973	134.9967	136.7423	135.9869	138.1355	135.9105	137.0523	135.8279	137.3582	136.0483	137.3957	133.4972	134.9967	136.7423	135.9869	138.1355	135.9105	137.0523	135.8279	137.3582	136.0483	137.3958	**131.615**
C2	132.8148	132.8487	133.5496	132.8076	133.4430	132.8239	133.7915	132.8337	133.6470	132.7821	133.7443	132.8148	132.8487	133.5496	132.8076	133.4430	132.8239	133.7915	132.8337	133.6470	132.7821	133.7444	**133.405**
C3	126.5599	127.8006	128.6789	128.1954	129.1589	128.1879	129.5213	128.1742	129.4129	128.1937	129.6445	126.5599	127.8006	128.6789	128.1954	129.1589	128.1879	129.5213	128.1742	129.4129	128.1936	129.6445	**126.19**
C4	167.7537	168.3736	168.9136	168.7044	169.3090	168.6971	169.8721	168.6845	169.7070	168.7031	169.9347	167.7538	168.3736	168.9136	168.7044	169.3090	168.6971	169.8721	168.6845	169.7070	168.7031	169.9348	**165.04**
C5	112.8194	113.7678	114.2270	114.2360	114.8109	114.2212	115.1488	114.2014	115.0169	114.2416	115.2399	112.8194	113.7678	114.2270	114.2360	114.8109	114.2212	115.1488	114.2014	115.0169	114.2417	115.2399	**116.425**
C6	125.1417	126.6345	127.4010	127.6455	128.7254	127.5959	129.3246	127.5396	129.0740	127.6825	129.5520	125.1417	126.6345	127.4011	127.6455	128.7254	127.5959	129.3246	127.5396	129.0740	127.6826	129.5520	**129.92**
C7	195.8448	200.6564	202.7457	203.5979	204.9396	203.3928	208.7989	203.1824	208.2210	203.7825	209.8532	195.8448	200.6564	202.7457	203.5979	204.9396	203.3928	208.7989	203.1824	208.2210	203.7826	209.8532	**195.9**
C8	65.8275	67.1728	68.3605	68.2452	69.2981	68.1620	69.7262	68.0754	69.7499	68.3160	69.9831	65.8275	67.1728	68.3605	68.2452	69.2981	68.1620	69.7262	68.0754	69.7499	68.3161	69.9831	**67.6**
C9	37.9207	37.6469	37.8141	37.5531	37.6981	37.5696	38.0419	37.5808	37.9519	37.5290	38.0099	37.9207	37.6469	37.8141	37.5531	37.6981	37.5696	38.0419	37.5808	37.9519	37.5291	38.0098	**32.2**
C10	20.3218	20.8147	21.1874	21.1758	21.6556	21.1624	21.5838	21.1436	21.5598	21.1798	21.6288	20.3217	20.8147	21.1874	21.1758	21.6556	21.1624	21.5838	21.1436	21.5598	21.1797	21.6288	**23.4**
C11	16.1889	16.2840	16.4723	16.4168	16.6185	16.4168	16.5822	16.4115	16.5846	16.4083	16.6990	16.1890	16.2840	16.4723	16.4168	16.6185	16.4168	16.5822	16.4115	16.5846	16.4083	16.6990	**17.9**
C1`	51.7583	52.4747	52.8734	53.0306	53.5856	53.0041	53.5789	52.9722	53.5340	53.0470	53.9720	56.3513	57.2514	57.6980	57.8094	58.3407	57.7827	58.4390	57.7503	58.3706	57.8255	58.6724	**52.4**
C2`	26.4821	26.8755	27.2199	27.1791	27.5358	27.1676	27.5686	27.1510	27.5718	27.1812	27.3888	26.5391	26.7441	27.1023	26.8670	27.4076	26.8703	27.1995	26.8677	27.2099	26.8549	26.9266	**14.5**
C3`	26.5391	26.7441	27.1023	26.8670	27.4076	26.8703	27.1995	26.8677	27.2099	26.8549	26.9266	26.4820	26.8755	27.2199	27.1791	27.5358	27.1676	27.5686	27.1510	27.5718	27.1812	27.3888	**14.2**
C4`	56.3514	57.2514	57.6980	57.8094	58.3407	57.7827	58.4390	57.7503	58.3706	57.8255	58.6723	51.7583	52.4747	52.8734	53.0306	53.5856	53.0041	53.5789	52.9722	53.5340	53.0469	53.9720	**53.9**
H2	8.1736	8.0277	7.9809	7.9241	7.8976	7.9339	7.9768	7.9436	7.9446	7.9146	7.9655	8.1736	8.0277	7.9809	7.9241	7.8976	7.9339	7.9768	7.9436	7.9446	7.9146	7.9655	**8.13**
H5	6.9912	7.1352	7.2110	7.1979	7.3065	7.1947	7.3280	7.1915	7.3164	7.2005	7.3432	6.9911	7.1352	7.2110	7.1979	7.3065	7.1947	7.3280	7.1915	7.3164	7.2005	7.3432	**8.03**
H6	7.6484	7.7595	7.7955	7.8198	7.9092	7.8178	7.9577	7.8157	7.9300	7.8213	7.9755	7.6484	7.7595	7.7955	7.8198	7.9092	7.8178	7.9577	7.8157	7.9300	7.8213	7.9755	**7.4**
H(3``A-3``C)	2.3288	2.3659	2.3819	2.3779	2.3962	2.3778	2.4072	2.3774	2.4030	2.3776	2.4093	2.3288	2.3659	2.3819	2.3779	2.3962	2.3778	2.4072	2.3774	2.4030	2.3776	2.4094	**2.32**
H8	4.9202	4.9332	4.9108	4.9278	4.9522	4.9297	4.9716	4.9315	4.9568	4.9257	4.9445	4.9202	4.9332	4.9108	4.9278	4.9522	4.9297	4.9716	4.9315	4.9568	4.9257	4.9445	**5.64**
H(9A-9B)	1.5841	1.6326	1.6229	1.6739	1.6596	1.6719	1.6974	1.6698	1.6832	1.6756	1.7146	1.5841	1.6326	1.6229	1.6739	1.6596	1.6719	1.6974	1.6698	1.6832	1.6756	1.7146	**1.92**
H(10A)	1.1064	1.0590	1.0269	1.0190	0.9745	1.0224	1.0070	1.0255	1.0042	1.0151	1.0107	1.1063	1.0590	1.0269	1.0190	0.9745	1.0224	1.0070	1.0255	1.0042	1.0151	1.0107	**1.26**
H(10B)	1.6864	1.6035	1.5696	1.5493	1.4876	1.5534	1.4877	1.5574	1.4940	1.5449	1.4596	1.6864	1.6035	1.5696	1.5493	1.4876	1.5534	1.4877	1.5574	1.4940	1.5449	1.4596	**1.07**
H(11A-11C)	0.7708	0.7853	0.7679	0.7981	0.7704	0.7976	0.7704	0.7970	0.7701	0.7980	0.7588	0.7707	0.7853	0.7679	0.7981	0.7704	0.7976	0.7704	0.7970	0.7701	0.7980	0.7588	**0.78**
H(1`A)	2.8205	2.8088	2.7881	2.7946	2.7464	2.7958	2.7504	2.7969	2.7540	2.7930	2.7192	2.9653	2.9586	2.9525	2.9425	2.9109	2.9439	2.9077	2.9453	2.9158	2.9407	2.7192	**3.47**
H(1`B)	3.3214	3.3554	3.3871	3.3900	3.4499	3.3877	3.4337	3.3854	3.4292	3.3919	3.4276	2.9696	2.8737	2.8750	2.8601	2.8805	2.8595	2.8750	2.8601	2.8805	2.8595	2.8590	**3.63**
H(4`A)	2.9696	2.8737	2.8750	2.8601	2.8805	2.8595	2.8590	2.8590	2.8647	2.8604	2.8510	3.3214	3.3554	3.3871	3.3900	3.4499	3.3877	3.4337	3.3854	3.4292	3.3919	2.8510	**3.07**
H(4`B)	2.9653	2.9586	2.9525	2.9425	2.9109	2.9439	2.9077	2.9453	2.9158	2.9407	2.8784	2.8205	2.8088	2.7881	2.7946	2.7464	2.7958	2.7504	2.7969	2.7540	2.7930	2.8784	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. X

Nuclei	R											S										Exp. [b]
	OPBE											OPBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	130.1638	131.8468	133.4651	132.7350	135.1447	132.6682	133.8744	132.5918	134.1630	132.8029	134.3068	130.1638	131.8468	133.4651	132.7350	135.1447	132.6682	133.8744	132.5918	134.1630	132.8029	134.3068	**131.615**
C2	131.6232	131.6706	132.3579	131.5537	132.2232	131.5803	132.5470	131.5885	132.4160	131.5220	132.5190	131.6232	131.6705	132.3579	131.5537	132.2232	131.5803	132.5470	131.5885	132.4160	131.5220	132.5190	**133.405**
C3	123.9490	125.4052	126.2792	125.8080	126.8467	125.8063	127.2134	125.7855	127.0967	125.8029	127.3817	123.9490	125.4053	126.2792	125.8080	126.8467	125.8063	127.2133	125.7855	127.0967	125.8029	127.3817	**126.19**
C4	164.2404	164.9405	165.3607	165.1529	165.5946	165.1622	166.2741	165.1523	166.1024	165.1374	166.3392	164.2404	164.9406	165.3607	165.1529	165.5946	165.1622	166.2741	165.1523	166.1024	165.1374	166.3392	**165.04**
C5	111.7064	112.8862	113.3260	113.3367	113.9238	113.3332	114.2926	113.3095	114.1480	113.3328	114.4223	111.7065	112.8861	113.3260	113.3367	113.9237	113.3332	114.2927	113.3095	114.1480	113.3328	114.4223	**116.425**
C6	123.7638	125.1525	125.8779	126.0227	126.9664	125.9846	127.7181	125.9280	127.4830	126.0529	127.9046	123.7639	125.1525	125.8779	126.0227	126.9664	125.9846	127.7181	125.9280	127.4830	126.0529	127.9046	**129.92**
C7	192.9939	197.7806	199.6398	200.4668	202.0434	200.2841	205.5210	200.0936	204.9348	200.6466	206.6364	192.9936	197.7807	199.6398	200.4668	202.0434	200.2841	205.5208	200.0936	204.9348	200.6466	206.6364	**195.9**
C8	63.1487	64.6985	65.6901	65.6289	66.8838	65.5642	67.1265	65.4883	67.1166	65.6927	67.5609	63.1486	64.6985	65.6901	65.6289	66.8838	65.5642	67.1265	65.4883	67.1166	65.6927	67.5609	**67.6**
C9	35.5355	35.4545	35.5555	35.3420	35.5403	35.3644	35.8125	35.3687	35.7183	35.3154	35.8714	35.5355	35.4545	35.5554	35.3420	35.5403	35.3644	35.8125	35.3687	35.7183	35.3155	35.8714	**32.2**
C10	18.3181	18.9088	19.1661	19.1859	19.6018	19.1867	19.5290	19.1692	19.4986	19.1796	19.6633	18.3183	18.9088	19.1661	19.1859	19.6018	19.1867	19.5290	19.1692	19.4986	19.1796	19.6633	**23.4**
C11	15.5201	15.6876	15.7560	15.7279	15.8915	15.7405	15.8367	15.7354	15.8377	15.7113	15.9874	15.5201	15.6876	15.7560	15.7279	15.8915	15.7405	15.8367	15.7354	15.8377	15.7113	15.9874	**17.9**
C1`	49.8449	50.6489	50.9230	51.1126	51.6517	51.1022	51.5608	51.0735	51.5300	51.1173	51.9938	54.2100	55.1987	55.5796	55.6591	56.1007	55.6493	56.2824	55.6210	56.2091	55.6631	56.4947	**52.4**
C2`	25.1051	25.5210	25.7450	25.6658	25.9852	25.6736	25.9823	25.6634	25.9874	25.6536	25.8054	24.9998	25.2327	25.5035	25.2396	25.6627	25.2517	25.5295	25.2468	25.5452	25.2242	25.2410	**14.5**
C3`	24.9998	25.2328	25.5035	25.2396	25.6627	25.2517	25.5295	25.2468	25.5452	25.2242	25.2410	25.1051	25.5210	25.7450	25.6658	25.9853	25.6736	25.9824	25.6634	25.9874	25.6536	25.8054	**14.2**
C4`	54.2099	55.1986	55.5796	55.6591	56.1007	55.6493	56.2823	55.6210	56.2091	55.6631	56.4947	49.8449	50.6489	50.9230	51.1126	51.6517	51.1022	51.5607	51.0735	51.5300	51.1173	51.9938	**53.9**
H2	8.2226	8.0701	8.0263	7.9709	7.9185	7.9810	8.0136	7.9894	7.9826	7.9594	7.9992	8.2226	8.0701	8.0263	7.9709	7.9185	7.9810	8.0136	7.9894	7.9826	7.9594	7.9992	**8.13**
H5	7.0052	7.1674	7.2404	7.2314	7.3342	7.2287	7.3618	7.2251	7.3489	7.2331	7.3776	7.0052	7.1674	7.2404	7.2314	7.3342	7.2287	7.3618	7.2251	7.3489	7.2331	7.3776	**8.03**
H6	7.7298	7.8332	7.8662	7.8914	7.9483	7.8899	8.0196	7.8872	7.9933	7.8914	8.0281	7.7298	7.8332	7.8662	7.8914	7.9483	7.8899	8.0196	7.8872	7.9933	7.8914	8.0281	**7.4**
H(3``A-3``C)	2.3006	2.3428	2.3510	2.3518	2.3659	2.3522	2.3764	2.3519	2.3715	2.3505	2.3813	2.3006	2.3428	2.3510	2.3518	2.3659	2.3522	2.3764	2.3519	2.3715	2.3505	2.3813	**2.32**
H8	4.9106	4.9232	4.9071	4.9234	4.9287	4.9245	4.9647	4.9246	4.9490	4.9212	4.9474	4.9106	4.9232	4.9071	4.9234	4.9287	4.9245	4.9647	4.9246	4.9490	4.9212	4.9474	**5.64**
H(9A-9B)	1.6061	1.6482	1.6221	1.6801	1.6675	1.6794	1.6867	1.6778	1.6719	1.6798	1.7115	1.6061	1.6482	1.6221	1.6801	1.6675	1.6794	1.6867	1.6778	1.6719	1.6798	1.7115	**1.92**
H(10A)	1.0122	0.9629	0.9456	0.9275	0.8788	0.9302	0.9235	0.9322	0.9209	0.9244	0.9279	1.0122	0.9628	0.9456	0.9275	0.8788	0.9302	0.9235	0.9322	0.9209	0.9244	0.9279	**1.26**
H(10B)	1.6375	1.5546	1.5068	1.4977	1.4315	1.5023	1.4226	1.5061	1.4293	1.4924	1.3981	1.6375	1.5546	1.5068	1.4977	1.4315	1.5023	1.4226	1.5061	1.4293	1.4924	1.3981	**1.07**
H(11A-11C)	0.7026	0.7182	0.6974	0.7270	0.6917	0.7270	0.6980	0.7262	0.6979	0.7263	0.6842	0.7026	0.7182	0.6974	0.7270	0.6917	0.7270	0.6981	0.7262	0.6979	0.7263	0.6842	**0.78**
H(1`A)	2.7472	2.7394	2.7126	2.7224	2.6764	2.7242	2.6780	2.7252	2.6813	2.7200	2.6524	2.8879	2.8909	2.8763	2.8749	2.8402	2.8764	2.8367	2.8772	2.8430	2.8728	2.8136	**3.47**
H(1`B)	3.2883	3.3208	3.3402	3.3493	3.4003	3.3476	3.3780	3.3453	3.3735	3.3501	3.3732	2.9521	2.8547	2.8367	2.8284	2.8570	2.8290	2.8114	2.8291	2.8174	2.8273	2.8045	**3.63**
H(4`A)	2.9521	2.8547	2.8367	2.8284	2.8570	2.8290	2.8114	2.8291	2.8174	2.8273	2.8045	3.2883	3.3208	3.3402	3.3493	3.4003	3.3476	3.3780	3.3453	3.3735	3.3501	3.3732	**3.07**
H(4`B)	2.8879	2.8909	2.8763	2.8749	2.8402	2.8764	2.8367	2.8772	2.8430	2.8728	2.8136	2.7472	2.7394	2.7126	2.7224	2.6764	2.7242	2.6780	2.7252	2.6813	2.7200	2.6524	**3.25**
Nuclei	OPW91											OPW91										
C1	130.4872	132.1627	133.7830	133.0487	135.4642	132.9727	134.1820	132.8880	134.4745	133.1116	134.6156	130.4872	132.1627	133.7830	133.0487	135.4641	132.9727	134.1820	132.8880	134.4745	133.1116	134.6156	**131.615**
C2	131.8399	131.8933	132.5753	131.7821	132.4372	131.7986	132.7664	131.7973	132.6340	131.7469	132.7412	131.8400	131.8933	132.5753	131.7821	132.4373	131.7986	132.7664	131.7973	132.6340	131.7469	132.7411	**133.405**
C3	124.2485	125.6989	126.5650	126.1025	127.1236	126.0910	127.4911	126.0613	127.3754	126.0935	127.6604	124.2486	125.6989	126.5650	126.1025	127.1236	126.0911	127.4911	126.0613	127.3754	126.0935	127.6605	**126.19**
C4	164.6458	165.3503	165.7686	165.5709	166.0012	165.5701	166.6838	165.5507	166.5122	165.5519	166.7513	164.6457	165.3503	165.7686	165.5709	166.0012	165.5700	166.6838	165.5507	166.5122	165.5518	166.7512	**165.04**
C5	111.9064	113.0842	113.5160	113.5387	114.1088	113.5251	114.4785	113.4923	114.3344	113.5311	114.6092	111.9064	113.0842	113.5160	113.5387	114.1089	113.5250	114.4785	113.4923	114.3344	113.5311	114.6091	**116.425**
C6	123.9800	125.3816	126.1047	126.2632	127.1914	126.2144	127.9521	126.1484	127.7162	126.2901	128.1430	123.9800	125.3816	126.1047	126.2632	127.1914	126.2145	127.9521	126.1484	127.7162	126.2900	128.1431	**129.92**
C7	193.3888	198.1862	200.0521	200.8824	202.4617	200.6902	205.9534	200.4907	205.3681	201.0577	207.0692	193.3888	198.1862	200.0521	200.8824	202.4619	200.6902	205.9534	200.4907	205.3681	201.0577	207.0694	**195.9**
C8	63.3801	64.9188	65.9103	65.8514	67.1072	65.7773	67.3391	65.6927	67.3318	65.9107	67.7714	63.3801	64.9188	65.9103	65.8514	67.1072	65.7773	67.3391	65.6927	67.3318	65.9107	67.7714	**67.6**
C9	35.6884	35.6061	35.7020	35.4965	35.6838	35.5092	35.9565	35.5047	35.8623	35.4660	36.0144	35.6884	35.6061	35.7020	35.4965	35.6839	35.5092	35.9565	35.5047	35.8623	35.4661	36.0144	**32.2**
C10	18.4459	19.0380	19.2952	19.3222	19.7305	19.3128	19.6580	19.2859	19.6278	19.3122	19.7884	18.4459	19.0380	19.2952	19.3222	19.7304	19.3128	19.6580	19.2859	19.6278	19.3122	19.7884	**23.4**
C11	15.5572	15.7287	15.7985	15.7763	15.9356	15.7785	15.8798	15.7642	15.8814	15.7559	16.0329	15.5572	15.7287	15.7985	15.7763	15.9355	15.7785	15.8798	15.7642	15.8814	15.7559	16.0329	**17.9**
C1`	49.9864	50.7893	51.0654	51.2601	51.7938	51.2391	51.7049	51.2009	51.6736	51.2612	52.1407	54.3601	55.3527	55.7326	55.8216	56.2547	55.8013	56.4372	55.7636	56.3648	55.8221	56.6561	**52.4**
C2`	25.2222	25.6425	25.8657	25.7984	26.1100	25.7957	26.1072	25.7760	26.1126	25.7823	25.9350	25.1193	25.3596	25.6290	25.3729	25.7903	25.3750	25.6570	25.3613	25.6731	25.3535	25.3721	**14.5**
C3`	25.1195	25.3596	25.6290	25.3729	25.7904	25.3751	25.6570	25.3613	25.6731	25.3535	25.3721	25.2221	25.6425	25.8657	25.7984	26.1099	25.7957	26.1072	25.7760	26.1126	25.7824	25.9350	**14.2**
C4`	54.3602	55.3527	55.7326	55.8216	56.2547	55.8013	56.4372	55.7636	56.3648	55.8221	56.6560	49.9865	50.7893	51.0654	51.2601	51.7938	51.2392	51.7049	51.2009	51.6736	51.2613	52.1407	**53.9**
H2	8.2239	8.0723	8.0276	7.9744	7.9196	7.9837	8.0152	7.9919	7.9838	7.9627	8.0010	8.2239	8.0723	8.0276	7.9744	7.9196	7.9837	8.0152	7.9919	7.9838	7.9627	8.0010	**8.13**
H5	7.0076	7.1691	7.2419	7.2337	7.3353	7.2303	7.3630	7.2265	7.3501	7.2351	7.3787	7.0076	7.1691	7.2419	7.2337	7.3353	7.2303	7.3630	7.2265	7.3501	7.2351	7.3787	**8.03**
H6	7.7289	7.8330	7.8657	7.8924	7.9477	7.8902	8.0198	7.8872	7.9932	7.8922	8.0288	7.7289	7.8330	7.8657	7.8924	7.9477	7.8902	8.0198	7.8872	7.9932	7.8922	8.0288	**7.4**
H(3``A-3``C)	2.3019	2.3440	2.3523	2.3538	2.3670	2.3535	2.3776	2.3529	2.3727	2.3523	2.3825	2.3019	2.3440	2.3523	2.3538	2.3670	2.3535	2.3776	2.3529	2.3727	2.3523	2.3825	**2.32**
H8	4.9094	4.9232	4.9062	4.9241	4.9280	4.9245	4.9641	4.9244	4.9483	4.9216	4.9466	4.9094	4.9232	4.9062	4.9241	4.9280	4.9245	4.9641	4.9244	4.9483	4.9216	4.9466	**5.64**
H(9A-9B)	1.6027	1.6455	1.6198	1.6791	1.6660	1.6777	1.6855	1.6758	1.6704	1.6786	1.7100	1.6027	1.6455	1.6198	1.6791	1.6659	1.6777	1.6855	1.6758	1.6704	1.6786	1.7100	**1.92**
H(10A)	1.0160	0.9672	0.9496	0.9321	0.8824	0.9341	0.9274	0.9359	0.9248	0.9286	0.9318	1.0160	0.9672	0.9496	0.9321	0.8824	0.9341	0.9274	0.9359	0.9248	0.9286	0.9318	**1.26**
H(10B)	1.6388	1.5556	1.5086	1.4994	1.4326	1.5033	1.4245	1.5069	1.4311	1.4938	1.3996	1.6388	1.5556	1.5086	1.4994	1.4326	1.5033	1.4245	1.5069	1.4311	1.4938	1.3996	**1.07**
H(11A-11C)	0.7047	0.7207	0.7001	0.7303	0.6945	0.7297	0.7010	0.7287	0.7009	0.7294	0.6874	0.7047	0.7207	0.7001	0.7303	0.6945	0.7297	0.7010	0.7287	0.7009	0.7294	0.6874	**0.78**
H(1`A)	2.7511	2.7432	2.7164	2.7269	2.6799	2.7279	2.6815	2.7287	2.6847	2.7241	2.6556	2.8918	2.8938	2.8795	2.8782	2.8432	2.8790	2.8395	2.8797	2.8459	2.8758	2.8164	**3.47**
H(1`B)	3.2846	3.3175	3.3376	3.3472	3.3979	3.3449	3.3761	3.3424	3.3713	3.3478	3.3710	2.9471	2.8504	2.8354	2.8543	2.8253	2.8089	2.8252	2.8147	2.8241	2.8024	2.8761	**3.63**
H(4`A)	2.9471	2.8504	2.8333	2.8254	2.8543	2.8253	2.8089	2.8252	2.8147	2.8241	2.8024	3.2846	3.3175	3.3376	3.3472	3.3979	3.3449	3.3761	3.3424	3.3713	3.3478	3.3709	**3.07**
H(4`B)	2.8918	2.8938	2.8795	2.8782	2.8432	2.8791	2.8395	2.8797	2.8459	2.8758	2.8164	2.7511	2.7432	2.7164	2.7269	2.6799	2.7279	2.6815	2.7287	2.6847	2.7241	2.6556	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. XI

Nuclei	R											S										Exp. [b]
	PBE											PBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	135.4010	136.2845	136.8305	136.8835	138.7209	136.8139	138.7494	136.7616	138.8051	136.9772	139.1750	135.4010	136.2844	136.8304	136.8835	138.7211	136.8139	138.7493	136.7616	138.8051	136.9772	139.1750	**131.615**
C2	137.0261	137.0017	137.4032	136.6842	137.4130	136.7058	137.6474	136.7372	137.5601	136.6803	137.6257	137.0261	137.0017	137.4031	136.6842	137.4129	136.7058	137.6475	136.7372	137.5602	136.6803	137.6255	**133.405**
C3	130.9970	132.4079	133.3882	132.7609	133.9682	132.7406	134.4025	132.7307	134.3005	132.7969	134.5973	130.9970	132.4078	133.3881	132.7609	133.9682	132.7406	134.4026	132.7307	134.3005	132.7969	134.5971	**126.19**
C4	173.1277	174.2088	174.9501	174.6799	175.5039	174.6454	176.2899	174.6222	176.1339	174.7308	176.4161	173.1277	174.2089	174.9502	174.6799	175.5038	174.6454	176.2899	174.6222	176.1339	174.7308	176.4160	**165.04**
C5	116.5915	117.8697	118.4805	118.4425	119.3445	118.4031	119.7919	118.3746	119.6678	118.4985	119.9365	116.5915	117.8696	118.4806	118.4425	119.3444	118.4031	119.7919	118.3746	119.6680	118.4985	119.9366	**116.425**
C6	129.8918	131.5631	132.5847	132.3833	133.8149	132.3343	134.0958	132.2944	133.8658	132.4455	134.4467	129.8918	131.5631	132.5847	132.3833	133.8148	132.3343	134.0958	132.2944	133.8658	132.4455	134.4466	**129.92**
C7	201.2817	205.3783	206.2869	207.7408	208.9029	207.5603	213.5375	207.3982	212.6731	207.9397	214.7818	201.2817	205.3782	206.2868	207.7408	208.9031	207.5603	213.5375	207.3982	212.6733	207.9397	214.7818	**195.9**
C8	67.1250	68.3943	68.7255	69.0038	70.1404	68.9496	70.7526	68.9098	70.6063	69.0772	71.3150	67.1250	68.3944	68.7257	69.0038	70.1404	68.9496	70.7527	68.9098	70.6062	69.0772	71.3150	**67.6**
C9	40.2194	40.0225	40.2384	39.8491	40.3239	39.8548	40.3308	39.8715	40.2350	39.8612	40.5180	40.2194	40.0226	40.2383	39.8491	40.3239	39.8548	40.3308	39.8715	40.2349	39.8612	40.5180	**32.2**
C10	19.9934	20.5540	20.7813	20.7722	21.3631	20.7558	21.2111	20.7500	21.1824	20.8051	21.4177	19.9934	20.5540	20.7813	20.7722	21.3631	20.7558	21.2111	20.7500	21.1825	20.8051	21.4176	**23.4**
C11	15.9004	16.1139	16.1849	16.0886	16.3844	16.0874	16.3096	16.0969	16.3049	16.1070	16.5319	15.9004	16.1139	16.1849	16.0886	16.3844	16.0874	16.3096	16.0969	16.3049	16.1070	16.5319	**17.9**
C1`	53.2603	54.2097	54.3587	54.6259	55.2663	54.5999	55.1848	54.5843	55.1514	54.6674	55.6879	57.7398	58.9407	59.3490	59.3547	59.9501	59.3273	60.2398	59.3107	60.1763	59.3987	60.4866	**52.4**
C2`	25.6456	26.2390	26.4721	26.3909	26.9067	26.3788	26.9324	26.3772	26.9298	26.4201	26.8990	25.3706	25.6351	26.0296	25.7333	26.3613	25.7222	26.3935	25.7221	26.3814	25.7617	26.2009	**14.5**
C3`	25.3706	25.6351	26.0296	25.7333	26.3612	25.7222	26.3935	25.7221	26.3814	25.7617	26.2008	25.6456	26.2389	26.4721	26.3909	26.9068	26.3788	26.9323	26.3772	26.9299	26.4201	26.8991	**14.2**
C4`	57.7398	58.9407	59.3491	59.3547	59.9501	59.3273	60.2398	59.3107	60.1762	59.3987	60.4867	53.2603	54.2097	54.3587	54.6259	55.2663	54.5999	55.1849	54.5843	55.1514	54.6674	55.6878	**53.9**
H2	8.3861	8.3075	8.3460	8.2342	8.2315	8.2413	8.2211	8.2483	8.2176	8.2274	8.2032	8.3861	8.3075	8.3460	8.2342	8.2314	8.2413	8.2211	8.2483	8.2176	8.2274	8.2032	**8.13**
H5	6.9781	7.1346	7.2290	7.1971	7.3190	7.1936	7.3430	7.1906	7.3320	7.2010	7.3626	6.9781	7.1346	7.2290	7.1971	7.3190	7.1936	7.3431	7.1906	7.3321	7.2010	7.3626	**8.03**
H6	7.7722	7.9285	8.0311	7.9996	8.1059	7.9963	8.1306	7.9933	8.1144	8.0031	8.1521	7.7722	7.9285	8.0311	7.9996	8.1059	7.9963	8.1306	7.9933	8.1144	8.0031	8.1521	**7.4**
H(3``A-3``C)	2.3186	2.3670	2.3850	2.3782	2.4062	2.3776	2.4178	2.3776	2.4150	2.3794	2.4234	2.3186	2.3670	2.3850	2.3782	2.4062	2.3776	2.4178	2.3776	2.4150	2.3794	2.4234	**2.32**
H8	4.9540	4.9847	5.0510	5.0028	5.0559	5.0023	5.0958	5.0020	5.0823	5.0038	5.0839	4.9540	4.9848	5.0510	5.0028	5.0559	5.0023	5.0958	5.0020	5.0823	5.0038	5.0839	**5.64**
H(9A-9B)	1.8410	1.8833	1.8635	1.9019	1.9155	1.9013	1.8587	1.9010	1.8520	1.9028	1.8902	1.8410	1.8833	1.8635	1.9019	1.9155	1.9013	1.8587	1.9010	1.8520	1.9028	1.8902	**1.92**
H(10A)	1.0625	0.9818	0.9807	0.9307	0.8674	0.9351	0.9267	0.9398	0.9205	0.9269	0.9362	1.0625	0.9818	0.9807	0.9307	0.8674	0.9351	0.9267	0.9398	0.9205	0.9269	0.9362	**1.26**
H(10B)	1.8358	1.7187	1.6709	1.6473	1.5798	1.6516	1.5635	1.6564	1.5706	1.6438	1.5277	1.8358	1.7187	1.6710	1.6473	1.5798	1.6516	1.5635	1.6564	1.5706	1.6438	1.5277	**1.07**
H(11A-11C)	0.7527	0.7636	0.7501	0.7651	0.7364	0.7653	0.7362	0.7658	0.7366	0.7656	0.7231	0.7527	0.7636	0.7501	0.7651	0.7364	0.7653	0.7362	0.7658	0.7366	0.7656	0.7231	**0.78**
H(1`A)	2.7877	2.7819	2.7641	2.7696	2.7330	2.7704	2.7317	2.7716	2.7338	2.7695	2.7135	2.8910	2.9062	2.8891	2.8946	2.8785	2.8951	2.8892	2.8962	2.8933	2.8948	2.8583	**3.47**
H(1`B)	3.3732	3.3999	3.4309	3.4219	3.4901	3.4203	3.4539	3.4193	3.4497	3.4240	3.4531	3.0558	2.8645	2.8252	2.8285	2.8430	2.8286	2.8064	2.8296	2.8036	2.8295	2.7991	**3.63**
H(4`A)	3.0558	2.8645	2.8252	2.8285	2.8430	2.8286	2.8064	2.8296	2.8036	2.8295	2.7991	3.3732	3.3999	3.4309	3.4219	3.4901	3.4203	3.4539	3.4193	3.4497	3.4240	3.4530	**3.07**
H(4`B)	2.8910	2.9062	2.8891	2.8946	2.8785	2.8951	2.8891	2.8962	2.8933	2.8948	2.8583	2.7877	2.7819	2.7641	2.7696	2.7331	2.7704	2.7317	2.7716	2.7338	2.7695	2.7134	**3.25**
Nuclei	PBE0																						
C1	136.2007	136.9147	137.5615	137.3512	138.9409	137.3039	139.2539	137.2630	138.1230	137.4045	139.5381	136.2008	136.9149	137.5615	137.3512	138.9409	137.3041	139.2540	137.2630	138.1230	137.4045	139.5381	**131.615**
C2	139.4557	139.3832	139.7713	139.1498	139.6996	139.1641	140.0174	139.1793	139.9414	139.1388	139.9259	139.4558	139.3832	139.7713	139.1499	139.6996	139.1642	140.0177	139.1793	139.9414	139.1388	139.9260	**133.405**
C3	131.5821	132.8494	133.7706	133.2264	134.3125	133.2015	134.7612	133.1780	134.5509	133.2529	134.8747	131.5821	132.8495	133.7705	133.2264	134.3126	133.2014	134.7612	133.1780	134.5509	133.2529	134.8748	**126.19**
C4	171.5776	172.4460	173.0738	172.8931	173.4817	172.8571	174.3616	172.8237	174.0700	172.9307	174.4196	171.5776	172.4460	173.0739	172.8931	173.4817	172.8571	174.3615	172.8237	174.0700	172.9307	174.4197	**165.04**
C5	118.1438	119.3874	119.9921	120.0197	120.8467	119.9746	121.3084	119.9316	121.0125	120.0661	121.4028	118.1437	119.3874	119.9922	120.0197	120.8467	119.9744	121.3085	119.9316	121.0125	120.0661	121.4028	**116.425**
C6	132.2745	133.9637	134.9490	134.9149	136.2680	134.8546	136.4989	134.7949	136.7876	134.9732	136.7704	132.2746	133.9636	134.9491	134.9149	136.2680	134.8545	136.4988	134.7949	136.7876	134.9732	136.7705	**129.92**
C7	201.3075	205.6698	206.5945	208.1217	208.7899	207.9497	214.6600	207.7847	212.3530	208.2937	215.7870	201.3076	205.6698	206.5945	208.1216	208.7899	207.9497	214.6602	207.7847	212.3530	208.2937	215.7870	**195.9**
C8	63.2461	64.4151	64.8221	64.9469	65.8253	64.9073	66.6518	64.8710	66.1021	64.9892	67.0631	63.2461	64.4152	64.8222	64.9469	65.8253	64.9073	66.6518	64.8710	66.1021	64.9891	67.0631	**67.6**
C9	36.7732	36.5863	36.7496	36.4519	36.8216	36.4569	36.7620	36.4636	36.8731	36.4500	36.8488	36.7734	36.5862	36.7498	36.4519	36.8216	36.4569	36.7620	36.4636	36.8731	36.4500	36.8488	**32.2**
C10	18.2181	18.7218	18.9479	18.9937	19.4770	18.9735	19.3649	18.9547	19.3386	19.0156	19.4816	18.2181	18.7218	18.9478	18.9937	19.4770	18.9735	19.3650	18.9547	19.3386	19.0156	19.4816	**23.4**
C11	15.6450	15.7854	15.8700	15.8237	16.0155	15.8164	16.0182	15.8107	15.9753	15.8334	16.1412	15.6450	15.7853	15.8700	15.8237	16.0155	15.8163	16.0182	15.8107	15.9753	15.8334	16.1412	**17.9**
C1`	50.4130	51.2513	51.4635	51.6937	52.2179	51.6631	52.2495	51.6338	52.1524	51.7256	52.6385	54.6200	55.6382	55.9981	56.0835	56.5847	56.0504	56.8847	56.0193	56.7286	56.1179	57.0767	**52.4**
C2`	24.3359	24.7427	25.0099	24.8926	25.3084	24.8789	25.3847	24.8668	25.3331	24.9084	25.2256	23.8225	23.9894	24.3470	24.1202	24.6026	24.1044	24.7082	24.0909	24.5231	24.1387	24.4528	**14.5**
C3`	23.8225	23.9894	24.3470	24.1202	24.6026	24.1044	24.7081	24.0909	24.5231	24.1386	24.4527	24.3359	24.7427	25.0099	24.8926	25.3084	24.8788	25.3847	24.8668	25.3331	24.9084	25.2256	**14.2**
C4`	54.6201	55.6382	55.9983	56.0835	56.5847	56.0504	56.8846	56.0193	56.7286	56.1179	57.0766	50.4130	51.2513	51.4635	51.6937	52.2179	51.6630	52.2494	51.6338	52.1524	51.7256	52.6384	**53.9**
H2	8.5916	8.5070	8.5428	8.4438	8.4492	8.4490	8.4073	8.4538	8.4910	8.4381	8.3888	8.5916	8.5070	8.5428	8.4438	8.4492	8.4490	8.4074	8.4538	8.4910	8.4381	8.3888	**8.13**
H5	7.1345	7.3011	7.3938	7.3709	7.4938	7.3670	7.5145	7.3630	7.5028	7.3742	7.5334	7.1345	7.3011	7.3938	7.3709	7.4938	7.3669	7.5146	7.3630	7.5028	7.3742	7.5334	**8.03**
H6	7.8890	8.0526	8.1579	8.1427	8.2720	8.1372	8.2843	8.1317	8.3261	8.1473	8.3064	7.8890	8.0526	8.1579	8.1427	8.2720	8.1372	8.2843	8.1317	8.3261	8.1473	8.3064	**7.4**
H(3``A-3``C)	2.3570	2.4017	2.4169	2.4136	2.4343	2.4129	2.4512	2.4123	2.4416	2.4140	2.4546	2.3569	2.4017	2.4169	2.4136	2.4343	2.4129	2.4512	2.4123	2.4416	2.4140	2.4546	**2.32**
H8	4.5366	4.5941	4.6639	4.6450	4.7167	4.6413	4.7588	4.6375	4.7612	4.6482	4.7512	4.5366	4.5940	4.6639	4.6450	4.7167	4.6413	4.7588	4.6375	4.7612	4.6482	4.7512	**5.64**
H(9A-9B)	1.7007	1.7415	1.7236	1.7637	1.7742	1.7630	1.7035	1.7622	1.7646	1.7637	1.7305	1.7007	1.7415	1.7236	1.7637	1.7742	1.7631	1.7035	1.7622	1.7646	1.7637	1.7305	**1.92**
H(10A)	1.0141	0.8933	0.8929	0.8433	0.7729	0.8466	0.8278	0.8497	0.8187	0.8397	0.8291	1.0141	0.8932	0.8928	0.8433	0.7729	0.8466	0.8278	0.8497	0.8187	0.8397	0.8292	**1.26**
H(10B)	1.7109	1.6058	1.5536	1.5331	1.4578	1.5374	1.4496	1.5417	1.4660	1.5287	1.4149	1.7108	1.6058	1.5536	1.5331	1.4578	1.5374	1.4496	1.5417	1.4660	1.5287	1.4149	**1.07**
H(11A-11C)	0.7296	0.7369	0.7204	0.7415	0.7072	0.7411	0.7083	0.7407	0.7173	0.7415	0.6945	0.7296	0.7369	0.7204	0.7415	0.7072	0.7411	0.7083	0.7407	0.7173	0.7415	0.6945	**0.78**
H(1`A)	2.6474	2.6430	2.6269	2.6349	2.5901	2.6354	2.6008	2.6359	2.6033	2.6340	2.5809	2.7682	2.7730	2.7551	2.7579	2.7292	2.7587	2.7564	2.7596	2.7392	2.7568	2.7255	**3.47**
H(1`B)	3.1638	3.2018	3.2264	3.2308	3.2894	3.2288	3.2616	3.2268	3.2681	3.2325	3.2635	2.8600	2.6934	2.6410	2.6557	2.6565	2.6568	2.6363	2.6582	2.5968	2.6546	2.6273	**3.63**
H(4`A)	2.8601	2.6934	2.6410	2.6557	2.6565	2.6568	2.6363	2.6582	2.5968	2.6546	2.6273	3.1638	3.2018	3.2264	3.2308	3.2894	3.2288	3.2615	3.2268	3.2681	3.2325	3.2634	**3.07**
H(4`B)	2.7681	2.7729	2.7551	2.7579	2.7292	2.7587	2.7564	2.7596	2.7392	2.7568	2.7255	2.6473	2.6430	2.6269	2.6349	2.5901	2.6354	2.6007	2.6359	2.6033	2.6340	2.5809	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. XII

Nuclei	R											S										Exp. [b]
	TPSS																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	132.1154	132.6981	133.4308	133.0960	134.7326	133.0650	133.9149	133.0485	133.5528	133.1391	134.1959	132.1154	132.6981	133.4308	133.0960	134.7326	133.0650	133.9149	133.0485	134.1611	133.1391	134.1959	**131.615**
C2	134.1276	134.0239	134.4897	133.8755	134.4383	133.8954	134.6701	133.9258	134.4336	133.8666	134.6754	134.1276	134.0239	134.4899	133.8755	134.4383	133.8954	134.6701	133.9258	135.0318	133.8666	134.6754	**133.405**
C3	128.4529	129.6100	130.6164	130.0088	131.0505	129.9952	131.4360	129.9925	130.4846	130.0321	131.5560	128.4529	129.6100	130.6165	130.0088	131.0505	129.9952	131.4360	129.9925	131.1280	130.0321	131.5560	**126.19**
C4	170.0230	170.8869	171.6752	171.3885	172.0710	171.3619	172.8875	171.3473	172.0048	171.4248	172.9799	170.0230	170.8869	171.6752	171.3885	172.0710	171.3619	172.8875	171.3473	172.1726	171.4248	172.9799	**165.04**
C5	113.9299	115.0019	115.6710	115.6200	116.3826	115.5886	116.7059	115.5687	116.0031	115.6603	116.8219	113.9299	115.0019	115.6709	115.6200	116.3826	115.5886	116.7059	115.5687	116.8124	115.6603	116.8219	**116.425**
C6	127.3100	128.8826	129.9133	129.8794	131.1746	129.8254	131.9183	129.7821	130.2733	129.9406	132.2412	127.3100	128.8826	129.9131	129.8794	131.1746	129.8254	131.9183	129.7821	130.9192	129.9406	132.2412	**129.92**
C7	197.4144	201.1916	202.2671	203.3678	204.2892	203.2251	208.3038	203.0973	203.8818	203.5173	209.3393	197.4144	201.1916	202.2672	203.3678	204.2892	203.2251	208.3038	203.0973	203.6845	203.5174	209.3393	**195.9**
C8	65.9602	67.0260	67.5026	67.6065	68.5603	67.5741	68.8519	67.5539	67.7962	67.6488	69.3297	65.9602	67.0260	67.5026	67.6065	68.5603	67.5741	68.8519	67.5539	69.1577	67.6488	69.3297	**67.6**
C9	39.0325	38.7522	39.0883	38.7323	39.1760	38.7395	39.3575	38.7582	38.8853	38.7364	39.5264	39.0325	38.7522	39.0883	38.7323	39.1760	38.7395	39.3575	38.7582	40.5780	38.7365	39.5264	**32.2**
C10	20.8238	21.1744	21.5479	21.4566	21.9344	21.4466	21.8461	21.4478	21.5057	21.4765	21.9460	20.8239	21.1744	21.5479	21.4566	21.9344	21.4466	21.8461	21.4478	23.3974	21.4765	21.9460	**23.4**
C11	16.7586	16.8356	17.0577	16.9276	17.1739	16.9286	17.1255	16.9409	16.9808	16.9372	17.2738	16.7586	16.8356	17.0577	16.9276	17.1739	16.9286	17.1255	16.9409	18.9243	16.9372	17.2738	**17.9**
C1`	53.1126	53.8236	54.1272	54.3471	54.8653	54.3207	54.8088	54.3057	54.4950	54.3824	55.2386	57.2363	58.2473	58.7417	58.7163	59.1883	58.6948	59.5114	58.6847	60.3550	58.7473	59.7122	**52.4**
C2`	26.3285	26.7518	27.1166	26.9700	27.3956	26.9629	27.4188	26.9674	27.0474	26.9873	27.2584	26.0732	26.1679	26.6933	26.3390	26.8670	26.3320	26.8299	26.3370	28.2499	26.3566	26.6387	**14.5**
C3`	26.0732	26.1679	26.6932	26.3390	26.8670	26.3320	26.8299	26.3370	26.4145	26.3566	26.6387	26.3285	26.7518	27.1166	26.9700	27.3956	26.9629	27.4188	26.9674	28.8756	26.9873	27.2584	**14.2**
C4`	57.2362	58.2473	58.7417	58.7163	59.1883	58.6948	59.5114	58.6847	58.8915	58.7473	59.7122	53.1126	53.8236	54.1272	54.3471	54.8653	54.3207	54.8088	54.3057	56.0088	54.3824	55.2386	**53.9**
H2	8.4087	8.3305	8.3664	8.2797	8.2797	8.2841	8.3180	8.2889	8.1285	8.2757	8.3031	8.4087	8.3305	8.3664	8.2797	8.2797	8.2841	8.3180	8.2889	8.3999	8.2757	8.3031	**8.13**
H5	6.9558	7.1161	7.2149	7.1870	7.3101	7.1833	7.3281	7.1801	7.0152	7.1909	7.3417	6.9558	7.1161	7.2149	7.1870	7.3101	7.1833	7.3281	7.1801	7.2995	7.1909	7.3417	**8.03**
H6	7.6857	7.8508	7.9491	7.9440	8.0661	7.9386	8.1409	7.9338	7.7719	7.9493	8.1611	7.6857	7.8508	7.9491	7.9440	8.0661	7.9386	8.1409	7.9338	8.0475	7.9493	8.1611	**7.4**
H(3``A-3``C)	2.3213	2.3642	2.3852	2.3791	2.4039	2.3785	2.4113	2.3785	2.1943	2.3801	2.4124	2.3213	2.3642	2.3852	2.3791	2.4039	2.3785	2.4113	2.3785	2.5338	2.3801	2.4124	**2.32**
H8	4.7279	4.7860	4.8488	4.8333	4.9046	4.8303	4.9639	4.8279	4.6536	4.8365	4.9601	4.7279	4.7860	4.8488	4.8333	4.9046	4.8303	4.9639	4.8279	4.9649	4.8365	4.9601	**5.64**
H(9A-9B)	1.7641	1.8094	1.7987	1.8472	1.8696	1.8450	1.8551	1.8434	1.6572	1.8496	1.8860	1.7641	1.8094	1.7987	1.8472	1.8696	1.8450	1.8551	1.8434	2.0028	1.8496	1.8860	**1.92**
H(10A)	1.0680	0.9690	0.9904	0.9298	0.8577	0.9329	0.9208	0.9365	1.1106	0.9270	0.9163	1.0681	0.9690	0.9905	0.9298	0.8577	0.9329	0.9208	0.9365	1.1106	0.9270	0.9163	**1.26**
H(10B)	1.8095	1.6801	1.6277	1.6073	1.5442	1.6113	1.5335	1.6161	1.9876	1.6040	1.4944	1.8095	1.6801	1.6277	1.6073	1.5442	1.6113	1.5335	1.6161	1.9876	1.6041	1.4944	**1.07**
H(11A-11C)	0.7555	0.7642	0.7535	0.7741	0.7461	0.7735	0.7561	0.7735	0.5830	0.7750	0.7414	0.7555	0.7642	0.7535	0.7741	0.7461	0.7735	0.7561	0.7735	0.9409	0.7750	0.7414	**0.78**
H(1`A)	2.7026	2.7050	2.6970	2.7012	2.6694	2.7016	2.6755	2.7025	2.6525	2.7012	2.6502	2.7981	2.8151	2.8087	2.8088	2.7947	2.8091	2.7956	2.8100	3.0026	2.8089	2.6502	**3.47**
H(1`B)	3.2696	3.3049	3.3388	3.3390	3.4081	3.3368	3.3898	3.3352	3.3248	3.3415	3.3849	3.0280	2.8216	2.7948	2.7819	2.8053	2.7830	2.7365	2.7849	2.8644	2.7816	3.3849	**3.63**
H(4`A)	3.0280	2.8216	2.7948	2.7819	2.8053	2.7830	2.7365	2.7849	2.8644	2.7816	2.7356	3.2696	3.3049	3.3388	3.3390	3.4081	3.3368	3.3898	3.3352	3.3248	3.3415	2.7356	**3.07**
H(4`B)	2.7981	2.8151	2.8087	2.8088	2.7947	2.8091	2.7956	2.8100	3.0026	2.8089	2.7709	2.7026	2.7050	2.6970	2.7012	2.6694	2.7016	2.6755	2.7025	2.6525	2.7012	2.7709	**3.25**
Nuclei	VSXC																						
C1	133.7089	134.0623	134.3904	134.2358	135.9678	134.2244	134.9923	134.2120	135.1654	134.2490	135.3549	133.7090	134.0623	134.3904	134.2358	135.9677	134.2245	134.9923	134.2121	135.1654	134.2490	135.3547	**131.615**
C2	131.0275	130.5956	131.3267	130.3155	130.7174	130.3370	131.1024	130.3562	131.0410	130.2964	131.1471	131.0274	130.5957	131.3267	130.3154	130.7174	130.3370	131.1024	130.3562	131.0410	130.2963	131.1472	**133.405**
C3	128.2955	129.8523	130.6098	130.3512	131.2930	130.3289	131.5435	130.3036	131.4760	130.3735	131.5973	128.2956	129.8523	130.6098	130.3512	131.2929	130.3289	131.5435	130.3037	131.4760	130.3734	131.5974	**126.19**
C4	166.2958	167.2811	167.9398	167.7958	168.4898	167.7669	169.1783	167.7358	169.0055	167.8252	169.3071	166.2958	167.2810	167.9398	167.7958	168.4898	167.7668	169.1783	167.7357	169.0055	167.8250	169.3071	**165.04**
C5	111.1342	112.3892	113.0735	113.1249	113.9026	113.0816	114.3287	113.0363	114.1744	113.1678	114.5223	111.1342	112.3892	113.0735	113.1249	113.9026	113.0816	114.3287	113.0362	114.1744	113.1678	114.5224	**116.425**
C6	126.0866	127.9182	128.9767	128.9941	130.1063	128.9310	130.7976	128.8655	130.5125	129.0555	131.0866	126.0865	127.9181	128.9767	128.9941	130.1063	128.9310	130.7976	128.8655	130.5125	129.0555	131.0864	**129.92**
C7	193.2388	197.7924	198.7855	200.1230	201.1223	199.9824	205.3983	199.8403	204.5527	200.2583	206.5185	193.2389	197.7924	198.7855	200.1229	201.1223	199.9824	205.3983	199.8403	204.5527	200.2584	206.5187	**195.9**
C8	71.8578	72.4767	73.0341	72.8352	73.6621	72.8137	73.9188	72.7904	73.8728	72.8577	74.4210	71.8577	72.4767	73.0341	72.8352	73.6621	72.8137	73.9188	72.7904	73.8728	72.8577	74.4210	**67.6**
C9	44.2072	44.7806	45.2319	45.0299	45.3275	45.0213	45.9109	45.0098	45.7706	45.0390	46.0933	44.2073	44.7806	45.2319	45.0299	45.3275	45.0213	45.9109	45.0098	45.7706	45.0391	46.0933	**32.2**
C10	24.9891	25.8370	26.0231	26.3259	26.7484	26.2987	26.8859	26.2694	26.7937	26.3533	27.0762	24.9890	25.8370	26.0231	26.3259	26.7485	26.2987	26.8859	26.2694	26.7937	26.3533	27.0763	**23.4**
C11	20.9345	20.9697	21.0762	20.9972	21.1076	20.9991	21.0676	20.9988	21.0796	20.9968	21.1670	20.9344	20.9696	21.0762	20.9972	21.1076	20.9991	21.0676	20.9988	21.0796	20.9967	21.1670	**17.9**
C1`	58.4455	58.9814	59.2906	59.3585	59.8879	59.3368	59.7529	59.3133	59.7237	59.3809	59.9371	61.7124	62.2969	62.6234	62.6433	63.1140	62.6232	62.9800	62.6013	62.9682	62.6642	63.3059	**52.4**
C2`	30.5271	31.0155	31.2698	31.2828	31.5322	31.2687	31.5100	31.2525	31.4957	31.2977	31.5937	28.6930	29.1390	29.4794	29.3495	29.7933	29.3402	29.8375	29.3287	29.7984	29.3598	29.6730	**14.5**
C3`	28.6930	29.1391	29.4794	29.3494	29.7932	29.3401	29.8375	29.3288	29.7984	29.3598	29.6730	30.5270	31.0155	31.2698	31.2827	31.5320	31.2686	31.5100	31.2526	31.4957	31.2976	31.5935	**14.2**
C4`	61.7125	62.2968	62.6234	62.6433	63.1140	62.6233	62.9800	62.6013	62.9682	62.6642	63.3060	58.4456	58.9814	59.2906	59.3585	59.8879	59.3369	59.7529	59.3133	59.7237	59.3809	59.9372	**53.9**
H2	8.3247	8.2475	8.3393	8.1901	8.1459	8.1945	8.2457	8.1988	8.2278	8.1858	8.2208	8.3247	8.2475	8.3393	8.1901	8.1460	8.1945	8.2457	8.1988	8.2278	8.1858	8.2208	**8.13**
H5	6.9926	7.1606	7.2527	7.2436	7.3628	7.2388	7.3899	7.2341	7.3764	7.2481	7.4107	6.9926	7.1606	7.2527	7.2436	7.3628	7.2388	7.3899	7.2341	7.3764	7.2481	7.4107	**8.03**
H6	7.6939	7.8705	7.9640	7.9698	8.0814	7.9637	8.1480	7.9577	8.1203	7.9756	8.1829	7.6939	7.8705	7.9640	7.9698	8.0814	7.9637	8.1480	7.9577	8.1203	7.9756	8.1829	**7.4**
H(3``A-3``C)	2.3252	2.4885	2.4814	2.5126	2.5143	2.5122	2.4891	2.5118	2.4963	2.5128	2.4515	2.3252	2.4885	2.4814	2.5126	2.5143	2.5122	2.4891	2.5118	2.4963	2.5128	2.4515	**2.32**
H8	4.3190	4.4318	4.4967	4.4928	4.5777	4.4891	4.6335	4.4856	4.6138	4.4963	4.6517	4.3189	4.4318	4.4967	4.4928	4.5777	4.4892	4.6335	4.4856	4.6138	4.4963	4.6517	**5.64**
H(9A-9B)	1.8546	1.8821	1.9136	1.9048	1.8818	1.9035	1.8943	1.9024	1.8903	1.9058	1.8918	1.8546	1.8821	1.9136	1.9048	1.8818	1.9035	1.8943	1.9024	1.8903	1.9059	1.8918	**1.92**
H(10A)	1.0056	1.0053	0.9968	1.0050	0.9784	1.0053	0.9766	1.0056	0.9872	1.0046	0.9712	1.0056	1.0054	0.9968	1.0049	0.9784	1.0052	0.9766	1.0056	0.9872	1.0046	0.9712	**1.26**
H(10B)	2.2840	2.1190	2.0705	1.9916	1.8793	2.0006	1.8503	2.0096	1.8642	1.9829	1.7764	2.2839	2.1190	2.0705	1.9916	1.8793	2.0006	1.8503	2.0096	1.8642	1.9829	1.7764	**1.07**
H(11A-11C)	0.9960	1.0168	1.0128	1.0267	0.9955	1.0263	0.9993	1.0259	0.9998	1.0271	0.9922	0.9960	1.0168	1.0128	1.0267	0.9955	1.0263	0.9993	1.0259	0.9998	1.0271	0.9922	**0.78**
H(1`A)	2.4656	2.5020	2.5219	2.5184	2.5119	2.5176	2.5318	2.5168	2.5291	2.5192	2.5484	2.9226	2.9016	2.8944	2.8967	2.8818	2.8969	2.8747	2.8972	2.8792	2.8965	2.8890	**3.47**
H(1`B)	3.1407	3.1350	3.1797	3.1401	3.2131	3.1396	3.2092	3.1393	3.2014	3.1405	3.2193	2.8613	2.7780	2.8159	2.7513	2.7751	2.7528	2.7295	2.7544	2.7410	2.7499	2.7383	**3.63**
H(4`A)	2.8613	2.7780	2.8159	2.7513	2.7751	2.7528	2.7295	2.7544	2.7410	2.7499	2.7384	3.1407	3.1350	3.1797	3.1401	3.2131	3.1396	3.2092	3.1393	3.2014	3.1405	3.2193	**3.07**
H(4`B)	2.9226	2.9016	2.8944	2.8967	2.8818	2.8969	2.8747	2.8972	2.8792	2.8965	2.8890	2.4656	2.5020	2.5219	2.5184	2.5119	2.5176	2.5318	2.5168	2.5291	2.5192	2.5484	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. XIII

Nuclei	R											S										Exp. [b]
	wB97											wB97										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.5685	137.2998	138.0458	137.5481	139.3513	137.5342	139.5815	137.5198	138.2796	137.5620	139.8130	136.5685	137.2999	138.0458	137.5481	139.3513	137.5344	139.5814	137.5197	138.2798	137.5619	139.8131	**131.615**
C2	140.4597	140.2803	140.7341	140.1078	140.6099	140.1179	140.8866	140.1271	140.9111	140.0988	140.8928	140.4597	140.2804	140.7341	140.1080	140.6099	140.1179	140.8868	140.1271	140.9110	140.0988	140.8929	**133.405**
C3	131.8491	132.8916	133.7579	133.2076	134.2702	133.1912	134.5709	133.1736	134.3426	133.2232	134.7015	131.8491	132.8916	133.7580	133.2076	134.2702	133.1911	134.5710	133.1736	134.3428	133.2231	134.7015	**126.19**
C4	172.6725	173.3200	173.9430	173.7031	174.2581	173.6773	174.6970	173.6509	174.7453	173.7281	174.8004	172.6725	173.3199	173.9431	173.7031	174.2580	173.6773	174.6971	173.6509	174.7452	173.7280	174.8004	**165.04**
C5	119.2416	120.4446	121.0584	121.0792	121.9447	121.0392	122.1559	120.9986	121.9530	121.1175	122.2990	119.2416	120.4446	121.0583	121.0792	121.9447	121.0392	122.1559	120.9986	121.9529	121.1175	122.2989	**116.425**
C6	133.7353	135.2434	136.1565	136.2387	137.5154	136.1726	137.6767	136.1065	137.9970	136.3022	138.0135	133.7353	135.2434	136.1565	136.2388	137.5153	136.1727	137.6765	136.1065	137.9968	136.3022	138.0133	**129.92**
C7	201.8010	206.7178	207.7402	209.2842	209.8800	209.1261	216.5903	208.9682	213.8414	209.4353	217.6960	201.8010	206.7175	207.7402	209.2842	209.8800	209.1262	216.5903	208.9677	213.8416	209.4353	217.6961	**195.9**
C8	61.8342	62.9820	63.4739	63.4435	64.2461	63.4181	65.1654	63.3917	64.4408	63.4676	65.4934	61.8342	62.9819	63.4739	63.4435	64.2461	63.4181	65.1654	63.3916	64.4408	63.4677	65.4934	**67.6**
C9	35.0243	34.8332	34.9958	34.6955	35.0458	34.7049	34.7826	34.7132	34.9627	34.6866	34.9646	35.0243	34.8332	34.9958	34.6955	35.0458	34.7049	34.7825	34.7132	34.9626	34.6865	34.9646	**32.2**
C10	18.2027	18.6531	18.8496	18.9099	19.3911	18.8932	19.2054	18.8758	19.1873	18.9260	19.3370	18.2028	18.6532	18.8496	18.9099	19.3910	18.8932	19.2054	18.8758	19.1872	18.9260	19.3371	**23.4**
C11	15.6995	15.7560	15.8801	15.8139	16.0215	15.8087	15.9265	15.8027	15.9471	15.8194	16.0957	15.6995	15.7560	15.8800	15.8140	16.0215	15.8087	15.9264	15.8027	15.9470	15.8194	16.0956	**17.9**
C1`	49.2258	49.8232	50.0620	50.2647	50.7891	50.2356	50.7958	50.2058	50.7027	50.2928	51.1399	52.8945	53.7467	54.0785	54.1592	54.6644	54.1319	54.8314	54.1044	54.6995	54.1857	55.1043	**52.4**
C2`	23.7756	24.1041	24.3533	24.2614	24.6818	24.2513	24.7299	24.2406	24.6529	24.2714	24.6392	23.1903	23.2947	23.6379	23.4229	23.9010	23.4127	23.8543	23.4017	23.8006	23.4334	23.7318	**14.5**
C3`	23.1903	23.2948	23.6380	23.4230	23.9011	23.4126	23.8544	23.4018	23.8006	23.4333	23.7318	23.7755	24.1041	24.3533	24.2613	24.6818	24.2513	24.7299	24.2406	24.6529	24.2714	24.6391	**14.2**
C4`	52.8945	53.7466	54.0785	54.1592	54.6643	54.1320	54.8313	54.1043	54.6996	54.1857	55.1043	49.2259	49.8232	50.0619	50.2647	50.7891	50.2355	50.7957	50.2057	50.7028	50.2929	51.1399	**53.9**
H2	8.6809	8.5744	8.6075	8.5183	8.5204	8.5212	8.4545	8.5240	8.5726	8.5156	8.4553	8.6809	8.5744	8.6075	8.5183	8.5204	8.5212	8.4545	8.5240	8.5726	8.5157	8.4553	**8.13**
H5	7.2542	7.4280	7.5179	7.5041	7.6322	7.4996	7.6357	7.4950	7.6366	7.5084	7.6595	7.2542	7.4280	7.5179	7.5041	7.6322	7.4996	7.6357	7.4950	7.6366	7.5084	7.6595	**8.03**
H6	7.9477	8.1022	8.2025	8.2030	8.3341	8.1962	8.3494	8.1894	8.3856	8.2096	8.3807	7.9477	8.1022	8.2025	8.2030	8.3342	8.1962	8.3494	8.1894	8.3856	8.2096	8.3807	**7.4**
H(3``A-3``C)	2.3549	2.3976	2.4124	2.4103	2.4336	2.4095	2.4577	2.4087	2.4403	2.4111	2.4663	2.3549	2.3976	2.4124	2.4103	2.4336	2.4096	2.4577	2.4087	2.4403	2.4111	2.4663	**2.32**
H8	4.2034	4.2712	4.3375	4.3387	4.4228	4.3334	4.4729	4.3282	4.4740	4.3440	4.4832	4.2034	4.2712	4.3375	4.3387	4.4227	4.3334	4.4729	4.3282	4.4740	4.3440	4.4832	**5.64**
H(9A-9B)	1.6611	1.7015	1.6840	1.7245	1.7275	1.7231	1.6535	1.7217	1.7210	1.7258	1.6931	1.6611	1.7015	1.6840	1.7245	1.7275	1.7231	1.6535	1.7217	1.7210	1.7258	1.6931	**1.92**
H(10A)	1.0493	0.8934	0.8871	0.8401	0.7823	0.8426	0.8036	0.8451	0.8313	0.8378	0.8170	1.0493	0.8934	0.8871	0.8401	0.7823	0.8426	0.8036	0.8451	0.8313	0.8378	0.8170	**1.26**
H(10B)	1.6872	1.5804	1.5359	1.5046	1.4271	1.5090	1.4210	1.5134	1.4409	1.5005	1.3992	1.6872	1.5804	1.5359	1.5046	1.4271	1.5090	1.4210	1.5134	1.4409	1.5005	1.3992	**1.07**
H(11A-11C)	0.7650	0.7661	0.7469	0.7725	0.7383	0.7717	0.7282	0.7709	0.7482	0.7734	0.7234	0.7650	0.7661	0.7469	0.7725	0.7383	0.7717	0.7282	0.7710	0.7482	0.7734	0.7234	**0.78**
H(1`A)	2.6078	2.6030	2.5890	2.5986	2.5571	2.5991	2.5722	2.5994	2.5745	2.5982	2.5473	2.7476	2.7543	2.7398	2.7341	2.7058	2.7357	2.7330	2.7371	2.7124	2.7326	2.7012	**3.47**
H(1`B)	3.0403	3.0692	3.0961	3.1040	3.1621	3.1014	3.1512	3.0988	3.1494	3.1065	3.1559	2.7254	2.5997	2.5452	2.5525	2.5629	2.5554	2.5567	2.5580	2.5054	2.5499	2.5531	**3.63**
H(4`A)	2.7253	2.5997	2.5452	2.5525	2.5629	2.5554	2.5567	2.5580	2.5054	2.5499	2.5531	3.0403	3.0692	3.0961	3.1039	3.1621	3.1014	3.1512	3.0988	3.1494	3.1065	3.1559	**3.07**
H(4`B)	2.7476	2.7543	2.7398	2.7341	2.7058	2.7357	2.7330	2.7371	2.7124	2.7326	2.7012	2.6078	2.6030	2.5889	2.5986	2.5571	2.5991	2.5722	2.5994	2.5745	2.5982	2.5473	**3.25**
Nuclei	wB97X																						
C1	137.9167	138.7291	139.4027	139.1862	140.8400	139.1410	141.1404	139.0995	139.8806	139.2327	141.3741	137.9167	138.7291	139.4025	139.1862	140.8401	139.1410	141.1404	139.0995	139.8809	139.2327	141.3740	**131.615**
C2	141.0494	140.9138	141.3464	140.7659	141.2763	140.7779	141.5666	140.7886	141.5609	140.7548	141.5438	141.0494	140.9138	141.3464	140.7660	141.2763	140.7779	141.5667	140.7886	141.5608	140.7550	141.5435	**133.405**
C3	132.8983	133.9883	134.8595	134.3501	135.3910	134.3308	135.7372	134.3109	135.4769	134.3691	135.8600	132.8983	133.9883	134.8594	134.3501	135.3908	134.3308	135.7371	134.3109	135.4769	134.3693	135.8600	**126.19**
C4	173.4290	174.0925	174.7321	174.4425	175.0116	174.4248	175.4899	174.4055	175.4614	174.4603	175.5807	173.4290	174.0925	174.7321	174.4425	175.0116	174.4248	175.4899	174.4055	175.4614	174.4604	175.5807	**165.04**
C5	119.9239	121.1094	121.7143	121.7414	122.5798	121.7041	122.8240	121.6659	122.5887	121.7782	122.9578	119.9239	121.1094	121.7143	121.7415	122.5798	121.7041	122.8240	121.6659	122.5887	121.7781	122.9578	**116.425**
C6	134.1177	135.6553	136.6069	136.6152	137.9383	136.5613	138.1354	136.5056	138.3862	136.6677	138.4562	134.1177	135.6553	136.6068	136.6153	137.9383	136.5613	138.1354	136.5056	138.3860	136.6675	138.4561	**129.92**
C7	203.4902	208.4617	209.3787	211.1218	211.5950	210.9424	218.2752	210.7679	215.5453	211.2963	219.3749	203.4902	208.4617	209.3790	211.1218	211.5948	210.9424	218.2752	210.7679	215.5457	211.2960	219.3747	**195.9**
C8	63.1447	64.2837	64.7138	64.7495	65.5120	64.7219	66.5338	64.6951	65.6891	64.7782	66.8394	63.1447	64.2837	64.7138	64.7495	65.5120	64.7218	66.5338	64.6951	65.6891	64.7781	66.8394	**67.6**
C9	35.8867	35.6553	35.7926	35.4652	35.8043	35.4843	35.6574	35.5015	35.6816	35.4482	35.7980	35.8867	35.6553	35.7927	35.4652	35.8045	35.4842	35.6574	35.5015	35.6816	35.4481	35.7980	**32.2**
C10	18.3267	18.7758	18.9867	19.0483	19.5211	19.0352	19.3979	19.0208	19.3074	19.0616	19.5186	18.3267	18.7758	18.9866	19.0483	19.5211	19.0352	19.3980	19.0208	19.3074	19.0616	19.5186	**23.4**
C11	15.7170	15.7824	15.9009	15.8356	16.0411	15.8344	15.9850	15.8321	15.9413	15.8373	16.1378	15.7170	15.7825	15.9008	15.8355	16.0412	15.8345	15.9851	15.8322	15.9413	15.8372	16.1378	**17.9**
C1`	49.9816	50.6681	50.9209	51.1061	51.6482	51.0811	51.6812	51.0548	51.5477	51.1309	52.0378	53.9090	54.7912	55.1324	55.2314	55.7325	55.2038	55.9347	55.1762	55.7634	55.2594	56.1763	**52.4**
C2`	24.2890	24.5786	24.8405	24.7246	25.1372	24.7177	25.2136	24.7101	25.0923	24.7322	25.1028	23.6801	23.7770	24.1376	23.9227	24.4125	23.9135	24.4023	23.9035	24.2810	23.9324	24.2369	**14.5**
C3`	23.6801	23.7770	24.1375	23.9227	24.4125	23.9135	24.4023	23.9035	24.2810	23.9324	24.2370	24.2890	24.5786	24.8404	24.7246	25.1372	24.7177	25.2137	24.7101	25.0924	24.7322	25.1028	**14.2**
C4`	53.9090	54.7912	55.1324	55.2314	55.7324	55.2039	55.9348	55.1762	55.7634	55.2594	56.1763	49.9816	50.6681	50.9208	51.1061	51.6481	51.0810	51.6813	51.0548	51.5477	51.1309	52.0377	**53.9**
H2	8.6573	8.5506	8.5924	8.4873	8.5035	8.4927	8.4297	8.4977	8.5448	8.4820	8.4250	8.6573	8.5506	8.5924	8.4873	8.5035	8.4927	8.4297	8.4977	8.5447	8.4820	8.4250	**8.13**
H5	7.2317	7.4023	7.4917	7.4772	7.6027	7.4732	7.6054	7.4691	7.6042	7.4810	7.6267	7.2317	7.4023	7.4917	7.4772	7.6027	7.4732	7.6054	7.4691	7.6042	7.4810	7.6267	**8.03**
H6	7.9266	8.0749	8.1830	8.1696	8.3042	8.1642	8.3142	8.1586	8.3490	8.1751	8.3438	7.9266	8.0749	8.1830	8.1696	8.3042	8.1642	8.3142	8.1586	8.3490	8.1751	8.3438	**7.4**
H(3``A-3``C)	2.3514	2.3974	2.4118	2.4128	2.4345	2.4120	2.4511	2.4111	2.4400	2.4138	2.4563	2.3514	2.3974	2.4118	2.4128	2.4345	2.4120	2.4511	2.4112	2.4400	2.4138	2.4563	**2.32**
H8	4.2964	4.3549	4.4302	4.4201	4.5025	4.4155	4.5433	4.4109	4.5481	4.4247	4.5434	4.2964	4.3549	4.4302	4.4201	4.5025	4.4155	4.5433	4.4109	4.5481	4.4247	4.5434	**5.64**
H(9A-9B)	1.6561	1.6953	1.6759	1.7062	1.7129	1.7071	1.6447	1.7075	1.6979	1.7055	1.6780	1.6561	1.6953	1.6760	1.7062	1.7129	1.7071	1.6447	1.7075	1.6978	1.7055	1.6780	**1.92**
H(10A)	1.0286	0.8865	0.8872	0.8404	0.7833	0.8434	0.8083	0.8463	0.8280	0.8376	0.8194	1.0286	0.8865	0.8872	0.8404	0.7833	0.8434	0.8083	0.8463	0.8280	0.8376	0.8194	**1.26**
H(10B)	1.6766	1.5661	1.5187	1.4915	1.4167	1.4961	1.4105	1.5007	1.4224	1.4873	1.3852	1.6766	1.5661	1.5187	1.4915	1.4167	1.4961	1.4105	1.5007	1.4224	1.4873	1.3852	**1.07**
H(11A-11C)	0.7565	0.7582	0.7409	0.7657	0.7337	0.7653	0.7245	0.7649	0.7398	0.7662	0.7170	0.7565	0.7582	0.7409	0.7657	0.7337	0.7653	0.7245	0.7649	0.7398	0.7662	0.7170	**0.78**
H(1`A)	2.6307	2.6257	2.6109	2.6226	2.5779	2.6232	2.5929	2.6237	2.5918	2.6222	2.5692	2.7666	2.7694	2.7512	2.7519	2.7214	2.7532	2.7532	2.7546	2.7278	2.7508	2.7188	**3.47**
H(1`B)	3.0645	3.0957	3.1234	3.1296	3.1868	3.1272	3.1722	3.1249	3.1715	3.1320	3.1753	2.7371	2.6172	2.5571	2.5764	2.5746	2.5784	2.5686	2.5805	2.5209	2.5748	2.5617	**3.63**
H(4`A)	2.7371	2.6172	2.5571	2.5764	2.5746	2.5784	2.5687	2.5805	2.5209	2.5748	2.5617	3.0645	3.0957	3.1234	3.1296	3.1868	3.1272	3.1722	3.1249	3.1715	3.1320	3.1753	**3.07**
H(4`B)	2.7666	2.7694	2.7513	2.7519	2.7214	2.7532	2.7533	2.7546	2.7278	2.7508	2.7188	2.6307	2.6257	2.6109	2.6226	2.5779	2.6232	2.5929	2.6237	2.5918	2.6222	2.5692	**3.25**

[a] methyl protons shifts are averaged

[b] according to [11]

Table S12. Cont. XIV

Nuclei	R											S											Exp. [b]
	X3LYP											X3LYP											
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.4041	140.0223	140.8129	140.5269	143.1312	140.4811	142.1658	140.4364	142.3764	140.5810	142.5466	139.4041	140.0223	140.8128	140.5269	143.1313	140.4811	142.1656	140.4364	142.3764	140.5811	142.5465	**131.615**
C2	140.5500	140.4125	140.7742	140.2073	140.7052	140.2265	141.0797	140.2422	140.9813	140.1926	141.0557	140.5502	140.4126	140.7740	140.2075	140.7050	140.2265	141.0797	140.2422	140.9813	140.1927	141.0559	**133.405**
C3	134.0323	135.1799	136.0888	135.5425	136.5779	135.5274	136.9165	135.5089	136.8432	135.5602	137.0649	134.0323	135.1799	136.0888	135.5424	136.5778	135.5274	136.9165	135.5089	136.8432	135.5603	137.0650	**126.19**
C4	175.0095	175.9667	176.6937	176.5244	177.1874	176.4907	177.8944	176.4543	177.7179	176.5608	177.9908	175.0093	175.9669	176.6938	176.5244	177.1874	176.4907	177.8944	176.4543	177.7179	176.5609	177.9907	**165.04**
C5	119.2391	120.4282	121.0066	121.0986	121.9322	121.0585	122.2322	121.0162	122.1290	121.1412	122.3575	119.2391	120.4281	121.0067	121.0986	121.9323	121.0585	122.2323	121.0162	122.1290	121.1413	122.3575	**116.425**
C6	133.4957	135.1735	136.1169	136.1069	136.9788	136.0579	137.7358	136.0047	137.4435	136.1542	138.0023	133.4956	135.1735	136.1169	136.1067	136.9787	136.0579	137.7358	136.0047	137.4435	136.1543	138.0022	**129.92**
C7	204.0680	208.6018	209.7906	211.2857	212.8613	211.1040	217.7497	210.9238	216.7862	211.4694	218.9551	204.0677	208.6014	209.7908	211.2857	212.8614	211.1040	217.7499	210.9238	216.7862	211.4694	218.9552	**195.9**
C8	66.0484	67.1131	67.4097	67.6924	68.8127	67.6555	69.2078	67.6167	69.1583	67.7330	69.6317	66.0484	67.1131	67.4096	67.6925	68.8127	67.6555	69.2079	67.6167	69.1583	67.7330	69.6317	**67.6**
C9	38.8515	38.4537	38.6398	38.3061	38.4752	38.3194	38.5849	38.3296	38.5301	38.2961	38.6638	38.8516	38.4537	38.6397	38.3060	38.4753	38.3194	38.5849	38.3296	38.5301	38.2962	38.6638	**32.2**
C10	19.8530	20.2980	20.5805	20.5917	21.0678	20.5777	20.9428	20.5605	20.9327	20.6084	21.0515	19.8530	20.2981	20.5805	20.5918	21.0678	20.5777	20.9429	20.5605	20.9327	20.6084	21.0515	**23.4**
C11	16.1311	16.2611	16.4069	16.3426	16.5437	16.3421	16.4790	16.3381	16.4858	16.3464	16.6472	16.1310	16.2611	16.4069	16.3427	16.5437	16.3421	16.4792	16.3381	16.4858	16.3464	16.6472	**17.9**
C1`	52.1870	53.0482	53.2659	53.5913	54.1404	53.5638	54.0666	53.5327	54.0389	53.6206	54.4972	56.7023	57.7867	58.1582	58.2874	58.7947	58.2596	58.9712	58.2291	58.9152	58.3175	59.2028	**52.4**
C2`	25.9147	26.3743	26.6079	26.5848	26.9763	26.5752	27.0117	26.5626	27.0228	26.5976	26.9096	25.5699	25.7049	26.1291	25.8844	26.4747	25.8740	26.4010	25.8609	26.3930	25.8987	26.1762	**14.5**
C3`	25.5699	25.7049	26.1291	25.8844	26.4747	25.8740	26.4010	25.8609	26.3930	25.8987	26.1764	25.9147	26.3743	26.6078	26.5849	26.9763	26.5752	27.0118	26.5626	27.0228	26.5976	26.9097	**14.2**
C4`	56.7024	57.7867	58.1582	58.2873	58.7947	58.2596	58.9712	58.2291	58.9152	58.3175	59.2028	52.1869	53.0481	53.2660	53.5913	54.1403	53.5638	54.0664	53.5327	54.0389	53.6205	54.4973	**53.9**
H2	8.5259	8.4459	8.4741	8.3825	8.3137	8.3882	8.3541	8.3930	8.3416	8.3765	8.3347	8.5259	8.4459	8.4741	8.3825	8.3136	8.3882	8.3541	8.3930	8.3416	8.3765	8.3347	**8.13**
H5	7.1012	7.2586	7.3480	7.3284	7.4453	7.3246	7.4665	7.3203	7.4558	7.3319	7.4859	7.1013	7.2586	7.3480	7.3284	7.4453	7.3246	7.4665	7.3203	7.4558	7.3319	7.4859	**8.03**
H6	7.7917	7.9695	8.0706	8.0644	8.1439	8.0593	8.2106	8.0535	8.1847	8.0691	8.2342	7.7917	7.9695	8.0706	8.0644	8.1439	8.0593	8.2106	8.0535	8.1847	8.0691	8.2342	**7.4**
H(3``A-3``C)	2.3710	2.4141	2.4315	2.4306	2.4536	2.4298	2.4622	2.4285	2.4596	2.4314	2.4669	2.3711	2.4141	2.4316	2.4306	2.4536	2.4298	2.4622	2.4285	2.4596	2.4314	2.4669	**2.32**
H8	4.5908	4.6521	4.7228	4.6993	4.7495	4.6964	4.8055	4.6929	4.7844	4.7019	4.7930	4.5908	4.6521	4.7228	4.6993	4.7495	4.6964	4.8055	4.6929	4.7844	4.7019	4.7930	**5.64**
H(9A-9B)	1.6700	1.7186	1.7006	1.7470	1.7128	1.7462	1.7045	1.7448	1.6977	1.7474	1.7295	1.6700	1.7186	1.7006	1.7470	1.7128	1.7462	1.7045	1.7448	1.6977	1.7474	1.7295	**1.92**
H(10A)	1.0788	0.9678	0.9721	0.9234	0.8482	0.9270	0.9015	0.9298	0.8938	0.9200	0.9082	1.0788	0.9678	0.9721	0.9234	0.8482	0.9270	0.9015	0.9298	0.8938	0.9200	0.9082	**1.26**
H(10B)	1.7441	1.6373	1.5950	1.5671	1.4883	1.5715	1.4882	1.5754	1.4926	1.5630	1.4528	1.7441	1.6374	1.5950	1.5672	1.4883	1.5715	1.4882	1.5754	1.4926	1.5630	1.4528	**1.07**
H(11A-11C)	0.7775	0.7888	0.7748	0.7980	0.7572	0.7975	0.7642	0.7966	0.7625	0.7983	0.7520	0.7775	0.7888	0.7748	0.7980	0.7572	0.7975	0.7642	0.7966	0.7625	0.7983	0.7520	**0.78**
H(1`A)	2.7254	2.7159	2.7001	2.7073	2.6580	2.7081	2.6654	2.7083	2.6679	2.7065	2.6483	2.8459	2.8443	2.8242	2.8320	2.8124	2.8329	2.8185	2.8334	2.8246	2.8312	2.7903	**3.47**
H(1`B)	3.1908	3.2308	3.2685	3.2671	3.3265	3.2649	3.3058	3.2623	3.2999	3.2690	3.3086	2.8710	2.6984	2.6765	2.6732	2.7143	2.6736	2.6619	2.6738	2.6654	2.6730	2.6605	**3.63**
H(4`A)	2.8709	2.6984	2.6765	2.6732	2.7143	2.6736	2.6619	2.6738	2.6654	2.6730	2.6605	3.1908	3.2308	3.2685	3.2671	3.3264	3.2649	3.3057	3.2623	3.2999	3.2690	3.3086	**3.07**
H(4`B)	2.8459	2.8443	2.8242	2.8320	2.8124	2.8329	2.8185	2.8334	2.8246	2.8312	2.7903	2.7254	2.7159	2.7001	2.7073	2.6580	2.7081	2.6654	2.7083	2.6679	2.7066	2.6483	**3.25**

[a] methyl protons shifts are averaged
[b] according to [11]

Table S13. Theoretical chemical shifts (in ppm) of *(R,S)*-4-fluoro-α-pyrrolidinooctanophenone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S										Exp. [b]
	B3LYP											B3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.7440	140.6555	142.0342	141.4602	143.3098	141.3148	142.4277	141.1275	142.5152	141.5693	142.9951	139.7439	140.6555	142.0341	141.4601	143.3098	141.3148	142.4277	141.1275	142.5152	141.5693	142.9952	**131.79**
C2	139.7404	139.8313	140.3450	139.5953	140.0872	139.6159	140.5636	139.6375	140.4349	139.5753	140.4849	139.7404	139.8313	140.3449	139.5953	140.0874	139.6158	140.5635	139.6375	140.4348	139.5751	140.4849	**131.93**
C3	122.0847	122.7996	123.3543	122.9484	123.5596	122.9391	123.8685	122.9308	123.7838	122.9561	123.8939	122.0848	122.7996	123.3542	122.9484	123.5597	122.9391	123.8685	122.9307	123.7837	122.9562	123.8939	**116.53**
C4	176.3853	177.2381	177.8754	177.5510	178.2024	177.5430	178.8558	177.5369	178.6824	177.5595	178.9299	176.3853	177.2381	177.8753	177.5509	178.2023	177.5430	178.8558	177.5369	178.6825	177.5595	178.9301	**168.1**
C5	119.8360	121.1437	121.7586	121.8151	122.5580	121.7557	122.8483	121.6924	122.7230	121.8667	123.0200	119.8360	121.1437	121.7585	121.8152	122.5580	121.7557	122.8483	121.6924	122.7232	121.8666	123.0200	**116.51**
C6	135.5687	137.4684	138.3866	138.4288	139.8539	138.3931	140.6351	138.3688	140.3514	138.4701	140.8634	135.5687	137.4684	138.3867	138.4288	139.8539	138.3930	140.6351	138.3688	140.3514	138.4700	140.8633	**131.88**
C7	203.6186	208.4436	210.2930	211.5325	212.4799	211.2330	217.4623	210.8895	216.3461	211.7872	218.9247	203.6186	208.4436	210.2931	211.5325	212.4799	211.2330	217.4623	210.8895	216.3462	211.7867	218.9249	**195.2**
C8	66.5090	67.7289	68.5733	68.3407	69.3202	68.2691	69.9581	68.1991	69.7954	68.4042	70.3423	66.5090	67.7289	68.5733	68.3407	69.3202	68.2691	69.9581	68.1991	69.7954	68.4042	70.3423	**54.87**
C9	37.1546	36.8932	36.9132	36.5849	36.8580	36.6191	37.0537	36.6673	36.9711	36.5582	37.0637	37.1546	36.8932	36.9132	36.5849	36.8580	36.6191	37.0537	36.6673	36.9710	36.5582	37.0638	**31.13**
C10	27.6112	28.1809	28.4922	28.3496	28.9997	28.3440	28.8458	28.3444	28.8208	28.3576	28.9233	27.6112	28.1809	28.4922	28.3497	28.9997	28.3440	28.8458	28.3444	28.8208	28.3576	28.9233	**30.82**
C11	37.1857	37.3183	37.6583	37.1831	37.7456	37.1935	37.7322	37.2080	37.7006	37.1728	37.8968	37.1857	37.3183	37.6582	37.1830	37.7456	37.1936	37.7322	37.2080	37.7007	37.1729	37.8968	**29.11**
C12	38.8215	39.1603	39.4656	39.3341	39.8093	39.3151	39.7210	39.2941	39.6945	39.3497	39.7747	38.8216	39.1603	39.4657	39.3340	39.8094	39.3151	39.7210	39.2941	39.6944	39.3497	39.7748	**25.52**
C13	29.8649	30.1122	30.3311	30.1260	30.4232	30.1224	30.4388	30.1191	30.4109	30.1278	30.4278	29.8650	30.1122	30.3312	30.1260	30.4231	30.1225	30.4388	30.1191	30.4109	30.1278	30.4278	**22.36**
C14	16.8464	17.0714	17.1281	17.1359	17.2139	17.1263	17.2234	17.1162	17.1938	17.1433	17.2338	16.8464	17.0714	17.1282	17.1359	17.2138	17.1263	17.2234	17.1162	17.1938	17.1432	17.2338	**13.85**
C1`	52.4430	53.2501	53.5796	53.7270	54.2978	53.6868	54.2682	53.6444	54.1816	53.7622	54.7742	56.8713	57.8585	58.3021	58.3786	58.8622	58.3368	59.1280	58.2937	59.0180	58.4156	59.4453	**51.23**
C2`	26.0864	26.6096	26.9407	26.7529	27.2069	26.7417	27.3157	26.7336	27.2752	26.7638	27.1542	25.8012	26.1795	26.5397	26.2972	26.8405	26.2786	26.7254	26.2545	26.7083	26.3104	26.5119	**23.85**
C3`	25.8012	26.1795	26.5398	26.2972	26.8405	26.2785	26.7254	26.2545	26.7084	26.3104	26.5120	26.0864	26.6096	26.9407	26.7529	27.2068	26.7417	27.3157	26.7336	27.2752	26.7638	27.1542	**23.66**
C4`	56.8713	57.8585	58.3021	58.3786	58.8622	58.3369	59.1280	58.2937	59.0180	58.4154	59.4454	52.4430	53.2501	53.5795	53.7270	54.2979	53.6869	54.2683	53.6444	54.1816	53.7622	54.7740	**52.72**
H2	8.6734	8.5716	8.5291	8.4413	8.4174	8.4598	8.4642	8.4844	8.4585	8.4273	8.4239	8.6734	8.5716	8.5291	8.4413	8.4174	8.4598	8.4642	8.4844	8.4585	8.4273	8.4239	**8.13**
H3	7.3212	7.4479	7.5248	7.4715	7.5851	7.4724	7.6015	7.4743	7.5911	7.4711	7.6161	7.3212	7.4479	7.5248	7.4715	7.5851	7.4724	7.6015	7.4742	7.5911	7.4711	7.6161	**7.22**
H5	7.1132	7.2968	7.3811	7.3806	7.5011	7.3731	7.5252	7.3659	7.5113	7.3874	7.5560	7.1132	7.2968	7.3811	7.3806	7.5011	7.3731	7.5252	7.3659	7.5113	7.3874	7.5560	**7.22**
H6	7.9527	8.1444	8.2339	8.2577	8.3717	8.2512	8.4472	8.2430	8.4253	8.2631	8.4517	7.9527	8.1444	8.2339	8.2577	8.3718	8.2512	8.4472	8.2430	8.4253	8.2631	8.4517	**8.13**
H8	4.6213	4.7003	4.7284	4.7485	4.8209	4.7447	4.8619	4.7397	4.8460	4.7514	4.8420	4.6213	4.7003	4.7284	4.7485	4.8209	4.7447	4.8619	4.7397	4.8460	4.7514	4.8420	**5.5**
H(9A-9B)	1.6744	1.7230	1.6952	1.7318	1.7394	1.7361	1.7440	1.7433	1.7352	1.7294	1.7633	1.6744	1.7230	1.6952	1.7318	1.7394	1.7361	1.7440	1.7433	1.7352	1.7294	1.7633	**2.08**
H(10-13A-10-13B)	1.2019	1.1748	1.1382	1.1621	1.1149	1.1624	1.1177	1.1622	1.1151	1.1615	1.1159	1.2019	1.1748	1.1382	1.1621	1.1149	1.1624	1.1177	1.1622	1.1151	1.1615	1.1159	**1.25**
H(14A-14C)	0.9542	0.9509	0.9274	0.9477	0.9189	0.9473	0.9196	0.9467	0.9167	0.9478	0.9209	0.9542	0.9509	0.9275	0.9477	0.9189	0.9473	0.9196	0.9467	0.9167	0.9478	0.9210	**0.79**
H(1`A-1`B)	2.9748	2.9963	2.9997	3.0082	3.0152	3.0070	3.0217	3.0057	3.0181	3.0092	3.0059	2.8861	2.8057	2.7806	2.7753	2.7692	2.7754	2.7470	2.7752	2.7466	2.7747	3.0059	**3.69**
H(2`-3`A-2`-3`B)	1.6646	1.7246	1.6943	1.7673	1.7228	1.7628	1.7410	1.7574	1.7327	1.7710	1.7734	1.6646	1.7246	1.6943	1.7673	1.7228	1.7628	1.7410	1.7574	1.7327	1.7710	1.7734	**2.18**
H(4`A)	2.8937	2.7424	2.7044	2.7040	2.7162	2.7035	2.6638	2.7024	2.6619	2.7039	2.6761	3.1957	3.2373	3.2700	3.2776	3.3397	3.2745	3.3374	3.2714	3.3312	3.2805	2.6761	**3.12**
H(4`B)	2.8784	2.8690	2.8569	2.8466	2.8222	2.8473	2.8302	2.8480	2.8313	2.8455	2.7966	2.7538	2.7552	2.7294	2.7387	2.6907	2.7394	2.7059	2.7399	2.7050	2.7378	2.7966	**3.86**
Nuclei	B3P86											B3P86										
C1	137.0834	137.8838	138.5950	138.1997	140.4007	138.1971	139.7281	138.1738	139.9163	138.2476	140.2401	137.0836	137.8838	138.5950	138.1997	140.4007	138.1971	139.7281	138.1738	139.9164	138.2476	140.2401	**131.79**
C2	138.7928	138.8426	139.4558	138.6348	139.1986	138.6691	139.6535	138.6809	139.6182	138.6455	139.6258	138.7927	138.8426	139.4557	138.6348	139.1985	138.6691	139.6535	138.6809	139.6181	138.6454	139.6258	**131.93**
C3	121.1615	121.9450	122.6230	122.2596	122.9450	122.2700	123.2610	122.2581	123.2718	122.2929	123.3166	121.1615	121.9450	122.6231	122.2596	122.9449	122.2700	123.2610	122.2581	123.2717	122.2928	123.3166	**116.53**
C4	173.9036	174.7161	175.4467	175.0930	175.7719	175.0900	176.4012	175.0650	176.3353	175.1398	176.5148	173.9036	174.7161	175.4468	175.0930	175.7718	175.0900	176.4013	175.0649	176.3352	175.1398	176.5148	**168.1**
C5	119.0932	120.4249	121.1457	121.1011	121.9976	121.0809	122.2909	121.0385	122.2654	121.1644	122.4717	119.0933	120.4249	121.1457	121.1011	121.9977	121.0809	122.2910	121.0384	122.2655	121.1644	122.4717	**116.51**
C6	134.7635	136.5921	137.7420	137.5435	138.9370	137.4931	139.5843	137.4212	139.4478	137.6355	139.8721	134.7635	136.5921	137.7420	137.5435	138.9370	137.4931	139.5844	137.4212	139.4478	137.6355	139.8721	**131.88**
C7	201.7091	206.1582	207.2235	208.6080	209.9808	208.4686	214.8876	208.3097	213.9505	208.7868	216.2023	201.7088	206.1582	207.2235	208.6080	209.9808	208.4686	214.8878	208.3097	213.9506	208.7865	216.2023	**195.2**
C8	64.8079	65.9343	66.5679	66.5613	67.5044	66.5388	68.2200	66.4954	68.2101	66.6277	68.6156	64.8079	65.9343	66.5680	66.5613	67.5045	66.5388	68.2201	66.4954	68.2101	66.6277	68.6156	**54.87**
C9	36.1125	35.8844	36.1431	35.7858	35.9382	35.8087	36.0235	35.8099	36.0965	35.8083	36.1250	36.1126	35.8844	36.1431	35.7858	35.9383	35.8087	36.0235	35.8099	36.0964	35.8083	36.1250	**31.13**
C10	26.4016	26.9937	27.3249	27.2664	27.8758	27.2696	27.6542	27.2513	27.7532	27.3075	27.7928	26.4017	26.9937	27.3250	27.2664	27.8759	27.2696	27.6541	27.2513	27.7533	27.3074	27.7928	**30.82**
C11	35.6753	35.7321	36.1663	35.7039	36.1700	35.7285	36.1437	35.7310	36.2176	35.7242	36.3336	35.6754	35.7321	36.1664	35.7039	36.1700	35.7285	36.1438	35.7310	36.2176	35.7242	36.3336	**29.11**
C12	37.2531	37.5794	37.8592	37.7441	38.2383	37.7533	38.1084	37.7409	38.2044	37.7796	38.1869	37.2531	37.5794	37.8592	37.7441	38.2383	37.7533	38.1084	37.7409	38.2043	37.7796	38.1869	**25.52**
C13	28.2609	28.4559	28.7123	28.5134	28.7908	28.5316	28.7900	28.5276	28.8713	28.5399	28.7979	28.2609	28.4559	28.7124	28.5134	28.7908	28.5316	28.7900	28.5276	28.8713	28.5399	28.7979	**22.36**
C14	16.4118	16.5961	16.6704	16.6782	16.7716	16.6932	16.7542	16.6863	16.8392	16.7079	16.7903	16.4118	16.5961	16.6704	16.6782	16.7717	16.6932	16.7541	16.6863	16.8392	16.7079	16.7903	**13.85**
C1`	51.4586	52.2270	52.4925	52.5680	53.2231	52.5592	53.1618	52.5291	53.1915	52.6207	53.6755	55.5406	56.5732	57.0357	57.1199	57.5941	57.1046	57.8900	57.0675	57.8765	57.1780	58.2123	**51.23**
C2`	24.8445	25.2727	25.6163	25.5167	25.8866	25.5220	25.9858	25.5055	26.0735	25.5557	25.8103	24.5386	24.8450	25.2192	24.8834	25.5159	24.9056	25.3966	24.9053	25.4888	24.9059	25.1849	**23.85**
C3`	24.5387	24.8450	25.2192	24.8834	25.5160	24.9056	25.3966	24.9053	25.4888	24.9060	25.1849	24.8445	25.2727	25.6162	25.5167	25.8865	25.5220	25.9859	25.5055	26.0735	25.5557	25.8103	**23.66**
C4`	55.5405	56.5732	57.0356	57.1199	57.5941	57.1046	57.8900	57.0675	57.8765	57.1780	58.2123	51.4586	52.2270	52.4925	52.5680	53.2230	52.5592	53.1620	52.5291	53.1916	52.6207	53.6755	**52.72**
H2	8.7392	8.6447	8.6970	8.5823	8.5070	8.5883	8.5348	8.5923	8.5317	8.5776	8.5038	8.7392	8.6447	8.6970	8.5823	8.5070	8.5883	8.5348	8.5923	8.5317	8.5776	8.5038	**8.13**
H3	7.3337	7.4702	7.5701	7.5138	7.6235	7.5132	7.6370	7.5107	7.6327	7.5155	7.6549	7.3337	7.4702	7.5701	7.5138	7.6235	7.5132	7.6370	7.5107	7.6327	7.5155	7.6549	**7.22**
H5	7.1474	7.3333	7.4302	7.4093	7.5333	7.4059	7.5590	7.4005	7.5500	7.4138	7.5840	7.1474	7.3333	7.4302	7.4093	7.5333	7.4059	7.5590	7.4005	7.5500	7.4138	7.5840	**7.22**
H6	8.0119	8.1936	8.2856	8.3051	8.4182	8.3001	8.4988	8.2933	8.4772	8.3111	8.5069	8.0119	8.1936	8.2856	8.3051	8.4182	8.3001	8.4988	8.2933	8.4771	8.3111	8.5069	**8.13**
H8	4.6254	4.6960	4.7298	4.7363	4.8181	4.7354	4.8719	4.7327	4.8546	4.7385	4.8647	4.6254	4.6960	4.7298	4.7363	4.8181	4.7354	4.8719	4.7327	4.8546	4.7385	4.8647	**5.5**
H(9A-9B)	1.7458	1.7919	1.7901	1.8253	1.7930	1.8234	1.7822	1.8197	1.7868	1.8284	1.8093	1.7458	1.7919	1.7901	1.8253	1.7930	1.8234	1.7822	1.8197	1.7868	1.8284	1.8093	**2.08**
H(10-13A-10-13B)	1.1889	1.1592	1.1310	1.1399	1.0947	1.1422	1.0973	1.1426	1.0997	1.1390	1.0966	1.1890	1.1592	1.1310	1.1399	1.0947	1.1422	1.0973	1.1426	1.0997	1.1390	1.0966	**1.25**
H(14A-14C)	0.9192	0.9158	0.8956	0.9098	0.8844	0.9113	0.8847	0.9111	0.8872	0.9095	0.8877	0.9192	0.9158	0.8956	0.9098	0.8844	0.9113	0.8847	0.9111	0.8872	0.9095	0.8877	**0.79**
H(1`A-1`B)	2.9539	2.9694	2.9771	2.9793	2.9882	2.9796	2.9930	2.9781	2.9949	2.9803	2.9820	2.8869	2.8015	2.7624	2.7622	2.7598	2.7653	2.7262	2.7668	2.7369	2.7606	2.7158	**3.69**
H(2`-3`A-2`-3`B)	1.6531	1.7111	1.6726	1.7411	1.7071	1.7403	1.7256	1.7378	1.7217	1.7432	1.7606	1.6531	1.7111	1.6726	1.7411	1.7071	1.7403	1.7256	1.7378	1.7217	1.7432	1.7606	**2.18**
H(4`A)	2.9440	2.7797	2.7181	2.7120	2.7345	2.7164	2.6580	2.7193	2.6678	2.7092	2.6662	3.1970	3.2311	3.2632	3.2664	3.3279	3.2646	3.3241	3.2610	3.3229	3.2695	3.3304	**3.12**
H(4`B)	2.8298	2.8233	2.8068	2.8125	2.7851	2.8142	2.7944	2.8142	2.8061	2.8120	2.7653	2.7109	2.7077	2.6911	2.6922	2.6485	2.6946	2.6619	2.6951	2.6669	2.6911	2.6335	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. I

Nuclei	R											S										Exp. [b]
	B3PW91											B3PW91										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.3645	138.2163	139.5596	138.6203	141.1688	138.5840	140.1980	138.5428	140.2522	138.6624	140.8332	137.3646	138.2164	139.5596	138.6209	140.8499	138.5840	140.1979	138.5429	140.2523	138.6624	140.8332	**131.79**
C2	138.8786	138.9320	139.4523	138.7409	139.6047	138.7629	139.7207	138.7751	139.6234	138.7210	139.7073	138.8786	138.9321	139.4523	138.7408	139.2858	138.7629	139.7206	138.7751	139.6233	138.7210	139.7073	**131.93**
C3	121.3464	122.1193	122.6939	122.3239	123.3407	122.3207	123.3300	122.3080	123.2511	122.3284	123.3858	121.3464	122.1193	122.6939	122.3239	123.0218	122.3207	123.3300	122.3080	123.2512	122.3284	123.3858	**116.53**
C4	173.9175	174.7530	175.3773	175.1270	176.0876	175.1110	176.3736	175.0858	176.2225	175.1436	176.4569	173.9174	174.7530	175.3773	175.1270	175.7686	175.1110	176.3736	175.0858	176.2225	175.1436	176.4568	**168.1**
C5	119.1873	120.5407	121.1755	121.1980	122.4166	121.1623	122.3683	121.1177	122.2464	121.2341	122.5596	119.1873	120.5408	121.1755	121.1979	122.0976	121.1623	122.3683	121.1178	122.2464	121.2341	122.5597	**116.51**
C6	134.5875	136.4784	137.3751	137.5710	139.2512	137.5080	139.5727	137.4362	139.3402	137.6323	139.8227	134.5876	136.4784	137.3751	137.5709	138.9321	137.5080	139.5728	137.4363	139.3404	137.6323	139.8227	**131.88**
C7	201.7750	206.3530	208.1156	208.9132	210.5822	208.7357	215.2564	208.5546	214.1387	209.0906	216.7068	201.7750	206.3531	208.1156	208.9134	210.2635	208.7357	215.2562	208.5546	214.1385	209.0906	216.7068	**195.2**
C8	64.8040	66.0074	66.8207	66.6379	67.9609	66.5916	68.3251	66.5385	68.1722	66.6879	68.7655	64.8040	66.0069	66.8207	66.6385	67.6419	66.5916	68.3251	66.5385	68.1722	66.6879	68.7655	**54.87**
C9	35.6465	35.4775	35.4913	35.3856	35.8745	35.3959	35.6827	35.3974	35.6386	35.3777	35.7426	35.6465	35.4776	35.4913	35.3856	35.5555	35.3959	35.6826	35.3974	35.6386	35.3777	35.7426	**31.13**
C10	26.1614	26.7547	26.9834	27.0064	27.9075	26.9959	27.4018	26.9765	27.3991	27.0185	27.5461	26.1613	26.7546	26.9834	27.0064	27.5885	26.9959	27.4018	26.9765	27.3990	27.0185	27.5461	**30.82**
C11	35.4336	35.5429	35.8310	35.4896	36.3003	35.5001	35.9266	35.5013	35.9047	35.4817	36.1113	35.4336	35.5428	35.8310	35.4898	35.9813	35.5001	35.9265	35.5013	35.9046	35.4817	36.1113	**29.11**
C12	36.9439	37.2879	37.5087	37.4449	38.2312	37.4390	37.7900	37.4244	37.7888	37.4530	37.8748	36.9440	37.2879	37.5087	37.4450	37.9123	37.4390	37.7901	37.4244	37.7887	37.4530	37.8748	**25.52**
C13	28.2326	28.4628	28.6279	28.5058	29.1001	28.5087	28.7676	28.5028	28.7548	28.5047	28.7787	28.2325	28.4628	28.6279	28.5057	28.7812	28.5087	28.7675	28.5027	28.7548	28.5048	28.7787	**22.36**
C14	16.4298	16.6433	16.6448	16.7183	17.1147	16.7179	16.7817	16.7088	16.7699	16.7208	16.8179	16.4299	16.6434	16.6448	16.7183	16.7958	16.7179	16.7816	16.7088	16.7699	16.7208	16.8178	**13.85**
C1`	51.2577	52.0600	52.3040	52.5115	53.3865	52.4856	53.0757	52.4515	53.0021	52.5388	53.6024	55.4709	56.4890	56.8905	57.0331	57.5091	57.0031	57.7631	56.9645	57.6619	57.0635	58.0933	**51.23**
C2`	25.1287	25.5832	25.8665	25.7707	26.5017	25.7620	26.2242	25.7445	26.2122	25.7820	26.0244	24.7778	25.0766	25.4001	25.1100	25.7222	25.1161	25.6045	25.1128	25.6091	25.1061	25.3792	**23.85**
C3`	24.7777	25.0765	25.4001	25.1105	26.0411	25.1160	25.6045	25.1127	25.6092	25.1061	25.3791	25.1288	25.5832	25.8665	25.7710	26.1827	25.7620	26.2242	25.7445	26.2123	25.7820	26.0244	**23.66**
C4`	55.4708	56.4889	56.8905	57.0326	57.8281	57.0031	57.7631	56.9644	57.6619	57.0635	58.0933	51.2577	52.0599	52.3040	52.5115	53.0676	52.4856	53.0756	52.4515	53.0022	52.5387	53.6024	**52.72**
H2	8.7103	8.6070	8.5673	8.5299	8.4699	8.5378	8.4926	8.5448	8.4922	8.5219	8.4533	8.7103	8.6070	8.5673	8.5299	8.4544	8.5378	8.4926	8.5448	8.4922	8.5219	8.4533	**8.13**
H3	7.3394	7.4704	7.5521	7.5077	7.6323	7.5067	7.6349	7.5053	7.6265	7.5087	7.6511	7.3394	7.4704	7.5521	7.5078	7.6168	7.5067	7.6349	7.5053	7.6265	7.5087	7.6511	**7.22**
H5	7.1369	7.3234	7.4096	7.4036	7.5461	7.3995	7.5606	7.3951	7.5472	7.4076	7.5861	7.1369	7.3234	7.4096	7.4036	7.5306	7.3995	7.5606	7.3951	7.5471	7.4076	7.5861	**7.22**
H6	8.0140	8.1968	8.2900	8.2999	8.4377	8.2941	8.4796	8.2881	8.4586	8.3052	8.4788	8.0140	8.1968	8.2900	8.2998	8.4223	8.2941	8.4796	8.2881	8.4587	8.3052	8.4788	**8.13**
H8	4.6225	4.6925	4.7350	4.7304	4.8337	4.7285	4.8595	4.7264	4.8415	4.7321	4.8437	4.6225	4.6925	4.7350	4.7303	4.8182	4.7285	4.8595	4.7264	4.8415	4.7321	4.8437	**5.5**
H(9A-9B)	1.6924	1.7398	1.7075	1.7804	1.7654	1.7782	1.7426	1.7757	1.7410	1.7826	1.7605	1.6924	1.7398	1.7075	1.7804	1.7499	1.7782	1.7426	1.7757	1.7410	1.7826	1.7605	**2.08**
H(10-13A-10-13B)	1.1619	1.1324	1.0979	1.1165	1.0864	1.1180	1.0759	1.1193	1.0754	1.1153	1.0725	1.1619	1.1324	1.0979	1.1165	1.0709	1.1180	1.0759	1.1193	1.0754	1.1153	1.0725	**1.25**
H(14A-14C)	0.9089	0.9041	0.8834	0.8995	0.8883	0.9002	0.8758	0.9007	0.8745	0.8989	0.8760	0.9089	0.9042	0.8834	0.8995	0.8728	0.9002	0.8758	0.9007	0.8745	0.8989	0.8760	**0.79**
H(1`A-1`B)	2.9352	2.9535	2.9613	2.9668	2.9890	2.9663	2.9814	2.9656	2.9796	2.9674	2.9660	2.8628	2.7786	2.7548	2.7425	2.7390	2.7444	2.7144	2.7462	2.7179	2.7411	2.7019	**3.69**
H(2`-3`A-2`-3`B)	1.6419	1.6981	1.6698	1.7314	1.7119	1.7295	1.7143	1.7274	1.7065	1.7334	1.7473	1.6419	1.6981	1.6698	1.7313	1.6964	1.7295	1.7143	1.7274	1.7064	1.7334	1.7473	**2.18**
H(4`A)	2.8969	2.7390	2.6984	2.6833	2.7181	2.6861	2.6443	2.6888	2.6460	2.6811	2.6520	3.1688	3.2062	3.2405	3.2479	3.3045	3.2453	3.3074	3.2424	3.3027	3.2506	3.3091	**3.12**
H(4`B)	2.8287	2.8182	2.8111	2.8018	2.7909	2.8027	2.7845	2.8034	2.7898	2.8012	2.7518	2.7017	2.7010	2.6820	2.6857	2.6424	2.6874	2.6555	2.6887	2.6566	2.6843	2.6229	**3.86**
Nuclei	B98											B98										
C1	138.3861	139.1649	140.4959	139.4943	141.7469	139.4786	140.9154	139.4636	141.0236	139.5145	141.5464	138.3859	139.1651	140.4960	139.4944	141.7468	139.4786	140.9153	139.4635	141.0237	139.5145	141.5464	**131.79**
C2	138.6697	138.6917	139.1617	138.4909	138.9633	138.5228	139.3950	138.5514	139.2860	138.4619	139.2967	138.6697	138.6918	139.1616	138.4909	138.9632	138.5229	139.3949	138.5516	139.2861	138.4619	139.2967	**131.93**
C3	121.0784	121.8156	122.4177	122.0425	122.7352	122.0473	123.0190	122.0490	122.9505	122.0395	123.0353	121.0785	121.8155	122.4178	122.0424	122.7354	122.0472	123.0190	122.0490	122.9507	122.0395	123.0353	**116.53**
C4	173.7000	174.5104	175.1610	174.9090	175.5572	174.9011	176.1754	174.8904	176.0258	174.9180	176.2418	173.7000	174.5102	175.1610	174.9088	175.5572	174.9011	176.1756	174.8904	176.0257	174.9180	176.2418	**168.1**
C5	118.9046	120.1908	120.8150	120.8450	121.7112	120.8201	121.9746	120.7925	121.8719	120.8711	122.1772	118.9047	120.1908	120.8150	120.8450	121.7112	120.8201	121.9746	120.7925	121.8717	120.8712	122.1772	**116.51**
C6	134.5982	136.4476	137.3328	137.5688	138.8504	137.5145	139.5600	137.4572	139.3090	137.6222	139.7331	134.5981	136.4477	137.3327	137.5689	138.8504	137.5145	139.5600	137.4572	139.3090	137.6223	139.7331	**131.88**
C7	200.2633	204.8889	206.6379	207.3940	208.7742	207.2367	213.7939	207.0820	212.6960	207.5500	215.3167	200.2632	204.8888	206.6385	207.3939	208.7741	207.2367	213.7938	207.0823	212.6960	207.5503	215.3167	**195.2**
C8	66.4691	67.6252	68.3963	68.1743	69.1924	68.1472	69.8314	68.1199	69.7053	68.2045	70.2790	66.4691	67.6251	68.3964	68.1742	69.1924	68.1472	69.8313	68.1199	69.7053	68.2045	70.2790	**54.87**
C9	36.8864	36.6288	36.6738	36.5274	36.7193	36.5483	36.8690	36.5668	36.8166	36.5103	36.9030	36.8864	36.6288	36.6737	36.5276	36.7191	36.5483	36.8691	36.5669	36.8166	36.5103	36.9030	**31.13**
C10	27.6385	28.1528	28.4190	28.3980	28.9752	28.3979	28.8124	28.3952	28.8117	28.4003	28.9096	27.6385	28.1528	28.4191	28.3979	28.9752	28.3979	28.8124	28.3952	28.8118	28.4003	28.9096	**30.82**
C11	36.8550	36.9202	37.2192	36.8523	37.3709	36.8743	37.3328	36.8934	37.3147	36.8331	37.5146	36.8549	36.9203	37.2192	36.8522	37.3709	36.8743	37.3329	36.8934	37.3147	36.8331	37.5146	**29.11**
C12	38.3761	38.6689	38.9421	38.8478	39.3324	38.8502	39.2296	38.8503	39.2294	38.8481	39.2872	38.3761	38.6689	38.9421	38.8478	39.3324	38.8502	39.2296	38.8503	39.2296	38.8480	39.2872	**25.52**
C13	29.5566	29.7397	29.9266	29.7837	30.0731	29.7970	30.0658	29.8076	30.0571	29.7733	30.0614	29.5566	29.7398	29.9266	29.7837	30.0731	29.7970	30.0657	29.8076	30.0572	29.7733	30.0614	**22.36**
C14	17.0197	17.1852	17.2176	17.2688	17.3571	17.2781	17.3471	17.2850	17.3394	17.2624	17.3623	17.0197	17.1853	17.2176	17.2688	17.3572	17.2781	17.3471	17.2850	17.3395	17.2624	17.3623	**13.85**
C1`	52.5177	53.2990	53.5734	53.7328	54.3305	53.7198	54.2589	53.7046	54.1936	53.7479	54.7567	56.8480	57.7803	58.1986	58.3161	58.8176	58.2952	59.0746	58.2721	58.9862	58.3384	59.3919	**51.23**
C2`	26.3044	26.7187	27.0115	26.9275	27.3424	26.9271	27.4333	26.9245	27.4151	26.9305	27.2806	25.9561	26.2650	26.6082	26.2868	26.9021	26.3055	26.7675	26.3213	26.7759	26.2708	26.5401	**23.85**
C3`	25.9562	26.2649	26.6082	26.2868	26.9021	26.3055	26.7676	26.3213	26.7759	26.2707	26.5401	26.3044	26.7186	27.0115	26.9275	27.3424	26.9271	27.4333	26.9245	27.4151	26.9305	27.2806	**23.66**
C4`	56.8479	57.7802	58.1987	58.3160	58.8176	58.2952	59.0746	58.2720	58.9861	58.3383	59.3919	52.5177	53.2991	53.5733	53.7329	54.3306	53.7198	54.2589	53.7046	54.1936	53.7479	54.7567	**52.72**
H2	8.7138	8.6192	8.5816	8.5493	8.4689	8.5557	8.5103	8.5617	8.5070	8.5430	8.4604	8.7138	8.6192	8.5815	8.5493	8.4689	8.5557	8.5103	8.5617	8.5070	8.5430	8.4604	**8.13**
H3	7.3308	7.4666	7.5545	7.5081	7.6197	7.5063	7.6370	7.5046	7.6287	7.5099	7.6479	7.3308	7.4666	7.5545	7.5081	7.6197	7.5063	7.6370	7.5046	7.6287	7.5099	7.6479	**7.22**
H5	7.1292	7.3142	7.4019	7.3959	7.5223	7.3913	7.5462	7.3867	7.5348	7.4004	7.5759	7.1292	7.3142	7.4019	7.3959	7.5223	7.3913	7.5462	7.3868	7.5348	7.4004	7.5759	**7.22**
H6	7.9721	8.1564	8.2591	8.2658	8.3991	8.2591	8.4756	8.2525	8.4559	8.2723	8.4782	7.9721	8.1564	8.2590	8.2658	8.3991	8.2591	8.4756	8.2525	8.4559	8.2723	8.4782	**8.13**
H8	4.5750	4.6530	4.6950	4.6953	4.7825	4.6930	4.8313	4.6907	4.8156	4.6978	4.8120	4.5750	4.6530	4.6950	4.6953	4.7825	4.6930	4.8313	4.6907	4.8156	4.6978	4.8120	**5.5**
H(9A-9B)	1.6864	1.7235	1.6967	1.7636	1.7394	1.7608	1.7401	1.7581	1.7363	1.7666	1.7530	1.6864	1.7235	1.6967	1.7636	1.7394	1.7608	1.7401	1.7581	1.7363	1.7666	1.7530	**2.08**
H(10-13A-10-13B)	1.1900	1.1580	1.1250	1.1423	1.0972	1.1434	1.1025	1.1446	1.1021	1.1416	1.0967	1.1900	1.1580	1.1250	1.1423	1.0972	1.1434	1.1025	1.1446	1.1021	1.1416	1.0967	**1.25**
H(14A-14C)	0.9310	0.9246	0.9047	0.9199	0.8935	0.9203	0.8961	0.9208	0.8954	0.9198	0.8946	0.9310	0.9246	0.9047	0.9199	0.8935	0.9203	0.8961	0.9208	0.8954	0.9198	0.8946	**0.79**
H(1`A-1`B)	2.9516	2.9712	2.9799	2.9851	2.9945	2.9841	2.9995	2.9833	2.9986	2.9863	2.9814	2.8644	2.7894	2.7693	2.7572	2.7536	2.7587	2.7353	2.7605	2.7377	2.7562	2.7249	**3.69**
H(2`-3`A-2`-3`B)	1.6594	1.7154	1.6872	1.7501	1.7151	1.7478	1.7358	1.7456	1.7293	1.7526	1.7695	1.6594	1.7154	1.6872	1.7500	1.7151	1.7478	1.7358	1.7456	1.7293	1.7526	1.7695	**2.18**
H(4`A)	2.8862	2.7447	2.7121	2.6974	2.7152	2.6997	2.6664	2.7022	2.6672	2.6957	2.6773	3.1819	3.2192	3.2560	3.2623	3.3244	3.2591	3.3205	3.2561	3.3176	3.2657	3.3173	**3.12**
H(4`B)	2.8427	2.8341	2.8265	2.8170	2.7920	2.8178	2.8042	2.8188	2.8081	2.8167	2.7724	2.7214	2.7233	2.7037	2.7079	2.6645	2.7092	2.6785	2.7106	2.6795	2.7069	2.6455	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. II

Nuclei	R											S										Exp. [b]
	B971											B971										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.9579	138.7472	140.0938	139.0723	141.3254	139.0511	140.5387	139.0325	140.6413	139.1010	141.1680	137.9579	138.7472	140.0938	139.0723	141.3253	139.0512	140.5387	139.0325	140.6414	139.1010	141.1681	**131.79**
C2	138.3790	138.4118	138.8725	138.2234	138.6679	138.2469	139.0987	138.2692	138.9878	138.2060	138.9993	138.3790	138.4117	138.8724	138.2234	138.6678	138.2470	139.0987	138.2692	138.9878	138.2059	138.9992	**131.93**
C3	120.8861	121.6303	122.2331	121.8686	122.5508	121.8653	122.8358	121.8608	122.7656	121.8770	122.8585	120.8861	121.6303	122.2331	121.8686	122.5508	121.8653	122.8357	121.8609	122.7654	121.8770	122.8584	**116.53**
C4	173.5870	174.4058	175.0620	174.8162	175.4697	174.8001	176.0781	174.7831	175.9292	174.8372	176.1579	173.5870	174.4059	175.0620	174.8162	175.4697	174.8002	176.0781	174.7830	175.9293	174.8372	176.1579	**168.1**
C5	118.7067	119.9991	120.6268	120.6631	121.5263	120.6301	121.7879	120.5967	121.6853	120.7004	121.9924	118.7067	119.9992	120.6268	120.6630	121.5264	120.6301	121.7879	120.5967	121.6852	120.7004	121.9925	**116.51**
C6	134.3132	136.1577	137.0294	137.2873	138.5643	137.2244	139.2420	137.1607	138.9968	137.3527	139.4332	134.3132	136.1576	137.0295	137.2873	138.5642	137.2243	139.2420	137.1608	138.9969	137.3528	139.4331	**131.88**
C7	200.1399	204.7116	206.4713	207.1825	208.5987	207.0220	213.5556	206.8653	212.4802	207.3455	215.0840	200.1399	204.7119	206.4711	207.1825	208.5990	207.0220	213.5556	206.8652	212.4801	207.3456	215.0840	**195.2**
C8	66.2700	67.4167	68.1726	67.9741	68.9802	67.9396	69.6005	67.9068	69.4827	68.0151	70.0458	66.2700	67.4167	68.1724	67.9741	68.9802	67.9396	69.6005	67.9069	69.4827	68.0152	70.0458	**54.87**
C9	36.8619	36.6248	36.6577	36.5434	36.7179	36.5549	36.8570	36.5661	36.8055	36.5388	36.9061	36.8619	36.6247	36.6578	36.5434	36.7179	36.5549	36.8570	36.5661	36.8054	36.5389	36.9061	**31.13**
C10	27.6649	28.1911	28.4444	28.4462	29.0102	28.4381	28.8356	28.4296	28.8361	28.4599	28.9396	27.6649	28.1911	28.4444	28.4462	29.0103	28.4381	28.8356	28.4296	28.8361	28.4599	28.9396	**30.82**
C11	36.8585	36.9218	37.2181	36.8639	37.3694	36.8775	37.3278	36.8904	37.3088	36.8566	37.5133	36.8585	36.9219	37.2181	36.8639	37.3696	36.8776	37.3278	36.8903	37.3088	36.8565	37.5132	**29.11**
C12	38.3909	38.6888	38.9535	38.8745	39.3479	38.8692	39.2394	38.8639	39.2396	38.8856	39.3057	38.3909	38.6887	38.9535	38.8744	39.3479	38.8693	39.2393	38.8638	39.2396	38.8856	39.3057	**25.52**
C13	29.5262	29.7114	29.8938	29.7636	30.0410	29.7689	30.0304	29.7736	30.0218	29.7645	30.0308	29.5262	29.7114	29.8938	29.7635	30.0411	29.7689	30.0304	29.7736	30.0218	29.7645	30.0308	**22.36**
C14	16.9704	17.1396	17.1657	17.2310	17.3068	17.2326	17.2929	17.2336	17.2853	17.2359	17.3134	16.9704	17.1396	17.1657	17.2311	17.3068	17.2326	17.2930	17.2336	17.2854	17.2358	17.3133	**13.85**
C1`	52.4411	53.2195	53.4844	53.6577	54.2418	53.6367	54.1675	53.6156	54.1020	53.6843	54.6682	56.7490	57.6864	58.1043	58.2296	58.7249	58.2010	58.9752	58.1722	58.8884	58.2627	59.2925	**51.23**
C2`	26.1067	26.5359	26.8246	26.7648	27.1656	26.7559	27.2507	26.7468	27.2329	26.7795	27.1086	25.7726	26.0821	26.4300	26.1125	26.7222	26.1234	26.5932	26.1329	26.5994	26.1079	26.3818	**23.85**
C3`	25.7726	26.0820	26.4300	26.1126	26.7222	26.1234	26.5932	26.1330	26.5994	26.1079	26.3817	26.1067	26.5358	26.8247	26.7649	27.1656	26.7560	27.2506	26.7468	27.2329	26.7796	27.1086	**23.66**
C4`	56.7490	57.6864	58.1043	58.2295	58.7248	58.2010	58.9752	58.1721	58.8883	58.2626	59.2925	52.4411	53.2195	53.4846	53.6578	54.2418	53.6367	54.1675	53.6157	54.1019	53.6843	54.6683	**52.72**
H2	8.7130	8.6205	8.5818	8.5548	8.4695	8.5605	8.5097	8.5658	8.5060	8.5492	8.4595	8.7130	8.6205	8.5818	8.5547	8.4695	8.5605	8.5097	8.5658	8.5060	8.5492	8.4595	**8.13**
H3	7.3267	7.4622	7.5503	7.5048	7.6156	7.5027	7.6328	7.5007	7.6245	7.5069	7.6441	7.3267	7.4621	7.5503	7.5047	7.6156	7.5027	7.6328	7.5007	7.6245	7.5069	7.6441	**7.22**
H5	7.1292	7.3125	7.3992	7.3941	7.5183	7.3894	7.5413	7.3846	7.5301	7.3990	7.5702	7.1292	7.3125	7.3992	7.3941	7.5183	7.3893	7.5413	7.3846	7.5301	7.3990	7.5702	**7.22**
H6	7.9816	8.1607	8.2609	8.2675	8.3993	8.2608	8.4733	8.2543	8.4537	8.2741	8.4750	7.9816	8.1607	8.2609	8.2675	8.3993	8.2608	8.4733	8.2543	8.4537	8.2741	8.4750	**8.13**
H8	4.5809	4.6550	4.7011	4.6960	4.7853	4.6937	4.8333	4.6913	4.8178	4.6985	4.8122	4.5809	4.6550	4.7011	4.6960	4.7853	4.6937	4.8333	4.6913	4.8178	4.6986	4.8122	**5.5**
H(9A-9B)	1.6950	1.7314	1.7009	1.7727	1.7457	1.7696	1.7438	1.7665	1.7404	1.7763	1.7578	1.6950	1.7314	1.7009	1.7727	1.7457	1.7696	1.7438	1.7665	1.7403	1.7763	1.7578	**2.08**
H(10-13A-10-13B)	1.1898	1.1569	1.1241	1.1418	1.0959	1.1427	1.1015	1.1437	1.1009	1.1414	1.0960	1.1898	1.1569	1.1241	1.1418	1.0959	1.1428	1.1015	1.1437	1.1009	1.1414	1.0960	**1.25**
H(14A-14C)	0.9262	0.9195	0.8998	0.9154	0.8883	0.9156	0.8910	0.9158	0.8902	0.9156	0.8896	0.9262	0.9195	0.8998	0.9154	0.8883	0.9156	0.8911	0.9158	0.8903	0.9156	0.8896	**0.79**
H(1`A-1`B)	2.9480	2.9666	2.9750	2.9807	2.9895	2.9797	2.9937	2.9786	2.9928	2.9822	2.9751	2.8620	2.7881	2.7681	2.7564	2.7524	2.7578	2.7328	2.7594	2.7356	2.7557	2.7222	**3.69**
H(2`-3`A-2`-3`B)	1.6590	1.7145	1.6864	1.7486	1.7137	1.7463	1.7340	1.7440	1.7275	1.7514	1.7675	1.6590	1.7145	1.6865	1.7487	1.7137	1.7463	1.7340	1.7440	1.7275	1.7514	1.7675	**2.18**
H(4`A)	2.8916	2.7505	2.7172	2.7005	2.7180	2.7029	2.6679	2.7055	2.6692	2.6990	2.6779	3.1854	3.2210	3.2569	3.2637	3.3248	3.2604	3.3200	3.2572	3.3172	3.2672	3.3168	**3.12**
H(4`B)	2.8325	2.8257	2.8192	2.8122	2.7869	2.8127	2.7977	2.8133	2.8020	2.8123	2.7665	2.7106	2.7123	2.6933	2.6978	2.6543	2.6989	2.6673	2.7000	2.6683	2.6971	2.6335	**3.86**
Nuclei	B972											B972											
C1	134.8089	135.7802	136.9805	137.1435	138.4018	137.0860	137.6594	137.0252	137.6561	137.1926	138.4940	134.8089	135.7802	136.9805	137.1435	138.4018	137.0861	137.6594	137.0251	137.6561	137.1925	138.4940	**131.79**
C2	136.3116	136.2928	136.8023	136.0499	136.6284	136.0667	136.9839	136.0811	136.9153	136.0297	136.9539	136.3116	136.2927	136.8023	136.0499	136.6284	136.0668	136.9839	136.0810	136.9154	136.0296	136.9539	**131.93**
C3	118.7780	119.4634	120.0489	119.7596	120.3977	119.7456	120.6719	119.7285	120.6023	119.7684	120.7324	118.7780	119.4634	120.0488	119.7596	120.3977	119.7457	120.6719	119.7284	120.6023	119.7685	120.7324	**116.53**
C4	170.5791	171.3249	171.9325	171.6078	172.2871	171.5891	172.8917	171.5681	172.7550	171.6213	172.9340	170.5791	171.3248	171.9324	171.6078	172.2870	171.5892	172.8917	171.5681	172.7551	171.6214	172.9341	**168.1**
C5	116.6218	117.8904	118.5100	118.6924	119.3953	118.6471	119.6764	118.5992	119.5557	118.7306	119.8804	116.6218	117.8903	118.5100	118.6925	119.3953	118.6472	119.6764	118.5992	119.5556	118.7306	119.8804	**116.51**
C6	132.0025	133.7516	134.6831	134.5632	136.1143	134.5041	136.7747	134.4435	136.5605	134.6155	136.9243	132.0025	133.7516	134.6832	134.5632	136.1143	134.5041	136.7747	134.4435	136.5605	134.6155	136.9243	**131.88**
C7	197.7084	202.3854	203.9953	205.9540	206.2360	205.7561	211.1804	205.5561	209.9691	206.1363	212.8165	197.7084	202.3858	203.9950	205.9540	206.2360	205.7561	211.1804	205.5560	209.9690	206.1363	212.8165	**195.2**
C8	63.4988	64.6959	65.5210	65.6629	66.3756	65.6036	67.0354	65.5423	66.8280	65.7148	67.5126	63.4988	64.6959	65.5210	65.6630	66.3756	65.6036	67.0354	65.5423	66.8280	65.7148	67.5126	**54.87**
C9	34.9897	34.7638	34.8547	34.5929	34.9074	34.6015	35.0731	34.6079	35.0157	34.5806	35.0839	34.9897	34.7637	34.8547	34.5929	34.9074	34.6016	35.0731	34.6079	35.0158	34.5806	35.0839	**31.13**
C10	26.0367	26.5440	26.8472	26.8206	27.4511	26.8013	27.2698	26.7800	27.2627	26.8350	27.4033	26.0367	26.5440	26.8472	26.8206	27.4511	26.8013	27.2698	26.7800	27.2627	26.8348	27.4034	**30.82**
C11	35.1774	35.2516	35.5671	35.2137	35.7190	35.2174	35.6745	35.2180	35.6527	35.2053	35.8517	35.1774	35.2516	35.5670	35.2137	35.7190	35.2174	35.6745	35.2180	35.6527	35.2054	35.8517	**29.11**
C12	36.6134	36.8984	37.1534	37.1431	37.5424	37.1282	37.4315	37.1115	37.4307	37.1534	37.5223	36.6134	36.8984	37.1535	37.1431	37.5425	37.1282	37.4315	37.1115	37.4308	37.1534	37.5223	**25.52**
C13	28.2326	28.4235	28.6155	28.5272	28.7792	28.5230	28.7619	28.5160	28.7482	28.5267	28.7781	28.2326	28.4234	28.6155	28.5271	28.7792	28.5230	28.7619	28.5161	28.7482	28.5266	28.7781	**22.36**
C14	16.5580	16.7272	16.7609	16.8870	16.9251	16.8784	16.9045	16.8677	16.8923	16.8908	16.9465	16.5580	16.7272	16.7608	16.8869	16.9250	16.8784	16.9045	16.8677	16.8923	16.8908	16.9465	**13.85**
C1`	50.4284	51.1614	51.4450	51.7720	52.2602	51.7409	52.2001	51.7073	52.1241	51.7971	52.7224	54.6531	55.5810	55.9895	56.1942	56.6326	56.1594	56.8078	56.1220	56.7158	56.2225	57.1181	**51.23**
C2`	25.0637	25.4848	25.8033	25.6862	26.1205	25.6707	26.1502	25.6530	26.1362	25.6968	25.9596	24.7216	24.9676	25.2925	25.1576	25.6280	25.1509	25.4971	25.1418	25.5048	25.1594	25.3054	**23.85**
C3`	24.7216	24.9675	25.2925	25.1576	25.6280	25.1510	25.4971	25.1418	25.5048	25.1594	25.3054	25.0637	25.4847	25.8033	25.6863	26.1205	25.6707	26.1502	25.6528	26.1361	25.6968	25.9596	**23.66**
C4`	54.6531	55.5809	55.9896	56.1941	56.6326	56.1594	56.8078	56.1221	56.7158	56.2225	57.1181	50.4285	51.1614	51.4451	51.7720	52.2603	51.7409	52.2001	51.7073	52.1241	51.7971	52.7224	**52.72**
H2	8.6878	8.5592	8.5417	8.3954	8.4285	8.4029	8.4611	8.4103	8.4688	8.3883	8.4115	8.6878	8.5592	8.5417	8.3954	8.4285	8.4029	8.4611	8.4103	8.4688	8.3884	8.4115	**8.13**
H3	7.3342	7.4591	7.5441	7.4876	7.6089	7.4859	7.6278	7.4839	7.6196	7.4892	7.6480	7.3342	7.4591	7.5441	7.4876	7.6088	7.4859	7.6278	7.4839	7.6196	7.4892	7.6480	**7.22**
H5	7.1246	7.3056	7.3964	7.4085	7.5202	7.4028	7.5507	7.3967	7.5365	7.4137	7.5813	7.1246	7.3056	7.3964	7.4085	7.5202	7.4027	7.5507	7.3967	7.5365	7.4137	7.5813	**7.22**
H6	8.0091	8.1941	8.2801	8.2570	8.3923	8.2524	8.4559	8.2476	8.4415	8.2613	8.4406	8.0091	8.1941	8.2801	8.2570	8.3923	8.2524	8.4559	8.2476	8.4415	8.2613	8.4406	**8.13**
H8	4.5979	4.6662	4.6965	4.6978	4.7701	4.6954	4.8178	4.6928	4.8038	4.6999	4.7959	4.5979	4.6662	4.6965	4.6978	4.7701	4.6954	4.8178	4.6928	4.8038	4.6999	4.7959	**5.5**
H(9A-9B)	1.6528	1.6966	1.6781	1.6882	1.7119	1.6868	1.7146	1.6853	1.7123	1.6895	1.7187	1.6528	1.6966	1.6781	1.6882	1.7119	1.6868	1.7146	1.6853	1.7123	1.6894	1.7187	**2.08**
H(10-13A-10-13B)	1.1634	1.1355	1.1013	1.1249	1.0761	1.1256	1.0792	1.1262	1.0798	1.1241	1.0761	1.1634	1.1355	1.1012	1.1249	1.0761	1.1256	1.0792	1.1262	1.0798	1.1241	1.0761	**1.25**
H(14A-14C)	0.9222	0.9177	0.8963	0.9192	0.8870	0.9193	0.8888	0.9192	0.8881	0.9190	0.8899	0.9222	0.9177	0.8963	0.9191	0.8870	0.9192	0.8888	0.9192	0.8881	0.9190	0.8900	**0.79**
H(1`A-1`B)	2.9360	2.9559	2.9627	2.9699	2.9748	2.9690	2.9825	2.9680	2.9811	2.9705	2.9660	2.8519	2.7754	2.7542	2.7578	2.7400	2.7588	2.7238	2.7598	2.7244	2.7568	2.7133	**3.69**
H(2`-3`A-2`-3`B)	1.6395	1.6971	1.6670	1.7420	1.6907	1.7395	1.7111	1.7367	1.7037	1.7443	1.7447	1.6395	1.6971	1.6670	1.7420	1.6907	1.7394	1.7111	1.7367	1.7037	1.7443	1.7447	**2.18**
H(4`A)	2.8705	2.7253	2.6920	2.7049	2.6985	2.7063	2.6585	2.7076	2.6567	2.7037	2.6715	3.1710	3.2128	3.2463	3.2573	3.3134	3.2546	3.3131	3.2518	3.3087	3.2596	3.3129	**3.12**
H(4`B)	2.8333	2.8255	2.8165	2.8106	2.7814	2.8114	2.7890	2.8120	2.7921	2.8098	2.7552	2.7011	2.6990	2.6790	2.6824	2.6363	2.6835	2.6518	2.6843	2.6535	2.6813	2.6192	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. III

Nuclei	R											S										Exp. [b]
	BHandH											BHandH										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	138.6392	139.2893	140.2741	139.4897	140.9812	139.4671	140.1446	139.4631	140.2254	139.4815	140.2996	138.6392	139.2892	140.2741	139.4897	140.2338	139.4672	140.1447	139.4631	140.2253	139.4815	140.2996	**131.79**
C2	143.6180	143.5853	144.1635	143.3967	143.9441	143.3976	144.4462	143.4166	144.3166	143.3660	144.4531	143.6180	143.5853	144.1635	143.3967	144.1408	143.3976	144.4462	143.4168	144.3166	143.3659	144.4531	**131.93**
C3	123.6791	124.4243	125.1207	124.6773	125.4049	124.6536	125.6146	124.6479	125.5729	124.6695	125.6917	123.6791	124.4242	125.1207	124.6773	125.4214	124.6537	125.6146	124.6479	125.5729	124.6693	125.6917	**116.53**
C4	174.8189	175.5463	176.2178	175.9829	176.5818	175.9460	177.2668	175.9274	177.1168	175.9878	177.4192	174.8190	175.5463	176.2178	175.9829	176.7270	175.9459	177.2667	175.9275	177.1168	175.9878	177.4192	**168.1**
C5	121.4880	122.8883	123.6214	123.6417	124.5170	123.5852	124.7004	123.5472	124.6068	123.6651	124.8658	121.4880	122.8883	123.6214	123.6417	124.3858	123.5851	124.7004	123.5472	124.6068	123.6651	124.8658	**116.51**
C6	139.7530	141.7171	142.7531	142.8378	144.4941	142.7554	145.1509	142.6914	144.9187	142.8863	145.6139	139.7530	141.7171	142.7531	142.8378	143.5819	142.7552	145.1510	142.6913	144.9187	142.8863	145.6139	**131.88**
C7	204.0200	208.5299	209.8118	211.0136	211.4334	210.8507	216.6692	210.7065	215.4841	211.1391	217.6266	204.0201	208.5300	209.8118	211.0136	211.7577	210.8508	216.6695	210.7068	215.4841	211.1388	217.6266	**195.2**
C8	60.0629	61.2181	61.7782	61.7237	62.4634	61.6795	63.1245	61.6541	62.9853	61.7361	63.5882	60.0629	61.2181	61.7782	61.7237	62.4678	61.6794	63.1245	61.6542	62.9853	61.7361	63.5882	**54.87**
C9	34.0304	33.8239	33.9730	33.6923	34.0343	33.6886	34.1544	33.7035	34.0820	33.6660	34.3061	34.0305	33.8240	33.9730	33.6923	34.4364	33.6886	34.1544	33.7035	34.0820	33.6661	34.3061	**31.13**
C10	25.2679	25.8006	26.1146	26.0254	26.7993	25.9980	26.5173	25.9890	26.5188	26.0215	26.7306	25.2679	25.8006	26.1146	26.0254	26.7695	25.9980	26.5173	25.9890	26.5188	26.0215	26.7306	**30.82**
C11	35.3003	35.3330	35.7168	35.2551	35.7623	35.2494	35.7712	35.2622	35.7494	35.2309	35.9759	35.3004	35.3329	35.7168	35.2551	35.9992	35.2493	35.7713	35.2622	35.7494	35.2310	35.9759	**29.11**
C12	37.3792	37.7038	38.0091	37.9152	38.4186	37.8914	38.2389	37.8858	38.2601	37.9077	38.3532	37.3791	37.7039	38.0091	37.9152	38.6593	37.8915	38.2389	37.8858	38.2601	37.9077	38.3532	**25.52**
C13	26.7117	26.9103	27.1369	26.9798	27.2221	26.9655	27.2254	26.9698	27.2194	26.9635	27.2471	26.7117	26.9104	27.1369	26.9798	27.7239	26.9656	27.2254	26.9698	27.2194	26.9634	27.2471	**22.36**
C14	15.7965	15.9832	16.0403	16.0871	16.1379	16.0698	16.1099	16.0708	16.1186	16.0737	16.1574	15.7965	15.9832	16.0403	16.0871	16.8312	16.0698	16.1100	16.0708	16.1186	16.0737	16.1574	**13.85**
C1`	48.3744	49.1967	49.4608	49.6885	50.1596	49.6499	50.2257	49.6302	50.1525	49.6953	50.6296	52.1935	53.2710	53.6481	53.7873	54.5314	53.7431	54.4348	53.7175	54.3940	53.7991	54.7570	**51.23**
C2`	21.5794	22.0519	22.3154	22.2316	22.6173	22.2086	22.7071	22.2043	22.7041	22.2235	22.6995	21.2208	21.4108	21.7851	21.5130	22.2571	21.4962	21.8977	21.4978	21.9033	21.4988	21.8255	**23.85**
C3`	21.2208	21.4108	21.7851	21.5130	22.0184	21.4962	21.8978	21.4978	21.9033	21.4987	21.8255	21.5794	22.0520	22.3154	22.2316	22.9757	22.2086	22.7071	22.2042	22.7041	22.2234	22.6995	**23.66**
C4`	52.1935	53.2710	53.6481	53.7873	54.2837	53.7431	54.4347	53.7176	54.3940	53.7990	54.7570	48.3744	49.1967	49.4608	49.6885	50.4326	49.6499	50.2257	49.6302	50.1525	49.6953	50.6296	**52.72**
H2	9.0235	8.9318	8.9487	8.8693	8.8865	8.8737	8.9047	8.8772	8.9024	8.8662	8.9029	9.0235	8.9318	8.9487	8.8693	8.7881	8.8737	8.9047	8.8772	8.9024	8.8662	8.9029	**8.13**
H3	7.4545	7.5964	7.6930	7.6419	7.7659	7.6405	7.7843	7.6383	7.7766	7.6442	7.7991	7.4545	7.5964	7.6930	7.6419	7.5607	7.6405	7.7843	7.6383	7.7766	7.6441	7.7991	**7.22**
H5	7.2781	7.4732	7.5675	7.5576	7.6925	7.5534	7.7041	7.5483	7.6934	7.5627	7.7271	7.2781	7.4732	7.5675	7.5576	7.4764	7.5534	7.7041	7.5483	7.6934	7.5627	7.7271	**7.22**
H6	8.1852	8.3700	8.4587	8.4675	8.6232	8.4616	8.6715	8.4549	8.6540	8.4741	8.7156	8.1852	8.3700	8.4587	8.4675	8.3863	8.4616	8.6715	8.4549	8.6540	8.4741	8.7156	**8.13**
H8	4.2740	4.3303	4.3803	4.3745	4.4715	4.3716	4.5023	4.3678	4.4886	4.3784	4.5298	4.2740	4.3303	4.3803	4.3745	4.2933	4.3716	4.5023	4.3678	4.4886	4.3784	4.5298	**5.5**
H(9A-9B)	1.7836	1.8237	1.7948	1.8463	1.8609	1.8451	1.8555	1.8432	1.8496	1.8485	1.8934	1.7836	1.8237	1.7948	1.8463	1.7651	1.8451	1.8555	1.8432	1.8496	1.8485	1.8934	**2.08**
H(10-13A-10-13B)	1.1768	1.1397	1.1063	1.1190	1.0697	1.1210	1.0701	1.1221	1.0702	1.1182	1.0666	1.1768	1.1397	1.1063	1.1190	1.0378	1.1210	1.0701	1.1221	1.0702	1.1182	1.0666	**1.25**
H(14A-14C)	0.9614	0.9531	0.9292	0.9453	0.9134	0.9466	0.9136	0.9469	0.9135	0.9450	0.9132	0.9614	0.9531	0.9292	0.9453	0.8640	0.9466	0.9136	0.9470	0.9135	0.9451	0.9132	**0.79**
H(1`A-1`B)	2.8481	2.8609	2.8597	2.8630	2.7618	2.8635	2.8669	2.8631	2.8659	2.8635	2.8610	2.8239	2.7243	2.6937	2.6794	2.6569	2.6829	2.6256	2.6855	2.6285	2.6772	2.6040	**3.69**
H(2`-3`A-2`-3`B)	1.6283	1.6812	1.6442	1.7104	1.6670	1.7091	1.6829	1.7069	1.6761	1.7127	1.7126	1.6283	1.6811	1.6442	1.7104	1.6292	1.7091	1.6829	1.7069	1.6761	1.7128	1.7126	**2.18**
H(4`A)	2.9163	2.7062	2.6663	2.6324	2.4855	2.6373	2.5520	2.6414	2.5551	2.6290	2.5375	3.0981	3.1297	3.1526	3.1513	3.2207	3.1501	3.1950	3.1483	3.1935	3.1534	3.2029	**3.12**
H(4`B)	2.7315	2.7424	2.7210	2.7264	2.5684	2.7284	2.6992	2.7296	2.7019	2.7255	2.6706	2.5982	2.5920	2.5668	2.5746	2.5276	2.5767	2.5387	2.5779	2.5383	2.5736	2.5191	**3.86**
Nuclei	BHandHLYP											BHandHLYP										
C1	139.1928	139.9013	140.7112	140.1569	142.5336	140.1385	141.5500	140.1233	141.7502	140.1750	142.0334	139.1929	139.9013	140.7111	140.1569	142.5334	140.1385	141.5501	140.1233	141.7502	140.1750	142.0331	**131.79**
C2	142.1655	142.1322	142.6342	141.9776	142.3637	141.9894	142.8794	142.0035	142.7529	141.9658	142.8286	142.1654	142.1322	142.6342	141.9776	142.3638	141.9896	142.8793	142.0035	142.7529	141.9658	142.8286	**131.93**
C3	122.5031	123.1334	123.7060	123.3234	124.0129	123.3150	124.2155	123.3087	124.1826	123.3306	124.2942	122.5030	123.1334	123.7061	123.3234	124.0130	123.3151	124.2155	123.3087	124.1826	123.3306	124.2943	**116.53**
C4	174.6361	175.2921	175.9223	175.6698	176.1555	175.6474	176.8358	175.6275	176.6732	175.6908	176.9422	174.6361	175.2922	175.9224	175.6698	176.1556	175.6475	176.8359	175.6274	176.6732	175.6907	176.9424	**168.1**
C5	120.2659	121.5074	122.1204	122.1537	122.9907	122.1148	123.1594	122.0783	123.0879	122.1906	123.3556	120.2659	121.5074	122.1204	122.1537	122.9907	122.1149	123.1594	122.0782	123.0879	122.1905	123.3556	**116.51**
C6	138.0345	139.8676	140.8657	141.0077	142.0466	140.9359	142.8027	140.8664	142.5355	141.0756	143.0370	138.0345	139.8675	140.8657	141.0077	142.0466	140.9358	142.8030	140.8664	142.5355	141.0756	143.0369	**131.88**
C7	202.1610	207.0232	208.2075	209.6662	210.9423	209.4976	216.5725	209.3331	215.3852	209.8275	217.9373	202.1614	207.0232	208.2072	209.6662	210.9423	209.4975	216.5725	209.3331	215.3852	209.8275	217.9374	**195.2**
C8	61.8693	62.8947	63.3940	63.3931	64.3258	63.3590	64.8884	63.3280	64.8140	63.4260	65.2323	61.8694	62.8947	63.3939	63.3931	64.3258	63.3591	64.8885	63.3281	64.8140	63.4260	65.2323	**54.87**
C9	34.0695	33.7412	33.8469	33.6151	33.7048	33.6229	33.6939	33.6332	33.7078	33.6073	33.7290	34.0694	33.7412	33.8469	33.6151	33.7048	33.6229	33.6939	33.6332	33.7078	33.6073	33.7290	**31.13**
C10	25.7789	26.2817	26.5863	26.5654	27.1335	26.5479	26.9323	26.5327	26.9407	26.5818	27.0472	25.7789	26.2817	26.5863	26.5654	27.1334	26.5478	26.9324	26.5327	26.9407	26.5818	27.0472	**30.82**
C11	35.1028	35.1280	35.5073	35.0932	35.5837	35.0978	35.5415	35.1046	35.5540	35.0881	35.7227	35.1029	35.1280	35.5073	35.0932	35.5838	35.0978	35.5414	35.1046	35.5540	35.0883	35.7227	**29.11**
C12	36.6734	36.9553	37.2405	37.1545	37.6318	37.1408	37.5146	37.1298	37.5133	37.1672	37.5952	36.6734	36.9553	37.2406	37.1545	37.6318	37.1409	37.5145	37.1298	37.5133	37.1672	37.5953	**25.52**
C13	27.8430	28.0148	28.2417	28.0882	28.3720	28.0846	28.3550	28.0833	28.3650	28.0912	28.3787	27.8430	28.0147	28.2418	28.0883	28.3721	28.0847	28.3550	28.0833	28.3650	28.0912	28.3788	**22.36**
C14	16.6334	16.7928	16.8568	16.9023	16.9934	16.8951	16.9712	16.8905	16.9770	16.9088	17.0098	16.6335	16.7928	16.8568	16.9023	16.9934	16.8952	16.9712	16.8905	16.9770	16.9088	17.0097	**13.85**
C1`	49.2159	49.9659	50.2127	50.4295	50.9631	50.3993	50.8971	50.3717	50.8545	50.4581	51.3450	53.3066	54.2167	54.6159	54.7419	55.1964	54.7107	55.3844	54.6815	55.3087	54.7711	55.6956	**51.23**
C2`	24.3806	24.7355	25.0468	24.9061	25.3240	24.8946	25.3705	24.8857	25.3842	24.9169	25.2014	23.9773	24.1581	24.5203	24.2206	24.8261	24.2173	24.6874	24.2165	24.7090	24.2235	24.4923	**23.85**
C3`	23.9774	24.1581	24.5203	24.2206	24.8261	24.2173	24.6874	24.2166	24.7090	24.2236	24.4923	24.3806	24.7355	25.0468	24.9061	25.3240	24.8947	25.3706	24.8856	25.3842	24.9169	25.2015	**23.66**
C4`	53.3066	54.2167	54.6158	54.7419	55.1963	54.7106	55.3845	54.6815	55.3087	54.7711	55.6956	49.2157	49.9659	50.2128	50.4295	50.9630	50.3992	50.8971	50.3717	50.8545	50.4582	51.3450	**52.72**
H2	8.9169	8.8163	8.8513	8.7600	8.6681	8.7642	8.7158	8.7683	8.7024	8.7557	8.6792	8.9169	8.8163	8.8513	8.7600	8.6681	8.7642	8.7158	8.7683	8.7024	8.7557	8.6792	**8.13**
H3	7.4454	7.5769	7.6704	7.6188	7.7282	7.6170	7.7465	7.6150	7.7375	7.6205	7.7606	7.4454	7.5769	7.6704	7.6188	7.7282	7.6170	7.7465	7.6150	7.7375	7.6205	7.7606	**7.22**
H5	7.2614	7.4455	7.5353	7.5273	7.6449	7.5229	7.6690	7.5182	7.6563	7.5315	7.6944	7.2614	7.4455	7.5353	7.5273	7.6449	7.5229	7.6690	7.5182	7.6563	7.5315	7.6944	**7.22**
H6	8.0527	8.2502	8.3488	8.3665	8.4936	8.3595	8.5791	8.3524	8.5490	8.3730	8.5954	8.0527	8.2502	8.3488	8.3665	8.4936	8.3595	8.5791	8.3524	8.5490	8.3730	8.5953	**8.13**
H8	4.2074	4.2966	4.3546	4.3558	4.4558	4.3521	4.5242	4.3483	4.4984	4.3594	4.5145	4.2074	4.2966	4.3546	4.3558	4.4557	4.3521	4.5242	4.3483	4.4984	4.3594	4.5144	**5.5**
H(9A-9B)	1.5691	1.6158	1.5988	1.6579	1.6068	1.6553	1.6070	1.6526	1.6026	1.6603	1.6274	1.5690	1.6158	1.5988	1.6579	1.6068	1.6553	1.6070	1.6526	1.6026	1.6603	1.6274	**2.08**
H(10-13A-10-13B)	1.1338	1.0990	1.0700	1.0854	1.0310	1.0864	1.0413	1.0873	1.0384	1.0843	1.0380	1.1338	1.0990	1.0700	1.0854	1.0309	1.0864	1.0413	1.0873	1.0384	1.0844	1.0380	**1.25**
H(14A-14C)	0.9551	0.9463	0.9245	0.9431	0.9122	0.9435	0.9176	0.9438	0.9158	0.9427	0.9177	0.9551	0.9463	0.9245	0.9431	0.9122	0.9435	0.9176	0.9438	0.9158	0.9427	0.9177	**0.79**
H(1`A-1`B)	2.8160	2.8373	2.8425	2.8531	2.8538	2.8523	2.8652	2.8514	2.8617	2.8538	2.8554	2.7349	2.6598	2.6184	2.6252	2.6227	2.6270	2.5982	2.6287	2.6043	2.6236	2.5875	**3.69**
H(2`-3`A-2`-3`B)	1.5840	1.6433	1.6048	1.6804	1.6404	1.6781	1.6638	1.6757	1.6557	1.6825	1.6923	1.5840	1.6433	1.6049	1.6804	1.6404	1.6781	1.6638	1.6758	1.6557	1.6825	1.6923	**2.18**
H(4`A)	2.7250	2.5834	2.5238	2.5377	2.5616	2.5398	2.5008	2.5420	2.5061	2.5358	2.5122	3.0171	3.0646	3.0971	3.1088	3.1630	3.1060	3.1649	3.1031	3.1581	3.1115	3.1696	**3.12**
H(4`B)	2.7449	2.7361	2.7129	2.7127	2.6836	2.7141	2.6956	2.7155	2.7024	2.7113	2.6629	2.6148	2.6099	2.5879	2.5974	2.5446	2.5986	2.5654	2.5997	2.5652	2.5961	2.5411	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. IV

Nuclei	R											S										Exp. [b]
	BLYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.6091	141.0335	141.7561	141.9121	143.2565	142.1359	142.2988	141.8987	142.5049	142.3276	142.9824	139.6091	141.0335	141.7561	141.9119	143.2565	142.1360	142.2988	141.8987	142.5050	142.3277	142.9824	**131.79**
C2	137.4832	137.5151	138.0115	137.2567	137.9429	137.5560	138.1711	137.3924	138.2743	137.5982	138.2031	137.4832	137.5151	138.0116	137.2567	137.9429	137.5561	138.1711	137.3924	138.2743	137.5982	138.2031	**131.93**
C3	120.8887	121.5245	122.0251	121.7467	122.3655	122.0116	122.5178	121.8149	122.6425	122.1226	122.6245	120.8887	121.5245	122.0252	121.7468	122.3655	122.0116	122.5178	121.8149	122.6425	122.1227	122.6245	**116.53**
C4	178.0063	178.8497	179.5600	179.1766	180.0903	179.4342	180.4946	179.2298	180.5444	179.5594	180.6774	178.0063	178.8497	179.5600	179.1767	180.0903	179.4341	180.4946	179.2298	180.5443	179.5594	180.6774	**168.1**
C5	118.7005	119.9642	120.4428	120.6576	121.3347	120.8935	121.4722	120.6674	121.5448	121.0607	121.7331	118.7005	119.9642	120.4429	120.6577	121.3347	120.8936	121.4722	120.6674	121.5448	121.0607	121.7331	**116.51**
C6	133.4320	135.1829	136.2363	136.1198	137.8295	136.3391	138.3709	136.0964	138.3047	136.5383	138.7340	133.4320	135.1829	136.2363	136.1198	137.8295	136.3392	138.3709	136.0964	138.3048	136.5384	138.7340	**131.88**
C7	203.9340	209.0041	210.2638	212.0040	212.6151	212.0927	216.8718	211.7208	216.0190	212.5486	218.4142	203.9340	209.0041	210.2637	212.0038	212.6151	212.0927	216.8718	211.7208	216.0191	212.5486	218.4142	**195.2**
C8	70.4214	71.7823	72.6560	72.5572	73.5816	72.7895	74.0549	72.5589	74.0361	72.9627	74.5550	70.4214	71.7823	72.6560	72.5572	73.5816	72.7895	74.0549	72.5589	74.0361	72.9628	74.5550	**54.87**
C9	39.9894	39.6157	39.7225	39.3191	39.7714	39.6231	39.9218	39.4633	39.9995	39.6560	39.9992	39.9894	39.6157	39.7224	39.3192	39.7714	39.6231	39.9218	39.4633	39.9994	39.6561	39.9992	**31.13**
C10	29.3739	29.8045	30.2251	29.9824	30.8272	30.2497	30.4966	30.0547	30.6746	30.3554	30.6518	29.3739	29.8045	30.2252	29.9824	30.8272	30.2497	30.4966	30.0547	30.6744	30.3554	30.6518	**30.82**
C11	39.0906	39.1884	39.4835	39.0427	39.7098	39.3344	39.4960	39.1632	39.6675	39.3920	39.7470	39.0906	39.1884	39.4836	39.0427	39.7098	39.3344	39.4960	39.1632	39.6675	39.3921	39.7470	**29.11**
C12	40.7888	41.0421	41.3481	41.2352	41.8084	41.4982	41.5172	41.3000	41.7029	41.6132	41.6686	40.7888	41.0421	41.3481	41.2352	41.8084	41.4982	41.5172	41.3000	41.7029	41.6131	41.6686	**25.52**
C13	31.8876	32.0852	32.2413	32.0972	32.4670	32.3764	32.2796	32.1932	32.4563	32.4590	32.3559	31.8876	32.0852	32.2413	32.0971	32.4670	32.3764	32.2796	32.1932	32.4562	32.4590	32.3559	**22.36**
C14	17.1634	17.3215	17.3350	17.3944	17.5443	17.6674	17.3535	17.4786	17.5317	17.7624	17.4539	17.1634	17.3215	17.3350	17.3944	17.5443	17.6674	17.3535	17.4786	17.5317	17.7624	17.4539	**13.85**
C1`	55.4135	56.1867	56.4431	56.7162	57.3333	56.9548	57.1063	56.7327	57.2310	57.1181	57.7471	60.0607	61.0163	61.3737	61.5481	62.1017	61.7899	62.1836	61.5703	62.2851	61.9459	62.6051	**51.23**
C2`	27.6364	28.1277	28.4947	28.3520	28.9347	28.6180	28.8639	28.4212	29.0152	28.7256	28.8135	27.5355	27.9777	28.2496	28.1832	28.7414	28.4485	28.4046	28.2520	28.5877	28.5588	28.3062	**23.85**
C3`	27.5355	27.9777	28.2496	28.1833	28.7414	28.4484	28.4046	28.2520	28.5877	28.5588	28.3062	27.6364	28.1277	28.4947	28.3519	28.9347	28.6180	28.8639	28.4212	29.0151	28.7256	28.8135	**23.66**
C4`	60.0607	61.0163	61.3738	61.5481	62.1017	61.7900	62.1836	61.5703	62.2851	61.9459	62.6051	55.4135	56.1867	56.4430	56.7162	57.3333	56.9547	57.1063	56.7327	57.2310	57.1181	57.7471	**52.72**
H2	8.4456	8.2914	8.3204	8.1864	8.2206	8.2400	8.4282	8.2011	8.2664	8.2357	8.4076	8.4456	8.2914	8.3204	8.1864	8.2206	8.2400	8.4282	8.2011	8.2664	8.2357	8.4076	**8.13**
H3	7.1848	7.2868	7.3787	7.3104	7.4359	7.3565	7.6219	7.3101	7.4480	7.3669	7.6461	7.1848	7.2868	7.3787	7.3104	7.4359	7.3565	7.6219	7.3101	7.4480	7.3669	7.6461	**7.22**
H5	6.9698	7.1544	7.2318	7.2558	7.3528	7.2970	7.5455	7.2457	7.3669	7.3170	7.5897	6.9698	7.1544	7.2318	7.2558	7.3528	7.2970	7.5455	7.2457	7.3669	7.3170	7.5897	**7.22**
H6	7.8379	8.0181	8.0910	8.1049	8.2229	8.1467	8.4574	8.0960	8.2779	8.1655	8.4752	7.8379	8.0181	8.0910	8.1049	8.2229	8.1467	8.4574	8.0960	8.2780	8.1655	8.4752	**8.13**
H8	4.9516	5.0023	5.0038	5.0252	5.0838	5.0711	5.2730	5.0244	5.0984	5.0821	5.2650	4.9516	5.0023	5.0038	5.0252	5.0838	5.0711	5.2730	5.0244	5.0984	5.0821	5.2650	**5.5**
H(9A-9B)	1.7580	1.7881	1.8062	1.7951	1.8478	1.8423	2.0274	1.7968	1.8524	1.8505	2.0566	1.7580	1.7881	1.8062	1.7951	1.8478	1.8423	2.0274	1.7968	1.8524	1.8505	2.0566	**2.08**
H(10-13A-10-13B)	1.2656	1.2387	1.1992	1.2249	1.1809	1.2730	1.3503	1.2286	1.1843	1.2796	1.3600	1.2656	1.2387	1.1992	1.2249	1.1809	1.2730	1.3503	1.2286	1.1843	1.2796	1.3600	**1.25**
H(14A-14C)	0.9625	0.9589	0.9331	0.9551	0.9275	1.0026	1.0965	0.9577	0.9296	1.0102	1.1087	0.9625	0.9589	0.9331	0.9551	0.9275	1.0026	1.0965	0.9577	0.9296	1.0101	1.1087	**0.79**
H(1`A-1`B)	3.1104	3.1271	3.1263	2.3128	3.1437	3.1822	3.3157	3.1366	3.1482	3.1907	3.3052	3.0069	2.9281	2.8991	2.0849	2.8873	2.9478	3.0387	2.9045	2.8714	2.9522	3.0365	**3.69**
H(2`-3`A-2`-3`B)	1.7292	1.7891	1.7535	1.8305	1.7840	1.8750	1.9690	1.8270	1.7970	1.8887	2.0143	1.7292	1.7891	1.7535	1.8305	1.7840	1.8750	1.9690	1.8270	1.7969	1.8887	2.0143	**2.18**
H(4`A)	3.0390	2.8875	2.8420	1.9974	2.8478	2.8981	2.9765	2.8552	2.8077	2.9021	2.9941	3.3579	3.3936	3.4186	2.5685	3.4891	3.4714	3.6522	3.4239	3.4821	3.4840	3.6582	**3.12**
H(4`B)	2.9749	2.9687	2.9562	2.1724	2.9267	2.9975	3.1009	2.9538	2.9350	3.0023	3.0790	2.8630	2.8607	2.8340	2.0571	2.7983	2.8930	2.9792	2.8494	2.8143	2.8976	2.9523	**3.86**
Nuclei	BMK																						
C1	154.7628	155.2412	156.0996	155.3902	156.9601	155.3645	156.0463	155.5496	156.1381	155.5766	156.6176	154.7626	155.2412	156.0996	155.3902	156.9601	155.3645	156.0463	155.5496	156.1381	155.5766	156.6176	**131.79**
C2	155.5428	155.2676	156.0638	154.9460	155.8212	154.9531	156.2002	155.1715	155.9140	155.1005	156.0044	155.5429	155.2675	156.0638	154.9460	155.8211	154.9531	156.2002	155.1715	155.9140	155.1005	156.0044	**131.93**
C3	136.1040	136.7626	137.6088	136.9946	138.0368	136.9656	138.3072	137.1477	138.0906	137.1833	137.9967	136.1038	136.7626	137.6088	136.9946	138.0368	136.9656	138.3072	137.1477	138.0906	137.1833	137.9967	**116.53**
C4	189.6047	190.2567	191.1020	190.6045	191.5969	190.5666	192.2410	190.7401	191.9495	190.8020	192.1636	189.6047	190.2566	191.1020	190.6045	191.5969	190.5666	192.2410	190.7401	191.9495	190.8020	192.1636	**168.1**
C5	133.4992	134.8983	135.6581	135.5731	136.6946	135.5164	136.8485	135.6709	136.6624	135.7886	136.9968	133.4994	134.8984	135.6581	135.5731	136.6946	135.5164	136.8485	135.6709	136.6624	135.7886	136.9968	**116.51**
C6	151.2388	153.0000	154.4171	154.2320	156.3033	154.1351	157.1478	154.2499	156.7099	154.4862	157.3021	151.2388	153.0001	154.4171	154.2320	156.3033	154.1351	157.1478	154.2499	156.7099	154.4862	157.3021	**131.88**
C7	218.2850	223.3781	224.3719	225.7748	226.1446	225.6024	232.0422	225.6438	230.7884	226.1019	233.8295	218.2853	223.3782	224.3719	225.7748	226.1446	225.6024	232.0422	225.6438	230.7884	226.1019	233.8295	**195.2**
C8	71.5254	73.0646	73.7488	73.7882	74.5456	73.7314	75.0997	73.8843	74.9236	74.0031	75.9921	71.5255	73.0647	73.7488	73.7882	74.5456	73.7314	75.0997	73.8843	74.9236	74.0031	75.9921	**54.87**
C9	39.0583	38.5435	38.7160	38.4136	38.9774	38.3944	39.1237	38.5878	39.0209	38.5948	39.4503	39.0583	38.5435	38.7160	38.4136	38.9774	38.3944	39.1237	38.5878	39.0209	38.5948	39.4503	**31.13**
C10	29.8532	30.1614	30.6113	30.3391	31.1543	30.3102	30.9005	30.4934	30.8267	30.5287	31.1104	29.8531	30.1614	30.6113	30.3391	31.1543	30.3102	30.9005	30.4934	30.8267	30.5288	31.1104	**30.82**
C11	39.0401	38.8641	39.3512	38.7731	39.5219	38.7637	39.4356	38.9647	39.3321	38.9428	39.5711	39.0401	38.8641	39.3512	38.7731	39.5219	38.7637	39.4356	38.9647	39.3321	38.9428	39.5711	**29.11**
C12	40.5806	40.8146	41.1751	40.9192	41.5867	40.8958	41.4176	41.0844	41.3188	41.1039	41.4364	40.5806	40.8145	41.1751	40.9192	41.5867	40.8957	41.4176	41.0844	41.3188	41.1039	41.4364	**25.52**
C13	30.9662	30.9782	31.2725	30.9590	31.4386	30.9450	31.3720	31.1418	31.2660	31.1337	31.3274	30.9663	30.9781	31.2725	30.9590	31.4386	30.9450	31.3720	31.1418	31.2660	31.1337	31.3274	**22.36**
C14	18.1325	18.1907	18.3060	18.2125	18.4520	18.1948	18.3887	18.3886	18.2933	18.3910	18.3836	18.1326	18.1907	18.3060	18.2125	18.4520	18.1948	18.3887	18.3886	18.2933	18.3910	18.3836	**13.85**
C1`	56.0789	56.7213	57.1191	57.0131	57.7800	56.9681	57.7027	57.1364	57.5327	57.2189	58.1918	60.5395	61.2398	61.7055	61.7555	62.3818	61.7207	62.5565	61.8939	62.3835	61.9472	62.6855	**51.23**
C2`	27.6957	28.1224	28.5016	28.4741	28.9656	28.4478	29.0152	28.6303	28.9166	28.6590	28.8898	27.1638	27.4561	27.9129	27.4105	28.0595	27.3771	27.9144	27.5598	27.8149	27.6075	27.8138	**23.85**
C3`	27.1639	27.4561	27.9129	27.4105	28.0595	27.3772	27.9144	27.5598	27.8149	27.6075	27.8138	27.6957	28.1223	28.5016	28.4741	28.9656	28.4479	29.0152	28.6303	28.9166	28.6590	28.8898	**23.66**
C4`	60.5394	61.2398	61.7055	61.7555	62.3818	61.7208	62.5565	61.8939	62.3835	61.9472	62.6855	56.0789	56.7212	57.1191	57.0131	57.7800	56.9681	57.7027	57.1364	57.5327	57.2189	58.1918	**52.72**
H2	9.1102	9.0152	9.0684	8.9549	8.9937	8.9556	9.0335	8.9562	9.0149	8.9448	8.9938	9.1102	9.0152	9.0684	8.9549	8.9937	8.9556	9.0335	8.9562	9.0149	8.9448	8.9938	**8.13**
H3	7.6269	7.7553	7.8601	7.8066	7.9398	7.8004	7.9774	7.7942	7.9619	7.8028	7.9586	7.6269	7.7553	7.8601	7.8066	7.9398	7.8004	7.9774	7.7942	7.9619	7.8028	7.9586	**7.22**
H5	7.4667	7.6906	7.7673	7.7866	7.9072	7.7775	7.9149	7.7684	7.9114	7.7857	7.9491	7.4667	7.6906	7.7673	7.7866	7.9072	7.7775	7.9149	7.7684	7.9114	7.7857	7.9491	**7.22**
H6	8.4055	8.5834	8.6734	8.6816	8.8134	8.6717	8.8515	8.6619	8.8335	8.6816	8.8621	8.4055	8.5834	8.6734	8.6816	8.8134	8.6717	8.8515	8.6619	8.8335	8.6816	8.8621	**8.13**
H8	4.4030	4.5004	4.5470	4.5709	4.6335	4.5626	4.6807	4.5544	4.6540	4.5694	4.6530	4.4030	4.5004	4.5470	4.5709	4.6335	4.5626	4.6807	4.5544	4.6540	4.5694	4.6530	**5.5**
H(9A-9B)	1.6844	1.6634	1.6400	1.6806	1.6983	1.6742	1.7132	1.6683	1.7132	1.6774	1.7764	1.6844	1.6634	1.6400	1.6806	1.6983	1.6742	1.7132	1.6683	1.7132	1.6774	1.7764	**2.08**
H(10-13A-10-13B)	1.1481	1.0926	1.0609	1.0673	1.0235	1.0653	1.0356	1.0635	1.0326	1.0598	1.0172	1.1481	1.0926	1.0609	1.0673	1.0235	1.0653	1.0356	1.0635	1.0326	1.0598	1.0172	**1.25**
H(14A-14C)	0.8768	0.8661	0.8384	0.8623	0.8259	0.8593	0.8301	0.8564	0.8306	0.8556	0.8270	0.8768	0.8661	0.8384	0.8623	0.8259	0.8593	0.8301	0.8564	0.8306	0.8556	0.8270	**0.79**
H(1`A-1`B)	2.8503	2.8506	2.8407	2.8621	2.8651	2.8586	2.8651	2.8553	2.8656	2.8558	2.8427	2.7257	2.6876	2.6498	2.6763	2.6386	2.6740	2.6140	2.6718	2.6239	2.6688	2.6217	**3.69**
H(2`-3`A-2`-3`B)	1.5999	1.6718	1.6311	1.7185	1.6599	1.7123	1.6787	1.7061	1.6729	1.7149	1.7022	1.5999	1.6718	1.6311	1.7185	1.6599	1.7123	1.6787	1.7061	1.6729	1.7149	1.7022	**2.18**
H(4`A)	2.7131	2.6174	2.5636	2.5803	2.5590	2.5780	2.4966	2.5760	2.5060	2.5732	2.5201	3.0782	3.0691	3.0810	3.0966	3.1568	3.0921	3.1516	3.0876	3.1519	3.0914	3.1518	**3.12**
H(4`B)	2.7382	2.7578	2.7360	2.7722	2.7183	2.7701	2.7315	2.7676	2.7419	2.7644	2.7233	2.6225	2.6323	2.6003	2.6275	2.5734	2.6252	2.5786	2.6229	2.5793	2.6201	2.5336	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. V

