Supplementary Material

Total synthesis of structures proposed for quinocitrinines A and B and their analogs. Microwave energy as efficient tool for generating heterocycles

Victoria Machtey, Hugo E. Gottlieb and Gerardo Byk*

Laboratory of Nano-Biotechnology, Department of Chemistry
Bar Ilan University 52900-Ramat Gan, Israel
E-mail: bykger@mail.biu.ac.il

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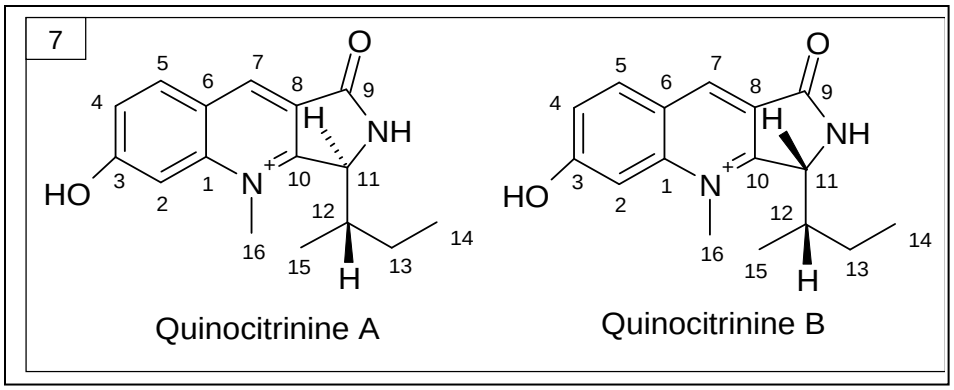

Figure S1. Arbitrary atom numbering of quinocitrinines 7 for NMR assignments.

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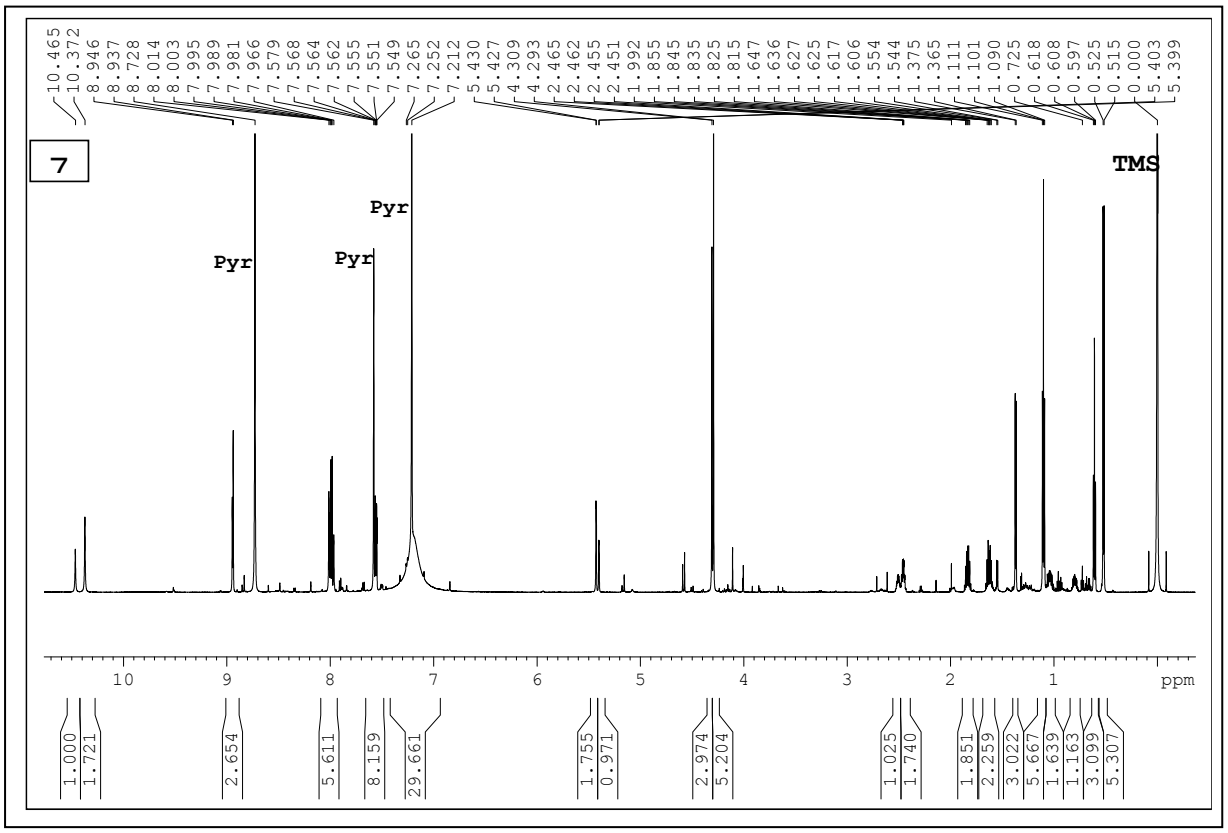

