Supplementary Materials

New Prenylated Indole Homodimeric and Pteridine Alkaloids from the Marine-Derived Fungus *Aspergillus austroafricanus* Y32-2

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† These authors contributed equally to this work.

List of Supplementary Materials

Table S1. All biological activities of isolated compounds

Compounds	Bioactivities (μg/mL)		
	Pro-angiogenesis	Anti-inflammatory	cytotoxicity against HepG2 (IC_{50})
1	-	-	>150
2	70, 120	-	>150
3	-	-	>150
4	120	-	>150
5	30, 70, 120	-	>150
6	-	-	30
7	30, 70, 120	70, 120	>150
8	-	70, 120	>150
9	-	-	>150
10	70, 120	70, 120	>150
11	-	30, 70, 120	>150
12	-	-	>150
13	-	-	>150
14	-	-	>150

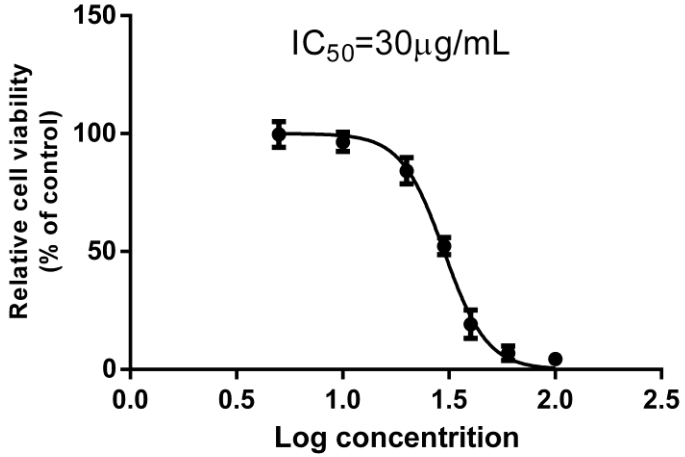
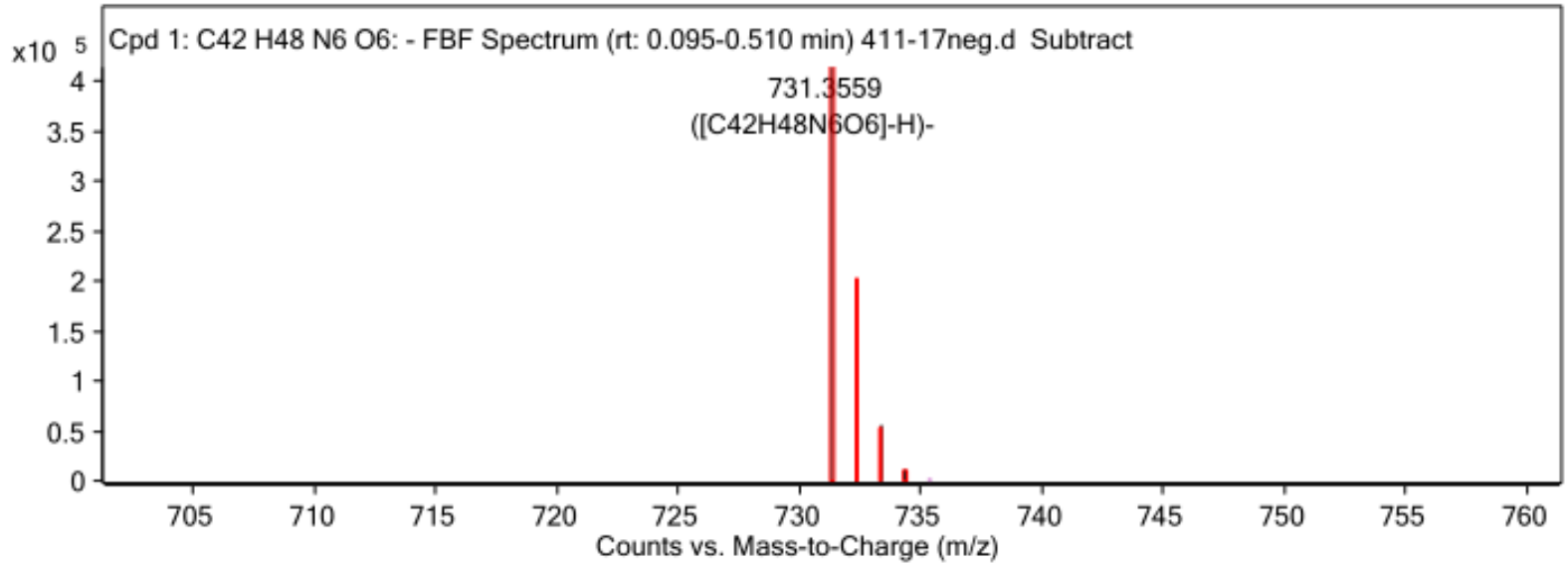


Figure S1. Dose–response curve of compound **6**



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
731.3559	1	413059.88	C42H48N6O6	(M-H)-
732.3593	1	201177.38	C42H48N6O6	(M-H)-
733.3622	1	55169.09	C42H48N6O6	(M-H)-
734.3649	1	11227.97	C42H48N6O6	(M-H)-

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Figure S2. HRESIMS data of compound **1**.

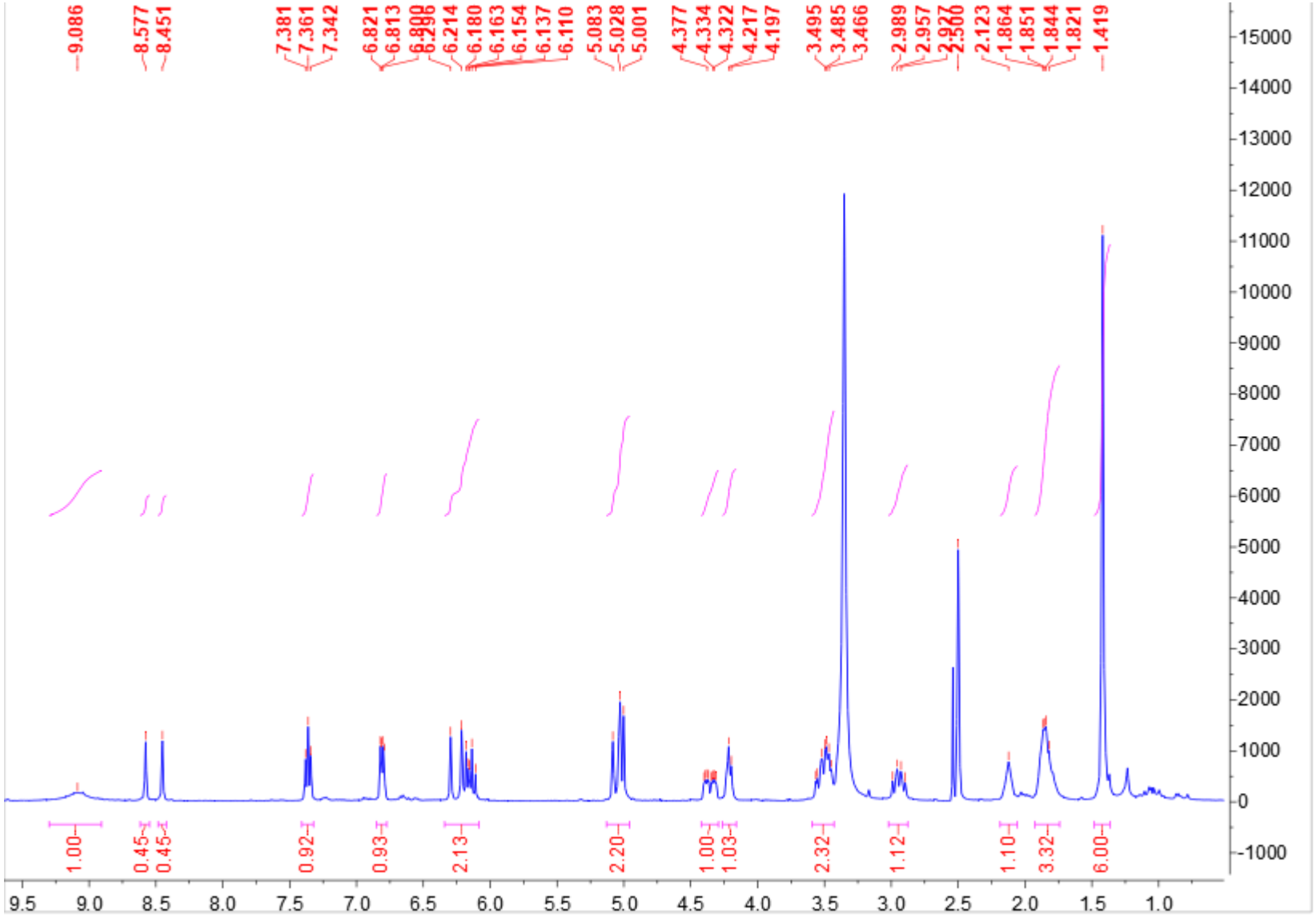

Figure S3. ^{1}H-NMR (400MHz) spectrum of compound **1** in DMSO-d_6.

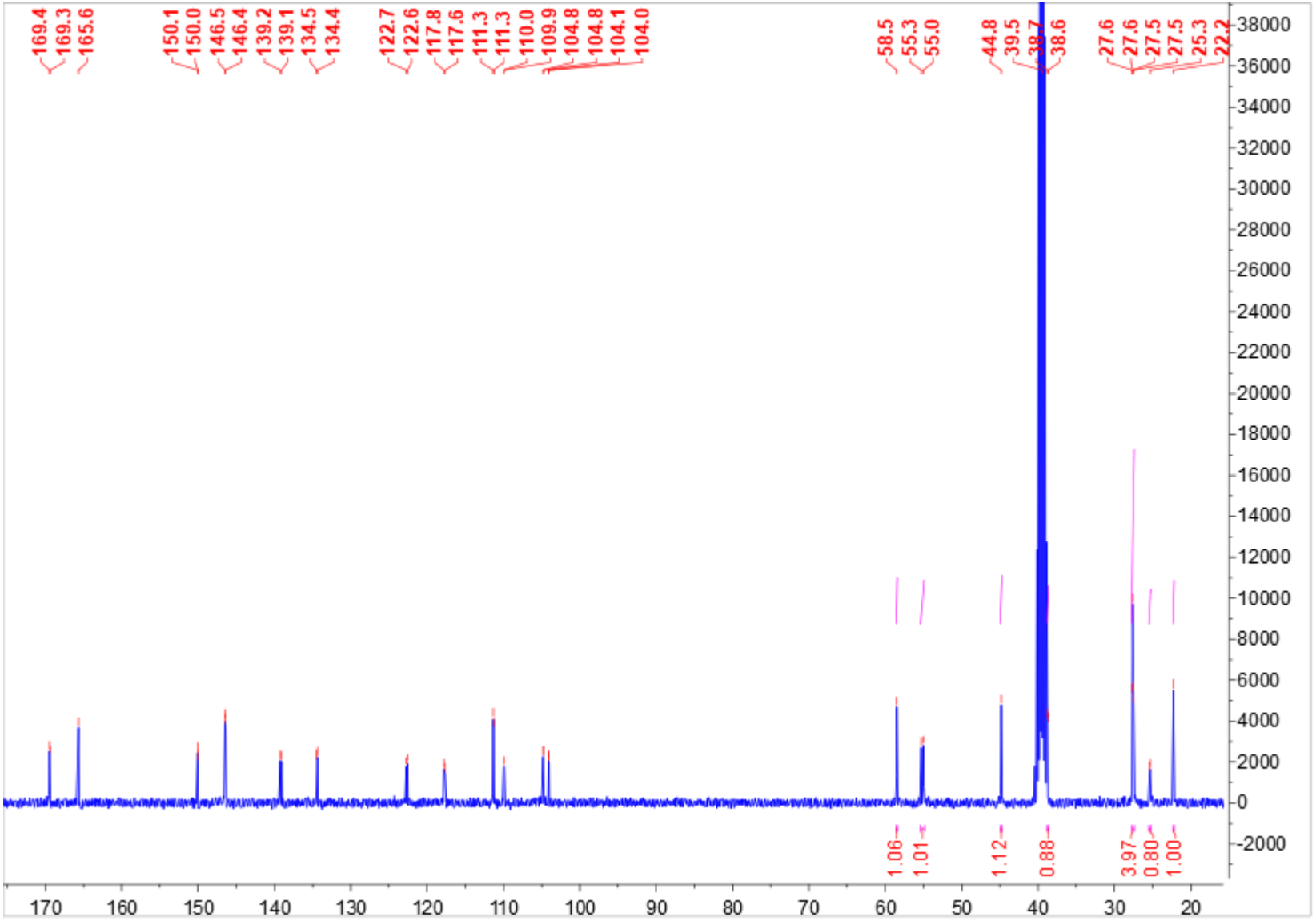

Figure S4. ^{13}C-NMR (150MHz) spectrum of compound **1** in DMSO-d_6.

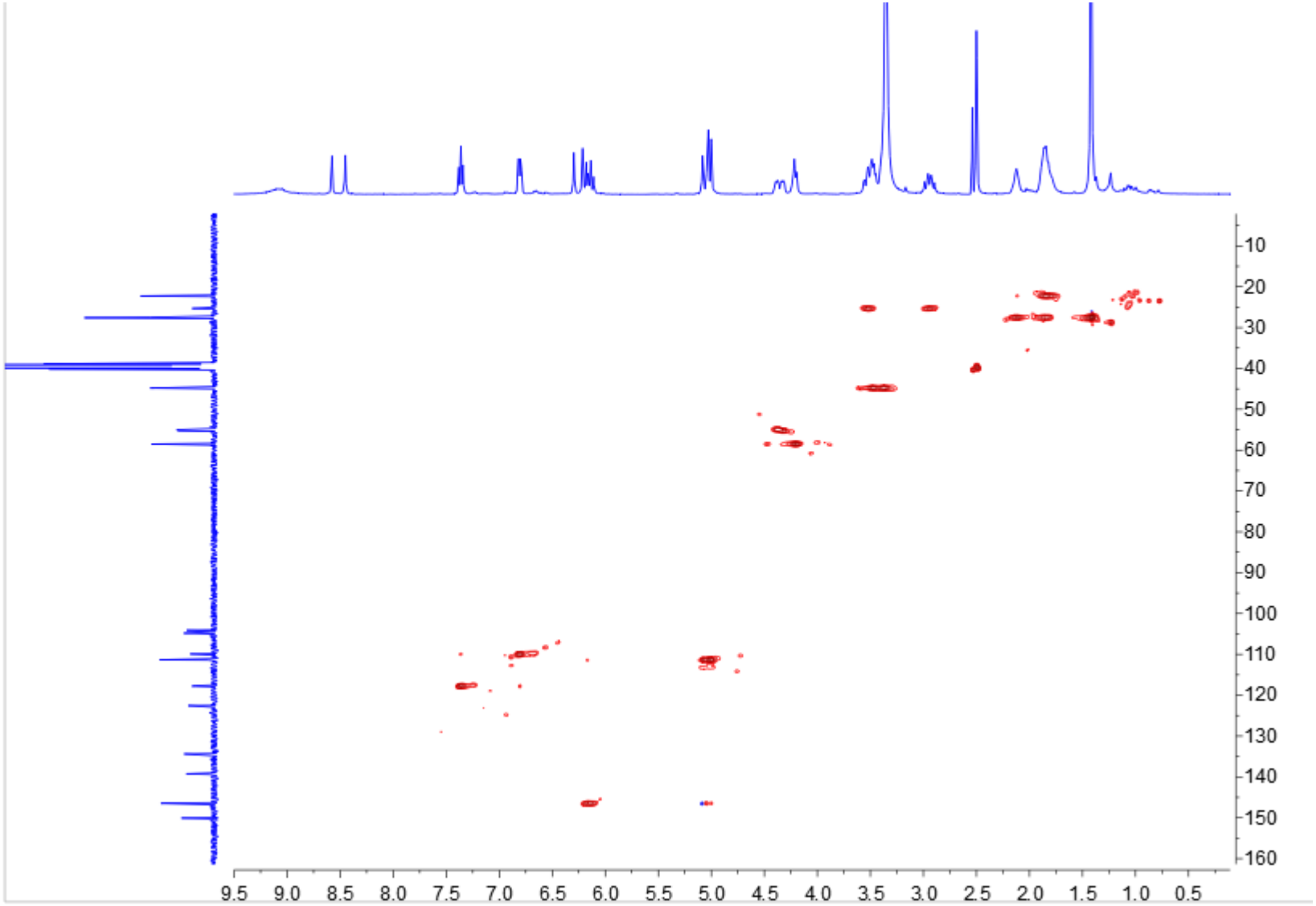

Figure S5. HSQC (400MHz) spectrum of compound **1** in DMSO-d_6.