Nuclei	R											S										Exp. [b]
	BP86											BP86										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.2321	137.2238	138.5261	137.6112	139.7629	137.5839	139.1691	137.5547	139.1902	137.6362	139.9830	136.2321	137.2238	138.5261	137.6112	139.7629	137.5839	139.1691	137.5547	139.1902	137.6361	139.9830	**131.79**
C2	136.0759	136.2532	136.7936	136.0369	136.5963	136.0629	137.0057	136.0828	136.9087	136.0065	137.1473	136.0759	136.2532	136.7936	136.0369	136.5963	136.0629	137.0057	136.0828	136.9087	136.0065	137.1473	**131.93**
C3	119.7505	120.6437	121.1724	120.8387	121.4424	120.8397	121.7912	120.8345	121.7083	120.8321	121.9703	119.7505	120.6437	121.1724	120.8387	121.4424	120.8397	121.7912	120.8345	121.7083	120.8321	121.9703	**116.53**
C4	174.5949	175.6154	176.2724	175.9947	176.6773	175.9818	177.2618	175.9629	177.1174	176.0015	177.5116	174.5949	175.6154	176.2724	175.9947	176.6773	175.9818	177.2618	175.9629	177.1174	176.0016	177.5116	**168.1**
C5	117.6308	119.0620	119.6482	119.6918	120.4940	119.6617	120.8350	119.6265	120.7092	119.7149	121.1578	117.6308	119.0620	119.6482	119.6918	120.4940	119.6617	120.8350	119.6265	120.7092	119.7151	121.1578	**116.51**
C6	132.0306	133.9623	134.8751	135.0256	136.4005	134.9656	137.0480	134.9008	136.8091	135.0775	137.4945	132.0306	133.9623	134.8751	135.0256	136.4006	134.9657	137.0480	134.9008	136.8091	135.0775	137.4945	**131.88**
C7	201.0410	205.3927	207.1230	207.7232	209.1847	207.5692	213.4787	207.4148	212.5240	207.8707	215.0883	201.0410	205.3927	207.1230	207.7232	209.1848	207.5692	213.4787	207.4148	212.5240	207.8707	215.0883	**195.2**
C8	68.1305	69.4688	70.2907	70.0812	71.0895	70.0403	71.8284	69.9974	71.6594	70.1194	72.4573	68.1305	69.4688	70.2907	70.0812	71.0896	70.0403	71.8284	69.9974	71.6594	70.1193	72.4573	**54.87**
C9	38.7037	38.5672	38.5201	38.4359	38.5330	38.4509	38.7492	38.4612	38.6584	38.4175	38.9866	38.7037	38.5672	38.5201	38.4359	38.5330	38.4509	38.7492	38.4612	38.6584	38.4176	38.9865	**31.13**
C10	27.9341	28.6185	28.8128	28.8373	29.3631	28.8311	29.1514	28.8198	29.1502	28.8386	29.4369	27.9341	28.6185	28.8128	28.8373	29.3631	28.8311	29.1514	28.8198	29.1502	28.8386	29.4369	**30.82**
C11	37.4166	37.5974	37.8544	37.4777	37.9244	37.4955	37.8867	37.5078	37.8582	37.4557	38.2358	37.4166	37.5974	37.8544	37.4777	37.9244	37.4955	37.8867	37.5078	37.8582	37.4556	38.2358	**29.11**
C12	39.0440	39.4512	39.6429	39.5778	39.9851	39.5768	39.8589	39.5707	39.8611	39.5739	40.0887	39.0440	39.4512	39.6429	39.5778	39.9851	39.5768	39.8589	39.5707	39.8611	39.5741	40.0887	**25.52**
C13	30.0622	30.3534	30.4831	30.3425	30.5556	30.3523	30.5470	30.3568	30.5325	30.3280	30.6960	30.0622	30.3534	30.4831	30.3425	30.5556	30.3523	30.5470	30.3568	30.5325	30.3280	30.6960	**22.36**
C14	16.6708	16.9480	16.8978	16.9780	16.9739	16.9838	16.9551	16.9846	16.9416	16.9678	17.1358	16.6708	16.9480	16.8978	16.9780	16.9739	16.9838	16.9552	16.9846	16.9416	16.9677	17.1357	**13.85**
C1`	53.8804	54.7724	54.9840	55.1753	55.7000	55.1572	55.6437	55.1342	55.5702	55.1877	56.3637	58.2661	59.4131	59.8086	59.9303	60.3455	59.9034	60.6832	59.8719	60.5898	59.9517	61.1879	**51.23**
C2`	26.1253	26.7421	26.9843	26.9475	27.2797	26.9396	27.3959	26.9275	27.3649	26.9511	27.4087	25.9219	26.4540	26.7334	26.5213	27.0486	26.5309	26.9363	26.5337	26.9285	26.5056	26.8449	**23.85**
C3`	25.9219	26.4540	26.7334	26.5213	27.0486	26.5309	26.9363	26.5337	26.9285	26.5056	26.8449	26.1253	26.7421	26.9843	26.9475	27.2797	26.9396	27.3959	26.9275	27.3649	26.9511	27.4087	**23.66**
C4`	58.2661	59.4131	59.8086	59.9303	60.3455	59.9033	60.6832	59.8719	60.5898	59.9517	61.1879	53.8804	54.7724	54.9840	55.1753	55.7000	55.1572	55.6437	55.1342	55.5702	55.1876	56.3637	**52.72**
H2	8.5234	8.4310	8.3850	8.3614	8.2790	8.3684	8.3139	8.3746	8.3150	8.3538	8.2872	8.5234	8.4310	8.3850	8.3614	8.2790	8.3684	8.3139	8.3746	8.3150	8.3538	8.2872	**8.13**
H3	7.1939	7.3249	7.3954	7.3623	7.4581	7.3616	7.4744	7.3605	7.4658	7.3625	7.5038	7.1939	7.3249	7.3954	7.3623	7.4581	7.3616	7.4744	7.3605	7.4658	7.3625	7.5038	**7.22**
H5	6.9895	7.1742	7.2496	7.2535	7.3697	7.2498	7.3979	7.2458	7.3849	7.2566	7.4369	6.9895	7.1742	7.2496	7.2535	7.3697	7.2498	7.3979	7.2458	7.3849	7.2566	7.4369	**7.22**
H6	7.9040	8.0756	8.1488	8.1731	8.2748	8.1683	8.3473	8.1629	8.3318	8.1771	8.3542	7.9040	8.0756	8.1488	8.1731	8.2748	8.1683	8.3473	8.1629	8.3318	8.1771	8.3542	**8.13**
H8	4.9624	5.0171	5.0267	5.0431	5.0997	5.0428	5.1307	5.0419	5.1199	5.0429	5.1193	4.9624	5.0171	5.0267	5.0431	5.0997	5.0428	5.1307	5.0419	5.1199	5.0429	5.1193	**5.5**
H(9A-9B)	1.8498	1.8952	1.8585	1.9364	1.9050	1.9340	1.9001	1.9315	1.8954	1.9385	1.9359	1.8498	1.8952	1.8585	1.9364	1.9050	1.9340	1.9001	1.9315	1.8954	1.9385	1.9359	**2.08**
H(10-13A-10-13B)	1.2593	1.2328	1.1896	1.2179	1.1644	1.2197	1.1661	1.2211	1.1657	1.2158	1.1754	1.2593	1.2328	1.1896	1.2179	1.1644	1.2197	1.1661	1.2211	1.1657	1.2158	1.1754	**1.25**
H(14A-14C)	0.9338	0.9320	0.9007	0.9273	0.8909	0.9284	0.8922	0.9293	0.8906	0.9258	0.9057	0.9338	0.9320	0.9007	0.9273	0.8909	0.9284	0.8922	0.9293	0.8906	0.9258	0.9057	**0.79**
H(1`A-1`B)	3.0868	3.0996	3.0959	3.1109	3.1092	3.1108	3.1133	3.1104	3.1121	3.1106	3.1074	3.0181	2.9246	2.8881	2.8864	2.8724	2.8890	2.8459	2.8914	2.8467	2.8838	2.8427	**3.69**
H(2`-3`A-2`-3`B)	1.7268	1.7828	1.7426	1.8139	1.7685	1.8126	1.7871	1.8111	1.7803	1.8148	1.8363	1.7268	1.7828	1.7426	1.8139	1.7685	1.8126	1.7871	1.8111	1.7803	1.8148	1.8363	**2.18**
H(4`A)	3.1049	2.9263	2.8699	2.8634	2.8681	2.8674	2.8045	2.8713	2.8037	2.8594	2.8197	3.3627	3.3857	3.4107	3.4248	3.4747	3.4225	3.4707	3.4200	3.4672	3.4267	3.4818	**3.12**
H(4`B)	2.9314	2.9230	2.9064	2.9095	2.8766	2.9106	2.8874	2.9116	2.8896	2.9082	2.8657	2.8110	2.8136	2.7811	2.7970	2.7436	2.7991	2.7560	2.8009	2.7569	2.7945	2.7329	**3.86**
Nuclei	CAM-B3LYP											CAM-B3LYP											
C1	140.9282	141.7944	143.3001	142.1583	144.6701	142.1313	143.8095	142.1077	143.9213	142.1899	144.4637	140.9282	141.7945	143.3003	142.1581	144.6702	142.1313	143.8094	142.1078	143.9212	142.1899	144.4638	**131.79**
C2	142.5117	142.5240	142.9418	142.3130	142.7791	142.3309	143.2584	142.3486	143.1407	142.2974	143.2194	142.5118	142.5240	142.9418	142.3129	142.7791	142.3310	143.2586	142.3486	143.1407	142.2974	143.2196	**131.93**
C3	123.8388	124.5284	125.1568	124.7622	125.4532	124.7589	125.6886	124.7556	125.6266	124.7671	125.7737	123.8389	124.5285	125.1567	124.7622	125.4534	124.7589	125.6886	124.7555	125.6265	124.7671	125.7737	**116.53**
C4	177.7941	178.5081	179.0686	178.8493	179.4281	178.8318	180.0541	178.8147	179.8952	178.8674	180.1392	177.7941	178.5081	179.0686	178.8493	179.4280	178.8319	180.0541	178.8147	179.8952	178.8673	180.1392	**168.1**
C5	121.7724	123.0645	123.6934	123.7054	124.5767	123.6695	124.7831	123.6344	124.6811	123.7417	124.9750	121.7724	123.0645	123.6933	123.7054	124.5767	123.6697	124.7832	123.6344	124.6812	123.7417	124.9749	**116.51**
C6	138.4383	140.3040	141.0010	141.3652	142.5633	141.3000	143.2030	141.2348	142.9652	141.4289	143.4117	138.4382	140.3040	141.0010	141.3652	142.5633	141.3001	143.2029	141.2348	142.9652	141.4289	143.4115	**131.88**
C7	206.1039	211.0612	212.9813	213.7932	215.2696	213.6136	220.6786	213.4387	219.5080	213.9711	222.2280	206.1036	211.0612	212.9810	213.7932	215.2692	213.6135	220.6787	213.4390	219.5080	213.9711	222.2276	**195.2**
C8	64.6013	65.7447	66.5120	66.3294	67.3255	66.2911	67.9295	66.2548	67.8194	66.3699	68.3706	64.6013	65.7446	66.5120	66.3295	67.3255	66.2911	67.9295	66.2548	67.8194	66.3699	68.3705	**54.87**
C9	35.3318	35.0465	34.9613	34.8735	34.9924	34.8858	35.0267	34.8985	35.0119	34.8635	35.0542	35.3318	35.0465	34.9613	34.8734	34.9924	34.8858	35.0267	34.8986	35.0120	34.8635	35.0541	**31.13**
C10	26.5810	27.1352	27.3679	27.3952	27.9953	27.3836	27.7848	27.3724	27.7788	27.4086	27.8989	26.5810	27.1352	27.3679	27.3952	27.9953	27.3836	27.7848	27.3723	27.7787	27.4086	27.8991	**30.82**
C11	36.1354	36.2004	36.5146	36.1549	36.6627	36.1648	36.6332	36.1750	36.6106	36.1473	36.8146	36.1355	36.2005	36.5145	36.1549	36.6627	36.1648	36.6333	36.1749	36.6106	36.1473	36.8145	**29.11**
C12	37.8378	38.1619	38.4092	38.3354	38.8460	38.3268	38.7204	38.3188	38.7131	38.3459	38.8078	37.8378	38.1619	38.4091	38.3354	38.8461	38.3268	38.7205	38.3188	38.7132	38.3459	38.8078	**25.52**
C13	28.4937	28.7030	28.8782	28.7557	29.0518	28.7573	29.0403	28.7592	29.0286	28.7561	29.0559	28.4937	28.7030	28.8781	28.7556	29.0518	28.7573	29.0403	28.7592	29.0286	28.7561	29.0559	**22.36**
C14	16.4442	16.6417	16.6533	16.7294	16.8275	16.7270	16.8087	16.7253	16.7971	16.7339	16.8441	16.4444	16.6417	16.6533	16.7294	16.8276	16.7270	16.8087	16.7252	16.7970	16.7339	16.8441	**13.85**
C1`	51.0019	51.8246	51.9724	52.2129	52.8555	52.1850	52.7762	52.1578	52.7042	52.2423	53.2630	55.1214	56.1291	56.4963	56.6661	57.1489	56.6367	57.3497	56.6075	57.2520	56.6960	57.6735	**51.23**
C2`	24.9465	25.3520	25.6480	25.5480	25.9499	25.5397	25.9956	25.5320	25.9904	25.5581	25.8215	24.5881	24.8130	25.1503	24.8404	25.4827	24.8433	25.3433	24.8466	25.3463	24.8398	25.1418	**23.85**
C3`	24.5882	24.8130	25.1503	24.8405	25.4828	24.8434	25.3433	24.8467	25.3463	24.8398	25.1418	24.9465	25.3519	25.6480	25.5481	25.9498	25.5397	25.9956	25.5320	25.9904	25.5581	25.8214	**23.66**
C4`	55.1213	56.1291	56.4964	56.6661	57.1489	56.6366	57.3499	56.6074	57.2520	56.6960	57.6734	51.0019	51.8245	51.9725	52.2130	52.8555	52.1850	52.7763	52.1578	52.7042	52.2423	53.2631	**52.72**
H2	8.8151	8.7078	8.6586	8.6372	8.5486	8.6433	8.5851	8.6489	8.5804	8.6309	8.5389	8.8151	8.7078	8.6586	8.6372	8.5487	8.6433	8.5851	8.6489	8.5804	8.6309	8.5389	**8.13**
H3	7.4066	7.5369	7.6238	7.5786	7.6900	7.5770	7.7070	7.5754	7.6992	7.5799	7.7229	7.4066	7.5369	7.6238	7.5786	7.6900	7.5770	7.7070	7.5754	7.6992	7.5799	7.7229	**7.22**
H5	7.2382	7.4199	7.5023	7.4959	7.6208	7.4914	7.6424	7.4870	7.6307	7.5001	7.6661	7.2382	7.4199	7.5023	7.4959	7.6208	7.4914	7.6424	7.4870	7.6307	7.5001	7.6661	**7.22**
H6	8.0282	8.2138	8.3196	8.3378	8.4424	8.3316	8.5141	8.3255	8.4898	8.3436	8.5205	8.0282	8.2138	8.3196	8.3378	8.4424	8.3316	8.5141	8.3254	8.4898	8.3436	8.5205	**8.13**
H8	4.4077	4.4833	4.5518	4.5367	4.6353	4.5337	4.6968	4.5309	4.6740	4.5395	4.6855	4.4077	4.4833	4.5518	4.5367	4.6353	4.5337	4.6968	4.5308	4.6740	4.5395	4.6855	**5.5**
H(9A-9B)	1.6636	1.7086	1.6564	1.7438	1.6990	1.7413	1.6927	1.7390	1.6918	1.7459	1.7073	1.6637	1.7086	1.6564	1.7438	1.6990	1.7413	1.6927	1.7390	1.6918	1.7459	1.7073	**2.08**
H(10-13A-10-13B)	1.1817	1.1491	1.1110	1.1331	1.0841	1.1342	1.0904	1.1354	1.0890	1.1319	1.0869	1.1817	1.1491	1.1110	1.1331	1.0841	1.1342	1.0905	1.1354	1.0890	1.1319	1.0869	**1.25**
H(14A-14C)	0.9689	0.9620	0.9403	0.9579	0.9303	0.9583	0.9335	0.9588	0.9324	0.9574	0.9334	0.9689	0.9620	0.9403	0.9579	0.9303	0.9583	0.9335	0.9588	0.9323	0.9574	0.9333	**0.79**
H(1`A-1`B)	2.9184	2.9382	2.9420	2.9510	2.9569	2.9501	2.9627	2.9494	2.9606	2.9517	2.9496	2.8300	2.7545	2.7330	2.7228	2.7192	2.7241	2.6960	2.7258	2.7013	2.7216	2.6849	**3.69**
H(2`-3`A-2`-3`B)	1.6537	1.7126	1.6853	1.7485	1.7123	1.7462	1.7330	1.7440	1.7251	1.7507	1.7633	1.6537	1.7126	1.6853	1.7485	1.7123	1.7462	1.7330	1.7440	1.7251	1.7507	1.7633	**2.18**
H(4`A)	2.8233	2.6801	2.6423	2.6326	2.6514	2.6345	2.5985	2.6367	2.6014	2.6312	2.6094	3.1207	3.1643	3.1936	3.2042	3.2636	3.2013	3.2602	3.1986	3.2549	3.2069	3.2626	**3.12**
H(4`B)	2.8365	2.8289	2.8238	2.8129	2.7870	2.8138	2.7935	2.8150	2.8012	2.8120	2.7603	2.7160	2.7121	2.6904	2.6978	2.6502	2.6990	2.6652	2.7003	2.6663	2.6965	2.6366	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. VI

Nuclei	R											S										Exp. [b]
	HF											HF										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.4035	137.1278	138.0461	138.4872	139.9277	138.4031	138.5011	138.3173	138.7464	138.5615	139.0624	136.4034	137.1278	138.0460	138.4871	139.9277	138.4032	138.5011	138.3173	138.7465	138.5615	139.0625	**131.79**
C2	144.3799	144.1940	144.6117	143.8110	144.2376	143.8387	144.8999	143.8673	144.7404	143.7843	144.8036	144.3800	144.1940	144.6118	143.8109	144.2376	143.8389	144.8999	143.8673	144.7404	143.7843	144.8035	**131.93**
C3	120.4241	120.9461	121.4129	121.2212	121.7448	121.2097	121.7134	121.1984	121.7225	121.2306	121.8327	120.4241	120.9463	121.4129	121.2212	121.7448	121.2096	121.7134	121.1984	121.7225	121.2306	121.8329	**116.53**
C4	171.1246	171.6259	172.1570	171.7650	172.2621	171.7599	173.0841	171.7556	172.8834	171.7699	173.1504	171.1246	171.6259	172.1571	171.7651	172.2621	171.7598	173.0841	171.7557	172.8834	171.7699	173.1503	**168.1**
C5	117.8580	119.0948	119.6067	119.8387	120.5249	119.7959	120.4836	119.7533	120.4426	119.8779	120.6979	117.8581	119.0948	119.6066	119.8387	120.5249	119.7961	120.4836	119.7532	120.4426	119.8779	120.6980	**116.51**
C6	139.8806	141.5815	142.5198	142.1624	143.6282	142.1252	144.6559	142.0906	144.3152	142.2001	144.7706	139.8807	141.5812	142.5197	142.1623	143.6282	142.1252	144.6559	142.0904	144.3152	142.2001	144.7706	**131.88**
C7	196.4816	201.8505	203.1192	205.7711	205.6536	205.5218	212.2035	205.2726	210.7097	206.0034	213.6470	196.4817	201.8506	203.1191	205.7712	205.6536	205.5218	212.2035	205.2726	210.7097	206.0034	213.6466	**195.2**
C8	55.7809	56.7123	57.1526	57.4317	58.0702	57.3775	58.5676	57.3217	58.4461	57.4800	58.9026	55.7810	56.7123	57.1526	57.4318	58.0702	57.3774	58.5676	57.3217	58.4461	57.4800	58.9025	**54.87**
C9	29.8996	29.5113	29.5627	29.1502	29.4549	29.1696	29.4271	29.1890	29.4288	29.1307	29.4061	29.8997	29.5113	29.5627	29.1501	29.4549	29.1696	29.4271	29.1891	29.4288	29.1307	29.4061	**31.13**
C10	23.2904	23.7279	24.0237	23.9132	24.5483	23.9023	24.3894	23.8917	24.3757	23.9233	24.5000	23.2903	23.7279	24.0237	23.9132	24.5483	23.9023	24.3894	23.8917	24.3757	23.9233	24.5001	**30.82**
C11	31.9658	31.9776	32.2737	31.8838	32.4266	31.8913	32.3529	31.8988	32.3537	31.8754	32.5134	31.9658	31.9775	32.2738	31.8838	32.4266	31.8914	32.3529	31.8988	32.3537	31.8754	32.5133	**29.11**
C12	33.2038	33.4266	33.7197	33.6077	34.0592	33.5944	33.9779	33.5822	33.9595	33.6206	34.0594	33.2038	33.4266	33.7196	33.6077	34.0592	33.5943	33.9779	33.5822	33.9595	33.6206	34.0594	**25.52**
C13	25.4897	25.6365	25.8280	25.6776	25.9818	25.6765	25.9469	25.6757	25.9433	25.6779	25.9788	25.4897	25.6364	25.8278	25.6776	25.9818	25.6766	25.9469	25.6757	25.9433	25.6779	25.9788	**22.36**
C14	16.3904	16.5117	16.5768	16.6005	16.7041	16.5939	16.6921	16.5881	16.6847	16.6061	16.7259	16.3904	16.5117	16.5768	16.6004	16.7041	16.5939	16.6921	16.5882	16.6848	16.6061	16.7259	**13.85**
C1`	44.7187	45.4339	45.6746	45.8521	46.3765	45.8201	46.3408	45.7884	46.2817	45.8817	46.6971	48.5589	49.3425	49.6846	49.8323	50.2795	49.8039	50.3316	49.7751	50.2617	49.8579	50.5880	**51.23**
C2`	22.8192	23.0499	23.3350	23.1165	23.5978	23.1132	23.5619	23.1098	23.5667	23.1188	23.3700	22.2374	22.3215	22.6524	22.3929	22.9300	22.3879	22.7818	22.3839	22.7996	22.3972	22.5805	**23.85**
C3`	22.2374	22.3214	22.6525	22.3929	22.9300	22.3879	22.7818	22.3838	22.7996	22.3972	22.5804	22.8192	23.0498	23.3350	23.1164	23.5978	23.1130	23.5619	23.1098	23.5667	23.1188	23.3700	**23.66**
C4`	48.5589	49.3424	49.6846	49.8323	50.2795	49.8038	50.3316	49.7751	50.2617	49.8579	50.5880	44.7187	45.4340	45.6745	45.8522	46.3765	45.8201	46.3408	45.7884	46.2817	45.8817	46.6972	**52.72**
H2	9.0701	8.9542	8.9762	8.7692	8.8084	8.7812	8.8743	8.7933	8.8631	8.7584	8.8267	9.0701	8.9542	8.9762	8.7692	8.8084	8.7812	8.8743	8.7933	8.8631	8.7584	8.8267	**8.13**
H3	7.4300	7.5696	7.6605	7.6188	7.7384	7.6167	7.7471	7.6143	7.7402	7.6208	7.7645	7.4300	7.5696	7.6605	7.6188	7.7384	7.6167	7.7471	7.6143	7.7402	7.6208	7.7645	**7.22**
H5	7.2460	7.4415	7.5333	7.5296	7.6528	7.5244	7.6636	7.5188	7.6531	7.5346	7.6900	7.2460	7.4415	7.5333	7.5296	7.6528	7.5244	7.6636	7.5188	7.6531	7.5346	7.6900	**7.22**
H6	8.0736	8.2925	8.4070	8.4017	8.5655	8.3964	8.6403	8.3911	8.6097	8.4070	8.6617	8.0736	8.2925	8.4070	8.4017	8.5655	8.3964	8.6403	8.3910	8.6097	8.4070	8.6617	**8.13**
H8	3.6324	3.7491	3.8285	3.8185	3.9415	3.8142	4.0156	3.8099	3.9891	3.8230	4.0086	3.6324	3.7491	3.8285	3.8186	3.9415	3.8142	4.0156	3.8099	3.9891	3.8230	4.0086	**5.5**
H(9A-9B)	1.3075	1.3449	1.3263	1.3155	1.3343	1.3164	1.3526	1.3171	1.3440	1.3149	1.3607	1.3075	1.3449	1.3263	1.3155	1.3343	1.3164	1.3526	1.3171	1.3440	1.3149	1.3607	**2.08**
H(10-13A-10-13B)	1.0044	0.9654	0.9376	0.9471	0.8968	0.9479	0.9043	0.9488	0.9031	0.9464	0.9008	1.0043	0.9654	0.9376	0.9471	0.8968	0.9479	0.9043	0.9488	0.9031	0.9464	0.9008	**1.25**
H(14A-14C)	0.9312	0.9202	0.8994	0.9193	0.8867	0.9193	0.8883	0.9192	0.8880	0.9193	0.8891	0.9312	0.9202	0.8994	0.9193	0.8867	0.9193	0.8883	0.9192	0.8880	0.9193	0.8891	**0.79**
H(1`A-1`B)	2.5533	2.5833	2.5875	4.0122	2.5938	2.5907	2.6105	2.5897	2.6069	2.5924	2.6046	2.4515	2.3988	2.3673	3.7878	2.3735	2.3901	2.3554	2.3902	2.3591	2.3894	2.3503	**3.69**
H(2`-3`A-2`-3`B)	1.4318	1.4977	1.4621	1.5540	1.4979	1.5504	1.5153	1.5467	1.5086	1.5574	1.5412	1.4318	1.4977	1.4621	1.5540	1.4979	1.5504	1.5153	1.5467	1.5086	1.5574	1.5412	**2.18**
H(4`A)	2.3740	2.2775	2.2423	3.7647	2.2922	2.2831	2.2448	2.2815	2.2477	2.2860	2.2620	2.7264	2.7907	2.8219	4.3261	2.8852	2.8224	2.8920	2.8198	2.8852	2.8273	2.8991	**3.12**
H(4`B)	2.5289	2.5200	2.4923	3.8108	2.4548	2.4972	2.4661	2.4990	2.4706	2.4928	2.4386	2.3801	2.3758	2.3530	3.6983	2.3024	2.3591	2.3291	2.3597	2.3287	2.3574	2.3100	**3.86**
Nuclei	LC-BLYP											LC-BLYP											
C1	144.3337	145.2525	146.1785	145.6373	148.5197	145.5838	147.4982	145.5603	147.5544	145.6745	147.9878	144.3338	145.2525	146.1784	145.6371	148.5198	145.5837	147.4981	145.5604	147.5545	145.6747	147.9879	**131.79**
C2	148.6496	148.4843	149.0546	148.3427	148.7114	148.3324	149.2174	148.3487	149.1040	148.3349	149.1780	148.6495	148.4842	149.0545	148.3428	148.7113	148.3324	149.2174	148.3486	149.1039	148.3350	149.1780	**131.93**
C3	128.2690	128.8816	129.5093	129.1027	129.9143	129.0701	130.1131	129.0648	130.0465	129.1164	130.2165	128.2689	128.8817	129.5093	129.1027	129.9141	129.0702	130.1130	129.0649	130.0462	129.1163	130.2166	**116.53**
C4	181.9798	182.4933	183.1107	182.8576	183.2651	182.8151	183.9702	182.7994	183.8042	182.8803	184.0980	181.9798	182.4933	183.1108	182.8578	183.2648	182.8149	183.9704	182.7994	183.8041	182.8802	184.0981	**168.1**
C5	126.1569	127.4600	128.1494	128.1739	129.0986	128.1091	129.2707	128.0714	129.1631	128.2181	129.4931	126.1568	127.4600	128.1495	128.1741	129.0987	128.1090	129.2708	128.0716	129.1631	128.2182	129.4930	**116.51**
C6	144.2894	146.1433	147.2813	147.3141	148.4182	147.2206	149.0102	147.1539	148.7911	147.3847	149.2672	144.2894	146.1434	147.2812	147.3142	148.4182	147.2207	149.0102	147.1540	148.7910	147.3848	149.2671	**131.88**
C7	211.8278	217.1487	218.4570	220.0985	221.7729	219.8831	227.5238	219.6985	226.1955	220.2906	228.9320	211.8278	217.1488	218.4569	220.0982	221.7726	219.8829	227.5238	219.6986	226.1955	220.2905	228.9321	**195.2**
C8	62.4909	63.6231	64.2597	64.2397	65.3892	64.1774	65.9514	64.1437	65.7846	64.2835	66.3958	62.4909	63.6233	64.2597	64.2397	65.3891	64.1773	65.9515	64.1438	65.7846	64.2834	66.3959	**54.87**
C9	33.0680	32.6961	32.9683	32.5839	32.7305	32.5691	32.6887	32.5814	32.6630	32.5807	32.7201	33.0680	32.6960	32.9684	32.5840	32.7304	32.5690	32.6887	32.5813	32.6630	32.5807	32.7202	**31.13**
C10	25.0507	25.5080	25.7804	25.7971	26.3215	25.7569	26.1723	25.7442	26.1362	25.8182	26.3359	25.0508	25.5079	25.7804	25.7972	26.3215	25.7569	26.1723	25.7442	26.1361	25.8182	26.3359	**30.82**
C11	34.5220	34.4735	34.9320	34.4506	34.9453	34.4311	34.9186	34.4392	34.8721	34.4519	35.0881	34.5220	34.4734	34.9321	34.4506	34.9454	34.4312	34.9185	34.4391	34.8721	34.4519	35.0881	**29.11**
C12	36.2808	36.5507	36.8178	36.7768	37.2355	36.7408	37.1366	36.7323	37.1251	36.7934	37.2658	36.2808	36.5507	36.8178	36.7768	37.2356	36.7409	37.1365	36.7323	37.1252	36.7934	37.2659	**25.52**
C13	26.2331	26.3735	26.6274	26.4658	26.7372	26.4395	26.7270	26.4405	26.7013	26.4731	26.7419	26.2331	26.3736	26.6275	26.4656	26.7372	26.4395	26.7270	26.4405	26.7012	26.4731	26.7418	**22.36**
C14	15.4616	15.5941	15.6570	15.7249	15.7857	15.6951	15.7837	15.6926	15.7615	15.7359	15.8362	15.4616	15.5940	15.6571	15.7249	15.7858	15.6951	15.7838	15.6927	15.7614	15.7360	15.8362	**13.85**
C1`	48.9243	49.7454	50.0229	50.2601	50.8108	50.2054	50.7778	50.1787	50.6826	50.2953	51.1597	52.7027	53.6594	54.0269	54.2002	54.7329	54.1469	54.8610	54.1209	54.7844	54.2335	55.1771	**51.23**
C2`	22.9721	23.2680	23.5662	23.4320	23.8331	23.4010	23.8693	23.3975	23.8636	23.4443	23.7302	22.4919	22.5698	22.9001	22.6625	23.1303	22.6356	23.0545	22.6358	23.0430	22.6706	22.9267	**23.85**
C3`	22.4919	22.5699	22.9002	22.6624	23.1302	22.6355	23.0545	22.6359	23.0430	22.6706	22.9267	22.9721	23.2680	23.5662	23.4319	23.8329	23.4010	23.8692	23.3975	23.8636	23.4442	23.7302	**23.66**
C4`	52.7027	53.6594	54.0269	54.2003	54.7329	54.1469	54.8611	54.1209	54.7844	54.2335	55.1771	48.9243	49.7454	50.0229	50.2601	50.8108	50.2054	50.7778	50.1787	50.6826	50.2954	51.1597	**52.72**
H2	9.0123	8.8795	8.9082	8.8108	8.6896	8.8153	8.7346	8.8210	8.7351	8.8051	8.7059	9.0123	8.8795	8.9082	8.8108	8.6896	8.8153	8.7346	8.8210	8.7351	8.8051	8.7059	**8.13**
H3	7.5402	7.6698	7.7636	7.7115	7.8303	7.7087	7.8492	7.7074	7.8413	7.7132	7.8687	7.5402	7.6699	7.7636	7.7115	7.8303	7.7087	7.8492	7.7074	7.8413	7.7132	7.8687	**7.22**
H5	7.3881	7.5726	7.6648	7.6567	7.7794	7.6510	7.7928	7.6468	7.7828	7.6611	7.8180	7.3881	7.5726	7.6648	7.6567	7.7794	7.6510	7.7928	7.6468	7.7828	7.6611	7.8180	**7.22**
H6	8.1915	8.3747	8.4717	8.4829	8.5778	8.4756	8.6442	8.4699	8.6229	8.4886	8.6675	8.1915	8.3747	8.4717	8.4829	8.5778	8.4757	8.6442	8.4699	8.6229	8.4886	8.6675	**8.13**
H8	4.2052	4.2789	4.3291	4.3443	4.4160	4.3392	4.5006	4.3357	4.4719	4.3480	4.5224	4.2052	4.2789	4.3291	4.3443	4.4160	4.3392	4.5006	4.3357	4.4719	4.3480	4.5224	**5.5**
H(9A-9B)	1.6608	1.6955	1.6938	1.7274	1.6824	1.7244	1.6683	1.7229	1.6685	1.7292	1.6815	1.6608	1.6955	1.6938	1.7274	1.6823	1.7243	1.6683	1.7229	1.6685	1.7292	1.6816	**2.08**
H(10-13A-10-13B)	1.1538	1.1143	1.0835	1.0982	1.0377	1.0985	1.0459	1.1003	1.0447	1.0969	1.0437	1.1538	1.1143	1.0835	1.0982	1.0377	1.0985	1.0459	1.1003	1.0447	1.0969	1.0437	**1.25**
H(14A-14C)	0.9733	0.9623	0.9406	0.9583	0.9256	0.9578	0.9296	0.9588	0.9286	0.9579	0.9313	0.9733	0.9623	0.9406	0.9583	0.9257	0.9578	0.9296	0.9588	0.9286	0.9579	0.9313	**0.79**
H(1`A-1`B)	2.8505	2.8672	2.8690	2.8796	2.8744	2.8780	2.8778	2.8779	2.8757	2.8801	2.8725	2.7669	2.6916	2.6662	2.6607	2.6645	2.6611	2.6373	2.6632	2.6427	2.6595	2.6263	**3.69**
H(2`-3`A-2`-3`B)	1.6417	1.7002	1.6646	1.7392	1.6998	1.7357	1.7212	1.7339	1.7125	1.7414	1.7515	1.6417	1.7003	1.6645	1.7392	1.6998	1.7357	1.7212	1.7339	1.7125	1.7415	1.7515	**2.18**
H(4`A)	2.7349	2.5890	2.5522	2.5471	2.5772	2.5473	2.5179	2.5493	2.5210	2.5462	2.5245	3.0212	3.0617	3.0878	3.0996	3.1453	3.0961	3.1358	3.0942	3.1312	3.1019	3.1452	**3.12**
H(4`B)	2.7989	2.7942	2.7803	2.7743	2.7517	2.7749	2.7567	2.7771	2.7644	2.7728	2.7282	2.6798	2.6728	2.6503	2.6595	2.6035	2.6597	2.6199	2.6615	2.6201	2.6583	2.5998	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. VII

Nuclei	R											S										Exp. [b]
	M06											M06										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.7395	137.4383	139.1872	139.7500	142.0626	139.7117	141.0007	139.6815	141.1315	139.8011	141.0203	136.7395	137.4383	139.1873	139.7500	142.0627	139.7119	141.0007	139.6817	141.1315	139.8011	141.0202	**131.79**
C2	140.3362	140.1738	140.8382	140.5152	141.1710	140.5096	141.5886	140.5117	141.4805	140.5343	141.5920	140.3362	140.1738	140.8382	140.5152	141.1710	140.5097	141.5887	140.5116	141.4805	140.5343	141.5918	**131.93**
C3	121.7301	122.5264	123.1854	122.5950	123.4710	122.5721	123.7068	122.5568	123.6508	122.6311	123.6545	121.7301	122.5264	123.1855	122.5950	123.4710	122.5720	123.7068	122.5565	123.6508	122.6311	123.6544	**116.53**
C4	173.6051	174.3515	174.9011	173.7989	174.4242	173.7727	175.0521	173.7545	174.8896	173.8386	175.3265	173.6051	174.3515	174.9010	173.7989	174.4241	173.7727	175.0521	173.7543	174.8896	173.8386	175.3266	**168.1**
C5	119.8470	121.1310	121.8720	121.8447	122.7079	121.7943	122.9654	121.7514	122.8696	121.9074	122.8272	119.8470	121.1310	121.8721	121.8447	122.7078	121.7943	122.9653	121.7514	122.8696	121.9074	122.8273	**116.51**
C6	136.5055	138.2404	139.2303	138.7073	140.0987	138.6322	140.7600	138.5651	140.5297	138.7932	141.3227	136.5055	138.2404	139.2303	138.7073	140.0987	138.6322	140.7600	138.5651	140.5297	138.7932	141.3226	**131.88**
C7	204.4927	209.2057	210.9794	212.9963	213.9539	212.8363	218.6410	212.6850	217.5696	213.1640	219.3307	204.4927	209.2057	210.9794	212.9963	213.9539	212.8362	218.6410	212.6849	217.5696	213.1640	219.3304	**195.2**
C8	62.3082	63.3776	64.7624	64.9615	66.0302	64.9170	66.3705	64.8807	66.2609	65.0187	66.5588	62.3082	63.3776	64.7625	64.9615	66.0303	64.9170	66.3706	64.8806	66.2609	65.0187	66.5588	**54.87**
C9	33.9746	33.6588	33.7535	33.1060	33.3277	33.1061	33.4541	33.1140	33.4109	33.1206	33.4528	33.9746	33.6588	33.7536	33.1060	33.3276	33.1061	33.4540	33.1140	33.4109	33.1206	33.4527	**31.13**
C10	24.2953	24.9543	25.5095	25.6106	26.5097	25.5760	26.4851	25.5488	26.4175	25.6577	26.7669	24.2953	24.9543	25.5095	25.6106	26.5096	25.5759	26.4851	25.5487	26.4175	25.6577	26.7668	**30.82**
C11	34.8467	34.7314	35.1637	34.5408	35.2789	34.5317	35.1177	34.5306	35.1156	34.5642	35.3094	34.8467	34.7314	35.1638	34.5408	35.2789	34.5318	35.1177	34.5306	35.1156	34.5642	35.3093	**29.11**
C12	36.4097	36.7323	37.0917	36.9663	37.5993	36.9423	37.5640	36.9262	37.5307	37.0036	37.6381	36.4097	36.7323	37.0917	36.9663	37.5993	36.9423	37.5641	36.9263	37.5307	37.0036	37.6382	**25.52**
C13	26.8520	26.9758	27.2556	26.9736	27.4054	26.9616	27.3243	26.9574	27.3210	26.9996	27.3574	26.8520	26.9758	27.2557	26.9736	27.4053	26.9616	27.3243	26.9574	27.3210	26.9996	27.3574	**22.36**
C14	15.7773	15.9410	16.1122	16.1076	16.2987	16.0880	16.2939	16.0763	16.3185	16.1411	16.3007	15.7773	15.9410	16.1122	16.1076	16.2986	16.0879	16.2939	16.0763	16.3185	16.1411	16.3008	**13.85**
C1`	50.6358	51.4709	52.0016	52.1078	52.8262	52.0713	52.6260	52.0428	52.6031	52.1574	52.7996	55.3156	56.3435	56.8201	56.9296	57.5812	56.8855	57.7505	56.8490	57.6713	56.9853	57.8463	**51.23**
C2`	23.4130	23.8827	24.3043	23.9912	24.5395	23.9728	24.4447	23.9622	24.4547	24.0233	24.4894	22.3000	22.9204	23.4016	23.1480	23.9340	23.1231	23.6949	23.1060	23.7548	23.1863	22.8523	**23.85**
C3`	22.3000	22.9204	23.4015	23.1480	23.9341	23.1231	23.6948	23.1060	23.7547	23.1863	22.8522	23.4130	23.8827	24.3043	23.9912	24.5395	23.9729	24.4446	23.9623	24.4547	24.0233	24.4894	**23.66**
C4`	55.3156	56.3435	56.8201	56.9296	57.5812	56.8856	57.7505	56.8491	57.6713	56.9853	57.8463	50.6358	51.4709	52.0015	52.1078	52.8263	52.0713	52.6260	52.0428	52.6030	52.1574	52.7997	**52.72**
H2	8.7458	8.6063	8.5389	8.3820	8.3631	8.3864	8.4368	8.3913	8.4245	8.3783	8.4346	8.7458	8.6063	8.5389	8.3820	8.3631	8.3864	8.4368	8.3913	8.4245	8.3783	8.4346	**8.13**
H3	7.3056	7.4123	7.4701	7.4308	7.5674	7.4280	7.6021	7.4258	7.5895	7.4339	7.5909	7.3056	7.4123	7.4701	7.4308	7.5674	7.4280	7.6021	7.4258	7.5895	7.4339	7.5909	**7.22**
H5	7.1471	7.3475	7.4562	7.4147	7.5406	7.4104	7.5526	7.4067	7.5431	7.4193	7.5372	7.1471	7.3475	7.4562	7.4147	7.5406	7.4104	7.5526	7.4067	7.5431	7.4193	7.5372	**7.22**
H6	8.0143	8.2403	8.3301	8.2337	8.3337	8.2291	8.3510	8.2251	8.3316	8.2385	8.4309	8.0143	8.2403	8.3301	8.2337	8.3337	8.2291	8.3510	8.2251	8.3316	8.2385	8.4309	**8.13**
H8	4.3873	4.4404	4.5343	4.5061	4.5536	4.5030	4.6173	4.5003	4.5881	4.5097	4.7136	4.3873	4.4404	4.5343	4.5061	4.5536	4.5030	4.6173	4.5003	4.5881	4.5097	4.7136	**5.5**
H(9A-9B)	1.8167	1.8196	1.7577	1.7271	1.7001	1.7266	1.6981	1.7266	1.6906	1.7282	1.7743	1.8167	1.8196	1.7577	1.7271	1.7001	1.7266	1.6981	1.7266	1.6906	1.7282	1.7742	**2.08**
H(10-13A-10-13B)	1.1913	1.1614	1.1081	1.1263	1.0823	1.1272	1.0890	1.1286	1.0867	1.1261	1.0894	1.1913	1.1614	1.1081	1.1263	1.0823	1.1272	1.0890	1.1286	1.0867	1.1261	1.0894	**1.25**
H(14A-14C)	0.8935	0.8845	0.8652	0.8810	0.8587	0.8809	0.8644	0.8814	0.8656	0.8816	0.8702	0.8935	0.8845	0.8652	0.8810	0.8587	0.8809	0.8644	0.8814	0.8656	0.8816	0.8702	**0.79**
H(1`A-1`B)	2.8882	2.8996	2.9026	2.8993	2.9034	2.8988	2.9098	2.8988	2.9053	2.9004	2.9533	2.8170	2.7641	2.7480	2.7688	2.7577	2.7691	2.7782	2.7700	2.7759	2.7691	2.7366	**3.69**
H(2`-3`A-2`-3`B)	1.6076	1.6738	1.6582	1.7262	1.6878	1.7240	1.7103	1.7223	1.7039	1.7289	1.7412	1.1913	1.1614	1.1081	1.1263	1.0823	1.1272	1.0890	1.1286	1.0867	1.1261	1.0894	**2.18**
H(4`A)	2.7136	2.6299	2.6049	2.6448	2.6561	2.6440	2.6651	2.6439	2.6588	2.6463	2.6526	3.0863	3.1159	3.1465	3.1458	3.1906	3.1441	3.1947	3.1429	3.1865	3.1480	3.2379	**3.12**
H(4`B)	2.9205	2.8983	2.8911	2.8927	2.8594	2.8941	2.8913	2.8962	2.8930	2.8918	2.8205	2.6901	2.6832	2.6587	2.6528	2.6163	2.6535	2.6250	2.6548	2.6241	2.6528	2.6687	**3.86**
Nuclei	M06-2X																						
C1	153.4197	154.5722	155.4853	154.9225	157.4968	154.9186	156.4566	154.9168	156.4545	154.9205	156.3853	153.4197	154.5722	155.4853	154.9225	157.4968	154.9186	156.4566	154.9168	156.4546	154.9205	156.3853	**131.79**
C2	155.1694	155.0797	155.7659	154.9067	155.5252	154.9406	155.9982	154.9758	155.8808	154.8674	156.0327	155.1694	155.0797	155.7659	154.9066	155.5252	154.9406	155.9982	154.9757	155.8808	154.8674	156.0327	**131.93**
C3	136.0211	136.8448	137.4934	137.0851	137.8625	137.0947	138.1302	137.1054	138.0647	137.0689	138.2095	136.0211	136.8448	137.4934	137.0851	137.8625	137.0947	138.1302	137.1052	138.0647	137.0689	138.2095	**116.53**
C4	187.1175	187.8325	188.4919	188.2201	188.7848	188.2181	189.4744	188.2173	189.3234	188.2154	189.6913	187.1175	187.8325	188.4919	188.2201	188.7848	188.2181	189.4744	188.2173	189.3234	188.2154	189.6913	**168.1**
C5	133.6444	135.1733	135.8765	135.9193	136.8070	135.8956	137.0657	135.8728	136.9525	135.9355	137.2247	133.6444	135.1733	135.8765	135.9193	136.8070	135.8956	137.0657	135.8728	136.9525	135.9355	137.2247	**116.51**
C6	151.2125	153.0661	154.2394	154.2054	155.7455	154.1545	156.3093	154.1051	156.0950	154.2477	157.0478	151.2125	153.0661	154.2394	154.2055	155.7455	154.1545	156.3093	154.1050	156.0949	154.2477	157.0478	**131.88**
C7	219.4178	225.2157	226.5468	228.1930	229.5552	228.0237	235.7021	227.8570	234.2369	228.3492	236.4504	219.4178	225.2157	226.5468	228.1930	229.5552	228.0237	235.7021	227.8571	234.2374	228.3492	236.4504	**195.2**
C8	67.2872	68.8639	69.5712	69.5554	70.9043	69.5317	71.5188	69.5099	71.2851	69.5720	71.7960	67.2872	68.8639	69.5712	69.5553	70.9043	69.5317	71.5188	69.5100	71.2850	69.5720	71.7960	**54.87**
C9	35.5238	35.2768	35.4231	35.1682	35.3427	35.1937	35.5447	35.2207	35.4242	35.1379	35.8854	35.5238	35.2768	35.4230	35.1681	35.3427	35.1937	35.5447	35.2207	35.4242	35.1379	35.8854	**31.13**
C10	26.3737	26.8258	27.0914	27.0936	27.6873	27.0961	27.5154	27.1001	27.4827	27.0853	27.7535	26.3737	26.8258	27.0913	27.0935	27.6873	27.0961	27.5154	27.1000	27.4828	27.0853	27.7535	**30.82**
C11	35.8549	35.8468	36.2837	35.7699	36.3578	35.7950	36.2981	35.8216	36.2898	35.7396	36.3506	35.8549	35.8468	36.2837	35.7699	36.3578	35.7950	36.2981	35.8216	36.2899	35.7396	36.3506	**29.11**
C12	37.5717	37.8909	38.1630	38.0950	38.6110	38.1039	38.4767	38.1137	38.4829	38.0803	38.5091	37.5717	37.8909	38.1630	38.0950	38.6110	38.1039	38.4767	38.1138	38.4829	38.0803	38.5091	**25.52**
C13	27.4100	27.5697	27.8054	27.6084	27.9427	27.6278	27.9092	27.6482	27.9205	27.5834	27.8205	27.4100	27.5697	27.8054	27.6084	27.9427	27.6278	27.9092	27.6482	27.9205	27.5834	27.8205	**22.36**
C14	15.9414	15.9867	15.9035	16.0207	16.0039	16.0384	15.9866	16.0576	15.9631	15.9979	16.2068	15.9414	15.9867	15.9035	16.0208	16.0039	16.0384	15.9866	16.0576	15.9631	15.9979	16.2068	**13.85**
C1`	52.9110	53.4208	53.6521	53.8296	54.4744	53.8210	54.4450	53.8141	54.3482	53.8323	54.9206	57.0977	58.1237	58.4890	58.5758	59.1546	58.5706	59.2285	58.5666	59.2046	58.5741	59.4819	**51.23**
C2`	24.5745	25.1092	25.3996	25.3261	25.7983	25.3339	25.7856	25.3429	25.7843	25.3126	25.5741	24.0916	24.2808	24.4796	24.3674	24.7211	24.3830	24.7199	24.3998	24.6828	24.3464	24.8957	**23.85**
C3`	24.0916	24.2808	24.4796	24.3674	24.7211	24.3830	24.7199	24.3997	24.6828	24.3464	24.8957	24.5745	25.1092	25.3996	25.3262	25.7983	25.3339	25.7856	25.3429	25.7843	25.3126	25.5741	**23.66**
C4`	57.0977	58.1237	58.4890	58.5757	59.1546	58.5706	59.2285	58.5666	59.2045	58.5741	59.4819	52.9110	53.4208	53.6521	53.8296	54.4744	53.8210	54.4450	53.8141	54.3483	53.8323	54.9206	**52.72**
H2	9.2660	9.1556	9.1885	9.1027	9.0318	9.1052	9.0789	9.1073	9.0814	9.1003	9.1208	9.2660	9.1556	9.1885	9.1027	9.0318	9.1052	9.0789	9.1073	9.0814	9.1003	9.1208	**8.13**
H3	7.8380	7.9580	8.0589	7.9934	8.0884	7.9907	8.1092	7.9876	8.1015	7.9961	8.1339	7.8380	7.9580	8.0589	7.9934	8.0884	7.9907	8.1092	7.9876	8.1015	7.9961	8.1339	**7.22**
H5	7.7366	7.9260	8.0189	8.0118	8.1296	8.0057	8.1461	7.9993	8.1371	8.0177	8.1506	7.7366	7.9260	8.0189	8.0118	8.1296	8.0057	8.1461	7.9993	8.1371	8.0177	8.1506	**7.22**
H6	8.5673	8.7324	8.8270	8.8445	8.9783	8.8363	9.0422	8.8277	9.0272	8.8524	9.0693	8.5673	8.7324	8.8270	8.8445	8.9783	8.8363	9.0422	8.8277	9.0272	8.8524	9.0693	**8.13**
H8	4.3040	4.3390	4.3774	4.3995	4.4501	4.3943	4.5274	4.3888	4.5096	4.4046	4.5325	4.3040	4.3390	4.3774	4.3995	4.4501	4.3943	4.5274	4.3888	4.5096	4.4046	4.5325	**5.5**
H(9A-9B)	1.7119	1.7083	1.6976	1.7305	1.7062	1.7272	1.7029	1.7236	1.6962	1.7339	1.7581	1.7119	1.7083	1.6976	1.7305	1.7062	1.7272	1.7029	1.7236	1.6962	1.7339	1.7581	**2.08**
H(10-13A-10-13B)	1.1135	1.0623	1.0350	1.0449	0.9906	1.0448	0.9954	1.0443	0.9967	1.0452	0.9881	1.1135	1.0623	1.0350	1.0449	0.9906	1.0448	0.9954	1.0443	0.9967	1.0452	0.9881	**1.25**
H(14A-14C)	0.9533	0.9288	0.8953	0.9192	0.8718	0.9185	0.8776	0.9174	0.8729	0.9201	0.8998	0.9533	0.9288	0.8953	0.9192	0.8718	0.9185	0.8776	0.9174	0.8729	0.9201	0.8998	**0.79**
H(1`A-1`B)	2.8296	2.8403	2.8435	2.8546	2.8541	2.8523	2.8612	2.8498	2.8580	2.8568	2.8528	2.7731	2.7297	2.7053	2.7016	2.6920	2.7020	2.6738	2.7020	2.6736	2.7015	2.6611	**3.69**
H(2`-3`A-2`-3`B)	1.6435	1.6988	1.6685	1.7408	1.7065	1.7368	1.7283	1.7324	1.7212	1.7449	1.7398	1.6435	1.6988	1.6685	1.7408	1.7065	1.7368	1.7283	1.7324	1.7212	1.7449	1.7398	**2.18**
H(4`A)	2.7447	2.6319	2.5902	2.5916	2.5962	2.5921	2.5511	2.5924	2.5457	2.5914	2.5591	3.0548	3.0671	3.0871	3.0996	3.1423	3.0959	3.1364	3.0920	3.1313	3.1034	3.1615	**3.12**
H(4`B)	2.8014	2.8274	2.8205	2.8117	2.7878	2.8119	2.7965	2.8117	2.8015	2.8117	2.7632	2.6044	2.6135	2.6000	2.6094	2.5658	2.6086	2.5859	2.6075	2.5847	2.6103	2.5442	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. VIII

Nuclei	R											S										Exp. [b]
	mpW1LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.9564	140.7835	142.2031	141.1581	143.4884	141.1218	142.5504	141.0900	142.6807	141.1946	143.0877	139.9564	140.7835	142.2031	141.1581	143.4884	141.1218	142.5502	141.0900	142.6808	141.1946	143.0877	**131.79**
C2	140.0869	140.1128	140.5989	139.9647	140.3317	139.9757	140.8095	139.9871	140.7017	139.9513	140.6988	140.0869	140.1128	140.5989	139.9647	140.3317	139.9757	140.8098	139.9871	140.7018	139.9513	140.6990	**131.93**
C3	122.1020	122.7540	123.3140	122.9669	123.5408	122.9548	123.8126	122.9436	123.7587	122.9758	123.8302	122.1021	122.7540	123.3140	122.9669	123.5408	122.9548	123.8129	122.9436	123.7587	122.9758	123.8302	**116.53**
C4	176.3414	177.1242	177.7564	177.5545	178.1089	177.5267	178.7385	177.5003	178.5908	177.5782	178.8000	176.3414	177.1242	177.7564	177.5545	178.1089	177.5267	178.7387	177.5003	178.5908	177.5782	178.8001	**168.1**
C5	119.8476	121.0787	121.6784	121.7389	122.5018	121.6958	122.7484	121.6543	122.6555	121.7781	122.9175	119.8476	121.0787	121.6784	121.7389	122.5018	121.6958	122.7481	121.6543	122.6556	121.7781	122.9175	**116.51**
C6	135.9743	137.8039	138.6879	138.9772	140.1969	138.9012	140.9518	138.8263	140.6930	139.0473	141.1671	135.9742	137.8039	138.6879	138.9772	140.1969	138.9012	140.9516	138.8263	140.6930	139.0473	141.1669	**131.88**
C7	203.3962	208.1939	210.0966	210.8527	212.3329	210.6699	217.3761	210.4927	216.2790	211.0298	218.8398	203.3962	208.1939	210.0966	210.8527	212.3329	210.6699	217.3759	210.4927	216.2790	211.0298	218.8394	**195.2**
C8	65.8383	66.9702	67.7779	67.5352	68.5552	67.4905	69.1310	67.4494	69.0094	67.5781	69.4798	65.8383	66.9702	67.7779	67.5352	68.5552	67.4905	69.1311	67.4494	69.0093	67.5781	69.4798	**54.87**
C9	36.8987	36.5656	36.5674	36.4418	36.5378	36.4484	36.6783	36.4565	36.6313	36.4332	36.6677	36.8987	36.5656	36.5674	36.4418	36.5377	36.4484	36.6784	36.4565	36.6313	36.4332	36.6677	**31.13**
C10	27.7123	28.2105	28.5088	28.4945	29.0481	28.4739	28.8709	28.4550	28.8715	28.5120	28.9354	27.7123	28.2105	28.5088	28.4945	29.0481	28.4739	28.8709	28.4550	28.8715	28.5120	28.9354	**30.82**
C11	37.4401	37.5086	37.8603	37.4671	37.9805	37.4706	37.9434	37.4751	37.9393	37.4614	38.1000	37.4401	37.5086	37.8603	37.4671	37.9805	37.4706	37.9432	37.4751	37.9392	37.4614	38.0998	**29.11**
C12	39.1710	39.4604	39.7735	39.6831	40.1557	39.6647	40.0461	39.6481	40.0446	39.6990	40.0900	39.1710	39.4604	39.7735	39.6831	40.1557	39.6647	40.0462	39.6481	40.0446	39.6990	40.0900	**25.52**
C13	30.0534	30.2462	30.4763	30.3292	30.6024	30.3225	30.5962	30.3173	30.5967	30.3334	30.5745	30.0534	30.2462	30.4763	30.3292	30.6024	30.3225	30.5963	30.3173	30.5967	30.3334	30.5745	**22.36**
C14	16.9568	17.1292	17.1924	17.2551	17.3117	17.2441	17.2998	17.2345	17.2979	17.2639	17.2966	16.9568	17.1292	17.1924	17.2551	17.3117	17.2441	17.2999	17.2345	17.2978	17.2639	17.2966	**13.85**
C1`	52.0596	52.8264	53.1517	53.3370	53.9059	53.3012	53.8501	53.2670	53.7906	53.3697	54.3351	56.5060	57.4407	57.8845	58.0141	58.4818	57.9734	58.7049	57.9346	58.6243	58.0510	59.0072	**51.23**
C2`	25.8538	26.3325	26.6606	26.5701	26.9727	26.5509	27.0562	26.5337	27.0426	26.5866	26.8914	25.5831	25.8965	26.2726	26.0203	26.6055	26.0119	26.4749	26.0047	26.4829	26.0259	26.2585	**23.85**
C3`	25.5831	25.8965	26.2726	26.0203	26.6055	26.0119	26.4748	26.0047	26.4828	26.0260	26.2585	25.8537	26.3325	26.6606	26.5701	26.9727	26.5509	27.0562	26.5337	27.0427	26.5866	26.8915	**23.66**
C4`	56.5060	57.4407	57.8845	58.0141	58.4818	57.9734	58.7049	57.9346	58.6243	58.0510	59.0071	52.0596	52.8264	53.1517	53.3370	53.9059	53.3012	53.8500	53.2670	53.7906	53.3697	54.3350	**52.72**
H2	8.7210	8.6206	8.5765	8.5556	8.4600	8.5618	8.5091	8.5673	8.5048	8.5489	8.4618	8.7210	8.6206	8.5765	8.5556	8.4600	8.5618	8.5091	8.5673	8.5048	8.5489	8.4618	**8.13**
H3	7.3462	7.4713	7.5539	7.5112	7.6133	7.5098	7.6306	7.5079	7.6232	7.5124	7.6404	7.3462	7.4713	7.5539	7.5112	7.6133	7.5098	7.6306	7.5079	7.6232	7.5124	7.6404	**7.22**
H5	7.1427	7.3226	7.4086	7.4041	7.5265	7.3998	7.5501	7.3950	7.5396	7.4082	7.5782	7.1427	7.3226	7.4086	7.4041	7.5265	7.3998	7.5501	7.3950	7.5396	7.4082	7.5782	**7.22**
H6	7.9614	8.1504	8.2514	8.2660	8.3906	8.2590	8.4685	8.2516	8.4484	8.2726	8.4704	7.9614	8.1504	8.2514	8.2660	8.3906	8.2590	8.4685	8.2516	8.4484	8.2726	8.4704	**8.13**
H8	4.5415	4.6186	4.6612	4.6667	4.7547	4.6638	4.7998	4.6606	4.7858	4.6693	4.7770	4.5415	4.6186	4.6612	4.6667	4.7547	4.6638	4.7998	4.6606	4.7858	4.6693	4.7770	**5.5**
H(9A-9B)	1.6545	1.7015	1.6735	1.7462	1.7185	1.7436	1.7227	1.7407	1.7170	1.7486	1.7376	1.6545	1.7015	1.6735	1.7462	1.7185	1.7436	1.7226	1.7407	1.7170	1.7486	1.7376	**2.08**
H(10-13A-10-13B)	1.1983	1.1681	1.1362	1.1578	1.1105	1.1588	1.1160	1.1594	1.1160	1.1569	1.1105	1.1983	1.1681	1.1362	1.1578	1.1105	1.1588	1.1160	1.1594	1.1160	1.1569	1.1105	**1.25**
H(14A-14C)	0.9688	0.9627	0.9437	0.9618	0.9332	0.9621	0.9357	0.9622	0.9356	0.9615	0.9331	0.9688	0.9627	0.9437	0.9618	0.9332	0.9621	0.9357	0.9622	0.9356	0.9615	0.9331	**0.79**
H(1`A-1`B)	2.9585	2.9773	2.9862	2.9942	3.0008	2.9932	3.0082	2.9920	3.0074	2.9951	2.9905	2.8716	2.7915	2.7698	2.7609	2.7570	2.7625	2.7361	2.7640	2.7391	2.7594	2.7217	**3.69**
H(2`-3`A-2`-3`B)	1.6621	1.7194	1.6938	1.7579	1.7212	1.7555	1.7413	1.7528	1.7359	1.7602	1.7702	1.6621	1.7194	1.6938	1.7579	1.7212	1.7555	1.7413	1.7528	1.7359	1.7602	1.7702	**2.18**
H(4`A)	2.8781	2.7280	2.6936	2.6866	2.7037	2.6885	2.6534	2.6903	2.6549	2.6849	2.6624	3.1784	3.2186	3.2572	3.2649	3.3267	3.2618	3.3253	3.2585	3.3219	3.2677	3.3221	**3.12**
H(4`B)	2.8652	2.8550	2.8460	2.8352	2.8103	2.8365	2.8187	2.8376	2.8233	2.8339	2.7810	2.7387	2.7359	2.7151	2.7236	2.6748	2.7247	2.6912	2.7255	2.6930	2.7225	2.6590	**3.86**
Nuclei	mpW1PW91																						
C1	137.0159	137.8241	139.1885	138.1931	140.4564	138.1609	139.7679	138.1367	139.8251	138.2259	140.3928	137.0160	137.8241	139.1885	138.1931	140.4565	138.1609	139.7677	138.1367	139.8251	138.2259	140.3928	**131.79**
C2	139.1128	139.1284	139.6291	138.8983	139.4168	138.9145	139.8285	138.9354	139.7236	138.8813	139.8026	139.1128	139.1283	139.6291	138.8983	139.4170	138.9145	139.8284	138.9354	139.7236	138.8813	139.8026	**131.93**
C3	121.1252	121.8940	122.5551	122.1904	122.9167	122.1808	123.2087	122.1767	123.1263	122.1982	123.2704	121.1252	121.8940	122.5550	122.1904	122.9168	122.1808	123.2086	122.1767	123.1263	122.1982	123.2704	**116.53**
C4	173.3567	174.1463	174.7634	174.5083	175.1361	174.4859	175.7471	174.4693	175.5926	174.5285	175.8225	173.3567	174.1463	174.7633	174.5083	175.1361	174.4859	175.7472	174.4693	175.5926	174.5285	175.8225	**168.1**
C5	119.0903	120.3998	121.0291	121.0612	121.9529	121.0209	122.2293	120.9863	122.1057	121.0991	122.4359	119.0903	120.3999	121.0291	121.0613	121.9529	121.0209	122.2294	120.9863	122.1057	121.0991	122.4359	**116.51**
C6	134.9413	136.7598	137.5390	137.7371	139.0919	137.6681	139.7237	137.6048	139.4973	137.8023	139.9696	134.9414	136.7597	137.5390	137.7371	139.0918	137.6681	139.7236	137.6048	139.4973	137.8023	139.9696	**131.88**
C7	201.2044	205.7347	207.5233	208.2837	209.6640	208.1101	214.7111	207.9462	213.5857	208.4517	216.1484	201.2044	205.7349	207.5233	208.2837	209.6640	208.1101	214.7112	207.9462	213.5857	208.4517	216.1484	**195.2**
C8	63.7059	64.8475	65.6612	65.4996	66.4682	65.4525	67.1640	65.4128	67.0290	65.5454	67.5846	63.7059	64.8475	65.6612	65.4996	66.4683	65.4525	67.1640	65.4127	67.0290	65.5454	67.5846	**54.87**
C9	35.0519	34.8561	34.8689	34.7499	34.9155	34.7537	35.0107	34.7633	34.9822	34.7457	35.0671	35.0519	34.8560	34.8689	34.7499	34.9155	34.7537	35.0107	34.7632	34.9822	34.7457	35.0671	**31.13**
C10	25.8847	26.4496	26.6898	26.7010	27.3112	26.6851	27.0929	26.6750	27.0915	26.7157	27.2331	25.8847	26.4496	26.6897	26.7010	27.3112	26.6851	27.0929	26.6750	27.0915	26.7157	27.2331	**30.82**
C11	35.2073	35.2765	35.5686	35.2493	35.7128	35.2539	35.6855	35.2639	35.6570	35.2442	35.8710	35.2073	35.2764	35.5685	35.2493	35.7129	35.2539	35.6857	35.2639	35.6570	35.2442	35.8710	**29.11**
C12	36.7949	37.1126	37.3511	37.2760	37.7612	37.2645	37.6307	37.2589	37.6294	37.2864	37.7181	36.7949	37.1124	37.3511	37.2760	37.7611	37.2645	37.6308	37.2590	37.6294	37.2865	37.7181	**25.52**
C13	27.9737	28.1746	28.3538	28.2299	28.5066	28.2275	28.4980	28.2307	28.4832	28.2314	28.5071	27.9737	28.1747	28.3537	28.2299	28.5066	28.2275	28.4980	28.2306	28.4832	28.2314	28.5071	**22.36**
C14	16.4221	16.6061	16.6266	16.6870	16.7802	16.6812	16.7589	16.6813	16.7471	16.6919	16.7931	16.4221	16.6061	16.6267	16.6870	16.7802	16.6812	16.7589	16.6813	16.7471	16.6919	16.7931	**13.85**
C1`	50.7171	51.4886	51.7262	51.8494	52.4818	51.8187	52.4073	51.7940	52.3348	51.8785	52.9195	54.8001	55.8037	56.1971	56.3298	56.8211	56.2963	57.0596	56.2685	56.9551	56.3608	57.3685	**51.23**
C2`	24.6416	25.0540	25.3471	25.2742	25.6576	25.2602	25.7206	25.2521	25.7135	25.2869	25.5187	24.3091	24.5560	24.9080	24.5878	25.2150	24.5875	25.0876	24.5928	25.0866	24.5874	24.8842	**23.85**
C3`	24.3091	24.5560	24.9080	24.5878	25.2150	24.5875	25.0875	24.5927	25.0866	24.5874	24.8842	24.6416	25.0540	25.3471	25.2742	25.6575	25.2602	25.7205	25.2521	25.7135	25.2869	25.5187	**23.66**
C4`	54.8001	55.8037	56.1971	56.3298	56.8211	56.2963	57.0596	56.2686	56.9551	56.3608	57.3685	50.7171	51.4885	51.7261	51.8494	52.4818	51.8187	52.4074	51.7940	52.3348	51.8786	52.9195	**52.72**
H2	8.7680	8.6702	8.6363	8.5996	8.5209	8.6062	8.5492	8.6125	8.5482	8.5931	8.5077	8.7680	8.6702	8.6363	8.5996	8.5209	8.6062	8.5493	8.6125	8.5482	8.5931	8.5077	**8.13**
H3	7.3664	7.5014	7.5904	7.5439	7.6558	7.5426	7.6729	7.5412	7.6646	7.5454	7.6882	7.3664	7.5014	7.5903	7.5439	7.6558	7.5426	7.6729	7.5412	7.6646	7.5454	7.6882	**7.22**
H5	7.1841	7.3673	7.4476	7.4421	7.5674	7.4379	7.5953	7.4337	7.5820	7.4464	7.6223	7.1841	7.3673	7.4476	7.4422	7.5674	7.4379	7.5953	7.4337	7.5820	7.4464	7.6223	**7.22**
H6	8.0386	8.2194	8.3083	8.3309	8.4422	8.3249	8.5163	8.3190	8.4926	8.3368	8.5162	8.0386	8.2193	8.3083	8.3309	8.4422	8.3249	8.5163	8.3190	8.4926	8.3368	8.5162	**8.13**
H8	4.5456	4.6113	4.6567	4.6527	4.7377	4.6506	4.7936	4.6485	4.7718	4.6551	4.7832	4.5456	4.6113	4.6567	4.6527	4.7376	4.6506	4.7936	4.6485	4.7718	4.6551	4.7832	**5.5**
H(9A-9B)	1.6871	1.7331	1.6874	1.7651	1.7289	1.7626	1.7220	1.7601	1.7228	1.7678	1.7375	1.6871	1.7330	1.6874	1.7651	1.7289	1.7626	1.7220	1.7601	1.7228	1.7678	1.7375	**2.08**
H(10-13A-10-13B)	1.1523	1.1213	1.0840	1.1026	1.0562	1.1041	1.0613	1.1055	1.0601	1.1015	1.0585	1.1523	1.1213	1.0840	1.1026	1.0562	1.1041	1.0613	1.1055	1.0601	1.1015	1.0585	**1.25**
H(14A-14C)	0.9138	0.9081	0.8865	0.9022	0.8756	0.9029	0.8784	0.9036	0.8768	0.9018	0.8791	0.9138	0.9081	0.8865	0.9022	0.8756	0.9029	0.8784	0.9036	0.8768	0.9018	0.8791	**0.79**
H(1`A-1`B)	2.9172	2.9331	2.9385	2.9418	2.9486	2.9412	2.9551	2.9407	2.9529	2.9426	2.9418	2.8413	2.7600	2.7351	2.7250	2.7185	2.7269	2.6940	2.7290	2.6992	2.7236	2.6830	**3.69**
H(2`-3`A-2`-3`B)	1.6368	1.6921	1.6615	1.7232	1.6875	1.7212	1.7087	1.7194	1.7000	1.7253	1.7422	1.6368	1.6921	1.6615	1.7232	1.6875	1.7212	1.7087	1.7194	1.7000	1.7253	1.7422	**2.18**
H(4`A)	2.8839	2.7282	2.6851	2.6684	2.6857	2.6713	2.6265	2.6745	2.6297	2.6662	2.6354	3.1547	3.1912	3.2218	3.2249	3.2847	3.2223	3.2824	3.2198	3.2770	3.2277	3.2862	**3.12**
H(4`B)	2.7987	2.7917	2.7851	2.7815	2.7513	2.7825	2.7616	2.7835	2.7688	2.7809	2.7306	2.6796	2.6749	2.6552	2.6586	2.6125	2.6601	2.6279	2.6616	2.6288	2.6574	2.5974	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. IX

Nuclei	R											S										Exp. [b]
	O3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	134.8069	136.8725	138.2604	137.4523	139.9273	137.4307	138.8371	137.4056	139.0108	137.4694	138.9821	134.8069	136.8725	138.2604	137.4523	139.9273	137.4307	138.8371	137.4056	139.0108	137.4694	138.9821	**131.79**
C2	134.3566	134.0195	134.5084	133.9055	134.5083	133.9255	134.8682	133.9400	134.7489	133.8797	135.0358	134.3566	134.0195	134.5086	133.9055	134.5083	133.9255	134.8683	133.9400	134.7489	133.8797	135.0358	**131.93**
C3	117.2995	117.9515	118.6167	118.2515	118.8991	118.2454	119.1305	118.2337	119.0837	118.2505	119.1191	117.2995	117.9515	118.6167	118.2514	118.8991	118.2454	119.1306	118.2337	119.0837	118.2505	119.1191	**116.53**
C4	169.4121	170.0003	170.6616	170.4585	171.0177	170.4384	171.6087	170.4134	171.4691	170.4715	171.6948	169.4121	170.0003	170.6619	170.4584	171.0177	170.4383	171.6086	170.4134	171.4690	170.4715	171.6948	**168.1**
C5	115.1868	116.4433	117.0470	117.0789	117.7639	117.0504	118.0270	117.0164	117.9192	117.0989	118.1826	115.1868	116.4433	117.0469	117.0790	117.7639	117.0503	118.0270	117.0164	117.9192	117.0989	118.1826	**116.51**
C6	129.8788	131.2176	131.9993	132.2893	133.3694	132.2264	134.0509	132.1592	133.8051	132.3425	134.4585	129.8788	131.2176	131.9992	132.2893	133.3694	132.2264	134.0508	132.1592	133.8051	132.3425	134.4585	**131.88**
C7	196.9625	202.8323	204.6364	205.5323	207.0811	205.3807	211.4363	205.2250	210.4879	205.6733	212.2084	196.9625	202.8323	204.6362	205.5324	207.0811	205.3804	211.4360	205.2250	210.4879	205.6733	212.2084	**195.2**
C8	64.5932	66.4169	67.2970	67.1314	68.4311	67.1078	68.9181	67.0788	68.7775	67.1476	68.9926	64.5932	66.4169	67.2970	67.1314	68.4311	67.1077	68.9181	67.0788	68.7774	67.1476	68.9926	**54.87**
C9	35.3938	35.1033	35.1909	34.9831	35.2124	35.0041	35.4764	35.0192	35.3825	34.9560	35.5008	35.3938	35.1033	35.1909	34.9831	35.2124	35.0040	35.4763	35.0192	35.3825	34.9560	35.5008	**31.13**
C10	26.5095	26.8856	27.2720	27.2006	27.8699	27.1918	27.7185	27.1776	27.6905	27.2020	27.8833	26.5095	26.8856	27.2719	27.2006	27.8699	27.1917	27.7185	27.1776	27.6904	27.2020	27.8833	**30.82**
C11	36.0380	36.1404	36.4382	36.1144	36.6658	36.1305	36.6082	36.1412	36.5979	36.0919	36.7780	36.0380	36.1404	36.4382	36.1144	36.6658	36.1306	36.6082	36.1412	36.5977	36.0919	36.7780	**29.11**
C12	37.5365	37.7943	38.1716	38.0776	38.5430	38.0655	38.4538	38.0493	38.4489	38.0834	38.5069	37.5365	37.7943	38.1717	38.0776	38.5430	38.0655	38.4538	38.0493	38.4488	38.0834	38.5069	**25.52**
C13	29.3869	29.5919	29.8005	29.7056	30.0014	29.7101	29.9806	29.7094	29.9703	29.6945	29.9811	29.3869	29.5919	29.8004	29.7054	30.0014	29.7101	29.9805	29.7094	29.9701	29.6945	29.9810	**22.36**
C14	16.7297	16.9022	16.9929	17.0711	17.1603	17.0698	17.1454	17.0635	17.1387	17.0661	17.1524	16.7297	16.9022	16.9929	17.0710	17.1603	17.0697	17.1454	17.0635	17.1386	17.0661	17.1524	**13.85**
C1`	50.8685	51.6425	52.0055	52.2069	52.7950	52.1774	52.7711	52.1438	52.7190	52.2296	53.2671	55.2479	56.1509	56.5936	56.7194	57.2536	56.6945	57.3616	56.6645	57.2883	56.7363	57.6069	**51.23**
C2`	25.8774	26.2974	26.6495	26.5689	27.0394	26.5671	27.0542	26.5594	27.0263	26.5628	26.8729	25.7276	26.0568	26.4043	26.2460	26.7295	26.2434	26.5565	26.2364	26.5726	26.2430	26.2988	**23.85**
C3`	25.7276	26.0568	26.4043	26.2459	26.7295	26.2433	26.5566	26.2364	26.5726	26.2430	26.2988	25.8774	26.2974	26.6494	26.5687	27.0394	26.5670	27.0541	26.5594	27.0263	26.5628	26.8729	**23.66**
C4`	55.2479	56.1509	56.5937	56.7194	57.2536	56.6946	57.3615	56.6645	57.2883	56.7363	57.6069	50.8685	51.6425	52.0056	52.2068	52.7950	52.1775	52.7711	52.1438	52.7190	52.2296	53.2671	**52.72**
H2	8.4791	8.2507	8.2358	8.1898	8.1362	8.1937	8.2067	8.1972	8.1901	8.1856	8.2337	8.4791	8.2507	8.2358	8.1898	8.1362	8.1937	8.2067	8.1972	8.1901	8.1856	8.2337	**8.13**
H3	7.2854	7.3930	7.4835	7.4418	7.5589	7.4396	7.5854	7.4371	7.5768	7.4438	7.6100	7.2854	7.3930	7.4835	7.4418	7.5589	7.4396	7.5854	7.4371	7.5768	7.4438	7.6100	**7.22**
H5	7.0850	7.3066	7.3982	7.3910	7.5045	7.3865	7.5247	7.3817	7.5133	7.3951	7.5447	7.0850	7.3066	7.3982	7.3910	7.5045	7.3865	7.5247	7.3817	7.5133	7.3951	7.5447	**7.22**
H6	7.9488	8.0390	8.1016	8.1351	8.1943	8.1286	8.2538	8.1218	8.2353	8.1411	8.2799	7.9488	8.0390	8.1016	8.1351	8.1943	8.1287	8.2538	8.1218	8.2353	8.1411	8.2799	**8.13**
H8	4.7502	4.7657	4.7716	4.8045	4.8375	4.8018	4.8690	4.7988	4.8553	4.8069	4.8595	4.7502	4.7657	4.7716	4.8045	4.8375	4.8018	4.8690	4.7988	4.8553	4.8069	4.8595	**5.5**
H(9A-9B)	1.5997	1.5990	1.5860	1.6295	1.6248	1.6281	1.6492	1.6262	1.6365	1.6307	1.6814	1.5997	1.5990	1.5860	1.6295	1.6248	1.6281	1.6492	1.6262	1.6365	1.6307	1.6814	**2.08**
H(10-13A-10-13B)	1.1725	1.1471	1.1215	1.1437	1.0998	1.1440	1.1041	1.1440	1.1060	1.1433	1.0993	1.1725	1.1471	1.1215	1.1437	1.0998	1.1440	1.1041	1.1440	1.1059	1.1433	1.0993	**1.25**
H(14A-14C)	0.9500	0.9464	0.9293	0.9479	0.9206	0.9481	0.9223	0.9480	0.9233	0.9476	0.9191	0.9500	0.9464	0.9293	0.9479	0.9206	0.9481	0.9223	0.9480	0.9233	0.9476	0.9191	**0.79**
H(1`A-1`B)	3.0178	3.0400	3.0452	3.0565	3.0601	3.0560	3.0651	3.0550	3.0639	3.0570	3.0437	2.9045	2.8565	2.8419	2.8320	2.8308	2.8336	2.8200	2.8350	2.8228	2.8303	2.7980	**3.69**
H(2`-3`A-2`-3`B)	1.6768	1.7395	1.7149	1.7803	1.7354	1.7778	1.7543	1.7750	1.7508	1.7827	1.7797	1.6768	1.7395	1.7149	1.7803	1.7354	1.7778	1.7543	1.7750	1.7508	1.7827	1.7797	**2.18**
H(4`A)	2.8948	2.8035	2.7894	2.7760	2.8046	2.7768	2.7770	2.7776	2.7803	2.7753	2.7695	3.2499	3.2973	3.3262	3.3408	3.3978	3.3381	3.3939	3.3352	3.3891	3.3434	3.3910	**3.12**
H(4`B)	2.9143	2.9095	2.8945	2.8879	2.8571	2.8904	2.8630	2.8925	2.8654	2.8853	2.8266	2.7858	2.7827	2.7643	2.7722	2.7224	2.7738	2.7364	2.7749	2.7388	2.7706	2.6964	**3.86**
Nuclei	OLYP																						
C1	133.9143	135.6081	136.9756	136.4141	138.5808	136.3815	137.5442	136.3420	137.7077	136.4355	137.7413	133.9144	135.6081	136.9756	136.4141	138.5808	136.3815	137.5442	136.3420	137.7077	136.4355	137.7413	**131.79**
C2	131.7284	131.5365	132.0652	131.4427	132.0847	131.4550	132.4506	131.4618	132.3401	131.4220	132.6095	131.7285	131.5365	132.0652	131.4427	132.0847	131.4550	132.4506	131.4618	132.3401	131.4220	132.6095	**131.93**
C3	115.5627	116.1423	116.7922	116.4183	117.0173	116.4135	117.2843	116.4029	117.2344	116.4136	117.2727	115.5628	116.1423	116.7923	116.4183	117.0173	116.4135	117.2843	116.4029	117.2344	116.4136	117.2727	**116.53**
C4	168.2340	168.9786	169.6997	169.4560	170.1067	169.4348	170.6303	169.4086	170.4930	169.4672	170.7229	168.2339	168.9786	169.6998	169.4560	170.1067	169.4348	170.6303	169.4086	170.4930	169.4672	170.7229	**168.1**
C5	113.5139	114.5783	115.1766	115.1531	115.8004	115.1262	116.1101	115.0937	116.0010	115.1697	116.2527	113.5139	114.5783	115.1766	115.1531	115.8003	115.1262	116.1101	115.0937	116.0010	115.1697	116.2527	**116.51**
C6	127.2730	128.7492	129.6100	129.8093	131.0424	129.7449	131.5987	129.6762	131.3625	129.8626	131.9684	127.2731	128.7492	129.6099	129.8093	131.0424	129.7449	131.5987	129.6762	131.3625	129.8626	131.9684	**131.88**
C7	195.6860	200.9953	202.7800	203.8061	205.1495	203.6514	209.0903	203.4895	208.2474	203.9428	209.8563	195.6860	200.9953	202.7800	203.8061	205.1495	203.6514	209.0903	203.4895	208.2474	203.9428	209.8563	**195.2**
C8	66.1971	67.9578	68.8446	68.7713	69.9082	68.7406	70.3827	68.7026	70.2515	68.7896	70.4557	66.1970	67.9578	68.8445	68.7713	69.9081	68.7406	70.3827	68.7026	70.2515	68.7896	70.4557	**54.87**
C9	36.3708	36.1285	36.2825	36.0221	36.2116	36.0390	36.5760	36.0503	36.4771	35.9964	36.5590	36.3707	36.1285	36.2825	36.0221	36.2116	36.0390	36.5760	36.0503	36.4771	35.9964	36.5590	**31.13**
C10	27.1170	27.5531	27.9746	27.8381	28.5226	27.8292	28.3927	27.8148	28.3689	27.8374	28.5079	27.1172	27.5531	27.9746	27.8381	28.5226	27.8292	28.3927	27.8148	28.3689	27.8374	28.5079	**30.82**
C11	36.7159	36.8143	37.1553	36.7897	37.3103	36.8028	37.2831	36.8100	37.2791	36.7679	37.4432	36.7159	36.8143	37.1554	36.7897	37.3104	36.8028	37.2831	36.8100	37.2791	36.7679	37.4432	**29.11**
C12	38.2245	38.4731	38.8738	38.7668	39.2451	38.7543	39.1386	38.7367	39.1335	38.7703	39.1821	38.2245	38.4731	38.8738	38.7668	39.2452	38.7543	39.1386	38.7367	39.1335	38.7703	39.1821	**25.52**
C13	30.2631	30.4702	30.6988	30.5877	30.8589	30.5903	30.8514	30.5873	30.8441	30.5761	30.8461	30.2630	30.4702	30.6988	30.5877	30.8589	30.5903	30.8514	30.5873	30.8441	30.5761	30.8461	**22.36**
C14	16.8687	17.0398	17.1445	17.2126	17.2821	17.2098	17.2701	17.2018	17.2662	17.2064	17.2681	16.8687	17.0398	17.1445	17.2126	17.2822	17.2098	17.2701	17.2018	17.2662	17.2064	17.2681	**13.85**
C1`	51.8347	52.5526	52.9343	53.1512	53.6872	53.1178	53.6952	53.0797	53.6495	53.1751	54.2033	56.3018	57.1619	57.5941	57.7168	58.2566	57.6916	58.3536	57.6610	58.2776	57.7318	58.5941	**51.23**
C2`	26.4651	26.9665	27.3139	27.2367	27.6648	27.2326	27.7188	27.2222	27.6925	27.2309	27.5191	26.4864	26.8084	27.1771	27.0485	27.5071	27.0423	27.2944	27.0308	27.3035	27.0458	27.0684	**23.85**
C3`	26.4865	26.8084	27.1771	27.0485	27.5070	27.0423	27.2944	27.0308	27.3035	27.0458	27.0684	26.4652	26.9665	27.3139	27.2367	27.6648	27.2326	27.7188	27.2222	27.6925	27.2309	27.5191	**23.66**
C4`	56.3018	57.1619	57.5941	57.7168	58.2567	57.6916	58.3536	57.6610	58.2776	57.7318	58.5941	51.8347	52.5526	52.9343	53.1512	53.6872	53.1178	53.6952	53.0797	53.6495	53.1751	54.2033	**52.72**
H2	8.2753	8.1071	8.0998	8.0311	8.0064	8.0353	8.0844	8.0394	8.0676	8.0269	8.1029	8.2753	8.1071	8.0998	8.0311	8.0064	8.0353	8.0844	8.0394	8.0676	8.0269	8.1029	**8.13**
H3	7.1893	7.3142	7.4060	7.3667	7.4860	7.3641	7.5062	7.3613	7.4976	7.3688	7.5301	7.1893	7.3142	7.4060	7.3667	7.4861	7.3641	7.5062	7.3613	7.4976	7.3688	7.5301	**7.22**
H5	7.0409	7.2336	7.3220	7.3096	7.4196	7.3057	7.4418	7.3017	7.4303	7.3128	7.4583	7.0409	7.2336	7.3220	7.3096	7.4196	7.3057	7.4418	7.3017	7.4303	7.3128	7.4583	**7.22**
H6	7.8329	7.9306	7.9994	8.0152	8.1030	8.0091	8.1490	8.0032	8.1303	8.0207	8.1672	7.8329	7.9306	7.9994	8.0152	8.1030	8.0091	8.1490	8.0032	8.1303	8.0207	8.1672	**8.13**
H8	4.9190	4.9190	4.9228	4.9401	4.9816	4.9390	4.9996	4.9377	4.9861	4.9408	4.9909	4.9190	4.9190	4.9228	4.9401	4.9816	4.9390	4.9996	4.9377	4.9861	4.9408	4.9909	**5.5**
H(9A-9B)	1.6178	1.6530	1.6472	1.6786	1.6790	1.6770	1.7133	1.6752	1.7021	1.6798	1.7344	1.6178	1.6530	1.6472	1.6786	1.6790	1.6770	1.7133	1.6752	1.7021	1.6798	1.7344	**2.08**
H(10-13A-10-13B)	1.2026	1.1790	1.1556	1.1788	1.1360	1.1790	1.1400	1.1790	1.1416	1.1782	1.1355	1.2026	1.1790	1.1556	1.1788	1.1360	1.1790	1.1400	1.1790	1.1416	1.1782	1.1355	**1.25**
H(14A-14C)	0.9619	0.9572	0.9414	0.9596	0.9322	0.9597	0.9332	0.9597	0.9343	0.9591	0.9295	0.9619	0.9572	0.9414	0.9596	0.9322	0.9597	0.9332	0.9597	0.9343	0.9591	0.9295	**0.79**
H(1`A-1`B)	3.0994	3.1220	3.1285	3.1357	3.1457	3.1353	3.1442	3.1346	3.1430	3.1357	3.1194	2.9786	2.9303	2.9199	2.9125	2.9075	2.9138	2.8962	2.9149	2.8990	2.9110	2.8768	**3.69**
H(2`-3`A-2`-3`B)	1.7192	1.7727	1.7485	1.8124	1.7695	1.8099	1.7843	1.8074	1.7809	1.8144	1.8117	1.7192	1.7727	1.7485	1.8124	1.7695	1.8099	1.7843	1.8074	1.7809	1.8144	1.8117	**2.18**
H(4`A)	2.9790	2.8873	2.8789	2.8718	2.8940	2.8721	2.8678	2.8724	2.8704	2.8712	2.8644	3.3473	3.3951	3.4282	3.4367	3.5030	3.4341	3.4912	3.4314	3.4861	3.4388	3.4847	**3.12**
H(4`B)	2.9783	2.9734	2.9610	2.9532	2.9210	2.9554	2.9247	2.9574	2.9275	2.9507	2.8892	2.8514	2.8489	2.8289	2.8347	2.7883	2.8364	2.7973	2.8379	2.7998	2.8326	2.7542	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. X

Nuclei	R											S										Exp. [b]
	OPBE											OPBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	130.6848	132.4678	133.6644	133.0546	135.2766	133.0179	134.2823	132.9696	134.4348	133.0881	134.4724	130.6849	132.4678	133.6644	133.0545	135.2766	133.0179	134.2823	132.9695	134.4348	133.0881	134.4724	**131.79**
C2	130.3966	130.3801	130.8450	130.2151	130.9235	130.2457	131.2300	130.2577	131.1175	130.1812	131.4493	130.3967	130.3801	130.8450	130.2150	130.9235	130.2457	131.2300	130.2577	131.1175	130.1812	131.4493	**131.93**
C3	114.3738	115.1133	115.7506	115.3627	116.0402	115.3674	116.3034	115.3535	116.2411	115.3523	116.3494	114.3739	115.1133	115.7506	115.3627	116.0402	115.3674	116.3034	115.3535	116.2411	115.3524	116.3494	**116.53**
C4	164.6889	165.4682	166.0941	165.8453	166.4106	165.8375	167.0019	165.8120	166.8600	165.8478	167.1289	164.6891	165.4682	166.0941	165.8452	166.4105	165.8375	167.0019	165.8119	166.8600	165.8479	167.1289	**168.1**
C5	112.4074	113.6666	114.2494	114.2214	114.9341	114.2073	115.2509	114.1740	115.1303	114.2291	115.4607	112.4073	113.6666	114.2494	114.2215	114.9341	114.2074	115.2508	114.1740	115.1303	114.2289	115.4607	**116.51**
C6	125.8324	127.4030	128.1932	128.3536	129.5143	128.3087	130.1392	128.2458	129.9186	128.3920	130.5624	125.8323	127.4030	128.1932	128.3537	129.5144	128.3087	130.1393	128.2458	129.9186	128.3919	130.5624	**131.88**
C7	192.9945	198.0837	199.6760	200.5343	201.9531	200.3816	205.7280	200.2170	204.9029	200.6783	206.4234	192.9944	198.0837	199.6760	200.5345	201.9531	200.3816	205.7280	200.2170	204.9029	200.6784	206.4234	**195.2**
C8	63.5491	65.3949	66.1671	66.0712	67.2523	66.0435	67.7674	65.9999	67.6336	66.0936	67.7988	63.5491	65.3949	66.1671	66.0712	67.2523	66.0435	67.7674	65.9998	67.6336	66.0937	67.7988	**54.87**
C9	34.1315	34.0942	34.1411	33.9493	34.1721	33.9789	34.5057	33.9895	34.4015	33.9156	34.5546	34.1315	34.0942	34.1411	33.9493	34.1721	33.9789	34.5057	33.9895	34.4015	33.9155	34.5546	**31.13**
C10	24.9878	25.5089	25.8025	25.7464	26.3699	25.7508	26.2152	25.7363	26.1911	25.7367	26.4489	24.9878	25.5089	25.8025	25.7465	26.3699	25.7508	26.2152	25.7362	26.1911	25.7368	26.4489	**30.82**
C11	34.1929	34.4299	34.6162	34.3257	34.8043	34.3534	34.7539	34.3623	34.7432	34.2937	34.9521	34.1929	34.4299	34.6162	34.3256	34.8043	34.3534	34.7539	34.3624	34.7432	34.2936	34.9521	**29.11**
C12	35.5773	35.9007	36.1700	36.0996	36.4589	36.0982	36.3817	36.0802	36.3782	36.0966	36.4632	35.5772	35.9007	36.1700	36.0996	36.4589	36.0982	36.3818	36.0803	36.3782	36.0966	36.4632	**25.52**
C13	27.8780	28.1641	28.2683	28.1927	28.4107	28.2087	28.3941	28.2066	28.3853	28.1724	28.4157	27.8780	28.1641	28.2683	28.1927	28.4107	28.2087	28.3941	28.2067	28.3853	28.1724	28.4157	**22.36**
C14	16.1540	16.3954	16.3877	16.4764	16.4899	16.4864	16.4794	16.4788	16.4747	16.4622	16.5092	16.1540	16.3954	16.3877	16.4764	16.4899	16.4864	16.4794	16.4789	16.4747	16.4622	16.5092	**13.85**
C1`	49.9630	50.7375	51.0021	51.1938	51.7067	51.1774	51.6936	51.1441	51.6426	51.2050	52.2338	54.1316	55.1255	55.4768	55.6036	56.0706	55.5903	56.1823	55.5591	56.1063	55.6112	56.4504	**51.23**
C2`	25.0520	25.5662	25.8133	25.7398	26.1486	25.7506	26.1320	25.7424	26.1172	25.7236	25.8908	25.0136	25.3315	25.5755	25.3984	25.7774	25.4063	25.6259	25.3981	25.6478	25.3870	25.3517	**23.85**
C3`	25.0136	25.3315	25.5755	25.3984	25.7774	25.4063	25.6259	25.3980	25.6478	25.3870	25.3517	25.0520	25.5662	25.8133	25.7397	26.1486	25.7506	26.1320	25.7424	26.1172	25.7235	25.8908	**23.66**
C4`	54.1315	55.1255	55.4768	55.6037	56.0706	55.5903	56.1824	55.5592	56.1063	55.6113	56.4504	49.9629	50.7375	51.0021	51.1938	51.7067	51.1774	51.6936	51.1441	51.6426	51.2051	52.2338	**52.72**
H2	8.3169	8.1594	8.1483	8.0949	8.0643	8.1016	8.1368	8.1069	8.1183	8.0874	8.1716	8.3169	8.1594	8.1483	8.0949	8.0643	8.1016	8.1368	8.1069	8.1183	8.0874	8.1716	**8.13**
H3	7.2140	7.3499	7.4365	7.3993	7.5156	7.3970	7.5443	7.3941	7.5348	7.4008	7.5733	7.2139	7.3499	7.4365	7.3993	7.5156	7.3970	7.5443	7.3941	7.5348	7.4008	7.5733	**7.22**
H5	7.0535	7.2614	7.3477	7.3402	7.4487	7.3364	7.4724	7.3318	7.4602	7.3429	7.4927	7.0535	7.2614	7.3477	7.3402	7.4487	7.3365	7.4724	7.3318	7.4602	7.3429	7.4927	**7.22**
H6	7.8887	7.9940	8.0604	8.0845	8.1494	8.0800	8.2051	8.0745	8.1870	8.0880	8.2283	7.8887	7.9940	8.0604	8.0845	8.1494	8.0800	8.2051	8.0745	8.1870	8.0880	8.2283	**8.13**
H8	4.9182	4.9269	4.9228	4.9535	4.9738	4.9523	5.0025	4.9502	4.9903	4.9539	4.9930	4.9182	4.9269	4.9228	4.9535	4.9738	4.9523	5.0025	4.9502	4.9903	4.9539	4.9930	**5.5**
H(9A-9B)	1.6305	1.6522	1.6364	1.6753	1.6713	1.6753	1.6965	1.6743	1.6842	1.6745	1.7284	1.6305	1.6522	1.6364	1.6754	1.6713	1.6753	1.6965	1.6743	1.6842	1.6745	1.7284	**2.08**
H(10-13A-10-13B)	1.1437	1.1226	1.0928	1.1166	1.0698	1.1172	1.0735	1.1172	1.0746	1.1153	1.0709	1.1437	1.1226	1.0928	1.1166	1.0698	1.1172	1.0735	1.1172	1.0746	1.1153	1.0709	**1.25**
H(14A-14C)	0.8958	0.8937	0.8711	0.8916	0.8594	0.8922	0.8613	0.8921	0.8619	0.8903	0.8591	0.8958	0.8937	0.8711	0.8916	0.8594	0.8922	0.8613	0.8921	0.8619	0.8903	0.8591	**0.79**
H(1`A-1`B)	3.0425	3.0640	3.0633	3.0745	3.0726	3.0745	3.0763	3.0738	3.0754	3.0738	3.0517	2.9372	2.8876	2.8644	2.8567	2.8457	2.8585	2.8361	2.8597	2.8390	2.8543	2.8118	**3.69**
H(2`-3`A-2`-3`B)	1.6727	1.7281	1.6979	1.7628	1.7126	1.7607	1.7335	1.7579	1.7290	1.7642	1.7674	1.6727	1.7281	1.6979	1.7628	1.7126	1.7607	1.7335	1.7579	1.7290	1.7642	1.7674	**2.18**
H(4`A)	2.9709	2.8708	2.8466	2.8346	2.8479	2.8354	2.8232	2.8359	2.8260	2.8333	2.8125	3.3124	3.3519	3.3741	3.3879	3.4370	3.3859	3.4324	3.3832	3.4281	3.3891	3.4268	**3.12**
H(4`B)	2.9033	2.9043	2.8821	2.8788	2.8435	2.8815	2.8490	2.8835	2.8519	2.8753	2.8112	2.7726	2.7760	2.7524	2.7612	2.7083	2.7631	2.7202	2.7642	2.7226	2.7586	2.6767	**3.86**
Nuclei	OPW91											OPW91											
C1	131.0036	132.7889	133.9841	133.3826	135.5941	133.3352	134.5944	133.2765	134.7477	133.4114	134.7895	131.0037	132.7889	133.9841	133.3826	135.5941	133.3352	134.5944	133.2765	134.7477	133.4114	134.7896	**131.79**
C2	130.6187	130.5947	131.0544	130.4335	131.1268	130.4541	131.4362	130.4572	131.3234	130.3959	131.6587	130.6187	130.5946	131.0544	130.4335	131.1268	130.4541	131.4362	130.4572	131.3234	130.3959	131.6588	**131.93**
C3	114.5772	115.3124	115.9445	115.5651	116.2263	115.5600	116.4911	115.5371	116.4297	115.5508	116.5349	114.5772	115.3124	115.9445	115.5651	116.2263	115.5600	116.4911	115.5371	116.4297	115.5508	116.5349	**116.53**
C4	165.0924	165.8748	166.4988	166.2589	166.8147	166.2409	167.4066	166.2062	167.2649	166.2578	167.5338	165.0924	165.8747	166.4988	166.2589	166.8147	166.2409	167.4066	166.2062	167.2649	166.2578	167.5338	**168.1**
C5	112.6030	113.8607	114.4382	114.4184	115.1164	114.3944	115.4332	114.3522	115.3139	114.4224	115.6414	112.6030	113.8608	114.4382	114.4184	115.1164	114.3944	115.4332	114.3522	115.3139	114.4224	115.6413	**116.51**
C6	126.0452	127.6221	128.4069	128.5815	129.7284	128.5263	130.3583	128.4543	130.1367	128.6166	130.7834	126.0453	127.6222	128.4069	128.5815	129.7284	128.5263	130.3583	128.4543	130.1367	128.6166	130.7834	**131.88**
C7	193.3815	198.4965	200.0893	200.9648	202.3693	200.8000	206.1644	200.6250	205.3351	201.1041	206.8693	193.3813	198.4966	200.0893	200.9648	202.3693	200.8000	206.1644	200.6250	205.3351	201.1041	206.8693	**195.2**
C8	63.7730	65.6220	66.3912	66.3027	67.4739	66.2649	67.9861	66.2120	67.8521	66.3204	68.0287	63.7730	65.6220	66.3912	66.3027	67.4739	66.2649	67.9861	66.2120	67.8521	66.3204	68.0287	**54.87**
C9	34.2862	34.2453	34.2901	34.1043	34.3170	34.1240	34.6510	34.1258	34.5473	34.0667	34.7022	34.2861	34.2453	34.2901	34.1043	34.3170	34.1240	34.6510	34.1258	34.5473	34.0667	34.7023	**31.13**
C10	25.1178	25.6416	25.9355	25.8823	26.4999	25.8767	26.3458	25.8534	26.3221	25.8688	26.5758	25.1180	25.6415	25.9355	25.8823	26.4999	25.8767	26.3458	25.8534	26.3221	25.8688	26.5757	**30.82**
C11	34.3038	34.5427	34.7309	34.4442	34.9170	34.4618	34.8662	34.4614	34.8564	34.4086	35.0651	34.3039	34.5428	34.7309	34.4442	34.9170	34.4618	34.8662	34.4614	34.8564	34.4086	35.0652	**29.11**
C12	35.6839	36.0112	36.2814	36.2166	36.5719	36.2053	36.4942	36.1780	36.4909	36.2098	36.5770	35.6839	36.0111	36.2814	36.2166	36.5719	36.2053	36.4942	36.1780	36.4909	36.2098	36.5770	**25.52**
C13	27.9839	28.2736	28.3789	28.3088	28.5215	28.3147	28.5050	28.3034	28.4967	28.2848	28.5289	27.9840	28.2737	28.3789	28.3087	28.5215	28.3147	28.5050	28.3034	28.4967	28.2848	28.5289	**22.36**
C14	16.1919	16.4370	16.4306	16.5246	16.5335	16.5245	16.5229	16.5077	16.5185	16.5066	16.5548	16.1919	16.4371	16.4306	16.5246	16.5335	16.5245	16.5229	16.5077	16.5185	16.5066	16.5548	**13.85**
C1`	50.1059	50.8803	51.1437	51.3439	51.8478	51.3169	51.8375	51.2739	51.7868	51.3520	52.3803	54.2844	55.2782	55.6284	55.7616	56.2208	55.7381	56.3347	55.6974	56.2589	55.7656	56.6058	**51.23**
C2`	25.1701	25.6880	25.9362	25.8678	26.2707	25.8686	26.2567	25.8512	26.2416	25.8479	26.0262	25.1309	25.4561	25.6993	25.5345	25.9081	25.5324	25.7532	25.5147	25.7749	25.5191	25.4847	**23.85**
C3`	25.1309	25.4560	25.6993	25.5345	25.9081	25.5324	25.7532	25.5147	25.7749	25.5191	25.4847	25.1700	25.6879	25.9362	25.8678	26.2707	25.8686	26.2567	25.8512	26.2416	25.8479	26.0261	**23.66**
C4`	54.2844	55.2783	55.6284	55.7616	56.2208	55.7381	56.3347	55.6974	56.2589	55.7656	56.6057	50.1059	50.8804	51.1437	51.3439	51.8478	51.3169	51.8375	51.2739	51.7868	51.3520	52.3803	**52.72**
H2	8.3181	8.1595	8.1486	8.0954	8.0638	8.1014	8.1365	8.1066	8.1181	8.0877	8.1706	8.3180	8.1595	8.1486	8.0954	8.0638	8.1014	8.1365	8.1066	8.1181	8.0877	8.1706	**8.13**
H3	7.2155	7.3507	7.4371	7.4006	7.5155	7.3976	7.5442	7.3945	7.5347	7.4017	7.5729	7.2154	7.3507	7.4371	7.4006	7.5155	7.3976	7.5442	7.3945	7.5347	7.4017	7.5729	**7.22**
H5	7.0557	7.2630	7.3492	7.3424	7.4499	7.3380	7.4736	7.3332	7.4614	7.3448	7.4936	7.0557	7.2630	7.3492	7.3424	7.4499	7.3380	7.4736	7.3332	7.4614	7.3448	7.4936	**7.22**
H6	7.8886	7.9943	8.0609	8.0855	8.1495	8.0802	8.2057	8.0746	8.1874	8.0887	8.2286	7.8886	7.9943	8.0609	8.0855	8.1495	8.0802	8.2057	8.0746	8.1874	8.0887	8.2286	**8.13**
H8	4.9166	4.9252	4.9213	4.9526	4.9726	4.9507	5.0013	4.9486	4.9889	4.9527	4.9922	4.9166	4.9252	4.9213	4.9526	4.9726	4.9507	5.0013	4.9486	4.9889	4.9527	4.9922	**5.5**
H(9A-9B)	1.6274	1.6502	1.6349	1.6743	1.6701	1.6736	1.6956	1.6724	1.6833	1.6733	1.7270	1.6274	1.6502	1.6349	1.6743	1.6701	1.6736	1.6956	1.6724	1.6833	1.6733	1.7271	**2.08**
H(10-13A-10-13B)	1.1454	1.1244	1.0948	1.1192	1.0718	1.1192	1.0756	1.1189	1.0767	1.1177	1.0729	1.1454	1.1244	1.0948	1.1192	1.0718	1.1192	1.0756	1.1189	1.0767	1.1177	1.0729	**1.25**
H(14A-14C)	0.8973	0.8953	0.8730	0.8940	0.8613	0.8939	0.8632	0.8936	0.8638	0.8925	0.8610	0.8973	0.8953	0.8730	0.8940	0.8613	0.8939	0.8632	0.8936	0.8638	0.8925	0.8610	**0.79**
H(1`A-1`B)	3.0428	3.0645	3.0641	3.0760	3.0737	3.0753	3.0775	3.0744	3.0765	3.0750	3.0530	2.9365	2.8873	2.8644	2.8575	2.8461	2.8587	2.8365	2.8597	2.8393	2.8548	2.8129	**3.69**
H(2`-3`A-2`-3`B)	1.6730	1.7288	1.6988	1.7643	1.7135	1.7615	1.7342	1.7585	1.7298	1.7655	1.7676	1.6730	1.7288	1.6988	1.7643	1.7135	1.7615	1.7342	1.7585	1.7298	1.7655	1.7676	**2.18**
H(4`A)	2.9663	2.8669	2.8431	2.8324	2.8454	2.8325	2.8207	2.8327	2.8233	2.8307	2.8108	3.3092	3.3493	3.3718	3.3864	3.4350	3.3837	3.4306	3.3808	3.4262	3.3873	3.4249	**3.12**
H(4`B)	2.9068	2.9077	2.8856	2.8827	2.8467	2.8848	2.8523	2.8866	2.8552	2.8789	2.8150	2.7764	2.7796	2.7564	2.7657	2.7123	2.7669	2.7244	2.7679	2.7267	2.7627	2.6810	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. XI

Nuclei	R											S										Exp. [b]
	PBE											PBE										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	135.9019	136.9008	138.2957	137.3275	139.6332	137.2822	139.1331	137.2518	139.1150	137.3924	139.8683	135.9019	136.9008	138.2956	137.3275	139.6332	137.2822	139.1332	137.2518	139.1150	137.3924	139.8683	**131.79**
C2	136.0916	136.2080	136.7329	135.9410	136.5703	135.9605	136.9597	135.9895	136.8757	135.9386	136.9479	136.0916	136.2080	136.7329	135.9410	136.5703	135.9605	136.9597	135.9895	136.8756	135.9386	136.9479	**131.93**
C3	119.6142	120.4697	121.0572	120.6436	121.4276	120.6347	121.7781	120.6356	121.6958	120.6691	121.8287	119.6142	120.4697	121.0572	120.6436	121.4276	120.6347	121.7782	120.6356	121.6957	120.6691	121.8287	**116.53**
C4	174.2298	175.2278	175.9319	175.5881	176.4354	175.5651	176.9991	175.5524	176.8616	175.6271	177.1010	174.2298	175.2278	175.9320	175.5881	176.4354	175.5651	176.9992	175.5524	176.8615	175.6271	177.1010	**168.1**
C5	117.5111	118.8939	119.5201	119.4968	120.4590	119.4571	120.8089	119.4283	120.6796	119.5520	121.0136	117.5111	118.8939	119.5203	119.4968	120.4590	119.4571	120.8088	119.4283	120.6796	119.5520	121.0136	**116.51**
C6	131.9239	133.8222	134.7858	134.8538	136.4172	134.7848	136.9985	134.7270	136.7804	134.9369	137.2761	131.9239	133.8222	134.7858	134.8538	136.4172	134.7848	136.9984	134.7270	136.7804	134.9369	137.2761	**131.88**
C7	200.9421	205.2157	207.0638	207.5666	209.2562	207.3936	213.4824	207.2379	212.5207	207.7553	214.9979	200.9421	205.2157	207.0637	207.5666	209.2562	207.3936	213.4827	207.2379	212.5207	207.7553	214.9979	**195.2**
C8	67.3324	68.6293	69.5269	69.2703	70.4597	69.2123	71.1693	69.1687	70.9985	69.3464	71.6226	67.3324	68.6293	69.5269	69.2703	70.4597	69.2123	71.1693	69.1687	70.9985	69.3464	71.6226	**54.87**
C9	38.3531	38.2197	38.2592	38.0778	38.3558	38.0819	38.5717	38.0973	38.4936	38.0916	38.6423	38.3531	38.2197	38.2592	38.0778	38.3557	38.0819	38.5717	38.0973	38.4936	38.0916	38.6423	**31.13**
C10	27.8784	28.5265	28.7604	28.7164	29.4057	28.7015	29.1818	28.6974	29.1837	28.7486	29.3306	27.8784	28.5265	28.7603	28.7164	29.4057	28.7015	29.1817	28.6974	29.1836	28.7486	29.3306	**30.82**
C11	37.6050	37.7486	38.0653	37.6161	38.2334	37.6228	38.1981	37.6400	38.1674	37.6270	38.4073	37.6050	37.7486	38.0652	37.6161	38.2334	37.6228	38.1982	37.6400	38.1673	37.6270	38.4073	**29.11**
C12	39.3005	39.6872	39.9269	39.7923	40.3697	39.7817	40.2421	39.7821	40.2443	39.8206	40.3451	39.3005	39.6872	39.9269	39.7923	40.3697	39.7817	40.2421	39.7821	40.2443	39.8206	40.3451	**25.52**
C13	30.0447	30.3064	30.4885	30.2793	30.6580	30.2786	30.6491	30.2885	30.6363	30.2976	30.6580	30.0447	30.3064	30.4885	30.2793	30.6580	30.2786	30.6492	30.2885	30.6362	30.2976	30.6580	**22.36**
C14	16.5687	16.8180	16.8201	16.8330	16.9916	16.8283	16.9743	16.8344	16.9624	16.8553	17.0126	16.5687	16.8180	16.8200	16.8330	16.9916	16.8283	16.9741	16.8344	16.9625	16.8553	17.0126	**13.85**
C1`	53.3410	54.2057	54.4627	54.6059	55.2859	54.5754	55.2319	54.5564	55.1513	54.6531	55.8136	57.6942	58.8135	59.2507	59.3342	59.9325	59.2955	60.2184	59.2681	60.1224	59.3891	60.5738	**51.23**
C2`	25.5924	26.2017	26.4942	26.4123	26.9175	26.3924	27.0070	26.3839	26.9795	26.4496	26.8801	25.4328	25.8990	26.2391	25.9202	26.6322	25.9227	26.5371	25.9345	26.5278	25.9344	26.3286	**23.85**
C3`	25.4328	25.8989	26.2390	25.9202	26.6321	25.9227	26.5370	25.9345	26.5278	25.9344	26.3286	25.5924	26.2017	26.4941	26.4123	26.9174	26.3924	27.0070	26.3839	26.9795	26.4496	26.8801	**23.66**
C4`	57.6942	58.8135	59.2507	59.3342	59.9325	59.2955	60.2183	59.2681	60.1224	59.3891	60.5738	53.3410	54.2057	54.4626	54.6059	55.2859	54.5754	55.2319	54.5564	55.1513	54.6531	55.8136	**52.72**
H2	8.5501	8.4545	8.4112	8.3736	8.3006	8.3812	8.3304	8.3887	8.3349	8.3665	8.2876	8.5501	8.4545	8.4112	8.3736	8.3006	8.3812	8.3304	8.3887	8.3349	8.3665	8.2876	**8.13**
H3	7.2135	7.3432	7.4259	7.3774	7.4896	7.3762	7.5074	7.3753	7.4996	7.3792	7.5233	7.2135	7.3431	7.4259	7.3774	7.4896	7.3762	7.5074	7.3753	7.4996	7.3792	7.5233	**7.22**
H5	7.0113	7.1898	7.2716	7.2632	7.3895	7.2592	7.4183	7.2556	7.4054	7.2677	7.4475	7.0113	7.1898	7.2716	7.2632	7.3895	7.2592	7.4183	7.2556	7.4055	7.2677	7.4475	**7.22**
H6	7.9378	8.1061	8.1901	8.1959	8.3117	8.1911	8.3764	8.1866	8.3627	8.2011	8.3581	7.9378	8.1061	8.1901	8.1959	8.3117	8.1911	8.3764	8.1866	8.3627	8.2011	8.3581	**8.13**
H8	4.9740	5.0192	5.0471	5.0353	5.1133	5.0351	5.1437	5.0352	5.1334	5.0360	5.1143	4.9740	5.0192	5.0472	5.0353	5.1133	5.0351	5.1437	5.0352	5.1335	5.0360	5.1143	**5.5**
H(9A-9B)	1.8490	1.8954	1.8711	1.9346	1.9160	1.9316	1.9057	1.9292	1.9042	1.9382	1.9204	1.8490	1.8954	1.8710	1.9346	1.9160	1.9316	1.9057	1.9292	1.9042	1.9382	1.9204	**2.08**
H(10-13A-10-13B)	1.2504	1.2243	1.1913	1.2067	1.1655	1.2080	1.1685	1.2096	1.1685	1.2062	1.1648	1.2504	1.2243	1.1913	1.2067	1.1655	1.2080	1.1685	1.2096	1.1685	1.2062	1.1648	**1.25**
H(14A-14C)	0.9368	0.9346	0.9144	0.9275	0.9039	0.9281	0.9068	0.9290	0.9056	0.9276	0.9063	0.9368	0.9346	0.9144	0.9275	0.9039	0.9281	0.9068	0.9290	0.9056	0.9276	0.9063	**0.79**
H(1`A-1`B)	3.0862	3.0998	3.1074	3.1086	3.1206	3.1079	3.1237	3.1078	3.1232	3.1099	3.1033	3.0106	2.9227	2.8986	2.8839	2.8812	2.8858	2.8586	2.8882	2.8601	2.8830	2.8422	**3.69**
H(2`-3`A-2`-3`B)	1.7347	1.7881	1.7588	1.8150	1.7837	1.8132	1.8040	1.8120	1.7968	1.8173	1.8402	1.7347	1.7881	1.7589	1.8150	1.7837	1.8132	1.8040	1.8120	1.7968	1.8173	1.8402	**2.18**
H(4`A)	3.0942	2.9249	2.8815	2.8586	2.8726	2.8621	2.8204	2.8662	2.8194	2.8561	2.8230	3.3629	3.3885	3.4236	3.4247	3.4880	3.4219	3.4829	3.4197	3.4799	3.4281	3.4801	**3.12**
H(4`B)	2.9269	2.9206	2.9157	2.9092	2.8898	2.9094	2.8969	2.9101	2.9008	2.9099	2.8614	2.8095	2.8112	2.7911	2.7924	2.7531	2.7938	2.7645	2.7958	2.7664	2.7916	2.7264	**3.86**
Nuclei	PBE0											PBE0										
C1	136.5457	137.3880	138.0044	137.7213	139.9579	137.6899	139.3775	137.6625	139.3773	137.7565	139.9307	136.5458	137.3880	138.0043	137.7214	139.9579	137.6899	139.3776	137.6625	139.3772	137.7565	139.9307	**131.79**
C2	138.8513	138.8867	139.4388	138.6562	139.1451	138.6663	139.6357	138.6774	139.4643	138.6487	139.5423	138.8513	138.8867	139.4389	138.6563	139.1451	138.6662	139.6359	138.6774	139.4645	138.6487	139.5422	**131.93**
C3	120.8921	121.6787	122.2812	121.9692	122.6796	121.9541	123.0508	121.9403	122.9093	121.9860	123.0642	120.8921	121.6787	122.2812	121.9692	122.6796	121.9541	123.0509	121.9403	122.9095	121.9860	123.0641	**116.53**
C4	172.9527	173.7585	174.4064	174.1223	174.7539	174.0941	175.4510	174.0677	175.2356	174.1521	175.4904	172.9527	173.7585	174.4064	174.1223	174.7540	174.0942	175.4509	174.0677	175.2356	174.1521	175.4903	**168.1**
C5	118.8295	120.1651	120.8200	120.8334	121.7198	120.7872	122.0756	120.7430	121.8958	120.8805	122.2257	118.8295	120.1651	120.8200	120.8333	121.7199	120.7872	122.0756	120.7430	121.8959	120.8805	122.2258	**116.51**
C6	134.7349	136.5641	137.6751	137.5320	138.8755	137.4577	139.5608	137.3855	139.2870	137.6058	139.7494	134.7350	136.5641	137.6750	137.5321	138.8754	137.4577	139.5608	137.3855	139.2869	137.6058	139.7494	**131.88**
C7	200.8618	205.3591	206.3219	207.8424	209.2278	207.6731	214.2812	207.5089	213.1349	208.0101	215.6372	200.8619	205.3591	206.3220	207.8427	209.2278	207.6731	214.2816	207.5089	213.1349	208.0101	215.6371	**195.2**
C8	63.3456	64.4869	65.0428	65.1229	66.0703	65.0754	66.8297	65.0308	66.6521	65.1727	67.1890	63.3457	64.4869	65.0429	65.1230	66.0702	65.0754	66.8298	65.0308	66.6521	65.1727	67.1889	**54.87**
C9	35.0955	34.9105	35.1221	34.7974	34.9278	34.7962	35.1022	34.7971	35.0220	34.8014	35.1211	35.0954	34.9105	35.1221	34.7974	34.9278	34.7962	35.1023	34.7971	35.0219	34.8014	35.1211	**31.13**
C10	25.9498	26.5331	26.8018	26.7923	27.3799	26.7704	27.2359	26.7507	27.1784	26.8163	27.3238	25.9498	26.5331	26.8017	26.7923	27.3800	26.7704	27.2359	26.7507	27.1785	26.8163	27.3238	**30.82**
C11	35.3946	35.4627	35.8243	35.4223	35.8597	35.4225	35.9099	35.4244	35.8218	35.4248	36.0386	35.3946	35.4627	35.8243	35.4221	35.8597	35.4225	35.9099	35.4244	35.8217	35.4248	36.0386	**29.11**
C12	37.0146	37.3450	37.5595	37.5061	37.9741	37.4892	37.9202	37.4745	37.8642	37.5252	37.9559	37.0146	37.3450	37.5596	37.5061	37.9741	37.4892	37.9203	37.4745	37.8643	37.5252	37.9559	**25.52**
C13	27.9507	28.1583	28.3390	28.2032	28.4525	28.1964	28.5231	28.1913	28.4488	28.2125	28.4762	27.9506	28.1583	28.3390	28.2032	28.4524	28.1964	28.5231	28.1913	28.4488	28.2125	28.4762	**22.36**
C14	16.3139	16.5070	16.5110	16.5814	16.6476	16.5708	16.7057	16.5622	16.6370	16.5946	16.6860	16.3139	16.5070	16.5110	16.5814	16.6476	16.5708	16.7058	16.5621	16.6370	16.5946	16.6860	**13.85**
C1`	50.5243	51.3153	51.5059	51.6688	52.2869	51.6333	52.2835	51.6005	52.1564	51.7060	52.7211	54.5933	55.6158	55.9855	56.1393	56.6218	56.1014	56.9350	56.0654	56.7710	56.1783	57.1741	**51.23**
C2`	24.2624	24.6947	24.9679	24.9194	25.2794	24.9009	25.4206	24.8845	25.3585	24.9402	25.1833	23.9347	24.1991	24.5048	24.2280	24.8203	24.2221	24.7795	24.2180	24.7178	24.2365	24.5447	**23.85**
C3`	23.9347	24.1991	24.5048	24.2281	24.8202	24.2221	24.7794	24.2180	24.7178	24.2365	24.5447	24.2623	24.6947	24.9680	24.9194	25.2796	24.9009	25.4207	24.8845	25.3586	24.9402	25.1834	**23.66**
C4`	54.5934	55.6158	55.9855	56.1393	56.6217	56.1014	56.9350	56.0654	56.7710	56.1783	57.1741	50.5243	51.3153	51.5059	51.6688	52.2869	51.6333	52.2835	51.6005	52.1564	51.7060	52.7211	**52.72**
H2	8.7741	8.6744	8.7276	8.6081	8.5263	8.6134	8.5584	8.6183	8.5528	8.6023	8.5147	8.7741	8.6744	8.7276	8.6081	8.5263	8.6134	8.5584	8.6183	8.5528	8.6023	8.5147	**8.13**
H3	7.3590	7.4941	7.5914	7.5376	7.6483	7.5358	7.6701	7.5338	7.6591	7.5389	7.6831	7.3589	7.4941	7.5914	7.5376	7.6483	7.5358	7.6702	7.5338	7.6591	7.5389	7.6831	**7.22**
H5	7.1746	7.3573	7.4534	7.4324	7.5546	7.4277	7.5848	7.4230	7.5694	7.4365	7.6080	7.1746	7.3573	7.4534	7.4324	7.5546	7.4277	7.5848	7.4230	7.5694	7.4365	7.6080	**7.22**
H6	8.0442	8.2217	8.3173	8.3339	8.4390	8.3277	8.5163	8.3215	8.4893	8.3395	8.5139	8.0442	8.2217	8.3173	8.3340	8.4390	8.3277	8.5163	8.3215	8.4893	8.3395	8.5139	**8.13**
H8	4.5487	4.6103	4.6487	4.6505	4.7317	4.6480	4.7922	4.6456	4.7666	4.6525	4.7815	4.5487	4.6103	4.6487	4.6505	4.7317	4.6480	4.7922	4.6456	4.7666	4.6525	4.7815	**5.5**
H(9A-9B)	1.7113	1.7539	1.7524	1.7853	1.7453	1.7826	1.7408	1.7798	1.7400	1.7877	1.7536	1.7113	1.7539	1.7524	1.7853	1.7453	1.7826	1.7408	1.7798	1.7400	1.7877	1.7536	**2.08**
H(10-13A-10-13B)	1.1616	1.1294	1.1007	1.1105	1.0608	1.1116	1.0702	1.1127	1.0660	1.1093	1.0643	1.1616	1.1294	1.1007	1.1105	1.0607	1.1116	1.0702	1.1127	1.0660	1.1093	1.0643	**1.25**
H(14A-14C)	0.9157	0.9095	0.8879	0.9032	0.8741	0.9035	0.8814	0.9040	0.8772	0.9026	0.8792	0.9157	0.9095	0.8880	0.9032	0.8741	0.9035	0.8814	0.9040	0.8772	0.9026	0.8792	**0.79**
H(1`A-1`B)	2.9186	2.9337	2.9387	2.9433	2.9462	2.9425	2.9560	2.9417	2.9511	2.9439	2.9406	2.8417	2.7623	2.7236	2.7267	2.7173	2.7284	2.6966	2.7302	2.7002	2.7250	2.6837	**3.69**
H(2`-3`A-2`-3`B)	1.6408	1.6949	1.6551	1.7247	1.6878	1.7226	1.7131	1.7206	1.7015	1.7266	1.7431	1.6408	1.6949	1.6552	1.7247	1.6878	1.7226	1.7131	1.7206	1.7015	1.7266	1.7431	**2.18**
H(4`A)	2.8936	2.7373	2.6776	2.6751	2.6869	2.6778	2.6327	2.6807	2.6344	2.6725	2.6390	3.1656	3.2005	3.2285	3.2348	3.2894	3.2320	3.2897	3.2293	3.2817	3.2372	3.2913	**3.12**
H(4`B)	2.7899	2.7873	2.7697	2.7784	2.7475	2.7791	2.7606	2.7798	2.7661	2.7774	2.7283	2.6717	2.6669	2.6490	2.6519	2.6029	2.6531	2.6223	2.6542	2.6206	2.6505	2.5899	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. XII

Nuclei	R											S										Exp. [b]
	TPSS																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	132.6431	133.3692	134.6530	133.6871	135.6963	133.6711	135.0989	133.6679	134.1747	133.7141	135.4892	132.6431	133.3692	134.6530	133.6872	135.6963	133.6711	135.0989	133.6679	134.7758	133.7141	135.4892	**131.79**
C2	133.1442	133.1763	133.8071	133.0800	133.5898	133.0942	134.0060	133.1197	133.6243	133.0766	133.8999	133.1442	133.1763	133.8072	133.0800	133.5898	133.0942	134.0060	133.1197	134.2317	133.0766	133.8999	**131.93**
C3	116.7789	117.4529	118.1353	117.7142	118.3710	117.7080	118.7172	117.7128	118.1558	117.7299	118.7330	116.7789	117.4529	118.1352	117.7142	118.3710	117.7080	118.7174	117.7127	118.9403	117.7299	118.7330	**116.53**
C4	170.8802	171.6960	172.4941	172.1468	172.8983	172.1270	173.5111	172.1181	172.7787	172.1761	173.6168	170.8803	171.6960	172.4940	172.1468	172.8983	172.1270	173.5111	172.1180	172.9376	172.1761	173.6168	**168.1**
C5	114.7362	115.9002	116.5875	116.5520	117.3692	116.5192	117.6735	116.4976	116.9357	116.5938	117.8249	114.7362	115.9002	116.5875	116.5520	117.3692	116.5192	117.6734	116.4976	117.7343	116.5938	117.8249	**116.51**
C6	129.0800	130.7781	131.8087	131.8789	133.2965	131.8151	133.9728	131.7627	132.2619	131.9507	134.2677	129.0799	130.7781	131.8088	131.8789	133.2965	131.8151	133.9728	131.7627	132.8849	131.9507	134.2677	**131.88**
C7	197.0469	200.9591	202.6423	203.1270	204.5358	202.9926	208.8170	202.8720	203.6556	203.2684	210.0679	197.0469	200.9591	202.6422	203.1270	204.5358	202.9926	208.8167	202.8721	203.4610	203.2684	210.0679	**195.2**
C8	66.1696	67.1861	68.0220	67.8051	68.7263	67.7677	69.4487	67.7436	67.9867	67.8532	69.8394	66.1696	67.1861	68.0220	67.8051	68.7263	67.7677	69.4487	67.7436	69.3460	67.8532	69.8394	**54.87**
C9	37.5030	37.2667	37.4312	37.2625	37.4754	37.2666	37.6827	37.2830	37.4042	37.2697	37.7671	37.5030	37.2667	37.4311	37.2625	37.4754	37.2667	37.6827	37.2831	39.1139	37.2697	37.7671	**31.13**
C10	27.8243	28.2961	28.6307	28.5745	29.1536	28.5633	28.9464	28.5637	28.6501	28.5959	29.0343	27.8243	28.2961	28.6307	28.5745	29.1536	28.5633	28.9464	28.5636	30.4598	28.5959	29.0343	**30.82**
C11	36.7157	36.7237	37.1380	36.7020	37.2158	36.7114	37.1875	36.7318	36.8508	36.7036	37.3744	36.7157	36.7237	37.1380	36.7020	37.2158	36.7114	37.1875	36.7318	38.5667	36.7036	37.3744	**29.11**
C12	38.0575	38.3083	38.6669	38.5109	39.0243	38.5040	38.9241	38.5086	38.6347	38.5282	38.9725	38.0576	38.3083	38.6668	38.5110	39.0243	38.5040	38.9240	38.5085	40.3301	38.5282	38.9725	**25.52**
C13	29.9782	30.1067	30.4070	30.1814	30.4937	30.1841	30.5018	30.1981	30.2910	30.1893	30.4865	29.9782	30.1067	30.4071	30.1814	30.4937	30.1841	30.5017	30.1981	32.0821	30.1893	30.4865	**22.36**
C14	17.4025	17.5248	17.6687	17.6412	17.7640	17.6400	17.7655	17.6503	17.6930	17.6530	17.7660	17.4025	17.5248	17.6687	17.6412	17.7640	17.6400	17.7656	17.6503	19.6284	17.6530	17.7660	**13.85**
C1`	53.1950	53.8980	54.2342	54.3618	54.9247	54.3378	54.8783	54.3256	54.5150	54.3954	55.3578	57.2279	58.1168	58.6670	58.6676	59.1270	58.6371	59.4942	58.6187	60.2895	58.7078	59.8143	**51.23**
C2`	26.2853	26.6610	27.0509	26.9332	27.2995	26.9200	27.4418	26.9190	26.9988	26.9570	27.2702	26.0917	26.4160	26.8595	26.5702	27.1629	26.5718	27.0823	26.5835	28.4946	26.5782	26.8115	**23.85**
C3`	26.0917	26.4160	26.8596	26.5702	27.1629	26.5718	27.0822	26.5835	26.6619	26.5782	26.8115	26.2853	26.6610	27.0510	26.9332	27.2995	26.9200	27.4419	26.9190	28.8275	26.9570	27.2702	**23.66**
C4`	57.2279	58.1168	58.6670	58.6676	59.1270	58.6371	59.4943	58.6188	58.8254	58.7078	59.8143	53.1950	53.8980	54.2342	54.3618	54.9247	54.3378	54.8783	54.3255	56.0285	54.3954	55.3578	**52.72**
H2	8.5634	8.4717	8.4568	8.4221	8.3504	8.4258	8.3826	8.4298	8.2699	8.4188	8.3378	8.5634	8.4717	8.4568	8.4221	8.3504	8.4258	8.3826	8.4298	8.5398	8.4188	8.3378	**8.13**
H3	7.1752	7.3069	7.4019	7.3509	7.4660	7.3489	7.4839	7.3473	7.1831	7.3532	7.4910	7.1752	7.3069	7.4019	7.3509	7.4660	7.3489	7.4839	7.3473	7.4654	7.3532	7.4910	**7.22**
H5	6.9831	7.1594	7.2434	7.2410	7.3584	7.2363	7.3795	7.2323	7.0676	7.2458	7.4006	6.9831	7.1594	7.2434	7.2410	7.3584	7.2363	7.3794	7.2323	7.3513	7.2458	7.4006	**7.22**
H6	7.8314	8.0028	8.1011	8.1065	8.2386	8.1005	8.3189	8.0950	7.9338	8.1124	8.3158	7.8314	8.0028	8.1011	8.1065	8.2386	8.1005	8.3189	8.0950	8.2075	8.1124	8.3158	**8.13**
H8	4.7401	4.7995	4.8477	4.8370	4.9324	4.8353	4.9749	4.8340	4.6597	4.8388	4.9472	4.7401	4.7995	4.8477	4.8370	4.9324	4.8353	4.9749	4.8340	4.9710	4.8388	4.9472	**5.5**
H(9A-9B)	1.7558	1.7977	1.7807	1.8477	1.8329	1.8439	1.8321	1.8408	1.6546	1.8518	1.8543	1.7558	1.7977	1.7807	1.8477	1.8329	1.8439	1.8321	1.8408	2.0002	1.8518	1.8543	**2.08**
H(10-13A-10-13B)	1.2065	1.1759	1.1500	1.1651	1.1240	1.1659	1.1281	1.1672	0.9783	1.1648	1.1193	1.2065	1.1759	1.1500	1.1651	1.1240	1.1659	1.1281	1.1672	1.3317	1.1648	1.1193	**1.25**
H(14A-14C)	0.9231	0.9174	0.9037	0.9167	0.8930	0.9169	0.8965	0.9176	0.7277	0.9169	0.8913	0.9231	0.9174	0.9037	0.9167	0.8930	0.9169	0.8966	0.9176	1.0839	0.9169	0.8913	**0.79**
H(1`A-1`B)	2.9922	3.0060	3.0214	3.0226	3.0358	3.0215	3.0431	3.0210	2.9618	3.0241	3.0256	2.9514	2.8647	2.8394	2.8272	2.8278	2.8293	2.7939	2.8321	2.9109	2.8257	2.7758	**3.69**
H(2`-3`A-2`-3`B)	1.6816	1.7385	1.7128	1.7726	1.7424	1.7705	1.7626	1.7691	1.5826	1.7748	1.7921	1.6816	1.7385	1.7128	1.7726	1.7424	1.7705	1.7626	1.7691	1.9290	1.7748	1.7921	**2.18**
H(4`A)	3.0666	2.8949	2.8478	2.8274	2.8512	2.8312	2.7738	2.8356	2.8344	2.8243	2.7664	3.2629	3.2878	3.3308	3.3296	3.3942	3.3266	3.3943	3.3242	3.3114	3.3329	3.3926	**3.12**
H(4`B)	2.8362	2.8345	2.8310	2.8270	2.8043	2.8274	2.8141	2.8285	2.9875	2.8271	2.7852	2.7215	2.7241	2.7120	2.7156	2.6773	2.7164	2.6919	2.7177	2.6123	2.7153	2.6587	**3.86**
Nuclei	VSXC																						
C1	132.9913	133.8687	134.2186	134.1798	135.8469	134.1613	134.7906	134.1414	134.9416	134.1995	135.3764	132.9912	133.8688	134.2187	134.1798	135.8469	134.1605	134.7906	134.1414	134.9416	134.1995	135.3764	**131.79**
C2	131.9016	132.4916	132.3087	132.5746	133.1440	132.5738	133.6235	132.5708	133.4960	132.5770	134.0213	131.9015	132.4915	132.3087	132.5745	133.1440	132.5728	133.6235	132.5708	133.4960	132.5771	134.0213	**131.93**
C3	114.2836	115.1112	115.8291	115.4866	116.1079	115.4687	116.4200	115.4483	116.3553	115.5049	116.4367	114.2836	115.1112	115.8291	115.4866	116.1079	115.4689	116.4200	115.4483	116.3553	115.5049	116.4367	**116.53**
C4	168.4847	169.2847	170.1404	169.7411	170.4527	169.7166	171.0396	169.6900	170.8966	169.7657	171.0774	168.4847	169.2846	170.1403	169.7411	170.4527	169.7169	171.0396	169.6900	170.8966	169.7659	171.0774	**168.1**
C5	112.7525	113.9731	114.8506	114.7206	115.3906	114.6768	115.8656	114.6310	115.7341	114.7638	115.9213	112.7524	113.9733	114.8505	114.7206	115.3906	114.6771	115.8656	114.6310	115.7341	114.7639	115.9213	**116.51**
C6	128.2883	129.8342	131.0689	130.8446	132.2272	130.7830	132.9675	130.7199	132.7013	130.9046	133.0916	128.2884	129.8345	131.0690	130.8445	132.2273	130.7835	132.9675	130.7199	132.7013	130.9045	133.0916	**131.88**
C7	192.0578	197.1385	198.7114	199.7272	200.7822	199.5698	205.0687	199.4106	204.2809	199.8787	206.3825	192.0578	197.1384	198.7114	199.7272	200.7822	199.5694	205.0687	199.4106	204.2809	199.8788	206.3825	**195.2**
C8	70.9636	71.8452	72.2988	72.3206	73.0868	72.2922	73.2077	72.2621	73.1865	72.3494	73.7289	70.9635	71.8453	72.2988	72.3205	73.0868	72.2921	73.2077	72.2621	73.1865	72.3494	73.7289	**54.87**
C9	41.8378	42.2481	42.6850	42.4824	42.7074	42.4716	43.3798	42.4586	43.2604	42.4943	43.5170	41.8378	42.2482	42.6850	42.4825	42.7075	42.4718	43.3798	42.4586	43.2604	42.4943	43.5170	**31.13**
C10	34.2844	35.1783	35.5087	35.7771	36.5291	35.7388	36.2073	35.6993	36.2122	35.8157	36.2373	34.2844	35.1783	35.5087	35.7771	36.5291	35.7389	36.2073	35.6993	36.2122	35.8157	36.2373	**30.82**
C11	44.2356	44.1076	44.5504	43.9961	44.4650	44.0076	44.4099	44.0168	44.4290	43.9867	44.4238	44.2356	44.1076	44.5504	43.9961	44.4650	44.0077	44.4099	44.0168	44.4290	43.9867	44.4238	**29.11**
C12	44.6745	45.1459	45.4750	45.5152	46.0875	45.4925	45.9143	45.4682	45.8827	45.5388	46.1113	44.6746	45.1459	45.4750	45.5151	46.0875	45.4928	45.9143	45.4682	45.8828	45.5387	46.1113	**25.52**
C13	34.2196	34.4402	34.5525	34.5069	34.7822	34.5062	34.7034	34.5035	34.7088	34.5090	34.7422	34.2196	34.4401	34.5524	34.5068	34.7822	34.5063	34.7034	34.5035	34.7088	34.5090	34.7422	**22.36**
C14	19.1790	19.4566	19.4615	19.6309	19.7023	19.6223	19.6772	19.6118	19.6576	19.6407	19.7427	19.1790	19.4567	19.4614	19.6309	19.7023	19.6224	19.6772	19.6118	19.6576	19.6407	19.7427	**13.85**
C1`	58.6628	59.1314	59.6320	59.5094	60.0212	59.4874	60.0324	59.4636	59.9928	59.5319	60.2583	60.3236	60.9500	61.3845	61.3694	61.9100	61.3458	61.9632	61.3200	61.8994	61.3937	62.3136	**51.23**
C2`	29.5483	29.9545	30.2674	30.2010	30.5179	30.1891	30.6085	30.1749	30.5444	30.2138	30.6036	29.5124	30.1971	30.3036	30.5294	30.9429	30.5112	30.7115	30.4912	30.7243	30.5483	30.7726	**23.85**
C3`	29.5125	30.1971	30.3035	30.5294	30.9429	30.5113	30.7115	30.4912	30.7243	30.5482	30.7726	29.5482	29.9545	30.2673	30.2010	30.5178	30.1893	30.6085	30.1749	30.5444	30.2139	30.6036	**23.66**
C4`	60.3235	60.9501	61.3846	61.3695	61.9100	61.3457	61.9632	61.3200	61.8994	61.3937	62.3136	58.6628	59.1314	59.6319	59.5094	60.0212	59.4876	60.0324	59.4637	59.9928	59.5318	60.2583	**52.72**
H2	8.6042	8.5849	8.5596	8.5442	8.5301	8.5474	8.5965	8.5505	8.5884	8.5411	8.5707	8.6042	8.5848	8.5596	8.5442	8.5301	8.5474	8.5965	8.5505	8.5884	8.5411	8.5707	**8.13**
H3	7.1677	7.3341	7.4127	7.3933	7.5076	7.3902	7.5365	7.3871	7.5258	7.3962	7.5631	7.1677	7.3341	7.4127	7.3933	7.5076	7.3901	7.5365	7.3871	7.5258	7.3962	7.5631	**7.22**
H5	7.1688	7.3794	7.4713	7.4763	7.6021	7.4706	7.6362	7.4650	7.6222	7.4817	7.6593	7.1688	7.3794	7.4713	7.4763	7.6021	7.4706	7.6362	7.4650	7.6222	7.4817	7.6593	**7.22**
H6	7.8106	7.9122	8.0739	7.9917	8.1152	7.9868	8.1860	7.9820	8.1628	7.9962	8.1820	7.8106	7.9123	8.0739	7.9916	8.1152	7.9869	8.1860	7.9820	8.1628	7.9962	8.1820	**8.13**
H8	4.3216	4.4280	4.4412	4.4988	4.5680	4.4940	4.6014	4.4894	4.5848	4.5034	4.6276	4.3216	4.4280	4.4412	4.4988	4.5680	4.4940	4.6014	4.4894	4.5848	4.5034	4.6276	**5.5**
H(9A-9B)	1.9578	1.9573	1.9925	1.9764	1.9549	1.9753	1.9848	1.9743	1.9748	1.9774	1.9738	1.9578	1.9573	1.9925	1.9764	1.9550	1.9753	1.9848	1.9743	1.9748	1.9775	1.9738	**2.08**
H(10-13A-10-13B)	1.4590	1.4284	1.4192	1.4185	1.3725	1.4191	1.3747	1.4198	1.3774	1.4178	1.3667	1.4590	1.4284	1.4192	1.4185	1.3725	1.4191	1.3747	1.4198	1.3774	1.4178	1.3667	**1.25**
H(14A-14C)	1.0509	1.0460	1.0293	1.0458	1.0153	1.0458	1.0177	1.0459	1.0184	1.0457	1.0201	1.0509	1.0460	1.0293	1.0458	1.0153	1.0458	1.0177	1.0459	1.0184	1.0457	1.0201	**0.79**
H(1`A-1`B)	2.7912	2.8035	2.8361	2.8146	2.8263	2.8140	2.8398	2.8136	2.8384	2.8151	2.8315	2.8090	2.7978	2.7791	2.7976	2.7849	2.7974	2.7857	2.7974	2.7875	2.7978	2.8029	**3.69**
H(2`-3`A-2`-3`B)	1.9592	2.0007	1.9765	2.0286	1.9894	2.0269	2.0025	2.0252	2.0001	2.0303	2.0158	1.9592	2.0007	1.9764	2.0286	1.9894	2.0268	2.0025	2.0252	2.0001	2.0303	2.0158	**2.18**
H(4`A)	2.7525	2.7231	2.6918	2.7244	2.7178	2.7239	2.7096	2.7235	2.7110	2.7250	2.7392	3.1565	3.1483	3.1855	3.1526	3.1911	3.1524	3.1933	3.1523	3.1880	3.1528	3.1709	**3.12**
H(4`B)	2.8655	2.8724	2.8665	2.8708	2.8521	2.8710	2.8617	2.8714	2.8641	2.8705	2.8666	2.4259	2.4587	2.4868	2.4766	2.4615	2.4757	2.4862	2.4749	2.4889	2.4774	2.4921	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. XIII

Nuclei	R											S										Exp. [b]
	wB97											wB97										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.5766	137.3594	138.1260	137.6724	140.4401	137.6450	139.4392	137.6186	139.4597	137.7009	139.9575	136.5766	137.3593	138.1260	137.6724	140.4401	137.6450	139.4392	137.6186	139.4596	137.7009	139.9574	**131.79**
C2	140.4685	140.3001	140.8566	140.1547	140.5969	140.1639	141.0458	140.1726	140.9313	140.1462	141.0183	140.4685	140.3002	140.8565	140.1547	140.5970	140.1639	141.0457	140.1726	140.9313	140.1462	141.0184	**131.93**
C3	121.5378	122.2517	122.8388	122.4590	123.2476	122.4476	123.4235	122.4354	123.3515	122.4698	123.5035	121.5378	122.2516	122.8389	122.4590	123.2477	122.4476	123.4234	122.4353	123.3514	122.4698	123.5035	**116.53**
C4	174.2773	174.7850	175.4147	175.1288	175.6400	175.1067	176.3065	175.0838	176.1345	175.1501	176.4401	174.2773	174.7849	175.4147	175.1288	175.6401	175.1067	176.3065	175.0836	176.1344	175.1501	176.4401	**168.1**
C5	119.5456	120.8101	121.4496	121.4743	122.3960	121.4321	122.5623	121.3893	122.4646	121.5149	122.7488	119.5456	120.8100	121.4497	121.4743	122.3960	121.4321	122.5621	121.3893	122.4646	121.5149	122.7488	**116.51**
C6	136.5805	138.2301	139.3700	139.2863	140.3915	139.2182	140.9173	139.1492	140.7461	139.3513	141.1652	136.5805	138.2302	139.3701	139.2863	140.3914	139.2182	140.9172	139.1493	140.7460	139.3513	141.1650	**131.88**
C7	201.6463	206.4608	207.5887	209.0875	210.6245	208.9109	215.9725	208.7363	214.7012	209.2585	217.3934	201.6463	206.4612	207.5888	209.0875	210.6245	208.9109	215.9722	208.7366	214.7013	209.2585	217.3938	**195.2**
C8	61.7455	62.8833	63.4808	63.4940	64.6671	63.4525	65.0662	63.4114	64.9445	63.5345	65.5074	61.7455	62.8834	63.4809	63.4940	64.6671	63.4525	65.0663	63.4113	64.9445	63.5345	65.5073	**54.87**
C9	33.5167	33.2336	33.4833	33.1151	33.3909	33.1202	33.1733	33.1248	33.2413	33.1108	33.2707	33.5167	33.2337	33.4833	33.1151	33.3909	33.1202	33.1733	33.1248	33.2413	33.1108	33.2707	**31.13**
C10	25.8672	26.3101	26.5752	26.5660	27.1186	26.5467	26.9017	26.5274	26.9138	26.5852	27.0669	25.8672	26.3101	26.5752	26.5660	27.1186	26.5467	26.9017	26.5274	26.9138	26.5852	27.0668	**30.82**
C11	34.2071	34.1679	34.5774	34.1229	34.6501	34.1256	34.5453	34.1275	34.5297	34.1208	34.6686	34.2071	34.1679	34.5774	34.1229	34.6501	34.1256	34.5453	34.1275	34.5297	34.1208	34.6684	**29.11**
C12	35.7033	35.9379	36.1713	36.1331	36.5655	36.1181	36.4807	36.1028	36.4464	36.1480	36.5998	35.7033	35.9380	36.1714	36.1331	36.5654	36.1181	36.4806	36.1028	36.4464	36.1480	36.5997	**25.52**
C13	26.6927	26.8320	27.0551	26.9015	27.2054	26.8962	27.1583	26.8904	27.1533	26.9068	27.1541	26.6928	26.8320	27.0552	26.9015	27.2053	26.8962	27.1584	26.8903	27.1533	26.9068	27.1541	**22.36**
C14	16.3113	16.4253	16.4646	16.5253	16.6006	16.5170	16.5818	16.5082	16.5514	16.5337	16.6294	16.3113	16.4252	16.4646	16.5253	16.6005	16.5170	16.5817	16.5082	16.5515	16.5337	16.6295	**13.85**
C1`	49.2269	49.8987	50.1374	50.3713	50.9952	50.3391	50.8596	50.3069	50.7986	50.4027	51.2045	52.9612	53.7707	54.0904	54.2507	54.8314	54.2195	54.8883	54.1880	54.8731	54.2810	55.1596	**51.23**
C2`	23.7270	24.0800	24.3404	24.2659	24.6995	24.2532	24.6453	24.2401	24.6806	24.2786	24.5276	23.2048	23.4265	23.7238	23.5664	24.0018	23.5579	23.9665	23.5483	23.9404	23.5747	23.8415	**23.85**
C3`	23.2048	23.4265	23.7237	23.5664	24.0019	23.5579	23.9666	23.5484	23.9404	23.5747	23.8415	23.7270	24.0799	24.3405	24.2659	24.6995	24.2532	24.6453	24.2402	24.6806	24.2786	24.5276	**23.66**
C4`	52.9612	53.7706	54.0904	54.2507	54.8314	54.2195	54.8883	54.1879	54.8730	54.2810	55.1595	49.2269	49.8988	50.1375	50.3713	50.9951	50.3391	50.8597	50.3069	50.7986	50.4027	51.2045	**52.72**
H2	8.8724	8.7491	8.7863	8.6793	8.5895	8.6843	8.6425	8.6890	8.6380	8.6746	8.6164	8.8724	8.7491	8.7863	8.6793	8.5895	8.6843	8.6425	8.6890	8.6380	8.6746	8.6164	**8.13**
H3	7.4319	7.5633	7.6560	7.6034	7.7299	7.6014	7.7489	7.5992	7.7407	7.6053	7.7719	7.4319	7.5633	7.6560	7.6034	7.7299	7.6014	7.7488	7.5992	7.7407	7.6053	7.7719	**7.22**
H5	7.2789	7.4716	7.5614	7.5532	7.6889	7.5484	7.7078	7.5434	7.6946	7.5579	7.7299	7.2789	7.4716	7.5614	7.5532	7.6889	7.5484	7.7078	7.5434	7.6946	7.5579	7.7299	**7.22**
H6	8.1395	8.3534	8.4518	8.4456	8.5192	8.4401	8.5680	8.4344	8.5513	8.4508	8.5743	8.1395	8.3534	8.4518	8.4456	8.5192	8.4401	8.5680	8.4344	8.5513	8.4508	8.5743	**8.13**
H8	4.2193	4.2959	4.3345	4.3559	4.3971	4.3521	4.4955	4.3482	4.4576	4.3595	4.4989	4.2193	4.2959	4.3345	4.3559	4.3971	4.3521	4.4955	4.3482	4.4576	4.3595	4.4989	**5.5**
H(9A-9B)	1.7181	1.7422	1.7461	1.7618	1.7278	1.7600	1.6924	1.7582	1.6997	1.7637	1.7137	1.7181	1.7423	1.7461	1.7618	1.7278	1.7600	1.6924	1.7582	1.6997	1.7637	1.7137	**2.08**
H(10-13A-10-13B)	1.1800	1.1362	1.1057	1.1138	1.0559	1.1151	1.0669	1.1164	1.0649	1.1125	1.0617	1.1800	1.1362	1.1057	1.1138	1.0559	1.1151	1.0669	1.1164	1.0649	1.1125	1.0616	**1.25**
H(14A-14C)	0.9509	0.9415	0.9189	0.9335	0.9024	0.9339	0.9073	0.9344	0.9045	0.9331	0.9088	0.9509	0.9415	0.9189	0.9335	0.9024	0.9339	0.9073	0.9344	0.9046	0.9331	0.9088	**0.79**
H(1`A-1`B)	2.8458	2.8628	2.8625	2.8691	2.8686	2.8686	2.8673	2.8681	2.8652	2.8696	2.8575	2.7570	2.6979	2.6726	2.6748	2.6892	2.6757	2.6583	2.6766	2.6689	2.6741	2.6447	**3.69**
H(2`-3`A-2`-3`B)	1.6371	1.6957	1.6590	1.7288	1.6911	1.7265	1.7123	1.7242	1.7035	1.7310	1.7349	1.6371	1.6957	1.6590	1.7288	1.6911	1.7265	1.7123	1.7242	1.7035	1.7310	1.7349	**2.18**
H(4`A)	2.7521	2.6218	2.5829	2.5857	2.6278	2.5867	2.5647	2.5876	2.5741	2.5851	2.5696	3.0727	3.1009	3.1242	3.1261	3.1760	3.1241	3.1560	3.1221	3.1557	3.1281	3.1587	**3.12**
H(4`B)	2.7619	2.7740	2.7622	2.7639	2.7506	2.7648	2.7519	2.7656	2.7636	2.7631	2.7198	2.6189	2.6247	2.6007	2.6121	2.5612	2.6131	2.5786	2.6140	2.5748	2.6111	2.5564	**3.86**
Nuclei	wB97X																						
C1	138.1299	138.9213	139.6895	139.2775	142.0220	139.2463	141.0530	139.2168	141.0141	139.3107	141.7243	138.1297	138.9213	139.6895	139.2775	142.0221	139.2463	141.0528	139.2168	141.0141	139.3108	141.7242	**131.79**
C2	140.9942	140.8612	141.4139	140.6949	141.0699	140.7095	141.5535	140.7231	141.3910	140.6817	141.4634	140.9940	140.8612	141.4140	140.6951	141.0700	140.7095	141.5534	140.7231	141.3908	140.6817	141.4634	**131.93**
C3	122.2386	122.9738	123.5544	123.1948	123.9888	123.1846	124.2448	123.1736	124.1140	123.2053	124.3187	122.2385	122.9738	123.5546	123.1949	123.9889	123.1846	124.2450	123.1736	124.1140	123.2054	124.3187	**116.53**
C4	174.9421	175.5141	176.1407	175.8751	176.4170	175.8547	177.1464	175.8334	176.9230	175.8955	177.2427	174.9421	175.5141	176.1407	175.8750	176.4170	175.8547	177.1466	175.8334	176.9230	175.8954	177.2427	**168.1**
C5	120.2375	121.5000	122.1360	122.1851	123.0981	122.1436	123.3186	122.1013	123.1528	122.2261	123.5110	120.2375	121.5000	122.1359	122.1852	123.0980	122.1436	123.3186	122.1013	123.1527	122.2261	123.5111	**116.51**
C6	136.9227	138.6345	139.7439	139.6857	140.7727	139.6224	141.3431	139.5581	141.0988	139.7464	141.5056	136.9227	138.6345	139.7437	139.6857	140.7726	139.6224	141.3430	139.5581	141.0986	139.7465	141.5056	**131.88**
C7	203.3192	208.1159	209.2399	210.7848	212.4050	210.6052	217.6835	210.4286	216.3531	210.9607	219.2110	203.3193	208.1159	209.2399	210.7848	212.4050	210.6052	217.6836	210.4286	216.3534	210.9607	219.2110	**195.2**
C8	63.0626	64.1293	64.7526	64.7950	66.0155	64.7516	66.3913	64.7083	66.1781	64.8382	66.8567	63.0626	64.1293	64.7526	64.7950	66.0154	64.7516	66.3914	64.7083	66.1780	64.8381	66.8566	**54.87**
C9	34.2852	33.9993	34.2357	33.8688	34.0983	33.8782	33.9536	33.8870	33.8705	33.8612	34.0173	34.2852	33.9993	34.2357	33.8688	34.0984	33.8782	33.9537	33.8870	33.8705	33.8612	34.0174	**31.13**
C10	26.1979	26.6938	26.9377	26.9426	27.4542	26.9269	27.2908	26.9110	27.2205	26.9591	27.4263	26.1980	26.6938	26.9377	26.9426	27.4543	26.9269	27.2909	26.9110	27.2205	26.9591	27.4263	**30.82**
C11	34.9115	34.8919	35.3008	34.8566	35.3866	34.8616	35.3189	34.8656	35.2187	34.8528	35.4505	34.9115	34.8919	35.3007	34.8565	35.3866	34.8616	35.3188	34.8656	35.2187	34.8528	35.4506	**29.11**
C12	36.4461	36.6968	36.9234	36.8833	37.3129	36.8714	37.2621	36.8589	37.1991	36.8958	37.3713	36.4463	36.6968	36.9234	36.8832	37.3129	36.8713	37.2622	36.8589	37.1992	36.8958	37.3714	**25.52**
C13	27.2122	27.3622	27.5893	27.4426	27.7508	27.4396	27.7362	27.4356	27.6582	27.4464	27.7069	27.2122	27.3622	27.5892	27.4426	27.7508	27.4396	27.7362	27.4356	27.6582	27.4464	27.7069	**22.36**
C14	16.3336	16.4536	16.4851	16.5547	16.6179	16.5490	16.6380	16.5426	16.5589	16.5613	16.6696	16.3336	16.4536	16.4850	16.5547	16.6179	16.5490	16.6380	16.5426	16.5589	16.5613	16.6696	**13.85**
C1`	50.0000	50.6871	50.9073	51.1813	51.7778	51.1500	51.6798	51.1185	51.5484	51.2125	52.0610	53.9250	54.7891	55.1185	55.3233	55.8958	55.2927	56.0245	55.2614	55.8655	55.3536	56.2672	**51.23**
C2`	24.2203	24.5256	24.7925	24.7476	25.1751	24.7362	25.1295	24.7238	25.0642	24.7597	24.9785	23.7235	23.8719	24.1660	23.9670	24.4078	23.9621	24.4086	23.9564	24.3464	23.9728	24.2873	**23.85**
C3`	23.7235	23.8719	24.1660	23.9671	24.4077	23.9621	24.4087	23.9564	24.3464	23.9727	24.2873	24.2204	24.5256	24.7925	24.7476	25.1752	24.7362	25.1295	24.7239	25.0642	24.7596	24.9785	**23.66**
C4`	53.9249	54.7891	55.1185	55.3232	55.8958	55.2927	56.0245	55.2614	55.8656	55.3535	56.2671	50.0000	50.6871	50.9073	51.1813	51.7777	51.1500	51.6798	51.1185	51.5485	51.2126	52.0610	**52.72**
H2	8.8468	8.7316	8.7702	8.6580	8.5595	8.6640	8.6180	8.6698	8.6173	8.6523	8.5723	8.8468	8.7316	8.7702	8.6580	8.5595	8.6640	8.6180	8.6698	8.6173	8.6523	8.5723	**8.13**
H3	7.4132	7.5501	7.6417	7.5927	7.7166	7.5908	7.7369	7.5888	7.7250	7.5946	7.7553	7.4132	7.5501	7.6417	7.5927	7.7166	7.5908	7.7369	7.5888	7.7250	7.5946	7.7553	**7.22**
H5	7.2592	7.4412	7.5320	7.5241	7.6575	7.5194	7.6768	7.5146	7.6634	7.5289	7.6969	7.2592	7.4412	7.5320	7.5242	7.6575	7.5194	7.6768	7.5146	7.6634	7.5289	7.6969	**7.22**
H6	8.1094	8.3185	8.4150	8.4119	8.4870	8.4067	8.5450	8.4014	8.5224	8.4169	8.5459	8.1094	8.3185	8.4150	8.4119	8.4870	8.4067	8.5450	8.4014	8.5224	8.4169	8.5459	**8.13**
H8	4.3111	4.3797	4.4205	4.4327	4.4761	4.4294	4.5807	4.4260	4.5524	4.4359	4.5771	4.3111	4.3797	4.4205	4.4327	4.4761	4.4294	4.5807	4.4260	4.5524	4.4359	4.5771	**5.5**
H(9A-9B)	1.6978	1.7311	1.7339	1.7520	1.7137	1.7507	1.6791	1.7493	1.6786	1.7534	1.6896	1.6978	1.7311	1.7339	1.7520	1.7138	1.7507	1.6791	1.7493	1.6786	1.7534	1.6896	**2.08**
H(10-13A-10-13B)	1.1724	1.1351	1.1039	1.1141	1.0560	1.1157	1.0690	1.1172	1.0651	1.1127	1.0621	1.1724	1.1351	1.1039	1.1141	1.0561	1.1157	1.0690	1.1172	1.0651	1.1127	1.0621	**1.25**
H(14A-14C)	0.9443	0.9364	0.9134	0.9301	0.8968	0.9306	0.9038	0.9313	0.8990	0.9295	0.9047	0.9443	0.9364	0.9134	0.9301	0.8968	0.9306	0.9038	0.9313	0.8990	0.9295	0.9047	**0.79**
H(1`A-1`B)	2.8683	2.8838	2.8843	2.8922	2.8893	2.8918	2.8928	2.8915	2.8882	2.8927	2.8800	2.7736	2.7098	2.6823	2.6866	2.6969	2.6875	2.6627	2.6885	2.6646	2.6858	2.6521	**3.69**
H(2`-3`A-2`-3`B)	1.6388	1.6963	1.6577	1.7307	1.6902	1.7285	1.7131	1.7263	1.7017	1.7329	1.7369	1.6388	1.6963	1.6577	1.7307	1.6902	1.7285	1.7131	1.7263	1.7017	1.7329	1.7370	**2.18**
H(4`A)	2.7697	2.6348	2.5915	2.5930	2.6285	2.5940	2.5664	2.5953	2.5648	2.5923	2.5784	3.0879	3.1206	3.1455	3.1477	3.1942	3.1459	3.1856	3.1443	3.1797	3.1496	3.1845	**3.12**
H(4`B)	2.7775	2.7848	2.7730	2.7802	2.7653	2.7810	2.7591	2.7818	2.7644	2.7795	2.7259	2.6488	2.6471	2.6232	2.6366	2.5845	2.6377	2.6000	2.6387	2.5967	2.6358	2.5756	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S13. Cont. XIV

Nuclei	R											S										Exp. [b]
	X3LYP											X3LYP										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.7752	140.6233	142.0342	140.9941	143.3465	140.9645	142.4467	140.9347	142.5664	141.0291	143.0033	139.7752	140.6233	142.0341	140.9941	143.3465	140.9645	142.4467	140.9347	142.5664	141.0291	143.0034	**131.79**
C2	139.9480	140.0001	140.5021	139.8489	140.2813	139.8661	140.7454	139.8792	140.6341	139.8353	140.6566	139.9480	140.0001	140.5022	139.8489	140.2813	139.8661	140.7455	139.8792	140.6340	139.8353	140.6567	**131.93**
C3	122.1645	122.8471	123.4040	123.0598	123.6653	123.0543	123.9468	123.0449	123.8840	123.0682	123.9781	122.1645	122.8471	123.4041	123.0598	123.6653	123.0543	123.9468	123.0449	123.8842	123.0682	123.9781	**116.53**
C4	176.3694	177.1817	177.8217	177.6088	178.2096	177.5876	178.8349	177.5629	178.6820	177.6321	178.9147	176.3694	177.1817	177.8216	177.6088	178.2096	177.5876	178.8347	177.5629	178.6821	177.6321	178.9145	**168.1**
C5	119.9157	121.1807	121.7927	121.8448	122.6528	121.8077	122.9102	121.7676	122.8089	121.8838	123.0895	119.9157	121.1807	121.7926	121.8448	122.6528	121.8077	122.9101	121.7676	122.8088	121.8838	123.0895	**116.51**
C6	135.8092	137.6619	138.5551	138.8279	140.0982	138.7580	140.8348	138.6852	140.5733	138.8979	141.0672	135.8092	137.6619	138.5549	138.8279	140.0982	138.7580	140.8349	138.6852	140.5735	138.8979	141.0672	**131.88**
C7	203.6220	208.3755	210.2577	210.9910	212.5015	210.8173	217.4697	210.6449	216.3878	211.1644	218.9304	203.6220	208.3755	210.2577	210.9910	212.5015	210.8173	217.4697	210.6448	216.3880	211.1644	218.9304	**195.2**
C8	66.1788	67.3414	68.1509	67.9113	68.9572	67.8723	69.5528	67.8325	69.4244	67.9544	69.9257	66.1788	67.3414	68.1510	67.9113	68.9572	67.8723	69.5527	67.8325	69.4242	67.9544	69.9258	**54.87**
C9	37.0947	36.7857	36.7812	36.6633	36.7889	36.6758	36.9304	36.6851	36.8767	36.6550	36.9461	37.0947	36.7857	36.7811	36.6633	36.7889	36.6758	36.9303	36.6851	36.8770	36.6550	36.9461	**31.13**
C10	27.6451	28.1769	28.4658	28.4595	29.0406	28.4452	28.8511	28.4277	28.8484	28.4767	28.9320	27.6451	28.1769	28.4658	28.4595	29.0406	28.4452	28.8511	28.4277	28.8483	28.4767	28.9320	**30.82**
C11	37.3161	37.3989	37.7411	37.3514	37.8849	37.3614	37.8431	37.3678	37.8343	37.3451	38.0150	37.3161	37.3989	37.7410	37.3514	37.8849	37.3614	37.8431	37.3678	37.8343	37.3451	38.0150	**29.11**
C12	39.0036	39.3104	39.6082	39.5235	40.0174	39.5121	39.8999	39.4976	39.8944	39.5385	39.9577	39.0036	39.3104	39.6082	39.5235	40.0174	39.5121	39.8998	39.4976	39.8945	39.5385	39.9578	**25.52**
C13	29.8878	30.0926	30.3116	30.1665	30.4610	30.1666	30.4498	30.1634	30.4449	30.1698	30.4417	29.8878	30.0926	30.3116	30.1665	30.4610	30.1666	30.4499	30.1634	30.4449	30.1698	30.4417	**22.36**
C14	16.8547	17.0413	17.0928	17.1574	17.2377	17.1532	17.2197	17.1459	17.2124	17.1650	17.2326	16.8547	17.0413	17.0927	17.1574	17.2377	17.1532	17.2196	17.1459	17.2123	17.1650	17.2325	**13.85**
C1`	52.2481	53.0282	53.3441	53.5289	54.1218	53.4999	54.0613	53.4681	53.9973	53.5604	54.5658	56.6734	57.6328	58.0744	58.2033	58.6935	58.1690	58.9314	58.1319	58.8436	58.2399	59.2528	**51.23**
C2`	25.8667	26.3543	26.6750	26.5823	27.0062	26.5698	27.0888	26.5548	27.0717	26.5981	26.9352	25.5836	25.9175	26.2849	26.0313	26.6417	26.0303	26.5072	26.0256	26.5110	26.0354	26.2969	**23.85**
C3`	25.5836	25.9175	26.2849	26.0313	26.6417	26.0303	26.5072	26.0256	26.5111	26.0354	26.2969	25.8667	26.3543	26.6749	26.5823	27.0062	26.5698	27.0889	26.5548	27.0718	26.5981	26.9352	**23.66**
C4`	56.6734	57.6328	58.0744	58.2033	58.6935	58.1690	58.9315	58.1319	58.8438	58.2399	59.2529	52.2481	53.0282	53.3442	53.5289	54.1218	53.4999	54.0613	53.4681	53.9972	53.5604	54.5657	**52.72**
H2	8.6986	8.5988	8.5569	8.5349	8.4425	8.5410	8.4901	8.5461	8.4856	8.5285	8.4461	8.6986	8.5988	8.5569	8.5349	8.4425	8.5410	8.4901	8.5461	8.4856	8.5285	8.4461	**8.13**
H3	7.3299	7.4564	7.5391	7.4967	7.5996	7.4952	7.6168	7.4931	7.6090	7.4980	7.6284	7.3299	7.4564	7.5391	7.4967	7.5996	7.4952	7.6169	7.4931	7.6090	7.4980	7.6285	**7.22**
H5	7.1252	7.3063	7.3933	7.3886	7.5115	7.3841	7.5362	7.3791	7.5250	7.3927	7.5645	7.1252	7.3063	7.3933	7.3886	7.5115	7.3841	7.5362	7.3791	7.5250	7.3927	7.5645	**7.22**
H6	7.9630	8.1497	8.2478	8.2632	8.3855	8.2563	8.4629	8.2489	8.4425	8.2696	8.4643	7.9630	8.1497	8.2478	8.2632	8.3855	8.2563	8.4629	8.2489	8.4426	8.2696	8.4643	**8.13**
H8	4.5959	4.6713	4.7112	4.7173	4.8026	4.7146	4.8465	4.7114	4.8324	4.7199	4.8238	4.5959	4.6713	4.7112	4.7173	4.8026	4.7146	4.8465	4.7114	4.8324	4.7199	4.8238	**5.5**
H(9A-9B)	1.6794	1.7257	1.6972	1.7704	1.7429	1.7678	1.7453	1.7645	1.7395	1.7730	1.7624	1.6794	1.7257	1.6971	1.7704	1.7429	1.7678	1.7453	1.7645	1.7395	1.7730	1.7624	**2.08**
H(10-13A-10-13B)	1.2032	1.1730	1.1413	1.1627	1.1164	1.1636	1.1212	1.1640	1.1210	1.1618	1.1168	1.2032	1.1730	1.1413	1.1627	1.1164	1.1636	1.1212	1.1640	1.1210	1.1618	1.1168	**1.25**
H(14A-14C)	0.9595	0.9537	0.9350	0.9530	0.9252	0.9533	0.9275	0.9531	0.9271	0.9528	0.9263	0.9595	0.9537	0.9350	0.9530	0.9252	0.9533	0.9275	0.9531	0.9271	0.9528	0.9263	**0.79**
H(1`A-1`B)	2.9708	2.9890	2.9979	3.0057	3.0129	3.0048	3.0200	3.0033	3.0189	3.0067	3.0025	2.8846	2.8020	2.7803	2.7707	2.7684	2.7723	2.7460	2.7736	2.7488	2.7694	2.7326	**3.69**
H(2`-3`A-2`-3`B)	1.6654	1.7225	1.6970	1.7606	1.7246	1.7582	1.7444	1.7553	1.7386	1.7630	1.7745	1.6654	1.7225	1.6970	1.7606	1.7246	1.7582	1.7444	1.7553	1.7386	1.7630	1.7745	**2.18**
H(4`A)	2.8965	2.7420	2.7067	2.6986	2.7177	2.7006	2.6639	2.7023	2.6652	2.6969	2.6736	3.1938	3.2320	3.2704	3.2779	3.3396	3.2748	3.3379	3.2713	3.3341	3.2808	3.3350	**3.12**
H(4`B)	2.8726	2.8619	2.8539	2.8429	2.8192	2.8441	2.8280	2.8449	2.8323	2.8419	2.7916	2.7478	2.7459	2.7254	2.7336	2.6862	2.7348	2.7021	2.7354	2.7037	2.7326	2.6701	**3.86**

[a] methyl protons shifts are averaged
[b] according to [12]