Figure S2. H-NMR of 7 in pyridine

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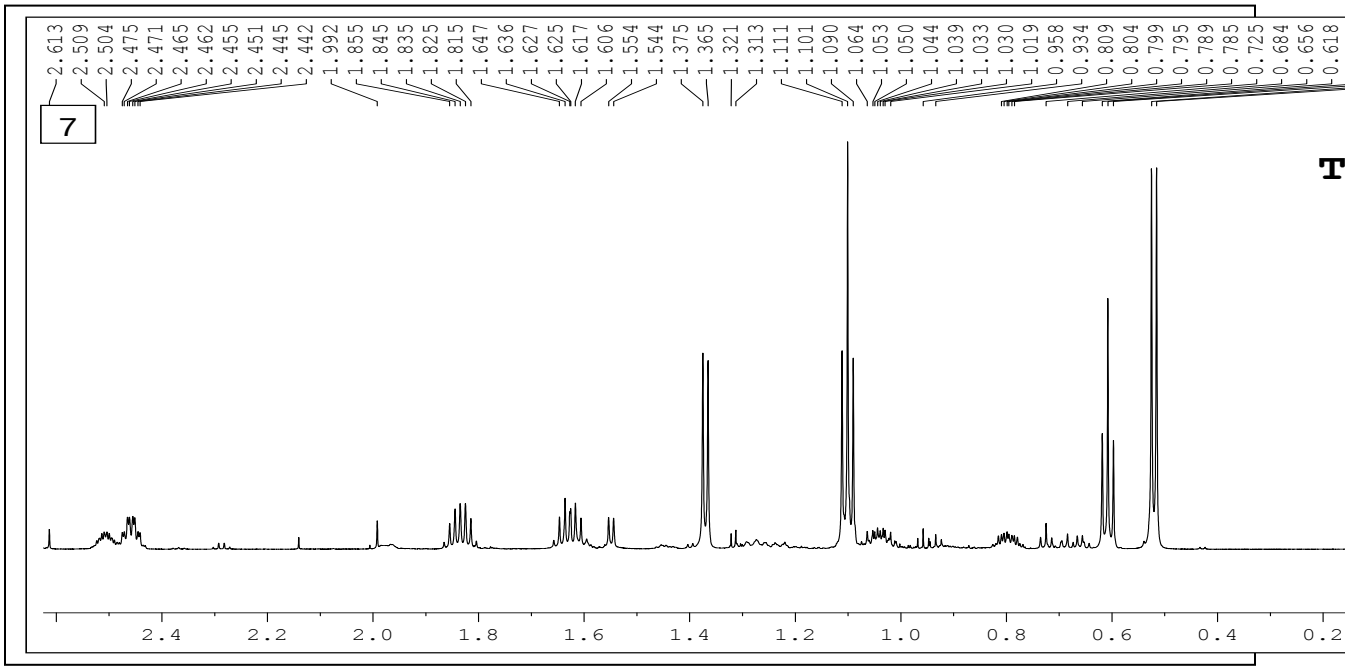

Figure S3. H-NMR of 7 in pyridine (enlarged)

