

Supplementary Materials

Short Note

1-Methyl-8-phenyl-1,3-diazaspiro[4.5]decane-2,4-dione

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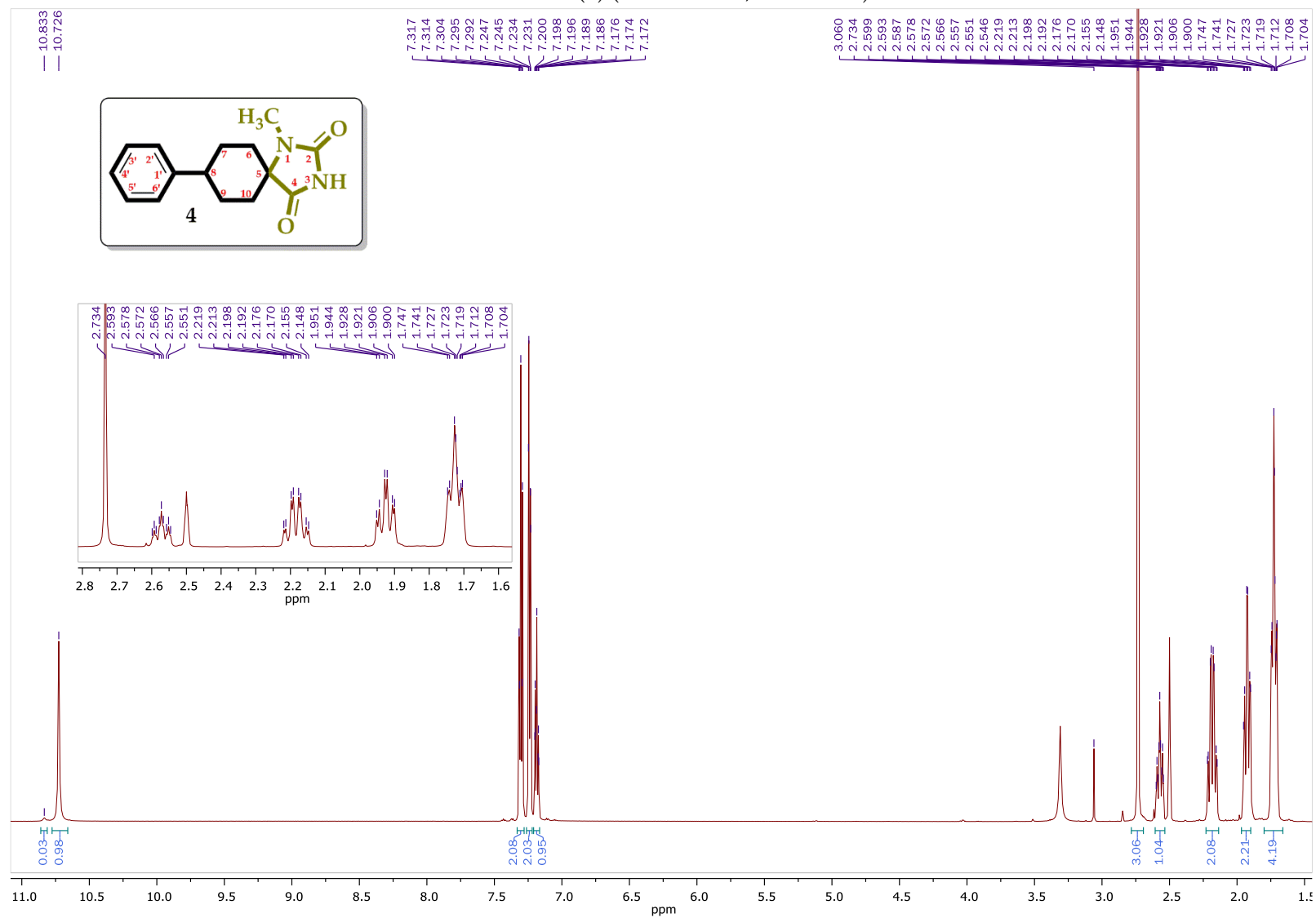
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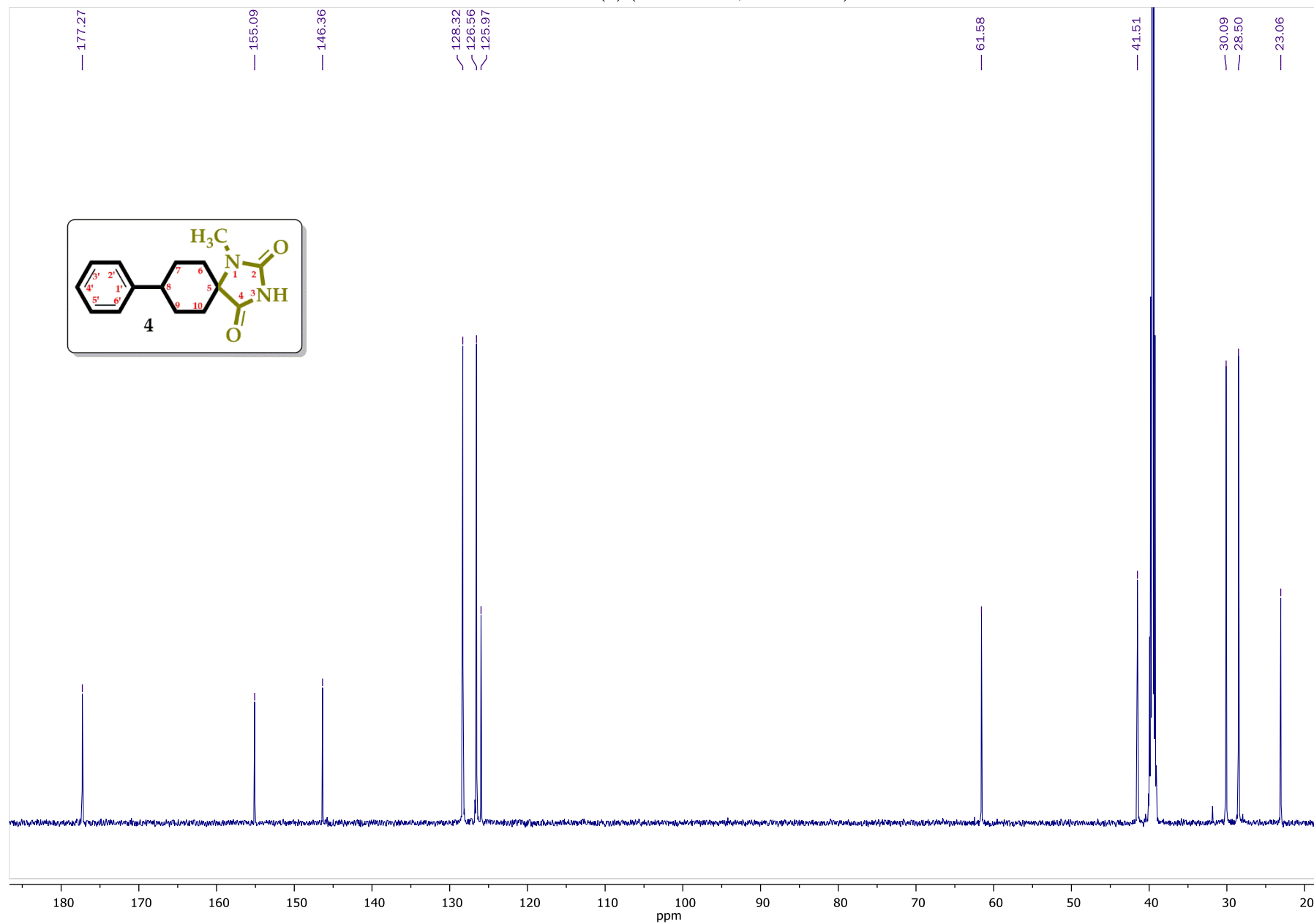
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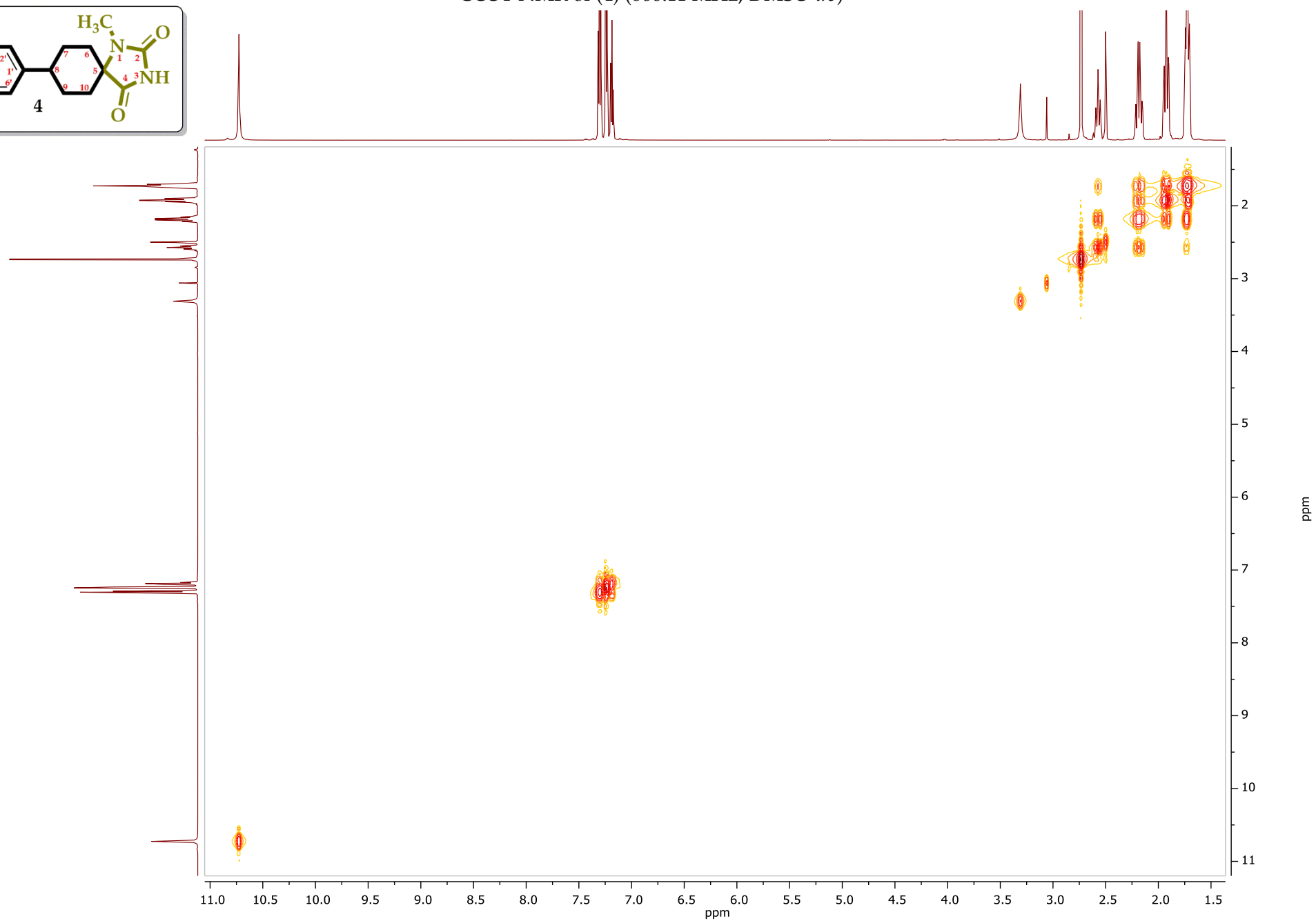
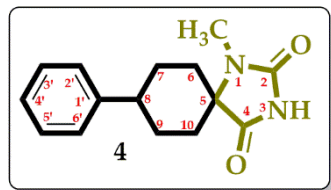
I Copies of NMR spectra
¹H NMR of (4) (600.11 MHz, DMSO-*d*₆)