Table S14. Theoretical chemical shifts (in ppm) of *(R,S)*-4-fluoro-α-pyrrolidinobutyrophenone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S									Exp. [b]
	B3LYP																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.4828	140.8601	141.0780	141.5114	143.5654	141.4590	142.9237	141.4086	142.8797	141.5624	143.1650	139.4828	140.8601	141.0780	141.5116	143.5655	141.4589	142.9237	141.4086	142.8797	141.5626	143.1650	**131.91**
C2	139.7139	139.6390	140.1816	139.5185	140.1697	139.5183	140.6491	139.5192	140.5332	139.5178	140.6883	139.7139	139.6390	140.1816	139.5185	140.1697	139.5186	140.6490	139.5193	140.5332	139.5180	140.6883	**131.65**
C3	121.7769	122.5971	123.1005	122.8272	123.5116	122.8103	123.8079	122.7933	123.7260	122.8413	123.8440	121.7769	122.5971	123.1005	122.8271	123.5116	122.8103	123.8080	122.7933	123.7260	122.8413	123.8440	**116.7**
C4	176.3708	177.2123	177.8981	177.5361	178.1936	177.5130	178.7872	177.4894	178.6329	177.5563	178.8941	176.3708	177.2123	177.8981	177.5359	178.1936	177.5129	178.7873	177.4895	178.6329	177.5562	178.8941	**166.84**
C5	119.9309	121.2165	121.8308	121.8184	122.5774	121.7765	122.8204	121.7346	122.7017	121.8569	122.9502	119.9309	121.2166	121.8308	121.8184	122.5774	121.7765	122.8204	121.7346	122.7017	121.8569	122.9502	**116.7**
C6	135.7473	137.5120	138.8314	138.4057	139.6223	138.3511	140.2599	138.2953	140.0273	138.4546	140.5977	135.7473	137.5120	138.8314	138.4057	139.6223	138.3512	140.2599	138.2952	140.0273	138.4545	140.5977	**131.65**
C7	203.5193	208.7924	209.4490	211.5358	212.4515	211.3577	217.7129	211.1810	216.4646	211.7052	218.7990	203.5193	208.7924	209.4490	211.5359	212.4515	211.3577	217.7129	211.1813	216.4645	211.7053	218.7990	**194.89**
C8	66.4139	67.8629	68.1923	68.4183	69.0761	68.3871	69.8726	68.3540	69.6357	68.4447	70.2526	66.4139	67.8629	68.1923	68.4185	69.0760	68.3870	69.8726	68.3540	69.6357	68.4447	70.2526	**65.05**
C9	29.6092	29.5091	29.6459	29.3733	29.2241	29.3864	29.6107	29.3971	29.5049	29.3567	29.6311	29.6092	29.5091	29.6459	29.3733	29.2240	29.3863	29.6106	29.3970	29.5049	29.3567	29.6311	**24.22**
C10	8.5219	8.8670	9.0241	8.9232	9.1226	8.9188	9.0844	8.9134	9.0590	8.9251	9.1520	8.5219	8.8670	9.0241	8.9233	9.1227	8.9189	9.0845	8.9135	9.0590	8.9250	9.1520	**10.45**
C1`	52.3002	53.1555	53.4631	53.6230	54.2265	53.5864	54.2406	53.5501	54.1597	53.6563	54.6389	56.7796	57.8268	58.2036	58.2917	58.9005	58.2547	59.0667	58.2187	58.9818	58.3264	59.2956	**50.48**
C2`	26.0777	26.5709	26.9149	26.7131	27.1346	26.7003	27.2250	26.6871	27.1920	26.7241	27.0507	25.8545	26.0027	26.3845	26.1079	26.6874	26.0941	26.5554	26.0810	26.5386	26.1200	26.3411	**23.91**
C3`	25.8545	26.0027	26.3845	26.1079	26.6874	26.0941	26.5553	26.0810	26.5386	26.1200	26.3411	26.0777	26.5709	26.9149	26.7132	27.1346	26.7001	27.2249	26.6872	27.1920	26.7240	27.0507	**23.74**
C4`	56.7796	57.8267	58.2036	58.2916	58.9006	58.2546	59.0667	58.2187	58.9818	58.3263	59.2956	52.3002	53.1555	53.4631	53.6230	54.2265	53.5865	54.2407	53.5502	54.1597	53.6563	54.6389	**52.48**
H2	8.6890	8.5481	8.6258	8.4698	8.4597	8.4744	8.4767	8.4790	8.4820	8.4651	8.4725	8.6890	8.5482	8.6258	8.4698	8.4597	8.4745	8.4767	8.4790	8.4820	8.4651	8.4725	**8.08**
H3	7.3023	7.4350	7.5184	7.4836	7.6081	7.4805	7.6278	7.4774	7.6168	7.4863	7.6439	7.3023	7.4350	7.5184	7.4836	7.6081	7.4805	7.6278	7.4774	7.6168	7.4863	7.6439	**7.23**
H5	7.1694	7.3383	7.4405	7.4027	7.5183	7.3988	7.5321	7.3948	7.5202	7.4062	7.5525	7.1694	7.3383	7.4405	7.4028	7.5183	7.3988	7.5321	7.3948	7.5202	7.4062	7.5525	**7.23**
H6	7.9686	8.1161	8.2330	8.2110	8.3323	8.2044	8.3665	8.1979	8.3506	8.2172	8.3915	7.9686	8.1161	8.2330	8.2110	8.3323	8.2044	8.3665	8.1979	8.3506	8.2172	8.3915	**8.08**
H8	4.6380	4.6871	4.7388	4.7267	4.8029	4.7234	4.8102	4.7202	4.7981	4.7298	4.7968	4.6380	4.6871	4.7388	4.7267	4.8028	4.7234	4.8101	4.7202	4.7981	4.7298	4.7968	**5.3**
H(9A)	1.9978	2.0755	2.0903	2.1231	2.1130	2.1204	2.1446	2.1174	2.1300	2.1254	2.1770	1.5791	1.5953	1.6173	1.5734	1.5114	1.5770	1.5144	1.5799	1.5168	1.5690	2.1770	**2.21**
H(9B)	1.5791	1.5953	1.6173	1.5734	1.5114	1.5770	1.5144	1.5799	1.5168	1.5690	1.5528	1.9978	2.0755	2.0903	2.1231	2.1130	2.1204	2.1446	2.1174	2.1300	2.1254	1.5528	**2.14**
H(10A-10C)	0.8519	0.7800	0.7565	0.7523	0.7089	0.7533	0.7233	0.7544	0.7216	0.7513	0.7188	0.8519	0.7800	0.7565	0.7523	0.7089	0.7533	0.7233	0.7544	0.7216	0.7513	0.7188	**1.01**
H(1`A-1`B)	2.9795	3.0097	3.0088	3.0181	3.0193	3.0176	3.0166	3.0170	3.0137	3.0183	3.0026	2.8907	2.8290	2.7850	2.7993	2.7740	2.8012	2.7632	2.8030	2.7608	2.7972	3.0026	**3.68**
H(2`-3`A-2`-3`B)	1.6689	1.7318	1.6874	1.7697	1.7328	1.7666	1.7477	1.7635	1.7395	1.7725	1.7726	1.6689	1.7318	1.6874	1.7697	1.7328	1.7666	1.7477	1.7635	1.7395	1.7725	1.7726	**2.19**
H(4`A)	2.9034	2.7715	2.7061	2.7345	2.7210	2.7367	2.6909	2.7388	2.6864	2.7321	2.6873	3.1978	3.2567	3.2807	3.2898	3.3392	3.2877	3.3234	3.2856	3.3181	3.2914	2.6873	**3.02**
H(4`B)	2.8780	2.8865	2.8640	2.8640	2.8270	2.8656	2.8354	2.8671	2.8352	2.8622	2.8054	2.7612	2.7627	2.7370	2.7464	2.6994	2.7475	2.7097	2.7485	2.7093	2.7452	2.8054	**3.83**
Nuclei	B3P86																						
C1	136.8836	137.9280	138.6491	138.4297	140.7966	138.4284	140.1803	138.4041	140.1661	138.4737	140.2584	136.8836	137.9280	138.6491	138.4298	140.7965	138.4284	140.1803	138.4042	140.1661	138.4735	140.2584	**131.91**
C2	138.7785	138.6776	139.3220	138.5641	139.1953	138.5910	139.7368	138.5961	139.7311	138.5827	139.7636	138.7785	138.6776	139.3221	138.5641	139.1953	138.5910	139.7368	138.5961	139.7311	138.5827	139.7636	**131.65**
C3	120.9580	121.7817	122.4305	122.0667	122.8867	122.0730	123.1998	122.0573	123.2260	122.1040	123.2547	120.9580	121.7817	122.4306	122.0666	122.8868	122.0730	123.1998	122.0572	123.2260	122.1041	123.2547	**116.7**
C4	173.8709	174.6917	175.3955	175.0637	175.6985	175.0611	176.3254	175.0371	176.3009	175.1100	176.4550	173.8709	174.6917	175.3955	175.0636	175.6988	175.0611	176.3254	175.0370	176.3009	175.1100	176.4550	**166.84**
C5	119.1744	120.5163	121.1913	121.1813	122.0259	121.1610	122.2923	121.1190	122.2841	121.2443	122.4529	119.1744	120.5163	121.1913	121.1814	122.0259	121.1610	122.2923	121.1190	122.2841	121.2443	122.4529	**116.7**
C6	134.8041	136.6574	137.7930	137.6415	138.8194	137.5983	139.3085	137.5337	139.2366	137.7268	139.7688	134.8041	136.6574	137.7930	137.6415	138.8194	137.5983	139.3085	137.5336	139.2366	137.7269	139.7688	**131.65**
C7	201.6813	206.4361	207.4719	208.9388	210.2428	208.8171	215.1444	208.6716	213.9615	209.0968	216.0874	201.6813	206.4361	207.4719	208.9388	210.2428	208.8171	215.1444	208.6715	213.9615	209.0968	216.0874	**194.89**
C8	64.7417	66.0406	66.5452	66.6565	67.5886	66.6470	68.1788	66.6143	67.9975	66.7082	68.6889	64.7417	66.0406	66.5452	66.6565	67.5886	66.6470	68.1788	66.6144	67.9975	66.7083	68.6889	**65.05**
C9	28.5917	28.5842	28.7161	28.5344	28.5430	28.5575	28.6966	28.5585	28.7070	28.5560	28.8688	28.5917	28.5842	28.7161	28.5344	28.5429	28.5575	28.6966	28.5584	28.7070	28.5560	28.8688	**24.22**
C10	8.2705	8.5859	8.7652	8.7053	8.9608	8.7199	8.8203	8.7125	8.8963	8.7352	8.9754	8.2705	8.5859	8.7652	8.7053	8.9608	8.7199	8.8203	8.7125	8.8963	8.7352	8.9754	**10.45**
C1`	51.1951	52.0169	52.3795	52.5015	53.1062	52.4938	53.0791	52.4647	53.0967	52.5531	53.5321	55.4732	56.4695	56.8838	56.9575	57.5094	56.9487	57.7645	56.9181	57.8008	57.0101	57.9944	**50.48**
C2`	24.8220	25.2420	25.6352	25.4398	25.8508	25.4488	25.8957	25.4359	25.9708	25.4749	25.7987	24.5100	24.6380	25.0628	24.7563	25.3156	24.7678	25.2120	24.7575	25.3165	24.7898	25.0252	**23.91**
C3`	24.5100	24.6380	25.0628	24.7564	25.3156	24.7678	25.2120	24.7575	25.3165	24.7897	25.0252	24.8220	25.2420	25.6351	25.4397	25.8507	25.4488	25.8957	25.4359	25.9708	25.4750	25.7987	**23.74**
C4`	55.4732	56.4695	56.8839	56.9575	57.5094	56.9487	57.7645	56.9182	57.8008	57.0101	57.9944	51.1951	52.0169	52.3795	52.5016	53.1062	52.4938	53.0791	52.4646	53.0967	52.5531	53.5321	**52.48**
H2	8.7555	8.6376	8.6808	8.5686	8.5162	8.5730	8.5499	8.5758	8.5686	8.5657	8.5528	8.7555	8.6376	8.6808	8.5686	8.5162	8.5730	8.5499	8.5758	8.5686	8.5657	8.5528	**8.08**
H3	7.3225	7.4583	7.5498	7.5058	7.6401	7.5045	7.6643	7.5014	7.6589	7.5082	7.6804	7.3225	7.4583	7.5498	7.5058	7.6401	7.5045	7.6643	7.5014	7.6589	7.5082	7.6804	**7.23**
H5	7.1886	7.3705	7.4676	7.4396	7.5546	7.4367	7.5671	7.4319	7.5622	7.4437	7.5896	7.1886	7.3705	7.4676	7.4396	7.5545	7.4367	7.5671	7.4319	7.5622	7.4437	7.5896	**7.23**
H6	8.0502	8.2070	8.3003	8.2985	8.4076	8.2935	8.4458	8.2867	8.4422	8.3047	8.4836	8.0502	8.2070	8.3003	8.2985	8.4077	8.2935	8.4458	8.2866	8.4422	8.3047	8.4836	**8.08**
H8	4.6395	4.6910	4.7319	4.7332	4.8065	4.7306	4.8259	4.7264	4.8261	4.7369	4.8276	4.6395	4.6910	4.7319	4.7332	4.8065	4.7306	4.8259	4.7264	4.8261	4.7369	4.8276	**5.3**
H(9A)	2.0257	2.1082	2.1131	2.1597	2.1529	2.1575	2.1676	2.1534	2.1607	2.1631	2.2096	1.6623	1.6878	1.6798	1.6839	1.6154	1.6858	1.5635	1.6858	1.5758	1.6832	1.6325	**2.21**
H(9B)	1.6623	1.6878	1.6798	1.6839	1.6154	1.6858	1.5635	1.6858	1.5758	1.6832	1.6325	2.0257	2.1082	2.1131	2.1597	2.1528	2.1575	2.1676	2.1534	2.1607	2.1631	2.2096	**2.14**
H(10A-10C)	0.8231	0.7544	0.7310	0.7225	0.6702	0.7254	0.6915	0.7265	0.6982	0.7211	0.6858	0.8231	0.7544	0.7310	0.7225	0.6702	0.7254	0.6915	0.7265	0.6982	0.7211	0.6858	**1.01**
H(1`A-1`B)	2.9570	2.9858	2.9886	2.9926	2.9995	2.9931	2.9912	2.9918	2.9958	2.9933	2.9774	2.8887	2.8143	2.7836	2.7793	2.7785	2.7825	2.7436	2.7837	2.7473	2.7776	2.7284	**3.68**
H(2`-3`A-2`-3`B)	1.6564	1.7176	1.6818	1.7538	1.7205	1.7526	1.7388	1.7497	1.7367	1.7562	1.7648	1.6564	1.7176	1.6818	1.7538	1.7205	1.7526	1.7388	1.7497	1.7367	1.7562	1.7648	**2.19**
H(4`A)	2.9482	2.7911	2.7413	2.7369	2.7627	2.7404	2.6863	2.7422	2.6887	2.7347	2.6789	3.2010	3.2556	3.2751	3.2836	3.3389	3.2828	3.3148	3.2802	3.3168	3.2856	3.3165	**3.02**
H(4`B)	2.8293	2.8376	2.8260	2.8218	2.7943	2.8245	2.8008	2.8252	2.8059	2.8205	2.7779	2.7130	2.7161	2.7022	2.7016	2.6601	2.7034	2.6675	2.7034	2.6748	2.7010	2.6382	**3.83**
Nuclei	B3PW91																						
C1	137.1378	138.4706	138.9735	139.1170	141.6407	139.0793	140.5527	139.0315	140.5116	139.1531	140.7674	137.1378	138.4705	138.9735	139.1170	141.3217	139.0793	140.5527	139.0315	140.5116	139.1531	140.7674	**131.91**
C2	138.8483	138.8029	139.3414	138.7073	139.7042	138.7176	139.8518	138.7187	139.7672	138.7001	139.9064	138.8483	138.8028	139.3415	138.7073	139.3852	138.7176	139.8518	138.7187	139.7672	138.7001	139.9064	**131.65**
C3	121.0799	121.9386	122.5010	122.2085	123.3019	122.1993	123.2678	122.1805	123.2010	122.2192	123.3341	121.0799	121.9386	122.5010	122.2085	122.9829	122.1993	123.2678	122.1805	123.2010	122.2192	123.3341	**116.7**
C4	173.9189	174.7305	175.3790	175.0539	176.0096	175.0392	176.3155	175.0159	176.1825	175.0705	176.4451	173.9189	174.7306	175.3790	175.0539	175.6906	175.0392	176.3155	175.0159	176.1825	175.0705	176.4451	**166.84**
C5	119.2605	120.6072	121.2018	121.2633	122.4151	121.2275	122.3409	121.1832	122.2382	121.2993	122.5062	119.2605	120.6072	121.2018	121.2633	122.0961	121.2275	122.3409	121.1832	122.2382	121.2993	122.5062	**116.7**
C6	134.8136	136.5906	137.7321	137.4819	139.0112	137.4336	139.2920	137.3773	139.0921	137.5305	139.6634	134.8136	136.5907	137.7320	137.4819	138.6922	137.4337	139.2920	137.3773	139.0921	137.5305	139.6634	**131.65**
C7	201.6923	206.7464	207.5948	209.4173	210.8576	209.2578	215.4231	209.0875	214.1917	209.5688	216.4735	201.6923	206.7465	207.5947	209.4173	210.5386	209.2578	215.4231	209.0875	214.1917	209.5688	216.4735	**194.89**
C8	64.6787	66.1211	66.5468	66.7686	67.9506	66.7401	68.2311	66.7009	67.9879	66.7957	68.6951	64.6787	66.1211	66.5469	66.7686	67.6316	66.7401	68.2311	66.7009	67.9879	66.7957	68.6951	**65.05**
C9	28.3648	28.3678	28.4671	28.2729	28.5966	28.2852	28.5082	28.2882	28.4130	28.2634	28.5963	28.3648	28.3678	28.4671	28.2729	28.2776	28.2852	28.5082	28.2882	28.4130	28.2634	28.5963	**24.22**
C10	8.3363	8.6767	8.7890	8.7744	9.3303	8.7761	8.8912	8.7685	8.8738	8.7744	9.0339	8.3363	8.6767	8.7890	8.7744	9.0113	8.7761	8.8912	8.7685	8.8738	8.7744	9.0339	**10.45**
C1`	51.1228	51.9598	52.2370	52.4487	53.3444	52.4272	52.9958	52.3963	52.9276	52.4707	53.4334	55.4114	56.4306	56.7432	56.9125	57.4594	56.8873	57.6785	56.8533	57.6166	56.9387	57.9183	**50.48**
C2`	25.0911	25.5313	25.8406	25.7001	26.4134	25.6951	26.1426	25.6810	26.1268	25.7067	25.9969	24.7692	24.9210	25.2534	25.0260	25.5638	25.0216	25.4362	25.0087	25.4454	25.0328	25.2379	**23.91**
C3`	24.7692	24.9209	25.2534	25.0260	25.8828	25.0216	25.4362	25.0087	25.4454	25.0328	25.2379	25.0911	25.5313	25.8406	25.7001	26.0944	25.6951	26.1426	25.6810	26.1268	25.7067	25.9969	**23.74**
C4`	55.4114	56.4306	56.7432	56.9125	57.7784	56.8873	57.6785	56.8533	57.6166	56.9387	57.9183	51.1228	51.9598	52.2369	52.4487	53.0254	52.4272	52.9958	52.3963	52.9276	52.4707	53.4334	**52.48**
H2	8.7299	8.5890	8.6433	8.5111	8.4939	8.5162	8.5209	8.5212	8.5306	8.5066	8.5163	8.7299	8.5890	8.6433	8.5111	8.4784	8.5162	8.5209	8.5212	8.5306	8.5066	8.5163	**8.08**
H3	7.3242	7.4615	7.5515	7.5113	7.6542	7.5090	7.6621	7.5064	7.6533	7.5135	7.6766	7.3242	7.4615	7.5515	7.5113	7.6387	7.5090	7.6621	7.5064	7.6533	7.5135	7.6766	**7.23**
H5	7.1834	7.3556	7.4545	7.4268	7.5614	7.4231	7.5634	7.4191	7.5533	7.4305	7.5832	7.1834	7.3556	7.4545	7.4268	7.5459	7.4231	7.5634	7.4191	7.5533	7.4305	7.5832	**7.23**
H6	8.0322	8.1803	8.2794	8.2709	8.3917	8.2655	8.4228	8.2599	8.4114	8.2763	8.4481	8.0322	8.1803	8.2794	8.2709	8.3762	8.2655	8.4228	8.2599	8.4114	8.2763	8.4481	**8.08**
H8	4.6317	4.6774	4.7215	4.7162	4.7983	4.7128	4.8076	4.7094	4.7995	4.7198	4.8012	4.6317	4.6774	4.7215	4.7162	4.7828	4.7128	4.8076	4.7094	4.7995	4.7198	4.8012	**5.3**
H(9A)	1.9896	2.0678	2.0784	2.1173	2.1286	2.1149	2.1377	2.1121	2.1250	2.1198	2.1719	1.6198	1.6299	1.6383	1.6131	1.5509	1.6166	1.5278	1.6196	1.5318	1.6097	1.5736	**2.21**
H(9B)	1.6198	1.6299	1.6383	1.6131	1.5664	1.6166	1.5278	1.6196	1.5318	1.6097	1.5736	1.9896	2.0678	2.0784	2.1173	2.1131	2.1149	2.1377	2.1121	2.1250	2.1198	2.1719	**2.14**
H(10A-10C)	0.8072	0.7381	0.7130	0.7090	0.6728	0.7110	0.6793	0.7129	0.6809	0.7073	0.6731	0.8072	0.7381	0.7130	0.7090	0.6574	0.7110	0.6793	0.7129	0.6809	0.7073	0.6731	**1.01**
H(1`A-1`B)	2.9415	2.9696	2.9717	2.9758	2.9962	2.9755	2.9774	2.9751	2.9770	2.9763	2.9608	2.8624	2.7980	2.7668	2.7664	2.7572	2.7684	2.7304	2.7701	2.7302	2.7648	2.7125	**3.68**
H(2`-3`A-2`-3`B)	1.6441	1.7050	1.6668	1.7431	1.7215	1.7410	1.7246	1.7387	1.7189	1.7453	1.7490	1.6441	1.7050	1.6668	1.7431	1.7060	1.7410	1.7246	1.7387	1.7189	1.7453	1.7490	**2.19**
H(4`A)	2.8992	2.7645	2.7144	2.7172	2.7472	2.7191	2.6694	2.7208	2.6678	2.7157	2.6612	3.1767	3.2312	3.2533	3.2604	3.3131	3.2588	3.2949	3.2570	3.2919	3.2620	3.2938	**3.02**
H(4`B)	2.8255	2.8316	2.8191	2.8157	2.7981	2.8177	2.7914	2.8193	2.7927	2.8139	2.7638	2.7062	2.7080	2.6900	2.6913	2.6483	2.6923	2.6600	2.6931	2.6622	2.6906	2.6278	**3.83**

[a] methyl protons shifts are averaged [b] according to [13] in $CDCl_3$

Table S14. Cont. I

Nuclei	R											S									Exp. [b]
	B98																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	138.0895	139.3262	139.5103	139.8526	142.0323	139.8370	141.3566	139.8180	141.3476	139.8684	141.5873	138.0895	139.3264	139.5103	139.8525	142.0323	139.8370	141.3566	139.8181	141.3476	139.8682	141.5873	**131.91**
C2	138.5327	138.4347	138.9651	138.3464	139.0357	138.3663	139.4705	138.3841	139.3869	138.3298	139.5112	138.5327	138.4346	138.9651	138.3463	139.0357	138.3663	139.4705	138.3840	139.3869	138.3298	139.5112	**131.65**
C3	120.8609	121.6536	122.1837	121.9011	122.6513	121.9036	122.9164	121.9033	122.8582	121.9008	122.9639	120.8609	121.6535	122.1836	121.9011	122.6513	121.9036	122.9165	121.9033	122.8582	121.9008	122.9639	**116.7**
C4	173.7300	174.5011	175.1988	174.8412	175.5050	174.8355	176.0816	174.8274	175.9511	174.8493	176.1984	173.7300	174.5011	175.1987	174.8413	175.5050	174.8355	176.0816	174.8274	175.9511	174.8494	176.1984	**166.84**
C5	119.0016	120.2696	120.8867	120.9271	121.7648	120.9014	121.9894	120.8732	121.8908	120.9541	122.1339	119.0016	120.2697	120.8867	120.9273	121.7648	120.9014	121.9894	120.8731	121.8908	120.9542	122.1339	**116.7**
C6	134.7500	136.4405	137.7513	137.3800	138.5556	137.3362	139.1668	137.2904	138.9572	137.4244	139.5057	134.7500	136.4405	137.7514	137.3802	138.5556	137.3362	139.1668	137.2904	138.9572	137.4245	139.5057	**131.65**
C7	200.0993	205.2330	205.8069	207.8907	208.8976	207.7449	214.1629	207.5954	212.9246	208.0286	215.2370	200.0993	205.2329	205.8071	207.8906	208.8976	207.7449	214.1629	207.5952	212.9246	208.0286	215.2370	**194.89**
C8	66.3027	67.6937	67.9568	68.3028	69.0056	68.2872	69.7561	68.2667	69.5333	68.3172	70.1746	66.3027	67.6936	67.9568	68.3029	69.0056	68.2872	69.7561	68.2668	69.5333	68.3171	70.1746	**65.05**
C9	29.4819	29.4579	29.5637	29.3921	29.2854	29.4139	29.6225	29.4333	29.5316	29.3737	29.6604	29.4819	29.4580	29.5637	29.3921	29.2854	29.4139	29.6226	29.4334	29.5316	29.3737	29.6604	**24.22**
C10	8.9753	9.2568	9.3695	9.3566	9.5471	9.3675	9.4943	9.3751	9.4823	9.3477	9.5852	8.9753	9.2567	9.3695	9.3566	9.5471	9.3675	9.4943	9.3751	9.4823	9.3477	9.5852	**10.45**
C1`	52.3942	53.1621	53.4348	53.6553	54.2356	53.6403	54.2196	53.6212	54.1613	53.6704	54.6249	56.8261	57.7455	58.1211	58.2175	58.8417	58.2019	58.9932	58.1838	58.9351	58.2347	59.2134	**50.48**
C2`	26.2704	26.6559	26.9849	26.8459	27.2546	26.8487	27.3257	26.8488	27.3121	26.8453	27.1787	25.9448	26.0723	26.4407	26.1998	26.7733	26.2044	26.6343	26.2073	26.6448	26.1983	26.4409	**23.91**
C3`	25.9448	26.0724	26.4406	26.1998	26.7733	26.2044	26.6342	26.2072	26.6448	26.1983	26.4409	26.2704	26.6559	26.9849	26.8459	27.2546	26.8487	27.3257	26.8488	27.3121	26.8453	27.1787	**23.74**
C4`	56.8261	57.7454	58.1212	58.2175	58.8417	58.2019	58.9933	58.1839	58.9351	58.2347	59.2134	52.3942	53.1621	53.4348	53.6553	54.2356	53.6403	54.2197	53.6212	54.1613	53.6704	54.6249	**52.48**
H2	8.7216	8.5873	8.6751	8.5166	8.4965	8.5207	8.5181	8.5251	8.5257	8.5132	8.5115	8.7216	8.5873	8.6751	8.5166	8.4965	8.5207	8.5181	8.5251	8.5257	8.5132	8.5115	**8.08**
H3	7.3168	7.4544	7.5474	7.5006	7.6285	7.4983	7.6496	7.4961	7.6411	7.5029	7.6640	7.3168	7.4545	7.5474	7.5006	7.6285	7.4983	7.6496	7.4961	7.6411	7.5030	7.6640	**7.23**
H5	7.1733	7.3507	7.4550	7.4251	7.5471	7.4209	7.5634	7.4167	7.5532	7.4294	7.5825	7.1733	7.3507	7.4550	7.4251	7.5471	7.4209	7.5634	7.4167	7.5532	7.4294	7.5825	**7.23**
H6	7.9950	8.1500	8.2746	8.2491	8.3721	8.2426	8.4103	8.2364	8.3968	8.2557	8.4333	7.9950	8.1499	8.2746	8.2491	8.3721	8.2426	8.4103	8.2363	8.3968	8.2557	8.4333	**8.08**
H8	4.5899	4.6436	4.7037	4.6864	4.7699	4.6827	4.7835	4.6795	4.7741	4.6906	4.7727	4.5899	4.6436	4.7037	4.6864	4.7699	4.6827	4.7835	4.6795	4.7741	4.6906	4.7727	**5.3**
H(9A)	1.9842	2.0572	2.0785	2.1113	2.0992	2.1080	2.1309	2.1048	2.1182	2.1147	2.1632	1.5975	1.6097	1.6275	1.6020	1.5214	1.6039	1.5200	1.6056	1.5229	1.6000	1.5564	**2.21**
H(9B)	1.5975	1.6097	1.6275	1.6020	1.5214	1.6039	1.5200	1.6055	1.5229	1.6000	1.5564	1.9842	2.0572	2.0785	2.1113	2.0992	2.1080	2.1309	2.1048	2.1182	2.1147	2.1632	**2.14**
H(10A-10C)	0.8434	0.7702	0.7522	0.7409	0.6955	0.7426	0.7118	0.7445	0.7133	0.7396	0.7055	0.8434	0.7702	0.7522	0.7409	0.6955	0.7426	0.7118	0.7445	0.7133	0.7396	0.7055	**1.01**
H(1`A-1`B)	2.9572	2.9812	2.9871	2.9893	2.9939	2.9887	2.9941	2.9884	2.9935	2.9903	2.9786	2.8718	2.8138	2.7688	2.7825	2.7627	2.7844	2.7530	2.7865	2.7532	2.7810	2.7344	**3.68**
H(2`-3`A-2`-3`B)	1.6625	1.7233	1.6816	1.7617	1.7266	1.7593	1.7434	1.7569	1.7381	1.7644	1.7668	1.6625	1.7233	1.6816	1.7618	1.7266	1.7593	1.7434	1.7569	1.7381	1.7644	1.7668	**2.19**
H(4`A)	2.8967	2.7767	2.7058	2.7316	2.7269	2.7337	2.6953	2.7363	2.6937	2.7301	2.6866	3.1881	3.2385	3.2670	3.2708	3.3225	3.2687	3.3092	3.2669	3.3061	3.2730	3.3094	**3.02**
H(4`B)	2.8469	2.8509	2.8318	2.8334	2.7985	2.8351	2.8107	2.8368	2.8126	2.8320	2.7822	2.7263	2.7240	2.7071	2.7079	2.6653	2.7088	2.6789	2.7099	2.6809	2.7076	2.6478	**3.83**
Nuclei	B971																						
C1	137.6687	138.8544	139.0766	139.3728	141.6380	139.3553	140.9588	139.3360	140.9511	139.3938	141.1916	137.6687	138.8544	139.0768	139.3728	141.6380	139.3553	140.9588	139.3360	140.9511	139.3938	141.1915	**131.91**
C2	138.2377	138.1469	138.6812	138.0613	138.7320	138.0739	139.1621	138.0860	139.0803	138.0553	139.2051	138.2377	138.1469	138.6814	138.0613	138.7319	138.0740	139.1621	138.0860	139.0804	138.0553	139.2051	**131.65**
C3	120.6642	121.4579	121.9890	121.7160	122.4641	121.7108	122.7275	121.7044	122.6690	121.7267	122.7808	120.6642	121.4578	121.9891	121.7160	122.4640	121.7106	122.7275	121.7044	122.6690	121.7267	122.7807	**116.7**
C4	173.6312	174.4204	175.1128	174.7758	175.4249	174.7610	175.9991	174.7460	175.8687	174.7963	176.1206	173.6312	174.4203	175.1127	174.7758	175.4250	174.7608	175.9991	174.7460	175.8686	174.7963	176.1206	**166.84**
C5	118.8046	120.0802	120.6931	120.7474	121.5819	120.7135	121.8073	120.6795	121.7080	120.7856	121.9573	118.8046	120.0803	120.6930	120.7474	121.5818	120.7136	121.8073	120.6795	121.7082	120.7856	121.9574	**116.7**
C6	134.4899	136.2162	137.4905	137.1701	138.3000	137.1159	138.8968	137.0617	138.6869	137.2285	139.2431	134.4899	136.2161	137.4905	137.1701	138.2999	137.1159	138.8968	137.0617	138.6870	137.2285	139.2432	**131.65**
C7	199.9842	205.0193	205.6279	207.6468	208.7697	207.5008	213.9201	207.3522	212.7096	207.7887	215.0113	199.9842	205.0193	205.6278	207.6468	208.7694	207.5007	213.9201	207.3522	212.7095	207.7887	215.0112	**194.89**
C8	66.1161	67.4695	67.7309	68.0894	68.8160	68.0678	69.5176	68.0429	69.3003	68.1132	69.9582	66.1161	67.4696	67.7309	68.0894	68.8160	68.0678	69.5176	68.0429	69.3004	68.1132	69.9582	**65.05**
C9	29.4609	29.4611	29.5569	29.4118	29.2916	29.4228	29.6107	29.4337	29.5204	29.4071	29.6678	29.4609	29.4611	29.5569	29.4118	29.2916	29.4229	29.6107	29.4337	29.5204	29.4071	29.6677	**24.22**
C10	8.9281	9.2106	9.3145	9.3222	9.5007	9.3249	9.4414	9.3263	9.4279	9.3252	9.5517	8.9281	9.2106	9.3144	9.3222	9.5007	9.3249	9.4414	9.3263	9.4279	9.3252	9.5516	**10.45**
C1`	52.3126	53.0808	53.3386	53.5778	54.1428	53.5568	54.1150	53.5342	54.0572	53.6026	54.5273	56.7306	57.6449	58.0249	58.1224	58.7397	58.0999	58.8856	58.0769	58.8293	58.1497	59.1022	**50.48**
C2`	26.0660	26.4604	26.7870	26.6700	27.0663	26.6645	27.1283	26.6580	27.1144	26.6809	27.0080	25.7585	25.8944	26.2639	26.0323	26.5977	26.0290	26.4603	26.0256	26.4705	26.0422	26.2861	**23.91**
C3`	25.7585	25.8943	26.2639	26.0323	26.5977	26.0289	26.4603	26.0256	26.4705	26.0422	26.2860	26.0660	26.4604	26.7870	26.6700	27.0663	26.6645	27.1283	26.6580	27.1144	26.6809	27.0079	**23.74**
C4`	56.7306	57.6449	58.0249	58.1224	58.7397	58.0999	58.8856	58.0769	58.8292	58.1497	59.1024	52.3126	53.0808	53.3387	53.5778	54.1428	53.5568	54.1150	53.5342	54.0572	53.6026	54.5272	**52.48**
H2	8.7211	8.5931	8.6773	8.5245	8.4941	8.5278	8.5180	8.5315	8.5253	8.5220	8.5110	8.7211	8.5931	8.6774	8.5245	8.4941	8.5279	8.5180	8.5315	8.5253	8.5220	8.5110	**8.08**
H3	7.3147	7.4516	7.5447	7.4978	7.6249	7.4953	7.6458	7.4929	7.6374	7.5004	7.6601	7.3147	7.4516	7.5447	7.4978	7.6249	7.4953	7.6458	7.4929	7.6374	7.5004	7.6601	**7.23**
H5	7.1717	7.3497	7.4523	7.4246	7.5453	7.4201	7.5616	7.4157	7.5514	7.4293	7.5804	7.1717	7.3497	7.4523	7.4246	7.5453	7.4201	7.5616	7.4157	7.5514	7.4293	7.5804	**7.23**
H6	7.9991	8.1539	8.2770	8.2522	8.3708	8.2455	8.4094	8.2390	8.3957	8.2590	8.4321	7.9991	8.1538	8.2770	8.2522	8.3708	8.2455	8.4094	8.2390	8.3957	8.2590	8.4321	**8.08**
H8	4.5927	4.6452	4.7066	4.6888	4.7722	4.6846	4.7871	4.6809	4.7777	4.6935	4.7762	4.5927	4.6452	4.7066	4.6888	4.7722	4.6846	4.7871	4.6809	4.7776	4.6935	4.7761	**5.3**
H(9A)	1.9902	2.0629	2.0828	2.1177	2.1030	2.1140	2.1334	2.1104	2.1206	2.1216	2.1664	1.6028	1.6182	1.6295	1.6137	1.5255	1.6149	1.5207	1.6160	1.5234	1.6126	1.5593	**2.21**
H(9B)	1.6028	1.6182	1.6295	1.6137	1.5255	1.6149	1.5207	1.6160	1.5234	1.6126	1.5593	1.9902	2.0629	2.0828	2.1177	2.1030	2.1140	2.1334	2.1104	2.1206	2.1216	2.1664	**2.14**
H(10A-10C)	0.8369	0.7633	0.7470	0.7342	0.6876	0.7358	0.7046	0.7374	0.7060	0.7333	0.6988	0.8369	0.7633	0.7470	0.7342	0.6876	0.7358	0.7046	0.7374	0.7060	0.7333	0.6988	**1.01**
H(1`A-1`B)	2.9539	2.9771	2.9832	2.9857	2.9903	2.9848	2.9889	2.9840	2.9885	2.9871	2.9730	2.8680	2.8102	2.7642	2.7797	2.7615	2.7813	2.7498	2.7831	2.7502	2.7786	2.7313	**3.68**
H(2`-3`A-2`-3`B)	1.6615	1.7214	1.6802	1.7600	1.7255	1.7575	1.7420	1.7550	1.7368	1.7629	1.7654	1.6615	1.7214	1.6801	1.7600	1.7255	1.7575	1.7420	1.7550	1.7368	1.7629	1.7654	**2.19**
H(4`A)	2.9002	2.7790	2.7061	2.7327	2.7307	2.7344	2.6969	2.7366	2.6956	2.7316	2.6870	3.1917	3.2403	3.2683	3.2724	3.3239	3.2701	3.3091	3.2680	3.3061	3.2750	3.3090	**3.02**
H(4`B)	2.8359	2.8415	2.8224	2.8267	2.7923	2.8281	2.8026	2.8296	2.8048	2.8255	2.7755	2.7162	2.7140	2.6981	2.6991	2.6567	2.6994	2.6687	2.7001	2.6709	2.6992	2.6369	**3.83**
Nuclei	B972																						
C1	134.5471	136.0569	137.2319	137.0535	138.7312	137.0179	138.0424	136.9791	137.9913	137.0831	138.4048	134.5471	136.0569	137.2317	137.0535	138.7313	137.0180	138.0424	136.9791	137.9914	137.0831	138.4048	**131.91**
C2	136.2193	136.1286	136.7989	136.1042	136.7370	136.1059	137.1406	136.1058	137.0645	136.0990	137.1838	136.2193	136.1286	136.7987	136.1042	136.7370	136.1061	137.1406	136.1058	137.0645	136.0990	137.1837	**131.65**
C3	118.5462	119.3398	120.0023	119.6719	120.3503	119.6577	120.6051	119.6406	120.5424	119.6808	120.6746	118.5462	119.3398	120.0023	119.6719	120.3503	119.6577	120.6051	119.6406	120.5424	119.6808	120.6746	**116.7**
C4	170.6043	171.2822	171.9307	171.6277	172.2676	171.6042	172.8520	171.5790	172.7150	171.6463	172.9820	170.6043	171.2822	171.9308	171.6277	172.2676	171.6043	172.8520	171.5790	172.7151	171.6463	172.9820	**166.84**
C5	116.7225	117.9683	118.6045	118.6711	119.4281	118.6304	119.6424	118.5875	119.5448	118.7050	119.8015	116.7225	117.9683	118.6045	118.6711	119.4281	118.6304	119.6424	118.5875	119.5448	118.7050	119.8015	**116.7**
C6	132.2452	133.7651	134.5263	134.5691	135.8913	134.5077	136.4830	134.4447	136.2871	134.6233	136.7864	132.2452	133.7651	134.5263	134.5691	135.8913	134.5077	136.4830	134.4447	136.2871	134.6233	136.7864	**131.65**
C7	197.6034	202.7854	204.0794	205.8061	206.3506	205.6446	211.3542	205.4784	210.1128	205.9538	212.5143	197.6034	202.7854	204.0795	205.8061	206.3506	205.6446	211.3542	205.4784	210.1126	205.9538	212.5141	**194.89**
C8	63.3681	64.8531	65.1088	65.6278	66.2153	65.5927	66.9131	65.5527	66.6849	65.6541	67.3267	63.3681	64.8531	65.1088	65.6278	66.2153	65.5928	66.9131	65.5527	66.6849	65.6541	67.3267	**65.05**
C9	27.9648	27.8951	27.7481	27.8108	27.7957	27.8174	28.0865	27.8218	28.0052	27.7998	28.1181	27.9648	27.8951	27.7480	27.8108	27.7957	27.8175	28.0865	27.8218	28.0052	27.7998	28.1181	**24.22**
C10	8.6203	8.9203	8.9599	9.0565	9.2694	9.0504	9.1647	9.0410	9.1608	9.0568	9.2781	8.6203	8.9203	8.9599	9.0565	9.2694	9.0505	9.1647	9.0410	9.1608	9.0568	9.2781	**10.45**
C1`	50.3107	51.0784	51.3663	51.6232	52.1519	51.5904	52.1250	51.5532	52.0677	51.6481	52.5263	54.5983	55.5236	56.0100	56.0833	56.5994	56.0494	56.7502	56.0134	56.6843	56.1113	56.9905	**50.48**
C2`	25.0389	25.4425	25.7339	25.6639	26.0348	25.6515	26.0735	25.6366	26.0631	25.6710	25.9136	24.7114	24.8248	25.2626	25.0090	25.5062	24.9983	25.3631	24.9860	25.3662	25.0157	25.1780	**23.91**
C3`	24.7114	24.8248	25.2625	25.0090	25.5061	24.9984	25.3631	24.9860	25.3663	25.0157	25.1780	25.0389	25.4425	25.7339	25.6639	26.0348	25.6516	26.0735	25.6366	26.0630	25.6711	25.9136	**23.74**
C4`	54.5983	55.5236	56.0100	56.0833	56.5994	56.0493	56.7502	56.0134	56.6841	56.1112	56.9905	50.3107	51.0784	51.3664	51.6232	52.1519	51.5905	52.1250	51.5532	52.0676	51.6480	52.5263	**52.48**
H2	8.7155	8.5493	8.5737	8.4504	8.4632	8.4542	8.4887	8.4580	8.5002	8.4468	8.4733	8.7155	8.5493	8.5737	8.4504	8.4632	8.4543	8.4887	8.4580	8.5002	8.4468	8.4733	**8.08**
H3	7.3211	7.4578	7.5556	7.5116	7.6318	7.5090	7.6525	7.5062	7.6443	7.5139	7.6664	7.3211	7.4578	7.5556	7.5116	7.6318	7.5090	7.6525	7.5062	7.6443	7.5139	7.6664	**7.23**
H5	7.1756	7.3408	7.4299	7.4172	7.5377	7.4126	7.5542	7.4078	7.5441	7.4214	7.5749	7.1756	7.3408	7.4299	7.4172	7.5377	7.4126	7.5542	7.4078	7.5441	7.4214	7.5748	**7.23**
H6	8.0068	8.1485	8.2381	8.2296	8.3522	8.2238	8.3882	8.2179	8.3777	8.2350	8.4045	8.0068	8.1485	8.2381	8.2296	8.3522	8.2238	8.3882	8.2179	8.3777	8.2350	8.4045	**8.08**
H8	4.6074	4.6427	4.6957	4.6760	4.7506	4.6729	4.7662	4.6701	4.7566	4.6792	4.7557	4.6074	4.6427	4.6956	4.6760	4.7506	4.6729	4.7662	4.6701	4.7566	4.6792	4.7557	**5.3**
H(9A)	1.9665	2.0401	2.0209	2.0808	2.0838	2.0777	2.1139	2.0743	2.1023	2.0836	2.1414	1.5730	1.5680	1.4735	1.5196	1.4883	1.5218	1.4808	1.5234	1.4890	1.5167	1.5069	**2.21**
H(9B)	1.5730	1.5680	1.4735	1.5196	1.4883	1.5218	1.4808	1.5234	1.4890	1.5167	1.5069	1.9665	2.0401	2.0209	2.0808	2.0838	2.0777	2.1139	2.0743	2.1023	2.0836	2.1414	**2.14**
H(10A-10C)	0.8179	0.7490	0.7391	0.7239	0.6755	0.7253	0.6936	0.7266	0.6943	0.7226	0.6884	0.8179	0.7490	0.7391	0.7239	0.6755	0.7253	0.6936	0.7266	0.6943	0.7226	0.6884	**1.01**
H(1`A-1`B)	2.9432	2.9707	2.9699	2.9774	2.9796	2.9771	2.9779	2.9767	2.9776	2.9778	2.9614	2.8519	2.8010	2.7614	2.7776	2.7511	2.7796	2.7386	2.7815	2.7381	2.7756	2.7227	**3.68**
H(2`-3`A-2`-3`B)	1.6424	1.7027	1.6763	1.7462	1.7039	1.7435	1.7212	1.7407	1.7152	1.7486	1.7458	1.6424	1.7027	1.6763	1.7462	1.7039	1.7435	1.7212	1.7407	1.7152	1.7486	1.7458	**2.19**
H(4`A)	2.8725	2.7623	2.7028	2.7301	2.7185	2.7325	2.6828	2.7350	2.6801	2.7280	2.6794	3.1774	3.2330	3.2520	3.2626	3.3131	3.2608	3.2981	3.2587	3.2955	3.2643	3.2966	**3.02**
H(4`B)	2.8314	2.8396	2.8199	2.8250	2.7837	2.8266	2.7943	2.8280	2.7960	2.8231	2.7661	2.7091	2.7084	2.6879	2.6921	2.6460	2.6934	2.6577	2.6947	2.6597	2.6911	2.6262	**3.83**

[a] methyl protons shifts are averaged [b] according to [13] in $CDCl_3$

Table S14. Cont. II

Nuclei	R											S									Exp. [b]
	BHandH											BHandH									
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	138.5212	138.9902	140.1763	139.3030	141.0047	139.2786	140.0248	139.2707	140.1939	139.2942	140.3266	138.5212	138.9902	140.1763	139.3031	140.0472	139.2786	140.0248	139.2707	140.1939	139.2942	140.3267	**131.91**
C2	143.5859	143.4645	144.0313	143.3188	143.8124	143.3172	144.3691	143.3342	144.2395	143.2907	144.4328	143.5859	143.4645	144.0313	143.3187	144.0628	143.3172	144.3691	143.3342	144.2395	143.2907	144.4329	**131.65**
C3	123.6774	124.4305	125.0975	124.6796	125.3939	124.6575	125.6117	124.6533	125.5821	124.6702	125.6970	123.6774	124.4305	125.0975	124.6796	125.4237	124.6575	125.6117	124.6533	125.5821	124.6702	125.6970	**116.7**
C4	174.8030	175.5798	176.2063	175.9857	176.5699	175.9506	177.2747	175.9337	177.1177	175.9891	177.4193	174.8030	175.5798	176.2063	175.9858	176.7299	175.9506	177.2747	175.9337	177.1177	175.9891	177.4194	**166.84**
C5	121.5533	122.9602	123.6643	123.6913	124.5795	123.6364	124.7656	123.5996	124.6801	123.7133	124.9300	121.5533	122.9602	123.6643	123.6914	124.4355	123.6364	124.7656	123.5996	124.6801	123.7133	124.9300	**116.7**
C6	139.7267	141.7737	142.8229	142.9213	144.5272	142.8372	145.2124	142.7725	144.9590	142.9718	145.5729	139.7267	141.7737	142.8229	142.9214	143.6655	142.8372	145.2124	142.7725	144.9590	142.9718	145.5729	**131.65**
C7	203.8767	208.2768	209.7734	210.7971	211.5325	210.6371	216.4807	210.4930	215.3771	210.9174	217.5695	203.8767	208.2768	209.7734	210.7970	211.5411	210.6371	216.4807	210.4930	215.3771	210.9174	217.5699	**194.89**
C8	60.1695	61.2113	61.9268	61.8637	62.6072	61.8124	63.1590	61.7790	63.0334	61.8817	63.6011	60.1695	61.2113	61.9268	61.8637	62.6078	61.8124	63.1590	61.7790	63.0334	61.8817	63.6011	**65.05**
C9	25.2929	25.2744	25.3505	25.2217	25.3832	25.2133	25.5416	25.2240	25.4660	25.2002	25.6283	25.2929	25.2744	25.3505	25.2217	25.9658	25.2133	25.5416	25.2240	25.4660	25.2002	25.6284	**24.22**
C10	6.8206	7.0835	7.2156	7.2207	7.5005	7.1990	7.3586	7.1962	7.3530	7.2120	7.4915	6.8206	7.0835	7.2156	7.2208	7.9649	7.1990	7.3586	7.1962	7.3530	7.2120	7.4915	**10.45**
C1`	48.0732	48.8651	49.2967	49.4024	49.9788	49.3579	49.9293	49.3318	49.8848	49.4151	50.3428	52.0603	53.0074	53.4703	53.5625	54.3066	53.5170	54.2364	53.4899	54.1747	53.5751	54.5228	**50.48**
C2`	21.5192	21.9011	22.2732	22.1414	22.5433	22.1153	22.6029	22.1075	22.5977	22.1362	22.5780	21.1146	21.3188	21.6815	21.4312	22.1753	21.4129	21.8669	21.4131	21.8834	21.4186	21.7649	**23.91**
C3`	21.1146	21.3188	21.6815	21.4312	21.9388	21.4129	21.8669	21.4131	21.8834	21.4186	21.7649	21.5192	21.9011	22.2732	22.1415	22.8856	22.1153	22.6029	22.1075	22.5977	22.1362	22.5780	**23.74**
C4`	52.0603	53.0074	53.4703	53.5624	54.0551	53.5170	54.2364	53.4899	54.1747	53.5751	54.5228	48.0732	48.8651	49.2967	49.4025	50.1466	49.3579	49.9293	49.3318	49.8848	49.4151	50.3428	**52.48**
H2	9.0450	8.9678	8.9601	8.9042	8.8849	8.9085	8.9332	8.9121	8.9273	8.9014	8.9210	9.0450	8.9678	8.9601	8.9042	8.8230	8.9085	8.9332	8.9121	8.9273	8.9014	8.9210	**8.08**
H3	7.4575	7.5997	7.6912	7.6424	7.7660	7.6412	7.7846	7.6390	7.7767	7.6446	7.8005	7.4575	7.5997	7.6912	7.6424	7.5612	7.6412	7.7846	7.6390	7.7767	7.6446	7.8005	**7.23**
H5	7.2908	7.4882	7.5789	7.5729	7.7023	7.5689	7.7160	7.5640	7.7051	7.5778	7.7354	7.2908	7.4882	7.5789	7.5729	7.4917	7.5689	7.7160	7.5640	7.7051	7.5778	7.7354	**7.23**
H6	8.1972	8.3935	8.4732	8.4945	8.6334	8.4887	8.6980	8.4821	8.6771	8.5012	8.7251	8.1972	8.3935	8.4732	8.4945	8.4133	8.4887	8.6980	8.4821	8.6771	8.5012	8.7251	**8.08**
H8	4.2733	4.3638	4.3954	4.4062	4.4953	4.4038	4.5488	4.4006	4.5345	4.4098	4.5541	4.2733	4.3638	4.3954	4.4062	4.3250	4.4038	4.5488	4.4006	4.5345	4.4098	4.5541	**5.3**
H(9A)	1.9600	2.0547	2.0355	2.1023	1.8708	2.0997	2.1414	2.0964	2.1260	2.1059	2.1696	1.7258	1.7468	1.7197	1.7626	1.7620	1.7625	1.7295	1.7618	1.7271	1.7637	1.7701	**2.21**
H(9B)	1.7258	1.7468	1.7197	1.7626	1.2753	1.7625	1.7295	1.7618	1.7271	1.7637	1.7701	1.9600	2.0547	2.0355	2.1023	2.1168	2.0997	2.1414	2.0964	2.1260	2.1059	2.1696	**2.14**
H(10A-10C)	0.8392	0.7759	0.7250	0.7295	0.6630	0.7332	0.6870	0.7360	0.6884	0.7271	0.6868	0.8392	0.7759	0.7250	0.7295	0.6483	0.7332	0.6870	0.7360	0.6884	0.7271	0.6868	**1.01**
H(1`A-1`B)	2.8373	2.8601	2.8579	2.8640	2.7665	2.8645	2.8676	2.8642	2.8667	2.8646	2.8596	2.8280	2.7309	2.7032	2.6857	2.6722	2.6893	2.6322	2.6921	2.6357	2.6834	2.6166	**3.68**
H(2`-3`A-2`-3`B)	1.6271	1.6798	1.6481	1.7172	1.4908	1.7155	1.6928	1.7130	1.6875	1.7198	1.7193	1.6271	1.6798	1.6481	1.7172	1.6718	1.7155	1.6928	1.7130	1.6875	1.7198	1.7194	**2.19**
H(4`A)	2.9174	2.7205	2.6790	2.6421	2.5055	2.6473	2.5593	2.6517	2.5643	2.6384	2.5516	3.0812	3.1274	3.1509	3.1551	3.2118	3.1541	3.1985	3.1523	3.1959	3.1571	3.2012	**3.02**
H(4`B)	2.7387	2.7413	2.7273	2.7293	2.5707	2.7313	2.7050	2.7325	2.7070	2.7284	2.6816	2.5935	2.5928	2.5648	2.5729	2.5242	2.5749	2.5366	2.5761	2.5374	2.5721	2.5181	**3.83**
Nuclei	BHandHLYP											BHandHLYP									
C1	139.1083	139.8726	140.5904	140.3953	141.4094	140.3823	142.0785	140.3697	140.8236	140.4052	142.2534	139.1082	139.8726	140.5904	140.3953	141.4093	140.3823	142.0785	140.3698	140.8236	140.4052	142.2532	**131.91**
C2	142.1831	142.0302	142.5305	141.8772	142.3344	141.8845	142.8844	141.8944	142.7416	141.8703	142.9307	142.1830	142.0302	142.5304	141.8774	142.3345	141.8845	142.8844	141.8945	142.7416	141.8703	142.9307	**131.65**
C3	122.4277	123.0603	123.5957	123.2820	123.8637	123.2729	124.2088	123.2657	124.0425	123.2902	124.2634	122.4276	123.0603	123.5957	123.2822	123.8639	123.2729	124.2088	123.2657	124.0425	123.2902	124.2634	**116.7**
C4	174.5933	175.2689	175.8601	175.6184	176.2622	175.5951	176.7432	175.5747	176.7571	175.6406	176.8767	174.5934	175.2689	175.8601	175.6184	176.2621	175.5951	176.7432	175.5746	176.7571	175.6406	176.8769	**166.84**
C5	120.3207	121.5907	122.1561	122.2421	122.9910	122.2033	123.1824	122.1670	123.0525	122.2782	123.3403	120.3207	121.5907	122.1560	122.2421	122.9909	122.2033	123.1824	122.1669	123.0525	122.2782	123.3404	**116.7**
C6	138.0425	139.8949	140.9966	140.9069	142.5888	140.8364	142.4604	140.7692	143.0045	140.9743	142.8273	138.0426	139.8949	140.9966	140.9069	142.5889	140.8364	142.4604	140.7691	143.0045	140.9743	142.8274	**131.65**
C7	202.0500	207.0643	208.1279	209.9315	209.7172	209.7777	216.9247	209.6234	214.3030	210.0743	217.9390	202.0500	207.0643	208.1279	209.9315	209.7171	209.7777	216.9247	209.6233	214.3030	210.0743	217.9391	**194.89**
C8	61.7828	62.8234	63.3429	63.4521	63.8268	63.4291	64.8957	63.4062	64.3758	63.4712	65.2587	61.7828	62.8234	63.3430	63.4521	63.8267	63.4291	64.8957	63.4062	64.3758	63.4712	65.2587	**65.05**
C9	26.5523	26.3705	26.4700	26.2778	26.3805	26.2817	26.3233	26.2878	26.5472	26.2734	26.3551	26.5523	26.3705	26.4701	26.2778	26.3806	26.2817	26.3233	26.2878	26.5472	26.2734	26.3551	**24.22**
C10	8.4702	8.6992	8.8741	8.8336	9.1031	8.8270	8.9481	8.8225	9.0209	8.8394	9.0345	8.4704	8.6992	8.8741	8.8337	9.1031	8.8271	8.9481	8.8224	9.0209	8.8394	9.0344	**10.45**
C1`	49.0156	49.7761	50.1008	50.3042	50.8136	50.2760	50.8593	50.2498	50.7864	50.3301	51.2588	53.2198	54.1039	54.4862	54.6111	55.1174	54.5821	55.3294	54.5555	55.2017	54.6382	55.5561	**50.48**
C2`	24.3612	24.6836	25.0620	24.8776	25.2998	24.8679	25.3219	24.8605	25.3484	24.8862	25.1915	23.9594	24.0570	24.4250	24.1596	24.7162	24.1503	24.5722	24.1439	24.5844	24.1687	24.4100	**23.91**
C3`	23.9594	24.0570	24.4251	24.1596	24.7161	24.1503	24.5722	24.1439	24.5844	24.1687	24.4100	24.3611	24.6836	25.0620	24.8775	25.2997	24.8679	25.3219	24.8604	25.3484	24.8862	25.1913	**23.74**
C4`	53.2198	54.1039	54.4862	54.6110	55.1174	54.5821	55.3294	54.5555	55.2017	54.6382	55.5561	49.0156	49.7761	50.1007	50.3040	50.8137	50.2760	50.8593	50.2498	50.7864	50.3301	51.2589	**52.48**
H2	8.9313	8.8229	8.8599	8.7433	8.8076	8.7463	8.7017	8.7493	8.8157	8.7408	8.7001	8.9313	8.8229	8.8599	8.7433	8.8077	8.7463	8.7017	8.7493	8.8157	8.7408	8.7001	**8.08**
H3	7.4402	7.5696	7.6580	7.6149	7.7285	7.6129	7.7642	7.6106	7.7418	7.6168	7.7790	7.4402	7.5696	7.6581	7.6149	7.7285	7.6129	7.7642	7.6106	7.7418	7.6168	7.7790	**7.23**
H5	7.2820	7.4697	7.5599	7.5450	7.6750	7.5408	7.6715	7.5363	7.6753	7.5491	7.6920	7.2820	7.4697	7.5599	7.5450	7.6751	7.5408	7.6715	7.5363	7.6753	7.5491	7.6920	**7.23**
H6	8.0832	8.2665	8.3686	8.3687	8.5376	8.3615	8.5314	8.3543	8.5639	8.3756	8.5619	8.0832	8.2665	8.3686	8.3687	8.5376	8.3615	8.5314	8.3543	8.5639	8.3756	8.5619	**8.08**
H8	4.2204	4.3077	4.3640	4.3667	4.4850	4.3614	4.4881	4.3562	4.5000	4.3720	4.4839	4.2204	4.3077	4.3640	4.3667	4.4850	4.3614	4.4881	4.3562	4.5000	4.3720	4.4839	**5.3**
H(9A)	1.8507	1.9379	1.9419	1.9923	2.0115	1.9885	1.9933	1.9846	2.0237	1.9959	2.0250	1.6707	1.7235	1.7290	1.7515	1.7703	1.7499	1.6996	1.7481	1.7748	1.7530	1.7325	**2.21**
H(9B)	1.4908	1.5091	1.5160	1.5107	1.5291	1.5113	1.4059	1.5117	1.5258	1.5100	1.4401	0.8656	0.7882	0.7602	0.7526	0.7100	0.7543	0.7229	0.7559	0.7275	0.7511	0.7182	**2.14**
H(10A-10C)	0.8655	0.7882	0.7602	0.7526	0.7100	0.7543	0.7229	0.7559	0.7275	0.7511	0.7182	2.7535	2.7480	2.7305	2.7294	2.6780	2.7315	2.7066	2.7335	2.6994	2.7273	2.6820	**1.01**
H(1`A-1`B)	2.8148	2.8437	2.8456	2.8555	2.8585	2.8547	2.8601	2.8537	2.8622	2.8563	2.8494	2.7365	2.6106	2.5587	2.5710	2.5307	2.5728	2.5378	2.5746	2.5025	2.5692	2.5338	**3.68**
H(2`-3`A-2`-3`B)	1.5887	1.6486	1.6090	1.6915	1.6376	1.6891	1.6761	1.6865	1.6545	1.6938	1.6974	1.5887	1.6486	1.6090	1.6915	1.6376	1.6891	1.6761	1.6865	1.6545	1.6938	1.6974	**2.19**
H(4`A)	2.7364	2.6106	2.5586	2.5710	2.5308	2.5728	2.5378	2.5746	2.5025	2.5692	2.5338	3.0114	3.0735	3.0977	3.1110	3.1652	3.1087	3.1512	3.1063	3.1533	3.1133	3.1560	**3.02**
H(4`B)	2.7535	2.7480	2.7305	2.7294	2.6780	2.7315	2.7066	2.7335	2.6994	2.7273	2.6820	2.6182	2.6138	2.5935	2.6000	2.5518	2.6006	2.5690	2.6012	2.5711	2.5993	2.5430	**3.83**
Nuclei	BLYP											BLYP									
C1	139.2705	140.9067	141.8858	141.8672	143.5912	142.0810	142.8045	141.8380	142.9624	142.2951	143.2638	139.2705	140.9067	141.8857	141.8672	143.5912	142.0810	142.8045	141.8380	142.9624	142.2951	143.2638	**131.91**
C2	137.3978	137.3570	137.9286	137.3759	138.0200	137.6572	138.3109	137.4769	138.3889	137.7363	138.4753	137.3978	137.3570	137.9284	137.3759	138.0200	137.6572	138.3109	137.4769	138.3889	137.7363	138.4753	**131.65**
C3	120.5341	121.3428	121.9216	121.6045	122.2834	121.8725	122.4338	121.6778	122.5466	121.9769	122.5690	120.5341	121.3428	121.9214	121.6045	122.2834	121.8725	122.4338	121.6778	122.5466	121.9769	122.5690	**116.7**
C4	178.0164	178.8916	179.6106	179.2458	180.0972	179.5054	180.4700	179.3025	180.5121	179.6263	180.6847	178.0164	178.8916	179.6107	179.2458	180.0972	179.5054	180.4700	179.3025	180.5121	179.6263	180.6847	**166.84**
C5	118.7984	119.9416	120.5141	120.5343	121.3266	120.7786	121.4220	120.5603	121.5015	120.9288	121.6469	118.7984	119.9416	120.5143	120.5343	121.3266	120.7786	121.4220	120.5603	121.5015	120.9288	121.6468	**116.7**
C6	133.6176	135.1910	136.0890	136.0511	137.5630	136.2700	137.9833	136.0265	137.9414	136.4700	138.4249	133.6176	135.1910	136.0891	136.0511	137.5630	136.2700	137.9833	136.0265	137.9414	136.4700	138.4250	**131.65**
C7	203.7891	208.8903	210.1713	211.6578	212.6539	211.7511	217.0183	211.3869	216.1579	212.2011	218.2860	203.7891	208.8903	210.1715	211.6578	212.6539	211.7511	217.0183	211.3869	216.1580	212.2011	218.2860	**194.89**
C8	70.3429	71.8475	72.1815	72.4218	73.3557	72.6518	73.8558	72.4209	73.8744	72.8315	74.2979	70.3429	71.8475	72.1814	72.4218	73.3557	72.6518	73.8558	72.4209	73.8744	72.8315	74.2979	**65.05**
C9	32.5579	32.2971	32.2284	32.1261	32.2136	32.4111	32.4952	32.2331	32.5914	32.4817	32.5782	32.5579	32.2971	32.2285	32.1261	32.2136	32.4111	32.4952	32.2331	32.5914	32.4817	32.5782	**24.22**
C10	8.8269	9.1055	9.1210	9.1156	9.4613	9.3928	9.2227	9.2069	9.4141	9.4788	9.3614	8.8269	9.1055	9.1210	9.1156	9.4613	9.3928	9.2227	9.2069	9.4141	9.4788	9.3614	**10.45**
C1`	55.2826	56.0393	56.3333	56.5290	57.2448	56.7763	57.0302	56.5616	57.1624	56.9214	57.5107	59.9281	61.0266	61.4308	61.5255	62.1534	61.7761	62.1404	61.5653	62.2487	61.9149	62.5011	**50.48**
C2`	27.6600	28.1718	28.4207	28.3269	28.8476	28.5940	28.7358	28.3994	28.9086	28.7004	28.6497	27.6842	27.7730	28.1627	27.9567	28.5331	28.2244	28.2249	28.0308	28.3996	28.3301	28.1119	**23.91**
C3`	27.6842	27.7730	28.1627	27.9567	28.5331	28.2244	28.2249	28.0308	28.3996	28.3301	28.1119	27.6600	28.1718	28.4207	28.3269	28.8476	28.5940	28.7358	28.3994	28.9086	28.7004	28.6497	**23.74**
C4`	59.9281	61.0266	61.4309	61.5255	62.1534	61.7761	62.1404	61.5653	62.2487	61.9149	62.5012	55.2826	56.0393	56.3333	56.5290	57.2448	56.7763	57.0302	56.5616	57.1624	56.9214	57.5107	**52.48**
H2	8.4741	8.3285	8.3494	8.2453	8.2530	8.2993	8.4500	8.2603	8.2861	8.2939	8.4557	8.4741	8.3285	8.3494	8.2453	8.2530	8.2993	8.4500	8.2603	8.2861	8.2939	8.4557	**8.08**
H3	7.1613	7.2946	7.3861	7.3452	7.4642	7.3903	7.6533	7.3428	7.4778	7.4025	7.6794	7.1613	7.2946	7.3861	7.3452	7.4642	7.3903	7.6533	7.3428	7.4778	7.4025	7.6794	**7.23**
H5	7.0469	7.1908	7.2751	7.2489	7.3699	7.2929	7.5533	7.2442	7.3771	7.3074	7.5843	7.0469	7.1908	7.2751	7.2489	7.3699	7.2929	7.5533	7.2442	7.3771	7.3074	7.5843	**7.23**
H6	7.8308	7.9672	8.0540	8.0515	8.1659	8.0949	8.3731	8.0455	8.1902	8.1104	8.4059	7.8308	7.9672	8.0540	8.0515	8.1659	8.0949	8.3731	8.0455	8.1902	8.1104	8.4059	**8.08**
H8	4.9639	4.9849	5.0165	5.0006	5.0516	5.0476	5.2282	5.0020	5.0512	5.0562	5.2230	4.9639	4.9849	5.0165	5.0006	5.0516	5.0476	5.2282	5.0020	5.0512	5.0562	5.2230	**5.3**
H(9A)	2.1100	2.1845	2.1750	1.4520	2.2360	2.2672	2.4411	2.2193	2.2613	2.2800	2.4825	1.6268	1.6332	1.5791	0.9704	1.5947	1.6303	1.7587	1.5873	1.5993	1.6327	1.7959	**2.21**
H(9B)	1.6268	1.6332	1.5791	0.9704	1.5947	1.6303	1.7587	1.5873	1.5993	1.6327	1.7959	2.1100	2.1845	2.1750	1.4520	2.2360	2.2672	2.4411	2.2193	2.2613	2.2800	2.4825	**2.14**
H(10A-10C)	0.8610	0.7948	0.7721	0.7727	0.7222	0.8220	0.9088	0.7788	0.7402	0.8261	0.9177	0.8610	0.7948	0.7721	0.7727	0.7222	0.8220	0.9088	0.7788	0.7402	0.8261	0.9177	**1.01**
H(1`A-1`B)	3.1102	3.1348	3.1350	2.3152	3.1470	3.1879	3.3112	3.1425	3.1440	3.1964	3.3048	3.0138	2.9400	2.9121	2.1099	2.8989	2.9628	3.0543	2.9186	2.8893	2.9692	3.0444	**3.68**
H(2`-3`A-2`-3`B)	1.7341	1.7919	1.7609	1.1511	1.7908	1.8748	1.9741	1.8273	1.8013	1.8877	2.0134	1.7341	1.7919	1.7609	1.1511	1.7908	1.8748	1.9741	1.8273	1.8013	1.8877	2.0134	**2.19**
H(4`A)	3.0552	2.8926	2.8543	2.0307	2.8600	2.9101	3.0004	2.8654	2.8335	2.9176	3.0053	3.3514	3.4019	3.4269	2.5707	3.4885	3.4775	3.6408	3.4305	3.4709	3.4890	3.6482	**3.02**
H(4`B)	2.9724	2.9875	2.9698	2.1891	2.9378	3.0156	3.1082	2.9718	2.9451	3.0208	3.0837	2.8690	2.8678	2.8432	2.0597	2.8054	2.8984	2.9816	2.8545	2.8170	2.9038	2.9614	**3.83**

[a] methyl protons shifts are averaged [b] according to [13] in $CDCl_3$

Table S14. Cont. III

Nuclei	R											S										Exp. [b]
	BMK																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	154.5298	155.4785	156.0406	155.7560	157.0506	155.7359	156.5758	155.9255	156.4939	155.9343	156.8108	154.5298	155.4786	156.0408	155.7560	157.0506	155.7359	156.5759	155.9255	156.4939	155.9343	156.8108	**131.91**
C2	155.3064	155.1890	155.9180	154.9647	155.6797	154.9632	156.0857	155.1726	155.8518	155.1275	156.1317	155.3064	155.1890	155.9179	154.9647	155.6797	154.9632	156.0858	155.1726	155.8518	155.1275	156.1317	**131.65**
C3	135.6633	136.4557	137.1229	136.6285	137.5262	136.6060	137.7354	136.7941	137.5870	136.8111	137.7325	135.6633	136.4556	137.1229	136.6285	137.5262	136.6060	137.7355	136.7941	137.5870	136.8111	137.7325	**116.7**
C4	189.3769	190.1320	190.9258	190.4806	191.4492	190.4433	192.0209	190.6171	191.7825	190.6780	192.0897	189.3769	190.1322	190.9257	190.4806	191.4492	190.4433	192.0209	190.6171	191.7825	190.6780	192.0897	**166.84**
C5	133.4305	134.7898	135.6266	135.4548	136.6015	135.3982	136.7114	135.5530	136.5273	135.6703	136.8089	133.4305	134.7898	135.6265	135.4548	136.6016	135.3982	136.7113	135.5530	136.5273	135.6703	136.8089	**116.7**
C6	151.4259	153.2342	154.7146	154.3487	156.4549	154.2578	156.9482	154.3796	156.6312	154.5973	157.2937	151.4259	153.2342	154.7145	154.3487	156.4549	154.2578	156.9483	154.3796	156.6312	154.5973	157.2937	**131.65**
C7	217.5517	223.2260	224.1611	226.0859	226.0934	225.9089	232.6506	225.9408	231.1493	226.4133	233.9081	217.5517	223.2262	224.1611	226.0859	226.0936	225.9089	232.6509	225.9408	231.1493	226.4133	233.9081	**194.89**
C8	71.7450	73.0889	73.2474	73.7070	74.1747	73.6614	75.3072	73.8259	74.9365	73.9104	75.9803	71.7450	73.0888	73.2475	73.7070	74.1747	73.6614	75.3072	73.8259	74.9365	73.9104	75.9803	**65.05**
C9	30.8307	30.8647	31.0333	30.9265	31.1266	30.9085	31.5970	31.1015	31.3694	31.1054	31.8452	30.8307	30.8648	31.0333	30.9265	31.1266	30.9085	31.5970	31.1015	31.3694	31.1054	31.8452	**24.22**
C10	9.9627	10.2044	10.2846	10.2178	10.6517	10.1966	10.4508	10.3876	10.3754	10.4000	10.5601	9.9627	10.2044	10.2846	10.2178	10.6517	10.1966	10.4507	10.3876	10.3754	10.4000	10.5601	**10.45**
C1`	55.9463	56.5701	56.9145	56.9479	57.6480	56.9075	57.6392	57.0784	57.4768	57.1484	57.9422	60.4793	61.2077	61.6687	61.5870	62.2695	61.5486	62.3987	61.7212	62.2400	61.7848	62.5841	**50.48**
C2`	27.6146	28.0616	28.3231	28.2761	28.6930	28.2492	28.8907	28.4332	28.7458	28.4628	28.8681	27.3316	27.4393	27.8678	27.5248	28.2368	27.5018	28.0684	27.6904	27.9701	27.7086	27.8920	**23.91**
C3`	27.3316	27.4393	27.8678	27.5248	28.2368	27.5018	28.0685	27.6904	27.9701	27.7086	27.8920	27.6146	28.0616	28.3231	28.2761	28.6930	28.2492	28.8905	28.4332	28.7458	28.4628	28.8681	**23.74**
C4`	60.4793	61.2078	61.6686	61.5870	62.2695	61.5486	62.3987	61.7212	62.2400	61.7848	62.5841	55.9463	56.5702	56.9146	56.9479	57.6480	56.9075	57.6392	57.0784	57.4768	57.1484	57.9422	**52.48**
H2	9.0586	9.0208	9.0552	8.9601	9.0144	8.9596	8.9975	8.9594	9.0063	8.9511	8.9835	9.0586	9.0208	9.0552	8.9601	9.0144	8.9596	8.9975	8.9594	9.0063	8.9511	8.9835	**8.08**
H3	7.6460	7.7871	7.8710	7.8390	7.9548	7.8334	7.9785	7.8277	7.9715	7.8347	7.9922	7.6460	7.7871	7.8711	7.8390	7.9548	7.8334	7.9785	7.8277	7.9715	7.8347	7.9922	**7.23**
H5	7.4734	7.6670	7.7595	7.7509	7.8826	7.7429	7.8927	7.7347	7.8861	7.7491	7.9062	7.4734	7.6670	7.7595	7.7509	7.8826	7.7429	7.8927	7.7347	7.8861	7.7491	7.9062	**7.23**
H6	8.3751	8.5662	8.6687	8.6756	8.8423	8.6652	8.8777	8.6548	8.8627	8.6760	8.9081	8.3751	8.5662	8.6686	8.6756	8.8423	8.6652	8.8777	8.6548	8.8627	8.6760	8.9081	**8.08**
H8	4.4066	4.4732	4.5296	4.5397	4.6401	4.5319	4.6811	4.5242	4.6669	4.5375	4.6664	4.4066	4.4732	4.5296	4.5397	4.6401	4.5319	4.6811	4.5242	4.6669	4.5375	4.6664	**5.3**
H(9A)	1.8670	1.9344	1.9495	2.0100	2.0131	2.0019	2.0452	1.9939	2.0318	2.0081	2.0976	1.5514	1.5988	1.5537	1.6246	1.5872	1.6201	1.6182	1.6157	1.6152	1.6193	1.6919	**2.21**
H(9B)	1.5514	1.5988	1.5537	1.6246	1.5872	1.6201	1.6182	1.6157	1.6152	1.6193	1.6919	1.8670	1.9344	1.9495	2.0100	2.0131	2.0019	2.0452	1.9939	2.0318	2.0081	2.0976	**2.14**
H(10A-10C)	0.8143	0.7380	0.7168	0.7013	0.6649	0.6997	0.6599	0.6983	0.6683	0.6934	0.6536	0.8143	0.7380	0.7169	0.7013	0.6649	0.6997	0.6599	0.6983	0.6683	0.6934	0.6536	**1.01**
H(1`A-1`B)	2.8438	2.8495	2.8627	2.8680	2.8667	2.8641	2.8685	2.8603	2.8675	2.8620	2.8573	2.7560	2.7065	2.6526	2.6866	2.6334	2.6850	2.6390	2.6834	2.6384	2.6785	2.6269	**3.68**
H(2`-3`A-2`-3`B)	1.6147	1.6770	1.6284	1.7183	1.6581	1.7125	1.6813	1.7067	1.6771	1.7143	1.7010	1.6147	1.6770	1.6284	1.7183	1.6581	1.7125	1.6813	1.7067	1.6771	1.7143	1.7010	**2.19**
H(4`A)	2.7311	2.6208	2.5487	2.5897	2.5418	2.5886	2.5284	2.5874	2.5261	2.5812	2.5236	3.0471	3.0743	3.1084	3.1196	3.1610	3.1141	3.1638	3.1085	3.1572	3.1153	3.1742	**3.02**
H(4`B)	2.7808	2.7922	2.7565	2.7835	2.7250	2.7814	2.7497	2.7793	2.7508	2.7758	2.7302	2.6405	2.6247	2.6170	2.6163	2.5725	2.6142	2.5733	2.6121	2.5778	2.6087	2.5405	**3.83**
Nuclei	BP86																						
C1	135.9057	137.4725	137.9145	138.0844	140.1573	138.0529	139.5683	138.0159	139.5315	138.1088	139.9956	135.9057	137.4725	137.9145	138.0844	140.1573	138.0529	139.5683	138.0159	139.5315	138.1088	139.9956	**131.91**
C2	136.0467	136.1128	136.6257	135.9936	136.6814	136.0078	137.1335	136.0175	137.0380	135.9751	137.3613	136.0467	136.1128	136.6258	135.9936	136.6814	136.0078	137.1335	136.0175	137.0380	135.9751	137.3613	**131.65**
C3	119.4011	120.3916	120.9160	120.6593	121.3650	120.6536	121.7076	120.6422	121.6277	120.6594	121.9242	119.4011	120.3916	120.9161	120.6593	121.3650	120.6536	121.7076	120.6422	121.6277	120.6594	121.9242	**116.7**
C4	174.5997	175.6012	176.2715	175.9436	176.6396	175.9318	177.2202	175.9147	177.0793	175.9501	177.4972	174.5997	175.6012	176.2715	175.9436	176.6396	175.9318	177.2202	175.9147	177.0793	175.9501	177.4972	**166.84**
C5	117.7092	119.0997	119.6750	119.7239	120.4804	119.6935	120.7775	119.6579	120.6613	119.7479	121.0864	117.7092	119.0997	119.6750	119.7239	120.4804	119.6935	120.7775	119.6579	120.6613	119.7479	121.0864	**116.7**
C6	132.2905	134.1084	135.2366	134.9827	136.1998	134.9384	136.7506	134.8888	136.5351	135.0201	137.2758	132.2905	134.1084	135.2364	134.9827	136.1998	134.9384	136.7506	134.8888	136.5351	135.0201	137.2758	**131.65**
C7	200.9264	205.7818	206.6785	208.1649	209.3460	208.0245	213.6166	207.8787	212.6074	208.2926	214.9040	200.9264	205.7818	206.6787	208.1649	209.3460	208.0245	213.6166	207.8787	212.6074	208.2926	214.9040	**194.89**
C8	68.0356	69.6466	70.1719	70.2389	71.0626	70.2126	71.6967	70.1806	71.4910	70.2583	72.3844	68.0356	69.6466	70.1720	70.2389	71.0626	70.2126	71.6967	70.1806	71.4910	70.2583	72.3844	**65.05**
C9	31.2980	31.3870	31.4867	31.2721	31.1250	31.2925	31.4864	31.3071	31.3766	31.2476	31.7540	31.2980	31.3870	31.4868	31.2721	31.1250	31.2925	31.4864	31.3071	31.3766	31.2476	31.7540	**24.22**
C10	8.4639	8.9095	8.9824	8.9561	9.1001	8.9633	8.9889	8.9649	8.9763	8.9443	9.2948	8.4639	8.9095	8.9825	8.9561	9.1001	8.9633	8.9889	8.9649	8.9763	8.9443	9.2948	**10.45**
C1`	53.7163	54.6257	54.8362	55.0632	55.6004	55.0418	55.5611	55.0150	55.5007	55.0785	56.1752	58.1982	59.3590	59.6658	59.8295	60.3766	59.8051	60.6039	59.7762	60.5339	59.8484	61.0062	**50.48**
C2`	26.1148	26.6908	26.9684	26.8555	27.2134	26.8518	27.2683	26.8435	27.2490	26.8547	27.3089	26.0005	26.2374	26.5081	26.3334	26.8210	26.3340	26.7008	26.3297	26.6987	26.3284	26.6554	**23.91**
C3`	26.0005	26.2374	26.5080	26.3334	26.8210	26.3340	26.7008	26.3297	26.6987	26.3284	26.6554	26.1148	26.6908	26.9684	26.8555	27.2134	26.8518	27.2683	26.8435	27.2490	26.8547	27.3089	**23.74**
C4`	58.1982	59.3590	59.6658	59.8295	60.3766	59.8051	60.6039	59.7762	60.5339	59.8484	61.0062	53.7163	54.6257	54.8362	55.0632	55.6004	55.0418	55.5611	55.0150	55.5007	55.0785	56.1752	**52.48**
H2	8.5445	8.4093	8.4460	8.3429	8.3113	8.3477	8.3452	8.3523	8.3487	8.3381	8.3531	8.5445	8.4093	8.4460	8.3429	8.3113	8.3477	8.3452	8.3523	8.3487	8.3381	8.3531	**8.08**
H3	7.1742	7.3133	7.3915	7.3647	7.4837	7.3627	7.5060	7.3604	7.4965	7.3662	7.5342	7.1742	7.3133	7.3915	7.3647	7.4837	7.3627	7.5060	7.3604	7.4965	7.3662	7.5342	**7.23**
H5	7.0502	7.2124	7.3043	7.2802	7.3879	7.2771	7.4042	7.2737	7.3936	7.2828	7.4362	7.0502	7.2124	7.3043	7.2802	7.3879	7.2771	7.4042	7.2737	7.3936	7.2828	7.4362	**7.23**
H6	7.9187	8.0504	8.1325	8.1375	8.2309	8.1326	8.2708	8.1274	8.2566	8.1419	8.3063	7.9187	8.0504	8.1325	8.1375	8.2309	8.1326	8.2708	8.1274	8.2566	8.1419	8.3063	**8.08**
H8	4.9722	4.9882	5.0094	5.0127	5.0576	5.0115	5.0681	5.0101	5.0590	5.0136	5.0689	4.9722	4.9882	5.0094	5.0127	5.0576	5.0115	5.0681	5.0101	5.0590	5.0136	5.0689	**5.3**
H(9A)	2.1703	2.2441	2.2444	2.2915	2.2767	2.2896	2.3041	2.2874	2.2902	2.2929	2.3521	1.7431	1.7646	1.7671	1.7487	1.6773	1.7516	1.6539	1.7540	1.6585	1.7455	1.7194	**2.21**
H(9B)	1.7431	1.7646	1.7671	1.7487	1.6773	1.7516	1.6539	1.7540	1.6585	1.7455	1.7194	2.1703	2.2441	2.2444	2.2915	2.2767	2.2896	2.3041	2.2874	2.2902	2.2929	2.3521	**2.14**
H(10A-10C)	0.8366	0.7729	0.7323	0.7463	0.6877	0.7487	0.7050	0.7508	0.7048	0.7437	0.7127	0.8366	0.7729	0.7324	0.7463	0.6877	0.7487	0.7050	0.7508	0.7048	0.7437	0.7127	**1.01**
H(1`A-1`B)	3.0937	3.1192	3.1108	3.1259	3.1209	3.1265	3.1122	3.1268	3.1118	3.1250	3.1054	3.0164	2.9437	2.9036	2.9092	2.8816	2.9123	2.8577	2.9151	2.8592	2.9058	2.8477	**3.68**
H(2`-3`A-2`-3`B)	1.7282	1.7873	1.7387	1.8226	1.7771	1.8209	1.7932	1.8190	1.7873	1.8238	1.8336	1.7282	1.7873	1.7387	1.8226	1.7771	1.8209	1.7932	1.8190	1.7873	1.8238	1.8336	**2.19**
H(4`A)	3.1134	2.9475	2.8853	2.8915	2.8747	2.8958	2.8231	2.8998	2.8237	2.8871	2.8211	3.3736	3.4207	3.4321	3.4471	3.4881	3.4464	3.4643	3.4455	3.4615	3.4473	3.4732	**3.02**
H(4`B)	2.9194	2.9399	2.9219	2.9269	2.8885	2.9289	2.8924	2.9305	2.8947	2.9245	2.8743	2.8139	2.8178	2.7896	2.8047	2.7537	2.8066	2.7602	2.8081	2.7621	2.8028	2.7375	**3.83**
Nuclei	CAM-B3LYP																						
C1	140.8178	141.9454	142.6315	142.5083	145.2055	142.4836	144.2823	142.4588	144.2735	142.5338	144.4838	140.8178	141.9454	142.6316	142.5083	145.2054	142.4835	144.2823	142.4588	144.2735	142.5338	144.4838	**131.91**
C2	142.4921	142.4056	142.8948	142.2784	142.8221	142.2900	143.3308	142.3021	143.2470	142.2697	143.3691	142.4921	142.4056	142.8948	142.2784	142.8221	142.2900	143.3308	142.3021	143.2470	142.2697	143.3691	**131.65**
C3	123.7767	124.4837	125.0050	124.6919	125.4486	124.6857	125.6608	124.6798	125.6104	124.6998	125.7179	123.7767	124.4837	125.0050	124.6919	125.4485	124.6858	125.6608	124.6798	125.6104	124.6998	125.7179	**116.7**
C4	177.7523	178.4739	179.0582	178.8040	179.3513	178.7868	179.9721	178.7702	179.8447	178.8226	180.0980	177.7523	178.4739	179.0582	178.8040	179.3513	178.7868	179.9721	178.7702	179.8447	178.8226	180.0980	**166.84**
C5	121.8226	123.1271	123.6669	123.7684	124.5871	123.7332	124.7607	123.6980	124.6689	123.8040	124.9200	121.8226	123.1271	123.6669	123.7684	124.5872	123.7330	124.7607	123.6980	124.6690	123.8040	124.9200	**116.7**
C6	138.4619	140.2889	141.3662	141.2699	142.2841	141.2111	142.8858	141.1526	142.6842	141.3278	143.2602	138.4619	140.2889	141.3662	141.2699	142.2841	141.2111	142.8858	141.1526	142.6842	141.3278	143.2602	**131.65**
C7	205.9601	211.2530	212.2857	214.1285	215.6078	213.9636	220.9578	213.7988	219.6416	214.2865	222.0385	205.9601	211.2530	212.2854	214.1285	215.6078	213.9637	220.9578	213.7988	219.6416	214.2865	222.0385	**194.89**
C8	64.5495	65.8213	66.2530	66.4417	67.3789	66.4169	67.9255	66.3913	67.6901	66.4664	68.3648	64.5495	65.8213	66.2529	66.4417	67.3789	66.4168	67.9255	66.3913	67.6902	66.4664	68.3648	**65.05**
C9	27.4431	27.2809	27.3562	27.1799	27.1272	27.1888	27.2673	27.1976	27.1929	27.1733	27.3228	27.4431	27.2809	27.3562	27.1799	27.1272	27.1888	27.2673	27.1976	27.1929	27.1733	27.3228	**24.22**
C10	8.0312	8.3181	8.4305	8.4258	8.6542	8.4248	8.5416	8.4241	8.5219	8.4287	8.6386	8.0312	8.3181	8.4305	8.4258	8.6543	8.4249	8.5416	8.4241	8.5220	8.4287	8.6386	**10.45**
C1`	50.7753	51.6280	51.9155	52.1364	52.7371	52.1121	52.7156	52.0883	52.6368	52.1618	53.1484	55.0409	56.0426	56.3382	56.5226	57.0816	56.4988	57.2659	56.4754	57.2040	56.5475	57.5005	**50.48**
C2`	24.9152	25.3130	25.6199	25.4842	25.8827	25.4795	25.9323	25.4749	25.9134	25.4908	25.8091	24.5473	24.6826	25.0241	24.7922	25.3474	24.7872	25.2230	24.7832	25.2311	24.7992	25.0590	**23.91**
C3`	24.5473	24.6826	25.0241	24.7922	25.3474	24.7874	25.2230	24.7832	25.2311	24.7992	25.0590	24.9152	25.3130	25.6199	25.4842	25.8827	25.4796	25.9323	25.4749	25.9134	25.4908	25.8091	**23.74**
C4`	55.0409	56.0426	56.3382	56.5226	57.0816	56.4989	57.2659	56.4754	57.2040	56.5475	57.5005	50.7753	51.6280	51.9155	52.1364	52.7371	52.1120	52.7156	52.0883	52.6368	52.1618	53.1484	**52.48**
H2	8.8310	8.6984	8.7389	8.6188	8.5418	8.6231	8.5834	8.6276	8.5944	8.6147	8.5784	8.8310	8.6984	8.7389	8.6188	8.5418	8.6231	8.5834	8.6276	8.5944	8.6147	8.5784	**8.08**
H3	7.4035	7.5336	7.6234	7.5777	7.7035	7.5755	7.7231	7.5735	7.7155	7.5796	7.7368	7.4035	7.5336	7.6234	7.5777	7.7035	7.5755	7.7231	7.5735	7.7155	7.5796	7.7368	**7.23**
H5	7.2558	7.4349	7.5269	7.5089	7.6252	7.5047	7.6407	7.5006	7.6307	7.5128	7.6611	7.2558	7.4349	7.5269	7.5089	7.6252	7.5047	7.6407	7.5006	7.6307	7.5128	7.6611	**7.23**
H6	8.0473	8.2152	8.3133	8.3127	8.4156	8.3063	8.4646	8.3001	8.4529	8.3187	8.4912	8.0473	8.2152	8.3133	8.3127	8.4156	8.3063	8.4646	8.3001	8.4529	8.3187	8.4912	**8.08**
H8	4.4165	4.4851	4.5384	4.5391	4.6212	4.5344	4.6550	4.5299	4.6464	4.5437	4.6509	4.4165	4.4851	4.5384	4.5391	4.6212	4.5344	4.6550	4.5299	4.6464	4.5437	4.6509	**5.3**
H(9A)	1.9297	2.0082	2.0161	2.0613	2.0461	2.0579	2.0684	2.0546	2.0559	2.0644	2.1025	1.5810	1.5949	1.5976	1.5893	1.5057	1.5908	1.4857	1.5921	1.4866	1.5878	1.5252	**2.21**
H(9B)	1.5810	1.5949	1.5976	1.5893	1.5057	1.5908	1.4857	1.5921	1.4866	1.5878	1.5252	1.9297	2.0082	2.0161	2.0613	2.0461	2.0579	2.0684	2.0546	2.0559	2.0644	2.1025	**2.14**
H(10A-10C)	0.8555	0.7808	0.7558	0.7486	0.6954	0.7504	0.7196	0.7523	0.7217	0.7469	0.7146	0.8555	0.7808	0.7558	0.7486	0.6954	0.7504	0.7196	0.7523	0.7217	0.7469	0.7146	**1.01**
H(1`A-1`B)	2.9176	2.9444	2.9488	2.9543	2.9591	2.9534	2.9573	2.9527	2.9567	2.9550	2.9450	2.8398	2.7734	2.7462	2.7463	2.7407	2.7476	2.7152	2.7491	2.7145	2.7449	2.7008	**3.68**
H(2`-3`A-2`-3`B)	1.6565	1.7188	1.6809	1.7586	1.7247	1.7562	1.7439	1.7538	1.7384	1.7610	1.7660	1.6565	1.7188	1.6809	1.7586	1.7247	1.7562	1.7439	1.7538	1.7384	1.7610	1.7660	**2.19**
H(4`A)	2.8345	2.7008	2.6612	2.6641	2.6868	2.6650	2.6282	2.6662	2.6254	2.6631	2.6245	3.1163	3.1734	3.1988	3.2069	3.2626	3.2046	3.2467	3.2025	3.2431	3.2091	3.2504	**3.02**
H(4`B)	2.8451	2.8459	2.8312	2.8285	2.7947	2.8302	2.8022	2.8320	2.8037	2.8268	2.7770	2.7188	2.7154	2.6989	2.7016	2.6557	2.7023	2.6679	2.7030	2.6704	2.7009	2.6395	**3.83**

[a] methyl protons shifts are averaged [b] according to [13] in $CDCl_3$

Table S14. Cont. IV

Nuclei	R											S										Exp. [b]
	HF																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.4209	136.9533	137.5981	138.5334	138.5267	138.4887	139.3247	138.4513	139.3910	138.5908	139.5972	136.4209	136.9533	137.5980	138.5334	138.5267	138.4887	139.3248	138.4513	139.3910	138.5909	139.5972	**131.91**
C2	144.4138	144.2278	144.6203	143.8669	144.3858	143.8853	144.7904	143.9028	144.7129	143.8463	144.7848	144.4138	144.2279	144.6200	143.8669	144.3858	143.8852	144.7904	143.9028	144.7129	143.8464	144.7848	**131.65**
C3	120.4960	120.9597	121.3813	121.2317	121.5829	121.2261	121.8485	121.2209	121.8373	121.2385	121.8914	120.4960	120.9597	121.3812	121.2317	121.5828	121.2259	121.8486	121.2209	121.8373	121.2386	121.8914	**116.7**
C4	171.1311	171.6692	172.2139	171.7713	172.5056	171.7582	172.9179	171.7444	172.7713	171.7806	173.0264	171.1311	171.6691	172.2140	171.7713	172.5055	171.7582	172.9179	171.7444	172.7713	171.7806	173.0264	**166.84**
C5	117.8436	119.0394	119.5217	119.8053	120.3440	119.7677	120.5617	119.7314	120.4936	119.8413	120.7260	117.8436	119.0394	119.5217	119.8053	120.3439	119.7678	120.5616	119.7314	120.4936	119.8412	120.7260	**116.7**
C6	139.9153	141.7457	142.9046	142.0537	144.3653	141.9987	144.0470	141.9415	143.8146	142.0972	144.3242	139.9153	141.7457	142.9045	142.0537	144.3653	141.9987	144.0470	141.9415	143.8146	142.0970	144.3242	**131.65**
C7	196.2929	201.5543	202.5554	205.7205	204.2234	205.5100	212.8199	205.3064	211.1460	205.9364	213.9640	196.2929	201.5542	202.5553	205.7205	204.2238	205.5099	212.8199	205.3064	211.1460	205.9362	213.9640	**194.89**
C8	55.6159	56.5268	57.0000	57.3279	57.3819	57.2945	58.6647	57.2631	58.4222	57.3642	58.9869	55.6159	56.5268	57.0001	57.3279	57.3818	57.2944	58.6647	57.2631	58.4222	57.3642	58.9869	**65.05**
C9	23.2421	22.8968	23.0461	22.5863	22.9066	22.5986	22.7730	22.6112	22.7403	22.5726	22.7380	23.2421	22.8969	23.0461	22.5863	22.9066	22.5986	22.7730	22.6112	22.7403	22.5726	22.7380	**24.22**
C10	8.9715	9.1464	9.3172	9.1897	9.5333	9.1871	9.3766	9.1845	9.3716	9.1904	9.4334	8.9715	9.1465	9.3173	9.1897	9.5334	9.1871	9.3765	9.1845	9.3716	9.1904	9.4334	**10.45**
C1`	44.5960	45.2986	45.5475	45.7442	46.2020	45.7185	46.2794	45.6925	46.2140	45.7675	46.6202	48.4651	49.2639	49.5856	49.7434	50.1174	49.7167	50.3465	49.6904	50.2785	49.7691	50.5722	**50.48**
C2`	22.7957	23.0336	23.3702	23.1061	23.5485	23.1020	23.5610	23.0981	23.5568	23.1088	23.4000	22.2330	22.2917	22.6174	22.3624	22.8829	22.3565	22.7390	22.3517	22.7556	22.3683	22.5673	**23.91**
C3`	22.2330	22.2917	22.6175	22.3624	22.8829	22.3565	22.7390	22.3517	22.7556	22.3681	22.5673	22.7957	23.0336	23.3702	23.1061	23.5484	23.1019	23.5609	23.0981	23.5568	23.1088	23.4000	**23.74**
C4`	48.4651	49.2639	49.5855	49.7434	50.1174	49.7167	50.3464	49.6904	50.2785	49.7692	50.5722	44.5960	45.2987	45.5475	45.7442	46.2020	45.7185	46.2793	45.6925	46.2140	45.7675	46.6202	**52.48**
H2	9.0962	8.9993	9.0463	8.7871	8.9824	8.7945	8.8162	8.8009	8.8269	8.7785	8.8030	9.0962	8.9993	9.0463	8.7871	8.9824	8.7945	8.8162	8.8009	8.8269	8.7785	8.8030	**8.08**
H3	7.4378	7.5763	7.6668	7.6214	7.7396	7.6193	7.7566	7.6170	7.7495	7.6234	7.7711	7.4378	7.5763	7.6668	7.6214	7.7396	7.6193	7.7566	7.6170	7.7495	7.6234	7.7711	**7.23**
H5	7.2415	7.4370	7.5282	7.5271	7.6509	7.5221	7.6651	7.5169	7.6542	7.5319	7.6884	7.2415	7.4370	7.5282	7.5271	7.6509	7.5221	7.6651	7.5169	7.6542	7.5319	7.6884	**7.23**
H6	8.0935	8.3199	8.4429	8.4012	8.6258	8.3940	8.6016	8.3865	8.5829	8.4074	8.6317	8.0935	8.3199	8.4429	8.4012	8.6257	8.3940	8.6016	8.3865	8.5829	8.4074	8.6317	**8.08**
H8	3.6381	3.7589	3.8433	3.8362	3.9911	3.8300	4.0000	3.8238	3.9821	3.8420	3.9970	3.6381	3.7589	3.8433	3.8362	3.9911	3.8300	4.0000	3.8238	3.9821	3.8420	3.9970	**5.3**
H(9A)	1.5893	1.6853	1.6955	3.1928	1.7638	1.6997	1.7350	1.6963	1.7228	1.7051	1.7600	1.2435	1.2683	1.2857	2.6500	1.2858	1.1595	1.1482	1.1620	1.1484	1.1515	1.1655	**2.21**
H(9B)	1.2435	1.2683	1.2856	2.6500	1.2858	1.1595	1.1482	1.1620	1.1484	1.1515	1.1655	1.5893	1.6853	1.6955	3.1928	1.7638	1.6997	1.7350	1.6963	1.7228	1.7051	1.7600	**2.14**
H(10A-10C)	0.8877	0.8064	0.7808	0.7653	0.7219	0.7666	0.7288	0.7680	0.7304	0.7642	0.7245	0.8877	0.8064	0.7808	0.7653	0.7219	0.7666	0.7287	0.7680	0.7304	0.7642	0.7245	**1.01**
H(1`A-1`B)	2.5468	2.5785	2.5858	4.0272	2.5992	2.5901	2.6070	2.5890	2.6041	2.5923	2.6001	2.4651	2.4064	2.3739	3.8105	2.3489	2.4083	2.3892	2.4096	2.3861	2.4062	2.3811	**3.68**
H(2`-3`A-2`-3`B)	1.4348	1.4984	1.4573	2.7239	1.4875	1.5556	1.5300	1.5523	1.5238	1.5623	1.5514	1.4348	1.4984	1.4573	2.7239	1.4875	1.5556	1.5300	1.5523	1.5238	1.5623	1.5514	**2.19**
H(4`A)	2.3921	2.2864	2.2444	3.7928	2.2572	2.3064	2.2933	2.3069	2.2874	2.3066	2.2994	2.7142	2.7866	2.8222	4.3484	2.8937	2.8228	2.8821	2.8200	2.8769	2.8280	2.8881	**3.02**
H(4`B)	2.5381	2.5264	2.5033	3.8282	2.4406	2.5103	2.4852	2.5124	2.4848	2.5058	2.4628	2.3794	2.3704	2.3494	3.7060	2.3047	2.3575	2.3319	2.3581	2.3314	2.3565	2.3120	**3.83**
Nuclei	LC-BLYP																						
C1	144.2529	145.2616	146.0982	145.7229	147.4123	145.6776	147.7476	145.6585	146.4741	145.7476	147.8148	144.2528	145.2616	146.0983	145.7229	147.4122	145.6776	147.7475	145.6586	146.4741	145.7477	147.8148	**131.91**
C2	148.6128	148.4513	148.9941	148.3396	148.7816	148.3261	149.2486	148.3398	149.2042	148.3349	149.2538	148.6127	148.4513	148.9940	148.3396	148.7817	148.3262	149.2486	148.3398	149.2041	148.3349	149.2538	**131.65**
C3	128.3160	128.9212	129.5334	129.1284	129.7954	129.0980	130.1137	129.0944	129.9243	129.1394	130.1492	128.3160	128.9212	129.5333	129.1284	129.7952	129.0980	130.1137	129.0943	129.9243	129.1394	130.1492	**116.7**
C4	181.9577	182.4979	183.0862	182.8533	183.3780	182.8102	183.9459	182.7944	183.8966	182.8768	184.0804	181.9578	182.4979	183.0860	182.8533	183.3780	182.8102	183.9459	182.7944	183.8967	182.8768	184.0804	**166.84**
C5	126.1783	127.4899	128.1045	128.2106	129.0230	128.1466	129.2994	128.1094	129.0650	128.2539	129.4517	126.1784	127.4899	128.1045	128.2106	129.0232	128.1465	129.2995	128.1096	129.0650	128.2538	129.4517	**116.7**
C6	144.3194	146.1352	147.3469	147.2631	148.9364	147.1686	148.7988	147.1020	149.3389	147.3369	149.3196	144.3193	146.1352	147.3470	147.2632	148.9364	147.1685	148.7988	147.1021	149.3388	147.3369	149.3196	**131.65**
C7	211.6149	217.1151	218.2887	220.0876	220.5887	219.8852	227.6215	219.7094	224.9662	220.2618	228.6511	211.6152	217.1151	218.2883	220.0876	220.5889	219.8853	227.6215	219.7095	224.9662	220.2618	228.6511	**194.89**
C8	62.4764	63.6690	64.3145	64.2818	65.1579	64.2186	65.8916	64.1836	65.5355	64.3257	66.4138	62.4765	63.6690	64.3146	64.2818	65.1580	64.2185	65.8916	64.1837	65.5356	64.3257	66.4138	**65.05**
C9	24.5842	24.3150	24.4913	24.2609	24.4714	24.2429	24.2742	24.2524	24.5261	24.2610	24.3976	24.5842	24.3150	24.4913	24.2609	24.4715	24.2429	24.2742	24.2524	24.5261	24.2610	24.3976	**24.22**
C10	7.0341	7.2218	7.4167	7.3717	7.6466	7.3397	7.4704	7.3357	7.5247	7.3851	7.5817	7.0341	7.2218	7.4166	7.3717	7.6467	7.3397	7.4704	7.3357	7.5248	7.3850	7.5817	**10.45**
C1`	48.6886	49.4728	49.9278	49.9914	50.6169	49.9322	50.6130	49.9014	50.5396	50.0316	51.0314	52.6020	53.5354	53.9311	54.0311	54.5350	53.9781	54.7405	53.9524	54.5842	54.0644	55.0135	**50.48**
C2`	22.9225	23.2154	23.5687	23.3886	23.8159	23.3548	23.8139	23.3489	23.8279	23.4035	23.7306	22.4210	22.5058	22.8663	22.6367	23.1256	22.6070	23.0621	22.6046	23.0308	22.6476	22.8960	**23.91**
C3`	22.4210	22.5059	22.8663	22.6367	23.1256	22.6071	23.0621	22.6046	23.0308	22.6477	22.8960	22.9225	23.2154	23.5685	23.3886	23.8159	23.3549	23.8139	23.3489	23.8279	23.4036	23.7306	**23.74**
C4`	52.6020	53.5354	53.9311	54.0311	54.5350	53.9780	54.7407	53.9524	54.5842	54.0645	55.0135	48.6886	49.4728	49.9277	49.9914	50.6168	49.9321	50.6129	49.9014	50.5397	50.0316	51.0314	**52.48**
H2	9.0351	8.8989	8.9306	8.8271	8.8216	8.8305	8.7459	8.8356	8.8602	8.8229	8.7488	9.0351	8.8989	8.9306	8.8271	8.8216	8.8305	8.7459	8.8356	8.8602	8.8229	8.7488	**8.08**
H3	7.5461	7.6769	7.7689	7.7183	7.8378	7.7155	7.8569	7.7141	7.8471	7.7200	7.8715	7.5461	7.6769	7.7689	7.7183	7.8377	7.7155	7.8569	7.7141	7.8472	7.7200	7.8715	**7.23**
H5	7.3885	7.5715	7.6624	7.6549	7.7793	7.6492	7.7928	7.6451	7.7821	7.6593	7.8161	7.3885	7.5715	7.6624	7.6549	7.7793	7.6492	7.7928	7.6451	7.7821	7.6593	7.8161	**7.23**
H6	8.1991	8.3809	8.4793	8.4872	8.6326	8.4797	8.6350	8.4737	8.6703	8.4935	8.6719	8.1991	8.3809	8.4793	8.4873	8.6326	8.4797	8.6350	8.4737	8.6703	8.4935	8.6719	**8.08**
H8	4.2134	4.3032	4.3439	4.3729	4.4571	4.3680	4.5214	4.3646	4.4972	4.3765	4.5227	4.2135	4.3032	4.3439	4.3729	4.4571	4.3680	4.5214	4.3646	4.4973	4.3765	4.5227	**5.3**
H(9A)	1.8596	1.9382	1.9396	1.9933	2.0119	1.9890	1.9942	1.9863	2.0235	1.9965	2.0313	1.6053	1.6091	1.6272	1.6086	1.6405	1.6071	1.4811	1.6074	1.6162	1.6094	1.5463	**2.21**
H(9B)	1.6053	1.6091	1.6272	1.6086	1.6405	1.6071	1.4811	1.6074	1.6162	1.6094	1.5463	1.8596	1.9382	1.9395	1.9933	2.0119	1.9890	1.9942	1.9863	2.0235	1.9964	2.0313	**2.14**
H(10A-10C)	0.8490	0.7679	0.7386	0.7333	0.6712	0.7346	0.6926	0.7374	0.6955	0.7311	0.6867	0.8490	0.7679	0.7386	0.7333	0.6712	0.7346	0.6926	0.7374	0.6955	0.7311	0.6867	**1.01**
H(1`A-1`B)	2.8440	2.8660	2.8680	2.8779	2.8810	2.8766	2.8783	2.8768	2.8821	2.8781	2.8712	2.7788	2.7068	2.6781	2.6811	2.6609	2.6819	2.6553	2.6843	2.6411	2.6793	2.6442	**3.68**
H(2`-3`A-2`-3`B)	1.6422	1.7028	1.6677	1.7438	1.6972	1.7402	1.7318	1.7382	1.7119	1.7462	1.7541	1.6422	1.7028	1.6677	1.7438	1.6972	1.7402	1.7318	1.7382	1.7119	1.7462	1.7541	**2.19**
H(4`A)	2.7478	2.6081	2.5674	2.5732	2.5693	2.5745	2.5435	2.5774	2.5178	2.5710	2.5419	3.0093	3.0606	3.0863	3.0971	3.1566	3.0940	3.1380	3.0925	3.1426	3.0990	3.1445	**3.02**
H(4`B)	2.8097	2.8055	2.7888	2.7890	2.7525	2.7893	2.7672	2.7912	2.7643	2.7877	2.7466	2.6786	2.6714	2.6497	2.6587	2.6054	2.6591	2.6186	2.6610	2.6215	2.6572	2.5979	**3.83**
Nuclei	M06																						
C1	136.2474	138.9328	140.1010	139.6813	141.8521	139.6218	140.5292	139.5718	140.7955	139.7541	140.8278	136.2474	138.9328	140.1009	139.6813	141.8522	139.6218	140.5292	139.5718	140.7955	139.7541	140.8278	**131.91**
C2	140.6132	140.1823	140.8258	140.1337	140.9103	140.1285	141.4100	140.1311	141.3103	140.1528	141.4049	140.6132	140.1823	140.8257	140.1336	140.9103	140.1285	141.4100	140.1311	141.3103	140.1528	141.4049	**131.65**
C3	121.5497	122.2466	122.9578	122.6056	123.5211	122.5748	123.6938	122.5516	123.6583	122.6495	123.8082	121.5497	122.2465	122.9578	122.6055	123.5212	122.5748	123.6938	122.5516	123.6583	122.6495	123.8082	**116.7**
C4	173.1448	173.6854	174.3788	174.0258	174.7546	173.9962	175.3869	173.9739	175.2162	174.0681	175.4981	173.1448	173.6853	174.3787	174.0259	174.7546	173.9962	175.3869	173.9739	175.2162	174.0682	175.4981	**166.84**
C5	119.8007	121.0074	121.6741	121.6898	122.5000	121.6376	122.7958	121.5930	122.6983	121.7542	122.9440	119.8007	121.0074	121.6739	121.6898	122.5000	121.6376	122.7958	121.5930	122.6983	121.7542	122.9440	**116.7**
C6	136.9225	138.0189	139.0688	138.7931	140.2370	138.7372	140.9027	138.6883	140.5797	138.8602	141.1852	136.9225	138.0189	139.0689	138.7933	140.2370	138.7372	140.9027	138.6883	140.5797	138.8600	141.1852	**131.65**
C7	202.9552	209.1736	210.6281	212.0370	212.9049	211.8430	217.5565	211.6588	216.5766	212.2388	218.7371	202.9552	209.1736	210.6280	212.0372	212.9048	211.8430	217.5565	211.6587	216.5766	212.2387	218.7371	**194.89**
C8	61.9334	63.9388	64.6742	64.6524	65.4872	64.5999	66.0984	64.5553	66.0271	64.7174	66.6463	61.9334	63.9388	64.6742	64.6524	65.4872	64.5999	66.0984	64.5553	66.0271	64.7174	66.6463	**65.05**
C9	25.7408	25.5771	25.7624	25.5069	25.7001	25.4997	25.9642	25.5006	25.8731	25.5283	26.0895	25.7408	25.5771	25.7624	25.5068	25.7000	25.4997	25.9642	25.5006	25.8731	25.5284	26.0895	**24.22**
C10	7.4812	8.1797	8.4921	8.4177	8.8321	8.3937	8.6899	8.3772	8.6937	8.4549	8.7511	7.4812	8.1797	8.4921	8.4177	8.8321	8.3936	8.6899	8.3772	8.6937	8.4549	8.7511	**10.45**
C1`	50.6217	51.3679	51.8756	51.9190	52.6685	51.8742	52.6179	51.8375	52.5886	51.9761	53.0993	54.9181	55.8619	56.2882	56.3888	57.0027	56.3493	57.2248	56.3171	57.1428	56.4404	57.6240	**50.48**
C2`	23.2425	23.7211	24.1482	23.9764	24.5914	23.9544	24.5998	23.9396	24.5811	24.0116	24.4541	21.8611	22.2788	22.7497	22.4626	23.1754	22.4437	22.9608	22.4324	22.9811	22.4950	22.6644	**23.91**
C3`	21.8611	22.2788	22.7497	22.4626	23.1754	22.4437	22.9608	22.4324	22.9811	22.4951	22.6644	23.2425	23.7211	24.1483	23.9765	24.5914	23.9544	24.5998	23.9396	24.5811	24.0116	24.4541	**23.74**
C4`	54.9181	55.8619	56.2882	56.3888	57.0027	56.3493	57.2248	56.3171	57.1428	56.4404	57.6240	50.6217	51.3679	51.8756	51.9189	52.6686	51.8742	52.6179	51.8375	52.5886	51.9761	53.0993	**52.48**
H2	8.7957	8.5103	8.5265	8.4158	8.4008	8.4211	8.4730	8.4270	8.4607	8.4112	8.4607	8.7957	8.5103	8.5265	8.4158	8.4008	8.4211	8.4730	8.4270	8.4607	8.4112	8.4607	**8.08**
H3	7.3187	7.4837	7.5786	7.4962	7.6094	7.4959	7.6333	7.4960	7.6220	7.4971	7.6379	7.3187	7.4837	7.5786	7.4962	7.6094	7.4959	7.6333	7.4960	7.6220	7.4971	7.6379	**7.23**
H5	7.1328	7.2675	7.3592	7.3456	7.4772	7.3405	7.4940	7.3361	7.4824	7.3511	7.5168	7.1328	7.2675	7.3592	7.3456	7.4773	7.3405	7.4940	7.3361	7.4824	7.3511	7.5168	**7.23**
H6	8.0836	8.1469	8.2265	8.2281	8.3434	8.2231	8.4147	8.2186	8.3857	8.2334	8.4451	8.0836	8.1469	8.2265	8.2281	8.3434	8.2231	8.4147	8.2186	8.3857	8.2334	8.4451	**8.08**
H8	4.4578	4.4522	4.4787	4.4904	4.5389	4.4874	4.6080	4.4849	4.5848	4.4939	4.6240	4.4578	4.4522	4.4787	4.4905	4.5389	4.4874	4.6080	4.4849	4.5848	4.4940	4.6240	**5.3**
H(9A)	2.0099	1.9945	2.0050	2.0343	2.0314	2.0314	2.0919	2.0291	2.0738	2.0375	2.1032	1.6933	1.5599	1.5480	1.5259	1.5099	1.5282	1.4957	1.5309	1.4894	1.5243	1.5153	**2.21**
H(9B)	1.6933	1.5599	1.5480	1.5260	1.5099	1.5282	1.4957	1.5309	1.4894	1.5243	1.5153	2.0099	1.9945	2.0050	2.0343	2.0314	2.0314	2.0919	2.0291	2.0738	2.0376	2.1032	**2.14**
H(10A-10C)	0.7943	0.7406	0.7102	0.7112	0.6556	0.7125	0.6747	0.7144	0.6748	0.7106	0.6592	0.7943	0.7406	0.7102	0.7112	0.6556	0.7125	0.6747	0.7144	0.6748	0.7106	0.6592	**1.01**
H(1`A-1`B)	2.8926	2.8920	2.8988	2.8914	2.9075	2.8912	2.9130	2.8916	2.9112	2.8921	2.9088	2.7986	2.7669	2.7538	2.7402	2.7167	2.7413	2.7187	2.7431	2.7224	2.7397	2.6959	**3.68**
H(2`-3`A-2`-3`B)	1.6369	1.6985	1.6704	1.7309	1.6906	1.7285	1.7115	1.7266	1.7063	1.7339	1.7403	1.6369	1.6985	1.6704	1.7309	1.6905	1.7285	1.7115	1.7266	1.7063	1.7339	1.7403	**2.19**
H(4`A)	2.7505	2.6531	2.6424	2.6224	2.6199	2.6228	2.6014	2.6240	2.6036	2.6228	2.5904	3.1090	3.1408	3.1707	3.1588	3.2246	3.1573	3.2175	3.1564	3.2135	3.1609	3.2236	**3.02**
H(4`B)	2.8468	2.8806	2.8651	2.8578	2.8136	2.8597	2.8360	2.8622	2.8412	2.8566	2.8013	2.6763	2.6432	2.6269	2.6238	2.5905	2.6250	2.6085	2.6268	2.6089	2.6232	2.5939	**3.83**

[a] methyl protons shifts are averaged [b] according to [13] in $CDCl_3$

Table S14. Cont. V

Nuclei	R											S									Exp. [b]
	M06-2X											M06-2X									
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	153.4338	154.4776	155.4189	154.8456	156.7849	154.8402	155.9729	154.8395	156.0038	154.8497	156.4893	153.4338	154.4776	155.4188	154.8456	156.7849	154.8402	155.9729	154.8395	156.0038	154.8497	156.4893	**131.91**
C2	155.2354	155.1784	155.7857	154.9519	155.5441	154.9895	155.9529	155.0277	155.8831	154.9086	155.9856	155.2354	155.1784	155.7857	154.9519	155.5441	154.9895	155.9529	155.0277	155.8831	154.9086	155.9856	**131.65**
C3	135.9486	136.8717	137.5122	137.1015	137.8641	137.1138	138.1032	137.1266	138.0470	137.0827	138.1772	135.9486	136.8717	137.5122	137.1015	137.8641	137.1138	138.1032	137.1266	138.0470	137.0827	138.1772	**116.7**
C4	186.7773	187.6456	188.2688	188.0569	188.7218	188.0543	189.3788	188.0529	189.2186	188.0524	189.5197	186.7773	187.6456	188.2688	188.0569	188.7218	188.0543	189.3788	188.0529	189.2186	188.0524	189.5197	**166.84**
C5	133.5954	135.0732	135.7386	135.8249	136.7706	135.7998	137.0170	135.7763	136.8845	135.8427	137.2270	133.5954	135.0732	135.7387	135.8249	136.7706	135.7998	137.0170	135.7763	136.8845	135.8427	137.2270	**116.7**
C6	151.2913	153.1749	154.4175	154.3788	156.1950	154.3215	156.7900	154.2649	156.5315	154.4258	157.1595	151.2913	153.1749	154.4175	154.3788	156.1950	154.3215	156.7900	154.2649	156.5315	154.4258	157.1595	**131.65**
C7	219.3619	224.9761	226.3223	227.9666	228.7428	227.7924	235.0017	227.6242	233.5317	228.1326	236.5080	219.3619	224.9761	226.3221	227.9666	228.7428	227.7924	235.0017	227.6242	233.5317	228.1326	236.5080	**194.89**
C8	67.2917	68.6496	69.4210	69.4181	70.4628	69.3861	71.1756	69.3556	70.9467	69.4434	71.8519	67.2917	68.6496	69.4211	69.4181	70.4628	69.3861	71.1756	69.3556	70.9467	69.4434	71.8519	**65.05**
C9	27.0091	27.0132	27.1644	26.9605	27.1410	26.9841	27.3958	27.0089	27.3306	26.9316	27.4365	27.0091	27.0132	27.1644	26.9605	27.1410	26.9841	27.3958	27.0089	27.3306	26.9316	27.4365	**24.22**
C10	7.5905	7.7559	7.8733	7.8899	8.1701	7.9007	8.0492	7.9125	8.0409	7.8727	8.1540	7.5905	7.7559	7.8733	7.8899	8.1701	7.9007	8.0492	7.9125	8.0409	7.8727	8.1540	**10.45**
C1`	52.7406	53.4619	53.8570	53.9723	54.5793	53.9591	54.5182	53.9463	54.4620	53.9777	54.8934	56.9951	57.8749	58.2466	58.3400	58.8654	58.3329	59.0246	58.3262	58.9266	58.3397	59.3241	**50.48**
C2`	24.5835	25.0035	25.3300	25.2318	25.6535	25.2384	25.7102	25.2457	25.6632	25.2191	25.6816	23.6110	23.8905	24.2292	24.0746	24.5966	24.0835	24.5159	24.0934	24.4995	24.0601	24.4839	**23.91**
C3`	23.6110	23.8905	24.2292	24.0746	24.5966	24.0835	24.5159	24.0934	24.4995	24.0601	24.4839	24.5835	25.0035	25.3299	25.2318	25.6535	25.2384	25.7102	25.2457	25.6632	25.2191	25.6816	**23.74**
C4`	56.9951	57.8749	58.2466	58.3400	58.8654	58.3329	59.0246	58.3262	58.9266	58.3397	59.3241	52.7406	53.4619	53.8570	53.9723	54.5793	53.9591	54.5182	53.9463	54.4620	53.9777	54.8934	**52.48**
H2	9.3040	9.2165	9.2445	9.1584	9.1396	9.1618	9.1608	9.1643	9.1716	9.1548	9.1314	9.3040	9.2165	9.2444	9.1584	9.1396	9.1618	9.1608	9.1643	9.1716	9.1548	9.1314	**8.08**
H3	7.8325	7.9654	8.0554	8.0245	8.1536	8.0198	8.1888	8.0148	8.1736	8.0294	8.2130	7.8325	7.9654	8.0554	8.0245	8.1536	8.0198	8.1888	8.0148	8.1736	8.0294	8.2130	**7.23**
H5	7.6919	7.8830	7.9791	7.9580	8.0778	7.9527	8.0845	7.9469	8.0770	7.9629	8.0959	7.6919	7.8830	7.9791	7.9580	8.0778	7.9527	8.0845	7.9469	8.0770	7.9629	8.0959	**7.23**
H6	8.5942	8.7612	8.8614	8.8561	8.9888	8.8492	9.0351	8.8418	9.0183	8.8626	9.0459	8.5942	8.7612	8.8615	8.8561	8.9888	8.8492	9.0351	8.8418	9.0183	8.8626	9.0459	**8.08**
H8	4.3087	4.3831	4.4222	4.4278	4.5074	4.4234	4.5592	4.4190	4.5438	4.4323	4.5575	4.3087	4.3831	4.4222	4.4278	4.5074	4.4234	4.5592	4.4190	4.5438	4.4323	4.5575	**5.3**
H(9A)	1.8680	1.9341	1.9354	1.9921	2.0080	1.9870	2.0308	1.9815	2.0226	1.9971	2.0617	1.6747	1.6572	1.6640	1.6683	1.6698	1.6664	1.6349	1.6638	1.6455	1.6699	1.6657	**2.21**
H(9B)	1.6747	1.6572	1.6640	1.6683	1.6698	1.6664	1.6349	1.6638	1.6455	1.6699	1.6657	1.8680	1.9341	1.9354	1.9921	2.0080	1.9870	2.0308	1.9815	2.0226	1.9971	2.0617	**2.14**
H(10A-10C)	0.8203	0.7411	0.7083	0.6976	0.6295	0.6993	0.6429	0.7005	0.6491	0.6960	0.6377	0.8203	0.7411	0.7083	0.6976	0.6295	0.6993	0.6429	0.7005	0.6491	0.6960	0.6377	**1.01**
H(1`A-1`B)	2.8555	2.8771	2.8821	2.8847	2.8887	2.8830	2.8879	2.8810	2.8892	2.8863	2.8704	2.7629	2.7088	2.6900	2.6819	2.6697	2.6817	2.6586	2.6815	2.6616	2.6824	2.6456	**3.68**
H(2`-3`A-2`-3`B)	1.6548	1.7084	1.6778	1.7476	1.7056	1.7436	1.7261	1.7394	1.7201	1.7516	1.7455	1.6548	1.7084	1.6778	1.7476	1.7056	1.7436	1.7261	1.7394	1.7201	1.7516	1.7455	**2.19**
H(4`A)	2.7505	2.6290	2.5941	2.5829	2.5883	2.5830	2.5485	2.5833	2.5544	2.5833	2.5511	3.0903	3.1386	3.1644	3.1671	3.2222	3.1639	3.2064	3.1605	3.2061	3.1702	3.2021	**3.02**
H(4`B)	2.7753	2.7886	2.7859	2.7810	2.7511	2.7805	2.7687	2.7797	2.7687	2.7816	2.7401	2.6207	2.6156	2.5998	2.6023	2.5551	2.6021	2.5693	2.6015	2.5723	2.6025	2.5387	**3.83**
Nuclei	mpW1LYP											mpW1LYP									
C1	139.7041	140.8993	141.2108	141.5353	143.7262	141.4950	143.0385	141.4551	143.0330	141.5703	143.2657	139.7041	140.8993	141.2108	141.5353	143.7262	141.4950	143.0388	141.4551	143.0330	141.5703	143.2657	**131.91**
C2	140.0691	139.8993	140.4439	139.8111	140.4109	139.8120	140.8782	139.8148	140.7887	139.8087	140.9050	140.0691	139.8993	140.4439	139.8111	140.4109	139.8119	140.8783	139.8150	140.7887	139.8087	140.9050	**131.65**
C3	121.8424	122.5770	123.0704	122.8466	123.4962	122.8298	123.7509	122.8143	123.7008	122.8601	123.7744	121.8424	122.5770	123.0704	122.8466	123.4962	122.8297	123.7509	122.8143	123.7008	122.8601	123.7744	**116.7**
C4	176.3048	177.0933	177.7491	177.4908	178.0943	177.4639	178.6610	177.4388	178.5349	177.5147	178.7537	176.3048	177.0933	177.7491	177.4908	178.0942	177.4640	178.6608	177.4388	178.5349	177.5147	178.7537	**166.84**
C5	119.9586	121.1812	121.7786	121.8382	122.5591	121.7948	122.7613	121.7532	122.6739	121.8775	122.8772	119.9586	121.1812	121.7786	121.8382	122.5590	121.7949	122.7613	121.7531	122.6739	121.8775	122.8772	**116.7**
C6	136.1411	137.8787	139.1770	138.8651	139.9640	138.8019	140.5812	138.7403	140.3736	138.9237	140.9067	136.1411	137.8787	139.1770	138.8651	139.9640	138.8020	140.5812	138.7404	140.3736	138.9237	140.9067	**131.65**
C7	203.2829	208.4843	209.2304	211.2866	212.2901	211.1153	217.6197	210.9439	216.3877	211.4459	218.6923	203.2829	208.4843	209.2304	211.2866	212.2901	211.1151	217.6200	210.9438	216.3877	211.4459	218.6923	**194.89**
C8	65.7471	67.0551	67.4443	67.6638	68.2910	67.6320	69.0594	67.5999	68.8541	67.6896	69.4214	65.7471	67.0551	67.4443	67.6638	68.2910	67.6321	69.0595	67.6000	68.8541	67.6896	69.4214	**65.05**
C9	29.2473	29.0780	29.2237	29.0100	28.8016	29.0174	29.1462	29.0253	29.0725	29.0002	29.1472	29.2473	29.0780	29.2237	29.0100	28.8016	29.0174	29.1463	29.0253	29.0725	29.0002	29.1472	**24.22**
C10	8.4703	8.7523	8.9179	8.8807	9.0432	8.8722	8.9862	8.8646	8.9862	8.8867	9.0419	8.4703	8.7523	8.9179	8.8807	9.0430	8.8721	8.9862	8.8646	8.9862	8.8867	9.0419	**10.45**
C1`	51.9302	52.7387	53.0511	53.2781	53.8438	53.2390	53.8361	53.2015	53.7816	53.3129	54.2245	56.4209	57.3952	57.7708	57.9189	58.5078	57.8812	58.6398	57.8456	58.5843	57.9535	58.8511	**50.48**
C2`	25.8290	26.2729	26.6313	26.4927	26.8887	26.4760	26.9615	26.4612	26.9546	26.5072	26.7956	25.6217	25.7331	26.1156	25.9026	26.4736	25.8869	26.3167	25.8733	26.3277	25.9161	26.1081	**23.91**
C3`	25.6217	25.7331	26.1156	25.9026	26.4737	25.8868	26.3167	25.8732	26.3277	25.9161	26.1081	25.8290	26.2729	26.6313	26.4927	26.8887	26.4760	26.9616	26.4611	26.9547	26.5072	26.7956	**23.74**
C4`	56.4209	57.3952	57.7708	57.9189	58.5077	57.8813	58.6397	57.8455	58.5843	57.9535	58.8511	51.9302	52.7387	53.0511	53.2781	53.8438	53.2391	53.8361	53.2015	53.7816	53.3129	54.2245	**52.48**
H2	8.7344	8.5973	8.6733	8.5256	8.5022	8.5297	8.5194	8.5337	8.5275	8.5218	8.5109	8.7344	8.5973	8.6733	8.5256	8.5022	8.5297	8.5194	8.5338	8.5275	8.5218	8.5109	**8.08**
H3	7.3318	7.4578	7.5481	7.5074	7.6321	7.5049	7.6524	7.5021	7.6445	7.5096	7.6648	7.3318	7.4578	7.5481	7.5074	7.6321	7.5049	7.6524	7.5021	7.6445	7.5096	7.6648	**7.23**
H5	7.1905	7.3618	7.4649	7.4327	7.5457	7.4289	7.5602	7.4247	7.5514	7.4363	7.5765	7.1905	7.3618	7.4649	7.4327	7.5457	7.4289	7.5602	7.4247	7.5514	7.4363	7.5765	**7.23**
H6	7.9770	8.1294	8.2484	8.2310	8.3508	8.2243	8.3865	8.2175	8.3729	8.2374	8.4082	7.9770	8.1294	8.2484	8.2310	8.3507	8.2243	8.3865	8.2175	8.3729	8.2374	8.4082	**8.08**
H8	4.5598	4.6136	4.6703	4.6608	4.7414	4.6574	4.7501	4.6539	4.7408	4.6642	4.7332	4.5598	4.6136	4.6703	4.6608	4.7414	4.6574	4.7501	4.6539	4.7408	4.6642	4.7332	**5.3**
H(9A)	1.9807	2.0574	2.0763	2.1117	2.0946	2.1087	2.1267	2.1054	2.1150	2.1144	2.1547	1.5649	1.5806	1.6077	1.5724	1.4929	1.5746	1.4993	1.5762	1.5036	1.5699	1.5326	**2.21**
H(9B)	1.5649	1.5806	1.6077	1.5724	1.4929	1.5746	1.4993	1.5762	1.5036	1.5699	1.5326	1.9807	2.0574	2.0763	2.1117	2.0946	2.1087	2.1267	2.1054	2.1150	2.1144	2.1547	**2.14**
H(10A-10C)	0.8626	0.7866	0.7675	0.7618	0.7184	0.7632	0.7337	0.7644	0.7351	0.7605	0.7257	0.8626	0.7866	0.7675	0.7618	0.7184	0.7632	0.7337	0.7644	0.7351	0.7605	0.7257	**1.01**
H(1`A-1`B)	2.9634	2.9912	2.9957	3.0042	3.0047	3.0039	3.0039	3.0033	3.0039	3.0044	2.9871	2.8756	2.8131	2.7748	2.7874	2.7610	2.7896	2.7528	2.7915	2.7532	2.7850	2.7329	**3.68**
H(2`-3`A-2`-3`B)	1.6666	1.7269	1.6867	1.7691	1.7319	1.7665	1.7481	1.7636	1.7430	1.7717	1.7684	1.6666	1.7269	1.6867	1.7691	1.7319	1.7665	1.7481	1.7636	1.7430	1.7717	1.7684	**2.19**
H(4`A)	2.8871	2.7565	2.6972	2.7224	2.7085	2.7251	2.6814	2.7273	2.6796	2.7197	2.6738	3.1823	3.2397	3.2688	3.2777	3.3264	3.2758	3.3124	3.2736	3.3099	3.2793	3.3116	**3.02**
H(4`B)	2.8642	2.8697	2.8524	2.8524	2.8134	2.8543	2.8242	2.8557	2.8269	2.8503	2.7921	2.7445	2.7426	2.7225	2.7308	2.6830	2.7320	2.6954	2.7330	2.6979	2.7295	2.6626	**3.83**
Nuclei	mpW1PW91											mpW1PW91									
C1	136.8100	137.9806	138.5386	138.5438	140.9037	138.5098	140.1336	138.4813	140.0843	138.5757	140.2635	136.8100	137.9806	138.5386	138.5438	140.9037	138.5098	140.1336	138.4813	140.0843	138.5757	140.2635	**131.91**
C2	139.0412	138.9314	139.5013	138.8207	139.4662	138.8270	139.9627	138.8392	139.8767	138.8140	139.9945	139.0412	138.9314	139.5013	138.8207	139.4662	138.8270	139.9627	138.8391	139.8767	138.8140	139.9946	**131.65**
C3	121.0157	121.8289	122.4065	122.0923	122.8849	122.0784	123.1551	122.0701	123.0903	122.1046	123.2168	121.0157	121.8289	122.4065	122.0923	122.8849	122.0784	123.1551	122.0701	123.0903	122.1046	123.2169	**116.7**
C4	173.3165	174.0978	174.7379	174.4372	175.0434	174.4164	175.6734	174.4013	175.5442	174.4564	175.8021	173.3165	174.0978	174.7379	174.4372	175.0434	174.4164	175.6734	174.4012	175.5442	174.4564	175.8020	**166.84**
C5	119.1703	120.4881	121.0927	121.1562	122.0098	121.1151	122.2414	121.0794	122.1406	121.1950	122.4078	119.1703	120.4881	121.0927	121.1562	122.0098	121.1151	122.2414	121.0795	122.1406	121.1950	122.4079	**116.7**
C6	135.0224	136.7980	137.9290	137.7268	138.8869	137.6698	139.4471	137.6183	139.2538	137.7801	139.8656	135.0224	136.7980	137.9290	137.7268	138.8869	137.6698	139.4471	137.6185	139.2538	137.7801	139.8657	**131.65**
C7	201.1226	206.0842	206.9648	208.7019	209.9730	208.5440	214.8896	208.3916	213.6284	208.8510	215.8666	201.1226	206.0842	206.9648	208.7019	209.9730	208.5440	214.8896	208.3915	213.6284	208.8510	215.8667	**194.89**
C8	63.6287	64.9779	65.4057	65.6030	66.5315	65.5705	67.0852	65.5429	66.8285	65.6322	67.5597	63.6287	64.9779	65.4057	65.6030	66.5315	65.5705	67.0852	65.5430	66.8285	65.6322	67.5597	**65.05**
C9	27.6971	27.6691	27.7767	27.6025	27.6219	27.6075	27.7916	27.6178	27.6991	27.5963	27.9184	27.6971	27.6691	27.7767	27.6025	27.6219	27.6075	27.7916	27.6177	27.6991	27.5963	27.9185	**24.22**
C10	8.2405	8.5463	8.6759	8.6535	8.9031	8.6486	8.7742	8.6490	8.7514	8.6574	8.9264	8.2405	8.5463	8.6759	8.6535	8.9031	8.6486	8.7742	8.6490	8.7514	8.6574	8.9264	**10.45**
C1`	50.4972	51.3180	51.6265	51.7888	52.3857	51.7612	52.3501	51.7396	52.2737	51.8147	52.7888	54.7343	55.7091	56.0448	56.1822	56.7373	56.1530	56.9493	56.1299	56.8896	56.2095	57.1799	**50.48**
C2`	24.5962	25.0060	25.3329	25.1856	25.5885	25.1752	25.6275	25.1705	25.6066	25.1947	25.5080	24.2688	24.4021	24.7516	24.5219	25.0670	24.5125	24.9468	24.5090	24.9547	24.5304	24.7611	**23.91**
C3`	24.2688	24.4021	24.7516	24.5219	25.0670	24.5125	24.9468	24.5090	24.9547	24.5304	24.7612	24.5962	25.0060	25.3329	25.1856	25.5885	25.1752	25.6275	25.1706	25.6066	25.1947	25.5080	**23.74**
C4`	54.7343	55.7091	56.0448	56.1822	56.7373	56.1530	56.9493	56.1299	56.8896	56.2095	57.1798	50.4972	51.3180	51.6265	51.7888	52.3857	51.7612	52.3501	51.7397	52.2737	51.8147	52.7888	**52.48**
H2	8.7931	8.6573	8.7109	8.5819	8.5316	8.5865	8.5778	8.5912	8.5894	8.5779	8.5762	8.7931	8.6573	8.7109	8.5819	8.5316	8.5865	8.5778	8.5912	8.5894	8.5779	8.5762	**8.08**
H3	7.3629	7.4973	7.5887	7.5438	7.6728	7.5416	7.6967	7.5394	7.6880	7.5461	7.7111	7.3629	7.4973	7.5887	7.5438	7.6728	7.5416	7.6967	7.5394	7.6880	7.5461	7.7111	**7.23**
H5	7.2138	7.3898	7.4873	7.4630	7.5830	7.4590	7.5997	7.4551	7.5898	7.4670	7.6200	7.2138	7.3898	7.4873	7.4630	7.5830	7.4590	7.5997	7.4551	7.5898	7.4670	7.6201	**7.23**
H6	8.0642	8.2199	8.3172	8.3125	8.4157	8.3067	8.4609	8.3012	8.4505	8.3182	8.4917	8.0642	8.2199	8.3172	8.3125	8.4157	8.3067	8.4609	8.3012	8.4505	8.3182	8.4917	**8.08**
H8	4.5552	4.6075	4.6487	4.6530	4.7204	4.6494	4.7473	4.6460	4.7406	4.6568	4.7450	4.5552	4.6075	4.6487	4.6530	4.7204	4.6494	4.7473	4.6460	4.7406	4.6568	4.7450	**5.3**
H(9A)	1.9698	2.0504	2.0584	2.1015	2.0941	2.0987	2.1156	2.0959	2.1030	2.1044	2.1529	1.6156	1.6295	1.6334	1.6159	1.5465	1.6183	1.5125	1.6206	1.5160	1.6138	1.5682	**2.21**
H(9B)	1.6156	1.6295	1.6334	1.6159	1.5465	1.6183	1.5125	1.6206	1.5160	1.6138	1.5682	1.9698	2.0504	2.0584	2.1015	2.0941	2.0987	2.1156	2.0959	2.1030	2.1044	2.1529	**2.14**
H(10A-10C)	0.8096	0.7385	0.7151	0.7072	0.6530	0.7092	0.6771	0.7112	0.6793	0.7056	0.6700	0.8096	0.7385	0.7151	0.7072	0.6530	0.7092	0.6771	0.7112	0.6793	0.7056	0.6700	**1.01**
H(1`A-1`B)	2.9178	2.9445	2.9469	2.9515	2.9556	2.9512	2.9527	2.9509	2.9526	2.9521	2.9375	2.8436	2.7772	2.7443	2.7465	2.7418	2.7483	2.7111	2.7502	2.7106	2.7449	2.6952	**3.68**
H(2`-3`A-2`-3`B)	1.6383	1.6989	1.6608	1.7358	1.7000	1.7336	1.7193	1.7315	1.7137	1.7382	1.7429	1.6383	1.6989	1.6608	1.7358	1.7000	1.7336	1.7193	1.7315	1.7137	1.7382	1.7429	**2.19**
H(4`A)	2.8867	2.7471	2.6964	2.7012	2.7228	2.7032	2.6529	2.7053	2.6513	2.6995	2.6453	3.1562	3.2102	3.2307	3.2391	3.2917	3.2374	3.2736	3.2358	3.2708	3.2410	3.2736	**3.02**
H(4`B)	2.8005	2.8073	2.7922	2.7917	2.7607	2.7934	2.7693	2.7951	2.7700	2.7903	2.7450	2.6794	2.6787	2.6631	2.6639	2.6195	2.6649	2.6318	2.6659	2.6344	2.6632	2.6014	**3.83**

[a] methyl protons shifts are averaged [b] according to [13] in $CDCl_3$

Table S14. Cont. VI

Nuclei	R											S									Exp. [b]
	O3LYP																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	134.6852	136.8207	137.1096	137.6206	139.3607	137.5893	138.3387	137.5522	138.5060	137.6429	138.5383	134.6851	136.8207	137.1096	137.6206	139.3607	137.5894	138.3387	137.5521	138.5060	137.6430	138.5383	**131.91**
C2	134.2200	134.2453	134.8776	134.2633	134.8477	134.2735	135.2336	134.2784	135.1484	134.2458	135.2345	134.2200	134.2453	134.8776	134.2633	134.8477	134.2736	135.2336	134.2783	135.1484	134.2459	135.2345	**131.65**
C3	117.1321	117.9019	118.4806	118.1484	118.8279	118.1468	119.0810	118.1397	119.0226	118.1431	119.1229	117.1320	117.9019	118.4806	118.1484	118.8279	118.1467	119.0810	118.1397	119.0226	118.1431	119.1229	**116.7**
C4	169.5264	170.0924	170.8213	170.5124	171.2149	170.4965	171.7802	170.4752	171.6254	170.5211	171.8946	169.5264	170.0924	170.8213	170.5124	171.2149	170.4963	171.7802	170.4753	171.6254	170.5211	171.8946	**166.84**
C5	115.2416	116.2916	116.9942	116.8973	117.6617	116.8703	117.9088	116.8382	117.8002	116.9169	118.0612	115.2416	116.2916	116.9942	116.8973	117.6617	116.8702	117.9088	116.8382	117.8002	116.9168	118.0612	**116.7**
C6	129.9224	131.2854	132.4315	132.4006	133.8108	132.3376	134.4252	132.2699	134.1495	132.4543	134.7239	129.9225	131.2854	132.4315	132.4006	133.8108	132.3376	134.4252	132.2699	134.1495	132.4542	134.7239	**131.65**
C7	196.8549	202.5909	203.1525	205.3974	206.1336	205.2395	210.4772	205.0767	209.5426	205.5412	211.4604	196.8550	202.5909	203.1525	205.3974	206.1336	205.2396	210.4772	205.0767	209.5426	205.5412	211.4604	**194.89**
C8	64.4100	66.2237	66.4509	66.9538	67.5942	66.9206	68.1364	66.8832	68.0238	66.9795	68.4155	64.4100	66.2237	66.4509	66.9538	67.5942	66.9207	68.1364	66.8831	68.0238	66.9796	68.4155	**65.05**
C9	28.5204	28.3499	28.4905	28.3340	28.3838	28.3453	28.7770	28.3520	28.6857	28.3171	28.7841	28.5205	28.3499	28.4905	28.3340	28.3838	28.3453	28.7770	28.3519	28.6857	28.3172	28.7841	**24.22**
C10	8.5924	8.8363	9.0684	8.9729	9.2485	8.9738	9.1996	8.9700	9.1884	8.9658	9.2938	8.5923	8.8363	9.0684	8.9729	9.2485	8.9739	9.1996	8.9701	9.1884	8.9658	9.2938	**10.45**
C1`	50.7604	51.5135	51.8645	52.0453	52.6526	52.0200	52.6148	51.9899	52.5713	52.0632	52.9703	55.2168	56.1221	56.5407	56.6385	57.1880	56.6160	57.2763	56.5886	57.2039	56.6532	57.5013	**50.48**
C2`	25.8590	26.2824	26.6436	26.4924	26.9122	26.4881	26.9437	26.4791	26.9283	26.4904	26.7395	25.7047	25.8528	26.1952	26.0666	26.6009	26.0633	26.4382	26.0547	26.4409	26.0632	26.1898	**23.91**
C3`	25.7047	25.8528	26.1952	26.0666	26.6009	26.0632	26.4382	26.0547	26.4409	26.0632	26.1898	25.8591	26.2824	26.6436	26.4924	26.9122	26.4881	26.9437	26.4792	26.9283	26.4904	26.7395	**23.74**
C4`	55.2168	56.1221	56.5407	56.6385	57.1880	56.6161	57.2763	56.5886	57.2039	56.6532	57.5013	50.7604	51.5135	51.8645	52.0453	52.6526	52.0200	52.6148	51.9899	52.5713	52.0632	52.9703	**52.48**
H2	8.5308	8.3196	8.4221	8.2448	8.2555	8.2493	8.3252	8.2535	8.3129	8.2404	8.3198	8.5308	8.3196	8.4221	8.2448	8.2555	8.2493	8.3252	8.2535	8.3129	8.2404	8.3198	**8.08**
H3	7.2883	7.4211	7.5238	7.4572	7.5730	7.4558	7.5974	7.4540	7.5883	7.4584	7.6113	7.2884	7.4211	7.5238	7.4572	7.5730	7.4558	7.5974	7.4540	7.5883	7.4584	7.6113	**7.23**
H5	7.1409	7.2961	7.3853	7.3784	7.4999	7.3741	7.5159	7.3694	7.5050	7.3824	7.5369	7.1409	7.2961	7.3853	7.3784	7.4999	7.3741	7.5159	7.3694	7.5050	7.3824	7.5369	**7.23**
H6	7.9048	8.0208	8.1410	8.0947	8.2285	8.0896	8.2785	8.0844	8.2530	8.0994	8.2976	7.9048	8.0208	8.1410	8.0947	8.2285	8.0896	8.2785	8.0844	8.2530	8.0994	8.2976	**8.08**
H8	4.7521	4.7485	4.7938	4.7718	4.8470	4.7701	4.8646	4.7682	4.8476	4.7734	4.8495	4.7522	4.7485	4.7938	4.7718	4.8470	4.7701	4.8646	4.7682	4.8476	4.7734	4.8495	**5.3**
H(9A)	1.9664	2.0280	2.0512	2.0822	2.0945	2.0788	2.1385	2.0752	2.1231	2.0853	2.1668	1.4792	1.4350	1.4604	1.4224	1.4164	1.4228	1.4371	1.4230	1.4335	1.4222	1.4705	**2.21**
H(9B)	1.4792	1.4350	1.4604	1.4224	1.4164	1.4228	1.4371	1.4229	1.4335	1.4222	1.4705	1.9664	2.0280	2.0512	2.0822	2.0945	2.0788	2.1385	2.0752	2.1231	2.0853	2.1668	**2.14**
H(10A-10C)	0.8069	0.7490	0.7302	0.7350	0.6882	0.7363	0.7069	0.7372	0.7060	0.7337	0.6989	0.8069	0.7490	0.7302	0.7350	0.6882	0.7363	0.7069	0.7372	0.7060	0.7337	0.6989	**1.01**
H(1`A-1`B)	3.0218	3.0401	3.0452	3.0476	3.0511	3.0475	3.0503	3.0470	3.0494	3.0475	3.0311	2.9150	2.8575	2.8342	2.8364	2.8196	2.8379	2.8075	2.8391	2.8109	2.8349	2.7910	**3.68**
H(2`-3`A-2`-3`B)	1.6809	1.7342	1.7006	1.7749	1.7343	1.7726	1.7483	1.7699	1.7436	1.7770	1.7711	1.6809	1.7342	1.7006	1.7749	1.7343	1.7726	1.7483	1.7699	1.7436	1.7770	1.7711	**2.19**
H(4`A)	2.9092	2.8074	2.7699	2.7873	2.7920	2.7884	2.7636	2.7894	2.7660	2.7862	2.7624	3.2472	3.2927	3.3272	3.3264	3.3834	3.3244	3.3722	3.3222	3.3685	3.3281	3.3655	**3.02**
H(4`B)	2.9209	2.9076	2.8986	2.8855	2.8473	2.8874	2.8515	2.8890	2.8558	2.8836	2.8196	2.7964	2.7875	2.7632	2.7687	2.7188	2.7705	2.7285	2.7720	2.7303	2.7669	2.6968	**3.83**
Nuclei	**OLYP**																						
C1	133.8351	135.6494	136.7395	136.4684	138.3119	136.4144	137.0878	136.3585	137.3217	136.5148	137.4066	133.8351	135.6494	136.7395	136.4684	138.3119	136.4144	137.0878	136.3586	137.3217	136.5148	137.4066	**131.91**
C2	131.8165	131.8666	132.5613	131.8889	132.4317	131.9005	132.8310	131.9059	132.7378	131.8683	132.8281	131.8165	131.8666	132.5614	131.8889	132.4317	131.9005	132.8310	131.9058	132.7378	131.8683	132.8281	**131.65**
C3	115.3675	116.0445	116.6770	116.2749	116.9243	116.2736	117.2202	116.2660	117.1513	116.2667	117.2580	115.3675	116.0445	116.6772	116.2749	116.9243	116.2736	117.2202	116.2659	117.1513	116.2667	117.2580	**116.7**
C4	168.3873	169.0642	169.8140	169.4983	170.2057	169.4832	170.7873	169.4620	170.6272	169.5032	170.8944	168.3873	169.0642	169.8141	169.4983	170.2057	169.4832	170.7873	169.4619	170.6272	169.5032	170.8944	**166.84**
C5	113.4391	114.4174	115.0512	115.0098	115.7200	114.9837	116.0289	114.9514	115.9097	115.0254	116.1576	113.4391	114.4174	115.0511	115.0098	115.7200	114.9837	116.0289	114.9514	115.9097	115.0254	116.1576	**116.7**
C6	127.3510	128.9229	129.9895	130.0369	131.3495	129.9778	132.0100	129.9124	131.7234	130.0834	132.2868	127.3510	128.9229	129.9895	130.0368	131.3495	129.9778	132.0100	129.9125	131.7234	130.0834	132.2868	**131.65**
C7	195.4633	200.7587	202.0891	203.5188	204.5384	203.3387	208.1627	203.1586	207.4247	203.6866	209.2319	195.4633	200.7587	202.0891	203.5188	204.5384	203.3387	208.1627	203.1586	207.4247	203.6866	209.2319	**194.89**
C8	65.9474	67.6652	68.1647	68.4705	69.3045	68.4195	69.6410	68.3655	69.5914	68.5126	69.8866	65.9474	67.6652	68.1647	68.4705	69.3045	68.4195	69.6410	68.3656	69.5914	68.5126	69.8866	**65.05**
C9	29.6624	29.4884	29.6242	29.5146	29.5588	29.5224	30.0305	29.5242	29.9292	29.4978	29.9896	29.6624	29.4884	29.6242	29.5146	29.5588	29.5224	30.0305	29.5242	29.9292	29.4978	29.9896	**24.22**
C10	8.7576	9.0274	9.1768	9.1836	9.4591	9.1834	9.4372	9.1777	9.4248	9.1743	9.4993	8.7576	9.0274	9.1768	9.1836	9.4591	9.1834	9.4372	9.1777	9.4248	9.1743	9.4993	**10.45**
C1`	51.7069	52.4585	52.8434	53.0117	53.6019	52.9846	53.5676	52.9522	53.5270	53.0288	53.9035	56.2414	57.1377	57.5367	57.6407	58.1548	57.6187	58.2570	57.5913	58.1780	57.6527	58.4958	**50.48**
C2`	26.4273	26.9302	27.2237	27.1732	27.5665	27.1678	27.6133	27.1568	27.5940	27.1691	27.3850	26.4685	26.5882	27.0514	26.8341	27.3255	26.8265	27.1736	26.8137	27.1757	26.8327	26.9495	**23.91**
C3`	26.4685	26.5882	27.0513	26.8341	27.3255	26.8265	27.1736	26.8137	27.1757	26.8327	26.9495	26.4273	26.9302	27.2237	27.1733	27.5665	27.1678	27.6133	27.1568	27.5940	27.1691	27.3850	**23.74**
C4`	56.2414	57.1377	57.5368	57.6407	58.1548	57.6187	58.2570	57.5913	58.1780	57.6527	58.4958	51.7069	52.4585	52.8433	53.0118	53.6019	52.9846	53.5676	52.9522	53.5270	53.0288	53.9035	**52.48**
H2	8.3451	8.1784	8.2118	8.1041	8.0993	8.1107	8.1998	8.1169	8.1779	8.0968	8.1842	8.3451	8.1784	8.2118	8.1041	8.0993	8.1107	8.1998	8.1169	8.1779	8.0968	8.1842	**8.08**
H3	7.2251	7.3362	7.4254	7.3700	7.4829	7.3688	7.5135	7.3675	7.5027	7.3705	7.5243	7.2251	7.3362	7.4254	7.3700	7.4829	7.3688	7.5135	7.3675	7.5027	7.3705	7.5243	**7.23**
H5	7.0535	7.2233	7.3156	7.3052	7.4261	7.3006	7.4407	7.2960	7.4304	7.3091	7.4611	7.0535	7.2233	7.3156	7.3052	7.4261	7.3006	7.4407	7.2960	7.4304	7.3091	7.4611	**7.23**
H6	7.8124	7.9126	8.0035	7.9844	8.1003	7.9806	8.1710	7.9766	8.1398	7.9874	8.1887	7.8124	7.9126	8.0035	7.9844	8.1003	7.9806	8.1710	7.9766	8.1398	7.9874	8.1887	**8.08**
H8	4.9123	4.8931	4.9173	4.9056	4.9642	4.9052	4.9892	4.9046	4.9723	4.9053	4.9719	4.9123	4.8931	4.9173	4.9056	4.9642	4.9052	4.9892	4.9046	4.9723	4.9053	4.9719	**5.3**
H(9A)	2.0161	2.0924	2.1000	2.1498	2.1655	2.1465	2.2138	2.1430	2.1978	2.1526	2.2408	1.4710	1.4659	1.4429	1.4662	1.4644	1.4666	1.4895	1.4668	1.4840	1.4653	1.5082	**2.21**
H(9B)	1.4710	1.4659	1.4429	1.4662	1.4644	1.4666	1.4895	1.4669	1.4840	1.4653	1.5082	2.0161	2.0924	2.1000	2.1498	2.1655	2.1465	2.2138	2.1430	2.1978	2.1526	2.2408	**2.14**
H(10A-10C)	0.8117	0.7606	0.7472	0.7487	0.7001	0.7496	0.7183	0.7505	0.7176	0.7474	0.7143	0.8117	0.7606	0.7472	0.7487	0.7001	0.7496	0.7183	0.7505	0.7176	0.7474	0.7143	**1.01**
H(1`A-1`B)	3.0956	3.1124	3.1161	3.1210	3.1260	3.1209	3.1246	3.1205	3.1240	3.1208	3.1031	2.9925	2.9258	2.9111	2.9113	2.9016	2.9118	2.8840	2.9124	2.8894	2.9104	2.8659	**3.68**
H(2`-3`A-2`-3`B)	1.7219	1.7678	1.7439	1.8060	1.7649	1.8035	1.7780	1.8011	1.7739	1.8078	1.8031	1.7219	1.7678	1.7439	1.8060	1.7649	1.8035	1.7780	1.8011	1.7739	1.8078	1.8031	**2.19**
H(4`A)	2.9962	2.8834	2.8672	2.8724	2.8868	2.8720	2.8538	2.8718	2.8587	2.8725	2.8528	3.3319	3.3770	3.4106	3.4139	3.4745	3.4118	3.4642	3.4095	3.4605	3.4156	3.4549	**3.02**
H(4`B)	2.9889	2.9682	2.9551	2.9501	2.9163	2.9516	2.9142	2.9530	2.9200	2.9483	2.8791	2.8594	2.8478	2.8215	2.8281	2.7774	2.8299	2.7851	2.8316	2.7874	2.8260	2.7514	**3.83**
Nuclei	**OPBE**																						
C1	130.5131	132.5342	133.5416	133.2638	135.1900	133.2330	133.9500	133.1867	134.1426	133.2924	134.2560	130.5130	132.5342	133.5417	133.2638	135.1900	133.2330	133.9500	133.1867	134.1426	133.2924	134.2560	**131.91**
C2	130.4654	130.5593	131.2646	130.5133	131.1427	130.5324	131.4958	130.5334	131.4169	130.4900	131.5188	130.4654	130.5593	131.2645	130.5133	131.1427	130.5324	131.4958	130.5333	131.4168	130.4900	131.5188	**131.65**
C3	114.2409	115.0778	115.6860	115.2694	115.9764	115.2769	116.2880	115.2657	116.2145	115.2567	116.3661	114.2409	115.0778	115.6859	115.2694	115.9764	115.2769	116.2880	115.2657	116.2145	115.2567	116.3661	**116.7**
C4	164.8191	165.5743	166.2518	165.9145	166.5739	165.9107	167.1865	165.8886	167.0297	165.9126	167.3162	164.8191	165.5743	166.2517	165.9145	166.5739	165.9107	167.1865	165.8887	167.0297	165.9126	167.3162	**166.84**
C5	112.3915	113.5120	114.0997	114.0481	114.7968	114.0322	115.1336	113.9981	115.0095	114.0579	115.3094	112.3915	113.5120	114.0998	114.0481	114.7968	114.0322	115.1336	113.9982	115.0096	114.0579	115.3094	**116.7**
C6	125.8932	127.4990	128.5138	128.4720	129.7852	128.4261	130.4324	128.3626	130.1682	128.5103	130.7223	125.8931	127.4990	128.5138	128.4720	129.7852	128.4262	130.4324	128.3625	130.1684	128.5103	130.7223	**131.65**
C7	192.7338	198.0357	199.1499	200.5675	201.6468	200.4240	205.0873	200.2661	204.3224	200.7036	206.1138	192.7338	198.0357	199.1501	200.5675	201.6468	200.4240	205.0873	200.2658	204.3223	200.7036	206.1138	**194.89**
C8	63.2927	65.2089	65.5222	65.9441	66.7821	65.9146	67.1347	65.8685	67.0426	65.9696	67.4768	63.2927	65.2089	65.5222	65.9441	66.7821	65.9146	67.1347	65.8685	67.0426	65.9696	67.4768	**65.05**
C9	27.7188	27.7819	27.7655	27.7587	27.7616	27.7791	28.2175	27.7810	28.1060	27.7333	28.2463	27.7188	27.7819	27.7654	27.7587	27.7616	27.7791	28.2175	27.7810	28.1059	27.7333	28.2463	**24.22**
C10	8.3107	8.6601	8.6766	8.7360	8.9559	8.7479	8.9088	8.7419	8.8948	8.7194	9.0637	8.3107	8.6601	8.6766	8.7360	8.9559	8.7479	8.9088	8.7419	8.8948	8.7194	9.0637	**10.45**
C1`	49.7994	50.6057	50.8749	51.0364	51.5932	51.0229	51.5367	50.9920	51.5017	51.0449	51.9169	54.1269	55.0800	55.4325	55.5005	55.9830	55.4885	56.1055	55.4591	56.0330	55.5076	56.3583	**50.48**
C2`	25.0597	25.5338	25.7242	25.6522	26.0222	25.6606	26.0182	25.6514	26.0055	25.6395	25.7853	24.9078	25.1189	25.4999	25.2113	25.6637	25.2209	25.5067	25.2129	25.5153	25.1978	25.2405	**23.91**
C3`	24.9078	25.1189	25.4999	25.2113	25.6637	25.2209	25.5066	25.2130	25.5153	25.1978	25.2405	25.0597	25.5338	25.7242	25.6522	26.0222	25.6606	26.0182	25.6514	26.0054	25.6395	25.7853	**23.74**
C4`	54.1269	55.0800	55.4325	55.5005	55.9830	55.4885	56.1055	55.4592	56.0330	55.5076	56.3583	49.7994	50.6057	50.8748	51.0364	51.5932	51.0229	51.5367	50.9921	51.5018	51.0449	51.9169	**52.48**
H2	8.4011	8.2161	8.2508	8.1423	8.1266	8.1477	8.2317	8.1521	8.2136	8.1360	8.2204	8.4011	8.2161	8.2508	8.1423	8.1266	8.1477	8.2317	8.1521	8.2136	8.1360	8.2204	**8.08**
H3	7.2498	7.3725	7.4570	7.4084	7.5185	7.4072	7.5500	7.4053	7.5393	7.4086	7.5643	7.2498	7.3725	7.4570	7.4084	7.5185	7.4072	7.5500	7.4053	7.5393	7.4086	7.5643	**7.23**
H5	7.0757	7.2539	7.3400	7.3316	7.4506	7.3277	7.4697	7.3231	7.4580	7.3344	7.4913	7.0757	7.2539	7.3400	7.3316	7.4506	7.3277	7.4697	7.3232	7.4580	7.3344	7.4913	**7.23**
H6	7.8852	7.9730	8.0618	8.0368	8.1461	8.0329	8.2155	8.0284	8.1883	8.0396	8.2315	7.8852	7.9730	8.0618	8.0368	8.1461	8.0329	8.2155	8.0284	8.1883	8.0396	8.2315	**8.08**
H8	4.9112	4.9002	4.9205	4.9122	4.9618	4.9118	4.9851	4.9106	4.9692	4.9118	4.9744	4.9112	4.9002	4.9205	4.9122	4.9618	4.9118	4.9851	4.9106	4.9693	4.9118	4.9744	**5.3**
H(9A)	2.0117	2.0819	2.0795	2.1355	2.1416	2.1326	2.1884	2.1290	2.1725	2.1374	2.2176	1.5133	1.4870	1.4386	1.4778	1.4593	1.4789	1.4799	1.4793	1.4756	1.4757	1.5126	**2.21**
H(9B)	1.5133	1.4870	1.4386	1.4778	1.4593	1.4789	1.4799	1.4793	1.4756	1.4757	1.5126	2.0117	2.0819	2.0794	2.1355	2.1416	2.1326	2.1884	2.1290	2.1725	2.1374	2.2176	**2.14**
H(10A-10C)	0.7402	0.6920	0.6764	0.6750	0.6264	0.6765	0.6434	0.6773	0.6431	0.6730	0.6385	0.7402	0.6920	0.6764	0.6750	0.6264	0.6765	0.6434	0.6773	0.6430	0.6730	0.6385	**1.01**
H(1`A-1`B)	3.0423	3.0608	3.0545	3.0638	3.0608	3.0643	3.0570	3.0642	3.0565	3.0624	3.0360	2.9475	2.8893	2.8557	2.8659	2.8477	2.8680	2.8287	2.8693	2.8329	2.8633	2.8133	**3.68**
H(2`-3`A-2`-3`B)	1.6770	1.7254	1.6974	1.7598	1.7175	1.7580	1.7315	1.7554	1.7272	1.7609	1.7597	1.6770	1.7254	1.6974	1.7598	1.7175	1.7580	1.7315	1.7555	1.7272	1.7609	1.7597	**2.19**
H(4`A)	2.9824	2.8765	2.8320	2.8523	2.8527	2.8542	2.8155	2.8554	2.8193	2.8498	2.8154	3.3033	3.3455	3.3652	3.3727	3.4196	3.3715	3.4051	3.3697	3.4022	3.3730	3.3958	**3.02**
H(4`B)	2.9125	2.9021	2.8794	2.8796	2.8428	2.8817	2.8418	2.8831	2.8464	2.8768	2.8112	2.7812	2.7760	2.7437	2.7549	2.7020	2.7571	2.7089	2.7586	2.7107	2.7519	2.6762	**3.83**