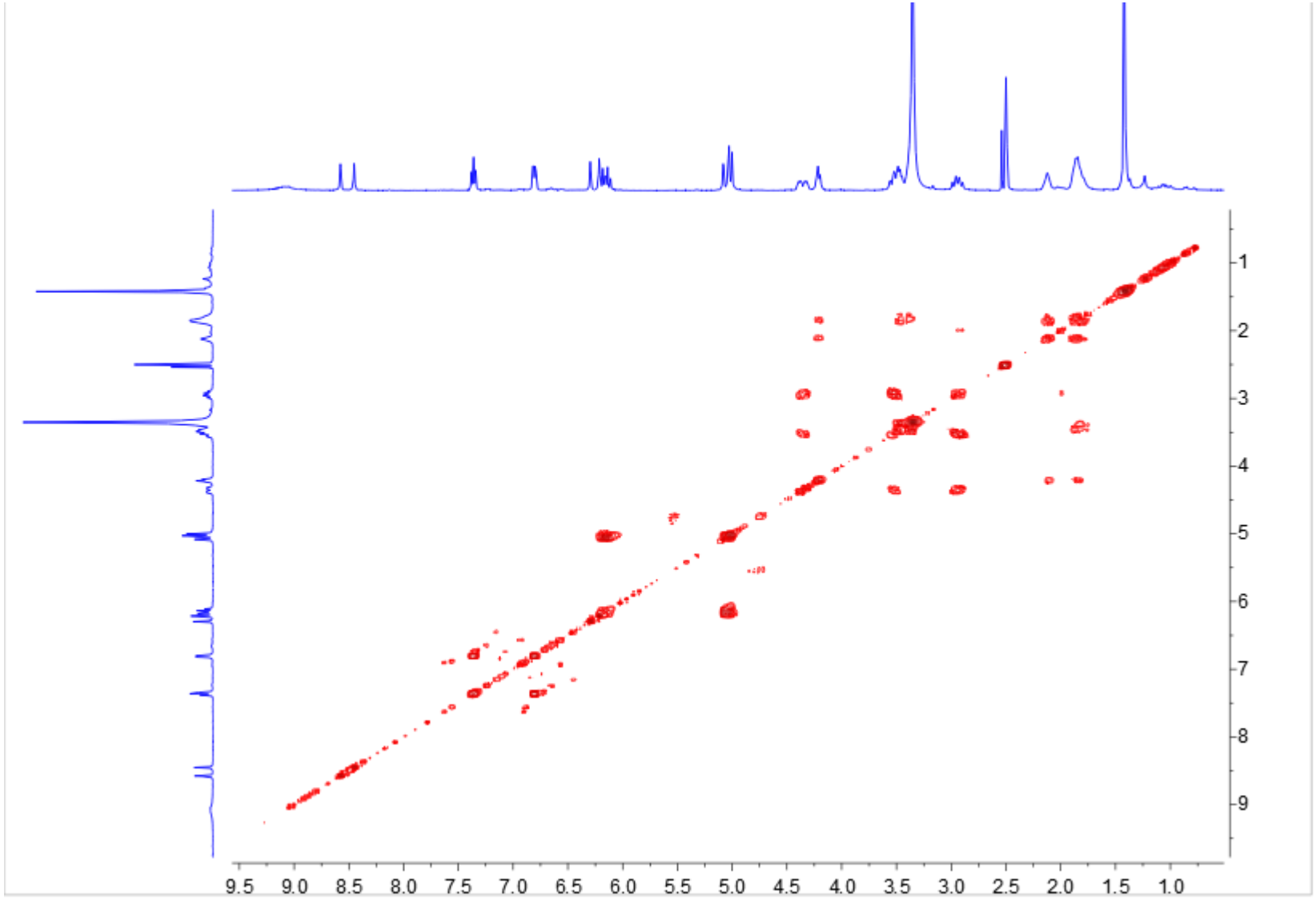

Figure S6. ^{1}H-^{1}H COSY (400MHz) spectrum of compound **1** in DMSO-d_6.

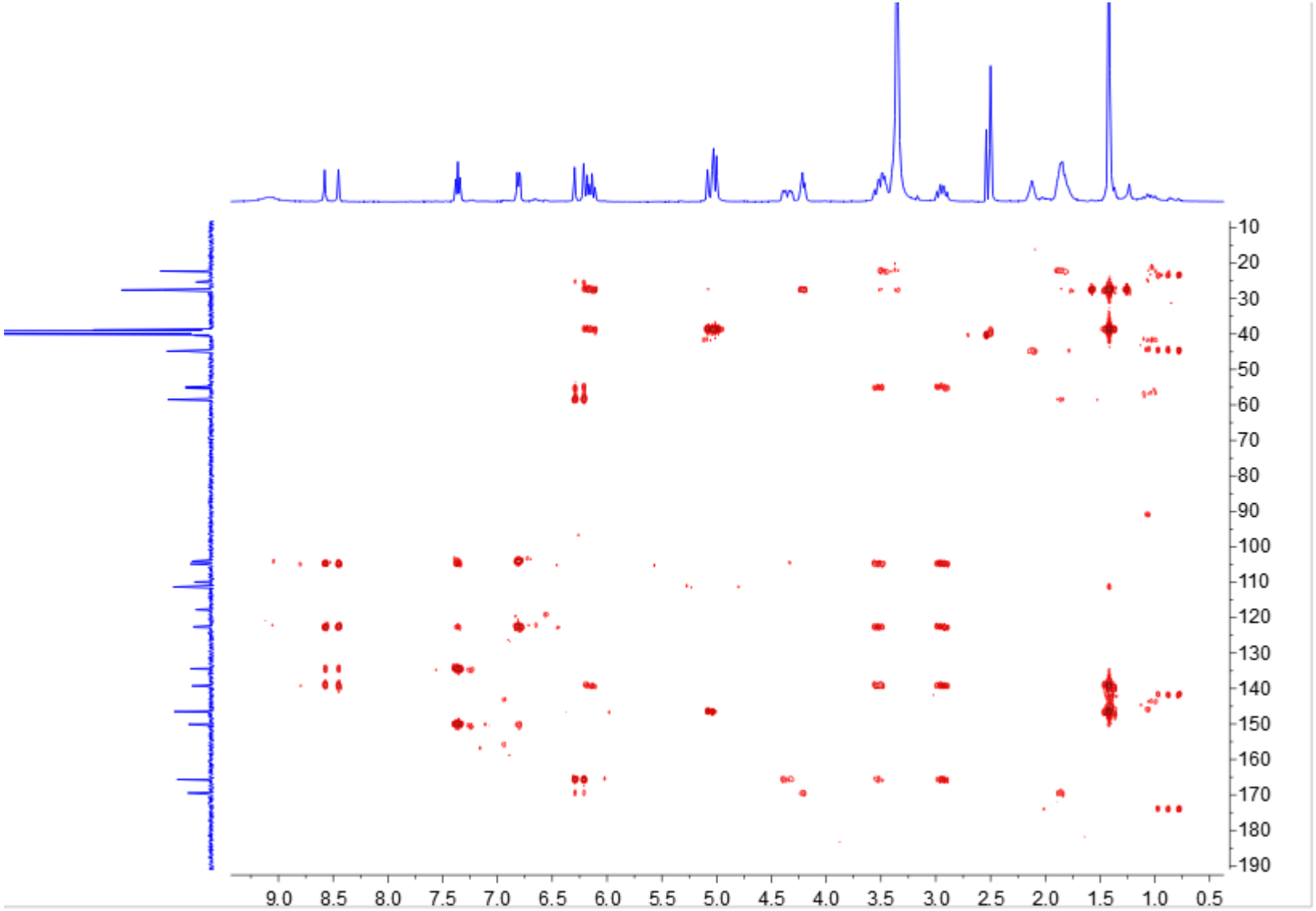

Figure S7. HMBC (400MHz) spectrum of compound **1** in DMSO-d_6.

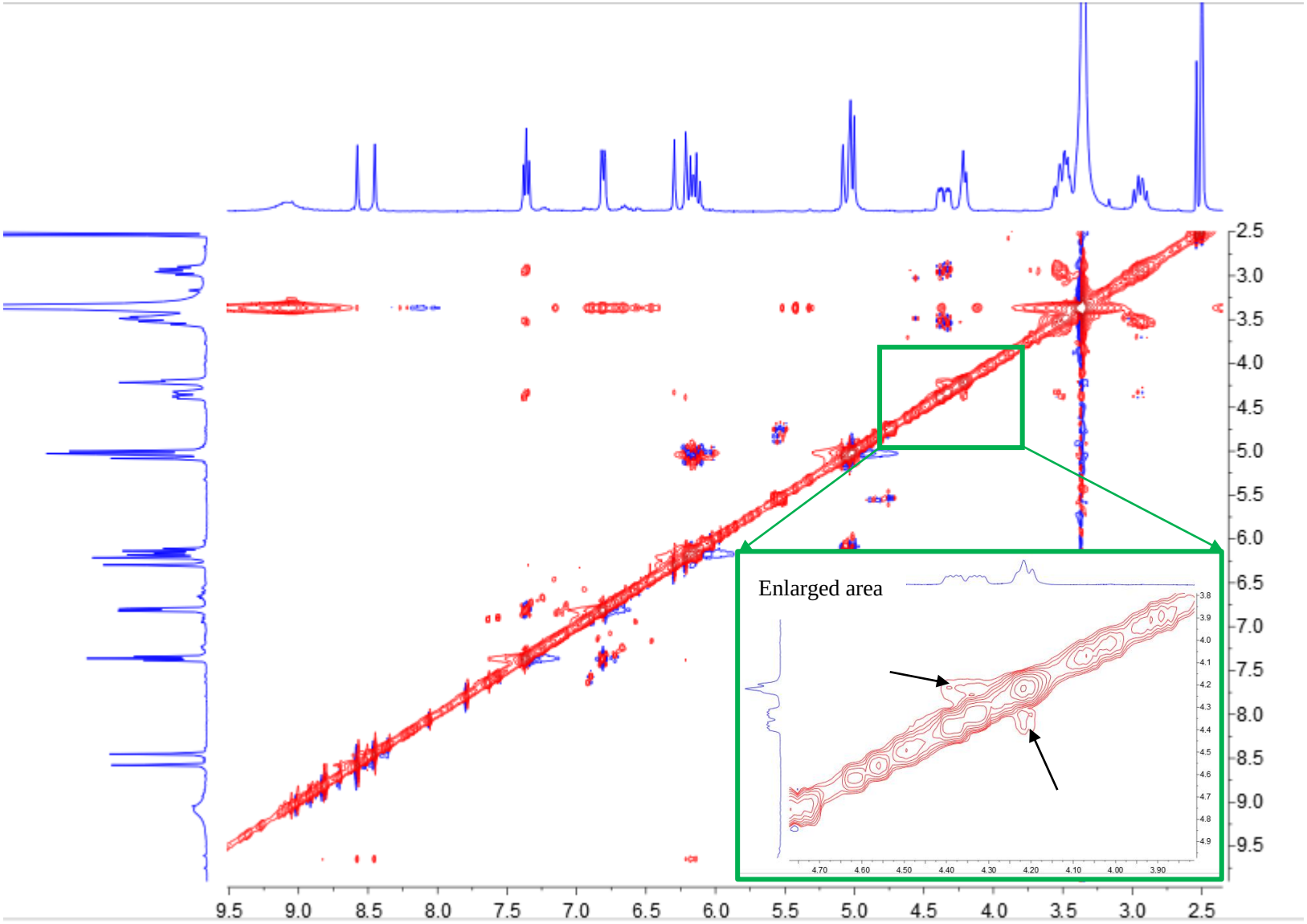

Figure S8. NOESY (400MHz) spectrum of compound **1** in DMSO-d_6. The NOESY correlations of H-11 and H-17 were indicated by black arrows in the enlarged area.