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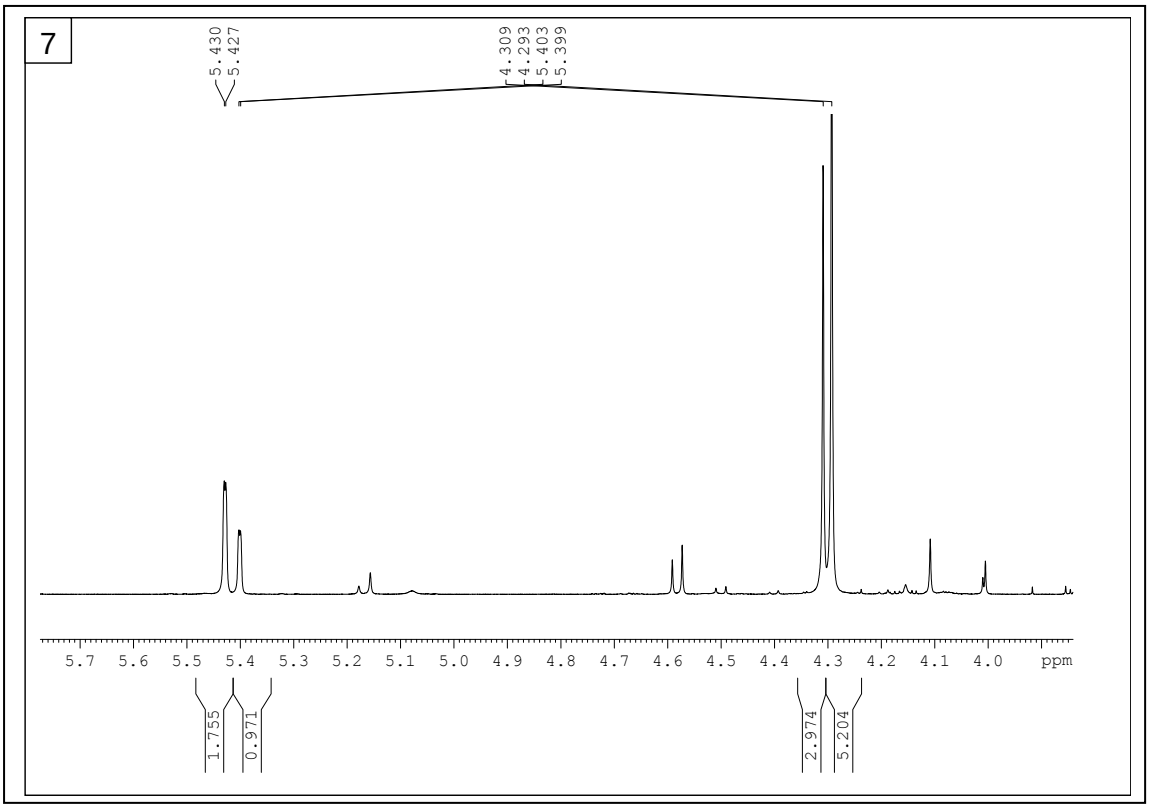

Figure S4. H-NMR of 7 in pyridine (enlarged)