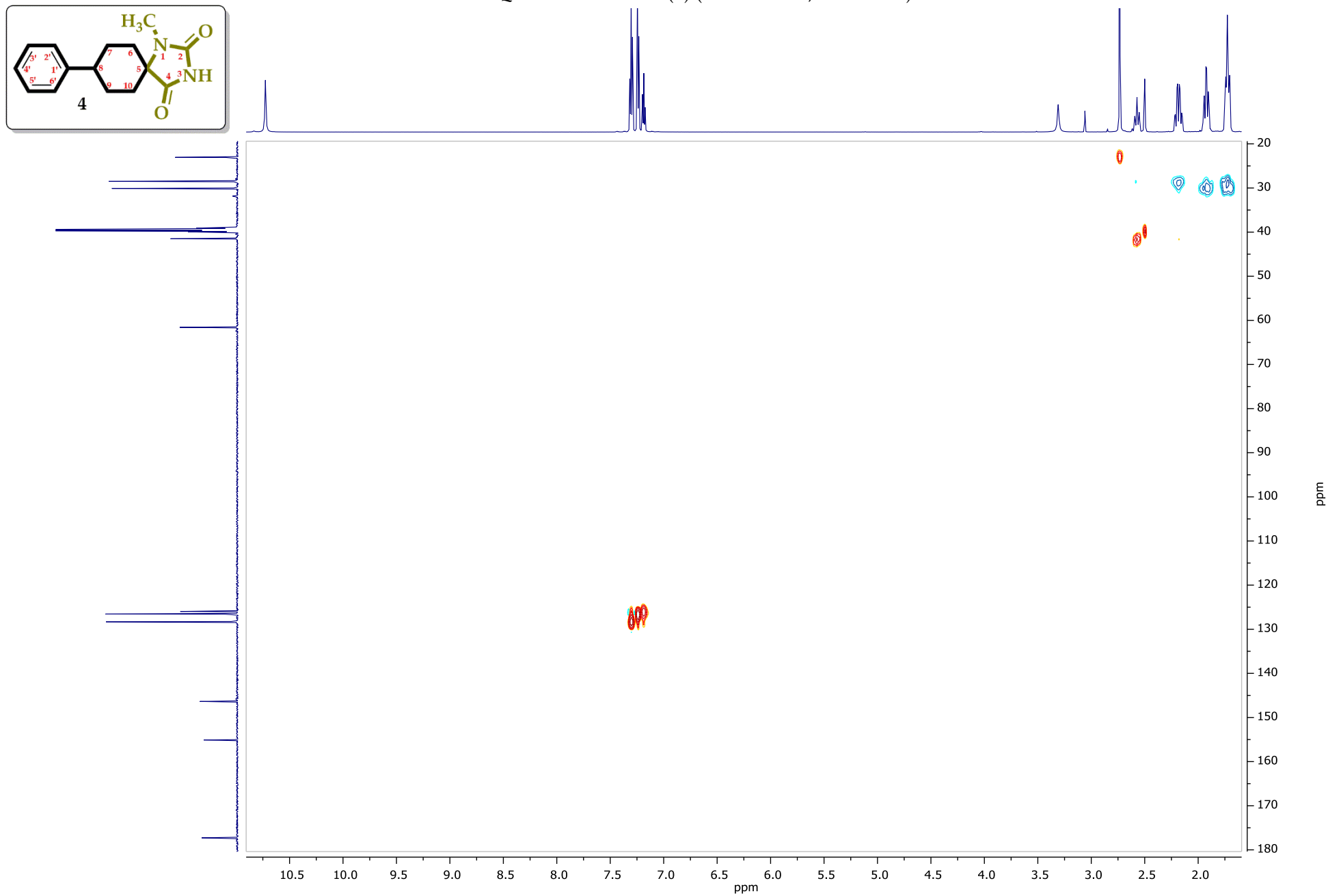
^{13}C NMR of (4) (150.9 MHz, DMSO-*d*₆)

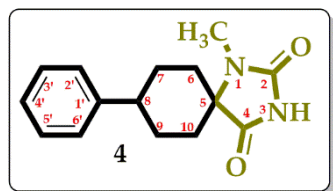


COSY NMR of (**4**) (600.11 MHz, DMSO-*d*₆)

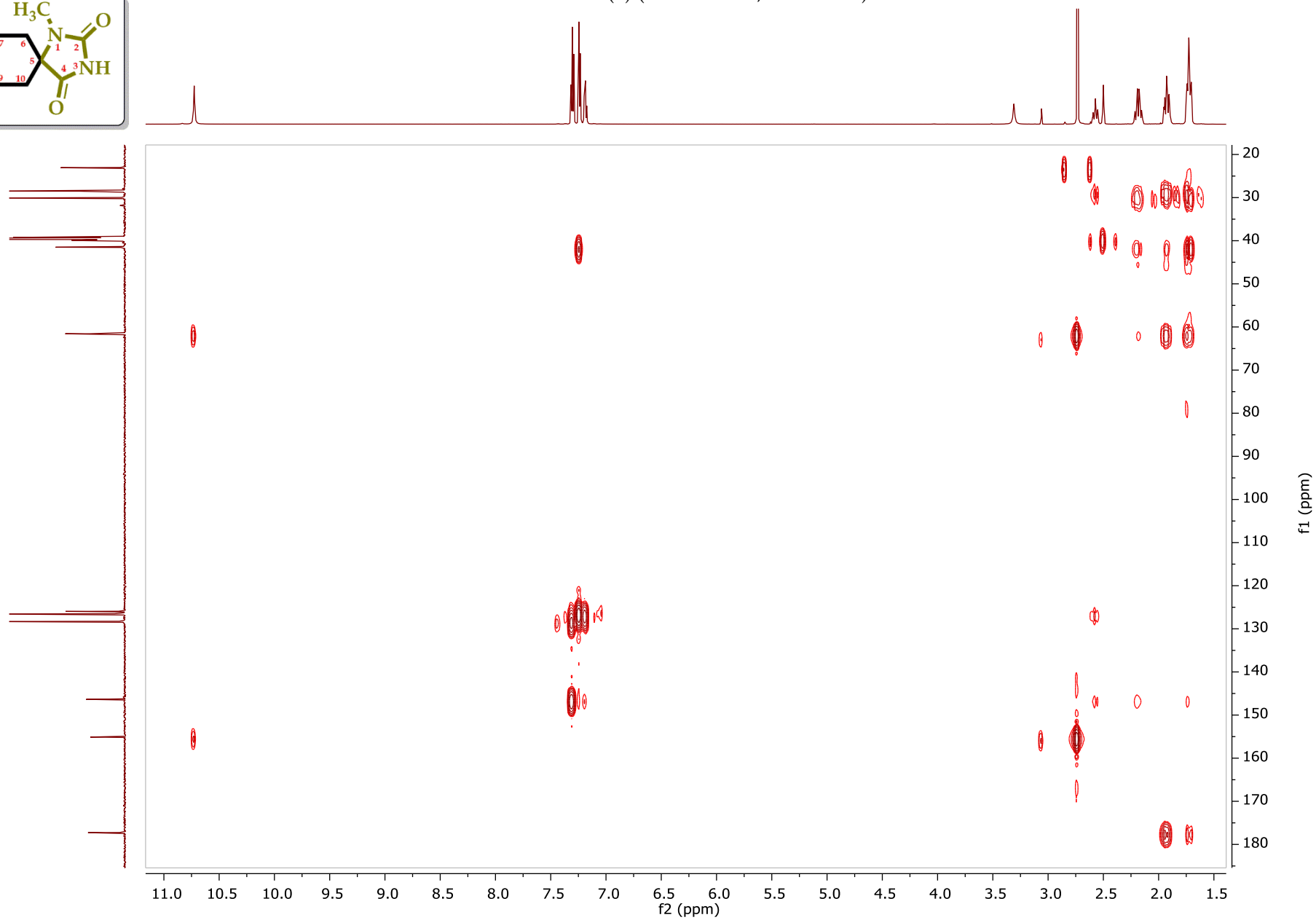


HSQC-DEPT NMR of (4) (600.11 MHz, DMSO-*d*₆)