[a] methyl protons shifts are averaged [b] according to [13] in $CDCl_3$

Table S14. Cont. VII

Nuclei	R											S									Exp. [b]
	OPW91																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	130.8334	132.8499	133.8571	133.5809	135.4758	133.5406	134.2542	133.4857	134.4481	133.6049	134.5635	130.8334	132.8499	133.8571	133.5809	135.4758	133.5406	134.2542	133.4857	134.4481	133.6049	134.5634	**131.91**
C2	130.6869	130.7809	131.4819	130.7413	131.3585	130.7502	131.7136	130.7421	131.6343	130.7145	131.7387	130.6869	130.7809	131.4819	130.7413	131.3585	130.7502	131.7136	130.7421	131.6343	130.7145	131.7387	**131.65**
C3	114.4375	115.2730	115.8749	115.4678	116.1604	115.4652	116.4717	115.4452	116.3987	115.4513	116.5506	114.4375	115.2730	115.8749	115.4678	116.1604	115.4652	116.4717	115.4452	116.3988	115.4513	116.5505	**116.7**
C4	165.2239	165.9795	166.6546	166.3272	166.9815	166.3131	167.5911	166.2816	167.4341	166.3216	167.7232	165.2238	165.9795	166.6546	166.3272	166.9815	166.3131	167.5911	166.2816	167.4342	166.3216	167.7232	**166.84**
C5	112.5854	113.7060	114.2881	114.2461	114.9833	114.2202	115.3172	114.1769	115.1938	114.2520	115.4937	112.5854	113.7060	114.2881	114.2461	114.9833	114.2202	115.3171	114.1769	115.1937	114.2520	115.4937	**116.7**
C6	126.1139	127.7231	128.7361	128.7081	130.0155	128.6517	130.6617	128.5782	130.3961	128.7432	130.9542	126.1140	127.7231	128.7361	128.7081	130.0155	128.6517	130.6616	128.5782	130.3961	128.7432	130.9542	**131.65**
C7	193.1215	198.4381	199.5572	200.9778	202.0184	200.8249	205.5061	200.6579	204.7375	201.1098	206.5369	193.1212	198.4380	199.5572	200.9778	202.0184	200.8249	205.5060	200.6579	204.7375	201.1098	206.5369	**194.89**
C8	63.5176	65.4318	65.7420	66.1658	66.9759	66.1270	67.3419	66.0724	67.2514	66.1867	67.6855	63.5175	65.4318	65.7419	66.1658	66.9759	66.1270	67.3419	66.0724	67.2514	66.1867	67.6855	**65.05**
C9	27.8629	27.9229	27.9054	27.9045	27.8985	27.9149	28.3552	27.9076	28.2444	27.8754	28.3853	27.8629	27.9229	27.9054	27.9045	27.8985	27.9149	28.3552	27.9076	28.2444	27.8754	28.3854	**24.22**
C10	8.3646	8.7176	8.7338	8.7982	9.0111	8.8002	8.9653	8.7850	8.9522	8.7779	9.1182	8.3646	8.7176	8.7339	8.7982	9.0111	8.8002	8.9653	8.7850	8.9520	8.7779	9.1182	**10.45**
C1`	49.9410	50.7530	51.0221	51.1910	51.7391	51.1673	51.6860	51.1272	51.6509	51.1958	52.0665	54.2763	55.2341	55.5835	55.6599	56.1365	55.6379	56.2572	55.5994	56.1845	55.6630	56.5133	**50.48**
C2`	25.1770	25.6592	25.8491	25.7847	26.1465	25.7830	26.1447	25.7643	26.1326	25.7681	25.9162	25.0261	25.2389	25.6194	25.3423	25.7885	25.3413	25.6326	25.3238	25.6410	25.3253	25.3716	**23.91**
C3`	25.0261	25.2389	25.6194	25.3423	25.7885	25.3413	25.6326	25.3238	25.6411	25.3253	25.3716	25.1770	25.6592	25.8491	25.7847	26.1465	25.7830	26.1447	25.7643	26.1326	25.7681	25.9161	**23.74**
C4`	54.2764	55.2341	55.5835	55.6599	56.1365	55.6379	56.2572	55.5994	56.1845	55.6630	56.5134	49.9409	50.7529	51.0221	51.1910	51.7391	51.1673	51.6860	51.1272	51.6509	51.1958	52.0665	**52.48**
H2	8.4015	8.2172	8.2517	8.1447	8.1303	8.1493	8.2333	8.1534	8.2152	8.1382	8.2218	8.4015	8.2172	8.2517	8.1447	8.1303	8.1493	8.2333	8.1534	8.2152	8.1382	8.2218	**8.08**
H3	7.2509	7.3736	7.4580	7.4100	7.5192	7.4082	7.5506	7.4061	7.5399	7.4099	7.5647	7.2509	7.3736	7.4580	7.4100	7.5192	7.4082	7.5506	7.4061	7.5399	7.4099	7.5647	**7.23**
H5	7.0782	7.2554	7.3413	7.3336	7.4516	7.3291	7.4707	7.3243	7.4589	7.3362	7.4921	7.0782	7.2554	7.3413	7.3336	7.4516	7.3291	7.4707	7.3243	7.4589	7.3362	7.4922	**7.23**
H6	7.8845	7.9736	8.0623	8.0385	8.1481	8.0339	8.2169	8.0291	8.1893	8.0411	8.2327	7.8845	7.9736	8.0623	8.0385	8.1481	8.0339	8.2169	8.0291	8.1893	8.0411	8.2327	**8.08**
H8	4.9104	4.8993	4.9197	4.9124	4.9620	4.9112	4.9850	4.9098	4.9690	4.9117	4.9739	4.9104	4.8993	4.9197	4.9124	4.9620	4.9112	4.9850	4.9098	4.9690	4.9117	4.9739	**5.3**
H(9A)	2.0089	2.0797	2.0772	2.1341	2.1396	2.1305	2.1866	2.1267	2.1706	2.1356	2.2155	1.5078	1.4834	1.4356	1.4751	1.4567	1.4756	1.4776	1.4757	1.4732	1.4728	1.5096	**2.21**
H(9B)	1.5078	1.4834	1.4356	1.4751	1.4567	1.4756	1.4776	1.4757	1.4732	1.4728	1.5096	2.0089	2.0797	2.0772	2.1341	2.1396	2.1305	2.1866	2.1267	2.1706	2.1356	2.2155	**2.14**
H(10A-10C)	0.7436	0.6951	0.6799	0.6790	0.6297	0.6798	0.6470	0.6803	0.6465	0.6767	0.6419	0.7436	0.6951	0.6799	0.6790	0.6297	0.6798	0.6470	0.6803	0.6465	0.6767	0.6419	**1.01**
H(1`A-1`B)	3.0424	3.0612	3.0551	3.0650	3.0615	3.0649	3.0581	3.0645	3.0574	3.0634	3.0370	2.9470	2.8887	2.8557	2.8662	2.8472	2.8676	2.8286	2.8687	2.8328	2.8633	2.8134	**3.68**
H(2`-3`A-2`-3`B)	1.6773	1.7260	1.6981	1.7610	1.7181	1.7585	1.7321	1.7558	1.7278	1.7619	1.7601	1.6773	1.7260	1.6981	1.7610	1.7181	1.7585	1.7321	1.7558	1.7278	1.7619	1.7601	**2.19**
H(4`A)	2.9778	2.8722	2.8287	2.8492	2.8489	2.8503	2.8124	2.8513	2.8162	2.8464	2.8127	3.2994	3.3423	3.3624	3.3707	3.4171	3.3688	3.4033	3.3667	3.4002	3.3707	3.3938	**3.02**
H(4`B)	2.9162	2.9052	2.8827	2.8833	2.8455	2.8848	2.8449	2.8860	2.8494	2.8802	2.8140	2.7854	2.7800	2.7478	2.7593	2.7058	2.7610	2.7129	2.7623	2.7145	2.7561	2.6802	**3.83**
Nuclei	PBE																						
C1	135.5027	137.0862	137.5815	137.7635	140.0277	137.7142	139.4466	137.6744	139.4065	137.8270	139.7153	135.5027	137.0862	137.5815	137.7635	140.0277	137.7142	139.4466	137.6744	139.4065	137.8270	139.7153	**131.91**
C2	135.9665	135.9788	136.5525	135.8311	136.6569	135.8362	137.1165	135.8525	137.0309	135.8442	137.1907	135.9667	135.9788	136.5525	135.8311	136.6569	135.8362	137.1165	135.8525	137.0309	135.8442	137.1907	**131.65**
C3	119.3235	120.2716	120.8385	120.5131	121.3639	120.4977	121.6981	120.4927	121.6228	120.5449	121.7767	119.3235	120.2716	120.8384	120.5131	121.3639	120.4977	121.6981	120.4927	121.6228	120.5449	121.7767	**116.7**
C4	174.2731	175.2247	175.9328	175.5311	176.3756	175.5099	176.9550	175.4997	176.8173	175.5691	177.0950	174.2731	175.2247	175.9328	175.5311	176.3756	175.5099	176.9550	175.4997	176.8173	175.5691	177.0950	**166.84**
C5	117.6189	118.9655	119.5711	119.5802	120.4993	119.5388	120.7932	119.5083	120.6809	119.6375	120.9648	117.6188	118.9655	119.5711	119.5802	120.4993	119.5388	120.7932	119.5083	120.6809	119.6375	120.9648	**116.7**
C6	132.2249	133.9873	135.1783	134.7972	136.2000	134.7461	136.7129	134.7061	136.5049	134.8645	137.1126	132.2249	133.9873	135.1783	134.7972	136.2000	134.7461	136.7129	134.7061	136.5049	134.8645	137.1126	**131.65**
C7	200.8114	205.6148	206.6166	208.0300	209.4645	207.8741	213.5761	207.7273	212.5852	208.1942	214.7106	200.8115	205.6148	206.6166	208.0300	209.4645	207.8741	213.5761	207.7273	212.5852	208.1942	214.7106	**194.89**
C8	67.2268	68.7774	69.4317	69.3737	70.3901	69.3341	70.9762	69.3036	70.7658	69.4272	71.5306	67.2268	68.7774	69.4317	69.3737	70.3901	69.3341	70.9762	69.3036	70.7658	69.4272	71.5306	**65.05**
C9	30.7959	30.8705	31.0388	30.7226	30.7906	30.7316	31.1310	30.7516	31.0214	30.7321	31.2757	30.7959	30.8705	31.0388	30.7226	30.7906	30.7316	31.1310	30.7516	31.0214	30.7321	31.2757	**24.22**
C10	8.1398	8.5496	8.7055	8.5833	8.9062	8.5797	8.7932	8.5864	8.7767	8.6037	8.9798	8.1399	8.5496	8.7054	8.5833	8.9062	8.5797	8.7932	8.5864	8.7767	8.6037	8.9798	**10.45**
C1`	53.1734	54.0696	54.3964	54.5000	55.1960	54.4706	55.1460	54.4508	55.0845	54.5444	55.6308	57.6512	58.7549	59.1195	59.2058	59.9064	59.1717	60.1273	59.1486	60.0614	59.2564	60.3789	**50.48**
C2`	25.5324	26.1048	26.4614	26.2639	26.7880	26.2483	26.8408	26.2436	26.8190	26.2964	26.7778	25.4524	25.6919	25.9861	25.7790	26.4314	25.7683	26.3160	25.7692	26.3163	25.8070	26.1595	**23.91**
C3`	25.4524	25.6919	25.9861	25.7790	26.4314	25.7683	26.3160	25.7692	26.3163	25.8070	26.1595	25.5323	26.1048	26.4614	26.2639	26.7879	26.2483	26.8408	26.2436	26.8190	26.2964	26.7778	**23.74**
C4`	57.6511	58.7549	59.1195	59.2058	59.9064	59.1717	60.1273	59.1486	60.0614	59.2564	60.3789	53.1734	54.0696	54.3964	54.5000	55.1960	54.4706	55.1460	54.4508	55.0845	54.5444	55.6308	**52.48**
H2	8.5716	8.4328	8.4794	8.3573	8.3335	8.3621	8.3735	8.3676	8.3788	8.3535	8.3666	8.5716	8.4328	8.4794	8.3573	8.3335	8.3621	8.3735	8.3676	8.3788	8.3535	8.3666	**8.08**
H3	7.1986	7.3342	7.4234	7.3804	7.5099	7.3780	7.5335	7.3760	7.5249	7.3833	7.5474	7.1986	7.3342	7.4235	7.3804	7.5099	7.3780	7.5335	7.3760	7.5249	7.3833	7.5474	**7.23**
H5	7.0682	7.2288	7.3293	7.2962	7.4194	7.2923	7.4365	7.2889	7.4264	7.3006	7.4553	7.0682	7.2288	7.3293	7.2962	7.4194	7.2923	7.4365	7.2889	7.4264	7.3006	7.4553	**7.23**
H6	7.9400	8.0735	8.1618	8.1551	8.2574	8.1499	8.2963	8.1454	8.2841	8.1606	8.3167	7.9400	8.0735	8.1618	8.1551	8.2574	8.1499	8.2963	8.1454	8.2841	8.1606	8.3167	**8.08**
H8	4.9767	4.9893	5.0066	5.0089	5.0670	5.0071	5.0780	5.0060	5.0709	5.0116	5.0660	4.9767	4.9893	5.0066	5.0089	5.0670	5.0071	5.0780	5.0060	5.0709	5.0116	5.0660	**5.3**
H(9A)	2.1739	2.2462	2.2582	2.2886	2.2914	2.2864	2.3162	2.2847	2.3032	2.2913	2.3517	1.7470	1.7630	1.7916	1.7398	1.6871	1.7428	1.6590	1.7459	1.6634	1.7374	1.7153	**2.21**
H(9B)	1.7470	1.7630	1.7916	1.7398	1.6871	1.7428	1.6590	1.7459	1.6634	1.7374	1.7153	2.1739	2.2462	2.2581	2.2886	2.2914	2.2864	2.3162	2.2847	2.3032	2.2913	2.3517	**2.14**
H(10A-10C)	0.8180	0.7571	0.7287	0.7279	0.6821	0.7298	0.7010	0.7322	0.7020	0.7268	0.6961	0.8180	0.7571	0.7286	0.7279	0.6821	0.7298	0.7010	0.7322	0.7020	0.7268	0.6961	**1.01**
H(1`A-1`B)	3.0949	3.1208	3.1226	3.1229	3.1330	3.1227	3.1242	3.1232	3.1247	3.1238	3.1022	3.0056	2.9396	2.9069	2.9050	2.8936	2.9071	2.8679	2.9098	2.8700	2.9037	2.8455	**3.68**
H(2`-3`A-2`-3`B)	1.7331	1.7913	1.7548	1.8238	1.7915	1.8216	1.8089	1.8200	1.8036	1.8266	1.8352	1.7331	1.7913	1.7548	1.8238	1.7915	1.8216	1.8089	1.8200	1.8036	1.8266	1.8352	**2.19**
H(4`A)	3.0969	2.9459	2.8885	2.8895	2.8922	2.8924	2.8382	2.8961	2.8393	2.8876	2.8222	3.3776	3.4250	3.4455	3.4469	3.5038	3.4457	3.4796	3.4451	3.4776	3.4488	3.4738	**3.02**
H(4`B)	2.9142	2.9333	2.9253	2.9204	2.8950	2.9217	2.8976	2.9234	2.9006	2.9197	2.8688	2.8121	2.8166	2.7997	2.7988	2.7621	2.7996	2.7688	2.8012	2.7718	2.7988	2.7305	**3.83**
Nuclei	PBE0																						
C1	136.3225	137.4483	138.0445	137.9533	140.3783	137.9237	139.7464	137.8949	139.6267	137.9832	139.7758	136.3223	137.4483	138.0445	137.9533	140.3783	137.9235	139.7464	137.8948	139.6267	137.9832	139.7758	**131.91**
C2	138.7485	138.6702	139.2371	138.5523	139.1555	138.5545	139.7372	138.5584	139.5959	138.5536	139.7005	138.7486	138.6702	139.2371	138.5524	139.1555	138.5544	139.7372	138.5583	139.5959	138.5536	139.7005	**131.65**
C3	120.7814	121.6015	122.1803	121.8604	122.6461	121.8420	123.0019	121.8253	122.8804	121.8805	123.0049	120.7814	121.6015	122.1803	121.8604	122.6462	121.8420	123.0019	121.8252	122.8804	121.8805	123.0049	**116.7**
C4	172.9514	173.7460	174.3773	174.0906	174.6703	174.0640	175.3773	174.0394	175.1937	174.1190	175.4543	172.9515	173.7460	174.3773	174.0906	174.6703	174.0641	175.3773	174.0394	175.1937	174.1190	175.4543	**166.84**
C5	118.9139	120.2549	120.8537	120.9266	121.7768	120.8803	122.0989	120.8356	121.9387	120.9735	122.2090	118.9139	120.2549	120.8537	120.9265	121.7767	120.8802	122.0989	120.8357	121.9387	120.9735	122.2090	**116.7**
C6	134.7999	136.6188	137.7302	137.5722	138.7078	137.5054	139.2967	137.4407	139.0528	137.6393	139.6976	134.7999	136.6188	137.7302	137.5721	138.7079	137.5053	139.2967	137.4410	139.0528	137.6393	139.6976	**131.65**
C7	200.7853	205.6553	206.5829	208.1828	209.5642	208.0297	214.5129	207.8770	213.2005	208.3297	215.4079	200.7855	205.6553	206.5829	208.1827	209.5641	208.0293	214.5129	207.8772	213.2005	208.3297	215.4079	**194.89**
C8	63.2907	64.6253	65.0671	65.2046	66.1463	65.1678	66.7741	65.1323	66.4548	65.2419	67.2010	63.2907	64.6253	65.0671	65.2046	66.1464	65.1677	66.7741	65.1322	66.4548	65.2419	67.2010	**65.05**
C9	27.5726	27.5554	27.6657	27.4965	27.4845	27.4951	27.7202	27.4956	27.5717	27.5005	27.8229	27.5726	27.5554	27.6657	27.4965	27.4845	27.4952	27.7202	27.4956	27.5717	27.5005	27.8229	**24.22**
C10	8.0284	8.3451	8.4650	8.4442	8.6722	8.4330	8.6226	8.4239	8.5413	8.4578	8.7211	8.0284	8.3451	8.4650	8.4442	8.6722	8.4331	8.6226	8.4238	8.5413	8.4578	8.7211	**10.45**
C1`	50.2914	51.1379	51.4460	51.5793	52.1694	51.5451	52.2113	51.5133	52.0753	51.6155	52.5912	54.5306	55.5111	55.8541	55.9689	56.5148	55.9354	56.8004	55.9038	56.6852	56.0041	56.9706	**50.48**
C2`	24.2105	24.6432	24.9602	24.8186	25.2087	24.8027	25.3255	24.7886	25.2434	24.8371	25.1779	23.8828	24.0346	24.3710	24.1538	24.6820	24.1399	24.6550	24.1283	24.6047	24.1701	24.4277	**23.91**
C3`	23.8829	24.0346	24.3710	24.1538	24.6820	24.1399	24.6550	24.1282	24.6047	24.1701	24.4277	24.2105	24.6432	24.9602	24.8187	25.2087	24.8026	25.3255	24.7885	25.2434	24.8371	25.1779	**23.74**
C4`	54.5306	55.5111	55.8541	55.9689	56.5148	55.9353	56.8004	55.9038	56.6852	56.0041	56.9706	50.2914	51.1379	51.4460	51.5793	52.1694	51.5451	52.2113	51.5134	52.0753	51.6155	52.5912	**52.48**
H2	8.7954	8.6671	8.7153	8.5963	8.5325	8.5999	8.5798	8.6036	8.5902	8.5926	8.5774	8.7955	8.6671	8.7153	8.5963	8.5325	8.5999	8.5798	8.6036	8.5902	8.5926	8.5774	**8.08**
H3	7.3536	7.4891	7.5804	7.5348	7.6620	7.5324	7.6909	7.5299	7.6796	7.5367	7.7020	7.3536	7.4891	7.5804	7.5348	7.6620	7.5324	7.6909	7.5299	7.6796	7.5367	7.7020	**7.23**
H5	7.2060	7.3840	7.4802	7.4583	7.5767	7.4538	7.5978	7.4494	7.5850	7.4621	7.6160	7.2060	7.3840	7.4802	7.4583	7.5767	7.4538	7.5978	7.4494	7.5850	7.4621	7.6160	**7.23**
H6	8.0673	8.2239	8.3184	8.3175	8.4200	8.3113	8.4671	8.3051	8.4550	8.3232	8.4978	8.0673	8.2239	8.3184	8.3175	8.4200	8.3113	8.4671	8.3051	8.4550	8.3232	8.4978	**8.08**
H8	4.5541	4.6040	4.6404	4.6530	4.7216	4.6493	4.7530	4.6457	4.7442	4.6561	4.7502	4.5541	4.6040	4.6404	4.6530	4.7216	4.6493	4.7530	4.6457	4.7442	4.6561	4.7502	**5.3**
H(9A)	1.9835	2.0636	2.0685	2.1147	2.1039	2.1113	2.1283	2.1080	2.1129	2.1176	2.1643	1.6364	1.6545	1.6552	1.6415	1.5659	1.6424	1.5286	1.6433	1.5296	1.6404	1.5888	**2.21**
H(9B)	1.6364	1.6545	1.6552	1.6415	1.5659	1.6424	1.5286	1.6433	1.5296	1.6404	1.5888	1.9835	2.0636	2.0685	2.1147	2.1038	2.1113	2.1283	2.1080	2.1129	2.1176	2.1643	**2.14**
H(10A-10C)	0.8056	0.7341	0.7102	0.7022	0.6445	0.7039	0.6731	0.7057	0.6730	0.7004	0.6634	0.8056	0.7341	0.7102	0.7022	0.6445	0.7039	0.6731	0.7057	0.6730	0.7004	0.6634	**1.01**
H(1`A-1`B)	2.9200	2.9444	2.9473	2.9529	2.9549	2.9523	2.9555	2.9517	2.9528	2.9531	2.9374	2.8444	2.7754	2.7434	2.7459	2.7405	2.7476	2.7138	2.7493	2.7104	2.7439	2.6953	**3.68**
H(2`-3`A-2`-3`B)	1.6415	1.7006	1.6633	1.7363	1.7002	1.7338	1.7248	1.7315	1.7164	1.7383	1.7452	1.6415	1.7006	1.6633	1.7362	1.7003	1.7338	1.7248	1.7315	1.7164	1.7383	1.7452	**2.19**
H(4`A)	2.8967	2.7498	2.7025	2.7060	2.7267	2.7083	2.6608	2.7106	2.6562	2.7034	2.6494	3.1675	3.2189	3.2384	3.2480	3.2988	3.2460	3.2847	3.2440	3.2791	3.2495	3.2813	**3.02**
H(4`B)	2.7921	2.8011	2.7843	2.7858	2.7543	2.7870	2.7669	2.7882	2.7647	2.7843	2.7411	2.6726	2.6699	2.6563	2.6579	2.6109	2.6587	2.6264	2.6595	2.6265	2.6567	2.5934	**3.83**

[a] methyl protons shifts are averaged [b] according to [13] in $CDCl_3$

Table S14. Cont. VIII

Nuclei	R											S									Exp. [b]
	TPSS																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	132.2641	133.0840	133.7897	133.6847	134.7535	133.6704	135.4801	133.6650	134.1718	133.7062	135.6403	132.2641	133.0840	133.7897	133.6847	134.7535	133.6704	135.4801	133.6650	134.7730	133.7062	135.6403	**131.91**
C2	133.0674	132.9479	133.5704	132.8784	133.4447	132.8875	134.0487	132.9080	133.4117	132.8806	134.0937	133.0674	132.9479	133.5704	132.8784	133.4447	132.8875	134.0486	132.9080	134.0216	132.8806	134.0937	**131.65**
C3	116.4718	117.1940	117.8453	117.5095	118.1711	117.5003	118.6061	117.5022	117.9443	117.5287	118.6500	116.4718	117.1940	117.8453	117.5095	118.1711	117.5003	118.6061	117.5022	118.7314	117.5287	118.6500	**116.7**
C4	170.9237	171.7366	172.5198	172.1547	172.9574	172.1349	173.4502	172.1270	172.7876	172.1844	173.5580	170.9237	171.7366	172.5198	172.1547	172.9574	172.1349	173.4502	172.1270	172.9465	172.1844	173.5580	**166.84**
C5	114.8428	116.0007	116.7003	116.6537	117.4628	116.6194	117.7545	116.5967	117.0352	116.6967	117.8907	114.8428	116.0007	116.7003	116.6537	117.4628	116.6194	117.7547	116.5967	117.8327	116.6967	117.8907	**116.7**
C6	129.4162	131.1766	132.3270	132.1441	133.7927	132.0860	133.7508	132.0404	132.5407	132.2105	134.1248	129.4162	131.1766	132.3270	132.1441	133.7927	132.0860	133.7508	132.0404	133.1605	132.2105	134.1248	**131.65**
C7	197.0373	201.1937	202.2474	203.5484	203.9345	203.4271	209.2336	203.3143	204.0997	203.6711	210.2340	197.0373	201.1937	202.2474	203.5484	203.9345	203.4271	209.2341	203.3143	203.8999	203.6711	210.2340	**194.89**
C8	66.0012	67.1549	67.7082	67.7955	68.4635	67.7715	69.2509	67.7570	68.0001	67.8268	69.7355	66.0012	67.1549	67.7082	67.7955	68.4635	67.7715	69.2514	67.7570	69.3593	67.8268	69.7355	**65.05**
C9	30.7677	30.7902	30.9685	30.8001	31.0228	30.8062	31.0432	30.8237	30.9191	30.8048	31.1659	30.7677	30.7902	30.9685	30.8001	31.0228	30.8062	31.0430	30.8237	32.7030	30.8048	31.1659	**24.22**
C10	9.7233	9.9403	10.1508	10.0708	10.3684	10.0697	10.2239	10.0799	10.0923	10.0820	10.3930	9.7233	9.9403	10.1508	10.0708	10.3684	10.0697	10.2239	10.0799	12.1147	10.0820	10.3930	**10.45**
C1`	53.0466	53.7459	54.0724	54.2546	54.8105	54.2292	54.8099	54.2152	54.4042	54.2892	55.2392	57.1640	58.1056	58.6056	58.6253	59.1425	58.5992	59.4957	58.5849	60.2560	58.6608	59.6823	**50.48**
C2`	26.2163	26.5883	27.0251	26.8269	27.2682	26.8177	27.3249	26.8201	26.8995	26.8464	27.1744	26.1514	26.2346	26.7011	26.3907	26.9232	26.3854	26.8882	26.3919	28.3044	26.4068	26.6826	**23.91**
C3`	26.1514	26.2346	26.7011	26.3907	26.9232	26.3854	26.8880	26.3919	26.4696	26.4068	26.6826	26.2163	26.5883	27.0251	26.8269	27.2682	26.8177	27.3249	26.8201	28.7294	26.8464	27.1744	**23.74**
C4`	57.1640	58.1056	58.6056	58.6253	59.1425	58.5992	59.4959	58.5849	58.7913	58.6608	59.6823	53.0466	53.7459	54.0724	54.2546	54.8105	54.2292	54.8103	54.2152	55.9190	54.2892	55.2392	**52.48**
H2	8.5746	8.4725	8.5182	8.4056	8.4493	8.4081	8.3993	8.4115	8.2515	8.4040	8.3901	8.5746	8.4725	8.5182	8.4056	8.4493	8.4081	8.3993	8.4115	8.5216	8.4040	8.3901	**8.08**
H3	7.1651	7.2945	7.3937	7.3411	7.4655	7.3387	7.5000	7.3369	7.1726	7.3436	7.5112	7.1651	7.2945	7.3937	7.3411	7.4655	7.3387	7.5000	7.3369	7.4551	7.3436	7.5112	**7.23**
H5	7.0301	7.2079	7.3097	7.2818	7.4197	7.2775	7.4185	7.2736	7.1091	7.2864	7.4330	7.0301	7.2079	7.3097	7.2818	7.4197	7.2775	7.4185	7.2736	7.3923	7.2864	7.4330	**7.23**
H6	7.8473	8.0023	8.1074	8.0934	8.2422	8.0870	8.2466	8.0813	7.9200	8.1001	8.2704	7.8473	8.0023	8.1074	8.0934	8.2422	8.0870	8.2466	8.0813	8.1939	8.1001	8.2704	**8.08**
H8	4.7474	4.7923	4.8456	4.8312	4.9158	4.8279	4.9258	4.8255	4.6512	4.8349	4.9134	4.7474	4.7923	4.8456	4.8312	4.9158	4.8279	4.9257	4.8255	4.9625	4.8349	4.9134	**5.3**
H(9A)	2.0821	2.1647	2.1746	2.2192	2.2444	2.2156	2.2359	2.2126	2.3357	2.2230	2.2683	1.6555	1.6924	1.6886	1.6958	1.7267	1.6957	1.5961	1.6962	1.8801	1.6961	1.6467	**2.21**
H(9B)	1.6555	1.6924	1.6886	1.6958	1.7267	1.6957	1.5961	1.6962	1.8801	1.6961	1.6467	2.0821	2.1647	2.1746	2.2192	2.2444	2.2156	2.2359	2.2126	2.3357	2.2230	2.2683	**2.14**
H(10A-10C)	0.8555	0.7841	0.7648	0.7554	0.7135	0.7569	0.7299	0.7589	0.5683	0.7544	0.7198	0.8555	0.7841	0.7648	0.7554	0.7135	0.7569	0.7299	0.7589	0.9264	0.7544	0.7198	**1.01**
H(1`A-1`B)	2.9988	3.0276	3.0374	3.0417	3.0542	3.0409	3.0477	3.0408	3.0672	3.0428	3.0246	2.9484	2.8717	2.8440	2.8430	2.8212	2.8451	2.8113	2.8479	3.0450	2.8412	2.7894	**3.68**
H(2`-3`A-2`-3`B)	1.6784	1.7377	1.7057	1.7805	1.7387	1.7779	1.7701	1.7760	2.1012	1.7833	1.7935	1.6784	1.7377	1.7057	1.7805	1.7387	1.7779	1.7701	1.7760	2.1012	1.7833	1.7935	**2.19**
H(4`A)	3.0769	2.9026	2.8523	2.8498	2.8339	2.8530	2.7996	2.8570	2.9589	2.8470	2.7814	3.2744	3.3257	3.3531	3.3597	3.4163	3.3578	3.3950	3.3565	3.5063	3.3620	3.3875	**3.02**
H(4`B)	2.8198	2.8408	2.8356	2.8361	2.8084	2.8372	2.8231	2.8388	3.1312	2.8354	2.7975	2.7231	2.7294	2.7217	2.7236	2.6920	2.7240	2.7005	2.7250	2.6282	2.7237	2.6618	**3.83**
Nuclei	VSXC																						
C1	133.7280	134.6932	135.5641	135.0028	136.7273	134.9834	135.5216	134.9625	135.6961	135.0234	135.9029	133.7280	134.6932	135.5641	135.0028	136.7273	134.9834	135.5216	134.9624	135.6960	135.0234	135.9029	**131.91**
C2	130.4484	130.4536	131.0013	130.2906	130.8229	130.3104	131.4948	130.3268	131.3582	130.2725	131.3842	130.4484	130.4536	131.0013	130.2906	130.8229	130.3104	131.4948	130.3268	131.3582	130.2725	131.3843	**131.65**
C3	115.0664	115.8768	116.4619	116.2108	116.7705	116.1954	117.1658	116.1776	117.0538	116.2268	117.1710	115.0663	115.8767	116.4619	116.2108	116.7705	116.1954	117.1658	116.1776	117.0537	116.2268	117.1710	**116.7**
C4	168.4331	169.3548	170.0092	169.8363	170.5115	169.8116	171.1646	169.7847	171.0105	169.8610	171.2657	168.4331	169.3548	170.0091	169.8363	170.5115	169.8116	171.1646	169.7847	171.0104	169.8610	171.2658	**166.84**
C5	112.6538	114.0697	114.6157	114.8678	115.5175	114.8218	115.8759	114.7736	115.7661	114.9129	116.0189	112.6537	114.0698	114.6157	114.8678	115.5175	114.8218	115.8759	114.7737	115.7662	114.9129	116.0189	**116.7**
C6	128.3780	129.9641	130.9113	130.9401	132.3261	130.8823	132.9018	130.8227	132.6820	130.9967	133.2067	128.3780	129.9641	130.9113	130.9401	132.3261	130.8823	132.9018	130.8227	132.6820	130.9967	133.2066	**131.65**
C7	193.7250	198.3258	199.6112	200.7729	201.7874	200.6184	205.4791	200.4637	204.7371	200.9227	206.6958	193.7248	198.3258	199.6113	200.7729	201.7874	200.6184	205.4791	200.4637	204.7371	200.9227	206.6956	**194.89**
C8	71.5690	72.7143	73.2527	73.3567	74.2081	73.3084	74.3399	73.2605	74.2578	73.4060	75.1245	71.5690	72.7143	73.2527	73.3567	74.2081	73.3084	74.3399	73.2605	74.2578	73.4060	75.1244	**65.05**
C9	34.1035	34.7466	34.9523	35.1716	35.3874	35.1428	35.7844	35.1127	35.6599	35.2008	36.1085	34.1034	34.7466	34.9523	35.1716	35.3874	35.1428	35.7844	35.1127	35.6599	35.2008	36.1085	**24.22**
C10	13.2393	13.8267	13.9208	14.0186	14.1425	14.0182	14.3826	14.0138	14.3677	14.0192	14.1232	13.2392	13.8267	13.9208	14.0186	14.1425	14.0182	14.3826	14.0138	14.3678	14.0192	14.1232	**10.45**
C1`	57.7470	58.3407	58.6804	58.7211	59.2365	58.7008	59.1402	58.6782	59.1025	58.7416	59.3076	61.3896	62.2048	62.5475	62.6521	63.1328	62.6279	63.1524	62.6011	63.1091	62.6764	63.3833	**50.48**
C2`	29.5603	30.0658	30.3268	30.3182	30.6584	30.3081	30.6963	30.2952	30.6602	30.3293	30.7793	28.1199	28.4650	28.7659	28.6490	29.0566	28.6415	29.0945	28.6315	29.0635	28.6574	29.0563	**23.91**
C3`	28.1198	28.4650	28.7659	28.6490	29.0566	28.6415	29.0945	28.6315	29.0635	28.6574	29.0564	29.5602	30.0658	30.3268	30.3182	30.6584	30.3081	30.6963	30.2952	30.6602	30.3293	30.7793	**23.74**
C4`	61.3898	62.2048	62.5475	62.6521	63.1328	62.6279	63.1524	62.6011	63.1091	62.6764	63.3834	57.7470	58.3407	58.6805	58.7211	59.2365	58.7008	59.1402	58.6782	59.1025	58.7416	59.3077	**52.48**
H2	8.3843	8.2653	8.2734	8.1867	8.1526	8.1942	8.2775	8.2014	8.2695	8.1792	8.2199	8.3843	8.2653	8.2734	8.1867	8.1526	8.1942	8.2775	8.2014	8.2695	8.1792	8.2199	**8.08**
H3	7.2851	7.4237	7.5085	7.4697	7.5820	7.4679	7.6070	7.4660	7.6001	7.4714	7.6202	7.2851	7.4237	7.5085	7.4697	7.5820	7.4679	7.6070	7.4660	7.6001	7.4714	7.6202	**7.23**
H5	7.0179	7.2122	7.2908	7.3003	7.4165	7.2952	7.4312	7.2902	7.4250	7.3051	7.4594	7.0179	7.2122	7.2908	7.3003	7.4165	7.2952	7.4312	7.2902	7.4250	7.3051	7.4594	**7.23**
H6	7.7692	7.9296	8.0043	8.0301	8.1595	8.0237	8.2165	8.0176	8.1960	8.0361	8.2605	7.7692	7.9296	8.0043	8.0301	8.1595	8.0237	8.2165	8.0176	8.1960	8.0361	8.2605	**8.08**
H8	4.2098	4.3417	4.3755	4.4324	4.5287	4.4254	4.5576	4.4187	4.5431	4.4392	4.6200	4.2098	4.3417	4.3755	4.4324	4.5287	4.4254	4.5576	4.4187	4.5431	4.4392	4.6200	**5.3**
H(9A)	2.0452	2.1139	2.1362	2.1752	2.1824	2.1714	2.2315	2.1675	2.2123	2.1787	2.2260	1.8576	1.8123	1.7953	1.8134	1.7941	1.8127	1.7627	1.8123	1.7567	1.8140	1.7863	**2.21**
H(9B)	1.8576	1.8123	1.7953	1.8134	1.7941	1.8127	1.7627	1.8123	1.7567	1.8140	1.7863	2.0452	2.1139	2.1363	2.1752	2.1824	2.1714	2.2315	2.1675	2.2123	2.1787	2.2260	**2.14**
H(10A-10C)	0.9526	0.9054	0.8739	0.8812	0.8194	0.8830	0.8336	0.8849	0.8353	0.8793	0.8036	0.9526	0.9054	0.8739	0.8812	0.8194	0.8830	0.8336	0.8849	0.8353	0.8793	0.8036	**1.01**
H(1`A-1`B)	2.8643	2.8823	2.9045	2.9155	2.9264	2.9132	2.9497	2.9112	2.9438	2.9173	2.9511	2.9479	2.9462	2.9455	2.9595	2.9661	2.9570	2.9206	2.9549	2.9216	2.9619	2.9380	**3.68**
H(2`-3`A-2`-3`B)	1.9324	1.9702	1.9427	2.0029	1.9645	2.0008	1.9833	1.9987	1.9778	2.0047	1.9946	1.9324	1.9702	1.9427	2.0029	1.9645	2.0008	1.9833	1.9987	1.9778	2.0047	1.9946	**2.19**
H(4`A)	2.8961	2.8655	2.8597	2.8807	2.9013	2.8775	2.8342	2.8748	2.8355	2.8838	2.8671	3.2877	3.2961	3.3325	3.3361	3.3750	3.3335	3.3892	3.3310	3.3829	3.3383	3.3923	**3.02**
H(4`B)	2.9999	3.0269	3.0314	3.0383	3.0310	3.0366	3.0070	3.0351	3.0078	3.0400	3.0088	2.4410	2.4684	2.4765	2.4948	2.4779	2.4930	2.5102	2.4914	2.5048	2.4962	2.5098	**3.83**
Nuclei	wB97																						
C1	136.4715	137.4982	138.3529	137.8181	139.4807	137.8005	139.5962	137.7822	138.5055	137.8359	139.7189	136.4715	137.4983	138.3529	137.8180	139.4808	137.8005	139.5962	137.7822	138.5056	137.8359	139.7189	**131.91**
C2	140.3386	140.3374	140.8427	140.2180	140.7137	140.2255	140.9867	140.2323	141.0674	140.2108	140.9901	140.3386	140.3375	140.8427	140.2179	140.7138	140.2255	140.9867	140.2323	141.0672	140.2109	140.9901	**131.65**
C3	121.5651	122.1795	122.7665	122.3744	123.0718	122.3643	123.3260	122.3534	123.1569	122.3841	123.3750	121.5650	122.1795	122.7665	122.3744	123.0718	122.3643	123.3260	122.3534	123.1568	122.3841	123.3750	**116.7**
C4	174.2914	174.8695	175.4567	175.2152	175.8180	175.1928	176.3449	175.1696	176.2762	175.2369	176.4646	174.2915	174.8694	175.4567	175.2153	175.8179	175.1928	176.3449	175.1696	176.2761	175.2368	176.4646	**166.84**
C5	119.5457	120.8019	121.3700	121.4824	122.2916	121.4403	122.5743	121.3972	122.3191	121.5231	122.7091	119.5458	120.8018	121.3700	121.4825	122.2916	121.4403	122.5744	121.3972	122.3192	121.5231	122.7091	**116.7**
C6	136.6600	138.3277	139.4365	139.3721	140.9844	139.3019	140.8865	139.2315	141.3412	139.4396	141.3315	136.6601	138.3277	139.4365	139.3721	140.9846	139.3019	140.8866	139.2315	141.3412	139.4397	141.3315	**131.65**
C7	201.2809	206.4139	207.5947	209.0989	209.5897	208.9323	216.0328	208.7653	213.6009	209.2593	217.0726	201.2809	206.4141	207.5947	209.0992	209.5896	208.9323	216.0330	208.7653	213.6005	209.2594	217.0726	**194.89**
C8	61.8494	62.9619	63.6230	63.5101	64.4230	63.4703	65.0089	63.4301	64.7011	63.5499	65.5141	61.8494	62.9619	63.6230	63.5102	64.4230	63.4703	65.0089	63.4301	64.7012	63.5499	65.5141	**65.05**
C9	25.9921	25.8024	25.9613	25.7593	26.0175	25.7596	25.7914	25.7598	26.0540	25.7593	25.9455	25.9921	25.8024	25.9613	25.7593	26.0175	25.7596	25.7914	25.7598	26.0539	25.7593	25.9455	**24.22**
C10	8.7286	8.9241	9.0919	9.0402	9.3256	9.0303	9.1445	9.0199	9.1755	9.0501	9.2966	8.7287	8.9240	9.0919	9.0402	9.3256	9.0303	9.1445	9.0199	9.1755	9.0501	9.2966	**10.45**
C1`	49.0447	49.7133	50.1226	50.1704	50.7840	50.1347	50.7071	50.0989	50.6714	50.2056	51.0474	52.8845	53.6761	54.0236	54.0964	54.6064	54.0680	54.7659	54.0392	54.6199	54.1238	55.0009	**50.48**
C2`	23.6938	24.0172	24.3561	24.2021	24.6518	24.1873	24.6242	24.1721	24.6351	24.2168	24.5827	23.1794	23.3501	23.6832	23.4969	23.9830	23.4857	23.9179	23.4735	23.8844	23.5084	23.7811	**23.91**
C3`	23.1794	23.3501	23.6832	23.4969	23.9829	23.4857	23.9179	23.4735	23.8843	23.5084	23.7811	23.6939	24.0172	24.3561	24.2021	24.6518	24.1873	24.6242	24.1721	24.6352	24.2168	24.5827	**23.74**
C4`	52.8844	53.6761	54.0236	54.0964	54.6064	54.0680	54.7659	54.0392	54.6199	54.1237	55.0009	49.0447	49.7133	50.1226	50.1703	50.7840	50.1347	50.7071	50.0989	50.6714	50.2056	51.0474	**52.48**
H2	8.8912	8.7744	8.7965	8.7066	8.7091	8.7108	8.6429	8.7148	8.7486	8.7025	8.6443	8.8912	8.7744	8.7965	8.7066	8.7091	8.7108	8.6429	8.7148	8.7485	8.7025	8.6443	**8.08**
H3	7.4478	7.5845	7.6762	7.6231	7.7464	7.6212	7.7598	7.6192	7.7544	7.6248	7.7750	7.4477	7.5845	7.6762	7.6231	7.7464	7.6212	7.7598	7.6192	7.7544	7.6248	7.7750	**7.23**
H5	7.2894	7.4691	7.5582	7.5493	7.6766	7.5446	7.6974	7.5397	7.6792	7.5538	7.7168	7.2894	7.4691	7.5582	7.5493	7.6766	7.5446	7.6974	7.5397	7.6792	7.5538	7.7168	**7.23**
H6	8.1426	8.3048	8.3975	8.4000	8.5390	8.3939	8.5509	8.3878	8.5772	8.4058	8.5860	8.1426	8.3048	8.3975	8.4000	8.5390	8.3939	8.5509	8.3878	8.5772	8.4058	8.5860	**8.08**
H8	4.2328	4.3054	4.3359	4.3584	4.4282	4.3554	4.5010	4.3522	4.4702	4.3612	4.5032	4.2328	4.3054	4.3359	4.3584	4.4282	4.3554	4.5010	4.3522	4.4702	4.3612	4.5032	**5.3**
H(9A)	1.8905	1.9588	1.9565	2.0087	2.0314	2.0054	2.0101	2.0020	2.0443	2.0120	2.0508	1.6348	1.6318	1.6452	1.6274	1.6622	1.6268	1.4972	1.6262	1.6394	1.6282	1.5636	**2.21**
H(9B)	1.6348	1.6318	1.6452	1.6275	1.6622	1.6268	1.4972	1.6262	1.6394	1.6282	1.5636	1.8905	1.9588	1.9565	2.0087	2.0314	2.0054	2.0101	2.0020	2.0443	2.0120	2.0508	**2.14**
H(10A-10C)	0.8698	0.7882	0.7561	0.7496	0.6888	0.7519	0.7139	0.7542	0.7134	0.7473	0.7068	0.8698	0.7882	0.7561	0.7496	0.6888	0.7519	0.7139	0.7542	0.7134	0.7473	0.7068	**1.01**
H(1`A-1`B)	2.8345	2.8556	2.8567	2.8639	2.8710	2.8634	2.8640	2.8630	2.8713	2.8644	2.8555	2.7611	2.7163	2.6917	2.6895	2.6738	2.6910	2.6736	2.6926	2.6563	2.6882	2.6585	**3.68**
H(2`-3`A-2`-3`B)	1.6369	1.6930	1.6588	1.7277	1.6862	1.7252	1.7182	1.7227	1.6991	1.7301	1.7380	1.6369	1.6930	1.6588	1.7277	1.6862	1.7252	1.7182	1.7227	1.6991	1.7301	1.7380	**2.19**
H(4`A)	2.7543	2.6469	2.6089	2.6056	2.6021	2.6078	2.5884	2.6101	2.5566	2.6037	2.5809	3.0470	3.0924	3.1134	3.1216	3.1806	3.1197	3.1609	3.1177	3.1667	3.1236	3.1676	**3.02**
H(4`B)	2.7679	2.7857	2.7744	2.7734	2.7454	2.7743	2.7589	2.7750	2.7559	2.7727	2.7361	2.6220	2.6189	2.6000	2.6062	2.5614	2.6072	2.5671	2.6082	2.5758	2.6051	2.5434	**3.83**

[a] methyl protons shifts are averaged [b] according to [13] in $CDCl_3$

Table S14. Cont. IX

Nuclei	R											S										Exp. [b]
	wB97X																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.9830	139.0482	139.8060	139.5364	141.1650	139.5166	141.2990	139.4954	141.2743	139.5564	141.3764	137.9830	139.0482	139.8059	139.5364	141.1651	139.5164	141.2989	139.4954	141.2743	139.5564	141.3764	**131.91**
C2	140.7860	140.7835	141.2973	140.6375	141.1362	140.6493	141.4998	140.6599	141.3622	140.6273	141.4804	140.7860	140.7835	141.2974	140.6375	141.1360	140.6492	141.4997	140.6599	141.3621	140.6273	141.4804	**131.65**
C3	122.2992	122.9286	123.5157	123.1405	123.8317	123.1319	124.1281	123.1221	124.0161	123.1493	124.1691	122.2992	122.9286	123.5157	123.1405	123.8318	123.1319	124.1281	123.1221	124.0162	123.1493	124.1691	**116.7**
C4	174.9955	175.6067	176.2121	175.9505	176.5643	175.9303	177.1378	175.9096	176.9404	175.9705	177.2458	174.9955	175.6067	176.2121	175.9505	176.5643	175.9305	177.1378	175.9096	176.9405	175.9705	177.2458	**166.84**
C5	120.2576	121.5322	122.0896	122.2505	123.0290	122.2094	123.3458	122.1674	123.1869	122.2903	123.4854	120.2576	121.5322	122.0897	122.2505	123.0291	122.2095	123.3457	122.1674	123.1867	122.2903	123.4854	**116.7**
C6	136.9905	138.6834	139.7981	139.6463	141.2466	139.5822	141.2105	139.5179	140.9330	139.7087	141.6533	136.9905	138.6834	139.7981	139.6463	141.2466	139.5821	141.2105	139.5179	140.9329	139.7087	141.6533	**131.65**
C7	202.9716	208.1012	209.1816	210.9432	211.4273	210.7756	217.8480	210.6072	216.5197	211.1040	218.8241	202.9716	208.1012	209.1818	210.9432	211.4273	210.7756	217.8480	210.6072	216.5199	211.1040	218.8241	**194.89**
C8	63.1303	64.3000	64.8617	64.8702	65.7803	64.8329	66.3427	64.7956	66.0749	64.9076	66.8277	63.1303	64.3000	64.8617	64.8702	65.7803	64.8329	66.3427	64.7956	66.0748	64.9076	66.8277	**65.05**
C9	26.6275	26.4303	26.5843	26.3609	26.5989	26.3647	26.4199	26.3679	26.2820	26.3585	26.5577	26.6275	26.4303	26.5842	26.3609	26.5988	26.3646	26.4199	26.3679	26.2820	26.3585	26.5577	**24.22**
C10	8.4666	8.6763	8.8401	8.7934	9.0797	8.7858	8.9301	8.7776	8.8457	8.8020	9.0521	8.4666	8.6763	8.8401	8.7934	9.0797	8.7858	8.9301	8.7776	8.8458	8.8020	9.0521	**10.45**
C1`	49.8215	50.5463	50.9191	50.9979	51.6134	50.9662	51.5712	50.9344	51.4424	51.0299	51.9289	53.8553	54.7231	55.0669	55.1617	55.6641	55.1351	55.8860	55.1079	55.7630	55.1881	56.0917	**50.48**
C2`	24.1830	24.5088	24.8229	24.6774	25.1231	24.6667	25.1168	24.6555	25.0332	24.6888	25.0304	23.6812	23.8106	24.1356	23.9541	24.4370	23.9459	24.4073	23.9370	24.3440	23.9630	24.2469	**23.91**
C3`	23.6812	23.8106	24.1356	23.9541	24.4371	23.9458	24.4073	23.9370	24.3441	23.9630	24.2469	24.1830	24.5088	24.8229	24.6774	25.1232	24.6668	25.1167	24.6555	25.0332	24.6888	25.0304	**23.74**
C4`	53.8553	54.7231	55.0668	55.1617	55.6640	55.1352	55.8861	55.1079	55.7630	55.1881	56.0917	49.8215	50.5463	50.9191	50.9979	51.6134	50.9660	51.5711	50.9344	51.4425	51.0299	51.9289	**52.48**
H2	8.8647	8.7427	8.7777	8.6608	8.6643	8.6655	8.6073	8.6702	8.6121	8.6564	8.6060	8.8647	8.7427	8.7777	8.6608	8.6642	8.6655	8.6073	8.6702	8.6121	8.6564	8.6060	**8.08**
H3	7.4264	7.5632	7.6561	7.6010	7.7238	7.5993	7.7352	7.5976	7.7243	7.6027	7.7481	7.4264	7.5632	7.6562	7.6010	7.7238	7.5993	7.7352	7.5976	7.7243	7.6026	7.7481	**7.23**
H5	7.2645	7.4481	7.5366	7.5331	7.6574	7.5284	7.6810	7.5236	7.6672	7.5377	7.6989	7.2645	7.4481	7.5366	7.5331	7.6574	7.5284	7.6810	7.5236	7.6672	7.5377	7.6989	**7.23**
H6	8.1139	8.2707	8.3651	8.3651	8.5022	8.3592	8.5158	8.3533	8.4994	8.3709	8.5478	8.1139	8.2707	8.3651	8.3651	8.5022	8.3592	8.5158	8.3533	8.4994	8.3709	8.5478	**8.08**
H8	4.3176	4.3805	4.4139	4.4376	4.5041	4.4344	4.5712	4.4313	4.5575	4.4406	4.5678	4.3176	4.3805	4.4139	4.4376	4.5041	4.4344	4.5712	4.4313	4.5575	4.4406	4.5678	**5.3**
H(9A)	1.8966	1.9671	1.9678	2.0146	2.0357	2.0114	2.0199	2.0083	2.0036	2.0177	2.0592	1.6027	1.6054	1.6177	1.5867	1.6220	1.5867	1.4661	1.5869	1.4626	1.5869	1.5256	**2.21**
H(9B)	1.6027	1.6054	1.6177	1.5867	1.6221	1.5867	1.4661	1.5869	1.4627	1.5869	1.5256	1.8966	1.9671	1.9678	2.0146	2.0357	2.0114	2.0199	2.0083	2.0036	2.0177	2.0592	**2.14**
H(10A-10C)	0.8498	0.7721	0.7445	0.7376	0.6776	0.7397	0.7077	0.7420	0.7064	0.7355	0.6982	0.8498	0.7721	0.7445	0.7376	0.6776	0.7397	0.7077	0.7420	0.7064	0.7355	0.6982	**1.01**
H(1`A-1`B)	2.8572	2.8763	2.8788	2.8863	2.8919	2.8861	2.8883	2.8857	2.8851	2.8866	2.8746	2.7824	2.7286	2.7021	2.7067	2.6895	2.7083	2.6827	2.7099	2.6788	2.7054	2.6682	**3.68**
H(2`-3`A-2`-3`B)	1.6367	1.6947	1.6589	1.7322	1.6883	1.7299	1.7211	1.7276	1.7132	1.7345	1.7393	1.6367	1.6947	1.6589	1.7322	1.6883	1.7299	1.7211	1.7276	1.7132	1.7345	1.7393	**2.19**
H(4`A)	2.7788	2.6588	2.6222	2.6275	2.6230	2.6297	2.5996	2.6318	2.5940	2.6258	2.5932	3.0657	3.1103	3.1314	3.1418	3.1997	3.1399	3.1815	3.1382	3.1753	3.1436	3.1835	**3.02**
H(4`B)	2.7860	2.7985	2.7820	2.7859	2.7560	2.7870	2.7658	2.7881	2.7636	2.7850	2.7433	2.6487	2.6424	2.6262	2.6308	2.5842	2.6321	2.5951	2.6333	2.5949	2.6297	2.5657	**3.83**
Nuclei	X3LYP																						
C1	139.5222	140.7607	141.1293	141.3841	143.5908	141.3514	142.9167	141.3142	142.8989	141.4174	143.1602	139.5222	140.7607	141.1292	141.3841	143.5908	141.3514	142.9167	141.3143	142.8989	141.4174	143.1602	**131.91**
C2	139.9181	139.7948	140.3308	139.7109	140.3553	139.7181	140.8143	139.7227	140.7218	139.7079	140.8575	139.9181	139.7948	140.3308	139.7109	140.3553	139.7181	140.8143	139.7227	140.7218	139.7080	140.8575	**131.65**
C3	121.8779	122.6466	123.1545	122.9205	123.6176	122.9097	123.8817	122.8955	123.8237	122.9339	123.9214	121.8779	122.6466	123.1545	122.9205	123.6176	122.9097	123.8817	122.8955	123.8237	122.9338	123.9215	**116.7**
C4	176.3560	177.1647	177.8267	177.5511	178.1892	177.5311	178.7567	177.5084	178.6257	177.5739	178.8657	176.3560	177.1647	177.8267	177.5511	178.1892	177.5311	178.7566	177.5083	178.6257	177.5739	178.8657	**166.84**
C5	120.0151	121.2676	121.8657	121.9258	122.6895	121.8889	122.9009	121.8487	122.8058	121.9650	123.0342	120.0151	121.2676	121.8656	121.9258	122.6895	121.8889	122.9008	121.8487	122.8058	121.9649	123.0342	**116.7**
C6	135.9756	137.7439	139.0035	138.7304	139.8686	138.6734	140.4766	138.6134	140.2661	138.7888	140.8151	135.9756	137.7439	139.0035	138.7304	139.8686	138.6734	140.4765	138.6134	140.2661	138.7888	140.8150	**131.65**
C7	203.5301	208.6866	209.4913	211.4296	212.4724	211.2679	217.7136	211.1015	216.4892	211.5846	218.8023	203.5301	208.6866	209.4912	211.4296	212.4723	211.2679	217.7137	211.1016	216.4892	211.5844	218.8023	**194.89**
C8	66.0902	67.4350	67.8541	68.0432	68.7185	68.0169	69.4778	67.9857	69.2630	68.0697	69.8630	66.0902	67.4350	67.8541	68.0432	68.7185	68.0169	69.4779	67.9857	69.2630	68.0698	69.8631	**65.05**
C9	29.4339	29.2958	29.4371	29.2287	29.0527	29.2418	29.3969	29.2509	29.3136	29.2193	29.4187	29.4339	29.2958	29.4372	29.2287	29.0528	29.2418	29.3969	29.2509	29.3136	29.2192	29.4187	**24.22**
C10	8.4213	8.7234	8.8794	8.8466	9.0380	8.8444	8.9694	8.8388	8.9640	8.8520	9.0427	8.4213	8.7234	8.8793	8.8466	9.0381	8.8444	8.9694	8.8387	8.9640	8.8519	9.0427	**10.45**
C1`	52.1043	52.9278	53.2322	53.4597	54.0550	53.4272	54.0405	53.3919	53.9804	53.4938	54.4469	56.5857	57.5886	57.9503	58.1088	58.7263	58.0776	58.8650	58.0439	58.8046	58.1428	59.0926	**50.48**
C2`	25.8450	26.2989	26.6477	26.5107	26.9310	26.5006	26.9968	26.4878	26.9852	26.5243	26.8383	25.6256	25.7431	26.1166	25.8996	26.4923	25.8912	26.3335	25.8800	26.3405	25.9118	26.1331	**23.91**
C3`	25.6256	25.7431	26.1166	25.8996	26.4924	25.8912	26.3335	25.8802	26.3405	25.9117	26.1331	25.8450	26.2989	26.6477	26.5107	26.9310	26.5006	26.9969	26.4878	26.9852	26.5241	26.8382	**23.74**
C4`	56.5857	57.5886	57.9503	58.1088	58.7263	58.0776	58.8650	58.0439	58.8046	58.1428	59.0925	52.1043	52.9278	53.2322	53.4597	54.0549	53.4272	54.0404	53.3918	53.9804	53.4939	54.4470	**52.48**
H2	8.7117	8.5765	8.6446	8.5069	8.4840	8.5109	8.5016	8.5146	8.5097	8.5032	8.4948	8.7117	8.5765	8.6446	8.5069	8.4840	8.5109	8.5016	8.5146	8.5097	8.5032	8.4948	**8.08**
H3	7.3131	7.4425	7.5320	7.4931	7.6189	7.4906	7.6397	7.4875	7.6313	7.4954	7.6535	7.3131	7.4425	7.5320	7.4931	7.6189	7.4906	7.6397	7.4875	7.6313	7.4954	7.6535	**7.23**
H5	7.1769	7.3467	7.4500	7.4173	7.5305	7.4134	7.5453	7.4091	7.5359	7.4209	7.5631	7.1769	7.3467	7.4500	7.4173	7.5305	7.4134	7.5453	7.4091	7.5359	7.4209	7.5631	**7.23**
H6	7.9778	8.1278	8.2412	8.2280	8.3470	8.2215	8.3829	8.2145	8.3694	8.2344	8.4056	7.9778	8.1278	8.2412	8.2280	8.3470	8.2215	8.3829	8.2145	8.3694	8.2344	8.4056	**8.08**
H8	4.6121	4.6620	4.7151	4.7073	4.7862	4.7040	4.7948	4.7004	4.7855	4.7106	4.7797	4.6121	4.6620	4.7151	4.7073	4.7862	4.7040	4.7948	4.7004	4.7855	4.7106	4.7797	**5.3**
H(9A)	1.9991	2.0753	2.0927	2.1300	2.1144	2.1270	2.1459	2.1234	2.1338	2.1329	2.1758	1.5856	1.6020	1.6259	1.5952	1.5166	1.5972	1.5197	1.5983	1.5238	1.5932	1.5553	**2.21**
H(9B)	1.5856	1.6020	1.6259	1.5952	1.5166	1.5972	1.5197	1.5983	1.5238	1.5932	1.5553	1.9991	2.0753	2.0927	2.1300	2.1144	2.1270	2.1459	2.1234	2.1338	2.1329	2.1758	**2.14**
H(10A-10C)	0.8536	0.7792	0.7576	0.7546	0.7110	0.7560	0.7265	0.7571	0.7277	0.7534	0.7200	0.8536	0.7792	0.7576	0.7546	0.7110	0.7560	0.7265	0.7571	0.7277	0.7534	0.7200	**1.01**
H(1`A-1`B)	2.9753	3.0033	3.0075	3.0163	3.0174	3.0160	3.0156	3.0152	3.0153	3.0166	2.9994	2.8890	2.8235	2.7898	2.7971	2.7722	2.7993	2.7621	2.8010	2.7622	2.7949	2.7430	**3.68**
H(2`-3`A-2`-3`B)	1.6692	1.7293	1.6903	1.7712	1.7349	1.7686	1.7512	1.7654	1.7458	1.7738	1.7734	1.6692	1.7293	1.6903	1.7712	1.7349	1.7686	1.7512	1.7654	1.7458	1.7738	1.7734	**2.19**
H(4`A)	2.9062	2.7698	2.7172	2.7339	2.7211	2.7366	2.6911	2.7387	2.6891	2.7313	2.6844	3.1966	3.2533	3.2813	3.2909	3.3399	3.2890	3.3249	3.2866	3.3220	3.2926	3.3248	**3.02**
H(4`B)	2.8717	2.8772	2.8625	2.8603	2.8233	2.8621	2.8330	2.8634	2.8353	2.8585	2.8016	2.7540	2.7532	2.7337	2.7418	2.6948	2.7430	2.7063	2.7438	2.7086	2.7406	2.6741	**3.83**

[a] methyl protons shifts are averaged [b] according to [13] in $CDCl_3$

Table S15. Theoretical chemical shifts (in ppm) of *(R,S)*-4-fluoro-α-pyrrolidinobutyrophenone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S									Exp. [b]
	B3LYP																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.4828	140.8601	141.0780	141.5114	143.5654	141.4590	142.9237	141.4086	142.8797	141.5624	143.1650	139.4828	140.8601	141.0780	141.5116	143.5655	141.4589	142.9237	141.4086	142.8797	141.5626	143.1650	**130.87**
C2	139.7139	139.6390	140.1816	139.5185	140.1697	139.5183	140.6491	139.5192	140.5332	139.5178	140.6883	139.7139	139.6390	140.1816	139.5185	140.1697	139.5186	140.6490	139.5193	140.5332	139.5180	140.6883	**132.98**
C3	121.7769	122.5971	123.1005	122.8272	123.5116	122.8103	123.8079	122.7933	123.7260	122.8413	123.8440	121.7769	122.5971	123.1005	122.8271	123.5116	122.8103	123.8080	122.7933	123.7260	122.8413	123.8440	**117.44**
C4	176.3708	177.2123	177.8981	177.5361	178.1936	177.5130	178.7872	177.4894	178.6329	177.5563	178.8941	176.3708	177.2123	177.8981	177.5359	178.1936	177.5129	178.7873	177.4895	178.6329	177.5562	178.8941	**167.85**
C5	119.9309	121.2165	121.8308	121.8184	122.5774	121.7765	122.8204	121.7346	122.7017	121.8569	122.9502	119.9309	121.2166	121.8308	121.8184	122.5774	121.7765	122.8204	121.7346	122.7017	121.8569	122.9502	**117.44**
C6	135.7473	137.5120	138.8314	138.4057	139.6223	138.3511	140.2599	138.2953	140.0273	138.4546	140.5977	135.7473	137.5120	138.8314	138.4057	139.6223	138.3512	140.2599	138.2952	140.0273	138.4545	140.5977	**132.98**
C7	203.5193	208.7924	209.4490	211.5358	212.4515	211.3577	217.7129	211.1810	216.4646	211.7052	218.7990	203.5193	208.7924	209.4490	211.5359	212.4515	211.3577	217.7129	211.1813	216.4645	211.7053	218.7990	**196.75**
C8	66.4139	67.8629	68.1923	68.4183	69.0761	68.3871	69.8726	68.3540	69.6357	68.4447	70.2526	66.4139	67.8629	68.1923	68.4185	69.0760	68.3870	69.8726	68.3540	69.6357	68.4447	70.2526	**70.92**
C9	29.6092	29.5091	29.6459	29.3733	29.2241	29.3864	29.6107	29.3971	29.5049	29.3567	29.6311	29.6092	29.5091	29.6459	29.3733	29.2240	29.3863	29.6106	29.3970	29.5049	29.3567	29.6311	**23.99**
C10	8.5219	8.8670	9.0241	8.9232	9.1226	8.9188	9.0844	8.9134	9.0590	8.9251	9.1520	8.5219	8.8670	9.0241	8.9233	9.1227	8.9189	9.0845	8.9135	9.0590	8.9250	9.1520	**8.05**
C1`	52.3002	53.1555	53.4631	53.6230	54.2265	53.5864	54.2406	53.5501	54.1597	53.6563	54.6389	56.7796	57.8268	58.2036	58.2917	58.9005	58.2547	59.0667	58.2187	58.9818	58.3264	59.2956	**52.76**
C2`	26.0777	26.5709	26.9149	26.7131	27.1346	26.7003	27.2250	26.6871	27.1920	26.7241	27.0507	25.8545	26.0027	26.3845	26.1079	26.6874	26.0941	26.5554	26.0810	26.5386	26.1200	26.3411	**23.74**
C3`	25.8545	26.0027	26.3845	26.1079	26.6874	26.0941	26.5553	26.0810	26.5386	26.1200	26.3411	26.0777	26.5709	26.9149	26.7132	27.1346	26.7001	27.2249	26.6872	27.1920	26.7240	27.0507	**23.57**
C4`	56.7796	57.8267	58.2036	58.2916	58.9006	58.2546	59.0667	58.2187	58.9818	58.3263	59.2956	52.3002	53.1555	53.4631	53.6230	54.2265	53.5865	54.2407	53.5502	54.1597	53.6563	54.6389	**56.17**
H2	8.6890	8.5481	8.6258	8.4698	8.4597	8.4744	8.4767	8.4790	8.4820	8.4651	8.4725	8.6890	8.5482	8.6258	8.4698	8.4597	8.4745	8.4767	8.4790	8.4820	8.4651	8.4725	**8.11**
H3	7.3023	7.4350	7.5184	7.4836	7.6081	7.4805	7.6278	7.4774	7.6168	7.4863	7.6439	7.3023	7.4350	7.5184	7.4836	7.6081	7.4805	7.6278	7.4774	7.6168	7.4863	7.6439	**7.34**
H5	7.1694	7.3383	7.4405	7.4027	7.5183	7.3988	7.5321	7.3948	7.5202	7.4062	7.5525	7.1694	7.3383	7.4405	7.4028	7.5183	7.3988	7.5321	7.3948	7.5202	7.4062	7.5525	**7.34**
H6	7.9686	8.1161	8.2330	8.2110	8.3323	8.2044	8.3665	8.1979	8.3506	8.2172	8.3915	7.9686	8.1161	8.2330	8.2110	8.3323	8.2044	8.3665	8.1979	8.3506	8.2172	8.3915	**8.11**
H8	4.6380	4.6871	4.7388	4.7267	4.8029	4.7234	4.8102	4.7202	4.7981	4.7298	4.7968	4.6380	4.6871	4.7388	4.7267	4.8028	4.7234	4.8101	4.7202	4.7981	4.7298	4.7968	**5.25**
H(9A)	1.7885	1.8354	1.8538	1.8483	1.8122	1.8487	1.8295	1.8487	1.8234	1.8472	1.8649	1.7885	1.8354	1.8538	1.8483	1.8122	1.8487	1.8295	1.8487	1.8234	1.8472	1.8649	**2.17**
H(9B)	0.8519	0.7800	0.7565	0.7523	0.7089	0.7533	0.7233	0.7544	0.7216	0.7513	0.7188	0.8519	0.7800	0.7565	0.7523	0.7089	0.7533	0.7233	0.7544	0.7216	0.7513	0.7188	**0.82**
H(10A-10C)	2.7612	2.7627	2.7370	2.7464	2.6994	2.7475	2.7097	2.7485	2.7093	2.7452	2.6799	2.8780	2.8865	2.8640	2.8640	2.8270	2.8656	2.8354	2.8671	2.8352	2.8622	2.6799	**3.38**
H(1`A-1`B)	3.1978	3.2567	3.2807	3.2898	3.3392	3.2877	3.3234	3.2855	3.3181	3.2914	3.3254	2.9034	2.7715	2.7061	2.7368	2.6909	2.7368	2.6909	2.7388	2.6864	2.7321	3.3254	**3.75**
H(2`-3`A-2`-3`B)	1.6689	1.7318	1.6874	1.7697	1.7328	1.7666	1.7477	1.7635	1.7395	1.7725	1.7726	1.6689	1.7318	1.6874	1.7697	1.7328	1.7666	1.7477	1.7635	1.7395	1.7725	1.7726	**2.125**
H(4`A)	2.9034	2.7715	2.7061	2.7345	2.7210	2.7367	2.6909	2.7388	2.6864	2.7321	2.6873	3.1978	3.2567	3.2807	3.2898	3.3392	3.2877	3.3234	3.2856	3.3181	3.2914	2.6873	**3.07**
H(4`B)	2.8780	2.8865	2.8640	2.8640	2.8270	2.8656	2.8354	2.8671	2.8352	2.8622	2.8054	2.7612	2.7627	2.7370	2.7464	2.6994	2.7475	2.7097	2.7485	2.7093	2.7452	2.8054	**3.71**
Nuclei	B3P86																						
C1	136.8836	137.9280	138.6491	138.4297	140.7966	138.4284	140.1803	138.4041	140.1661	138.4737	140.2584	136.8836	137.9280	138.6491	138.4298	140.7965	138.4284	140.1803	138.4042	140.1661	138.4735	140.2584	**130.87**
C2	138.7785	138.6776	139.3220	138.5641	139.1953	138.5910	139.7368	138.5961	139.7311	138.5827	139.7636	138.7785	138.6776	139.3221	138.5641	139.1953	138.5910	139.7368	138.5961	139.7311	138.5827	139.7636	**132.98**
C3	120.9580	121.7817	122.4305	122.0667	122.8867	122.0730	123.1998	122.0573	123.2260	122.1040	123.2547	120.9580	121.7817	122.4306	122.0666	122.8868	122.0730	123.1998	122.0572	123.2260	122.1041	123.2547	**117.44**
C4	173.8709	174.6917	175.3955	175.0637	175.6985	175.0611	176.3254	175.0371	176.3009	175.1100	176.4550	173.8709	174.6917	175.3955	175.0636	175.6988	175.0611	176.3254	175.0370	176.3009	175.1100	176.4550	**167.85**
C5	119.1744	120.5163	121.1913	121.1813	122.0259	121.1610	122.2923	121.1190	122.2841	121.2443	122.4529	119.1744	120.5163	121.1913	121.1814	122.0259	121.1610	122.2923	121.1190	122.2841	121.2443	122.4529	**117.44**
C6	134.8041	136.6574	137.7930	137.6415	138.8194	137.5983	139.3085	137.5337	139.2366	137.7268	139.7688	134.8041	136.6574	137.7930	137.6415	138.8194	137.5983	139.3085	137.5336	139.2366	137.7269	139.7688	**132.98**
C7	201.6813	206.4361	207.4719	208.9388	210.2428	208.8171	215.1444	208.6716	213.9615	209.0968	216.0874	201.6813	206.4361	207.4719	208.9388	210.2428	208.8171	215.1444	208.6715	213.9615	209.0968	216.0874	**196.75**
C8	64.7417	66.0406	66.5452	66.6565	67.5886	66.6470	68.1788	66.6143	67.9975	66.7082	68.6889	64.7417	66.0406	66.5452	66.6565	67.5886	66.6470	68.1788	66.6144	67.9975	66.7083	68.6889	**70.92**
C9	28.5917	28.5842	28.7161	28.5344	28.5430	28.5575	28.6966	28.5585	28.7070	28.5560	28.8688	28.5917	28.5842	28.7161	28.5344	28.5429	28.5575	28.6966	28.5584	28.7070	28.5560	28.8688	**23.99**
C10	8.2705	8.5859	8.7652	8.7053	8.9608	8.7199	8.8203	8.7125	8.8963	8.7352	8.9754	8.2705	8.5859	8.7652	8.7053	8.9608	8.7199	8.8203	8.7125	8.8963	8.7352	8.9754	**8.05**
C1`	51.1951	52.0169	52.3795	52.5015	53.1062	52.4938	53.0791	52.4647	53.0967	52.5531	53.5321	55.4732	56.4695	56.8838	56.9577	57.5094	56.9487	57.7645	56.9181	57.8008	57.0101	57.9944	**52.76**
C2`	24.8220	25.2420	25.6352	25.4398	25.8508	25.4488	25.8957	25.4359	25.9708	25.4749	25.7987	24.5100	24.6380	25.0628	24.7563	25.3156	24.7678	25.2120	24.7575	25.3165	24.7898	25.0252	**23.74**
C3`	24.5100	24.6380	25.0628	24.7564	25.3156	24.7678	25.2120	24.7575	25.3165	24.7897	25.0252	24.8220	25.2420	25.6351	25.4397	25.8507	25.4488	25.8957	25.4359	25.9708	25.4750	25.7987	**23.57**
C4`	55.4732	56.4695	56.8839	56.9575	57.5094	56.9487	57.7645	56.9182	57.8008	57.0101	57.9944	51.1951	52.0169	52.3795	52.5016	53.1062	52.4938	53.0791	52.4646	53.0967	52.5531	53.5321	**56.17**
H2	8.7555	8.6376	8.6808	8.5686	8.5162	8.5730	8.5499	8.5758	8.5686	8.5657	8.5528	8.7555	8.6376	8.6808	8.5686	8.5162	8.5730	8.5499	8.5758	8.5686	8.5657	8.5528	**8.11**
H3	7.3225	7.4583	7.5498	7.5058	7.6401	7.5045	7.6643	7.5014	7.6589	7.5082	7.6804	7.3225	7.4583	7.5498	7.5058	7.6401	7.5045	7.6643	7.5014	7.6589	7.5082	7.6804	**7.34**
H5	7.1886	7.3705	7.4676	7.4396	7.5546	7.4367	7.5671	7.4319	7.5622	7.4437	7.5896	7.1886	7.3705	7.4676	7.4396	7.5545	7.4367	7.5671	7.4319	7.5622	7.4437	7.5896	**7.34**
H6	8.0502	8.2070	8.3003	8.2985	8.4076	8.2935	8.4458	8.2867	8.4422	8.3047	8.4836	8.0502	8.2070	8.3003	8.2985	8.4077	8.2935	8.4458	8.2866	8.4422	8.3047	8.4836	**8.11**
H8	4.6395	4.6910	4.7319	4.7332	4.8065	4.7306	4.8259	4.7264	4.8261	4.7369	4.8276	4.6395	4.6910	4.7319	4.7332	4.8065	4.7306	4.8259	4.7264	4.8261	4.7369	4.8276	**5.25**
H(9A)	1.8440	1.8980	1.8964	1.9218	1.8842	1.9217	1.8656	1.9196	1.8682	1.9232	1.9211	1.8440	1.8980	1.8964	1.9218	1.8841	1.9217	1.8656	1.9196	1.8682	1.9232	1.9211	**2.17**
H(9B)	0.8231	0.7544	0.7310	0.7225	0.6702	0.7254	0.6915	0.7265	0.6982	0.7211	0.6858	0.8231	0.7544	0.7310	0.7225	0.6702	0.7254	0.6915	0.7265	0.6982	0.7211	0.6858	**0.82**
H(10A-10C)	2.7130	2.7161	2.7022	2.7016	2.6601	2.7034	2.6675	2.7034	2.6748	2.7010	2.6382	2.8293	2.8376	2.8260	2.8219	2.7943	2.8245	2.8008	2.8252	2.8059	2.8205	2.7779	**3.38**
H(1`A-1`B)	3.2010	3.2556	3.2751	3.2836	3.3389	3.2828	3.3148	3.2802	3.3168	3.2856	3.3165	2.9482	2.7911	2.7413	2.7368	2.7627	2.7404	2.6863	2.7422	2.6887	2.7347	2.6789	**3.75**
H(2`-3`A-2`-3`B)	1.6564	1.7176	1.6818	1.7538	1.7205	1.7526	1.7388	1.7497	1.7367	1.7562	1.7648	1.6564	1.7176	1.6818	1.7538	1.7205	1.7526	1.7388	1.7497	1.7367	1.7562	1.7648	**2.125**
H(4`A)	2.9482	2.7911	2.7413	2.7369	2.7627	2.7404	2.6863	2.7422	2.6887	2.7347	2.6789	3.2010	3.2556	3.2751	3.2836	3.3389	3.2828	3.3148	3.2802	3.3168	3.2856	3.3165	**3.07**
H(4`B)	2.8293	2.8376	2.8260	2.8218	2.7943	2.8245	2.8008	2.8252	2.8059	2.8205	2.7779	2.7130	2.7161	2.7022	2.7016	2.6601	2.7034	2.6675	2.7034	2.6748	2.7010	2.6382	**3.71**
Nuclei	B3PW91																						
C1	137.1378	138.4706	138.9735	139.1170	141.6407	139.0793	140.5527	139.0315	140.5116	139.1531	140.7674	137.1378	138.4705	138.9735	139.1170	141.3217	139.0793	140.5527	139.0315	140.5116	139.1531	140.7674	**130.87**
C2	138.8483	138.8029	139.3414	138.7073	139.7042	138.7176	139.8518	138.7187	139.7672	138.7001	139.9064	138.8483	138.8028	139.3415	138.7073	139.3852	138.7176	139.8518	138.7187	139.7672	138.7001	139.9064	**132.98**
C3	121.0799	121.9386	122.5010	122.2085	123.3019	122.1993	123.2678	122.1805	123.2010	122.2192	123.3341	121.0799	121.9386	122.5010	122.2085	122.9829	122.1993	123.2678	122.1805	123.2010	122.2192	123.3341	**117.44**
C4	173.9189	174.7305	175.3790	175.0539	176.0096	175.0392	176.3155	175.0159	176.1825	175.0705	176.4451	173.9189	174.7306	175.3790	175.0539	175.6906	175.0392	176.3155	175.0159	176.1825	175.0705	176.4451	**167.85**
C5	119.2605	120.6072	121.2018	121.2633	122.4151	121.2275	122.3409	121.1832	122.2382	121.2993	122.5062	119.2605	120.6072	121.2018	121.2633	122.0961	121.2275	122.3409	121.1832	122.2382	121.2993	122.5062	**117.44**
C6	134.8136	136.5906	137.7321	137.4819	139.0112	137.4336	139.2920	137.3773	139.0921	137.5305	139.6634	134.8136	136.5907	137.7320	137.4819	138.6922	137.4337	139.2920	137.3773	139.0921	137.5305	139.6634	**132.98**
C7	201.6923	206.7464	207.5948	209.4173	210.8576	209.2578	215.4231	209.0875	214.1917	209.5688	216.4735	201.6923	206.7465	207.5947	209.4173	210.5386	209.2578	215.4231	209.0875	214.1917	209.5688	216.4735	**196.75**
C8	64.6787	66.1211	66.5468	66.7686	67.9506	66.7401	68.2311	66.7009	67.9879	66.7957	68.6951	64.6787	66.1211	66.5469	66.7686	67.6316	66.7401	68.2311	66.7009	67.9879	66.7957	68.6951	**70.92**
C9	28.3648	28.3678	28.4671	28.2729	28.5966	28.2852	28.5082	28.2882	28.4130	28.2634	28.5963	28.3648	28.3678	28.4671	28.2729	28.2776	28.2852	28.5082	28.2882	28.4130	28.2634	28.5963	**23.99**
C10	8.3363	8.6767	8.7890	8.7744	9.3303	8.7761	8.8912	8.7685	8.8738	8.7744	9.0339	8.3363	8.6767	8.7890	8.7744	9.0113	8.7761	8.8912	8.7685	8.8738	8.7744	9.0339	**8.05**
C1`	51.1228	51.9598	52.2370	52.4487	53.3444	52.4272	52.9958	52.3963	52.9276	52.4707	53.4334	55.4114	56.4306	56.7432	56.9125	57.4594	56.8873	57.6785	56.8533	57.6166	56.9387	57.9183	**52.76**
C2`	25.0911	25.5313	25.8406	25.7001	26.4134	25.6951	26.1426	25.6810	26.1268	25.7067	25.9969	24.7692	24.9210	25.2534	25.0260	25.5638	25.0216	25.4362	25.0087	25.4454	25.0328	25.2379	**23.74**
C3`	24.7692	24.9209	25.2534	25.0260	25.8828	25.0216	25.4362	25.0087	25.4454	25.0328	25.2379	25.0911	25.5313	25.8406	25.7001	26.0944	25.6951	26.1426	25.6810	26.1268	25.7067	25.9969	**23.57**
C4`	55.4114	56.4306	56.7432	56.9125	57.7784	56.8873	57.6785	56.8533	57.6166	56.9387	57.9183	51.1228	51.9598	52.2369	52.4487	53.0254	52.4272	52.9958	52.3963	52.9276	52.4707	53.4334	**56.17**
H2	8.7299	8.5890	8.6433	8.5111	8.4939	8.5162	8.5209	8.5212	8.5306	8.5066	8.5163	8.7299	8.5890	8.6433	8.5111	8.4784	8.5162	8.5209	8.5212	8.5306	8.5066	8.5163	**8.11**
H3	7.3242	7.4615	7.5515	7.5113	7.6542	7.5090	7.6621	7.5064	7.6533	7.5135	7.6766	7.3242	7.4615	7.5515	7.5113	7.6387	7.5090	7.6621	7.5064	7.6533	7.5135	7.6766	**7.34**
H5	7.1834	7.3556	7.4545	7.4268	7.5614	7.4231	7.5634	7.4191	7.5533	7.4305	7.5832	7.1834	7.3556	7.4545	7.4268	7.5459	7.4231	7.5634	7.4191	7.5533	7.4305	7.5832	**7.34**
H6	8.0322	8.1803	8.2794	8.2709	8.3917	8.2655	8.4228	8.2599	8.4114	8.2763	8.4481	8.0322	8.1803	8.2794	8.2709	8.3762	8.2655	8.4228	8.2599	8.4114	8.2763	8.4481	**8.11**
H8	4.6317	4.6774	4.7215	4.7162	4.7983	4.7128	4.8076	4.7094	4.7995	4.7198	4.8012	4.6317	4.6774	4.7215	4.7162	4.7828	4.7128	4.8076	4.7094	4.7995	4.7198	4.8012	**5.25**
H(9A)	1.8047	1.8488	1.8584	1.8652	1.8475	1.8657	1.8327	1.8659	1.8284	1.8647	1.8728	1.8047	1.8488	1.8584	1.8652	1.8320	1.8657	1.8327	1.8659	1.8284	1.8647	1.8728	**2.17**
H(9B)	0.8072	0.7381	0.7130	0.7090	0.6728	0.7110	0.6793	0.7129	0.6809	0.7073	0.6731	0.8072	0.7381	0.7130	0.7090	0.6574	0.7110	0.6793	0.7129	0.6809	0.7073	0.6731	**0.82**
H(10A-10C)	2.7062	2.7080	2.6900	2.6913	2.6638	2.6923	2.6600	2.6931	2.6622	2.6906	2.6278	2.8255	2.8316	2.8191	2.8157	2.7826	2.8177	2.7914	2.8193	2.7927	2.8139	2.7638	**3.38**
H(1`A-1`B)	3.1767	3.2312	3.2533	3.2604	3.3286	3.2588	3.2949	3.2570	3.2919	3.2620	3.2938	2.8992	2.7645	2.7144	2.7172	2.7317	2.7191	2.6694	2.7208	2.6678	2.7157	2.6612	**3.75**
H(2`-3`A-2`-3`B)	1.6441	1.7050	1.6668	1.7431	1.7215	1.7410	1.7246	1.7387	1.7189	1.7453	1.7490	1.6441	1.7050	1.6668	1.7431	1.7060	1.7410	1.7246	1.7387	1.7189	1.7453	1.7490	**2.125**
H(4`A)	2.8992	2.7645	2.7144	2.7172	2.7472	2.7191	2.6694	2.7208	2.6678	2.7157	2.6612	3.1767	3.2312	3.2533	3.2604	3.3131	3.2588	3.2949	3.2570	3.2919	3.2620	3.2938	**3.07**
H(4`B)	2.8255	2.8316	2.8191	2.8157	2.7981	2.8177	2.7914	2.8193	2.7927	2.8139	2.7638	2.7062	2.7080	2.6900	2.6913	2.6483	2.6923	2.6600	2.6931	2.6622	2.6906	2.6278	**3.71**

[a] methyl protons shifts are averaged [b] according to [13] in D_2O

Table S15. Cont. I

Nuclei	R											S									Exp. [b]
	B98											B98									
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	138.0895	139.3262	139.5103	139.8526	142.0323	139.8370	141.3566	139.8180	141.3476	139.8684	141.5873	138.0895	139.3264	139.5103	139.8525	142.0323	139.8370	141.3566	139.8181	141.3476	139.8682	141.5873	**130.87**
C2	138.5327	138.4347	138.9651	138.3464	139.0357	138.3663	139.4705	138.3841	139.3869	138.3298	139.5112	138.5327	138.4346	138.9651	138.3463	139.0357	138.3663	139.4705	138.3840	139.3869	138.3298	139.5112	**132.98**
C3	120.8609	121.6536	122.1837	121.9011	122.6513	121.9036	122.9164	121.9033	122.8582	121.9008	122.9639	120.8609	121.6535	122.1836	121.9011	122.6513	121.9036	122.9165	121.9033	122.8582	121.9008	122.9639	**117.44**
C4	173.7300	174.5011	175.1988	174.8412	175.5050	174.8355	176.0816	174.8274	175.9511	174.8493	176.1984	173.7300	174.5011	175.1987	174.8413	175.5050	174.8355	176.0816	174.8274	175.9511	174.8494	176.1984	**167.85**
C5	119.0016	120.2696	120.8867	120.9271	121.7648	120.9014	121.9894	120.8732	121.8908	120.9541	122.1339	119.0016	120.2697	120.8867	120.9273	121.7648	120.9014	121.9894	120.8731	121.8908	120.9542	122.1339	**117.44**
C6	134.7500	136.4405	137.7513	137.3800	138.5556	137.3362	139.1668	137.2904	138.9572	137.4244	139.5057	134.7500	136.4405	137.7514	137.3802	138.5556	137.3362	139.1668	137.2904	138.9572	137.4245	139.5057	**132.98**
C7	200.0993	205.2330	205.8069	207.8907	208.8976	207.7449	214.1629	207.5954	212.9246	208.0286	215.2370	200.0993	205.2329	205.8071	207.8906	208.8976	207.7449	214.1629	207.5952	212.9246	208.0286	215.2370	**196.75**
C8	66.3027	67.6937	67.9568	68.3028	69.0056	68.2872	69.7561	68.2667	69.5333	68.3172	70.1746	66.3027	67.6936	67.9568	68.3029	69.0056	68.2872	69.7561	68.2668	69.5333	68.3171	70.1746	**70.92**
C9	29.4819	29.4579	29.5637	29.3921	29.2854	29.4139	29.6225	29.4333	29.5316	29.3737	29.6604	29.4819	29.4580	29.5637	29.3921	29.2854	29.4139	29.6226	29.4334	29.5316	29.3737	29.6604	**23.99**
C10	8.9753	9.2568	9.3695	9.3566	9.5471	9.3675	9.4943	9.3751	9.4823	9.3477	9.5852	8.9753	9.2567	9.3695	9.3566	9.5471	9.3675	9.4943	9.3751	9.4823	9.3477	9.5852	**8.05**
C1`	52.3942	53.1621	53.4348	53.6553	54.2356	53.6403	54.2196	53.6212	54.1613	53.6704	54.6249	56.8261	57.7455	58.1211	58.2175	58.8417	58.2019	58.9932	58.1838	58.9351	58.2347	59.2134	**52.76**
C2`	26.2704	26.6559	26.9849	26.8459	27.2546	26.8487	27.3257	26.8488	27.3121	26.8453	27.1787	25.9448	26.0723	26.4407	26.1998	26.7733	26.2044	26.6343	26.2073	26.6448	26.1983	26.4409	**23.74**
C3`	25.9448	26.0724	26.4406	26.1998	26.7733	26.2044	26.6342	26.2072	26.6448	26.1983	26.4409	26.2704	26.6559	26.9849	26.8459	27.2546	26.8487	27.3257	26.8488	27.3121	26.8453	27.1787	**23.57**
C4`	56.8261	57.7454	58.1212	58.2175	58.8417	58.2019	58.9933	58.1839	58.9351	58.2347	59.2134	52.3942	53.1621	53.4348	53.6553	54.2356	53.6403	54.2197	53.6212	54.1613	53.6704	54.6249	**56.17**
H2	8.7216	8.5873	8.6751	8.5166	8.4965	8.5207	8.5181	8.5251	8.5257	8.5132	8.5115	8.7216	8.5873	8.6751	8.5166	8.4965	8.5207	8.5181	8.5251	8.5257	8.5132	8.5115	**8.11**
H3	7.3168	7.4544	7.5474	7.5006	7.6285	7.4983	7.6496	7.4961	7.6411	7.5029	7.6640	7.3168	7.4545	7.5474	7.5006	7.6285	7.4983	7.6496	7.4961	7.6411	7.5030	7.6640	**7.34**
H5	7.1733	7.3507	7.4550	7.4251	7.5471	7.4209	7.5634	7.4167	7.5532	7.4294	7.5825	7.1733	7.3507	7.4550	7.4251	7.5471	7.4209	7.5634	7.4167	7.5532	7.4294	7.5825	**7.34**
H6	7.9950	8.1500	8.2746	8.2491	8.3721	8.2426	8.4103	8.2364	8.3968	8.2557	8.4333	7.9950	8.1499	8.2746	8.2491	8.3721	8.2426	8.4103	8.2363	8.3968	8.2557	8.4333	**8.11**
H8	4.5899	4.6436	4.7037	4.6864	4.7699	4.6827	4.7835	4.6795	4.7741	4.6906	4.7727	4.5899	4.6436	4.7037	4.6864	4.7699	4.6827	4.7835	4.6795	4.7741	4.6906	4.7727	**5.25**
H(9A)	1.7908	1.8334	1.8530	1.8566	1.8103	1.8559	1.8255	1.8551	1.8206	1.8573	1.8598	1.7908	1.8334	1.8530	1.8566	1.8103	1.8559	1.8255	1.8552	1.8206	1.8573	1.8598	**2.17**
H(9B)	0.8434	0.7702	0.7522	0.7409	0.6955	0.7426	0.7118	0.7445	0.7133	0.7396	0.7055	0.8434	0.7702	0.7522	0.7409	0.6955	0.7426	0.7118	0.7445	0.7133	0.7396	0.7055	**0.82**
H(10A-10C)	2.7263	2.7240	2.7071	2.7079	2.6653	2.7088	2.6789	2.7099	2.6809	2.7076	2.6478	2.8469	2.8509	2.8318	2.8334	2.7985	2.8351	2.8107	2.8368	2.8126	2.8320	2.7822	**3.38**
H(1`A-1`B)	3.1881	3.2385	3.2670	3.2707	3.3225	3.2687	3.3092	3.2669	3.3061	3.2730	3.3094	2.8967	2.7767	2.7057	2.7316	2.7269	2.7337	2.6953	2.7363	2.6937	2.7301	2.6866	**3.75**
H(2`-3`A-2`-3`B)	1.6625	1.7233	1.6816	1.7617	1.7266	1.7593	1.7434	1.7569	1.7381	1.7644	1.7668	1.6625	1.7233	1.6816	1.7618	1.7266	1.7593	1.7434	1.7569	1.7381	1.7644	1.7668	**2.125**
H(4`A)	2.8967	2.7767	2.7058	2.7316	2.7269	2.7337	2.6953	2.7363	2.6937	2.7301	2.6866	3.1881	3.2385	3.2670	3.2708	3.3225	3.2687	3.3092	3.2669	3.3061	3.2730	3.3094	**3.07**
H(4`B)	2.8469	2.8509	2.8318	2.8334	2.7985	2.8351	2.8107	2.8368	2.8126	2.8320	2.7822	2.7263	2.7240	2.7071	2.7079	2.6653	2.7088	2.6789	2.7099	2.6809	2.7076	2.6478	**3.71**
Nuclei	B971											B971											
C1	137.6687	138.8544	139.0766	139.3728	141.6380	139.3553	140.9588	139.3360	140.9511	139.3938	141.1916	137.6687	138.8544	139.0768	139.3728	141.6380	139.3553	140.9588	139.3360	140.9511	139.3938	141.1915	**130.87**
C2	138.2377	138.1469	138.6812	138.0613	138.7320	138.0739	139.1621	138.0860	139.0803	138.0553	139.2051	138.2377	138.1469	138.6814	138.0613	138.7319	138.0740	139.1621	138.0860	139.0804	138.0553	139.2051	**132.98**
C3	120.6642	121.4579	121.9890	121.7160	122.4641	121.7108	122.7275	121.7044	122.6690	121.7267	122.7808	120.6642	121.4578	121.9891	121.7160	122.4640	121.7106	122.7275	121.7044	122.6690	121.7267	122.7807	**117.44**
C4	173.6312	174.4204	175.1128	174.7758	175.4249	174.7610	175.9991	174.7460	175.8687	174.7963	176.1206	173.6312	174.4203	175.1127	174.7758	175.4250	174.7608	175.9991	174.7460	175.8686	174.7963	176.1206	**167.85**
C5	118.8046	120.0802	120.6931	120.7474	121.5819	120.7135	121.8073	120.6795	121.7080	120.7856	121.9573	118.8046	120.0803	120.6930	120.7474	121.5818	120.7136	121.8073	120.6795	121.7082	120.7856	121.9574	**117.44**
C6	134.4899	136.2162	137.4905	137.1701	138.3000	137.1159	138.8968	137.0617	138.6869	137.2285	139.2431	134.4899	136.2161	137.4905	137.1701	138.2999	137.1159	138.8968	137.0617	138.6870	137.2285	139.2432	**132.98**
C7	199.9842	205.0193	205.6279	207.6468	208.7697	207.5008	213.9201	207.3522	212.7096	207.7887	215.0113	199.9842	205.0193	205.6278	207.6468	208.7694	207.5007	213.9201	207.3522	212.7095	207.7887	215.0112	**196.75**
C8	66.1161	67.4695	67.7309	68.0894	68.8160	68.0678	69.5176	68.0429	69.3003	68.1132	69.9582	66.1161	67.4696	67.7309	68.0894	68.8160	68.0678	69.5176	68.0429	69.3004	68.1132	69.9582	**70.92**
C9	29.4609	29.4611	29.5569	29.4118	29.2916	29.4228	29.6107	29.4337	29.5204	29.4071	29.6678	29.4609	29.4611	29.5569	29.4118	29.2916	29.4229	29.6107	29.4337	29.5204	29.4071	29.6677	**23.99**
C10	8.9281	9.2106	9.3145	9.3222	9.5007	9.3249	9.4414	9.3263	9.4279	9.3252	9.5517	8.9281	9.2106	9.3144	9.3222	9.5007	9.3249	9.4414	9.3263	9.4279	9.3252	9.5516	**8.05**
C1`	52.3126	53.0808	53.3386	53.5778	54.1428	53.5568	54.1150	53.5342	54.0572	53.6026	54.5273	56.7306	57.6449	58.0249	58.1224	58.7397	58.0999	58.8856	58.0769	58.8293	58.1497	59.1022	**52.76**
C2`	26.0660	26.4604	26.7870	26.6700	27.0663	26.6645	27.1283	26.6580	27.1144	26.6809	27.0080	25.7585	25.8944	26.2639	26.0323	26.5977	26.0290	26.4603	26.0256	26.4705	26.0422	26.2861	**23.74**
C3`	25.7585	25.8943	26.2639	26.0323	26.5977	26.0289	26.4603	26.0256	26.4705	26.0422	26.2860	26.0660	26.4604	26.7870	26.6700	27.0663	26.6645	27.1283	26.6580	27.1144	26.6809	27.0079	**23.57**
C4`	56.7306	57.6449	58.0249	58.1224	58.7397	58.0999	58.8856	58.0769	58.8292	58.1497	59.1024	52.3126	53.0808	53.3387	53.5778	54.1428	53.5568	54.1150	53.5342	54.0572	53.6026	54.5272	**56.17**
H2	8.7211	8.5931	8.6773	8.5245	8.4941	8.5278	8.5180	8.5315	8.5253	8.5220	8.5110	8.7211	8.5931	8.6774	8.5245	8.4941	8.5279	8.5180	8.5315	8.5253	8.5220	8.5110	**8.11**
H3	7.3147	7.4516	7.5447	7.4978	7.6249	7.4953	7.6458	7.4929	7.6374	7.5004	7.6601	7.3147	7.4516	7.5447	7.4978	7.6249	7.4953	7.6458	7.4929	7.6374	7.5004	7.6601	**7.34**
H5	7.1717	7.3497	7.4523	7.4246	7.5453	7.4201	7.5616	7.4157	7.5514	7.4293	7.5804	7.1717	7.3497	7.4523	7.4246	7.5453	7.4201	7.5616	7.4157	7.5514	7.4293	7.5804	**7.34**
H6	7.9991	8.1539	8.2770	8.2522	8.3708	8.2455	8.4094	8.2390	8.3957	8.2590	8.4321	7.9991	8.1538	8.2770	8.2522	8.3708	8.2455	8.4094	8.2390	8.3957	8.2590	8.4321	**8.11**
H8	4.5927	4.6452	4.7066	4.6888	4.7722	4.6846	4.7871	4.6809	4.7777	4.6935	4.7762	4.5927	4.6452	4.7066	4.6888	4.7722	4.6846	4.7871	4.6809	4.7776	4.6935	4.7761	**5.25**
H(9A)	1.7965	1.8405	1.8561	1.8657	1.8142	1.8645	1.8271	1.8632	1.8220	1.8671	1.8629	1.7965	1.8405	1.8561	1.8657	1.8142	1.8645	1.8271	1.8632	1.8220	1.8671	1.8629	**2.17**
H(9B)	0.8369	0.7633	0.7470	0.7342	0.6876	0.7358	0.7046	0.7374	0.7060	0.7333	0.6988	0.8369	0.7633	0.7470	0.7342	0.6876	0.7358	0.7046	0.7374	0.7060	0.7333	0.6988	**0.82**
H(10A-10C)	2.7162	2.7140	2.6981	2.6991	2.6567	2.6994	2.6686	2.7001	2.6709	2.6992	2.6369	2.8359	2.8415	2.8224	2.8267	2.7923	2.8281	2.8026	2.8296	2.8048	2.8255	2.7755	**3.38**
H(1`A-1`B)	3.1917	3.2403	3.2683	3.2724	3.3239	3.2701	3.3091	3.2680	3.3061	3.2750	3.3090	2.9002	2.7790	2.7061	2.7327	2.7307	2.7344	2.6969	2.7366	2.6956	2.7316	2.6870	**3.75**
H(2`-3`A-2`-3`B)	1.6615	1.7214	1.6802	1.7600	1.7255	1.7575	1.7420	1.7550	1.7368	1.7629	1.7654	1.6615	1.7214	1.6801	1.7600	1.7255	1.7575	1.7420	1.7550	1.7368	1.7629	1.7654	**2.125**
H(4`A)	2.9002	2.7790	2.7061	2.7327	2.7307	2.7344	2.6969	2.7366	2.6956	2.7316	2.6870	3.1917	3.2403	3.2683	3.2724	3.3239	3.2701	3.3091	3.2680	3.3061	3.2750	3.3090	**3.07**
H(4`B)	2.8359	2.8415	2.8224	2.8267	2.7923	2.8281	2.8026	2.8296	2.8048	2.8255	2.7755	2.7162	2.7140	2.6981	2.6991	2.6567	2.6994	2.6687	2.7001	2.6709	2.6992	2.6369	**3.71**
Nuclei	B972											B972											
C1	134.5471	136.0569	137.2319	137.0535	138.7312	137.0179	138.0424	136.9791	137.9913	137.0831	138.4048	134.5471	136.0569	137.2317	137.0535	138.7313	137.0180	138.0424	136.9791	137.9914	137.0831	138.4048	**130.87**
C2	136.2193	136.1286	136.7989	136.1042	136.7370	136.1059	137.1406	136.1058	137.0645	136.0990	137.1838	136.2193	136.1286	136.7987	136.1042	136.7370	136.1061	137.1406	136.1058	137.0645	136.0990	137.1837	**132.98**
C3	118.5462	119.3398	120.0023	119.6719	120.3503	119.6577	120.6051	119.6406	120.5424	119.6808	120.6746	118.5462	119.3398	120.0023	119.6719	120.3503	119.6577	120.6051	119.6406	120.5424	119.6808	120.6746	**117.44**
C4	170.6043	171.2822	171.9307	171.6277	172.2676	171.6042	172.8520	171.5790	172.7150	171.6463	172.9820	170.6043	171.2822	171.9308	171.6277	172.2676	171.6043	172.8520	171.5790	172.7151	171.6463	172.9820	**167.85**
C5	116.7225	117.9683	118.6045	118.6711	119.4281	118.6304	119.6424	118.5875	119.5448	118.7050	119.8015	116.7225	117.9683	118.6045	118.6711	119.4281	118.6304	119.6424	118.5875	119.5448	118.7050	119.8015	**117.44**
C6	132.2452	133.7651	134.5263	134.5691	135.8913	134.5077	136.4830	134.4447	136.2871	134.6233	136.7864	132.2452	133.7651	134.5263	134.5691	135.8913	134.5077	136.4830	134.4447	136.2871	134.6233	136.7864	**132.98**
C7	197.6034	202.7854	204.0794	205.8061	206.3506	205.6446	211.3542	205.4784	210.1128	205.9538	212.5143	197.6034	202.7854	204.0795	205.8061	206.3506	205.6446	211.3542	205.4784	210.1126	205.9538	212.5141	**196.75**
C8	63.3681	64.8531	65.1088	65.6278	66.2153	65.5927	66.9131	65.5527	66.6849	65.6541	67.3267	63.3681	64.8531	65.1088	65.6278	66.2153	65.5928	66.9131	65.5527	66.6849	65.6541	67.3267	**70.92**
C9	27.9648	27.8951	27.7481	27.8108	27.7957	27.8174	28.0865	27.8218	28.0052	27.7998	28.1181	27.9648	27.8951	27.7480	27.8108	27.7957	27.8175	28.0865	27.8218	28.0052	27.7998	28.1181	**23.99**
C10	8.6203	8.9203	8.9599	9.0565	9.2694	9.0504	9.1647	9.0410	9.1608	9.0568	9.2781	8.6203	8.9203	8.9599	9.0565	9.2694	9.0505	9.1647	9.0410	9.1608	9.0568	9.2781	**8.05**
C1`	50.3107	51.0784	51.3663	51.6232	52.1519	51.5904	52.1250	51.5532	52.0677	51.6481	52.5263	54.5983	55.5236	56.0100	56.0833	56.5994	56.0494	56.7502	56.0134	56.6843	56.1113	56.9905	**52.76**
C2`	25.0389	25.4425	25.7339	25.6639	26.0348	25.6515	26.0735	25.6366	26.0631	25.6710	25.9136	24.7114	24.8248	25.2626	25.0090	25.5062	24.9983	25.3631	24.9860	25.3662	25.0157	25.1780	**23.74**
C3`	24.7114	24.8248	25.2625	25.0090	25.5061	24.9984	25.3631	24.9860	25.3663	25.0157	25.1780	25.0389	25.4425	25.7339	25.6639	26.0348	25.6516	26.0735	25.6366	26.0630	25.6711	25.9136	**23.57**
C4`	54.5983	55.5236	56.0100	56.0833	56.5994	56.0493	56.7502	56.0134	56.6841	56.1112	56.9905	50.3107	51.0784	51.3664	51.6232	52.1519	51.5905	52.1250	51.5532	52.0676	51.6480	52.5263	**56.17**
H2	8.7155	8.5493	8.5737	8.4504	8.4632	8.4542	8.4887	8.4580	8.5002	8.4468	8.4733	8.7155	8.5493	8.5737	8.4504	8.4632	8.4543	8.4887	8.4580	8.5002	8.4468	8.4733	**8.11**
H3	7.3211	7.4578	7.5556	7.5116	7.6318	7.5090	7.6525	7.5062	7.6443	7.5139	7.6664	7.3211	7.4578	7.5556	7.5116	7.6318	7.5090	7.6525	7.5062	7.6443	7.5139	7.6664	**7.34**
H5	7.1756	7.3408	7.4299	7.4172	7.5377	7.4126	7.5542	7.4078	7.5441	7.4214	7.5749	7.1756	7.3408	7.4299	7.4172	7.5377	7.4126	7.5542	7.4078	7.5441	7.4214	7.5748	**7.34**
H6	8.0068	8.1485	8.2381	8.2296	8.3522	8.2238	8.3882	8.2179	8.3777	8.2350	8.4045	8.0068	8.1485	8.2381	8.2296	8.3522	8.2238	8.3882	8.2179	8.3777	8.2350	8.4045	**8.11**
H8	4.6074	4.6427	4.6957	4.6760	4.7506	4.6729	4.7662	4.6701	4.7566	4.6792	4.7557	4.6074	4.6427	4.6956	4.6760	4.7506	4.6729	4.7662	4.6701	4.7566	4.6792	4.7557	**5.25**
H(9A)	1.7697	1.8041	1.7472	1.8002	1.7861	1.7997	1.7974	1.7988	1.7957	1.8002	1.8241	1.7697	1.8041	1.7472	1.8002	1.7861	1.7997	1.7974	1.7988	1.7957	1.8002	1.8241	**2.17**
H(9B)	0.8179	0.7490	0.7391	0.7239	0.6755	0.7253	0.6936	0.7266	0.6943	0.7226	0.6884	0.8179	0.7490	0.7391	0.7239	0.6755	0.7253	0.6936	0.7266	0.6943	0.7226	0.6884	**0.82**
H(10A-10C)	2.7091	2.7084	2.6879	2.6921	2.6460	2.6934	2.6577	2.6947	2.6597	2.6911	2.6262	2.8314	2.8396	2.8199	2.8250	2.7837	2.8266	2.7943	2.8280	2.7960	2.8231	2.7661	**3.38**
H(1`A-1`B)	3.1774	3.2330	3.2519	3.2626	3.3131	3.2608	3.2981	3.2587	3.2954	3.2644	3.2966	2.8725	2.7623	2.7028	2.7301	2.7185	2.7325	2.6828	2.7350	2.6801	2.7280	2.6794	**3.75**
H(2`-3`A-2`-3`B)	1.6424	1.7027	1.6763	1.7462	1.7039	1.7435	1.7212	1.7407	1.7152	1.7486	1.7458	1.6424	1.7027	1.6763	1.7462	1.7039	1.7435	1.7212	1.7407	1.7152	1.7486	1.7458	**2.125**
H(4`A)	2.8725	2.7623	2.7028	2.7301	2.7185	2.7325	2.6828	2.7350	2.6801	2.7280	2.6794	3.1774	3.2330	3.2520	3.2626	3.3131	3.2608	3.2981	3.2587	3.2955	3.2643	3.2966	**3.07**
H(4`B)	2.8314	2.8396	2.8199	2.8250	2.7837	2.8266	2.7943	2.8280	2.7960	2.8231	2.7661	2.7091	2.7084	2.6879	2.6921	2.6460	2.6934	2.6577	2.6947	2.6597	2.6911	2.6262	**3.71**

[a] methyl protons shifts are averaged [b] according to [13] in D_2O

Table S15. Cont. II

Nuclei	R											S									Exp. [b]
	BHandH											BHandH									
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	138.5212	138.9902	140.1763	139.3030	141.0047	139.2786	140.0248	139.2707	140.1939	139.2942	140.3266	138.5212	138.9902	140.1763	139.3031	140.0472	139.2786	140.0248	139.2707	140.1939	139.2942	140.3267	**130.87**
C2	143.5859	143.4645	144.0313	143.3188	143.8124	143.3172	144.3691	143.3342	144.2395	143.2907	144.4328	143.5859	143.4645	144.0313	143.3187	144.0628	143.3172	144.3691	143.3342	144.2395	143.2907	144.4329	**132.98**
C3	123.6774	124.4305	125.0975	124.6796	125.3939	124.6575	125.6117	124.6533	125.5821	124.6702	125.6970	123.6774	124.4305	125.0975	124.6796	125.4237	124.6575	125.6117	124.6533	125.5821	124.6702	125.6970	**117.44**
C4	174.8030	175.5798	176.2063	175.9857	176.5699	175.9506	177.2747	175.9337	177.1177	175.9891	177.4193	174.8030	175.5798	176.2063	175.9858	176.7299	175.9506	177.2747	175.9337	177.1177	175.9891	177.4194	**167.85**
C5	121.5533	122.9602	123.6643	123.6913	124.5795	123.6364	124.7656	123.5996	124.6801	123.7133	124.9300	121.5533	122.9602	123.6643	123.6914	124.4355	123.6364	124.7656	123.5996	124.6801	123.7133	124.9300	**117.44**
C6	139.7267	141.7737	142.8229	142.9213	144.5272	142.8372	145.2124	142.7725	144.9590	142.9718	145.5729	139.7267	141.7737	142.8229	142.9214	143.6655	142.8372	145.2124	142.7725	144.9590	142.9718	145.5729	**132.98**
C7	203.8767	208.2768	209.7734	210.7971	211.5325	210.6371	216.4807	210.4930	215.3771	210.9174	217.5695	203.8767	208.2768	209.7734	210.7970	211.5411	210.6371	216.4807	210.4930	215.3771	210.9174	217.5699	**196.75**
C8	60.1695	61.2113	61.9268	61.8637	62.6072	61.8124	63.1590	61.7790	63.0334	61.8817	63.6011	60.1695	61.2113	61.9268	61.8637	62.6078	61.8124	63.1590	61.7790	63.0334	61.8817	63.6011	**70.92**
C9	25.2929	25.2744	25.3505	25.2217	25.3832	25.2133	25.5416	25.2240	25.4660	25.2002	25.6283	25.2929	25.2744	25.3505	25.2217	25.9658	25.2133	25.5416	25.2240	25.4660	25.2002	25.6284	**23.99**
C10	6.8206	7.0835	7.2156	7.2207	7.5005	7.1990	7.3586	7.1962	7.3530	7.2120	7.4915	6.8206	7.0835	7.2156	7.2208	7.9649	7.1990	7.3586	7.1962	7.3530	7.2120	7.4915	**8.05**
C1`	48.0732	48.8651	49.2967	49.4024	49.9788	49.3579	49.9293	49.3318	49.8848	49.4151	50.3428	52.0603	53.0074	53.4703	53.5625	54.3066	53.5170	54.2364	53.4899	54.1747	53.5751	54.5228	**52.76**
C2`	21.5192	21.9011	22.2732	22.1414	22.5433	22.1153	22.6029	22.1075	22.5977	22.1362	22.5780	21.1146	21.3188	21.6815	21.4312	22.1753	21.4129	21.8669	21.4131	21.8834	21.4186	21.7649	**23.74**
C3`	21.1146	21.3188	21.6815	21.4312	21.9388	21.4129	21.8669	21.4131	21.8834	21.4186	21.7649	21.5192	21.9011	22.2732	22.1415	22.8856	22.1153	22.6029	22.1075	22.5977	22.1362	22.5780	**23.57**
C4`	52.0603	53.0074	53.4703	53.5624	54.0551	53.5170	54.2364	53.4899	54.1747	53.5751	54.5228	48.0732	48.8651	49.2967	49.4025	50.1466	49.3579	49.9293	49.3318	49.8848	49.4151	50.3428	**56.17**
H2	9.0450	8.9678	8.9601	8.9042	8.8849	8.9085	8.9332	8.9121	8.9273	8.9014	8.9210	9.0450	8.9678	8.9601	8.9042	8.8230	8.9085	8.9332	8.9121	8.9273	8.9014	8.9210	**8.11**
H3	7.4575	7.5997	7.6912	7.6424	7.7660	7.6412	7.7846	7.6390	7.7767	7.6446	7.8005	7.4575	7.5997	7.6912	7.6424	7.5612	7.6412	7.7846	7.6390	7.7767	7.6446	7.8005	**7.34**
H5	7.2908	7.4882	7.5789	7.5729	7.7023	7.5689	7.7160	7.5640	7.7051	7.5778	7.7354	7.2908	7.4882	7.5789	7.5729	7.4917	7.5689	7.7160	7.5640	7.7051	7.5778	7.7354	**7.34**
H6	8.1972	8.3935	8.4732	8.4945	8.6334	8.4887	8.6980	8.4821	8.6771	8.5012	8.7251	8.1972	8.3935	8.4732	8.4945	8.4133	8.4887	8.6980	8.4821	8.6771	8.5012	8.7251	**8.11**
H8	4.2733	4.3638	4.3954	4.4062	4.4953	4.4038	4.5488	4.4006	4.5345	4.4098	4.5541	4.2733	4.3638	4.3954	4.4062	4.3250	4.4038	4.5488	4.4006	4.5345	4.4098	4.5541	**5.25**
H(9A)	1.8429	1.9008	1.8776	1.9325	1.5730	1.9311	1.9355	1.9291	1.9266	1.9348	1.9698	1.8429	1.9008	1.8776	1.9325	1.9394	1.9311	1.9355	1.9291	1.9266	1.9348	1.9698	**2.17**
H(9B)	0.8392	0.7759	0.7250	0.7295	0.6630	0.7332	0.6870	0.7360	0.6884	0.7271	0.6868	0.8392	0.7759	0.7250	0.7295	0.6483	0.7332	0.6870	0.7360	0.6884	0.7271	0.6868	**0.82**
H(10A-10C)	2.5935	2.5928	2.5648	2.5729	2.4330	2.5749	2.5366	2.5761	2.5374	2.5721	2.5181	2.7387	2.7413	2.7273	2.7293	2.6918	2.7313	2.7050	2.7325	2.7070	2.7284	2.6816	**3.38**
H(1`A-1`B)	3.0812	3.1274	3.1509	3.1551	3.1001	3.1541	3.1985	3.1523	3.1959	3.1571	3.2012	2.9174	2.7205	2.6790	2.6421	2.6527	2.6473	2.5593	2.6517	2.5643	2.6384	2.5516	**3.75**
H(2`-3`A-2`-3`B)	1.6271	1.6798	1.6481	1.7172	1.4908	1.7155	1.6928	1.7130	1.6875	1.7198	1.7193	1.6271	1.6798	1.6481	1.7172	1.6718	1.7155	1.6928	1.7130	1.6875	1.7198	1.7194	**2.125**
H(4`A)	2.9174	2.7205	2.6790	2.6421	2.5055	2.6473	2.5593	2.6517	2.5643	2.6384	2.5516	3.0812	3.1274	3.1509	3.1551	3.2118	3.1541	3.1985	3.1523	3.1959	3.1571	3.2012	**3.07**
H(4`B)	2.7387	2.7413	2.7273	2.7293	2.5707	2.7313	2.7050	2.7325	2.7070	2.7284	2.6816	2.5935	2.5928	2.5648	2.5729	2.5242	2.5749	2.5366	2.5761	2.5374	2.5721	2.5181	**3.71**
Nuclei	BHandHLYP											BHandHLYP									
C1	139.1083	139.8726	140.5904	140.3953	141.4094	140.3823	142.0785	140.3697	140.8236	140.4052	142.2534	139.1082	139.8726	140.5904	140.3953	141.4093	140.3823	142.0785	140.3698	140.8236	140.4052	142.2532	**130.87**
C2	142.1831	142.0302	142.5305	141.8772	142.3344	141.8845	142.8844	141.8944	142.7416	141.8703	142.9307	142.1830	142.0302	142.5304	141.8774	142.3345	141.8845	142.8844	141.8945	142.7416	141.8703	142.9307	**132.98**
C3	122.4277	123.0603	123.5957	123.2820	123.8637	123.2729	124.2088	123.2657	124.0425	123.2902	124.2634	122.4276	123.0603	123.5957	123.2822	123.8639	123.2729	124.2088	123.2657	124.0425	123.2902	124.2634	**117.44**
C4	174.5933	175.2689	175.8601	175.6184	176.2622	175.5951	176.7432	175.5747	176.7571	175.6406	176.8767	174.5934	175.2689	175.8601	175.6184	176.2621	175.5951	176.7432	175.5746	176.7571	175.6406	176.8769	**167.85**
C5	120.3207	121.5907	122.1561	122.2421	122.9910	122.2033	123.1824	122.1670	123.0525	122.2782	123.3403	120.3207	121.5907	122.1560	122.2421	122.9909	122.2033	123.1824	122.1669	123.0525	122.2782	123.3404	**117.44**
C6	138.0425	139.8949	140.9966	140.9069	142.5888	140.8364	142.4604	140.7692	143.0045	140.9743	142.8273	138.0426	139.8949	140.9966	140.9069	142.5889	140.8364	142.4604	140.7691	143.0045	140.9743	142.8274	**132.98**
C7	202.0500	207.0643	208.1279	209.9315	209.7172	209.7777	216.9247	209.6234	214.3030	210.0743	217.9390	202.0500	207.0643	208.1279	209.9315	209.7171	209.7777	216.9247	209.6233	214.3030	210.0743	217.9391	**196.75**
C8	61.7828	62.8234	63.3429	63.4521	63.8268	63.4291	64.8957	63.4062	64.3758	63.4712	65.2587	61.7828	62.8234	63.3430	63.4521	63.8267	63.4291	64.8957	63.4062	64.3758	63.4712	65.2587	**70.92**
C9	26.5523	26.3705	26.4700	26.2778	26.3805	26.2817	26.3233	26.2878	26.5472	26.2734	26.3551	26.5523	26.3705	26.4701	26.2778	26.3806	26.2817	26.3233	26.2878	26.5472	26.2734	26.3551	**23.99**
C10	8.4702	8.6992	8.8741	8.8336	9.1031	8.8270	8.9481	8.8225	9.0209	8.8394	9.0345	8.4704	8.6992	8.8741	8.8337	9.1031	8.8271	8.9481	8.8224	9.0209	8.8394	9.0344	**8.05**
C1`	49.0156	49.7761	50.1008	50.3042	50.8136	50.2760	50.8593	50.2498	50.7864	50.3301	51.2588	53.2198	54.1039	54.4862	54.6111	55.1174	54.5821	55.3294	54.5555	55.2017	54.6382	55.5561	**52.76**
C2`	24.3612	24.6836	25.0620	24.8776	25.2998	24.8679	25.3219	24.8605	25.3484	24.8862	25.1915	23.9594	24.0570	24.4250	24.1596	24.7162	24.1503	24.5722	24.1439	24.5844	24.1687	24.4100	**23.74**
C3`	23.9594	24.0570	24.4251	24.1596	24.7161	24.1503	24.5722	24.1439	24.5844	24.1687	24.4100	24.3611	24.6836	25.0620	24.8775	25.2997	24.8679	25.3219	24.8604	25.3484	24.8862	25.1913	**23.57**
C4`	53.2198	54.1039	54.4862	54.6110	55.1174	54.5821	55.3294	54.5555	55.2017	54.6382	55.5561	49.0156	49.7761	50.1007	50.3040	50.8137	50.2760	50.8593	50.2498	50.7864	50.3301	51.2589	**56.17**
H2	8.9313	8.8229	8.8599	8.7433	8.8076	8.7463	8.7017	8.7493	8.8157	8.7408	8.7001	8.9313	8.8229	8.8599	8.7433	8.8077	8.7463	8.7017	8.7493	8.8157	8.7408	8.7001	**8.11**
H3	7.4402	7.5696	7.6580	7.6149	7.7285	7.6129	7.7642	7.6106	7.7418	7.6168	7.7790	7.4402	7.5696	7.6581	7.6149	7.7285	7.6129	7.7642	7.6106	7.7418	7.6168	7.7790	**7.34**
H5	7.2820	7.4697	7.5599	7.5450	7.6750	7.5408	7.6715	7.5363	7.6753	7.5491	7.6920	7.2820	7.4697	7.5599	7.5450	7.6751	7.5408	7.6715	7.5363	7.6753	7.5491	7.6920	**7.34**
H6	8.0832	8.2665	8.3686	8.3687	8.5376	8.3615	8.5314	8.3543	8.5639	8.3756	8.5619	8.0832	8.2665	8.3686	8.3687	8.5376	8.3615	8.5314	8.3543	8.5639	8.3756	8.5619	**8.11**
H8	4.2204	4.3077	4.3640	4.3667	4.4850	4.3614	4.4881	4.3562	4.5000	4.3720	4.4839	4.2204	4.3077	4.3640	4.3667	4.4850	4.3614	4.4881	4.3562	4.5000	4.3720	4.4839	**5.25**
H(9A)	1.6707	1.7235	1.7290	1.7515	1.7703	1.7499	1.6996	1.7481	1.7748	1.7530	1.7325	1.6707	1.7235	1.7290	1.7515	1.7703	1.7499	1.6996	1.7481	1.7748	1.7530	1.7325	**2.17**
H(9B)	0.8655	0.7882	0.7602	0.7526	0.7100	0.7543	0.7229	0.7559	0.7275	0.7511	0.7182	0.8656	0.7882	0.7602	0.7526	0.7100	0.7543	0.7229	0.7559	0.7275	0.7511	0.7182	**0.82**
H(10A-10C)	2.6182	2.6138	2.5935	2.6000	2.5518	2.6006	2.5690	2.6012	2.5711	2.5993	2.5430	2.7535	2.7480	2.7305	2.7294	2.6780	2.7315	2.7066	2.7335	2.6994	2.7273	2.6820	**3.38**
H(1`A-1`B)	3.0114	3.0735	3.0977	3.1110	3.1652	3.1087	3.1512	3.1063	3.1533	3.1133	3.1559	2.7365	2.6106	2.5587	2.5710	2.5307	2.5728	2.5378	2.5746	2.5025	2.5692	2.5338	**3.75**
H(2`-3`A-2`-3`B)	1.5887	1.6486	1.6090	1.6915	1.6376	1.6891	1.6761	1.6865	1.6545	1.6938	1.6974	1.5887	1.6486	1.6090	1.6915	1.6376	1.6891	1.6761	1.6865	1.6545	1.6938	1.6974	**2.125**
H(4`A)	2.7364	2.6106	2.5586	2.5710	2.5308	2.5728	2.5378	2.5746	2.5025	2.5692	2.5338	3.0114	3.0735	3.0977	3.1110	3.1652	3.1087	3.1512	3.1063	3.1533	3.1133	3.1560	**3.07**
H(4`B)	2.7535	2.7480	2.7305	2.7294	2.6780	2.7315	2.7066	2.7335	2.6994	2.7273	2.6820	2.6182	2.6138	2.5935	2.5930	2.6000	2.5518	2.6006	2.5690	2.6012	2.5711	2.5993	2.5430	**3.71**
Nuclei	BLYP											BLYP									
C1	139.2705	140.9067	141.8858	141.8672	143.5912	142.0810	142.8045	141.8380	142.9624	142.2951	143.2638	139.2705	140.9067	141.8857	141.8672	143.5912	142.0810	142.8045	141.8380	142.9624	142.2951	143.2638	**130.87**
C2	137.3978	137.3570	137.9286	137.3759	138.0200	137.6572	138.3109	137.4769	138.3889	137.7363	138.4753	137.3978	137.3570	137.9284	137.3759	138.0200	137.6572	138.3109	137.4769	138.3889	137.7363	138.4753	**132.98**
C3	120.5341	121.3428	121.9216	121.6045	122.2834	121.8725	122.4338	121.6778	122.5466	121.9769	122.5690	120.5341	121.3428	121.9214	121.6045	122.2834	121.8725	122.4338	121.6778	122.5466	121.9769	122.5690	**117.44**
C4	178.0164	178.8916	179.6106	179.2458	180.0972	179.5054	180.4700	179.3025	180.5121	179.6263	180.6847	178.0164	178.8916	179.6107	179.2458	180.0972	179.5054	180.4700	179.3025	180.5121	179.6263	180.6847	**167.85**
C5	118.7984	119.9416	120.5141	120.5343	121.3266	120.7786	121.4220	120.5603	121.5015	120.9288	121.6469	118.7984	119.9416	120.5143	120.5343	121.3266	120.7786	121.4220	120.5603	121.5015	120.9288	121.6468	**117.44**
C6	133.6176	135.1910	136.0890	136.0511	137.5630	136.2700	137.9833	136.0265	137.9414	136.4700	138.4249	133.6176	135.1910	136.0891	136.0511	137.5630	136.2700	137.9833	136.0265	137.9414	136.4700	138.4250	**132.98**
C7	203.7891	208.8903	210.1713	211.6578	212.6539	211.7511	217.0183	211.3869	216.1579	212.2011	218.2860	203.7891	208.8903	210.1715	211.6578	212.6539	211.7511	217.0183	211.3869	216.1580	212.2011	218.2860	**196.75**
C8	70.3429	71.8475	72.1815	72.4218	73.3557	72.6518	73.8558	72.4209	73.8744	72.8315	74.2979	70.3429	71.8475	72.1814	72.4218	73.3557	72.6518	73.8558	72.4209	73.8744	72.8315	74.2979	**70.92**
C9	32.5579	32.2971	32.2284	32.1261	32.2136	32.4111	32.4952	32.2331	32.5914	32.4817	32.5782	32.5579	32.2971	32.2285	32.1261	32.2136	32.4111	32.4952	32.2331	32.5914	32.4817	32.5782	**23.99**
C10	8.8269	9.1055	9.1210	9.1156	9.4613	9.3928	9.2227	9.2069	9.4141	9.4788	9.3614	8.8269	9.1055	9.1210	9.1156	9.4613	9.3928	9.2227	9.2069	9.4141	9.4788	9.3614	**8.05**
C1`	55.2826	56.0393	56.3333	56.5290	57.2448	56.7763	57.0302	56.5616	57.1624	56.9214	57.5107	59.9281	61.0266	61.4308	61.5255	62.1534	61.7761	62.1404	61.5653	62.2487	61.9149	62.5011	**52.76**
C2`	27.6600	28.1718	28.4207	28.3269	28.8476	28.5940	28.7358	28.3994	28.9086	28.7004	28.6497	27.6842	27.7730	28.1627	28.0269	28.5331	28.2244	28.2249	28.0308	28.3996	28.3301	28.1119	**23.74**
C3`	27.6842	27.7730	28.1627	27.9567	28.5331	28.2244	28.2249	28.0308	28.3996	28.3301	28.1119	27.6600	28.1718	28.4207	28.3269	28.8476	28.5940	28.7358	28.3994	28.9086	28.7004	28.6497	**23.57**
C4`	59.9281	61.0266	61.4309	61.5255	62.1534	61.7761	62.1404	61.5653	62.2487	61.9149	62.5012	55.2826	56.0393	56.3333	56.5290	57.2448	56.7763	57.0302	56.5616	57.1624	56.9214	57.5107	**56.17**
H2	8.4741	8.3285	8.3494	8.2453	8.2530	8.2993	8.4500	8.2603	8.2861	8.2939	8.4557	8.4741	8.3285	8.3494	8.2453	8.2530	8.2993	8.4500	8.2603	8.2861	8.2939	8.4557	**8.11**
H3	7.1613	7.2946	7.3861	7.3452	7.4642	7.3903	7.6533	7.3428	7.4778	7.4025	7.6794	7.1613	7.2946	7.3861	7.3452	7.4642	7.3903	7.6533	7.3428	7.4778	7.4025	7.6794	**7.34**
H5	7.0469	7.1908	7.2751	7.2489	7.3699	7.2929	7.5533	7.2442	7.3771	7.3074	7.5843	7.0469	7.1908	7.2751	7.2489	7.3699	7.2929	7.5533	7.2442	7.3771	7.3074	7.5843	**7.34**
H6	7.8308	7.9672	8.0540	8.0515	8.1659	8.0949	8.3731	8.0455	8.1902	8.1104	8.4059	7.8308	7.9672	8.0540	8.0515	8.1659	8.0949	8.3731	8.0455	8.1902	8.1104	8.4059	**8.11**
H8	4.9639	4.9849	5.0165	5.0006	5.0516	5.0476	5.2282	5.0020	5.0512	5.0562	5.2230	4.9639	4.9849	5.0165	5.0006	5.0516	5.0476	5.2282	5.0020	5.0512	5.0562	5.2230	**5.25**
H(9A)	1.8684	1.9088	1.8771	1.2112	1.9154	1.9487	2.0999	1.9033	1.9303	1.9563	2.1392	1.8684	1.9088	1.8771	1.2112	1.9154	1.9487	2.0999	1.9033	1.9303	1.9563	2.1392	**2.17**
H(9B)	0.8610	0.7948	0.7721	0.7727	0.7222	0.8220	0.9088	0.7788	0.7402	0.8261	0.9177	0.8610	0.7948	0.7721	0.7727	0.7222	0.8220	0.9088	0.7788	0.7402	0.8261	0.9177	**0.82**
H(10A-10C)	2.8690	2.8678	2.8432	2.0597	2.8054	2.8984	2.9816	2.8545	2.8170	2.9038	2.9614	2.9724	2.9875	2.9698	2.1891	2.9378	3.0156	3.1082	2.9718	2.9451	3.0208	3.0836	**3.38**
H(1`A-1`B)	3.3514	3.4019	3.4268	2.5707	3.4885	3.4775	3.6408	3.4305	3.4709	3.4890	3.6482	3.0552	2.8926	2.8543	2.1891	3.0004	3.0156	3.1082	2.9718	2.9451	3.0208	3.0836	**3.75**
H(2`-3`A-2`-3`B)	1.7341	1.7919	1.7609	1.1511	1.7908	1.8748	1.9741	1.8273	1.8013	1.8877	2.0134	1.7341	1.7919	1.7609	1.1511	1.7908	1.8748	1.9741	1.8273	1.8013	1.8877	2.0134	**2.125**
H(4`A)	3.0552	2.8926	2.8543	2.0307	2.8600	2.9101	3.0004	2.8654	2.8335	2.9176	3.0053	3.3514	3.4019	3.4269	2.5707	3.4885	3.4775	3.6408	3.4305	3.4709	3.4890	3.6482	**3.07**
H(4`B)	2.9724	2.9875	2.9698	2.1891	2.9378	3.0156	3.1082	2.9718	2.9451	3.0208	3.0837	2.8690	2.8678	2.8432	2.0597	2.8054	2.8984	2.9816	2.8545	2.8170	2.9038	2.9614	**3.71**

[a] methyl protons shifts are averaged [b] according to [13] in D_2O

Table S15. Cont. III

Nuclei	R											S										Exp. [b]
	BMK																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	154.5298	155.4785	156.0406	155.7560	157.0506	155.7359	156.5758	155.9255	156.4939	155.9343	156.8108	154.5298	155.4786	156.0408	155.7560	157.0506	155.7359	156.5759	155.9255	156.4939	155.9343	156.8108	**130.87**
C2	155.3064	155.1890	155.9180	154.9647	155.6797	154.9632	156.0857	155.1726	155.8518	155.1275	156.1317	155.3064	155.1890	155.9179	154.9647	155.6797	154.9632	156.0858	155.1726	155.8518	155.1275	156.1317	**132.98**
C3	135.6633	136.4557	137.1229	136.6285	137.5262	136.6060	137.7354	136.7941	137.5870	136.8111	137.7325	135.6633	136.4556	137.1229	136.6285	137.5262	136.6060	137.7355	136.7941	137.5870	136.8111	137.7325	**117.44**
C4	189.3769	190.1320	190.9258	190.4806	191.4492	190.4433	192.0209	190.6171	191.7825	190.6780	192.0897	189.3769	190.1322	190.9257	190.4806	191.4492	190.4433	192.0209	190.6171	191.7825	190.6780	192.0897	**167.85**
C5	133.4305	134.7898	135.6266	135.4548	136.6015	135.3982	136.7114	135.5530	136.5273	135.6703	136.8089	133.4305	134.7898	135.6265	135.4548	136.6016	135.3982	136.7113	135.5530	136.5273	135.6703	136.8089	**117.44**
C6	151.4259	153.2342	154.7146	154.3487	156.4549	154.2578	156.9482	154.3796	156.6312	154.5973	157.2937	151.4259	153.2342	154.7145	154.3487	156.4549	154.2578	156.9483	154.3796	156.6312	154.5973	157.2937	**132.98**
C7	217.5517	223.2260	224.1611	226.0859	226.0934	225.9089	232.6506	225.9408	231.1493	226.4133	233.9081	217.5517	223.2262	224.1611	226.0859	226.0936	225.9089	232.6509	225.9408	231.1493	226.4133	233.9081	**196.75**
C8	71.7450	73.0889	73.2474	73.7070	74.1747	73.6614	75.3072	73.8259	74.9365	73.9104	75.9803	71.7450	73.0888	73.2475	73.7070	74.1747	73.6614	75.3072	73.8259	74.9365	73.9104	75.9803	**70.92**
C9	30.8307	30.8647	31.0333	30.9265	31.1266	30.9085	31.5970	31.1015	31.3694	31.1054	31.8452	30.8307	30.8648	31.0333	30.9265	31.1266	30.9085	31.5970	31.1015	31.3694	31.1054	31.8452	**23.99**
C10	9.9627	10.2044	10.2846	10.2178	10.6517	10.1966	10.4508	10.3876	10.3754	10.4000	10.5601	9.9627	10.2044	10.2846	10.2178	10.6517	10.1966	10.4507	10.3876	10.3754	10.4000	10.5601	**8.05**
C1`	55.9463	56.5701	56.9145	56.9479	57.6480	56.9075	57.6392	57.0784	57.4768	57.1484	57.9422	60.4793	61.2077	61.6687	61.5870	62.2695	61.5486	62.3987	61.7212	62.2400	61.7848	62.5841	**52.76**
C2`	27.6146	28.0616	28.3231	28.2761	28.6930	28.2492	28.8907	28.4332	28.7458	28.4628	28.8681	27.3316	27.4393	27.8678	27.5248	28.2368	27.5018	28.0684	27.6904	27.9701	27.7086	27.8920	**23.74**
C3`	27.3316	27.4393	27.8678	27.5248	28.2368	27.5018	28.0685	27.6904	27.9701	27.7086	27.8920	27.6146	28.0616	28.3231	28.2761	28.6930	28.2492	28.8905	28.4332	28.7458	28.4628	28.8681	**23.57**
C4`	60.4793	61.2078	61.6686	61.5870	62.2695	61.5486	62.3987	61.7212	62.2400	61.7848	62.5841	55.9463	56.5702	56.9146	56.9479	57.6480	56.9075	57.6392	57.0784	57.4768	57.1484	57.9422	**56.17**
H2	9.0586	9.0208	9.0552	8.9601	9.0144	8.9596	8.9975	8.9594	9.0063	8.9511	8.9835	9.0586	9.0208	9.0552	8.9601	9.0144	8.9596	8.9975	8.9594	9.0063	8.9511	8.9835	**8.11**
H3	7.6460	7.7871	7.8710	7.8390	7.9548	7.8334	7.9785	7.8277	7.9715	7.8347	7.9922	7.6460	7.7871	7.8711	7.8390	7.9548	7.8334	7.9785	7.8277	7.9715	7.8347	7.9922	**7.34**
H5	7.4734	7.6670	7.7595	7.7509	7.8826	7.7429	7.8927	7.7347	7.8861	7.7491	7.9062	7.4734	7.6670	7.7595	7.7509	7.8826	7.7429	7.8927	7.7347	7.8861	7.7491	7.9062	**7.34**
H6	8.3751	8.5662	8.6687	8.6756	8.8423	8.6652	8.8777	8.6548	8.8627	8.6760	8.9081	8.3751	8.5662	8.6686	8.6756	8.8423	8.6652	8.8777	8.6548	8.8627	8.6760	8.9081	**8.11**
H8	4.4066	4.4732	4.5296	4.5397	4.6401	4.5319	4.6811	4.5242	4.6669	4.5375	4.6664	4.4066	4.4732	4.5296	4.5397	4.6401	4.5319	4.6811	4.5242	4.6669	4.5375	4.6664	**5.25**
H(9A)	1.7092	1.7666	1.7516	1.8173	1.8001	1.8110	1.8317	1.8048	1.8235	1.8137	1.8947	1.7092	1.7666	1.7516	1.8173	1.8001	1.8110	1.8317	1.8048	1.8235	1.8137	1.8947	**2.17**
H(9B)	0.8143	0.7380	0.7168	0.7013	0.6649	0.6997	0.6599	0.6983	0.6683	0.6934	0.6536	0.8143	0.7380	0.7169	0.7013	0.6649	0.6997	0.6599	0.6983	0.6683	0.6934	0.6536	**0.82**
H(10A-10C)	2.6405	2.6247	2.6170	2.6163	2.5725	2.6142	2.5733	2.6121	2.5778	2.6087	2.5405	2.7808	2.7922	2.7565	2.7835	2.7250	2.7814	2.7497	2.7793	2.7508	2.7758	2.7302	**3.38**
H(1`A-1`B)	3.0471	3.0744	3.1084	3.1196	3.1610	3.1141	3.1638	3.1085	3.1572	3.1153	3.1742	2.7311	2.6208	2.5487	2.5897	2.5418	2.5886	2.5284	2.5874	2.5261	2.5812	2.5236	**3.75**
H(2`-3`A-2`-3`B)	1.6147	1.6770	1.6284	1.7183	1.6581	1.7125	1.6813	1.7067	1.6771	1.7143	1.7010	1.6147	1.6770	1.6284	1.7183	1.6581	1.7125	1.6813	1.7067	1.6771	1.7143	1.7010	**2.125**
H(4`A)	2.7311	2.6208	2.5487	2.5897	2.5418	2.5886	2.5284	2.5874	2.5261	2.5812	2.5236	3.0471	3.0743	3.1084	3.1196	3.1610	3.1141	3.1638	3.1085	3.1572	3.1153	3.1742	**3.07**
H(4`B)	2.7808	2.7922	2.7565	2.7835	2.7250	2.7814	2.7497	2.7793	2.7508	2.7758	2.7302	2.6405	2.6247	2.6170	2.6163	2.5725	2.6142	2.5733	2.6121	2.5778	2.6087	2.5405	**3.71**
Nuclei	BP86																						
C1	135.9057	137.4725	137.9145	138.0844	140.1573	138.0529	139.5683	138.0159	139.5315	138.1088	139.9956	135.9057	137.4725	137.9145	138.0844	140.1573	138.0529	139.5683	138.0159	139.5315	138.1088	139.9956	**130.87**
C2	136.0467	136.1128	136.6257	135.9936	136.6814	136.0078	137.1335	136.0175	137.0380	135.9751	137.3613	136.0467	136.1128	136.6258	135.9936	136.6814	136.0078	137.1335	136.0175	137.0380	135.9751	137.3613	**132.98**
C3	119.4011	120.3916	120.9160	120.6593	121.3650	120.6536	121.7076	120.6422	121.6277	120.6594	121.9242	119.4011	120.3916	120.9161	120.6593	121.3650	120.6536	121.7076	120.6422	121.6277	120.6594	121.9242	**117.44**
C4	174.5997	175.6012	176.2715	175.9436	176.6396	175.9318	177.2202	175.9147	177.0793	175.9501	177.4972	174.5997	175.6012	176.2715	175.9436	176.6396	175.9318	177.2202	175.9147	177.0793	175.9501	177.4972	**167.85**
C5	117.7092	119.0997	119.6750	119.7239	120.4804	119.6935	120.7775	119.6579	120.6613	119.7479	121.0864	117.7092	119.0997	119.6750	119.7239	120.4804	119.6935	120.7775	119.6579	120.6613	119.7479	121.0864	**117.44**
C6	132.2905	134.1084	135.2366	134.9827	136.1998	134.9384	136.7506	134.8888	136.5351	135.0201	137.2758	132.2905	134.1084	135.2364	134.9827	136.1998	134.9384	136.7506	134.8888	136.5351	135.0201	137.2758	**132.98**
C7	200.9264	205.7818	206.6785	208.1649	209.3460	208.0245	213.6166	207.8787	212.6074	208.2926	214.9040	200.9264	205.7818	206.6787	208.1649	209.3460	208.0245	213.6166	207.8787	212.6074	208.2926	214.9040	**196.75**
C8	68.0356	69.6466	70.1719	70.2389	71.0626	70.2126	71.6967	70.1806	71.4910	70.2583	72.3844	68.0356	69.6466	70.1720	70.2389	71.0626	70.2126	71.6967	70.1806	71.4910	70.2583	72.3844	**70.92**
C9	31.2980	31.3870	31.4867	31.2721	31.1250	31.2925	31.4864	31.3071	31.3766	31.2476	31.7540	31.2980	31.3870	31.4868	31.2721	31.1250	31.2925	31.4864	31.3071	31.3766	31.2476	31.7540	**23.99**
C10	8.4639	8.9095	8.9824	8.9561	9.1001	8.9633	8.9889	8.9649	8.9763	8.9443	9.2948	8.4639	8.9095	8.9825	8.9561	9.1001	8.9633	8.9889	8.9649	8.9763	8.9443	9.2948	**8.05**
C1`	53.7163	54.6257	54.8362	55.0632	55.6004	55.0418	55.5611	55.0150	55.5007	55.0785	56.1752	58.1982	59.3590	59.6658	59.8295	60.3766	59.8051	60.6039	59.7762	60.5339	59.8484	61.0062	**52.76**
C2`	26.1148	26.6908	26.9684	26.8555	27.2134	26.8518	27.2683	26.8435	27.2490	26.8547	27.3089	26.0005	26.2374	26.5081	26.3334	26.8210	26.3340	26.7008	26.3297	26.6987	26.3284	26.6554	**23.74**
C3`	26.0005	26.2374	26.5080	26.3334	26.8210	26.3340	26.7008	26.3297	26.6987	26.3284	26.6554	26.1148	26.6908	26.9684	26.8555	27.2134	26.8518	27.2683	26.8435	27.2490	26.8547	27.3089	**23.57**
C4`	58.1982	59.3590	59.6658	59.8295	60.3766	59.8051	60.6039	59.7762	60.5339	59.8484	61.0062	53.7163	54.6257	54.8362	55.0632	55.6004	55.0418	55.5611	55.0150	55.5007	55.0785	56.1752	**56.17**
H2	8.5445	8.4093	8.4460	8.3429	8.3113	8.3477	8.3452	8.3523	8.3487	8.3381	8.3531	8.5445	8.4093	8.4460	8.3429	8.3113	8.3477	8.3452	8.3523	8.3487	8.3381	8.3531	**8.11**
H3	7.1742	7.3133	7.3915	7.3647	7.4837	7.3627	7.5060	7.3604	7.4965	7.3662	7.5342	7.1742	7.3133	7.3915	7.3647	7.4837	7.3627	7.5060	7.3604	7.4965	7.3662	7.5342	**7.34**
H5	7.0502	7.2124	7.3043	7.2802	7.3879	7.2771	7.4042	7.2737	7.3936	7.2828	7.4362	7.0502	7.2124	7.3043	7.2802	7.3879	7.2771	7.4042	7.2737	7.3936	7.2828	7.4362	**7.34**
H6	7.9187	8.0504	8.1325	8.1375	8.2309	8.1326	8.2708	8.1274	8.2566	8.1419	8.3063	7.9187	8.0504	8.1325	8.1375	8.2309	8.1326	8.2708	8.1274	8.2566	8.1419	8.3063	**8.11**
H8	4.9722	4.9882	5.0094	5.0127	5.0576	5.0115	5.0681	5.0101	5.0590	5.0136	5.0689	4.9722	4.9882	5.0094	5.0127	5.0576	5.0115	5.0681	5.0101	5.0590	5.0136	5.0689	**5.25**
H(9A)	1.9567	2.0043	2.0057	2.0201	1.9770	2.0206	1.9790	2.0207	1.9744	2.0192	2.0358	1.9567	2.0043	2.0057	2.0201	1.9770	2.0206	1.9790	2.0207	1.9744	2.0192	2.0358	**2.17**
H(9B)	0.8366	0.7729	0.7323	0.7463	0.6877	0.7487	0.7050	0.7508	0.7048	0.7437	0.7127	0.8366	0.7729	0.7324	0.7463	0.6877	0.7487	0.7050	0.7508	0.7048	0.7437	0.7127	**0.82**
H(10A-10C)	2.8139	2.8178	2.7896	2.8047	2.7537	2.8066	2.7602	2.8081	2.7621	2.8028	2.7375	2.9194	2.9399	2.9219	2.9269	2.8885	2.9289	2.8924	2.9305	2.8947	2.9245	2.8743	**3.38**
H(1`A-1`B)	3.3736	3.4207	3.4321	3.4471	3.4881	3.4464	3.4643	3.4455	3.4615	3.4473	3.4732	3.1134	2.9475	2.8853	2.8915	2.8747	2.8958	2.8231	2.8998	2.8237	2.8871	2.8211	**3.75**
H(2`-3`A-2`-3`B)	1.7282	1.7873	1.7387	1.8226	1.7771	1.8209	1.7932	1.8190	1.7873	1.8238	1.8336	1.7282	1.7873	1.7387	1.8226	1.7771	1.8209	1.7932	1.8190	1.7873	1.8238	1.8336	**2.125**
H(4`A)	3.1134	2.9475	2.8853	2.8915	2.8747	2.8958	2.8231	2.8998	2.8237	2.8871	2.8211	3.3736	3.4207	3.4321	3.4471	3.4881	3.4464	3.4643	3.4455	3.4615	3.4473	3.4732	**3.07**
H(4`B)	2.9194	2.9399	2.9219	2.9269	2.8885	2.9289	2.8924	2.9305	2.8947	2.9245	2.8743	2.8139	2.8178	2.7896	2.8047	2.7537	2.8066	2.7602	2.8081	2.7621	2.8028	2.7375	**3.71**
Nuclei	CAM-B3LYP																						
C1	140.8178	141.9454	142.6315	142.5083	145.2055	142.4836	144.2823	142.4588	144.2735	142.5338	144.4838	140.8178	141.9454	142.6316	142.5083	145.2054	142.4835	144.2823	142.4588	144.2735	142.5338	144.4838	**130.87**
C2	142.4921	142.4056	142.8948	142.2784	142.8221	142.2900	143.3308	142.3021	143.2470	142.2697	143.3691	142.4921	142.4056	142.8948	142.2784	142.8221	142.2900	143.3308	142.3021	143.2470	142.2697	143.3691	**132.98**
C3	123.7767	124.4837	125.0050	124.6919	125.4486	124.6857	125.6608	124.6798	125.6104	124.6998	125.7179	123.7767	124.4837	125.0050	124.6919	125.4485	124.6858	125.6608	124.6798	125.6104	124.6998	125.7179	**117.44**
C4	177.7523	178.4739	179.0582	178.8040	179.3513	178.7868	179.9721	178.7702	179.8447	178.8226	180.0980	177.7523	178.4739	179.0582	178.8040	179.3513	178.7868	179.9721	178.7702	179.8447	178.8226	180.0980	**167.85**
C5	121.8226	123.1271	123.6669	123.7684	124.5871	123.7332	124.7607	123.6980	124.6689	123.8040	124.9200	121.8226	123.1271	123.6669	123.7684	124.5872	123.7330	124.7607	123.6980	124.6690	123.8040	124.9200	**117.44**
C6	138.4619	140.2889	141.3662	141.2699	142.2841	141.2111	142.8858	141.1526	142.6842	141.3278	143.2602	138.4619	140.2889	141.3662	141.2699	142.2841	141.2111	142.8858	141.1526	142.6842	141.3278	143.2602	**132.98**
C7	205.9601	211.2530	212.2857	214.1285	215.6078	213.9636	220.9578	213.7988	219.6416	214.2865	222.0385	205.9601	211.2530	212.2854	214.1285	215.6078	213.9637	220.9578	213.7988	219.6416	214.2865	222.0385	**196.75**
C8	64.5495	65.8213	66.2530	66.4417	67.3789	66.4169	67.9255	66.3913	67.6901	66.4664	68.3648	64.5495	65.8213	66.2529	66.4417	67.3789	66.4168	67.9255	66.3913	67.6902	66.4664	68.3648	**70.92**
C9	27.4431	27.2809	27.3562	27.1799	27.1272	27.1888	27.2673	27.1976	27.1929	27.1733	27.3228	27.4431	27.2809	27.3562	27.1799	27.1272	27.1888	27.2673	27.1976	27.1929	27.1733	27.3228	**23.99**
C10	8.0312	8.3181	8.4305	8.4258	8.6542	8.4248	8.5416	8.4241	8.5219	8.4287	8.6386	8.0312	8.3181	8.4305	8.4258	8.6543	8.4249	8.5416	8.4241	8.5220	8.4287	8.6386	**8.05**
C1`	50.7753	51.6280	51.9155	52.1364	52.7371	52.1121	52.7156	52.0883	52.6368	52.1618	53.1484	55.0409	56.0426	56.3382	56.5226	57.0816	56.4988	57.2659	56.4754	57.2040	56.5475	57.5005	**52.76**
C2`	24.9152	25.3130	25.6199	25.4842	25.8827	25.4795	25.9323	25.4749	25.9134	25.4908	25.8091	24.5473	24.6826	25.0241	24.7922	25.3474	24.7872	25.2230	24.7832	25.2311	24.7992	25.0590	**23.74**
C3`	24.5473	24.6826	25.0241	24.7922	25.3474	24.7874	25.2230	24.7832	25.2311	24.7992	25.0590	24.9152	25.3130	25.6199	25.4842	25.8827	25.4796	25.9323	25.4749	25.9134	25.4908	25.8091	**23.57**
C4`	55.0409	56.0426	56.3382	56.5226	57.0816	56.4989	57.2659	56.4754	57.2040	56.5475	57.5005	50.7753	51.6280	51.9155	52.1364	52.7371	52.1120	52.7156	52.0883	52.6368	52.1618	53.1484	**56.17**
H2	8.8310	8.6984	8.7389	8.6188	8.5418	8.6231	8.5834	8.6276	8.5944	8.6147	8.5784	8.8310	8.6984	8.7389	8.6188	8.5418	8.6231	8.5834	8.6276	8.5944	8.6147	8.5784	**8.11**
H3	7.4035	7.5336	7.6234	7.5777	7.7035	7.5755	7.7231	7.5735	7.7155	7.5796	7.7368	7.4035	7.5336	7.6234	7.5777	7.7035	7.5755	7.7231	7.5735	7.7155	7.5796	7.7368	**7.34**
H5	7.2558	7.4349	7.5269	7.5089	7.6252	7.5047	7.6407	7.5006	7.6307	7.5128	7.6611	7.2558	7.4349	7.5269	7.5089	7.6252	7.5047	7.6407	7.5006	7.6307	7.5128	7.6611	**7.34**
H6	8.0473	8.2152	8.3133	8.3127	8.4156	8.3063	8.4646	8.3001	8.4529	8.3187	8.4912	8.0473	8.2152	8.3133	8.3127	8.4156	8.3063	8.4646	8.3001	8.4529	8.3187	8.4912	**8.11**
H8	4.4165	4.4851	4.5384	4.5391	4.6212	4.5344	4.6550	4.5299	4.6464	4.5437	4.6509	4.4165	4.4851	4.5384	4.5391	4.6212	4.5344	4.6550	4.5299	4.6464	4.5437	4.6509	**5.25**
H(9A)	1.7554	1.8016	1.8068	1.8253	1.7759	1.8243	1.7771	1.8233	1.7712	1.8261	1.8139	1.7554	1.8016	1.8068	1.8253	1.7759	1.8243	1.7771	1.8233	1.7712	1.8261	1.8139	**2.17**
H(9B)	0.8555	0.7808	0.7558	0.7486	0.6954	0.7504	0.7196	0.7523	0.7217	0.7469	0.7146	0.8555	0.7808	0.7558	0.7486	0.6954	0.7504	0.7196	0.7523	0.7217	0.7469	0.7146	**0.82**
H(10A-10C)	2.7188	2.7154	2.6989	2.7016	2.6557	2.7023	2.6679	2.7030	2.6704	2.7009	2.6395	2.8451	2.8459	2.8312	2.8285	2.7947	2.8302	2.8022	2.8320	2.8037	2.8268	2.7770	**3.38**
H(1`A-1`B)	3.1163	3.1734	3.1988	3.2069	3.2626	3.2046	3.2467	3.2025	3.2431	3.2091	3.2504	2.8345	2.7008	2.6612	2.6641	2.6868	2.6650	2.6282	2.6662	2.6254	2.6631	2.6245	**3.75**
H(2`-3`A-2`-3`B)	1.6565	1.7188	1.6809	1.7586	1.7247	1.7562	1.7439	1.7538	1.7384	1.7610	1.7660	1.6565	1.7188	1.6809	1.7586	1.7247	1.7562	1.7439	1.7538	1.7384	1.7610	1.7660	**2.125**
H(4`A)	2.8345	2.7008	2.6612	2.6641	2.6868	2.6650	2.6282	2.6662	2.6254	2.6631	2.6245	3.1163	3.1734	3.1988	3.2069	3.2626	3.2046	3.2467	3.2025	3.2431	3.2091	3.2504	**3.07**
H(4`B)	2.8451	2.8459	2.8312	2.8285	2.7947	2.8302	2.8022	2.8320	2.8037	2.8268	2.7770	2.7188	2.7154	2.6989	2.7016	2.6557	2.7023	2.6679	2.7030	2.6704	2.7009	2.6395	**3.71**

[a] methyl protons shifts are averaged [b] according to [13] in D_2O

Table S15. Cont. IV

Nuclei	R											S										Exp. [b]
	HF																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.4209	136.9533	137.5981	138.5334	138.5267	138.4887	139.3247	138.4513	139.3910	138.5908	139.5972	136.4209	136.9533	137.5980	138.5334	138.5267	138.4887	139.3248	138.4513	139.3910	138.5909	139.5972	**130.87**
C2	144.4138	144.2278	144.6203	143.8669	144.3858	143.8853	144.7904	143.9028	144.7129	143.8463	144.7848	144.4138	144.2279	144.6200	143.8669	144.3858	143.8852	144.7904	143.9028	144.7129	143.8464	144.7848	**132.98**
C3	120.4960	120.9597	121.3813	121.2317	121.5829	121.2261	121.8485	121.2209	121.8373	121.2385	121.8914	120.4960	120.9597	121.3812	121.2317	121.5828	121.2259	121.8486	121.2209	121.8373	121.2386	121.8914	**117.44**
C4	171.1311	171.6692	172.2139	171.7713	172.5056	171.7582	172.9179	171.7444	172.7713	171.7806	173.0264	171.1311	171.6691	172.2140	171.7713	172.5055	171.7582	172.9179	171.7444	172.7713	171.7806	173.0264	**167.85**
C5	117.8436	119.0394	119.5217	119.8053	120.3440	119.7677	120.5617	119.7314	120.4936	119.8413	120.7260	117.8436	119.0394	119.5217	119.8053	120.3439	119.7678	120.5616	119.7314	120.4936	119.8412	120.7260	**117.44**
C6	139.9153	141.7457	142.9046	142.0537	144.3653	141.9987	144.0470	141.9415	143.8146	142.0972	144.3242	139.9153	141.7457	142.9045	142.0537	144.3653	141.9987	144.0470	141.9415	143.8146	142.0970	144.3242	**132.98**
C7	196.2929	201.5543	202.5554	205.7205	204.2234	205.5100	212.8199	205.3064	211.1460	205.9364	213.9640	196.2929	201.5542	202.5553	205.7205	204.2238	205.5099	212.8199	205.3064	211.1460	205.9362	213.9640	**196.75**
C8	55.6159	56.5268	57.0000	57.3279	57.3819	57.2945	58.6647	57.2631	58.4222	57.3642	58.9869	55.6159	56.5268	57.0001	57.3279	57.3818	57.2944	58.6647	57.2631	58.4222	57.3642	58.9869	**70.92**
C9	23.2421	22.8968	23.0461	22.5863	22.9066	22.5986	22.7730	22.6112	22.7403	22.5726	22.7380	23.2421	22.8969	23.0461	22.5863	22.9066	22.5986	22.7730	22.6112	22.7403	22.5726	22.7380	**23.99**
C10	8.9715	9.1464	9.3172	9.1897	9.5333	9.1871	9.3766	9.1845	9.3716	9.1904	9.4334	8.9715	9.1465	9.3173	9.1897	9.5334	9.1871	9.3765	9.1845	9.3716	9.1904	9.4334	**8.05**
C1`	44.5960	45.2986	45.5475	45.7442	46.2020	45.7185	46.2794	45.6925	46.2140	45.7675	46.6202	48.4651	49.2639	49.5856	49.7434	50.1174	49.7167	50.3465	49.6904	50.2785	49.7691	50.5722	**52.76**
C2`	22.7957	23.0336	23.3702	23.1061	23.5485	23.1020	23.5610	23.0981	23.5568	23.1088	23.4000	22.2330	22.2917	22.6174	22.3624	22.8829	22.3565	22.7390	22.3517	22.7556	22.3683	22.5673	**23.74**
C3`	22.2330	22.2917	22.6175	22.3624	22.8829	22.3565	22.7390	22.3517	22.7556	22.3681	22.5673	22.7957	23.0336	23.3702	23.1061	23.5484	23.1019	23.5609	23.0981	23.5568	23.1088	23.4000	**23.57**
C4`	48.4651	49.2639	49.5855	49.7434	50.1174	49.7167	50.3464	49.6904	50.2785	49.7692	50.5722	44.5960	45.2987	45.5475	45.7442	46.2020	45.7185	46.2793	45.6925	46.2140	45.7675	46.6202	**56.17**
H2	9.0962	8.9993	9.0463	8.7871	8.9824	8.7945	8.8162	8.8009	8.8269	8.7785	8.8030	9.0962	8.9993	9.0463	8.7871	8.9824	8.7945	8.8162	8.8009	8.8269	8.7785	8.8030	**8.11**
H3	7.4378	7.5763	7.6668	7.6214	7.7396	7.6193	7.7566	7.6170	7.7495	7.6234	7.7711	7.4378	7.5763	7.6668	7.6214	7.7396	7.6193	7.7566	7.6170	7.7495	7.6234	7.7711	**7.34**
H5	7.2415	7.4370	7.5282	7.5271	7.6509	7.5221	7.6651	7.5169	7.6542	7.5319	7.6884	7.2415	7.4370	7.5282	7.5271	7.6509	7.5221	7.6651	7.5169	7.6542	7.5319	7.6884	**7.34**
H6	8.0935	8.3199	8.4429	8.4012	8.6258	8.3940	8.6016	8.3865	8.5829	8.4074	8.6317	8.0935	8.3199	8.4429	8.4012	8.6257	8.3940	8.6016	8.3865	8.5829	8.4074	8.6317	**8.11**
H8	3.6381	3.7589	3.8433	3.8362	3.9911	3.8300	4.0000	3.8238	3.9821	3.8420	3.9970	3.6381	3.7589	3.8433	3.8362	3.9911	3.8300	4.0000	3.8238	3.9821	3.8420	3.9970	**5.25**
H(9A)	1.4164	1.4768	1.4906	2.9214	1.5248	1.4296	1.4416	1.4291	1.4356	1.4283	1.4628	1.4164	1.4768	1.4906	2.9214	1.5248	1.4296	1.4416	1.4291	1.4356	1.4283	1.4628	**2.17**
H(9B)	0.8877	0.8064	0.7808	0.7653	0.7219	0.7666	0.7288	0.7680	0.7304	0.7642	0.7245	0.8877	0.8064	0.7808	0.7653	0.7219	0.7666	0.7287	0.7680	0.7304	0.7642	0.7245	**0.82**
H(10A-10C)	2.3794	2.3704	2.3494	3.7060	2.3047	2.3575	2.3319	2.3581	2.3314	2.3565	2.3120	2.5381	2.5264	2.5033	3.8282	2.4406	2.5103	2.4852	2.5124	2.4848	2.5058	2.4628	**3.38**
H(1`A-1`B)	2.7142	2.7865	2.8222	4.3484	2.8937	2.8228	2.8821	2.8200	2.8769	2.8280	2.8881	2.3921	2.2864	2.2444	3.7928	2.2572	2.3064	2.2933	2.3069	2.2874	2.3066	2.2994	**3.75**
H(2`-3`A-2`-3`B)	1.4348	1.4984	1.4573	2.7239	1.4875	1.5556	1.5300	1.5523	1.5238	1.5623	1.5514	1.4348	1.4984	1.4573	2.7239	1.4875	1.5556	1.5300	1.5523	1.5238	1.5623	1.5514	**2.125**
H(4`A)	2.3921	2.2864	2.2444	3.7928	2.2572	2.3064	2.2933	2.3069	2.2874	2.3066	2.2994	2.7142	2.7866	2.8222	4.3484	2.8937	2.8228	2.8821	2.8200	2.8769	2.8280	2.8881	**3.07**
H(4`B)	2.5381	2.5264	2.5033	3.8282	2.4406	2.5103	2.4852	2.5124	2.4848	2.5058	2.4628	2.3794	2.3704	2.3494	3.7060	2.3047	2.3575	2.3319	2.3581	2.3314	2.3565	2.3120	**3.71**
Nuclei	LC-BLYP																						
C1	144.2529	145.2616	146.0982	145.7229	147.4123	145.6776	147.7476	145.6585	146.4741	145.7476	147.8148	144.2528	145.2616	146.0983	145.7229	147.4122	145.6776	147.7475	145.6586	146.4741	145.7477	147.8148	**130.87**
C2	148.6128	148.4513	148.9941	148.3396	148.7816	148.3261	149.2486	148.3398	149.2042	148.3349	149.2538	148.6127	148.4513	148.9940	148.3396	148.7817	148.3262	149.2486	148.3398	149.2041	148.3349	149.2538	**132.98**
C3	128.3160	128.9212	129.5334	129.1284	129.7954	129.0980	130.1137	129.0944	129.9243	129.1394	130.1492	128.3160	128.9212	129.5333	129.1284	129.7952	129.0980	130.1137	129.0943	129.9243	129.1394	130.1492	**117.44**
C4	181.9577	182.4979	183.0862	182.8533	183.3780	182.8102	183.9459	182.7944	183.8966	182.8768	184.0804	181.9578	182.4979	183.0860	182.8533	183.3780	182.8102	183.9459	182.7944	183.8967	182.8768	184.0804	**167.85**
C5	126.1783	127.4899	128.1045	128.2106	129.0230	128.1466	129.2994	128.1094	129.0650	128.2539	129.4517	126.1784	127.4899	128.1045	128.2106	129.0232	128.1465	129.2995	128.1096	129.0650	128.2538	129.4517	**117.44**
C6	144.3194	146.1352	147.3469	147.2631	148.9364	147.1686	148.7988	147.1020	149.3389	147.3369	149.3196	144.3193	146.1352	147.3470	147.2632	148.9364	147.1685	148.7988	147.1021	149.3388	147.3369	149.3196	**132.98**
C7	211.6149	217.1151	218.2887	220.0876	220.5887	219.8852	227.6215	219.7094	224.9662	220.2618	228.6511	211.6152	217.1151	218.2883	220.0876	220.5889	219.8853	227.6215	219.7095	224.9662	220.2618	228.6511	**196.75**
C8	62.4764	63.6690	64.3145	64.2818	65.1579	64.2186	65.8916	64.1836	65.5355	64.3257	66.4138	62.4765	63.6690	64.3146	64.2818	65.1580	64.2185	65.8916	64.1837	65.5356	64.3257	66.4138	**70.92**
C9	24.5842	24.3150	24.4913	24.2609	24.4714	24.2429	24.2742	24.2524	24.5261	24.2610	24.3976	24.5842	24.3150	24.4913	24.2609	24.4715	24.2429	24.2742	24.2524	24.5261	24.2610	24.3976	**23.99**
C10	7.0341	7.2218	7.4167	7.3717	7.6466	7.3397	7.4704	7.3357	7.5247	7.3851	7.5817	7.0341	7.2218	7.4166	7.3717	7.6467	7.3397	7.4704	7.3357	7.5248	7.3850	7.5817	**8.05**
C1`	48.6886	49.4728	49.9278	49.9914	50.6169	49.9322	50.6130	49.9014	50.5396	50.0316	51.0314	52.6020	53.5354	53.9311	54.0311	54.5350	53.9781	54.7405	53.9524	54.5842	54.0644	55.0135	**52.76**
C2`	22.9225	23.2154	23.5687	23.3886	23.8159	23.3548	23.8139	23.3489	23.8279	23.4035	23.7306	22.4210	22.5058	22.8663	22.6367	23.1256	22.6070	23.0621	22.6046	23.0308	22.6476	22.8960	**23.74**
C3`	22.4210	22.5059	22.8663	22.6367	23.1256	22.6071	23.0621	22.6046	23.0308	22.6477	22.8960	22.9225	23.2154	23.5685	23.3886	23.8159	23.3549	23.8139	23.3489	23.8279	23.4036	23.7306	**23.57**
C4`	52.6020	53.5354	53.9311	54.0311	54.5350	53.9780	54.7407	53.9524	54.5842	54.0645	55.0135	48.6886	49.4728	49.9277	49.9914	50.6168	49.9321	50.6129	49.9014	50.5397	50.0316	51.0314	**56.17**
H2	9.0351	8.8989	8.9306	8.8271	8.8216	8.8305	8.7459	8.8356	8.8602	8.8229	8.7488	9.0351	8.8989	8.9306	8.8271	8.8216	8.8305	8.7459	8.8356	8.8602	8.8229	8.7488	**8.11**
H3	7.5461	7.6769	7.7689	7.7183	7.8378	7.7155	7.8569	7.7141	7.8471	7.7200	7.8715	7.5461	7.6769	7.7689	7.7183	7.8377	7.7155	7.8569	7.7141	7.8472	7.7200	7.8715	**7.34**
H5	7.3885	7.5715	7.6624	7.6549	7.7793	7.6492	7.7928	7.6451	7.7821	7.6593	7.8161	7.3885	7.5715	7.6624	7.6549	7.7793	7.6492	7.7928	7.6451	7.7821	7.6593	7.8161	**7.34**
H6	8.1991	8.3809	8.4793	8.4872	8.6326	8.4797	8.6350	8.4737	8.6703	8.4935	8.6719	8.1991	8.3809	8.4793	8.4873	8.6326	8.4797	8.6350	8.4737	8.6703	8.4935	8.6719	**8.11**
H8	4.2134	4.3032	4.3439	4.3729	4.4571	4.3680	4.5214	4.3646	4.4972	4.3765	4.5227	4.2135	4.3032	4.3439	4.3729	4.4571	4.3680	4.5214	4.3646	4.4973	4.3765	4.5227	**5.25**
H(9A)	1.7325	1.7736	1.7834	1.8010	1.8262	1.7981	1.7376	1.7969	1.8199	1.8029	1.7888	1.7325	1.7736	1.7833	1.8010	1.8262	1.7981	1.7376	1.7969	1.8199	1.8029	1.7888	**2.17**
H(9B)	0.8490	0.7679	0.7386	0.7333	0.6712	0.7346	0.6926	0.7374	0.6955	0.7311	0.6867	0.8490	0.7679	0.7386	0.7333	0.6712	0.7346	0.6926	0.7374	0.6955	0.7311	0.6867	**0.82**
H(10A-10C)	2.6786	2.6714	2.6497	2.6587	2.6054	2.6591	2.6186	2.6610	2.6215	2.6572	2.5979	2.8097	2.8055	2.7888	2.7890	2.7525	2.7893	2.7672	2.7912	2.7643	2.7877	2.7466	**3.38**
H(1`A-1`B)	3.0093	3.0606	3.0863	3.0971	3.1566	3.0940	3.1380	3.0925	3.1426	3.0990	3.1445	2.7478	2.6081	2.5674	2.5732	2.5692	2.5745	2.5435	2.5774	2.5178	2.5709	2.5419	**3.75**
H(2`-3`A-2`-3`B)	1.6422	1.7028	1.6677	1.7438	1.6972	1.7402	1.7318	1.7382	1.7119	1.7462	1.7541	1.6422	1.7028	1.6677	1.7438	1.6972	1.7402	1.7318	1.7382	1.7119	1.7462	1.7541	**2.125**
H(4`A)	2.7478	2.6081	2.5674	2.5732	2.5693	2.5745	2.5435	2.5774	2.5178	2.5710	2.5419	3.0093	3.0606	3.0863	3.0971	3.1566	3.0940	3.1380	3.0925	3.1426	3.0990	3.1445	**3.07**
H(4`B)	2.8097	2.8055	2.7888	2.7890	2.7525	2.7893	2.7672	2.7912	2.7643	2.7877	2.7466	2.6786	2.6714	2.6497	2.6587	2.6054	2.6591	2.6186	2.6610	2.6215	2.6572	2.5979	**3.71**
Nuclei	M06																						
C1	136.2474	138.9328	140.1010	139.6813	141.8521	139.6218	140.5292	139.5718	140.7955	139.7541	140.8278	136.2474	138.9328	140.1009	139.6813	141.8522	139.6218	140.5292	139.5718	140.7955	139.7541	140.8278	**130.87**
C2	140.6132	140.1823	140.8258	140.1337	140.9103	140.1285	141.4100	140.1311	141.3103	140.1528	141.4049	140.6132	140.1823	140.8257	140.1336	140.9103	140.1285	141.4100	140.1311	141.3103	140.1528	141.4049	**132.98**
C3	121.5497	122.2466	122.9578	122.6056	123.5211	122.5748	123.6938	122.5516	123.6583	122.6495	123.8082	121.5497	122.2465	122.9578	122.6055	123.5212	122.5748	123.6938	122.5516	123.6583	122.6495	123.8082	**117.44**
C4	173.1448	173.6854	174.3788	174.0258	174.7546	173.9962	175.3869	173.9739	175.2162	174.0681	175.4981	173.1448	173.6853	174.3787	174.0259	174.7546	173.9962	175.3869	173.9739	175.2162	174.0682	175.4981	**167.85**
C5	119.8007	121.0074	121.6741	121.6898	122.5000	121.6376	122.7958	121.5930	122.6983	121.7542	122.9440	119.8007	121.0074	121.6739	121.6898	122.5000	121.6376	122.7958	121.5930	122.6983	121.7542	122.9440	**117.44**
C6	136.9225	138.0189	139.0688	138.7931	140.2370	138.7372	140.9027	138.6883	140.5797	138.8602	141.1852	136.9225	138.0189	139.0689	138.7933	140.2370	138.7372	140.9027	138.6883	140.5797	138.8600	141.1852	**132.98**
C7	202.9552	209.1736	210.6281	212.0370	212.9049	211.8430	217.5565	211.6588	216.5766	212.2388	218.7371	202.9552	209.1736	210.6280	212.0372	212.9048	211.8430	217.5565	211.6587	216.5766	212.2387	218.7371	**196.75**
C8	61.9334	63.9388	64.6742	64.6524	65.4872	64.5999	66.0984	64.5553	66.0271	64.7174	66.6463	61.9334	63.9388	64.6742	64.6524	65.4872	64.5999	66.0984	64.5553	66.0271	64.7174	66.6463	**70.92**
C9	25.7408	25.5771	25.7624	25.5069	25.7001	25.4997	25.9642	25.5006	25.8731	25.5283	26.0895	25.7408	25.5771	25.7624	25.5068	25.7000	25.4997	25.9642	25.5006	25.8731	25.5284	26.0895	**23.99**
C10	7.4812	8.1797	8.4921	8.4177	8.8321	8.3937	8.6899	8.3772	8.6937	8.4549	8.7511	7.4812	8.1797	8.4921	8.4177	8.8321	8.3936	8.6899	8.3772	8.6937	8.4549	8.7511	**8.05**
C1`	50.6217	51.3679	51.8756	51.9190	52.6685	51.8742	52.6179	51.8375	52.5886	51.9761	53.0993	54.9181	55.8619	56.2882	56.3888	57.0027	56.3493	57.2248	56.3171	57.1428	56.4404	57.6240	**52.76**
C2`	23.2425	23.7211	24.1482	23.9764	24.5914	23.9544	24.5998	23.9396	24.5811	24.0116	24.4541	21.8611	22.2788	22.7497	22.4626	23.1754	22.4437	22.9608	22.4324	22.9811	22.4950	22.6644	**23.74**
C3`	21.8611	22.2788	22.7497	22.4626	23.1754	22.4437	22.9608	22.4324	22.9811	22.4951	22.6644	23.2425	23.7211	24.1483	23.9765	24.5914	23.9544	24.5998	23.9396	24.5811	24.0116	24.4541	**23.57**
C4`	54.9181	55.8619	56.2882	56.3888	57.0027	56.3493	57.2248	56.3171	57.1428	56.4404	57.6240	50.6217	51.3679	51.8756	51.9189	52.6686	51.8742	52.6179	51.8375	52.5886	51.9761	53.0993	**56.17**
H2	8.7957	8.5103	8.5265	8.4158	8.4008	8.4211	8.4730	8.4270	8.4607	8.4112	8.4607	8.7957	8.5103	8.5265	8.4158	8.4008	8.4211	8.4730	8.4270	8.4607	8.4112	8.4607	**8.11**
H3	7.3187	7.4837	7.5786	7.4962	7.6094	7.4959	7.6333	7.4960	7.6220	7.4971	7.6379	7.3187	7.4837	7.5786	7.4962	7.6094	7.4959	7.6333	7.4960	7.6220	7.4971	7.6379	**7.34**
H5	7.1328	7.2675	7.3592	7.3456	7.4772	7.3405	7.4940	7.3361	7.4824	7.3511	7.5168	7.1328	7.2675	7.3592	7.3456	7.4773	7.3405	7.4940	7.3361	7.4824	7.3511	7.5168	**7.34**
H6	8.0836	8.1469	8.2265	8.2281	8.3434	8.2231	8.4147	8.2186	8.3857	8.2334	8.4451	8.0836	8.1469	8.2265	8.2281	8.3434	8.2231	8.4147	8.2186	8.3857	8.2334	8.4451	**8.11**
H8	4.4578	4.4522	4.4787	4.4904	4.5389	4.4874	4.6080	4.4849	4.5848	4.4939	4.6240	4.4578	4.4522	4.4787	4.4905	4.5389	4.4874	4.6080	4.4849	4.5848	4.4940	4.6240	**5.25**
H(9A)	1.8516	1.7772	1.7765	1.7802	1.7706	1.7798	1.7938	1.7800	1.7816	1.7809	1.8093	1.8516	1.7772	1.7765	1.7801	1.7706	1.7798	1.7938	1.7800	1.7816	1.7810	1.8093	**2.17**
H(9B)	0.7943	0.7406	0.7102	0.7112	0.6556	0.7125	0.6747	0.7144	0.6748	0.7106	0.6592	0.7943	0.7406	0.7102	0.7112	0.6556	0.7125	0.6747	0.7144	0.6748	0.7106	0.6592	**0.82**
H(10A-10C)	2.6763	2.6432	2.6269	2.6238	2.5905	2.6250	2.6085	2.6268	2.6089	2.6232	2.5939	2.8468	2.8806	2.8651	2.8578	2.8136	2.8597	2.8360	2.8622	2.8412	2.8566	2.8013	**3.38**
H(1`A-1`B)	3.1090	3.1408	3.1707	3.1589	3.2246	3.1573	3.2175	3.1564	3.2135	3.1609	3.2236	2.7505	2.6531	2.6424	2.6224	2.6199	2.6228	2.6014	2.6240	2.6036	2.6228	2.5904	**3.75**
H(2`-3`A-2`-3`B)	1.6369	1.6985	1.6704	1.7309	1.6906	1.7285	1.7115	1.7266	1.7063	1.7339	1.7403	1.6369	1.6985	1.6704	1.7309	1.6905	1.7285	1.7115	1.7266	1.7063	1.7339	1.7403	**2.125**
H(4`A)	2.7505	2.6531	2.6424	2.6224	2.6199	2.6228	2.6014	2.6240	2.6036	2.6228	2.5904	3.1090	3.1408	3.1707	3.1588	3.2246	3.1573	3.2175	3.1564	3.2135	3.1609	3.2236	**3.07**
H(4`B)	2.8468	2.8806	2.8651	2.8578	2.8136	2.8597	2.8360	2.8622	2.8412	2.8566	2.8013	2.6763	2.6432	2.6269	2.6238	2.5905	2.6250	2.6085	2.6268	2.6089	2.6232	2.5939	**3.71**