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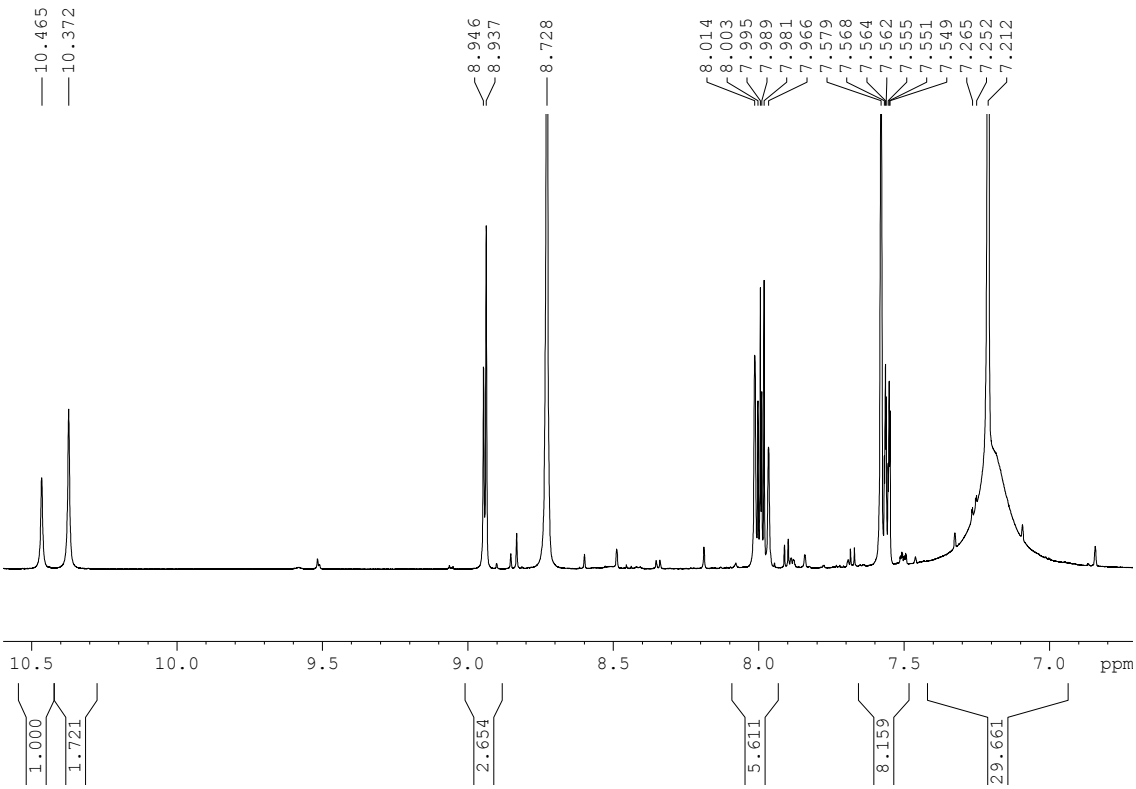

Figure S5. H-NMR of 7 in pyridine (enlarged)

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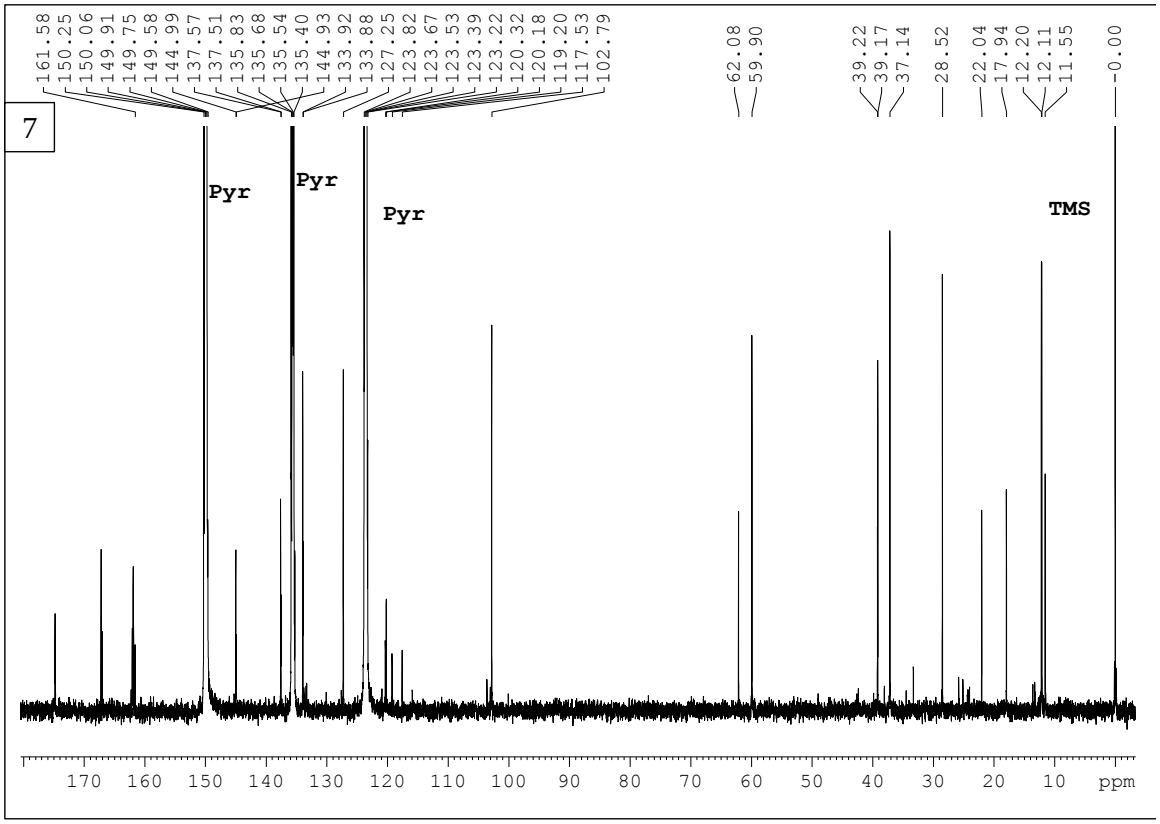