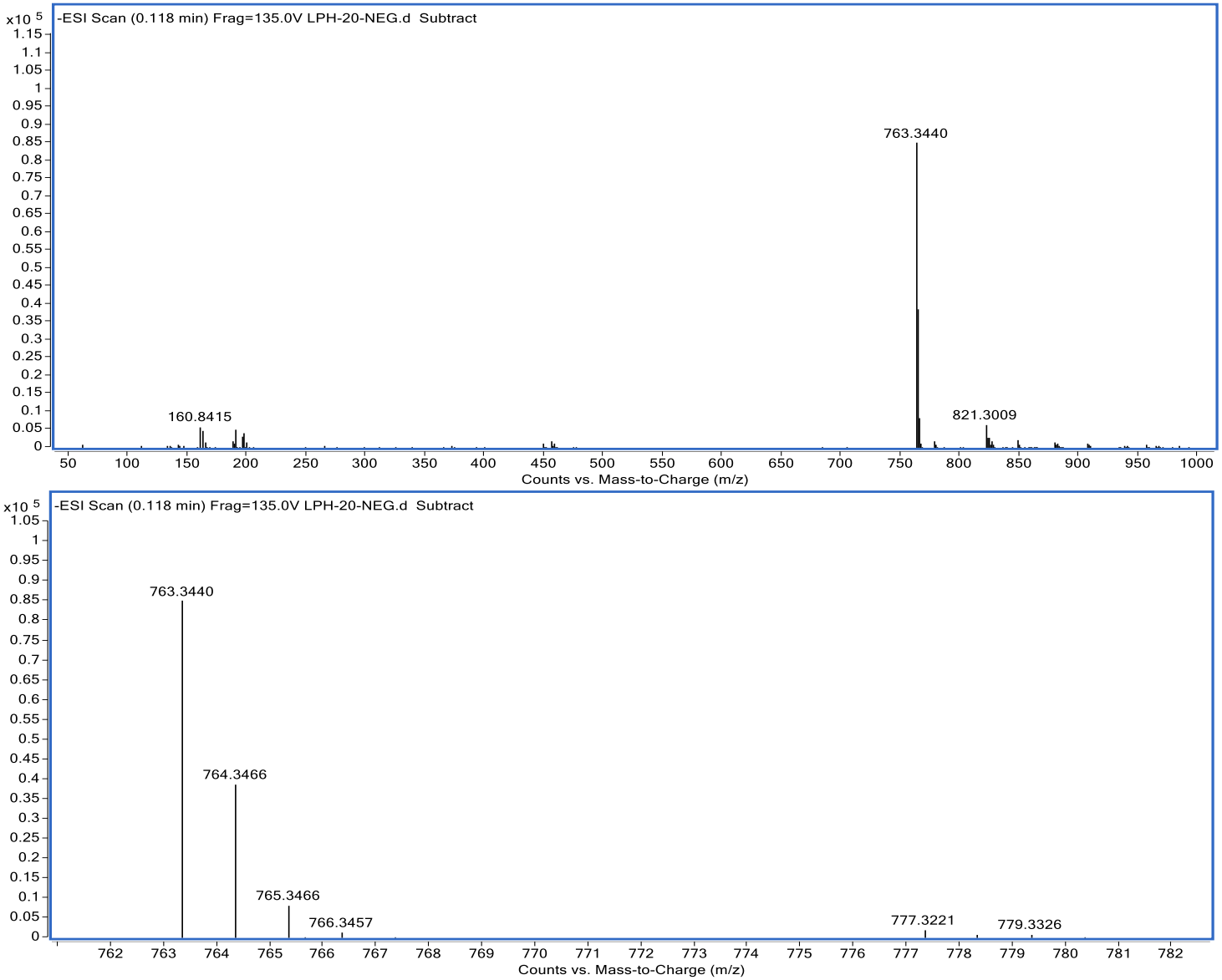

Figure S9. HRESIMS data of compound **2**

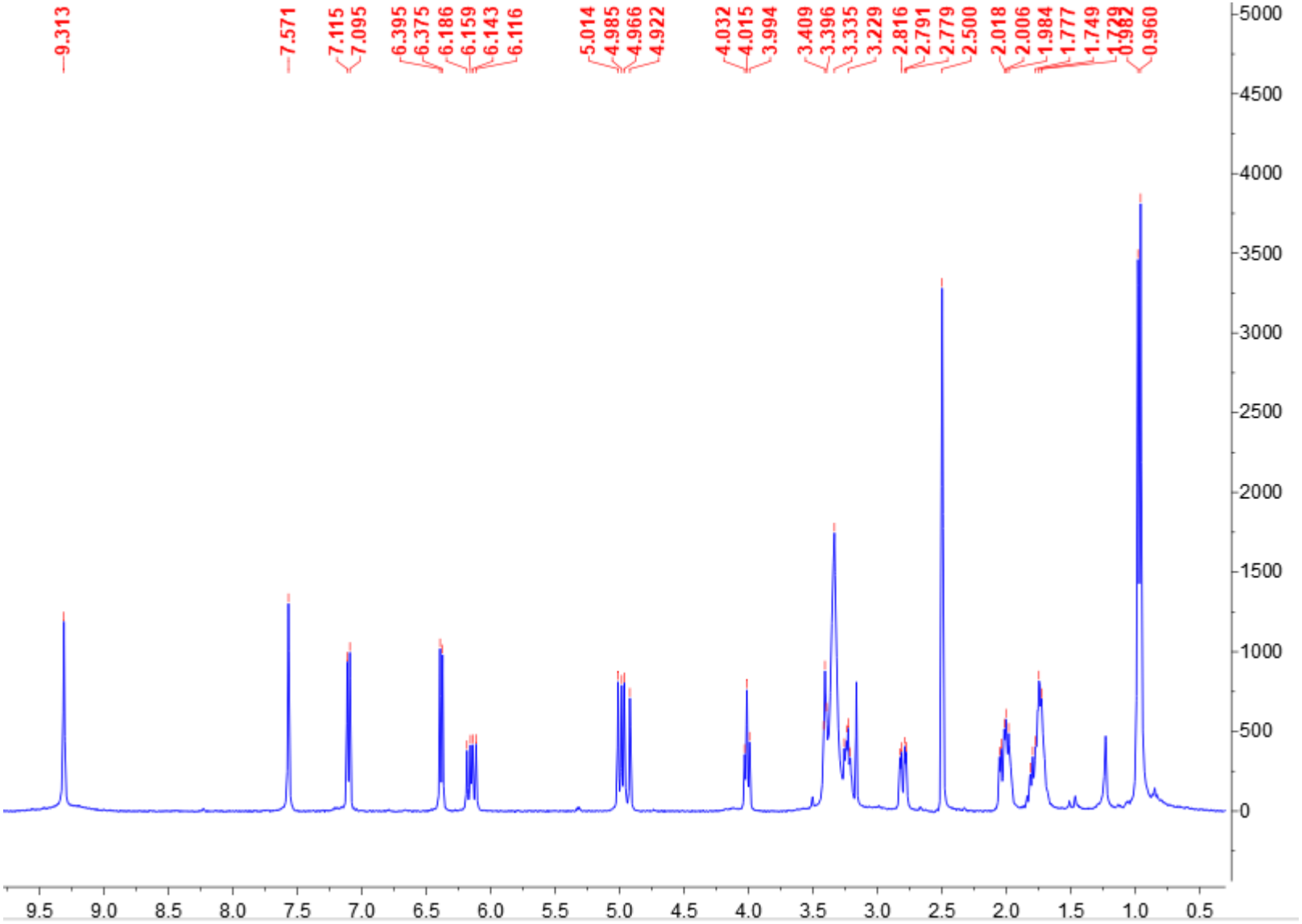

Figure S10. ^{1}H-NMR (400MHz) spectrum of compound **2** in DMSO-d_6.

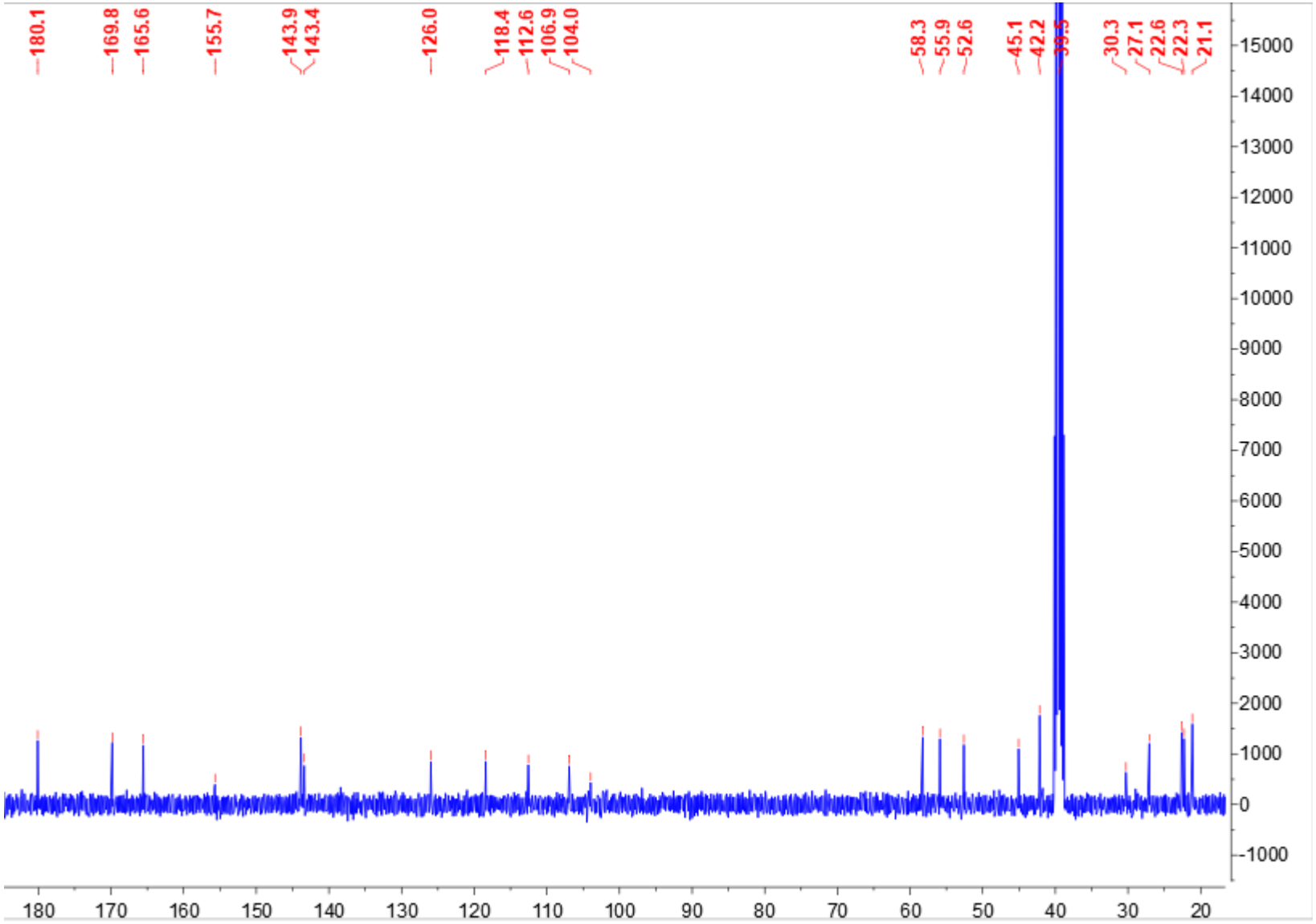

Figure S11. ^{13}C-NMR (150MHz) spectrum of compound **2** in DMSO-d_6.

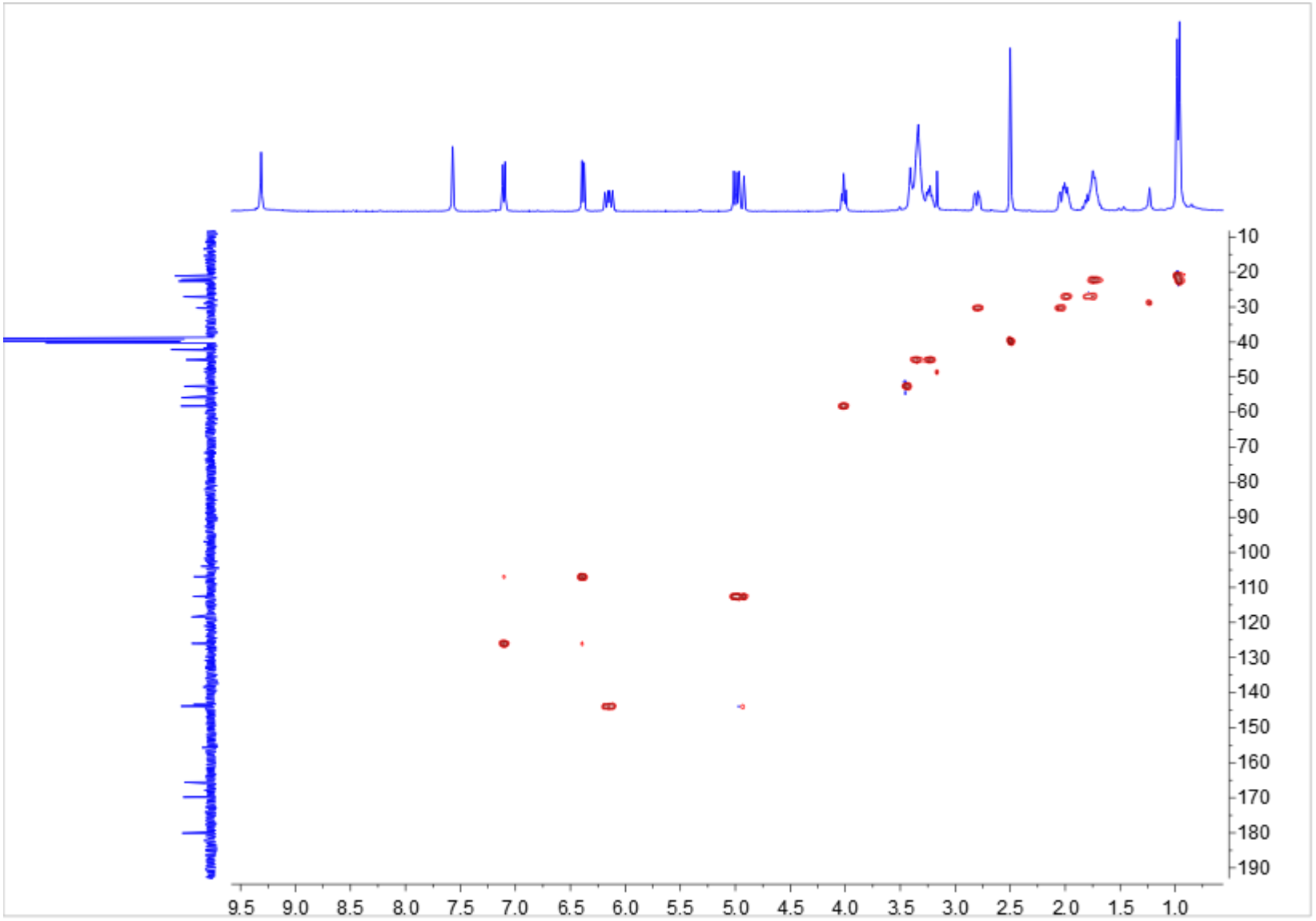

Figure S12. HSQC (400MHz) spectrum of compound **2** in DMSO-d_6.

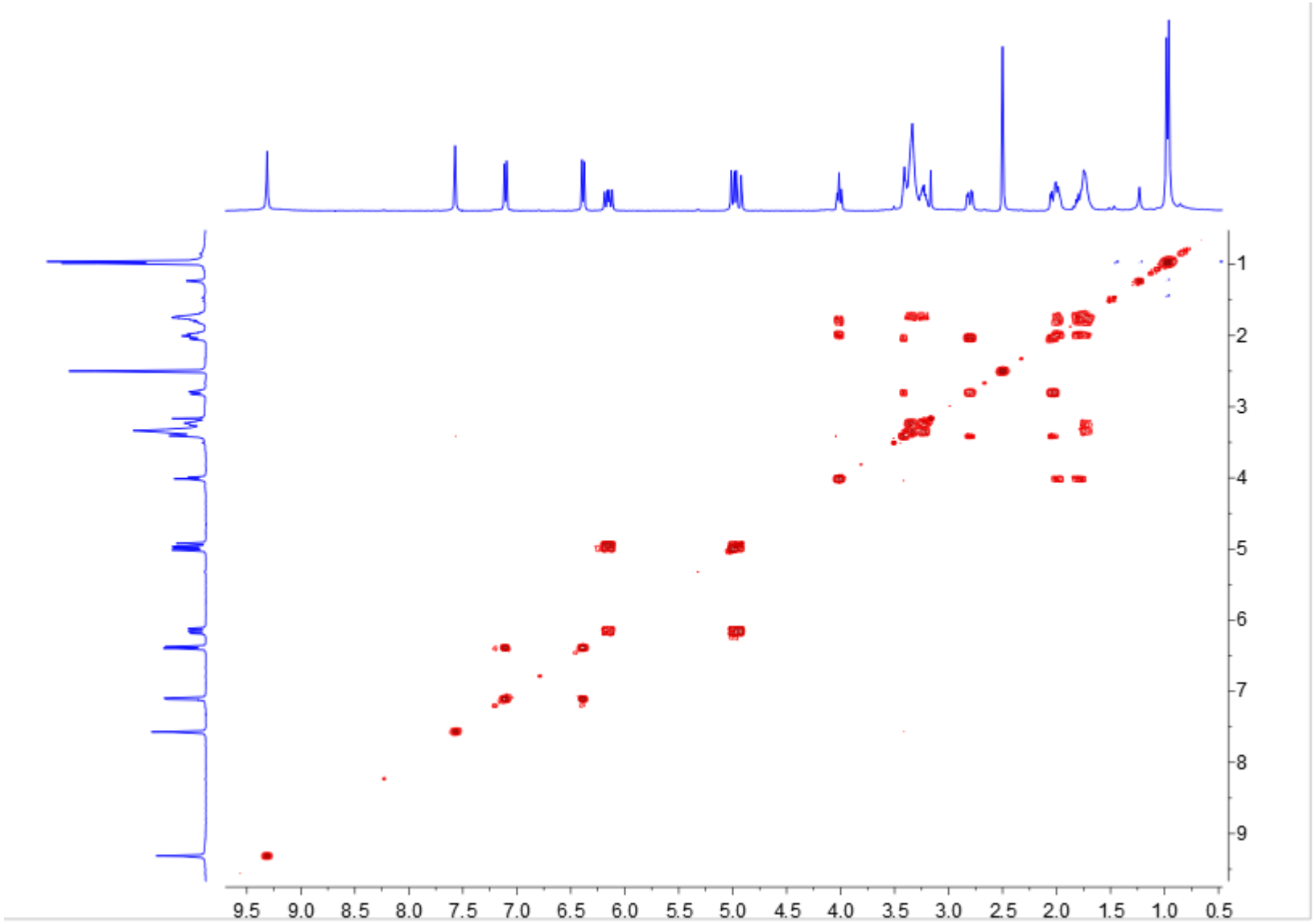

Figure S13. ^{1}H-^{1}H COSY (400MHz) spectrum of compound **2** in DMSO-d_6.