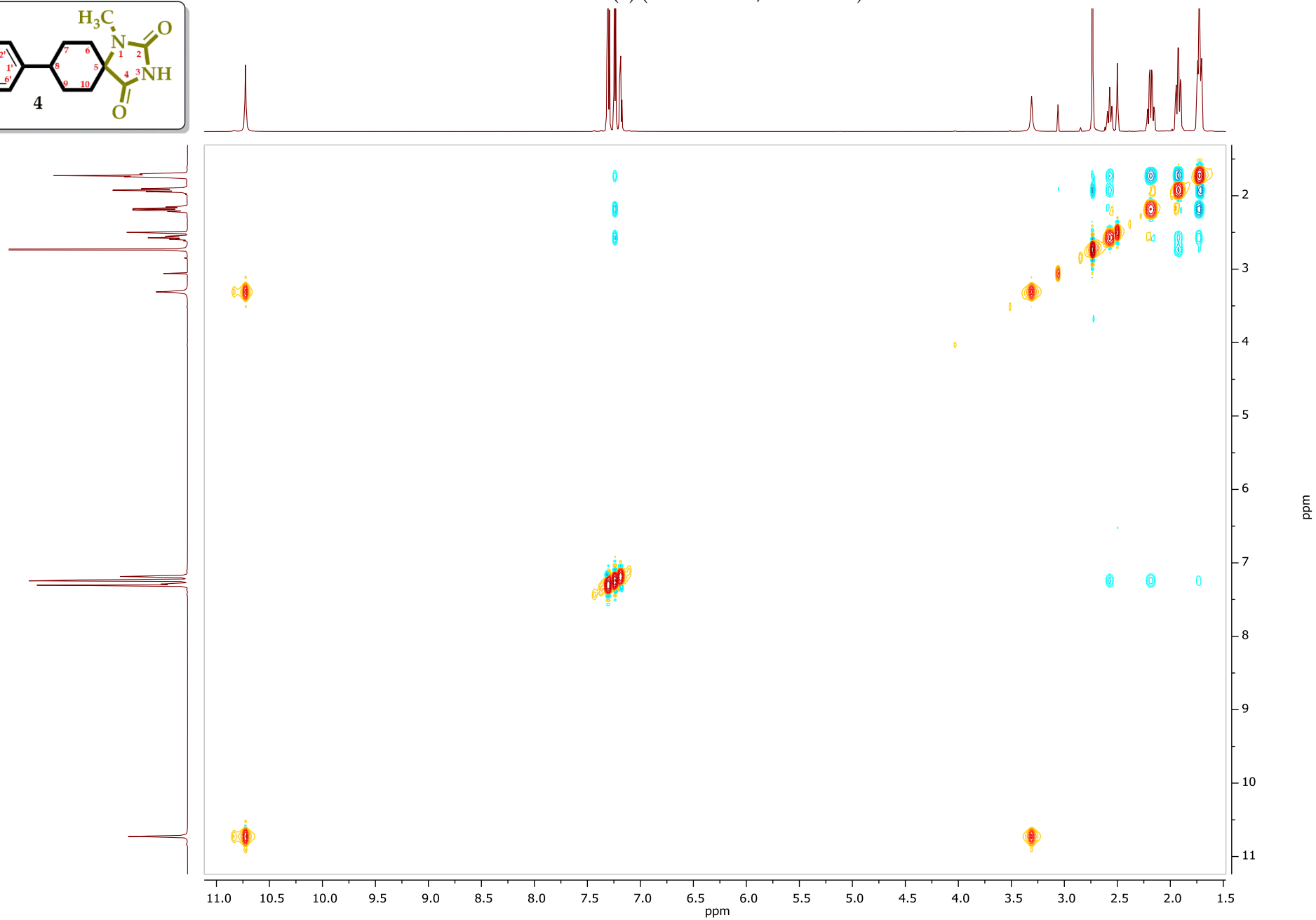
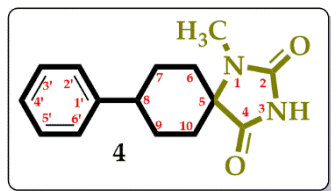




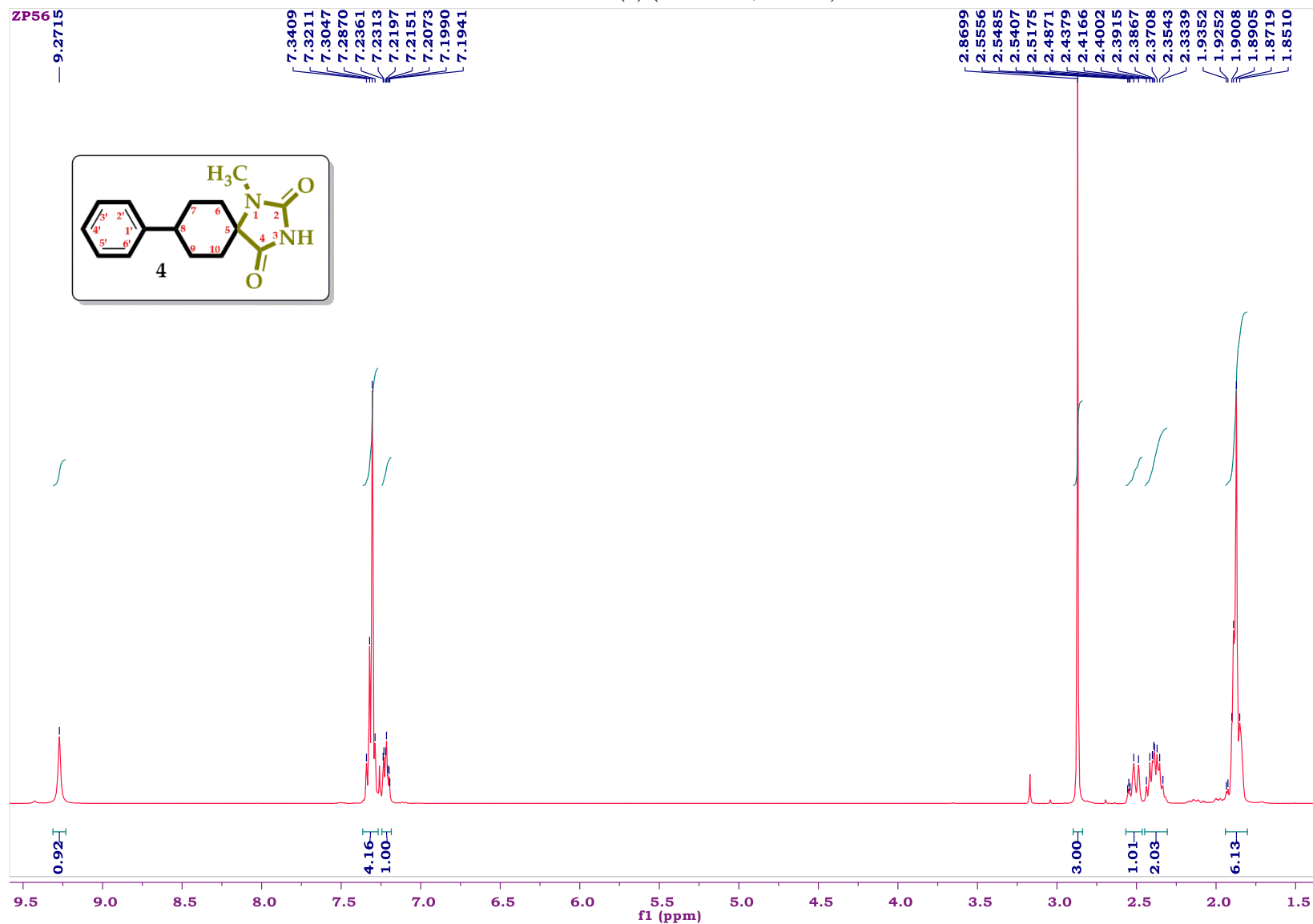
HMBC NMR of (4) (600.11 MHz, DMSO-*d*₆)



NOESY NMR of (4) (600.11 MHz, DMSO-*d*₆)