[a] methyl protons shifts are averaged [b] according to [13] in D_2O

Table S15. Cont. V

Nuclei	R											S										Exp. [b]
	M06-2X											M06-2X										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	153.4338	154.4776	155.4189	154.8456	156.7849	154.8402	155.9729	154.8395	156.0038	154.8497	156.4893	153.4338	154.4776	155.4188	154.8456	156.7849	154.8402	155.9729	154.8395	156.0038	154.8497	156.4893	**130.87**
C2	155.2354	155.1784	155.7857	154.9519	155.5441	154.9895	155.9529	155.0277	155.8831	154.9086	155.9856	155.2354	155.1784	155.7857	154.9519	155.5441	154.9895	155.9529	155.0277	155.8831	154.9086	155.9856	**132.98**
C3	135.9486	136.8717	137.5122	137.1015	137.8641	137.1138	138.1032	137.1266	138.0470	137.0827	138.1772	135.9486	136.8717	137.5122	137.1015	137.8641	137.1138	138.1032	137.1266	138.0470	137.0827	138.1772	**117.44**
C4	186.7773	187.6456	188.2688	188.0569	188.7218	188.0543	189.3788	188.0529	189.2186	188.0524	189.5197	186.7773	187.6456	188.2688	188.0569	188.7218	188.0543	189.3788	188.0529	189.2186	188.0524	189.5197	**167.85**
C5	133.5954	135.0732	135.7386	135.8249	136.7706	135.7998	137.0170	135.7763	136.8845	135.8427	137.2270	133.5954	135.0732	135.7387	135.8249	136.7706	135.7998	137.0170	135.7763	136.8845	135.8427	137.2270	**117.44**
C6	151.2913	153.1749	154.4175	154.3788	156.1950	154.3215	156.7900	154.2649	156.5315	154.4258	157.1595	151.2913	153.1749	154.4175	154.3788	156.1950	154.3215	156.7900	154.2649	156.5315	154.4258	157.1595	**132.98**
C7	219.3619	224.9761	226.3223	227.9666	228.7428	227.7924	235.0017	227.6242	233.5317	228.1326	236.5080	219.3619	224.9761	226.3221	227.9666	228.7428	227.7924	235.0017	227.6242	233.5317	228.1326	236.5080	**196.75**
C8	67.2917	68.6496	69.4210	69.4181	70.4628	69.3861	71.1756	69.3556	70.9467	69.4434	71.8519	67.2917	68.6496	69.4211	69.4181	70.4628	69.3861	71.1756	69.3556	70.9467	69.4434	71.8519	**70.92**
C9	27.0091	27.0132	27.1644	26.9605	27.1410	26.9841	27.3958	27.0089	27.3306	26.9316	27.4365	27.0091	27.0132	27.1644	26.9605	27.1410	26.9841	27.3958	27.0089	27.3306	26.9316	27.4365	**23.99**
C10	7.5905	7.7559	7.8733	7.8899	8.1701	7.9007	8.0492	7.9125	8.0409	7.8727	8.1540	7.5905	7.7559	7.8733	7.8899	8.1701	7.9007	8.0492	7.9125	8.0409	7.8727	8.1540	**8.05**
C1`	52.7406	53.4619	53.8570	53.9723	54.5793	53.9591	54.5182	53.9463	54.4620	53.9777	54.8934	56.9951	57.8749	58.2466	58.3400	58.8654	58.3329	59.0246	58.3262	58.9266	58.3397	59.3241	**52.76**
C2`	24.5835	25.0035	25.3300	25.2318	25.6535	25.2384	25.7102	25.2457	25.6632	25.2191	25.6816	23.6110	23.8905	24.2292	24.0746	24.5966	24.0835	24.5159	24.0934	24.4995	24.0601	24.4839	**23.74**
C3`	23.6110	23.8905	24.2292	24.0746	24.5966	24.0835	24.5159	24.0934	24.4995	24.0601	24.4839	24.5835	25.0035	25.3299	25.2318	25.6535	25.2384	25.7102	25.2457	25.6632	25.2191	25.6816	**23.57**
C4`	56.9951	57.8749	58.2466	58.3400	58.8654	58.3329	59.0246	58.3262	58.9266	58.3397	59.3241	52.7406	53.4619	53.8570	53.9723	54.5793	53.9591	54.5182	53.9463	54.4620	53.9777	54.8934	**56.17**
H2	9.3040	9.2165	9.2445	9.1584	9.1396	9.1618	9.1608	9.1643	9.1716	9.1548	9.1314	9.3040	9.2165	9.2444	9.1584	9.1396	9.1618	9.1608	9.1643	9.1716	9.1548	9.1314	**8.11**
H3	7.8325	7.9654	8.0554	8.0245	8.1536	8.0198	8.1888	8.0148	8.1736	8.0294	8.2130	7.8325	7.9654	8.0554	8.0245	8.1536	8.0198	8.1888	8.0148	8.1736	8.0294	8.2130	**7.34**
H5	7.6919	7.8830	7.9791	7.9580	8.0778	7.9527	8.0845	7.9469	8.0770	7.9629	8.0959	7.6919	7.8830	7.9791	7.9580	8.0778	7.9527	8.0845	7.9469	8.0770	7.9629	8.0959	**7.34**
H6	8.5942	8.7612	8.8614	8.8561	8.9888	8.8492	9.0351	8.8418	9.0183	8.8626	9.0459	8.5942	8.7612	8.8615	8.8561	8.9888	8.8492	9.0351	8.8418	9.0183	8.8626	9.0459	**8.11**
H8	4.3087	4.3831	4.4222	4.4278	4.5074	4.4234	4.5592	4.4190	4.5438	4.4323	4.5575	4.3087	4.3831	4.4222	4.4278	4.5074	4.4234	4.5592	4.4190	4.5438	4.4323	4.5575	**5.25**
H(9A)	1.7714	1.7957	1.7997	1.8302	1.8389	1.8267	1.8329	1.8227	1.8341	1.8335	1.8637	1.7714	1.7957	1.7997	1.8302	1.8389	1.8267	1.8329	1.8227	1.8341	1.8335	1.8637	**2.17**
H(9B)	0.8203	0.7411	0.7083	0.6976	0.6295	0.6993	0.6429	0.7005	0.6491	0.6960	0.6377	0.8203	0.7411	0.7083	0.6976	0.6295	0.6993	0.6429	0.7005	0.6491	0.6960	0.6377	**0.82**
H(10A-10C)	2.6207	2.6156	2.5998	2.6023	2.5551	2.6021	2.5693	2.6015	2.5723	2.6025	2.5387	2.7753	2.7886	2.7859	2.7810	2.7511	2.7805	2.7687	2.7797	2.7687	2.7816	2.7401	**3.38**
H(1`A-1`B)	3.0903	3.1386	3.1644	3.1671	3.2222	3.1639	3.2064	3.1605	3.2061	3.1702	3.2021	2.7505	2.6290	2.5941	2.5829	2.5883	2.5830	2.5485	2.5833	2.5544	2.5833	2.5511	**3.75**
H(2`-3`A-2`-3`B)	1.6548	1.7084	1.6778	1.7476	1.7056	1.7436	1.7261	1.7394	1.7201	1.7516	1.7455	1.6548	1.7084	1.6778	1.7476	1.7056	1.7436	1.7261	1.7394	1.7201	1.7516	1.7455	**2.125**
H(4`A)	2.7505	2.6290	2.5941	2.5829	2.5883	2.5830	2.5485	2.5833	2.5544	2.5833	2.5511	3.0903	3.1386	3.1644	3.1671	3.2222	3.1639	3.2064	3.1605	3.2061	3.1702	3.2021	**3.07**
H(4`B)	2.7753	2.7886	2.7859	2.7810	2.7511	2.7805	2.7687	2.7797	2.7687	2.7816	2.7401	2.6207	2.6156	2.5998	2.6023	2.5551	2.6021	2.5693	2.6015	2.5723	2.6025	2.5387	**3.71**
Nuclei	**mpW1LYP**											**mpW1LYP**										
C1	139.7041	140.8993	141.2108	141.5353	143.7262	141.4950	143.0385	141.4551	143.0330	141.5703	143.2657	139.7041	140.8993	141.2108	141.5353	143.7262	141.4950	143.0388	141.4551	143.0330	141.5703	143.2657	**130.87**
C2	140.0691	139.8993	140.4439	139.8111	140.4109	139.8120	140.8782	139.8148	140.7887	139.8087	140.9050	140.0691	139.8993	140.4439	139.8111	140.4109	139.8119	140.8783	139.8150	140.7887	139.8087	140.9050	**132.98**
C3	121.8424	122.5770	123.0704	122.8466	123.4962	122.8298	123.7509	122.8143	123.7008	122.8601	123.7744	121.8424	122.5770	123.0704	122.8466	123.4962	122.8297	123.7509	122.8143	123.7008	122.8601	123.7744	**117.44**
C4	176.3048	177.0933	177.7491	177.4908	178.0943	177.4639	178.6610	177.4388	178.5349	177.5147	178.7537	176.3048	177.0933	177.7491	177.4908	178.0942	177.4640	178.6608	177.4388	178.5349	177.5147	178.7537	**167.85**
C5	119.9586	121.1812	121.7786	121.8382	122.5591	121.7948	122.7613	121.7532	122.6739	121.8775	122.8772	119.9586	121.1812	121.7786	121.8382	122.5590	121.7949	122.7613	121.7531	122.6739	121.8775	122.8772	**117.44**
C6	136.1411	137.8787	139.1770	138.8651	139.9640	138.8019	140.5812	138.7403	140.3736	138.9237	140.9067	136.1411	137.8787	139.1770	138.8651	139.9640	138.8020	140.5812	138.7404	140.3736	138.9237	140.9067	**132.98**
C7	203.2829	208.4843	209.2304	211.2866	212.2901	211.1153	217.6197	210.9439	216.3877	211.4459	218.6923	203.2829	208.4843	209.2304	211.2866	212.2901	211.1151	217.6200	210.9438	216.3877	211.4459	218.6923	**196.75**
C8	65.7471	67.0551	67.4443	67.6638	68.2910	67.6320	69.0594	67.5999	68.8541	67.6896	69.4214	65.7471	67.0551	67.4443	67.6638	68.2910	67.6321	69.0595	67.6000	68.8541	67.6896	69.4214	**70.92**
C9	29.2473	29.0780	29.2237	29.0100	28.8016	29.0174	29.1462	29.0253	29.0725	29.0002	29.1472	29.2473	29.0780	29.2237	29.0100	28.8016	29.0174	29.1463	29.0253	29.0725	29.0002	29.1472	**23.99**
C10	8.4703	8.7523	8.9179	8.8807	9.0432	8.8722	8.9862	8.8646	8.9862	8.8867	9.0419	8.4703	8.7523	8.9179	8.8807	9.0430	8.8721	8.9862	8.8646	8.9862	8.8867	9.0419	**8.05**
C1`	51.9302	52.7387	53.0511	53.2781	53.8438	53.2390	53.8361	53.2015	53.7816	53.3129	54.2245	56.4209	57.3952	57.7708	57.9189	58.5078	57.8812	58.6398	57.8456	58.5843	57.9535	58.8511	**52.76**
C2`	25.8290	26.2729	26.6313	26.4927	26.8887	26.4760	26.9615	26.4612	26.9546	26.5072	26.7956	25.6217	25.7331	26.1156	25.9026	26.4736	25.8869	26.3167	25.8733	26.3277	25.9161	26.1081	**23.74**
C3`	25.6217	25.7331	26.1156	25.9026	26.4737	25.8868	26.3167	25.8732	26.3277	25.9161	26.1081	25.8290	26.2729	26.6313	26.4927	26.8887	26.4760	26.9616	26.4611	26.9547	26.5072	26.7956	**23.57**
C4`	56.4209	57.3952	57.7708	57.9189	58.5077	57.8813	58.6397	57.8455	58.5843	57.9535	58.8511	51.9302	52.7387	53.0511	53.2781	53.8438	53.2391	53.8361	53.2015	53.7816	53.3129	54.2245	**56.17**
H2	8.7344	8.5973	8.6733	8.5256	8.5022	8.5297	8.5194	8.5337	8.5275	8.5218	8.5109	8.7344	8.5973	8.6733	8.5256	8.5022	8.5297	8.5194	8.5338	8.5275	8.5218	8.5109	**8.11**
H3	7.3318	7.4578	7.5481	7.5074	7.6321	7.5049	7.6524	7.5021	7.6445	7.5096	7.6648	7.3318	7.4578	7.5481	7.5074	7.6321	7.5049	7.6524	7.5021	7.6445	7.5096	7.6648	**7.34**
H5	7.1905	7.3618	7.4649	7.4327	7.5457	7.4289	7.5602	7.4247	7.5514	7.4363	7.5765	7.1905	7.3618	7.4649	7.4327	7.5457	7.4289	7.5602	7.4247	7.5514	7.4363	7.5765	**7.34**
H6	7.9770	8.1294	8.2484	8.2310	8.3508	8.2243	8.3865	8.2175	8.3729	8.2374	8.4082	7.9770	8.1294	8.2484	8.2310	8.3507	8.2243	8.3865	8.2175	8.3729	8.2374	8.4082	**8.11**
H8	4.5598	4.6136	4.6703	4.6608	4.7414	4.6574	4.7501	4.6539	4.7408	4.6642	4.7332	4.5598	4.6136	4.6703	4.6608	4.7414	4.6574	4.7501	4.6539	4.7408	4.6642	4.7332	**5.25**
H(9A)	1.7728	1.8190	1.8420	1.8420	1.7938	1.8416	1.8130	1.8408	1.8093	1.8422	1.8436	1.7728	1.8190	1.8420	1.8420	1.7938	1.8416	1.8130	1.8408	1.8093	1.8422	1.8436	**2.17**
H(9B)	0.8626	0.7866	0.7675	0.7618	0.7184	0.7632	0.7337	0.7644	0.7351	0.7605	0.7257	0.8626	0.7866	0.7675	0.7618	0.7184	0.7632	0.7337	0.7644	0.7351	0.7605	0.7257	**0.82**
H(10A-10C)	2.7445	2.7426	2.7225	2.7308	2.6830	2.7320	2.6954	2.7330	2.6979	2.7295	2.6626	2.8642	2.8697	2.8524	2.8524	2.8134	2.8542	2.8242	2.8557	2.8503	2.7921	**3.38**
H(1`A-1`B)	3.1823	3.2397	3.2688	3.2777	3.3264	3.2758	3.3124	3.2736	3.3099	3.2793	3.3116	2.8871	2.7565	2.6972	2.7224	2.7085	2.7251	2.6814	2.7273	2.6796	2.7197	2.6738	**3.75**
H(2`-3`A-2`-3`B)	1.6666	1.7269	1.6867	1.7691	1.7319	1.7665	1.7481	1.7636	1.7430	1.7717	1.7684	1.6666	1.7269	1.6867	1.7691	1.7319	1.7665	1.7481	1.7636	1.7430	1.7717	1.7684	**2.125**
H(4`A)	2.8871	2.7565	2.6972	2.7224	2.7085	2.7251	2.6814	2.7273	2.6796	2.7197	2.6738	3.1823	3.2397	3.2688	3.2777	3.3264	3.2758	3.3124	3.2736	3.3099	3.2793	3.3116	**3.07**
H(4`B)	2.8642	2.8697	2.8524	2.8524	2.8134	2.8543	2.8242	2.8557	2.8269	2.8503	2.7921	2.7445	2.7426	2.7225	2.7308	2.6830	2.7320	2.6954	2.7330	2.6979	2.7295	2.6626	**3.71**
Nuclei	**mpW1PW91**											**mpW1PW91**										
C1	136.8100	137.9806	138.5386	138.5438	140.9037	138.5098	140.1336	138.4813	140.0843	138.5757	140.2635	136.8100	137.9806	138.5386	138.5438	140.9037	138.5098	140.1336	138.4813	140.0843	138.5757	140.2635	**130.87**
C2	139.0412	138.9314	139.5013	138.8207	139.4662	138.8270	139.9627	138.8392	139.8767	138.8140	139.9945	139.0412	138.9314	139.5013	138.8207	139.4662	138.8270	139.9627	138.8391	139.8767	138.8140	139.9946	**132.98**
C3	121.0157	121.8289	122.4065	122.0923	122.8849	122.0784	123.1551	122.0701	123.0903	122.1046	123.2168	121.0157	121.8289	122.4065	122.0923	122.8849	122.0784	123.1551	122.0701	123.0903	122.1046	123.2169	**117.44**
C4	173.3165	174.0978	174.7379	174.4372	175.0434	174.4164	175.6734	174.4013	175.5442	174.4564	175.8021	173.3165	174.0978	174.7379	174.4372	175.0434	174.4164	175.6734	174.4012	175.5442	174.4564	175.8020	**167.85**
C5	119.1703	120.4881	121.0927	121.1562	122.0098	121.1151	122.2414	121.0794	122.1406	121.1950	122.4078	119.1703	120.4881	121.0927	121.1562	122.0098	121.1151	122.2414	121.0795	122.1406	121.1950	122.4079	**117.44**
C6	135.0224	136.7980	137.9290	137.7268	138.8869	137.6698	139.4471	137.6183	139.2538	137.7801	139.8656	135.0224	136.7980	137.9290	137.7268	138.8869	137.6698	139.4471	137.6185	139.2538	137.7801	139.8657	**132.98**
C7	201.1226	206.0842	206.9648	208.7019	209.9730	208.5440	214.8896	208.3916	213.6284	208.8510	215.8666	201.1226	206.0842	206.9648	208.7019	209.9730	208.5440	214.8896	208.3915	213.6284	208.8510	215.8667	**196.75**
C8	63.6287	64.9779	65.4057	65.6030	66.5315	65.5705	67.0852	65.5429	66.8285	65.6322	67.5597	63.6287	64.9779	65.4057	65.6030	66.5315	65.5705	67.0852	65.5430	66.8285	65.6322	67.5597	**70.92**
C9	27.6971	27.6691	27.7767	27.6025	27.6219	27.6075	27.7916	27.6178	27.6991	27.5963	27.9184	27.6971	27.6691	27.7767	27.6025	27.6219	27.6075	27.7916	27.6177	27.6991	27.5963	27.9185	**23.99**
C10	8.2405	8.5463	8.6759	8.6535	8.9031	8.6486	8.7742	8.6490	8.7514	8.6574	8.9264	8.2405	8.5463	8.6759	8.6535	8.9031	8.6486	8.7742	8.6490	8.7514	8.6574	8.9264	**8.05**
C1`	50.4972	51.3180	51.6265	51.7888	52.3857	51.7612	52.3501	51.7396	52.2737	51.8147	52.7888	54.7343	55.7091	56.0448	56.1822	56.7373	56.1530	56.9493	56.1299	56.8896	56.2095	57.1798	**52.76**
C2`	24.5962	25.0060	25.3329	25.1856	25.5885	25.1752	25.6275	25.1705	25.6066	25.1947	25.5080	24.2688	24.4021	24.7516	24.5219	25.0670	24.5125	24.9468	24.5090	24.9547	24.5304	24.7611	**23.74**
C3`	24.2688	24.4021	24.7516	24.5219	25.0670	24.5125	24.9468	24.5090	24.9547	24.5304	24.7612	24.5962	25.0060	25.3329	25.1856	25.5885	25.1752	25.6275	25.1706	25.6066	25.1947	25.5080	**23.57**
C4`	54.7343	55.7091	56.0448	56.1822	56.7373	56.1530	56.9493	56.1299	56.8896	56.2095	57.1798	50.4972	51.3180	51.6265	51.7888	52.3857	51.7612	52.3501	51.7397	52.2737	51.8147	52.7888	**56.17**
H2	8.7931	8.6573	8.7109	8.5819	8.5316	8.5865	8.5778	8.5912	8.5894	8.5779	8.5762	8.7931	8.6573	8.7109	8.5819	8.5316	8.5865	8.5778	8.5912	8.5894	8.5779	8.5762	**8.11**
H3	7.3629	7.4973	7.5887	7.5438	7.6728	7.5416	7.6967	7.5394	7.6880	7.5461	7.7111	7.3629	7.4973	7.5887	7.5438	7.6728	7.5416	7.6967	7.5394	7.6880	7.5461	7.7111	**7.34**
H5	7.2138	7.3898	7.4873	7.4630	7.5830	7.4590	7.5997	7.4551	7.5898	7.4670	7.6200	7.2138	7.3898	7.4873	7.4630	7.5830	7.4590	7.5997	7.4551	7.5898	7.4670	7.6201	**7.34**
H6	8.0642	8.2199	8.3172	8.3125	8.4157	8.3067	8.4609	8.3012	8.4505	8.3182	8.4917	8.0642	8.2199	8.3172	8.3125	8.4157	8.3067	8.4609	8.3012	8.4505	8.3182	8.4917	**8.11**
H8	4.5552	4.6075	4.6487	4.6530	4.7204	4.6494	4.7473	4.6460	4.7406	4.6568	4.7450	4.5552	4.6075	4.6487	4.6530	4.7204	4.6494	4.7473	4.6460	4.7406	4.6568	4.7450	**5.25**
H(9A)	1.7927	1.8400	1.8459	1.8587	1.8203	1.8585	1.8140	1.8582	1.8095	1.8591	1.8606	1.7927	1.8400	1.8459	1.8587	1.8203	1.8585	1.8140	1.8582	1.8095	1.8591	1.8606	**2.17**
H(9B)	0.8096	0.7385	0.7151	0.7072	0.6530	0.7092	0.6771	0.7112	0.6793	0.7056	0.6700	0.8096	0.7385	0.7151	0.7072	0.6530	0.7092	0.6771	0.7112	0.6793	0.7056	0.6700	**0.82**
H(10A-10C)	2.6794	2.6787	2.6631	2.6639	2.6195	2.6649	2.6318	2.6660	2.6344	2.6632	2.6014	2.8005	2.8073	2.7922	2.7917	2.7607	2.7934	2.7693	2.7951	2.7700	2.7903	2.7450	**3.38**
H(1`A-1`B)	3.1562	3.2102	3.2307	3.2391	3.2917	3.2374	3.2736	3.2358	3.2708	3.2410	3.2736	2.8867	2.7471	2.6964	2.7012	2.7228	2.7032	2.6529	2.7053	2.6513	2.6995	2.6453	**3.75**
H(2`-3`A-2`-3`B)	1.6383	1.6989	1.6608	1.7358	1.7000	1.7336	1.7193	1.7315	1.7137	1.7382	1.7429	1.6383	1.6989	1.6608	1.7358	1.7000	1.7336	1.7193	1.7315	1.7137	1.7382	1.7429	**2.125**
H(4`A)	2.8867	2.7471	2.6964	2.7012	2.7228	2.7032	2.6529	2.7053	2.6513	2.6995	2.6453	3.1562	3.2102	3.2307	3.2391	3.2917	3.2374	3.2736	3.2358	3.2708	3.2410	3.2736	**3.07**
H(4`B)	2.8005	2.8073	2.7922	2.7917	2.7607	2.7934	2.7693	2.7951	2.7700	2.7903	2.7450	2.6794	2.6787	2.6631	2.6639	2.6195	2.6649	2.6318	2.6659	2.6344	2.6632	2.6014	**3.71**

[a] methyl protons shifts are averaged [b] according to [13] in D_2O

Table S15. Cont. VI

Nuclei	R											S									Exp. [b]
	O3LYP																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	134.6852	136.8207	137.1096	137.6206	139.3607	137.5893	138.3387	137.5522	138.5060	137.6429	138.5383	134.6851	136.8207	137.1096	137.6206	139.3607	137.5894	138.3387	137.5521	138.5060	137.6430	138.5383	**130.87**
C2	134.2200	134.2453	134.8776	134.2633	134.8477	134.2735	135.2336	134.2784	135.1484	134.2458	135.2345	134.2200	134.2453	134.8776	134.2633	134.8477	134.2736	135.2336	134.2783	135.1484	134.2459	135.2345	**132.98**
C3	117.1321	117.9019	118.4806	118.1484	118.8279	118.1468	119.0810	118.1397	119.0226	118.1431	119.1229	117.1320	117.9019	118.4806	118.1484	118.8279	118.1467	119.0810	118.1397	119.0226	118.1431	119.1229	**117.44**
C4	169.5264	170.0924	170.8213	170.5124	171.2149	170.4965	171.7802	170.4752	171.6254	170.5211	171.8946	169.5264	170.0924	170.8213	170.5124	171.2149	170.4963	171.7802	170.4753	171.6254	170.5211	171.8946	**167.85**
C5	115.2416	116.2916	116.9942	116.8973	117.6617	116.8703	117.9088	116.8382	117.8002	116.9169	118.0612	115.2416	116.2916	116.9942	116.8973	117.6617	116.8702	117.9088	116.8382	117.8002	116.9168	118.0612	**117.44**
C6	129.9224	131.2854	132.4315	132.4006	133.8108	132.3376	134.4252	132.2699	134.1495	132.4543	134.7239	129.9225	131.2854	132.4315	132.4006	133.8108	132.3376	134.4252	132.2699	134.1495	132.4542	134.7239	**132.98**
C7	196.8549	202.5909	203.1525	205.3974	206.1336	205.2395	210.4772	205.0767	209.5426	205.5412	211.4604	196.8550	202.5909	203.1525	205.3974	206.1336	205.2396	210.4772	205.0767	209.5426	205.5412	211.4604	**196.75**
C8	64.4100	66.2237	66.4509	66.9538	67.5942	66.9206	68.1364	66.8832	68.0238	66.9795	68.4155	64.4100	66.2237	66.4509	66.9538	67.5942	66.9207	68.1364	66.8831	68.0238	66.9796	68.4155	**70.92**
C9	28.5204	28.3499	28.4905	28.3340	28.3838	28.3453	28.7770	28.3520	28.6857	28.3171	28.7841	28.5205	28.3499	28.4905	28.3340	28.3838	28.3453	28.7770	28.3519	28.6857	28.3172	28.7841	**23.99**
C10	8.5924	8.8363	9.0684	8.9729	9.2485	8.9738	9.1996	8.9700	9.1884	8.9658	9.2938	8.5923	8.8363	9.0684	8.9729	9.2485	8.9739	9.1996	8.9701	9.1884	8.9658	9.2938	**8.05**
C1`	50.7604	51.5135	51.8645	52.0453	52.6526	52.0200	52.6148	51.9899	52.5713	52.0632	52.9703	55.2168	56.1221	56.5407	56.6385	57.1880	56.6160	57.2763	56.5886	57.2039	56.6532	57.5013	**52.76**
C2`	25.8590	26.2824	26.6436	26.4924	26.9122	26.4881	26.9437	26.4791	26.9283	26.4904	26.7395	25.7047	25.8528	26.1952	26.0666	26.6009	26.0633	26.4382	26.0547	26.4409	26.0632	26.1898	**23.74**
C3`	25.7047	25.8528	26.1952	26.0666	26.6009	26.0632	26.4382	26.0547	26.4409	26.0632	26.1898	25.8591	26.2824	26.6436	26.4924	26.9122	26.4881	26.9437	26.4792	26.9283	26.4904	26.7395	**23.57**
C4`	55.2168	56.1221	56.5407	56.6385	57.1880	56.6161	57.2763	56.5886	57.2039	56.6532	57.5013	50.7604	51.5135	51.8645	52.0453	52.6526	52.0200	52.6148	51.9899	52.5713	52.0632	52.9703	**56.17**
H2	8.5308	8.3196	8.4221	8.2448	8.2555	8.2493	8.3252	8.2535	8.3129	8.2404	8.3198	8.5308	8.3196	8.4221	8.2448	8.2555	8.2493	8.3252	8.2535	8.3129	8.2404	8.3198	**8.11**
H3	7.2883	7.4211	7.5238	7.4572	7.5730	7.4558	7.5974	7.4540	7.5883	7.4584	7.6113	7.2884	7.4211	7.5238	7.4572	7.5730	7.4558	7.5974	7.4540	7.5883	7.4584	7.6113	**7.34**
H5	7.1409	7.2961	7.3853	7.3784	7.4999	7.3741	7.5159	7.3694	7.5050	7.3824	7.5369	7.1409	7.2961	7.3853	7.3784	7.4999	7.3741	7.5159	7.3694	7.5050	7.3824	7.5369	**7.34**
H6	7.9048	8.0208	8.1410	8.0947	8.2285	8.0896	8.2785	8.0844	8.2530	8.0994	8.2976	7.9048	8.0208	8.1410	8.0947	8.2285	8.0896	8.2785	8.0844	8.2530	8.0994	8.2976	**8.11**
H8	4.7521	4.7485	4.7938	4.7718	4.8470	4.7701	4.8646	4.7682	4.8476	4.7734	4.8495	4.7522	4.7485	4.7938	4.7718	4.8470	4.7701	4.8646	4.7682	4.8476	4.7734	4.8495	**5.25**
H(9A)	1.7228	1.7315	1.7558	1.7523	1.7554	1.7508	1.7878	1.7490	1.7783	1.7538	1.8186	1.7228	1.7315	1.7558	1.7523	1.7554	1.7508	1.7878	1.7491	1.7783	1.7538	1.8186	**2.17**
H(9B)	0.8069	0.7490	0.7302	0.7350	0.6882	0.7363	0.7069	0.7372	0.7060	0.7337	0.6989	0.8069	0.7490	0.7302	0.7350	0.6882	0.7363	0.7069	0.7372	0.7060	0.7337	0.6989	**0.82**
H(10A-10C)	2.7964	2.7875	2.7632	2.7687	2.7188	2.7705	2.7285	2.7720	2.7303	2.7669	2.6968	2.9209	2.9076	2.8986	2.8855	2.8473	2.8874	2.8515	2.8890	2.8558	2.8836	2.8196	**3.38**
H(1`A-1`B)	3.2472	3.2927	3.3272	3.3264	3.3834	3.3244	3.3722	3.3221	3.3685	3.3281	3.3655	2.9092	2.8074	2.7699	2.7873	2.7920	2.7884	2.7636	2.7893	2.7660	2.7862	2.7624	**3.75**
H(2`-3`A-2`-3`B)	1.6809	1.7342	1.7006	1.7749	1.7343	1.7726	1.7483	1.7699	1.7436	1.7770	1.7711	1.6809	1.7342	1.7006	1.7749	1.7343	1.7726	1.7483	1.7699	1.7436	1.7770	1.7711	**2.125**
H(4`A)	2.9092	2.8074	2.7699	2.7873	2.7920	2.7884	2.7636	2.7894	2.7660	2.7862	2.7624	3.2472	3.2927	3.3272	3.3264	3.3834	3.3244	3.3722	3.3222	3.3685	3.3281	3.3655	**3.07**
H(4`B)	2.9209	2.9076	2.8986	2.8855	2.8473	2.8874	2.8515	2.8890	2.8558	2.8836	2.8196	2.7964	2.7875	2.7632	2.7687	2.7188	2.7705	2.7285	2.7720	2.7303	2.7669	2.6968	**3.71**
Nuclei	OLYP																						
C1	133.8351	135.6494	136.7395	136.4684	138.3119	136.4144	137.0878	136.3585	137.3217	136.5148	137.4066	133.8351	135.6494	136.7395	136.4684	138.3119	136.4144	137.0878	136.3586	137.3217	136.5148	137.4066	**130.87**
C2	131.8165	131.8666	132.5613	131.8889	132.4317	131.9005	132.8310	131.9059	132.7378	131.8683	132.8281	131.8165	131.8666	132.5614	131.8889	132.4317	131.9005	132.8310	131.9058	132.7378	131.8683	132.8281	**132.98**
C3	115.3675	116.0445	116.6770	116.2749	116.9243	116.2736	117.2202	116.2660	117.1513	116.2667	117.2580	115.3675	116.0445	116.6772	116.2749	116.9243	116.2736	117.2202	116.2659	117.1513	116.2667	117.2580	**117.44**
C4	168.3873	169.0642	169.8140	169.4983	170.2057	169.4832	170.7873	169.4620	170.6272	169.5032	170.8944	168.3873	169.0642	169.8141	169.4983	170.2057	169.4832	170.7873	169.4619	170.6272	169.5032	170.8944	**167.85**
C5	113.4391	114.4174	115.0512	115.0098	115.7200	114.9837	116.0289	114.9514	115.9097	115.0254	116.1576	113.4391	114.4174	115.0511	115.0098	115.7200	114.9837	116.0289	114.9514	115.9097	115.0254	116.1576	**117.44**
C6	127.3510	128.9229	129.9895	130.0369	131.3495	129.9778	132.0100	129.9124	131.7234	130.0834	132.2868	127.3510	128.9229	129.9895	130.0368	131.3495	129.9778	132.0100	129.9125	131.7234	130.0834	132.2868	**132.98**
C7	195.4633	200.7587	202.0891	203.5188	204.5384	203.3387	208.1627	203.1586	207.4247	203.6866	209.2319	195.4633	200.7587	202.0891	203.5188	204.5384	203.3387	208.1627	203.1586	207.4247	203.6866	209.2319	**196.75**
C8	65.9474	67.6652	68.1647	68.4705	69.3045	68.4195	69.6410	68.3655	69.5914	68.5126	69.8866	65.9474	67.6652	68.1647	68.4705	69.3045	68.4195	69.6410	68.3656	69.5914	68.5126	69.8866	**70.92**
C9	29.6624	29.4884	29.6242	29.5146	29.5588	29.5224	30.0305	29.5242	29.9292	29.4978	29.9896	29.6624	29.4884	29.6242	29.5146	29.5588	29.5224	30.0305	29.5242	29.9292	29.4978	29.9896	**23.99**
C10	8.7576	9.0274	9.1768	9.1836	9.4591	9.1834	9.4372	9.1777	9.4248	9.1743	9.4993	8.7576	9.0274	9.1768	9.1836	9.4591	9.1834	9.4372	9.1777	9.4248	9.1743	9.4993	**8.05**
C1`	51.7069	52.4585	52.8434	53.0117	53.6019	52.9846	53.5676	52.9522	53.5270	53.0288	53.9035	56.2414	57.1377	57.5367	57.6407	58.1548	57.6187	58.2570	57.5913	58.1780	57.6527	58.4958	**52.76**
C2`	26.4273	26.9302	27.2237	27.1732	27.5665	27.1678	27.6133	27.1568	27.5940	27.1691	27.3850	26.4685	26.5882	27.0514	26.8341	27.3255	26.8265	27.1736	26.8137	27.1757	26.8327	26.9495	**23.74**
C3`	26.4685	26.5882	27.0513	26.8341	27.3255	26.8265	27.1736	26.8137	27.1757	26.8327	26.9495	26.4273	26.9302	27.2237	27.1733	27.5665	27.1678	27.6133	27.1568	27.5940	27.1691	27.3850	**23.57**
C4`	56.2414	57.1377	57.5368	57.6407	58.1548	57.6187	58.2570	57.5913	58.1780	57.6527	58.4958	51.7069	52.4585	52.8433	53.0118	53.6019	52.9846	53.5676	52.9522	53.5270	53.0288	53.9035	**56.17**
H2	8.3451	8.1784	8.2118	8.1041	8.0993	8.1107	8.1998	8.1169	8.1779	8.0968	8.1842	8.3451	8.1784	8.2118	8.1041	8.0993	8.1107	8.1998	8.1169	8.1779	8.0968	8.1842	**8.11**
H3	7.2251	7.3362	7.4254	7.3700	7.4829	7.3688	7.5135	7.3675	7.5027	7.3705	7.5243	7.2251	7.3362	7.4254	7.3700	7.4829	7.3688	7.5135	7.3675	7.5027	7.3705	7.5243	**7.34**
H5	7.0535	7.2233	7.3156	7.3052	7.4261	7.3006	7.4407	7.2960	7.4304	7.3091	7.4611	7.0535	7.2233	7.3156	7.3052	7.4261	7.3006	7.4407	7.2960	7.4304	7.3091	7.4611	**7.34**
H6	7.8124	7.9126	8.0035	7.9844	8.1003	7.9806	8.1710	7.9766	8.1398	7.9874	8.1887	7.8124	7.9126	8.0035	7.9844	8.1003	7.9806	8.1710	7.9766	8.1398	7.9874	8.1887	**8.11**
H8	4.9123	4.8931	4.9173	4.9056	4.9642	4.9052	4.9892	4.9046	4.9723	4.9053	4.9719	4.9123	4.8931	4.9173	4.9056	4.9642	4.9052	4.9892	4.9046	4.9723	4.9053	4.9719	**5.25**
H(9A)	1.7435	1.7791	1.7714	1.8080	1.8150	1.8066	1.8516	1.8049	1.8409	1.8090	1.8745	1.7435	1.7791	1.7714	1.8080	1.8150	1.8066	1.8516	1.8049	1.8409	1.8090	1.8745	**2.17**
H(9B)	0.8117	0.7606	0.7472	0.7487	0.7001	0.7496	0.7183	0.7505	0.7176	0.7474	0.7143	0.8117	0.7606	0.7472	0.7487	0.7001	0.7496	0.7183	0.7505	0.7176	0.7474	0.7143	**0.82**
H(10A-10C)	2.8594	2.8478	2.8216	2.8281	2.7774	2.8299	2.7851	2.8316	2.7874	2.8260	2.7514	2.9889	2.9682	2.9551	2.9501	2.9163	2.9516	2.9142	2.9530	2.9200	2.9483	2.8791	**3.38**
H(1`A-1`B)	3.3319	3.3770	3.4106	3.4139	3.4745	3.4118	3.4642	3.4095	3.4605	3.4156	3.4549	2.9962	2.8834	2.8672	2.8724	2.8868	2.8720	2.8538	2.8718	2.8587	2.8725	2.8528	**3.75**
H(2`-3`A-2`-3`B)	1.7219	1.7678	1.7439	1.8060	1.7649	1.8035	1.7780	1.8011	1.7739	1.8078	1.8031	1.7219	1.7678	1.7439	1.8060	1.7649	1.8035	1.7780	1.8011	1.7739	1.8078	1.8031	**2.125**
H(4`A)	2.9962	2.8834	2.8672	2.8724	2.8868	2.8720	2.8538	2.8718	2.8587	2.8725	2.8528	3.3319	3.3770	3.4106	3.4139	3.4745	3.4118	3.4642	3.4095	3.4605	3.4156	3.4549	**3.07**
H(4`B)	2.9889	2.9682	2.9551	2.9501	2.9163	2.9516	2.9142	2.9530	2.9200	2.9483	2.8791	2.8594	2.8478	2.8215	2.8281	2.7774	2.8299	2.7851	2.8316	2.7874	2.8260	2.7514	**3.71**
Nuclei	OPBE																						
C1	130.5131	132.5342	133.5416	133.2638	135.1900	133.2330	133.9500	133.1867	134.1426	133.2924	134.2560	130.5130	132.5342	133.5417	133.2638	135.1900	133.2330	133.9500	133.1867	134.1426	133.2924	134.2560	**130.87**
C2	130.4654	130.5593	131.2646	130.5133	131.1427	130.5324	131.4958	130.5334	131.4169	130.4900	131.5188	130.4654	130.5593	131.2645	130.5133	131.1427	130.5324	131.4958	130.5333	131.4168	130.4900	131.5188	**132.98**
C3	114.2409	115.0778	115.6860	115.2694	115.9764	115.2769	116.2880	115.2657	116.2145	115.2567	116.3661	114.2409	115.0778	115.6859	115.2694	115.9764	115.2769	116.2880	115.2657	116.2145	115.2567	116.3661	**117.44**
C4	164.8191	165.5743	166.2518	165.9145	166.5739	165.9107	167.1865	165.8886	167.0297	165.9126	167.3162	164.8191	165.5743	166.2517	165.9145	166.5739	165.9107	167.1865	165.8887	167.0297	165.9126	167.3162	**167.85**
C5	112.3915	113.5120	114.0997	114.0481	114.7968	114.0322	115.1336	113.9981	115.0095	114.0579	115.3094	112.3915	113.5120	114.0998	114.0481	114.7968	114.0322	115.1336	113.9982	115.0096	114.0579	115.3094	**117.44**
C6	125.8932	127.4990	128.5138	128.4720	129.7852	128.4261	130.4324	128.3626	130.1682	128.5103	130.7223	125.8931	127.4990	128.5138	128.4720	129.7852	128.4262	130.4324	128.3625	130.1684	128.5103	130.7223	**132.98**
C7	192.7338	198.0357	199.1499	200.5675	201.6468	200.4240	205.0873	200.2661	204.3224	200.7036	206.1138	192.7338	198.0357	199.1501	200.5675	201.6468	200.4240	205.0873	200.2658	204.3223	200.7036	206.1138	**196.75**
C8	63.2927	65.2089	65.5222	65.9441	66.7821	65.9146	67.1347	65.8685	67.0426	65.9696	67.4768	63.2927	65.2089	65.5222	65.9441	66.7821	65.9146	67.1347	65.8685	67.0426	65.9696	67.4768	**70.92**
C9	27.7188	27.7819	27.7655	27.7587	27.7616	27.7791	28.2175	27.7810	28.1060	27.7333	28.2463	27.7188	27.7819	27.7654	27.7587	27.7616	27.7791	28.2175	27.7810	28.1059	27.7333	28.2463	**23.99**
C10	8.3107	8.6601	8.6766	8.7360	8.9559	8.7479	8.9088	8.7419	8.8948	8.7194	9.0637	8.3107	8.6601	8.6766	8.7360	8.9559	8.7479	8.9088	8.7419	8.8948	8.7194	9.0637	**8.05**
C1`	49.7994	50.6057	50.8749	51.0364	51.5932	51.0229	51.5367	50.9920	51.5017	51.0449	51.9169	54.1269	55.0800	55.4325	55.5005	55.9830	55.4885	56.1055	55.4591	56.0330	55.5076	56.3583	**52.76**
C2`	25.0597	25.5338	25.7242	25.6522	26.0222	25.6606	26.0182	25.6514	26.0055	25.6395	25.7853	24.9078	25.1189	25.4999	25.2113	25.6637	25.2209	25.5067	25.2129	25.5153	25.1978	25.2405	**23.74**
C3`	24.9078	25.1189	25.4999	25.2113	25.6637	25.2209	25.5066	25.2130	25.5153	25.1978	25.2405	25.0597	25.5338	25.7242	25.6522	26.0222	25.6606	26.0182	25.6514	26.0054	25.6395	25.7853	**23.57**
C4`	54.1269	55.0800	55.4325	55.5005	55.9830	55.4885	56.1055	55.4592	56.0330	55.5076	56.3583	49.7994	50.6057	50.8748	51.0364	51.5932	51.0229	51.5367	50.9921	51.5018	51.0449	51.9169	**56.17**
H2	8.4011	8.2161	8.2508	8.1423	8.1266	8.1477	8.2317	8.1521	8.2136	8.1360	8.2204	8.4011	8.2161	8.2508	8.1423	8.1266	8.1477	8.2317	8.1521	8.2136	8.1360	8.2204	**8.11**
H3	7.2498	7.3725	7.4570	7.4084	7.5185	7.4072	7.5500	7.4053	7.5393	7.4086	7.5643	7.2498	7.3725	7.4570	7.4084	7.5185	7.4072	7.5500	7.4053	7.5393	7.4086	7.5643	**7.34**
H5	7.0757	7.2539	7.3400	7.3316	7.4506	7.3277	7.4697	7.3231	7.4580	7.3344	7.4913	7.0757	7.2539	7.3400	7.3316	7.4506	7.3277	7.4697	7.3232	7.4580	7.3344	7.4913	**7.34**
H6	7.8852	7.9730	8.0618	8.0368	8.1461	8.0329	8.2155	8.0284	8.1883	8.0396	8.2315	7.8852	7.9730	8.0618	8.0368	8.1461	8.0329	8.2155	8.0284	8.1883	8.0396	8.2315	**8.11**
H8	4.9112	4.9002	4.9205	4.9122	4.9618	4.9118	4.9851	4.9106	4.9692	4.9118	4.9744	4.9112	4.9002	4.9205	4.9122	4.9618	4.9118	4.9851	4.9106	4.9693	4.9118	4.9744	**5.25**
H(9A)	1.7625	1.7845	1.7591	1.8066	1.8004	1.8058	1.8342	1.8042	1.8241	1.8065	1.8651	1.7625	1.7845	1.7590	1.8066	1.8004	1.8058	1.8342	1.8042	1.8241	1.8065	1.8651	**2.17**
H(9B)	0.7402	0.6920	0.6764	0.6750	0.6264	0.6765	0.6434	0.6773	0.6431	0.6730	0.6385	0.7402	0.6920	0.6764	0.6750	0.6264	0.6765	0.6434	0.6773	0.6430	0.6730	0.6385	**0.82**
H(10A-10C)	2.7812	2.7760	2.7437	2.7549	2.7020	2.7571	2.7089	2.7586	2.7107	2.7609	2.6762	2.9125	2.9021	2.8794	2.8796	2.8428	2.8817	2.8418	2.8832	2.8464	2.8768	2.8112	**3.38**
H(1`A-1`B)	3.3033	3.3455	3.3652	3.3727	3.4196	3.3715	3.4051	3.3697	3.4022	3.3730	3.3958	2.9824	2.8765	2.8320	2.8523	2.8527	2.8542	2.8155	2.8554	2.8193	2.8498	2.8154	**3.75**
H(2`-3`A-2`-3`B)	1.6770	1.7254	1.6974	1.7598	1.7175	1.7580	1.7315	1.7554	1.7272	1.7609	1.7597	1.6770	1.7254	1.6974	1.7598	1.7175	1.7580	1.7315	1.7555	1.7272	1.7609	1.7597	**2.125**
H(4`A)	2.9824	2.8765	2.8320	2.8523	2.8527	2.8542	2.8155	2.8554	2.8193	2.8498	2.8154	3.3033	3.3455	3.3652	3.3727	3.4196	3.3715	3.4051	3.3697	3.4022	3.3730	3.3958	**3.07**
H(4`B)	2.9125	2.9021	2.8794	2.8796	2.8428	2.8817	2.8418	2.8831	2.8464	2.8768	2.8112	2.7812	2.7760	2.7437	2.7549	2.7020	2.7571	2.7089	2.7586	2.7107	2.7519	2.6762	**3.71**

[a] methyl protons shifts are averaged [b] according to [13] in D_2O

Table S15. Cont. VII

Nuclei	R											S									Exp. [b]
	OPW91																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	130.8334	132.8499	133.8571	133.5809	135.4758	133.5406	134.2542	133.4857	134.4481	133.6049	134.5635	130.8334	132.8499	133.8571	133.5809	135.4758	133.5406	134.2542	133.4857	134.4481	133.6049	134.5634	**130.87**
C2	130.6869	130.7809	131.4819	130.7413	131.3585	130.7502	131.7136	130.7421	131.6343	130.7145	131.7387	130.6869	130.7809	131.4819	130.7413	131.3585	130.7502	131.7136	130.7421	131.6343	130.7145	131.7387	**132.98**
C3	114.4375	115.2730	115.8749	115.4678	116.1604	115.4652	116.4717	115.4452	116.3987	115.4513	116.5506	114.4375	115.2730	115.8749	115.4678	116.1604	115.4652	116.4717	115.4452	116.3988	115.4513	116.5505	**117.44**
C4	165.2239	165.9795	166.6546	166.3272	166.9815	166.3131	167.5911	166.2816	167.4341	166.3216	167.7232	165.2238	165.9795	166.6546	166.3272	166.9815	166.3131	167.5911	166.2816	167.4342	166.3216	167.7232	**167.85**
C5	112.5854	113.7060	114.2881	114.2461	114.9833	114.2202	115.3172	114.1769	115.1938	114.2520	115.4937	112.5854	113.7060	114.2881	114.2461	114.9833	114.2202	115.3171	114.1769	115.1937	114.2520	115.4937	**117.44**
C6	126.1139	127.7231	128.7361	128.7081	130.0155	128.6517	130.6617	128.5782	130.3961	128.7432	130.9542	126.1140	127.7231	128.7361	128.7081	130.0155	128.6517	130.6616	128.5782	130.3961	128.7432	130.9542	**132.98**
C7	193.1215	198.4381	199.5572	200.9778	202.0184	200.8249	205.5061	200.6579	204.7375	201.1098	206.5369	193.1212	198.4380	199.5572	200.9778	202.0184	200.8249	205.5060	200.6579	204.7375	201.1098	206.5369	**196.75**
C8	63.5176	65.4318	65.7420	66.1658	66.9759	66.1270	67.3419	66.0724	67.2514	66.1867	67.6855	63.5175	65.4318	65.7419	66.1658	66.9759	66.1270	67.3419	66.0724	67.2514	66.1867	67.6855	**70.92**
C9	27.8629	27.9229	27.9054	27.9045	27.8985	27.9149	28.3552	27.9076	28.2444	27.8754	28.3853	27.8629	27.9229	27.9054	27.9045	27.8985	27.9149	28.3552	27.9076	28.2444	27.8754	28.3854	**23.99**
C10	8.3646	8.7176	8.7338	8.7982	9.0111	8.8002	8.9653	8.7850	8.9522	8.7779	9.1182	8.3646	8.7176	8.7339	8.7982	9.0111	8.8002	8.9653	8.7850	8.9520	8.7779	9.1182	**8.05**
C1`	49.9410	50.7530	51.0221	51.1910	51.7391	51.1673	51.6860	51.1272	51.6509	51.1958	52.0665	54.2763	55.2341	55.5835	55.6599	56.1365	55.6379	56.2572	55.5994	56.1845	55.6630	56.5133	**52.76**
C2`	25.1770	25.6592	25.8491	25.7847	26.1465	25.7830	26.1447	25.7643	26.1326	25.7681	25.9162	25.0261	25.2389	25.6194	25.3423	25.7885	25.3413	25.6326	25.3238	25.6410	25.3253	25.3716	**23.74**
C3`	25.0261	25.2389	25.6194	25.3423	25.7885	25.3413	25.6326	25.3238	25.6411	25.3253	25.3716	25.1770	25.6592	25.8491	25.7847	26.1465	25.7830	26.1447	25.7643	26.1326	25.7681	25.9161	**23.57**
C4`	54.2764	55.2341	55.5835	55.6599	56.1365	55.6379	56.2572	55.5994	56.1845	55.6630	56.5134	49.9409	50.7529	51.0221	51.1910	51.7391	51.1673	51.6860	51.1272	51.6509	51.1958	52.0665	**56.17**
H2	8.4015	8.2172	8.2517	8.1447	8.1303	8.1493	8.2333	8.1534	8.2152	8.1382	8.2218	8.4015	8.2172	8.2517	8.1447	8.1303	8.1493	8.2333	8.1534	8.2152	8.1382	8.2218	**8.11**
H3	7.2509	7.3736	7.4580	7.4100	7.5192	7.4082	7.5506	7.4061	7.5399	7.4099	7.5647	7.2509	7.3736	7.4580	7.4100	7.5192	7.4082	7.5506	7.4061	7.5399	7.4099	7.5647	**7.34**
H5	7.0782	7.2554	7.3413	7.3336	7.4516	7.3291	7.4707	7.3243	7.4589	7.3362	7.4921	7.0782	7.2554	7.3413	7.3336	7.4516	7.3291	7.4707	7.3243	7.4589	7.3362	7.4922	**7.34**
H6	7.8845	7.9736	8.0623	8.0385	8.1481	8.0339	8.2169	8.0291	8.1893	8.0411	8.2327	7.8845	7.9736	8.0623	8.0385	8.1481	8.0339	8.2169	8.0291	8.1893	8.0411	8.2327	**8.11**
H8	4.9104	4.8993	4.9197	4.9124	4.9620	4.9112	4.9850	4.9098	4.9690	4.9117	4.9739	4.9104	4.8993	4.9197	4.9124	4.9620	4.9112	4.9850	4.9098	4.9690	4.9117	4.9739	**5.25**
H(9A)	1.7583	1.7816	1.7564	1.8046	1.7982	1.8031	1.8321	1.8012	1.8219	1.8042	1.8626	1.7583	1.7816	1.7564	1.8046	1.7982	1.8031	1.8321	1.8012	1.8219	1.8042	1.8626	**2.17**
H(9B)	0.7436	0.6951	0.6799	0.6790	0.6297	0.6798	0.6470	0.6803	0.6465	0.6767	0.6419	0.7436	0.6951	0.6799	0.6790	0.6297	0.6798	0.6470	0.6803	0.6465	0.6767	0.6419	**0.82**
H(10A-10C)	2.7854	2.7800	2.7478	2.7593	2.7058	2.7610	2.7129	2.7623	2.7145	2.7561	2.6802	2.9162	2.9052	2.8827	2.8833	2.8455	2.8848	2.8449	2.8860	2.8494	2.8802	2.8140	**3.38**
H(1`A-1`B)	3.2994	3.3423	3.3624	3.3707	3.4171	3.3688	3.4033	3.3667	3.4002	3.3707	3.3938	2.9778	2.8722	2.8287	2.8492	2.8489	2.8503	2.8124	2.8513	2.8162	2.8464	2.8127	**3.75**
H(2`-3`A-2`-3`B)	1.6773	1.7260	1.6981	1.7610	1.7181	1.7585	1.7321	1.7558	1.7278	1.7619	1.7601	1.6773	1.7260	1.6981	1.7610	1.7181	1.7585	1.7321	1.7558	1.7278	1.7619	1.7601	**2.125**
H(4`A)	2.9778	2.8722	2.8287	2.8492	2.8489	2.8503	2.8124	2.8513	2.8162	2.8464	2.8127	3.2994	3.3423	3.3624	3.3707	3.4171	3.3688	3.4033	3.3667	3.4002	3.3707	3.3938	**3.07**
H(4`B)	2.9162	2.9052	2.8827	2.8833	2.8455	2.8848	2.8449	2.8860	2.8494	2.8802	2.8140	2.7854	2.7800	2.7478	2.7593	2.7058	2.7610	2.7129	2.7623	2.7145	2.7561	2.6802	**3.71**
Nuclei	PBE																						
C1	135.5027	137.0862	137.5815	137.7635	140.0277	137.7142	139.4466	137.6744	139.4065	137.8270	139.7153	135.5027	137.0862	137.5815	137.7635	140.0277	137.7142	139.4466	137.6744	139.4065	137.8270	139.7153	**130.87**
C2	135.9665	135.9788	136.5525	135.8311	136.6569	135.8362	137.1165	135.8525	137.0309	135.8442	137.1907	135.9667	135.9788	136.5525	135.8311	136.6569	135.8362	137.1165	135.8525	137.0309	135.8442	137.1907	**132.98**
C3	119.3235	120.2716	120.8385	120.5131	121.3639	120.4977	121.6981	120.4927	121.6228	120.5449	121.7767	119.3235	120.2716	120.8384	120.5131	121.3639	120.4977	121.6981	120.4927	121.6228	120.5449	121.7767	**117.44**
C4	174.2731	175.2247	175.9328	175.5311	176.3756	175.5099	176.9550	175.4997	176.8173	175.5691	177.0950	174.2731	175.2247	175.9328	175.5311	176.3756	175.5099	176.9550	175.4997	176.8173	175.5691	177.0950	**167.85**
C5	117.6189	118.9655	119.5711	119.5802	120.4993	119.5388	120.7932	119.5083	120.6809	119.6375	120.9648	117.6188	118.9655	119.5711	119.5802	120.4993	119.5388	120.7932	119.5083	120.6809	119.6375	120.9648	**117.44**
C6	132.2249	133.9873	135.1783	134.7972	136.2000	134.7461	136.7129	134.7061	136.5049	134.8645	137.1126	132.2249	133.9873	135.1783	134.7972	136.2000	134.7461	136.7129	134.7061	136.5049	134.8645	137.1126	**132.98**
C7	200.8114	205.6148	206.6166	208.0300	209.4645	207.8741	213.5761	207.7273	212.5852	208.1942	214.7106	200.8115	205.6148	206.6166	208.0300	209.4645	207.8741	213.5761	207.7273	212.5852	208.1942	214.7106	**196.75**
C8	67.2268	68.7774	69.4317	69.3737	70.3901	69.3341	70.9762	69.3036	70.7658	69.4272	71.5306	67.2268	68.7774	69.4317	69.3737	70.3901	69.3341	70.9762	69.3036	70.7658	69.4272	71.5306	**70.92**
C9	30.7959	30.8705	31.0388	30.7226	30.7906	30.7316	31.1310	30.7516	31.0214	30.7321	31.2757	30.7959	30.8705	31.0388	30.7226	30.7906	30.7316	31.1310	30.7516	31.0214	30.7321	31.2757	**23.99**
C10	8.1398	8.5496	8.7055	8.5833	8.9062	8.5797	8.7932	8.5864	8.7767	8.6037	8.9798	8.1399	8.5496	8.7054	8.5833	8.9062	8.5797	8.7932	8.5864	8.7767	8.6037	8.9798	**8.05**
C1`	53.1734	54.0696	54.3964	54.5000	55.1960	54.4706	55.1460	54.4508	55.0845	54.5444	55.6308	57.6512	58.7549	59.1195	59.2058	59.9064	59.1717	60.1273	59.1486	60.0614	59.2564	60.3789	**52.76**
C2`	25.5324	26.1048	26.4614	26.2639	26.7880	26.2483	26.8408	26.2436	26.8190	26.2964	26.7778	25.4524	25.6919	25.9861	25.7790	26.4314	25.7683	26.3160	25.7692	26.3163	25.8070	26.1595	**23.74**
C3`	25.4524	25.6919	25.9861	25.7790	26.4314	25.7683	26.3160	25.7692	26.3163	25.8070	26.1595	25.5323	26.1048	26.4614	26.2639	26.7879	26.2483	26.8408	26.2436	26.8190	26.2964	26.7778	**23.57**
C4`	57.6511	58.7549	59.1195	59.2058	59.9064	59.1717	60.1273	59.1486	60.0614	59.2564	60.3789	53.1734	54.0696	54.3964	54.5000	55.1960	54.4706	55.1460	54.4508	55.0845	54.5444	55.6308	**56.17**
H2	8.5716	8.4328	8.4794	8.3573	8.3335	8.3621	8.3735	8.3676	8.3788	8.3535	8.3666	8.5716	8.4328	8.4794	8.3573	8.3335	8.3621	8.3735	8.3676	8.3788	8.3535	8.3666	**8.11**
H3	7.1986	7.3342	7.4234	7.3804	7.5099	7.3780	7.5335	7.3760	7.5249	7.3833	7.5474	7.1986	7.3342	7.4235	7.3804	7.5099	7.3780	7.5335	7.3760	7.5249	7.3833	7.5474	**7.34**
H5	7.0682	7.2288	7.3293	7.2962	7.4194	7.2923	7.4365	7.2889	7.4264	7.3006	7.4553	7.0682	7.2288	7.3293	7.2962	7.4194	7.2923	7.4365	7.2889	7.4264	7.3006	7.4553	**7.34**
H6	7.9400	8.0735	8.1618	8.1551	8.2574	8.1499	8.2963	8.1454	8.2841	8.1606	8.3167	7.9400	8.0735	8.1618	8.1551	8.2574	8.1499	8.2963	8.1454	8.2841	8.1606	8.3167	**8.11**
H8	4.9767	4.9893	5.0066	5.0089	5.0670	5.0071	5.0780	5.0060	5.0709	5.0116	5.0660	4.9767	4.9893	5.0066	5.0089	5.0670	5.0071	5.0780	5.0060	5.0709	5.0116	5.0660	**5.25**
H(9A)	1.9605	2.0046	2.0249	2.0142	1.9893	2.0146	1.9876	2.0153	1.9833	2.0144	2.0335	1.9605	2.0046	2.0249	2.0142	1.9893	2.0146	1.9876	2.0153	1.9833	2.0144	2.0335	**2.17**
H(9B)	0.8180	0.7571	0.7287	0.7279	0.6821	0.7298	0.7010	0.7322	0.7020	0.7268	0.6961	0.8180	0.7571	0.7286	0.7279	0.6821	0.7298	0.7010	0.7322	0.7020	0.7268	0.6961	**0.82**
H(10A-10C)	2.8121	2.8166	2.7997	2.7988	2.7621	2.7996	2.7688	2.8012	2.7718	2.7988	2.7305	2.9142	2.9333	2.9253	2.9204	2.8950	2.9217	2.8976	2.9234	2.9006	2.9197	2.8688	**3.38**
H(1`A-1`B)	3.3776	3.4250	3.4455	3.4469	3.5038	3.4457	3.4796	3.4451	3.4776	3.4488	3.4738	3.0969	2.9459	2.8885	2.8895	2.8922	2.8924	2.8382	2.8961	2.8393	2.8876	2.8222	**3.75**
H(2`-3`A-2`-3`B)	1.7331	1.7913	1.7548	1.8238	1.7915	1.8216	1.8089	1.8200	1.8036	1.8266	1.8352	1.7331	1.7913	1.7548	1.8238	1.7915	1.8216	1.8089	1.8200	1.8036	1.8266	1.8352	**2.125**
H(4`A)	3.0969	2.9459	2.8885	2.8895	2.8922	2.8924	2.8382	2.8961	2.8393	2.8876	2.8222	3.3776	3.4250	3.4455	3.4469	3.5038	3.4457	3.4796	3.4451	3.4776	3.4488	3.4738	**3.07**
H(4`B)	2.9142	2.9333	2.9253	2.9204	2.8950	2.9217	2.8976	2.9234	2.9006	2.9197	2.8688	2.8121	2.8166	2.7997	2.7988	2.7621	2.7996	2.7688	2.8012	2.7718	2.7988	2.7305	**3.71**
Nuclei	PBE0																						
C1	136.3225	137.4483	138.0445	137.9533	140.3783	137.9237	139.7464	137.8949	139.6267	137.9832	139.7758	136.3223	137.4483	138.0445	137.9533	140.3783	137.9235	139.7464	137.8948	139.6267	137.9832	139.7758	**130.87**
C2	138.7485	138.6702	139.2371	138.5523	139.1555	138.5545	139.7372	138.5584	139.5959	138.5536	139.7005	138.7486	138.6702	139.2371	138.5524	139.1555	138.5544	139.7372	138.5583	139.5959	138.5536	139.7005	**132.98**
C3	120.7814	121.6015	122.1803	121.8604	122.6461	121.8420	123.0019	121.8253	122.8804	121.8805	123.0049	120.7814	121.6015	122.1803	121.8604	122.6462	121.8420	123.0019	121.8252	122.8804	121.8805	123.0049	**117.44**
C4	172.9514	173.7460	174.3773	174.0906	174.6703	174.0640	175.3773	174.0394	175.1937	174.1190	175.4543	172.9515	173.7460	174.3773	174.0906	174.6703	174.0641	175.3773	174.0394	175.1937	174.1190	175.4543	**167.85**
C5	118.9139	120.2549	120.8537	120.9266	121.7768	120.8803	122.0989	120.8356	121.9387	120.9735	122.2090	118.9139	120.2549	120.8537	120.9265	121.7767	120.8802	122.0989	120.8357	121.9387	120.9735	122.2090	**117.44**
C6	134.7999	136.6188	137.7302	137.5722	138.7078	137.5054	139.2967	137.4407	139.0528	137.6393	139.6976	134.7999	136.6188	137.7302	137.5721	138.7079	137.5053	139.2967	137.4410	139.0528	137.6393	139.6976	**132.98**
C7	200.7853	205.6553	206.5829	208.1828	209.5642	208.0297	214.5129	207.8770	213.2005	208.3297	215.4079	200.7855	205.6553	206.5829	208.1827	209.5641	208.0293	214.5129	207.8772	213.2005	208.3297	215.4079	**196.75**
C8	63.2907	64.6253	65.0671	65.2046	66.1463	65.1678	66.7741	65.1323	66.4548	65.2419	67.2010	63.2907	64.6253	65.0671	65.2046	66.1464	65.1677	66.7741	65.1322	66.4548	65.2419	67.2010	**70.92**
C9	27.5726	27.5554	27.6657	27.4965	27.4845	27.4951	27.7202	27.4956	27.5717	27.5005	27.8229	27.5726	27.5554	27.6657	27.4965	27.4845	27.4952	27.7202	27.4956	27.5717	27.5005	27.8229	**23.99**
C10	8.0284	8.3451	8.4650	8.4442	8.6722	8.4330	8.6226	8.4239	8.5413	8.4578	8.7211	8.0284	8.3451	8.4650	8.4442	8.6722	8.4331	8.6226	8.4238	8.5413	8.4578	8.7211	**8.05**
C1`	50.2914	51.1379	51.4460	51.5793	52.1694	51.5451	52.2113	51.5133	52.0753	51.6155	52.5912	54.5306	55.5111	55.8541	55.9689	56.5148	55.9354	56.8004	55.9038	56.6852	56.0041	56.9706	**52.76**
C2`	24.2105	24.6432	24.9602	24.8186	25.2087	24.8027	25.3255	24.7886	25.2434	24.8371	25.1779	23.8828	24.0346	24.3710	24.1539	24.6820	24.1399	24.6550	24.1283	24.6047	24.1701	24.4277	**23.74**
C3`	23.8829	24.0346	24.3710	24.1538	24.6820	24.1399	24.6550	24.1282	24.6047	24.1701	24.4277	24.2105	24.6432	24.9602	24.8187	25.2087	24.8026	25.3255	24.7885	25.2434	24.8371	25.1779	**23.57**
C4`	54.5306	55.5111	55.8541	55.9689	56.5148	55.9353	56.8004	55.9038	56.6852	56.0041	56.9706	50.2914	51.1379	51.4460	51.5793	52.1694	51.5451	52.2113	51.5134	52.0753	51.6155	52.5912	**56.17**
H2	8.7954	8.6671	8.7153	8.5963	8.5325	8.5999	8.5798	8.6036	8.5902	8.5926	8.5774	8.7955	8.6671	8.7153	8.5963	8.5325	8.5999	8.5798	8.6036	8.5902	8.5926	8.5774	**8.11**
H3	7.3536	7.4891	7.5804	7.5348	7.6620	7.5324	7.6909	7.5299	7.6796	7.5367	7.7020	7.3536	7.4891	7.5804	7.5348	7.6620	7.5324	7.6909	7.5299	7.6796	7.5367	7.7020	**7.34**
H5	7.2060	7.3840	7.4802	7.4583	7.5767	7.4538	7.5978	7.4494	7.5850	7.4621	7.6160	7.2060	7.3840	7.4802	7.4583	7.5767	7.4538	7.5978	7.4494	7.5850	7.4621	7.6160	**7.34**
H6	8.0673	8.2239	8.3184	8.3175	8.4200	8.3113	8.4671	8.3051	8.4550	8.3232	8.4978	8.0673	8.2239	8.3184	8.3175	8.4200	8.3113	8.4671	8.3051	8.4550	8.3232	8.4978	**8.11**
H8	4.5541	4.6040	4.6404	4.6530	4.7216	4.6493	4.7530	4.6457	4.7442	4.6561	4.7502	4.5541	4.6040	4.6404	4.6530	4.7216	4.6493	4.7530	4.6457	4.7442	4.6561	4.7502	**5.25**
H(9A)	1.8099	1.8590	1.8618	1.8781	1.8349	1.8768	1.8284	1.8756	1.8212	1.8790	1.8766	1.8099	1.8590	1.8618	1.8781	1.8349	1.8768	1.8284	1.8756	1.8212	1.8790	1.8766	**2.17**
H(9B)	0.8056	0.7341	0.7102	0.7022	0.6445	0.7039	0.6731	0.7057	0.6730	0.7004	0.6634	0.8056	0.7341	0.7102	0.7022	0.6445	0.7039	0.6731	0.7057	0.6730	0.7004	0.6634	**0.82**
H(10A-10C)	2.6726	2.6699	2.6563	2.6579	2.6109	2.6587	2.6264	2.6595	2.6265	2.6567	2.5934	2.7921	2.8011	2.7843	2.7858	2.7543	2.7870	2.7669	2.7882	2.7647	2.7843	2.7411	**3.38**
H(1`A-1`B)	3.1675	3.2189	3.2384	3.2480	3.2988	3.2460	3.2847	3.2440	3.2791	3.2495	3.2813	2.8967	2.7498	2.7025	2.7060	2.7267	2.7083	2.6608	2.7106	2.6562	2.7034	2.6494	**3.75**
H(2`-3`A-2`-3`B)	1.6415	1.7006	1.6633	1.7363	1.7002	1.7338	1.7248	1.7315	1.7164	1.7383	1.7452	1.6415	1.7006	1.6633	1.7362	1.7003	1.7338	1.7248	1.7315	1.7164	1.7383	1.7452	**2.125**
H(4`A)	2.8967	2.7498	2.7025	2.7060	2.7267	2.7083	2.6608	2.7106	2.6562	2.7034	2.6494	3.1675	3.2189	3.2384	3.2480	3.2988	3.2460	3.2847	3.2440	3.2791	3.2495	3.2813	**3.07**
H(4`B)	2.7921	2.8011	2.7843	2.7858	2.7543	2.7870	2.7669	2.7882	2.7647	2.7843	2.7411	2.6726	2.6699	2.6563	2.6579	2.6109	2.6587	2.6264	2.6595	2.6265	2.6567	2.5934	**3.71**

[a] methyl protons shifts are averaged [b] according to [13] in D_2O

Table S15. Cont. VIII

Nuclei	R											S									Exp. [b]
	TPSS																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	132.2641	133.0840	133.7897	133.6847	134.7535	133.6704	135.4801	133.6650	134.1718	133.7062	135.6403	132.2641	133.0840	133.7897	133.6847	134.7535	133.6704	135.4801	133.6650	134.7730	133.7062	135.6403	**130.87**
C2	133.0674	132.9479	133.5704	132.8784	133.4447	132.8875	134.0487	132.9080	133.4117	132.8806	134.0937	133.0674	132.9479	133.5704	132.8784	133.4447	132.8875	134.0486	132.9080	134.0216	132.8806	134.0937	**132.98**
C3	116.4718	117.1940	117.8453	117.5095	118.1711	117.5003	118.6061	117.5022	117.9443	117.5287	118.6500	116.4718	117.1940	117.8453	117.5095	118.1711	117.5003	118.6061	117.5022	118.7314	117.5287	118.6500	**117.44**
C4	170.9237	171.7366	172.5198	172.1547	172.9574	172.1349	173.4502	172.1270	172.7876	172.1844	173.5580	170.9237	171.7366	172.5198	172.1547	172.9574	172.1349	173.4502	172.1270	172.9465	172.1844	173.5580	**167.85**
C5	114.8428	116.0007	116.7003	116.6537	117.4628	116.6194	117.7545	116.5967	117.0352	116.6967	117.8907	114.8428	116.0007	116.7003	116.6537	117.4628	116.6194	117.7547	116.5967	117.8327	116.6967	117.8907	**117.44**
C6	129.4162	131.1766	132.3270	132.1441	133.7927	132.0860	133.7508	132.0404	132.5407	132.2105	134.1248	129.4162	131.1766	132.3270	132.1441	133.7927	132.0860	133.7508	132.0404	133.1605	132.2105	134.1248	**132.98**
C7	197.0373	201.1937	202.2474	203.5484	203.9345	203.4271	209.2336	203.3143	204.0997	203.6711	210.2340	197.0373	201.1937	202.2474	203.5484	203.9345	203.4271	209.2341	203.3143	203.8999	203.6711	210.2340	**196.75**
C8	66.0012	67.1549	67.7082	67.7955	68.4635	67.7715	69.2509	67.7570	68.0001	67.8268	69.7355	66.0012	67.1549	67.7082	67.7955	68.4635	67.7715	69.2514	67.7570	69.3593	67.8268	69.7355	**70.92**
C9	30.7677	30.7902	30.9685	30.8001	31.0228	30.8062	31.0432	30.8237	30.9191	30.8048	31.1659	30.7677	30.7902	30.9685	30.8001	31.0228	30.8062	31.0430	30.8237	32.7030	30.8048	31.1659	**23.99**
C10	9.7233	9.9403	10.1508	10.0708	10.3684	10.0697	10.2239	10.0799	10.0923	10.0820	10.3930	9.7233	9.9403	10.1508	10.0708	10.3684	10.0697	10.2239	10.0799	12.1147	10.0820	10.3930	**8.05**
C1`	53.0466	53.7459	54.0724	54.2546	54.8105	54.2292	54.8099	54.2152	54.4042	54.2892	55.2392	57.1640	58.1056	58.6056	58.6253	59.1425	58.5992	59.4957	58.5849	60.2560	58.6608	59.6823	**52.76**
C2`	26.2163	26.5883	27.0251	26.8269	27.2682	26.8177	27.3249	26.8201	26.8995	26.8464	27.1744	26.1514	26.2346	26.7011	26.3907	26.9232	26.3854	26.8882	26.3919	28.3044	26.4068	26.6826	**23.74**
C3`	26.1514	26.2346	26.7011	26.3907	26.9232	26.3854	26.8880	26.3919	26.4696	26.4068	26.6826	26.2163	26.5883	27.0251	26.8269	27.2682	26.8177	27.3249	26.8201	28.7294	26.8464	27.1744	**23.57**
C4`	57.1640	58.1056	58.6056	58.6253	59.1425	58.5992	59.4959	58.5849	58.7913	58.6608	59.6823	53.0466	53.7459	54.0724	54.2546	54.8105	54.2292	54.8103	54.2152	55.9190	54.2892	55.2392	**56.17**
H2	8.5746	8.4725	8.5182	8.4056	8.4493	8.4081	8.3993	8.4115	8.2515	8.4040	8.3901	8.5746	8.4725	8.5182	8.4056	8.4493	8.4081	8.3993	8.4115	8.5216	8.4040	8.3901	**8.11**
H3	7.1651	7.2945	7.3937	7.3411	7.4655	7.3387	7.5000	7.3369	7.1726	7.3436	7.5112	7.1651	7.2945	7.3937	7.3411	7.4655	7.3387	7.5000	7.3369	7.4551	7.3436	7.5112	**7.34**
H5	7.0301	7.2079	7.3097	7.2818	7.4197	7.2775	7.4185	7.2736	7.1091	7.2864	7.4330	7.0301	7.2079	7.3097	7.2818	7.4197	7.2775	7.4185	7.2736	7.3923	7.2864	7.4330	**7.34**
H6	7.8473	8.0023	8.1074	8.0934	8.2422	8.0870	8.2466	8.0813	7.9200	8.1001	8.2704	7.8473	8.0023	8.1074	8.0934	8.2422	8.0870	8.2466	8.0813	8.1939	8.1001	8.2704	**8.11**
H8	4.7474	4.7923	4.8456	4.8312	4.9158	4.8279	4.9258	4.8255	4.6512	4.8349	4.9134	4.7474	4.7923	4.8456	4.8312	4.9158	4.8279	4.9257	4.8255	4.9625	4.8349	4.9134	**5.25**
H(9A)	1.8688	1.9286	1.9316	1.9575	1.9856	1.9557	1.9160	1.9544	2.1079	1.9595	1.9575	1.8688	1.9286	1.9316	1.9575	1.9856	1.9557	1.9160	1.9544	2.1079	1.9595	1.9575	**2.17**
H(9B)	0.8555	0.7841	0.7648	0.7554	0.7135	0.7569	0.7299	0.7589	0.5683	0.7544	0.7198	0.8555	0.7841	0.7648	0.7554	0.7135	0.7569	0.7299	0.7589	0.9264	0.7544	0.7198	**0.82**
H(10A-10C)	2.7231	2.7294	2.7217	2.7236	2.6920	2.7240	2.7005	2.7250	2.6282	2.7237	2.6618	2.8198	2.8408	2.8356	2.8361	2.8084	2.8372	2.8232	2.8388	3.1312	2.8354	2.7975	**3.38**
H(1`A-1`B)	3.2744	3.3257	3.3531	3.3597	3.4163	3.3578	3.3950	3.3565	3.5063	3.3620	3.3875	3.0769	2.9026	2.8523	2.8498	2.8339	2.8530	2.7995	2.8570	2.9589	2.8470	2.7814	**3.75**
H(2`-3`A-2`-3`B)	1.6784	1.7377	1.7057	1.7805	1.7387	1.7779	1.7701	1.7760	2.1012	1.7833	1.7935	1.6784	1.7377	1.7057	1.7805	1.7387	1.7779	1.7701	1.7760	2.1012	1.7833	1.7935	**2.125**
H(4`A)	3.0769	2.9026	2.8523	2.8498	2.8339	2.8530	2.7996	2.8570	2.9589	2.8470	2.7814	3.2744	3.3257	3.3531	3.3597	3.4163	3.3578	3.3950	3.3565	3.5063	3.3620	3.3875	**3.07**
H(4`B)	2.8198	2.8408	2.8356	2.8361	2.8084	2.8372	2.8231	2.8388	3.1312	2.8354	2.7975	2.7231	2.7294	2.7217	2.7236	2.6920	2.7240	2.7005	2.7250	2.6282	2.7237	2.6618	**3.71**
Nuclei	VSXC																						
C1	133.7280	134.6932	135.5641	135.0028	136.7273	134.9834	135.5216	134.9625	135.6961	135.0234	135.9029	133.7280	134.6932	135.5641	135.0028	136.7273	134.9834	135.5216	134.9624	135.6960	135.0234	135.9029	**130.87**
C2	130.4484	130.4536	131.0013	130.2906	130.8229	130.3104	131.4948	130.3268	131.3582	130.2725	131.3842	130.4484	130.4536	131.0013	130.2906	130.8229	130.3104	131.4948	130.3268	131.3582	130.2725	131.3843	**132.98**
C3	115.0664	115.8768	116.4619	116.2108	116.7705	116.1954	117.1658	116.1776	117.0538	116.2268	117.1710	115.0663	115.8767	116.4619	116.2108	116.7705	116.1954	117.1658	116.1776	117.0537	116.2268	117.1710	**117.44**
C4	168.4331	169.3548	170.0092	169.8363	170.5115	169.8116	171.1646	169.7847	171.0105	169.8610	171.2657	168.4331	169.3548	170.0091	169.8363	170.5115	169.8116	171.1646	169.7847	171.0104	169.8610	171.2658	**167.85**
C5	112.6538	114.0697	114.6157	114.8678	115.5175	114.8218	115.8759	114.7736	115.7661	114.9129	116.0189	112.6537	114.0698	114.6157	114.8678	115.5175	114.8218	115.8759	114.7737	115.7662	114.9129	116.0189	**117.44**
C6	128.3780	129.9641	130.9113	130.9401	132.3261	130.8823	132.9018	130.8227	132.6820	130.9967	133.2067	128.3780	129.9641	130.9113	130.9401	132.3261	130.8823	132.9018	130.8227	132.6820	130.9967	133.2066	**132.98**
C7	193.7250	198.3258	199.6112	200.7729	201.7874	200.6184	205.4791	200.4637	204.7371	200.9227	206.6958	193.7248	198.3258	199.6113	200.7729	201.7874	200.6184	205.4791	200.4637	204.7371	200.9227	206.6956	**196.75**
C8	71.5690	72.7143	73.2527	73.3567	74.2081	73.3084	74.3399	73.2605	74.2578	73.4060	75.1245	71.5690	72.7143	73.2527	73.3567	74.2081	73.3084	74.3399	73.2605	74.2578	73.4060	75.1244	**70.92**
C9	34.1035	34.7466	34.9523	35.1716	35.3874	35.1428	35.7844	35.1127	35.6599	35.2008	36.1085	34.1034	34.7466	34.9523	35.1716	35.3874	35.1428	35.7844	35.1127	35.6599	35.2008	36.1085	**23.99**
C10	13.2393	13.8267	13.9208	14.0186	14.1425	14.0182	14.3826	14.0138	14.3677	14.0192	14.1232	13.2392	13.8267	13.9208	14.0186	14.1425	14.0182	14.3826	14.0138	14.3678	14.0192	14.1232	**8.05**
C1`	57.7470	58.3407	58.6804	58.7211	59.2365	58.7008	59.1402	58.6782	59.1025	58.7416	59.3076	61.3896	62.2048	62.5475	62.6521	63.1328	62.6279	63.1524	62.6011	63.1091	62.6764	63.3833	**52.76**
C2`	29.5603	30.0658	30.3268	30.3182	30.6584	30.3081	30.6963	30.2952	30.6602	30.3293	30.7793	28.1199	28.4650	28.7659	28.6490	29.0566	28.6415	29.0945	28.6315	29.0635	28.6574	29.0563	**23.74**
C3`	28.1198	28.4650	28.7659	28.6490	29.0566	28.6415	29.0945	28.6315	29.0635	28.6574	29.0564	29.5602	30.0658	30.3268	30.3182	30.6584	30.3081	30.6963	30.2952	30.6602	30.3293	30.7793	**23.57**
C4`	61.3898	62.2048	62.5475	62.6521	63.1328	62.6279	63.1524	62.6011	63.1091	62.6764	63.3834	57.7470	58.3407	58.6805	58.7211	59.2365	58.7008	59.1402	58.6782	59.1025	58.7416	59.3077	**56.17**
H2	8.3843	8.2653	8.2734	8.1867	8.1526	8.1942	8.2775	8.2014	8.2695	8.1792	8.2199	8.3843	8.2653	8.2734	8.1867	8.1526	8.1942	8.2775	8.2014	8.2695	8.1792	8.2199	**8.11**
H3	7.2851	7.4237	7.5085	7.4697	7.5820	7.4679	7.6070	7.4660	7.6001	7.4714	7.6202	7.2851	7.4237	7.5085	7.4697	7.5820	7.4679	7.6070	7.4660	7.6001	7.4714	7.6202	**7.34**
H5	7.0179	7.2122	7.2908	7.3003	7.4165	7.2952	7.4312	7.2902	7.4250	7.3051	7.4594	7.0179	7.2122	7.2908	7.3003	7.4165	7.2952	7.4312	7.2902	7.4250	7.3051	7.4594	**7.34**
H6	7.7692	7.9296	8.0043	8.0301	8.1595	8.0237	8.2165	8.0176	8.1960	8.0361	8.2605	7.7692	7.9296	8.0043	8.0301	8.1595	8.0237	8.2165	8.0176	8.1960	8.0361	8.2605	**8.11**
H8	4.2098	4.3417	4.3755	4.4324	4.5287	4.4254	4.5576	4.4187	4.5431	4.4392	4.6200	4.2098	4.3417	4.3755	4.4324	4.5287	4.4254	4.5576	4.4187	4.5431	4.4392	4.6200	**5.25**
H(9A)	1.9514	1.9631	1.9657	1.9943	1.9882	1.9920	1.9971	1.9899	1.9845	1.9964	2.0062	1.9514	1.9631	1.9658	1.9943	1.9882	1.9920	1.9971	1.9899	1.9845	1.9964	2.0062	**2.17**
H(9B)	0.9526	0.9054	0.8739	0.8812	0.8194	0.8830	0.8336	0.8849	0.8353	0.8793	0.8036	0.9526	0.9054	0.8739	0.8812	0.8194	0.8830	0.8336	0.8849	0.8353	0.8793	0.8036	**0.82**
H(10A-10C)	2.4410	2.4684	2.4765	2.4948	2.4779	2.4930	2.5102	2.4914	2.5048	2.4962	2.5098	2.9999	3.0269	3.0314	3.0383	3.0310	3.0366	3.0070	3.0351	3.0078	3.0400	3.0088	**3.38**
H(1`A-1`B)	3.2877	3.2961	3.3325	3.3361	3.3750	3.3335	3.3892	3.3310	3.3829	3.3383	3.3923	2.8960	2.8655	2.8597	2.8807	2.9013	2.8775	2.8342	2.8748	2.8355	2.8838	2.8671	**3.75**
H(2`-3`A-2`-3`B)	1.9324	1.9702	1.9427	2.0029	1.9645	2.0008	1.9833	1.9987	1.9778	2.0047	1.9946	1.9324	1.9702	1.9427	2.0029	1.9645	2.0008	1.9833	1.9987	1.9778	2.0047	1.9946	**2.125**
H(4`A)	2.8961	2.8655	2.8597	2.8807	2.9013	2.8775	2.8342	2.8748	2.8355	2.8838	2.8671	3.2877	3.2961	3.3325	3.3361	3.3750	3.3335	3.3892	3.3310	3.3829	3.3383	3.3923	**3.07**
H(4`B)	2.9999	3.0269	3.0314	3.0383	3.0310	3.0366	3.0070	3.0351	3.0078	3.0400	3.0088	2.4410	2.4684	2.4765	2.4948	2.4779	2.4930	2.5102	2.4914	2.5048	2.4962	2.5098	**3.71**
Nuclei	wB97																						
C1	136.4715	137.4982	138.3529	137.8181	139.4807	137.8005	139.5962	137.7822	138.5055	137.8359	139.7189	136.4715	137.4983	138.3529	137.8180	139.4808	137.8005	139.5962	137.7822	138.5056	137.8359	139.7189	**130.87**
C2	140.3386	140.3374	140.8427	140.2180	140.7137	140.2255	140.9867	140.2323	141.0674	140.2108	140.9901	140.3386	140.3375	140.8427	140.2179	140.7138	140.2255	140.9867	140.2323	141.0672	140.2109	140.9901	**132.98**
C3	121.5651	122.1795	122.7665	122.3744	123.0718	122.3643	123.3260	122.3534	123.1569	122.3841	123.3750	121.5650	122.1795	122.7665	122.3744	123.0718	122.3643	123.3260	122.3534	123.1568	122.3841	123.3750	**117.44**
C4	174.2914	174.8695	175.4567	175.2152	175.8180	175.1928	176.3449	175.1696	176.2762	175.2369	176.4646	174.2915	174.8694	175.4567	175.2153	175.8179	175.1928	176.3449	175.1696	176.2761	175.2368	176.4646	**167.85**
C5	119.5457	120.8019	121.3700	121.4824	122.2916	121.4403	122.5743	121.3972	122.3191	121.5231	122.7091	119.5458	120.8018	121.3700	121.4825	122.2916	121.4403	122.5744	121.3972	122.3192	121.5231	122.7091	**117.44**
C6	136.6600	138.3277	139.4365	139.3721	140.9844	139.3019	140.8865	139.2315	141.3412	139.4396	141.3315	136.6601	138.3277	139.4365	139.3721	140.9846	139.3019	140.8866	139.2315	141.3412	139.4397	141.3315	**132.98**
C7	201.2809	206.4139	207.5947	209.0989	209.5897	208.9323	216.0328	208.7653	213.6009	209.2593	217.0726	201.2809	206.4141	207.5947	209.0992	209.5896	208.9323	216.0330	208.7653	213.6005	209.2594	217.0726	**196.75**
C8	61.8494	62.9619	63.6230	63.5101	64.4230	63.4703	65.0089	63.4301	64.7011	63.5499	65.5141	61.8494	62.9619	63.6230	63.5102	64.4230	63.4703	65.0089	63.4301	64.7012	63.5499	65.5141	**70.92**
C9	25.9921	25.8024	25.9613	25.7593	26.0175	25.7596	25.7914	25.7598	26.0540	25.7593	25.9455	25.9921	25.8024	25.9613	25.7593	26.0175	25.7596	25.7914	25.7598	26.0539	25.7593	25.9455	**23.99**
C10	8.7286	8.9241	9.0919	9.0402	9.3256	9.0303	9.1445	9.0199	9.1755	9.0501	9.2966	8.7287	8.9240	9.0919	9.0402	9.3256	9.0303	9.1445	9.0199	9.1755	9.0501	9.2966	**8.05**
C1`	49.0447	49.7133	50.1226	50.1704	50.7840	50.1347	50.7071	50.0989	50.6714	50.2056	51.0474	52.8845	53.6761	54.0236	54.0964	54.6064	54.0680	54.7659	54.0392	54.6199	54.1238	55.0009	**52.76**
C2`	23.6938	24.0172	24.3561	24.2021	24.6518	24.1873	24.6242	24.1721	24.6351	24.2168	24.5827	23.1794	23.3501	23.6832	23.4969	23.9830	23.4857	23.9179	23.4735	23.8844	23.5084	23.7811	**23.74**
C3`	23.1794	23.3501	23.6832	23.4969	23.9829	23.4857	23.9179	23.4735	23.8843	23.5084	23.7811	23.6939	24.0172	24.3561	24.2021	24.6518	24.1873	24.6242	24.1721	24.6352	24.2168	24.5827	**23.57**
C4`	52.8844	53.6761	54.0236	54.0964	54.6064	54.0680	54.7659	54.0392	54.6199	54.1237	55.0009	49.0447	49.7133	50.1226	50.1703	50.7840	50.1347	50.7071	50.0989	50.6714	50.2056	51.0474	**56.17**
H2	8.8912	8.7744	8.7965	8.7066	8.7091	8.7108	8.6429	8.7148	8.7486	8.7025	8.6443	8.8912	8.7744	8.7965	8.7066	8.7091	8.7108	8.6429	8.7148	8.7485	8.7025	8.6443	**8.11**
H3	7.4478	7.5845	7.6762	7.6231	7.7464	7.6212	7.7598	7.6192	7.7544	7.6248	7.7750	7.4477	7.5845	7.6762	7.6231	7.7464	7.6212	7.7598	7.6192	7.7544	7.6248	7.7750	**7.34**
H5	7.2894	7.4691	7.5582	7.5493	7.6766	7.5446	7.6974	7.5397	7.6792	7.5538	7.7168	7.2894	7.4691	7.5582	7.5493	7.6766	7.5446	7.6974	7.5397	7.6792	7.5538	7.7168	**7.34**
H6	8.1426	8.3048	8.3975	8.4000	8.5390	8.3939	8.5509	8.3878	8.5772	8.4058	8.5860	8.1426	8.3048	8.3975	8.4000	8.5390	8.3939	8.5509	8.3878	8.5772	8.4058	8.5860	**8.11**
H8	4.2328	4.3054	4.3359	4.3584	4.4282	4.3554	4.5010	4.3522	4.4702	4.3612	4.5032	4.2328	4.3054	4.3359	4.3584	4.4282	4.3554	4.5010	4.3522	4.4702	4.3612	4.5032	**5.25**
H(9A)	1.7626	1.7953	1.8009	1.8181	1.8468	1.8161	1.7536	1.8141	1.8419	1.8201	1.8072	1.7626	1.7953	1.8009	1.8181	1.8468	1.8161	1.7536	1.8141	1.8419	1.8201	1.8072	**2.17**
H(9B)	0.8698	0.7882	0.7561	0.7496	0.6888	0.7519	0.7139	0.7542	0.7134	0.7473	0.7068	0.8698	0.7882	0.7561	0.7496	0.6888	0.7519	0.7139	0.7542	0.7134	0.7473	0.7068	**0.82**
H(10A-10C)	2.6220	2.6189	2.6000	2.6061	2.5613	2.6072	2.5671	2.6082	2.5759	2.6051	2.5434	2.7679	2.7857	2.7744	2.7734	2.7454	2.7743	2.7589	2.7750	2.7559	2.7727	2.7361	**3.38**
H(1`A-1`B)	3.0470	3.0923	3.1134	3.1216	3.1806	3.1197	3.1609	3.1177	3.1667	3.1236	3.1676	2.7543	2.6470	2.6089	2.6056	2.6021	2.6078	2.5884	2.6101	2.5566	2.6037	2.5809	**3.75**
H(2`-3`A-2`-3`B)	1.6369	1.6930	1.6588	1.7277	1.6862	1.7252	1.7182	1.7227	1.6991	1.7301	1.7380	1.6369	1.6930	1.6588	1.7277	1.6862	1.7252	1.7182	1.7227	1.6991	1.7301	1.7380	**2.125**
H(4`A)	2.7543	2.6469	2.6089	2.6056	2.6021	2.6078	2.5884	2.6101	2.5566	2.6037	2.5809	3.0470	3.0924	3.1134	3.1216	3.1806	3.1197	3.1609	3.1177	3.1667	3.1236	3.1676	**3.07**
H(4`B)	2.7679	2.7857	2.7744	2.7734	2.7454	2.7743	2.7589	2.7750	2.7559	2.7727	2.7361	2.6220	2.6189	2.6000	2.6062	2.5614	2.6072	2.5671	2.6082	2.5758	2.6051	2.5434	**3.71**

[a] methyl protons shifts are averaged [b] according to [13] in D_2O

Table S15. Cont. IX

Nuclei	R											S										Exp. [b]
	wB97X																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	137.9830	139.0482	139.8060	139.5364	141.1650	139.5166	141.2990	139.4954	141.2743	139.5564	141.3764	137.9830	139.0482	139.8059	139.5364	141.1651	139.5164	141.2989	139.4954	141.2743	139.5564	141.3764	**130.87**
C2	140.7860	140.7835	141.2973	140.6375	141.1362	140.6493	141.4998	140.6599	141.3622	140.6273	141.4804	140.7860	140.7835	141.2974	140.6375	141.1360	140.6492	141.4997	140.6599	141.3621	140.6273	141.4804	**132.98**
C3	122.2992	122.9286	123.5157	123.1405	123.8317	123.1319	124.1281	123.1221	124.0161	123.1493	124.1691	122.2992	122.9286	123.5157	123.1405	123.8318	123.1319	124.1281	123.1221	124.0162	123.1493	124.1691	**117.44**
C4	174.9955	175.6067	176.2121	175.9505	176.5643	175.9303	177.1378	175.9096	176.9404	175.9705	177.2458	174.9955	175.6067	176.2121	175.9505	176.5643	175.9305	177.1378	175.9096	176.9405	175.9705	177.2458	**167.85**
C5	120.2576	121.5322	122.0896	122.2505	123.0290	122.2094	123.3458	122.1674	123.1869	122.2903	123.4854	120.2576	121.5322	122.0897	122.2505	123.0291	122.2095	123.3457	122.1674	123.1867	122.2903	123.4854	**117.44**
C6	136.9905	138.6834	139.7981	139.6463	141.2466	139.5822	141.2105	139.5179	140.9330	139.7087	141.6533	136.9905	138.6834	139.7981	139.6463	141.2466	139.5821	141.2105	139.5179	140.9329	139.7087	141.6533	**132.98**
C7	202.9716	208.1012	209.1816	210.9432	211.4273	210.7756	217.8480	210.6072	216.5197	211.1040	218.8241	202.9716	208.1012	209.1818	210.9432	211.4273	210.7756	217.8480	210.6072	216.5199	211.1040	218.8241	**196.75**
C8	63.1303	64.3000	64.8617	64.8702	65.7803	64.8329	66.3427	64.7956	66.0749	64.9076	66.8277	63.1303	64.3000	64.8617	64.8702	65.7803	64.8329	66.3427	64.7956	66.0748	64.9076	66.8277	**70.92**
C9	26.6275	26.4303	26.5843	26.3609	26.5989	26.3647	26.4199	26.3679	26.2820	26.3585	26.5577	26.6275	26.4303	26.5842	26.3609	26.5988	26.3646	26.4199	26.3679	26.2820	26.3585	26.5577	**23.99**
C10	8.4666	8.6763	8.8401	8.7934	9.0797	8.7858	8.9301	8.7776	8.8457	8.8020	9.0521	8.4666	8.6763	8.8401	8.7934	9.0797	8.7858	8.9301	8.7776	8.8458	8.8020	9.0521	**8.05**
C1`	49.8215	50.5463	50.9191	50.9979	51.6134	50.9662	51.5712	50.9344	51.4424	51.0299	51.9289	53.8553	54.7231	55.0669	55.1617	55.6641	55.1351	55.8860	55.1079	55.7630	55.1881	56.0917	**52.76**
C2`	24.1830	24.5088	24.8229	24.6774	25.1231	24.6667	25.1168	24.6555	25.0332	24.6888	25.0304	23.6812	23.8106	24.1356	23.9541	24.4370	23.9459	24.4073	23.9370	24.3440	23.9630	24.2469	**23.74**
C3`	23.6812	23.8106	24.1356	23.9541	24.4371	23.9458	24.4073	23.9370	24.3441	23.9630	24.2469	24.1830	24.5088	24.8229	24.6774	25.1232	24.6668	25.1167	24.6555	25.0332	24.6888	25.0304	**23.57**
C4`	53.8553	54.7231	55.0668	55.1617	55.6640	55.1352	55.8861	55.1079	55.7630	55.1881	56.0917	49.8215	50.5463	50.9191	50.9979	51.6134	50.9660	51.5711	50.9344	51.4425	51.0299	51.9289	**56.17**
H2	8.8647	8.7427	8.7777	8.6608	8.6643	8.6655	8.6073	8.6702	8.6121	8.6564	8.6060	8.8647	8.7427	8.7777	8.6608	8.6642	8.6655	8.6073	8.6702	8.6121	8.6564	8.6060	**8.11**
H3	7.4264	7.5632	7.6561	7.6010	7.7238	7.5993	7.7352	7.5976	7.7243	7.6027	7.7481	7.4264	7.5632	7.6562	7.6010	7.7238	7.5993	7.7352	7.5976	7.7243	7.6026	7.7481	**7.34**
H5	7.2645	7.4481	7.5366	7.5331	7.6574	7.5284	7.6810	7.5236	7.6672	7.5377	7.6989	7.2645	7.4481	7.5366	7.5331	7.6574	7.5284	7.6810	7.5236	7.6672	7.5377	7.6989	**7.34**
H6	8.1139	8.2707	8.3651	8.3651	8.5022	8.3592	8.5158	8.3533	8.4994	8.3709	8.5478	8.1139	8.2707	8.3651	8.3651	8.5022	8.3592	8.5158	8.3533	8.4994	8.3709	8.5478	**8.11**
H8	4.3176	4.3805	4.4139	4.4376	4.5041	4.4344	4.5712	4.4313	4.5575	4.4406	4.5678	4.3176	4.3805	4.4139	4.4376	4.5041	4.4344	4.5712	4.4313	4.5575	4.4406	4.5678	**5.25**
H(9A)	1.7496	1.7862	1.7928	1.8007	1.8289	1.7991	1.7430	1.7976	1.7331	1.8023	1.7924	1.7496	1.7862	1.7928	1.8007	1.8288	1.7991	1.7430	1.7976	1.7331	1.8023	1.7924	**2.17**
H(9B)	0.8498	0.7721	0.7445	0.7376	0.6776	0.7397	0.7077	0.7420	0.7064	0.7355	0.6982	0.8498	0.7721	0.7445	0.7376	0.6776	0.7397	0.7077	0.7420	0.7064	0.7355	0.6982	**0.82**
H(10A-10C)	2.6487	2.6424	2.6262	2.6308	2.5842	2.6321	2.5951	2.6333	2.5949	2.6297	2.5657	2.7860	2.7985	2.7819	2.7859	2.7560	2.7870	2.7658	2.7881	2.7636	2.7850	2.7433	**3.38**
H(1`A-1`B)	3.0657	3.1103	3.1314	3.1418	3.1997	3.1400	3.1815	3.1382	3.1753	3.1436	3.1835	2.7788	2.6588	2.6222	2.6275	2.6230	2.6296	2.5996	2.6318	2.5941	2.6258	2.5932	**3.75**
H(2`-3`A-2`-3`B)	1.6367	1.6947	1.6589	1.7322	1.6883	1.7299	1.7211	1.7276	1.7132	1.7345	1.7393	1.6367	1.6947	1.6589	1.7322	1.6883	1.7299	1.7211	1.7276	1.7132	1.7345	1.7393	**2.125**
H(4`A)	2.7788	2.6588	2.6222	2.6275	2.6230	2.6297	2.5996	2.6318	2.5940	2.6258	2.5932	3.0657	3.1103	3.1314	3.1418	3.1997	3.1399	3.1815	3.1382	3.1753	3.1436	3.1835	**3.07**
H(4`B)	2.7860	2.7985	2.7820	2.7859	2.7560	2.7870	2.7658	2.7881	2.7636	2.7850	2.7433	2.6487	2.6424	2.6262	2.6308	2.5842	2.6321	2.5951	2.6333	2.5949	2.6297	2.5657	**3.71**
Nuclei	X3LYP																						
C1	139.5222	140.7607	141.1293	141.3841	143.5908	141.3514	142.9167	141.3142	142.8989	141.4174	143.1602	139.5222	140.7607	141.1292	141.3841	143.5908	141.3514	142.9167	141.3143	142.8989	141.4174	143.1602	**130.87**
C2	139.9181	139.7948	140.3308	139.7109	140.3553	139.7181	140.8143	139.7227	140.7218	139.7079	140.8575	139.9181	139.7948	140.3308	139.7109	140.3553	139.7181	140.8143	139.7227	140.7218	139.7080	140.8575	**132.98**
C3	121.8779	122.6466	123.1545	122.9205	123.6176	122.9097	123.8817	122.8955	123.8237	122.9339	123.9214	121.8779	122.6466	123.1545	122.9205	123.6176	122.9097	123.8817	122.8955	123.8237	122.9338	123.9215	**117.44**
C4	176.3560	177.1647	177.8267	177.5511	178.1892	177.5311	178.7567	177.5084	178.6257	177.5739	178.8657	176.3560	177.1647	177.8267	177.5511	178.1892	177.5311	178.7566	177.5083	178.6257	177.5739	178.8657	**167.85**
C5	120.0151	121.2676	121.8657	121.9258	122.6895	121.8889	122.9009	121.8487	122.8058	121.9650	123.0342	120.0151	121.2676	121.8656	121.9258	122.6895	121.8889	122.9008	121.8487	122.8058	121.9649	123.0342	**117.44**
C6	135.9756	137.7439	139.0035	138.7304	139.8686	138.6734	140.4766	138.6134	140.2661	138.7888	140.8151	135.9756	137.7439	139.0035	138.7304	139.8686	138.6734	140.4765	138.6134	140.2661	138.7888	140.8150	**132.98**
C7	203.5301	208.6866	209.4913	211.4296	212.4724	211.2679	217.7136	211.1015	216.4892	211.5846	218.8023	203.5301	208.6866	209.4912	211.4296	212.4723	211.2679	217.7137	211.1016	216.4892	211.5844	218.8023	**196.75**
C8	66.0902	67.4350	67.8541	68.0432	68.7185	68.0169	69.4778	67.9857	69.2630	68.0697	69.8630	66.0902	67.4350	67.8541	68.0432	68.7185	68.0169	69.4779	67.9857	69.2630	68.0698	69.8631	**70.92**
C9	29.4339	29.2958	29.4371	29.2287	29.0527	29.2418	29.3969	29.2509	29.3136	29.2193	29.4187	29.4339	29.2958	29.4372	29.2287	29.0528	29.2418	29.3969	29.2509	29.3136	29.2192	29.4187	**23.99**
C10	8.4213	8.7234	8.8794	8.8466	9.0380	8.8444	8.9694	8.8388	8.9640	8.8520	9.0427	8.4213	8.7234	8.8793	8.8466	9.0381	8.8444	8.9694	8.8387	8.9640	8.8519	9.0427	**8.05**
C1`	52.1043	52.9278	53.2322	53.4597	54.0550	53.4272	54.0405	53.3919	53.9804	53.4938	54.4469	56.5857	57.5886	57.9503	58.1088	58.7263	58.0776	58.8650	58.0439	58.8046	58.1428	59.0926	**52.76**
C2`	25.8450	26.2989	26.6477	26.5107	26.9310	26.5006	26.9968	26.4878	26.9852	26.5243	26.8383	25.6256	25.7431	26.1166	25.8996	26.4923	25.8912	26.3335	25.8800	26.3405	25.9118	26.1331	**23.74**
C3`	25.6256	25.7431	26.1166	25.8996	26.4924	25.8912	26.3335	25.8802	26.3405	25.9117	26.1331	25.8450	26.2989	26.6477	26.5107	26.9310	26.5006	26.9969	26.4878	26.9852	26.5241	26.8382	**23.57**
C4`	56.5857	57.5886	57.9503	58.1088	58.7263	58.0776	58.8650	58.0439	58.8046	58.1428	59.0925	52.1043	52.9278	53.2322	53.4597	54.0549	53.4272	54.0404	53.3918	53.9804	53.4939	54.4470	**56.17**
H2	8.7117	8.5765	8.6446	8.5069	8.4840	8.5109	8.5016	8.5146	8.5097	8.5032	8.4948	8.7117	8.5765	8.6446	8.5069	8.4840	8.5109	8.5016	8.5146	8.5097	8.5032	8.4948	**8.11**
H3	7.3131	7.4425	7.5320	7.4931	7.6189	7.4906	7.6397	7.4875	7.6313	7.4954	7.6535	7.3131	7.4425	7.5320	7.4931	7.6189	7.4906	7.6397	7.4875	7.6313	7.4954	7.6535	**7.34**
H5	7.1769	7.3467	7.4500	7.4173	7.5305	7.4134	7.5453	7.4091	7.5359	7.4209	7.5631	7.1769	7.3467	7.4500	7.4173	7.5305	7.4134	7.5453	7.4091	7.5359	7.4209	7.5631	**7.34**
H6	7.9778	8.1278	8.2412	8.2280	8.3470	8.2215	8.3829	8.2145	8.3694	8.2344	8.4056	7.9778	8.1278	8.2412	8.2280	8.3470	8.2215	8.3829	8.2145	8.3694	8.2344	8.4056	**8.11**
H8	4.6121	4.6620	4.7151	4.7073	4.7862	4.7040	4.7948	4.7004	4.7855	4.7106	4.7797	4.6121	4.6620	4.7151	4.7073	4.7862	4.7040	4.7948	4.7004	4.7855	4.7106	4.7797	**5.25**
H(9A)	1.7924	1.8387	1.8593	1.8626	1.8155	1.8621	1.8328	1.8608	1.8288	1.8631	1.8655	1.7924	1.8387	1.8593	1.8626	1.8155	1.8621	1.8328	1.8608	1.8288	1.8631	1.8655	**2.17**
H(9B)	0.8536	0.7792	0.7576	0.7546	0.7110	0.7560	0.7265	0.7571	0.7277	0.7534	0.7200	0.8536	0.7792	0.7576	0.7546	0.7110	0.7560	0.7265	0.7571	0.7277	0.7534	0.7200	**0.82**
H(10A-10C)	2.7540	2.7532	2.7337	2.7418	2.6949	2.7430	2.7063	2.7438	2.7086	2.7406	2.6741	2.8717	2.8772	2.8625	2.8603	2.8233	2.8621	2.8330	2.8634	2.8353	2.8585	2.8016	**3.38**
H(1`A-1`B)	3.1966	3.2533	3.2813	3.2909	3.3399	3.2890	3.3249	3.2866	3.3220	3.2926	3.3248	2.9062	2.7698	2.7172	2.7339	2.7211	2.7366	2.6911	2.7387	2.6891	2.7313	2.6844	**3.75**
H(2`-3`A-2`-3`B)	1.6692	1.7293	1.6903	1.7712	1.7349	1.7686	1.7512	1.7654	1.7458	1.7738	1.7734	1.6692	1.7293	1.6903	1.7712	1.7349	1.7686	1.7512	1.7654	1.7458	1.7738	1.7734	**2.125**
H(4`A)	2.9062	2.7698	2.7172	2.7339	2.7211	2.7366	2.6911	2.7387	2.6891	2.7313	2.6844	3.1966	3.2533	3.2813	3.2909	3.3399	3.2890	3.3249	3.2866	3.3220	3.2926	3.3248	**3.07**
H(4`B)	2.8717	2.8772	2.8625	2.8603	2.8233	2.8621	2.8330	2.8634	2.8353	2.8585	2.8016	2.7540	2.7532	2.7337	2.7418	2.6948	2.7430	2.7063	2.7438	2.7086	2.7406	2.6741	**3.71**

[a] methyl protons shifts are averaged [b] according to [13] in D_2O

Table S16. Theoretical chemical shifts (in ppm) of *(R,S)*-2-trifluoromethylmethcathinone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S									Exp. [b]
	B3LYP																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	150.1404	149.4187	150.4884	148.9518	150.8615	148.9716	149.4613	148.9921	149.6921	148.9331	149.5826	149.7819	149.3390	150.2812	149.0096	150.7252	149.0235	149.1859	149.0364	149.6472	148.9942	149.5506	**135.7**
C2	138.5752	136.9781	137.0701	136.1928	136.1651	136.2369	136.3873	136.2807	136.3935	136.1488	136.2514	138.4510	136.6988	136.7466	135.9706	135.9954	136.0068	136.3808	136.0439	136.2022	135.9358	136.1504	**126.6**
C3	134.2983	135.1413	135.8856	135.4137	136.3975	135.3954	136.5042	135.3764	136.4255	135.4284	136.5526	134.3488	135.0734	135.8497	135.3445	136.3957	135.3248	136.5817	135.3053	136.4115	135.3617	136.5256	**128.9**
C4	135.3264	137.6361	138.3471	138.6413	139.2052	138.5810	140.1885	138.5197	139.9450	138.6959	140.2980	135.3803	137.3481	137.9498	138.1955	138.8127	138.1435	139.7546	138.0917	139.3533	138.2432	139.7127	**129.8**
C5	136.6391	138.9217	139.6736	139.9095	140.9873	139.8488	141.0939	139.7873	140.9620	139.9647	141.2989	136.9379	139.1987	140.0497	140.1523	141.2779	140.0925	141.3818	140.0322	141.2506	140.2069	141.5481	**133.8**
C6	133.0544	134.8758	136.0239	135.8531	137.1403	135.7865	137.6984	135.7203	137.5257	135.9160	137.8220	132.4974	133.9032	134.7515	134.5636	135.8551	134.5198	136.5894	134.4768	136.1382	134.6045	136.4793	**133.9**
C7	210.2010	215.8142	217.6258	218.8241	219.9250	218.6221	224.9995	218.4232	223.8953	219.0186	225.9935	212.9008	218.1524	219.7527	220.8932	221.8488	220.7255	226.1166	220.5578	225.3923	221.0504	227.1695	**199.2**
C8	69.5880	70.6990	71.3328	71.1238	71.9389	71.0887	72.4351	71.0545	72.2827	71.1570	73.1970	65.3805	66.6140	67.2477	67.1013	67.9001	67.0659	67.9000	67.0297	68.0435	67.1322	68.5138	**62.9**
C9	21.0797	21.4456	21.6750	21.6726	21.9546	21.6513	22.1225	21.6306	22.0586	21.6922	22.2345	18.1325	18.1892	18.2839	18.1981	18.3444	18.1889	18.5253	18.1807	18.4361	18.2063	18.8830	**14.1**
C2``	134.7806	136.2639	137.1862	136.8809	138.2210	136.8400	138.0970	136.7988	138.0284	136.9180	138.1923	135.0163	136.4804	137.4469	137.0319	138.4030	136.9956	138.3207	136.9589	138.2467	137.0647	138.4111	**123**
C8`	36.6417	37.2927	37.5076	37.6235	37.9729	37.5963	38.1725	37.5691	38.1592	37.6486	38.5899	30.7846	31.2067	31.4593	31.5085	31.8103	31.4853	32.0142	31.4624	31.9236	31.5293	31.9935	**31.6**
H(3-4)	7.8412	7.9975	8.0479	8.0599	8.1272	8.0562	8.1610	8.0524	8.1465	8.0632	8.1808	7.8272	7.9696	8.0187	8.0293	8.0989	8.0256	8.1334	8.0219	8.1125	8.0325	8.1455	**7.93**
H(5-6)	7.6114	7.8480	7.9338	7.9630	8.0699	7.9559	8.1199	7.9488	8.1030	7.9696	8.1431	7.6028	7.7957	7.8638	7.8818	7.9910	7.8767	8.0344	7.8714	8.0017	7.8866	8.0438	**7.835**
H8	4.0912	4.2484	4.3184	4.3513	4.4380	4.3443	4.5006	4.3374	4.4733	4.3579	4.5181	4.3344	4.5084	4.5650	4.6018	4.7236	4.5959	4.8125	4.5900	4.7617	4.6074	4.8141	**5.01**
H(9A-9C)	1.2145	1.2326	1.2321	1.2371	1.2203	1.2364	1.2483	1.2357	1.2429	1.2377	1.2572	1.3042	1.3258	1.3087	1.3412	1.3194	1.3398	1.3412	1.3384	1.3322	1.3425	1.3573	**1.46**
H(8`A-8`C)	2.6298	2.5658	2.5235	2.5414	2.5103	2.5422	2.4988	2.5430	2.4965	2.5406	2.4859	2.8023	2.6593	2.6048	2.5851	2.5436	2.5899	2.4943	2.5948	2.4931	2.5806	2.4545	**2.83**
Nuclei	B3P86																						
C1	147.6344	146.9587	147.9807	146.5242	148.4608	146.5733	147.0474	146.6004	147.3577	146.5214	147.2229	147.4022	147.0096	147.7838	146.7052	148.3706	146.7453	146.7390	146.7636	147.4406	146.7111	147.2830	**135.7**
C2	136.9546	135.4167	135.5319	134.7099	134.7237	134.7709	134.9318	134.8105	135.0427	134.6961	134.8264	136.8498	135.1794	135.4682	134.5461	134.7056	134.6011	135.0703	134.6346	134.9580	134.5385	134.7910	**126.6**
C3	133.2428	134.0816	134.8613	134.4093	135.4108	134.4111	135.5445	134.3909	135.5756	134.4511	135.6149	133.2909	133.9834	134.8800	134.2976	135.4296	134.2991	135.6535	134.2790	135.5214	134.3399	135.5527	**128.9**
C4	134.5226	136.8094	137.5962	137.8797	138.5172	137.8371	139.4790	137.7724	139.3389	137.9638	139.6122	134.5194	136.4942	137.3203	137.3986	138.1765	137.3661	139.1679	137.3115	138.7924	137.4731	139.0433	**129.8**
C5	135.6000	137.8823	138.7445	138.9230	140.1010	138.8831	140.2236	138.8210	140.2067	139.0041	140.4450	135.9007	138.1487	139.0655	139.1531	140.3537	139.1158	140.4703	139.0559	140.4347	139.2321	140.6411	**133.8**
C6	132.0421	133.7728	134.9215	134.7854	136.0807	134.7401	136.5917	134.6737	136.5264	134.8735	136.7269	131.3931	132.8120	133.9150	133.5458	134.9807	133.5203	135.8027	133.4725	135.3504	133.6140	135.5338	**133.9**
C7	208.6257	213.8924	215.5287	216.6799	217.8161	216.5302	222.6038	216.3589	221.5348	216.8660	223.6272	210.8173	216.0216	217.2873	218.6237	219.4589	218.4819	223.6680	218.3198	223.1257	218.8029	224.8729	**199.2**
C8	67.8554	68.9518	69.6414	69.4143	70.2654	69.4087	70.7910	69.3814	70.7013	69.4635	71.6196	63.5458	64.6615	65.0216	65.1559	65.8482	65.1455	65.8415	65.1137	66.1904	65.2096	66.6421	**62.9**
C9	20.7243	21.0379	21.1990	21.3081	21.5590	21.3106	21.6502	21.2914	21.6702	21.3496	21.8323	17.6703	17.7569	17.8911	17.9177	18.0784	17.9286	18.2357	17.9170	18.3066	17.9506	18.6454	**14.1**
C2``	131.6986	133.0497	133.9810	133.6432	134.9610	133.6288	134.8350	133.5923	134.8866	133.7008	134.9449	131.9400	133.2456	134.2197	133.7821	135.1281	133.7717	135.0302	133.7392	135.0648	133.8357	135.1410	**123**
C8`	36.0737	36.6814	36.9086	36.9949	37.3311	36.9955	37.5330	36.9745	37.5981	37.0386	37.9850	29.9899	30.4783	30.7451	30.7950	31.0877	30.7906	31.3835	30.7648	31.3567	30.8435	31.3817	**31.6**
H(3-4)	7.8930	8.0524	8.1076	8.1176	8.1874	8.1151	8.2232	8.1107	8.2147	8.1212	8.2438	7.8748	8.0205	8.0802	8.0826	8.1595	8.0803	8.1979	8.0760	8.1789	8.0861	8.2063	**7.93**
H(5-6)	7.6703	7.9049	7.9892	8.0212	8.1258	8.0152	8.1741	8.0075	8.1614	8.0281	8.1984	7.6487	7.8473	7.9337	7.9365	8.0568	7.9324	8.1062	7.9265	8.0717	7.9416	8.1055	**7.835**
H8	4.1450	4.2944	4.3520	4.4033	4.4756	4.3971	4.5401	4.3892	4.5153	4.4106	4.5609	4.4008	4.5733	4.6644	4.6687	4.8075	4.6643	4.8964	4.6580	4.8436	4.6742	4.8841	**5.01**
H(9A-9C)	1.2043	1.2231	1.2132	1.2265	1.2073	1.2275	1.2317	1.2268	1.2291	1.2268	1.2465	1.2804	1.3082	1.2934	1.3227	1.3028	1.3229	1.3277	1.3213	1.3231	1.3239	1.3460	**1.46**
H(8`A-8`C)	2.6055	2.5401	2.4996	2.5122	2.4810	2.5148	2.4639	2.5155	2.4679	2.5111	2.4529	2.7300	2.5999	2.5469	2.5289	2.4859	2.5341	2.4488	2.5377	2.4500	2.5252	2.4091	**2.83**
Nuclei	B3PW91																						
C1	147.8171	147.2010	148.1502	146.7667	149.0034	146.7956	147.2556	146.8162	147.4786	146.7422	147.4144	147.6071	147.2558	148.0265	146.9542	148.5960	146.9795	147.0832	146.9956	147.5302	146.9322	147.5041	**135.7**
C2	136.9686	135.4458	135.5379	134.7398	135.0911	134.7875	134.9717	134.8263	134.9905	134.6968	134.8729	136.7993	135.1370	135.3047	134.4983	134.6610	134.5370	134.9568	134.5676	134.8180	134.4641	134.7316	**126.6**
C3	133.4069	134.2500	134.9691	134.5540	135.8862	134.5425	135.6769	134.5215	135.6085	134.5668	135.7504	133.4308	134.1455	134.9687	134.4508	135.5779	134.4371	135.7302	134.4147	135.5767	134.4659	135.6754	**128.9**
C4	134.5445	136.8415	137.5626	137.8908	138.8325	137.8357	139.4696	137.7711	139.2420	137.9444	139.6130	134.5295	136.4914	137.2103	137.3838	138.1584	137.3354	139.0482	137.2781	138.6784	137.4316	138.9985	**129.8**
C5	135.6484	137.9449	138.7264	138.9653	140.4463	138.9114	140.2472	138.8481	140.1329	139.0178	140.4701	135.9492	138.2122	139.0450	139.1925	140.3783	139.1408	140.4750	139.0799	140.3602	139.2430	140.6612	**133.8**
C6	132.2155	133.9788	135.0466	134.9672	136.5458	134.9083	136.7129	134.8411	136.5703	135.0260	136.8709	131.5281	132.9207	133.9015	133.6323	135.0717	133.5909	135.7299	133.5408	135.3408	133.6738	135.5840	**133.9**
C7	208.4633	213.8940	215.4564	216.7544	218.1369	216.5743	222.6876	216.3879	221.5323	216.9295	223.7177	210.6843	215.9997	217.3767	218.7049	219.5089	218.5426	223.8830	218.3720	223.1109	218.8619	225.0123	**199.2**
C8	67.7192	68.8892	69.4234	69.3329	70.4661	69.3070	70.6298	69.2731	70.4542	69.3605	71.4522	63.6150	64.8249	65.2063	65.3144	65.9837	65.2901	66.0927	65.2572	66.2157	65.3396	66.7965	**62.9**
C9	20.4840	20.8435	20.9580	21.0984	21.6757	21.0867	21.4680	21.0664	21.4051	21.1120	21.6362	17.4189	17.5144	17.5985	17.6515	17.8121	17.6469	17.9980	17.6333	17.9493	17.6569	18.3791	**14.1**
C2``	131.8964	133.2808	134.1427	133.8688	135.4915	133.8389	135.0448	133.7999	134.9967	133.8992	135.1521	132.1301	133.4739	134.3690	133.9976	135.3307	133.9722	135.2301	133.9378	135.1737	134.0235	135.3389	**123**
C8`	36.0178	36.6764	36.8243	37.0022	37.6556	36.9838	37.5064	36.9573	37.4794	37.0220	37.9635	30.0710	30.5535	30.8023	30.8874	31.2085	30.8663	31.4050	30.8374	31.3376	30.9100	31.4282	**31.6**
H(3-4)	7.8882	8.0453	8.1013	8.1113	8.1954	8.1081	8.2193	8.1046	8.2068	8.1144	8.2377	7.8703	8.0132	8.0715	8.0767	8.1520	8.0734	8.1900	8.0699	8.1711	8.0799	8.1989	**7.93**
H(5-6)	7.6671	7.9007	7.9873	8.0184	8.1359	8.0119	8.1722	8.0050	8.1570	8.0248	8.1954	7.6425	7.8359	7.9188	7.9266	8.0461	7.9216	8.0908	7.9163	8.0608	7.9315	8.0942	**7.835**
H8	4.1160	4.2686	4.3322	4.3787	4.4624	4.3721	4.5163	4.3652	4.4911	4.3851	4.5341	4.3645	4.5301	4.6129	4.6285	4.7649	4.6228	4.8496	4.6169	4.8027	4.6339	4.8415	**5.01**
H(9A-9C)	1.1911	1.2094	1.2027	1.2153	1.2107	1.2153	1.2216	1.2151	1.2162	1.2155	1.2334	1.2618	1.2883	1.2743	1.3063	1.2830	1.3055	1.3113	1.3045	1.3022	1.3073	1.3268	**1.46**
H(8`A-8`C)	2.5773	2.5138	2.4731	2.4891	2.4720	2.4908	2.4449	2.4922	2.4441	2.4878	2.4311	2.6989	2.5654	2.5222	2.5011	2.4601	2.5050	2.4215	2.5087	2.4202	2.4976	2.3824	**2.83**
Nuclei	B98																						
C1	148.8028	148.0638	149.1372	147.6537	149.5759	147.6900	148.1239	147.7252	148.3790	147.6232	148.2652	148.5364	148.0565	148.9652	147.8017	149.5300	147.8371	148.0429	147.8690	148.4469	147.7700	148.3913	**135.7**
C2	137.8782	136.2959	136.4042	135.5700	135.6370	135.6282	135.8153	135.6838	135.8437	135.5164	135.6910	137.6028	135.8885	135.9775	135.2187	135.3382	135.2673	135.5944	135.3143	135.4912	135.1755	135.3860	**126.6**
C3	133.0239	133.8261	134.5631	134.1296	135.1631	134.1290	135.2509	134.1250	135.1950	134.1317	135.3001	133.0821	133.7597	134.5564	134.0537	135.1580	134.0497	135.2791	134.0429	135.1447	134.0603	135.2303	**128.9**
C4	134.2148	136.4509	137.1496	137.4662	138.0820	137.4241	139.0602	137.3786	138.8354	137.5073	139.1683	134.2163	136.1256	136.7678	136.9836	137.6842	136.9455	138.5270	136.9048	138.1999	137.0222	138.4970	**129.8**
C5	135.4329	137.6263	138.3835	138.6225	139.7468	138.5807	139.8525	138.5355	139.7474	138.6635	140.0569	135.7490	137.9207	138.7541	138.8895	140.0432	138.8491	140.1044	138.8059	140.0096	138.9294	140.2863	**133.8**
C6	132.0419	133.7402	134.8789	134.7340	136.0384	134.6841	136.6242	134.6328	136.4700	134.7848	136.7280	131.3444	132.6899	133.6005	133.3417	134.7114	133.3095	135.3424	133.2759	134.9690	133.3748	135.2124	**133.9**
C7	206.6319	212.1485	213.9690	215.1873	216.2510	215.0030	221.3177	214.8195	220.2121	215.3712	222.3159	208.8974	214.2039	215.8427	216.9627	217.9781	216.8064	222.3571	216.6475	221.5473	217.1131	223.4052	**199.2**
C8	69.5363	70.5575	71.2601	71.0417	71.9068	71.0230	72.3072	71.0036	72.1792	71.0642	73.0805	65.4239	66.5030	67.0850	67.0286	67.8212	67.0169	67.8914	67.0024	67.9782	67.0419	68.5071	**62.9**
C9	21.4035	21.7151	21.9356	21.9563	22.2721	21.9540	22.3869	21.9500	22.3415	21.9623	22.5201	18.4601	18.4550	18.5522	18.5862	18.7079	18.5915	18.8908	18.5941	18.8259	18.5833	19.2509	**14.1**
C2``	130.4863	131.8174	132.7161	132.4290	133.7576	132.4078	133.6295	132.3838	133.5881	132.4512	133.7198	130.7415	132.0500	132.9748	132.5928	133.9413	132.5768	133.8298	132.5582	133.7806	132.6101	133.9327	**123**
C8`	36.8265	37.4261	37.6560	37.7913	38.1360	37.7820	38.3029	37.7708	38.3045	37.8037	38.7269	30.8870	31.3280	31.6071	31.6774	32.0365	31.6657	32.1587	31.6514	32.1297	31.6908	32.1810	**31.6**
H(3-4)	7.8668	8.0217	8.0742	8.0835	8.1595	8.0802	8.1948	8.0770	8.1825	8.0868	8.2116	7.8511	7.9961	8.0537	8.0603	8.1369	8.0566	8.1684	8.0531	8.1516	8.0640	8.1788	**7.93**
H(5-6)	7.6456	7.8770	7.9687	7.9939	8.1073	7.9870	8.1602	7.9802	8.1448	8.0008	8.1808	7.6275	7.8236	7.9035	7.9121	8.0317	7.9067	8.0687	7.9014	8.0427	7.9174	8.0753	**7.835**
H8	4.0775	4.2323	4.2997	4.3347	4.4236	4.3279	4.4887	4.3213	4.4635	4.3416	4.5029	4.3151	4.4879	4.5599	4.5830	4.7164	4.5768	4.7946	4.5708	4.7502	4.5892	4.7880	**5.01**
H(9A-9C)	1.2059	1.2200	1.2252	1.2256	1.2132	1.2251	1.2391	1.2248	1.2353	1.2265	1.2466	1.2805	1.3032	1.2924	1.3216	1.3033	1.3203	1.3219	1.3191	1.3157	1.3232	1.3365	**1.46**
H(8`A-8`C)	2.6013	2.5425	2.5020	2.5191	2.4889	2.5202	2.4785	2.5215	2.4783	2.5183	2.4642	2.7431	2.6059	2.5665	2.5338	2.4977	2.5372	2.4549	2.5410	2.4567	2.5308	2.4153	**2.83**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S16. Cont. I

Nuclei	R											S										Exp. [b]
	B971											B971										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	148.4478	147.7260	148.7779	147.3389	149.2197	147.3651	147.8059	147.3915	148.0715	147.3219	147.9364	148.1803	147.7243	148.5998	147.4675	149.1684	147.4933	147.8109	147.5182	148.1138	147.4484	148.0947	**135.7**
C2	137.4844	135.9074	136.0136	135.1815	135.2465	135.2334	135.4184	135.2846	135.4339	135.1383	135.3045	137.2093	135.4884	135.5708	134.8338	134.9341	134.8751	135.1242	134.9169	135.0825	134.8013	134.9656	**126.6**
C3	132.7330	133.5520	134.2870	133.8686	134.8947	133.8602	134.9863	133.8507	134.9145	133.8817	135.0461	132.7996	133.4751	134.2717	133.7921	134.8829	133.7798	134.9558	133.7672	134.8699	133.8097	134.9512	**128.9**
C4	133.9911	136.2334	136.9392	137.2535	137.8786	137.2048	138.8355	137.1548	138.6004	137.3047	138.9580	133.9988	135.9085	136.5626	136.7875	137.4889	136.7418	138.2443	136.6955	137.9894	136.8370	138.2769	**129.8**
C5	135.1983	137.4029	138.1593	138.4132	139.5310	138.3633	139.6372	138.3119	139.5283	138.4657	139.8482	135.5244	137.7057	138.5335	138.6850	139.8302	138.6366	139.8877	138.5872	139.7944	138.7365	140.0781	**133.8**
C6	131.7918	133.4851	134.6256	134.4610	135.7844	134.4073	136.3412	134.3537	136.1754	134.5191	136.4625	131.0815	132.4123	133.3504	133.0914	134.4668	133.0522	134.9720	133.0130	134.7124	133.1349	134.9327	**133.9**
C7	206.6976	212.1726	213.9636	215.1944	216.2497	215.0021	221.2396	214.8131	220.1789	215.3868	222.2346	208.9123	214.1853	215.8231	216.9224	217.9539	216.7580	222.3774	216.5933	221.4572	217.0851	223.3512	**199.2**
C8	69.4792	70.4962	71.1773	70.9906	71.8169	70.9620	72.2372	70.9342	72.1346	71.0250	73.0003	65.3097	66.3933	66.9480	66.9081	67.6827	66.8875	67.8633	66.8659	67.8442	66.9336	68.3976	**62.9**
C9	21.4144	21.7362	21.9313	22.0128	22.2725	21.9991	22.3947	21.9857	22.3700	22.0327	22.5185	18.4507	18.4735	18.5527	18.6129	18.7106	18.6103	18.9211	18.6068	18.8435	18.6208	19.2805	**14.1**
C2``	131.0475	132.3863	133.2740	133.0076	134.3194	132.9787	134.2083	132.9492	134.1558	133.0407	134.2942	131.3094	132.6256	133.5405	133.1797	134.5109	133.1554	134.4041	133.1301	134.3549	133.2084	134.5127	**123**
C8`	36.8355	37.4218	37.6402	37.7854	38.1142	37.7683	38.2771	37.7510	38.2766	37.8079	38.7073	30.8230	31.2520	31.5329	31.5939	31.9526	31.5724	32.0551	31.5511	32.0376	31.6205	32.0964	**31.6**
H(3-4)	7.8625	8.0170	8.0693	8.0794	8.1540	8.0761	8.1907	8.0726	8.1774	8.0831	8.2070	7.8494	7.9937	8.0499	8.0586	8.1328	8.0548	8.1618	8.0510	8.1485	8.0627	8.1749	**7.93**
H(5-6)	7.6451	7.8745	7.9656	7.9904	8.1026	7.9836	8.1560	7.9768	8.1388	7.9974	8.1766	7.6273	7.8220	7.9021	7.9118	8.0298	7.9063	8.0607	7.9008	8.0408	7.9174	8.0720	**7.835**
H8	4.0782	4.2314	4.2981	4.3337	4.4195	4.3269	4.4874	4.3205	4.4596	4.3406	4.4996	4.3193	4.4894	4.5608	4.5870	4.7173	4.5809	4.7833	4.5749	4.7512	4.5933	4.7863	**5.01**
H(9A-9C)	1.2019	1.2151	1.2199	1.2214	1.2072	1.2207	1.2330	1.2201	1.2297	1.2226	1.2416	1.2779	1.3006	1.2884	1.3193	1.2997	1.3179	1.3168	1.3165	1.3128	1.3210	1.3340	**1.46**
H(8`A-8`C)	2.5978	2.5375	2.4956	2.5142	2.4823	2.5151	2.4708	2.5162	2.4712	2.5137	2.4565	2.7353	2.5969	2.5617	2.5284	2.4933	2.5318	2.4465	2.5354	2.4510	2.5257	2.4081	**2.83**
Nuclei	B972																						
C1	145.0264	144.3657	145.3567	144.0311	145.8130	144.0475	144.4428	144.0631	144.6784	144.0124	144.5752	144.8374	144.4111	145.2356	144.1889	145.8029	144.2051	144.5150	144.2186	144.7619	144.1691	144.7282	**135.7**
C2	134.2247	132.6890	132.8683	132.0782	132.1195	132.1176	132.2941	132.1542	132.3104	132.0366	132.2056	133.9717	132.2902	132.4530	131.7417	131.8289	131.7717	132.0098	131.8000	131.9875	131.7094	131.8984	**126.6**
C3	130.7087	131.4630	132.1941	131.8141	132.7839	131.7972	132.8471	131.7771	132.7844	131.8250	132.9304	130.7202	131.3558	132.1654	131.7331	132.7659	131.7116	132.8030	131.6877	132.7469	131.7490	132.8447	**128.9**
C4	131.7020	133.8660	134.6098	134.9339	135.5280	134.8761	136.4524	134.8150	136.2309	134.9837	136.5940	131.6628	133.4923	134.1839	134.4248	135.0827	134.3706	135.7994	134.3140	135.5800	134.4716	135.8861	**129.8**
C5	132.8738	135.0318	135.7933	136.0751	137.1429	136.0172	137.2271	135.9557	137.1184	136.1244	137.4491	133.1704	135.2997	136.1250	136.3066	137.4048	136.2498	137.4652	136.1902	137.3705	136.3557	137.6646	**133.8**
C6	129.5894	131.2352	132.3338	132.2267	133.4620	132.1664	133.9392	132.1040	133.7968	132.2814	134.0901	128.8049	130.0576	131.0054	130.8004	132.1138	130.7541	132.5265	130.7058	132.3375	130.8404	132.5886	**133.9**
C7	204.1492	209.5155	211.1323	212.4722	213.3397	212.2782	218.2446	212.0860	217.1723	212.6562	219.1800	206.3120	211.4754	212.9936	214.2430	215.0064	214.0746	219.5346	213.9041	218.5630	214.3982	220.4240	**199.2**
C8	66.5125	67.5754	68.1130	68.0759	68.7647	68.0420	69.2290	68.0073	69.0955	68.1051	69.9634	62.6133	63.7266	64.1931	64.2541	64.9257	64.2242	65.2021	64.1918	65.1212	64.2782	65.6769	**62.9**
C9	20.3347	20.6406	20.8841	20.9552	21.2170	20.9343	21.3665	20.9116	21.3202	20.9725	21.4785	17.3667	17.3801	17.4971	17.5528	17.6704	17.5412	17.8682	17.5269	17.8011	17.5594	18.1940	**14.1**
C2``	128.8703	130.1523	131.0070	130.7880	132.0044	130.7518	131.8674	130.7131	131.8220	130.8176	131.9784	129.0931	130.3438	131.2293	130.9233	132.1691	130.8910	132.0628	130.8562	132.0189	130.9494	132.1804	**123**
C8`	35.7650	36.3677	36.5741	36.7878	37.0724	36.7604	37.2205	36.7314	37.2129	36.8097	37.6422	30.0111	30.4272	30.7371	30.8199	31.1218	30.7934	31.1990	30.7656	31.2040	30.8413	31.2613	**31.6**
H(3-4)	7.8722	8.0284	8.0863	8.0977	8.1661	8.0940	8.2040	8.0901	8.1917	8.1010	8.2227	7.8548	7.9956	8.0528	8.0620	8.1331	8.0582	8.1642	8.0542	8.1517	8.0655	8.1795	**7.93**
H(5-6)	7.6558	7.8857	7.9770	8.0037	8.1092	7.9969	8.1612	7.9898	8.1461	8.0100	8.1841	7.6284	7.8175	7.8982	7.9106	8.0228	7.9050	8.0542	7.8993	8.0371	7.9156	8.0706	**7.835**
H8	4.0632	4.2114	4.2855	4.3184	4.3974	4.3117	4.4692	4.3049	4.4435	4.3249	4.4860	4.3059	4.4653	4.5401	4.5686	4.6916	4.5622	4.7596	4.5556	4.7323	4.5745	4.7717	**5.01**
H(9A-9C)	1.1933	1.2103	1.2130	1.2210	1.1994	1.2202	1.2297	1.2192	1.2260	1.2218	1.2385	1.2633	1.2862	1.2739	1.3091	1.2811	1.3076	1.3056	1.3059	1.2996	1.3105	1.3226	**1.46**
H(8`A-8`C)	2.5683	2.5098	2.4700	2.4923	2.4571	2.4931	2.4488	2.4936	2.4486	2.4915	2.4348	2.6908	2.5569	2.5272	2.5019	2.4602	2.5048	2.4161	2.5075	2.4206	2.4992	2.3814	**2.83**
Nuclei	BHandH																						
C1	150.6655	149.9794	150.6172	149.3715	151.1732	149.4042	149.6732	149.4549	149.9018	149.3105	149.8576	150.4812	150.0138	150.6758	149.5676	150.3117	149.5923	149.9930	149.6348	150.3258	149.5134	150.2383	**135.7**
C2	140.0366	138.4006	138.6706	137.7100	137.7934	137.7393	138.0005	137.7873	138.0225	137.6524	137.9018	139.8248	138.0552	138.4366	137.4225	138.1666	137.4439	137.6423	137.4845	137.6483	137.3724	137.4722	**126.6**
C3	136.7470	137.5520	138.3724	137.9072	138.8533	137.8771	138.9670	137.8649	138.9570	137.9057	139.0686	136.8453	137.5305	138.4161	137.9007	138.6448	137.8662	138.9355	137.8502	138.8968	137.9039	139.0149	**128.9**
C4	138.4981	140.7664	141.7153	141.9279	142.6066	141.8469	143.6289	141.7841	143.3793	141.9741	143.7784	138.5284	140.4906	141.4429	141.5116	142.2557	141.4361	143.0027	141.3794	142.7605	141.5532	143.0860	**129.8**
C5	140.2174	142.5413	143.4071	143.5937	144.8072	143.5216	144.8288	143.4674	144.7498	143.6318	145.0789	140.4827	142.8397	143.7000	143.8746	144.6187	143.8047	145.1015	143.7528	145.0197	143.9105	145.3520	**133.8**
C6	135.3153	136.8885	138.2191	138.0077	139.3777	137.9229	139.9744	137.8570	139.7541	138.0586	140.1169	134.6122	135.9698	137.3016	136.8613	137.6054	136.7889	138.7909	136.7356	138.5704	136.9006	138.8736	**133.9**
C7	211.2840	216.8745	218.1594	219.6744	220.6358	219.4952	225.5859	219.3345	224.3345	219.8141	226.6307	213.0159	218.0720	219.6144	220.8704	221.6145	220.6917	226.6226	220.5308	225.6282	221.0104	227.5293	**199.2**
C8	64.2954	65.3939	65.8454	65.8779	66.6213	65.8398	67.1983	65.8196	66.9996	65.8837	68.0150	59.1856	60.1692	60.3527	60.5718	61.3159	60.5409	61.5529	60.5284	61.5189	60.5711	62.1009	**62.9**
C9	20.4911	20.7338	20.8342	20.9965	21.2154	20.9675	21.1223	20.9571	21.0714	20.9945	21.2690	17.1529	17.3369	17.3104	17.4616	18.2057	17.4452	17.5426	17.4469	17.5554	17.4469	18.0469	**14.1**
C2``	121.1386	122.3881	123.2655	122.9458	124.1379	122.9026	124.0483	122.8777	124.0289	122.9567	124.1832	121.3972	122.6313	123.5248	123.1473	123.8914	123.1075	124.2680	123.0857	124.2440	123.1552	124.4138	**123**
C8`	33.8708	34.4998	34.6644	34.8054	35.1703	34.7749	35.3503	34.7628	35.2898	34.8044	35.8543	27.3477	27.8080	28.1373	28.2135	28.9576	28.1741	28.7792	28.1536	28.7445	28.2215	28.8782	**31.6**
H(3-4)	8.0318	8.1902	8.2499	8.2611	8.3309	8.2578	8.3670	8.2537	8.3552	8.2651	8.3878	8.0208	8.1697	8.2308	8.2381	8.1568	8.2348	8.3398	8.2308	8.3270	8.2422	8.3582	**7.93**
H(5-6)	7.8114	8.0365	8.1355	8.1591	8.2718	8.1523	8.3215	8.1447	8.3008	8.1666	8.3467	7.7876	7.9889	8.0890	8.0910	8.0098	8.0855	8.2411	8.0792	8.2229	8.0973	8.2616	**7.835**
H8	3.9128	4.0609	4.1509	4.1924	4.2766	4.1844	4.3661	4.1756	4.3287	4.2010	4.3851	4.2528	4.4358	4.5545	4.5489	4.4677	4.5423	4.7478	4.5349	4.7224	4.5563	4.7621	**5.01**
H(9A-9C)	1.1920	1.2062	1.1814	1.2008	1.1699	1.2023	1.1996	1.2029	1.1933	1.2003	1.2119	1.2730	1.2845	1.2739	1.2984	1.2172	1.2984	1.2961	1.2974	1.2928	1.2995	1.3119	**1.46**
H(8`A-8`C)	2.6601	2.5875	2.5366	2.5534	2.5162	2.5559	2.4853	2.5577	2.4892	2.5521	2.4760	2.7371	2.5789	2.5596	2.5288	2.4476	2.5320	2.4451	2.5344	2.4526	2.5269	2.4054	**2.83**
Nuclei	HHandHLYP																						
C1	150.5718	149.5723	150.5469	149.0483	150.8687	149.0751	149.3804	149.1058	149.6706	149.0237	149.5170	150.3269	149.6776	150.4241	149.2357	150.9317	149.2604	149.3688	149.2879	149.8568	149.2123	149.7452	**135.7**
C2	139.2357	137.6039	137.7027	136.9021	136.9100	136.9446	137.0904	136.9894	137.1179	136.8615	136.9768	139.0625	137.2268	137.4189	136.6083	136.6895	136.6431	136.9247	136.6811	136.8410	136.5754	136.7224	**126.6**
C3	135.8001	136.4928	137.2012	136.7792	137.7063	136.7653	137.7371	136.7531	137.7155	136.7911	137.8119	135.7867	136.4069	137.1686	136.7392	137.7575	136.7200	137.8082	136.7030	137.7112	136.7565	137.8227	**128.9**
C4	136.4914	138.6958	139.3773	139.7369	140.2441	139.6785	141.2041	139.6215	140.9814	139.7914	141.3300	136.5348	138.3605	139.0330	139.2819	139.8538	139.2308	140.7011	139.1816	140.3815	139.3295	140.6931	**129.8**
C5	138.4066	140.5302	141.2448	141.4991	142.5530	141.4443	142.5362	141.3910	142.4589	141.5497	142.7625	138.6100	140.7823	141.5869	141.7419	142.8224	141.6858	142.8189	141.6316	142.7649	141.7941	143.0439	**133.8**
C6	133.9985	135.7086	136.8743	136.7712	138.0240	136.7016	138.6062	136.6357	138.4629	136.8385	138.7314	133.6201	134.8277	135.7885	135.5785	136.8383	135.5345	137.4065	135.4930	137.0809	135.6200	137.3381	**133.9**
C7	207.7002	213.4895	215.1725	216.6503	217.4665	216.4450	223.1053	216.2452	221.8650	216.8488	224.1393	210.3212	215.6075	216.9805	218.4176	219.1662	218.2556	224.0628	218.0950	223.0463	218.5719	225.0572	**199.2**
C8	65.0497	65.9911	66.6015	66.4368	67.1547	66.4047	67.6710	66.3761	67.5549	66.4683	68.3813	60.9477	61.9350	62.3088	62.3231	63.0196	62.2975	63.1094	62.2744	63.1841	62.3472	63.6702	**62.9**
C9	20.4633	20.6251	20.8057	20.8419	21.0966	20.8249	21.0871	20.8113	21.0777	20.8585	21.1901	17.4936	17.4263	17.4945	17.4581	17.6068	17.4516	17.6365	17.4485	17.6534	17.4647	17.9840	**14.1**
C2``	123.4531	124.7149	125.5654	125.3063	126.5275	125.2718	126.3837	125.2396	126.3599	125.3385	126.5078	123.6652	124.9062	125.7827	125.4432	126.6889	125.4116	126.5879	125.3823	126.5445	125.4727	126.7140	**123**
C8`	34.8963	35.5021	35.6768	35.8598	36.1804	35.8356	36.3780	35.8142	36.3598	35.8829	36.8093	29.4352	29.7905	30.0800	30.1377	30.4442	30.1159	30.6252	30.0972	30.5715	30.1591	30.6681	**31.6**
H(3-4)	7.9839	8.1410	8.1939	8.2080	8.2735	8.2046	8.3116	8.2009	8.2983	8.2111	8.3299	7.9698	8.1145	8.1709	8.1816	8.2514	8.1780	8.2858	8.1743	8.2687	8.1849	8.2984	**7.93**
H(5-6)	7.7443	7.9837	8.0733	8.1062	8.2167	8.0990	8.2683	8.0918	8.2506	8.1130	8.2909	7.7427	7.9358	8.0180	8.0314	8.1441	8.0263	8.1811	8.0209	8.1561	8.0363	8.1921	**7.835**
H8	3.7922	3.9734	4.0567	4.1007	4.1948	4.0926	4.2707	4.0844	4.2408	4.1086	4.2863	4.0660	4.2496	4.3300	4.3618	4.4910	4.3555	4.5707	4.3491	4.5315	4.3677	4.5705	**5.01**
H(9A-9C)	1.1760	1.1905	1.1880	1.1974	1.1717	1.1969	1.2067	1.1964	1.2028	1.1978	1.2130	1.2505	1.2656	1.2479	1.2820	1.2569	1.2812	1.2801	1.2802	1.2753	1.2829	1.2938	**1.46**
H(8`A-8`C)	2.5678	2.5078	2.4637	2.4885	2.4518	2.4896	2.4468	2.4906	2.4448	2.4874	2.4364	2.7275	2.5808	2.5356	2.5192	2.4737	2.5243	2.4290	2.5290	2.4308	2.5145	2.3901	**2.83**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S16. Cont. II

Nuclei	R											S									Exp. [b]
	BLYP																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	149.5835	148.9860	150.0653	148.6057	150.6296	148.9033	149.0732	148.7401	149.4896	148.9512	149.3039	148.9530	148.5880	149.6265	148.3759	150.2629	148.6597	148.6346	148.4825	149.1442	148.7340	148.9113	**135.7**
C2	137.6273	135.9123	135.9363	135.0958	135.1005	135.4249	135.1328	135.2918	135.3503	135.4097	135.0960	137.5844	135.7582	135.6548	134.9778	134.9551	135.3031	135.1457	135.1668	135.2370	135.2961	135.0918	**126.6**
C3	132.6643	133.5019	134.2224	133.8140	134.9252	134.0768	134.8119	133.8768	134.9430	134.1906	134.9603	132.8102	133.5085	134.2061	133.7989	134.9176	134.0627	134.8947	133.8640	134.9742	134.1751	135.0194	**128.9**
C4	133.6934	135.9614	136.6488	136.9914	137.6715	137.2126	138.4730	136.9711	138.4301	137.4073	138.6920	133.8543	135.7948	136.2816	136.6471	137.2790	136.8819	138.0265	136.6534	137.8965	137.0503	138.2059	**129.8**
C5	134.6309	136.9173	137.6631	137.9724	139.1327	138.1900	139.0973	137.9449	139.1655	138.3922	139.3927	135.0553	137.2739	138.0873	138.2612	139.4807	138.4828	139.4366	138.2421	139.4949	138.6774	139.7069	**133.8**
C6	131.6852	133.4734	134.5327	134.4263	135.8367	134.6460	136.1466	134.4040	136.1569	134.8451	136.4143	131.1125	132.5068	133.1977	133.1894	134.4598	133.4347	134.9918	133.2168	134.8697	133.5832	135.2003	**133.9**
C7	211.2373	216.5749	218.5213	219.5078	220.9727	219.5924	225.2655	219.2191	224.4996	220.0586	226.3546	214.4128	219.1230	220.7577	221.8069	223.0180	221.9186	226.6789	221.5684	226.1425	222.3278	227.6469	**199.2**
C8	73.3912	74.5527	75.1710	75.0248	75.9562	75.2699	76.2014	75.0543	76.2601	75.4207	77.0946	68.9532	70.4051	71.1947	71.0599	72.0771	71.2899	71.9229	71.0592	72.1586	71.4690	72.4696	**62.9**
C9	21.7164	22.1512	22.4084	22.4456	22.8580	22.7035	22.9554	22.4997	23.0579	22.8287	23.2041	18.8527	18.9676	19.0140	19.0100	19.2155	19.2839	19.3190	19.0965	19.3798	19.3777	19.7893	**14.1**
C2``	144.7732	146.3761	147.3333	147.0984	148.6350	147.3342	148.2880	147.1077	148.4253	147.5013	148.4652	145.0067	146.5905	147.6091	147.2423	148.8215	147.4825	148.5105	147.2605	148.6467	147.6410	148.6786	**123**
C8`	38.3320	38.8983	39.1232	39.2501	39.7130	39.5036	39.6800	39.2961	39.8791	39.6375	40.1874	32.4034	32.6112	32.7406	32.9054	33.2278	33.1676	33.2557	32.9673	33.3570	33.2832	33.3300	**31.6**
H(3-4)	7.6902	7.8414	7.8911	7.9028	7.9717	7.9468	8.1732	7.8983	7.9947	7.9611	8.2045	7.6838	7.8201	7.8625	7.8760	7.9411	7.9205	8.1462	7.8724	7.9636	7.9340	8.1749	**7.93**
H(5-6)	7.4651	7.6952	7.7799	7.8057	7.9159	7.8467	8.1359	7.7952	7.9533	7.8671	8.1720	7.4628	7.6473	7.7059	7.7296	7.8307	7.7728	8.0464	7.7233	7.8551	7.7888	8.0786	**7.835**
H8	4.3197	4.4492	4.5036	4.5309	4.6187	4.5732	4.8389	4.5229	4.6487	4.5912	4.8720	4.5382	4.7032	4.7447	4.7850	4.8936	4.8280	5.1492	4.7783	4.9451	4.8444	5.1822	**5.01**
H(9A-9C)	1.2606	1.2764	1.2786	1.2810	1.2728	1.3281	1.4663	1.2826	1.2960	1.3367	1.4892	1.3726	1.3868	1.3722	1.4017	1.3851	1.4480	1.5768	1.4017	1.4035	1.4581	1.6083	**1.46**
H(8`A-8`C)	2.6858	2.6141	2.5748	2.5881	2.5608	2.6367	2.7156	2.5929	2.5507	2.6423	2.7102	2.8952	2.7376	2.6721	2.6581	2.6137	2.7112	2.7341	2.6716	2.5693	2.7078	2.7094	**2.83**
Nuclei	BMK																						
C1	167.2174	166.3396	167.6654	165.8546	167.9921	165.8630	166.3916	166.0840	166.7322	166.0096	166.5374	166.8655	166.1414	167.1622	165.6730	167.7383	165.6876	165.7479	165.9696	166.6400	165.8889	166.7300	**135.7**
C2	154.4771	152.5240	152.5713	151.5675	151.8432	151.6106	151.9294	151.8648	151.7620	151.6879	151.7331	154.7645	152.8439	153.1162	152.0809	152.4114	152.1093	152.6982	152.3171	152.2528	152.1824	152.1457	**126.6**
C3	149.1095	149.9555	150.8659	150.2593	151.5103	150.2299	151.5705	150.4105	151.3574	150.4475	151.5859	149.2026	149.8210	150.7968	150.1469	151.5089	150.1138	151.7924	150.2533	151.2680	150.2966	151.4123	**128.9**
C4	150.9057	153.4960	154.2812	154.5431	155.4201	154.4693	156.3532	154.6062	155.9243	154.7737	156.4511	150.8984	152.9779	153.8755	153.9291	154.9406	153.8569	156.0145	153.9668	155.2354	154.1251	155.5800	**129.8**
C5	152.5460	154.9196	155.7954	155.9768	157.3591	155.9049	157.4762	156.0423	157.2005	156.2049	157.6851	152.9234	155.2744	156.3048	156.3177	157.7687	156.2436	157.7645	156.3820	157.5639	156.5502	157.9461	**133.8**
C6	147.9297	149.6318	150.9183	150.6228	152.2942	150.5413	152.7808	150.6727	152.4546	150.8636	152.9658	147.2377	148.6816	149.9351	149.5140	151.1875	149.4450	152.2957	149.4987	151.2245	149.6290	151.4440	**133.9**
C7	224.6751	231.1745	233.4355	234.7200	235.8652	234.4781	242.0647	234.4509	240.7958	235.1148	243.2304	226.9764	233.1864	234.9836	236.0477	237.3854	235.8451	242.0137	235.9294	241.5172	236.5199	244.1957	**199.2**
C8	75.3840	76.4694	77.4631	76.8993	78.0251	76.8504	78.5323	77.0149	78.4542	77.1096	79.3196	70.3367	71.4407	72.0558	71.8607	72.9338	71.8190	72.6134	72.0421	73.0264	72.1288	73.7573	**62.9**
C9	23.7267	24.0358	24.2491	24.2834	24.6486	24.2462	24.6823	24.4213	24.6148	24.4808	24.7374	20.3046	20.4095	20.3658	20.4568	20.6317	20.4341	20.8394	20.7083	20.6949	20.7188	21.2821	**14.1**
C2``	132.7906	134.2266	135.2435	134.8343	136.3604	134.7813	136.2025	134.9398	136.0514	135.0462	136.2820	133.1360	134.3627	135.4231	134.8665	136.4475	134.8206	136.3985	134.9784	136.1439	135.0587	136.3506	**123**
C8`	38.9059	39.4536	39.9854	39.7662	40.4554	39.7267	40.6039	39.9000	40.4868	39.9670	41.0318	32.7787	33.2350	33.5414	33.2330	33.8542	33.2039	34.2358	33.3801	33.9430	33.4217	34.1016	**31.6**
H(3-4)	8.2201	8.4578	8.4682	8.5092	8.5606	8.5046	8.5992	8.4997	8.5910	8.5038	8.6213	8.2218	8.3784	8.4375	8.4489	8.5228	8.4416	8.5692	8.4317	8.5352	8.4428	8.5573	**7.93**
H(5-6)	8.0437	8.3149	8.3905	8.4348	8.5437	8.4243	8.5911	8.4140	8.5719	8.4353	8.6203	7.9953	8.2073	8.2936	8.3111	8.4291	8.3018	8.4869	8.2882	8.4301	8.3048	8.4591	**7.835**
H8	3.9687	4.2497	4.2934	4.3846	4.4507	4.3717	4.5120	4.3592	4.4907	4.3878	4.5363	4.2514	4.4422	4.5414	4.5708	4.7105	4.5609	4.8073	4.5459	4.7084	4.5643	4.7414	**5.01**
H(9A-9C)	1.1669	1.2118	1.2138	1.2321	1.1899	1.2277	1.2271	1.2233	1.2266	1.2267	1.2395	1.2359	1.2570	1.2312	1.2701	1.2455	1.2652	1.2590	1.2575	1.2578	1.2621	1.2735	**1.46**
H(8`A-8`C)	2.5399	2.4914	2.4377	2.4807	2.4297	2.4782	2.4177	2.4757	2.4230	2.4734	2.4126	2.6767	2.5657	2.5146	2.4889	2.4498	2.4886	2.4074	2.4875	2.4024	2.4801	2.3503	**2.83**
Nuclei	BP86																						
C1	146.3649	146.0170	146.9758	145.6156	147.5468	145.6497	146.1721	145.6787	146.3689	145.5778	146.4822	145.9486	145.7677	146.6934	145.5832	147.2245	145.6048	145.6760	145.6206	146.0935	145.5577	146.1678	**135.7**
C2	135.5253	134.0560	134.0685	133.2819	133.1891	133.3357	133.3980	133.3847	133.4244	133.2260	133.4578	135.4633	133.9390	133.9199	133.1909	133.1913	133.2394	133.5700	133.2833	133.4406	133.1408	133.5556	**126.6**
C3	131.2097	132.2027	132.9003	132.5071	133.4805	132.4980	133.6098	132.4833	133.5320	132.5106	133.8387	131.3311	132.1922	132.9216	132.4354	133.5067	132.4289	133.7450	132.4173	133.5766	132.4364	133.8830	**128.9**
C4	132.5683	134.9682	135.6850	136.0101	136.5924	135.9573	137.5764	135.8989	137.3484	136.0552	137.8791	132.6120	134.7656	135.3475	135.5818	136.2907	135.5414	137.2868	135.4957	136.8971	135.6152	137.4593	**129.8**
C5	133.2441	135.6854	136.4704	136.7289	137.8495	136.6761	138.0392	136.6176	137.9129	136.7738	138.4195	133.6507	136.0164	136.8443	136.9900	138.1581	136.9419	138.3441	136.8881	138.1874	137.0300	138.6683	**133.8**
C6	130.3642	132.2271	133.2467	133.1552	134.3625	133.1036	134.8401	133.0476	134.6894	133.2001	135.1704	129.5479	131.2021	131.9976	131.8342	133.1898	131.8002	134.0096	131.7617	133.6129	131.8617	134.1435	**133.9**
C7	208.6406	213.7925	215.4146	216.4262	217.7454	216.2699	221.9642	216.1094	220.9358	216.5703	223.1082	211.0970	216.1548	217.6211	218.6463	219.6146	218.4978	223.2456	218.3454	222.6086	218.7835	224.3964	**199.2**
C8	71.1649	72.5032	73.0793	72.9356	73.7804	72.9178	74.2818	72.8951	74.0834	72.9478	75.3110	66.7663	68.0549	68.6707	68.6798	69.4081	68.6515	69.4218	68.6178	69.5450	68.7019	70.1815	**62.9**
C9	21.2395	21.7630	21.8501	22.0440	22.2187	22.0339	22.4559	22.0187	22.3650	22.0487	22.8199	18.2189	18.4539	18.4958	18.5881	18.6631	18.5847	19.0011	18.5758	18.8871	18.5860	19.5902	**14.1**
C2``	140.0339	141.6180	142.4965	142.2243	143.5654	142.1963	143.4169	142.1632	143.3619	142.2457	143.6718	140.2862	141.8184	142.7525	142.3587	143.7329	142.3360	143.6205	142.3077	143.5594	142.3750	143.8644	**123**
C8`	37.6421	38.2966	38.4026	38.5600	38.8214	38.5499	38.9860	38.5350	38.9626	38.5652	39.5934	31.1741	31.7800	31.8864	32.0025	32.2265	31.9909	32.4771	31.9752	32.3652	32.0100	32.6313	**31.6**
H(3-4)	7.7340	7.8910	7.9361	7.9567	8.0151	7.9538	8.0523	7.9506	8.0394	7.9591	8.0852	7.7202	7.8650	7.9056	7.9238	7.9867	7.9212	8.0275	7.9183	8.0080	7.9259	8.0534	**7.93**
H(5-6)	7.5219	7.7508	7.8250	7.8648	7.9520	7.8587	8.0050	7.8523	7.9899	7.8702	8.0421	7.4945	7.6951	7.7538	7.7786	7.8827	7.7744	7.9358	7.7699	7.9045	7.7821	7.9607	**7.835**
H8	4.3877	4.5115	4.5543	4.6027	4.6528	4.5975	4.7098	4.5921	4.6887	4.6074	4.7441	4.6207	4.7847	4.8327	4.8665	4.9837	4.8622	5.0707	4.8577	5.0268	4.8701	5.0945	**5.01**
H(9A-9C)	1.2590	1.2776	1.2607	1.2822	1.2568	1.2828	1.2792	1.2830	1.2732	1.2812	1.3059	1.3515	1.3807	1.3574	1.3969	1.3673	1.3966	1.3913	1.3960	1.3822	1.3968	1.4261	**1.46**
H(8`A-8`C)	2.6656	2.5940	2.5420	2.5638	2.5230	2.5661	2.5040	2.5682	2.5045	2.5612	2.5007	2.8032	2.6788	2.6086	2.5976	2.5434	2.6029	2.5020	2.6080	2.4999	2.5924	2.4789	**2.83**
Nuclei	CAM-B3LYP																						
C1	152.0111	151.2043	152.1365	150.6664	152.5766	150.6962	151.0522	150.7279	151.3272	150.6418	151.2113	151.7820	151.2361	152.0084	150.8472	152.5732	150.8770	151.2054	150.9067	151.5571	150.8209	151.5375	**135.7**
C2	140.3520	138.7154	138.7917	138.0050	138.0213	138.0522	138.2363	138.0997	138.2413	137.9623	138.1198	140.1849	138.4103	138.5289	137.7478	137.8560	137.7855	137.9954	137.8248	137.9710	137.7150	137.8244	**126.6**
C3	136.6791	137.4583	138.1279	137.7578	138.7391	137.7460	138.8077	137.7344	138.7373	137.7704	138.8701	136.6924	137.3634	138.1308	137.6879	138.7611	137.6723	138.7874	137.6570	138.6917	137.7047	138.7902	**128.9**
C4	137.5929	139.8162	140.5139	140.8642	141.4586	140.8097	142.3970	140.7544	142.1766	140.9173	142.5204	137.6356	139.5512	140.2176	140.4516	141.1311	140.4014	141.8386	140.3515	141.5853	140.5014	141.8643	**129.8**
C5	139.5481	141.7848	142.4989	142.7787	143.8983	142.7259	143.9245	142.6725	143.8104	142.8302	144.1510	139.7726	142.0346	142.8314	143.0129	144.1544	142.9612	144.1804	142.9091	144.0922	143.0636	144.4044	**133.8**
C6	135.0049	136.6895	137.8587	137.7177	139.0716	137.6560	139.5932	137.5954	139.4974	137.7793	139.7223	134.4714	135.7807	136.7711	136.5091	137.9020	136.4643	138.3408	136.4207	138.0760	136.5541	138.2985	**133.9**
C7	212.3165	218.1866	219.8867	221.2589	222.3095	221.0612	227.4914	220.8674	226.4073	221.4528	228.5754	214.6414	220.1162	221.6878	222.9477	223.9746	222.7782	228.6867	222.6098	227.6915	223.1119	229.6995	**199.2**
C8	67.9105	69.0591	69.6854	69.4869	70.3190	69.4576	70.7399	69.4305	70.6437	69.5184	71.5335	63.5745	64.6814	65.1005	65.1372	65.8822	65.1157	66.1155	65.0941	66.0746	65.1594	66.6858	**62.9**
C9	20.6178	20.8624	21.0445	21.0903	21.3827	21.0772	21.3428	21.0650	21.3470	21.1057	21.4856	17.7587	17.7015	17.7133	17.7608	17.8509	17.7586	17.9527	17.7569	17.9152	17.7646	18.3326	**14.1**
C2``	132.5900	133.9738	134.8223	134.5905	135.8974	134.5581	135.7697	134.5260	135.7042	134.6231	135.8871	132.8327	134.1920	135.0776	134.7480	136.0745	134.7197	135.9787	134.6913	135.9110	134.7769	136.1008	**123**
C8`	35.6818	36.3394	36.4345	36.6578	37.0045	36.6376	37.1777	36.6187	37.1554	36.6800	37.6638	29.7588	30.1978	30.4982	30.5477	30.9217	30.5234	31.0317	30.5008	31.0053	30.5742	31.1212	**31.6**
H(3-4)	7.9375	8.0906	8.1447	8.1567	8.2241	8.1532	8.2600	8.1498	8.2482	8.1598	8.2775	7.9256	8.0676	8.1234	8.1317	8.2038	8.1281	8.2311	8.1246	8.2179	8.1349	8.2442	**7.93**
H(5-6)	7.6965	7.9259	8.0157	8.0461	8.1562	8.0391	8.2069	8.0323	8.1934	8.0526	8.2286	7.6907	7.8829	7.9660	7.9749	8.0915	7.9694	8.1190	7.9641	8.1002	7.9799	8.1309	**7.835**
H8	3.9333	4.0975	4.1886	4.2251	4.3210	4.2172	4.3992	4.2094	4.3760	4.2327	4.4131	4.2111	4.3880	4.4697	4.4934	4.6291	4.4870	4.6912	4.4806	4.6620	4.4995	4.6938	**5.01**
H(9A-9C)	1.2097	1.2252	1.2209	1.2295	1.2102	1.2291	1.2354	1.2289	1.2346	1.2298	1.2451	1.2863	1.3074	1.2928	1.3234	1.3046	1.3223	1.3230	1.3213	1.3218	1.3244	1.3397	**1.46**
H(8`A-8`C)	2.6398	2.5755	2.5281	2.5504	2.5168	2.5519	2.5040	2.5535	2.5033	2.5489	2.4923	2.7689	2.6249	2.5921	2.5584	2.5294	2.5622	2.4733	2.5663	2.4826	2.5547	2.4366	**2.83**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S16. Cont. III

Nuclei	R											S										Exp. [b]
	HF																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	149.8993	148.6345	149.6354	147.9591	149.8617	147.9937	148.0953	148.0306	148.4103	147.9271	148.2087	149.7551	148.9261	149.7360	148.4242	150.1725	148.4560	148.6104	148.4879	148.9715	148.3925	148.7861	**135.7**
C2	138.2185	136.6013	136.7010	135.9884	135.9788	136.0381	136.1867	136.0866	136.2008	135.9389	136.0847	137.9296	136.0212	136.1637	135.3690	135.4961	135.4031	135.6319	135.4391	135.5821	135.3370	135.4998	**126.6**
C3	136.2132	136.7492	137.3684	136.9241	137.8332	136.9128	137.7163	136.9016	137.7063	136.9338	137.7922	136.0928	136.7343	137.4616	137.0069	138.0033	136.9903	137.9084	136.9744	137.8956	137.0219	137.9919	**128.9**
C4	135.4724	137.5271	138.0581	138.5226	138.8289	138.4784	139.8917	138.4325	139.6490	138.5623	140.0138	135.5183	137.1113	137.6232	137.9103	138.3075	137.8626	139.1158	137.8153	138.8577	137.9555	139.2017	**129.8**
C5	138.6209	140.5432	141.1826	141.3323	142.3567	141.2819	142.1875	141.2318	142.1383	141.3792	142.3898	138.7449	140.8467	141.5565	141.7050	142.7334	141.6568	142.6374	141.6082	142.6072	141.7498	142.8629	**133.8**
C6	133.2179	134.8031	135.7962	135.8646	136.9752	135.8204	137.6377	135.7752	137.4557	135.9057	137.7811	133.0704	133.9381	134.7368	134.5251	135.6391	134.4879	136.0194	134.4516	135.8131	134.5606	136.0833	**133.9**
C7	200.0236	206.3647	208.1368	209.8184	210.4286	209.6092	216.8733	209.4016	215.3751	210.0180	217.9744	202.9675	208.1728	209.7299	211.2004	211.7764	211.0201	217.6257	210.8380	216.3117	211.3681	218.5630	**199.2**
C8	58.9755	59.7634	60.4464	60.1195	60.8726	60.0997	61.2680	60.0822	61.1391	60.1401	61.8389	55.3630	56.1233	56.5160	56.4920	57.1204	56.4713	57.4076	56.4502	57.3731	56.5103	57.7699	**62.9**
C9	19.1886	19.1955	19.3781	19.3261	19.6492	19.3218	19.4681	19.3177	19.4735	19.3292	19.5440	16.4305	16.2371	16.2673	16.1970	16.3688	16.1956	16.3516	16.1955	16.3403	16.1989	16.6005	**14.1**
C2``	108.3897	109.4699	110.2203	109.9653	111.0720	109.9359	110.9395	109.9068	110.9083	109.9924	111.0621	108.5362	109.6155	110.4031	110.0563	111.2016	110.0308	111.0951	110.0056	111.0623	110.0798	111.2209	**123**
C8`	32.7977	33.4049	33.6321	33.7009	34.0556	33.6769	34.2058	33.6545	34.1742	33.7240	34.5466	28.2973	28.5088	28.8305	28.7907	29.1525	28.7742	29.1970	28.7580	29.1866	28.8054	29.2724	**31.6**
H(3-4)	7.9960	8.1608	8.2191	8.2306	8.3037	8.2270	8.3398	8.2232	8.3274	8.2339	8.3596	7.9850	8.1409	8.2003	8.2106	8.2863	8.2066	8.3153	8.2024	8.3020	8.2144	8.3341	**7.93**
H(5-6)	7.7490	7.9971	8.0906	8.1268	8.2493	8.1204	8.2930	8.1137	8.2756	8.1328	8.3193	7.7625	7.9547	8.0405	8.0492	8.1722	8.0437	8.1943	8.0380	8.1761	8.0545	8.2165	**7.835**
H8	3.3144	3.5135	3.5992	3.6711	3.7756	3.6648	3.8509	3.6582	3.8206	3.6770	3.8714	3.5836	3.7816	3.8644	3.8931	4.0274	3.8861	4.0915	3.8790	4.0600	3.8999	4.1015	**5.01**
H(9A-9C)	1.1168	1.1287	1.1379	1.1456	1.1208	1.1462	1.1470	1.1466	1.1434	1.1450	1.1547	1.1708	1.1715	1.1580	1.1884	1.1609	1.1873	1.1834	1.1859	1.1772	1.1897	1.1936	**1.46**
H(8`A-8`C)	2.4000	2.3629	2.3250	2.3537	2.3189	2.3535	2.3225	2.3531	2.3206	2.3540	2.3147	2.5694	2.4216	2.3925	2.3689	2.3373	2.3719	2.2929	2.3747	2.2967	2.3659	2.2588	**2.83**
Nuclei	**LC-BLYP**																					
C1	156.6791	155.7863	156.6082	155.1891	156.9978	155.2065	155.4340	155.2518	155.7081	155.1567	155.5940	156.5916	155.8451	156.7113	155.4300	157.2955	155.4394	155.9857	155.4751	156.2063	155.4027	156.1520	**135.7**
C2	144.4659	142.7181	142.9191	142.0267	142.1253	142.0446	142.3436	142.0900	142.3054	141.9927	142.2422	144.2076	142.3418	142.6494	141.6999	141.7963	141.7110	141.8152	141.7505	141.8450	141.6731	141.6883	**126.6**
C3	142.0648	142.7522	143.5073	143.1154	144.0788	143.0731	144.1087	143.0577	144.0417	143.1382	144.1949	142.0762	142.7296	143.5202	143.1091	144.1431	143.0656	144.0957	143.0488	144.0447	143.1332	144.1881	**128.9**
C4	142.6580	144.8087	145.6619	145.9106	146.5991	145.8236	147.5370	145.7632	147.2872	145.9750	147.6753	142.6814	144.6049	145.3942	145.5792	146.1954	145.4977	146.8484	145.4437	146.6530	145.6396	146.9606	**129.8**
C5	145.4779	147.7323	148.5237	148.7854	149.9082	148.7038	149.8922	148.6489	149.7845	148.8450	150.1346	145.7098	148.0184	148.8609	149.0625	150.2416	148.9821	150.2664	148.9287	150.1629	149.1208	150.5107	**133.8**
C6	139.6494	141.1295	142.5422	142.1908	143.8013	142.0982	144.2563	142.0331	144.1402	142.2612	144.4042	139.0555	140.3343	141.4801	141.1355	142.4639	141.0603	142.8183	141.0136	142.6689	141.1907	142.8997	**133.9**
C7	218.1301	224.3916	226.0181	227.6227	228.5317	227.4041	234.0250	227.2141	232.8605	227.8141	235.1286	219.9507	225.7172	227.5887	228.8873	229.8852	228.6699	235.2389	228.4795	234.0052	229.0755	236.2062	**199.2**
C8	65.7217	66.8955	67.6384	67.4353	68.2910	67.3814	68.7559	67.3552	68.6735	67.4697	69.5314	61.0858	62.1036	62.5068	62.6448	63.4112	62.5940	63.8309	62.5698	63.6868	62.6751	64.3267	**62.9**
C9	19.8394	20.0014	20.2206	20.2365	20.5485	20.1980	20.3938	20.1875	20.3975	20.2564	20.5241	17.0029	16.9180	16.9050	17.0069	17.0756	16.9816	17.1413	16.9833	17.1157	17.0137	17.5194	**14.1**
C2``	131.8678	133.1363	134.0369	133.7813	135.0271	133.7214	134.9294	133.6884	134.8601	133.8207	135.0543	132.1276	133.3864	134.2998	133.9689	135.2466	133.9145	135.1484	133.8872	135.0924	134.0027	135.2829	**123**
C8`	33.7936	34.4865	34.5784	34.8436	35.1554	34.8011	35.3523	34.7862	35.2856	34.8667	35.8718	27.8828	28.3421	28.7741	28.7725	29.1088	28.7228	29.2524	28.7010	29.1918	28.8029	29.4168	**31.6**
H(3-4)	8.0922	8.2409	8.2976	8.3088	8.3766	8.3041	8.4098	8.3009	8.3983	8.3122	8.4297	8.0839	8.2265	8.2816	8.2925	8.3590	8.2877	8.3833	8.2846	8.3729	8.2959	8.4027	**7.93**
H(5-6)	7.8372	8.0592	8.1552	8.1785	8.3015	8.1703	8.3456	8.1637	8.3289	8.1852	8.3707	7.8314	8.0282	8.1183	8.1242	8.2370	8.1175	8.2577	8.1124	8.2449	8.1296	8.2789	**7.835**
H8	3.8037	3.9675	4.0883	4.1033	4.2399	4.0931	4.3223	4.0845	4.2909	4.1121	4.3408	4.1164	4.3033	4.4077	4.4137	4.5513	4.4056	4.5935	4.3992	4.5747	4.4205	4.6074	**5.01**
H(9A-9C)	1.2090	1.2246	1.2142	1.2274	1.2035	1.2264	1.2279	1.2270	1.2242	1.2274	1.2416	1.2711	1.2894	1.2806	1.3088	1.2868	1.3066	1.3067	1.3059	1.3022	1.3099	1.3252	**1.46**
H(8`A-8`C)	2.6319	2.5705	2.5152	2.5492	2.5025	2.5495	2.4885	2.5514	2.4877	2.5479	2.4820	2.7054	2.5622	2.5540	2.5096	2.4762	2.5110	2.4274	2.5140	2.4377	2.5073	2.3977	**2.83**
Nuclei	**M06**																					
C1	148.2752	146.7806	147.6418	146.2529	148.8653	146.2772	146.5664	146.3090	146.9418	146.2441	146.7329	148.4749	147.7212	148.5530	147.1174	149.5965	147.1392	147.6025	147.1698	147.8691	147.1127	147.6418	**135.7**
C2	134.8015	133.7860	134.1480	133.0954	133.2511	133.1236	133.4997	133.1602	133.4942	133.0836	133.3579	135.4417	133.7770	134.3203	133.4709	133.4504	133.4928	133.7280	133.5219	133.7631	133.4643	133.6496	**126.6**
C3	134.3789	134.9925	135.8763	135.3609	136.5445	135.3291	136.5802	135.3052	136.5583	135.4057	136.6442	134.6543	135.2307	136.1857	135.6789	137.0569	135.6456	136.8139	135.6200	136.7715	135.7243	136.9156	**128.9**
C4	135.7585	138.2681	139.2393	139.3602	140.0097	139.2858	141.1800	139.2188	140.8875	139.4451	141.2984	135.1243	137.1157	138.0497	138.2561	138.8367	138.1856	139.7445	138.1221	139.5493	138.3367	139.9297	**129.8**
C5	137.8199	139.5516	140.4951	140.5721	141.9840	140.5025	141.9621	140.4403	141.8678	140.6526	142.1511	137.8373	139.9460	140.8197	140.9165	142.2773	140.8483	142.1823	140.7875	142.0977	140.9957	142.3847	**133.8**
C6	132.8963	135.3983	136.7780	136.2459	137.7233	136.1830	138.4141	136.1279	138.1439	136.3196	138.6475	131.0022	132.4584	133.8652	133.6108	134.6578	133.5411	135.5963	133.4779	135.4194	133.6902	135.8630	**133.9**
C7	209.9118	216.9702	218.9930	219.7747	221.6258	219.6006	226.0864	219.4314	225.0095	219.9520	227.1452	210.9477	216.6905	218.5156	219.9144	220.9409	219.7249	225.8806	219.5420	224.7973	220.1084	226.7358	**199.2**
C8	65.4210	67.3863	67.9641	67.7205	69.1247	67.6955	68.9727	67.6774	68.8929	67.7580	69.8126	60.6260	61.4919	62.0164	61.8441	63.1167	61.8093	63.0851	61.7830	62.9823	61.8933	63.4352	**62.9**
C9	20.6503	20.8591	21.3932	21.1956	22.0903	21.1636	21.8763	21.1392	21.7676	21.2403	21.8513	17.8501	18.0159	18.0989	17.9462	18.4481	17.9334	18.2241	17.9305	18.2115	17.9726	18.5295	**14.1**
C2``	125.5166	126.5578	127.6467	127.1715	128.9826	127.1243	128.5181	127.0850	128.4893	127.2309	128.5805	125.8952	127.0314	127.9940	127.5486	129.2806	127.5062	128.8304	127.4720	128.7860	127.6035	128.9831	**123**
C8`	37.2875	38.0469	38.4874	38.3819	39.1299	38.3540	39.1495	38.3333	39.0719	38.4225	39.6935	30.5256	31.2595	31.7185	31.7531	32.1269	31.7187	32.3287	31.6918	32.3121	31.8007	32.5980	**31.6**
H(3-4)	7.9617	8.0660	8.1095	8.1278	8.2370	8.1240	8.2271	8.1207	8.2178	8.1320	8.2462	7.8246	7.9675	8.0402	8.0448	8.1639	8.0405	8.1551	8.0367	8.1448	8.0493	8.1727	**7.93**
H(5-6)	7.6990	7.9251	8.0332	8.0222	8.1742	8.0163	8.2038	8.0108	8.1815	8.0284	8.2291	7.5462	7.7466	7.8426	7.8540	7.9657	7.8478	8.0043	7.8421	7.9898	7.8603	8.0307	**7.835**
H8	4.0318	4.2395	4.2694	4.3052	4.4177	4.3001	4.4011	4.2957	4.3837	4.3107	4.4174	4.2976	4.4391	4.5494	4.5448	4.7031	4.5387	4.7336	4.5331	4.7171	4.5511	4.7546	**5.01**
H(9A-9C)	1.2036	1.2675	1.2788	1.2625	1.2655	1.2628	1.2912	1.2637	1.2940	1.2625	1.3058	1.2876	1.2976	1.2839	1.3043	1.3215	1.3036	1.3083	1.3034	1.3089	1.3056	1.3144	**1.46**
H(8`A-8`C)	2.6132	2.5513	2.5232	2.5421	2.5466	2.5426	2.5004	2.5436	2.5044	2.5422	2.4871	2.6244	2.5302	2.4658	2.4459	2.4386	2.4483	2.3910	2.4515	2.3951	2.4443	2.3590	**2.83**
Nuclei	**M06-2X**																					
C1	166.3068	165.2781	166.3208	164.6832	166.6474	164.7360	165.0366	164.7912	165.3282	164.6277	165.1999	166.2554	165.4213	166.1443	164.8924	166.7644	164.9498	165.3989	165.0075	165.5950	164.8306	165.5939	**135.7**
C2	152.2648	150.3830	150.5372	149.5428	149.6849	149.6124	149.7901	149.6838	149.8008	149.4705	149.6987	152.3205	150.4733	150.7316	149.7116	149.8773	149.7753	149.8424	149.8412	149.9335	149.6453	149.7269	**126.6**
C3	149.1004	149.9258	150.7983	150.2987	151.4444	150.3002	151.5521	150.3024	151.4966	150.2905	151.6565	149.0953	149.9130	150.7077	150.2623	151.3718	150.2630	151.3766	150.2648	151.3116	150.2554	151.5273	**128.9**
C4	151.5325	154.0257	154.8903	155.2120	156.0625	155.1636	157.0287	155.1155	156.7626	155.2516	157.2340	151.3338	153.5948	154.5087	154.6686	155.5358	154.6249	156.1982	154.5824	156.0189	154.7037	156.3332	**129.8**
C5	153.3345	155.9061	156.8229	157.0689	158.4100	157.0238	158.4992	156.9789	158.3717	157.1045	158.7579	153.5002	156.0190	156.9478	157.1549	158.4667	157.1093	158.5321	157.0645	158.4058	157.1914	158.7908	**133.8**
C6	148.3774	150.0922	151.5309	151.2688	152.8730	151.2089	153.2900	151.1513	153.1596	151.3199	153.5106	147.0702	148.6188	149.9407	149.5064	151.1854	149.4705	151.4156	149.4363	151.3015	149.5348	151.5329	**133.9**
C7	226.7932	233.3962	235.4764	237.0143	237.9621	236.7993	244.1817	236.5895	242.8289	237.2146	245.4208	227.9933	234.2399	235.8896	237.6651	238.6373	237.4792	244.6092	237.2933	243.2089	237.8344	245.8155	**199.2**
C8	71.2904	72.3876	73.1475	72.8879	73.6940	72.8800	74.1836	72.8731	74.0730	72.8890	75.0064	66.1287	67.1236	67.4906	67.7140	68.5560	67.6975	69.0278	67.6823	68.8233	67.7230	69.5740	**62.9**
C9	21.6354	21.9278	22.1117	22.2468	22.4778	22.2422	22.5127	22.2393	22.4501	22.2452	22.6319	18.3877	18.6179	18.6019	18.7681	18.8889	18.7789	18.8997	18.7910	18.8478	18.7518	19.3742	**14.1**
C2``	128.5335	129.8520	130.7749	130.4651	131.7929	130.4502	131.6342	130.4363	131.5959	130.4727	131.7794	128.7982	130.1352	131.0000	130.6608	131.9941	130.6519	131.8528	130.6438	131.7975	130.6628	132.0275	**123**
C8`	36.1388	36.7784	37.0064	37.1451	37.4698	37.1406	37.7471	37.1380	37.6782	37.1441	38.2322	29.8644	30.3961	30.7270	30.7557	31.1324	30.7512	31.2633	30.7482	31.2510	30.7543	31.4595	**31.6**
H(3-4)	8.4841	8.6330	8.6989	8.7052	8.7857	8.6997	8.8210	8.6938	8.8100	8.7106	8.8402	8.4344	8.5828	8.6430	8.6535	8.7280	8.6481	8.7504	8.6424	8.7400	8.6588	8.7692	**7.93**
H(5-6)	8.2828	8.5108	8.6069	8.6373	8.7548	8.6280	8.7969	8.6185	8.7796	8.6463	8.8237	8.2100	8.4139	8.5091	8.5169	8.6367	8.5095	8.6557	8.5017	8.6440	8.5241	8.6769	**7.835**
H8	4.0420	4.2087	4.3072	4.3547	4.4488	4.3429	4.5252	4.3310	4.4960	4.3661	4.5527	4.2898	4.4728	4.5787	4.5781	4.7122	4.5705	4.7457	4.5625	4.7338	4.5856	4.7475	**5.01**
H(9A-9C)	1.2140	1.2147	1.2221	1.2195	1.2028	1.2175	1.2284	1.2153	1.2268	1.2216	1.2374	1.2418	1.2663	1.2529	1.2870	1.2626	1.2846	1.2880	1.2819	1.2863	1.2893	1.3022	**1.46**
H(8`A-8`C)	2.5801	2.5297	2.4839	2.5097	2.4740	2.5095	2.4599	2.5091	2.4613	2.5101	2.4480	2.6067	2.4942	2.4735	2.4569	2.4180	2.4576	2.3967	2.4581	2.4049	2.4563	2.3540	**2.83**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S16. Cont. IV