Figure S6. C-NMR of 7 in pyridine

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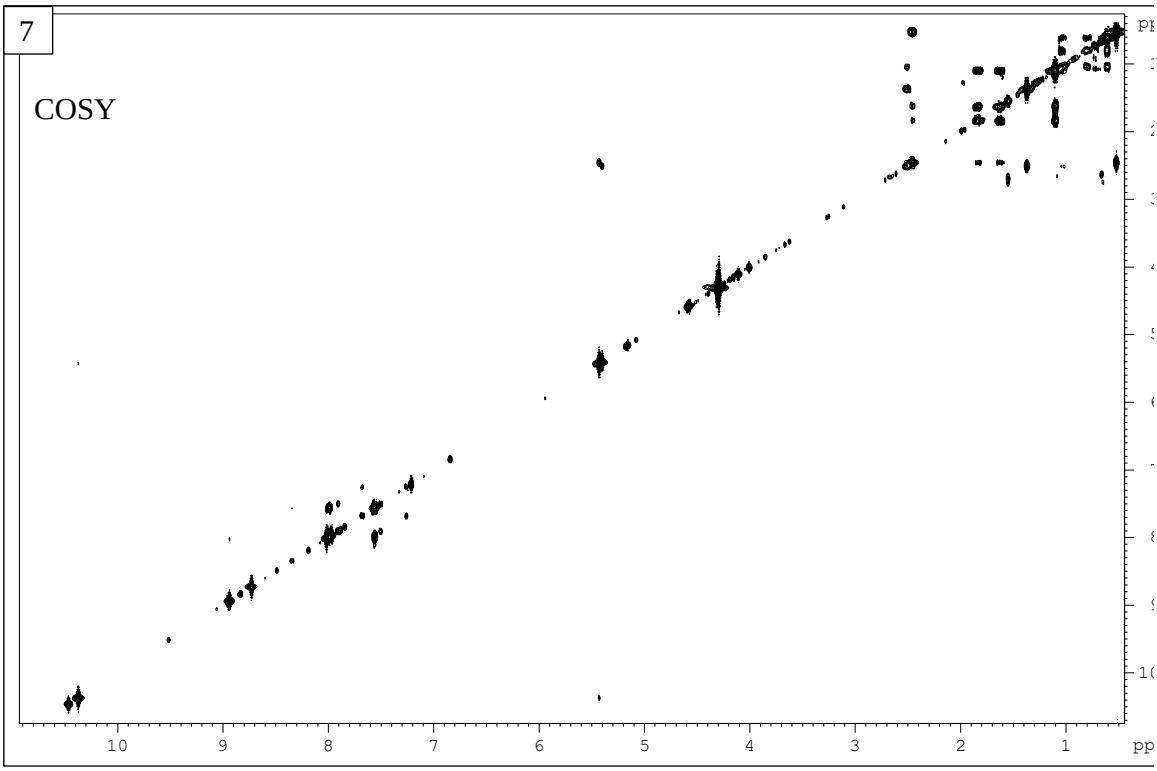