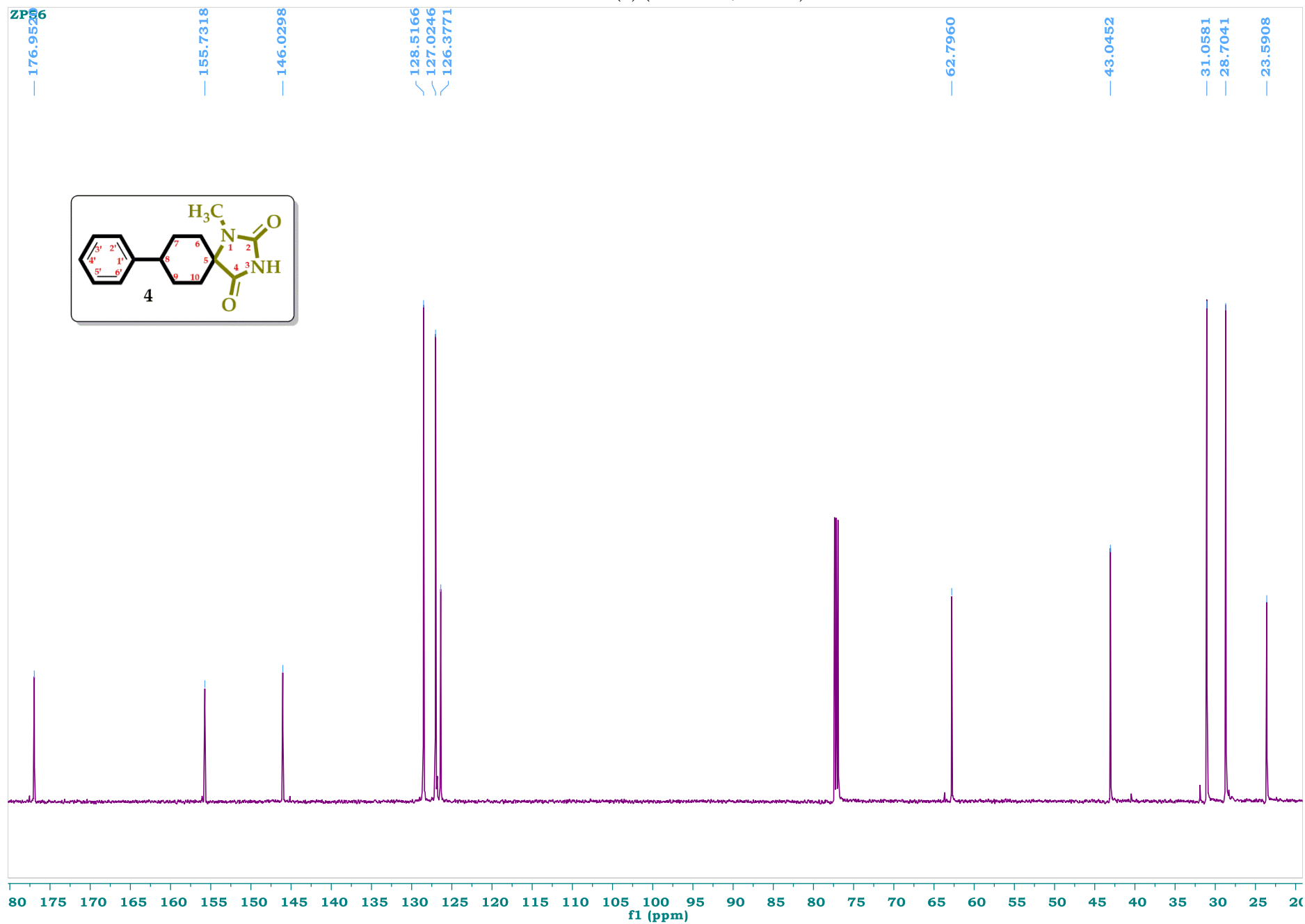


¹H NMR of (4) (400 MHz, CDCl₃)

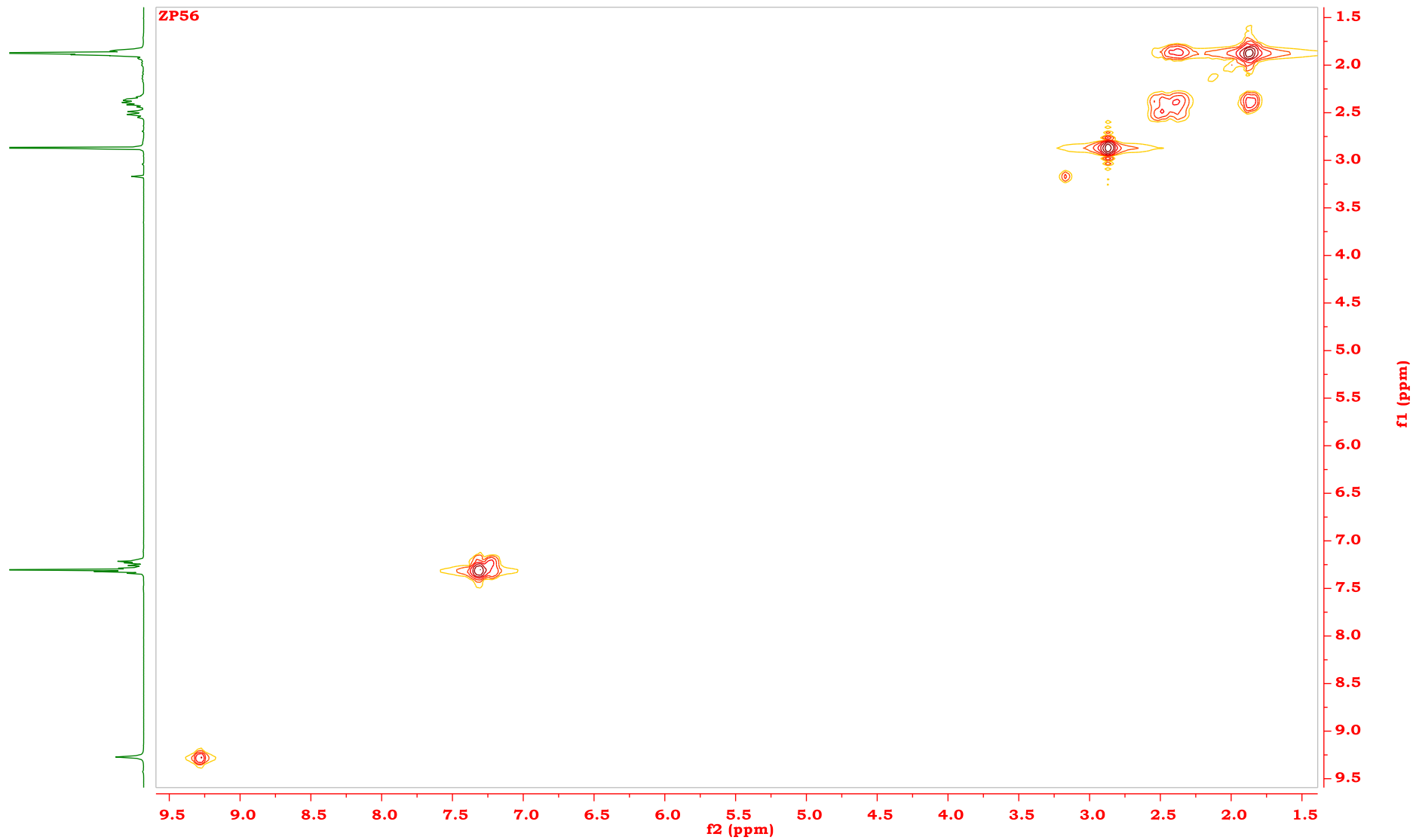
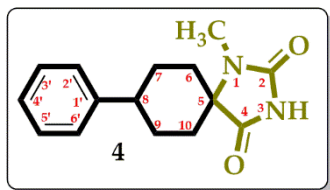


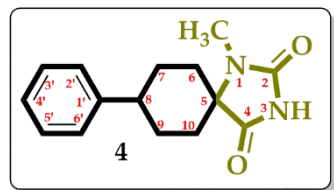
¹H NMR (400 MHz, CDCl₃) δ (ppm): 1.80-1.94 (complex m, 6H, H_6 , H_7 , H_9 , H_{10}), 2.31-2.44 (m, 2H, H_7 , H_9), 2.53 (t, 1H, $J=12.2$ Hz, H_8), 2.87 (s, 3H, CH_3), 7.22 (td, 1H, $J_1=1.9$ Hz, $J_2=6.5$ Hz, $H_{4'}$), 7.30 (d, 2H, $J=7.1$ Hz, $H_{2'}$, $H_{6'}$), 7.32 (t, 2H, $J=7.9$ Hz, $H_{3'}$, $H_{5'}$), 9.27 (s, 1H, H_3); ¹³C NMR (150 MHz, CDCl₃) δ (ppm): 23.6 (CH_3), 28.7 (C_7 , C_9), 31.0 (C_6 , C_{10}), 43.0 (C_8), 62.8 (C_5), 126.4 ($C_{4'}$), 127.0 ($C_{2'}$, $C_{6'}$), 128.5 ($C_{3'}$, $C_{5'}$), 146.0 ($C_{1'}$), 155.7 ($C_{2=O}$), 177.0 ($C_{4=O}$).

^{13}C NMR of (**4**) (100 MHz, CDCl_3)

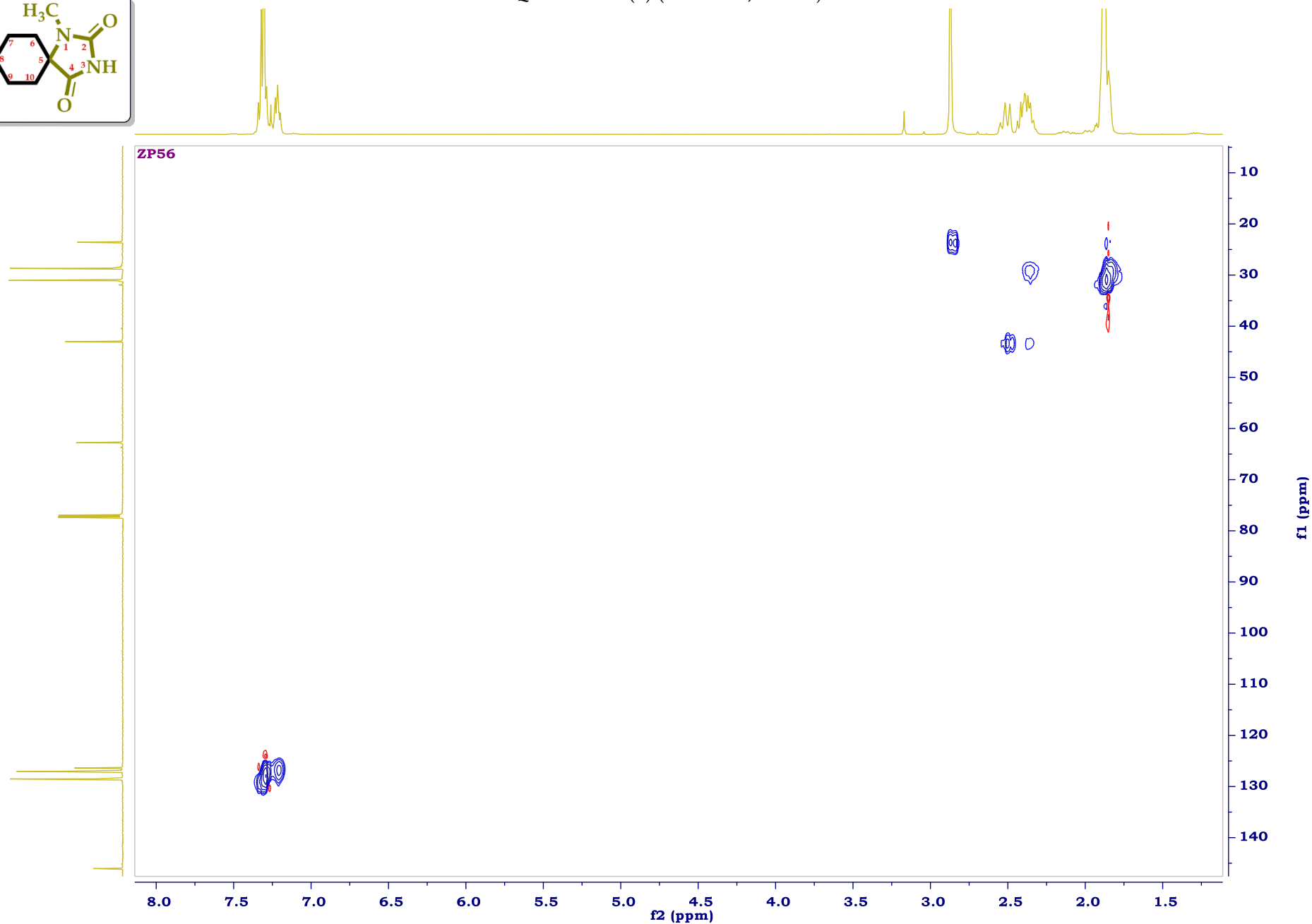


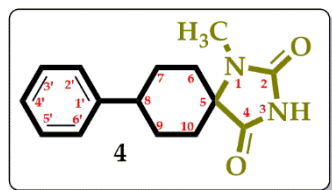
COSY NMR of (4) (400 MHz, CDCl₃)