Nuclei	R											S										Exp. [b]
	mpW1LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	150.5091	149.6736	150.7559	149.2455	151.1158	149.2633	149.6909	149.2838	149.9556	149.2283	149.7969	150.1319	149.5964	150.4983	149.2921	150.9844	149.3069	149.5218	149.3228	149.9363	149.2758	149.8358	**135.7**
C2	138.7818	137.1098	137.1958	136.3862	136.3195	136.4281	136.5180	136.4714	136.5471	136.3442	136.3674	138.6259	136.7837	136.8363	136.1193	136.1012	136.1523	136.3857	136.1880	136.2884	136.0870	136.1767	**126.6**
C3	134.4498	135.2269	135.9617	135.5638	136.4985	135.5438	136.5804	135.5245	136.5297	135.5803	136.6160	134.5063	135.1597	135.9388	135.4997	136.5078	135.4766	136.6182	135.4554	136.5168	135.5193	136.5805	**128.9**
C4	135.5356	137.7772	138.4755	138.8418	139.3649	138.7797	140.3099	138.7181	140.0896	138.8979	140.4083	135.5960	137.4874	138.1038	138.4042	138.9742	138.3491	139.8069	138.2952	139.4951	138.4546	139.7825	**129.8**
C5	137.0213	139.2303	139.9685	140.2689	141.3036	140.2070	141.3614	140.1456	141.2628	140.3249	141.5532	137.2939	139.4927	140.3338	140.5023	141.5825	140.4409	141.6312	140.3803	141.5449	140.5581	141.7978	**133.8**
C6	133.2160	134.9625	136.1368	136.0141	137.2885	135.9439	137.8213	135.8760	137.6720	136.0800	137.9358	132.6852	133.9899	134.8849	134.7235	135.9836	134.6756	136.5717	134.6301	136.2383	134.7677	136.4971	**133.9**
C7	209.9059	215.5240	217.3916	218.6202	219.7024	218.4137	224.8153	218.2125	223.7236	218.8180	225.8100	212.6499	217.8362	219.4360	220.6376	221.6238	220.4706	226.0036	220.3041	225.1790	220.7935	226.9453	**199.2**
C8	69.1714	70.1976	70.8853	70.6694	71.4647	70.6326	71.9334	70.5984	71.8179	70.7038	72.6594	64.9808	66.1022	66.6973	66.6099	67.3917	66.5765	67.4494	66.5439	67.5366	66.6390	67.9982	**62.9**
C9	21.1582	21.4374	21.6747	21.7216	21.9723	21.6977	22.0798	21.6764	22.0484	21.7432	22.1744	18.1884	18.1470	18.2267	18.2034	18.3051	18.1931	18.4350	18.1854	18.3795	18.2125	18.7818	**14.1**
C2``	132.9566	134.3735	135.2839	135.0505	136.3415	135.0079	136.2032	134.9665	136.1603	135.0890	136.2895	133.1931	134.5897	135.5439	135.2018	136.5230	135.1632	136.4265	135.1259	136.3751	135.2364	136.5138	**123**
C8`	36.4618	37.0540	37.2852	37.4418	37.7717	37.4124	37.9489	37.3849	37.9500	37.4683	38.3536	30.5956	30.9409	31.2080	31.3041	31.5939	31.2781	31.7576	31.2541	31.7012	31.3273	31.7278	**31.6**
H(3-4)	7.8610	8.0149	8.0696	8.0819	8.1478	8.0785	8.1823	8.0749	8.1708	8.0850	8.1982	7.8442	7.9839	8.0388	8.0489	8.1172	8.0454	8.1485	8.0418	8.1335	8.0520	8.1584	**7.93**
H(5-6)	7.6306	7.8634	7.9528	7.9829	8.0897	7.9762	8.1394	7.9691	8.1244	7.9893	8.1595	7.6214	7.8113	7.8873	7.9034	8.0117	7.8983	8.0490	7.8930	8.0247	7.9081	8.0569	**7.835**
H8	4.0309	4.1889	4.2640	4.3005	4.3889	4.2936	4.4527	4.2864	4.4269	4.3072	4.4675	4.2816	4.4550	4.5216	4.5565	4.6783	4.5505	4.7572	4.5443	4.7183	4.5621	4.7582	**5.01**
H(9A-9C)	1.2129	1.2270	1.2327	1.2354	1.2164	1.2349	1.2465	1.2342	1.2439	1.2358	1.2510	1.3057	1.3222	1.3088	1.3408	1.3185	1.3398	1.3384	1.3385	1.3346	1.3418	1.3504	**1.46**
H(8`A-8`C)	2.6428	2.5767	2.5377	2.5564	2.5237	2.5576	2.5140	2.5585	2.5147	2.5553	2.4974	2.8149	2.6662	2.6194	2.5979	2.5569	2.6030	2.5044	2.6079	2.5098	2.5931	2.4599	**2.83**
Nuclei	mpW1PW91																					
C1	147.6545	146.9673	147.9183	146.5229	148.4312	146.5479	146.9982	146.5792	147.2221	146.4993	147.1629	147.4611	147.0520	147.7775	146.7218	148.3667	146.7434	146.9739	146.7706	147.3546	146.7002	147.3254	**135.7**
C2	136.8216	135.2817	135.3758	134.5866	134.6284	134.6277	134.8290	134.6749	134.8378	134.5467	134.7214	136.6041	134.9099	135.1216	134.2900	134.4668	134.3231	134.6634	134.3625	134.5825	134.2589	134.4867	**126.6**
C3	133.3727	134.1804	134.9077	134.4953	135.5046	134.4781	135.6177	134.4661	135.5475	134.5105	135.6866	133.3998	134.0759	134.9206	134.3951	135.5270	134.3753	135.6135	134.3612	135.4957	134.4137	135.6046	**128.9**
C4	134.6057	136.8667	137.5949	137.9184	138.5596	137.8578	139.5008	137.8022	139.2666	137.9748	139.6359	134.5841	136.5074	137.2741	137.4162	138.2013	137.3617	138.9887	137.3128	138.6805	137.4673	138.9949	**129.8**
C5	135.8202	138.0706	138.8634	139.0895	140.2623	139.0308	140.3611	138.9769	140.2499	139.1442	140.5816	136.1053	138.3367	139.1722	139.3181	140.5038	139.2615	140.5691	139.2099	140.4660	139.3705	140.7684	**133.8**
C6	132.1991	133.9109	134.9959	134.9069	136.2022	134.8418	136.6811	134.7832	136.5353	134.9690	136.8245	131.5069	132.8414	133.8964	133.5735	135.0310	133.5266	135.5504	133.4855	135.2407	133.6180	135.4810	**133.9**
C7	207.8840	213.2797	214.8409	216.1301	217.1913	215.9485	222.0872	215.7749	220.9181	216.3034	223.1193	209.9992	215.2702	216.6292	217.9744	218.7896	217.8056	223.3746	217.6431	222.4847	218.1345	224.4053	**199.2**
C8	66.8699	67.9746	68.5438	68.4182	69.2367	68.3884	69.7228	68.3651	69.5550	68.4468	70.5319	62.7690	63.8917	64.2223	64.3583	65.0250	64.3308	65.2625	64.3083	65.2902	64.3833	65.8742	**62.9**
C9	20.4173	20.7206	20.8386	20.9739	21.2398	20.9570	21.3086	20.9461	21.2458	20.9895	21.4726	17.3143	17.3840	17.4687	17.5329	17.6935	17.5258	17.8427	17.5236	17.8001	17.5381	18.2071	**14.1**
C2``	129.5660	130.8882	131.7488	131.4696	132.7545	131.4352	132.6366	131.4063	132.5874	131.5015	132.7420	129.7992	131.0772	131.9687	131.5980	132.9130	131.5680	132.8107	131.5433	132.7544	131.6257	132.9244	**123**
C8`	35.6827	36.3094	36.4690	36.6313	36.9791	36.6087	37.1565	36.5923	37.1206	36.6527	37.6085	29.7197	30.1666	30.4380	30.5186	30.8460	30.4924	31.0261	30.4719	30.9780	30.5430	31.0811	**31.6**
H(3-4)	7.9255	8.0829	8.1387	8.1489	8.2183	8.1455	8.2574	8.1422	8.2449	8.1522	8.2757	7.9048	8.0483	8.1075	8.1120	8.1878	8.1086	8.2211	8.1053	8.2051	8.1155	8.2331	**7.93**
H(5-6)	7.7064	7.9393	8.0239	8.0558	8.1604	8.0491	8.2109	8.0424	8.1946	8.0625	8.2336	7.6781	7.8719	7.9591	7.9640	8.0850	7.9588	8.1208	7.9536	8.0965	7.9693	8.1295	**7.835**
H8	4.0646	4.2218	4.2840	4.3345	4.4059	4.3274	4.4774	4.3205	4.4494	4.3415	4.4945	4.3230	4.4904	4.5817	4.5911	4.7310	4.5851	4.8009	4.5793	4.7640	4.5971	4.8006	**5.01**
H(9A-9C)	1.1865	1.2040	1.1949	1.2083	1.1867	1.2082	1.2140	1.2083	1.2079	1.2086	1.2260	1.2542	1.2791	1.2643	1.2957	1.2730	1.2948	1.2991	1.2939	1.2930	1.2970	1.3161	**1.46**
H(8`A-8`C)	2.5795	2.5159	2.4748	2.4908	2.4573	2.4924	2.4454	2.4940	2.4449	2.4896	2.4325	2.6891	2.5540	2.5148	2.4924	2.4513	2.4959	2.4125	2.4995	2.4150	2.4896	2.3760	**2.83**
Nuclei	O3LYP																					
C1	143.9885	143.4161	144.4621	143.1675	145.0085	143.1855	143.6512	143.2004	143.8743	143.1455	143.7749	143.6907	143.3752	144.2614	143.1973	144.9506	143.2185	143.8211	143.2351	143.9555	143.1707	143.8920	**135.7**
C2	132.8117	131.2279	131.4338	130.6488	130.6843	130.6929	130.8608	130.7316	130.8827	130.5981	130.7709	132.5135	130.7935	131.0064	130.2586	130.3525	130.2962	130.4615	130.3294	130.4981	130.2172	130.3978	**126.6**
C3	129.0323	129.7326	130.5217	130.1181	131.1238	130.1087	131.1448	130.0931	131.0986	130.1189	131.2066	129.0630	129.6693	130.4714	130.0512	131.0755	130.0373	131.0221	130.0184	131.0167	130.0581	131.0969	**128.9**
C4	129.9513	131.9929	132.7634	133.0132	133.6469	132.9655	134.5528	132.9123	134.3342	133.0497	134.6696	129.9167	131.6152	132.3514	132.5255	133.1551	132.4808	133.7264	132.4308	133.6015	132.5610	133.8733	**129.8**
C5	130.9884	133.0959	133.8944	134.1177	135.1947	134.0710	135.2917	134.0177	135.1887	134.1544	135.4728	131.3412	133.3720	134.2318	134.3525	135.4758	134.3055	135.5157	134.2530	135.4354	134.3902	135.6926	**133.8**
C6	128.1485	129.6259	130.7103	130.5532	131.8642	130.4996	132.3100	130.4438	132.1457	130.5965	132.4584	127.3471	128.4855	129.4998	129.2180	130.5246	129.1819	130.7273	129.1407	130.6610	129.2457	130.9021	**133.9**
C7	203.1538	208.5495	210.3134	211.4715	212.6227	211.2877	217.0890	211.1034	216.1028	211.6447	217.9759	205.6839	210.6526	212.2505	213.5100	214.3817	213.3484	218.8780	213.1810	217.8908	213.6562	219.5616	**199.2**
C8	67.2957	68.4271	69.0334	68.9118	69.7654	68.8896	70.0493	68.8638	69.9353	68.9304	70.7311	63.7515	65.1120	65.5860	65.6944	66.4842	65.6714	66.8821	65.6431	66.6916	65.7096	67.1856	**62.9**
C9	20.2280	20.5713	20.9769	20.9283	21.3549	20.9072	21.5232	20.8838	21.4610	20.9396	21.6402	17.1708	17.1359	17.3159	17.2537	17.4353	17.2527	17.5654	17.2473	17.5065	17.2485	17.8237	**14.1**
C2``	130.9035	132.2105	133.1307	132.8881	134.1700	132.8586	134.0197	132.8237	133.9780	132.9095	134.1013	131.1279	132.4361	133.3625	133.0467	134.3605	133.0209	134.2167	132.9901	134.1859	133.0645	134.3043	**123**
C8`	35.9436	36.6052	36.8830	36.9992	37.4071	36.9860	37.4721	36.9679	37.4576	37.0077	37.8267	30.3616	30.6500	31.0025	31.0777	31.4125	31.0622	31.4385	31.0417	31.4736	31.0857	31.4363	**31.6**
H(3-4)	7.8249	7.9739	8.0319	8.0400	8.1099	8.0369	8.1466	8.0333	8.1347	8.0427	8.1638	7.8066	7.9388	7.9980	8.0032	8.0730	7.9998	8.0968	7.9961	8.0886	8.0062	8.1156	**7.93**
H(5-6)	7.5969	7.8153	7.9081	7.9286	8.0401	7.9220	8.0928	7.9153	8.0755	7.9345	8.1147	7.5724	7.7481	7.8334	7.8390	7.9475	7.8340	7.9684	7.8286	7.9596	7.8436	7.9918	**7.835**
H8	4.1076	4.2213	4.2945	4.3275	4.4124	4.3193	4.4812	4.3114	4.4564	4.3347	4.5027	4.3614	4.5055	4.5879	4.6029	4.7225	4.5967	4.7680	4.5902	4.7524	4.6086	4.7951	**5.01**
H(9A-9C)	1.2022	1.2168	1.2232	1.2326	1.2175	1.2314	1.2410	1.2300	1.2374	1.2334	1.2518	1.2866	1.3047	1.2968	1.3283	1.3051	1.3269	1.3257	1.3252	1.3213	1.3296	1.3422	**1.46**
H(8`A-8`C)	2.5997	2.5499	2.5171	2.5356	2.5043	2.5367	2.4945	2.5375	2.4964	2.5344	2.4748	2.7488	2.5961	2.5738	2.5506	2.5083	2.5531	2.4709	2.5553	2.4783	2.5481	2.4323	**2.83**
Nuclei	OLYP																					
C1	142.1867	141.7073	142.7765	141.5423	143.3665	141.5562	142.0714	141.5650	142.3079	141.5206	142.1981	141.7642	141.5940	142.4863	141.4602	143.2060	141.4776	142.1692	141.4900	142.2723	141.4347	142.1927	**135.7**
C2	130.9111	129.3732	129.5508	128.7815	128.7491	128.8334	128.9288	128.8797	128.9542	128.7237	128.8380	130.6480	128.9244	129.1482	128.3908	128.4390	128.4274	128.5454	128.4590	128.5875	128.3477	128.4774	**126.6**
C3	126.9177	127.5970	128.4369	128.0035	129.0337	127.9927	129.0284	127.9760	129.0084	128.0045	129.0916	126.9851	127.5902	128.3769	127.9703	128.9662	127.9548	128.8849	127.9337	128.8860	127.9761	128.9611	**128.9**
C4	127.7910	129.8207	130.5829	130.8176	131.4081	130.7776	132.3101	130.7315	132.0750	130.8462	132.4115	127.7753	129.4151	130.1941	130.3143	130.9341	130.2695	131.4497	130.2186	131.3619	130.3477	131.6139	**129.8**
C5	128.6174	130.7120	131.5458	131.7332	132.8038	131.6832	132.9174	131.6269	132.8098	131.7706	133.0833	129.0274	131.0058	131.8953	131.9811	133.0923	131.9329	133.1287	131.8789	133.0639	132.0174	133.3048	**133.8**
C6	126.1900	127.6398	128.6533	128.5422	129.7465	128.5051	130.1878	128.4633	129.9953	128.5694	130.3324	125.3206	126.4272	127.4953	127.1644	128.4678	127.1273	128.6332	127.0849	128.6022	127.1903	128.8510	**133.9**
C7	201.8182	206.9595	208.8300	209.8562	211.1882	209.6814	215.2061	209.5027	214.3755	210.0146	216.0589	204.4607	209.2565	210.8071	212.0407	212.9361	211.8813	217.1460	211.7153	216.2755	212.1826	217.7774	**199.2**
C8	68.4330	69.5695	70.2519	70.1126	71.0309	70.0793	71.2687	70.0415	71.1998	70.1359	71.9585	64.9786	66.5450	67.0090	67.1875	67.9712	67.1589	68.4406	67.1248	68.2203	67.2057	68.6971	**62.9**
C9	20.3986	20.8289	21.2666	21.2228	21.6110	21.2187	21.8544	21.2093	21.7727	21.2181	21.9833	17.3578	17.3416	17.5542	17.4762	17.6433	17.4726	17.8007	17.4642	17.7474	17.4710	18.0630	**14.1**
C2``	134.2621	135.6024	136.5820	136.3144	137.6435	136.2812	137.4588	136.2423	137.4283	136.3368	137.5312	134.4850	135.8555	136.8065	136.4955	137.8203	136.4667	137.6657	136.4322	137.6357	136.5140	137.7322	**123**
C8`	36.5554	37.1800	37.4868	37.5879	38.0064	37.5691	38.0331	37.5452	38.0256	37.5970	38.3671	30.9740	31.2175	31.5758	31.6311	31.9486	31.6150	31.9586	31.5933	32.0160	31.6374	31.9374	**31.6**
H(3-4)	7.7457	7.8931	7.9511	7.9568	8.0266	7.9538	8.0611	7.9505	8.0492	7.9592	8.0769	7.7279	7.8552	7.9164	7.9175	7.9865	7.9142	8.0086	7.9107	8.0022	7.9202	8.0275	**7.93**
H(5-6)	7.5164	7.7331	7.8200	7.8423	7.9450	7.8373	7.9987	7.8321	7.9780	7.8467	8.0187	7.4894	7.6580	7.7469	7.7468	7.8544	7.7419	7.8737	7.7367	7.8677	7.7511	7.8988	**7.835**
H8	4.2170	4.3239	4.3792	4.4196	4.4813	4.4167	4.5489	4.4139	4.5232	4.4223	4.5700	4.4699	4.6018	4.6871	4.6922	4.8118	4.6864	4.8489	4.6805	4.8367	4.6974	4.8799	**5.01**
H(9A-9C)	1.2295	1.2447	1.2506	1.2611	1.2472	1.2608	1.2678	1.2604	1.2656	1.2609	1.2791	1.3266	1.3425	1.3359	1.3639	1.3426	1.3625	1.3631	1.3610	1.3588	1.3648	1.3797	**1.46**
H(8`A-8`C)	2.6320	2.5840	2.5558	2.5678	2.5400	2.5687	2.5274	2.5694	2.5310	2.5666	2.5030	2.7879	2.6308	2.6107	2.5861	2.5446	2.5884	2.5076	2.5906	2.5173	2.5835	2.4693	**2.83**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S16. Cont. V

Nuclei	R											S										Exp. [b]
	OPBE																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	139.0185	138.7212	139.6807	138.5115	140.2860	138.5349	139.0334	138.5415	139.2556	138.4855	139.1698	138.8287	138.7399	139.6053	138.5632	140.2847	138.5889	139.2405	138.5971	139.3455	138.5343	139.3261	**135.7**
C2	128.5909	127.2701	127.4469	126.6562	126.7589	126.7087	126.8868	126.7436	126.9051	126.6016	126.8558	128.2009	126.8391	126.9811	126.3048	126.4277	126.3506	126.4783	126.3790	126.5259	126.2567	126.4347	**126.6**
C3	125.4980	126.2609	127.0455	126.5897	127.6334	126.5879	127.6632	126.5677	127.6359	126.5861	127.7586	125.5003	126.2230	126.9087	126.5441	127.5353	126.5407	127.4590	126.5195	127.4673	126.5425	127.5381	**128.9**
C4	126.4890	128.5851	129.3400	129.4780	130.1660	129.4450	131.0545	129.3935	130.8184	129.5037	131.1992	126.3273	128.1420	128.8139	128.9662	129.6328	128.9347	130.1604	128.8848	130.0718	128.9909	130.3080	**129.8**
C5	127.1118	129.2788	130.0723	130.2179	131.3234	130.1810	131.4687	130.1254	131.3517	130.2471	131.6745	127.4844	129.5411	130.3662	130.4270	131.5753	130.3917	131.6242	130.3382	131.5532	130.4554	131.8236	**133.8**
C6	124.8557	126.3443	127.3206	127.0846	128.3648	127.0546	128.7502	127.0074	128.5809	127.1094	128.9296	123.7703	125.0825	126.0053	125.7063	127.0068	125.6850	127.1557	125.6456	127.1390	125.7213	127.3243	**133.9**
C7	199.3570	204.3664	205.9228	207.0056	208.0425	206.8494	212.0925	206.6781	211.2472	207.1514	212.8847	201.5145	206.5437	207.9307	209.1043	209.8680	208.9648	214.1430	208.8067	213.2432	209.2321	214.7423	**199.2**
C8	65.6847	66.9767	67.4506	67.4641	68.2365	67.4485	68.5754	67.4157	68.4791	67.4742	69.3275	62.6359	63.9933	64.4536	64.5085	65.2658	64.4920	65.7800	64.4579	65.5391	64.5196	66.1620	**62.9**
C9	19.5299	20.0217	20.3678	20.2781	20.6616	20.2754	20.9240	20.2561	20.8421	20.2775	21.0554	16.3525	16.4875	16.6335	16.5902	16.7324	16.5971	16.8913	16.5866	16.8506	16.5791	17.1779	**14.1**
C2``	129.8822	131.1572	132.0035	131.7065	132.9397	131.6901	132.7671	131.6557	132.7404	131.7169	132.8670	130.1248	131.3974	132.2094	131.8834	133.1103	131.8711	132.9503	131.8408	132.9247	131.8901	133.0605	**123**
C8`	35.5082	36.2167	36.3771	36.5077	36.8287	36.5057	36.8712	36.4859	36.8585	36.5040	37.2504	29.7474	30.2884	30.5220	30.5908	30.9001	30.5872	30.8991	30.5660	30.9636	30.5896	30.8877	**31.6**
H(3-4)	7.7991	7.9524	8.0082	8.0152	8.0868	8.0124	8.1213	8.0088	8.1085	8.0170	8.1401	7.7758	7.9158	7.9693	7.9771	8.0464	7.9742	8.0683	7.9706	8.0614	7.9791	8.0869	**7.93**
H(5-6)	7.5809	7.7986	7.8853	7.8997	8.0063	7.8945	8.0579	7.8886	8.0376	7.9039	8.0807	7.5280	7.7151	7.7938	7.8017	7.9080	7.7974	7.9261	7.7923	7.9206	7.8051	7.9476	**7.835**
H8	4.2468	4.3502	4.4152	4.4331	4.5103	4.4277	4.5763	4.4219	4.5511	4.4380	4.5993	4.4923	4.6369	4.7079	4.7301	4.8407	4.7249	4.8732	4.7190	4.8643	4.7342	4.8972	**5.01**
H(9A-9C)	1.1898	1.2086	1.2073	1.2220	1.2031	1.2214	1.2257	1.2202	1.2226	1.2220	1.2392	1.2618	1.2914	1.2770	1.3137	1.2851	1.3127	1.3036	1.3111	1.2985	1.3139	1.3221	**1.46**
H(8`A-8`C)	2.5501	2.5043	2.4654	2.4863	2.4478	2.4878	2.4360	2.4886	2.4389	2.4841	2.4149	2.6312	2.5159	2.4852	2.4764	2.4239	2.4793	2.3935	2.4814	2.4015	2.4730	2.3513	**2.83**
Nuclei	**OPW91**																						
C1	139.3496	139.0451	140.0025	138.8363	140.6012	138.8498	139.3442	138.8477	139.5674	138.8064	139.4832	139.1454	139.0562	139.9127	138.8802	140.5914	138.8963	139.5416	138.8956	139.6488	138.8470	139.6281	**135.7**
C2	128.8472	127.5146	127.6854	126.9002	126.9857	126.9431	127.1179	126.9691	127.1372	126.8414	127.0866	128.4639	127.0817	127.2241	126.5482	126.6557	126.5843	126.7137	126.6035	126.7612	126.4962	126.6718	**126.6**
C3	125.7244	126.4902	127.2696	126.8238	127.8542	126.8122	127.8837	126.7828	127.8558	126.8164	127.9812	125.7289	126.4523	127.1381	126.7788	127.7585	126.7652	127.6850	126.7347	127.6932	126.7733	127.7675	**128.9**
C4	126.6860	128.7892	129.5382	129.6900	130.3629	129.6469	131.2551	129.5858	131.0198	129.7120	131.4013	126.5338	128.3486	129.0208	129.1810	129.8323	129.1390	130.3664	129.0797	130.2765	129.2021	130.5179	**129.8**
C5	127.3301	129.5045	130.2920	130.4513	131.5424	130.4041	131.6870	130.3392	131.5710	130.4769	131.8944	127.7042	129.7681	130.5895	130.6617	131.7960	130.6162	131.8461	130.5532	131.7752	130.6863	132.0479	**133.8**
C6	125.0541	126.5518	127.5255	127.3030	128.5717	127.2624	128.9639	127.2056	128.7941	127.3245	129.1451	123.9835	125.2944	126.2195	125.9288	127.2168	125.8969	127.3730	125.8480	127.3544	125.9405	127.5467	**133.9**
C7	199.7166	204.7481	206.3099	207.4032	208.4364	207.2359	212.5019	207.0543	211.6511	207.5457	213.2997	201.8837	206.9227	208.3087	209.4998	210.2547	209.3494	214.5357	209.1818	213.6332	209.6242	215.1387	**199.2**
C8	65.8719	67.1625	67.6378	67.6541	68.4188	67.6287	68.7554	67.5866	68.6581	67.6606	69.5063	62.8050	64.1804	64.6285	64.7008	65.4485	64.6744	65.9537	64.6314	65.7155	64.7079	66.3315	**62.9**
C9	19.5949	20.0909	20.4362	20.3556	20.7333	20.3423	20.9964	20.3134	20.9148	20.3515	21.1310	16.4469	16.5817	16.7280	16.6898	16.8244	16.6864	16.9872	16.6666	16.9446	16.6749	17.2750	**14.1**
C2``	130.3892	131.6800	132.5280	132.2413	133.4709	132.2145	133.2980	132.1705	133.2709	132.2482	133.4002	130.6305	131.9201	132.7338	132.4173	133.6415	132.3944	133.4806	132.3546	133.4556	132.4204	133.5918	**123**
C8`	35.5736	36.2871	36.4491	36.5857	36.9016	36.5737	36.9452	36.5446	36.9330	36.5786	37.3255	29.8378	30.3742	30.6073	30.6856	30.9852	30.6719	30.9883	30.6414	31.0523	30.6808	30.9774	**31.6**
H(3-4)	7.7992	7.9524	8.0081	8.0158	8.0863	8.0124	8.1210	8.0086	8.1083	8.0173	8.1398	7.7762	7.9156	7.9693	7.9776	8.0459	7.9741	8.0680	7.9702	8.0610	7.9793	8.0867	**7.93**
H(5-6)	7.5803	7.7984	7.8849	7.9003	8.0061	7.8945	8.0580	7.8883	8.0379	7.9043	8.0808	7.5291	7.7155	7.7946	7.8030	7.9083	7.7980	7.9269	7.7926	7.9212	7.8061	7.9487	**7.835**
H8	4.2451	4.3489	4.4138	4.4329	4.5093	4.4267	4.5758	4.4207	4.5505	4.4375	4.5987	4.4883	4.6321	4.7045	4.7263	4.8363	4.7204	4.8704	4.7142	4.8608	4.7302	4.8948	**5.01**
H(9A-9C)	1.1909	1.2098	1.2088	1.2239	1.2043	1.2226	1.2272	1.2211	1.2240	1.2237	1.2406	1.2633	1.2928	1.2789	1.3156	1.2866	1.3140	1.3054	1.3122	1.3003	1.3156	1.3239	**1.46**
H(8`A-8`C)	2.5515	2.5059	2.4675	2.4887	2.4499	2.4896	2.4382	2.4902	2.4410	2.4863	2.4173	2.6376	2.5202	2.4908	2.4812	2.4285	2.4835	2.3981	2.4853	2.4059	2.4776	2.3562	**2.83**
Nuclei	**PBE**																						
C1	146.2354	145.8752	146.8740	145.4573	147.5365	145.4780	146.1770	145.5100	146.3906	145.4559	146.3571	145.8600	145.7116	146.5822	145.4509	147.2385	145.4641	145.9713	145.4881	146.2434	145.4562	146.3091	**135.7**
C2	135.1174	133.6307	133.7235	132.8552	132.9468	132.8985	133.1577	132.9526	133.1612	132.8320	133.0747	134.8920	133.2897	133.3599	132.5667	132.7315	132.6036	132.9518	132.6519	132.9045	132.5497	132.8183	**126.6**
C3	130.9412	131.9177	132.6663	132.2215	133.3536	132.2015	133.5034	132.1919	133.4073	132.2580	133.5903	131.0720	131.8521	132.6794	132.1142	133.3538	132.0951	133.4614	132.0870	133.3629	132.1501	133.4521	**128.9**
C4	132.5104	134.8608	135.6381	135.8789	136.6510	135.8170	137.6097	135.7653	137.3697	135.9547	137.7687	132.5330	134.5770	135.2992	135.4294	136.3254	135.3759	137.0948	135.3330	136.8303	135.4974	137.1348	**129.8**
C5	133.2771	135.6663	136.4956	136.6864	137.9688	136.6238	138.1547	136.5715	138.0272	136.7628	138.3929	133.7042	136.0241	136.9043	136.9718	138.3020	136.9139	138.4163	136.8662	138.2939	137.0442	138.6100	**133.8**
C6	130.3227	132.1171	133.2073	133.0114	134.4435	132.9508	134.8801	132.9017	134.7328	133.0875	135.0644	129.3451	130.8385	131.8390	131.5159	133.0933	131.4699	133.6240	131.4346	133.3606	131.5774	133.6044	**133.9**
C7	209.0511	214.1499	215.7955	216.7096	218.2177	216.5431	222.2785	216.3891	221.3319	216.8871	223.2768	211.3485	216.3252	218.0028	218.8339	220.0730	218.6717	223.8796	218.5213	223.1112	219.0060	224.8637	**199.2**
C8	70.7155	72.0400	72.6355	72.4276	73.4257	72.3988	73.9247	72.3813	73.7657	72.4734	74.8159	66.3656	67.6814	68.2485	68.1875	69.0733	68.1524	69.3739	68.1286	69.3269	68.2387	70.0020	**62.9**
C9	21.2116	21.7083	21.8768	21.9726	22.3435	21.9518	22.5339	21.9419	22.4554	22.0102	22.7655	18.1122	18.2820	18.3976	18.4145	18.6297	18.4031	18.9686	18.4023	18.8563	18.4425	19.4011	**14.1**
C2``	139.4621	140.9988	141.9192	141.5876	143.0648	141.5496	142.9467	141.5223	142.8825	141.6409	143.0612	139.7373	141.2276	142.1876	141.7457	143.2592	141.7128	143.1533	141.6905	143.0971	141.7943	143.2755	**123**
C8`	37.2326	37.8587	37.9944	38.0856	38.5276	38.0652	38.6762	38.0562	38.6521	38.1234	39.1490	30.6164	31.1108	31.4155	31.3948	31.8401	31.3680	31.9720	31.3528	31.9208	31.4389	32.0327	**31.6**
H(3-4)	7.7485	7.9044	7.9607	7.9684	8.0392	7.9649	8.0789	7.9619	8.0662	7.9723	8.0974	7.7354	7.8765	7.9317	7.9358	8.0115	7.9325	8.0440	7.9296	8.0299	7.9396	8.0566	**7.93**
H(5-6)	7.5412	7.7655	7.8496	7.8755	7.9769	7.8690	8.0302	7.8630	8.0140	7.8823	8.0533	7.5087	7.7020	7.7811	7.7887	7.9072	7.7837	7.9440	7.7792	7.9231	7.7941	7.9540	**7.835**
H8	4.3652	4.4904	4.5492	4.5816	4.6468	4.5758	4.7083	4.5705	4.6843	4.5878	4.7281	4.6115	4.7644	4.8329	4.8520	4.9850	4.8469	5.0503	4.8422	5.0198	4.8575	5.0569	**5.01**
H(9A-9C)	1.2527	1.2702	1.2651	1.2718	1.2596	1.2717	1.2838	1.2721	1.2777	1.2726	1.2970	1.3497	1.3770	1.3653	1.3918	1.3757	1.3908	1.3953	1.3904	1.3906	1.3933	1.4172	**1.46**
H(8`A-8`C)	2.6765	2.6050	2.5643	2.5726	2.5438	2.5744	2.5251	2.5766	2.5270	2.5715	2.5073	2.7908	2.6549	2.6225	2.5883	2.5532	2.5920	2.5052	2.5963	2.5115	2.5854	2.4668	**2.83**
Nuclei	**PBE0**																						
C1	147.3202	146.6657	147.6117	146.2203	148.0993	146.2400	146.7655	146.2623	146.9345	146.2052	146.8797	147.1480	146.7559	147.4708	146.4195	148.0668	146.4368	146.8523	146.4555	147.1086	146.4057	147.1220	**135.7**
C2	136.5315	135.0181	135.1040	134.3208	134.3574	134.3568	134.6351	134.3947	134.5766	134.2898	134.4755	136.2734	134.6125	134.8183	133.9848	134.1356	134.0128	134.3521	134.0434	134.2684	133.9621	134.1443	**126.6**
C3	133.0301	133.8620	134.5785	134.1804	135.1719	134.1577	135.3717	134.1365	135.2392	134.2045	135.3876	133.0699	133.7588	134.5855	134.0811	135.1855	134.0557	135.3219	134.0322	135.1677	134.1084	135.2685	**128.9**
C4	134.4123	136.6797	137.4071	137.7257	138.3721	137.6600	139.3852	137.5958	139.0898	137.7903	139.4636	134.3914	136.3317	137.1107	137.2401	138.0130	137.1799	138.8119	137.1216	138.5015	137.3004	138.7909	**129.8**
C5	135.6156	137.8728	138.6642	138.8884	140.0469	138.8246	140.2295	138.7620	140.0601	138.9513	140.3947	135.9181	138.1627	138.9971	139.1392	140.3138	139.0776	140.4540	139.0175	140.2960	139.2001	140.6043	**133.8**
C6	131.9609	133.6592	134.7353	134.6327	135.9506	134.5642	136.4870	134.4985	136.2874	134.7018	136.5730	131.2018	132.5478	133.6327	133.2828	134.7362	133.2302	135.2522	133.1799	134.9563	133.3361	135.1629	**133.9**
C7	207.8292	213.2085	214.7665	216.0253	217.0820	215.8418	221.9627	215.6617	220.7813	216.2046	222.9364	209.8795	215.0946	216.4790	217.7846	218.6283	217.6111	223.3149	217.4399	222.2910	217.9525	224.2432	**199.2**
C8	66.8042	67.9176	68.4864	68.3435	69.1331	68.3098	69.6985	68.2788	69.4931	68.3794	70.4524	62.5315	63.6274	63.9404	64.0846	64.7402	64.0533	65.1396	64.0233	65.0241	64.1166	65.6473	**62.9**
C9	20.4451	20.7542	20.8702	21.0061	21.2500	20.9835	21.3847	20.9630	21.2680	21.0311	21.4954	17.2893	17.3807	17.4424	17.5177	17.6464	17.5067	17.8711	17.4972	17.7660	17.5306	18.1886	**14.1**
C2``	129.1379	130.4541	131.3032	131.0223	132.2798	130.9835	132.2511	130.9467	132.1420	131.0618	132.3011	129.3826	130.6587	131.5369	131.1710	132.4595	131.1363	132.4393	131.1032	132.3233	131.2067	132.4988	**123**
C8`	35.5895	36.2059	36.3447	36.5031	36.8277	36.4769	37.0817	36.4533	36.9931	36.5315	37.4773	29.4450	29.9008	30.1744	30.2498	30.5598	30.2198	30.7943	30.1917	30.7061	30.2815	30.8112	**31.6**
H(3-4)	7.9144	8.0714	8.1265	8.1374	8.2051	8.1338	8.2487	8.1300	8.2332	8.1406	8.2641	7.8992	8.0433	8.1024	8.1070	8.1805	8.1033	8.2153	8.0995	8.1992	8.1103	8.2265	**7.93**
H(5-6)	7.6983	7.9286	8.0119	8.0441	8.1483	8.0371	8.2029	8.0302	8.1834	8.0504	8.2228	7.6730	7.8667	7.9556	7.9586	8.0779	7.9531	8.1121	7.9475	8.0905	7.9637	8.1212	**7.835**
H8	4.0583	4.2132	4.2738	4.3251	4.3971	4.3178	4.4738	4.3105	4.4414	4.3318	4.4883	4.3302	4.4975	4.5901	4.5973	4.7355	4.5908	4.7989	4.5846	4.7690	4.6031	4.8012	**5.01**
H(9A-9C)	1.1845	1.2010	1.1910	1.2040	1.1808	1.2038	1.2126	1.2035	1.2035	1.2041	1.2221	1.2569	1.2813	1.2667	1.2970	1.2734	1.2957	1.3010	1.2946	1.2952	1.2980	1.3170	**1.46**
H(8`A-8`C)	2.5856	2.5207	2.4794	2.4948	2.4587	2.4961	2.4497	2.4975	2.4471	2.4934	2.4337	2.6876	2.5512	2.5160	2.4918	2.4492	2.4946	2.4130	2.4976	2.4167	2.4890	2.3752	**2.83**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S16. Cont. VI

Nuclei	R											S										Exp. [b]
	TPSS																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	142.7454	142.1281	143.1696	141.7815	143.6429	141.8129	142.3712	141.8554	142.3949	141.7612	142.5002	142.2502	141.7697	142.6501	141.5379	143.3507	141.5568	141.7444	141.5877	142.6362	141.5312	141.9914	**135.7**
C2	132.4076	130.7279	130.8886	130.0201	130.0001	130.0677	130.1974	130.1269	130.6195	129.9859	130.0729	132.0883	130.3452	130.5625	129.7113	129.6496	129.7509	130.0347	129.8025	130.9394	129.6846	129.9011	**126.6**
C3	128.0993	128.8816	129.7194	129.2562	130.2457	129.2409	130.4037	129.2367	129.7258	129.2812	130.4579	128.1954	128.8696	129.7689	129.2243	130.2177	129.2101	130.5099	129.2072	130.3486	129.2479	130.5293	**128.9**
C4	129.2547	131.4058	132.2327	132.4883	133.1063	132.4298	134.0580	132.3828	132.8844	132.5544	134.1784	129.3298	131.2717	132.0452	132.2081	132.7707	132.1615	133.8245	132.1259	133.2454	132.2620	133.8960	**129.8**
C5	129.9647	132.1405	133.0222	133.2092	134.3421	133.1527	134.5100	133.1073	133.6118	133.2732	134.7088	130.3510	132.4556	133.3864	133.4727	134.6215	133.4202	134.7896	133.3783	134.4884	133.5324	134.9550	**133.8**
C6	127.1504	128.7938	129.9401	129.8182	131.0507	129.7574	131.5209	129.7092	130.2001	129.8876	131.6742	126.5353	128.0094	128.9888	128.7932	129.9385	128.7523	130.8116	128.7225	129.8675	128.8421	130.8638	**133.9**
C7	204.0109	208.7805	210.4304	211.4126	212.6481	211.2586	216.9415	211.1158	211.9324	211.5697	217.9255	206.3317	210.9649	212.2191	213.2995	214.3678	213.1679	217.9230	213.0500	213.5626	213.4389	218.7930	**199.2**
C8	68.8505	69.8967	70.5928	70.3940	71.2316	70.3727	71.7843	70.3624	70.6160	70.4248	72.5879	65.0206	65.9821	66.4981	66.5022	67.5141	66.4742	67.4406	66.4585	68.0705	66.5402	67.8701	**62.9**
C9	21.8652	22.2140	22.4842	22.5637	22.8330	22.5474	23.0698	22.5427	22.6050	22.5900	23.2090	18.8494	18.9583	19.1723	19.1772	19.3820	19.1658	19.7099	19.1655	21.1322	19.1977	20.0665	**14.1**
C2``	137.0986	138.5158	139.5097	139.2024	140.5263	139.1680	140.4379	139.1449	139.6736	139.2455	140.5137	137.3170	138.6550	139.7081	139.2736	140.6399	139.2439	140.5811	139.2250	140.2913	139.3123	140.6520	**123**
C8`	37.6356	38.1557	38.4253	38.5101	38.8458	38.4935	39.0564	38.4886	38.6147	38.5370	39.4633	31.8488	32.2786	32.5127	32.5538	32.7507	32.5420	33.0571	32.5433	34.4097	32.5781	33.0647	**31.6**
H(3-4)	7.7080	7.8631	7.9253	7.9340	8.0035	7.9300	8.0473	7.9265	7.7646	7.9382	8.0617	7.7015	7.8461	7.9081	7.9141	7.9802	7.9103	8.0278	7.9071	8.0210	7.9179	8.0399	**7.93**
H(5-6)	7.4987	7.7305	7.8214	7.8520	7.9542	7.8446	8.0074	7.8378	7.6755	7.8595	8.0270	7.4798	7.6851	7.7698	7.7824	7.8836	7.7769	7.9447	7.7720	7.8869	7.7878	7.9587	**7.835**
H8	4.2877	4.4162	4.4807	4.5202	4.5910	4.5133	4.6468	4.5071	4.3315	4.5273	4.6632	4.4865	4.6626	4.7520	4.7694	4.8770	4.7632	4.9742	4.7574	4.8949	4.7755	4.9882	**5.01**
H(9A-9C)	1.2405	1.2589	1.2616	1.2709	1.2532	1.2705	1.2877	1.2706	1.0820	1.2718	1.2932	1.3234	1.3529	1.3480	1.3754	1.3543	1.3740	1.3914	1.3733	1.5361	1.3772	1.4060	**1.46**
H(8`A-8`C)	2.6271	2.5614	2.5244	2.5377	2.5083	2.5390	2.4948	2.5408	2.3573	2.5370	2.4779	2.7857	2.6630	2.6059	2.5945	2.5355	2.5996	2.5002	2.6052	2.7588	2.5903	2.4633	**2.83**
Nuclei	VSXC																						
C1	141.2506	140.7850	141.6608	140.5291	142.1799	140.5467	141.0950	140.5620	141.2097	140.5145	141.2013	141.7150	141.3659	142.1074	141.2186	142.6032	141.2307	141.5926	141.2405	141.7980	141.2085	141.7306	**135.7**
C2	130.2115	128.5985	128.4946	127.7998	127.7593	127.8520	127.7582	127.9020	127.7894	127.7518	127.7659	130.6695	128.9312	129.1364	128.2615	128.2905	128.2985	128.4255	128.3344	128.4741	128.2290	128.1923	**126.6**
C3	125.4834	126.5792	127.1505	127.0185	127.8867	126.9996	128.1204	126.9779	127.9644	127.0373	128.2302	126.0572	126.8038	127.5339	127.2395	128.1249	127.2145	128.2472	127.1875	128.1903	127.2650	128.3318	**128.9**
C4	129.0210	131.4010	131.9157	132.4842	133.0505	132.4262	133.8803	132.3653	133.6121	132.5400	134.0820	127.9139	130.1072	130.8190	131.1715	131.8891	131.1106	132.6219	131.0475	132.3905	131.2308	132.7944	**129.8**
C5	129.4158	131.6267	132.5370	132.6770	133.9262	132.6199	133.9780	132.5601	133.8703	132.7318	134.1556	128.8191	131.0669	131.7901	132.1613	133.1802	132.0991	133.2984	132.0347	133.1768	132.2216	133.5013	**133.8**
C6	128.2855	129.4949	130.8957	130.4414	132.0835	130.3790	132.2758	130.3154	132.2771	130.5031	132.5856	125.8312	127.5822	128.5326	128.5271	129.9129	128.4717	130.4412	128.4143	130.1702	128.5813	130.6400	**133.9**
C7	207.9468	212.6363	213.8850	215.0659	215.7540	214.9196	219.8564	214.7717	218.8402	215.2059	220.5683	199.9030	205.0382	206.4336	207.6675	208.7481	207.5131	212.4636	207.3562	211.6447	207.8149	213.5229	**199.2**
C8	77.3460	77.9862	78.2612	78.2367	78.5047	78.2233	78.9439	78.2081	78.8518	78.2514	79.5424	66.9570	68.1483	68.6966	68.7775	69.6213	68.7460	69.8202	68.7116	69.7018	68.8084	70.4019	**62.9**
C9	30.3306	30.8820	31.2701	31.2948	31.7369	31.2714	31.8956	31.2460	31.8244	31.3187	31.7712	29.5957	29.5692	29.5868	29.5510	29.8108	29.5565	29.5737	29.5599	29.5518	29.5469	30.1229	**14.1**
C2``	134.9707	136.4118	136.9988	137.0158	138.1248	136.9854	138.0142	136.9525	137.9155	137.0457	138.2135	135.8310	137.2242	138.1334	137.8824	139.1610	137.8464	139.0312	137.8081	138.9859	137.9182	139.1507	**123**
C8`	43.3212	43.9896	45.0340	44.4291	45.4283	44.3995	45.2883	44.3687	45.3920	44.4598	45.7845	34.5012	35.2519	35.4494	35.6842	35.9779	35.6607	36.1124	35.6350	36.0452	35.7080	36.4117	**31.6**
H(3-4)	7.8385	8.0048	8.0527	8.0765	8.1390	8.0726	8.1698	8.0687	8.1544	8.0802	8.1899	7.7285	7.8826	7.9369	7.9563	8.0167	7.9519	8.0578	7.9477	8.0417	7.9603	8.0733	**7.93**
H(5-6)	7.9162	8.0953	8.1843	8.1846	8.3210	8.1793	8.3250	8.1741	8.3181	8.1896	8.3598	7.5835	7.7936	7.8622	7.8993	8.0046	7.8929	8.0420	7.8866	8.0214	7.9053	8.0612	**7.835**
H8	4.5522	4.6185	4.5640	4.6767	4.6857	4.6727	4.6869	4.6689	4.6759	4.6806	4.7394	4.6798	4.8395	4.9053	4.9432	5.0473	4.9363	5.1133	4.9296	5.0861	4.9498	5.1239	**5.01**
H(9A-9C)	1.6060	1.5951	1.5555	1.5817	1.5326	1.5827	1.5588	1.5838	1.5512	1.5807	1.5750	1.5807	1.5852	1.5755	1.5980	1.5829	1.5968	1.6000	1.5959	1.5988	1.5991	1.6153	**1.46**
H(8`A-8`C)	2.8995	2.8741	2.8636	2.8720	2.8637	2.8716	2.8319	2.8713	2.8407	2.8725	2.8270	2.8114	2.7426	2.7040	2.6911	2.6829	2.6949	2.6030	2.6987	2.6202	2.6874	2.6218	**2.83**
Nuclei	wB97																						
C1	148.2604	147.4068	148.2998	146.8229	148.6688	146.8541	147.1422	146.8856	147.4099	146.7953	147.2359	148.3102	147.5605	148.3776	147.1235	148.9615	147.1498	147.7219	147.1753	147.9552	147.0987	147.8994	**135.7**
C2	136.7882	135.1263	135.3285	134.5022	134.5594	134.5357	134.7844	134.5687	134.7633	134.4711	134.7075	136.6602	134.9600	135.2273	134.3340	134.3800	134.3672	134.4070	134.4002	134.4161	134.3037	134.2380	**126.6**
C3	134.3884	135.0809	135.7909	135.4080	136.4173	135.3880	136.4070	135.3670	136.3270	135.4273	136.5019	134.3666	135.0099	135.7623	135.3710	136.4246	135.3482	136.3229	135.3245	136.2958	135.3929	136.4132	**128.9**
C4	134.9773	137.0361	137.8362	138.0891	138.7442	138.0252	139.6397	137.9605	139.3962	138.1501	139.7798	134.9419	136.8066	137.5437	137.7398	138.3582	137.6828	138.9170	137.6250	138.7191	137.7942	138.9820	**129.8**
C5	137.4750	139.6067	140.3754	140.5983	141.7448	140.5399	141.7069	140.4803	141.6109	140.6533	141.9288	137.7165	139.8801	140.6770	140.8559	142.0330	140.7977	142.0237	140.7384	141.9334	140.9112	142.2583	**133.8**
C6	132.1860	133.6957	135.0209	134.6930	136.1305	134.6237	136.6058	134.5557	136.4628	134.7618	136.7266	131.4234	132.6622	133.7613	133.4414	134.6802	133.3908	134.9493	133.3396	134.7739	133.4901	134.9628	**133.9**
C7	207.2679	213.0734	214.8477	216.0988	217.1340	215.9054	222.2525	215.7136	221.1643	216.2863	223.2047	208.6931	214.0751	215.8678	217.0793	218.1030	216.8950	223.0607	216.7098	221.9541	217.2538	224.0330	**199.2**
C8	65.3601	66.4062	67.1394	66.7830	67.6079	66.7571	67.9933	66.7318	67.9036	66.8099	68.6338	60.7893	61.6146	62.0282	62.0612	62.8953	62.0313	63.2145	62.0009	63.1150	62.0900	63.6187	**62.9**
C9	20.4813	20.6415	20.7572	20.8457	21.0969	20.8290	20.9965	20.8120	20.9680	20.8624	21.0716	17.9694	17.9535	17.8680	18.0040	18.0967	17.9974	18.1981	17.9906	18.1537	18.0113	18.5917	**14.1**
C2``	130.2606	131.4547	132.2984	132.0283	133.2680	131.9924	133.1457	131.9557	133.0728	132.0629	133.2575	130.5021	131.6757	132.5296	132.2007	133.4758	132.1686	133.3511	132.1359	133.3096	132.2314	133.4826	**123**
C8`	35.3106	35.8295	36.0067	36.1004	36.4455	36.0790	36.6298	36.0579	36.5747	36.1226	37.0500	29.4550	29.8573	30.2405	30.2069	30.5682	30.1807	30.6154	30.1543	30.5649	30.2327	30.6929	**31.6**
H(3-4)	7.9980	8.1490	8.2076	8.2133	8.2864	8.2096	8.3211	8.2059	8.3089	8.2168	8.3397	7.9835	8.1285	8.1833	8.1921	8.2635	8.1883	8.2855	8.1845	8.2751	8.1956	8.3030	**7.93**
H(5-6)	7.7653	7.9871	8.0884	8.1026	8.2229	8.0953	8.2728	8.0880	8.2554	8.1097	8.2957	7.7464	7.9424	8.0291	8.0361	8.1467	8.0305	8.1675	8.0248	8.1522	8.0415	8.1872	**7.835**
H8	3.8115	3.9749	4.0818	4.1052	4.2110	4.0959	4.2962	4.0867	4.2670	4.1146	4.3178	4.0813	4.2602	4.3539	4.3666	4.4855	4.3602	4.5231	4.3536	4.5010	4.3728	4.5237	**5.01**
H(9A-9C)	1.2105	1.2221	1.2248	1.2211	1.2067	1.2208	1.2307	1.2207	1.2281	1.2214	1.2369	1.2654	1.2811	1.2717	1.2999	1.2807	1.2985	1.2998	1.2972	1.2956	1.3012	1.3176	**1.46**
H(8`A-8`C)	2.5896	2.5298	2.4740	2.5066	2.4681	2.5080	2.4509	2.5093	2.4514	2.5052	2.4424	2.6412	2.5158	2.5155	2.4669	2.4360	2.4694	2.3903	2.4719	2.3965	2.4645	2.3597	**2.83**
Nuclei	wB97X																						
C1	149.4483	148.6076	149.5410	148.0456	149.9155	148.0749	148.4277	148.1045	148.6298	148.0205	148.5260	149.4539	148.7689	149.5708	148.3862	150.1648	148.4114	148.9806	148.4355	149.1422	148.3631	149.1407	**135.7**
C2	138.1359	136.5161	136.6962	135.9122	135.9480	135.9501	136.1809	135.9876	136.1104	135.8764	136.0846	137.9275	136.1829	136.4117	135.5359	135.6356	135.5718	135.6703	135.6077	135.6413	135.5037	135.5130	**126.6**
C3	134.9681	135.6761	136.3673	135.9896	136.9985	135.9743	137.0264	135.9575	136.8865	136.0047	137.1031	134.9539	135.5793	136.3603	135.9272	136.9827	135.9073	136.9318	135.8863	136.8310	135.9472	136.9872	**128.9**
C4	135.7085	137.8120	138.5878	138.8863	139.5174	138.8251	140.4398	138.7631	140.1420	138.9446	140.5624	135.7295	137.5886	138.3229	138.5053	139.1587	138.4518	139.7692	138.3973	139.5196	138.5573	139.8440	**129.8**
C5	137.9339	140.0747	140.8493	141.0663	142.2083	141.0113	142.2210	140.9545	142.0638	141.1189	142.4276	138.1751	140.3477	141.1517	141.3256	142.4826	141.2703	142.5220	141.2137	142.3647	141.3788	142.7269	**133.8**
C6	133.1589	134.7216	135.9441	135.7358	137.0864	135.6683	137.5485	135.6027	137.3582	135.8019	137.6620	132.3605	133.5896	134.6705	134.3342	135.6455	134.2888	135.9599	134.2431	135.7469	134.3788	135.9849	**133.9**
C7	209.0314	214.8511	216.6102	217.9193	218.8841	217.7181	224.1132	217.5202	222.9286	218.1150	225.0748	210.7205	216.0674	217.8298	219.0654	220.0369	218.8822	225.0750	218.6971	223.8685	219.2399	226.0241	**199.2**
C8	66.5806	67.6294	68.3463	68.0187	68.8259	67.9875	69.2781	67.9578	69.1153	68.0519	69.9401	61.9900	62.9076	63.3222	63.3840	64.1527	63.3562	64.5388	63.3275	64.3504	63.4113	64.9556	**62.9**
C9	20.5445	20.6968	20.8893	20.9206	21.2010	20.9043	21.1760	20.8877	21.0938	20.9372	21.2596	17.9052	17.9120	17.8609	17.9952	18.0382	17.9916	18.2148	17.9873	18.1044	17.9999	18.5504	**14.1**
C2``	130.2582	131.4765	132.3138	132.0400	133.2940	132.0076	133.1908	131.9741	133.0620	132.0717	133.2933	130.4860	131.6791	132.5483	132.2097	133.4792	132.1798	133.3991	132.1490	133.2866	132.2390	133.5106	**123**
C8`	35.5749	36.1174	36.3021	36.4232	36.7599	36.3994	36.9770	36.3763	36.8651	36.4490	37.3980	29.6052	29.9933	30.3608	30.3706	30.7235	30.3451	30.8401	30.3193	30.7432	30.3964	30.9272	**31.6**
H(3-4)	7.9680	8.1209	8.1790	8.1876	8.2586	8.1840	8.2928	8.1803	8.2777	8.1910	8.3099	7.9590	8.1042	8.1608	8.1689	8.2411	8.1653	8.2651	8.1616	8.2515	8.1725	8.2796	**7.93**
H(5-6)	7.7399	7.9656	8.0601	8.0833	8.1966	8.0762	8.2446	8.0691	8.2253	8.0902	8.2661	7.7249	7.9198	8.0061	8.0129	8.1262	8.0076	8.1478	8.0022	8.1311	8.0181	8.1653	**7.835**
H8	3.8670	4.0301	4.1181	4.1568	4.2490	4.1481	4.3256	4.1398	4.2948	4.1652	4.3458	4.1319	4.3047	4.3942	4.4072	4.5314	4.4011	4.5756	4.3950	4.5530	4.4133	4.5822	**5.01**
H(9A-9C)	1.2018	1.2157	1.2143	1.2142	1.1979	1.2140	1.2226	1.2139	1.2160	1.2145	1.2279	1.2615	1.2760	1.2666	1.2966	1.2741	1.2953	1.2974	1.2940	1.2909	1.2978	1.3111	**1.46**
H(8`A-8`C)	2.5951	2.5336	2.4808	2.5074	2.4732	2.5092	2.4575	2.5110	2.4551	2.5057	2.4457	2.6652	2.5348	2.5238	2.4848	2.4520	2.4875	2.4041	2.4902	2.4097	2.4824	2.3711	**2.83**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S16. Cont. VII

Nuclei	R											S										Exp. [b]
	X3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	150.2726	149.4948	150.5489	149.0720	150.9801	149.0966	149.5534	149.1195	149.8118	149.0533	149.6779	149.9162	149.4261	150.3356	149.1328	150.8491	149.1530	149.2947	149.1697	149.7832	149.1169	149.6876	**135.7**
C2	138.6869	137.0492	137.1314	136.3229	136.2857	136.3711	136.4847	136.4160	136.5100	136.2806	136.3492	138.5386	136.7378	136.7898	136.0701	136.0929	136.1099	136.4260	136.1475	136.2793	136.0369	136.1956	**126.6**
C3	134.4067	135.2132	135.9506	135.5472	136.5187	135.5334	136.6069	135.5156	136.5480	135.5632	136.6569	134.4621	135.1408	135.9186	135.4714	136.5213	135.4557	136.6711	135.4368	136.5257	135.4899	136.6146	**128.9**
C4	135.5124	137.7852	138.4936	138.8517	139.4125	138.7953	140.3646	138.7347	140.1430	138.9080	140.4768	135.5650	137.4949	138.1103	138.4081	139.0296	138.3597	139.9245	138.3080	139.5513	138.4578	139.8732	**129.8**
C5	136.8805	139.1224	139.8679	140.1642	141.2439	140.1080	141.3151	140.0482	141.2048	140.2204	141.5239	137.1733	139.3986	140.2448	140.4094	141.5329	140.3541	141.5999	140.2952	141.4958	140.4649	141.7722	**133.8**
C6	133.1941	134.9668	136.1244	136.0080	137.2990	135.9443	137.8315	135.8786	137.6886	136.0732	137.9559	132.6113	133.9740	134.8556	134.7041	136.0096	134.6628	136.6964	134.6194	136.2694	134.7475	136.5706	**133.9**
C7	210.2828	215.8543	217.6489	218.9026	220.0153	218.7064	225.0491	218.5106	223.9799	219.0960	226.0565	212.9423	218.1779	219.7672	220.9509	221.9382	220.7901	226.1784	220.6259	225.4616	221.1075	227.2252	**199.2**
C8	69.3935	70.4595	71.0933	70.9288	71.7478	70.8991	72.2235	70.8671	72.0998	70.9621	72.9916	65.1572	66.3107	66.9123	66.8256	67.6248	66.7972	67.6125	66.7653	67.7696	66.8555	68.2459	**62.9**
C9	21.1300	21.4406	21.6557	21.7222	21.9927	21.7057	22.1119	21.6865	22.0772	21.7426	22.2292	18.1552	18.1503	18.2316	18.2154	18.3506	18.2105	18.4961	18.2035	18.4344	18.2248	18.8640	**14.1**
C2``	133.9834	135.4180	136.3298	136.0866	137.4175	136.0508	137.2720	136.0113	137.2236	136.1243	137.3717	134.2221	135.6350	136.5902	136.2383	137.5986	136.2067	137.4947	136.1717	137.4398	136.2720	137.5940	**123**
C8`	36.5310	37.1399	37.3326	37.5161	37.8613	37.4936	38.0369	37.4686	38.0441	37.5415	38.4674	30.5913	30.9893	31.2459	31.3447	31.6558	31.3250	31.8300	31.3029	31.7602	31.3676	31.8110	**31.6**
H(3-4)	7.8494	8.0039	8.0593	8.0714	8.1378	8.0680	8.1730	8.0640	8.1611	8.0746	8.1903	7.8352	7.9757	8.0304	8.0407	8.1100	8.0372	8.1446	8.0333	8.1266	8.0440	8.1538	**7.93**
H(5-6)	7.6213	7.8547	7.9444	7.9745	8.0802	7.9676	8.1310	7.9602	8.1168	7.9810	8.1520	7.6109	7.8026	7.8777	7.8946	8.0039	7.8896	8.0468	7.8840	8.0173	7.8994	8.0525	**7.835**
H8	4.0746	4.2300	4.3062	4.3402	4.4255	4.3333	4.4900	4.3260	4.4652	4.3469	4.5047	4.3236	4.4958	4.5606	4.5962	4.7194	4.5904	4.8061	4.5841	4.7591	4.6018	4.8033	**5.01**
H(9A-9C)	1.2143	1.2293	1.2323	1.2379	1.2192	1.2375	1.2487	1.2366	1.2464	1.2383	1.2551	1.3048	1.3244	1.3116	1.3438	1.3219	1.3427	1.3432	1.3411	1.3378	1.3449	1.3568	**1.46**
H(8`A-8`C)	2.6391	2.5716	2.5332	2.5509	2.5189	2.5521	2.5078	2.5528	2.5081	2.5499	2.4925	2.8062	2.6615	2.6137	2.5925	2.5508	2.5975	2.5009	2.6022	2.5034	2.5879	2.4575	**2.83**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S17. Theoretical chemical shifts (in ppm) of *(R,S)*-3-trifluoromethylmethcathinone calculated with HF and selected functionals combined with 6-311++G** basis set[a]

Nuclei	R											S										Exp. [b]
	B3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	143.3809	143.2119	146.2093	144.4948	146.8949	144.4762	146.2557	143.1929	146.3862	144.5137	146.3332	141.9336	143.0651	144.0610	143.9600	143.7659	143.9061	144.9250	143.8626	144.7479	144.0756	145.0528	**135.1**
C2	134.3510	133.6748	136.1292	133.5156	135.7224	133.5281	136.2198	133.3720	136.1094	133.5026	136.1875	133.9053	133.7574	135.6309	133.5465	133.8590	133.5382	135.7587	133.5395	135.6362	133.6453	135.6920	**131.6**
C3	140.1802	138.9763	139.1748	138.5194	138.6247	138.5429	138.8142	138.5129	138.7949	138.4959	138.8132	140.0810	138.8720	138.9058	138.2979	138.2703	138.3191	138.5038	138.3411	138.4778	138.2820	138.5033	**126.5**
C4	136.2477	138.1137	137.2355	138.5819	138.1059	138.5362	139.0128	138.7490	138.7668	138.6231	139.2209	136.4258	137.6378	137.4580	138.1383	139.4759	138.1199	138.9388	138.0915	138.7520	138.0617	139.1517	**132.3**
C5	133.6981	135.8268	135.6032	136.6647	136.6950	136.6075	136.8118	136.6261	136.7022	136.7168	136.9566	134.0260	135.9850	135.9975	136.7815	137.6538	136.7396	137.0357	136.6924	136.9472	136.7752	137.1802	**133.1**
C6	136.5463	139.1227	139.8443	140.0581	141.5456	139.9828	141.8800	140.1804	141.6456	140.1276	142.2665	136.8483	139.3637	140.6920	140.4274	142.8172	140.3639	142.7658	140.2972	142.6108	140.4672	143.1100	**133.7**
C7	203.7460	208.7036	211.4160	212.2252	213.5526	212.0468	218.6038	210.9650	217.6309	212.3963	219.3736	208.5019	212.7953	213.9428	215.1427	215.4246	214.9965	220.0517	214.8499	218.9374	215.2690	220.6734	**196.3**
C8	65.6514	66.6733	67.3659	67.3487	68.0464	67.3338	68.6671	67.0314	68.4701	67.3621	69.3430	60.1351	62.1511	62.7470	63.1511	63.7316	63.0853	64.7021	63.0242	64.4026	63.2405	64.9626	**60.8**
C9	22.7277	23.1140	22.9968	23.1827	23.3498	23.1603	23.4131	23.2908	23.3481	23.2025	23.5454	19.4123	19.8451	20.0955	20.0166	20.4380	20.0015	20.5846	19.9875	20.5211	20.0376	20.9151	**15.9**
C3``	135.4312	136.7764	137.6575	137.2551	138.5795	137.2235	138.4366	137.1944	138.3844	137.2832	138.5085	135.4310	136.8097	137.6059	137.3038	138.7087	137.2707	138.3471	137.2382	138.2988	137.3361	138.4175	**123.3**
C8`	36.5575	37.3334	37.6315	37.7290	38.0960	37.7102	38.3248	37.6613	38.2612	37.7452	38.7491	31.9892	32.3390	32.6379	32.4030	32.9664	32.3958	32.8494	32.3861	32.8553	32.3957	32.9066	**31.7**
H(2-4)	8.4518	8.4960	8.4770	8.4338	8.4830	8.4338	8.5234	8.4974	8.5113	8.4334	8.5377	8.4870	8.4402	8.5006	8.4182	8.5222	8.4200	8.4942	8.4215	8.4965	8.4158	8.5064	**8.32**
H5	7.6301	7.8580	7.8476	7.9424	7.9633	7.9366	7.9795	7.9431	7.9676	7.9477	8.0040	7.6486	7.8581	7.8674	7.9335	8.0253	7.9290	7.9815	7.9240	7.9720	7.9353	8.0054	**7.84**
H6	8.2039	8.4564	8.4859	8.4989	8.6473	8.4912	8.6798	8.5539	8.6636	8.5060	8.7161	8.0193	8.2375	8.3475	8.3168	8.5573	8.3115	8.5185	8.3058	8.5097	8.3197	8.5646	**8.05**
H8	4.4195	4.5402	4.5589	4.5750	4.6767	4.5675	4.7008	4.5971	4.6920	4.5820	4.7244	4.5421	4.7095	4.7633	4.7786	4.9091	4.7738	4.9252	4.7688	4.9079	4.7817	4.9628	**5.2**
H(9A-9C)	1.3258	1.3522	1.2700	1.3006	1.2527	1.3017	1.2799	1.3485	1.2669	1.2994	1.2993	1.4098	1.4405	1.4465	1.4592	1.4812	1.4579	1.4799	1.4565	1.4750	1.4594	1.5033	**1.59**
H(8`A-8`C)	2.5475	2.4742	2.4590	2.4832	2.4407	2.4842	2.4314	2.4545	2.4313	2.4822	2.4146	2.9731	2.8059	2.7657	2.7101	2.7063	2.7144	2.5881	2.7184	2.6122	2.7041	2.5595	**2.8**
Nuclei	B3P86																					
C1	141.0246	141.0285	142.2192	140.9808	144.0980	141.0001	144.0222	140.9986	144.3420	141.0084	143.1385	139.8964	140.8617	141.9652	141.7869	142.7801	141.6874	142.9257	141.6351	142.7723	141.8909	143.0928	**135.1**
C2	133.3419	132.8514	133.5894	132.5496	134.5756	132.5891	135.1223	132.6069	135.1312	132.5563	134.9428	132.9824	132.6985	134.5664	132.5814	134.1904	132.5034	134.6895	132.5005	134.6726	132.6137	134.6395	**131.6**
C3	138.5303	137.3927	137.5490	136.9504	137.2547	136.9950	137.4605	137.0181	137.5479	136.9524	137.4563	138.4328	137.3126	137.4445	136.8682	136.9767	136.8993	137.1581	136.9188	137.2374	136.8764	137.1919	**126.5**
C4	135.2382	136.8298	137.7510	137.5843	137.2848	137.5599	138.1357	137.5136	137.9912	137.6510	138.4865	135.3148	136.6452	136.5866	137.1157	137.4508	137.2009	138.0496	137.1780	138.0059	137.1497	138.2798	**132.3**
C5	132.7772	134.8277	135.5349	135.7819	136.0038	135.7463	136.1312	135.6883	136.1284	135.8594	136.2880	133.0553	135.0469	135.1490	135.8694	136.2797	135.8921	136.2408	135.8468	136.2789	135.9296	136.4179	**133.1**
C6	135.4735	137.9484	139.1542	139.1822	140.6163	139.1291	140.7289	139.0535	140.5966	139.2761	141.4820	135.7432	138.2117	139.5726	139.2691	141.3244	139.2492	141.5619	139.1883	141.5508	139.3386	141.9124	**133.7**
C7	201.9404	206.6323	208.3710	209.0122	210.6942	208.8858	216.0891	208.7387	215.3367	209.1770	215.8162	206.0529	210.2712	211.4714	212.6512	213.0740	212.5359	217.5253	212.3909	216.5474	212.8258	218.1559	**196.3**
C8	64.0940	65.1702	65.8791	65.6186	66.6690	65.6117	67.1210	65.5832	67.0594	65.6691	67.8322	58.7896	60.4490	61.0607	61.3411	62.0808	61.2807	62.9060	61.2216	62.6739	61.4342	63.1859	**60.8**
C9	22.5302	22.8563	23.0723	23.1370	23.3630	23.1395	23.1769	23.1200	23.2262	23.1783	23.6467	19.2841	19.7543	20.0391	19.9464	20.3448	19.9491	20.5175	19.9359	20.5472	19.9836	20.8886	**15.9**
C3``	132.3483	133.5663	134.5747	134.0381	135.2815	134.0321	135.1243	134.0038	135.1909	134.0874	135.2149	132.3610	133.5677	134.3569	134.0520	135.2009	134.0443	135.0489	134.0157	135.1172	134.0999	135.1386	**123.3**
C8`	35.9490	36.7031	36.9804	37.0613	37.4118	37.0588	37.6519	37.0348	37.7040	37.1080	38.1017	31.2547	31.6225	31.9388	31.6981	32.1255	31.7254	32.1182	31.7189	32.2851	31.7170	32.1970	**31.7**
H(2-4)	8.5100	8.5562	8.5899	8.5650	8.5612	8.5662	8.5838	8.5653	8.5745	8.5651	8.6327	8.5260	8.4922	8.5518	8.4757	8.5476	8.4785	8.5429	8.4798	8.5559	8.4722	8.5557	**8.32**
H5	7.6775	7.9061	7.9566	8.0050	8.0240	8.0005	8.0388	7.9941	8.0325	8.0104	8.0695	7.6948	7.9119	7.9261	7.9912	8.0439	7.9905	8.0424	7.9853	8.0402	7.9950	8.0678	**7.84**
H6	8.2874	8.5373	8.5961	8.6512	8.7102	8.6460	8.7362	8.6388	8.7244	8.6573	8.8108	8.0866	8.3122	8.4280	8.3930	8.6013	8.3911	8.5915	8.3855	8.5954	8.3961	8.6382	**8.05**
H8	4.4547	4.5765	4.5824	4.6449	4.6871	4.6420	4.7274	4.6372	4.7250	4.6489	4.7513	4.5918	4.7602	4.8202	4.8371	4.9632	4.8346	4.9840	4.8293	4.9761	4.8414	5.0244	**5.2**
H(9A-9C)	1.3436	1.3677	1.3340	1.3701	1.2922	1.3714	1.2855	1.3709	1.2767	1.3700	1.3521	1.4212	1.4509	1.4561	1.4667	1.4666	1.4681	1.4844	1.4667	1.4864	1.4667	1.5095	**1.59**
H(8`A-8`C)	2.5289	2.4511	2.4329	2.4258	2.4245	2.4280	2.4004	2.4285	2.4075	2.4251	2.3813	2.9163	2.7528	2.7167	2.6663	2.6404	2.6740	2.5360	2.6782	2.5689	2.6608	2.5099	**2.8**
Nuclei	B3PW91																					
C1	141.3665	142.2479	143.6084	142.4891	145.2212	142.4800	144.3851	142.4677	144.5144	142.5065	144.5299	140.3459	141.2776	142.3130	142.4822	143.4298	142.2778	143.4991	142.0699	143.6044	142.5099	143.6539	**135.1**
C2	133.4659	132.9115	133.0908	132.5985	135.1484	132.6216	135.2675	132.6369	135.1765	132.5798	135.2519	133.1117	132.5153	134.7192	132.8402	134.4245	132.8311	134.9159	132.6916	134.8450	132.8305	134.8569	**131.6**
C3	138.5674	137.5142	137.7208	137.0827	137.6259	137.1115	137.4752	137.1319	137.4702	137.0580	137.5073	138.5069	137.3295	137.4871	136.9460	137.0621	136.9639	137.2306	136.9672	137.2259	136.9247	137.2694	**126.5**
C4	135.2834	136.9226	138.3217	137.6460	137.6192	137.6075	138.1432	137.5588	137.9191	137.6831	138.3596	135.4184	136.9845	136.5284	137.0394	137.4026	137.0640	137.9922	137.1759	137.7663	137.0640	138.2325	**132.3**
C5	132.9207	135.0365	135.8351	135.9932	136.4750	135.9415	136.2500	135.8806	136.1541	136.0438	136.4270	133.2549	135.2780	135.1853	135.9055	136.3138	135.8833	136.2905	135.9019	136.1906	135.9457	136.4705	**133.1**
C6	135.3571	137.6772	138.7126	138.8335	140.6604	138.7676	140.6086	138.6913	140.4131	138.8971	140.9970	135.6672	138.1101	139.3986	139.1092	141.1786	139.1019	141.3766	139.0801	141.1726	139.1650	141.7422	**133.7**
C7	202.1308	207.5751	209.8770	210.3142	211.9053	210.1551	216.5838	209.9920	215.6066	210.4734	217.3609	206.2532	210.6531	211.6663	213.0725	213.3836	212.8501	217.9456	212.6803	217.0163	213.2051	218.5993	**196.3**
C8	63.8840	65.2124	65.6464	65.6677	66.6858	65.6571	67.0135	65.6370	66.8195	65.6800	67.7602	58.7186	60.5791	61.0235	61.5540	62.2884	61.4264	63.0889	61.3017	62.9539	61.6006	63.3565	**60.8**
C9	22.2521	22.5347	22.5116	22.7246	23.2272	22.7109	22.9238	22.6885	22.8859	22.7395	23.0827	19.0481	19.4926	19.6513	19.6482	20.0631	19.6379	20.1848	19.6144	20.1541	19.6569	20.5398	**15.9**
C3``	132.5601	133.7959	134.6065	134.2500	135.8438	134.2289	135.3630	134.1989	135.3334	134.2717	135.4554	132.5792	133.7642	134.5614	134.2903	135.4452	134.2719	135.2894	134.2410	135.2617	134.3112	135.3813	**123.3**
C8`	35.9131	36.7029	36.9462	37.0938	37.7765	37.0847	37.6614	37.0657	37.5977	37.1037	38.1205	31.2888	31.6181	31.9036	31.6680	32.0708	31.7110	32.0878	31.7359	32.0566	31.6769	32.1766	**31.7**
H(2-4)	8.4862	8.4769	8.5099	8.4725	8.5392	8.4731	8.5592	8.4733	8.5495	8.4717	8.5696	8.5067	8.4580	8.5288	8.4362	8.5094	8.4477	8.5139	8.4537	8.5038	8.4348	8.5250	**8.32**
H5	7.6813	7.9030	7.9658	8.0014	8.0401	7.9961	8.0418	7.9905	8.0316	8.0064	8.0651	7.7006	7.9150	7.9187	7.9820	8.0323	7.9798	8.0359	7.9796	8.0245	7.9863	8.0593	**7.84**
H6	8.2615	8.4397	8.5265	8.5505	8.7111	8.5439	8.7214	8.5369	8.7076	8.5567	8.7537	8.0706	8.2744	8.3974	8.3568	8.5613	8.3596	8.5548	8.3599	8.5345	8.3619	8.6003	**8.05**
H8	4.4364	4.5121	4.5696	4.5877	4.7011	4.5814	4.7069	4.5751	4.7021	4.5941	4.7264	4.5733	4.7336	4.7938	4.8074	4.9331	4.8044	4.9509	4.8018	4.9330	4.8116	4.9897	**5.2**
H(9A-9C)	1.3055	1.2971	1.2372	1.2809	1.2440	1.2825	1.2549	1.2836	1.2448	1.2792	1.2734	1.3871	1.4091	1.4166	1.4274	1.4233	1.4308	1.4479	1.4327	1.4364	1.4283	1.4695	**1.59**
H(8`A-8`C)	2.4984	2.4562	2.4101	2.4330	2.4034	2.4345	2.3812	2.4359	2.3837	2.4318	2.3652	2.8799	2.7098	2.6837	2.6282	2.5927	2.6393	2.5052	2.6487	2.5115	2.6244	2.4766	**2.8**
Nuclei	B98																					
C1	142.1982	141.9669	144.1984	142.0420	144.8674	142.0505	144.9873	142.0576	145.1501	142.0373	145.0532	141.1096	142.0845	143.0857	142.9281	143.4651	142.8135	143.9814	142.7785	143.7680	143.0080	144.1270	**135.1**
C2	133.0467	132.3009	132.6563	132.2841	132.9095	132.3132	134.8511	132.3400	134.7701	132.2588	134.8226	132.6630	132.4850	134.3335	132.3605	133.0766	132.2606	134.5182	132.2743	134.4116	132.3595	134.4574	**131.6**
C3	139.4225	138.2570	138.4263	137.7845	137.9862	137.8241	138.2128	137.8617	138.2162	137.7500	138.2230	139.3706	138.2019	138.2748	137.7084	137.7568	137.7452	137.9912	137.7807	137.9810	137.6784	138.0054	**126.5**
C4	134.9827	136.7915	137.9780	137.2703	138.2620	137.2444	137.7931	137.2158	137.5668	137.2972	138.0108	135.1236	136.2819	136.1293	136.7549	137.8596	136.8545	137.6528	136.8443	137.5065	136.7458	137.8643	**132.3**
C5	132.6752	134.7602	135.5073	135.5788	136.5349	135.5405	135.8795	135.4996	135.7899	135.6171	136.0357	133.0159	134.8183	134.8475	135.6051	136.3944	135.6303	135.9367	135.5992	135.8698	135.6256	136.0853	**133.1**
C6	135.3055	137.7956	138.6713	139.0036	140.4824	138.9469	140.5142	138.8871	140.3114	139.0594	140.9100	135.5888	137.9722	139.2496	139.0681	141.2969	139.0403	141.3152	138.9917	141.2119	139.0973	141.6501	**133.7**
C7	200.3555	205.2101	208.0993	207.7094	209.9057	207.5649	215.0847	207.4193	214.1046	207.8494	215.8313	204.6286	208.9282	210.1019	211.3253	211.7324	211.2036	216.3908	211.0697	215.2327	211.4724	217.0184	**196.3**
C8	65.5508	66.5480	67.2033	67.0036	68.0128	66.9925	68.5298	66.9787	68.3616	67.0161	69.1999	60.3677	62.1656	62.6866	63.0767	63.7521	63.0039	64.6272	62.9576	64.3366	63.1413	64.8966	**60.8**
C9	22.9956	23.3864	23.2560	23.6277	23.7106	23.6285	23.6703	23.6266	23.6320	23.6291	23.8162	19.8802	20.2359	20.4125	20.4164	20.8619	20.4148	20.9084	20.4172	20.8784	20.4157	21.2641	**15.9**
C3``	131.1330	132.3393	133.1564	132.8309	134.2022	132.8189	133.9273	132.8041	133.9009	132.8443	134.0055	131.1507	132.3639	133.1188	132.8547	134.2238	132.8385	133.8810	132.8236	133.8580	132.8669	133.9589	**123.3**
C8`	36.7438	37.4702	37.7480	37.8396	38.2341	37.8306	38.4592	37.8193	38.4113	37.8506	38.8857	32.1182	32.4552	32.7206	32.5466	32.9885	32.5743	32.9243	32.5823	32.9902	32.5205	32.9771	**31.7**
H(2-4)	8.4701	8.5154	8.5065	8.5263	8.5173	8.5265	8.5570	8.5266	8.5469	8.5264	8.5700	8.4991	8.4573	8.5211	8.4419	8.5451	8.4451	8.5186	8.4472	8.5263	8.4374	8.5280	**8.32**
H5	7.6614	7.8938	7.9490	7.9874	8.0562	7.9819	8.0248	7.9765	8.0146	7.9928	8.0477	7.6800	7.8823	7.8969	7.9615	8.0420	7.9604	8.0146	7.9560	8.0073	7.9653	8.0377	**7.84**
H6	8.2231	8.4784	8.5128	8.6002	8.6829	8.5934	8.7146	8.5867	8.7003	8.6068	8.7517	8.0394	8.2523	8.3706	8.3412	8.5640	8.3384	8.5416	8.3336	8.5393	8.3436	8.5842	**8.05**
H8	4.4062	4.5248	4.5521	4.5957	4.6643	4.5914	4.6998	4.5872	4.6925	4.6001	4.7203	4.5356	4.7006	4.7625	4.7732	4.9091	4.7710	4.9262	4.7669	4.9145	4.7769	4.9574	**5.2**
H(9A-9C)	1.3254	1.3525	1.2633	1.3544	1.2539	1.3550	1.2766	1.3556	1.2665	1.3541	1.2942	1.4122	1.4307	1.4373	1.4502	1.4619	1.4504	1.4728	1.4498	1.4720	1.4502	1.4926	**1.59**
H(8`A-8`C)	2.5183	2.4482	2.4394	2.4281	2.4241	2.4290	2.4124	2.4300	2.4151	2.4277	2.3937	2.9174	2.7519	2.7209	2.6684	2.6510	2.6754	2.5463	2.6804	2.5719	2.6626	2.5152	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S17. Cont. I

Nuclei	R											S										Exp. [b]
	B971											B971										
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	141.7902	141.5959	143.6299	141.6467	144.2046	141.6502	144.6140	141.6547	144.7778	141.6505	144.6556	140.7285	141.6901	142.6890	142.5299	143.1149	142.4190	143.6191	142.3784	143.4007	142.6143	143.7594	**135.1**
C2	132.7339	131.9908	132.3262	131.9586	132.5062	131.9813	134.5328	132.0037	134.4542	131.9434	134.5052	132.3420	132.1752	134.0183	132.0414	132.7537	131.9467	134.2060	131.9536	134.0974	132.0528	134.1505	**131.6**
C3	139.0827	137.9211	138.0713	137.4618	137.6332	137.4935	137.8721	137.5252	137.8751	137.4383	137.8880	139.0337	137.8734	137.9353	137.3899	137.4318	137.4186	137.6634	137.4482	137.6538	137.3704	137.6839	**126.5**
C4	134.7191	136.5213	137.7341	137.0250	138.0684	136.9904	137.5254	136.9550	137.3002	137.0637	137.7545	134.8480	136.0351	135.8801	136.5226	137.5962	136.5996	137.3903	136.5835	137.2465	136.5260	137.6112	**132.3**
C5	132.4904	134.5848	135.3297	135.4256	136.3866	135.3787	135.7299	135.3309	135.6385	135.4759	135.8935	132.8209	134.6407	134.6745	135.4436	136.2275	135.4538	135.7674	135.4164	135.7026	135.4760	135.9233	**133.1**
C6	135.0709	137.5471	138.4604	138.7692	140.3274	138.7037	140.2628	138.6371	140.0636	138.8367	140.6775	135.3524	137.7431	139.0229	138.8485	141.0546	138.8100	141.0768	138.7556	140.9690	138.8918	141.4202	**133.7**
C7	200.2685	205.0866	207.7765	207.5416	209.5139	207.3948	214.8511	207.2481	213.8889	207.6882	215.5745	204.4951	208.7789	209.9745	211.1750	211.6193	211.0443	216.1928	210.9057	215.0609	211.3293	216.8255	**196.3**
C8	65.5157	66.5153	67.1673	66.9749	67.9811	66.9553	68.4342	66.9351	68.2689	66.9995	69.1023	60.3640	62.0885	62.6076	62.9828	63.6780	62.9086	64.5198	62.8580	64.2272	63.0542	64.7833	**60.8**
C9	22.9855	23.3892	23.2848	23.6617	23.8000	23.6528	23.6564	23.6430	23.6217	23.6757	23.8175	19.9005	20.2802	20.4527	20.4597	20.8992	20.4527	20.9518	20.4501	20.9142	20.4692	21.3178	**15.9**
C3``	131.6907	132.9033	133.7216	133.4012	134.7654	133.3811	134.4811	133.3604	134.4552	133.4259	134.5638	131.7032	132.9268	133.6783	133.4234	134.7827	133.3992	134.4448	133.3782	134.4212	133.4469	134.5281	**123.3**
C8`	36.7401	37.4576	37.7194	37.8241	38.1821	37.8085	38.4188	37.7929	38.3647	37.8451	38.8429	32.0649	32.4026	32.6646	32.4921	32.9131	32.5106	32.8312	32.5133	32.9011	32.4787	32.8924	**31.7**
H(2-4)	8.4656	8.5103	8.5070	8.5239	8.5209	8.5237	8.5524	8.5235	8.5421	8.5244	8.5666	8.4929	8.4552	8.5168	8.4400	8.5382	8.4430	8.5118	8.4449	8.5197	8.4363	8.5222	**8.32**
H5	7.6643	7.8951	7.9505	7.9897	8.0592	7.9840	8.0262	7.9783	8.0159	7.9954	8.0493	7.6821	7.8830	7.8979	7.9637	8.0424	7.9620	8.0141	7.9574	8.0070	7.9678	8.0371	**7.84**
H6	8.2272	8.4793	8.5105	8.6017	8.6838	8.5948	8.7133	8.5878	8.6987	8.6087	8.7513	8.0413	8.2558	8.3763	8.3456	8.5635	8.3423	8.5430	8.3374	8.5399	8.3486	8.5866	**8.05**
H8	4.4041	4.5217	4.5420	4.5936	4.6556	4.5891	4.6985	4.5847	4.6917	4.5982	4.7196	4.5359	4.7036	4.7667	4.7765	4.9091	4.7741	4.9249	4.7700	4.9136	4.7803	4.9567	**5.2**
H(9A-9C)	1.3260	1.3527	1.2695	1.3572	1.2663	1.3574	1.2749	1.3575	1.2652	1.3574	1.2935	1.4154	1.4340	1.4405	1.4536	1.4631	1.4536	1.4744	1.4527	1.4734	1.4540	1.4946	**1.59**
H(8`A-8`C)	2.5150	2.4438	2.4377	2.4229	2.4220	2.4237	2.4057	2.4245	2.4087	2.4227	2.3865	2.9098	2.7466	2.7165	2.6636	2.6430	2.6702	2.5401	2.6749	2.5663	2.6582	2.5095	**2.8**
Nuclei	B972											B972										
C1	138.7706	138.4094	140.8568	138.6809	141.4708	138.6412	141.7491	138.6126	141.8955	139.9870	142.0464	137.6805	138.8900	139.6026	139.9598	140.8664	139.9457	141.1642	139.9264	140.9711	139.9665	141.2492	**135.1**
C2	130.9160	130.1983	130.5139	130.2945	130.8866	130.3032	132.7048	130.3100	132.6009	130.1245	132.6910	130.5902	130.3971	132.2344	130.4015	130.9747	130.4076	132.4342	130.4109	132.3405	130.3909	132.3518	**131.6**
C3	135.8638	134.7281	134.9316	134.3396	134.5002	134.3593	134.7121	134.3777	134.7068	134.3852	134.7461	135.7990	134.6829	134.7861	134.2844	134.3355	134.3020	134.5425	134.3178	134.5285	134.2639	134.5891	**126.5**
C4	132.6371	134.4209	135.5550	134.8962	135.8077	134.8584	135.2817	134.8165	135.0826	134.9437	135.4680	132.7783	133.8413	133.7125	134.2457	135.3562	134.2111	135.0306	134.1749	134.8843	134.2751	135.2983	**132.3**
C5	130.1701	132.1910	132.9036	133.0386	133.9193	132.9859	133.2877	132.9301	133.2092	133.1496	133.4630	130.5070	132.2577	132.3057	133.0375	133.8532	132.9893	133.3561	132.9389	133.2720	133.0788	133.5408	**133.1**
C6	132.6624	135.1356	135.9316	136.3610	137.7163	136.2940	137.7051	136.2214	137.4948	136.1375	138.0165	132.9854	135.1839	136.5550	136.2548	138.2141	136.1861	138.2528	136.1155	138.1789	136.3160	138.6366	**133.7**
C7	198.1762	202.6737	205.7436	205.2069	207.4271	205.0358	212.4738	204.8702	211.6119	206.5091	213.3962	202.1576	206.5084	207.4152	208.9849	209.7171	208.8516	213.9743	208.7139	212.8146	209.1051	214.6327	**196.3**
C8	62.6251	63.5136	64.2879	64.0118	64.9722	63.9815	65.6963	63.9506	65.5014	64.3463	66.4399	57.6244	59.5046	59.9244	60.5523	61.1091	60.5089	62.0846	60.4618	61.8362	60.5880	62.2633	**60.8**
C9	21.9469	22.2913	22.2159	22.5618	22.6189	22.5472	22.6068	22.5291	22.5551	22.4293	22.7399	18.8405	19.1229	19.3523	19.3787	19.6381	19.3660	19.7834	19.3512	19.7731	19.3866	20.0877	**15.9**
C3``	129.4870	130.6378	131.4407	131.1822	132.4592	131.1542	132.1873	131.1232	132.1571	131.1718	132.2829	129.5097	130.6624	131.4150	131.1901	132.4772	131.1625	132.1219	131.1322	132.0936	131.2115	132.2168	**123.3**
C8`	35.6763	36.3861	36.6825	36.8494	37.1848	36.8249	37.3423	36.7969	37.3055	36.8559	37.7536	31.1725	31.4166	31.7388	31.5456	31.8795	31.5247	31.8641	31.5020	31.8923	31.5615	31.9849	**31.7**
H(2-4)	8.4648	8.5175	8.4916	8.5257	8.5103	8.5273	8.5315	8.5279	8.5217	8.4505	8.5349	8.4899	8.4323	8.5103	8.4113	8.4853	8.4112	8.4783	8.4112	8.4817	8.4113	8.4932	**8.32**
H5	7.6745	7.9039	7.9559	7.9973	8.0628	7.9921	8.0286	7.9864	8.0201	7.9963	8.0513	7.6903	7.8882	7.9019	7.9678	8.0400	7.9627	8.0152	7.9573	8.0072	7.9725	8.0395	**7.84**
H6	8.2318	8.4876	8.5093	8.6042	8.6844	8.5991	8.6889	8.5930	8.6779	8.5381	8.7146	8.0540	8.2484	8.3716	8.3336	8.5222	8.3269	8.5031	8.3200	8.5009	8.3400	8.5541	**8.05**
H8	4.4010	4.5217	4.5331	4.5938	4.6542	4.5895	4.6650	4.5848	4.6641	4.5633	4.6853	4.5414	4.6912	4.7512	4.7683	4.9053	4.7631	4.8999	4.7578	4.8879	4.7730	4.9465	**5.2**
H(9A-9C)	1.2826	1.3129	1.2227	1.3133	1.2136	1.3147	1.2358	1.3153	1.2223	1.2576	1.2471	1.3732	1.3887	1.4026	1.4134	1.3876	1.4117	1.4173	1.4099	1.4159	1.4150	1.4364	**1.59**
H(8`A-8`C)	2.4878	2.4165	2.4075	2.4032	2.3889	2.4027	2.3883	2.4027	2.3892	2.4321	2.3738	2.8716	2.7007	2.6790	2.6262	2.5910	2.6289	2.4976	2.6316	2.5133	2.6237	2.4741	**2.8**
Nuclei	BHandH											BHandH										
C1	142.8677	142.7805	144.4921	142.7388	144.7821	142.7320	143.9348	142.7436	144.1404	142.7151	144.1711	142.0256	142.4747	143.9047	143.1771	143.9212	143.1260	144.3644	143.0932	144.3728	143.1955	144.5020	**135.1**
C2	137.6181	136.9948	139.0004	136.6343	138.4920	136.6460	138.9552	136.6764	138.8648	136.5931	138.9400	137.3606	136.8577	138.8042	136.7465	137.4906	136.7406	138.9206	136.7528	138.8517	136.7223	138.9137	**131.6**
C3	141.2982	140.0645	140.2567	139.6192	139.7929	139.6330	139.8987	139.6656	139.9188	139.5763	139.9343	141.2577	140.0065	140.1483	139.6194	140.3635	139.6293	139.8073	139.6581	139.8197	139.5808	139.8431	**126.5**
C4	139.3478	140.9814	140.8626	141.8156	141.8575	141.7548	142.8318	141.7122	142.5748	141.8431	143.0612	139.4426	140.9543	140.8833	141.5297	142.2738	141.4881	142.5117	141.4649	142.3058	141.5390	142.7552	**132.3**
C5	135.9496	138.0302	138.0583	139.0699	139.2894	138.9972	139.3588	138.9426	139.2743	139.1087	139.5369	136.1093	138.1298	138.1344	139.0118	139.7559	138.9529	139.2632	138.9120	139.1963	139.0373	139.4460	**133.1**
C6	140.6621	143.2930	144.2895	144.5438	146.1874	144.4581	146.5831	144.3908	146.3731	144.5951	146.9938	140.8983	143.6801	144.8955	144.9318	145.6759	144.8541	147.1763	144.7941	146.9724	144.9746	147.5558	**133.7**
C7	203.3030	208.0563	209.7179	210.5816	211.4848	210.4193	216.3049	210.2749	215.2733	210.7050	217.2111	207.4410	211.6134	213.1833	213.9093	214.6534	213.7575	219.2447	213.6239	218.2066	214.0240	219.8444	**196.3**
C8	60.3294	61.5453	62.2345	61.9897	62.8010	61.9570	63.2805	61.9421	63.1296	61.9901	64.0049	54.5397	55.8254	56.4258	56.6054	57.3495	56.5446	57.9823	56.5021	57.7833	56.6335	58.3242	**60.8**
C9	22.1541	22.4612	22.5855	22.7246	23.0132	22.6950	22.9262	22.6843	22.9051	22.7229	23.1098	18.8257	19.2673	19.3105	19.5291	20.2732	19.5073	19.8206	19.5037	19.7389	19.5198	20.2579	**15.9**
C3``	121.7093	122.8276	123.6110	123.2860	124.4195	123.2493	124.2815	123.2307	124.2627	123.2906	124.3923	121.7259	122.8449	123.5839	123.2942	124.0383	123.2590	124.2536	123.2418	124.2369	123.2974	124.3657	**123.3**
C8`	33.7765	34.5427	34.8487	34.8968	35.2667	34.8668	35.4932	34.8548	35.4345	34.8949	35.9847	28.6108	29.0571	29.3365	29.2685	30.0126	29.2480	29.7434	29.2459	29.7469	29.2575	29.8858	**31.7**
H(2-4)	8.7662	8.7973	8.8384	8.8029	8.8632	8.8034	8.9064	8.8032	8.8939	8.8033	8.9134	8.7781	8.7679	8.8053	8.7467	8.6654	8.7494	8.8171	8.7513	8.8169	8.7450	8.8304	**8.32**
H5	7.7888	8.0228	8.0247	8.1260	8.1520	8.1209	8.1687	8.1150	8.1569	8.1319	8.1934	7.7924	8.0186	8.0193	8.1130	8.0318	8.1089	8.1502	8.1039	8.1398	8.1179	8.1751	**7.84**
H6	8.5045	8.7582	8.8106	8.8775	9.0142	8.8712	9.0623	8.8640	9.0394	8.8846	9.1015	8.3032	8.5453	8.6514	8.6545	8.5733	8.6501	8.8511	8.6447	8.8353	8.6597	8.8969	**8.05**
H8	4.2188	4.3429	4.3402	4.4334	4.5060	4.4281	4.5528	4.4221	4.5357	4.4396	4.5856	4.4499	4.6319	4.7117	4.7245	4.6433	4.7202	4.8884	4.7152	4.8701	4.7295	4.9215	**5.2**
H(9A-9C)	1.4151	1.4382	1.4000	1.4345	1.3904	1.4356	1.4140	1.4359	1.4067	1.4344	1.4277	1.4970	1.5307	1.4900	1.5440	1.4628	1.5448	1.5191	1.5447	1.5147	1.5443	1.5447	**1.59**
H(8`A-8`C)	2.5827	2.5017	2.4736	2.4732	2.4342	2.4756	2.4015	2.4770	2.4082	2.4720	2.3915	2.9268	2.7638	2.7152	2.6753	2.5941	2.6813	2.5394	2.6866	2.5581	2.6707	2.5120	**2.8**
Nuclei	BHandHLYP											BHandHLYP										
C1	143.1003	142.9680	144.9046	142.8124	145.7143	142.8202	145.4271	142.8311	145.5798	142.8055	144.4832	141.8932	142.7532	143.6265	143.6304	144.2842	143.5767	144.3651	143.4725	144.3483	143.6862	144.5199	**135.1**
C2	136.7887	136.2944	138.3209	136.0000	137.9612	136.0184	138.5217	136.0395	138.4373	135.9825	138.4019	136.4297	136.1869	138.0753	136.0668	137.6553	136.0571	138.1609	135.9423	138.0827	136.0698	138.1367	**131.6**
C3	140.3325	138.9752	139.1792	138.4754	138.7044	138.5028	138.8352	138.5329	138.8634	138.4498	138.7766	140.2558	138.9550	138.9715	138.4820	138.4506	138.5017	138.5863	138.5192	138.6060	138.4638	138.6111	**126.5**
C4	138.1445	139.6685	139.2697	140.4518	140.1113	140.4052	141.0057	140.3607	140.7916	140.4957	141.4088	138.3698	139.5279	139.3422	139.9687	140.3223	139.9578	140.9266	140.0438	140.7450	139.9825	141.1574	**132.3**
C5	134.2147	136.0635	135.9556	136.9536	137.0286	136.9010	137.0931	136.8504	137.0380	137.0029	137.1905	134.4056	136.2093	136.0303	136.9854	137.1514	136.9496	137.0523	136.9654	137.0049	137.0214	137.2127	**133.1**
C6	138.7770	141.3442	142.1435	142.6680	143.8820	142.5891	144.0181	142.5119	143.8243	142.7418	144.8886	139.0844	141.6340	142.9150	142.7367	144.7672	142.6804	145.0355	142.6398	144.8832	142.7874	145.3817	**133.7**
C7	201.5461	206.7559	208.6075	209.3801	210.8158	209.2211	217.0016	209.0649	215.8662	209.5311	216.7100	206.1267	210.5230	211.6403	213.0116	213.2530	212.8594	218.2438	212.7324	217.0833	213.1616	218.9374	**196.3**
C8	61.0818	62.0471	62.7312	62.4765	63.3706	62.4510	63.7993	62.4279	63.5934	62.5005	64.3945	55.9241	57.5600	58.0957	58.4960	59.0566	58.4371	59.8728	58.3680	59.6572	58.5540	60.1530	**60.8**
C9	21.9709	22.1570	22.2162	22.4037	22.5749	22.3878	22.3163	22.3742	22.3213	22.4183	22.7171	18.7860	19.0442	19.2014	19.1865	19.4824	19.1779	19.5554	19.1682	19.5482	19.1944	19.8361	**15.9**
C3``	124.0475	125.2149	125.9871	125.7048	126.8629	125.6770	126.7112	125.6513	126.6975	125.7306	126.8169	124.0521	125.2207	125.9606	125.7147	126.8113	125.6881	126.6565	125.6569	126.6452	125.7390	126.7610	**123.3**
C8`	34.7962	35.5438	35.8497	35.9266	36.2677	35.9024	36.4952	35.8811	36.4451	35.9494	36.8899	30.4909	30.8057	31.0888	30.9442	31.4158	30.9368	31.3791	30.9348	31.3930	30.9485	31.4865	**31.7**
H(2-4)	8.6777	8.7121	8.7287	8.7227	8.7276	8.7226	8.7552	8.7222	8.7468	8.7228	8.8090	8.6903	8.6595	8.7244	8.6344	8.7319	8.6368	8.7239	8.6374	8.7236	8.6315	8.7345	**8.32**
H5	7.7406	7.9631	7.9579	8.0626	8.0717	8.0571	8.0898	8.0515	8.0797	8.0678	8.1165	7.7546	7.9630	7.9634	8.0475	8.0848	8.0435	8.0870	8.0420	8.0774	8.0514	8.1096	**7.84**
H6	8.3351	8.5986	8.6426	8.7285	8.8124	8.7210	8.8533	8.7135	8.8397	8.7354	8.9249	8.1786	8.4131	8.5255	8.5028	8.7208	8.4979	8.7156	8.4934	8.7024	8.5070	8.7581	**8.05**
H8	4.1367	4.2808	4.2874	4.3707	4.4348	4.3654	4.4960	4.3599	4.4917	4.3758	4.5124	4.3070	4.4846	4.5459	4.5620	4.6969	4.5576	4.7227	4.5541	4.7056	4.5662	4.7549	**5.2**
H(9A-9C)	1.3151	1.3337	1.2789	1.3400	1.2533	1.3400	1.2505	1.3399	1.2406	1.3398	1.3152	1.3839	1.4098	1.4083	1.4244	1.4305	1.4242	1.4415	1.4237	1.4364	1.4244	1.4590	**1.59**
H(8`A-8`C)	2.4768	2.4107	2.3966	2.3933	2.3837	2.3942	2.3723	2.3949	2.3707	2.3925	2.3497	2.8849	2.7228	2.6884	2.6334	2.6225	2.6382	2.5193	2.6435	2.5399	2.6287	2.4922	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S17. Cont. II

Nuclei	R											S										Exp. [b]
	BLYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	143.2283	144.6193	145.6228	144.6604	146.7462	144.9286	146.3425	144.7387	146.5952	145.0405	146.6935	141.3488	143.1513	143.4252	143.9101	144.3827	144.1470	144.5918	143.9232	144.7195	144.3159	144.7570	**135.1**
C2	131.9769	131.6006	131.9152	131.3143	133.5842	131.6108	133.8542	131.4457	133.9533	131.6610	133.9135	131.3814	132.5977	133.2092	132.2823	132.9672	132.5818	133.3679	132.4196	133.4747	132.6254	133.3710	**131.6**
C3	139.5189	138.2730	138.3723	137.7509	137.8742	138.0585	137.8701	137.9042	138.0528	138.0861	137.9542	139.4546	138.0532	138.0758	137.5212	137.6404	137.8263	137.5602	137.6701	137.8272	137.8593	137.6483	**126.5**
C4	134.4372	135.8860	137.1636	136.6197	136.2325	136.8553	136.8469	136.6280	136.8496	137.0216	137.1266	134.6974	134.6273	135.4412	135.2542	136.4272	135.4934	136.7867	135.2705	136.8025	135.6531	137.1123	**132.3**
C5	132.5125	134.4568	135.1534	135.3916	135.5560	135.6156	135.5079	135.3771	135.6121	135.8045	135.7560	133.1292	134.4344	134.9576	135.2437	136.1813	135.4736	135.9582	135.2413	136.0934	135.6515	136.2065	**133.1**
C6	134.3827	136.5914	137.7275	137.8312	139.4936	138.0358	139.4922	137.7774	139.4549	138.2619	139.9348	134.7182	136.9265	138.4002	137.9965	140.3032	138.2130	140.2829	137.9662	140.2593	138.4165	140.7538	**133.7**
C7	204.7842	210.4897	212.6605	213.0114	214.3694	213.1218	219.0361	212.7761	218.4541	213.5441	220.0585	209.9224	213.7338	214.8375	215.8772	216.5990	216.0178	220.5409	215.6969	219.9114	216.3726	221.1963	**196.3**
C8	69.6639	71.0195	71.3880	71.4179	72.1646	71.6661	72.7616	71.4538	72.7346	71.8112	73.6349	63.5996	66.0740	66.6855	67.2750	67.9191	67.4888	68.7476	67.2413	68.5948	67.7006	69.0861	**60.8**
C9	23.4760	23.6981	23.7339	23.9778	24.2607	24.2428	24.2141	24.0444	24.3278	24.3503	24.4468	20.0449	20.5625	20.8971	20.8340	21.2940	21.0977	21.3771	20.8992	21.4302	21.2109	21.8665	**15.9**
C3``	145.4705	146.8938	147.8283	147.4511	149.0085	147.6981	148.6366	147.4827	148.7876	147.8436	148.7942	145.4713	146.7036	147.7699	147.2851	148.9374	147.5308	148.5267	147.3142	148.7422	147.6789	148.6786	**123.3**
C8`	38.2642	39.0050	39.2441	39.3502	39.8190	39.5980	39.8171	39.3862	39.9806	39.7451	40.3287	33.6265	33.7435	34.0307	33.8338	34.3956	34.1076	34.1148	33.9190	34.3428	34.1995	34.2563	**31.7**
H(2-4)	8.2355	8.2129	8.2620	8.2177	8.2809	8.2653	8.4733	8.2203	8.3006	8.2725	8.4917	8.2989	8.2320	8.3055	8.1964	8.3116	8.2458	8.4594	8.2027	8.3029	8.2496	8.4850	**8.32**
H5	7.4986	7.7025	7.7638	7.7974	7.8305	7.8392	8.0143	7.7886	7.8397	7.8578	8.0496	7.5386	7.6937	7.7418	7.7691	7.8509	7.8121	8.0192	7.7625	7.8403	7.8285	8.0553	**7.84**
H6	8.0459	8.2083	8.3170	8.3224	8.4840	8.3628	8.6631	8.3106	8.4882	8.3843	8.7033	7.8624	8.0414	8.1589	8.1200	8.3310	8.1626	8.4827	8.1126	8.3016	8.1797	8.5444	**8.05**
H8	4.6281	4.6678	4.7287	4.7329	4.8355	4.7769	5.0162	4.7281	4.8470	4.7914	5.0490	4.7149	4.8618	4.9098	4.9257	5.0527	4.9686	5.2346	4.9191	5.0556	4.9852	5.2856	**5.2**
H(9A-9C)	1.3410	1.3206	1.2827	1.3175	1.2862	1.3654	1.4756	1.3207	1.2969	1.3719	1.5010	1.4277	1.4705	1.4844	1.4887	1.5018	1.5350	1.6839	1.4887	1.5082	1.5450	1.7224	**1.59**
H(8`A-8`C)	2.6134	2.5606	2.5156	2.5348	2.4961	2.5837	2.6601	2.5401	2.4943	2.5885	2.6527	3.0567	2.8770	2.8394	2.7755	2.7702	2.8273	2.8265	2.7866	2.6851	2.8265	2.8072	**2.8**
Nuclei	**BMK**																					
C1	159.2960	159.1916	160.9952	158.9541	162.3394	158.9548	161.1326	159.1664	161.2208	159.1149	161.1863	158.7672	159.3662	160.7112	160.3071	161.4932	160.2109	161.9209	160.9167	161.8805	160.5435	161.9819	**135.1**
C2	148.8840	147.9813	150.6996	147.4996	150.3703	147.5135	150.7005	147.7389	150.5311	147.6478	150.6177	148.6710	147.9469	150.5535	147.7702	150.0620	147.7671	150.6823	149.4785	150.5197	147.9324	150.5547	**131.6**
C3	156.4150	154.9946	155.5657	154.4422	155.1617	154.4565	155.2376	154.6829	155.1543	154.5905	155.2051	156.6487	155.2915	155.3084	154.6204	154.8555	154.6239	154.9682	154.8307	154.8798	154.7789	154.9413	**126.5**
C4	151.6598	153.3572	152.5433	154.1474	153.4740	154.0844	154.4045	154.2325	154.0575	154.3689	154.6088	151.4222	153.3871	152.7359	153.2177	153.6969	153.1763	154.2203	152.4396	153.9124	153.4221	154.4377	**132.3**
C5	149.3469	151.5273	151.4617	152.5577	152.8224	152.4806	152.8577	152.6148	152.6637	152.7920	152.9849	149.3897	151.5492	151.4037	152.3632	152.7412	152.2922	152.6874	151.8059	152.4973	152.5903	152.8244	**133.1**
C6	152.3887	154.6837	155.7989	156.0199	157.7845	155.9213	158.0892	156.0343	157.7684	156.2750	158.4555	152.4545	155.0713	156.5666	156.3498	158.5334	156.2715	158.8891	156.1696	158.5978	156.5914	159.2066	**133.7**
C7	217.6740	222.9923	224.5732	225.7947	227.4299	225.6115	232.7462	225.6387	231.4607	226.1299	233.6811	221.8360	226.7446	228.1199	229.5634	229.8882	229.3447	235.7102	229.2112	234.4296	229.9267	236.4000	**196.3**
C8	71.0813	72.2548	73.0645	72.6883	73.7521	72.6478	74.2130	72.8184	73.9326	72.8881	74.8668	65.2621	66.9214	67.6686	67.9466	68.7698	67.8260	69.8244	67.9777	69.5563	68.2093	70.0163	**60.8**
C9	25.4161	25.3309	25.6261	25.6007	26.2224	25.5641	26.1751	25.7394	26.0305	25.7977	26.2694	22.1652	22.4008	22.6230	22.3512	22.8577	22.3154	22.9795	22.4510	22.8721	22.5508	23.3784	**15.9**
C3``	133.6238	134.7509	135.6679	135.1873	136.6714	135.1469	136.4548	135.3173	136.3353	135.3872	136.5110	133.6887	134.6179	135.6774	135.2599	136.7086	135.2219	136.5098	135.1516	136.3874	135.4590	136.5810	**123.3**
C8`	38.9693	39.5434	39.8853	39.8094	40.3907	39.7777	40.4900	39.9573	40.3413	40.0009	40.8823	33.8492	34.2209	34.6861	33.8249	34.9097	33.8164	34.4181	34.0358	34.2921	34.0161	34.4808	**31.7**
H(2-4)	8.8771	8.9060	8.9548	8.9198	8.9511	8.9159	9.0050	8.9122	8.9958	8.9138	9.0172	8.8793	8.8637	8.9055	8.8164	8.9031	8.8190	8.8824	8.7972	8.8767	8.8063	8.8926	**8.32**
H5	8.0657	8.3023	8.2865	8.4105	8.4019	8.4012	8.4192	8.3917	8.4092	8.4099	8.4477	8.0690	8.2721	8.2718	8.3666	8.4050	8.3550	8.4030	8.2963	8.3921	8.3674	8.4258	**7.84**
H6	8.6258	8.8858	8.9215	9.0185	9.0936	9.0073	9.1525	8.9962	9.1376	9.0195	9.1978	8.4628	8.6634	8.7944	8.7590	8.9181	8.7481	8.9682	8.7236	8.9497	8.7614	9.0117	**8.05**
H8	4.3342	4.4820	4.4791	4.5700	4.6026	4.5611	4.6588	4.5522	4.6431	4.5690	4.6884	4.4995	4.6788	4.7415	4.7132	4.8039	4.7052	4.8519	4.6879	4.8337	4.7111	4.8947	**5.2**
H(9A-9C)	1.3383	1.3598	1.3394	1.3711	1.2850	1.3674	1.3270	1.3638	1.3189	1.3651	1.3450	1.3994	1.3969	1.3979	1.4267	1.3817	1.4199	1.4187	1.4016	1.4114	1.4222	1.4430	**1.59**
H(8`A-8`C)	2.4695	2.3871	2.3646	2.3733	2.3742	2.3707	2.3421	2.3682	2.3463	2.3663	2.3243	2.8324	2.6718	2.6348	2.5829	2.5231	2.5859	2.4567	2.5855	2.4667	2.5708	2.4398	**2.8**
Nuclei	**BP86**																					
C1	140.0893	141.1465	142.5682	141.6204	143.8499	141.6035	143.4875	141.5881	143.5679	141.6378	143.7806	138.7460	140.2133	140.9194	140.8140	141.5051	140.7523	142.0423	140.6996	141.7096	140.8868	142.3566	**135.1**
C2	130.4744	130.0866	130.3254	129.7896	131.9711	129.8146	132.4209	129.8362	132.3389	129.7619	132.5506	129.9815	129.9364	131.7521	129.7403	131.3484	129.7526	131.9477	129.7625	131.8113	129.7286	132.0350	**131.6**
C3	137.3816	136.4355	136.6390	135.9752	136.0987	136.0094	136.3048	136.0385	136.2950	135.9382	136.4881	137.3167	136.2290	136.3293	135.7638	135.8058	135.7954	135.9988	135.8228	135.9837	135.7299	136.1824	**126.5**
C4	132.9701	134.6824	136.0071	135.3431	134.8950	135.3120	135.7259	135.2743	135.5090	135.3667	136.1027	133.1176	134.4511	134.2309	134.9591	135.1298	134.9468	135.6344	134.9252	135.5035	134.9601	136.0190	**132.3**
C5	131.3030	133.5214	134.2806	134.4542	134.6067	134.4072	134.7404	134.3541	134.6296	134.4937	135.0747	131.7873	133.7916	133.8721	134.6021	135.0294	134.5683	134.9674	134.5270	134.9051	134.6256	135.2970	**133.1**
C6	132.9023	135.2497	136.2914	136.3127	137.8949	136.2551	138.0939	136.1912	137.9078	136.3617	138.6593	133.1379	135.6178	136.8881	136.6561	138.7437	136.6121	138.8666	136.5591	138.7767	136.6875	139.3860	**133.7**
C7	201.9286	207.0657	209.3319	209.7693	211.0265	209.6186	215.5391	209.4684	214.6856	209.9125	216.4427	206.3893	210.4194	211.5108	212.5565	212.9340	212.4229	217.0211	212.2894	216.0154	212.6863	217.7508	**196.3**
C8	67.6594	69.0649	69.5001	69.5515	70.2045	69.5454	70.8230	69.5329	70.6293	69.5511	71.7743	62.1289	64.1379	64.6022	65.0016	65.6738	64.9417	66.6008	64.8828	66.2619	65.0622	67.0400	**60.8**
C9	23.2140	23.6440	23.5876	23.8240	23.9793	23.8127	24.0502	23.7963	23.9925	23.8296	24.3919	19.9694	20.6499	20.8140	20.8427	21.2265	20.8380	21.4684	20.8284	21.4082	20.8426	22.0714	**15.9**
C3``	140.7321	142.1320	142.9574	142.5807	143.8907	142.5635	143.7102	142.5411	143.6779	142.5920	143.9426	140.7366	142.1665	142.8984	142.6264	143.7871	142.6087	143.6189	142.5857	143.5861	142.6382	143.8503	**123.3**
C8`	37.5215	38.3125	38.4971	38.6456	38.9061	38.6432	39.1451	38.6344	39.0816	38.6415	39.7715	32.5672	32.8950	33.1569	32.9613	33.3881	32.9754	33.2668	32.9797	33.3437	32.9370	33.4665	**31.7**
H(2-4)	8.2892	8.2926	8.3165	8.2815	8.3257	8.2829	8.3602	8.2836	8.3514	8.2797	8.3856	8.3248	8.2974	8.3377	8.2735	8.3406	8.2775	8.3270	8.2805	8.3361	8.2684	8.3511	**8.32**
H5	7.5394	7.7576	7.8099	7.8530	7.8749	7.8483	7.8918	7.8431	7.8810	7.8571	7.9295	7.5730	7.7682	7.7827	7.8518	7.9026	7.8484	7.8960	7.8444	7.8903	7.8544	7.9325	**7.84**
H6	8.1325	8.2989	8.3673	8.3899	8.5303	8.3847	8.5561	8.3791	8.5435	8.3944	8.6024	7.9125	8.1062	8.2187	8.1978	8.4042	8.1947	8.3795	8.1907	8.3809	8.1995	8.4391	**8.05**
H8	4.6689	4.7291	4.7614	4.7785	4.8627	4.7738	4.8804	4.7692	4.8753	4.7828	4.9151	4.7766	4.9235	4.9712	5.0012	5.1088	4.9974	5.1264	4.9932	5.1128	5.0044	5.1792	**5.2**
H(9A-9C)	1.3730	1.3699	1.3025	1.3491	1.2951	1.3514	1.3181	1.3531	1.3085	1.3464	1.3513	1.4621	1.5003	1.4899	1.5192	1.5164	1.5194	1.5291	1.5190	1.5275	1.5183	1.5697	**1.59**
H(8`A-8`C)	2.5997	2.5457	2.4897	2.5197	2.4650	2.5217	2.4492	2.5235	2.4518	2.5174	2.4436	2.9937	2.8165	2.7819	2.7400	2.7116	2.7465	2.5929	2.7522	2.6235	2.7328	2.5744	**2.8**
Nuclei	**CAM-B3LYP**																					
C1	144.8458	144.7518	146.9508	144.6012	147.7154	144.6121	147.5744	144.6242	147.7809	144.4611	146.5822	143.6539	144.6285	145.5612	145.5870	146.4746	145.5188	146.5949	145.4656	146.3196	145.6751	146.7663	**135.1**
C2	137.0062	136.5291	138.5134	136.2102	138.2028	136.2336	138.7572	136.2580	138.6589	135.8530	138.6263	136.6829	136.4430	138.2494	136.3454	137.9417	136.3495	138.4680	136.3552	138.3493	136.3447	138.4342	**131.6**
C3	141.9908	140.6697	140.8161	140.1467	140.3668	140.1793	140.5201	140.2127	140.5320	140.1366	140.4738	141.9306	140.6574	140.6449	140.1567	140.1752	140.1821	140.3140	140.2094	140.3018	140.1366	140.3400	**126.5**
C4	138.7052	140.2634	139.8082	141.0189	140.7371	140.9776	141.5394	140.9363	141.3042	141.3747	141.9184	138.8523	140.1314	139.9540	140.5335	140.8792	140.5206	141.4316	140.5047	141.3067	140.5436	141.6612	**132.3**
C5	135.7666	137.7439	137.6566	138.6585	138.8373	138.6083	138.9265	138.5579	138.8451	138.8741	139.0425	135.9639	137.8687	137.7743	138.6291	138.8973	138.5926	138.8154	138.5552	138.7647	138.6641	138.9776	**133.1**
C6	139.3422	141.9300	142.7277	143.2250	144.5752	143.1509	144.6095	143.0768	144.3905	143.3101	145.4800	139.6514	142.2482	143.5678	143.3376	145.4457	143.2884	145.6526	143.2347	145.5590	143.3798	146.0081	**133.7**
C7	205.6264	210.7823	212.9172	213.3799	215.1700	213.2260	221.0961	213.0724	220.1085	213.6045	220.7301	210.1374	214.6546	215.8406	217.2116	217.5601	217.0507	222.3558	216.8964	221.2014	217.3763	223.0677	**196.3**
C8	63.8913	64.9712	65.6977	65.4192	66.4160	65.3960	66.8751	65.3734	66.7190	65.4413	67.5249	58.4451	60.1923	60.7114	61.1574	61.8765	61.0917	62.7008	61.0329	62.3677	61.2316	63.0075	**60.8**
C9	22.1545	22.4188	22.4177	22.6756	22.8725	22.6622	22.6097	22.6490	22.5898	22.6979	23.0522	19.1056	19.4142	19.5689	19.5312	19.9110	19.5268	19.9558	19.5235	19.9195	19.5388	20.2782	**15.9**
C3``	133.2628	134.5492	135.3347	135.0502	136.2940	135.0255	136.1386	135.0010	136.1044	135.0466	136.2397	133.2705	134.5502	135.2999	135.0561	136.2396	135.0334	136.0848	135.0105	136.0549	135.0790	136.1813	**123.3**
C8`	35.5706	36.3658	36.6253	36.7420	37.1010	36.7224	37.3210	36.7033	37.2616	36.7645	37.7599	30.9380	31.3224	31.5752	31.4149	31.8431	31.4191	31.8278	31.4191	31.8986	31.4065	31.9508	**31.7**
H(2-4)	8.5922	8.6290	8.6303	8.6379	8.6365	8.6378	8.6555	8.6377	8.6433	8.6310	8.7099	8.6200	8.5753	8.6381	8.5463	8.6318	8.5500	8.6242	8.5531	8.6356	8.5412	8.6342	**8.32**
H5	7.7201	7.9409	7.9381	8.0385	8.0532	8.0330	8.0664	8.0276	8.0566	8.0522	8.0945	7.7300	7.9372	7.9458	8.0195	8.0593	8.0154	8.0598	8.0111	8.0538	8.0230	8.0819	**7.84**
H6	8.3025	8.5624	8.5945	8.6873	8.7676	8.6801	8.7929	8.6730	8.7758	8.6890	8.8667	8.1322	8.3603	8.4822	8.4440	8.6565	8.4403	8.6434	8.4359	8.6457	8.4464	8.6855	**8.05**
H8	4.2793	4.4177	4.4203	4.5011	4.5695	4.4961	4.6207	4.4913	4.6117	4.5040	4.6336	4.4395	4.6189	4.6864	4.6963	4.8284	4.6920	4.8438	4.6877	4.8350	4.7000	4.8781	**5.2**
H(9A-9C)	1.3434	1.3652	1.3050	1.3708	1.2879	1.3707	1.2805	1.3707	1.2700	1.3668	1.3462	1.4214	1.4427	1.4494	1.4584	1.4612	1.4584	1.4750	1.4582	1.4757	1.4576	1.4942	**1.59**
H(8`A-8`C)	2.5515	2.4777	2.4702	2.4570	2.4538	2.4579	2.4377	2.4590	2.4407	2.4578	2.4150	2.9462	2.7753	2.7422	2.6874	2.6625	2.6929	2.5634	2.6981	2.5917	2.6812	2.5345	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S17. Cont. III

Nuclei	R											S										Exp. [b]
	HF																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	140.8278	141.1937	142.8361	139.9673	143.6160	139.9859	142.7014	141.0017	143.0674	139.9487	142.6932	139.5755	140.7117	141.4701	141.1040	141.8866	141.0545	143.3926	141.0200	141.7381	141.1814	142.2602	**135.1**
C2	138.4017	137.8232	140.4222	137.6174	140.0701	137.6300	140.6246	137.7074	140.4718	137.6046	140.6518	138.0895	138.2233	140.3607	137.5845	139.9453	137.6152	140.1094	137.6421	140.3888	137.5469	140.4259	**131.6**
C3	138.2978	136.8833	137.0732	136.1761	136.5680	136.2087	136.5170	136.3988	136.5968	136.1444	136.4994	138.1790	136.9157	136.8960	136.3955	136.3311	136.4162	136.6643	136.4399	136.4041	136.3801	136.4582	**126.5**
C4	139.5381	141.0293	140.4048	142.0272	141.2290	141.9824	142.2812	141.6424	141.9814	142.0689	142.5321	139.9765	140.7119	140.5085	141.4178	141.5090	141.3893	141.6669	141.3584	141.9730	141.4371	142.2852	**132.3**
C5	132.2665	133.9598	133.6011	134.6202	134.5105	134.5771	134.4047	134.6180	134.4129	134.6603	134.5169	132.3389	133.8129	133.3638	134.6275	134.2754	134.5793	134.3492	134.5339	134.0418	134.6773	134.2423	**133.1**
C6	139.9066	142.3091	142.9399	144.0792	144.6153	143.9956	145.0791	143.4061	144.7523	144.1586	145.5045	140.3299	142.7131	143.9926	143.9081	145.9229	143.8601	145.1264	143.8039	145.9782	143.9359	146.2681	**133.7**
C7	195.3869	201.7578	203.5923	204.0590	205.8794	203.8830	212.5884	204.5116	211.3796	204.2238	213.3855	199.9121	204.6836	205.4858	207.3320	207.0653	207.1476	214.6281	206.9752	211.5677	207.5307	214.0084	**196.3**
C8	54.9068	55.9282	56.2153	56.0418	56.8456	56.0233	57.4630	56.1507	57.2731	56.0585	57.9945	50.1948	51.9492	52.4634	52.7474	53.2717	52.6943	54.3266	52.6456	53.8641	52.8052	54.4616	**60.8**
C9	20.5039	20.4972	20.4270	20.6814	20.7443	20.6712	20.5347	20.5528	20.5330	20.6913	20.6357	17.6970	17.6231	17.8107	17.6838	17.9858	17.6833	17.6601	17.6829	17.8875	17.6825	18.0740	**15.9**
C3``	108.9207	109.9188	110.6419	110.3342	111.4438	110.3104	111.3134	110.2836	111.2855	110.3559	111.4268	108.9087	109.9592	110.6547	110.3446	111.4699	110.3246	111.2751	110.3043	111.2705	110.3613	111.4017	**123.3**
C8`	32.7337	33.4970	33.7069	33.7873	34.1267	33.7662	34.3141	33.7487	34.2386	33.8062	34.6548	29.0442	29.2734	29.5193	29.4245	29.8376	29.4194	29.7249	29.4127	29.8212	29.4240	29.8505	**31.7**
H(2-4)	8.7806	8.7727	8.8335	8.8312	8.8332	8.8305	8.8716	8.7732	8.8525	8.8319	8.8901	8.8108	8.7577	8.8482	8.7250	8.8696	8.7289	8.7737	8.7317	8.8602	8.7192	8.8522	**8.32**
H5	7.7037	7.9295	7.9151	8.0305	8.0276	8.0250	8.0390	8.0143	8.0316	8.0358	8.0611	7.7044	7.9099	7.9010	8.0142	8.0227	8.0088	8.0203	8.0032	8.0103	8.0194	8.0424	**7.84**
H6	8.3234	8.5762	8.6931	8.7696	8.8758	8.7605	8.9125	8.7106	8.8891	8.7783	8.9552	8.2100	8.4555	8.5786	8.5628	8.7887	8.5578	8.7048	8.5519	8.7676	8.5661	8.8012	**8.05**
H8	3.6860	3.8268	3.9210	3.9762	4.0835	3.9686	4.1198	3.9484	4.1071	3.9834	4.1471	3.8586	4.0564	4.1300	4.1427	4.2894	4.1378	4.3016	4.1326	4.2947	4.1470	4.3271	**5.2**
H(9A-9C)	1.2259	1.2028	1.1485	1.2416	1.1141	1.2417	1.1334	1.1868	1.1193	1.2416	1.1518	1.3007	1.2859	1.2995	1.3056	1.3153	1.3062	1.2413	1.3060	1.3180	1.3037	1.3185	**1.59**
H(8`A-8`C)	2.2978	2.2822	2.2389	2.2445	2.2342	2.2449	2.2413	2.2698	2.2409	2.2442	2.2306	2.7123	2.5415	2.5075	2.4736	2.4544	2.4774	2.3619	2.4809	2.3863	2.4694	2.3366	**2.8**
Nuclei	**LC-BLYP**																						
C1	148.5640	148.8119	150.4574	148.2000	151.0246	148.1929	150.0845	148.2125	150.2138	148.1893	150.0518	147.5491	148.6307	149.3773	149.6239	150.5251	149.5662	150.5855	149.2982	150.6738	149.6407	150.7596	**135.1**
C2	142.8139	142.0141	144.3820	141.9539	143.9837	141.9526	144.4888	141.9786	144.3695	141.9376	144.4777	142.5785	142.0993	144.2244	142.2005	143.8902	142.1850	144.3920	142.1780	144.2911	142.1959	144.3680	**131.6**
C3	146.1506	144.6931	144.8577	144.1580	144.3214	144.1656	144.3928	144.2009	144.4001	144.1337	144.3917	146.1311	144.6885	144.7513	144.2748	144.2724	144.2752	144.3940	144.2909	144.3970	144.2563	144.4258	**126.5**
C4	144.3805	145.9953	145.6102	146.7287	146.5742	146.6559	147.4930	146.6106	147.2491	146.7801	147.7631	144.5423	145.8508	145.7033	146.1774	146.5979	146.1218	147.1836	146.1556	146.9578	146.2182	147.4241	**132.3**
C5	140.5110	142.5435	142.4335	143.4262	143.5883	143.3474	143.6186	143.2957	143.5329	143.4832	143.7678	140.6187	142.5096	142.3415	143.2562	143.4329	143.1870	143.3421	143.1584	143.2549	143.3059	143.5092	**133.1**
C6	145.2817	147.8730	148.8915	149.3678	150.7941	149.2594	151.1750	149.1784	150.9571	149.4535	151.6745	145.6126	148.3553	149.7134	149.4516	151.5827	149.3627	151.8245	149.3645	151.6204	149.5239	152.1930	**133.7**
C7	210.8885	216.6604	218.3845	219.0911	220.5895	218.9043	225.9128	218.7437	224.7449	219.2503	226.6778	215.1680	220.0712	221.2711	222.8812	223.1966	222.6887	228.4185	222.4325	227.3517	223.0381	229.1873	**196.3**
C8	61.6833	62.9513	63.5901	63.3872	64.3338	63.3355	64.8266	63.3108	64.6150	63.4185	65.5093	56.0441	57.6908	58.2591	58.7145	59.3711	58.6392	60.2152	58.4962	60.0514	58.7600	60.5653	**60.8**
C9	21.2576	21.4270	21.5314	21.6788	21.9414	21.6337	21.8098	21.6168	21.7918	21.7049	22.0200	18.4449	18.6538	18.7595	18.7641	19.0332	18.7343	19.0292	18.7187	19.0287	18.7737	19.3453	**15.9**
C3``	132.5945	133.7527	134.6132	134.3152	135.5094	134.2634	135.3806	134.2386	135.3364	134.3468	135.4899	132.5991	133.7872	134.5993	134.3059	135.4894	134.2558	135.3587	134.2363	135.3142	134.3360	135.4649	**123.3**
C8`	33.6771	34.5420	34.8032	34.9276	35.3123	34.8808	35.5261	34.8611	35.4293	34.9543	35.9995	29.0308	29.3681	29.7090	29.5607	29.9764	29.5248	30.0366	29.5707	29.9856	29.5820	30.2368	**31.7**
H(2-4)	8.7984	8.7985	8.8415	8.8312	8.8503	8.8299	8.8944	8.8302	8.8864	8.8314	8.9139	8.8218	8.7704	8.8374	8.7278	8.8221	8.7286	8.8137	8.7435	8.8067	8.7272	8.8256	**8.32**
H5	7.8634	8.0849	8.0784	8.1820	8.1935	8.1754	8.2067	8.1703	8.1970	8.1872	8.2328	7.8631	8.0764	8.0691	8.1557	8.1823	8.1500	8.1846	8.1479	8.1751	8.1602	8.2086	**7.84**
H6	8.4772	8.7059	8.7878	8.8748	8.9734	8.8658	9.0139	8.8585	8.9987	8.8822	9.0651	8.3170	8.5455	8.6704	8.6302	8.8468	8.6236	8.8343	8.6297	8.8164	8.6365	8.8775	**8.05**
H8	4.1642	4.2762	4.3247	4.4143	4.4856	4.4071	4.5302	4.4015	4.5227	4.4202	4.5614	4.3656	4.5573	4.6274	4.6357	4.7773	4.6296	4.7878	4.6296	4.7716	4.6408	4.8234	**5.2**
H(9A-9C)	1.3650	1.3758	1.3295	1.3886	1.3167	1.3872	1.3383	1.3874	1.3324	1.3888	1.3669	1.4338	1.4508	1.4412	1.4549	1.4503	1.4531	1.4640	1.4595	1.4549	1.4561	1.4833	**1.59**
H(8`A-8`C)	2.5391	2.4885	2.4559	2.4437	2.4369	2.4437	2.4175	2.4453	2.4174	2.4427	2.4037	2.8979	2.7165	2.6877	2.6294	2.6058	2.6320	2.5120	2.6471	2.5195	2.6269	2.4873	**2.8**
Nuclei	**M06**																						
C1	140.6491	140.4250	142.2226	140.5525	143.0385	140.5210	141.7607	140.5008	142.8327	140.6019	141.7656	138.8786	140.5186	140.7921	141.1968	142.2043	141.0879	142.1886	141.0118	142.2011	141.3331	142.3650	**135.1**
C2	136.6890	135.9481	136.8159	135.5267	136.4473	135.5429	136.8921	135.5670	136.8668	135.5259	136.8433	136.1824	135.5818	136.3510	135.2048	136.0228	135.2173	136.4955	135.2375	136.4075	135.2078	136.4344	**131.6**
C3	137.8361	136.5503	136.7736	136.1189	136.3635	136.1312	136.4831	136.1517	136.5151	136.1224	136.4835	137.4869	135.9022	136.0304	135.4814	135.5701	135.4901	135.6973	135.5083	135.7083	135.4890	135.7235	**126.5**
C4	135.2475	137.0526	137.8121	137.9626	138.8039	137.9004	139.8537	137.8450	139.5134	138.0356	140.0876	135.3039	136.5809	137.6304	137.3095	138.5058	137.2686	139.1019	137.2300	138.9141	137.3588	139.3524	**132.3**
C5	133.0910	134.9994	135.6662	135.9675	136.8971	135.9000	136.9643	135.8399	136.9682	136.0462	137.1002	133.9360	135.7784	136.3675	136.6612	137.5005	136.6032	137.4180	136.5510	137.3508	136.7291	137.6036	**133.1**
C6	137.1403	139.6024	140.7536	140.8149	142.6002	140.7344	143.0945	140.6612	142.6208	140.9051	143.5559	137.4035	139.7481	141.4307	140.7666	143.0614	140.7185	143.2380	140.6689	143.0733	140.8203	143.5987	**133.7**
C7	202.4331	206.9955	208.8904	209.4459	210.9080	209.2834	215.2788	209.1291	215.2119	209.6164	215.9895	206.7488	210.9602	212.0872	213.3086	213.9033	213.1339	218.2407	212.9762	217.3157	213.4968	219.0003	**196.3**
C8	61.2319	62.2885	63.0501	62.6941	63.7613	62.6646	64.0914	62.6424	63.9447	62.7362	64.8433	54.8410	56.7126	57.3050	57.5206	58.5465	57.4475	59.1918	57.3885	59.0177	57.6090	59.5061	**60.8**
C9	21.6312	22.1230	22.3762	22.4463	22.9315	22.4160	23.0850	22.3934	23.1914	22.4894	23.1768	19.0415	19.4918	19.7963	19.7495	20.3903	19.7101	20.4755	19.6843	20.4454	19.8055	20.8598	**15.9**
C3``	125.9986	127.2616	128.3327	127.8053	129.3247	127.7643	129.1871	127.7308	129.1683	127.8588	129.2883	125.9172	126.7270	127.8100	127.2787	128.7136	127.2360	128.5695	127.2012	128.5472	127.3340	128.6597	**123.3**
C8`	36.8414	37.4652	37.8986	37.8175	38.3280	37.7840	38.4158	37.7586	38.5505	37.8643	38.9564	31.7364	31.8162	32.2613	32.1344	32.6209	32.1052	32.8945	32.0832	32.8597	32.1771	33.0910	**31.7**
H(2-4)	8.5680	8.6173	8.6240	8.6090	8.6235	8.6104	8.6979	8.6121	8.6550	8.6079	8.7068	8.5738	8.5556	8.6423	8.5279	8.6124	8.5318	8.6281	8.5353	8.6223	8.5239	8.6341	**8.32**
H5	7.5793	7.8108	7.8393	7.9050	7.9530	7.8998	7.9863	7.8950	7.9662	7.9104	8.0088	7.6255	7.8489	7.9022	7.9340	8.0095	7.9293	8.0152	7.9250	8.0040	7.9389	8.0390	**7.84**
H6	8.3103	8.5722	8.5707	8.6653	8.7208	8.6611	8.8145	8.6572	8.7647	8.6693	8.8547	8.1443	8.3575	8.4953	8.4422	8.6501	8.4400	8.6257	8.4370	8.6149	8.4440	8.6826	**8.05**
H8	4.4269	4.5301	4.5029	4.5825	4.6112	4.5794	4.6825	4.5769	4.6840	4.5859	4.6968	4.4383	4.5847	4.6561	4.6812	4.8132	4.6728	4.8373	4.6660	4.8171	4.6905	4.8900	**5.2**
H(9A-9C)	1.3059	1.3367	1.2709	1.3200	1.2540	1.3219	1.2916	1.3242	1.2448	1.3185	1.3153	1.3945	1.4105	1.4140	1.4184	1.4139	1.4180	1.4163	1.4180	1.4083	1.4192	1.4452	**1.59**
H(8`A-8`C)	2.5166	2.4434	2.4389	2.4277	2.4157	2.4280	2.3927	2.4290	2.3899	2.4281	2.3737	2.9388	2.7196	2.6883	2.6402	2.5936	2.6457	2.5043	2.6512	2.5146	2.6350	2.4760	**2.8**
Nuclei	**M06-2X**																						
C1	157.9679	157.9169	159.5908	157.8512	160.6719	157.8792	159.7741	157.9081	159.8604	157.8180	159.9717	157.4138	158.9904	160.0458	159.7049	160.9557	159.7255	160.9567	159.0370	160.8839	159.6773	161.0591	**135.1**
C2	148.6045	147.7652	150.4384	147.3061	149.9718	147.3561	150.3774	147.4071	150.2903	147.2524	150.3763	148.4444	149.5530	150.3807	148.0878	149.9505	148.1256	150.4205	148.0164	150.3311	148.0449	150.3922	**131.6**
C3	154.8631	153.5379	153.7958	153.0265	153.3473	153.0755	153.4917	153.1261	153.4873	152.9742	153.5323	154.8098	153.3070	153.4273	152.9644	152.9304	153.0099	153.0721	152.9988	153.0730	152.9155	153.1187	**126.5**
C4	151.7277	153.4378	152.6915	154.2466	153.6548	154.2184	154.5756	154.1917	154.3261	154.2669	154.8335	151.5967	151.8536	152.6668	153.1769	153.6859	153.1553	154.3230	153.4131	154.1263	153.1917	154.6115	**132.3**
C5	149.6606	152.0592	151.9115	153.2002	153.3449	153.1535	153.4533	153.1076	153.3331	153.2377	153.6637	149.8578	151.4029	151.9518	152.8755	153.3214	152.8384	153.2856	152.9171	153.1910	152.9045	153.5087	**133.1**
C6	152.6398	155.3558	156.4377	156.7143	158.3546	156.6517	158.6878	156.5902	158.4779	156.7672	159.1149	152.8177	155.4374	156.9420	156.6680	158.9948	156.6127	159.1732	156.7068	159.0079	156.7145	159.6068	**133.7**
C7	218.8166	224.3852	225.8516	227.3019	228.6015	227.1490	234.0980	226.9964	232.7988	227.4404	235.1701	222.6202	227.8696	229.3870	230.9114	231.4419	230.7728	237.0437	230.5486	235.8167	231.0357	237.8405	**196.3**
C8	66.7882	68.0182	68.7538	68.5122	69.4226	68.5071	69.8690	68.5028	69.6748	68.5099	70.5960	60.8178	62.5090	63.3640	63.5939	64.4429	63.5743	65.2221	63.3271	64.9826	63.6055	65.5468	**60.8**
C9	22.9968	23.3627	23.3741	23.6190	23.6570	23.6185	23.6753	23.6198	23.6432	23.6140	23.8626	20.0627	20.2874	20.5306	20.6548	20.8916	20.6732	20.9166	20.5206	20.8936	20.6307	21.2942	**15.9**
C3``	129.1339	130.3791	131.2465	130.8630	132.1677	130.8564	132.0175	130.8509	131.9834	130.8626	132.1410	129.2626	130.1730	131.0711	130.8166	132.0034	130.8141	131.8487	130.8286	131.8148	130.8129	131.9765	**123.3**
C8`	35.9708	36.6123	36.8874	36.9430	37.3854	36.9457	37.4978	36.9492	37.4123	36.9338	37.9733	30.5971	31.0932	31.2403	31.3267	31.6599	31.3280	31.7328	31.3437	31.6927	31.3192	31.9997	**31.7**
H(2-4)	9.1049	9.1409	9.1869	9.1508	9.1794	9.1490	9.2301	9.1469	9.2224	9.1526	9.2377	9.0944	9.0382	9.0906	9.0370	9.0932	9.0353	9.1014	9.0348	9.0993	9.0388	9.1156	**8.32**
H5	8.3089	8.5493	8.5289	8.6578	8.6483	8.6503	8.6662	8.6424	8.6558	8.6650	8.6881	8.3074	8.4740	8.5153	8.5915	8.6390	8.5846	8.6422	8.5906	8.6333	8.5981	8.6657	**7.84**
H6	8.9135	9.1653	9.2380	9.2922	9.3978	9.2832	9.4432	9.2739	9.4270	9.3008	9.4746	8.7189	8.9501	9.0549	9.0193	9.2399	9.0107	9.2317	9.0421	9.2220	9.0277	9.2751	**8.05**
H8	4.3057	4.4524	4.4500	4.5505	4.5978	4.5427	4.6450	4.5347	4.6343	4.5581	4.6676	4.5197	4.6698	4.7301	4.7528	4.8766	4.7461	4.8956	4.7470	4.8835	4.7593	4.9226	**5.2**
H(9A-9C)	1.3792	1.3966	1.3746	1.3976	1.3186	1.3963	1.3459	1.3947	1.3429	1.3989	1.3596	1.4229	1.4259	1.4092	1.4399	1.4224	1.4369	1.4465	1.4366	1.4402	1.4430	1.4637	**1.59**
H(8`A-8`C)	2.4915	2.4180	2.4047	2.3996	2.4024	2.3991	2.3749	2.3984	2.3764	2.4002	2.3586	2.7922	2.6402	2.5770	2.5580	2.5161	2.5584	2.4517	2.5804	2.4666	2.5578	2.4241	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S17. Cont. IV

Nuclei	R											S										Exp. [b]
	mpW1LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	143.4937	143.2988	145.5486	143.3690	146.9811	143.3594	146.2821	143.3532	146.4272	143.3786	146.3131	142.0647	143.0536	144.0686	144.0664	144.6196	143.9596	144.8722	143.9158	144.7799	144.1274	144.9837	**135.1**
C2	134.6551	133.8937	134.2512	133.8950	135.9395	133.9046	136.4339	133.9160	136.3507	133.8846	136.3858	134.2232	133.9841	135.8620	133.9351	135.4219	133.8340	135.9907	133.8313	135.9007	133.9431	135.9177	**131.6**
C3	140.3651	139.0710	139.2823	138.5494	138.7359	138.5724	138.8905	138.5975	138.9035	138.5262	138.8735	140.2611	138.9747	138.9948	138.4455	138.3899	138.4627	138.5629	138.4852	138.5701	138.4279	138.5474	**126.5**
C4	136.5197	138.3289	139.4833	138.8347	138.3517	138.7888	139.2441	138.7443	139.0272	138.8758	139.4461	136.6883	137.8572	137.6670	138.3192	138.6152	138.3896	139.1734	138.3645	139.0014	138.3326	139.3767	**132.3**
C5	133.7985	135.8508	136.5668	136.6845	136.7219	136.6278	136.7993	136.5723	136.7191	136.7359	136.9298	134.1066	136.0038	135.9814	136.8235	137.0816	136.8235	137.0142	136.7778	136.9518	136.8611	137.1459	**133.1**
C6	137.0491	139.5694	140.4428	140.8685	142.0133	140.7898	142.3152	140.7115	142.1174	140.9405	142.7030	137.3190	139.8074	141.1381	140.9168	143.0421	140.8638	143.2504	140.7962	143.1038	140.9717	143.5799	**133.7**
C7	203.3316	208.3367	211.2711	210.8956	213.2082	210.7297	218.3027	210.5671	217.3103	211.0534	219.0491	208.2378	212.4889	213.6892	214.8855	215.2430	214.7545	219.7828	214.6086	218.7178	215.0294	220.4091	**196.3**
C8	65.1759	66.1570	66.7803	66.6316	67.5224	66.6007	68.0643	66.5713	67.8795	66.6588	68.7075	59.7684	61.6160	62.2155	62.6690	63.2640	62.5842	64.1033	62.5241	63.8600	62.7347	64.3470	**60.8**
C9	22.7553	23.0602	22.9779	23.3476	23.3276	23.3280	23.3311	23.3091	23.3065	23.3637	23.4555	19.4438	19.8049	20.0209	20.0084	20.3328	19.9863	20.4976	19.9731	20.4661	20.0216	20.8017	**15.9**
C3``	133.5911	134.8797	135.7351	135.4530	136.7015	135.4188	136.5434	135.3858	136.5182	135.4835	136.6067	133.5900	134.9049	135.7018	135.4716	136.6006	135.4330	136.4419	135.3995	136.4208	135.5009	136.5026	**123.3**
C8`	36.3698	37.0904	37.3919	37.5056	37.8788	37.4746	38.0899	37.4460	38.0395	37.5339	38.4954	31.7935	32.0918	32.3925	32.2098	32.6980	32.2075	32.6149	32.1965	32.6322	32.2143	32.6709	**31.7**
H(2-4)	8.4920	8.5299	8.5169	8.5447	8.5195	8.5448	8.5632	8.5445	8.5551	8.5444	8.5747	8.5272	8.4774	8.5423	8.4597	8.5479	8.4615	8.5382	8.4630	8.5411	8.4568	8.5469	**8.32**
H5	7.6434	7.8683	7.9203	7.9633	7.9730	7.9580	7.9906	7.9522	7.9818	7.9683	8.0113	7.6616	7.8692	7.8820	7.9474	7.9992	7.9454	7.9958	7.9406	7.9886	7.9511	8.0158	**7.84**
H6	8.2268	8.4762	8.5076	8.6016	8.6697	8.5949	8.7070	8.5878	8.6942	8.6078	8.7408	8.0439	8.2668	8.3827	8.3504	8.5712	8.3465	8.5572	8.3408	8.5483	8.3543	8.5989	**8.05**
H8	4.3632	4.4845	4.5171	4.5620	4.6317	4.5576	4.6616	4.5528	4.6570	4.5662	4.6821	4.4951	4.6669	4.7283	4.7398	4.8701	4.7364	4.8898	4.7314	4.8751	4.7440	4.9224	**5.2**
H(9A-9C)	1.3349	1.3564	1.2692	1.3644	1.2568	1.3648	1.2835	1.3648	1.2745	1.3639	1.2994	1.4239	1.4495	1.4580	1.4685	1.4804	1.4681	1.4902	1.4668	1.4873	1.4688	1.5088	**1.59**
H(8`A-8`C)	2.5583	2.4833	2.4730	2.4650	2.4555	2.4659	2.4452	2.4667	2.4475	2.4640	2.4246	2.9829	2.8149	2.7789	2.7195	2.7120	2.7253	2.6010	2.7293	2.6269	2.7146	2.5688	**2.8**
Nuclei	mpW1PW91																					
C1	141.0178	140.9179	142.2811	140.9112	144.4928	142.3310	143.9737	140.8970	144.1465	140.9262	144.0626	139.6492	141.0733	141.9439	142.0308	142.9881	141.8443	143.0508	141.7570	142.7069	142.0888	143.2085	**135.1**
C2	133.6080	133.1087	133.7809	132.8180	134.8788	132.9327	135.3247	132.8572	135.2319	132.8025	135.3080	133.1736	133.0200	134.8319	132.9374	134.5201	132.9274	135.0022	132.9282	134.8851	132.9321	134.9468	**131.6**
C3	138.3972	137.2373	137.3487	136.7901	137.1245	136.8707	137.2847	136.8435	137.2807	136.7677	137.3139	138.3102	137.2076	137.3030	136.7461	136.8646	136.7592	137.0253	136.7826	137.0030	136.7289	137.0608	**126.5**
C4	135.3733	136.9523	137.7934	137.6861	137.4027	137.4540	138.2476	137.6060	138.0118	137.7250	138.4742	135.5726	136.7108	136.6137	137.1181	137.5202	137.1316	138.1073	137.1290	137.9935	137.1376	138.3436	**132.3**
C5	132.8529	134.8667	135.5140	135.8022	136.0673	135.6921	136.1523	135.6972	136.0561	135.8535	136.3255	133.1169	135.0334	135.0630	135.8098	136.2086	135.7793	136.1721	135.7467	136.1175	135.8498	136.3489	**133.1**
C6	135.6189	138.1321	139.2052	139.3484	140.5776	139.0740	140.8250	139.2122	140.6207	139.4132	141.2240	135.9201	138.2926	139.6412	139.3394	141.4293	139.3216	141.6310	139.2822	141.5709	139.3888	141.9883	**133.7**
C7	201.4241	206.0975	208.0047	208.5501	210.8035	209.3477	215.8594	208.2424	214.8943	208.7026	216.5942	205.4639	209.8907	210.9381	212.3099	212.6473	212.0979	217.2124	211.9383	216.0470	212.4596	217.8718	**196.3**
C8	62.9943	64.0386	64.7173	64.4916	65.4659	64.7235	66.0476	64.4397	65.8772	64.5191	66.7543	57.8887	59.6373	60.1189	60.5624	61.2995	60.4421	62.0758	60.3703	61.7220	60.6227	62.3466	**60.8**
C9	22.1716	22.5081	22.5899	22.7526	22.8049	22.6068	22.7610	22.7307	22.7312	22.7638	22.9223	18.9435	19.3563	19.5597	19.5220	19.9370	19.5078	20.0407	19.5021	19.9955	19.5325	20.3889	**15.9**
C3``	130.2132	131.4143	132.3374	131.8774	133.1048	131.8524	132.9497	131.8305	132.9190	131.9013	133.0423	130.2022	131.4034	132.1606	131.8835	133.0160	131.8602	132.8632	131.8414	132.8355	131.9057	132.9546	**123.3**
C8`	35.5659	36.3162	36.5781	36.6919	37.0683	36.7193	37.2869	36.6463	37.2192	36.7168	37.7311	30.9660	31.2463	31.5380	31.3187	31.7279	31.3513	31.7319	31.3640	31.8242	31.3214	31.8234	**31.7**
H(2-4)	8.5422	8.5905	8.6111	8.5969	8.5756	8.5329	8.6116	8.5982	8.5997	8.5962	8.6246	8.5473	8.5123	8.5813	8.4921	8.5670	8.5025	8.5698	8.5075	8.5827	8.4891	8.5808	**8.32**
H5	7.7122	7.9394	7.9877	8.0376	8.0528	8.0264	8.0702	8.0271	8.0597	8.0428	8.0940	7.7321	7.9362	7.9484	8.0144	8.0645	8.0118	8.0680	8.0082	8.0623	8.0185	8.0915	**7.84**
H6	8.3070	8.5620	8.6125	8.6751	8.7328	8.5840	8.7619	8.6635	8.7452	8.6806	8.7971	8.1205	8.3307	8.4526	8.4125	8.6199	8.4147	8.6133	8.4123	8.6192	8.4165	8.6580	**8.05**
H8	4.3875	4.5137	4.5194	4.5830	4.6399	4.5284	4.6666	4.5756	4.6590	4.5867	4.6891	4.5382	4.7048	4.7639	4.7786	4.9041	4.7753	4.9239	4.7713	4.9142	4.7830	4.9615	**5.2**
H(9A-9C)	1.3132	1.3404	1.2908	1.3404	1.2300	1.2980	1.2529	1.3422	1.2424	1.3394	1.2726	1.3900	1.4136	1.4224	1.4316	1.4287	1.4347	1.4518	1.4355	1.4527	1.4318	1.4731	**1.59**
H(8`A-8`C)	2.4992	2.4229	2.4075	2.4008	2.3918	2.4349	2.3815	2.4029	2.3850	2.4002	2.3649	2.8784	2.7054	2.6753	2.6220	2.5884	2.6326	2.4995	2.6394	2.5283	2.6172	2.4707	**2.8**
Nuclei	O3LYP																					
C1	139.0310	140.5715	141.7475	140.5429	142.8188	140.5032	141.5126	140.4849	142.7700	141.0085	141.5782	137.2160	139.4420	141.3766	139.9279	141.9581	139.9150	141.8815	139.8971	141.9441	139.9331	141.9220	**135.1**
C2	129.0182	128.6607	130.7414	128.4800	128.5563	128.4949	128.8782	128.5071	128.7903	128.5009	128.9031	128.7042	128.4753	130.4083	128.5610	129.1531	128.5764	130.4782	128.5864	130.2308	128.5401	130.4387	**131.6**
C3	134.7570	133.4012	133.6490	133.0495	133.0577	133.0876	133.2610	133.1181	133.2835	132.9445	133.2994	134.6108	133.3773	133.7025	133.0406	133.1815	133.0661	133.4209	133.0871	133.5017	133.0104	133.4364	**126.5**
C4	130.7599	131.8661	131.5087	132.6479	133.8301	132.6329	134.8105	132.6026	134.3224	132.4852	134.9697	130.9388	131.7708	131.3225	132.1269	133.0950	132.1027	132.7287	132.0737	132.5981	132.1439	132.9500	**132.3**
C5	128.7515	130.5276	130.6093	131.4786	132.5395	131.4321	132.6687	131.3797	132.4907	131.5135	132.7794	129.1875	130.8027	130.9302	131.5682	132.3611	131.5293	132.0251	131.4852	132.0314	131.5983	132.1829	**133.1**
C6	130.3844	132.3364	133.3338	133.5421	134.7525	133.4933	135.2548	133.4300	134.9011	133.4089	135.6883	130.7554	132.6317	133.4819	133.7880	135.4318	133.7293	135.4420	133.6649	135.2517	133.8370	135.7992	**133.7**
C7	198.1557	204.4179	205.8488	207.2993	209.3100	207.0939	213.2599	206.9099	214.5209	208.0678	213.6395	202.2144	207.1134	209.5992	209.2644	211.2589	209.1466	215.2975	209.0240	214.4096	209.3704	215.7515	**196.3**
C8	63.4164	64.7242	65.3485	65.1490	66.5127	65.1147	66.7915	65.0882	66.9100	65.3968	67.4551	58.3500	60.7875	61.4391	61.7595	62.4397	61.7101	63.3318	61.6554	63.1209	61.7993	63.5534	**60.8**
C9	21.5802	21.8850	22.0241	22.1561	22.4264	22.1497	22.5651	22.1364	22.5794	22.1402	22.7215	18.2919	18.5258	18.5522	18.7786	18.8763	18.7719	18.9891	18.7600	18.9062	18.7783	19.2723	**15.9**
C3``	131.5754	132.7796	133.6338	133.2874	134.5943	133.2650	134.4361	133.2377	134.4042	133.2981	134.5106	131.6024	132.7904	133.6345	133.3528	134.7300	133.3314	134.3739	133.3047	134.4261	133.3666	134.4441	**123.3**
C8`	35.9563	36.6903	37.0036	37.1364	37.4771	37.1180	37.5953	37.0959	37.6523	37.1790	37.9769	31.4490	31.5356	31.8314	31.8081	32.1976	31.7991	32.1822	31.7856	32.2065	31.8105	32.2189	**31.7**
H(2-4)	8.3185	8.2950	8.3450	8.2825	8.2858	8.2854	8.3620	8.2862	8.2943	8.2543	8.3812	8.3842	8.2887	8.2889	8.2842	8.3132	8.2847	8.3258	8.2849	8.3204	8.2836	8.3432	**8.32**
H5	7.6474	7.8555	7.8672	7.9545	8.0180	7.9499	8.0408	7.9447	8.0303	7.9523	8.0631	7.6649	7.8424	7.8595	7.9235	7.9872	7.9191	7.9730	7.9143	7.9686	7.9276	7.9951	**7.84**
H6	8.1170	8.2939	8.3933	8.4380	8.4984	8.4325	8.5597	8.4253	8.5024	8.4254	8.5874	7.9545	8.1052	8.1888	8.2090	8.3738	8.2032	8.3498	8.1970	8.3292	8.2144	8.3943	**8.05**
H8	4.4415	4.5266	4.5455	4.6257	4.6700	4.6212	4.7042	4.6156	4.6520	4.6271	4.7127	4.6101	4.7490	4.8243	4.8277	4.9747	4.8233	4.9749	4.8187	4.9566	4.8318	5.0124	**5.2**
H(9A-9C)	1.2188	1.2058	1.1911	1.1965	1.1433	1.1985	1.1937	1.1993	1.1517	1.1782	1.2144	1.3300	1.3429	1.2925	1.3731	1.3151	1.3714	1.3388	1.3693	1.3280	1.3746	1.3593	**1.59**
H(8`A-8`C)	2.5264	2.4890	2.4625	2.4768	2.4593	2.4764	2.4475	2.4763	2.4605	2.4844	2.4267	2.9202	2.7394	2.7161	2.6803	2.6527	2.6840	2.5746	2.6874	2.5840	2.6769	2.5382	**2.8**
Nuclei	OLYP																					
C1	138.2128	139.1714	140.6753	139.7602	142.4518	139.7392	141.8981	139.7137	142.0924	139.7742	141.8925	134.9370	138.2941	140.0368	138.7842	140.9221	138.8062	140.6230	138.8214	140.8429	137.6006	140.6383	**135.1**
C2	126.4951	125.8112	127.5601	126.2011	127.8856	126.2137	128.3859	126.2194	128.3905	126.1809	128.3367	126.0158	125.9726	128.0267	126.1183	127.8074	126.1289	127.9022	126.1339	127.8105	125.7378	127.4197	**131.6**
C3	132.9292	131.5110	131.5990	131.1067	131.3234	131.1383	131.4505	131.1651	131.4880	131.0682	131.4279	131.8925	131.6398	131.9737	131.3249	131.6090	131.3472	131.7616	131.3649	131.7481	130.7519	131.6861	**126.5**
C4	128.5306	129.8829	129.6853	130.0306	129.8521	130.0070	130.3136	129.9787	130.0785	130.0435	130.5612	128.7743	129.4704	128.9726	129.7763	129.7244	129.7423	130.3624	129.7032	130.1513	130.0661	131.5687	**132.3**
C5	126.8377	128.7753	129.1657	129.6124	129.9027	129.5653	130.0015	129.5125	129.8323	129.6477	130.2130	127.0074	128.8659	129.0366	129.6246	130.0618	129.5805	130.1781	129.5306	130.0785	129.1450	130.5817	**133.1**
C6	127.7814	129.6271	130.7764	130.7470	132.2541	130.6825	132.4128	130.6132	132.2607	130.7989	132.7027	132.4372	130.1093	131.0563	131.2232	132.6961	131.1538	132.9190	131.0790	132.6975	133.5321	133.6072	**133.7**
C7	197.6323	203.6287	205.2814	206.9513	209.4010	206.7558	213.3386	206.5536	212.6884	207.1343	213.7365	196.1881	206.1640	208.4918	208.1652	210.0417	208.0789	213.8707	207.9865	213.0759	205.7736	211.7689	**196.3**
C8	64.7557	66.1004	66.7446	66.7782	67.5880	66.7479	68.3226	66.7118	68.1625	66.7973	68.9808	62.7854	62.2294	62.8103	63.2471	63.8847	63.2127	64.7644	63.1727	64.6704	62.9109	63.4824	**60.8**
C9	21.7367	22.0446	22.2649	22.3766	22.7513	22.3628	22.8548	22.3437	22.8627	22.3810	22.8871	15.5332	18.7279	18.8073	18.9693	19.0455	18.9628	19.2569	18.9512	19.1851	14.6057	14.6826	**15.9**
C3``	134.9073	136.0664	137.1836	136.7122	138.0743	136.6881	137.8335	136.6579	137.8127	136.7257	137.8824	135.1089	136.2451	137.1015	136.8348	138.0524	136.8103	137.9465	136.7801	137.9319	136.8858	138.0870	**123.3**
C8`	36.5960	37.3542	37.6067	37.7897	38.3230	37.7697	38.1947	37.7446	38.2289	37.8005	38.5043	31.5049	32.1343	32.4891	32.3950	32.7821	32.3800	32.7451	32.3595	32.7293	31.7140	32.1418	**31.7**
H(2-4)	8.1543	8.1233	8.2052	8.1298	8.1574	8.1301	8.2001	8.1302	8.1858	8.1290	8.2203	8.2661	8.1538	8.1670	8.1529	8.1823	8.1511	8.2128	8.1493	8.1978	8.1934	8.2893	**8.32**
H5	7.5880	7.7890	7.8231	7.8735	7.9109	7.8687	7.9204	7.8637	7.9082	7.8776	7.9426	7.6253	7.7706	7.7880	7.8469	7.8870	7.8423	7.8979	7.8376	7.8868	7.8277	7.9645	**7.84**
H6	8.0017	8.1894	8.2944	8.3137	8.3991	8.3070	8.4123	8.3001	8.3911	8.3194	8.4517	8.8774	8.0043	8.0946	8.0985	8.2416	8.0914	8.2320	8.0843	8.2099	8.3469	8.3650	**8.05**
H8	4.5516	4.6181	4.6508	4.7019	4.7077	4.6979	4.7279	4.6936	4.7104	4.7050	4.7609	4.5148	4.8442	4.9096	4.9130	5.0503	4.9081	5.0522	4.9031	5.0317	4.8042	4.9598	**5.2**
H(9A-9C)	1.2089	1.1989	1.1919	1.1883	1.1416	1.1888	1.1805	1.1892	1.1792	1.1874	1.1908	1.3093	1.3569	1.3179	1.3859	1.3301	1.3832	1.3565	1.3804	1.3443	1.3150	1.3244	**1.59**
H(8`A-8`C)	2.5661	2.5321	2.5134	2.5236	2.5134	2.5244	2.4989	2.5249	2.5057	2.5226	2.4680	2.3594	2.7834	2.7594	2.7186	2.6881	2.7214	2.6190	2.7241	2.6224	2.2253	2.1866	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S17. Cont. V