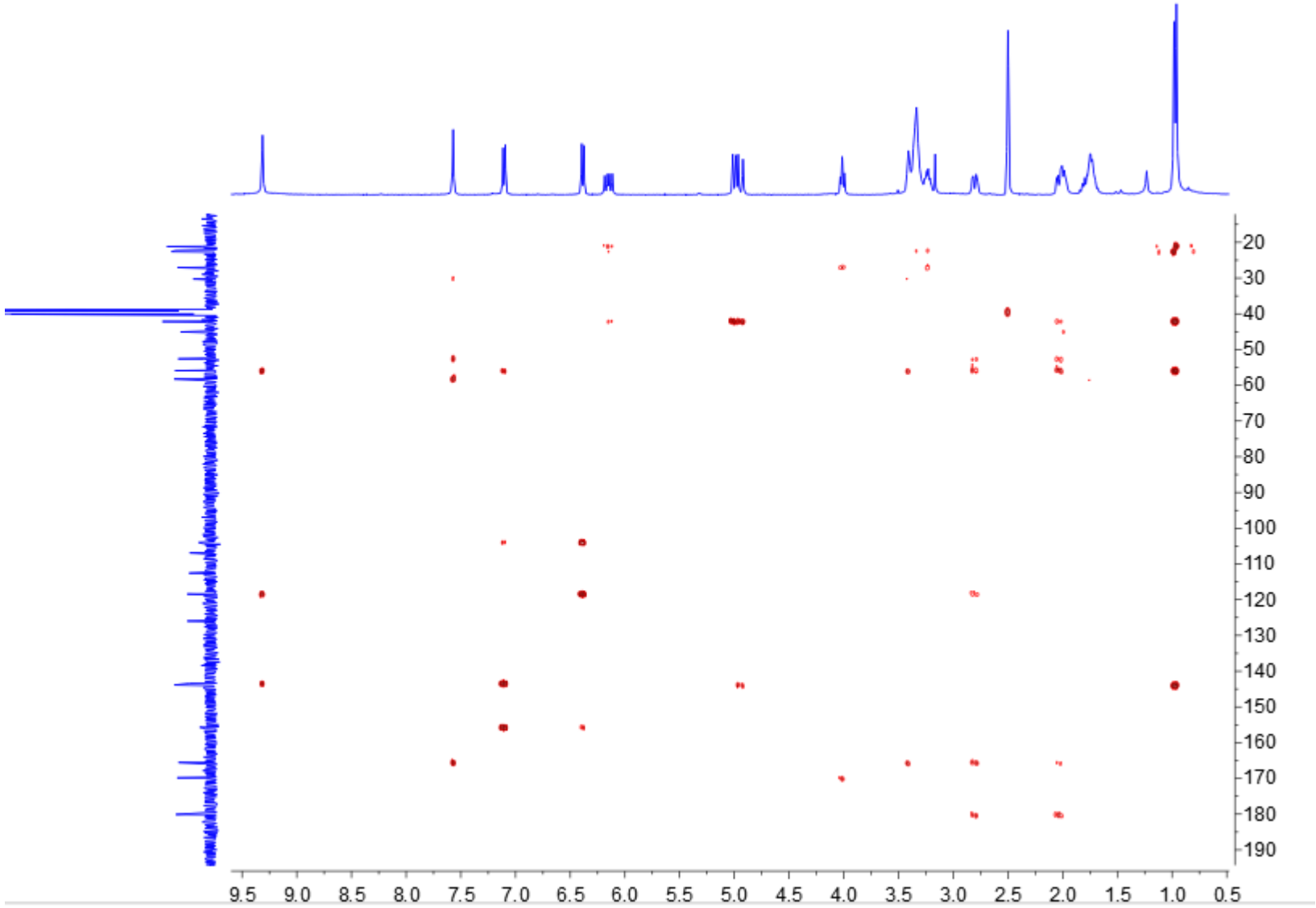

Figure S14. HMBC (400MHz) spectrum of compound **2** in DMSO-d_6.

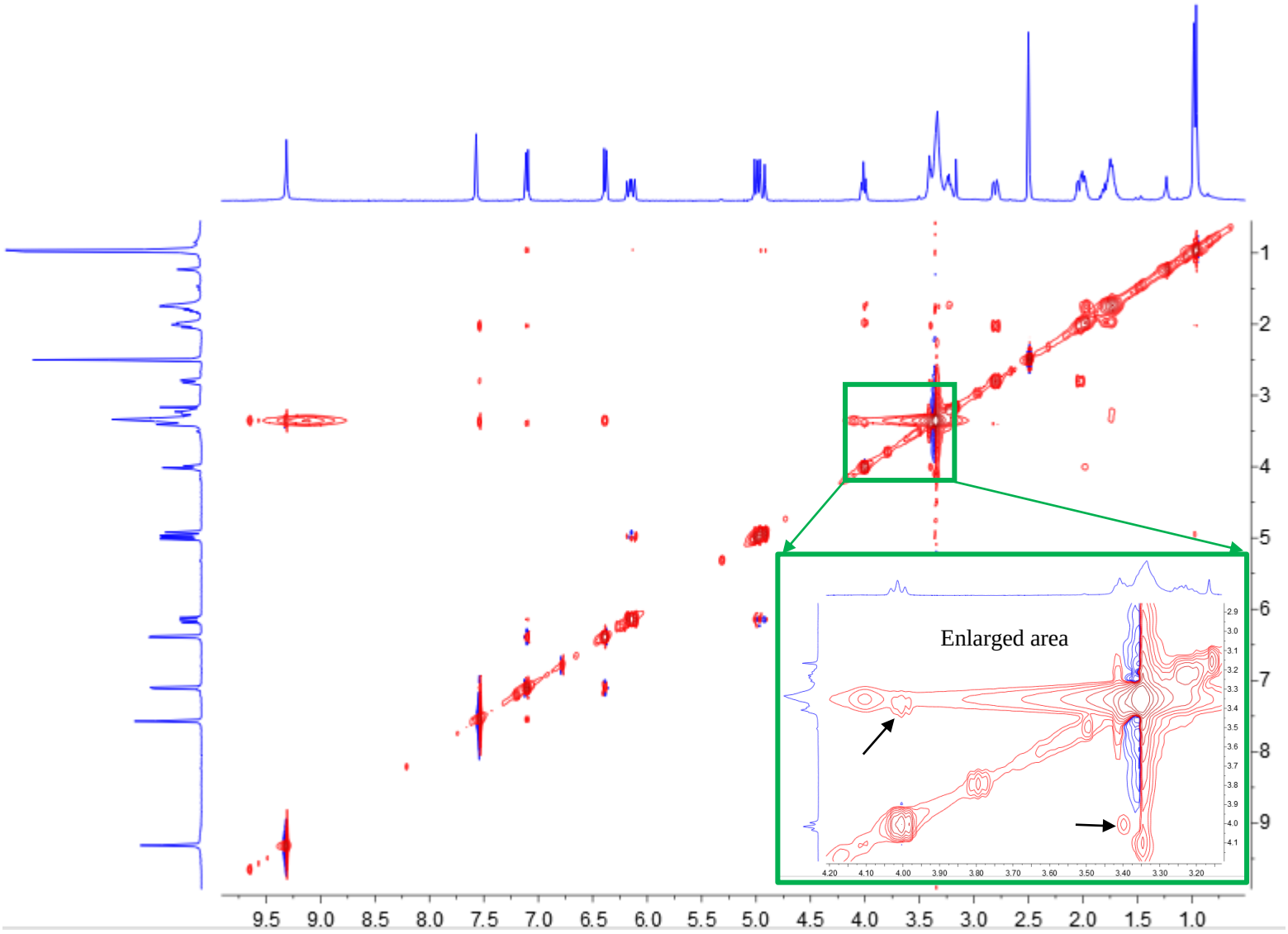

Figure S15. NOESY (400MHz) spectrum of compound **2** in DMSO-d_6. The NOESY correlations of H-11 and H-17 were indicated by black arrows in the enlarged area.

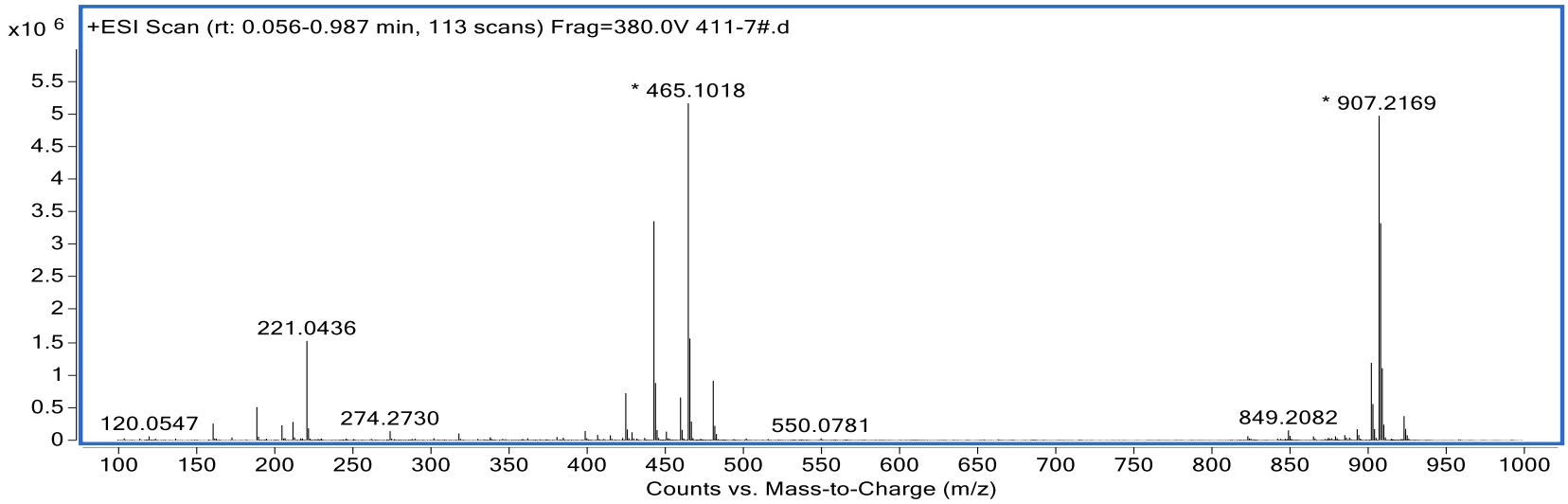

Figure S16. HRESIMS data of compound **3**

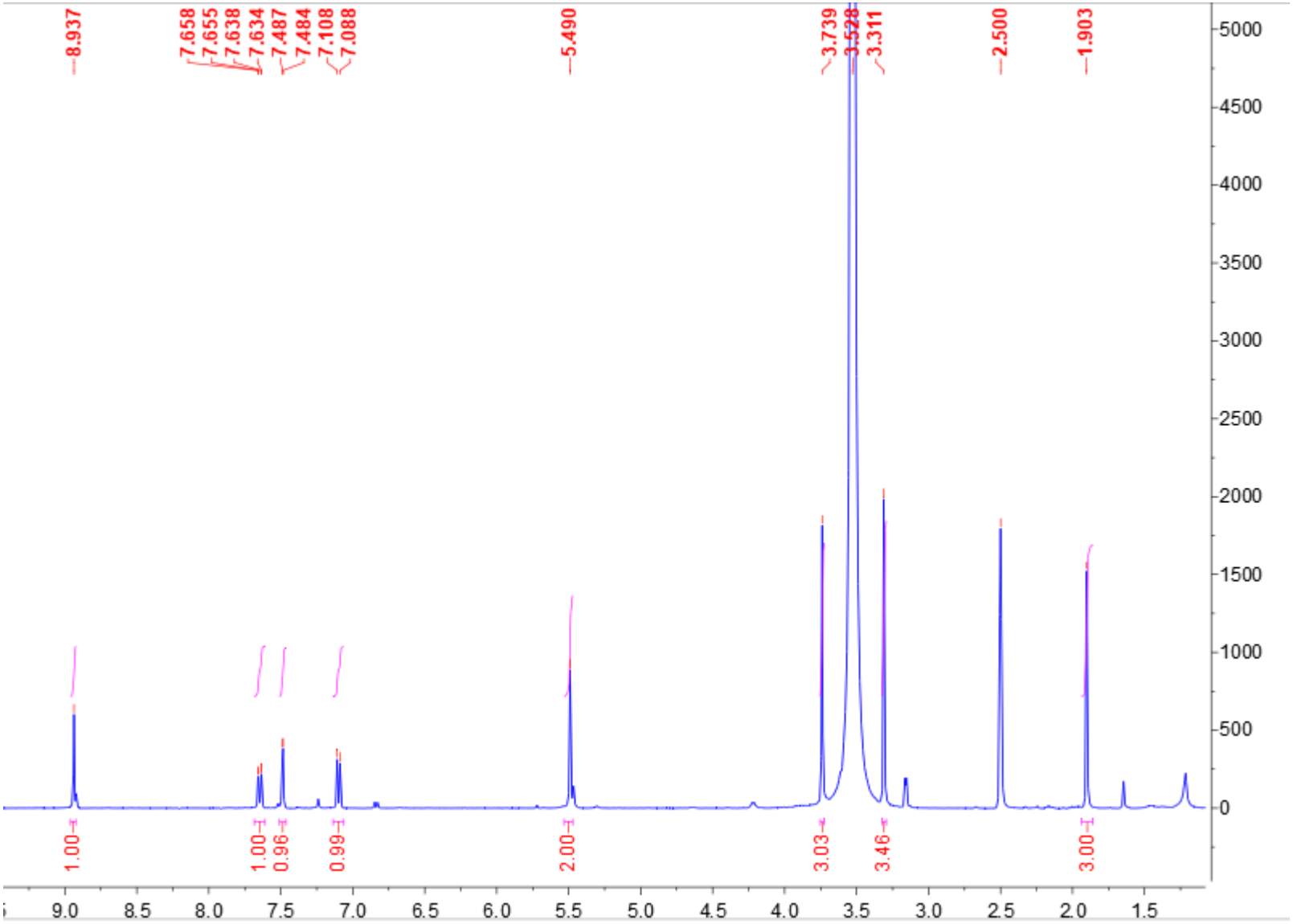

Figure S17. ^{1}H-NMR (400MHz) spectrum of compound **3** in DMSO-d_6.

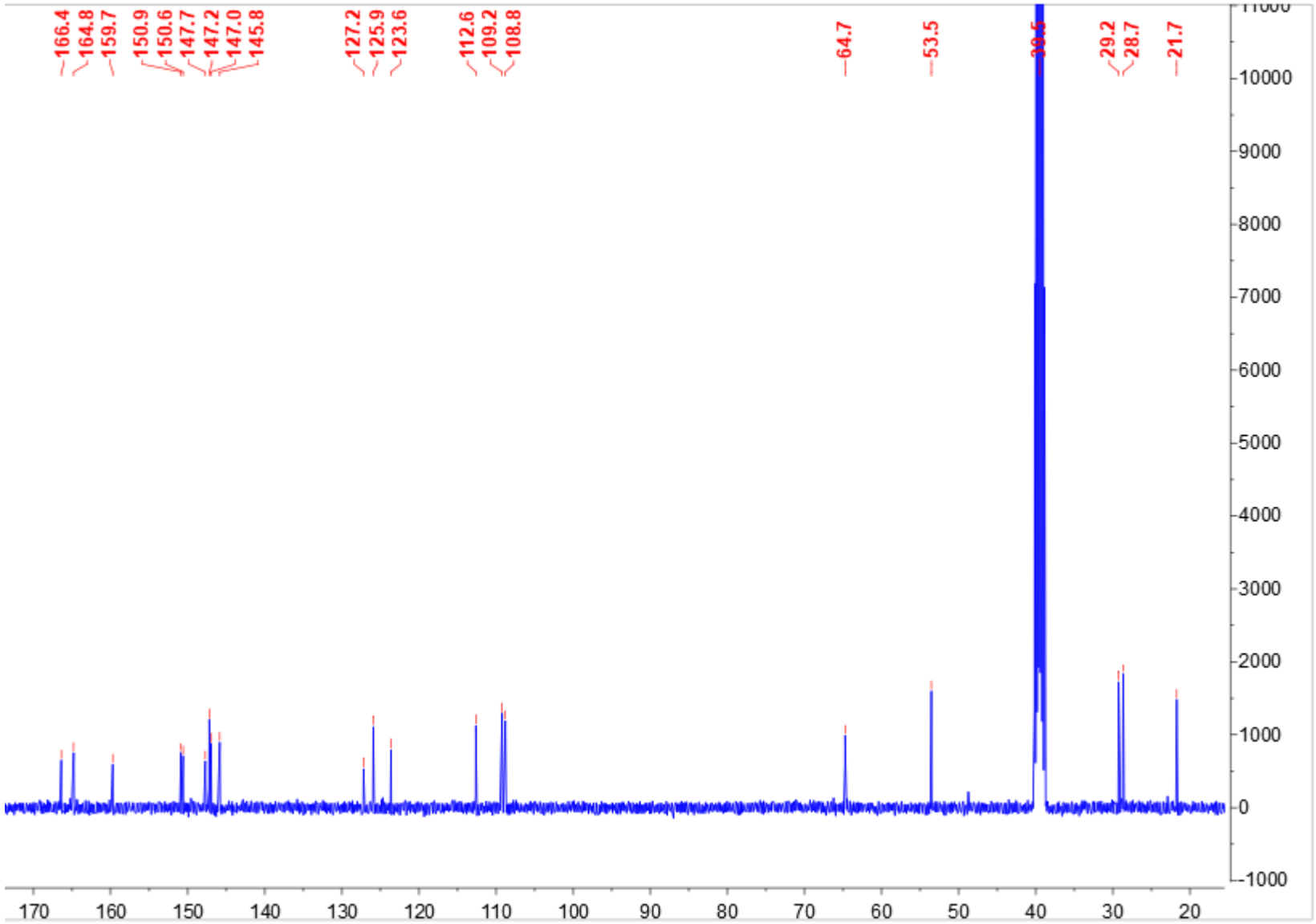

Figure S18. ^{13}C-NMR (150MHz) spectrum of compound **3** in DMSO-d_6.