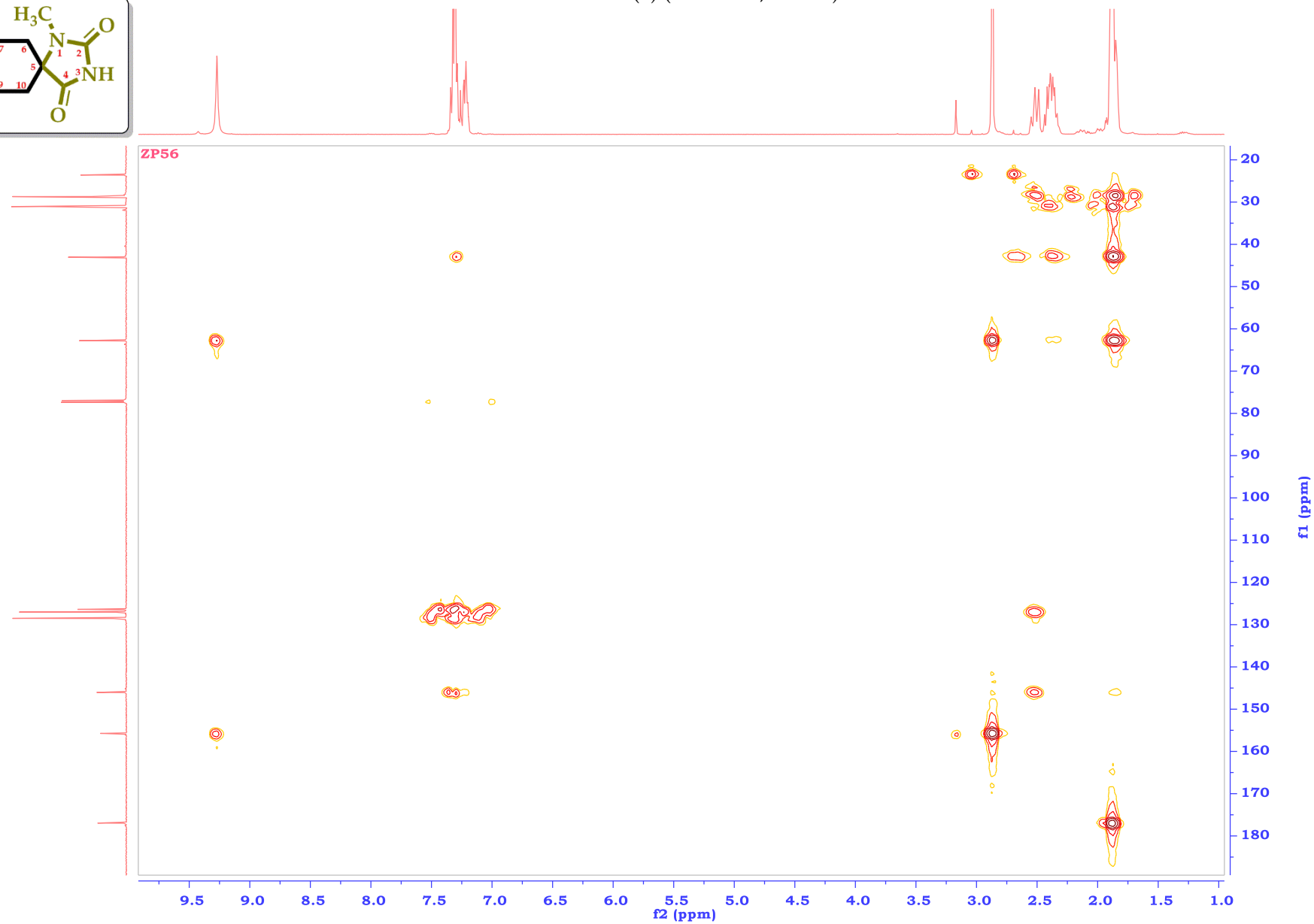


HSQC NMR of (4) (400 MHz, CDCl₃)

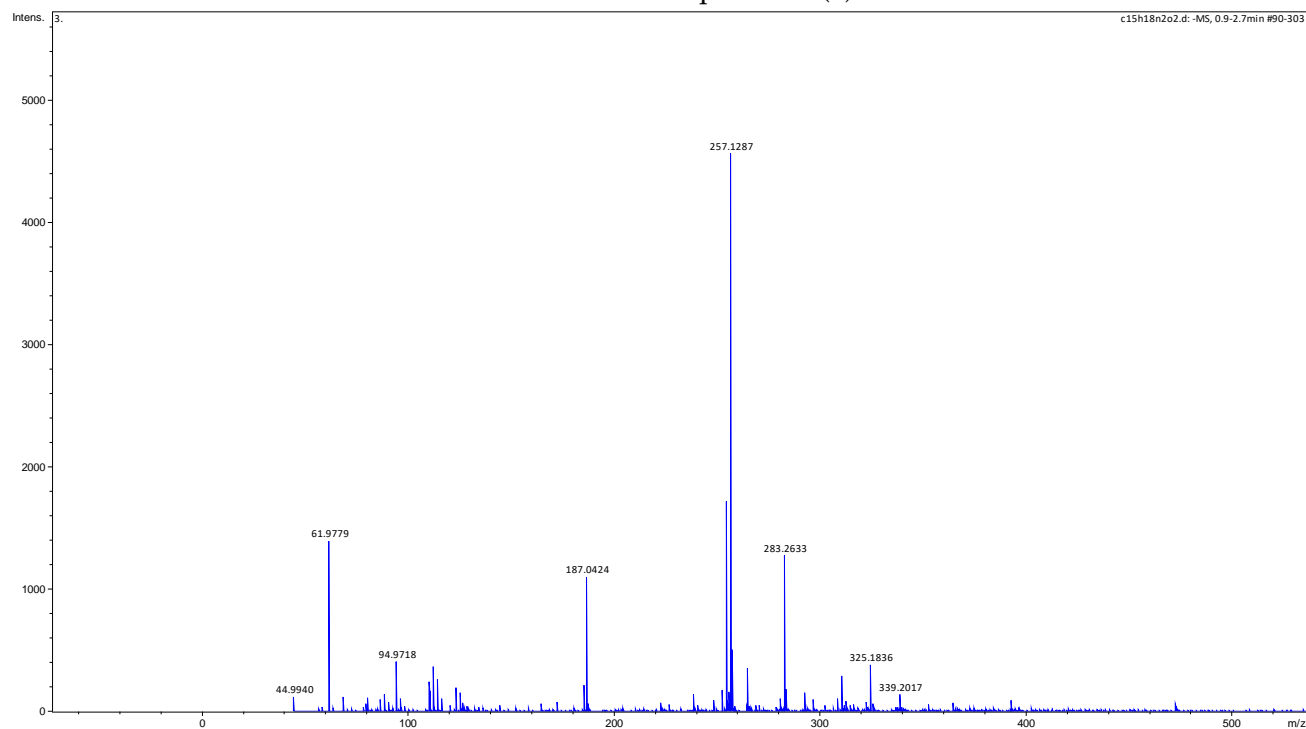
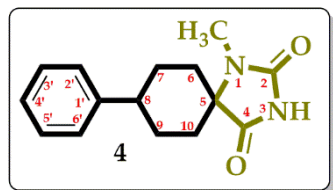