Figure S7. COSY spectrum of 7 in pyridine

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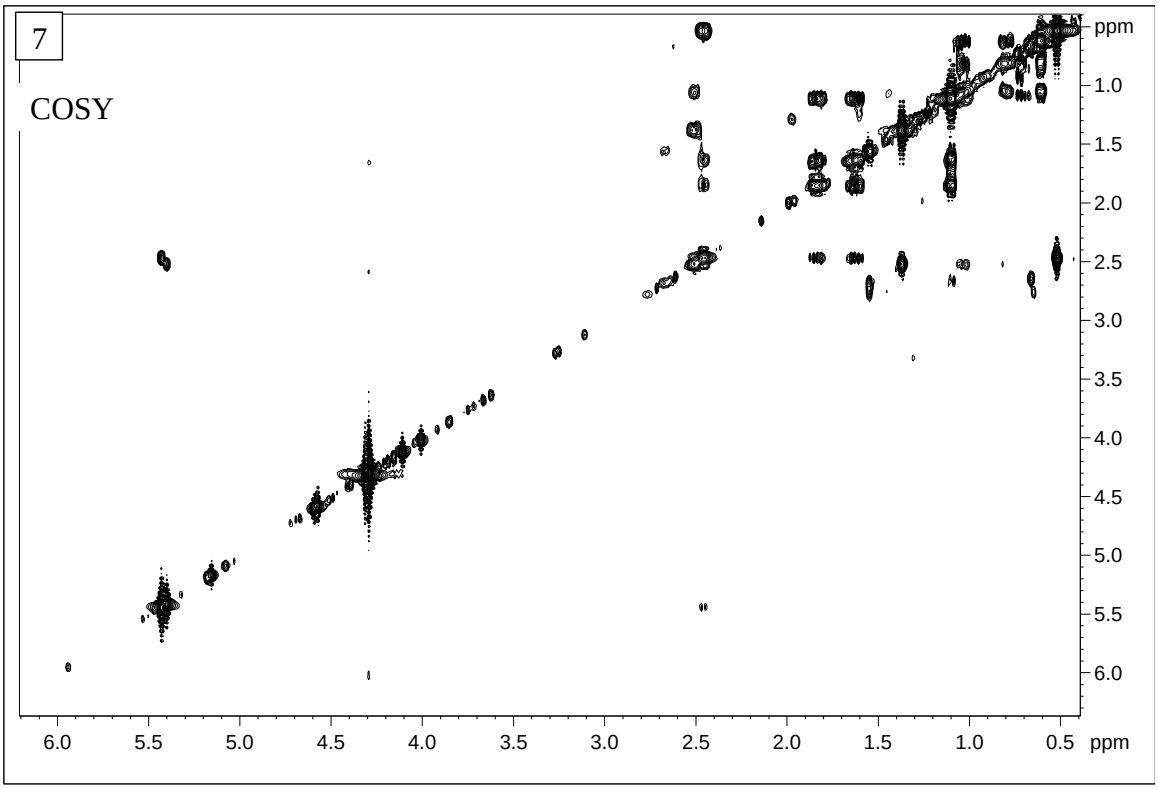

Figure S8. COSY spectrum of 7 in pyridine (enlarged)