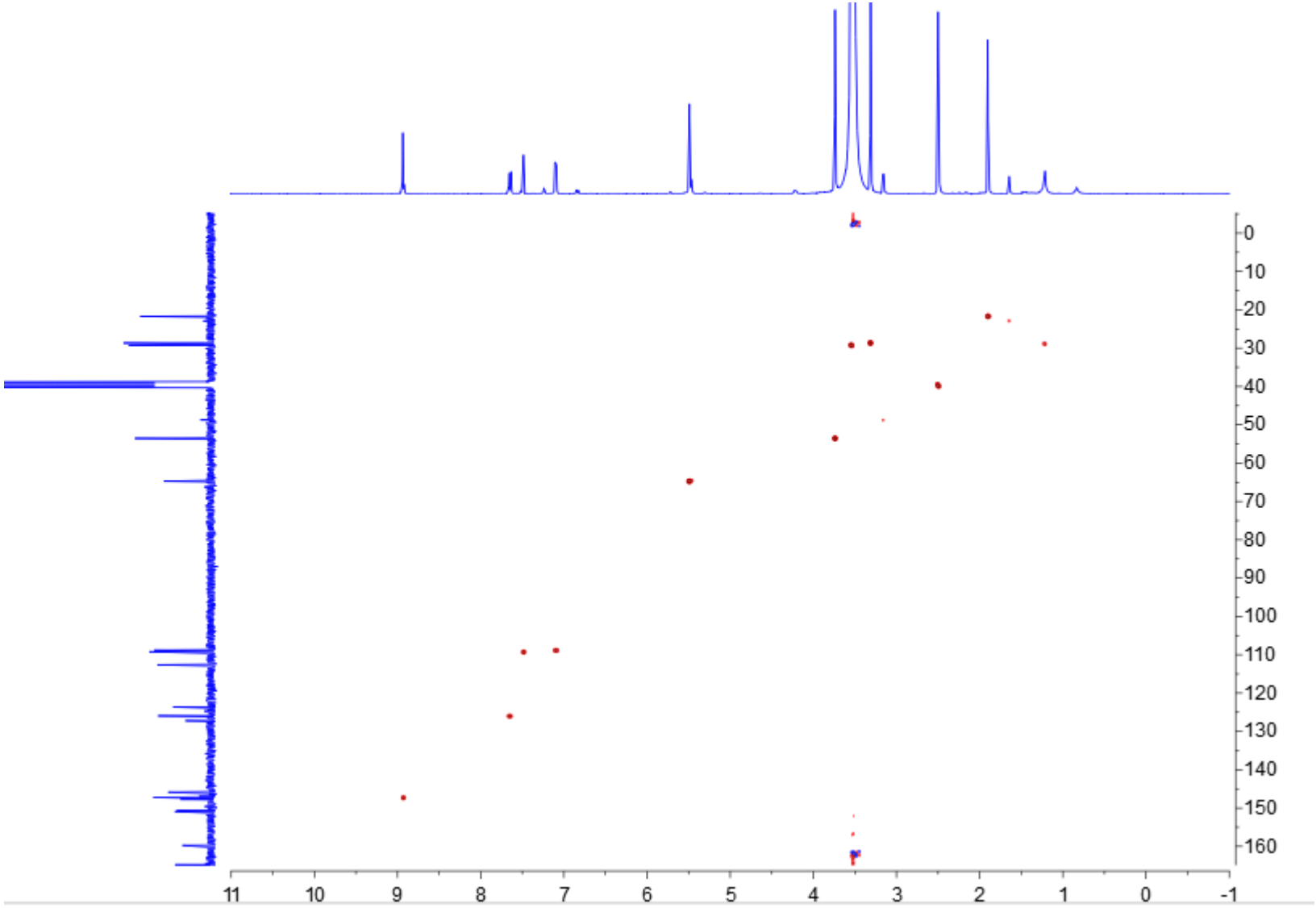

Figure S19. HSQC (400MHz) spectrum of compound **3** in DMSO-d_6.

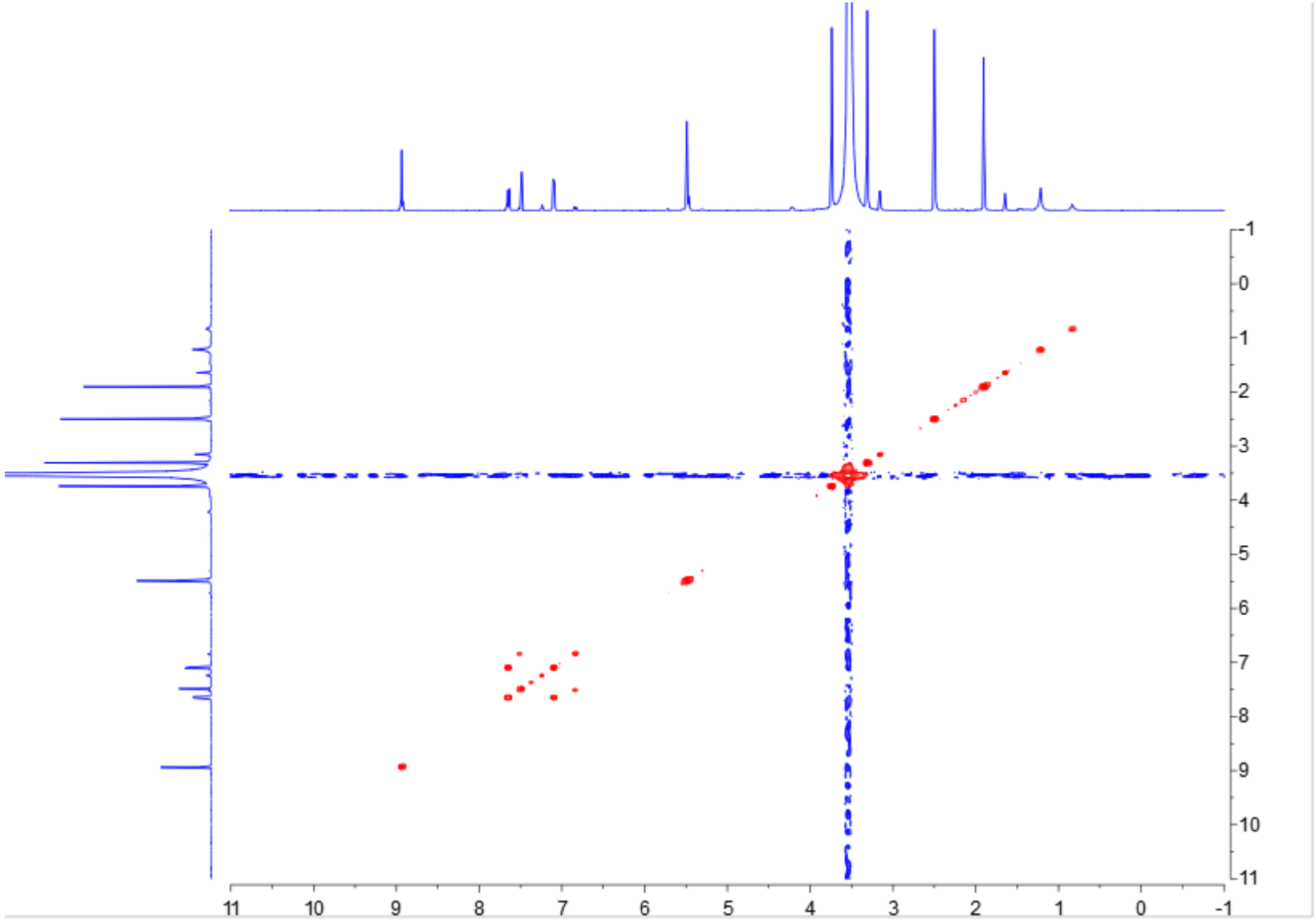

Figure S20. ^{1}H-^{1}H COSY (400MHz) spectrum of compound **3** in DMSO-d_6.

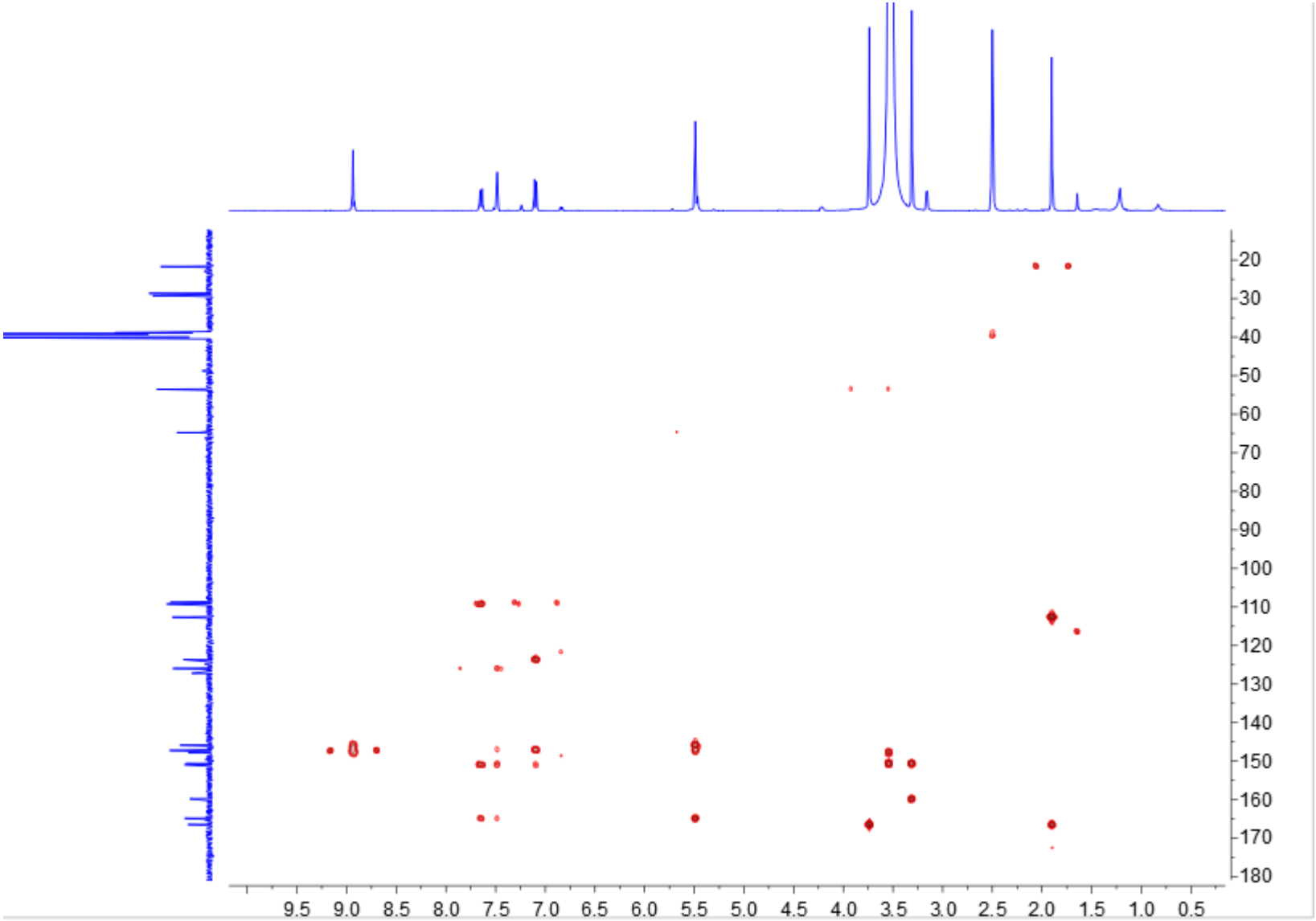

Figure S21. HMBC (400MHz) spectrum of compound **3** in DMSO-d_6.

Table S2. Cartesian coordinates for the low-energy reoptimized random research conformers of compound **1** at PBE0-D3/def2-SVP level of theory in methanol.

1_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.971659	5.001589	-4.928552
1	6	0	-2.562483	2.763244	-5.024116
2	6	0	-2.244555	1.238525	-2.88973
3	6	0	-3.60612	1.976663	-0.74059
4	6	0	-5.127973	4.171291	-0.63029
5	6	0	-5.216738	5.733186	-2.755218
6	7	0	-3.827081	0.808554	1.549416
7	6	0	-5.454488	2.132863	3.124941
8	6	0	-6.311218	4.23465	1.822717
9	6	0	-5.880523	0.992344	5.720776
10	7	0	-11.797681	3.191132	2.077738
11	6	0	-10.922251	5.721989	1.508938
12	6	0	-8.217132	6.173438	2.564608
13	6	0	-12.053577	1.271648	0.456935
14	6	0	-12.023475	1.89659	-2.302352
15	7	0	-11.530177	4.533464	-2.913704
16	6	0	-11.059034	6.38204	-1.269409
17	8	0	-12.490312	-0.924589	1.146112
18	8	0	-10.659627	8.599979	-1.927474
19	6	0	-10.138839	0.50456	-3.972473
20	6	0	-10.23853	2.054204	-6.417011
21	6	0	-11.029992	4.741683	-5.628877

22	8	0	-1.427475	2.188954	-7.291502
23	1	0	-12.16358	7.055328	2.468487
24	1	0	-13.931206	1.445168	-2.962467
25	6	0	-3.299161	0.417534	6.818816
26	6	0	-2.385671	-1.838298	7.416754
27	6	0	-7.16384	2.796005	7.581828
28	6	0	-7.494537	-1.394924	5.463962
29	6	0	4.934368	0.242011	6.625641
30	6	0	4.255604	4.162949	4.141641
31	6	0	10.147687	1.211153	5.025768
32	6	0	8.228644	1.88616	3.563706
33	1	0	14.331178	-2.610539	-3.344456
34	1	0	10.12125	-1.477233	0.4822
35	8	0	-2.519195	-2.898296	-6.270211
36	6	0	15.792067	-7.082573	-0.279757
37	6	0	17.208271	-6.954608	-2.784483
38	6	0	15.168665	-6.340911	-4.7246
39	8	0	11.992952	-5.819256	3.25128
40	8	0	10.354369	-4.27775	-6.562926
41	6	0	11.820608	-5.033559	1.048362
42	7	0	13.574994	-5.471888	-0.70238
43	6	0	13.48957	-4.502745	-3.292947
44	6	0	10.83264	-4.216216	-4.27152
45	6	0	7.231989	-3.987577	1.76421
46	6	0	9.586302	-3.448127	0.179293
47	7	0	9.074461	-3.841332	-2.4979
48	6	0	5.446771	1.516228	4.082265

49	6	0	5.004069	-2.409649	1.053322
50	6	0	4.317846	-0.069063	1.984331
51	7	0	2.163664	0.714785	0.719153
52	6	0	2.890005	-5.121665	-2.497141
53	6	0	3.195735	-3.062683	-0.866888
54	6	0	1.450677	-1.039355	-1.036919
55	6	0	-0.517574	-0.9401	-2.803493
56	6	0	-0.665066	-2.995691	-4.443917
57	6	0	0.980961	-5.062204	-4.279067
58	1	0	-4.084783	6.141652	-6.620591
59	1	0	-6.292639	7.466825	-2.743106
60	1	0	-2.889973	-0.754169	2.089715
61	1	0	-11.938801	2.73755	3.925713
62	1	0	-7.636713	8.039591	1.915203
63	1	0	-8.391825	6.313562	4.599051
64	1	0	-10.655407	-1.461722	-4.24824
65	1	0	-8.271053	0.579361	-3.117447
66	1	0	-11.630091	1.260944	-7.704534
67	1	0	-8.424714	2.066146	-7.37801
68	1	0	-9.563412	6.141684	-5.926649
69	1	0	-12.720242	5.366898	-6.621949
70	1	0	-1.450648	0.359937	-7.500384
71	1	0	-2.140218	2.08083	7.140713
72	1	0	-0.527106	-2.035587	8.244168
73	1	0	-3.431338	-3.573068	7.145674
74	1	0	-9.11174	3.193744	7.066165
75	1	0	-6.151494	4.576948	7.750102

76	1	0	-7.204909	1.919802	9.442877
77	1	0	-7.800695	-2.263507	7.30446
78	1	0	-9.328626	-0.945383	4.658911
79	1	0	-6.617764	-2.794175	4.237691
80	1	0	5.740289	-1.642361	6.739564
81	1	0	5.698108	1.36312	8.173337
82	1	0	2.908723	0.068751	6.914386
83	1	0	5.16203	5.286598	5.604899
84	1	0	2.248222	4.084577	4.596265
85	1	0	4.488222	5.158126	2.355265
86	1	0	12.075033	1.607544	4.465793
87	1	0	9.906295	0.224608	6.799352
88	1	0	8.623307	2.848864	1.794177
89	1	0	-2.339651	-4.330454	-7.389151
90	1	0	15.160193	-8.992049	0.163615
91	1	0	16.893751	-6.390923	1.311863
92	1	0	18.603094	-5.442097	-2.730056
93	1	0	18.191395	-8.709652	-3.195286
94	1	0	14.09099	-8.026447	-5.2135
95	1	0	15.90828	-5.521117	-6.453146
96	1	0	7.759107	-3.685373	3.719719
97	1	0	6.765141	-5.986271	1.586838
98	1	0	7.317954	-3.409202	-3.111778
99	1	0	1.35066	2.417439	0.921889
100	1	0	4.130899	-6.743937	-2.405922
101	1	0	0.735518	-6.627536	-5.572767
5_tddft_		Standard Orientation (Ångstroms)			

Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.992226	5.231552	-4.571074
1	6	0	-2.498397	3.061909	-4.832434
2	6	0	-2.109642	1.395582	-2.815875
3	6	0	-3.463272	1.945506	-0.605211
4	6	0	-5.07509	4.057932	-0.337539
5	6	0	-5.255796	5.75541	-2.349282
6	7	0	-3.598258	0.62381	1.608575
7	6	0	-5.262501	1.770846	3.285595
8	6	0	-6.235012	3.901657	2.121444
9	6	0	-5.457215	0.607599	5.899105
10	7	0	-11.60009	2.41111	2.374389
11	6	0	-10.933622	5.025849	1.914761
12	6	0	-8.265447	5.64656	2.989853
13	6	0	-11.545279	0.525107	0.692924
14	6	0	-11.615254	1.250408	-2.041364
15	7	0	-11.425787	3.950163	-2.550167
16	6	0	-11.131876	5.774261	-0.8367
17	8	0	-11.664957	-1.731652	1.308518
18	8	0	-10.951194	8.043221	-1.412315
19	6	0	-9.623585	0.139436	-3.793074
20	6	0	-9.952689	1.755941	-6.172353
21	6	0	-10.96528	4.324155	-5.255751
22	8	0	-1.361288	2.696787	-7.142057
23	1	0	-12.275935	6.213174	2.927038
24	1	0	-13.473885	0.616743	-2.695334

25	6	0	-7.350365	1.942921	7.55447
26	6	0	-6.880109	3.311066	9.599927
27	6	0	-6.356315	-2.155342	5.677768
28	6	0	-2.820007	0.630775	7.101762
29	6	0	4.849846	-0.572606	6.722574
30	6	0	4.289269	3.590669	4.616572
31	6	0	10.111858	0.545615	5.412349
32	6	0	8.247609	1.324253	3.930842
33	1	0	14.212138	-2.039687	-2.610045
34	1	0	10.318272	-1.890206	0.741264
35	8	0	-2.317766	-2.404857	-6.568164
36	6	0	15.551805	-7.576636	-1.242707
37	6	0	15.9749	-7.767662	-4.074543
38	6	0	15.652104	-5.052794	-4.989868
39	8	0	11.691381	-7.027605	2.527666
40	8	0	10.648191	-3.284064	-6.646532
41	6	0	11.732199	-5.633671	0.644845
42	7	0	13.580069	-5.652358	-1.071205
43	6	0	13.648662	-3.925144	-3.242757
44	6	0	11.029947	-3.603828	-4.361347
45	6	0	7.222631	-4.359347	1.527192
46	6	0	9.643702	-3.730312	0.088726
47	7	0	9.190024	-3.614607	-2.628259
48	6	0	5.447808	0.943175	4.332885
49	6	0	5.055319	-2.65827	0.919333
50	6	0	4.367879	-0.411413	2.05565
51	7	0	2.259922	0.522026	0.812829

52	6	0	3.020474	-4.984978	-2.930986
53	6	0	3.295412	-3.09416	-1.104602
54	6	0	1.574006	-1.044024	-1.123734
55	6	0	-0.360669	-0.76528	-2.910909
56	6	0	-0.485468	-2.663628	-4.735296
57	6	0	1.150949	-4.74271	-4.737685
58	1	0	-4.162112	6.478802	-6.180692
59	1	0	-6.417742	7.426998	-2.211616
60	1	0	-2.702274	-1.017601	1.926946
61	1	0	-11.693944	1.875223	4.201857
62	1	0	-7.846306	7.589572	2.452478
63	1	0	-8.422422	5.630036	5.033497
64	1	0	-9.921929	-1.861237	-4.134549
65	1	0	-7.759091	0.398695	-2.970571
66	1	0	-11.310791	0.877897	-7.44097
67	1	0	-8.186045	1.97372	-7.194637
68	1	0	-9.624433	5.856685	-5.490316
69	1	0	-12.708514	4.850925	-6.213711
70	1	0	-1.371039	0.888398	-7.502211
71	1	0	-9.311671	1.617144	7.062771
72	1	0	-8.415985	4.109287	10.690418
73	1	0	-4.991702	3.718088	10.267101
74	1	0	-5.024062	-3.305726	4.6125
75	1	0	-8.182093	-2.272112	4.740041
76	1	0	-6.531333	-2.987859	7.551729
77	1	0	-1.506195	-0.489331	5.990517
78	1	0	-2.063844	2.53721	7.243543

79	1	0	-2.880545	-0.187204	8.987739
80	1	0	5.573218	0.384844	8.394413
81	1	0	2.815807	-0.767495	6.945047
82	1	0	5.65237	-2.462021	6.671735
83	1	0	5.145416	4.540738	6.225541
84	1	0	2.263529	3.502768	4.974175
85	1	0	4.615324	4.761688	2.955974
86	1	0	12.058546	0.97239	4.94975
87	1	0	9.805636	-0.548679	7.111487
88	1	0	8.706703	2.40087	2.244519
89	1	0	-2.112803	-3.720153	-7.818854
90	1	0	14.903567	-9.313919	-0.365379
91	1	0	17.251202	-6.942982	-0.260941
92	1	0	17.81901	-8.544987	-4.536114
93	1	0	14.534853	-8.98337	-4.90494
94	1	0	15.079181	-4.921676	-6.956039
95	1	0	17.407456	-4.006214	-4.770628
96	1	0	7.683547	-4.292199	3.523363
97	1	0	6.704503	-6.310665	1.120776
98	1	0	7.434988	-3.135804	-3.207878
99	1	0	1.45498	2.203362	1.167283
100	1	0	4.252131	-6.616501	-2.970365
101	1	0	0.923729	-6.176731	-6.178429
6_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.248479	4.31597	-4.634769

1	6	0	-1.453865	2.37189	-4.5184
2	6	0	-1.24633	0.799473	-2.407669
3	6	0	-2.90962	1.308574	-0.416323
4	6	0	-4.786351	3.208947	-0.508104
5	6	0	-4.89848	4.739808	-2.659271
6	7	0	-3.09539	0.169373	1.888739
7	6	0	-5.041979	1.231475	3.285647
8	6	0	-6.161294	3.098049	1.832969
9	6	0	-5.42143	0.463681	6.023084
10	7	0	-11.321444	1.06861	1.571565
11	6	0	-10.896782	3.730988	1.093028
12	6	0	-8.442352	4.63408	2.4327
13	6	0	-10.824047	-0.818212	-0.037907
14	6	0	-10.790682	-0.165499	-2.792803
15	7	0	-10.856786	2.528698	-3.365228
16	6	0	-10.886849	4.405042	-1.683071
17	8	0	-10.634297	-3.052416	0.637985
18	8	0	-10.855655	6.669266	-2.304426
19	6	0	-8.56899	-1.0818	-4.371738
20	6	0	-8.928142	0.417687	-6.819412
21	6	0	-10.214957	2.904116	-6.035539
22	8	0	0.137451	2.115527	-6.550525
23	1	0	-12.453044	4.789973	1.926382
24	1	0	-12.516783	-1.017723	-3.552983
25	6	0	-8.066324	-0.529794	6.403486
26	6	0	-9.82976	0.377114	7.938762
27	6	0	-3.648384	-1.720201	6.746539

28	6	0	-4.799464	2.717231	7.727179
29	6	0	3.729795	1.625131	6.79122
30	6	0	6.196493	4.532374	3.991174
31	6	0	8.741834	0.184589	8.445486
32	6	0	8.395967	1.100983	6.139904
33	1	0	11.540918	0.459841	-5.301616
34	1	0	12.493508	-3.920722	1.390137
35	8	0	-1.253369	-3.702447	-5.527948
36	6	0	8.916028	-3.845837	-6.332618
37	6	0	7.366998	-1.607265	-7.35874
38	6	0	7.510339	0.457917	-5.332433
39	8	0	10.354027	-6.680722	-2.024277
40	8	0	10.593276	3.47201	-1.443174
41	6	0	10.40473	-4.335029	-1.949087
42	7	0	10.01535	-2.8923	-3.978115
43	6	0	10.011325	-0.139172	-4.043003
44	6	0	10.584656	1.134869	-1.579376
45	6	0	8.587833	-3.553643	2.396239
46	6	0	10.828492	-3.039569	0.562187
47	7	0	11.320295	-0.357523	0.324734
48	6	0	5.924307	1.77764	4.902272
49	6	0	6.218662	-2.18069	1.745823
50	6	0	5.295682	0.083177	2.677337
51	7	0	3.141051	0.703205	1.305701
52	6	0	4.355269	-5.100054	-1.78942
53	6	0	4.510488	-2.98276	-0.219556
54	6	0	2.626543	-1.10599	-0.452689

55	6	0	0.674264	-1.20526	-2.232601
56	6	0	0.614843	-3.356107	-3.763903
57	6	0	2.427374	-5.272408	-3.540357
58	1	0	-3.297657	5.497095	-6.300603
59	1	0	-6.250932	6.261915	-2.790602
60	1	0	-2.036194	-1.30209	2.448561
61	1	0	-11.310908	0.578637	3.421145
62	1	0	-8.171651	6.613122	1.931953
63	1	0	-8.839021	4.591608	4.444886
64	1	0	-8.599257	-3.112793	-4.656478
65	1	0	-6.813797	-0.566578	-3.432604
66	1	0	-10.140234	-0.62632	-8.11001
67	1	0	-7.146783	0.769106	-7.777789
68	1	0	-8.986864	4.537897	-6.195702
69	1	0	-11.911777	3.27726	-7.137275
70	1	0	1.411025	0.86401	-6.139357
71	1	0	-8.4805	-2.220236	5.315839
72	1	0	-11.643599	-0.55502	8.109026
73	1	0	-9.564298	2.053649	9.077891
74	1	0	-3.994194	-2.25919	8.699238
75	1	0	-1.669884	-1.171566	6.610414
76	1	0	-3.954121	-3.391397	5.584825
77	1	0	-4.945473	2.18911	9.710863
78	1	0	-2.872953	3.3474	7.379146
79	1	0	-6.0395	4.321184	7.401802
80	1	0	4.088772	2.834105	8.416042
81	1	0	1.979079	2.264609	5.927016

82	1	0	3.437724	-0.297164	7.460103
83	1	0	6.704104	5.74581	5.573438
84	1	0	4.440193	5.25652	3.200619
85	1	0	7.656576	4.698597	2.551832
86	1	0	10.631154	-0.134395	9.162389
87	1	0	7.204154	-0.304129	9.699737
88	1	0	10.059803	1.562526	5.038777
89	1	0	-2.50503	-2.378729	-5.327095
90	1	0	7.778123	-5.49713	-5.910557
91	1	0	10.40119	-4.413327	-7.638806
92	1	0	8.187578	-0.929537	-9.116331
93	1	0	5.430871	-2.167813	-7.75037
94	1	0	5.981144	0.283809	-3.969029
95	1	0	7.476469	2.353934	-6.114943
96	1	0	9.234041	-3.059557	4.277346
97	1	0	8.276672	-5.58866	2.400137
98	1	0	11.836758	0.545539	1.92422
99	1	0	2.11325	2.280927	1.54582
100	1	0	5.72805	-6.603622	-1.662639
101	1	0	2.273857	-6.905041	-4.758191

Table S3. The atom energies of the low-energy conformers of compound **1**.

Conformers	Gibbs free energies (ΔG) [a]	Final single point energy (a.u.)
1_tddft_	0.00000	-2406.554720381671
5_tddft_	0.00137	-2406.553355177897
6_tddft_	0.00134	-2406.553380015092

[a] CAM-B3LYP-D3/def2-SVP, in kcal/mol.

Table S4.Cartesian coordinates for the low-energy reoptimized random research conformers of compound **2** at PBE0-D3/def2-SVP level of theory in methanol.

8_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-1.599355	-0.505127	7.018406
1	6	0	-2.63135	0.646473	4.889392
2	6	0	-1.180445	0.932653	2.675219
3	6	0	1.234472	-0.085401	2.735331
4	6	0	2.275349	-1.307588	4.815193
5	6	0	0.84553	-1.468649	6.993646
6	7	0	3.040111	0.064928	0.829757
7	6	0	5.287053	-1.012793	1.504945
8	6	0	4.951584	-2.108866	4.193946
9	7	0	4.798878	3.117249	6.638121
10	6	0	7.207186	1.862678	6.220102
11	6	0	6.901851	-1.031155	6.057623
12	6	0	3.734016	4.929761	5.259182
13	6	0	5.380774	6.210503	3.349185
14	7	0	7.629952	4.775116	2.657199
15	6	0	8.677074	2.909429	3.986255
16	8	0	1.533403	5.666829	5.642211
17	8	0	10.756185	1.979273	3.448246
18	6	0	4.233773	6.872497	0.802466
19	6	0	6.586155	7.437518	-0.770531
20	6	0	8.599096	5.59673	0.191393
21	8	0	-5.038415	1.515613	5.07134

22	1	0	8.403638	2.198317	7.866755
23	1	0	5.976987	7.969986	4.265956
24	1	0	-10.252097	-3.596	0.517611
25	1	0	-9.89171	-1.417576	-6.37634
26	8	0	-2.48332	6.32815	2.333682
27	6	0	-6.854083	-7.38252	-1.297674
28	6	0	-6.627438	-7.054529	1.566878
29	6	0	-6.551091	-4.202077	2.001459
30	8	0	-7.565131	-5.861131	-6.345016
31	8	0	-8.198937	1.145254	1.005404
32	6	0	-7.795154	-4.283989	-4.631283
33	7	0	-7.701242	-4.897338	-2.190188
34	6	0	-8.296397	-3.242238	-0.066321
35	6	0	-8.220211	-0.483496	-0.693661
36	6	0	-6.061318	-0.593351	-7.133627
37	6	0	-8.130142	-1.514815	-5.307127
38	7	0	-8.35977	0.133979	-3.12352
39	6	0	-3.381182	-0.139607	-6.098961
40	6	0	-2.371555	-2.460605	-4.635666
41	7	0	-1.820244	-1.680865	-2.233624
42	6	0	-4.057716	4.390534	-4.075814
43	6	0	-3.300731	1.891655	-4.086191
44	6	0	-2.340915	0.874721	-1.861242
45	6	0	-2.091611	2.210127	0.383422
46	6	0	-2.752843	4.786468	0.2979
47	6	0	-3.759066	5.831817	-1.896507
48	8	0	7.154019	-1.065045	0.146691

49	6	0	5.118537	-5.121802	3.981094
50	6	0	4.817179	-6.348122	6.581527
51	6	0	7.640069	-6.004747	2.891719
52	6	0	2.911641	-5.987486	2.373445
53	6	0	2.929464	-6.457589	-0.090069
54	8	0	-2.047739	-4.61685	-5.397322
55	6	0	-1.419838	0.495892	-8.317738
56	6	0	-1.239536	-1.634533	-10.273699
57	6	0	1.197009	0.894323	-7.172755
58	6	0	-2.329454	2.800249	-9.716585
59	6	0	-1.247518	5.059445	-9.781138
60	1	0	-2.753332	-0.661352	8.695765
61	1	0	1.595163	-2.296382	8.702191
62	1	0	2.773467	0.852428	-0.881879
63	1	0	3.675887	2.348851	7.977685
64	1	0	8.766825	-1.778988	5.648127
65	1	0	6.404164	-1.684686	7.939866
66	1	0	2.934246	8.452982	0.921666
67	1	0	3.21196	5.257018	0.044408
68	1	0	7.187532	9.37616	-0.441954
69	1	0	6.255824	7.21323	-2.784117
70	1	0	8.80035	3.935916	-1.005493
71	1	0	10.449243	6.472906	0.382313
72	1	0	-5.913013	1.513169	3.428348
73	1	0	-1.149733	5.734963	3.481889
74	1	0	-5.057354	-7.814094	-2.202643
75	1	0	-8.194468	-8.850439	-1.822728