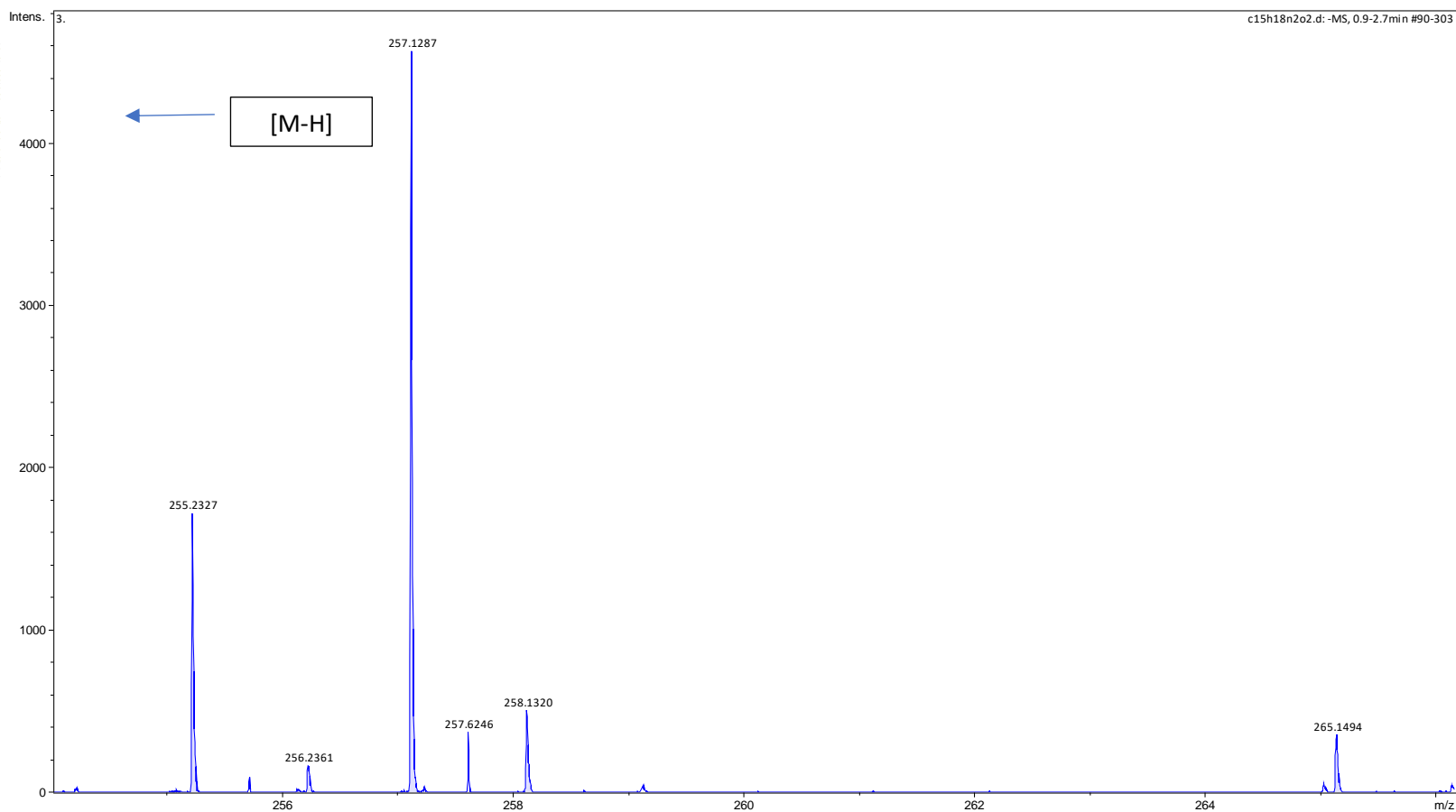
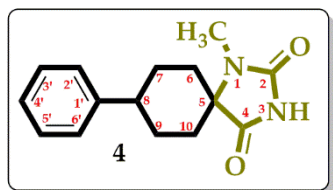


HMBC NMR of (4) (400 MHz, CDCl_3)



HRMS Spectra of (4)





Meas. m/z	Ion Formula	m/z	Err(ppm)	mSigma	rdb	Adduct Type
257.1287	C ₁₅ H ₁₇ N ₂ O ₂	257.1296	3.1	37.2	9.0	M-H

HRMS m/z calc. for C₁₅H₁₈N₂O₂: 258.136279

HRMS m/z calc. for [C₁₅H₁₈N₂O₂-H]: 257.1285

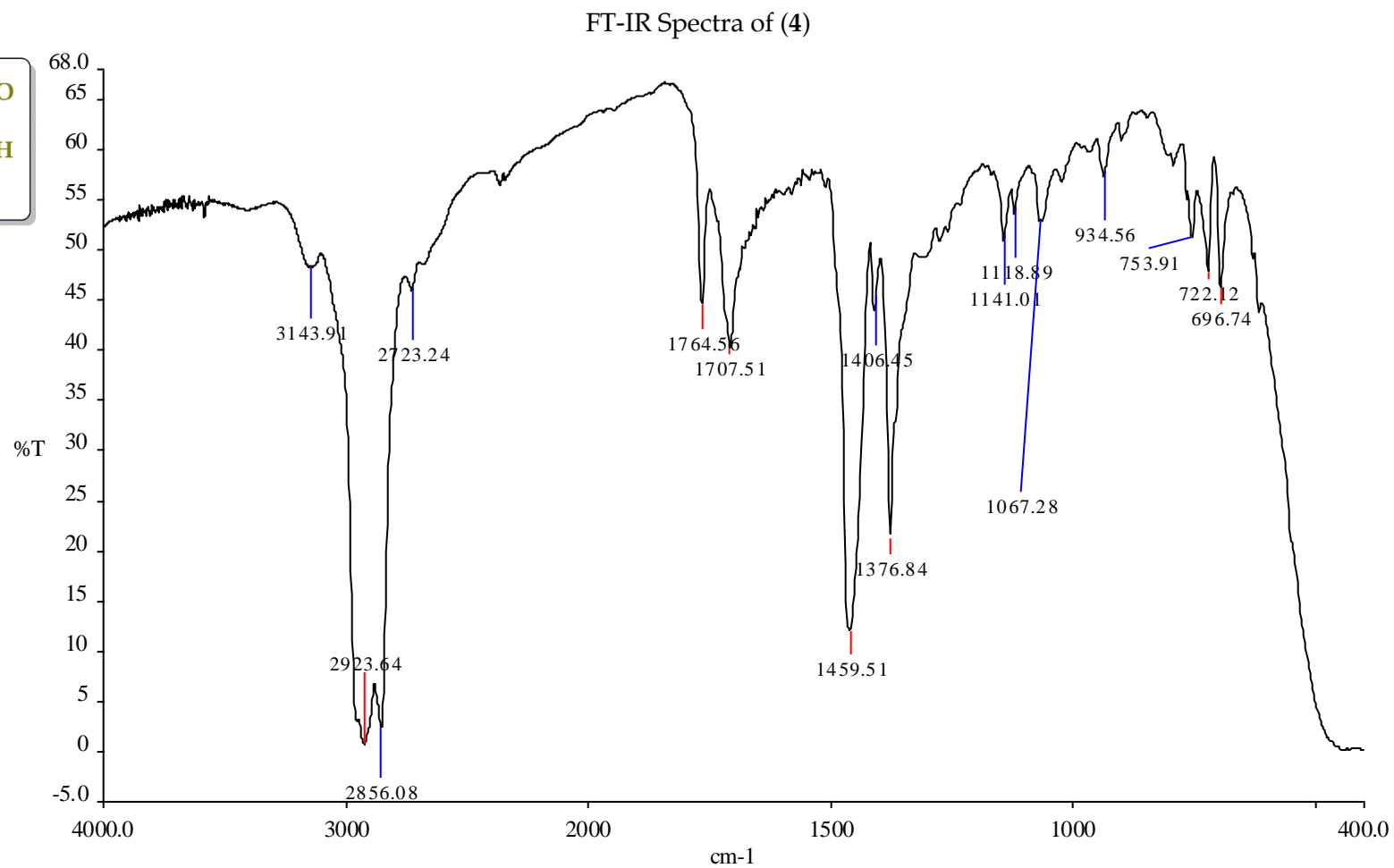
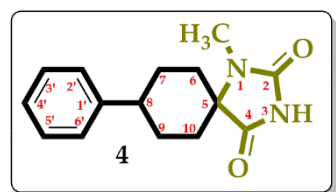
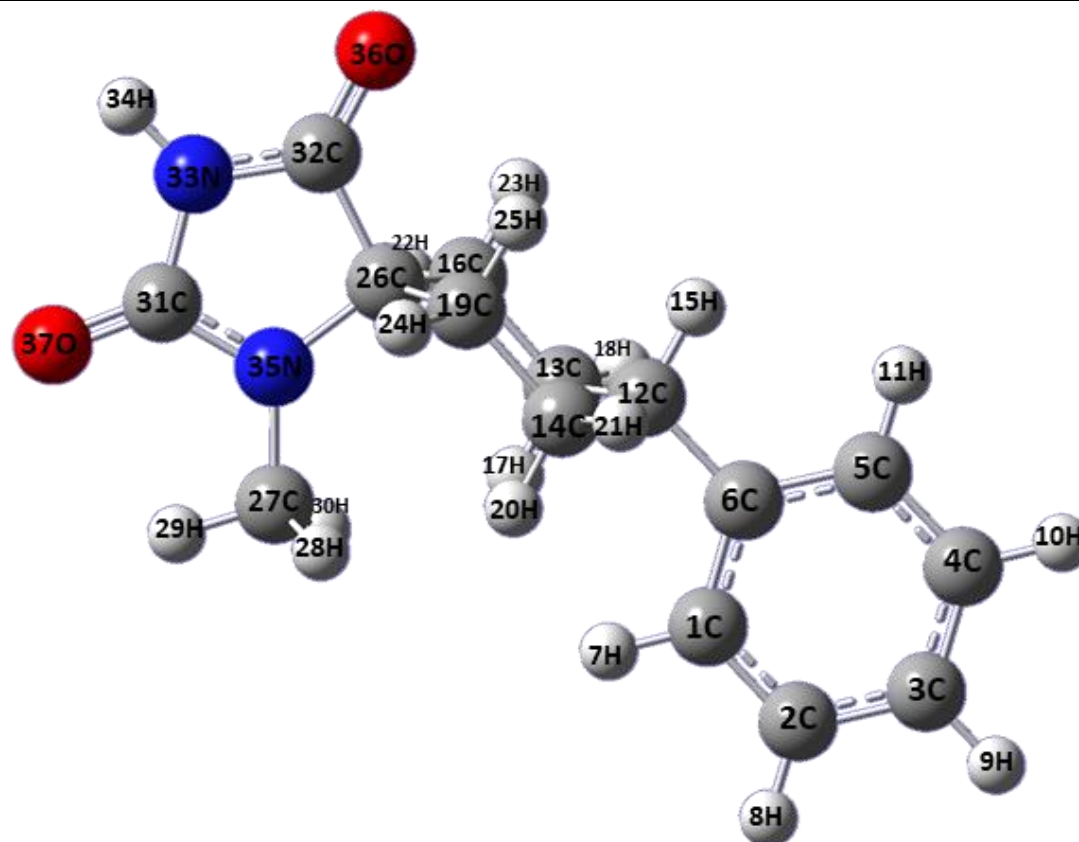