Nuclei	R											S										Exp. [b]
	OPBE																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	135.3971	136.5604	136.9534	137.1954	139.6633	137.1733	139.2015	136.9154	139.5136	137.2144	139.2936	133.9333	136.1148	138.1393	136.7483	139.0108	136.7262	138.1921	136.6889	138.8615	136.7676	138.3696	**135.1**
C2	125.1445	124.5514	125.4539	124.8329	126.4349	124.8585	126.9201	124.1934	126.9007	124.8027	126.9252	125.0423	124.7489	125.9117	124.8052	126.4718	124.8305	126.7273	124.8380	126.6064	124.7760	126.7128	**131.6**
C3	130.5712	129.4695	129.7816	129.1290	129.3728	129.1665	129.5142	129.1028	129.5045	129.0891	129.5694	130.5310	129.6043	129.8017	129.2826	129.5847	129.3153	129.7496	129.3307	129.7040	129.2472	129.8106	**126.5**
C4	127.0007	128.4618	129.2152	128.5458	128.5364	128.5385	128.9571	129.1120	128.6656	128.5471	129.2055	127.0046	127.9916	127.8699	128.1629	128.0892	128.1559	128.8202	128.1301	128.4060	128.1636	129.0282	**132.3**
C5	125.6435	127.6155	128.2173	128.3264	128.7940	128.2955	128.8395	128.4526	128.6881	128.3503	129.0443	125.9221	127.5615	127.8823	128.2209	128.7160	128.1951	128.8766	128.1510	128.6830	128.2396	129.0653	**133.1**
C6	126.0300	127.9687	129.1641	128.9734	130.4486	128.9266	130.6030	128.8240	130.3828	129.0128	130.9203	126.3485	128.3317	129.1681	129.2533	130.5580	129.2187	130.9109	129.1647	130.5335	129.2798	131.2162	**133.7**
C7	195.3728	201.1355	201.9317	204.1825	206.4213	204.0100	210.2272	203.9115	209.6004	204.3391	210.7009	198.5929	203.3675	205.5808	205.4118	207.1523	205.3001	210.7934	205.1717	210.3329	205.5139	211.3042	**196.3**
C8	62.2083	63.6747	63.9950	64.3330	65.0025	64.3053	65.8629	64.2669	65.8113	64.3570	66.5668	57.7409	60.0630	60.8801	61.0123	61.7808	60.9693	62.2391	60.9103	62.4262	61.0499	62.4947	**60.8**
C9	20.9606	21.3698	21.5205	21.5712	21.8971	21.5736	21.9528	21.5653	21.8626	21.5643	22.0901	17.7174	18.1185	18.1580	18.2777	18.3204	18.2825	18.4683	18.2697	18.4048	18.2687	18.7827	**15.9**
C3``	130.5403	131.6414	132.5649	132.1243	133.4007	132.1160	133.1379	132.0464	133.1166	132.1270	133.2241	130.5859	131.7904	132.6565	132.2248	133.3325	132.2168	133.1831	132.1907	133.1658	132.2271	133.2727	**123.3**
C8`	35.5335	36.3794	36.5237	36.7094	37.1647	36.7059	37.0152	36.6792	37.0256	36.7074	37.3851	30.7818	31.0050	31.1280	31.1766	31.4627	31.1821	31.5754	31.1695	31.4781	31.1660	31.5973	**31.7**
H(2-4)	8.1891	8.1651	8.2569	8.1655	8.1986	8.1669	8.2405	8.1495	8.2206	8.1634	8.2592	8.2404	8.1739	8.1749	8.1653	8.1843	8.1666	8.2368	8.1670	8.1994	8.1631	8.2514	**8.32**
H5	7.6504	7.8582	7.9137	7.9389	7.9776	7.9346	7.9862	7.9380	7.9707	7.9421	8.0101	7.6537	7.8272	7.8562	7.9010	7.9459	7.8973	7.9654	7.8929	7.9443	7.9036	7.9880	**7.84**
H6	8.0569	8.2400	8.3543	8.3517	8.4534	8.3469	8.4584	8.3288	8.4285	8.3551	8.4945	7.8646	8.0354	8.0892	8.1185	8.2352	8.1146	8.2658	8.1098	8.2154	8.1212	8.3042	**8.05**
H8	4.5711	4.6421	4.6596	4.7172	4.7299	4.7146	4.7454	4.7061	4.7196	4.7188	4.7769	4.7429	4.8750	4.9113	4.9288	5.0442	4.9262	5.0749	4.9227	5.0304	4.9304	5.1138	**5.2**
H(9A-9C)	1.1643	1.1602	1.1600	1.1463	1.0942	1.1473	1.1340	1.1472	1.1281	1.1446	1.1491	1.2795	1.3079	1.2506	1.3292	1.2532	1.3283	1.2953	1.3267	1.2713	1.3293	1.3137	**1.59**
H(8`A-8`C)	2.4874	2.4566	2.4154	2.4451	2.4173	2.4463	2.4083	2.4440	2.4142	2.4433	2.3835	2.8211	2.6617	2.6031	2.5933	2.5405	2.5976	2.5017	2.6011	2.4887	2.5885	2.4663	**2.8**
Nuclei	OPW91																					
C1	135.6804	137.1089	138.0169	137.4687	139.9443	137.4374	139.4745	137.1653	139.7720	137.9444	139.5666	134.1835	136.3790	137.3757	136.9815	139.2667	136.9531	138.4392	136.9079	139.1264	136.9904	138.6067	**135.1**
C2	125.3805	125.0789	126.4168	125.0743	126.6691	125.0894	127.1516	124.4178	127.1346	124.8128	127.1590	125.2678	124.9801	125.2746	125.0463	126.7004	125.0616	126.9604	125.0599	126.8359	125.0139	126.9496	**131.6**
C3	130.8226	129.7168	129.8806	129.3579	129.5857	129.3861	129.7266	129.3184	129.7198	129.2184	129.7819	130.7786	129.8371	129.9712	129.5168	129.7969	129.5395	129.9624	129.5459	129.9175	129.4772	130.0245	**126.5**
C4	127.2344	128.4054	128.5764	128.7900	128.7567	128.7723	129.1849	129.3373	128.9000	128.8372	129.4362	127.2494	128.2337	129.3282	128.4176	128.3236	128.3992	129.0604	128.3638	128.6389	128.4166	129.2756	**132.3**
C5	125.8328	127.7478	128.1164	128.5349	128.9817	128.4934	129.0324	128.6416	128.8837	128.6045	129.2391	126.1304	127.7715	128.5024	128.4399	128.9163	128.4034	129.0780	128.3499	128.8827	128.4556	129.2701	**133.1**
C6	126.2765	128.2385	129.3782	129.2355	130.6958	129.1781	130.8520	129.0653	130.6368	129.2553	131.1724	126.6000	128.5868	129.5812	129.5324	130.8134	129.4858	131.1716	129.4220	130.7883	129.5579	131.4840	**133.7**
C7	195.7082	201.5050	202.5029	204.5659	206.8089	204.3813	210.6247	204.2695	209.9897	205.1022	211.1052	198.9601	203.7529	205.7840	205.7803	207.5326	205.6607	211.1889	205.5234	210.7286	205.8750	211.6967	**196.3**
C8	62.3877	63.8546	64.3269	64.5090	65.1815	64.4720	66.0409	64.4218	65.9761	64.6762	66.7427	57.8887	60.2324	60.5846	61.1745	61.9542	61.1234	62.4084	61.0556	62.6070	61.2050	62.6591	**60.8**
C9	21.0221	21.4859	21.6126	21.6458	21.9631	21.6378	22.0194	21.6207	21.9331	21.6324	22.1579	17.7935	18.1992	18.2308	18.3648	18.4031	18.3597	18.5490	18.3377	18.4883	18.3520	18.8631	**15.9**
C3``	131.0456	132.2737	133.1183	132.6560	133.9284	132.6373	133.6656	132.5566	133.6450	132.6983	133.7537	131.0918	132.3110	133.1875	132.7574	133.8600	132.7391	133.7087	132.7036	133.6923	132.7564	133.7999	**123.3**
C8`	35.5989	36.4311	36.5509	36.7876	37.2365	36.7738	37.0851	36.7380	37.0986	36.7553	37.4577	30.8794	31.0987	31.3667	31.2814	31.5524	31.2761	31.6712	31.2541	31.5688	31.2681	31.6998	**31.7**
H(2-4)	8.1917	8.1893	8.2564	8.1682	8.1995	8.1688	8.2414	8.1516	8.2223	8.1558	8.2602	8.2446	8.1762	8.2088	8.1697	8.1858	8.1701	8.2386	8.1703	8.2004	8.1676	8.2537	**8.32**
H5	7.6496	7.8495	7.8853	7.9390	7.9766	7.9341	7.9855	7.9373	7.9703	7.9447	8.0092	7.6540	7.8275	7.8786	7.9023	7.9457	7.8979	7.9654	7.8932	7.9439	7.9046	7.9880	**7.84**
H6	8.0569	8.2381	8.3348	8.3546	8.4535	8.3490	8.4592	8.3310	8.4307	8.3306	8.4952	7.8676	8.0378	8.1322	8.1238	8.2375	8.1190	8.2689	8.1139	8.2173	8.1266	8.3079	**8.05**
H8	4.5703	4.6481	4.6510	4.7185	4.7292	4.7150	4.7455	4.7067	4.7204	4.6966	4.7767	4.7387	4.8718	4.9428	4.9282	5.0408	4.9247	5.0725	4.9209	5.0268	4.9298	5.1117	**5.2**
H(9A-9C)	1.1662	1.1664	1.1569	1.1486	1.0959	1.1490	1.1357	1.1487	1.1298	1.1489	1.1508	1.2808	1.3092	1.2729	1.3322	1.2550	1.3305	1.2975	1.3286	1.2729	1.3322	1.3161	**1.59**
H(8`A-8`C)	2.4885	2.4588	2.4297	2.4470	2.4192	2.4476	2.4102	2.4449	2.4159	2.4463	2.3855	2.8265	2.6669	2.6433	2.5996	2.5458	2.6031	2.5067	2.6063	2.4932	2.5947	2.4719	**2.8**
Nuclei	PBE																					
C1	139.7212	140.7632	142.1457	141.4743	143.5609	141.1869	143.3656	141.1793	143.4527	141.2507	143.5034	138.3280	139.8329	140.5514	140.4901	141.7122	140.3782	141.9188	140.3135	141.5510	140.7038	142.0914	**135.1**
C2	130.3305	129.8674	130.0482	129.5391	131.8664	129.5348	132.3357	129.5642	132.2550	129.5179	132.3267	129.8530	129.7585	131.6375	129.5729	131.4067	129.5557	131.9388	129.5650	131.8009	129.6832	131.8851	**131.6**
C3	137.1494	136.1486	136.3006	135.6275	135.9210	135.6924	136.1263	135.7269	136.1188	135.6647	136.1719	137.0705	135.9455	136.1142	135.4458	135.6811	135.4699	135.8641	135.5052	135.8515	135.4420	135.9108	**126.5**
C4	132.8389	134.5246	135.9659	135.1836	134.9124	135.1365	135.6976	135.1032	135.4895	135.2380	135.9383	133.0118	134.3126	134.1013	134.7613	135.0361	134.7599	135.5955	134.7517	135.4778	134.6996	135.8433	**132.3**
C5	131.3419	133.5450	134.3628	134.4015	134.8016	134.4135	134.9318	134.3654	134.8226	134.5448	135.1250	131.8109	133.7938	133.9277	134.5692	135.1258	134.5360	135.1150	134.5044	135.0624	134.5782	135.3069	**133.1**
C6	132.9334	135.2235	136.3727	136.3569	138.0607	136.1938	138.1937	136.1365	138.0091	136.3428	138.6271	133.1571	135.5863	136.9326	136.5934	138.7812	136.5466	138.9608	136.5024	138.8838	136.6365	139.3423	**133.7**
C7	201.9109	206.9944	209.1963	209.6217	211.0232	209.4796	215.4697	209.3379	214.6811	209.8020	216.2122	206.4050	210.4319	211.5806	212.5481	213.2485	212.3959	217.1109	212.2649	216.1395	212.7236	217.6895	**196.3**
C8	67.0880	68.4594	69.0193	68.9220	69.8106	68.9057	70.3829	68.8959	70.1978	68.9588	71.1858	61.7296	63.5682	64.1013	64.4006	65.4169	64.3171	66.1541	64.2596	65.8115	64.5340	66.4515	**60.8**
C9	23.0890	23.4910	23.5423	23.6944	24.0232	23.6363	24.0451	23.6270	23.9887	23.6955	24.2548	19.8844	20.4915	20.7285	20.6424	21.2207	20.6283	21.4190	20.6258	21.3652	20.6780	21.8846	**15.9**
C3``	140.1590	141.5263	142.3805	141.9316	143.4044	141.9277	143.2302	141.9111	143.1977	141.9986	143.3249	140.1654	141.5555	142.3363	141.9959	143.3201	141.9674	143.1545	141.9500	143.1230	142.0404	143.2476	**123.3**
C8`	37.1164	37.8677	38.1063	38.1800	38.6066	38.1575	38.8094	38.1503	38.7595	38.2057	39.2865	32.0619	32.3521	32.6756	32.3899	32.8439	32.4045	32.8393	32.4193	32.9322	32.3724	32.9077	**31.7**
H(2-4)	8.3075	8.3096	8.3407	8.2959	8.3535	8.2965	8.3837	8.2974	8.3754	8.2960	8.3960	8.3464	8.3182	8.3659	8.2891	8.3498	8.2942	8.3547	8.2982	8.3662	8.2818	8.3655	**8.32**
H5	7.5705	7.7875	7.8504	7.8833	7.9131	7.8746	7.9292	7.8697	7.9192	7.8855	7.9531	7.5992	7.7927	7.8157	7.8721	7.9273	7.8689	7.9290	7.8654	7.9243	7.8733	7.9517	**7.84**
H6	8.1643	8.3298	8.4040	8.4091	8.5661	8.4112	8.5869	8.4058	8.5757	8.4231	8.6198	7.9431	8.1366	8.2606	8.2233	8.4222	8.2211	8.4163	8.2180	8.4206	8.2230	8.4615	**8.05**
H8	4.6554	4.7164	4.7510	4.7569	4.8606	4.7620	4.8808	4.7580	4.8762	4.7724	4.9024	4.7808	4.9353	4.9938	5.0119	5.1320	5.0075	5.1496	5.0034	5.1377	5.0160	5.1884	**5.2**
H(9A-9C)	1.3721	1.3683	1.3170	1.3547	1.3072	1.3474	1.3262	1.3492	1.3166	1.3451	1.3460	1.4764	1.5081	1.5100	1.5225	1.5232	1.5228	1.5461	1.5230	1.5456	1.5214	1.5723	**1.59**
H(8`A-8`C)	2.6103	2.5557	2.5183	2.5277	2.4906	2.5299	2.4737	2.5319	2.4769	2.5278	2.4533	2.9909	2.8165	2.7933	2.7360	2.6984	2.7435	2.6045	2.7500	2.6367	2.7264	2.5711	**2.8**
Nuclei	PBE0																					
C1	140.5602	140.5509	141.6746	140.4848	143.5480	140.4784	143.6254	140.4755	143.7903	140.4956	142.6458	139.6478	140.8335	141.5449	141.5087	142.5468	141.3957	142.7246	141.3175	142.3501	141.6368	142.8257	**135.1**
C2	133.2397	132.7487	133.4008	132.4234	134.4110	132.4379	135.0190	132.4547	134.8730	132.4126	134.8057	132.9015	132.5882	134.4704	132.5386	134.1461	132.5296	134.7112	132.5240	134.5383	132.5493	134.6038	**131.6**
C3	138.1782	137.0541	137.1414	136.6074	136.8655	136.6264	137.1331	136.6476	137.0718	136.5929	137.0660	138.1137	136.9552	137.0917	136.5412	136.6720	136.5543	136.9147	136.5710	136.8361	136.5332	136.8956	**126.5**
C4	135.0939	136.6706	137.5406	137.4178	137.1733	137.3681	138.0539	137.3201	137.7576	137.4674	138.3566	135.2197	136.5201	136.3574	136.9196	137.2511	136.9069	137.9101	136.8894	137.7326	136.9321	138.0892	**132.3**
C5	132.6932	134.7329	135.3872	135.6778	135.9322	135.6166	136.1323	135.5568	135.9793	135.7387	136.2229	132.9871	134.9064	134.9103	135.6697	136.0553	135.6270	136.0897	135.5835	135.9809	135.7119	136.2108	**133.1**
C6	135.4259	137.9112	139.0499	139.1297	140.5457	139.0517	140.6692	138.9752	140.3874	139.2062	141.4005	135.7146	138.1546	139.4803	139.2078	141.2434	139.1610	141.5318	139.1063	141.3942	139.2502	141.8339	**133.7**
C7	201.0615	205.7581	207.4669	208.1424	209.8819	207.9895	215.4183	207.8392	214.4993	208.2916	215.0527	205.1470	209.5177	210.5774	211.8608	212.2819	211.6833	216.8381	211.5239	215.6654	212.0439	217.4307	**196.3**
C8	62.8991	63.9623	64.6008	64.3964	65.4144	64.3642	65.9555	64.3342	65.7533	64.4305	66.5831	57.7640	59.3848	59.8772	60.2288	60.9856	60.1418	61.8321	60.0713	61.4354	60.3225	62.0499	**60.8**
C9	22.1584	22.4931	22.6317	22.7534	22.9482	22.7313	22.8069	22.7109	22.7103	22.7770	23.2142	18.9640	19.3534	19.5418	19.4996	19.8767	19.4826	20.0672	19.4684	19.9573	19.5201	20.3735	**15.9**
C3``	129.7732	130.9674	131.8879	131.4176	132.6100	131.3868	132.5359	131.3576	132.4478	131.4496	132.5753	129.7928	130.9840	131.6975	131.4248	132.5531	131.3961	132.4833	131.3685	132.3980	131.4545	132.5196	**123.3**
C8`	35.4663	36.2100	36.4263	36.5551	36.8973	36.5274	37.1897	36.5019	37.0920	36.5851	37.5716	30.6967	30.9918	31.3003	31.1132	31.4843	31.1205	31.5527	31.1197	31.5881	31.1051	31.5860	**31.7**
H(2-4)	8.5382	8.5824	8.6154	8.5911	8.5866	8.5911	8.6109	8.5909	8.5946	8.5908	8.6577	8.5537	8.5217	8.5759	8.4943	8.5648	8.4998	8.5697	8.5035	8.5789	8.4877	8.5783	**8.32**
H5	7.7113	7.9374	7.9874	8.0361	8.0534	8.0304	8.0727	8.0247	8.0594	8.0411	8.0994	7.7264	7.9310	7.9437	8.0132	8.0583	8.0094	8.0656	8.0051	8.0569	8.0164	8.0862	**7.84**
H6	8.3132	8.5629	8.6249	8.6779	8.7455	8.6713	8.7692	8.6647	8.7494	8.6836	8.8427	8.1220	8.3274	8.4549	8.4192	8.6202	8.4172	8.6178	8.4135	8.6190	8.4199	8.6594	**8.05**
H8	4.3787	4.5044	4.5123	4.5758	4.6236	4.5716	4.6690	4.5672	4.6577	4.5795	4.6874	4.5428	4.7084	4.7712	4.7876	4.9105	4.7835	4.9347	4.7791	4.9225	4.7911	4.9687	**5.2**
H(9A-9C)	1.3225	1.3453	1.3087	1.3475	1.2637	1.3476	1.2603	1.3477	1.2451	1.3469	1.3245	1.4102	1.4322	1.4339	1.4449	1.4377	1.4458	1.4638	1.4459	1.4612	1.4433	1.4828	**1.59**
H(8`A-8`C)	2.5055	2.4287	2.4088	2.4045	2.3993	2.4054	2.3868	2.4065	2.3878	2.4034	2.3597	2.8750	2.7058	2.6779	2.6289	2.5927	2.6361	2.5053	2.6419	2.5310	2.6212	2.4731	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S17. Cont. VI

Nuclei	R											S										Exp. [b]
	TPSS																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	136.2276	136.2094	137.3098	136.2059	139.2726	136.2094	139.0314	136.2249	136.7419	136.2145	138.4227	135.0557	135.7714	136.9182	136.7179	137.4137	136.6766	137.8582	136.6530	137.7385	136.7741	137.9431	**135.1**
C2	127.9563	127.4469	128.1664	127.2008	129.1294	127.2223	129.6418	127.2554	127.7365	127.1911	129.4682	127.4671	127.2217	129.0185	127.1497	128.6211	127.1490	129.1980	127.1653	128.3220	127.1643	129.1209	**131.6**
C3	133.6187	132.4099	132.5662	131.9841	132.1677	132.0138	132.4039	132.0553	132.5556	131.9669	132.3877	133.5387	132.3161	132.4986	131.8098	131.9284	131.8391	132.1433	131.8801	133.0014	131.7934	132.1477	**126.5**
C4	129.9020	131.3789	132.2994	132.1371	131.9798	132.0986	132.8498	132.0712	132.5716	132.1841	133.1241	130.1075	131.1625	131.2461	131.7788	132.2079	131.7647	132.7424	131.7561	132.8784	131.7990	132.9623	**132.3**
C5	127.7575	129.6791	130.4090	130.6302	130.8438	130.5807	130.9832	130.5423	131.0366	130.6873	131.1460	128.1696	129.8982	130.1207	130.7335	131.2338	130.6987	131.1793	130.6720	131.8024	130.7746	131.3345	**133.1**
C6	130.0581	132.3184	133.5465	133.5338	134.9679	133.4665	135.1596	133.4104	133.9161	133.6078	135.7595	130.2504	132.5177	133.8564	133.6109	135.6396	133.5554	135.8234	133.5095	134.6186	133.6717	136.1650	**133.7**
C7	197.7434	202.0372	203.6815	204.2731	206.0727	204.1432	210.7412	204.0244	204.8126	204.4081	210.7497	201.9311	205.5667	206.8712	207.7552	208.3020	207.6321	212.3135	207.5205	208.0745	207.8847	212.8487	**196.3**
C8	65.5897	66.5806	67.3103	67.0380	68.0808	67.0167	68.4635	67.0072	67.2473	67.0688	69.1963	60.9016	62.4784	63.1309	63.3943	64.0970	63.3429	64.9028	63.3055	64.9411	63.4562	65.1087	**60.8**
C9	23.7353	24.0320	24.2797	24.3692	24.5131	24.3535	24.4605	24.3491	24.4186	24.3947	24.8716	20.5884	21.0897	21.3994	21.3502	21.7344	21.3399	22.0163	21.3415	23.2919	21.3709	22.3953	**15.9**
C3``	137.7590	138.9978	140.0662	139.5338	140.7961	139.5098	140.6370	139.4970	140.0271	139.5669	140.6984	137.7703	138.9926	139.8267	139.5357	140.7263	139.5131	140.5718	139.5013	140.5655	139.5670	140.6341	**123.3**
C8`	37.5149	38.1757	38.4508	38.5584	38.9028	38.5411	39.2010	38.5354	38.6616	38.5859	39.5557	33.1578	33.3756	33.7244	33.4332	33.9624	33.4341	33.8075	33.4448	35.3044	33.4407	33.8352	**31.7**
H(2-4)	8.3127	8.3571	8.4007	8.3714	8.3656	8.3711	8.4015	8.3712	8.2110	8.3720	8.4310	8.3384	8.3119	8.3653	8.2950	8.3762	8.2967	8.3622	8.2988	8.4098	8.2933	8.3711	**8.32**
H5	7.5053	7.7295	7.7855	7.8320	7.8547	7.8262	7.8738	7.8210	7.6587	7.8378	7.8974	7.5276	7.7329	7.7509	7.8127	7.8747	7.8081	7.8699	7.8039	7.9186	7.8171	7.8898	**7.84**
H6	8.0669	8.3074	8.3776	8.4240	8.4937	8.4174	8.5357	8.4112	8.2512	8.4306	8.5873	7.8732	8.0874	8.2087	8.1837	8.4014	8.1781	8.3891	8.1729	8.2848	8.1890	8.4325	**8.05**
H8	4.5279	4.6310	4.6406	4.6975	4.7476	4.6934	4.7915	4.6900	4.5152	4.7017	4.8029	4.6265	4.7937	4.8547	4.8778	4.9976	4.8729	5.0280	4.8685	5.0052	4.8828	5.0594	**5.2**
H(9A-9C)	1.3684	1.3912	1.3707	1.3997	1.3239	1.3996	1.3338	1.4000	1.2119	1.4002	1.3800	1.4600	1.4940	1.5033	1.5192	1.5327	1.5180	1.5452	1.5172	1.6790	1.5206	1.5682	**1.59**
H(8`A-8`C)	2.5613	2.4782	2.4636	2.4571	2.4590	2.4581	2.4345	2.4597	2.2759	2.4566	2.4099	2.9628	2.8058	2.7752	2.7178	2.7163	2.7225	2.5972	2.7277	2.8804	2.7135	2.5642	**2.8**
Nuclei	VSXC																						
C1	133.8726	133.8822	134.5524	133.9143	135.1026	133.9159	134.6551	133.9150	134.7437	133.9145	134.7773	134.6019	135.1754	136.0201	135.5406	136.9371	135.5270	136.5090	135.5057	136.5196	135.5509	136.6355	**135.1**
C2	127.2397	126.4623	127.0306	126.0199	126.5115	126.0500	126.9394	126.0778	126.8673	125.9932	126.9113	127.3474	126.6316	127.2114	126.2381	126.7713	126.2672	127.1453	126.2931	127.0874	126.2115	127.0827	**131.6**
C3	133.3160	132.2729	132.3354	131.9207	131.9071	131.9418	132.0871	131.9610	132.0770	131.9028	132.1134	133.2605	132.1654	132.2376	131.8130	131.8561	131.8329	132.0131	131.8515	132.0076	131.7964	132.0567	**126.5**
C4	126.1898	127.8989	128.6840	128.8296	129.8709	128.7759	130.6634	128.7203	130.4322	128.8819	130.9519	126.3941	128.0768	128.8978	128.9320	129.8986	128.8828	130.5830	128.8317	130.3845	128.9805	130.8327	**132.3**
C5	126.0132	128.1416	128.8416	129.2199	130.1338	129.1574	130.2437	129.0930	130.1222	129.2804	130.4091	126.2691	128.2259	128.8071	129.1982	130.0299	129.1422	130.1018	129.0847	129.9982	129.2535	130.2712	**133.1**
C6	130.5489	132.7393	133.8176	133.8536	135.5423	133.7888	135.8309	133.7222	135.6461	133.9162	136.1608	130.4348	132.7583	133.9294	133.8311	135.5894	133.7687	135.8802	133.7061	135.7187	133.8932	136.1847	**133.7**
C7	191.7166	196.0578	197.4091	198.2677	199.1236	198.1366	202.7695	198.0034	201.9858	198.3934	203.4967	192.4827	196.5355	198.0255	198.7902	200.0493	198.6576	203.5430	198.5185	202.7411	198.9139	204.2825	**196.3**
C8	71.1842	71.9764	72.5848	72.3009	73.0596	72.2876	73.4495	72.2715	73.3379	72.3146	73.9461	64.0590	65.2486	65.8658	65.9620	66.9743	65.9232	67.2192	65.8805	67.0874	65.9991	67.7128	**60.8**
C9	27.1294	28.0449	28.3270	28.6593	29.1118	28.6202	29.2882	28.5795	29.1804	28.6989	29.3713	28.0895	28.2536	28.3564	28.4656	28.7720	28.4546	28.6626	28.4395	28.6156	28.4766	28.9483	**15.9**
C3``	135.6437	136.9150	137.8650	137.4685	138.7968	137.4394	138.6317	137.4080	138.5961	137.4974	138.7282	135.4944	136.8394	137.8426	137.4087	138.8820	137.3790	138.7230	137.3468	138.6853	137.4385	138.8435	**123.3**
C8`	40.8549	41.1026	41.2744	41.2185	41.4097	41.2137	41.3715	41.2070	41.3509	41.2248	41.7201	35.7106	36.1566	36.3597	36.4200	36.8169	36.4054	36.8375	36.3893	36.8068	36.4357	37.1806	**31.7**
H(2-4)	8.4249	8.4631	8.5289	8.4662	8.5283	8.4662	8.5505	8.4662	8.5436	8.4662	8.5582	8.3688	8.3760	8.4310	8.3676	8.4342	8.3682	8.4553	8.3690	8.4516	8.3671	8.4635	**8.32**
H5	7.5778	7.8017	7.8552	7.9020	7.9775	7.8963	7.9863	7.8906	7.9748	7.9073	8.0093	7.5618	7.7748	7.8230	7.8692	7.9423	7.8637	7.9504	7.8583	7.9413	7.8744	7.9714	**7.84**
H6	8.2872	8.4871	8.5859	8.5902	8.7307	8.5838	8.7751	8.5776	8.7548	8.5962	8.7815	7.9281	8.1366	8.2471	8.2399	8.4131	8.2336	8.4456	8.2275	8.4269	8.2460	8.4703	**8.05**
H8	4.4363	4.5262	4.5452	4.5968	4.6679	4.5918	4.6758	4.5871	4.6622	4.6015	4.7066	4.6145	4.8078	4.8839	4.9091	5.0400	4.9029	5.0765	4.8969	5.0621	4.9151	5.1027	**5.2**
H(9A-9C)	1.6263	1.6474	1.6420	1.6472	1.6253	1.6475	1.6423	1.6478	1.6369	1.6469	1.6579	1.7030	1.7055	1.6713	1.7102	1.6704	1.7096	1.6936	1.7094	1.6892	1.7111	1.7004	**1.59**
H(8`A-8`C)	2.6925	2.6334	2.5879	2.6160	2.5839	2.6169	2.5636	2.6180	2.5677	2.6150	2.5449	2.8653	2.7461	2.6915	2.6877	2.6177	2.6904	2.5943	2.6936	2.6045	2.6856	2.5561	**2.8**
Nuclei	wB97																						
C1	140.7810	140.4612	141.9677	140.2266	143.1351	140.2398	142.0269	140.2524	142.2749	140.2148	142.0870	140.1262	140.9586	141.8277	141.9675	143.1059	141.9619	143.0247	141.9525	142.9931	141.9706	143.1096	**135.1**
C2	134.6863	133.9274	136.3692	133.6079	136.0447	133.6265	136.4704	133.6445	136.3705	133.5907	136.4641	134.4790	134.1495	136.3082	134.3000	136.0490	134.3024	136.4835	134.3035	136.3945	134.2970	136.4524	**131.6**
C3	138.5562	137.2220	137.4288	136.7310	137.0220	136.7566	137.0593	136.7819	137.0733	136.7077	137.0694	138.6814	137.3259	137.3986	136.9867	137.0056	137.0079	137.0765	137.0288	137.0782	136.9673	137.1020	**126.5**
C4	136.6437	138.3682	137.6807	139.1492	138.5118	139.1009	139.3610	139.0519	139.1145	139.1954	139.5939	137.0010	137.9300	137.7786	138.2114	138.5751	138.1737	139.1115	138.1367	138.9334	138.2489	139.3506	**132.3**
C5	133.2434	135.2053	135.0698	136.1462	136.2313	136.0890	136.2421	136.0309	136.1641	136.2008	136.3947	133.3753	135.0472	134.9355	135.7402	135.9622	135.6930	135.8756	135.6453	135.7992	135.7854	136.0323	**133.1**
C6	137.2908	139.7299	140.7819	141.0309	142.4265	140.9499	142.8009	140.8681	142.5547	141.1083	143.2149	137.5927	140.1136	141.3995	141.0895	143.1177	141.0173	143.3083	140.9448	143.1533	141.1585	143.6761	**133.7**
C7	200.7714	205.7742	207.0972	208.3519	209.7185	208.1956	214.4197	208.0382	213.4545	208.5009	215.2501	204.2602	208.8353	210.0277	211.5331	211.9435	211.3860	216.8549	211.2364	215.7992	211.6716	217.5626	**196.3**
C8	61.4996	62.4307	63.0825	62.8281	63.7829	62.8046	64.1025	62.7801	63.9586	62.8507	64.7254	56.1105	57.5259	58.0184	58.5101	59.2249	58.4722	59.8814	58.4324	59.6991	58.5456	60.1375	**60.8**
C9	21.8146	21.9764	22.1468	22.2456	22.4537	22.2231	22.3542	22.2007	22.3150	22.2679	22.5214	19.3687	19.5118	19.6119	19.6436	19.9575	19.6368	19.9216	19.6291	19.9099	19.6503	20.2231	**15.9**
C3``	130.8106	131.9016	132.7921	132.3765	133.6522	132.3477	133.5075	132.3182	133.4684	132.4041	133.6044	130.8799	131.9507	132.7544	132.4171	133.5867	132.3904	133.4394	132.3632	133.4032	132.4425	133.5311	**123.3**
C8`	35.2152	35.8390	36.0586	36.1539	36.4860	36.1344	36.6232	36.1143	36.5492	36.1728	37.0329	30.5306	30.8469	31.1512	30.9562	31.3187	30.9373	31.2965	30.9184	31.2860	30.9750	31.4707	**31.7**
H(2-4)	8.6632	8.6905	8.7455	8.6971	8.7286	8.6967	8.7808	8.6964	8.7663	8.6973	8.7952	8.6713	8.6405	8.6970	8.5977	8.6772	8.5976	8.6747	8.5976	8.6723	8.5980	8.6905	**8.32**
H5	7.7918	8.0166	8.0119	8.1130	8.1235	8.1075	8.1377	8.1017	8.1265	8.1184	8.1622	7.7766	7.9889	7.9799	8.0615	8.0931	8.0566	8.0982	8.0517	8.0894	8.0661	8.1227	**7.84**
H6	8.3915	8.6490	8.7161	8.7756	8.8713	8.7681	8.9235	8.7604	8.9014	8.7828	8.9670	8.2398	8.4620	8.5875	8.5340	8.7330	8.5270	8.7248	8.5201	8.7147	8.5408	8.7673	**8.05**
H8	4.1528	4.2975	4.2995	4.3879	4.4435	4.3820	4.4961	4.3761	4.4834	4.3935	4.5251	4.3338	4.4989	4.5655	4.5636	4.6997	4.5583	4.7149	4.5530	4.7030	4.5688	4.7447	**5.2**
H(9A-9C)	1.3607	1.3746	1.3603	1.3766	1.3139	1.3764	1.3389	1.3762	1.3285	1.3767	1.3613	1.4186	1.4415	1.4343	1.4361	1.4278	1.4344	1.4489	1.4328	1.4434	1.4378	1.4685	**1.59**
H(8`A-8`C)	2.4952	2.4265	2.4027	2.4051	2.4037	2.4059	2.3770	2.4067	2.3806	2.4045	2.3629	2.8267	2.6592	2.6319	2.5685	2.5373	2.5702	2.4651	2.5722	2.4768	2.5670	2.4415	**2.8**
Nuclei	wB97X																						
C1	142.2012	141.8956	143.9605	141.8371	144.6823	141.8505	143.6289	141.8255	143.7966	141.8256	143.6097	141.4689	142.3442	143.2209	143.4299	144.4670	143.4259	144.4817	143.4160	144.4128	143.4311	144.5527	**135.1**
C2	135.2231	134.3883	136.7654	134.4170	136.4284	134.4373	136.8921	134.1884	136.7348	134.3987	136.8621	134.9888	134.7810	136.6915	134.7332	136.4221	134.7407	136.9181	134.7460	136.7675	134.7256	136.8686	**131.6**
C3	139.8665	138.5312	138.7368	138.0895	138.3111	138.1166	138.4074	138.0982	138.3557	138.0651	138.4028	139.9510	138.6470	138.6924	138.2299	138.3049	138.2532	138.4327	138.2759	138.3714	138.2093	138.4492	**126.5**
C4	136.9960	138.7622	138.0689	139.2080	138.9897	139.1630	139.8889	139.3351	139.5847	139.2517	140.1174	137.3209	138.4035	138.2145	138.6604	139.0288	138.6243	139.5994	138.5896	139.3518	138.6971	139.8295	**132.3**
C5	134.0640	136.0814	135.9736	136.8903	137.1548	136.8367	137.2206	136.8787	137.0778	136.9421	137.3560	134.2177	135.9479	135.8651	136.6442	136.9093	136.5984	136.8587	136.5522	136.7173	136.6894	137.0093	**133.1**
C6	137.6500	140.0836	140.9621	141.3510	142.7281	141.2733	143.1401	141.2281	142.8406	141.4257	143.5689	137.9486	140.4391	141.7776	141.4430	143.4663	141.3733	143.6932	141.3033	143.4711	141.5105	144.0505	**133.7**
C7	202.4973	207.5472	209.3902	210.0448	211.5953	209.8930	216.3947	209.7994	215.3464	210.1891	217.1294	206.2368	210.8170	211.9463	213.5009	213.8546	213.3567	218.7892	213.2091	217.6806	213.6371	219.4751	**196.3**
C8	62.5616	63.5040	64.2145	63.9202	64.9020	63.8977	65.3032	63.9041	65.0858	63.9423	65.9192	57.1762	58.6657	59.1593	59.6529	60.3443	59.6162	61.1017	59.5765	60.8634	59.6871	61.3404	**60.8**
C9	22.0178	22.1731	22.2513	22.4332	22.6611	22.4130	22.6108	22.4260	22.5112	22.4542	22.7792	19.4556	19.6201	19.7406	19.7263	20.0456	19.7212	20.0846	19.7149	20.0125	19.7319	20.3690	**15.9**
C3``	130.7941	131.8745	132.7648	132.4276	133.6414	132.4006	133.5268	132.2509	133.4295	132.4540	133.6100	130.8465	131.9457	132.7222	132.3997	133.5601	132.3757	133.4428	132.3509	133.3488	132.4236	133.5192	**123.3**
C8`	35.4567	36.1265	36.3509	36.4672	36.7733	36.4485	36.9792	36.4272	36.8438	36.4859	37.3845	30.7272	31.0264	31.3204	31.1389	31.5203	31.1209	31.5403	31.1034	31.4718	31.1580	31.7033	**31.7**
H(2-4)	8.6204	8.6500	8.6752	8.6620	8.6830	8.6617	8.7356	8.6641	8.7199	8.6623	8.7503	8.6383	8.5996	8.6573	8.5580	8.6419	8.5581	8.6405	8.5584	8.6342	8.5582	8.6548	**8.32**
H5	7.7693	7.9974	7.9922	8.0856	8.1095	8.0802	8.1251	8.0801	8.1113	8.0909	8.1478	7.7582	7.9628	7.9627	8.0491	8.0791	8.0443	8.0851	8.0395	8.0735	8.0538	8.1076	**7.84**
H6	8.3578	8.6149	8.6631	8.7426	8.8347	8.7352	8.8863	8.7292	8.8632	8.7497	8.9299	8.1996	8.4251	8.5484	8.4947	8.6937	8.4879	8.6871	8.4811	8.6725	8.5015	8.7312	**8.05**
H8	4.2049	4.3449	4.3472	4.4311	4.4941	4.4258	4.5407	4.4148	4.5283	4.4363	4.5652	4.3800	4.5456	4.6056	4.6187	4.7514	4.6137	4.7634	4.6087	4.7481	4.6237	4.7940	**5.2**
H(9A-9C)	1.3432	1.3571	1.3105	1.3628	1.2924	1.3627	1.3196	1.3724	1.3071	1.3631	1.3437	1.4096	1.4231	1.4293	1.4354	1.4280	1.4340	1.4471	1.4326	1.4381	1.4369	1.4648	**1.59**
H(8`A-8`C)	2.5029	2.4322	2.4193	2.4103	2.4071	2.4113	2.3844	2.4140	2.3843	2.4095	2.3662	2.8536	2.6823	2.6507	2.5925	2.5637	2.5946	2.4839	2.5970	2.4917	2.5908	2.4569	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S17. Cont. VII

Nuclei	R											S										Exp. [b]
	X3LYP																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	
C1	143.3841	143.2105	145.4881	143.2916	146.1036	143.2857	146.2623	143.2791	146.4040	143.3034	146.3144	141.9748	142.9958	144.0136	144.0098	144.4086	143.9148	144.8935	143.8731	144.7657	144.0762	145.0294	**135.1**
C2	134.5087	133.7699	134.1395	133.7623	134.3471	133.7775	136.3379	133.7902	136.2505	133.7519	136.3031	134.0694	133.8567	135.7246	133.7884	134.4778	133.7014	135.8852	133.7029	135.7869	133.8030	135.8249	**131.6**
C3	140.2977	139.0463	139.2491	138.5337	138.6811	138.5625	138.9085	138.5891	138.9136	138.5106	138.9088	140.1981	138.9459	138.9714	138.4256	138.3717	138.4499	138.5907	138.4739	138.5894	138.4074	138.5930	**126.5**
C4	136.4144	138.2433	139.3969	138.7507	139.7115	138.7122	139.1941	138.6705	138.9713	138.7907	139.4093	136.5839	137.7827	137.6013	138.2625	139.3312	138.3290	139.1229	138.3033	138.9529	138.2689	139.3387	**132.3**
C5	133.8318	135.9239	136.6399	136.7650	137.6410	136.7145	136.9432	136.6606	136.8551	136.8160	137.0910	134.1514	136.0805	136.0774	136.9009	137.6286	136.9025	137.1499	136.8574	137.0834	136.9349	137.2985	**133.1**
C6	136.8386	139.3699	140.2458	140.6500	142.1291	140.5790	142.1376	140.5038	141.9346	140.7201	142.5403	137.1181	139.6242	140.9454	140.7304	143.0106	140.6814	143.0701	140.6158	142.9272	140.7830	143.4117	**133.7**
C7	203.6635	208.6220	211.5586	211.1578	213.3582	210.9979	218.5340	210.8375	217.5569	211.3150	219.2808	208.4725	212.7074	213.9044	215.1062	215.5457	214.9815	219.9970	214.8369	218.9270	215.2494	220.6289	**196.3**
C8	65.4420	66.4492	67.0884	66.9217	67.9217	66.8970	68.4051	66.8693	68.2174	66.9486	69.0792	59.9694	61.8514	62.4360	62.8961	63.5265	62.8195	64.3842	62.7613	64.1209	62.9639	64.6462	**60.8**
C9	22.7610	23.0953	23.0090	23.3779	23.4790	23.3652	23.4036	23.3486	23.3712	23.3930	23.5468	19.4405	19.8391	20.0594	20.0535	20.4847	20.0376	20.5861	20.0258	20.5464	20.0673	20.9151	**15.9**
C3``	134.6231	135.9246	136.7792	136.4861	137.8796	136.4587	137.6021	136.4280	137.5727	136.5154	137.6781	134.6242	135.9553	136.7422	136.5061	137.8983	136.4738	137.5121	136.4428	137.4863	136.5346	137.5862	**123.3**
C8`	36.4443	37.1820	37.4733	37.5924	37.9722	37.5676	38.1918	37.5406	38.1369	37.6206	38.6194	31.8218	32.1478	32.4430	32.2552	32.7283	32.2585	32.6814	32.2498	32.7025	32.2575	32.7467	**31.7**
H(2-4)	8.4713	8.5102	8.4981	8.5251	8.5070	8.5253	8.5449	8.5248	8.5362	8.5249	8.5576	8.5046	8.4587	8.5218	8.4403	8.5451	8.4419	8.5173	8.4432	8.5212	8.4374	8.5271	**8.32**
H5	7.6374	7.8634	7.9165	7.9591	8.0211	7.9537	7.9889	7.9477	7.9795	7.9641	8.0111	7.6550	7.8629	7.8765	7.9421	8.0165	7.9397	7.9913	7.9346	7.9841	7.9457	8.0127	**7.84**
H6	8.2199	8.4687	8.4986	8.5922	8.6668	8.5856	8.6977	8.5784	8.6846	8.5983	8.7323	8.0329	8.2532	8.3696	8.3370	8.5578	8.3328	8.5427	8.3268	8.5350	8.3409	8.5858	**8.05**
H8	4.4014	4.5208	4.5509	4.5959	4.6600	4.5915	4.6933	4.5867	4.6885	4.6000	4.7149	4.5307	4.6990	4.7600	4.7737	4.9013	4.7701	4.9229	4.7649	4.9081	4.7779	4.9579	**5.2**
H(9A-9C)	1.3345	1.3568	1.2712	1.3642	1.2667	1.3646	1.2860	1.3645	1.2765	1.3636	1.3036	1.4213	1.4491	1.4579	1.4696	1.4816	1.4690	1.4915	1.4674	1.4886	1.4700	1.5119	**1.59**
H(8`A-8`C)	2.5563	2.4802	2.4700	2.4616	2.4570	2.4625	2.4407	2.4630	2.4429	2.4608	2.4215	2.9791	2.8112	2.7759	2.7172	2.7034	2.7229	2.5966	2.7267	2.6233	2.7122	2.5657	**2.8**

[a] methyl protons shifts are averaged
[b] according to [2]

Table S18. RMS values of proton chemical shifts of *S*-cathinone and its selected fluorinated synthetic derivatives calculated with HF and selected functionals combined with 6-311++G** basis set. The most accurate methods and their smallest RMS values are in boald and marked in green, the worst methods with their highests RMS values are in italic font and marked in orange

Method	R											S									
	Cathinone																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP												0.4383	0.4179	0.4324	0.4204	0.4588	0.4200	0.4600	0.4195	0.4544	0.4208	0.4752
B3P86												0.4574	0.4520	0.4717	0.4602	0.5077	0.4602	0.5074	0.4593	0.5050	0.4609	0.5241
B3PW91												0.4562	0.4471	0.4679	0.4546	0.5010	0.4543	0.5023	0.4539	0.4973	0.4550	0.5170
B98												0.4505	0.4373	0.4566	0.4434	0.4880	0.4430	0.4909	0.4426	0.4866	0.4440	0.5051
B971												0.4517	0.4392	0.4574	0.4455	0.4891	0.4449	0.4914	0.4444	0.4871	0.4462	0.5056
B972												0.4589	0.4452	0.4654	0.4523	0.4942	0.4518	0.4955	0.4513	0.4910	0.4526	0.5098
BHandH												0.5867	0.5953	0.6234	0.6085	0.5630	0.6080	0.6626	0.6071	0.6590	0.6096	0.6784
BHandHLYP												0.5607	0.5522	0.5685	0.5584	0.5984	0.5580	0.6015	0.5576	0.5967	0.5587	0.6159
BLYP												0.3495	0.3024	0.3097	0.2956	0.3273	0.3165	0.4494	0.2969	0.3238	0.3208	0.4767
BMK												0.6797	0.7212	0.7487	0.7465	0.8051	0.7427	0.8142	0.7389	0.8084	0.7436	0.8299
BP86												0.3547	0.3278	0.3383	0.3312	0.3665	0.3312	0.3658	0.3310	0.3608	0.3310	0.3897
CAM-B3LYP												0.5050	0.4952	0.5115	0.5007	0.5440	0.5003	0.5435	0.5000	0.5395	0.5010	0.5578
HF												0.6753	0.6528	0.6685	0.6509	0.6870	0.6510	0.6894	0.6511	0.6865	0.6507	0.7026
LC-BLYP												0.6049	0.6104	0.6304	0.6229	0.6711	0.6215	0.6674	0.6210	0.6631	0.6236	0.6835
M06												0.4679	0.4588	0.4822	0.4637	0.5135	0.4632	0.5169	0.4631	0.5121	0.4644	0.5292
M06-2X												0.8423	0.8958	0.9352	0.9267	0.9914	0.9239	0.9990	0.9209	0.9919	0.9295	*1.0144*
mpW1LYP												0.4603	0.4400	0.4555	0.4439	0.4812	0.4437	0.4833	0.4433	0.4796	0.4441	0.4957
mpW1PW91												0.4859	0.4807	0.5018	0.4887	0.5369	0.4883	0.5379	0.4879	0.5329	0.4893	0.5528
O3LYP												0.4179	0.3950	0.4109	0.3779	0.4170	0.3781	0.4116	0.3780	0.4031	**0.3777**	0.4227
OLYP												0.3607	0.3091	0.3221	0.3000	0.3326	0.2999	0.3320	**0.2998**	0.3271	0.3000	0.3430
OPBE												0.3718	0.3398	0.3619	0.3409	0.3832	0.3404	0.3795	**0.3398**	0.3721	0.3411	0.3919
OPW91												0.3727	0.3404	0.3618	0.3409	0.3831	0.3403	0.3790	**0.3396**	0.3716	0.3410	0.3913
PBE												0.3665	0.3461	0.3612	0.3493	0.3936	0.3490	0.3930	0.3489	0.3885	0.3499	0.4074
PBE0												0.4850	0.4809	0.5005	0.4891	0.5354	0.4885	0.5385	0.4878	0.5318	0.4895	0.5517
TPSS												0.3927	0.3440	0.3514	0.3373	0.3689	0.3375	0.3655	0.3379	0.3872	0.3373	0.3765
VSXC												0.4090	0.3926	0.4138	0.3998	0.4392	0.3992	0.4541	0.3986	0.4488	0.4004	0.4753
wB97												0.5606	0.5592	0.5780	0.5664	0.6139	0.5657	0.6118	0.5650	0.6068	0.5672	0.6263
wB97X												0.5409	0.5384	0.5550	0.5459	0.5912	0.5453	0.5904	0.5447	0.5839	0.5465	0.6038
X3LYP												0.4470	0.4272	0.4434	0.4319	0.4705	0.4316	0.4722	0.4310	0.4683	0.4322	0.4857
Method	4-trifluoromethylmethcathinone																				
B3LYP	0.3514	0.3288	0.3366	0.3053	0.3146	0.3065	0.3204	0.3076	0.3167	0.3040	0.3292	0.3205	0.2251	0.2192	0.1978	0.2066	0.1980	0.2131	0.1992	0.2112	0.1969	0.2205
B3P86	0.3526	0.3472	0.3581	0.3299	0.3583	0.3298	0.3620	0.3300	0.3634	0.3299	0.3677	0.3041	0.2308	0.2369	0.2131	0.2461	0.2137	0.2497	0.2143	0.2455	0.2126	0.2606
B3PW91	0.3594	0.3419	0.3647	0.3327	0.3617	0.3332	0.3513	0.3338	0.3489	0.3321	0.3603	0.3086	0.2357	0.2392	0.2187	0.2433	0.2188	0.2528	0.2194	0.2494	0.2183	0.2623
B98	0.3632	0.3479	0.3579	0.3277	0.3364	0.3283	0.3558	0.3290	0.3573	0.3272	0.3596	0.3195	0.2353	0.2338	0.2136	0.2331	0.2138	0.2402	0.2146	0.2370	0.2130	0.2487
B971	0.3643	0.3489	0.3584	0.3295	0.3545	0.3302	0.3576	0.3309	0.3419	0.3289	0.3618	0.3172	0.2353	0.2336	0.2132	0.2336	0.2136	0.2406	0.2147	0.2371	0.2125	0.2488
B972	0.3705	0.3478	0.3629	0.3291	0.3502	0.3298	0.3511	0.3306	0.3497	0.3285	0.3581	0.3191	0.2430	0.2448	0.2246	0.2418	0.2246	0.2508	0.2252	0.2484	0.2242	0.2585
BHandH	0.4941	0.4962	0.5158	0.4945	0.5274	0.4950	0.5368	0.4953	0.5287	0.4942	0.5431	0.4172	0.3718	0.3973	0.3620	0.3391	0.3626	0.4081	0.3629	0.4121	0.3617	0.4194
BHandHLYP	0.4922	0.4752	0.4831	0.4519	0.4689	0.4530	0.4720	0.4540	0.4730	0.4507	0.4747	0.4292	0.3572	0.3593	0.3387	0.3566	0.3391	0.3551	0.3400	0.3514	0.3379	0.3639
BLYP	0.2761	0.2296	0.2254	0.2024	0.2207	0.1777	0.2180	0.2017	0.2128	**0.1742**	0.2434	0.2848	0.1701	0.1432	0.1318	0.3160	0.1078	0.1608	0.1318	0.1155	**0.1026**	0.1840
BMK	0.5398	0.5665	0.5863	0.5676	0.6206	0.5672	0.6160	0.5668	0.6196	0.5648	0.6263	0.4731	0.4594	0.4910	0.4568	0.5070	0.4553	0.5237	0.4538	0.5142	0.4540	0.5220
BP86	0.2529	0.2216	0.2303	0.2065	0.2312	0.2068	0.2299	0.2072	0.2286	**0.2064**	0.2383	0.2501	0.1380	0.1292	0.1041	0.1116	0.1048	0.1312	0.1057	0.1277	**0.1037**	0.1406
CAM-B3LYP	0.4191	0.4041	0.4123	0.3813	0.4023	0.3820	0.3863	0.3827	0.3859	0.3806	0.4083	0.3698	0.2911	0.2898	0.2687	0.2906	0.2697	0.2900	0.2707	0.2872	0.2679	0.2992
HF	0.6695	0.6232	0.6335	0.5906	0.5931	0.5922	0.5863	0.5939	0.5906	0.5890	0.5901	0.5938	0.5126	0.5063	0.4859	0.4880	0.4871	0.4898	0.4884	0.4910	0.4867	0.4933
LC-BLYP	0.5141	0.5106	0.5253	0.4916	0.5160	0.4914	0.5171	0.4915	0.5253	0.4917	0.5228	0.4505	0.3949	0.4031	0.3805	0.4071	0.3809	0.4067	0.3821	0.4033	0.3798	0.4186
M06	0.3731	0.3601	0.3799	0.3441	0.3767	0.3446	0.3801	0.3452	0.3779	0.3437	0.3848	0.3384	0.2483	0.2569	0.2324	0.2626	0.2330	0.2748	0.2335	0.2719	0.2320	0.2885
M06-2X	0.6676	0.7157	0.7428	0.7221	0.7799	0.7222	0.7799	0.7094	0.7786	0.7220	*0.7895*	0.6082	0.6164	0.6363	0.6122	0.6754	0.6100	0.6671	0.6078	0.6585	0.6144	0.6866
mpW1LYP	0.3744	0.3526	0.3579	0.3277	0.3325	0.3286	0.3413	0.3297	0.3515	0.3268	0.3489	0.3399	0.2453	0.2389	0.2175	0.2276	0.2178	0.2308	0.2191	0.2286	0.2165	0.2380
mpW1PW91	0.3862	0.3831	0.3947	0.3637	0.3925	0.3640	0.3830	0.3644	0.3816	0.3633	0.3987	0.3271	0.2620	0.2682	0.2468	0.2767	0.2473	0.2819	0.2479	0.2780	0.2465	0.2922
O3LYP	0.3383	0.3067	0.3234	0.3049	0.3215	0.3058	0.3165	0.3076	0.3174	0.3039	0.3184	0.3015	0.2190	0.2097	0.2000	0.2136	0.2013	0.2125	0.2026	0.2117	0.1991	0.2153
OLYP	0.3119	0.2982	0.2973	0.2822	0.3047	0.2831	0.2783	0.2841	0.2855	0.2819	**0.2766**	0.2920	0.2311	0.2060	0.1993	0.1976	0.2014	0.1855	0.2035	0.1885	0.1975	**0.1829**
OPBE	0.3160	0.3039	0.3167	0.2999	0.3243	0.3003	0.3091	0.3010	0.3143	0.2999	0.3105	0.2745	0.2298	0.2258	0.2093	0.2331	0.2100	0.2219	0.2112	0.2280	0.2091	0.2257
OPW91	0.3156	0.3034	0.3161	0.2985	0.3234	0.2994	0.3082	0.3002	0.3133	0.2987	0.3092	0.2750	0.2294	0.2227	0.2034	0.2316	0.2046	0.2204	0.2060	0.2239	0.2033	0.2239
PBE	0.2535	0.2266	0.2370	0.2159	0.2400	0.2164	0.2408	0.2168	0.2435	**0.2153**	0.2493	0.2443	0.1353	0.1280	0.1041	0.1219	0.1050	0.1370	0.1059	0.1327	**0.1032**	0.1501
PBE0	0.3875	0.3834	0.3952	0.3658	0.3936	0.3660	0.3966	0.3662	0.3979	0.3657	0.4003	0.3252	0.2594	0.2646	0.2431	0.2746	0.2437	0.2782	0.2443	0.2736	0.2427	0.2886
TPSS	0.3151	0.2697	0.2672	0.2473	0.2550	0.2489	0.2562	0.2501	0.3688	0.2458	**0.2598**	0.3002	0.1861	0.1655	0.1451	**0.1269**	0.1468	0.1397	0.1484	0.1378	0.1434	0.1458
VSXC	0.3462	0.3186	0.3283	0.3050	0.3262	0.3058	0.3294	0.3066	0.3296	0.3043	0.3374	0.3035	0.2148	0.2154	0.1593	0.1807	0.1898	0.2163	0.1909	0.2114	0.1583	0.2057
wB97	0.4839	0.4724	0.4830	0.4500	0.4714	0.4503	0.4728	0.4506	0.4810	0.4500	0.4783	0.4084	0.3573	0.3576	0.3388	0.3585	*0.9023*	0.3654	0.3404	0.3632	0.3384	0.3710
wB97X	0.4582	0.4468	0.4571	0.4251	0.4468	0.4253	0.4505	0.4257	0.4574	0.4250	0.4549	0.3909	0.3315	0.3318	0.3125	0.3318	0.3134	0.3377	0.3143	0.3351	0.3119	0.3454
X3LYP	0.3589	0.3384	0.3441	0.3142	0.3206	0.3151	0.3376	0.3161	0.3255	0.3134	0.3406	0.3263	0.2315	0.2254	0.2038	0.2156	0.2042	0.2198	0.2054	0.2174	0.2028	0.2277

Table S18. Cont. I

Method	R	S
	3-fluoromethcathinone	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	0.3181	0.3261	0.3894	0.3472	0.4058	0.3456	0.4350	0.3440	0.4241	0.3488	0.4516	0.3128	0.2490	0.2968	0.2506	0.3214	0.2495	0.3238	0.2485	0.3178	0.2514	0.3430
B3P86	0.3330	0.3562	0.4173	0.3796	0.4423	0.3783	0.4697	0.3763	0.4668	0.3814	0.4901	0.3017	0.2679	0.3234	0.2793	0.3614	0.2790	0.3647	0.2774	0.3645	0.2804	0.3861
B3PW91	0.3303	0.3473	0.3843	0.3723	0.4413	0.3707	0.4604	0.3692	0.4421	0.3738	0.4805	0.2942	0.2532	0.3113	0.2691	0.3492	0.2683	0.3503	0.2672	0.3480	0.2699	0.3701
B98	0.3295	0.3414	0.4037	0.3651	0.4271	0.3636	0.4561	0.3621	0.4479	0.3668	0.4722	0.3039	0.2509	0.3071	0.2631	0.3398	0.2620	0.3442	0.2609	0.3400	0.2643	0.3624
B971	0.3299	0.3430	0.4028	0.3664	0.4273	0.3647	0.4549	0.3631	0.4476	0.3681	0.4715	0.3009	0.2510	0.3060	0.2636	0.3395	0.2623	0.3447	0.2611	0.3405	0.2650	0.3631
B972	0.3322	0.3469	0.3828	0.3707	0.4301	0.3689	0.4508	0.3672	0.4340	0.3722	0.4485	0.2965	0.2476	0.3040	0.2638	0.3376	0.2627	0.3374	0.2615	0.3298	0.2644	0.3548
BHandH	0.4903	0.5200	0.5689	0.5407	0.6063	0.5396	0.6315	0.5382	0.6240	0.5422	0.6469	0.4329	0.4315	0.4744	0.4345	0.3835	0.4342	0.5199	0.4335	0.5179	0.4354	0.5393
BHandHLYP	0.4723	0.4821	0.5389	0.4977	0.5524	0.4966	0.5794	0.4954	0.5763	0.4987	0.5941	0.4285	0.3922	0.4360	0.3940	0.4589	0.3934	0.4663	0.3927	0.4631	0.3946	0.4826
BLYP	0.2068	**0.1969**	0.2296	0.2204	0.2806	0.2371	0.4214	0.2173	0.2954	0.2453	0.4500	0.2608	0.1593	0.1816	**0.1371**	0.2100	0.1785	0.3617	0.1378	0.2024	0.1875	0.3931
BMK	0.5392	0.6020	0.6597	0.6293	0.7003	0.6254	0.7242	0.6216	0.7250	0.6280	0.7428	0.4721	0.4937	0.5543	0.5289	0.6135	0.5247	0.6214	0.5205	0.6184	0.5261	0.6410
BP86	**0.2109**	0.2157	0.2481	0.2448	0.3038	0.2430	0.3319	0.2413	0.3183	0.2463	0.3593	0.2315	**0.1523**	0.1956	0.1632	0.2373	0.1626	0.2389	0.1618	0.2334	0.1635	0.2727
CAM-B3LYP	0.4032	0.4162	0.4737	0.4341	0.4925	0.4327	0.5174	0.4314	0.5091	0.4354	0.5337	0.3743	0.3307	0.3817	0.3370	0.4097	0.3364	0.4107	0.3358	0.4083	0.3375	0.4266
HF	0.6295	0.6168	0.6426	0.6133	0.6613	0.6125	0.6570	0.6117	0.6523	0.6141	0.6674	0.5664	0.5088	0.5478	0.5072	0.5500	0.5074	0.5490	0.5074	0.5389	0.5067	0.5613
LC-BLYP	0.5136	0.5405	0.5925	0.5585	0.6166	0.5570	0.3945	0.5561	0.6482	0.5596	0.6600	0.4667	0.4459	0.5036	0.4591	0.5340	0.4580	0.5349	0.4576	0.5292	0.4594	0.5514
M06	0.3455	0.3655	0.4241	0.3884	0.4625	0.3868	0.4867	0.3853	0.4850	0.3903	0.5006	0.2946	0.2358	0.2904	0.2497	0.3308	0.2482	0.3408	0.2471	0.3337	0.2514	0.3599
M06-2X	0.6691	0.7383	0.8021	0.7770	0.8502	0.7740	0.8782	0.7707	0.8753	0.7800	*0.8945*	0.6055	0.6522	0.7214	0.6850	0.7691	0.6826	0.7783	0.6798	0.7725	0.6871	*0.7947*
mpW1LYP	0.3485	0.3520	0.4159	0.3731	0.4298	0.3717	0.4590	0.3703	0.4528	0.3744	0.4768	0.3373	0.2764	0.3243	0.2792	0.3467	0.2785	0.3501	0.2778	0.3463	0.2798	0.3659
mpW1PW91	0.3623	0.3845	0.4485	0.4090	0.4708	0.4075	0.4974	0.4060	0.4855	0.4106	0.5139	0.3180	0.2868	0.3444	0.3022	0.3825	0.3013	0.3860	0.3004	0.3826	0.3030	0.4040
O3LYP	0.2702	0.2776	0.3135	0.3030	0.3583	0.3022	0.3883	0.3021	0.3697	0.3046	0.3960	0.2657	0.1946	0.2166	0.1935	0.2582	0.1921	0.2697	0.1915	0.2586	0.1951	0.2881
OLYP	**0.2019**	0.2075	0.2529	0.2428	0.2892	0.2407	0.3012	0.2387	0.2983	0.2447	0.3169	0.2189	**0.1239**	0.1459	0.1287	0.1962	0.1269	0.2040	0.1251	0.1938	0.1303	0.2228
OPBE	**0.2138**	0.2355	0.2827	0.2713	0.3253	0.2692	0.3340	0.2671	0.3240	0.2731	0.3507	0.1744	**0.1177**	0.1620	0.1519	0.2285	0.1494	0.2375	0.1467	0.2273	0.1539	0.2588
OPW91	**0.2142**	0.2357	0.2831	0.2719	0.3245	0.2698	0.3340	0.2676	0.3245	0.2738	0.3505	0.1775	**0.1190**	0.1631	0.1526	0.2286	0.1500	0.2376	0.1472	0.2275	0.1546	0.2588
PBE	**0.2189**	0.2304	0.2694	0.2596	0.3245	0.2576	0.3503	0.2558	0.3385	0.2617	0.3708	0.2329	**0.1665**	0.2200	0.1772	0.2639	0.1761	0.2642	0.1754	0.2603	0.1787	0.2861
PBE0	0.3635	0.3865	0.4452	0.4083	0.4684	0.4066	0.4964	0.4050	0.4891	0.4097	0.5129	0.3164	0.2864	0.3420	0.2999	0.3787	0.2988	0.3857	0.2977	0.3807	0.3006	0.4022
TPSS	0.2495	**0.2335**	0.2843	0.2501	0.3163	0.2486	0.3356	0.2474	0.2681	0.2516	0.3562	0.2585	0.1725	0.2003	0.1556	0.2309	0.1550	0.2397	**0.1549**	0.2641	0.1566	0.2593
VSXC	0.3181	0.3193	0.3577	0.3398	0.4000	0.3382	0.4179	0.3367	0.4163	0.3414	0.4304	0.2762	0.2315	0.2541	0.2412	0.3064	0.2404	0.3244	0.2397	0.3160	0.2418	0.3414
wB97	0.4620	0.4834	0.5302	0.4978	0.5567	0.4969	0.5809	0.4960	0.5806	0.4987	0.5943	0.4087	0.3869	0.4362	0.3970	0.4659	0.3966	0.4642	0.3960	0.4550	0.3969	0.4795
wB97X	0.4360	0.4564	0.5051	0.4703	0.5298	0.4694	0.5558	0.4685	0.5563	0.4713	0.5707	0.3868	0.3610	0.4103	0.3723	0.4429	0.3717	0.4445	0.3710	0.4384	0.3727	0.4588
X3LYP	0.3317	0.3362	0.4007	0.3588	0.4167	0.3573	0.4461	0.3556	0.4395	0.3602	0.4650	0.3212	0.2600	0.3096	0.2647	0.3348	0.2639	0.3380	0.2628	0.3340	0.2654	0.3552
Method	**4-fluoro-α-pyrrolidinopentiophenone**																					
B3LYP	0.2408	0.2401	0.2657	0.2490	0.2886	0.2484	0.2912	0.2479	0.2887	0.2496	0.3003	0.2684	0.2781	0.3043	0.2890	0.3280	0.2883	0.3304	0.2877	0.3280	0.2897	0.3379
B3P86	0.2433	0.2468	0.2763	0.2612	0.3017	0.2600	0.3082	0.2591	0.3084	0.2621	0.3196	0.2684	0.2819	0.3113	0.2986	0.3370	0.2974	0.3442	0.2963	0.3449	0.2997	0.3547
B3PW91	0.2504	0.2545	0.2826	0.2670	0.3049	0.2660	0.3115	0.2651	0.3120	0.2679	0.3224	0.2761	0.2891	0.3175	0.3037	0.3420	0.3026	0.3471	0.3016	0.3479	0.3047	0.3569
B98	0.2497	0.2517	0.2764	0.2628	0.3039	0.2621	0.3052	0.2613	0.3046	0.2635	0.3146	0.2759	0.2867	0.3117	0.2996	0.3401	0.2987	0.3413	0.2978	0.3409	0.3005	0.3496
B971	0.2492	0.2518	0.2763	0.2630	0.3020	0.2622	0.3053	0.2614	0.3056	0.2637	0.3155	0.2756	0.2866	0.3115	0.2999	0.3376	0.2990	0.3411	0.2981	0.3417	0.3007	0.3505
B972	0.2553	0.2584	0.2824	0.2682	0.3074	0.2674	0.3101	0.2668	0.3097	0.2689	0.3202	0.2822	0.2931	0.3176	0.3051	0.3433	0.3042	0.3461	0.3034	0.3460	0.3059	0.3550
BHandH	0.3561	0.3658	0.3959	0.3779	0.4192	0.3768	0.4318	0.3758	0.4280	0.3788	0.4391	0.3701	0.3883	0.4201	0.4038	0.4068	0.4025	0.4592	0.4014	0.4553	0.4050	0.4662
BHandHLYP	0.3782	0.3780	0.4010	0.3828	0.4150	0.3824	0.4134	0.3820	0.4150	0.3832	0.4208	0.3959	0.4023	0.4263	0.4095	0.4423	0.4090	0.4410	0.4085	0.4427	0.4100	0.4478
BLYP	0.1962	**0.1827**	0.1967	0.1920	0.2242	0.1875	0.2792	0.1897	0.2203	0.1903	0.2939	**0.2286**	0.2323	0.2474	0.2434	0.2743	0.2397	0.3213	0.2413	0.2708	0.2422	0.3337
BMK	0.3827	0.4168	0.4525	0.4345	0.4845	0.4333	0.4919	0.4322	0.4889	0.4356	0.5028	0.4010	0.4386	0.4743	0.4578	0.5070	0.4565	0.5149	0.4553	0.5120	0.4590	0.5256
BP86	0.1880	**0.1723**	0.1929	0.1853	0.2283	0.1842	0.2317	0.1832	0.2307	0.1863	0.2431	**0.2200**	0.2211	0.2420	0.2364	0.2755	0.2352	0.2792	0.2341	0.2788	0.2375	0.2887
CAM-B3LYP	0.2998	0.3021	0.3280	0.3095	0.3431	0.3090	0.3464	0.3086	0.3455	0.3100	0.3561	0.3218	0.3317	0.3586	0.3285	0.3747	0.3409	0.3784	0.3403	0.3775	0.3421	0.3561
HF	0.5979	0.5827	0.5948	0.5725	0.5916	0.5732	0.5848	0.5740	0.5871	0.5718	0.5900	0.6105	0.5999	0.6123	0.5907	0.4987	0.5913	0.6047	0.5921	0.6069	0.5900	0.6096
LC-BLYP	0.3836	0.3909	0.4225	0.3981	0.4374	0.3978	0.4367	0.3972	0.4346	0.3986	0.4432	0.3998	0.4129	0.4458	0.4226	0.4622	0.4221	0.4617	0.4213	0.4596	0.4232	0.4680
M06	0.2768	0.2893	0.3070	0.2934	0.3220	0.2933	0.3197	0.2929	0.3179	0.2933	0.3260	0.3065	0.3228	0.3421	0.3293	0.3572	0.3289	0.3566	0.3285	0.3548	0.3293	0.3619
M06-2X	0.4726	0.5057	0.5477	0.5264	0.5768	0.5248	0.5924	0.5236	0.5891	0.5277	*0.6022*	0.4899	0.5255	0.5766	0.5474	0.5996	0.5457	0.6133	0.5445	0.6101	0.5488	*0.6228*
mpW1LYP	0.2587	0.2577	0.2801	0.2658	0.3045	0.2652	0.3062	0.2647	0.3041	0.2663	0.3155	0.2848	0.2934	0.3164	0.3035	0.3420	0.3028	0.3436	0.3022	0.3415	0.3042	0.3515
mpW1PW91	0.2710	0.2774	0.3068	0.2897	0.3297	0.2888	0.3345	0.2879	0.3325	0.2904	0.3449	0.2945	0.3091	0.3388	0.3236	0.3622	0.3226	0.3677	0.3216	0.3657	0.3245	0.3774
O3LYP	0.2282	0.2352	0.2557	0.2444	0.2787	0.2437	0.2758	0.2432	0.2734	0.2451	0.2838	0.2597	0.2742	0.2938	0.2838	0.3167	0.2831	0.3150	0.2826	0.3121	0.2845	0.3214
OLYP	0.2173	0.2183	0.2290	0.2236	0.2546	0.2227	0.2463	0.2218	0.2457	0.2247	0.2529	0.2511	0.2603	0.2718	0.2665	0.2961	0.2657	0.2895	0.2649	0.2884	0.2675	0.2529
OPBE	0.2169	0.2257	0.2432	0.2353	0.2729	0.2342	0.2672	0.2335	0.2657	0.2366	0.2756	0.2489	0.2645	0.2823	0.2754	0.3106	0.2744	0.3064	0.2736	0.3046	0.2767	0.3132
OPW91	0.2168	0.2255	0.2429	0.2347	0.2723	0.2338	0.2667	0.2332	0.2651	0.2360	0.2749	0.2489	0.2644	0.2821	0.2749	0.3102	0.2741	0.3060	0.2734	0.3041	0.2762	0.3126
PBE	0.1829	**0.1738**	0.1965	0.1881	0.2328	0.1871	0.2376	0.1861	0.2357	0.1890	0.2489	**0.2167**	0.2218	0.2448	0.2378	0.2785	0.2368	0.2834	0.2357	0.2821	0.2388	0.2932
PBE0	0.2690	0.2753	0.3050	0.2881	0.3288	0.2873	0.3334	0.2865	0.3313	0.2888	0.3444	0.2926	0.3073	0.3371	0.3223	0.3614	0.3214	0.3668	0.3205	0.3647	0.3232	0.3771
TPSS	0.2236	**0.1990**	0.2121	0.2033	0.2431	0.2027	0.2456	0.2019	0.2254	0.2039	0.2522	0.2467	**0.2385**	0.2530	0.2473	0.2857	0.2465	0.2886	0.2455	0.2586	0.2481	0.2522
VSXC	0.2890	0.2710	0.2717	0.2661	0.2747	0.2663	0.2774	0.2665	0.2743	0.2660	0.2784	0.3261	0.3108	0.3123	0.3063	0.3170	0.3065	0.3185	0.3067	0.3154	0.3062	0.3192
wB97	0.3516	0.3586	0.3841	0.3647	0.3994	0.3644	0.3988	0.3640	0.3969	0.3651	0.4070	0.3713	0.3837	0.4104	0.3922	0.4271	0.3917	0.4267	0.3911	0.4248	0.3927	0.4347
wB97X	0.3275	0.3357	0.3621	0.3428	0.3777	0.3423	0.3815	0.3419	0.3803	0.3433	0.3904	0.3486	0.3624	0.3899	0.3716	0.4061	0.3710	0.4105	0.3705	0.4093	0.3721	0.4191
X3LYP	0.2452	0.2444	0.2675	0.2536	0.2938	0.2529	0.2960	0.2524	0.2938	0.2542	0.3051	0.2723	0.2816	0.3052	0.2929	0.3326	0.2921	0.3345	0.2914	0.3325	0.2937	0.3422

Table S18. Cont. II

Method	R	S
	4-fluoro-α-pyrrolidinohexiophenone [5]	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	0.4408	0.4071	0.4192	0.3942	0.4123	0.3953	0.3999	0.3965	0.4022	0.3932	0.4091	0.4702	0.4546	0.4700	0.4471	0.4689	0.4480	0.4563	0.4488	0.4649	0.4463	0.4673
B3P86	0.4504	0.4238	0.4344	0.4112	0.4318	0.4113	0.4273	0.4124	0.4266	0.4104	0.4287	0.4759	0.4676	0.4810	0.4616	0.4847	0.4614	0.4830	0.4622	0.4821	0.4611	0.4846
B3PW91	0.4571	0.4308	0.4426	0.4185	0.4311	0.4190	0.4328	0.4197	0.4347	0.4178	0.4369	0.4840	0.4746	0.4889	0.4682	0.4923	0.4685	0.4874	0.4689	0.4889	0.4678	0.4916
B98	0.4523	0.4240	0.4335	0.4096	0.4287	0.4105	0.4207	0.4114	0.4224	0.4086	0.4255	0.4806	0.4690	0.4813	0.4603	0.4822	0.4609	0.4762	0.4615	0.4776	0.4595	0.4808
B971	0.4534	0.4261	0.4353	0.4112	0.4305	0.4122	0.4231	0.4132	0.4246	0.4100	0.4276	0.4817	0.4710	0.4829	0.4618	0.4839	0.4625	0.4785	0.4632	0.4796	0.4609	0.4827
B972	0.4612	0.4333	0.4445	0.4175	0.4326	0.4185	0.4257	0.4196	0.4270	0.4166	0.4290	0.4898	0.4775	0.4908	0.4666	0.4820	0.4674	0.4777	0.4682	0.4782	0.4658	0.4806
BHandH	0.5415	0.5230	0.5398	0.5161	0.5395	0.5160	0.5355	0.5164	0.5370	0.5156	0.5353	0.5584	0.5554	0.5757	0.5545	0.5781	0.5541	0.5801	0.5541	0.5809	0.5544	0.5801
BHandHLYP	0.5609	0.5373	0.5481	0.5218	0.5433	0.5227	0.5348	0.5237	0.5373	0.5211	0.5374	0.5837	0.5732	0.5860	0.5620	0.5860	0.5627	0.5796	0.5634	0.5815	0.5614	0.5821
BLYP	0.3715	0.3271	0.3333	0.3132	0.3201	0.2830	**0.2421**	0.3132	0.3139	0.2769	0.2488	0.4057	0.3845	0.3967	0.3780	0.3886	0.3533	**0.3288**	0.3778	0.3835	0.3486	0.3337
BMK	0.5331	0.5264	0.5498	0.5174	0.5536	0.5195	0.5515	0.5216	0.5511	0.5197	0.5616	0.5617	0.5649	0.5895	0.5605	0.5976	0.5623	0.5968	0.5640	0.5961	0.5628	0.6057
BP86	0.3770	0.3363	0.3483	0.3214	0.3431	0.3218	0.3350	0.3224	0.3368	**0.3212**	0.3316	0.4075	0.3914	0.4064	**0.3854**	0.4097	0.3855	0.4051	0.3857	0.4061	0.3854	0.4026
CAM-B3LYP	0.4865	0.4615	0.4724	0.4464	0.4660	0.4473	0.4596	0.4482	0.4617	0.4457	0.4627	0.5128	0.5030	0.5166	0.4931	0.5155	0.4937	0.5110	0.4943	0.5127	0.4926	0.5145
HF	*0.7648*	0.7334	0.7426	0.7135	0.7195	0.7151	0.7092	0.7166	0.7108	0.7120	0.7101	*0.7839*	0.7601	0.7719	0.7422	0.7484	0.7437	0.7400	0.7452	0.7406	0.7407	*0.7410*
LC-BLYP	0.5467	0.5292	0.5424	0.5151	0.5384	0.5163	0.5327	0.5167	0.5351	0.5145	0.5332	0.5691	0.5635	0.5796	0.5540	0.5804	0.5549	0.5756	0.5550	0.5781	0.5537	0.5766
M06	0.4966	0.4801	0.4849	0.4694	0.4702	0.4702	0.4621	0.4708	0.4622	0.4682	0.4557	0.5282	0.5214	0.5291	0.5147	0.5183	0.5152	0.5107	0.5155	0.5120	0.5139	0.5030
M06-2X	0.5802	0.5837	0.6052	0.5805	0.6153	0.5811	0.6141	0.5817	0.6156	0.5798	0.6141	0.4899	0.5255	0.5766	0.5474	0.5996	0.5457	0.6133	0.5445	0.6101	0.5488	0.6228
mpW1LYP	0.4555	0.4245	0.4336	0.4086	0.4275	0.4095	0.4193	0.4106	0.4211	0.4077	0.4261	0.4841	0.4701	0.4827	0.4598	0.4822	0.4605	0.4759	0.4613	0.4773	0.4591	0.4823
mpW1PW91	0.4748	0.4511	0.4641	0.4395	0.4620	0.4401	0.4561	0.4406	0.4578	0.4388	0.4589	0.5002	0.4925	0.5080	0.4866	0.5115	0.4869	0.5080	0.4872	0.5093	0.4862	0.5111
O3LYP	0.4125	0.3878	0.3950	0.3763	0.3895	0.3768	0.3828	0.3776	0.3839	0.3759	0.3856	0.4465	0.4362	0.4452	0.4281	0.4445	0.4285	0.4396	0.4291	0.4397	0.4278	0.4422
OLYP	0.3733	0.3503	0.3513	0.3370	0.3488	0.3377	0.3391	0.3384	0.3410	**0.3367**	0.3417	0.4106	0.4024	0.4070	0.3944	0.4083	0.3949	0.4011	0.3954	0.4019	**0.3943**	0.4034
OPBE	0.3956	0.3727	0.3836	0.3650	0.3863	0.3650	0.3743	0.3657	0.3761	0.3654	0.3769	0.4297	0.4216	0.4346	0.4177	0.4409	0.4177	0.4316	0.4181	0.4325	0.4182	0.4338
OPW91	0.3953	0.3722	0.3829	0.3637	0.3854	0.3643	0.3734	0.3651	0.3752	0.3643	0.3758	0.4294	0.4211	0.4340	0.4166	0.4401	0.4170	0.4309	0.4176	0.4317	0.4172	0.4330
PBE	0.3726	0.3369	0.3421	0.3244	0.3398	0.3252	0.3324	0.3256	0.3336	**0.3233**	0.3370	0.4047	0.3921	0.4008	0.3876	0.4067	0.3880	0.4023	0.3881	0.4031	**0.3870**	0.4067
PBE0	0.4744	0.4522	0.4642	0.4400	0.4633	0.4408	0.3313	0.4415	0.4584	0.4395	0.4591	0.5001	0.4936	0.5081	0.4872	0.5128	0.4876	0.5075	0.4880	0.5100	0.4869	0.5114
TPSS	0.4344	0.3931	0.3914	0.3726	0.3815	0.3737	0.3727	0.3745	0.5143	0.3713	0.3766	0.4561	0.4364	0.4394	0.4242	0.4371	0.4250	0.4325	0.4254	0.3854	0.4233	0.4357
VSXC	0.5075	0.4491	0.4348	0.4180	0.3970	0.4199	0.3919	0.4218	0.3977	0.4163	0.3800	0.5434	0.4893	0.4791	0.4610	0.4461	0.4627	0.4416	0.4644	0.4471	0.4594	0.4293
wB97	0.5358	0.5157	0.5263	0.5024	0.5201	0.5033	0.5140	0.5042	0.5159	0.5016	0.5152	0.5614	0.5529	0.5660	0.5444	0.5645	0.5450	0.5590	0.5455	0.5608	0.5439	0.5594
wB97X	0.5192	0.4989	0.5099	0.4839	0.5038	0.4847	0.4976	0.4856	0.5005	0.4830	0.5000	0.5452	0.5369	0.5506	0.5269	0.5494	0.5274	0.5452	0.5279	0.5468	0.5264	0.5469
X3LYP	0.4450	0.4140	0.4232	0.3982	0.4170	0.3992	0.4093	0.4004	0.4109	0.3973	0.4151	0.4739	0.4607	0.4733	0.4508	0.4730	0.4514	0.4674	0.4524	0.4686	0.4501	0.4727
Method	**4-fluoro-α-pyrrolidinohexiophenone [6]**																					
B3LYP	0.3839	0.3571	0.3713	0.3489	0.3687	0.3497	0.3599	0.3505	0.3602	0.3482	0.3739	0.4266	0.4245	0.4423	0.4227	0.4468	0.4232	0.4374	0.4237	0.4458	0.4222	0.4527
B3P86	0.3934	0.3757	0.3874	0.3689	0.3920	0.3687	0.3936	0.3694	0.3916	0.3685	0.3986	0.4312	0.4379	0.4528	0.4388	0.4647	0.4384	0.4688	0.4387	0.4669	0.4388	0.4735
B3PW91	0.3997	0.3817	0.3948	0.3751	0.3921	0.3753	0.3973	0.3757	0.3977	0.3748	0.4052	0.4392	0.4439	0.4597	0.4442	0.4707	0.4442	0.4713	0.4442	0.4714	0.4442	0.4786
B98	0.3956	0.3747	0.3858	0.3660	0.3872	0.3665	0.3847	0.3670	0.3851	0.3654	0.3930	0.4699	0.4674	0.4801	0.4620	0.4840	0.4625	0.4827	0.4629	0.4832	0.4614	0.4894
B971	0.3965	0.3766	0.3871	0.3674	0.3886	0.3679	0.3868	0.3686	0.3869	0.3666	0.3947	0.4378	0.4403	0.4539	0.4379	0.4622	0.4381	0.4622	0.4384	0.4620	0.4374	0.4692
B972	0.4037	0.3826	0.3948	0.3714	0.3856	0.3722	0.3847	0.3730	0.3845	0.3707	0.3904	0.4457	0.4456	0.4602	0.4404	0.4551	0.4409	0.4566	0.4415	0.4556	0.4399	0.4616
BHandH	0.4957	0.4870	0.5046	0.4860	0.5120	0.4857	0.5132	0.4857	0.5131	0.4860	0.5159	0.5209	0.5320	0.5541	0.5382	0.5544	0.5375	0.5726	0.5370	0.5718	0.5385	0.5751
BHandHLYP	0.5123	0.4975	0.5090	0.4877	0.5101	0.4882	0.5070	0.4888	0.5077	0.4872	0.5122	0.5446	0.5468	0.5605	0.5419	0.5674	0.5422	0.5664	0.5425	0.5666	0.5416	0.5712
BLYP	0.3122	0.2685	0.2761	0.2567	0.2642	0.2321	0.2303	0.2565	0.2617	**0.2274**	0.2418	0.3621	0.3529	0.3678	0.3510	0.3632	0.3334	0.3407	0.3507	0.3612	**0.3303**	0.3485
BMK	0.4941	0.4985	0.5271	0.4985	0.5375	0.4996	0.5416	0.5007	0.5400	0.5005	0.5545	0.5684	0.5803	0.6087	0.5816	0.6210	0.5828	0.6246	0.5840	0.6232	0.5837	0.6366
BP86	0.3173	0.2800	0.2906	**0.2693**	0.2909	0.2695	0.2894	0.2698	0.2894	0.2693	0.2920	0.3630	**0.3609**	0.3754	0.3614	0.3860	0.3613	0.3875	0.3612	0.3871	0.3617	0.3899
CAM-B3LYP	0.4363	0.4202	0.4322	0.4106	0.4320	0.4111	0.4308	0.4116	0.4314	0.4101	0.4370	0.4740	0.4777	0.4927	0.4741	0.4989	0.4743	0.4995	0.4745	0.4997	0.4739	0.5056
HF	*0.7212*	0.6972	0.7066	0.6819	0.6869	0.6832	0.6808	0.6845	0.6809	0.6807	0.6844	*0.7477*	0.7334	0.7458	0.7204	0.7257	0.7216	0.7216	0.7229	0.7207	0.7191	0.7253
LC-BLYP	0.5075	0.5001	0.5149	0.4917	0.5179	0.4924	0.5155	0.4925	0.5172	0.4915	0.5189	0.5389	0.5464	0.5647	0.5433	0.5730	0.5436	0.5716	0.5434	0.5736	0.5434	0.5754
M06	0.4399	0.4282	0.4340	0.4208	0.4213	0.4214	0.4178	0.4217	0.4171	0.4200	0.4152	0.4871	0.4884	0.4977	0.4861	0.4902	0.4862	0.4868	0.4862	0.4870	0.4856	0.4825
M06-2X	0.5589	0.5750	0.5999	0.5789	0.6175	0.5789	0.6195	0.5789	0.6210	0.5788	0.6205	0.5947	0.6199	0.6469	0.6272	0.6677	0.6270	0.6696	0.6268	0.6720	0.6274	0.6693
mpW1LYP	0.4004	0.3765	0.3879	0.3659	0.3862	0.3665	0.3834	0.3673	0.3838	0.3654	0.3929	0.4418	0.4410	0.4561	0.4369	0.4614	0.4373	0.4601	0.4377	0.4603	0.4365	0.4685
mpW1PW91	0.4197	0.4052	0.4194	0.3993	0.4244	0.3995	0.4241	0.3998	0.4242	0.3990	0.4303	0.4569	0.4635	0.4805	0.4644	0.4919	0.4643	0.4940	0.4642	0.4938	0.4644	0.5000
O3LYP	0.3531	0.3307	0.3392	0.3227	0.3388	0.3229	0.3370	0.3234	0.3363	0.3225	0.3415	0.4033	0.4014	0.4118	0.3974	0.4169	0.3976	0.4166	0.3979	0.4150	0.3973	0.4207
OLYP	0.3108	0.2877	0.2896	0.2772	0.2903	0.2777	0.2855	0.2782	0.2852	**0.2771**	0.2901	0.3666	0.3656	0.3720	**0.3621**	0.3775	0.3623	0.3750	0.3626	0.3738	0.3621	0.3789
OPBE	0.3312	0.3106	0.3220	0.3065	0.3297	0.3064	0.3224	0.3067	0.3226	0.3072	0.3283	0.3831	0.3835	0.3973	0.3840	0.4087	0.3838	0.4043	0.3839	0.4037	0.3846	0.4094
OPW91	0.3310	0.3101	0.3214	0.3054	0.3288	0.3057	0.3217	0.3062	0.3219	0.3062	0.3273	0.3829	0.3832	0.3969	0.3831	0.4080	0.3832	0.4037	0.3835	0.4031	0.3838	0.4086
PBE	0.3139	0.2822	0.2880	0.2738	0.2918	0.2743	0.2909	0.2745	0.2906	**0.2731**	0.2994	**0.3620**	0.3630	0.3730	0.3646	0.3865	0.3646	0.3879	0.3644	0.3875	0.3644	0.3951
PBE0	0.4192	0.4059	0.4190	0.3993	0.4249	0.3997	0.3063	0.4000	0.4243	0.3991	0.4300	0.4568	0.4643	0.4803	0.4645	0.4926	0.4645	0.4936	0.4645	0.4941	0.4646	0.5000
TPSS	0.3722	0.3349	0.3348	0.3191	0.3291	0.3199	0.3269	0.3204	0.4499	0.3181	0.3334	0.4047	0.3982	0.4040	0.3933	0.4085	0.3937	0.4104	0.3937	0.3814	0.3929	0.4154
VSXC	0.4610	0.4057	0.3913	0.3763	0.3552	0.3781	0.3569	0.3799	0.3618	0.3747	0.3458	0.5179	0.4686	0.4595	0.4432	0.4304	0.4447	0.4314	0.4462	0.4361	0.4418	0.4204
wB97	0.4877	0.4761	0.4882	0.4682	0.4885	0.4687	0.4858	0.4691	0.4865	0.4678	0.4894	0.5244	0.5277	0.5426	0.5254	0.5486	0.5255	0.5466	0.5257	0.5473	0.5254	0.5488
wB97X	0.4697	0.4581	0.4704	0.4482	0.4706	0.4486	0.4693	0.4490	0.4693	0.4477	0.4736	0.5070	0.5110	0.5262	0.5070	0.5324	0.5070	0.5332	0.5071	0.5320	0.5070	0.5365
X3LYP	0.3888	0.3648	0.3761	0.3544	0.3747	0.3550	0.3726	0.3559	0.3728	0.3539	0.3813	0.4308	0.4309	0.4460	0.4275	0.4518	0.4278	0.4515	0.4283	0.4514	0.4271	0.4591

Table S18. Cont. III

	R	S

Method	4-fluoro-α-pyrrolidinononanophenone																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	0.4482	0.4420	0.4607	0.4375	0.4568	0.4380	0.4531	0.4385	0.4563	0.4371	0.4661	0.4426	0.4385	0.4557	0.4349	0.4527	0.4354	0.4509	0.4360	0.4516	0.4345	0.4643
B3P86	0.4532	0.4564	0.4678	0.4532	0.4704	0.4532	0.4723	0.4540	0.4780	0.4524	0.4829	0.4471	0.4541	0.4643	0.4506	0.4671	0.4508	0.4789	0.4517	0.4756	0.4496	0.4805
B3PW91	0.4634	0.4619	0.4786	0.4596	0.4740	0.4598	0.4782	0.4600	0.4866	0.4593	0.4892	0.4578	0.4591	0.4747	0.4568	0.4768	0.4570	0.4832	0.4573	0.4841	0.4563	0.4855
B98	0.4585	0.4573	0.4713	0.4534	0.4721	0.4537	0.4781	0.4539	0.4684	0.4529	0.4805	0.4523	0.4535	0.4661	0.4500	0.4679	0.4504	0.4644	0.4506	0.4639	0.4494	0.4780
B971	0.4586	0.4594	0.4716	0.4548	0.4731	0.4553	0.4794	0.4556	0.4693	0.4541	0.4819	0.4523	0.4555	0.4664	0.4512	0.4688	0.4517	0.4647	0.4521	0.4642	0.4505	0.4790
B972	0.4689	0.4635	0.4820	0.4588	0.4789	0.4591	0.4785	0.4595	0.4785	0.4584	0.4825	0.4628	0.4588	0.4768	0.4538	0.4731	0.4542	0.4728	0.4547	0.4725	0.4534	0.4771
BHandH	0.5410	0.5474	0.5646	0.5497	0.5715	0.5493	0.5723	0.5491	0.5790	0.5498	0.5843	0.5331	0.5386	0.5593	0.5423	0.5587	0.5417	0.5763	0.5414	0.5741	0.5426	0.5798
BHandHLYP	0.5731	0.5720	0.5836	0.5632	0.5806	0.5639	0.5761	0.5646	0.5859	0.5625	0.5880	0.5672	0.5691	0.5789	0.5608	0.5770	0.5615	0.5839	0.5623	0.5835	0.5599	0.5860
BLYP	0.3654	0.3578	0.3740	0.3552	0.3658	0.3351	**0.3279**	0.3545	0.3686	0.3320	0.3382	0.3612	0.3535	0.3683	0.3528	0.3615	0.3325	**0.3288**	0.3519	0.3639	0.3296	0.3344
BMK	0.5672	0.5960	0.6093	0.5962	0.6202	0.5974	0.6362	0.5985	0.6330	0.5978	0.6408	0.5637	0.5924	0.6044	0.5921	0.6170	0.5932	0.6329	0.5941	0.6293	0.5939	0.6357
BP86	0.3645	0.3597	0.3787	0.3598	0.3805	0.3596	0.3822	**0.3594**	0.3889	0.3602	0.3885	0.3585	**0.3560**	0.3742	0.3568	0.3759	0.3565	0.3852	0.3564	0.3855	0.3570	0.3858
CAM-B3LYP	0.4999	0.5010	0.5113	0.4916	0.5095	0.4922	0.5059	0.4926	0.5151	0.4911	0.5150	0.4942	0.4985	0.5071	0.4704	0.5057	0.4891	0.5116	0.4897	0.5124	0.4877	0.5159
HF	*0.7754*	0.7615	0.7729	0.7444	0.7550	0.7454	0.7499	0.7464	0.7519	0.7433	0.7510	*0.7700*	0.7576	0.7685	0.7400	0.5738	0.7410	0.7446	0.7421	0.7464	0.7389	0.7461
LC-BLYP	0.5665	0.5726	0.5808	0.5641	0.5821	0.5642	0.5823	0.5677	0.5808	0.5997	0.5838	0.5611	0.5697	0.5771	0.5586	0.5778	0.5584	0.5771	0.5634	0.5752	0.5587	0.5787
M06	0.5133	0.4900	0.5024	0.4844	0.5001	0.4850	0.4934	0.4852	0.4984	0.4836	0.5036	0.5009	0.4835	0.4924	0.4794	0.4961	0.4799	0.4924	0.4801	0.4917	0.4786	0.5011
M06-2X	0.6191	0.6431	0.6606	0.6398	0.6754	0.6397	0.6728	0.6399	0.6655	0.6397	0.6751	0.6117	0.6379	0.6668	0.6303	0.6676	0.6298	0.6618	0.6300	0.6587	0.6305	0.6690
mpW1LYP	0.4632	0.4583	0.4736	0.4514	0.4704	0.4518	0.4663	0.4522	0.4680	0.4510	0.4807	0.4572	0.4547	0.4681	0.4483	0.4659	0.4488	0.4633	0.4493	0.4629	0.4478	0.4784
mpW1PW91	0.4810	0.4843	0.4968	0.4789	0.4990	0.4792	0.4980	0.4793	0.5060	0.4785	0.5097	0.4750	0.4816	0.4927	0.4753	0.4951	0.4756	0.5027	0.4758	0.5030	0.4746	0.5053
O3LYP	0.4279	0.4253	0.4369	0.4188	0.4372	0.4190	0.4375	0.4198	0.4373	0.4185	0.4410	0.4202	0.4187	0.4288	0.4138	0.4315	0.4140	0.4322	0.4144	0.4315	0.4137	0.4358
OLYP	0.3849	0.3801	0.3873	0.3728	0.3840	0.3732	0.3816	0.3736	0.3837	**0.3727**	0.3902	0.3754	0.3718	0.3781	**0.3661**	0.3743	0.3663	0.3753	0.3666	0.3755	0.3661	0.3913
OPBE	0.4049	0.4031	0.4167	0.3995	0.4216	0.3995	0.4175	0.3999	0.4212	0.4000	0.4240	0.3954	0.3949	0.4076	0.3934	0.4156	0.3932	0.4153	0.3935	0.4148	0.3940	0.4162
OPW91	0.4052	0.4032	0.4167	0.3991	0.4177	0.3995	0.4171	0.4000	0.4210	0.3997	0.4237	0.3958	0.3951	0.4076	0.3930	0.4088	0.3932	0.4152	0.3936	0.4147	0.3938	0.4162
PBE	0.3636	**0.3605**	0.3743	0.3625	0.3778	0.3625	0.3807	0.3623	0.3857	0.3621	0.3907	0.3577	**0.3565**	0.3698	0.3585	0.3721	0.3586	0.3826	0.3584	0.3815	0.3580	0.3856
PBE0	0.4785	0.4828	0.4944	0.4791	0.4987	0.4796	0.4970	0.4801	0.5048	0.4786	0.5081	0.4725	0.4797	0.4904	0.4750	0.4944	0.4757	0.5005	0.4763	0.5015	0.4743	0.5034
TPSS	0.4132	0.4057	0.4109	0.4007	0.4098	0.4011	0.4117	0.4011	0.4670	0.4001	0.4224	0.4075	0.4024	0.4073	0.3979	0.4054	0.3983	0.4162	0.3983	0.3550	0.3971	0.4244
VSXC	0.4889	0.4742	0.4712	0.4665	0.4648	0.4670	0.4641	0.4675	0.4664	0.4660	0.4612	0.4397	0.4285	0.4303	0.4182	0.4198	0.4188	0.4192	0.4193	0.4203	0.4177	0.4125
wB97	0.5503	0.5553	0.5628	0.5493	0.5599	0.5504	0.5606	0.5512	0.5577	0.5480	0.5594	0.5426	0.5491	0.5560	0.5425	0.5531	0.5437	0.5492	0.5447	0.5485	0.5410	0.5503
wB97X	0.5319	0.5364	0.5458	0.5319	0.5459	0.5330	0.5447	0.5337	0.5445	0.5307	0.5458	0.5248	0.5319	0.5405	0.5255	0.5396	0.5270	0.5365	0.5279	0.5367	0.5241	0.5383
X3LYP	0.4519	0.4479	0.4632	0.4416	0.4604	0.4419	0.4572	0.4425	0.4580	0.4411	0.4706	0.4461	0.4445	0.4580	0.4389	0.4561	0.4393	0.4536	0.4399	0.4531	0.4384	0.4686
Method	3,5-difluoromethcathinone																					
B3LYP	0.4948	0.3998	0.3781	0.3651	0.3276	0.3680	0.3221	0.3709	0.3248	0.3623	0.3170	0.4979	0.3575	0.2910	0.2992	0.2044	0.3026	0.1877	0.3059	0.1971	0.2962	0.1745
B3P86	0.4870	0.3982	0.3824	0.3602	0.3330	0.3618	0.3248	0.3644	0.3224	0.3578	0.3219	0.4769	0.3386	0.2700	0.2783	0.1899	0.2808	0.1766	0.2845	0.1826	0.2751	0.1694
B3PW91	0.4974	0.4108	0.3848	0.3705	0.3303	0.3729	0.3271	0.3754	0.3297	0.3681	0.3213	0.4830	0.3454	0.2783	0.2888	0.1957	0.2916	0.1853	0.2947	0.1912	0.2861	0.1740
B98	0.5034	0.4095	0.3861	0.3715	0.3346	0.3742	0.3278	0.3768	0.3291	0.3686	0.3238	0.4959	0.3546	0.2845	0.2956	0.1993	0.2987	0.1864	0.3018	0.1934	0.2924	0.1761
B971	0.5046	0.4131	0.3889	0.3734	0.3371	0.3761	0.3300	0.3788	0.3311	0.3705	0.3264	0.4951	0.3549	0.2847	0.2960	0.2002	0.2992	0.1864	0.3025	0.1937	0.2926	0.1770
B972	0.5101	0.4273	0.3931	0.3816	0.3445	0.3846	0.3357	0.3876	0.3376	0.3789	0.3291	0.4944	0.3580	0.2935	0.3056	0.2099	0.3085	0.2059	0.3116	0.2200	0.3030	0.1931
BHandH	0.5552	0.4858	0.4904	0.4530	0.4631	0.4549	0.4666	0.4569	0.4686	0.4509	0.4679	0.4966	0.3742	0.3293	0.3115	0.3379	0.3138	0.2739	0.3164	0.2729	0.3091	0.2758
BHandHLYP	0.5762	0.4956	0.4959	0.4527	0.4458	0.4552	0.4434	0.4598	0.4395	0.4504	0.4423	0.5345	0.4089	0.3673	0.3489	0.3063	0.3516	0.2876	0.3543	0.2952	0.3465	0.2855
BLYP	0.4767	0.3896	0.3334	0.3466	0.2702	0.3129	**0.2036**	0.3501	0.2653	0.3019	0.2038	0.5151	0.3791	0.2990	0.3327	0.2085	0.3080	0.1438	0.3372	0.2029	0.2981	0.1423
BMK	0.5113	0.4625	0.4743	0.4383	0.4636	0.4407	0.4741	0.4432	0.4742	0.4381	0.4781	0.4556	0.3433	0.3124	0.2756	0.2894	0.2780	0.2851	0.2804	0.2869	0.2749	0.2992
BP86	0.4711	0.3679	0.3343	0.3350	0.2718	0.3370	0.2577	0.3392	0.2664	0.3333	**0.2423**	0.5017	0.3622	0.2823	0.3128	0.1906	0.3155	0.1812	0.3183	0.1854	0.3106	0.1543
CAM-B3LYP	0.5255	0.4420	0.4312	0.3988	0.3830	0.4021	0.3766	0.4049	0.3739	0.3943	0.3750	0.5014	0.3686	0.3144	0.3045	0.2457	0.3074	0.2220	0.3104	0.2301	0.3018	0.2182
HF	*0.7597*	0.6708	0.6510	0.6273	0.5988	0.6296	0.5853	0.6311	0.5912	0.6249	0.5814	*0.6823*	0.5615	0.5279	0.5294	0.4714	0.5316	0.4672	0.5340	0.4752	0.5275	0.4645
LC-BLYP	0.5622	0.4995	0.4994	0.4590	0.4716	0.4617	0.4702	0.4640	0.4544	0.4569	0.4723	0.5061	0.3916	0.3595	0.3278	0.3202	0.3306	0.2894	0.3332	0.3106	0.3254	0.2947
M06	0.5210	0.4294	0.4061	0.3937	0.3571	0.3958	0.3471	0.3975	0.3482	0.3913	0.3431	0.5439	0.4058	0.3412	0.3667	0.2621	0.3699	0.2670	0.3727	0.2707	0.3634	0.2418
M06-2X	0.5401	0.5131	0.5482	0.4987	0.5502	0.4999	0.5687	0.5009	0.5711	0.4976	0.5729	0.4679	0.4108	0.4156	0.3604	0.4159	0.3615	0.4067	0.3625	0.4101	0.3595	0.4144
mpW1LYP	0.5036	0.4134	0.3928	0.3742	0.3447	0.3768	0.3410	0.3795	0.3408	0.3717	0.3382	0.5010	0.3626	0.2985	0.3000	0.2174	0.3031	0.1978	0.3064	0.2066	0.2971	0.1896
mpW1PW91	0.5036	0.4177	0.4016	0.3807	0.3573	0.3831	0.3491	0.3854	0.3487	0.3783	0.3454	0.4779	0.3435	0.2816	0.2851	0.2068	0.2880	0.1931	0.2909	0.1991	0.2823	0.1871
O3LYP	0.5054	0.4247	0.3866	0.3932	0.3346	0.3949	0.3199	0.3969	0.3309	0.3918	0.3124	0.4950	0.3743	0.3021	0.3427	0.2212	0.3447	0.2140	0.3471	0.2296	0.3412	0.2002
OLYP	0.5083	0.4401	0.3737	0.4143	0.3511	0.4077	0.3349	0.4087	0.3348	0.4129	0.3207	0.5112	0.4032	0.3205	0.3803	0.2481	0.3821	0.2463	0.3842	0.2584	0.3791	0.2315
OPBE	0.5190	0.4485	0.3862	0.4245	0.3710	0.4240	0.3536	0.4243	0.3566	0.4251	0.3381	0.5080	0.4139	0.3180	0.3857	0.2927	0.3843	0.2726	0.3843	0.2699	0.3888	0.2531
OPW91	0.5169	0.4461	0.3846	0.4204	0.3687	0.4204	0.3516	0.4212	0.3543	0.4214	0.3361	0.5066	0.4123	0.3168	0.3814	0.2901	0.3811	0.2690	0.3817	0.2674	0.3837	0.2497
PBE	0.4664	0.3662	0.3267	0.3356	0.2676	0.3378	0.2536	0.3394	0.2604	0.3329	**0.2479**	0.4934	0.3544	0.2680	0.3038	0.1764	0.3068	0.1625	0.3096	0.1688	0.3006	0.1493
PBE0	0.5082	0.4237	0.4099	0.3863	0.3636	0.3887	0.3526	0.3910	0.3525	0.3841	0.3508	0.4814	0.3469	0.2825	0.2874	0.2077	0.2905	0.1916	0.2937	0.2018	0.2845	0.1895
TPSS	0.5104	0.4111	0.3617	0.3660	0.2980	0.3681	0.2850	0.3699	0.5101	0.3636	**0.2802**	0.5300	0.3890	0.3010	0.3302	0.2038	0.3337	0.1874	0.3368	0.2832	0.3266	0.1747
VSXC	0.5194	0.4300	0.3935	0.3838	0.3404	0.3868	0.3335	0.3898	0.3393	0.3810	0.3299	0.5185	0.3909	0.3184	0.3280	0.2102	0.3316	0.2011	0.3352	0.2110	0.3247	0.1901
wB97	0.5778	0.5012	0.4885	0.4630	0.4504	0.4657	0.4485	0.4685	0.4432	0.4604	0.4470	0.5182	0.4018	0.3529	0.3436	0.2992	0.3463	0.2909	0.3491	0.2976	0.3411	0.2879
wB97X	0.5606	0.4837	0.4683	0.4407	0.4272	0.4432	0.4208	0.4458	0.4088	0.4384	0.4213	0.5122	0.3919	0.3394	0.3305	0.2780	0.3333	0.2599	0.3361	0.2755	0.3279	0.2605
X3LYP	0.4970	0.4050	0.3825	0.3659	0.3325	0.3685	0.3277	0.3715	0.3282	0.3634	0.3242	0.4984	0.3591	0.2912	0.2962	0.2067	0.2994	0.1869	0.3029	0.1959	0.2933	0.1770

Table S18. Cont. IV

Method	R	S
	Flephedrone [9]	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	0.3848	0.3629	0.3797	0.3509	0.3783	0.3513	0.3863	0.3518	0.3861	0.3507	0.3908	0.3473	0.2437	0.2556	0.2152	0.2406	0.2165	0.2471	0.2177	0.2451	0.2141	0.2598
B3P86	0.3918	0.3821	0.4055	0.3772	0.4080	0.3776	0.4201	0.3780	0.4152	0.3768	0.4253	0.3328	0.2497	0.2724	0.2317	0.2743	0.2326	0.2822	0.2333	0.2827	0.2309	0.2974
B3PW91	0.3971	0.3855	0.4033	0.3782	0.4098	0.3786	0.4153	0.3790	0.4179	0.3779	0.4215	0.3367	0.2516	0.2748	0.2341	0.2730	0.2349	0.2798	0.2356	0.2794	0.2334	0.2931
B98	0.3989	0.3797	0.4026	0.3718	0.4027	0.3722	0.4189	0.3727	0.4111	0.3714	0.4199	0.3453	0.2532	0.2716	0.2311	0.2660	0.2319	0.2750	0.2328	0.2739	0.2304	0.2881
B971	0.3995	0.3816	0.4056	0.3733	0.4045	0.3738	0.4230	0.3743	0.4114	0.3728	0.4214	0.3429	0.2536	0.2717	0.2317	0.2669	0.2325	0.2764	0.2334	0.2752	0.2310	0.2893
B972	0.4074	0.3875	0.4075	0.3818	0.4100	0.3820	0.4112	0.3822	0.4047	0.3817	0.4190	0.3481	0.2593	0.2795	0.2395	0.2717	0.2404	0.2764	0.2413	0.2757	0.2386	0.2880
BHandH	0.5244	0.5236	0.5524	0.5238	0.5662	0.5239	0.5861	0.5239	0.5835	0.5239	0.5955	0.4400	0.3937	0.4168	0.3822	0.3604	0.3832	0.4363	0.3838	0.4365	0.3816	0.4495
BHandHLYP	0.5254	0.5101	0.5397	0.4996	0.5249	0.5004	0.5411	0.5011	0.5293	0.4989	0.5393	0.4558	0.3852	0.4045	0.3649	0.3969	0.3658	0.4025	0.3666	0.4027	0.3641	0.4141
BLYP	0.2975	0.2505	0.2621	0.2376	0.2571	0.2253	0.2988	0.2381	0.2664	**0.2241**	0.3199	0.4766	0.1730	0.1542	0.1204	0.1078	0.1126	0.2109	0.1250	0.1142	**0.1075**	0.2417
BMK	0.5606	0.5895	0.6406	0.6006	0.6492	0.5989	0.6881	0.5973	0.6728	0.5992	0.7035	0.4820	0.4639	0.5099	0.4743	0.5393	0.4722	0.5434	0.4700	0.5496	0.4720	0.5595
BP86	0.2943	0.2634	0.2783	0.2520	0.2768	0.2524	0.2879	0.2528	0.2886	**0.2517**	0.2953	0.2824	0.1558	0.1510	0.1112	0.1302	0.1132	0.1439	0.1153	0.1402	**0.1095**	0.1643
CAM-B3LYP	0.4510	0.4377	0.4622	0.4282	0.4556	0.4290	0.4638	0.4297	0.4595	0.4274	0.4679	0.3943	0.3126	0.3372	0.2937	0.3313	0.2947	0.3328	0.2956	0.3351	0.2927	0.3453
HF	0.7132	0.6780	0.7001	0.6559	0.6712	0.6571	0.6883	0.6581	0.6756	0.6548	0.6736	0.6318	0.5571	0.5680	0.5284	0.5431	0.5296	0.5401	0.5308	0.5426	0.5273	0.5484
LC-BLYP	0.5438	0.5411	0.5685	0.5389	0.5774	0.5392	0.5973	0.5397	0.5686	0.5384	0.5783	0.4718	0.4171	0.4517	0.4065	0.4580	0.4072	0.4556	0.4082	0.4602	0.4054	0.4682
M06	0.4226	0.4044	0.4254	0.4046	0.4365	0.4046	0.4648	0.4044	0.4445	0.4048	0.4667	0.3728	0.2743	0.2946	0.2515	0.2875	0.2525	0.2941	0.2536	0.2919	0.2506	0.3066
M06-2X	0.6785	0.7235	0.7679	0.7446	0.8059	0.7429	0.8305	0.7410	0.8200	0.7463	*0.8417*	0.5883	0.6037	0.6607	0.6141	0.6906	0.6136	0.6913	0.6128	0.6924	0.6143	*0.7051*
mpW1LYP	0.4068	0.3868	0.4075	0.3747	0.4011	0.3756	0.4128	0.3764	0.4080	0.3738	0.4153	0.3658	0.2661	0.2797	0.2385	0.2652	0.2397	0.2720	0.2408	0.2708	0.2374	0.2833
mpW1PW91	0.4230	0.4159	0.4354	0.4101	0.4407	0.4106	0.4489	0.4110	0.4483	0.4097	0.4551	0.3541	0.2782	0.3052	0.2642	0.3071	0.2649	0.3132	0.2655	0.3135	0.2635	0.3267
O3LYP	0.3633	0.3283	0.3664	0.3185	0.3498	0.3189	0.3574	0.3188	0.3549	0.3182	0.3641	0.3281	0.2195	0.2216	0.1896	0.2120	0.1908	0.2190	0.1922	0.2163	0.1886	0.2284
OLYP	0.3134	0.2777	0.2812	0.2737	0.2926	0.2744	0.2950	0.2749	0.2925	**0.2733**	0.3008	0.4451	0.1834	0.1648	0.1442	0.1448	0.1457	0.1530	0.1474	0.1512	**0.1433**	0.1610
OPBE	0.3306	**0.3003**	0.3122	0.3011	0.3305	0.3008	0.3314	0.3008	0.3302	0.3033	0.3408	0.2812	0.1842	0.1879	0.1650	0.1914	0.1641	0.2012	**0.1638**	0.1999	0.1660	0.2117
OPW91	0.3303	**0.2998**	0.3115	0.3018	0.3298	0.3017	0.3329	0.3019	0.3293	0.3025	0.3404	0.2823	0.1848	0.1880	0.1639	0.1905	**0.1636**	0.2005	0.1637	0.1990	0.1651	0.2109
PBE	0.2968	0.2728	0.2884	0.2654	0.2911	0.2659	0.3027	0.2663	0.3014	**0.2649**	0.3098	0.2782	0.1559	0.1591	0.1161	0.1477	0.1180	0.1583	0.1200	0.1554	**0.1142**	0.1757
PBE0	0.4241	0.4166	0.4406	0.4110	0.4414	0.4115	0.4513	0.4119	0.4468	0.4106	0.4566	0.3523	0.2777	0.3028	0.2622	0.3044	0.2630	0.3123	0.2637	0.3119	0.2613	0.3251
TPSS	0.3449	0.3030	0.3142	0.2838	0.3025	0.2849	0.3184	0.2859	0.3774	0.2826	0.3214	0.3266	0.2016	0.1864	0.1539	0.1535	0.1562	0.1669	0.1584	0.1658	0.1518	0.1770
VSXC	0.3724	0.3430	0.3557	0.3353	0.3626	0.3355	0.3729	0.3358	0.3704	0.3350	0.3812	0.3223	0.2381	0.2262	0.2060	0.2269	0.2080	0.2328	0.2100	0.2319	0.2040	0.2449
wB97	0.5138	0.5050	0.5298	0.5001	0.5371	0.5006	0.5561	0.5011	0.5405	0.4995	0.5623	0.4322	0.3816	0.4084	0.3682	0.4127	0.3694	0.4119	0.3704	0.4138	0.3669	0.4220
wB97X	0.4880	0.4789	0.5040	0.4737	0.5087	0.4744	0.5280	0.4750	0.5026	0.4730	0.5123	0.4150	0.3552	0.3818	0.3406	0.3833	0.3418	0.3820	0.3428	0.3849	0.3394	0.3927
X3LYP	0.3923	0.3724	0.3915	0.3608	0.3876	0.3617	0.3989	0.3625	0.3953	0.3600	0.4025	0.3527	0.2516	0.2647	0.2235	0.2510	0.2247	0.2581	0.2259	0.2568	0.2224	0.2702
Method	**Flephedrone [10]**																					
B3LYP	0.4377	0.4301	0.4509	0.4219	0.4527	0.4221	0.4609	0.4225	0.4603	0.4219	0.4656	0.3915	0.3085	0.3291	0.2886	0.3197	0.2894	0.3248	0.2901	0.3231	0.2878	0.3373
B3P86	0.4485	0.4516	0.4785	0.4498	0.4831	0.4502	0.4949	0.4504	0.4899	0.4495	0.5003	0.3812	0.3188	0.3479	0.3076	0.3527	0.3084	0.3588	0.3087	0.3600	0.3071	0.3731
B3PW91	0.4524	0.4535	0.4748	0.4494	0.4845	0.4497	0.4895	0.4500	0.4915	0.4492	0.4956	0.3849	0.3196	0.3497	0.3088	0.3508	0.3093	0.3556	0.3098	0.3559	0.3082	0.3682
B98	0.4533	0.4475	0.4747	0.4436	0.4776	0.4439	0.4939	0.4442	0.4860	0.4434	0.4950	0.3921	0.3204	0.3465	0.3059	0.3450	0.3065	0.3523	0.3070	0.3517	0.3055	0.3649
B971	0.4538	0.4493	0.4776	0.4450	0.4793	0.4454	0.4978	0.4456	0.4862	0.4448	0.4964	0.3898	0.3208	0.3465	0.3066	0.3458	0.3070	0.3536	0.3076	0.3528	0.3061	0.3660
B972	0.4616	0.4542	0.4783	0.4524	0.4832	0.4524	0.4847	0.4524	0.4776	0.4524	0.4927	0.3957	0.3257	0.3535	0.3130	0.3494	0.3137	0.3522	0.3143	0.3521	0.3123	0.3635
BHandH	0.5913	0.5990	0.6299	0.6014	0.6457	0.6015	0.6650	0.6013	0.6624	0.6016	0.6744	0.5028	0.4694	0.4951	0.4613	0.4368	0.4621	0.5148	0.4626	0.5152	0.4608	0.5272
BHandHLYP	0.5877	0.5819	0.6145	0.5747	0.6021	0.5754	0.6184	0.5759	0.6066	0.5741	0.6169	0.5152	0.4583	0.4817	0.4424	0.4772	0.4431	0.4821	0.4437	0.4824	0.4418	0.4935
BLYP	0.3283	0.3015	0.3232	0.2951	0.3236	**0.2910**	0.3752	0.2955	0.3341	0.2913	0.3947	0.5248	0.2079	0.2101	**0.1696**	0.1811	0.1739	0.2797	0.1731	0.1855	0.1725	0.3078
BMK	0.6335	0.6674	0.7191	0.6794	0.7280	0.6776	0.7660	0.6759	0.7509	0.6778	0.7813	0.5550	0.5432	0.5890	0.5540	0.6169	0.5518	0.6206	0.5497	0.6268	0.5516	0.6359
BP86	0.3315	0.3215	0.3421	0.3150	0.3447	0.3153	0.3563	0.3156	0.3562	**0.3148**	0.3650	0.3020	0.2004	0.2140	0.1730	0.2044	0.1743	0.2139	0.1756	0.2112	**0.1718**	0.2332
CAM-B3LYP	0.5124	0.5100	0.5376	0.5037	0.5333	0.5044	0.5417	0.5050	0.5371	0.5031	0.5458	0.4507	0.3853	0.4149	0.3718	0.4119	0.3726	0.4122	0.3733	0.4149	0.3710	0.4242
HF	0.7723	0.7459	0.7713	0.7273	0.7457	0.7283	0.7637	0.7291	0.7506	0.7264	0.7494	0.6911	0.6267	0.6416	0.6013	0.6203	0.6023	0.6170	0.6033	0.6195	0.6003	0.6258
LC-BLYP	0.6131	0.6177	0.6470	0.6175	0.6574	0.6177	0.6768	0.6182	0.6481	0.6171	0.6579	0.5392	0.4952	0.5315	0.4871	0.5386	0.4877	0.5354	0.4885	0.5402	0.4861	0.5474
M06	0.4803	0.4737	0.4983	0.4767	0.5112	0.4765	0.5385	0.4763	0.5186	0.4770	0.5404	0.4234	0.3431	0.3705	0.3265	0.3670	0.3273	0.3718	0.3282	0.3703	0.3259	0.3838
M06-2X	0.7570	0.8037	0.8480	0.8245	0.8852	0.8228	0.9089	0.8209	0.8987	0.8261	*0.9197*	0.6657	0.6833	0.7394	0.6935	0.7680	0.6931	0.7684	0.6923	0.7696	0.6937	*0.7815*
mpW1LYP	0.4625	0.4556	0.4806	0.4477	0.4770	0.4484	0.4889	0.4491	0.4839	0.4470	0.4914	0.4134	0.3332	0.3545	0.3136	0.3452	0.3144	0.3510	0.3152	0.3501	0.3128	0.3619
mpW1PW91	0.4819	0.4862	0.5086	0.4833	0.5161	0.4837	0.5244	0.4840	0.5233	0.4830	0.5305	0.4070	0.3493	0.3814	0.3406	0.3856	0.3411	0.3901	0.3416	0.3910	0.3400	0.4029
O3LYP	0.4121	0.3888	0.4355	0.3826	0.4182	0.3828	0.4279	0.3825	0.4249	0.3824	0.4348	0.3690	0.2779	0.2908	0.2570	0.2869	0.2580	0.2920	0.2591	0.2895	0.2561	0.3011
OLYP	0.3486	0.3263	0.3366	0.3261	0.3495	0.3262	0.3606	0.3262	0.3569	**0.3260**	0.3667	0.4950	0.2229	0.2213	0.1936	0.2120	0.1948	0.2187	0.1962	0.2163	**0.1926**	0.2262
OPBE	0.3693	**0.3517**	0.3677	0.3543	0.3868	0.3537	0.3950	0.3533	0.3930	0.3568	0.4050	0.3094	0.2324	0.2426	0.2173	0.2493	**0.2169**	0.2627	0.2170	0.2583	0.2178	0.2725
OPW91	0.3692	**0.3513**	0.3672	0.3554	0.3862	0.3549	0.3968	0.3547	0.3923	0.3562	0.4048	0.3110	0.2334	0.2430	0.2173	0.2490	**0.2173**	0.2625	0.2176	0.2580	0.2179	0.2721
PBE	0.3384	0.3343	0.3562	0.3313	0.3622	0.3316	0.3740	0.3319	0.3722	**0.3310**	0.3808	0.3019	0.2059	0.2263	0.1817	0.2228	0.1829	0.2300	0.1842	0.2283	**0.1807**	0.2451
PBE0	0.4829	0.4867	0.5139	0.4841	0.5168	0.4845	0.5270	0.4848	0.5221	0.4838	0.5321	0.4048	0.3484	0.3789	0.3384	0.3829	0.3390	0.3893	0.3395	0.3893	0.3377	0.4012
TPSS	0.3805	0.3576	0.3779	0.3455	0.3721	0.3463	0.3885	0.3471	0.4126	**0.3447**	0.3916	0.3266	0.2016	0.1864	0.1539	0.1535	0.1562	0.1669	0.1584	0.1658	**0.1518**	0.1770
VSXC	0.4256	0.4111	0.4295	0.4085	0.4406	0.4085	0.4505	0.4085	0.4480	0.4085	0.4586	0.3573	0.2944	0.2930	0.2715	0.3002	0.2731	0.3042	0.2747	0.3038	0.2700	0.3152
wB97	0.5780	0.5783	0.6057	0.5761	0.6155	0.5765	0.6343	0.5768	0.6188	0.5756	0.6406	0.4953	0.4572	0.4873	0.4468	0.4933	0.4479	0.4913	0.4488	0.4937	0.4456	0.5012
wB97X	0.5506	0.5513	0.5793	0.5490	0.5866	0.5496	0.6058	0.5501	0.5801	0.5485	0.5902	0.4757	0.4298	0.4601	0.4190	0.4637	0.4200	0.4612	0.4209	0.4645	0.4178	0.4715
X3LYP	0.4466	0.4403	0.4638	0.4331	0.4629	0.4338	0.4744	0.4344	0.4704	0.4325	0.4780	0.3983	0.3174	0.3391	0.2980	0.3307	0.2989	0.3366	0.2996	0.3356	0.2973	0.3481

Table S18. Cont. V

Method	R	S
	Flephedrone [3]	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	0.3643	0.3607	0.3851	0.3580	0.3952	0.3578	0.4082	0.3577	0.4067	0.3583	0.4150	0.3457	0.2579	0.2848	0.2369	0.2822	0.2377	0.2860	0.2385	0.2832	0.2361	0.3035
B3P86	0.3796	0.3879	0.4182	0.3917	0.4309	0.3919	0.4474	0.3916	0.4417	0.3919	0.4550	0.3369	0.2722	0.3098	0.2625	0.3221	0.2637	0.3263	0.2639	0.3289	0.2619	0.3450
B3PW91	0.3800	0.3865	0.4111	0.3880	0.4312	0.3881	0.4374	0.3880	0.4401	0.3881	0.4459	0.3357	0.2662	0.3056	0.2571	0.3141	0.2578	0.3170	0.2584	0.3180	0.2563	0.3339
B98	0.3807	0.3790	0.4110	0.3811	0.4217	0.3810	0.4444	0.3809	0.4340	0.3813	0.4463	0.3436	0.2680	0.3024	0.2548	0.3083	0.2553	0.3144	0.2558	0.3133	0.2543	0.3307
B971	0.3810	0.3805	0.4140	0.3822	0.4233	0.3821	0.4484	0.3820	0.4334	0.3824	0.4474	0.3408	0.2681	0.3021	0.2554	0.3091	0.2559	0.3157	0.2563	0.3143	0.2551	0.3318
B972	0.3870	0.3845	0.4128	0.3888	0.4253	0.3884	0.4294	0.3879	0.4198	0.3892	0.4402	0.3438	0.2679	0.3050	0.2568	0.3076	0.2575	0.3082	0.2581	0.3086	0.2560	0.3236
BHandH	0.5308	0.5433	0.5771	0.5502	0.5992	0.5500	0.6223	0.5495	0.6189	0.5507	0.6337	0.4628	0.4327	0.4629	0.4266	0.3875	0.4275	0.4876	0.4279	0.4894	0.4262	0.5028
BHandHLYP	0.5166	0.5151	0.5525	0.5131	0.5452	0.5134	0.5677	0.5136	0.5530	0.5128	0.5664	0.4621	0.4048	0.4334	0.3899	0.4342	0.3905	0.4396	0.3910	0.4401	0.3892	0.4540
BLYP	0.2528	0.2232	0.2509	0.2228	0.2616	0.2293	0.3559	**0.2224**	0.2773	0.2332	0.3808	0.4741	0.1651	0.1721	**0.1194**	0.1495	0.1463	0.2952	0.1249	0.1489	0.1483	0.3271
BMK	0.5763	0.6184	0.6752	0.6374	0.6893	0.6348	0.7321	0.6322	0.7157	0.6354	0.7487	0.5148	0.5106	0.5605	0.5253	0.5948	0.5225	0.5951	0.5197	0.6033	0.5221	0.6132
BP86	0.2619	0.2538	0.2753	0.2527	0.2875	0.2527	0.3053	0.2527	0.3045	**0.2526**	0.3199	0.2718	0.1632	0.1806	0.1340	0.1817	0.1360	0.1881	0.1378	0.1837	**0.1318**	0.2184
CAM-B3LYP	0.4424	0.4449	0.4767	0.4443	0.4792	0.4446	0.4914	0.4448	0.4861	0.4439	0.4974	0.4031	0.3357	0.3728	0.3239	0.3764	0.3247	0.3748	0.3255	0.3785	0.3229	0.3901
HF	0.6947	0.6712	0.7010	0.6563	0.6787	0.6569	0.7027	0.6575	0.6865	0.6556	0.6868	0.6245	0.5589	0.5771	0.5326	0.5586	0.5336	0.5555	0.5345	0.5581	0.5316	0.5665
LC-BLYP	0.5496	0.5601	0.5924	0.5651	0.6097	0.5648	0.6337	0.5650	0.6018	0.5650	0.6143	0.4940	0.4516	0.4948	0.4457	0.5073	0.4461	0.5019	0.4471	0.5082	0.4447	0.5166
M06	0.4116	0.4107	0.4394	0.4199	0.4610	0.4193	0.4972	0.4187	0.4733	0.4207	0.5002	0.3741	0.2892	0.3245	0.2721	0.3278	0.2730	0.3298	0.2741	0.3299	0.2715	0.3461
M06-2X	0.7115	0.7646	0.8119	0.7901	0.8547	0.7880	0.8814	0.7856	0.8701	0.7922	*0.8936*	0.6357	0.6573	0.7179	0.6694	0.7497	0.6688	0.7487	0.6678	0.7504	0.6697	*0.7630*
mpW1LYP	0.3901	0.3871	0.4168	0.3852	0.4205	0.3856	0.4382	0.3858	0.4314	0.3849	0.4415	0.3675	0.2837	0.3117	0.2643	0.3085	0.2652	0.3138	0.2659	0.3126	0.2634	0.3281
mpW1PW91	0.4114	0.4213	0.4466	0.4240	0.4619	0.4240	0.4738	0.4240	0.4729	0.4240	0.4822	0.3583	0.2983	0.3391	0.2913	0.3501	0.2920	0.3528	0.2926	0.3547	0.2906	0.3693
O3LYP	0.3328	0.3098	0.3685	0.3069	0.3562	0.3066	0.3698	0.3059	0.3646	0.3070	0.3800	0.3199	0.2163	0.2375	0.1949	0.2433	0.1963	0.2454	0.1975	0.2417	0.1935	0.2584
OLYP	0.2654	**0.2397**	0.2540	0.2424	0.2756	0.2418	0.2976	0.2411	0.2902	0.2430	0.3076	0.4324	0.1590	0.1634	0.1242	0.1681	0.1259	0.1708	0.1277	0.1662	**0.1225**	0.1829
OPBE	0.2866	**0.2691**	0.2869	0.2735	0.3134	0.2725	0.3324	0.2716	0.3279	0.2763	0.3476	0.2552	0.1651	0.1738	0.1447	0.1952	0.1452	0.2144	0.1461	0.2039	**0.1445**	0.2291
OPW91	0.2865	**0.2686**	0.2865	0.2747	0.3129	0.2737	0.3346	0.2730	0.3273	0.2758	0.3475	0.2570	0.1661	0.1744	0.1457	0.1951	0.1463	0.2142	0.1471	0.2038	**0.1453**	0.2288
PBE	0.2698	**0.2689**	0.2936	0.2713	0.3096	0.2713	0.3267	0.2713	0.3240	0.2715	0.3364	0.2727	0.1715	0.2006	0.1458	0.2074	0.1475	0.2111	0.1492	0.2088	**0.1446**	0.2315
PBE0	0.4125	0.4216	0.4520	0.4244	0.4620	0.4243	0.4769	0.4243	0.4708	0.4243	0.4838	0.3565	0.2983	0.3370	0.2896	0.3477	0.2903	0.3532	0.2908	0.3536	0.2887	0.3682
TPSS	0.3065	0.2820	0.3078	0.2747	0.3104	0.2752	0.3349	0.2757	0.3225	**0.2744**	0.3400	0.3059	0.1927	0.2027	0.1554	0.1933	0.1572	0.2064	0.1592	0.2296	**0.1537**	0.2194
VSXC	0.3708	0.3586	0.3803	0.3602	0.3999	0.3599	0.4134	0.3596	0.4091	0.3605	0.4235	0.3294	0.2708	0.2713	0.2534	0.2913	0.2547	0.2982	0.2559	0.2967	0.2521	0.3105
wB97	0.5074	0.5135	0.5445	0.5159	0.5618	0.5160	0.5852	0.5160	0.5671	0.5158	0.5934	0.4409	0.4036	0.4408	0.3940	0.4522	0.3952	0.4479	0.3961	0.4512	0.3926	0.4604
wB97X	0.4794	0.4858	0.5175	0.4885	0.5321	0.4887	0.5565	0.4889	0.5269	0.4882	0.5403	0.4221	0.3765	0.4140	0.3666	0.4236	0.3678	0.4186	0.3687	0.4227	0.3653	0.4314
X3LYP	0.3741	0.3717	0.3996	0.3706	0.4067	0.3709	0.4237	0.3710	0.4184	0.3704	0.4287	0.3531	0.2680	0.2968	0.2490	0.2951	0.2499	0.3002	0.2505	0.2989	0.2482	0.3158
Method	**4-fluoro-3-methyl-α-pyrrolidinopentiophenone**																					
B3LYP	0.5338	0.5113	0.4847	0.5018	0.4909	0.5025	0.4916	0.5033	0.4929	0.5011	0.4938	0.5556	0.5505	0.5313	0.5464	0.5370	0.5469	0.5402	0.5474	0.5405	0.5458	0.5430
B3P86	0.5465	0.5242	0.5157	0.5155	0.5116	0.5156	0.5152	0.5165	0.5157	0.5149	0.5169	0.5652	0.5612	0.5584	0.5585	0.5583	0.5584	0.5645	0.5589	0.5653	0.5581	0.5667
B3PW91	0.5470	0.5273	0.5204	0.5185	0.5053	0.5189	0.5092	0.5194	0.5107	0.5180	0.5122	0.5671	0.5645	0.5631	0.5610	0.5556	0.5612	0.5557	0.5615	0.5567	0.5606	0.5592
B98	0.5462	0.5253	0.5157	0.5159	0.5081	0.5164	0.5042	0.5169	0.5053	0.5152	0.5079	0.5676	0.5622	0.5588	0.5582	0.5522	0.5585	0.5505	0.5588	0.5507	0.5578	0.5547
B971	0.5473	0.5266	0.5168	0.5167	0.5115	0.5174	0.5056	0.5180	0.5068	0.5159	0.5096	0.5690	0.5635	0.5600	0.5592	0.5567	0.5596	0.5518	0.5600	0.5522	0.5587	0.5562
B972	0.5493	0.5301	0.5234	0.5180	0.5105	0.5188	0.5099	0.5196	0.5109	0.5172	0.5123	0.5708	0.5670	0.5642	0.5588	0.5535	0.5594	0.5557	0.5601	0.5560	0.5582	0.5582
BHandH	0.6408	0.6270	0.6285	0.6202	0.6232	0.6203	0.6221	0.6207	0.6266	0.6198	0.6246	0.6494	0.6518	0.6565	0.6518	0.6662	0.6516	0.6604	0.6516	0.6662	0.6518	0.6636
BHandHLYP	0.6436	0.6256	0.6195	0.6141	0.6109	0.6148	0.6118	0.6156	0.6124	0.6135	0.6075	0.6598	0.6564	0.6548	0.6504	0.6494	0.6508	0.6539	0.6513	0.6533	0.6499	0.6471
BLYP	0.4773	0.4474	0.4378	0.4355	0.4223	0.4203	**0.3950**	0.4361	0.4213	0.4165	0.3973	0.5021	0.4926	0.4875	0.4858	0.4765	0.4721	**0.4544**	0.4860	0.4765	0.4690	0.4574
BMK	0.6242	0.6162	0.6275	0.6118	0.6240	0.6130	0.6281	0.6141	0.6280	0.6135	0.6334	0.6427	0.6445	0.6605	0.6468	0.6613	0.6475	0.6679	0.6483	0.6676	0.6487	0.6752
BP86	0.4905	0.4590	0.4508	0.4493	0.4432	0.4495	0.4390	0.4499	0.4399	0.4492	**0.4361**	0.5122	0.5020	0.5002	0.4990	0.4970	0.4990	0.4938	0.4990	0.4939	0.4990	**0.4922**
CAM-B3LYP	0.5782	0.5589	0.5521	0.5466	0.5416	0.5475	0.5340	0.5483	0.5366	0.5458	0.5380	0.5971	0.5940	0.5928	0.5762	0.5854	0.5875	0.5783	0.5881	0.5806	0.5862	0.5380
HF	*0.8408*	0.8172	0.8095	0.7988	0.7915	0.7999	0.7849	0.8010	0.7872	0.7976	0.7861	*0.8545*	0.8403	0.8352	0.8252	0.6863	0.8261	0.8151	0.8270	0.8163	0.8242	0.8163
LC-BLYP	0.6361	0.6191	0.6163	0.6090	0.6107	0.6099	0.5968	0.6103	0.6127	0.6084	0.5983	0.6515	0.6472	0.6499	0.6432	0.6485	0.6437	0.6341	0.6437	0.6536	0.6431	0.6365
M06	0.6033	0.5846	0.5760	0.5731	0.5637	0.5741	0.5602	0.5750	0.5624	0.5718	0.5576	0.6180	0.6103	0.6042	0.6042	0.5983	0.6049	0.5959	0.6053	0.5967	0.6032	0.5954
M06-2X	0.6672	0.6670	0.6742	0.6646	0.6776	0.6651	0.6793	0.6656	0.6735	0.6642	0.6811	0.6841	0.6915	0.7139	0.6940	0.7092	0.6939	0.7140	0.6943	0.7061	0.6939	0.7175
mpW1LYP	0.5485	0.5276	0.5180	0.5159	0.5055	0.5166	0.5051	0.5173	0.5054	0.5153	0.5089	0.5695	0.5654	0.5612	0.5593	0.5502	0.5597	0.5524	0.5602	0.5518	0.5589	0.5566
mpW1PW91	0.5648	0.5463	0.5411	0.5375	0.5357	0.5380	0.5282	0.5384	0.5387	0.5369	0.5315	0.5836	0.5816	0.5819	0.5779	0.5797	0.5782	0.5724	0.5785	0.5853	0.5775	0.5765
O3LYP	0.5025	0.4746	0.4684	0.4666	0.4613	0.4668	**0.4577**	0.4672	0.4588	0.4665	0.4636	0.5274	0.5117	0.5082	0.5084	0.5060	0.5083	0.5040	0.5085	**0.5040**	0.5084	0.5095
OLYP	0.4629	0.4373	0.4322	0.4317	0.4248	0.4316	**0.4195**	0.4316	0.4212	0.4319	0.4269	0.4896	0.4771	0.4747	0.4764	0.4733	0.4762	0.4692	0.4760	0.4696	0.4768	**0.4269**
OPBE	0.4781	0.4519	0.4495	0.4481	0.4456	0.4478	**0.4412**	0.4480	0.4427	0.4487	0.4461	0.5028	0.4892	0.4898	0.4904	0.4897	0.4900	**0.4879**	0.4900	0.4882	0.4911	0.4925
OPW91	0.4776	0.4513	0.4489	0.4470	0.4448	0.4471	**0.4405**	0.4474	0.4420	0.4477	0.4455	0.5024	0.4887	0.4893	0.4895	0.4890	0.4894	**0.4874**	0.4895	0.4877	0.4903	0.4919
PBE	0.4863	0.4583	0.4480	0.4501	0.4412	0.4506	**0.4346**	0.4509	0.4359	0.4495	0.4372	0.5102	0.5020	0.4986	0.4995	0.4955	0.4998	**0.4892**	0.4999	0.4902	0.4990	0.4926
PBE0	0.5661	0.5472	0.5424	0.5384	0.5379	0.5390	0.5280	0.5395	0.5406	0.5379	0.5325	0.5852	0.5821	0.5834	0.5790	0.5824	0.5793	0.5722	0.5796	0.5878	0.5788	0.5775
TPSS	0.5319	0.4978	0.4807	0.4835	0.4715	0.4843	0.4710	0.4848	0.5543	0.4827	0.4746	0.5482	0.5345	0.5236	0.5274	0.5196	0.5278	0.5235	0.5280	0.5299	0.5269	0.4746
VSXC	0.6756	0.6258	0.6023	0.5979	0.5665	0.5996	0.5600	0.6013	0.5622	0.5963	0.5467	0.6820	0.6394	0.6177	0.6150	0.5884	0.6165	0.5859	0.6179	0.5864	0.6135	0.5734
wB97	0.6340	0.6145	0.6107	0.6043	0.5998	0.6049	0.5893	0.6055	0.6012	0.6037	0.5928	0.6514	0.6426	0.6445	0.6388	0.6375	0.6390	0.6269	0.6392	0.6421	0.6386	0.6310
wB97X	0.6114	0.5919	0.5881	0.5806	0.5789	0.5813	0.5685	0.5820	0.5803	0.5799	0.5735	0.6304	0.6219	0.6245	0.6167	0.6189	0.6171	0.6081	0.6174	0.6231	0.6164	0.6138
X3LYP	0.5390	0.5176	0.5079	0.5062	0.4959	0.5068	0.4959	0.5077	0.4962	0.5056	0.4991	0.5603	0.5562	0.5520	0.5506	0.5417	0.5510	0.5442	0.5515	0.5437	0.5502	0.5478

Table S18. Cont. VI

Method	**R**	**S**
	4-fluoro-α-pyrrolidinooctanophenone	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	0.5088	0.4886	0.4963	0.4792	0.4890	0.4806	0.4927	0.4825	0.4931	0.4784	0.4991	0.5366	0.5224	0.5344	0.5172	0.5353	0.5182	0.5375	0.5197	0.5375	0.5167	0.4991
B3P86	0.5174	0.5023	0.5205	0.4995	0.5072	0.4992	0.5120	0.4997	0.5086	0.4991	0.5160	0.5439	0.5360	0.5568	0.5378	0.5528	0.5373	0.5565	0.5374	0.5537	0.5378	0.5618
B3PW91	0.5233	0.5087	0.5155	0.5043	0.5067	0.5047	0.5169	0.5051	0.5161	0.5038	0.5225	0.5501	0.5411	0.5520	0.5410	0.5562	0.5409	0.5596	0.5410	0.5589	0.5408	0.5662
B98	0.5265	0.5088	0.5140	0.5027	0.5089	0.5032	0.5111	0.5036	0.5104	0.5020	0.5168	0.5533	0.5408	0.5504	0.5391	0.5528	0.5392	0.5541	0.5392	0.5535	0.5388	0.5604
B971	0.5265	0.5096	0.5142	0.5035	0.5091	0.5040	0.5117	0.5045	0.5109	0.5027	0.5175	0.5537	0.5422	0.5512	0.5407	0.5539	0.5408	0.5555	0.5409	0.5548	0.5403	0.5620
B972	0.5281	0.5101	0.5190	0.5006	0.5163	0.5010	0.5172	0.5016	0.5176	0.5002	0.5237	0.5560	0.5440	0.5566	0.5393	0.5615	0.5394	0.5612	0.5396	0.5613	0.5392	0.5683
BHandH	0.6334	0.6282	0.6440	0.6287	0.6884	0.6284	0.6541	0.6285	0.6533	0.6285	0.6594	0.6540	0.6563	0.6740	0.6589	0.6735	0.6586	0.6875	0.6585	0.6869	0.6590	0.6928
BHandHLYP	0.6563	0.6417	0.6573	0.6357	0.6406	0.6361	0.6420	0.6366	0.6410	0.6353	0.6461	0.6757	0.6639	0.6808	0.6597	0.6708	0.6599	0.6706	0.6602	0.6699	0.6594	0.6750
BLYP	0.4095	0.3794	0.3874	0.7346	0.3799	0.3497	**0.3420**	0.3733	0.3812	0.3461	0.3518	0.4476	0.4297	0.4431	0.7417	0.4469	0.4109	0.4232	0.4287	0.4465	**0.4091**	0.4332
BMK	0.6523	0.6539	0.6844	0.6509	0.6905	0.6517	0.6977	0.6525	0.6934	0.6524	0.6966	0.6733	0.6754	0.7069	0.6752	0.7179	0.6759	0.7245	0.6765	0.7211	0.6766	0.7277
BP86	0.4138	0.3890	0.3982	**0.3835**	0.3945	0.3836	0.3975	0.3837	0.3973	0.3836	0.4004	0.4508	**0.4381**	0.4536	0.4405	0.4601	0.4400	0.4630	0.4396	0.4625	0.4411	0.4677
CAM-B3LYP	0.5720	0.5577	0.5616	0.5518	0.5569	0.5524	0.5590	0.5527	0.5582	0.5513	0.5637	0.5947	0.5849	0.5925	0.5822	0.5944	0.5825	0.5949	0.5826	0.5942	0.5820	0.6001
HF	*0.8792*	0.8552	0.8626	0.6565	0.8442	0.8387	0.8400	0.8399	0.8414	0.8364	0.8417	*0.8914*	0.8672	0.8747	0.7153	0.8614	0.8518	0.8549	0.8530	0.8565	0.8495	0.8570
LC-BLYP	0.6504	0.6429	0.6592	0.6383	0.6464	0.6391	0.6476	0.6393	0.6481	0.6379	0.6496	0.6679	0.6630	0.6810	0.6600	0.6744	0.6606	0.6733	0.6606	0.6741	0.6597	0.6758
M06	0.5587	0.5436	0.5388	0.5232	0.5377	0.5237	0.5268	0.5238	0.5303	0.5225	0.5164	0.6349	0.6311	0.6369	0.6265	0.6467	0.6265	0.6396	0.6263	0.6420	0.6261	0.6256
M06-2X	0.7089	0.7221	0.7501	0.7270	0.7515	0.7270	0.7576	0.7270	0.7572	0.7270	0.7691	0.7332	0.7477	0.7763	0.7532	0.7813	0.7531	0.7854	0.7530	0.7852	0.7533	0.7995
mpW1LYP	0.5312	0.5128	0.5171	0.5052	0.5093	0.5057	0.5125	0.5064	0.5117	0.5046	0.5198	0.5577	0.5450	0.5537	0.5413	0.5538	0.5416	0.5556	0.5419	0.5547	0.5410	0.5627
mpW1PW91	0.5479	0.5360	0.5445	0.5325	0.5416	0.5328	0.5442	0.5330	0.5433	0.5320	0.5485	0.5729	0.5667	0.5789	0.5672	0.5831	0.5672	0.5845	0.5672	0.5837	0.5671	0.5899
O3LYP	0.4701	0.4552	0.4652	0.4499	0.4642	0.4500	0.4613	0.4502	0.4619	0.4500	0.4715	0.5035	0.4956	0.5085	0.4944	0.5158	0.4942	0.5120	0.4942	0.5119	0.4946	0.5230
OLYP	0.4167	0.4012	0.4065	**0.3965**	0.4069	0.3966	0.4025	0.3967	0.4036	0.3968	0.4118	0.4576	**0.4512**	0.4612	0.4520	0.4713	0.4517	0.4659	0.4515	0.4662	0.4525	0.4760
OPBE	0.4376	0.4231	0.4364	0.4221	0.4409	**0.4216**	0.4370	0.4216	0.4374	0.4230	0.4473	0.4767	**0.4702**	0.4861	0.4733	0.4987	0.4727	0.4942	0.4725	0.4940	0.4743	0.5053
OPW91	0.4375	0.4229	0.4361	0.4214	0.4404	**0.4213**	0.4365	0.4215	0.4370	0.4224	0.4466	0.4764	**0.4697**	0.4854	0.4723	0.4978	0.4721	0.4934	0.4720	0.4932	0.4734	0.5043
PBE	0.4126	0.3906	0.3938	0.3864	0.3920	0.3868	0.3958	0.3869	0.3950	**0.3857**	0.4042	0.4501	**0.4400**	0.4503	0.4438	0.4593	0.4436	0.4623	0.4431	0.4614	0.4438	0.4712
PBE0	0.5470	0.5346	0.5532	0.5315	0.5411	0.5318	0.5422	0.5321	0.5420	0.5312	0.5470	0.5725	0.5665	0.5871	0.5675	0.5839	0.5675	0.5839	0.5675	0.5837	0.5675	0.5896
TPSS	0.4851	0.4566	0.4544	0.4457	0.4431	0.4463	0.4439	0.4465	0.4811	0.4451	0.4509	0.5122	0.4942	0.4986	0.4903	0.4966	0.4903	0.4979	0.4901	0.4911	0.4901	0.5059
VSXC	0.5648	0.5405	0.5357	0.5258	0.5243	0.5267	0.5242	0.5276	0.5244	0.5249	0.5198	0.6279	0.6019	0.5961	0.5865	0.5885	0.5874	0.5860	0.5883	0.5856	0.5856	0.5798
wB97	0.6292	0.6165	0.6323	0.6105	0.6205	0.6110	0.6199	0.6115	0.6203	0.6101	0.6244	0.6525	0.6429	0.6609	0.6390	0.6560	0.6393	0.6522	0.6396	0.6540	0.6387	0.6568
wB97X	0.6059	0.5946	0.6104	0.5885	0.5988	0.5890	0.5993	0.5895	0.6006	0.5881	0.6033	0.6287	0.6213	0.6394	0.6178	0.6351	0.6181	0.6327	0.6184	0.6343	0.6175	0.6366
X3LYP	0.5154	0.4973	0.5021	0.4904	0.4949	0.4909	0.4987	0.4916	0.4978	0.4898	0.5058	0.5429	0.5307	0.5401	0.5279	0.5409	0.5281	0.5433	0.5284	0.5423	0.5276	0.5504
Method	**4-fluoro-α-pyrrolidinobutyrophenone [13] in $CDCl_3$**																					
B3LYP	0.4914	0.4680	0.4874	0.4669	0.4931	0.4667	0.4950	0.4666	0.4955	0.4673	0.5003	0.5277	0.5175	0.5399	0.5215	0.5531	0.5210	0.5536	0.5205	0.5536	0.5221	0.5003
B3P86	0.5012	0.4824	0.5010	0.4814	0.5026	0.4807	0.5136	0.4810	0.5115	0.4814	0.5166	0.5357	0.5305	0.5515	0.5348	0.5618	0.5340	0.5716	0.5340	0.5691	0.5351	0.5759
B3PW91	0.5091	0.4901	0.5077	0.4894	0.5071	0.4891	0.5207	0.4889	0.5203	0.4896	0.5253	0.5438	0.5368	0.5572	0.5414	0.5707	0.5409	0.5766	0.5405	0.5757	0.5418	0.5823
B98	0.5074	0.4868	0.5065	0.4844	0.5106	0.4843	0.5122	0.4842	0.5118	0.4843	0.5178	0.5431	0.5340	0.5567	0.5370	0.5685	0.5367	0.5692	0.5363	0.5683	0.5372	0.5757
B971	0.5086	0.4886	0.5084	0.4855	0.5111	0.4855	0.5137	0.4856	0.5132	0.4852	0.5189	0.5445	0.5360	0.5588	0.5386	0.5695	0.5384	0.5710	0.5382	0.5701	0.5386	0.5774
B972	0.5148	0.4944	0.5182	0.4943	0.5199	0.4940	0.5223	0.4939	0.5220	0.4946	0.5273	0.5507	0.5420	0.5683	0.5470	0.5775	0.5465	0.5788	0.5460	0.5781	0.5475	0.5847
BHandH	0.6155	0.6060	0.6240	0.6065	0.7228	0.6061	0.6377	0.6059	0.6357	0.6066	0.6414	0.6407	0.6420	0.6633	0.6473	0.6551	0.6467	0.6833	0.6463	0.6811	0.6476	0.6871
BHandHLYP	0.6363	0.6189	0.6350	0.6119	0.6389	0.6121	0.6344	0.6124	0.6370	0.6117	0.6386	0.6623	0.6520	0.6700	0.6486	0.6793	0.6487	0.6752	0.6489	0.6764	0.6486	0.6804
BLYP	0.4014	0.3725	0.3874	0.8536	0.3894	0.3484	**0.3446**	0.3736	0.3898	0.3450	0.3549	0.4488	0.4414	0.4609	0.8698	0.4728	0.4301	0.4434	0.4485	0.4713	**0.4285**	0.4530
BMK	0.6319	0.6415	0.6732	0.6398	0.6891	0.6405	0.6836	0.6411	0.6836	0.6417	0.6864	0.6597	0.6747	0.7062	0.6768	0.7271	0.6771	0.7237	0.6774	0.7228	0.6787	0.7288
BP86	0.4051	0.3749	0.3916	0.3741	0.4018	0.3734	0.4086	**0.3729**	0.4071	0.3749	0.4093	0.4514	**0.4443**	0.4651	0.4513	0.4844	0.4503	0.4892	0.4495	0.4874	0.4523	0.4922
CAM-B3LYP	0.5524	0.5341	0.5499	0.5290	0.5488	0.5292	0.5547	0.5295	0.5551	0.5288	0.5585	0.5827	0.5742	0.5923	0.5736	0.5991	0.5736	0.6038	0.5736	0.6035	0.5736	0.6088
HF	*0.8641*	0.8390	0.8471	0.6631	0.8390	0.8231	0.8258	0.8239	0.8289	0.8215	0.8278	*0.8820*	0.8593	0.8682	0.7321	0.8636	0.8461	0.8518	0.8468	0.8545	0.8446	0.8545
LC-BLYP	0.6312	0.6195	0.6394	0.6147	0.6381	0.6152	0.6363	0.6151	0.6422	0.6146	0.6385	0.6545	0.6494	0.6710	0.6479	0.6765	0.6481	0.6747	0.6478	0.6792	0.6480	0.6776
M06	0.5393	0.5266	0.5377	0.5250	0.5439	0.5251	0.5400	0.5250	0.5399	0.5245	0.5438	0.5767	0.5765	0.5900	0.5781	0.6014	0.5781	0.5977	0.5778	0.5974	0.5779	0.6008
M06-2X	0.6978	0.7106	0.7384	0.7173	0.7509	0.7173	0.7578	0.7172	0.7556	0.7173	0.7611	0.7253	0.7443	0.7739	0.7539	0.7918	0.7537	0.7978	0.7533	0.7952	0.7541	0.8018
mpW1LYP	0.5117	0.4896	0.5062	0.4847	0.5114	0.4846	0.5123	0.4846	0.5118	0.4850	0.5189	0.5468	0.5370	0.5568	0.5374	0.5694	0.5370	0.5691	0.5367	0.5682	0.5379	0.5764
mpW1PW91	0.5336	0.5157	0.5354	0.5141	0.5372	0.5140	0.5460	0.5139	0.5458	0.5142	0.5494	0.5664	0.5602	0.5817	0.5634	0.5918	0.5630	0.5994	0.5627	0.5986	0.5637	0.6041
O3LYP	0.4667	0.4580	0.4678	0.4569	0.4752	0.4568	0.4754	0.4569	0.4746	0.4571	0.4812	0.5095	0.5110	0.5262	0.5150	0.5400	0.5146	0.5392	0.5144	0.5381	0.5155	0.5448
OLYP	0.4200	0.4090	0.4172	0.4054	0.4194	**0.4053**	0.4180	0.4054	0.4171	0.4058	0.4255	**0.4704**	0.4719	0.4860	0.4752	0.4975	0.4747	0.4955	0.4744	0.4942	0.4758	0.5021
OPBE	0.4410	**0.4316**	0.4500	0.4331	0.4544	0.4325	0.4553	0.4325	0.4541	0.4341	0.4601	**0.4891**	0.4912	0.5138	0.4979	0.5253	0.4971	0.5252	0.4966	0.5238	0.4991	0.5298
OPW91	0.4410	**0.4315**	0.4498	0.4325	0.4541	0.4323	0.4549	0.4324	0.4538	0.4337	0.4598	**0.4888**	0.4908	0.5132	0.4971	0.5247	0.4965	0.5246	0.4963	0.5232	0.4984	0.5291
PBE	0.4063	0.3787	0.3914	0.3796	0.4012	0.3792	0.4094	**0.3787**	0.4076	0.3796	0.4149	0.4540	**0.4477**	0.4652	0.4562	0.4847	0.4555	0.4907	0.4547	0.4885	0.4566	0.4975
PBE0	0.5324	0.5153	0.5350	0.5134	0.5358	0.5134	0.5432	0.5134	0.5442	0.5135	0.5473	0.5657	0.5608	0.5819	0.5634	0.5915	0.5632	0.5981	0.5629	0.5983	0.5638	0.6033
TPSS	0.4719	0.4377	0.4437	0.4277	0.4411	0.4280	0.4464	0.4279	**0.3706**	0.4273	0.4512	0.5058	0.4920	0.5032	0.4903	0.5105	0.4902	0.5156	0.4898	**0.4695**	0.4903	0.5220
VSXC	0.4977	0.4559	0.4517	0.4300	0.4275	0.4321	0.4333	0.4340	0.4351	0.4281	**0.4237**	0.5892	0.5553	0.5553	0.5355	0.5394	0.5371	0.5423	0.5385	0.5437	0.5340	**0.5338**
wB97	0.6088	0.5938	0.6101	0.5900	0.6093	0.5902	0.6082	0.5904	0.6116	0.5898	0.6101	0.6374	0.6304	0.6486	0.6302	0.6550	0.6301	0.6544	0.6301	0.6561	0.6302	0.6574
wB97X	0.5892	0.5750	0.5924	0.5696	0.5897	0.5698	0.5913	0.5700	0.5928	0.5695	0.5939	0.6181	0.6124	0.6311	0.6110	0.6367	0.6109	0.6379	0.6108	0.6386	0.6111	0.6419
X3LYP	0.4973	0.4757	0.4914	0.4714	0.4980	0.4712	0.4998	0.4713	0.4992	0.4716	0.5061	0.5333	0.5245	0.5436	0.5256	0.5578	0.5252	0.5582	0.5250	0.5573	0.5261	0.5652

Table S18. Cont. VII

Method	R	S
	4-fluoro-α-pyrrolidinobutyrophenone [13] in D_2O	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	0.4585	0.4260	0.4436	0.4197	0.4381	0.4199	0.4398	0.4202	0.4413	0.4196	0.4487	0.5000	0.4932	0.5186	0.4955	0.5186	0.4953	0.5215	0.4951	0.5227	0.4959	0.4487
B3P86	0.4725	0.4457	0.4605	0.4413	0.4541	0.4409	0.4630	0.4414	0.4615	0.4411	0.4710	0.5082	0.5079	0.5285	0.5131	0.5281	0.5123	0.5412	0.5123	0.5398	0.5134	0.5493
B3PW91	0.4793	0.4518	0.4665	0.4470	0.4558	0.4471	0.4690	0.4473	0.4694	0.4469	0.4779	0.5174	0.5136	0.5346	0.5179	0.5364	0.5177	0.5460	0.5175	0.5461	0.5181	0.5546
B98	0.4768	0.4475	0.4648	0.4412	0.4583	0.4415	0.4593	0.4416	0.4595	0.4408	0.4684	0.5167	0.5095	0.5353	0.5125	0.5337	0.5123	0.5364	0.5120	0.5364	0.5125	0.5453
B971	0.4784	0.4501	0.4671	0.4433	0.4594	0.4437	0.4613	0.4441	0.4614	0.4427	0.4703	0.5182	0.5117	0.5374	0.5145	0.5346	0.5145	0.5381	0.5143	0.5380	0.5143	0.5471
B972	0.4830	0.4532	0.4685	0.4467	0.4667	0.4468	0.4682	0.4469	0.4689	0.4466	0.4764	0.5240	0.5157	0.5376	0.5169	0.5411	0.5165	0.5445	0.5162	0.5451	0.5172	0.5519
BHandH	0.5944	0.5796	0.5937	0.5786	0.6755	0.5782	0.6055	0.5782	0.6036	0.5786	0.6111	0.6163	0.6247	0.6441	0.6337	0.6403	0.6328	0.6696	0.6322	0.6673	0.6341	0.6753
BHandHLYP	0.6083	0.5844	0.5981	0.5745	0.5994	0.5749	0.5871	0.5754	0.5972	0.5741	0.5943	0.6392	0.6336	0.6530	0.6312	0.6619	0.6313	0.6495	0.6314	0.6614	0.6311	0.6568
BLYP	0.3674	0.3266	0.3328	0.8411	0.3297	0.2897	**0.2742**	0.3194	0.3293	0.2846	0.2869	0.4175	0.4134	0.4273	0.8808	0.4327	0.3933	0.3933	0.4153	0.4333	**0.3901**	0.4024
BMK	0.5975	0.6048	0.6318	0.6013	0.6471	0.6021	0.6430	0.6029	0.6430	0.6034	0.6497	0.6329	0.6530	0.6857	0.6564	0.7052	0.6567	0.7036	0.6571	0.7032	0.6586	0.7115
BP86	0.3771	0.3360	0.3493	0.3295	0.3494	0.3291	0.3537	**0.3290**	0.3533	0.3301	0.3584	0.4213	**0.4162**	0.4373	0.4222	0.4461	0.4212	0.4528	0.4205	0.4521	0.4233	0.4581
CAM-B3LYP	0.5216	0.4957	0.5082	0.4869	0.4972	0.4875	0.5025	0.4880	0.5033	0.4865	0.5097	0.5576	0.5535	0.5714	0.5528	0.5658	0.5530	0.5745	0.5532	0.5750	0.5527	0.5816
HF	*0.8439*	0.8144	0.8205	0.6180	0.8094	0.7895	0.7869	0.7906	0.7904	0.7871	0.7906	*0.8703*	0.8535	0.8644	0.6720	0.8572	0.8308	0.8333	0.8317	0.8366	0.8288	0.8367
LC-BLYP	0.6030	0.5850	0.6027	0.5772	0.5980	0.5779	0.5889	0.5779	0.6020	0.5771	0.5950	0.6328	0.6331	0.6555	0.6323	0.6575	0.6324	0.6499	0.6321	0.6641	0.6325	0.6561
M06	0.5193	0.4951	0.5010	0.4895	0.5014	0.4899	0.4952	0.4900	0.4953	0.4888	0.5001	0.5654	0.5599	0.5692	0.5597	0.5764	0.5599	0.5723	0.5598	0.5720	0.5592	0.5773
M06-2X	0.6633	0.6713	0.6975	0.6770	0.7084	0.6771	0.7145	0.6771	0.7127	0.6768	0.7200	0.6979	0.7196	0.7493	0.7310	0.7645	0.7308	0.7721	0.7305	0.7698	0.7311	0.7767
mpW1LYP	0.4788	0.4482	0.4630	0.4387	0.4568	0.4389	0.4576	0.4392	0.4578	0.4387	0.4679	0.5190	0.5125	0.5350	0.5120	0.5347	0.5116	0.5366	0.5114	0.5367	0.5124	0.5462
mpW1PW91	0.5043	0.4788	0.4955	0.4735	0.4884	0.4737	0.4955	0.4738	0.4960	0.4733	0.5036	0.5399	0.5374	0.5596	0.5406	0.5575	0.5404	0.5687	0.5402	0.5689	0.5407	0.5768
O3LYP	0.4232	0.4016	0.4093	0.3957	0.4095	0.3958	0.4102	0.3961	0.4097	0.3957	0.4201	0.4735	0.4721	0.4880	0.4734	0.4917	0.4731	0.4940	0.4730	0.4930	0.4737	0.5016
OLYP	0.3729	0.3507	0.3521	**0.3426**	0.3515	0.3427	0.3498	0.3430	0.3492	0.3428	0.3605	**0.4293**	0.4308	0.4392	0.4306	0.4447	0.4305	0.4457	0.4305	0.4443	0.4310	0.4530
OPBE	0.3982	0.3768	0.3890	0.3744	0.3913	**0.3740**	0.3920	0.3741	0.3911	0.3753	0.4009	**0.4496**	0.4496	0.4682	0.4539	0.4744	0.4531	0.4772	0.4529	0.4759	0.4550	0.4837
OPW91	0.3978	0.3764	0.3884	**0.3733**	0.3906	0.3734	0.3912	0.3737	0.3905	0.3745	0.4002	0.4493	**0.4493**	0.4678	0.4531	0.4740	0.4528	0.4768	0.4526	0.4755	0.4544	0.4831
PBE	0.3767	0.3379	0.3476	0.3334	0.3466	0.3335	0.3522	0.3333	0.3513	**0.3330**	0.3633	0.4235	**0.4182**	0.4369	0.4255	0.4435	0.4250	0.4514	0.4243	0.4504	0.4256	0.4620
PBE0	0.5042	0.4799	0.4964	0.4742	0.4885	0.4744	0.4937	0.4747	0.4954	0.4742	0.5029	0.5399	0.5392	0.5605	0.5416	0.5580	0.5414	0.5676	0.5412	0.5689	0.5420	0.5767
TPSS	0.4477	0.4050	0.4054	0.3905	0.3994	0.3910	0.3964	0.3912	0.3577	0.3898	0.4066	0.4777	0.4670	0.4769	0.4653	0.4816	0.4651	0.4810	0.4647	0.4415	0.4652	0.4914
VSXC	0.5093	0.4587	0.4478	0.4272	0.4175	0.4296	0.4168	0.4318	0.4196	0.4251	0.4069	0.5784	0.5384	0.5335	0.5138	0.5083	0.5159	0.5138	0.5178	0.5155	0.5120	0.5025
wB97	0.5862	0.5643	0.5780	0.5577	0.5741	0.5580	0.5655	0.5583	0.5760	0.5574	0.5717	0.6203	0.6149	0.6332	0.6154	0.6366	0.6153	0.6287	0.6152	0.6410	0.6155	0.6356
wB97X	0.5635	0.5425	0.5573	0.5332	0.5507	0.5335	0.5443	0.5339	0.5462	0.5329	0.5516	0.5980	0.5950	0.6139	0.5926	0.6149	0.5925	0.6096	0.5924	0.6112	0.5927	0.6172
X3LYP	0.4648	0.4345	0.4479	0.4255	0.4435	0.4256	0.4450	0.4261	0.4452	0.4254	0.4550	0.5054	0.5004	0.5212	0.5007	0.5234	0.5003	0.5261	0.5002	0.5262	0.5011	0.5354
Method	**2-trifluoromethylmethcathinone**																					
B3LYP	0.4478	0.3758	0.3600	0.3464	0.3409	0.3483	0.3312	0.3501	0.3362	0.3447	0.3345	0.3304	0.2457	0.2368	0.2248	0.2176	0.2256	0.2222	0.2264	0.2248	0.2242	0.2366
B3P86	0.4225	0.3666	0.3629	0.3445	0.3527	0.3452	0.3487	0.3467	0.3512	0.3433	0.3521	0.3004	0.2345	0.2279	0.2279	0.2392	0.2271	0.2534	0.2273	0.2485	0.2280	0.2667
B3PW91	0.4394	0.3821	0.3756	0.3581	0.3609	0.3591	0.3595	0.3603	0.3627	0.3571	0.3637	0.3206	0.2595	0.2506	0.2479	0.2538	0.2480	0.2637	0.2482	0.2627	0.2478	0.2778
B98	0.4531	0.3886	0.3757	0.3623	0.3600	0.3639	0.3521	0.3654	0.3557	0.3607	0.3565	0.3382	0.2653	0.2530	0.2499	0.2460	0.2506	0.2520	0.2513	0.2530	0.2490	0.2669
B971	0.4537	0.3901	0.3776	0.3635	0.3620	0.3651	0.3534	0.3666	0.3573	0.3617	0.3581	0.3373	0.2665	0.2538	0.2499	0.2465	0.2506	0.2544	0.2513	0.2539	0.2490	0.2683
B972	0.4629	0.4037	0.3899	0.3758	0.3777	0.3773	0.3667	0.3789	0.3705	0.3743	0.3708	0.3470	0.2850	0.2706	0.2639	0.2633	0.2649	0.2686	0.2660	0.2685	0.2632	0.2810
BHandH	0.5129	0.4759	0.4678	0.4532	0.4631	0.4541	0.4536	0.4554	0.4581	0.4520	0.4580	0.3543	0.3177	0.3066	0.3130	0.3410	0.3128	0.3396	0.3129	0.3350	0.3130	0.3547
BHandHLYP	0.5734	0.5133	0.4987	0.4823	0.4805	0.4841	0.4671	0.4860	0.4721	0.4806	0.4706	0.4372	0.3801	0.3703	0.3606	0.3568	0.3611	0.3557	0.3617	0.3578	0.3602	0.3681
BLYP	0.3825	0.2906	0.2680	0.2536	0.2319	0.2218	**0.1960**	0.2560	0.2252	0.2135	0.2112	0.2945	0.1763	0.1576	0.1397	0.1150	0.1013	0.1635	0.1400	0.1240	**0.0944**	0.1926
BMK	0.5257	0.5026	0.5150	0.5020	0.5378	0.5025	0.5462	0.5030	0.5422	0.5017	0.5553	0.3899	0.3932	0.4097	0.4102	0.4438	0.4089	0.4677	0.4076	0.4550	0.4108	0.4733
BP86	0.3439	0.2631	0.2571	0.2324	0.2383	0.2334	0.2336	0.2346	0.2367	**0.2317**	0.2323	0.2546	0.1440	0.1401	0.1279	0.1392	0.1275	0.1647	**0.1273**	0.1589	0.1287	0.1803
CAM-B3LYP	0.5054	0.4442	0.4247	0.4107	0.4062	0.4125	0.3942	0.4143	0.3973	0.4090	0.3980	0.3723	0.3077	0.2936	0.2897	0.2830	0.2904	0.2895	0.2911	0.2878	0.2891	0.3018
HF	*0.7987*	0.7276	0.7068	0.6773	0.6650	0.6790	0.6445	0.6807	0.6521	0.6758	0.6441	*0.6625*	0.6029	0.5848	0.5759	0.5547	0.5775	0.5452	0.5791	0.5517	0.5744	0.5534
LC-BLYP	0.5628	0.5209	0.4994	0.4932	0.4864	0.4952	0.4763	0.4968	0.4802	0.4917	0.4803	0.4180	0.3809	0.3674	0.3731	0.3771	0.3737	0.3856	0.3740	0.3827	0.3728	0.3969
M06	0.4667	0.3834	0.3865	0.3722	0.3683	0.3731	0.3827	0.3737	0.3818	0.3712	0.3867	0.3672	0.3005	0.2786	0.2835	0.2602	0.2845	0.2726	0.2852	0.2713	0.2822	0.2848
M06-2X	0.5599	0.5905	0.6095	0.6057	0.6459	0.6046	0.6549	0.6035	0.6513	0.6068	0.6649	0.4497	0.4899	0.5136	0.5185	0.5616	0.5164	0.5716	0.5143	0.5653	0.5205	0.5888
mpW1LYP	0.4693	0.4002	0.3813	0.3671	0.3609	0.3688	0.3500	0.3707	0.3544	0.3654	0.3538	0.3486	0.2673	0.2531	0.2419	0.2328	0.2427	0.2359	0.2436	0.2370	0.2412	0.2505
mpW1PW91	0.4578	0.4049	0.4007	0.3824	0.3918	0.3836	0.3849	0.3846	0.3885	0.3813	0.3891	0.3345	0.2808	0.2713	0.2706	0.2775	0.2708	0.2865	0.2710	0.2845	0.2703	0.2998
O3LYP	0.4476	0.3904	0.3692	0.3536	0.3454	0.3562	0.3327	0.3588	0.3368	0.3514	0.3346	0.3291	0.2611	0.2346	0.2309	0.2206	0.2324	0.2241	0.2342	0.2236	0.2296	0.2355
OLYP	0.4139	0.3433	0.3218	0.3025	0.2934	0.3035	0.2776	0.3045	0.2824	0.3018	0.2788	0.3071	0.2268	0.1875	0.1885	0.1662	0.1905	0.1714	0.1927	0.1699	0.1869	0.1828
OPBE	0.4038	0.3483	0.3344	0.3222	0.3212	0.3235	0.3113	0.3253	0.3140	0.3212	0.3144	0.3049	0.2370	0.2222	0.2136	0.2205	0.2142	0.2285	0.2153	0.2260	0.2136	0.2442
OPW91	0.4042	0.3483	0.3342	0.3215	0.3207	0.3233	0.3106	0.3252	0.3134	0.3207	0.3137	0.3050	0.2371	0.2210	0.2127	0.2192	0.2138	0.2269	0.2152	0.2246	0.2129	0.2424
PBE	0.3469	0.2691	0.2538	0.2401	0.2392	0.2415	**0.2347**	0.2427	0.2374	0.2384	0.2391	0.2517	0.1539	**0.1314**	0.1343	0.1387	0.1346	0.1650	0.1347	0.1576	0.1336	0.1823
PBE0	0.4605	0.4066	0.4018	0.3831	0.3912	0.3844	0.3822	0.3857	0.3871	0.3820	0.3867	0.3319	0.2779	0.2671	0.2676	0.2745	0.2680	0.2835	0.2684	0.2807	0.2673	0.2969
TPSS	0.3933	0.3100	0.2874	0.2688	0.2613	0.2711	**0.2520**	0.2729	0.4194	0.2665	0.2555	0.3076	0.1947	0.1637	0.1572	0.1552	0.1582	0.1651	0.1590	**0.0838**	0.1560	0.1818
VSXC	0.2239	**0.2222**	0.2632	0.2329	0.2798	0.2321	0.2870	0.2314	0.2842	0.2337	0.2931	0.2134	0.1062	**0.0905**	0.0976	0.1220	0.0962	0.1679	0.0950	0.1525	0.0991	0.1744
wB97	0.5596	0.5078	0.4868	0.4758	0.4714	0.4780	0.4583	0.4801	0.4625	0.4737	0.4603	0.4351	0.3857	0.3651	0.3689	0.3663	0.3697	0.3723	0.3705	0.3725	0.3682	0.3850
wB97X	0.5364	0.4819	0.4670	0.4518	0.4503	0.4536	0.4389	0.4554	0.4438	0.4500	0.4411	0.4125	0.3622	0.3444	0.3458	0.3430	0.3465	0.3483	0.3472	0.3479	0.3451	0.3598
X3LYP	0.4525	0.3832	0.3644	0.3508	0.3463	0.3525	0.3363	0.3545	0.3403	0.3492	0.3404	0.3332	0.2507	0.2378	0.2267	0.2202	0.2273	0.2256	0.2283	0.2264	0.2261	0.2406