76	1	0	-8.274892	-7.854729	2.50094
77	1	0	-4.964563	-8.003653	2.308931
78	1	0	-4.653646	-3.465474	1.719459
79	1	0	-7.18364	-3.651833	3.871484
80	1	0	-6.730705	1.169283	-7.948122
81	1	0	-6.005045	-1.965146	-8.655357
82	1	0	-8.384875	2.008822	-3.485563
83	1	0	-0.9323	-2.812018	-0.982512
84	1	0	-4.868004	5.252691	-5.73725
85	1	0	-4.280696	7.806248	-1.886219
86	1	0	4.835853	-8.394339	6.357545
87	1	0	6.358417	-5.858088	7.849353
88	1	0	3.041294	-5.856201	7.483718
89	1	0	7.638839	-8.060337	2.793279
90	1	0	9.209792	-5.450694	4.096879
91	1	0	8.016776	-5.283606	1.013957
92	1	0	1.148779	-6.231144	3.392141
93	1	0	1.241634	-7.107444	-1.050047
94	1	0	4.59937	-6.258651	-1.25268
95	1	0	-3.021822	-1.981275	-11.235506
96	1	0	0.128716	-1.090919	-11.712391
97	1	0	-0.60952	-3.395737	-9.433623
98	1	0	2.54996	1.373985	-8.644449
99	1	0	1.882015	-0.820671	-6.265867
100	1	0	1.223056	2.41273	-5.788908
101	1	0	-4.019012	2.51321	-10.841475
102	1	0	-2.050519	6.566092	-10.909535

103	1	0	0.4413	5.526172	-8.728875
10_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-0.71577	-2.140656	6.991739
1	6	0	-2.129368	-0.72659	5.282592
2	6	0	-1.011255	0.19821	3.048322
3	6	0	1.480338	-0.499223	2.627312
4	6	0	2.90153	-1.975067	4.271432
5	6	0	1.792179	-2.753501	6.502835
6	7	0	2.993974	0.247879	0.609291
7	6	0	5.400318	-0.672894	0.779885
8	6	0	5.537513	-2.299183	3.20628
9	7	0	5.170181	2.267696	6.75495
10	6	0	7.604735	1.472036	5.758407
11	6	0	7.601181	-1.349212	5.019278
12	6	0	3.699901	4.141088	5.946143
13	6	0	4.868775	5.988957	4.151626
14	7	0	7.108102	5.033787	2.858312
15	6	0	8.570747	3.130391	3.622541
16	8	0	1.515872	4.460929	6.757788
17	8	0	10.631185	2.634774	2.630658
18	6	0	3.249614	6.978379	1.998917
19	6	0	5.231953	8.12654	0.243307
20	6	0	7.561271	6.433254	0.50841
21	8	0	-4.575307	-0.247008	5.891038
22	1	0	9.004971	1.642805	7.263354

23	1	0	5.426389	7.594389	5.336906
24	1	0	-9.613317	-5.036098	0.763776
25	1	0	-10.456331	-1.395165	-5.426076
26	8	0	-2.979886	5.277768	4.10368
27	6	0	-5.944386	-7.71924	-2.172589
28	6	0	-5.428588	-7.99222	0.659376
29	6	0	-5.712352	-5.33324	1.743953
30	8	0	-7.585349	-5.318905	-6.637243
31	8	0	-8.169542	-0.241417	2.158342
32	6	0	-7.785406	-4.19895	-4.592822
33	7	0	-7.251913	-5.283574	-2.382291
34	6	0	-7.810595	-4.250671	0.112122
35	6	0	-8.195686	-1.448033	0.138432
36	6	0	-6.889018	0.156614	-6.324723
37	6	0	-8.578029	-1.438575	-4.574958
38	7	0	-8.748449	-0.357306	-2.05624
39	6	0	-4.173314	0.762265	-5.486294
40	6	0	-2.687564	-1.639993	-4.726829
41	7	0	-1.921839	-1.330971	-2.276272
42	6	0	-5.170204	4.557506	-2.372984
43	6	0	-4.082161	2.285689	-3.064189
44	6	0	-2.711441	0.964473	-1.253273
45	6	0	-2.345673	1.793672	1.211016
46	6	0	-3.33708	4.191042	1.80567
47	6	0	-4.770771	5.515871	0.041635
48	8	0	7.058977	-0.243387	-0.76755
49	6	0	5.980156	-5.168347	2.356988

50	6	0	6.026325	-6.921614	4.656041
51	6	0	8.468074	-5.514641	0.940727
52	6	0	3.728405	-5.930341	0.762698
53	6	0	3.60239	-6.01133	-1.740361
54	8	0	-2.184219	-3.496486	-6.003506
55	6	0	-2.640747	2.140173	-7.70308
56	6	0	-2.591295	0.572696	-10.121113
57	6	0	0.090345	2.573486	-6.839226
58	6	0	-3.792689	4.707766	-8.15562
59	6	0	-5.278673	5.390733	-10.055373
60	1	0	-1.620729	-2.786784	8.704184
61	1	0	2.840488	-3.811121	7.898561
62	1	0	2.429658	1.335779	-0.845977
63	1	0	4.36333	1.096719	8.02986
64	1	0	9.459504	-1.738517	4.244865
65	1	0	7.451317	-2.416364	6.768258
66	1	0	1.854519	8.336725	2.638901
67	1	0	2.254182	5.424922	1.09023
68	1	0	5.6763	10.036239	0.863148
69	1	0	4.588791	8.232947	-1.703291
70	1	0	7.741461	5.074826	-1.025765
71	1	0	9.312125	7.505859	0.616287
72	1	0	-5.646667	-0.034368	4.385172
73	1	0	-1.445933	4.648197	4.939172
74	1	0	-4.221218	-7.625598	-3.294263
75	1	0	-7.100814	-9.246127	-2.919588
76	1	0	-6.823122	-9.238844	1.512792

77	1	0	-3.572688	-8.79319	1.020612
78	1	0	-3.98901	-4.238112	1.495138
79	1	0	-6.19504	-5.323326	3.735907
80	1	0	-7.84674	1.944914	-6.657287
81	1	0	-6.861733	-0.827724	-8.121505
82	1	0	-9.074911	1.522161	-1.969042
83	1	0	-0.76839	-2.581776	-1.418527
84	1	0	-6.336236	5.610707	-3.676237
85	1	0	-5.545605	7.328581	0.573895
86	1	0	4.257428	-6.890028	5.696116
87	1	0	6.319097	-8.85584	4.015567
88	1	0	7.558867	-6.463812	5.945518
89	1	0	8.612958	-7.466972	0.307186
90	1	0	10.076649	-5.15522	2.168541
91	1	0	8.647912	-4.29882	-0.6968
92	1	0	2.060509	-6.453778	1.836103
93	1	0	1.893123	-6.616644	-2.691385
94	1	0	5.173892	-5.523223	-2.953734
95	1	0	-1.71882	-1.255034	-9.808076
96	1	0	-4.453529	0.246698	-10.919262
97	1	0	-1.48619	1.569168	-11.542423
98	1	0	0.173003	3.673447	-5.102163
99	1	0	1.115236	3.627605	-8.277985
100	1	0	1.094846	0.79997	-6.553839
101	1	0	-3.277512	6.133984	-6.779223
102	1	0	-5.96484	7.313313	-10.199258
103	1	0	-5.878333	4.106535	-11.528809

Table S5. The atom energies of low-energy conformers of compound **2**.

Conformers	Gibbs free energies (ΔG) [a]	Final single point energy (a.u.)
8_tddft_	0.0000	-2556.903699068551
10_tddft_	0.0004	-2556.903301112253

[a] CAM-B3LYP-D3/def2-TZVP, in kcal/mol.

Table S6. Cartesian coordinates for the low-energy reoptimized random reseach conformers of comound **3** at PBE0-D3/def2-SVP level of theory in methanol.

2_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	4.240471	1.518117	-2.434761
1	6	0	3.160243	2.276234	-0.146012
2	7	0	3.344619	4.62105	0.711118
3	6	0	4.64091	6.25574	-0.711634
4	6	0	5.761771	5.505642	-2.984991
5	7	0	5.539735	3.144969	-3.829769
6	7	0	4.850657	8.704158	0.1208
7	6	0	6.179905	10.500817	-1.22316
8	7	0	7.296647	9.738651	-3.484732
9	6	0	7.196697	7.322246	-4.499653
10	8	0	8.23369	6.781543	-6.50155
11	8	0	6.394838	12.688125	-0.494605
12	6	0	8.68087	11.705431	-4.845488
13	6	0	3.651349	9.425782	2.504491

14	6	0	4.071846	-1.136979	-3.400183
15	8	0	1.984554	-2.511978	-2.341082
16	6	0	-0.342208	-1.87591	-3.193103
17	6	0	-2.358634	-3.366249	-2.004518
18	8	0	-0.669646	-0.228223	-4.775731
19	6	0	-1.812033	-5.225101	-0.176289
20	6	0	-3.82319	-6.502501	0.820307
21	6	0	-6.293197	-6.021522	0.079817
22	6	0	-6.867938	-4.221278	-1.70528
23	6	0	-4.848434	-2.890474	-2.736696
24	8	0	-3.79682	-8.433734	2.549737
25	6	0	-6.376915	-8.919007	3.20363
26	8	0	-7.904182	-7.609072	1.314764
27	6	0	-6.910958	-11.692416	3.177134
28	6	0	-6.951641	-7.584419	5.738667
29	8	0	-9.229779	-8.211353	6.568091
30	6	0	-10.072061	-6.987594	8.869101
31	8	0	-5.516191	-6.113845	6.751713
32	1	0	2.121284	0.955986	1.017714
33	1	0	7.421679	13.25932	-5.299476
34	1	0	10.2275	12.401878	-3.691465
35	1	0	9.419867	10.893306	-6.567554
36	1	0	4.472204	8.361978	4.054897
37	1	0	3.964229	11.421006	2.801882
38	1	0	1.637799	9.049369	2.414501
39	1	0	3.969954	-1.134418	-5.450938
40	1	0	5.73115	-2.207021	-2.828821

41	1	0	0.096532	-5.630844	0.408947
42	1	0	-8.791828	-3.861491	-2.279856
43	1	0	-5.212689	-1.452492	-4.137263
44	1	0	-5.814725	-12.623923	4.645073
45	1	0	-8.902242	-12.03889	3.524503
46	1	0	-6.390298	-12.466331	1.347087
47	1	0	-8.812279	-7.461378	10.418445
48	1	0	-10.138043	-4.953795	8.600453
49	1	0	-11.947816	-7.726876	9.21897
3_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	4.224626	1.545024	-2.334327
1	6	0	2.275535	3.327347	-2.234926
2	7	0	2.691632	5.742841	-1.730301
3	6	0	5.091066	6.425301	-1.333652
4	6	0	7.057991	4.664341	-1.467289
5	7	0	6.60312	2.236257	-1.953911
6	7	0	5.58037	8.915347	-0.79588
7	6	0	8.009353	9.783776	-0.409898
8	7	0	9.96108	8.019271	-0.548691
9	6	0	9.6751	5.462487	-1.058917
10	8	0	11.48353	4.014802	-1.156267
11	8	0	8.474776	12.006526	0.041342
12	6	0	12.499653	9.023096	-0.119474
13	6	0	3.477898	10.704747	-0.656646
14	6	0	3.745095	-1.175729	-2.946221

15	8	0	1.274003	-1.993846	-2.16146
16	6	0	0.922268	-2.27189	0.356068
17	6	0	-1.671156	-3.022822	0.997296
18	8	0	2.611443	-1.909675	1.887257
19	6	0	-3.539891	-3.29162	-0.881917
20	6	0	-5.899285	-3.97861	-0.086008
21	6	0	-6.456779	-4.39434	2.442968
22	6	0	-4.663589	-4.136051	4.307616
23	6	0	-2.248496	-3.439196	3.537944
24	8	0	-8.04604	-4.278543	-1.508229
25	6	0	-9.937072	-5.282881	0.147258
26	8	0	-8.950175	-4.986424	2.706747
27	6	0	-12.374118	-3.886817	-0.155621
28	6	0	-10.130753	-8.162477	-0.309034
29	8	0	-11.977847	-9.14364	1.068114
30	6	0	-12.312544	-11.857389	0.913108
31	8	0	-8.728202	-9.328993	-1.694767
32	1	0	0.334645	2.781771	-2.571204
33	1	0	12.610589	9.871355	1.744499
34	1	0	13.829875	7.479276	-0.2537
35	1	0	12.941921	10.439551	-1.535879
36	1	0	2.116917	10.071217	0.739543
37	1	0	4.221875	12.526588	-0.113462
38	1	0	2.556407	10.854525	-2.483514
39	1	0	3.750538	-1.461855	-4.981259
40	1	0	5.201681	-2.356297	-2.111317
41	1	0	-3.140062	-2.962784	-2.852466

42	1	0	-5.111291	-4.451459	6.272625
43	1	0	-0.78094	-3.217931	4.937489
44	1	0	-12.05275	-1.881665	0.152164
45	1	0	-13.104105	-4.173842	-2.05546
46	1	0	-13.761007	-4.571809	1.191223
47	1	0	-10.597082	-12.814926	1.506922
48	1	0	-13.852548	-12.285574	2.190648
49	1	0	-12.800854	-12.395279	-1.006552
4_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	4.21574	1.438416	-2.700383
1	6	0	3.169277	2.2571	-0.417611
2	7	0	3.514955	4.577007	0.458999
3	6	0	4.942205	6.122464	-0.936781
4	6	0	6.027863	5.309076	-3.205614
5	7	0	5.644287	2.976965	-4.06959
6	7	0	5.322359	8.542781	-0.082307
7	6	0	6.787313	10.249215	-1.402299
8	7	0	7.879688	9.419574	-3.652111
9	6	0	7.606877	7.027091	-4.691823
10	8	0	8.617059	6.428541	-6.690911
11	8	0	7.141501	12.414448	-0.662053
12	6	0	9.422022	11.287592	-4.981026
13	6	0	4.152836	9.332121	2.294834
14	6	0	3.869871	-1.18541	-3.704567
15	8	0	1.806266	-2.502391	-2.536124

16	6	0	-0.546562	-1.777737	-3.233699
17	6	0	-2.533577	-3.214141	-1.934379
18	8	0	-0.915446	-0.09643	-4.770509
19	6	0	-1.93641	-5.167114	-0.223892
20	6	0	-3.922951	-6.379755	0.895379
21	6	0	-6.416869	-5.744254	0.388298
22	6	0	-7.041574	-3.850035	-1.279034
23	6	0	-5.046797	-2.586291	-2.435512
24	8	0	-3.855168	-8.376169	2.547863
25	6	0	-6.393124	-8.758349	3.403122
26	8	0	-8.001745	-7.290649	1.706462
27	6	0	-7.077843	-11.496653	3.313221
28	6	0	-6.67985	-7.506923	6.027506
29	8	0	-8.900723	-8.072445	7.036611
30	6	0	-9.480647	-6.903722	9.44465
31	8	0	-5.096505	-6.13729	6.958273
32	1	0	2.025955	1.009888	0.728421
33	1	0	8.274958	12.909014	-5.495165
34	1	0	10.965276	11.904636	-3.77897
35	1	0	10.171402	10.414956	-6.668682
36	1	0	2.113003	9.165514	2.161232
37	1	0	4.829997	8.15574	3.832501
38	1	0	4.660824	11.278133	2.644134
39	1	0	3.630316	-1.131455	-5.743586
40	1	0	5.521693	-2.329785	-3.272666
41	1	0	-0.010431	-5.690966	0.18318
42	1	0	-8.984535	-3.368486	-1.671211

43	1	0	-5.448735	-1.077615	-3.748722
44	1	0	-5.912847	-12.546684	4.641607
45	1	0	-9.047948	-11.756411	3.820829
46	1	0	-6.759203	-12.214306	1.415369
47	1	0	-8.111283	-7.487623	10.857486
48	1	0	-9.479434	-4.860206	9.252843
49	1	0	-11.349167	-7.577481	9.936423
5_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	4.203413	0.701089	-4.204111
1	6	0	6.695306	0.052238	-3.62416
2	7	0	8.338864	1.701375	-2.704219
3	6	0	7.492071	4.049519	-2.321612
4	6	0	4.991508	4.718027	-2.877514
5	7	0	3.37516	3.040526	-3.823055
6	7	0	9.143076	5.803144	-1.363973
7	6	0	8.422556	8.273727	-0.92407
8	7	0	5.935325	8.928423	-1.49231
9	6	0	4.106954	7.302867	-2.436919
10	8	0	1.938658	8.001734	-2.864636
11	8	0	9.880945	9.855421	-0.070581
12	6	0	5.259437	11.563276	-1.004033
13	6	0	11.739814	5.04236	-0.795381
14	6	0	2.391585	-1.188557	-5.261225
15	8	0	0.261296	-1.600414	-3.595159
16	6	0	0.731417	-2.913332	-1.459904