Table S1. Conformation A properties



a/a	Atom	NA	NB	NC	Bond length	Bond angle	Dihedral
1	1C	-	-	-	-	-	-
2	2C	1	-	-	1.3963903	-	-

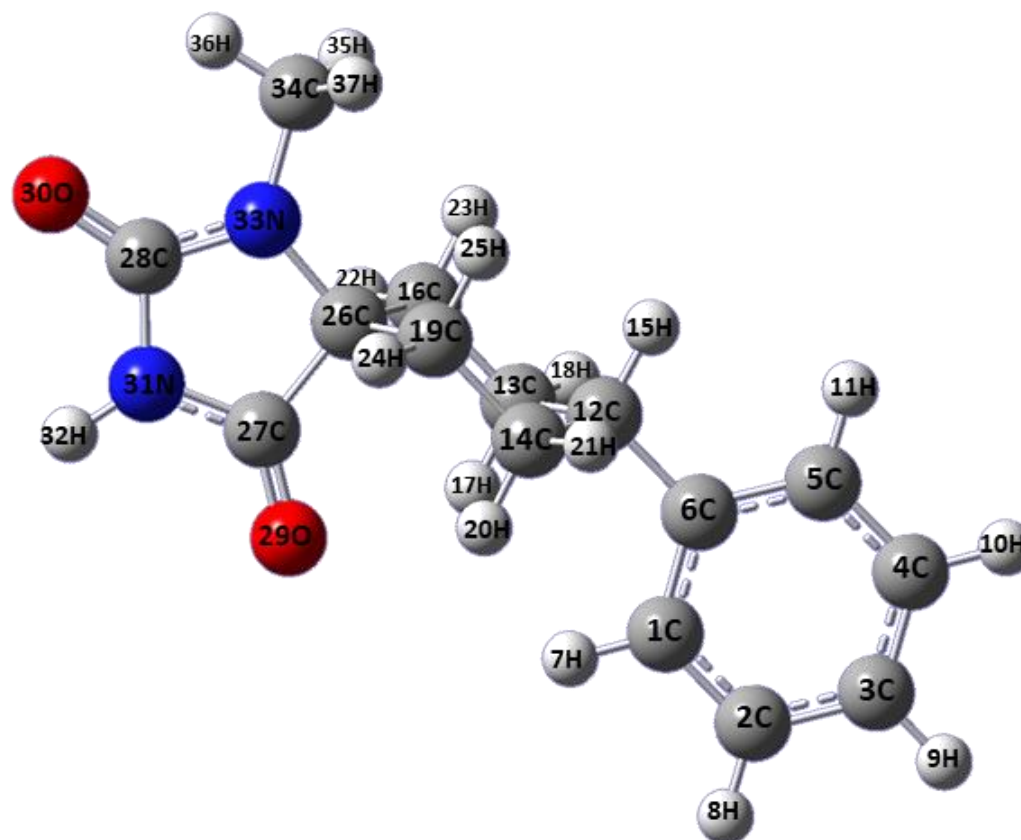
(Table S1) contd....

3	3C	2	1	-	1.3980104	120.2413079	-
4	4C	3	2	1	1.3963342	119.4036692	0.0000000
5	5C	4	3	2	1.3979700	120.0909880	0.0000000
6	6C	5	4	3	1.4024263	121.2218800	0.0000000
7	7H	1	2	3	1.0870031	118.9797019	180.0000000
8	8H	2	1	6	1.0865131	119.7119005	-180.0000000
9	9H	3	2	1	1.0860979	120.2547510	-180.0000000
10	10H	4	3	2	1.0863995	120.1633823	180.0000000
11	11H	5	4	3	1.0875661	119.4983030	180.0000000
12	12C	6	5	4	1.5201539	120.3774719	-180.0000000
13	13C	12	6	5	1.5431293	112.6419435	117.7767399
14	14C	12	6	5	1.5431294	112.6422074	-117.7764074
15	15H	12	6	5	1.0997481	107.1887602	0.0000000
16	16C	13	12	6	1.5375469	111.9638783	-177.0747506
17	17H	13	12	6	1.0960612	109.3236770	59.6580974
18	18H	13	12	6	1.0961953	109.6981001	-56.3308002
19	19C	14	12	6	1.5375465	111.9640667	177.0739064
20	20H	14	12	6	1.0960620	109.3237291	-59.6583363

(Table S1) contd....

21	21H	14	12	6	1.0961955	109.6980729	56.3304351
22	22H	16	13	12	1.0961561	110.6117705	-176.5402286
23	23H	16	13	12	1.0966912	108.6535525	66.4286190
24	24H	19	14	12	1.0961557	110.6120399	176.5412455
25	25H	19	14	12	1.0966905	108.6542859	-66.4270936
26	26C	19	14	12	1.5514818	115.0596033	52.6109215
27	27C	26	19	14	2.6263877	100.9562467	61.0718887
28	28C	27	26	19	1.0942563	97.2274323	-1.8541559
29	29O	27	26	19	1.0910722	133.8802954	122.9296124
30	30O	27	26	19	1.0942568	97.2253847	-112.2888267
31	31N	26	19	14	2.3724554	123.6459452	120.2088080
32	32H	26	19	14	1.5469430	108.0900075	-163.6596844
33	33N	32	26	19	1.3694450	106.7444745	-119.9172095
34	34C	33	32	26	1.0107234	124.8369448	-179.9689890
35	35H	31	26	19	1.3692384	35.1192436	-81.8383804
36	36H	32	26	19	1.2173196	126.2377544	60.1494127
37	37H	31	26	19	1.2208567	163.6747913	-81.8923235
38	-	13	12	6	1.3881169	59.7421356	131.7372944

Table S2. Conformation **B** properties



a/a	Atom	NA	NB	NC	Bond length	Bond angle	Dihedral
1	1C	-	-	-	-	-	-
2	2C	1	-	-	1.3963172	-	-
3	3C	2	1	-	1.3983524	120.3254840	-

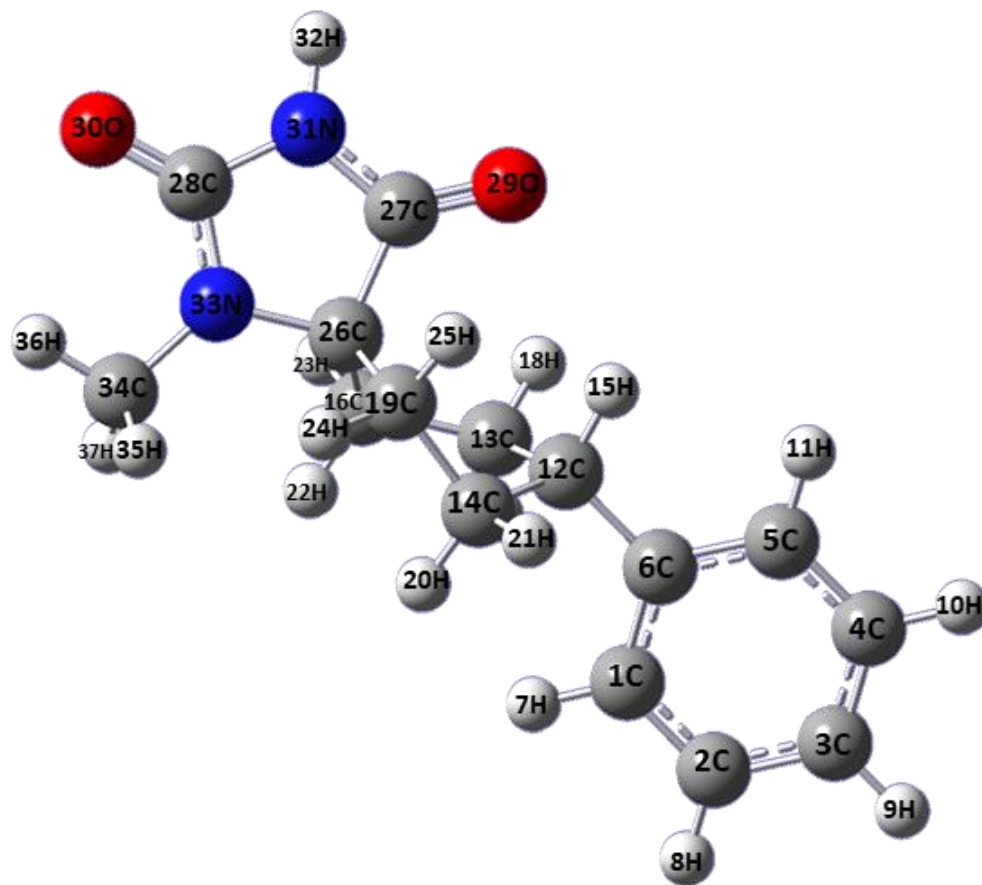
(Table S2) contd....

4	4C	3	2	1	1.3962568	119.4186736	0.0000000
5	5C	4	3	2	1.3982528	120.0399774	0.0000000
6	6C	5	4	3	1.4022061	121.2046436	0.0000000
7	7H	1	2	3	1.0868635	119.2390416	-180.0000000
8	8H	2	1	6	1.0865227	119.6437569	-180.0000000
9	9H	3	2	1	1.0862034	120.2626130	180.0000000
10	10H	4	3	2	1.0865232	120.1860546	-180.0000000
11	11H	5	4	3	1.0878616	119.4951791	-180.0000000
12	12C	6	5	4	1.5201338	120.5265471	180.0000000
13	13C	12	6	5	1.5446317	112.3079028	117.7115710
14	14C	12	6	5	1.5446329	112.3078149	-117.7120856
15	15H	12	6	5	1.1009459	107.1063248	0.0000000
16	16C	13	12	6	1.5364564	111.9432557	-178.7867604
17	17H	13	12	6	1.0943895	109.5233114	59.5390017
18	18H	13	12	6	1.0961717	109.7112831	-57.6626457
19	19C	14	12	6	1.5364558	111.9436766	178.7875853
20	20H	14	12	6	1.0943900	109.5231594	-59.5381737

(Table S2) contd....