Table S18. Cont. VIII

Method	**R**	**S**
	3-trifluoromethylmethcathinone	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	0.3714	0.3639	0.3752	0.3651	0.3906	0.3651	0.3955	0.3736	0.3932	0.3651	0.4036	0.3057	0.2284	0.2361	0.2207	0.2701	0.2209	0.2590	0.2211	0.2562	0.2207	0.2734
B3P86	0.3671	0.3780	0.4013	0.3969	0.4124	0.3956	0.4195	0.3944	0.4152	0.3980	0.4402	0.2819	0.2304	0.2494	0.2343	0.2870	0.2339	0.2919	0.2333	0.2908	0.2346	0.3096
B3PW91	0.3769	0.3781	0.3985	0.3884	0.4185	0.3878	0.4242	0.3873	0.4208	0.3887	0.4324	0.2872	0.2357	0.2513	0.2373	0.2817	0.2378	0.2887	0.2379	0.2830	0.2379	0.3045
B98	0.3795	0.3787	0.3910	0.3928	0.4138	0.3919	0.4145	0.3909	0.4114	0.3937	0.4244	0.3013	0.2376	0.2475	0.2357	0.2825	0.2354	0.2783	0.2351	0.2761	0.2356	0.2936
B971	0.3803	0.3801	0.3929	0.3942	0.4152	0.3933	0.4153	0.3923	0.4119	0.3951	0.4255	0.2996	0.2367	0.2469	0.2358	0.2821	0.2353	0.2789	0.2350	0.2763	0.2359	0.2945
B972	0.3898	0.3913	0.4057	0.4033	0.4276	0.4029	0.4222	0.4023	0.4200	0.3939	0.4275	0.2992	0.2462	0.2565	0.2425	0.2774	0.2422	0.2806	0.2420	0.2791	0.2429	0.2938
BHandH	0.4914	0.5179	0.5421	0.5352	0.5741	0.5342	0.5895	0.5330	0.5827	0.5362	0.5991	0.3794	0.3664	0.3840	0.3799	0.3648	0.3793	0.4388	0.3784	0.4333	0.3807	0.4569
BHandHLYP	0.5049	0.5053	0.5203	0.5144	0.5281	0.5137	0.5309	0.5130	0.5278	0.5151	0.5526	0.4099	0.3680	0.3826	0.3672	0.4061	0.3671	0.4074	0.3669	0.4043	0.3672	0.4195
BLYP	0.3021	0.2795	0.2822	0.2736	0.2908	0.2507	0.2876	0.2718	0.2876	**0.2495**	0.3035	0.2751	0.1652	0.1406	0.1362	0.1351	0.1128	0.2039	0.1373	0.1319	**0.1086**	0.2390
BMK	0.5188	0.5766	0.5964	0.6124	0.6370	0.6094	0.6572	0.6066	0.6523	0.6130	0.6734	0.4211	0.4442	0.4757	0.4721	0.5307	0.4692	0.5392	0.4534	0.5325	0.4727	0.5539
BP86	0.2791	**0.2596**	0.2807	0.2682	0.3014	0.2676	0.3054	0.2670	0.3034	0.2689	0.3116	0.2322	0.1249	0.1257	0.1098	0.1588	0.1093	0.1652	**0.1091**	0.1607	0.1104	0.1883
CAM-B3LYP	0.4325	0.4349	0.4473	0.4474	0.4599	0.4464	0.4616	0.4455	0.4575	0.4475	0.4852	0.3505	0.2975	0.3125	0.2951	0.3383	0.2952	0.3389	0.2952	0.3391	0.2947	0.3522
HF	0.7050	0.6823	0.6866	0.6762	0.6799	0.6765	0.6801	0.6686	0.6774	0.6759	0.6853	0.6022	0.5520	0.5593	0.5420	0.5635	0.5426	0.5459	0.5431	0.5628	0.5413	0.5685
LC-BLYP	0.5170	0.5347	0.5516	0.5543	0.5738	0.5530	0.5848	0.5519	0.5802	0.5554	0.5989	0.4191	0.3966	0.4218	0.4018	0.4546	0.4009	0.4558	0.4033	0.4504	0.4027	0.4703
M06	0.3992	0.4087	0.4246	0.4202	0.4401	0.4197	0.4603	0.4191	0.4458	0.4204	0.4719	0.3552	0.3075	0.3280	0.2972	0.3410	0.2990	0.3431	0.3001	0.3412	0.2951	0.3560
M06-2X	0.6482	0.7261	0.7531	0.7661	0.7961	0.7632	0.8165	0.7602	0.8100	0.7688	*0.8289*	0.5410	0.5862	0.6275	0.6191	0.6911	0.6160	0.6934	0.6239	0.6885	0.6220	*0.7129*
mpW1LYP	0.3923	0.3859	0.3939	0.3958	0.4071	0.3950	0.4130	0.3943	0.4101	0.3966	0.4213	0.3248	0.2506	0.2589	0.2430	0.2821	0.2430	0.2813	0.2432	0.2785	0.2428	0.2946
mpW1PW91	0.3998	0.4125	0.4339	0.4299	0.4447	0.4153	0.4506	0.4277	0.4464	0.4309	0.4595	0.3034	0.2615	0.2816	0.2664	0.3148	0.2672	0.3208	0.2671	0.3206	0.2668	0.3366
O3LYP	0.3718	0.3555	0.3698	0.3545	0.3720	0.3542	0.3717	0.3540	0.3762	0.3548	0.3786	0.2811	0.2130	0.2071	0.1973	0.2139	0.1975	0.2130	0.1980	0.2117	0.1971	0.2236
OLYP	0.3449	0.3225	0.3203	0.3143	0.3364	0.3141	0.3249	**0.3141**	0.3251	0.3148	0.3277	0.4960	0.1896	0.1771	0.1638	0.1635	0.1655	**0.1618**	0.1674	0.1648	0.3334	0.3215
OPBE	0.3482	**0.3352**	0.3480	0.3368	0.3674	0.3360	0.3565	0.3374	0.3567	0.3379	0.3599	0.2520	0.1941	0.2082	0.1900	0.2117	**0.1895**	0.2084	0.1896	0.2160	0.1911	0.2184
OPW91	0.3478	**0.3299**	0.3448	0.3359	0.3667	0.3354	0.3558	0.3369	0.3561	0.3391	0.3592	0.2526	0.1937	**0.1879**	0.1882	0.2108	0.1882	0.2074	0.1885	0.2152	0.1893	0.2173
PBE	0.2787	**0.2658**	0.2832	0.2761	0.3065	0.2756	0.3104	0.2748	0.3081	0.2765	0.3193	0.2218	0.1203	0.1265	0.1126	0.1666	0.1122	0.1761	**0.1118**	0.1728	0.1129	0.1986
PBE0	0.4013	0.4129	0.4368	0.4303	0.4471	0.4292	0.4505	0.4280	0.4464	0.4314	0.4720	0.3007	0.2586	0.2779	0.2637	0.3116	0.2636	0.3185	0.2633	0.3172	0.2636	0.3343
TPSS	0.3342	0.3019	0.3138	0.3025	0.3138	0.3021	0.3188	**0.3015**	0.4025	0.3027	0.3312	0.2891	0.1767	0.1646	0.1499	0.1728	0.1506	0.1781	0.1513	**0.1424**	0.1492	0.1946
VSXC	0.3493	0.3411	0.3669	0.3459	0.3779	0.3455	0.3945	0.3451	0.3895	0.3464	0.3945	0.2752	0.1756	0.1682	0.1586	0.1918	0.1587	0.2063	0.1590	0.1986	0.1585	0.2220
wB97	0.4965	0.5046	0.5285	0.5171	0.5366	0.5163	0.5479	0.5154	0.5422	0.5179	0.5582	0.3966	0.3715	0.3885	0.3748	0.4090	0.3742	0.4113	0.3737	0.4085	0.3753	0.4247
wB97X	0.4707	0.4784	0.4959	0.4919	0.5101	0.4909	0.5218	0.4916	0.5162	0.4928	0.5332	0.3738	0.3425	0.3602	0.3423	0.3783	0.3417	0.3829	0.3411	0.3793	0.3429	0.3971
X3LYP	0.3775	0.3719	0.3809	0.3831	0.4004	0.3823	0.4022	0.3815	0.3992	0.3839	0.4107	0.3101	0.2352	0.2435	0.2274	0.2739	0.2274	0.2685	0.2275	0.2656	0.2273	0.2826

Table S19. RMS values of carbon-13 chemical shifts of *S*-cathinone and its selected fluorinated synthetic derivatives calculated with HF and selected functionals combined with 6-311++G** basis set. The most accurate methods and their smallest RMS values in boald and marked in green, the the worst methods with its highests RMS values are in italic font and marked in orange

Method	R											S										
	Cathinone																					
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP												7.7581	9.1108	9.9160	9.6807	10.4286	9.6432	11.8179	9.6053	11.5003	9.7149	12.0449
B3P86												6.5266	7.8217	8.6603	8.4046	9.1630	8.3889	10.5313	8.3534	10.3162	8.4586	10.7717
B3PW91												6.5690	7.9254	8.6874	8.5127	9.2615	8.4822	10.6341	8.4437	10.3326	8.5435	10.8802
B98												6.4910	7.7334	8.5118	8.3111	9.0761	8.2905	10.4010	8.2676	10.1044	8.3325	10.6285
B971												6.3344	7.5719	8.3502	8.1560	8.9105	8.1284	10.2274	8.1002	9.9344	8.1875	10.4617
B972												4.2829	5.4733	6.1850	6.0962	6.7337	6.0592	8.1085	6.0203	7.8044	6.1280	8.3469
BHandH												8.9393	10.2256	11.0229	10.8223	11.5007	10.7782	12.8319	10.7505	12.5360	10.8366	13.0859
BHandHLYP												7.6857	8.9357	9.7106	9.5410	10.2446	9.5056	11.6023	9.4722	11.2983	9.5744	11.8471
BLYP												7.7871	9.0238	9.7861	9.5870	10.4100	9.7936	11.5941	9.6003	11.4883	9.9333	11.8915
BMK												20.9172	22.1870	23.1999	22.7823	23.8697	22.7333	25.1204	22.8848	24.7388	22.9825	25.3137
BP86												6.1818	7.4638	8.1965	7.9704	8.6762	7.9473	10.0141	7.9196	9.7407	7.9884	10.3755
CAM-B3LYP												9.2983	10.6604	11.4496	11.2728	12.0403	11.2404	13.4002	11.2081	13.0971	11.3054	13.6522
HF												6.4837	7.4860	8.1443	8.0026	8.6560	7.9713	9.9670	7.9406	9.6283	8.0318	10.2104
LC-BLYP												13.4714	14.8101	15.6858	15.4594	16.2380	15.4026	17.6095	15.3704	17.2986	15.4971	17.8657
M06												6.8878	8.1490	8.9959	8.7549	9.5678	8.7104	10.8855	8.6725	10.5960	8.8097	11.1240
M06-2X												20.7391	22.2014	23.0875	22.8387	23.7357	22.8220	25.0854	22.8062	24.7781	22.8484	*25.3727*
mpW1LYP												7.8037	9.0962	9.9032	9.7257	10.4452	9.6861	11.8034	9.6475	11.5090	9.7617	12.0230
mpW1PW91												**6.3658**	7.6850	8.4593	8.2790	9.0294	8.2439	10.3900	8.2138	10.0869	8.3115	10.6353
O3LYP												**3.7832**	4.8949	5.6248	5.8237	6.4500	5.7848	7.9142	5.7433	7.7178	5.8572	8.1713
OLYP												**3.7787**	4.8303	5.4382	5.6255	6.1612	5.5888	7.5034	5.5475	7.2862	5.6540	7.7188
OPBE												**3.5569**	4.0717	4.3214	4.5847	4.7879	4.5638	6.1655	4.5377	6.0326	4.6030	6.3918
OPW91												3.5185	4.1211	4.4167	4.6722	4.8969	4.6472	6.2982	4.6164	6.1656	4.6897	6.5313
PBE												6.1166	7.3734	8.1646	7.8689	8.7210	7.8367	10.0385	7.8134	9.7689	7.9143	10.2891
PBE0												6.1700	7.4845	8.2646	8.0673	8.8118	8.0285	10.2300	7.9911	9.8818	8.1066	10.4255
TPSS												4.5055	5.2647	5.8828	5.7045	6.2248	5.6819	7.5504	5.6667	6.5270	5.7330	7.7544
VSXC												5.6904	6.0283	6.3075	6.2920	6.5839	6.2763	7.3558	6.2596	7.1569	6.3079	7.5186
wB97												6.5044	7.7290	8.5106	8.3300	9.0495	8.2942	10.3571	8.2575	10.0633	8.3640	10.6128
wB97X												7.3917	8.6497	9.4366	9.2562	9.9843	9.2225	11.3388	9.1878	10.9877	9.2888	11.5727
X3LYP												7.8307	9.1430	9.9478	9.7636	10.5132	9.7301	11.8695	9.6936	11.5725	9.7986	12.1001
Method	**4-trifluoromethylmethcathinone**																					
B3LYP	7.5276	8.3804	9.0612	9.2135	10.3497	9.1691	11.1568	9.1262	11.1036	9.2572	11.4450	7.4077	8.4599	9.1795	9.1101	9.8469	9.0826	10.9745	9.0395	10.7365	9.1492	11.1747
B3P86	6.2624	6.9815	7.6321	7.7018	8.4390	7.6891	9.4699	7.6594	9.2678	7.7470	9.8198	6.1872	7.0521	7.7148	7.6756	8.2821	7.6515	9.4688	7.6132	9.3270	7.7267	9.6537
B3PW91	6.3119	7.2990	7.6511	7.8735	8.8429	7.8359	9.9364	7.7916	9.7341	7.9116	10.1680	6.2410	7.1624	7.8892	7.8206	8.5409	7.7999	9.6581	7.7568	9.4078	7.8536	9.8405
B98	6.4536	7.0600	7.6371	7.8070	8.9191	7.7839	9.4501	7.7597	9.1761	7.8317	9.8114	6.0769	6.9656	7.6529	7.5586	8.2288	7.5360	9.3665	7.5041	9.1322	7.5874	9.5683
B971	6.4013	7.0078	7.5756	7.7327	8.4064	7.7052	9.3397	7.6777	9.5102	7.7638	9.6976	6.0355	6.9003	7.5793	7.4904	8.1334	7.4620	9.2549	7.4221	9.0284	7.5263	9.4640
B972	**5.2045**	5.6943	5.9629	6.4858	7.0683	6.4554	7.9524	6.4227	7.8091	6.5109	8.1852	**5.0470**	5.5234	6.0474	6.0783	6.6073	6.0678	7.6579	6.0331	7.4030	6.1046	7.8266
BHandH	6.7631	7.5232	8.1523	8.0868	8.7280	8.0394	9.7168	8.0071	9.5270	8.1096	10.0359	7.2804	8.0296	8.5449	8.5616	9.0396	8.5206	10.1651	8.4912	9.8429	8.5822	10.3933
BHandHLYP	6.3085	6.9597	7.5460	7.6996	8.3938	7.6608	9.5029	7.6271	9.2109	7.7420	9.8410	6.5513	7.3219	7.9337	7.8766	8.4348	7.8543	9.7476	7.8182	9.5384	7.9124	9.9471
BLYP	9.7444	10.7485	11.1382	11.3387	12.4062	11.4946	12.9384	11.3214	12.9454	11.6535	13.2179	9.3724	10.4168	11.0828	10.9991	12.5132	11.1533	12.5559	10.9933	12.5025	11.2769	12.8293
BMK	17.4838	18.5988	19.4928	19.2095	20.2432	19.1539	21.3782	19.2938	20.9910	19.4123	*21.6664*	17.4455	18.6740	19.4672	19.3271	20.3482	19.2698	21.5916	19.3968	21.2933	19.5227	*21.7737*
BP86	7.9515	8.8569	9.1583	9.2998	9.9772	9.2710	10.9793	9.2416	10.8281	9.3254	11.1666	7.5844	8.4636	9.0464	8.9608	9.5964	8.9439	10.4753	8.9040	10.2841	8.9826	10.7540
CAM-B3LYP	7.9844	8.9264	9.6208	9.7642	10.5983	9.7320	12.1017	9.7005	11.8491	9.7973	11.3270	8.1317	9.2220	9.9784	9.9323	10.6764	9.8924	11.8922	9.8526	11.6516	9.9714	12.0916
HF	7.3773	7.3925	7.4710	7.8750	8.3847	7.8571	9.3978	7.8394	8.9251	7.8919	9.3165	7.7534	7.8043	8.0281	8.1136	8.3481	8.0876	9.3523	8.0615	9.0967	8.1096	9.5193
LC-BLYP	10.7976	11.8254	12.6382	12.7026	13.5821	12.6500	14.7073	12.6197	14.2948	12.7364	15.0608	11.2545	12.3812	13.1902	13.1124	14.0115	13.0566	15.2014	13.0043	14.9406	13.1587	15.4168
M06	5.4731	6.2064	6.9128	6.9723	7.7711	6.9305	8.8634	6.8951	8.6261	7.0229	9.1878	5.9173	6.6232	7.2915	7.2205	7.8499	7.1579	9.0019	7.1211	8.7595	7.2678	9.1884
M06-2X	16.6864	17.8347	18.6868	18.5852	19.4307	18.5440	20.5689	18.6452	20.2710	18.6186	20.9331	16.8016	18.1218	19.0025	18.9798	19.8856	18.9572	21.0967	18.9350	20.8452	18.9955	21.3803
mpW1LYP	7.2732	8.0669	8.7445	8.9364	10.0863	8.8933	10.9120	8.8522	10.3711	8.9768	11.1389	7.1897	8.1764	8.8986	8.8650	9.5592	8.8329	10.6943	8.7893	10.4833	8.9060	10.8913
mpW1PW91	5.8536	6.5205	7.1090	7.3112	8.0346	7.2710	9.3933	7.2369	9.1477	7.3511	9.4509	5.8445	6.6885	7.3390	7.3302	7.9702	7.2925	9.1641	7.2577	8.9174	7.3651	9.3464
O3LYP	5.7518	6.2836	6.8838	6.9810	7.5296	6.9528	8.3833	6.9501	8.2112	7.0189	8.6036	5.4665	6.0024	6.2977	6.4579	7.2967	6.4675	7.8732	6.4416	7.6563	6.4770	8.0682
OLYP	6.8507	7.3044	7.6942	7.7107	8.3933	7.6884	8.8923	7.6659	8.7736	7.7333	9.0416	6.4989	6.9366	7.3461	7.2339	7.7887	7.2226	8.2734	7.2088	8.1083	7.2412	8.4407
OPBE	6.4444	**6.4380**	6.5601	6.6612	6.9213	6.6510	7.4405	6.6307	7.3274	6.6697	7.5202	6.2162	**6.1696**	6.2893	6.2477	6.5354	6.2396	6.9790	6.2330	6.8742	6.2560	7.1237
OPW91	**6.4182**	6.4774	6.6354	6.7254	7.0264	6.7128	7.5583	6.6910	7.4457	6.7340	7.7410	**6.1788**	6.2043	6.3598	6.3071	6.6357	6.2991	7.0882	6.2921	6.9948	6.3154	7.2378
PBE	7.6957	8.5721	8.9110	8.9880	9.7675	8.9560	10.6130	8.9324	10.3494	9.0313	10.9012	7.3985	8.2470	8.8705	8.7319	9.4863	8.7067	10.3372	8.6742	10.1494	8.7717	10.5229
PBE0	5.6652	6.3227	6.8957	7.0355	7.7278	7.0023	8.8425	6.9705	8.4976	7.0690	9.1719	5.6853	6.4917	7.1824	7.1124	7.6978	7.0719	8.9559	7.0325	8.6840	7.1521	9.1044
TPSS	7.1790	7.4269	7.7529	7.7992	8.2402	7.7862	8.8401	7.7777	7.9611	7.8154	9.1114	6.7844	7.1064	7.4664	7.4238	7.7650	7.4030	8.5545	7.3867	7.8598	7.4474	8.6940
VSXC	8.4475	8.4078	8.4777	8.5175	8.7146	8.5095	8.9289	8.5011	8.8790	8.5258	9.1271	7.6174	7.4377	7.4531	7.5033	7.6467	7.4978	7.9158	7.4921	7.8565	7.5101	8.0946
wB97	5.9293	6.5199	7.1338	7.1843	7.9170	7.1600	8.8573	7.1335	8.4792	7.2055	9.1861	6.0806	6.8196	7.4716	7.4375	8.1201	8.3756	9.2227	7.3521	8.9750	7.4732	9.4298
wB97X	6.5036	7.2284	7.8715	7.9492	8.7123	7.9231	9.7287	7.8953	9.2915	7.9734	10.0760	6.6140	7.5123	8.2185	8.1625	8.8899	8.1262	10.0473	8.0736	9.7475	8.2021	10.2445
X3LYP	7.4169	8.2388	8.9165	9.1050	10.2764	9.0667	10.8409	9.0269	10.9569	9.1454	11.1973	7.3245	8.3361	9.0582	9.0228	9.7418	8.9953	10.8653	8.9530	10.6520	9.0631	11.0679

Table S19. Cont. I

Method	R	S
	3-fluoromethcathinone	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	7.2098	8.4953	9.0244	9.1375	9.9865	9.0926	10.9648	9.0474	10.7056	9.1780	11.2730	9.9838	8.3405	9.0415	9.0352	9.8385	8.9892	10.9781	8.9431	10.6767	9.0779	11.1997
B3P86	5.8730	6.9905	7.6145	7.6844	8.5166	7.6627	9.5112	7.6204	9.3096	7.7468	9.7990	5.6115	6.8523	7.5834	7.5636	8.3634	7.5370	9.4825	7.4924	9.2562	7.6259	9.7193
B3PW91	5.9073	7.1292	7.8672	7.7843	8.9350	7.7466	9.6260	7.7005	9.4273	7.8221	9.9418	5.6752	6.9954	7.6350	7.6850	8.4659	7.6451	9.6369	7.5987	9.3216	7.7255	9.8819
B98	6.1347	7.1902	7.6912	7.8102	8.6505	7.7843	9.5655	7.7561	9.3164	7.8370	9.8772	5.5306	6.7822	7.4598	7.4845	8.3038	7.4533	9.4283	7.4204	9.1319	7.5166	9.6745
B971	5.9952	7.0222	7.5387	7.6537	8.4737	7.6203	9.3910	7.5868	9.1380	7.6916	9.7035	5.3730	6.6130	7.2980	7.3270	8.1403	7.2887	9.2458	7.2503	8.9524	7.3689	9.4984
B972	**4.1316**	4.9409	5.6167	5.5841	6.3332	5.5447	7.2867	5.5034	7.1435	5.6182	7.7838	**3.5770**	4.6638	5.2340	5.3612	6.0392	5.3157	7.2480	5.2696	6.9659	5.4030	7.4927
BHandH	7.2919	8.4356	9.1528	9.1020	9.9441	9.0511	10.8987	9.0171	10.6176	9.1222	11.2318	7.6516	8.7882	9.5139	9.4813	10.0745	9.4305	11.2748	9.3941	10.9821	9.5060	11.5031
BHandHLYP	6.7451	7.8270	8.3719	8.5102	9.2754	8.4678	10.3398	8.4282	10.0284	8.5504	10.6274	6.8691	7.9914	8.6789	8.6940	9.4096	8.6522	10.5334	8.6124	10.2333	8.7336	10.7643
BLYP	7.8095	8.9850	9.7173	9.6263	10.5662	9.8433	11.2316	9.6379	11.2509	9.9934	11.6519	7.2278	8.5185	9.2330	9.2610	10.1862	9.4533	11.0892	9.2547	10.9957	9.6095	11.3860
BMK	18.8090	20.0883	20.9091	20.7944	21.8703	20.7380	22.8039	20.8818	22.4079	21.0010	*23.1059*	18.7251	20.0552	20.9238	20.8437	21.9065	20.7828	22.9874	20.9125	22.5877	21.0479	*23.2293*
BP86	6.0695	7.2352	7.8908	7.8022	8.5783	7.7725	9.4458	7.7385	9.2456	7.8261	9.9205	5.2935	6.6338	7.2722	7.2857	8.0628	7.2514	9.1134	7.2132	8.8435	7.3146	9.4887
CAM-B3LYP	8.3187	9.6041	10.1604	10.3342	11.1752	10.2942	12.2145	10.2548	11.9325	10.3748	12.5038	8.4104	9.7353	10.4169	10.4544	11.2480	10.4135	12.3743	10.3733	12.0719	10.4958	12.6248
HF	5.7578	6.3016	6.9039	6.8674	7.5063	6.8373	8.7428	6.8079	8.4269	6.8959	8.9727	6.0785	6.7671	7.2531	7.2539	7.8818	7.2190	8.9963	7.1862	8.7473	7.2895	9.2140
LC-BLYP	11.8255	13.1009	13.8124	13.8790	14.7479	13.8107	13.2864	13.7669	15.3886	13.9279	16.0593	12.2553	13.5594	14.2902	14.3107	15.0965	14.2454	16.2357	14.2033	15.9340	14.3599	16.4770
M06	5.8276	6.9837	7.6666	7.7339	8.5262	7.6771	9.6861	7.6282	9.2895	7.8019	9.9656	5.9843	7.2122	7.9050	7.8986	8.7147	7.8476	9.8162	7.8037	9.5266	7.9597	10.0671
M06-2X	17.8943	19.3712	20.0880	20.1349	21.0808	20.1063	22.1109	20.0792	21.7674	20.1564	22.4703	18.1123	19.6060	20.3522	20.4010	21.3317	20.3663	22.4678	20.3342	22.1434	20.4305	22.7708
mpW1LYP	7.1856	8.4098	8.9333	9.1038	9.9053	9.0569	10.8836	9.0115	10.6209	9.1466	11.1729	7.0041	8.2843	9.0042	9.0296	9.8061	8.9818	10.9105	8.9353	10.6343	9.0736	11.1244
mpW1PW91	5.6210	6.7766	7.2717	7.4313	8.2714	7.3890	9.2716	7.3525	9.0116	7.4710	9.5752	5.4467	6.6991	7.3528	7.3883	8.1721	7.3445	9.3167	7.3060	9.0038	7.4304	9.5643
O3LYP	3.9825	4.8057	5.5495	5.5390	6.4086	5.4671	7.2136	5.3862	7.0488	5.5753	7.5604	3.1232	4.1586	4.9672	5.0736	5.8218	5.0408	6.8758	4.9891	6.6617	5.0951	7.0765
OLYP	**4.3240**	4.9068	5.2547	5.4070	6.1294	5.3750	6.8461	5.3406	6.6736	5.4328	7.1129	**3.0868**	3.9227	4.4850	4.6412	5.2066	4.6159	6.2116	4.5872	6.0004	4.6600	6.3844
OPBE	4.0107	**3.9406**	3.9536	4.2356	4.6582	4.2168	5.3346	4.1905	5.1692	4.2508	5.6111	**3.1184**	3.2119	3.2346	3.4684	3.6731	3.4549	4.7502	3.4380	4.5498	3.4796	4.9035
OPW91	**3.9503**	3.9840	4.0342	4.3088	4.7750	4.2845	5.4733	4.2527	5.3021	4.3233	5.7542	**3.0266**	3.2475	3.3181	3.5461	3.7998	3.5293	4.8888	3.5083	4.6833	3.5572	5.0482
PBE	5.8121	6.9301	7.6274	7.5059	8.4354	7.4671	9.2923	7.4386	9.0877	7.5592	9.6262	5.1320	6.4361	7.1276	7.0752	7.9953	7.0322	9.0219	6.9983	8.7572	7.1311	9.2799
PBE0	5.3845	6.4848	7.0370	7.1665	7.9899	7.1204	9.0421	7.0764	8.7014	7.2133	9.2849	5.2105	6.4466	7.1095	7.1345	7.9132	7.0866	9.1014	7.0412	8.7454	7.1833	9.2996
TPSS	**4.6841**	5.1555	5.5923	5.6431	6.2101	5.6162	7.0731	5.5984	5.9048	5.6772	7.3480	**3.4978**	4.2047	4.8739	4.8572	5.5323	4.8225	6.5464	4.7962	5.7101	4.8980	6.7615
VSXC	6.7880	6.8400	7.0264	7.0522	7.4501	7.0368	7.7520	7.0209	7.6543	7.0681	8.0278	5.2699	5.1821	5.4195	5.3918	5.8101	5.3724	6.1606	5.3533	6.0308	5.4127	6.4301
wB97	5.8909	6.8262	7.4636	7.4732	8.3011	7.4296	9.1799	7.3855	8.8783	7.5153	9.4999	5.8820	6.9544	7.5989	7.6366	8.4123	7.5880	9.5134	7.5412	9.2524	7.6866	9.7726
wB97X	6.6024	7.6476	8.2784	8.3477	9.1716	8.3030	10.1285	8.2580	9.7377	8.3913	10.4219	6.5878	7.7558	8.4241	8.4672	9.2409	8.4208	10.3985	8.3753	10.0457	8.5144	10.6449
X3LYP	7.2147	8.4675	8.9912	9.1575	9.9905	9.1167	10.9655	9.0733	10.7013	9.1998	11.2683	7.0209	8.3267	9.0408	9.0667	9.8692	9.0243	10.9711	8.9794	10.6895	9.1100	11.1982
Method	**4-fluoro-α-pyrrolidinopentiophenone**																					
B3LYP	5.2278	6.1941	6.7561	6.7202	7.3578	6.6823	8.2389	6.6446	7.9881	6.7552	8.5138	5.2278	6.1941	6.7561	6.7202	7.3578	6.6823	8.2389	6.6446	7.9880	6.7552	8.5138
B3P86	4.1878	4.9452	5.4647	5.4229	6.1250	5.4065	6.9794	5.3737	6.7844	5.4728	7.2430	4.1878	4.9452	5.4647	5.4229	6.1249	5.4065	6.9794	5.3738	6.7844	5.4729	7.2429
B3PW91	4.1874	4.9911	5.4440	5.5274	6.4505	5.4976	7.0572	5.4613	6.7798	5.5577	7.3394	4.1874	4.9911	5.4440	5.5274	6.1882	5.4976	7.0572	5.4613	6.7798	5.5577	7.3394
B98	4.3422	5.0620	5.5562	5.5850	6.2579	5.5666	7.0704	5.5462	6.8209	5.6045	7.3494	4.3422	5.0620	5.5562	5.5850	6.2579	5.5666	7.0704	5.5462	6.8209	5.6045	7.3494
B971	4.2172	4.9232	5.4102	5.4267	6.1280	5.4012	6.9228	5.3751	6.6639	5.4560	7.1996	4.2172	4.9232	5.4102	5.4267	6.1281	5.4012	6.9228	5.3751	6.6639	5.4560	7.1996
B972	2.9476	3.3032	3.7135	3.7546	4.2645	3.7240	5.0766	3.6921	4.8153	3.7812	5.3455	2.9476	3.3032	3.7134	3.7546	4.2645	3.7240	5.0765	3.6921	4.8153	3.7812	5.3455
BHandH	6.0860	6.7388	7.2052	7.1656	7.6912	7.1333	8.4638	7.1112	8.2594	7.1795	8.7115	6.0860	6.7388	7.2052	7.1656	7.6057	7.1333	8.4638	7.1112	8.2594	7.1795	8.7116
BHandHLYP	5.2088	5.8696	6.3152	6.3283	6.9277	6.2971	7.8405	6.2683	7.5843	6.3585	8.1164	5.2088	5.8696	6.3152	6.3283	6.9278	6.2971	7.8405	6.2683	7.5842	6.3585	8.1164
BLYP	5.9078	6.8342	7.3429	7.3509	8.0945	7.5608	8.6446	7.3632	8.6401	7.7063	8.9842	5.9078	6.8342	7.3429	7.3509	8.0945	7.5608	8.6447	7.3632	8.6401	7.7063	8.9842
BMK	14.7148	15.7195	16.4223	16.2435	17.1400	16.1989	17.9522	16.3306	17.6302	16.4205	*18.2064*	14.7148	15.7195	16.4223	16.2435	17.1400	16.1989	17.9523	16.3306	17.6302	16.4205	*18.2064*
BP86	4.3374	5.1699	5.5865	5.6214	6.2482	5.6001	6.9883	5.5746	6.7456	5.6379	7.4099	4.3374	5.1699	5.5865	5.6214	6.2482	5.6001	6.9883	5.5746	6.7456	5.6379	7.4100
CAM-B3LYP	6.1868	7.1223	7.5994	7.7164	8.4084	7.6787	9.3540	7.6397	9.0821	7.7532	9.6461	6.1868	7.1223	7.5994	7.7164	8.4084	7.6787	9.3540	7.6397	9.0821	7.7532	9.6461
HF	5.8976	5.9723	6.2169	6.1610	6.4542	6.1469	7.2174	6.1336	6.9807	6.1749	7.3981	5.8976	5.9723	6.2169	6.1610	6.4542	6.1469	7.2174	6.1336	6.9806	6.1749	7.3981
LC-BLYP	9.3338	10.3021	10.7855	10.8990	11.4360	10.8459	12.5223	10.8110	12.2748	10.9393	12.8152	9.3338	10.3021	10.7855	10.8990	11.4361	10.8458	12.5223	10.8110	12.2748	10.9393	12.8152
M06	4.7284	5.5127	6.0657	6.0809	6.7381	6.0365	7.5961	5.9978	7.3613	6.1334	7.8917	4.7284	5.5127	6.0657	6.0809	6.7381	6.0365	7.5961	5.9978	7.3613	6.1334	7.8917
M06-2X	14.0732	15.3170	15.8437	15.9457	16.6500	15.9226	17.5123	15.9006	17.2348	15.9630	17.8368	14.0732	15.3170	15.8437	15.9457	16.6500	15.9226	17.5123	15.9006	17.2348	15.9630	17.8368
mpW1LYP	5.2420	6.0870	6.6031	6.7005	7.3161	6.6621	8.1872	6.6249	7.9526	6.7357	8.4553	5.2420	6.0870	6.6032	6.7005	7.3161	6.6621	8.1872	6.6249	7.9526	6.7357	8.4553
mpW1PW91	4.0578	4.7682	5.2185	5.2751	5.9295	5.2409	6.7913	5.2107	6.5398	5.3071	7.0688	4.0578	4.7682	5.2185	5.2751	5.9295	5.2409	6.7913	5.2107	6.5398	5.3071	7.0688
O3LYP	**2.7466**	2.9604	3.4243	3.4665	4.0857	3.4413	4.7136	3.4134	4.5404	3.4868	4.9484	**2.7465**	2.9604	3.4243	3.4665	4.0857	3.4413	4.7136	3.4134	4.5404	3.4868	4.9483
OLYP	3.1276	**3.0554**	3.3304	3.3524	3.8639	3.3312	4.3463	3.3078	4.2165	3.3674	4.5443	3.1276	**3.0554**	3.3305	3.3524	3.8639	3.3312	4.3463	3.3078	4.2165	3.3674	4.5443
OPBE	3.3814	2.4438	**2.2828**	2.3190	2.3597	2.3219	2.7365	2.3238	2.6276	2.3165	2.9255	3.3814	2.4438	**2.2828**	2.3190	2.3597	2.3219	2.7365	2.3238	2.6276	2.3165	2.9255
OPW91	3.2568	2.4026	**2.2942**	2.3326	2.4467	2.3313	2.8552	2.3279	2.7400	2.3310	3.0566	3.2568	2.4026	**2.2942**	2.3326	2.4467	2.3313	2.8552	2.3279	2.7400	2.3310	3.0567
PBE	4.1211	4.9043	5.3506	5.3599	6.1084	5.3271	6.8404	5.3038	6.6107	5.4062	7.1466	4.1212	4.9043	5.3506	5.3599	6.1084	5.3271	6.8404	5.3038	6.6107	5.4062	7.1466
PBE0	3.9246	4.5981	5.0370	5.0622	5.7089	5.0247	6.6118	4.9898	6.3284	5.1012	6.8407	3.9246	4.5981	5.0370	5.0622	5.7089	5.0247	6.6119	4.9898	6.3284	5.1012	6.8407
TPSS	3.3957	3.5754	3.9230	3.8689	4.3200	3.8523	4.9594	3.8443	4.0744	3.8925	5.2231	3.3957	3.5754	3.9230	3.8689	4.3200	3.8523	4.9594	3.8443	5.0182	3.8925	5.2231
VSXC	5.9525	6.0963	6.2824	6.3164	6.6487	6.3023	6.9352	6.2872	6.8369	6.3311	7.1599	5.9525	6.0963	6.2824	6.3164	6.6487	6.3023	6.9352	6.2872	6.8369	6.3311	7.1598
wB97	4.4867	5.0959	5.5194	5.5765	6.0838	5.5421	7.0485	5.5082	6.8076	5.6104	7.3298	4.4867	5.0959	5.5194	5.5765	6.0838	5.5421	7.0485	5.5082	6.8076	5.6104	7.3298
wB97X	4.8569	5.6247	6.0779	6.1939	6.8246	6.1498	7.7455	6.1064	7.4408	6.2355	8.0168	4.8569	5.6247	6.0779	6.1939	6.8246	6.1498	7.7455	6.1064	7.4408	6.2354	8.0168
X3LYP	5.2508	6.1252	6.6399	6.7259	7.3754	6.6934	8.2409	6.6585	8.0023	6.7598	8.5258	5.2508	6.1252	6.6399	6.7259	7.3754	6.6934	8.2409	6.6585	8.0023	6.7598	8.5258

Table S19. Cont. II

Method	R	S
	4-fluoro-α-pyrrolidinohexiophenone [5]	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	4.7643	5.7395	6.2266	6.2829	6.8344	6.2442	8.0678	6.2058	7.8372	6.3187	8.0044	4.9393	5.8963	6.3723	6.4239	6.9641	6.3864	8.1809	6.3491	7.6608	6.4586	8.1121
B3P86	3.7430	4.5038	4.9985	5.0092	5.5575	4.9924	6.4438	4.9604	6.2832	5.0556	6.7157	3.9555	4.6948	5.1749	5.1791	5.7104	5.1632	6.5807	5.1325	6.4242	5.2236	6.8407
B3PW91	3.7650	4.5908	5.0298	5.0987	5.8716	5.0700	6.5448	5.0353	6.3019	5.1275	6.7900	3.9766	4.7781	5.2051	5.2656	5.7799	5.2382	6.6794	5.2049	6.4422	5.2931	6.9128
B98	3.8158	4.6002	5.0680	5.1011	5.6931	5.0815	6.5634	5.0600	6.3256	5.1215	6.8105	4.0295	4.7894	5.2438	5.2687	5.8440	5.2502	6.6987	5.2298	6.4661	5.2881	6.9349
B971	3.7076	4.4656	4.9216	4.9692	5.5554	4.9440	6.4092	4.9183	6.1757	4.9979	6.6668	3.9266	4.6598	5.1021	5.1409	5.7094	5.1169	6.5473	5.0925	6.3193	5.1681	6.7935
B972	2.8397	3.1805	3.4990	3.6450	4.2996	3.6122	5.1584	3.5792	4.9421	3.6752	5.4113	3.1135	3.4424	3.7435	3.8730	4.4958	3.8425	5.3269	3.8118	5.1173	3.9010	5.5640
BHandH	5.7641	6.3815	6.8206	6.7934	7.2484	6.7619	8.1297	6.7392	7.9060	6.8091	8.3809	5.8916	6.5032	6.9386	6.9081	7.2843	6.8773	8.2312	6.8550	8.0094	6.9235	8.4752
BHandHLYP	4.9468	5.6228	6.0383	6.1160	6.5343	6.0857	7.4797	6.0567	7.2432	6.1446	7.7291	5.1055	5.7714	6.1771	6.2495	6.6593	6.2202	7.5916	6.1923	7.3587	6.2772	7.8322
BLYP	5.3511	6.3148	6.7862	6.8782	7.7840	7.0820	8.3596	6.8886	8.3750	7.2235	8.6774	5.5134	6.4646	6.9271	7.0150	7.9039	7.2152	8.4744	7.0258	8.4888	7.3536	8.7838
BMK	13.7854	14.7526	15.3958	15.2618	16.1758	15.2177	17.0536	15.3449	16.7140	15.4344	*17.3541*	13.8464	14.8108	15.4507	15.3144	16.2257	15.2707	17.1030	15.3977	16.7639	15.4861	17.4057
BP86	3.7394	4.5997	5.0308	5.0474	5.5994	5.0265	6.3653	5.0013	6.1569	5.0633	6.7582	3.9613	4.7986	5.2179	5.2276	5.7610	5.2078	6.5141	5.1838	6.3112	5.2425	6.8913
CAM-B3LYP	5.7415	6.6996	7.1522	7.2741	7.8357	7.2420	8.7902	7.2100	8.5405	7.3061	9.0454	5.8812	6.8265	7.2737	7.3887	7.9415	7.3574	8.8874	7.3262	8.6407	7.4200	9.1351
HF	5.9827	6.0884	6.2841	6.3445	6.6162	6.3232	7.4887	6.3029	7.2707	6.3652	7.6476	6.1044	6.2125	6.4043	6.4614	6.7271	6.4407	7.5887	6.4210	7.3728	6.4814	7.7424
LC-BLYP	8.8115	9.7653	10.2858	10.3827	10.8963	10.3341	11.9259	10.3009	11.6547	10.4183	12.1911	8.8945	9.8441	10.3624	10.4558	10.9651	10.4077	11.9910	10.3748	11.7213	10.4911	12.2519
M06	4.2339	5.1153	5.5912	5.6738	6.4887	5.6323	7.3861	5.5946	7.1544	5.7210	7.6800	4.4194	5.2737	5.7363	5.8184	6.6164	5.7778	7.5051	5.7408	7.2768	5.8645	7.7937
M06-2X	13.2380	14.3737	14.9951	15.0304	15.7390	15.0028	16.8187	14.9764	16.4887	15.0524	17.1993	14.0732	15.3170	15.8437	15.9457	16.6500	15.9226	17.5123	15.9006	17.2348	15.9630	*17.8368*
mpW1LYP	4.8329	5.7277	6.1983	6.3025	6.8321	6.2643	7.7495	6.2272	7.5086	6.3378	7.9723	5.0060	5.8843	6.3443	6.4421	6.9612	6.4050	7.8663	6.3691	7.6292	6.4762	8.0796
mpW1PW91	3.7154	4.4265	4.8438	4.9078	5.4206	4.8772	6.3176	4.8503	6.0808	4.9365	6.5697	3.9278	4.6175	5.0227	5.0780	5.5744	5.0488	6.4542	5.0231	6.2233	5.1054	6.6946
O3LYP	**2.8660**	3.1543	3.6039	3.6651	4.1457	3.6398	4.8673	3.6102	4.6969	3.6847	5.0709	**3.1436**	3.4224	3.8397	3.8944	4.3475	3.8709	5.0442	3.8435	4.8789	3.9123	5.2353
OLYP	**3.2802**	3.3450	3.5820	3.6388	4.0728	3.6227	4.6120	3.6043	4.5089	3.6499	4.7826	**3.5288**	3.6021	3.8207	3.8721	4.2804	3.8574	4.7999	3.8405	4.7000	3.8822	4.9600
OPBE	3.6942	3.0317	**2.8425**	2.9760	2.9056	2.9746	3.3443	2.9754	3.2340	2.9779	3.4418	3.9062	3.3015	**3.1324**	3.2469	3.1856	3.2460	3.5929	3.2471	3.4901	3.2484	3.6740
OPW91	3.5595	2.9641	**2.8174**	2.9525	2.9404	2.9501	3.4134	2.9488	3.2960	2.9554	3.5229	3.7794	3.2401	**3.1099**	3.2259	3.2177	3.2241	3.6576	3.2232	3.5476	3.2283	3.7507
PBE	3.6155	4.4029	4.8738	4.8230	5.5093	4.7939	6.2539	4.7733	6.0467	4.8645	6.5305	3.8445	4.6077	5.0643	5.0090	5.6710	4.9813	6.4028	4.9618	6.2015	5.0486	6.6655
PBE0	3.6207	4.2753	4.6854	4.7411	5.2371	4.7089	6.1691	4.6778	5.9012	4.7737	6.3887	3.8378	4.4719	4.8696	4.9167	5.3954	4.8859	6.3084	4.8563	6.0471	4.9478	6.5167
TPSS	**3.1456**	3.2860	3.5777	3.5729	3.9441	3.5567	4.6387	3.5477	3.7383	3.5949	4.8890	**3.3861**	3.5369	3.8100	3.8018	4.1515	3.7872	4.8236	3.7792	4.8228	3.8219	5.0575
VSXC	5.8605	6.0658	6.2422	6.3087	6.6760	6.2936	6.9707	6.2775	6.8480	6.3243	7.2076	5.9278	6.1410	6.3149	6.3841	6.7498	6.3690	7.0436	6.3529	6.9200	6.3996	7.2833
wB97	4.2485	4.8497	5.2567	5.3309	5.7999	5.3006	6.7730	5.2695	6.5287	5.3593	7.0503	4.4128	5.0002	5.4006	5.4672	5.9250	5.4378	6.8841	5.4076	6.6435	5.4947	7.1510
wB97X	4.5439	5.2980	5.7444	5.8515	6.3621	5.8215	7.3188	5.7906	7.0858	5.8799	7.5944	4.7084	5.4458	5.8852	5.9843	6.4826	5.9551	7.4284	5.9252	7.1980	6.0118	7.6942
X3LYP	4.8063	5.7286	6.2015	6.3005	6.8625	6.2674	7.7644	6.2321	7.5264	6.3347	8.0043	4.9800	5.8855	6.3481	6.4407	6.9914	6.4087	7.8815	6.3745	7.6474	6.4738	8.1116
Method	**4-fluoro-α-pyrrolidinohexiophenone [6]**																					
B3LYP	4.8545	5.8352	6.3290	6.3762	6.9382	6.3377	8.1685	6.2997	7.9350	6.4116	8.1197	5.0826	6.0406	6.5200	6.5612	7.1086	6.5244	8.3176	6.4877	7.8105	6.5953	8.2614
B3P86	3.8072	4.5835	5.0960	5.0904	5.6541	5.0739	6.5538	5.0417	6.3924	5.1371	6.8280	4.0841	4.8329	5.3263	5.3128	5.8543	5.2974	6.7332	5.2671	6.5771	5.3571	6.9920
B3PW91	3.8266	4.6688	5.1236	5.1786	5.9700	5.1501	6.6539	5.1154	6.4090	5.2072	6.9012	4.1026	4.9136	5.3527	5.3973	5.9219	5.3704	6.8303	5.3376	6.5929	5.4243	7.0624
B98	3.8726	4.6748	5.1575	5.1781	5.7844	5.1588	6.6697	5.1375	6.4294	5.1982	6.9184	4.1518	4.9222	5.3873	5.3979	5.9823	5.3800	6.8472	5.3600	6.6138	5.4166	7.0818
B971	3.7594	4.5365	5.0094	5.0430	5.6445	5.0180	6.5133	4.9924	6.2773	5.0717	6.7727	4.0455	4.7905	5.2452	5.2681	5.8463	5.2446	6.6945	5.2207	6.4655	5.2948	6.9391
B972	**2.7703**	3.1571	3.5100	3.6391	4.3103	3.6057	5.2008	3.5719	4.9773	3.6696	5.4585	**3.1389**	3.5052	3.8325	3.9413	4.5699	3.9110	5.4231	3.8804	5.2087	3.9689	5.6599
BHandH	5.8192	6.4510	6.9036	6.8673	7.3313	6.8355	8.2269	6.8128	8.0013	6.8829	8.4807	5.9874	6.6115	7.0590	7.0187	7.4025	6.9877	8.3608	6.9655	8.1377	7.0339	8.6052
BHandHLYP	4.9904	5.6794	6.1066	6.1743	6.6038	6.1440	7.5638	6.1150	7.3253	6.2030	7.8150	5.1997	5.8753	6.2894	6.3506	6.7687	6.3215	7.7115	6.2938	7.4777	6.3780	7.9511
BLYP	5.4594	6.4260	6.9007	6.9861	7.8865	7.1918	8.4733	6.9979	8.4879	7.3329	8.7907	5.6707	6.6219	7.0853	7.1656	8.0441	7.3666	8.6243	7.1778	8.6376	7.5037	8.9308
BMK	13.9464	14.9147	15.5588	15.4226	16.3398	15.3787	17.2196	15.5059	16.8792	15.5950	*17.5223*	14.0269	14.9917	15.6315	15.4922	16.4058	15.4488	17.2851	15.5758	16.9453	15.6635	*17.5907*
BP86	3.8203	4.6951	5.1408	5.1430	5.7122	5.1224	6.4902	5.0974	6.2798	5.1585	6.8855	4.1079	4.9540	5.3842	5.3781	5.9231	5.3589	6.6845	5.3355	6.4813	5.3923	7.0596
CAM-B3LYP	5.8417	6.8018	7.2636	7.3740	7.9427	7.3421	8.9058	7.3104	8.6549	7.4058	9.1621	6.0246	6.9685	7.4231	7.5248	8.0820	7.4939	9.0339	7.4632	8.7869	7.5556	9.2804
HF	5.9425	6.0625	6.2717	6.3235	6.5973	6.3021	7.4973	6.2817	7.2734	6.3442	7.6587	6.1056	6.2287	6.4323	6.4798	6.7456	6.4593	7.6306	6.4397	7.4096	6.4997	7.7850
LC-BLYP	8.9383	9.8912	10.4161	10.5059	11.0225	10.4574	12.0581	10.4244	11.7860	10.5414	12.3243	9.0475	9.9950	10.5170	10.6025	11.1134	10.5546	12.1442	10.5220	11.8741	10.6375	12.4047
M06	4.2625	5.1507	5.6487	5.7128	6.5296	5.6710	7.4475	5.6330	7.2117	5.7607	7.7424	4.5077	5.3606	5.8404	5.9045	6.6990	5.8639	7.6054	5.8270	7.3740	5.9510	7.8934
M06-2X	13.3863	14.5235	15.1467	15.1790	15.8893	15.1515	16.9710	15.1254	16.6415	15.2008	17.3520	13.4715	14.6044	15.2258	15.2543	15.9616	15.2271	17.0397	15.2012	16.7127	15.2758	17.4166
mpW1LYP	4.9115	5.8129	6.2928	6.3870	6.9268	6.3490	7.8554	6.3121	7.6129	6.4221	8.0794	5.1379	6.0184	6.4843	6.5705	7.0965	6.5340	8.0091	6.4986	7.7715	6.6041	8.2206
mpW1PW91	3.7539	4.4864	4.9234	4.9724	5.5021	4.9417	6.4154	4.9148	6.1763	5.0012	6.6703	4.0324	4.7368	5.1576	5.1959	5.7039	5.1670	6.5948	5.1416	6.3632	5.2230	6.8343
O3LYP	**2.7379**	3.0779	3.5567	3.6167	4.1165	3.5904	4.8813	3.5597	4.7031	3.6367	5.0911	**3.1180**	3.4394	3.8722	3.9237	4.3857	3.9001	5.1157	3.8723	4.9444	3.9416	5.3088
OLYP	**3.1265**	3.2387	3.5057	3.5612	4.0204	3.5442	4.6044	3.5245	4.4950	3.5728	4.7794	**3.4688**	3.5879	3.8272	3.8759	4.2986	3.8608	4.8541	3.8432	4.7494	3.8860	5.0151
OPBE	3.4729	2.8117	**2.6442**	2.7741	2.7368	2.7723	3.2517	2.7720	3.1258	2.7762	3.3589	3.7697	3.1918	**3.0504**	3.1541	3.1255	3.1531	3.5887	3.1532	3.4745	3.1556	3.6730
OPW91	3.3419	2.7540	**2.6323**	2.7644	2.7882	2.7611	3.3347	2.7580	3.2020	2.7674	3.4539	3.6499	3.1419	**3.0406**	3.1463	3.1711	3.1439	3.6643	3.1416	3.5431	3.1484	3.7609
PBE	3.6820	4.4875	4.9752	4.9089	5.6156	4.8800	6.3734	4.8598	6.1639	4.9505	6.6517	3.9797	4.7544	5.2234	5.1518	5.8269	5.1247	6.5680	5.1058	6.3661	5.1909	6.8282
PBE0	3.6477	4.3269	4.7582	4.7978	5.3121	4.7653	6.2626	4.7339	5.9914	4.8307	6.4846	3.9331	4.5848	4.9993	5.0285	5.5199	4.9979	6.4455	4.9684	6.1829	5.0594	6.6527
TPSS	**3.0726**	3.2521	3.5768	3.5557	3.9633	3.5390	4.6887	3.5298	3.7410	3.5786	4.9454	**3.3967**	3.5864	3.8840	3.8598	4.2368	3.8452	4.9317	3.8374	4.8952	3.8802	5.1668
VSXC	5.7885	6.0193	6.2160	6.2734	6.6553	6.2577	6.9770	6.2410	6.8478	6.2894	7.2184	5.8799	6.1209	6.3140	6.3751	6.7545	6.3595	7.0748	6.3428	6.9444	6.3910	7.3197
wB97	4.2885	4.9112	5.3330	5.3964	5.8787	5.3660	6.8659	5.3349	6.6190	5.4249	7.1473	4.5050	5.1091	5.5220	5.5759	6.0432	5.5467	7.0122	5.5167	6.7701	5.6031	7.2799
wB97X	4.6080	5.3750	5.8345	5.9296	6.4515	5.8998	7.4198	5.8690	7.1856	5.9579	7.7003	4.8237	5.5692	6.0192	6.1043	6.6099	6.0756	7.5641	6.0460	7.3333	6.1314	7.8317
X3LYP	4.8935	5.8211	6.3032	6.3917	6.9638	6.3589	7.8763	6.3238	7.6368	6.4256	8.1174	5.1202	6.0268	6.4954	6.5758	7.1332	6.5444	8.0304	6.5107	7.7959	6.6084	8.2587

Table S19. Cont. III

Method	**R**	**S**
	3,5-difluoromethcathinone	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	7.9601	9.1832	9.9798	9.9771	10.6351	9.9315	11.6213	9.8866	11.4573	10.0194	11.9450	7.7366	8.9608	9.7071	9.6830	10.4446	9.6480	11.6674	9.6122	11.3378	9.7140	11.8325
B3P86	6.4356	7.5736	8.3328	8.2676	9.0445	8.2417	10.0489	8.1964	9.9905	8.3366	10.3680	6.1619	7.3100	8.1000	8.0420	8.7978	8.0232	9.9251	7.9856	9.7010	8.0971	10.1431
B3PW91	6.4647	7.7326	8.4135	8.4906	9.4816	8.4530	10.1660	8.4078	10.0021	8.5290	10.5516	6.2213	7.4157	8.1376	8.1765	8.9220	8.1472	10.2048	8.1101	9.8826	8.2057	10.3841
B98	6.6574	7.7125	8.4787	8.4978	9.1699	8.4730	10.1021	8.4461	9.9650	8.5242	10.4306	6.0803	7.2230	7.9758	8.0025	8.7809	7.9824	10.0166	7.9598	9.7018	8.0230	10.1917
B971	6.5215	7.5565	8.3214	8.3379	9.0063	8.3064	9.9341	8.2742	9.7991	8.3733	10.2636	5.9310	7.0699	7.8164	7.8440	8.6121	7.8167	9.8251	7.7887	9.4822	7.8750	9.9985
B972	4.4531	5.5623	6.0805	6.2494	6.8839	6.2052	7.9702	6.1592	7.6378	6.2887	8.3208	3.8916	4.9896	5.6990	5.8337	6.4792	5.7928	7.8146	5.7504	7.6202	5.8706	8.0212
BHandH	7.3045	8.4474	9.1188	9.0888	9.8899	9.0382	10.7795	9.0050	10.5297	9.1089	11.1060	7.6117	8.6838	9.4882	9.3525	9.9540	9.3094	11.1665	9.2806	10.9366	9.3694	11.4048
BHandHLYP	7.0613	8.1265	8.7312	8.9507	9.5932	8.9055	10.6103	8.7931	10.4619	8.9921	10.9154	7.1301	8.2007	8.9104	8.9159	9.6141	8.8838	10.8563	8.8534	10.5361	8.9462	11.0566
BLYP	8.8083	10.0765	10.6793	10.7139	11.4773	10.9257	12.1931	10.7136	12.2079	11.0950	12.6247	8.2966	9.4711	10.2613	10.2118	11.1572	10.4175	12.0370	10.2224	11.9342	10.5598	12.2791
BMK	19.0033	20.1416	20.9803	20.7891	21.8584	20.7333	22.7499	20.8783	22.3396	20.9953	*23.0639*	18.8327	19.9487	20.8894	20.7452	21.7363	20.6947	22.8058	20.8346	22.4087	20.9389	*22.9744*
BP86	6.7952	7.9841	8.6699	8.6790	9.3079	8.6511	10.1853	8.6186	10.0463	8.7013	10.6766	6.1072	7.3386	8.0197	8.0198	8.7481	7.9964	9.8420	7.9681	9.5085	8.0378	10.1393
CAM-B3LYP	8.9704	10.1644	10.8739	10.9558	11.6866	10.8975	12.6973	10.8488	12.5576	11.0479	13.0162	9.0127	10.1774	10.8940	10.9203	11.6669	10.8896	12.9416	10.8590	12.6012	10.9512	13.1227
HF	5.3982	6.1163	6.5606	6.9259	7.2642	6.8711	8.6368	6.8015	8.3870	6.9730	8.9119	5.5904	6.2911	7.1704	7.2139	7.7936	7.1719	8.8781	7.1320	8.6251	7.2555	9.1139
LC-BLYP	12.2498	13.3972	14.1920	14.1509	14.9360	14.0865	15.9501	14.0464	15.8581	14.1959	16.2468	12.6136	13.7086	14.5066	14.4957	15.2204	14.4368	16.5566	14.4006	16.0576	14.5376	16.7357
M06	6.2460	7.4007	8.0740	8.1240	8.9669	8.0630	9.9773	8.0119	9.8427	8.1985	10.2971	6.3462	7.3993	8.1403	8.0974	8.8470	8.0532	10.1706	8.0155	9.8597	8.1516	10.3377
M06-2X	17.7407	19.0515	19.7688	19.7408	20.6202	19.7157	21.5877	19.6925	21.2766	19.7593	21.9604	17.9143	19.1665	20.0127	19.9896	20.8342	19.9655	22.0211	19.9429	21.6831	20.0072	22.3168
mpW1LYP	7.8960	9.0311	9.8408	9.8892	10.5205	9.8429	11.4781	9.7982	11.3403	9.9321	11.7837	7.7056	8.8639	9.6048	9.6301	10.3618	9.5944	11.5509	9.5594	11.2307	9.6615	11.7082
mpW1PW91	6.0882	7.2453	7.9918	8.0463	8.7217	8.0044	9.7151	7.9673	9.5686	8.0852	10.0504	5.8899	7.0331	7.7658	7.7904	8.5254	7.7557	9.8081	7.7256	9.4596	7.8226	9.9776
O3LYP	4.1885	5.2956	5.8774	6.1052	6.7787	6.0540	7.7020	6.0036	7.5937	6.1600	7.9971	3.3637	4.6574	5.4566	5.6433	6.2712	5.5967	7.3850	5.5481	7.1811	5.6843	7.5965
OLYP	4.2988	5.2659	5.6689	6.0801	6.7772	5.9137	7.6076	5.8565	7.4212	6.1140	7.8392	3.0483	4.2072	4.8153	5.1378	5.6153	5.0974	6.7175	5.0546	6.5031	5.1716	6.9227
OPBE	**3.5811**	4.0669	4.1488	4.5792	5.0722	4.5352	5.9261	4.4871	5.7205	4.6161	6.1603	**2.4643**	3.0495	3.1890	3.6900	4.1529	3.6344	5.1301	3.5786	4.8017	3.7499	5.2814
OPW91	**3.5468**	4.1337	4.2541	4.6712	5.2069	4.6212	6.0776	4.5692	5.8680	4.7097	6.3133	**2.4091**	3.1301	3.3181	3.7915	4.3026	3.7354	5.2829	3.6775	4.9594	3.8418	5.4415
PBE	6.5115	7.6569	8.3732	8.3119	9.1059	8.2607	9.9806	8.2182	9.8569	8.3681	10.3368	5.9095	7.1029	7.8326	7.7680	8.6272	7.7343	9.6872	7.7094	9.3557	7.8148	9.8461
PBE0	5.8152	6.9378	7.6333	7.6399	8.3821	7.5880	9.4571	7.5401	9.2605	7.6953	9.7309	5.6106	6.7530	7.4850	7.4956	8.2174	7.4544	9.4936	7.4147	9.0807	7.5370	9.6248
TPSS	4.9837	5.6904	6.2543	6.2573	6.8978	6.2253	7.7546	6.2032	6.5524	6.2975	8.0722	3.9036	4.8266	5.5155	5.4885	6.1618	5.4583	7.1464	5.4371	6.4079	5.5255	7.3561
VSXC	6.8671	7.1197	7.3867	7.4234	7.8602	7.4013	8.1719	7.3788	8.0639	7.4462	8.4308	5.2043	5.3564	5.5918	5.8035	6.3481	5.7864	6.6589	5.7685	6.5143	5.8210	6.9188
wB97	6.3957	7.2974	8.0356	7.9321	8.7195	7.8885	9.6068	7.8442	9.4447	7.9737	9.9208	6.3017	7.2529	7.9869	7.9907	8.7016	7.9511	9.8060	7.9111	9.4633	8.0288	10.0509
wB97X	7.1335	8.1256	8.8784	8.8204	9.5987	8.7779	10.5615	8.7339	10.4216	8.8608	10.8578	7.0475	8.0778	8.8216	8.8497	9.5578	8.8119	10.9186	8.7735	10.3389	8.8867	11.0517
X3LYP	7.9415	9.1098	9.9170	9.9590	10.6248	9.9190	11.5813	9.8764	11.4396	10.0015	11.9003	7.7419	8.9212	9.6620	9.6819	10.4424	9.6518	11.6247	9.6184	11.2980	9.7130	11.7920
Method	**Flephedrone [9]**																					
B3LYP	6.9621	8.2667	9.0183	8.9824	9.8376	8.9292	10.9925	8.8775	10.7155	9.0327	11.3611	6.7742	8.1984	8.8497	8.9106	9.6984	8.8632	10.8960	8.8162	10.5662	8.9547	11.0973
B3P86	5.6548	6.8435	7.6244	7.5299	8.4309	7.5064	9.5145	7.4622	9.3753	7.5945	9.8879	5.4053	6.7447	7.4387	7.4632	8.2445	7.4348	9.4140	7.3887	9.1621	7.5280	9.6399
B3PW91	5.6709	6.9114	7.6427	7.6194	8.8316	7.5763	9.6495	7.5256	9.3783	7.6632	10.0258	5.4646	6.8666	7.4706	7.5793	8.3588	7.5375	9.5777	7.4892	9.2304	7.6222	9.8012
B98	5.8795	6.9725	7.6541	7.6175	8.5084	7.5902	9.5214	7.5606	9.3098	7.6463	9.9031	5.2838	6.6313	7.2802	7.3643	8.1775	7.3312	9.3523	7.2965	9.0341	7.3984	9.5749
B971	5.7310	6.8151	7.4842	7.4591	8.3271	7.4250	9.3117	7.3907	9.1196	7.4975	9.7169	5.1144	6.4585	7.1091	7.1987	7.9995	7.1584	9.1537	7.1185	8.8424	7.2429	9.3857
B972	3.8209	4.7299	5.3649	5.4567	6.2224	5.4088	7.4158	5.3602	7.2216	5.4987	7.7259	3.2800	4.4871	5.0451	5.2327	5.9159	5.1848	7.1761	5.1358	6.8284	5.2765	7.4008
BHandH	7.3494	8.5170	9.2758	9.1925	10.0179	9.1407	10.9873	9.1060	10.7203	9.2139	11.3024	7.7522	8.9152	9.6517	9.5719	10.1621	9.5225	11.3873	9.4878	11.1049	9.5956	11.6306
BHandHLYP	6.6983	7.8109	8.4627	8.4976	9.3211	8.4536	10.4465	8.4122	10.2322	8.5395	10.8067	6.8863	8.0463	8.6775	8.7409	9.4415	8.6987	10.6111	8.6587	10.2946	8.7811	10.8329
BLYP	7.3747	8.6706	9.2773	9.4332	10.2622	9.6468	11.2217	9.4283	11.0747	9.8103	11.6702	6.7703	8.2475	8.9377	8.9948	9.9115	9.1898	10.8475	8.9850	10.7532	9.3526	11.1247
BMK	18.7282	20.0567	20.9890	20.8038	21.8435	20.7442	22.8706	20.8846	22.5295	21.0130	*23.1170*	18.6410	20.0378	20.8954	20.7687	21.8367	20.7077	22.9343	20.8376	22.5511	20.9729	*23.1596*
BP86	5.6385	6.8651	7.5044	7.4625	8.2778	7.4301	9.2675	7.3932	9.0535	7.4892	9.8084	4.8233	6.3052	6.8941	6.9991	7.7548	6.9629	8.8618	6.9229	8.5721	7.0301	9.2290
CAM-B3LYP	8.1687	9.4878	10.1924	10.2221	11.1372	10.1787	12.2650	10.1361	12.0229	10.2657	12.6403	8.3275	9.7084	10.3313	10.4379	11.2118	10.3953	12.4138	10.3536	12.0658	10.4814	12.6387
HF	6.0616	6.6339	7.1424	7.1823	7.7992	7.1453	8.9135	7.1104	8.6320	7.2179	9.2317	6.5382	7.1455	7.6222	7.6002	8.1730	7.5708	9.3173	7.5419	8.9991	7.6280	9.5244
LC-BLYP	11.8205	13.1267	13.9252	13.9122	14.7258	13.8429	15.8014	13.7985	15.7304	13.9629	16.3440	12.3345	13.6443	14.3552	14.4000	15.1371	14.3332	16.3465	14.2896	15.9924	14.4505	16.5840
M06	5.8510	7.0352	7.8612	7.7436	8.7126	7.6898	9.7626	7.6437	9.5597	7.8084	10.0951	6.0772	7.2690	7.9305	7.9499	8.7436	7.8977	9.9052	7.8523	9.5865	8.0119	10.1033
M06-2X	17.9861	19.4351	20.2578	20.1922	21.1235	20.1645	22.1862	20.1382	21.9243	20.2127	22.5420	18.1652	19.6661	20.4205	20.4610	21.3298	20.4250	22.5360	20.3917	22.1954	20.4916	22.8326
mpW1LYP	6.9762	8.2024	8.9320	8.9425	9.7914	8.8914	10.8948	8.8424	10.6701	8.9903	11.2447	6.8284	8.1766	8.8334	8.9393	9.6912	8.8904	10.8456	8.8430	10.5454	8.9846	11.0461
mpW1PW91	5.4323	6.6009	7.3476	7.2884	8.2046	7.2444	9.3072	7.2061	9.0533	7.3300	9.6765	5.2827	6.6143	7.2340	7.3206	8.0924	7.2746	9.2912	7.2344	8.9409	7.3652	9.5140
O3LYP	**3.4590**	4.4324	4.7494	5.2130	5.9242	5.1779	6.9428	5.1485	6.7096	5.2417	7.2246	**2.5566**	3.8083	4.4897	4.6190	5.3223	4.5697	6.5328	4.5187	6.2422	4.6634	6.7521
OLYP	**3.7095**	4.3230	4.9222	5.0871	5.8913	5.0637	6.3246	5.0371	6.1388	5.1050	6.5916	**1.6149**	3.2794	3.8195	4.0329	4.5939	3.9844	5.6780	3.9336	5.4368	4.0745	5.9004
OPBE	3.6197	**3.4297**	3.6726	3.8872	4.4041	3.8761	4.8018	3.8583	4.6099	3.8865	5.0120	2.6750	**2.4194**	2.6260	2.8627	3.2026	2.8242	4.1035	2.7818	3.9853	2.8922	4.3156
OPW91	3.5251	**3.4559**	3.7507	3.9599	4.5265	3.9433	4.9261	3.9202	4.7463	3.9676	5.1591	2.5336	**2.4261**	2.7083	2.9248	3.3300	2.8833	4.2532	2.8372	4.1231	2.9570	4.4713
PBE	5.3752	6.5570	7.2642	7.1477	8.1470	7.1070	9.0948	7.0767	8.8745	7.2031	9.5151	4.6486	6.1033	6.7441	6.7762	7.6721	6.7302	8.7611	6.6941	8.4727	6.8359	9.0100
PBE0	5.1914	6.3508	7.0627	7.0246	7.9147	6.9767	9.0590	6.9309	8.7678	7.0733	9.3715	5.0435	6.3625	6.9950	7.0656	7.8208	7.0153	9.0613	6.9676	8.6730	7.1171	9.2429
TPSS	**4.2746**	4.8733	5.4131	5.3741	6.0164	5.3463	6.8900	5.3280	5.6333	5.4094	7.2540	**2.9760**	3.9390	4.5261	4.6038	5.2417	4.5662	6.3167	4.5377	5.5046	4.6479	6.5536
VSXC	6.4872	6.6136	6.8206	6.8364	7.2130	6.8216	7.5641	6.8060	7.4433	6.8517	7.8250	4.9917	4.9776	5.1434	5.1994	5.5620	5.1817	6.0065	5.1638	5.8416	5.2179	6.2602
wB97	5.7671	6.8158	7.5311	7.4985	8.2896	7.4529	9.2674	7.4070	9.0517	7.5426	9.5899	5.8436	6.9866	7.6468	7.6862	8.4015	7.6370	9.5596	7.5889	9.2295	7.7351	9.8165
wB97X	6.4494	7.5984	8.3216	8.3098	9.1141	8.2655	10.1262	8.2210	9.9721	8.3533	10.6126	6.5188	7.7680	8.4245	8.4922	9.2235	8.4436	10.4450	8.3958	10.0438	8.5411	10.6769
X3LYP	6.9888	8.2453	8.9851	8.9820	9.8643	8.9369	10.9657	8.8898	10.7351	9.0291	11.3284	6.8267	8.2046	8.8575	8.9613	9.7434	8.9179	10.8959	8.8721	10.5898	9.0062	11.1078

Table S19. Cont. IV

Method	**R**	**S**
	Flephedrone [10]	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	5.8263	7.2032	7.9620	7.9661	8.7999	7.9098	10.0557	7.8550	9.7651	8.0197	10.4340	5.8890	7.3281	7.9621	8.0582	8.8061	8.0101	10.0837	7.9623	9.7401	8.1030	10.2841
B3P86	4.5132	5.7758	6.5579	6.5083	7.3832	6.4814	8.5805	6.4344	8.4217	6.5747	8.9620	4.5636	5.9056	6.5748	6.6400	7.3645	6.6093	8.6234	6.5626	8.3497	6.7037	8.8455
B3PW91	4.5273	5.8454	6.5839	6.6040	7.7821	6.5573	8.7224	6.5033	8.4358	6.6512	9.1074	4.6224	6.0283	6.6108	6.7575	7.4825	6.7146	8.7937	6.6659	8.4292	6.8012	9.0133
B98	4.7111	5.8681	6.5546	6.5584	7.4289	6.5278	8.5557	6.4950	8.3259	6.5903	8.9476	4.3234	5.7119	6.3472	6.4721	7.2403	6.4366	8.5170	6.3996	8.1792	6.5082	8.7394
B971	4.5734	5.7189	6.3908	6.4068	7.2525	6.3697	8.3508	6.3324	8.1400	6.4479	8.7667	4.1700	5.5512	6.1875	6.3174	7.0711	6.2752	8.3266	6.2334	7.9962	6.3630	8.5583
B972	2.8190	3.7360	4.3493	4.5167	5.2223	4.4647	6.5700	4.4124	6.3583	4.5629	6.8832	2.6841	3.7993	4.2933	4.5357	5.1226	4.4881	6.5009	4.4398	6.1335	4.5797	6.7178
BHandH	6.2133	7.4371	8.1974	8.1487	8.9484	8.0950	10.0129	8.0579	9.7268	8.1728	10.3316	6.9234	8.0797	8.7991	8.7393	9.2870	8.6905	10.5773	8.6552	10.2857	8.7643	10.8175
BHandHLYP	5.5261	6.7119	7.3678	7.4460	8.2500	7.3990	9.4991	7.3545	9.2630	7.4908	9.8649	6.0092	7.1787	7.7915	7.8871	8.5428	7.8441	9.8044	7.8030	9.4702	7.9280	10.0251
BLYP	6.3560	7.6992	8.2963	8.4989	9.2899	8.7002	10.3360	8.4860	10.1685	8.8645	10.7884	5.8743	7.4279	8.1079	8.1877	9.0604	8.3656	10.0691	8.1707	9.9552	8.5253	10.3384
BMK	17.5677	18.9328	19.8687	19.6993	20.7313	19.6386	21.8063	19.7764	21.4567	19.9084	*22.0571*	17.5685	18.9918	19.8505	19.7381	20.7943	19.6764	21.9359	19.8028	21.5449	19.9408	*22.1641*
BP86	4.6567	5.9000	6.5262	6.5255	7.3030	6.4908	8.3812	6.4519	8.1581	6.5548	8.9231	4.0748	5.5211	6.0819	6.2237	6.9198	6.1864	8.1035	6.1456	7.8017	6.2561	8.4559
CAM-B3LYP	7.0277	8.4199	9.1301	9.1955	10.0939	9.1495	11.3170	9.1042	11.0605	9.2415	11.7003	7.4255	8.8250	9.4397	9.5724	10.3110	9.5287	11.5895	9.4860	11.2269	9.6166	11.8127
HF	5.1207	5.6642	6.1573	6.2470	6.8024	6.2074	8.0648	6.1698	7.7499	6.2853	8.3789	5.9016	6.4456	6.8766	6.8836	7.3831	6.8546	8.6244	6.8262	8.2888	6.9110	8.8297
LC-BLYP	10.7354	12.0919	12.8910	12.9056	13.6984	12.8350	14.8474	12.7888	14.7700	12.9579	15.4000	11.4299	12.7559	13.4605	13.5217	14.2323	13.4550	15.4992	13.4106	15.1351	13.5726	15.7351
M06	4.7305	5.9977	6.8225	6.7511	7.6855	6.6951	8.8492	6.6463	8.6268	6.8176	9.1865	5.3296	6.5057	7.1299	7.1842	7.9088	7.1331	9.1466	7.0882	8.8164	7.2438	9.3380
M06-2X	16.8649	18.3510	19.1776	19.1280	20.0494	19.0989	21.1622	19.0710	20.8907	19.1500	21.5214	17.1454	18.6697	19.4257	19.4780	20.3326	19.4408	21.5840	19.4062	21.2342	19.5098	21.8820
mpW1LYP	5.8277	7.1287	7.8652	7.9126	8.7455	7.8586	9.9532	7.8068	9.7131	7.9631	10.3120	5.9372	7.3053	7.9454	8.0824	8.7966	8.0328	10.0326	7.9847	9.7174	8.1283	10.2337
mpW1PW91	4.2760	5.5243	6.2786	6.2628	7.1534	6.2157	8.3765	6.1740	8.1066	6.3075	8.7550	4.4530	5.7857	6.3821	6.5068	7.2200	6.4602	8.5136	6.4189	8.1458	6.5520	8.7323
O3LYP	**2.7754**	3.6640	3.8871	4.4515	5.0681	4.4147	6.2057	4.3830	5.9559	4.4828	6.4864	**2.3712**	3.3540	3.9231	4.1134	4.6754	4.0646	5.9776	4.0151	5.6745	4.1586	6.1879
OLYP	**3.5068**	3.8881	4.3521	4.5956	5.2662	4.5733	5.7465	4.5490	5.5532	4.6141	6.0038	**1.9548**	3.2110	3.5366	3.8217	4.1770	3.7781	5.2973	3.7339	5.0552	3.8611	5.5040
OPBE	3.9817	**3.4912**	3.5150	3.8067	4.0685	3.7966	4.4932	3.7850	4.3069	3.8063	4.6666	3.6100	3.0555	**2.9506**	3.2515	3.2326	3.2243	4.0948	3.2007	3.9862	3.2744	4.2566
OPW91	3.8308	**3.4432**	3.5260	3.8128	4.1413	3.7999	4.5735	3.7853	4.3963	3.8224	4.7725	3.4344	2.9752	**2.9391**	3.2280	3.2845	3.2004	4.1853	3.1755	4.0632	3.2550	4.3569
PBE	4.3983	5.5973	6.2887	6.2174	7.1726	6.1751	8.2067	6.1425	7.9752	6.2736	8.6353	3.9406	5.3503	5.9570	6.0322	6.8518	5.9862	8.0133	5.9491	7.7134	6.0901	8.2555
PBE0	4.0394	5.2764	5.9912	6.0015	6.8638	5.9507	8.1267	5.9019	7.8201	6.0528	8.4499	4.2398	5.5506	6.1589	6.2672	6.9608	6.2168	8.2898	6.1688	7.8888	6.3188	8.4707
TPSS	**3.7267**	4.2020	4.6441	4.6762	5.2047	4.6485	6.1659	4.6289	4.8807	4.7100	6.5319	**2.9760**	3.9390	4.5261	4.6038	5.2417	4.5662	6.3167	4.5377	5.5046	4.6479	6.5536
VSXC	6.1502	6.1249	6.2393	6.2859	6.5521	6.2741	6.9070	6.2617	6.7895	6.2983	7.1592	4.7587	4.5391	4.5681	4.6745	4.8838	4.6612	5.3505	4.6481	5.1852	4.6886	5.5944
wB97	4.6034	5.7374	6.4568	6.4738	7.2300	6.4250	8.3321	6.3758	8.0960	6.5209	8.6635	4.9870	6.1427	6.7864	6.8598	7.5177	6.8095	8.7770	6.7604	8.4297	6.9097	9.0329
wB97X	5.2871	6.5221	7.2499	7.2837	8.0580	7.2363	9.1818	7.1887	9.0178	7.3300	9.6844	5.6314	6.9059	7.5487	7.6478	8.3312	7.5979	9.6459	7.5488	9.2301	7.6978	9.8773
X3LYP	5.8470	7.1767	7.9235	7.9561	8.8211	7.9081	10.0240	7.8582	9.7793	8.0060	10.3953	5.9391	7.3346	7.9709	8.1059	8.8485	8.0614	10.0815	8.0148	9.7608	8.1514	10.2927
Method	**Flephedrone [3]**																					
B3LYP	6.8602	8.1601	8.9128	8.8738	9.7318	8.8207	10.8854	8.7690	10.6083	8.9241	11.2557	6.6616	8.0892	8.7411	8.8032	9.5927	8.7557	10.7910	8.7085	10.4608	8.8474	10.9915
B3P86	5.5389	6.7241	7.5073	7.4092	8.3141	7.3858	9.3978	7.3416	9.2587	7.4738	9.7735	5.2775	6.6212	7.3168	7.3426	8.1259	7.3139	9.2981	7.2675	9.0450	7.4076	9.5233
B3PW91	5.5555	6.7922	7.5259	7.4992	8.7154	7.4561	9.5340	7.4054	9.2620	7.5430	9.9123	5.3385	6.7455	7.3506	7.4608	8.2425	7.4188	9.4644	7.3703	9.1159	7.5040	9.6872
B98	5.7757	6.8615	7.5440	7.5036	8.3979	7.4765	9.4088	7.4470	9.1979	7.5323	9.7929	5.1609	6.5132	7.1637	7.2489	8.0647	7.2156	9.2412	7.1807	8.9223	7.2832	9.4631
B971	5.6275	6.7043	7.3740	7.3453	8.2165	7.3113	9.1989	7.2772	9.0078	7.3836	9.6067	4.9911	6.3398	6.9922	7.0828	7.8862	7.0423	9.0421	7.0021	8.7301	7.1272	9.2734
B972	3.7078	4.6031	5.2403	5.3286	6.0995	5.2808	7.2958	5.2322	7.1022	5.3706	7.6080	3.1372	4.3539	4.9137	5.1049	5.7916	5.0566	7.0586	5.0072	6.7088	5.1492	7.2827
BHandH	7.2117	8.3794	9.1407	9.0551	9.8838	9.0032	10.8546	8.9685	10.5869	9.0765	11.1712	7.6170	8.7804	9.5192	9.4383	10.0280	9.3889	11.2582	9.3541	10.9749	9.4622	11.5010
BHandHLYP	6.5701	7.6801	8.3339	8.3662	9.1943	8.3222	10.3201	8.2808	10.1061	8.4081	10.6826	6.7547	7.9173	8.5506	8.6146	9.3178	8.5722	10.4897	8.5320	10.1721	8.6549	10.7110
BLYP	7.3028	8.5896	9.1950	9.3483	10.1775	9.5612	11.1345	9.3436	10.9868	9.7239	11.5834	6.7287	8.1608	8.8502	8.9085	9.8255	9.1023	10.7604	8.8982	10.6661	9.2649	11.0360
BMK	18.6243	19.9506	20.8828	20.6966	21.7374	20.6371	22.7628	20.7775	22.4222	20.9057	*23.0098*	18.5342	19.9312	20.7891	20.6623	21.7311	20.6013	22.8282	20.7310	22.4450	20.8664	*23.0531*
BP86	5.5599	6.7751	7.4137	7.3682	8.1846	7.3361	9.1713	7.2994	8.9576	7.3948	9.7134	4.7222	6.2045	6.7930	6.8994	7.6558	6.8630	8.7629	6.8229	8.4731	6.9306	9.1283
CAM-B3LYP	8.0561	9.3732	10.0792	10.1065	11.0246	10.0632	12.1523	10.0206	11.9102	10.1501	12.5290	8.2101	9.5935	10.2173	10.3247	11.1000	10.2819	12.3036	10.2401	11.9547	10.3683	12.5279
HF	5.9246	6.4830	6.9937	7.0294	7.6515	6.9924	8.7669	6.9575	8.4851	7.0650	9.0879	6.4022	7.0043	7.4826	7.4596	8.0354	7.4301	9.1826	7.4012	8.8632	7.4875	9.3896
LC-BLYP	11.7049	13.0101	13.8097	13.7951	14.6102	13.7258	15.6857	13.6815	15.6157	13.8458	16.2301	12.2182	13.5289	14.2403	14.2854	15.0233	14.2185	16.2338	14.1749	15.8790	14.3360	16.4708
M06	5.7096	6.8956	7.7259	7.6051	8.5797	7.5513	9.6305	7.5051	9.4282	7.6701	9.9658	5.9294	7.1271	7.7914	7.8116	8.6082	7.7591	9.7746	7.7135	9.4544	7.8738	9.9719
M06-2X	17.8761	19.3240	20.1472	20.0804	21.0127	20.0528	22.0744	20.0264	21.8129	20.1009	22.4307	18.0541	19.5554	20.3100	20.3509	21.2202	20.3148	22.4265	20.2814	22.0857	20.3816	22.7228
mpW1LYP	6.8714	8.0933	8.8241	8.8314	9.6833	8.7804	10.7854	8.7314	10.5610	8.8791	11.1370	6.7139	8.0653	8.7231	8.8299	9.5838	8.7809	10.7388	8.7334	10.4382	8.8753	10.9387
mpW1PW91	5.3093	6.4749	7.2249	7.1619	8.0829	7.1179	9.1868	7.0795	8.9322	7.2035	9.5582	5.1509	6.4876	7.1089	7.1970	7.9712	7.1507	9.1736	7.1102	8.8218	7.2419	9.3958
O3LYP	**3.3795**	4.3306	4.6398	5.1085	5.8184	5.0738	6.8356	5.0444	6.6028	5.1371	7.1196	**2.4360**	3.6979	4.3793	4.5131	5.2167	4.4632	6.4321	4.4118	6.1408	4.5581	6.6507
OLYP	**3.6851**	4.2632	4.8538	5.0127	5.8147	4.9900	6.2376	4.9642	6.0539	5.0300	6.5059	**1.7120**	3.2114	3.7420	3.9607	4.5147	3.9121	5.5986	3.8613	5.5382	4.0027	5.8196
OPBE	3.6195	**3.3788**	3.6072	3.8151	4.3246	3.8047	4.7083	3.7879	4.5183	3.8143	4.9198	2.6770	**2.3668**	2.5558	2.7980	3.1233	2.7590	4.0186	2.7166	3.9045	2.8281	4.2282
OPW91	3.5199	**3.4001**	3.6818	3.8847	4.4451	3.8689	4.8315	3.8468	4.6534	3.8921	5.0659	2.5278	**2.3653**	2.6329	2.8543	3.2479	2.8125	4.1667	2.7667	4.0403	2.8873	4.3826
PBE	5.2926	6.4637	7.1703	7.0505	8.0507	7.0100	8.9961	6.9799	8.7761	7.1057	9.4182	4.5443	5.9999	6.6403	6.6745	7.5704	6.6284	8.6601	6.5921	8.3714	6.7343	8.9078
PBE0	5.0668	6.2233	6.9383	6.8965	7.7915	6.8485	8.9371	6.8027	8.6456	6.9451	9.2518	4.9092	6.2334	6.8680	6.9399	7.6976	6.8893	8.9419	6.8414	8.5521	6.9918	9.1228
TPSS	**4.2149**	4.7909	5.3244	5.2827	5.9225	5.2553	6.7904	5.2374	5.5400	5.3176	7.1569	**2.8817**	3.8357	4.4195	4.5009	5.1369	4.4631	6.2125	4.4344	5.3915	4.5451	6.4482
VSXC	6.4698	6.5694	6.7676	6.7788	7.1481	6.7648	7.4872	6.7499	7.3692	6.7933	7.7481	4.9235	4.8816	5.0388	5.0936	5.4516	5.0764	5.8895	5.0589	5.7255	5.1117	6.1436
wB97	5.6385	6.6838	7.4022	7.3665	8.1615	7.3209	9.1401	7.2750	8.9248	7.4106	9.4644	5.7065	6.8524	7.5152	7.5553	8.2731	7.5058	9.4353	7.4574	9.1037	7.6046	9.6921
wB97X	6.3261	7.4727	8.1982	8.1838	8.9914	8.1395	10.0037	8.0950	9.8508	8.2272	10.4932	6.3875	7.6402	8.2986	8.3673	9.1007	8.3184	10.3256	8.2703	9.9231	8.4164	10.5571
X3LYP	6.8849	8.1371	8.8781	8.8718	9.7570	8.8268	10.8571	8.7798	10.6267	8.9189	11.2215	6.7128	8.0938	8.7475	8.8524	9.6362	8.8088	10.7895	8.7629	10.4829	8.8973	11.0006

Table S19. Cont. V

Method	**R**	**S**
	4-fluoro-3-methyl-α-pyrrolidinopentiophenone	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	6.8090	7.6553	8.6474	8.1669	8.9320	8.1234	9.7202	8.0821	9.5274	8.2105	9.9581	6.8760	7.7190	8.7024	8.2263	8.9851	8.1830	9.7718	8.1421	9.5799	8.2696	10.0068
B3P86	5.7119	6.4128	6.8938	6.8624	7.4496	6.8451	8.2033	6.8129	8.0547	6.9112	8.4258	5.7879	6.4852	6.9631	6.9297	7.5108	6.9125	8.2627	6.8807	8.1148	6.9779	8.4814
B3PW91	5.7857	6.5143	6.9333	6.9920	7.9279	6.9589	8.4885	6.9212	8.2938	7.0272	8.7303	5.8610	6.5855	7.0022	7.0583	7.7457	7.0255	8.5460	6.9881	8.3524	7.0932	8.7840
B98	6.0246	6.6996	7.1551	7.1581	7.8714	7.1360	8.6285	7.1129	8.4547	7.1824	8.8587	6.0995	6.7701	7.2235	7.2236	7.9304	7.2015	8.6855	7.1787	8.5125	7.2477	8.9120
B971	5.8887	6.5527	6.9996	7.0110	7.6414	6.9829	8.4679	6.9555	8.2934	7.0432	8.7052	5.9649	6.6243	7.0691	7.0773	7.7017	7.0496	8.5259	7.0224	8.3522	7.1093	8.7592
B972	**4.7955**	5.1841	5.5774	5.6462	6.1426	5.6139	6.8148	5.5814	6.6460	5.6762	7.0251	**4.8861**	5.2725	5.6622	5.7281	6.2163	5.6963	6.8852	5.6641	6.7180	5.7578	7.0910
BHandH	6.6488	7.3601	7.8645	7.7980	8.3199	7.7650	9.1848	7.7425	8.8975	7.8119	9.4099	6.7080	7.4175	7.9185	7.8520	8.3039	7.8192	9.2325	7.7970	8.9466	7.8658	9.4549
BHandHLYP	6.4430	7.1132	7.5544	7.5698	8.0901	7.5380	8.9236	7.5086	8.7311	7.6008	9.3306	6.5096	7.1767	7.6149	7.6289	8.1443	7.5974	8.9757	7.5682	8.7838	7.6597	9.3788
BLYP	7.5611	8.3789	8.8756	8.9421	9.7323	9.1328	10.2376	8.9451	10.2508	9.2777	10.5593	7.6234	8.4408	8.9346	9.0004	9.7838	9.1899	10.2894	9.0034	10.3023	9.3339	10.6081
BMK	15.7311	16.6727	17.3502	17.2045	18.1117	17.1580	18.9495	17.2877	18.6137	17.3837	*19.1825*	15.7584	16.6991	17.3744	17.2302	18.1365	17.1837	18.9737	17.3133	18.6379	17.4090	*19.2063*
BP86	5.9796	6.7456	7.1415	7.1634	7.7356	7.1383	8.5020	7.1103	8.3486	7.1850	8.8752	6.0555	6.8186	7.2137	7.2322	7.7981	7.2073	8.5638	7.1796	8.4110	7.2536	8.9321
CAM-B3LYP	7.4337	8.3244	8.7858	8.8883	9.5061	8.8492	10.5540	8.8114	10.3254	8.9282	10.8175	7.4921	8.3792	8.8385	8.9394	9.5531	8.9004	10.5986	8.8629	10.3708	8.9790	10.8595
HF	6.5031	6.7237	7.0223	7.0328	7.3232	7.0102	8.1482	6.9894	7.9331	7.0559	8.3091	6.5641	6.7852	7.0816	7.0912	7.3783	7.0689	8.1995	7.0482	7.9856	7.1142	8.3579
LC-BLYP	9.9751	10.9612	11.5093	11.5424	12.1286	11.4916	13.3808	11.4591	12.7942	11.5796	13.6232	10.0150	10.9995	11.5464	11.5787	12.1629	11.5281	13.4131	11.4957	12.8278	11.6158	13.6540
M06	5.7508	6.6691	7.2942	7.2274	7.8573	7.1853	8.6807	7.1477	8.4935	7.2764	8.8848	5.8294	6.7411	7.3605	7.2951	7.9183	7.2533	8.7390	7.2161	8.5519	7.3437	8.9410
M06-2X	14.8471	16.0881	16.7005	16.7086	17.3834	16.6881	18.4002	16.6681	18.2539	16.7227	18.7144	14.8762	16.1172	16.7291	16.7367	17.4101	16.7162	18.4264	16.6962	18.2803	16.7507	18.7391
mpW1LYP	6.7667	7.5632	8.0740	8.1118	8.8576	8.0701	9.6430	8.0311	9.4666	8.1517	9.8710	6.8342	7.6272	8.1353	8.1710	8.9109	8.1296	9.6946	8.0909	9.5190	8.2106	9.9197
mpW1PW91	5.5693	6.2355	6.6582	6.6992	7.2554	6.6645	8.1987	6.6346	7.8024	6.7327	8.4311	5.6465	6.3084	6.7283	6.7670	7.3174	6.7326	8.2570	6.7031	7.8631	6.8003	8.4857
O3LYP	**4.8901**	5.2662	5.7480	5.6973	6.2644	5.6719	6.8222	5.6448	6.7197	5.7187	6.9873	**4.9817**	5.3556	5.8315	5.7807	6.3397	5.7557	6.8938	5.7290	6.7921	5.8019	7.0548
OLYP	**5.1494**	5.3343	5.7008	5.6525	6.1024	5.6294	6.5217	5.6041	6.4495	5.6700	6.6483	**5.2376**	5.4236	5.7852	5.7375	6.1803	5.7147	6.5969	5.6897	6.5252	5.7548	6.7200
OPBE	5.0180	**4.7222**	4.7694	4.7466	4.9407	4.7411	5.2247	4.7337	5.1705	4.7525	5.3053	5.1047	**4.8188**	4.8671	4.8432	5.0312	4.8378	5.3160	4.8305	5.2619	4.8490	5.3916
OPW91	4.9659	**4.7317**	4.8142	4.7892	5.0210	4.7800	5.3248	4.7684	5.2668	4.7953	5.4165	5.0535	**4.8284**	4.9111	4.8853	5.1103	4.8762	5.4146	4.8648	5.3568	4.8913	5.5013
PBE	5.7131	6.4418	6.8552	6.8544	7.5492	6.8199	8.3159	6.7949	8.1492	6.9024	8.5835	5.7919	6.5167	6.9289	6.9249	7.6124	6.8907	8.3777	6.8660	8.2120	6.9725	8.6408
PBE0	5.3715	6.0245	6.4360	6.4542	6.9869	6.4199	8.0036	6.3880	7.5352	6.4900	8.1917	5.4512	6.0994	6.5082	6.5243	7.0511	6.4903	8.0631	6.4587	7.5979	6.5597	8.2476
TPSS	**5.1374**	5.4292	5.7878	5.7210	6.1582	5.7030	6.7004	5.6929	5.8928	5.7455	6.8546	**5.2180**	5.5122	5.8685	5.7991	6.2297	5.7814	6.7719	5.7715	6.7920	5.8232	6.9214
VSXC	7.3228	7.5867	7.8103	7.8192	8.1755	7.8051	8.4788	7.7900	8.3877	7.8338	8.6599	7.3722	7.6352	7.8574	7.8661	8.2190	7.8520	8.5207	7.8370	8.4304	7.8805	8.7031
wB97	5.6150	6.2800	6.7005	6.7238	7.2366	6.6942	8.3243	6.6645	7.8190	6.7525	8.5424	5.6820	6.3447	6.7623	6.7839	7.2921	6.7546	8.3747	6.7252	7.8721	6.8123	8.5908
wB97X	6.0909	6.8716	7.3088	7.3747	7.9031	7.3402	9.0299	7.3063	8.4840	7.4090	9.2480	6.1570	6.9337	7.3681	7.4326	7.9564	7.3983	9.0787	7.3647	8.5355	7.4666	9.2944
X3LYP	6.7816	7.5960	8.1015	8.1352	8.9094	8.0996	9.6886	8.0626	9.5104	8.1735	9.9298	6.8489	7.6599	8.1628	8.1945	8.9627	8.1590	9.7404	8.1224	9.5629	8.2325	9.9786
Method	**4-fluoro-α-pyrrolidinooctanophenone**																					
B3LYP	6.8195	7.6949	8.2952	8.2281	8.8757	8.1727	9.6051	8.1114	9.4000	8.2753	9.9112	6.8735	7.7449	8.3427	8.2754	8.9187	8.2203	9.6476	8.1594	9.4432	8.3222	9.9509
B3P86	5.5908	6.3620	6.8506	6.8146	7.5041	6.8002	8.2503	6.7686	8.1442	6.8641	8.5508	5.6515	6.4190	6.9059	6.8706	7.5527	6.8562	8.2984	6.8248	8.1924	6.9198	8.5954
B3PW91	5.5628	6.3765	6.9317	6.8495	7.8104	6.8187	8.3006	6.7820	8.1008	6.8819	8.6289	5.6258	6.4346	6.9869	6.9050	7.5948	6.8743	8.3480	6.8378	8.1490	6.9371	8.6727
B98	6.1220	6.8388	7.3781	7.2623	7.9676	7.2448	8.6311	7.2263	8.4560	7.2816	8.9436	6.1809	6.8935	7.4305	7.3152	8.0147	7.2978	8.6779	7.2793	8.5036	7.3346	8.9873
B971	6.0124	6.7192	7.2509	7.1432	7.8377	7.1197	8.4932	7.0967	8.3213	7.1714	8.8101	6.0720	6.7748	7.3040	7.1969	7.8855	7.1735	8.5407	7.1506	8.3695	7.2250	8.8543
B972	**4.5138**	5.0763	5.5373	5.6668	6.0946	5.6313	6.7791	5.5942	6.5731	5.6975	7.1278	**4.5914**	5.1489	5.6058	5.7320	6.1546	5.6969	6.8362	5.6601	6.6317	5.7624	7.1796
BHandH	6.3760	7.1604	7.6691	7.6206	8.1508	7.5838	8.9325	7.5598	8.7282	7.6350	9.1726	6.4260	7.2083	7.7149	7.6660	8.1954	7.6293	8.9725	7.6054	8.7692	7.6803	9.2108
BHandHLYP	5.8895	6.6586	7.1296	7.1306	7.7901	7.0995	8.6100	7.0707	8.4153	7.1602	8.9007	5.9474	6.7122	7.1813	7.1815	7.8356	7.1507	8.6539	7.1220	8.4599	7.2109	8.9419
BLYP	7.9940	8.8477	9.3165	9.3709	10.0073	9.5762	10.4534	9.3846	10.4367	9.7153	10.8335	8.0421	8.8930	9.3605	9.4136	10.0468	9.6181	10.4940	9.4273	10.4772	9.7565	10.8710
BMK	14.9033	15.8414	16.4836	16.3214	17.1289	16.2769	17.8911	16.4117	17.6139	16.5008	*18.2021*	14.9285	15.8654	16.5070	16.3461	17.1517	16.3018	17.9142	16.4363	17.6374	16.5252	*18.2232*
BP86	6.3842	7.1599	7.6362	7.5412	8.1655	7.5200	8.7727	7.4956	8.6069	7.5586	9.2220	6.4412	7.2138	7.6886	7.5938	8.2128	7.5727	8.8207	7.5483	8.6556	7.6113	9.2658
CAM-B3LYP	7.1341	8.0656	8.6703	8.5862	9.3388	8.5535	10.1539	8.5220	9.9467	8.6200	10.4994	7.1823	8.1104	8.7140	8.6298	9.3772	8.5973	10.1918	8.5660	9.9851	8.6635	10.5347
HF	**5.1281**	5.5185	5.8580	5.9594	6.2951	5.9279	7.1666	5.8973	6.9289	5.9892	7.4078	**5.1909**	5.5782	5.9156	6.0157	6.3473	5.9846	7.2137	5.9542	6.9775	6.0452	7.4522
LC-BLYP	9.2979	10.2783	10.8305	10.8684	11.6449	10.8145	12.5312	10.7803	12.2889	10.9086	12.8468	9.3320	10.3106	10.8617	10.8991	11.6734	10.8453	12.5588	10.8113	12.3172	10.9392	12.8734
M06	5.5872	6.4238	7.0972	7.2136	7.9122	7.1738	8.6403	7.1400	8.4429	7.2621	8.8110	5.6582	6.4879	7.1545	7.2700	7.9626	7.2304	8.6902	7.1968	8.4933	7.3182	8.8602
M06-2X	13.8241	15.0004	15.5963	15.5962	16.4377	15.5742	17.3060	15.5535	17.0536	15.6126	17.5199	13.8495	15.0269	15.6225	15.6221	16.4619	15.6000	17.3295	15.5794	17.0779	15.6384	17.5418
mpW1LYP	6.8225	7.6355	8.2368	8.1338	8.8400	8.0971	9.5494	8.0625	9.3685	8.1681	9.8425	6.8766	7.6860	8.2847	8.1819	8.8832	8.1455	9.5921	8.1110	9.4118	8.2161	9.8824
mpW1PW91	5.3000	6.0629	6.6164	6.5261	7.2163	6.4933	7.9789	6.4658	7.7780	6.5576	8.3005	5.3640	6.1224	6.6727	6.5838	7.2665	6.5512	8.0278	6.5239	7.8278	6.6151	8.3455
O3LYP	**4.8444**	5.5000	5.9734	5.9261	6.5822	5.9068	7.1058	5.8843	6.9613	5.9406	7.2552	**4.9190**	5.5679	6.0371	5.9894	6.6385	5.9703	7.1598	5.9481	7.0161	6.0037	7.3054
OLYP	**5.3969**	5.8401	6.2286	6.2129	6.7228	6.1957	7.1172	6.1747	7.0074	6.2233	7.2424	**5.4649**	5.9053	6.2905	6.2738	6.7790	6.2568	7.1718	6.2362	7.0624	6.2840	7.2930
OPBE	**4.5098**	4.6188	4.7737	4.7798	5.1056	4.7716	5.4609	4.7575	5.3633	4.7863	5.5516	**4.5858**	4.6973	4.8512	4.8563	5.1766	4.8483	5.5295	4.8344	5.4326	4.8626	5.6151
OPW91	**4.5004**	4.6659	4.8454	4.8522	5.2020	4.8386	5.5718	4.8189	5.4703	4.8574	5.6717	**4.5767**	4.7438	4.9219	4.9276	5.2718	4.9144	5.6392	4.8950	5.5385	4.9327	5.7340
PBE	6.2152	6.9489	7.4713	7.3219	8.0853	7.2906	8.6823	7.2695	8.5154	7.3674	9.0193	6.2732	7.0040	7.5245	7.3759	8.1331	7.3447	8.7303	7.3236	8.5641	7.4211	9.0636
PBE0	5.1809	5.9263	6.3457	6.3683	7.0347	6.3338	7.8456	6.3014	7.6071	6.4043	8.1187	5.2462	5.9870	6.4047	6.4274	7.0862	6.3930	7.8955	6.3609	7.6581	6.4630	8.1648
TPSS	**5.3922**	5.7497	6.1823	6.0581	6.5735	6.0408	7.1095	6.0326	6.2255	6.0831	7.3496	**5.4542**	5.8106	6.2417	6.1173	6.6264	6.1000	7.1635	6.0918	7.3242	6.1421	7.4003
VSXC	8.7359	8.9779	9.2299	9.2072	9.6069	9.1929	9.8022	9.1776	9.7382	9.2221	10.0214	8.7517	8.9943	9.2456	9.2235	9.6227	9.2093	9.8184	9.1940	9.7542	9.2384	10.0382
wB97	5.1002	5.8539	6.3261	6.3438	7.0742	6.3092	7.8722	6.2749	7.6417	6.3776	8.1915	5.1616	5.9096	6.3787	6.3954	7.1200	6.3611	7.9153	6.3270	7.6867	6.4289	8.2323
wB97X	5.7315	6.5434	7.0277	7.0624	7.8308	7.0276	8.6306	6.9931	8.3530	7.0971	8.9681	5.7888	6.5961	7.0780	7.1120	7.8752	7.0774	8.6731	7.0431	8.3966	7.1464	9.0077
X3LYP	6.8271	7.6611	8.2595	8.1553	8.8877	8.1242	9.5938	8.0913	9.4102	8.1890	9.8995	6.8810	7.7113	8.3073	8.2034	8.9306	8.1723	9.6364	8.1395	9.4534	8.2369	9.9393

Table S19. Cont. VI

Method	R	S
	4-fluoro-α-pyrrolidinobutyrophenone [13] in $CDCl_3$	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	5.3869	6.6583	7.1163	7.3306	8.0516	7.2836	9.0972	7.2369	8.8020	7.3745	9.3880	5.5049	6.7588	7.2117	7.4220	8.1348	7.3756	9.1736	7.3296	8.8808	7.4654	9.4595
B3P86	4.1417	5.2806	5.8526	5.9272	6.7290	5.9051	7.7435	5.8656	7.5174	5.9822	8.0234	4.2877	5.4011	5.9627	6.0350	6.8228	6.0133	7.8305	5.9744	7.6073	6.0891	8.1036
B3PW91	4.1792	5.3949	5.8834	6.0710	7.0963	6.0322	7.8325	5.9862	7.5448	6.1092	8.1328	4.3242	5.5134	5.9930	6.1765	6.9297	6.1383	7.9185	6.0930	7.6341	6.2141	8.2123
B98	4.2828	5.4161	5.8592	6.0646	6.8355	6.0371	7.8334	6.0072	7.5589	6.0922	8.1267	4.4291	5.5369	5.9735	6.1724	6.9319	6.1454	7.9210	6.1160	7.6497	6.1996	8.2081
B971	4.1223	5.2431	5.6889	5.8937	6.6759	5.8608	7.6594	5.8272	7.3886	5.9295	7.9614	4.2735	5.3673	5.8065	6.0041	6.7743	5.9718	7.7489	5.9388	7.4813	6.0393	8.0442
B972	2.3914	3.3954	3.9781	4.1727	4.7426	4.1294	5.7975	4.0841	5.4970	4.2106	6.1255	2.6366	3.5797	4.1429	4.3245	4.8761	4.2828	5.9119	4.2391	5.6172	4.3613	6.2301
BHandH	6.1210	7.0036	7.5853	7.5568	8.1488	7.5166	9.0812	7.4867	8.8470	7.5775	9.3570	6.2141	7.0886	7.6644	7.6362	8.0830	7.5964	9.1497	7.5667	8.9170	7.6566	9.4217
BHandHLYP	5.2365	6.2062	6.7159	6.8385	7.2776	6.8021	8.6443	6.7670	8.1023	6.8725	8.9092	5.3509	6.3062	6.8096	6.9292	7.3626	6.8932	8.7189	6.8586	8.1809	6.9628	8.9789
BLYP	6.1098	7.3241	7.8745	8.0154	8.7686	8.2075	9.4903	8.0044	9.4091	8.3721	9.8828	6.2174	7.4214	7.9668	8.1045	8.8486	8.2946	9.5676	8.0938	9.4867	8.4574	9.9553
BMK	15.4286	16.6721	17.3028	17.2927	18.0380	17.2439	19.0885	17.3715	18.7365	17.4738	*19.3851*	15.4707	16.7123	17.3423	17.3315	18.0749	17.2829	19.1246	17.4101	18.7733	17.5122	*19.4198*
BP86	4.2826	5.5099	5.9585	6.1022	6.8124	6.0713	7.6804	6.0360	7.4381	6.1276	8.1389	4.4299	5.6322	6.0741	6.2138	6.9125	6.1833	7.7746	6.1487	7.5350	6.2388	8.2242
CAM-B3LYP	6.4700	7.6876	8.2031	8.3767	9.2157	8.3382	10.2414	8.2998	9.9516	8.4150	10.5340	6.5642	7.7702	8.2806	8.4522	9.2835	8.4140	10.3055	8.3760	10.0178	8.4901	10.5937
HF	5.5682	5.9345	6.2478	6.3780	6.6014	6.3482	7.7851	6.3196	7.4939	6.4080	8.0074	5.6678	6.0307	6.3408	6.4683	6.6869	6.4389	7.8607	6.4108	7.5723	6.4980	8.0789
LC-BLYP	9.8488	10.9927	11.5505	11.6668	12.2546	11.6113	13.5553	11.5735	13.0117	11.7083	13.8181	9.9061	11.0461	11.6006	11.7170	12.3009	11.6617	13.5994	11.6242	13.0568	11.7582	13.8600
M06	4.5955	5.8889	6.5389	6.6211	7.3519	6.5670	8.2957	6.5186	8.0661	6.6829	8.6291	4.7307	5.9999	6.6371	6.7197	7.4379	6.6664	8.3770	6.6188	8.1487	6.7804	8.7062
M06-2X	14.8915	16.2040	16.8559	16.8890	17.6718	16.8604	18.7194	16.8337	18.4299	16.9127	19.1013	14.9331	16.2436	16.8938	16.9268	17.7072	16.8983	18.7545	16.8717	18.4652	16.9503	19.1352
mpW1LYP	5.3680	6.5549	7.0320	7.2642	7.9861	7.2183	9.0208	7.1733	8.7475	7.3061	9.3002	5.4867	6.6566	7.1281	7.3559	8.0698	7.3106	9.0975	7.2662	8.8264	7.3973	9.3718
mpW1PW91	3.9673	5.0942	5.5936	5.7471	6.5361	5.7064	7.5380	5.6700	7.2447	5.7853	7.8176	4.1181	5.2173	5.7066	5.8567	6.6315	5.8167	7.6257	5.7809	7.3363	5.8942	7.8986
O3LYP	**2.2081**	3.2507	3.5803	3.9694	4.5572	3.9318	5.4266	3.8909	5.2076	4.0006	5.6883	**2.4805**	3.4488	3.7637	4.1327	4.6980	4.0967	5.5491	4.0575	5.3342	4.1625	5.8022
OLYP	**2.6735**	3.2288	3.6246	3.8041	4.3332	3.7658	4.9647	3.7257	4.8119	3.8367	5.2277	**2.9056**	3.4308	3.8057	3.9752	4.4814	3.9387	5.0989	3.9006	4.9491	4.0062	5.3527
OPBE	2.6133	2.2414	**2.2381**	2.4826	2.7231	2.4631	3.3480	2.4416	3.1851	2.5017	3.6008	2.8407	**2.5124**	2.5133	2.7294	2.9459	2.7118	3.5393	2.6922	3.3840	2.7467	3.7747
OPW91	2.4967	**2.2554**	2.3122	2.5549	2.8411	2.5310	3.4904	2.5039	3.3234	2.5741	3.7510	2.7342	**2.5253**	2.5798	2.7955	3.0557	2.7738	3.6744	2.7492	3.5146	2.8130	3.9184
PBE	3.9892	5.1881	5.6942	5.7832	6.6450	5.7419	7.4959	5.7091	7.2554	5.8366	7.8394	4.1467	5.3165	5.8124	5.8993	6.7461	5.8587	7.5910	5.8265	7.3536	5.9518	7.9264
PBE0	3.7606	4.8614	5.3627	5.4913	6.2813	5.4492	7.3444	5.4083	7.0091	5.5333	7.5783	3.9194	4.9898	5.4801	5.6057	6.3803	5.5645	7.4342	5.5246	7.1035	5.6469	7.6616
TPSS	**2.8770**	3.4980	3.9368	4.0293	4.4750	4.0024	5.5477	3.9838	4.2778	4.0626	5.8300	**3.0749**	3.6729	4.0990	4.1827	4.6121	4.1567	5.6681	4.1388	5.2432	4.2148	5.9389
VSXC	5.1385	5.5760	5.8591	5.9601	6.3975	5.9342	6.7901	5.9075	6.6712	5.9863	7.1047	5.2421	5.6775	5.9558	6.0570	6.4869	6.0314	6.8768	6.0050	6.7593	6.0828	7.1891
wB97	4.3791	5.3904	5.9193	6.0038	6.5752	5.9639	7.8254	5.9240	7.3133	6.0424	8.1019	4.5040	5.4959	6.0141	6.0979	6.6589	6.0588	7.9003	6.0196	7.3911	6.1357	8.1725
wB97X	4.9318	6.0437	6.5764	6.7153	7.3102	6.6751	8.5880	6.6345	8.2586	6.7544	8.8499	5.0485	6.1431	6.6672	6.8046	7.3901	6.7650	8.6604	6.7250	8.3340	6.8431	8.9179
X3LYP	5.3931	6.6074	7.0956	7.3083	8.0567	7.2680	9.0801	7.2249	8.8039	7.3492	9.3731	5.5110	6.7084	7.1908	7.3997	8.1398	7.3599	9.1566	7.3174	8.8827	7.4400	9.4445
Method	**4-fluoro-α-pyrrolidinobutyrophenone [13] in D_2O**																					
B3LYP	4.8843	5.9493	6.3632	6.5607	7.2534	6.5169	8.2421	6.4737	7.9586	6.6017	8.5086	5.1034	6.1387	6.5431	6.7329	7.4094	6.6902	8.3845	6.6482	8.1058	6.7729	8.6418
B3P86	3.9047	4.7358	5.2320	5.2801	6.0219	5.2608	6.9670	5.2267	6.7509	5.3279	7.2066	4.1639	4.9610	5.4389	5.4833	6.1985	5.4647	7.1301	5.4317	6.9197	5.5294	7.3571
B3PW91	3.9605	4.8593	5.2803	5.4347	6.3775	5.4002	7.0664	5.3596	6.7950	5.4688	7.3310	4.2169	5.0799	5.4855	5.6327	6.3172	5.5993	7.2272	5.5600	6.9623	5.6657	7.4798
B98	3.8818	4.7386	5.1289	5.2996	6.0371	5.2751	6.9669	5.2488	6.7054	5.3243	7.2308	4.1516	4.9701	5.3481	5.5067	6.2211	5.4831	7.1331	5.4578	6.8778	5.5305	7.3850
B971	3.7491	4.5814	4.9721	5.1392	5.8856	5.1101	6.8023	5.0806	6.5446	5.1712	7.0737	4.0268	4.8194	5.1979	5.3517	6.0738	5.3237	6.9722	5.2953	6.7210	5.3825	7.2307
B972	2.9182	3.2739	3.7155	3.8172	4.2776	3.7849	5.1939	3.7516	4.9228	3.8461	5.4728	3.2577	3.5915	4.0098	4.0938	4.5252	4.0637	5.4081	4.0327	5.1478	4.1210	5.6695
BHandH	6.2112	6.8432	7.3234	7.2765	7.7912	7.2445	8.6222	7.2206	8.4093	7.2932	8.8568	6.3664	6.9901	7.4619	7.4156	7.7742	7.3842	8.7440	7.3607	8.5337	7.4320	8.9722
BHandHLYP	5.3347	6.0175	6.4384	6.5232	6.9059	6.4928	8.1455	6.4636	7.6352	6.5518	8.3728	5.5242	6.1915	6.6034	6.6834	7.0571	6.6537	8.2791	6.6251	7.7759	6.7114	8.4980
BLYP	5.2231	6.3144	6.8532	6.9769	7.7086	7.1642	8.4074	6.9673	8.3264	7.3236	8.7842	5.4354	6.5047	7.0325	7.1498	7.8626	7.3328	8.5549	7.1407	8.4746	7.4885	8.9222
BMK	14.6175	15.8097	16.4341	16.4065	17.1465	16.3593	18.1615	16.4843	17.8183	16.5830	*18.4428*	14.6931	15.8816	16.5048	16.4758	17.2124	16.4288	18.2258	16.5533	17.8839	16.6516	*18.5046*
BP86	3.5919	4.5853	4.9843	5.1191	5.8022	5.0909	6.6344	5.0586	6.3980	5.1422	7.0622	3.8843	4.8313	5.2161	5.3423	6.0001	5.3151	6.8180	5.2841	6.5878	5.3646	7.2280
CAM-B3LYP	6.1050	7.1314	7.6045	7.7491	8.5497	7.7137	9.5168	7.6786	9.2413	7.7843	9.7810	6.2736	7.2817	7.7457	7.8869	8.6734	7.8521	9.6335	7.8176	9.3618	7.9214	9.8897
HF	6.5161	6.5902	6.7853	6.8442	7.0116	6.8246	7.9130	6.8062	7.6790	6.8641	8.0798	6.6602	6.7365	6.9300	6.9863	7.1475	6.9672	8.0385	6.9491	7.8081	7.0059	8.1993
LC-BLYP	9.5269	10.5363	11.0474	11.1507	11.6962	11.1002	12.9443	11.0658	12.4104	11.1884	13.1782	9.6271	10.6306	11.1360	11.2394	11.7783	11.1895	13.0225	11.1554	12.4903	11.2766	13.2524
M06	4.5133	5.4868	6.0440	6.1117	6.7719	6.0643	7.6272	6.0220	7.4126	6.1655	7.9145	4.7431	5.6859	6.2220	6.2903	6.9285	6.2444	7.7755	6.2034	7.5634	6.3423	8.0553
M06-2X	14.2346	15.4792	16.1075	16.1303	16.8927	16.1032	17.9073	16.0780	17.6259	16.1528	18.2717	14.3080	15.5494	16.1745	16.1970	16.9552	16.1701	17.9693	16.1451	17.6882	16.2193	18.3314
mpW1LYP	4.9431	5.9155	6.3417	6.5504	7.2438	6.5085	8.2154	6.4674	7.9542	6.5889	8.4696	5.1601	6.1052	6.5214	6.7218	7.3997	6.6810	8.3576	6.6411	8.1009	6.7593	8.6026
mpW1PW91	3.9308	4.6976	5.1130	5.2294	5.9405	5.1947	6.8571	5.1638	6.5850	5.2621	7.0944	4.1861	4.9215	5.3206	5.4316	6.1174	5.3982	7.0197	5.3684	6.7547	5.4632	7.2449
O3LYP	**2.8074**	3.1107	3.2892	3.5877	4.0508	3.5603	4.7918	3.5308	4.5994	3.6108	5.0098	**3.1712**	3.4543	3.6204	3.8884	4.3157	3.8633	5.0244	3.8363	4.8397	3.9095	5.2268
OLYP	3.1421	**3.0620**	3.2619	3.3750	3.7490	3.3492	4.2560	3.3231	4.1296	3.3977	4.4766	3.4757	**3.4152**	3.5959	3.6951	4.0347	3.6719	4.5176	3.6485	4.3966	3.7155	4.7210
OPBE	3.8390	2.9920	**2.7790**	2.8769	2.8048	2.8743	3.1414	2.8761	3.0436	2.8815	3.2850	4.1049	3.3379	**3.1541**	3.2345	3.1645	3.2322	3.4794	3.2340	3.3886	3.2385	3.6011
OPW91	3.6903	2.9128	**2.7450**	2.8463	2.8325	2.8428	3.2128	2.8427	3.1054	2.8530	3.3718	3.9666	3.2677	**3.1246**	3.2077	3.1897	3.2047	3.5442	3.2048	3.4444	3.2135	3.6808
PBE	3.3951	4.3312	4.7687	4.8602	5.6788	4.8226	6.4920	4.7929	6.2589	4.9093	6.8062	3.7027	4.5883	5.0053	5.0918	5.8781	5.0556	6.6772	5.0271	6.4506	5.1389	6.9751
PBE0	3.7995	4.5097	4.9171	5.0123	5.7148	4.9776	6.6815	4.9440	6.3740	5.0469	6.8749	4.0631	4.7415	5.1323	5.2227	5.8982	5.1895	6.8479	5.1574	6.5489	5.2560	7.0297
TPSS	**2.9113**	3.0362	3.3136	3.3803	3.7013	3.3613	4.6906	3.3490	3.5734	3.4045	4.9261	**3.2378**	3.3691	3.6326	3.6833	3.9773	3.6658	4.9291	3.6544	4.5814	3.7056	5.1422
VSXC	4.7065	4.8733	5.0582	5.1405	5.4917	5.1216	5.8115	5.1019	5.7098	5.1598	6.0745	4.8949	5.0665	5.2447	5.3273	5.6653	5.3089	5.9805	5.2897	5.8815	5.3461	6.2391
wB97	4.5829	5.2515	5.6629	5.7271	6.1929	5.6957	7.3399	5.6644	6.8500	5.7576	7.5691	4.7839	5.4337	5.8297	5.8932	6.3427	5.8630	7.4745	5.8328	6.9902	5.9225	7.6965
wB97X	4.8620	5.6947	6.1451	6.2610	6.7761	6.2269	7.9813	6.1925	7.6767	6.2943	8.2045	5.0612	5.8720	6.3087	6.4224	6.9214	6.3893	8.1129	6.3559	7.8136	6.4545	8.3283
X3LYP	4.9206	5.9283	6.3683	6.5595	7.2795	6.5225	8.2451	6.4831	7.9802	6.5971	8.5129	5.1382	6.1179	6.5472	6.7311	7.4348	6.6951	8.3874	6.6567	8.1271	6.7676	8.6458

Table S19. Cont. VII

Method	**R**	**S**
	2-trifluoromethylmethcathinone	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	8.5230	9.6417	10.4156	10.3063	11.1738	10.2569	12.1001	10.2083	11.8544	10.3529	12.4171	8.3480	9.4572	10.1696	10.0892	10.8898	10.0462	11.6943	10.0033	11.5160	10.1288	11.9867
B3P86	7.0740	8.1162	8.8607	8.7797	9.6485	8.7557	10.5607	8.7125	10.3790	8.8418	10.9126	6.9077	7.9655	8.6199	8.6010	9.3685	8.5758	10.1994	8.5343	10.1135	8.6589	10.5384
B3PW91	7.0830	8.1722	8.8568	8.8410	9.9845	8.8003	10.6095	8.7525	10.3493	8.8823	10.9603	6.9286	8.0200	8.6592	8.6700	9.4308	8.6321	10.2857	8.5877	10.0987	8.7078	10.6084
B98	7.2455	8.1241	8.8689	8.7608	9.6250	8.7300	10.5040	8.6980	10.2781	8.7939	10.8335	6.8292	7.7464	8.4364	8.3657	9.1778	8.3376	9.9710	8.3077	9.7924	8.3942	10.2757
B971	7.1656	8.0551	8.7854	8.7035	9.5475	8.6647	10.4228	8.6266	10.2048	8.7468	10.7527	6.7472	7.6750	8.3547	8.2994	9.1000	8.2646	9.9126	8.2295	9.7085	8.3375	10.2056
B972	5.2194	5.9454	6.5877	6.6040	7.3112	6.5582	8.2364	6.5118	7.9974	6.6453	8.5631	4.9722	5.7396	6.3302	6.3763	7.0028	6.3357	7.9132	6.2936	7.6846	6.4123	8.1918
BHandH	8.4335	9.5108	10.1525	10.1680	10.9418	10.1179	11.8916	10.0833	11.6138	10.1905	12.2189	8.5944	9.5321	10.2064	10.1610	10.6929	10.1140	11.7864	10.0799	11.5742	10.1848	12.0406
BHandHLYP	7.5250	8.3849	9.0734	9.0382	9.7737	8.9931	10.7920	8.9511	10.5414	9.0820	11.1043	7.5642	8.3973	8.9936	8.9932	9.6732	8.9566	10.5735	8.9219	10.3588	9.0281	10.8469
BLYP	10.3644	11.4196	12.1570	12.0627	13.0377	12.2522	13.5996	12.0554	13.5693	12.4097	13.9955	10.0588	11.1014	11.7920	11.7292	12.6265	11.9007	13.1224	11.7199	13.1131	12.0453	13.4398
BMK	19.5850	20.8939	21.8651	21.6179	22.7282	21.5562	23.6810	21.6908	23.3682	21.8267	*23.9855*	19.3881	20.6036	21.4843	21.2219	22.3539	21.1680	23.0950	21.3069	22.8484	21.4281	*23.4642*
BP86	8.2807	9.3486	9.9732	9.9190	10.7484	9.8886	11.4668	9.8543	11.2452	9.9441	11.9422	7.9132	8.9953	9.6129	9.5732	10.3101	9.5419	10.9504	9.5070	10.8070	9.5998	11.3603
CAM-B3LYP	9.3368	10.5284	11.2631	11.2367	12.1145	11.1919	13.0431	11.1485	12.8140	11.2823	13.3838	9.3110	10.4437	11.1293	11.1092	11.9408	11.0702	12.8057	11.0317	12.5854	11.1483	13.0951
HF	7.9934	8.0249	8.3961	8.3208	8.7480	8.3003	9.5608	8.2804	9.3269	8.3405	9.7845	8.1577	8.2455	8.5627	8.5178	8.8861	8.4979	9.6343	8.4785	9.4278	8.5365	9.8168
LC-BLYP	12.6134	13.8933	14.6775	14.6646	15.5301	14.5974	16.4938	14.5546	16.2444	14.7137	16.8164	12.7703	13.9410	14.7398	14.6834	15.5183	14.6197	16.4518	14.5778	16.1922	14.7301	16.7147
M06	6.8142	8.2813	9.1953	9.0371	10.2683	8.9827	11.0735	8.9346	10.8098	9.1007	11.4308	6.7035	7.7990	8.5814	8.5889	9.4965	8.5358	10.4035	8.4885	10.1519	8.6499	10.6670
M06-2X	19.0854	20.4823	21.3955	21.3109	22.2695	21.2745	23.3018	21.2402	23.0361	21.3405	23.6615	18.8843	20.2030	20.9775	20.9633	21.8938	20.9339	22.8509	20.9055	22.5793	20.9859	23.1730
mpW1LYP	8.3600	9.4034	10.1910	10.1204	10.9581	10.0689	11.8788	10.0197	11.6534	10.1688	12.1855	8.1935	9.2255	9.9287	9.8980	10.6787	9.8544	11.4938	9.8118	11.3122	9.9381	11.7599
mpW1PW91	6.6629	7.6906	8.3782	8.3585	9.2090	8.3138	10.1420	8.2749	9.8737	8.4010	10.4900	6.5319	7.5602	8.1915	8.2068	8.9599	8.1649	9.8661	8.1276	9.6543	8.2463	10.1698
O3LYP	5.2410	5.8383	6.4716	6.4353	7.1833	6.3990	7.9539	6.3606	7.7446	6.4664	8.2530	4.9326	5.6011	6.1559	6.2108	6.8317	6.1768	7.7149	6.1402	7.4828	6.2393	7.9210
OLYP	5.9042	6.2822	6.8057	6.7632	7.4220	6.7335	7.9983	6.7013	7.8517	6.7866	8.2721	5.4956	5.9999	6.4087	6.4877	6.9918	6.4587	7.7355	6.4275	7.5423	6.5113	7.8987
OPBE	4.8985	**4.8783**	5.1032	5.1562	5.5221	5.1381	6.1380	5.1143	5.9841	5.1723	6.4019	**4.7017**	4.7498	4.9127	5.0440	5.2609	5.0242	6.0592	5.0017	5.8529	5.0624	6.2219
OPW91	**4.9354**	4.9859	5.2466	5.2938	5.6936	5.2705	6.3169	5.2412	6.1601	5.3091	6.5852	**4.7253**	4.8469	5.0429	5.1694	5.4243	5.1466	6.2235	5.1208	6.0166	5.1873	6.3899
PBE	8.0879	9.1572	9.8217	9.7157	10.6848	9.6757	11.3942	9.6451	11.1854	9.7687	11.7537	7.7561	8.8263	9.4933	9.3999	10.2641	9.3602	10.9637	9.3286	10.7889	9.4504	11.2711
PBE0	6.4850	7.5207	8.1991	8.1811	9.0109	8.1323	10.0085	8.0860	9.6976	8.2307	10.3103	6.3576	7.3796	8.0038	8.0204	8.7584	7.9748	9.7400	7.9310	9.4683	8.0660	9.9952
TPSS	6.7327	7.2617	7.8150	7.7474	8.4316	7.7197	9.1345	7.7002	8.0119	7.7814	9.4471	6.1999	6.7863	7.2755	7.2560	7.9000	7.2290	8.4825	7.2092	7.9028	7.2887	8.7303
VSXC	9.2254	9.9319	10.3579	10.4114	10.8996	10.3815	11.5363	10.3507	11.3492	10.4410	11.7966	7.2889	7.4223	7.7039	7.7021	8.1758	7.6840	8.5241	7.6650	8.4068	7.7204	8.8475
wB97	6.8310	7.8102	8.5521	8.4852	9.3313	8.4382	10.2428	8.3916	9.9974	8.5315	10.5438	6.7987	7.6963	8.3935	8.3526	9.1391	8.3094	10.0307	8.2659	9.7888	8.3941	10.3074
wB97X	7.5780	8.6245	9.3813	9.3237	10.1620	9.2759	11.1251	9.2287	10.8215	9.3712	11.4259	7.5006	8.4629	9.1736	9.1411	9.9273	9.0983	10.8741	9.0549	10.5735	9.1826	11.1392
X3LYP	8.4786	9.5625	10.3290	10.2754	11.1422	10.2301	12.0490	10.1831	11.8251	10.3226	12.3715	8.3076	9.3852	10.0896	10.0567	10.8614	10.0178	11.6480	9.9765	11.4844	10.0967	11.9435
Method	**3-trifluoromethylmethcathinone**																					
B3LYP	7.2844	8.2580	9.2257	9.0936	9.9606	9.0488	10.9211	8.7702	10.6886	9.1357	11.1999	7.2184	8.3255	8.9063	8.9874	9.5730	8.9432	10.5689	8.8996	10.2769	9.0275	10.7811
B3P86	5.8875	6.7527	7.5079	7.3306	8.3127	7.3109	9.3641	7.2722	9.2528	7.3887	9.4297	5.8269	6.8087	7.4006	7.4753	8.0612	7.4507	9.0634	7.4084	8.8572	7.5375	9.2947
B3PW91	5.9345	7.0121	7.8409	7.6666	8.8064	7.6302	9.4980	7.5872	9.2692	7.7047	9.8027	5.9327	6.9471	7.4728	7.6364	8.2034	7.5727	9.2157	7.5195	8.9863	7.6725	9.4508
B98	6.0721	6.8027	7.7280	7.3354	8.4320	7.3122	9.3491	7.2873	9.1373	7.3598	9.6344	5.7338	6.6498	7.2002	7.2974	7.9248	7.2686	8.8982	7.2378	8.6072	7.3337	9.1212
B971	6.0035	6.7349	7.6037	7.2668	8.2996	7.2373	9.2367	7.2079	9.0291	7.3005	9.5188	5.6626	6.5749	7.1189	7.2221	7.8525	7.1875	8.8008	7.1525	8.5153	7.2657	9.0270
B972	**4.3579**	4.7924	5.6677	5.3298	6.2852	5.2903	7.2564	5.2508	7.0543	5.6339	7.5945	**4.1941**	4.8488	5.2414	5.4881	6.0577	5.4532	6.9894	5.4164	6.6906	5.5182	7.2156
BHandH	6.8558	7.7101	8.4157	8.3217	9.0588	8.2737	9.9946	8.2414	9.7618	8.3419	10.3118	7.3529	8.2132	8.8499	8.8261	9.3574	8.7813	10.4224	8.7492	10.1706	8.8481	10.6403
BHandHLYP	6.1647	6.9384	7.6848	7.5306	8.4079	7.4920	9.6213	7.4558	9.3686	7.5675	9.6539	6.4450	7.3035	7.8291	7.9409	8.4357	7.9011	9.5376	7.8683	9.2617	7.9803	9.7718
BLYP	9.4563	10.5697	11.2636	11.1114	11.9712	11.2991	12.6410	11.1139	12.6265	11.4439	13.0274	9.1431	10.1009	10.6547	10.7056	11.4362	10.8744	12.0988	10.6993	12.0594	11.0137	12.3507
BMK	18.0394	19.0913	19.9541	19.7003	20.9564	19.6477	21.7554	19.7926	21.4331	19.9013	*22.0200*	18.0076	19.2303	19.9719	19.8997	20.7408	19.8302	21.8657	19.9377	21.5343	20.1064	*22.0609*
BP86	7.5007	8.4658	9.1418	9.0165	9.7324	8.9899	10.4878	8.9602	10.3063	9.0391	10.9067	7.1384	8.1060	8.5344	8.6416	9.1266	8.6094	9.9507	8.5756	9.7050	8.6713	10.2699
CAM-B3LYP	7.9432	8.9893	9.8327	9.6193	10.6670	9.5826	11.8126	9.5464	11.5892	9.6791	11.8338	8.1517	9.2841	9.8666	9.9961	10.6107	9.9525	11.6443	9.9114	11.3505	10.0425	11.8879
HF	7.2266	7.3341	7.7444	7.6059	8.1118	7.5829	9.1394	7.6171	8.9129	7.6279	9.3300	7.6569	7.8149	8.0959	8.1028	8.3572	8.0798	9.5049	8.0583	9.0353	8.1270	9.4905
LC-BLYP	11.1223	12.3293	13.1291	12.9411	13.9205	12.8786	14.9128	12.8405	14.6448	12.9850	15.1807	11.6302	12.8233	13.4422	13.5778	14.2148	13.5150	15.2806	13.4463	15.0298	13.6212	15.5279
M06	5.3093	6.1317	7.0031	6.7794	7.8135	6.7273	8.7110	6.6828	8.7203	6.8426	8.9993	5.5664	6.4101	7.0191	7.0674	7.7640	7.0115	8.7843	6.9644	8.5407	7.1337	9.0527
M06-2X	17.2481	18.4859	19.2328	19.1837	20.1694	19.1596	21.1182	19.1366	20.8416	19.2009	21.4608	17.4476	18.7518	19.5258	19.5798	20.3577	19.5571	21.4223	19.4702	21.1463	19.5959	21.6872
mpW1LYP	7.0378	7.9594	8.9732	8.5794	9.6887	8.5352	10.6446	8.4928	10.4240	8.6204	10.9083	7.0075	8.0566	8.6487	8.7642	9.3033	8.7219	10.3181	8.6781	10.0538	8.8076	10.5255
mpW1PW91	5.4517	6.2749	7.0253	6.8656	7.9701	7.0886	8.9741	6.7905	8.7474	6.9044	9.2641	5.4622	6.4703	6.9962	7.1381	7.7049	7.0758	8.7344	7.0329	8.4258	7.1803	8.9715
O3LYP	4.7837	5.4502	5.9336	5.9800	6.8824	5.9391	7.5671	5.9023	7.9276	6.1586	7.7648	4.4739	5.1921	5.9508	5.6894	6.5230	5.6624	7.3808	5.6332	7.1846	5.7118	7.5284
OLYP	5.8444	6.2584	6.6635	6.7839	7.6051	6.7518	8.2293	6.7174	8.1256	6.8113	8.3782	4.8149	5.8947	6.4237	6.2621	6.8643	6.2487	7.6044	6.2334	7.4589	5.7193	7.0630
OPBE	5.1911	5.1463	**5.1215**	5.4444	5.9313	5.4236	6.5227	5.4256	6.4425	5.4635	6.6904	4.9181	**4.8957**	5.2136	5.0988	5.4208	5.0829	6.0152	5.0666	6.0096	5.1143	6.1383
OPW91	**5.1838**	5.2318	5.2886	5.5430	6.0742	5.5180	6.6760	5.5132	6.5893	5.6629	6.8493	**4.9014**	4.9578	5.2003	5.1827	5.5530	5.1655	6.1597	5.1468	6.1527	5.1969	6.2857
PBE	7.2401	8.1828	8.8814	8.7312	9.5583	8.6852	10.3134	8.6595	10.1435	8.7670	10.6131	6.9485	7.8927	8.3534	8.4167	9.0676	8.3747	9.8378	8.3436	9.5963	8.4733	10.0518
PBE0	5.2411	6.0601	6.7526	6.6316	7.5947	6.5889	8.7570	6.5483	8.5049	6.6754	8.7579	5.3077	6.2687	6.7672	6.8942	7.4620	6.8412	8.5420	6.7948	8.2004	6.9507	8.7346
TPSS	6.3394	6.6653	7.1000	7.0168	7.6464	6.9962	8.3036	6.9826	7.2207	7.0430	8.4380	5.8220	6.2601	6.6101	6.6794	7.0627	6.6553	7.7872	6.6371	7.2886	6.7082	7.9510
VSXC	7.7200	7.7008	7.8902	7.8587	8.2046	7.8472	8.4111	7.8351	8.3273	7.8706	8.5983	6.7069	6.5706	6.7426	6.7139	7.1414	6.7027	7.3220	6.6905	7.2336	6.7251	7.5280
wB97	5.5854	6.3761	7.0210	6.9855	7.8714	6.9446	8.7129	6.9034	8.4883	7.0251	9.0038	5.8425	6.6818	7.2521	7.3603	7.9780	7.3222	8.9819	7.2833	8.7261	7.3967	9.2140
wB97X	6.2524	7.1120	7.8842	7.7204	8.6681	7.6819	9.5717	7.6504	9.2878	7.7579	9.8369	6.4660	7.4178	7.9748	8.1168	8.7198	8.0796	9.7804	8.0411	9.4759	8.1527	10.0035
X3LYP	7.1880	8.1368	9.1481	8.7525	9.8841	8.7139	10.8279	8.6734	10.6077	8.7931	11.1037	7.1464	8.2161	8.8039	8.9231	9.5609	8.8857	10.4903	8.8434	10.2214	8.9661	10.7077

Table S20. Deviations of calculated fluorine-19 chemical shifts from experimental data of selected fluorinated synthetic derivatives of cathinone calculated with HF and selected functionals combined with 6-311++G** basis set. Smallest deviations of most accurate methods are in boald and marked in green, highests deviations of the worst methods are in italic font and marked in orange

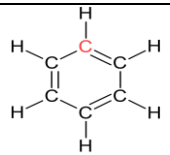
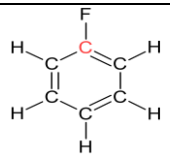
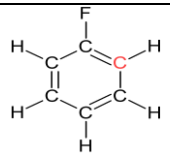
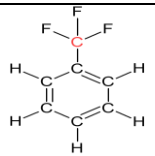
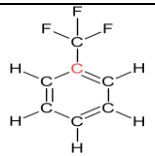
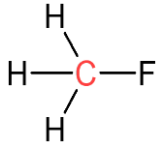
Method	R											S									
	3-fluoromethcathinone																				
	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	-16.9194	-20.2618	-22.6749	-21.5329	-25.0130	-21.4611	-24.5830	-21.3878	-24.5380	-21.6010	-24.5597	-16.7659	-20.1639	-22.7834	-21.5639	-25.0737	-21.4971	-24.7075	-21.4285	-24.6516	-21.6270	-24.6655
B3P86	-9.6177	-12.6307	-15.0279	-13.7665	-17.0268	-13.7028	-16.5656	-13.6389	-16.5312	-13.8256	-16.5379	-9.6731	-12.7355	-15.1737	-13.8234	-17.1082	-13.7638	-16.7032	-13.7048	-16.6667	-13.8780	-16.6590
B3PW91	-8.9719	-12.2387	-14.6600	-13.3865	-15.5020	-13.3220	-16.1849	-13.2573	-16.1591	-13.4467	-15.9611	-9.0037	-12.1223	-14.5704	-13.2193	-16.5159	-13.1599	-16.3305	-13.0999	-16.0753	-13.2750	-16.0634
B98	-11.9852	-14.9829	-17.4945	-16.1167	-19.4622	-16.0534	-19.0366	-15.9887	-18.9997	-16.1765	-18.9921	-11.8701	-15.0984	-17.6175	-16.1832	-19.5565	-16.1249	-19.1911	-16.0650	-19.1478	-16.2379	-19.1253
B971	-12.6156	-15.6388	-18.1535	-16.7791	-20.1394	-16.7148	-19.7060	-16.6499	-19.6675	-16.8390	-19.6649	-12.5180	-15.7546	-18.2785	-16.8515	-20.2343	-16.7923	-19.8667	-16.7325	-19.8224	-16.9066	-19.8042
B972	-6.4494	-9.6661	-12.0064	-10.7924	-13.9638	-10.7291	-13.5215	-10.6668	-13.4918	-10.8517	-13.4895	-6.4863	-9.5564	-11.9406	-10.6300	-13.8401	-10.5721	-13.6745	-10.5144	-13.6409	-10.6836	-13.6334
BHandH	2.2488	**-0.4354**	-2.4564	-1.4365	-4.1430	-1.3815	-3.8662	-1.3250	-3.8061	-1.4883	-3.8823	2.1877	**-0.5406**	-2.6027	-1.5074	-1.8441	-1.4558	-3.9588	-1.4028	-3.9202	-1.5557	-3.9582
BHandHLYP	**-0.8424**	-3.8067	-5.9956	-4.9512	-7.8207	-4.8864	-7.5233	-4.8213	-7.4701	-5.0122	-7.5507	**-0.9380**	-3.9152	-6.0990	-4.9870	-7.8897	-4.9285	-7.5985	-4.8696	-7.5505	-5.0415	-7.5985
BLYP	-35.2810	-39.0351	-42.0813	-40.4865	*-44.5930*	-40.1969	-43.0613	-40.3229	-44.0425	-40.4981	-43.5253	-35.1211	-38.9915	-42.0955	-40.4370	*-44.5676*	-40.1528	-43.1688	-40.2834	-44.1131	-40.4431	-43.6058
BMK	-9.8036	-12.8968	-15.3884	-14.0504	-17.3947	-13.9875	-16.9845	-13.9232	-16.9335	-14.1101	-16.9567	-9.6957	-13.0220	-15.5340	-14.1001	-17.4483	-14.0440	-17.0541	-13.9858	-17.0213	-14.1526	-17.0069
BP86	-26.8067	-30.1016	-32.9425	-31.3351	-35.1426	-31.2653	-34.6031	-31.1949	-34.5849	-31.4011	-34.5218	-26.6979	-30.1329	-32.9549	-31.3423	-35.1753	-31.2762	-34.7500	-31.2091	-34.6997	-31.4046	-34.6612
CAM-B3LYP	-7.1520	-10.4651	-12.8374	-11.7286	-14.8868	-11.6570	-14.5218	-11.5846	-14.4621	-11.7967	-14.5516	-7.2074	-10.5609	-12.9399	-11.7709	-14.9581	-11.7050	-14.6235	-11.6379	-14.5684	-11.8336	-14.6236
HF	14.4990	11.8759	10.1409	10.8435	8.5115	10.9092	8.7475	10.9759	8.8334	10.7817	8.6882	14.2763	11.7390	9.8580	10.8155	8.4719	10.8612	8.6654	10.9100	8.7959	10.7770	8.6532
LC-BLYP	5.6555	2.2478	**0.1272**	0.9367	-1.8684	1.0096	-3.3669	1.0834	-1.5413	0.8680	-1.6695	5.6056	2.1669	**0.0316**	0.9038	-1.9454	0.9718	-1.6589	1.0415	-1.5948	0.8401	-1.7086
M06	-10.7488	-14.1326	-16.1259	-14.6752	-17.9390	-14.6146	-17.5565	-14.5533	-17.5880	-14.7327	-17.5321	-10.7574	-14.2262	-16.1018	-14.7427	-17.9652	-14.6862	-17.6111	-14.6287	-17.5779	-14.7957	-17.5781
M06-2X	-6.0083	-9.1231	-11.5058	-10.2832	-13.4026	-10.2193	-13.0490	-10.1540	-13.0197	-10.3431	-13.0487	-6.0520	-9.2137	-11.5766	-10.2952	-13.4337	-10.2397	-13.0227	-10.1813	-12.9991	-10.3466	-12.9888
mpW1LYP	-15.5075	-19.0136	-21.4018	-20.3003	-23.6971	-20.2282	-23.3150	-20.1543	-23.2609	-20.3683	-23.1277	-15.5541	-18.9341	-21.5131	-20.1751	-23.6156	-20.1080	-23.4808	-20.0391	-23.4170	-20.2376	-23.4495
mpW1PW91	-5.8262	-8.8094	-11.1651	-9.9318	-13.0790	-9.8698	-12.6539	-9.8062	-12.6180	-9.9912	-12.6323	-5.8782	-8.9338	-11.2996	-10.0128	-13.2021	-9.9551	-12.8226	-9.8955	-12.7859	-10.0686	-12.7868
O3LYP	-11.2402	-14.4639	-16.9742	-15.6478	-18.9683	-15.5860	-18.4498	-15.5192	-18.4657	-15.7073	-18.4185	-10.9862	-14.4767	-17.0642	-15.6703	-19.0949	-15.6081	-18.7074	-15.5414	-18.6678	-15.7281	-18.6450
OLYP	-19.0110	-22.3391	-24.9995	-23.4978	-27.1765	-23.4307	-26.6821	-23.3633	-26.6036	-23.5611	-26.6020	-18.7865	-22.3402	-25.1057	-23.6234	-27.2980	-23.5593	-26.9052	-23.4940	-26.8672	-23.6832	-26.8239
OPBE	-8.3832	-11.2245	-13.6053	-12.1864	-15.4560	-12.1310	-14.9264	-12.0756	-14.9501	-12.2373	-14.8212	-8.2107	-11.3422	-13.7587	-12.3261	-15.6199	-12.2753	-15.1951	-12.2237	-15.1741	-12.3722	-15.0974
OPW91	-8.9834	-11.8739	-14.2687	-12.8530	-16.1545	-12.7968	-15.6198	-12.7406	-15.6378	-12.9058	-15.5190	-8.8103	-11.9874	-14.4189	-12.9909	-16.3070	-12.9392	-15.8808	-12.8866	-15.8591	-13.0388	-15.7863
PBE	-24.4976	-27.7934	-30.5989	-29.0251	-32.7870	-28.9565	-32.2541	-28.8864	-32.2286	-29.0905	-32.1807	-24.3877	-27.8466	-30.6316	-29.0769	-32.8679	-29.0097	-32.4651	-28.9414	-32.4086	-29.1407	-32.3901
PBE0	-5.7898	-8.7207	-11.0490	-9.8152	-12.9524	-9.7537	-12.5226	-9.6925	-12.4900	-9.8724	-12.5052	-5.8500	-8.8388	-11.1928	-9.8940	-13.0608	-9.8367	-12.6822	-9.7791	-12.6467	-9.9474	-12.6462
TPSS	-18.5308	-21.9701	-24.6397	-23.2722	-26.8869	-23.1992	-26.3758	-23.1260	-24.6836	-23.3406	-26.3150	-18.3284	-22.0225	-24.7487	-23.3492	-26.9957	-23.2786	-26.5739	-23.2079	-21.5877	-23.4153	-26.5076
VSXC	-19.0512	-22.5518	-25.2693	-23.8599	-27.5265	-23.7878	-27.0466	-23.7059	-26.9952	-23.9271	-27.0168	-19.7775	-23.4449	-26.2580	-24.7888	-28.5119	-24.7146	-28.0452	-24.6307	-28.0030	-24.8580	-27.9927
wB97	**0.6195**	-2.8061	-5.0140	-4.1376	-7.0645	-4.0640	-6.7653	-3.9896	-6.6966	-4.2067	-6.8176	**0.5542**	-2.9082	-5.1223	-4.1747	-7.1229	-4.1085	-6.9110	-4.0403	-6.8431	-4.2355	-6.9407
wB97X	-1.6611	-4.8713	-7.1059	-6.0925	-9.0684	-6.0246	-8.7470	-5.9561	-8.6997	-6.1564	-8.7760	-1.7198	-4.9703	-7.2136	-6.1453	-9.1473	-6.0825	-8.8147	-6.0183	-8.7634	-6.2039	-8.8234
X3LYP	-16.0732	-19.5687	-21.9637	-20.8449	-24.2756	-20.7729	-23.8560	-20.7002	-23.8056	-20.9126	-23.6736	-16.1047	-19.4706	-22.0678	-20.6974	-24.1671	-20.6308	-23.9914	-20.5632	-23.9332	-20.7599	-23.9546
Method	4-fluoro-α-pyrrolidinohexiophenone [6]																					
B3LYP	-20.3149	-21.8152	-24.5636	-22.0914	-26.4346	-22.0786	-24.7811	-22.0649	-25.1710	-22.1047	-23.9774	-20.3149	-21.8152	-24.5636	-22.0914	-26.4347	-22.0786	-24.7810	-22.0649	-24.6519	-22.1046	-23.9774
B3P86	-12.8895	-13.8317	-16.4580	-13.8711	-17.9835	-13.8770	-15.6128	-13.8824	-16.0248	-13.8637	-15.3815	-12.8895	-13.8317	-16.4580	-13.8712	-17.9835	-13.8770	-15.6130	-13.8824	-16.0248	-13.8636	-15.3817
B3PW91	-12.2959	-13.4095	-16.0427	-13.5094	-16.4748	-13.5111	-15.3565	-13.5120	-15.7252	-13.5064	-15.0682	-12.2958	-13.4095	-16.0429	-13.5094	-17.6115	-13.5112	-15.3566	-13.5121	-15.7252	-13.5064	-15.0682
B98	-15.4176	-16.5442	-19.2574	-16.6149	-20.8354	-16.6187	-18.6429	-16.6210	-19.0029	-16.6108	-18.3648	-15.4177	-16.5442	-19.2575	-16.6149	-20.8354	-16.6187	-18.6431	-16.6210	-19.0029	-16.6108	-18.3649
B971	-16.0398	-17.1484	-19.8709	-17.2179	-21.4690	-17.2225	-19.2522	-17.2262	-19.6160	-17.2121	-18.9809	-16.0398	-17.1485	-19.8711	-17.2180	-21.4690	-17.2225	-19.2523	-17.2262	-19.6161	-17.2121	-18.9809
B972	-9.8977	-11.1364	-13.7166	-11.3900	-15.9650	-11.3748	-13.7436	-11.3631	-14.1277	-11.4061	-13.6036	-9.8977	-11.1364	-13.7168	-11.3901	-15.9650	-11.3748	-13.7438	-11.3631	-14.1278	-11.4061	-13.6037
BHandH	**-0.9115**	-1.5759	-3.7201	-1.4738	-4.8505	-1.4854	-2.7526	-1.4960	-3.1314	-1.4624	-2.6068	**-0.9115**	-1.5759	-3.7201	-1.4738	-1.8105	-1.4854	-2.7526	-1.4960	-3.1314	-1.4624	-2.6068
BHandHLYP	-4.5357	-5.7556	-8.0349	-5.9787	-9.5316	-5.9726	-7.5026	-5.9662	-7.8770	-5.9837	-7.3763	-4.5357	-5.7556	-8.0350	-5.9787	-9.5316	-5.9726	-7.5026	-5.9662	-7.8770	-5.9836	-7.3763
BLYP	-38.0703	-39.9267	-43.2209	-40.3583	*-45.9862*	-40.1289	-42.3437	-40.3151	-43.8973	-40.3127	-42.5218	-38.0703	-39.9267	-43.2209	-40.3583	*-45.9862*	-40.1289	-42.3437	-40.3151	-43.8973	-40.3126	-42.5218
BMK	-13.5260	-14.6096	-17.2794	-14.6175	-18.7437	-14.6250	-16.5201	-14.6311	-16.8999	-14.6100	-16.2181	-13.5260	-14.6096	-17.2793	-14.6175	-18.7437	-14.6250	-16.5200	-14.6311	-16.8999	-14.6101	-16.2181
BP86	-29.2224	-30.2487	-33.4211	-30.2351	-35.1524	-30.2459	-32.4829	-30.2552	-32.9182	-30.2242	-32.0988	-29.2224	-30.2487	-33.4211	-30.2351	-35.1524	-30.2459	-32.4829	-30.2552	-32.9182	-30.2242	-32.0988
CAM-B3LYP	-11.2732	-12.8132	-15.3083	-13.1410	-17.0488	-13.1299	-15.0812	-13.1175	-15.3864	-13.1514	-14.8760	-11.2731	-12.8132	-15.3084	-13.1410	-17.0487	-13.1299	-15.0812	-13.1176	-15.3864	-13.1513	-14.8760
HF	12.0231	10.7243	9.0880	10.3515	6.9420	10.3867	8.8882	10.4178	8.4401	10.3184	9.0165	12.0232	10.7243	9.0880	10.3515	6.9420	10.3867	8.8882	10.4177	8.4400	10.3184	9.0165
LC-BLYP	1.7354	**-0.0332**	-2.2278	-0.4953	-3.9054	-0.4782	-2.1670	-0.4590	-2.3896	-0.5099	-2.0740	1.7354	**-0.0332**	-2.2278	-0.4953	-3.9055	-0.4782	-2.1671	-0.4589	-2.3897	-0.5099	-2.0740
M06	-13.1983	-14.7994	-16.8029	-14.4567	-19.3039	-14.4528	-17.2203	-14.4471	-17.5604	-14.4592	-17.0181	-13.1983	-14.7994	-16.8029	-14.4567	-19.3038	-14.4528	-17.2203	-14.4472	-17.5604	-14.4592	-17.0182
M06-2X	-9.9379	-11.0001	-13.4210	-11.0535	-14.7724	-11.0557	-12.8185	-11.0562	-13.0468	-11.0516	-12.7639	-9.9381	-11.0001	-13.4210	-11.0535	-14.7724	-11.0556	-12.8185	-11.0562	-13.0468	-11.0516	-12.7639
mpW1LYP	-19.1800	-20.6567	-23.3792	-20.9417	-25.2061	-20.9315	-23.0801	-20.9197	-23.4117	-20.9509	-22.8327	-19.1800	-20.6568	-23.3792	-20.9416	-25.2063	-20.9315	-23.0801	-20.9197	-23.4118	-20.9509	-22.8325
mpW1PW91	-9.1339	-10.1702	-12.7070	-10.2395	-14.2138	-10.2443	-11.9756	-10.2472	-12.3590	-10.2353	-11.7551	-9.1339	-10.1702	-12.7070	-10.2395	-14.2138	-10.2443	-11.9758	-10.2472	-12.3590	-10.2353	-11.7551
O3LYP	-14.6850	-16.7457	-19.7185	-17.3398	-21.6256	-17.3215	-19.4355	-17.2987	-19.8373	-17.3539	-19.2649	-14.6848	-16.7457	-19.7185	-17.3396	-21.6256	-17.3216	-19.4355	-17.2987	-19.8373	-17.3539	-19.2646
OLYP	-22.3941	-24.7746	-27.7452	-25.1606	-29.9154	-25.1500	-27.5547	-25.1387	-28.0484	-25.1690	-27.2814	-22.3941	-24.7745	-27.7452	-25.1605	-29.9155	-25.1500	-27.5547	-25.1385	-28.0484	-25.1690	-27.2814
OPBE	-11.2719	-12.9650	-15.7202	-13.2317	-17.6750	-13.2322	-15.1997	-13.2324	-15.6322	-13.2293	-14.8803	-11.2717	-12.9650	-15.7200	-13.2317	-17.6749	-13.2322	-15.1998	-13.2324	-15.6322	-13.2293	-14.8804
OPW91	-11.8894	-13.6382	-16.4029	-13.9211	-18.3862	-13.9208	-15.9042	-13.9200	-16.3382	-13.9199	-15.5932	-11.8894	-13.6382	-16.4028	-13.9211	-18.3863	-13.9208	-15.9042	-13.9200	-16.3382	-13.9199	-15.5932
PBE	-26.8443	-27.8866	-31.0345	-27.8677	-32.7648	-27.8799	-30.1625	-27.8899	-30.5650	-27.8559	-29.7918	-26.8443	-27.8863	-31.0345	-27.8677	-32.7648	-27.8799	-30.1625	-27.8899	-30.5650	-27.8559	-29.7918
PBE0	-9.1775	-10.1292	-12.6471	-10.1715	-14.1310	-10.1782	-11.8951	-10.1840	-12.2842	-10.1635	-11.6705	-9.1775	-10.1293	-12.6472	-10.1715	-14.1310	-10.1782	-11.8951	-10.1840	-12.2840	-10.1635	-11.6704
TPSS	-20.4440	-21.6785	-24.6128	-21.7557	-26.4715	-21.7608	-23.7470	-21.7651	-23.2783	-21.7491	-23.5382	-20.4440	-21.6785	-24.6129	-21.7557	-26.4715	-21.7608	-23.7470	-21.7651	-20.2287	-21.7491	-23.5382
VSXC	-22.2028	-23.3970	-26.3935	-23.2985	-28.2002	-23.3157	-25.3887	-23.3226	-25.7655	-23.2806	-25.1275	-22.2030	-23.3970	-26.3935	-23.2985	-28.2001	-23.3157	-25.3888	-23.3226	-25.7654	-23.2806	-25.1275
wB97	-3.5081	-5.1688	-7.4384	-5.5751	-9.1828	-5.5627	-7.4416	-5.5477	-7.6966	-5.5845	-7.4270	-3.5083	-5.1688	-7.4384	-5.5751	-9.1827	-5.5627	-7.4418	-5.5477	-7.6966	-5.5845	-7.4269
wB97X	-5.8425	-7.3026	-9.6109	-7.6812	-11.3382	-7.6764	-9.4559	-7.6690	-9.8523	-7.6830	-9.4045	-5.8428	-7.3023	-9.6108	-7.6812	-11.3382	-7.6764	-9.4558	-7.6689	-9.8524	-7.6830	-9.4045
X3LYP	-19.6700	-21.1079	-23.8558	-21.3662	-25.6796	-21.3578	-23.4823	-21.3489	-23.8359	-21.3737	-23.2278	-19.6700	-21.1079	-23.8558	-21.3663	-25.6796	-21.3578	-23.4823	-21.3489	-23.8359	-21.3737	-23.2277

Table S20. Cont.

Method	R	S
	Flephedrone [9]	

	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)	Gas	$CHCl_3$ (PCM)	$CHCl_3$ (SMD)	DMSO (PCM)	DMSO (SMD)	CH_3OH (PCM)	CH_3OH (SMD)	C_2H_5OH (PCM)	C_2H_5OH (SMD)	H_2O (PCM)	H_2O (SMD)
B3LYP	-22.4867	-23.6404	-26.5276	-23.6622	-28.1938	-23.6680	-25.9611	-23.6715	-26.2171	-23.6554	-25.7310	-22.1856	-24.0284	-26.7884	-24.4189	-28.6445	-24.3983	-26.9169	-24.3776	-27.1395	-24.4402	-26.5511
B3P86	-15.0651	-15.7836	-18.4922	-15.6226	-19.8927	-15.6352	-17.5541	-15.6485	-17.9548	-15.6094	-17.3165	-14.9081	-16.2431	-18.7782	-16.4063	-20.3355	-16.3942	-18.5607	-16.3844	-18.7650	-16.4187	-18.2178
B3PW91	-14.4680	-15.2601	-18.0088	-15.1553	-18.3514	-15.1656	-17.2899	-15.1753	-17.4897	-15.1446	-17.0158	-14.2972	-15.7565	-18.2794	-15.9672	-19.9110	-15.9509	-18.2403	-15.9375	-18.4104	-15.9852	-17.8935
B98	-17.5030	-18.3442	-21.0898	-18.2267	-22.5696	-18.2380	-20.2243	-18.2491	-20.6908	-18.2158	-20.0756	-17.3577	-18.7773	-21.4272	-19.0015	-23.0436	-18.9896	-21.3668	-18.9780	-21.5940	-19.0150	-21.0078
B971	-18.1351	-18.9807	-21.7156	-18.8622	-23.1909	-18.8730	-20.8021	-18.8844	-21.3531	-18.8506	-20.7061	-18.0050	-19.4166	-22.0797	-19.6361	-23.6875	-19.6233	-21.9920	-19.6123	-22.2270	-19.6490	-21.6384
B972	-12.0394	-12.8916	-15.5165	-12.7823	-17.0303	-12.7982	-14.9933	-12.8144	-15.4459	-12.7661	-14.6899	-11.8897	-13.3937	-15.8379	-13.6417	-17.4861	-13.6233	-15.9262	-13.6090	-16.0925	-13.6622	-15.5994
BHandH	**-3.1660**	-3.7310	-5.8761	-3.5345	-6.9248	-3.5521	-4.7723	-3.5688	-5.1259	-3.5171	-4.5144	**-3.0037**	-3.9291	-6.0331	-4.0131	-4.3498	-4.0094	-5.6443	-4.0061	-5.8144	-4.0172	-5.3800
BHandHLYP	-6.6738	-7.7192	-9.9485	-7.7454	-11.4515	-7.7482	-9.2452	-7.7508	-9.7572	-7.7427	-9.2217	-6.3921	-7.9709	-10.2417	-8.3795	-11.8112	-8.3590	-10.2617	-8.3396	-10.4235	-8.4005	-9.9844
BLYP	-40.3546	-41.6783	-44.9938	-41.6711	*-47.0057*	-41.4779	-43.6067	-41.6967	-44.7744	-41.5896	-43.7209	-39.0875	-42.1745	-45.4672	-42.5769	*-47.6768*	-42.3505	-44.6327	-42.5396	-46.0049	-42.5295	-44.6999
BMK	-15.7305	-16.7370	-19.3737	-16.6660	-20.7911	-16.6769	-18.5770	-16.6873	-18.9954	-16.6564	-18.2901	-15.2179	-16.6955	-19.3641	-16.9073	-20.8757	-16.8968	-19.3127	-16.8864	-19.4751	-16.9189	-18.9973
BP86	-31.4336	-32.0591	-35.2936	-31.8827	-36.9671	-31.9019	-34.3323	-31.9203	-34.6655	-31.8638	-33.9779	-31.2260	-32.5989	-35.6252	-32.8784	-37.5686	-32.8729	-35.4976	-32.8689	-35.8175	-32.8853	-35.0579
CAM-B3LYP	-13.4485	-14.7719	-17.3187	-14.8933	-18.9302	-14.8892	-16.9882	-14.8849	-17.2688	-14.8983	-16.8035	-13.1826	-15.0929	-17.5136	-15.5345	-19.2475	-15.5057	-17.8108	-15.4789	-17.9081	-15.5651	-17.5376
HF	9.8988	8.9756	7.2508	8.9840	5.8240	8.9766	8.1551	8.9698	7.4947	8.9912	7.8336	10.2725	8.8144	6.9272	8.2666	5.3877	8.2902	6.7289	8.3136	6.5991	8.2437	6.9684
LC-BLYP	**-0.4915**	-2.0036	-4.2783	-2.2438	-5.7530	-2.2346	-3.7842	-2.2254	-4.3778	-2.2524	-3.9793	**-0.2680**	-2.2796	-4.3884	-2.8374	-6.0733	-2.8008	-4.8030	-2.7663	-4.8326	-2.8747	-4.6271
M06	-15.8861	-17.1076	-19.1891	-16.4282	-20.4446	-16.4433	-18.0915	-16.4580	-18.5873	-16.4136	-17.8422	-15.0236	-16.5403	-18.4867	-16.1581	-19.9157	-16.1436	-18.4752	-16.1316	-18.5654	-16.1748	-18.1123
M06-2X	-12.3865	-13.4461	-15.9466	-13.4383	-17.1719	-13.4463	-15.1772	-13.4522	-15.5551	-13.4307	-14.9120	-11.9898	-13.4429	-15.7876	-13.7591	-17.3131	-13.7335	-15.9296	-13.7097	-16.0523	-13.7875	-15.6694
mpW1LYP	-21.4335	-22.6384	-25.4322	-22.7079	-27.0894	-22.7085	-24.8584	-22.7080	-25.2233	-22.7073	-24.6826	-21.1212	-22.8948	-25.6245	-23.3158	-27.4143	-23.2951	-25.7153	-23.2738	-25.9377	-23.3361	-25.3735
mpW1PW91	-11.3956	-12.1818	-14.8359	-12.0722	-16.2272	-12.0834	-14.0885	-12.0934	-14.3533	-12.0628	-13.8268	-11.2010	-12.5367	-14.9827	-12.7267	-16.5086	-12.7120	-14.8763	-12.6988	-15.0332	-12.7441	-14.5468
O3LYP	-16.6922	-18.0360	-20.3287	-18.3098	-22.5326	-18.3123	-20.3604	-18.4582	-20.7366	-18.3073	-20.0699	-16.4618	-18.3429	-21.0971	-18.7378	-22.8656	-18.7070	-21.3420	-18.6796	-21.5814	-18.7716	-21.0412
OLYP	-24.1399	-25.7764	-29.0829	-26.0328	-31.1759	-26.0639	-28.2061	-26.0920	-28.6905	-26.0043	-27.8584	-23.0106	-25.8468	-28.9095	-26.3021	-30.7593	-26.2693	-29.2222	-26.2392	-29.4975	-26.3363	-28.9041
OPBE	-13.0642	-14.1433	-17.2426	-14.2765	-19.0136	-14.3067	-16.0552	-14.3377	-16.4815	-14.1483	-15.5067	-12.9982	-14.2610	-17.3888	-14.6532	-19.1078	-14.6051	-16.9436	-14.5554	-17.5253	-14.6819	-16.6471
OPW91	-13.6848	-14.8206	-17.9301	-14.8646	-19.7199	-14.8928	-16.6228	-14.9127	-17.1902	-14.8380	-16.2062	-13.6012	-14.9262	-18.0651	-15.3050	-19.7965	-15.2613	-17.6414	-15.2169	-18.2065	-15.3400	-17.3445
PBE	-29.0424	-29.6563	-32.8700	-29.4194	-34.4599	-29.4379	-31.9199	-29.4553	-32.2640	-29.4024	-31.5741	-28.8917	-30.2049	-33.1933	-30.3127	-34.9364	-30.3049	-33.0822	-30.2985	-33.3687	-30.3236	-32.6644
PBE0	-11.3353	-12.0433	-14.6497	-11.8892	-16.0064	-11.9013	-13.8498	-11.9142	-14.1896	-11.8770	-13.5973	-11.2277	-12.4966	-14.9322	-12.6673	-16.4219	-12.6530	-14.7851	-12.6415	-14.9489	-12.6824	-14.4622
TPSS	-22.6102	-23.5695	-26.5489	-23.4433	-28.2088	-23.4555	-25.3659	-23.4685	-24.9790	-23.4312	-25.0658	-22.5252	-24.0659	-27.0136	-24.3163	-28.8115	-24.3042	-26.6170	-24.2932	-22.7559	-24.3283	-26.2327
VSXC	-23.3361	-24.0598	-27.0323	-23.8174	-28.3800	-23.8405	-25.7419	-23.8540	-26.2085	-23.7941	-25.3076	-23.6847	-24.7972	-27.8759	-24.8215	-29.3340	-24.8246	-27.1349	-24.8188	-27.4967	-24.8184	-26.7423
wB97	-5.6949	-7.2040	-9.5571	-7.4462	-11.0227	-7.4381	-9.0741	-7.4298	-9.5029	-7.4542	-8.8940	-5.5757	-7.5708	-9.7955	-8.1470	-11.5052	-8.1079	-10.2236	-8.0720	-10.2996	-8.1883	-10.0601
wB97X	-8.0038	-9.2687	-11.6560	-9.3876	-13.0632	-9.3851	-11.0412	-9.3826	-11.6242	-9.3904	-11.1461	-7.9121	-9.6897	-11.9512	-10.1600	-13.5866	-10.1271	-12.2918	-10.0969	-12.3583	-10.1953	-12.0696
X3LYP	-21.8446	-22.9794	-25.8228	-23.0110	-27.4643	-23.0134	-25.1940	-23.0155	-25.5376	-23.0089	-24.9904	-21.5606	-23.3316	-26.0731	-23.7293	-27.8814	-23.7093	-26.1500	-23.6897	-26.3739	-23.7494	-25.8006

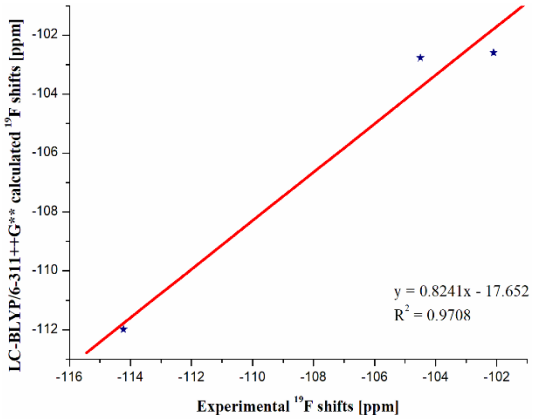
Table S21. Theoretical chemical shifts [ppm] of some nuclei of model fluorinated compounds calculated in the gas phase using OLYP/6-311++G** level of the theory compared with available experimental data

Model compound with marked studied atom	δ_C (teor.)	δ_C (exp.)	δ_C (teor.) – δ_C (exp.)
	127.2058	128.36[a]	-1.1542
	166.0380	163.20[b]	2.8380
	114.4092	115.50[b]	-1.091
	135.4101	124.50[b]	10.910
	131.7743	130.80[b]	0.9743
	73.7298	71.57[c]	2.1598

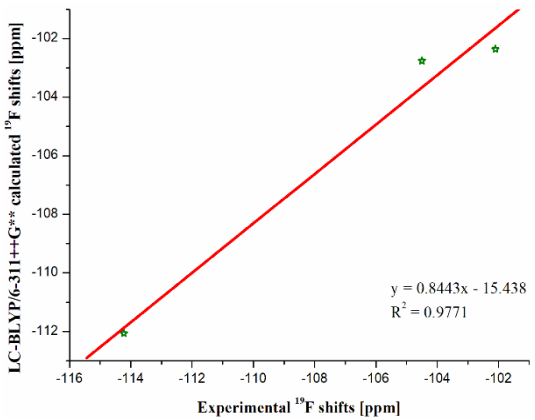
[a] according to [14]

[b] according to [15]

[c] according to [16]



A



B

Figure S1. Correlation between theoretical and experimental ^{19}F NMR chemical shifts for (A) R-configurations and (B) S-configurations of the studied cathinones. Parameters of linear correlations are also given.

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