17	6	0	-1.522629	-3.20031	0.138357
18	8	0	2.822802	-3.753407	-0.953451
19	6	0	-3.879299	-2.201977	-0.601251
20	6	0	-5.860397	-2.57842	1.013042
21	6	0	-5.592602	-3.866144	3.281666
22	6	0	-3.309737	-4.846186	4.044407
23	6	0	-1.26927	-4.4942	2.422692
24	8	0	-8.306754	-1.752187	0.761777
25	6	0	-9.708419	-2.870029	2.843511
26	8	0	-7.842382	-3.917636	4.533045
27	6	0	-11.262759	-0.922932	4.166819
28	6	0	-11.308682	-4.987689	1.633884
29	8	0	-10.083129	-7.168552	1.564396
30	6	0	-11.344866	-9.235209	0.285568
31	8	0	-13.391144	-4.594937	0.756168
32	1	0	7.36803	-1.85574	-3.915892
33	1	0	6.500472	12.807948	-2.059906
34	1	0	3.327222	11.848482	-1.600727
35	1	0	5.430361	11.974838	0.998844
36	1	0	12.728166	6.656378	-0.030907
37	1	0	11.735531	3.520007	0.578439
38	1	0	12.675163	4.409139	-2.507367
39	1	0	1.540075	-0.475681	-6.985867
40	1	0	3.324797	-2.973506	-5.652479
41	1	0	-4.115778	-1.1853	-2.350576
42	1	0	-3.111358	-5.841933	5.813567
43	1	0	0.55628	-5.243013	2.940332

44	1	0	-12.601943	-0.079895	2.861651
45	1	0	-12.305133	-1.795004	5.708235
46	1	0	-10.02753	0.53511	4.918798
47	1	0	-13.128697	-9.652667	1.210721
48	1	0	-11.659938	-8.753828	-1.68484
49	1	0	-10.067131	-10.825864	0.441498
6_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	3.62957	0.842379	-5.075244
1	6	0	3.149029	2.732488	-6.853928
2	7	0	3.627001	5.150564	-6.413998
3	6	0	4.582461	5.721292	-4.147345
4	6	0	5.061776	3.843736	-2.343842
5	7	0	4.589089	1.422664	-2.828505
6	7	0	5.092528	8.208731	-3.626951
7	6	0	6.083152	8.957966	-1.330921
8	7	0	6.560359	7.079275	0.452578
9	6	0	6.112116	4.516052	0.126514
10	8	0	6.568371	2.963779	1.786541
11	8	0	6.540926	11.17373	-0.843191
12	6	0	7.607579	7.960614	2.853419
13	6	0	4.572151	10.12399	-5.552036
14	6	0	3.079233	-1.873292	-5.613874
15	8	0	1.166591	-2.87013	-3.929166
16	6	0	-1.22188	-2.07493	-4.334264
17	6	0	-3.026548	-3.127744	-2.503314

18	8	0	-1.777569	-0.636493	-6.054608
19	6	0	-2.224851	-4.743128	-0.542083
20	6	0	-4.048092	-5.612247	1.067677
21	6	0	-6.573497	-4.955432	0.807945
22	6	0	-7.398076	-3.391163	-1.095991
23	6	0	-5.570899	-2.479899	-2.754192
24	8	0	-3.771582	-7.239246	3.07065
25	6	0	-6.213134	-7.325807	4.326168
26	8	0	-7.973559	-6.109864	2.635419
27	6	0	-6.995516	-9.989928	4.822526
28	6	0	-5.874092	-5.753362	6.760604
29	8	0	-6.266347	-3.314835	6.3578
30	6	0	-5.792362	-1.63678	8.469153
31	8	0	-5.198909	-6.690177	8.742343
32	1	0	2.355933	2.266962	-8.67912
33	1	0	9.392071	8.917831	2.528937
34	1	0	6.298078	9.256496	3.755957
35	1	0	7.905559	6.33634	4.054741
36	1	0	5.669647	9.734405	-7.240028
37	1	0	2.576401	10.118112	-6.023551
38	1	0	5.094568	11.948148	-4.799098
39	1	0	2.499399	-2.143637	-7.563333
40	1	0	4.728942	-3.029921	-5.229692
41	1	0	-0.270698	-5.272614	-0.315871
42	1	0	-9.365754	-2.89007	-1.291268
43	1	0	-6.132296	-1.235161	-4.269718
44	1	0	-5.613732	-10.922275	6.018129

45	1	0	-8.814754	-10.015699	5.777394
46	1	0	-7.147549	-10.99588	3.038906
47	1	0	-7.047416	-2.095219	10.027053
48	1	0	-3.833663	-1.789131	9.063373
49	1	0	-6.185527	0.242758	7.761521
7_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	4.555816	-0.068539	-3.916376
1	6	0	7.110096	-0.443522	-3.364997
2	7	0	8.635837	1.42968	-2.710288
3	6	0	7.60762	3.73215	-2.572783
4	6	0	5.047531	4.129039	-3.110093
5	7	0	3.548506	2.226124	-3.786003
6	7	0	9.132767	5.711704	-1.881386
7	6	0	8.22695	8.154111	-1.721006
8	7	0	5.681019	8.538934	-2.283947
9	6	0	3.96448	6.670958	-2.947261
10	8	0	1.732678	7.138465	-3.365168
11	8	0	9.571233	9.937878	-1.114456
12	6	0	4.805105	11.153419	-2.094869
13	6	0	11.796452	5.228059	-1.314898
14	6	0	2.881825	-2.214359	-4.671953
15	8	0	0.693861	-2.425835	-3.048732
16	6	0	1.133075	-3.222748	-0.665955
17	6	0	-1.184149	-3.362753	0.861162
18	8	0	3.246986	-3.765307	0.091395

19	6	0	-3.554695	-2.699117	-0.157319
20	6	0	-5.595721	-2.909796	1.410764
21	6	0	-5.375256	-3.722745	3.893793
22	6	0	-3.080157	-4.368889	4.928278
23	6	0	-0.97682	-4.178618	3.360354
24	8	0	-8.072641	-2.346153	0.893893
25	6	0	-9.520203	-3.090635	3.069072
26	8	0	-7.684223	-3.703852	5.035972
27	6	0	-11.209066	-0.995069	3.911813
28	6	0	-10.946933	-5.582452	2.540522
29	8	0	-9.591481	-7.126509	1.11166
30	6	0	-10.661449	-9.600324	0.626413
31	8	0	-13.004794	-6.050157	3.437766
32	1	0	7.931954	-2.313172	-3.455434
33	1	0	2.855185	11.221762	-2.69826
34	1	0	4.947025	11.808626	-0.15523
35	1	0	5.944954	12.35762	-3.300413
36	1	0	12.753847	4.524491	-2.987051
37	1	0	12.656031	6.981166	-0.719756
38	1	0	11.948042	3.8415	0.187677
39	1	0	2.089239	-1.88867	-6.53619
40	1	0	3.914661	-3.987373	-4.679613
41	1	0	-3.759595	-2.05498	-2.078973
42	1	0	-2.918472	-4.993937	6.863417
43	1	0	0.860867	-4.676181	4.093472
44	1	0	-12.21507	-1.534014	5.616645
45	1	0	-10.075311	0.676026	4.284282

46	1	0	-12.583449	-0.570654	2.444933
47	1	0	-10.940795	-10.604256	2.394781
48	1	0	-12.443071	-9.410971	-0.374409
49	1	0	-9.282746	-10.565259	-0.537802
8_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	4.923385	-0.389809	-3.36952
1	6	0	7.287579	-0.746442	-2.251815
2	7	0	8.706192	1.159017	-1.461064
3	6	0	7.75533	3.478677	-1.76232
4	6	0	5.386051	3.860636	-2.880597
5	7	0	3.997069	1.92377	-3.679753
6	7	0	9.166528	5.493139	-0.945069
7	6	0	8.331096	7.953216	-1.204178
8	7	0	5.97859	8.320058	-2.330103
9	6	0	4.392058	6.423328	-3.205572
10	8	0	2.335532	6.884155	-4.169537
11	8	0	9.578571	9.766391	-0.488332
12	6	0	5.175266	10.953269	-2.569187
13	6	0	11.624796	5.029115	0.231737
14	6	0	3.350043	-2.568569	-4.233757
15	8	0	1.012136	-2.743922	-2.8209
16	6	0	1.204321	-3.571124	-0.415934
17	6	0	-1.241671	-3.618557	0.900294
18	8	0	3.217797	-4.203197	0.5236
19	6	0	-3.478891	-2.816695	-0.303228

20	6	0	-5.65441	-2.939072	1.084229
21	6	0	-5.689182	-3.798237	3.561533
22	6	0	-3.528308	-4.580658	4.774547
23	6	0	-1.292725	-4.479583	3.392947
24	8	0	-8.044151	-2.218174	0.376535
25	6	0	-9.709072	-2.968747	2.42859
26	8	0	-8.083204	-3.673594	4.501709
27	6	0	-11.401982	-0.838985	3.173861
28	6	0	-11.159476	-5.295018	1.430089
29	8	0	-9.882589	-7.416541	1.797949
30	6	0	-10.980177	-9.697713	0.755772
31	8	0	-13.165383	-5.114529	0.333475
32	1	0	8.043853	-2.627588	-1.994583
33	1	0	5.029607	11.814355	-0.713006
34	1	0	6.53342	11.99925	-3.695444
35	1	0	3.351132	10.983877	-3.486684
36	1	0	11.393945	3.816216	1.868775
37	1	0	12.88668	4.125227	-1.109345
38	1	0	12.408221	6.823068	0.80993
39	1	0	2.73983	-2.29165	-6.17201
40	1	0	4.383047	-4.335412	-4.089676
41	1	0	-3.483317	-2.130567	-2.221418
42	1	0	-3.564892	-5.242622	6.703663
43	1	0	0.447862	-5.086053	4.267143
44	1	0	-12.538857	-0.247823	1.571982
45	1	0	-12.65742	-1.440184	4.685386
46	1	0	-10.260184	0.739666	3.823229

47	1	0	-12.812703	-10.051467	1.609959
48	1	0	-11.166765	-9.521501	-1.280834
49	1	0	-9.666799	-11.193372	1.230578
9_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	2.361419	2.234714	-5.177862
1	6	0	4.748204	1.637326	-6.132855
2	7	0	6.823131	2.851441	-5.432985
3	6	0	6.53707	4.688263	-3.72412
4	6	0	4.155544	5.290596	-2.737082
5	7	0	2.090431	4.06638	-3.481982
6	7	0	8.648181	5.97821	-2.951571
7	6	0	8.517929	7.895355	-1.184378
8	7	0	6.141578	8.491299	-0.217573
9	6	0	3.891117	7.307203	-0.860169
10	8	0	1.863308	7.919578	0.08099
11	8	0	10.392096	9.051683	-0.471875
12	6	0	6.095971	10.534281	1.642921
13	6	0	11.107853	5.301326	-4.017677
14	6	0	0.04635	0.848491	-6.009113
15	8	0	-1.162819	-0.442084	-3.923038
16	6	0	0.025709	-2.515338	-3.033274
17	6	0	-1.277591	-3.64446	-0.854662
18	8	0	1.975105	-3.327667	-3.969376
19	6	0	-3.451587	-2.516936	0.192316
20	6	0	-4.52146	-3.711335	2.217624

21	6	0	-3.530201	-5.921775	3.222771
22	6	0	-1.406296	-7.049326	2.234734
23	6	0	-0.292028	-5.867979	0.166335
24	8	0	-6.574754	-2.966817	3.614498
25	6	0	-7.111401	-4.983855	5.336987
26	8	0	-4.917	-6.655746	5.267345
27	6	0	-7.528911	-3.984125	7.945341
28	6	0	-9.328346	-6.551697	4.257894
29	8	0	-10.086483	-8.264919	5.919645
30	6	0	-12.082542	-9.955343	5.108821
31	8	0	-10.174611	-6.268103	2.147724
32	1	0	4.97575	0.13402	-7.499039
33	1	0	4.157619	10.842518	2.206963
34	1	0	7.217328	10.017255	3.281207
35	1	0	6.857208	12.249779	0.815908
36	1	0	12.519154	6.533705	-3.207477
37	1	0	11.553998	3.350591	-3.56692
38	1	0	11.074387	5.536377	-6.054341
39	1	0	-1.379927	2.165407	-6.671545
40	1	0	0.481093	-0.489853	-7.502647
41	1	0	-4.232944	-0.789728	-0.553293
42	1	0	-0.639474	-8.765063	3.028088
43	1	0	1.372852	-6.693763	-0.675198
44	1	0	-7.792861	-5.528224	9.26932
45	1	0	-5.901432	-2.866101	8.51162
46	1	0	-9.209306	-2.800871	7.972896
47	1	0	-11.469879	-11.038715	3.476432

48	1	0	-12.423588	-11.192067	6.702948
49	1	0	-13.772695	-8.881999	4.657523
10_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	4.706044	-0.145528	-3.724174
1	6	0	7.215532	-0.578372	-3.030518
2	7	0	8.744335	1.259913	-2.287997
3	6	0	7.760482	3.583966	-2.199467
4	6	0	5.241335	4.037533	-2.872498
5	7	0	3.742499	2.170516	-3.64089
6	7	0	9.289552	5.529933	-1.427016
7	6	0	8.42105	7.987027	-1.284614
8	7	0	5.910604	8.423916	-1.95246
9	6	0	4.20196	6.599077	-2.744977
10	8	0	2.008937	7.117488	-3.289057
11	8	0	9.769943	9.740595	-0.604109
12	6	0	5.073242	11.050784	-1.767116
13	6	0	11.913226	4.99251	-0.739707
14	6	0	3.032554	-2.250789	-4.585435
15	8	0	0.755126	-2.435897	-3.087885
16	6	0	1.046511	-3.248249	-0.687853
17	6	0	-1.354434	-3.362067	0.704303
18	8	0	3.106952	-3.819616	0.186617
19	6	0	-3.660757	-2.709681	-0.458763
20	6	0	-5.789805	-2.8979	0.991542
21	6	0	-5.7146	-3.678215	3.493894

22	6	0	-3.484905	-4.310758	4.669369
23	6	0	-1.294748	-4.144273	3.222664
24	8	0	-8.231762	-2.327139	0.327558
25	6	0	-9.801437	-3.097724	2.447131
26	8	0	-8.086746	-3.649545	4.495025
27	6	0	-11.586147	-1.037596	3.173397
28	6	0	-11.149154	-5.528063	1.559845
29	8	0	-9.754738	-7.567337	1.96185
30	6	0	-10.759272	-9.936483	1.026646
31	8	0	-13.189062	-5.487241	0.512529
32	1	0	7.998815	-2.466002	-3.076778
33	1	0	6.222944	12.238542	-2.981139
34	1	0	3.121554	11.144262	-2.361282
35	1	0	5.235967	11.704353	0.170626
36	1	0	12.923354	4.241181	-2.359105
37	1	0	12.788054	6.734405	-0.133861
38	1	0	11.967625	3.625685	0.787922
39	1	0	2.347484	-1.8898	-6.48588
40	1	0	4.02953	-4.044228	-4.559321
41	1	0	-3.750679	-2.089696	-2.397176
42	1	0	-3.437102	-4.910646	6.618473
43	1	0	0.496544	-4.635788	4.066277
44	1	0	-12.79698	-0.560866	1.587345
45	1	0	-12.765615	-1.65516	4.738741
46	1	0	-10.515265	0.620434	3.739959
47	1	0	-9.357808	-11.345881	1.513276
48	1	0	-12.547758	-10.353637	1.943185

49	1	0	-11.008094	-9.839157	-1.00852

Table S7. The atom energies of low-energy conformers of comound **3**.

Conformers	Gibbs free energies (ΔG) [a]	Final single point energy (a.u.)
2_tddft_	0.00028	-1593.792780676491
3_tddft_	0.00007	-1593.792987083299
4_tddft_	0.00032	-1593.792735343297
5_tddft_	0.00016	-1593.792902050109
6_tddft_	0.0002	-1593.792862655066
7_tddft_	0.00028	-1593.792774643712
8_tddft_	0.00012	-1593.792934170733
9_tddft_	0.00000	-1593.793058492482
10_tddft_	0.00015	-1593.792905237641

[a] CAM-B3LYP-D3/def2-TZVP, in kcal/mol.