21	21H	14	12	6	1.0961724	109.7111680	57.6632478
22	22H	16	13	12	1.0963677	110.6693777	-177.9955865
23	23H	16	13	12	1.0980768	109.0915947	64.8161257
24	24H	19	14	12	1.0963671	110.6694307	177.9937092
25	25H	19	14	12	1.0980758	109.0916588	-64.8179542
26	26C	19	14	12	1.5483942	113.2953786	54.6615711
27	27C	26	19	14	1.5442977	111.0610818	72.2514731
28	28C	27	26	19	2.3245244	72.5466405	118.4402362
29	29O	27	26	19	1.2191566	127.4379499	-61.5676994
30	30O	28	27	26	1.2202293	157.9131405	179.9859491
31	31N	27	26	19	1.3726973	106.3952610	118.4440324
32	32H	31	27	26	1.0108212	124.4542057	179.9953663
33	33N	28	27	26	1.3675961	73.2928861	-0.0030008
34	34C	33	28	27	1.4516288	121.5496516	179.9881700
35	35H	34	33	28	1.0952805	111.4864412	-118.9865124
36	36H	34	33	28	1.0909595	107.3537553	0.0310747
37	37H	34	33	28	1.0952747	111.4837802	119.0476723
38	-	13	12	6	1.3992598	59.8072848	132.8672009

Table S3. Conformation C properties



a/a	Atom	NA	NB	NC	Bond length	Bond angle	Dihedral
1	1C	-	-	-	-	-	-
2	2C	1	-	-	1.3961913	-	-

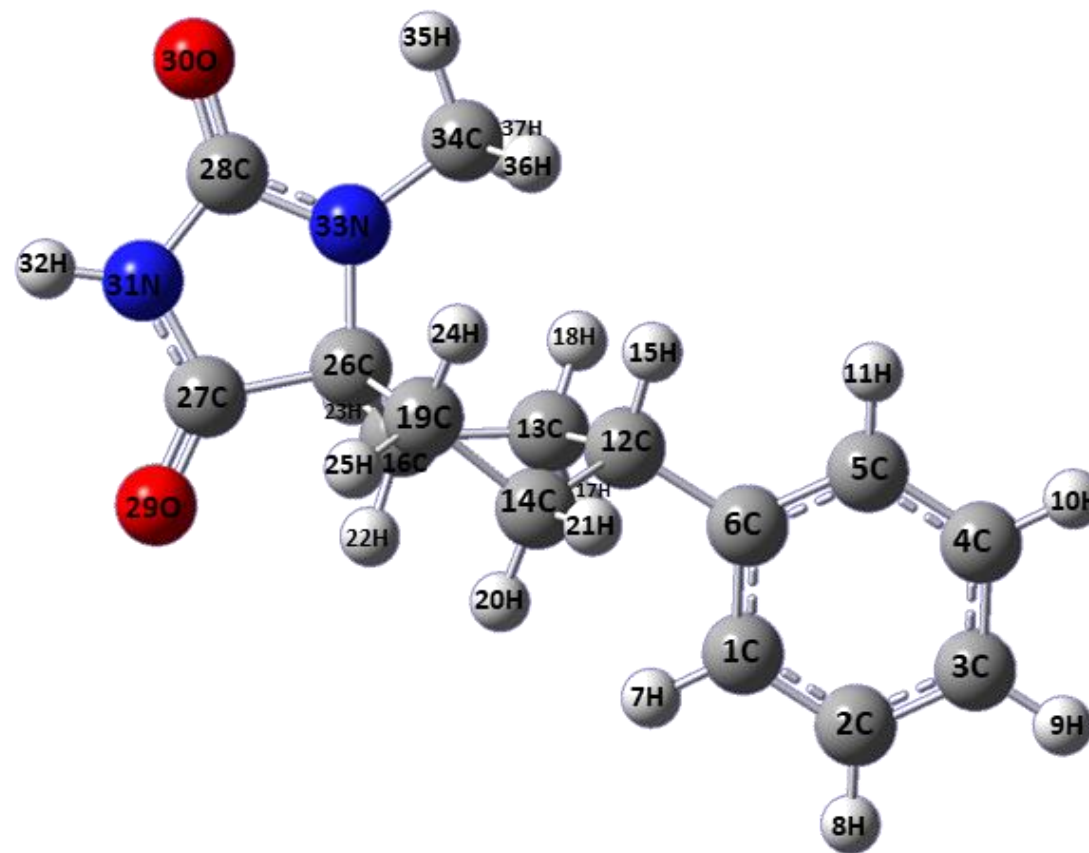
(Table S3) contd....

3	3C	2	1		1.3984113	120.2097804	-
4	4C	3	2	1	1.3962317	119.3856733	0.0108290
5	5C	4	3	2	1.3983677	120.1297883	0.1180891
6	6C	5	4	3	1.4022516	121.1954182	-0.1192828
7	7H	1	2	3	1.0874165	119.0443809	179.8037376
8	8H	2	1	6	1.0866117	119.7398224	179.8910050
9	9H	3	2	1	1.0861669	120.2672664	-179.9139306
10	10H	4	3	2	1.0864995	120.1369250	-179.8331195
11	11H	5	4	3	1.0873744	119.6026942	-179.9755799
12	12C	6	5	4	1.5198894	120.3851933	179.2647747
13	13C	12	6	5	1.5586819	112.9015297	117.1961648
14	14C	12	6	5	1.5433197	112.6281129	-117.3435596
15	15H	12	6	5	1.0957741	107.3828157	-0.5064645
16	16C	13	12	6	1.5423826	113.4806811	146.7531508
17	17H	13	12	6	1.0953634	110.0178467	26.0288593
18	18H	13	12	6	1.0935746	108.7506085	-90.3887781
19	19C	14	12	6	1.5396173	111.0029529	170.2044441
20	20H	14	12	6	1.0979037	110.1035986	-67.2395854

(Table S3) contd....

21	21H	14	12	6	1.0953287	110.0213478	49.5081790
22	22H	16	13	12	1.0963345	109.3764791	-81.5106427
23	23H	16	13	12	1.0960111	110.3956248	161.7108104
24	24H	19	14	12	1.0951459	108.9745922	-75.6450071
25	25H	19	14	12	1.0944543	109.9127247	167.9416744
26	26C	16	13	12	1.5491306	114.0595645	37.9569750
27	27C	26	16	13	1.5435155	110.1930641	68.6160066
28	28C	27	26	16	2.3223019	72.5941442	114.9125600
29	29O	27	26	16	1.2182354	126.9844307	-66.8199846
30	30O	28	27	26	1.2201324	158.0650724	-177.6130814
31	31N	27	26	16	1.3724798	106.5015854	113.2811782
32	32H	31	27	26	1.0108073	124.5680354	179.1155658
33	33N	28	27	26	1.3681537	73.2568924	2.8675047
34	34C	33	28	27	1.4512164	121.4948768	-174.2619056
35	35H	34	33	28	1.0944997	110.6894997	-135.6045356
36	36H	34	33	28	1.0908763	107.6967995	-16.6214649
37	37H	34	33	28	1.0966394	111.9869332	102.7504376
38	-	12	6	5	1.2792208	160.4533133	169.9976098

Table S4. Conformation D properties



a/a	Atom	NA	NB	NC	Bond length	Bond angle	Dihedral
1	1C	-	-	-	-	-	-
2	2C	1	-	-	1.3960115	-	-
3	3C	2	1	-	1.3984523	120.2457009	-

(Table S4) contd....

4	4C	3	2	1	1.3960488	119.4019995	0.0549980
5	5C	4	3	2	1.3983812	120.0866429	0.0628501
6	6C	5	4	3	1.4019630	121.2052946	-0.1204022
7	7H	1	2	3	1.0872467	119.0893671	179.9277053
8	8H	2	1	6	1.0864564	119.6945349	179.8725527
9	9H	3	2	1	1.0860792	120.2666552	-179.9254038
10	10H	4	3	2	1.0864454	120.1578368	-179.9127891
11	11H	5	4	3	1.0876838	119.4722530	179.9155418
12	12C	6	5	4	1.5203400	120.5663465	179.1135361
13	13C	12	6	5	1.5596952	113.0041752	118.8456699
14	14C	12	6	5	1.5431978	112.6066473	-115.3713486
15	15H	12	6	5	1.0981659	106.5408952	0.6443803
16	16C	13	12	6	1.5430324	113.8599110	143.4317371
17	17H	13	12	6	1.0949963	109.6661523	23.0864283
18	18H	13	12	6	1.0948372	109.1879993	-92.1932716
19	19C	14	12	6	1.5364435	111.1202892	171.3602549
20	20H	14	12	6	1.0966541	110.3307588	-66.1534582

(Table S4) contd....

21	21H	14	12	6	1.0955492	109.7400023	50.7420598
22	22H	16	13	12	1.0953924	109.1760339	-80.4653389
23	23H	16	13	12	1.0959142	110.2076113	162.9518676
24	24H	19	14	12	1.0956290	109.3334766	-70.0247273
25	25H	19	14	12	1.0942255	109.3050575	173.4486614
26	26C	16	13	12	1.5487856	115.7543908	38.4773357
27	27C	26	16	13	1.5440496	107.7427142	-169.1077164
28	28C	27	26	16	2.3185543	72.6856777	-118.6683784
29	29O	27	26	16	1.2173980	126.2154470	61.7979177
30	30O	28	27	26	1.2205025	157.9883302	179.4504282
31	31N	27	26	16	1.3706361	106.7312095	-118.1189680
32	32H	31	27	26	1.0107201	124.8279926	-179.5991546
33	33N	28	27	26	1.3682227	73.4215410	-0.8950393
34	34C	33	28	27	1.4516350	120.9941676	178.4497062
35	35H	34	33	28	1.0909961	107.6706760	12.8220762
36	36H	34	33	28	1.0943622	110.7583672	131.8078912
37	37H	34	33	28	1.0955866	111.8935795	-106.5087911
38	-	12	6	5	1.2655778	160.3079155	170.4912801