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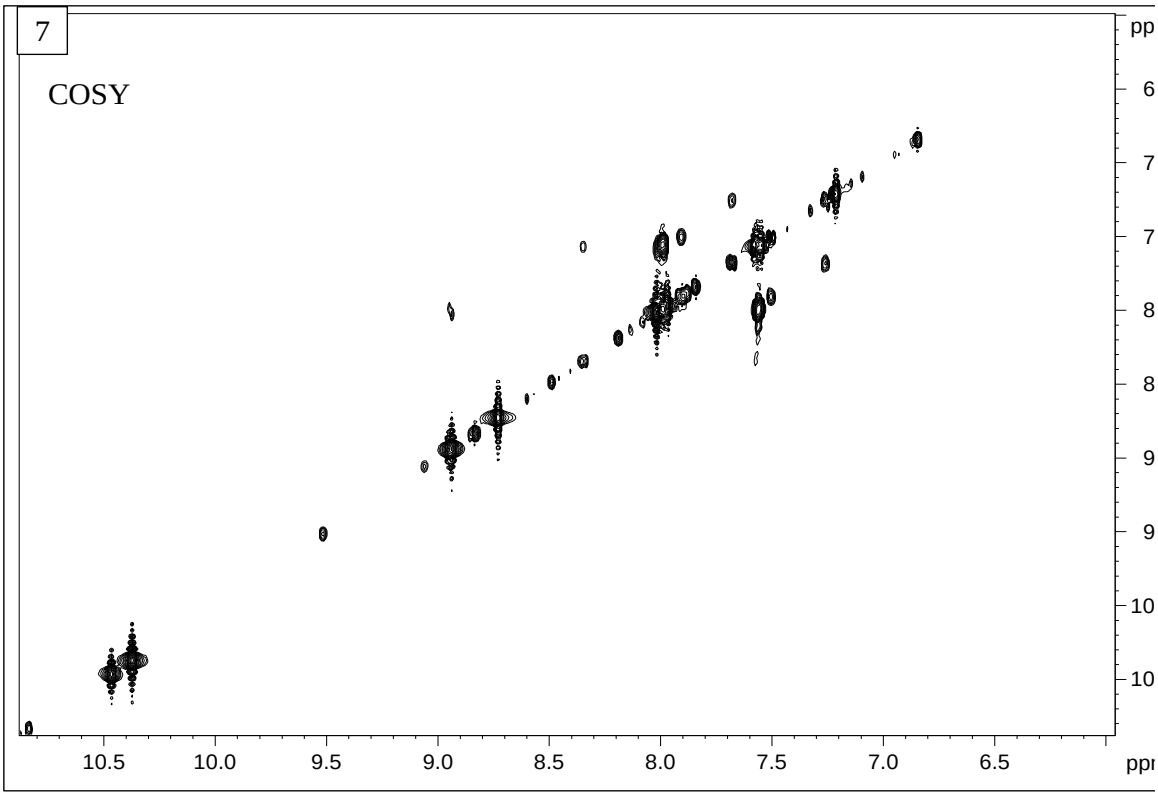

Figure S9. COSY spectrum of 7 in pyridine (enlarged)

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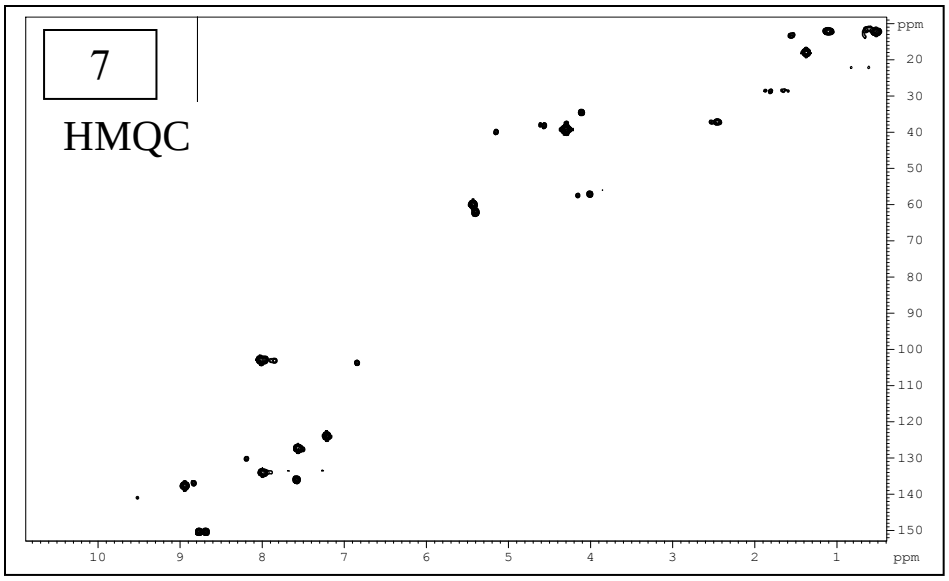

Figure S10. HMQC spectrum of 7 in pyridine

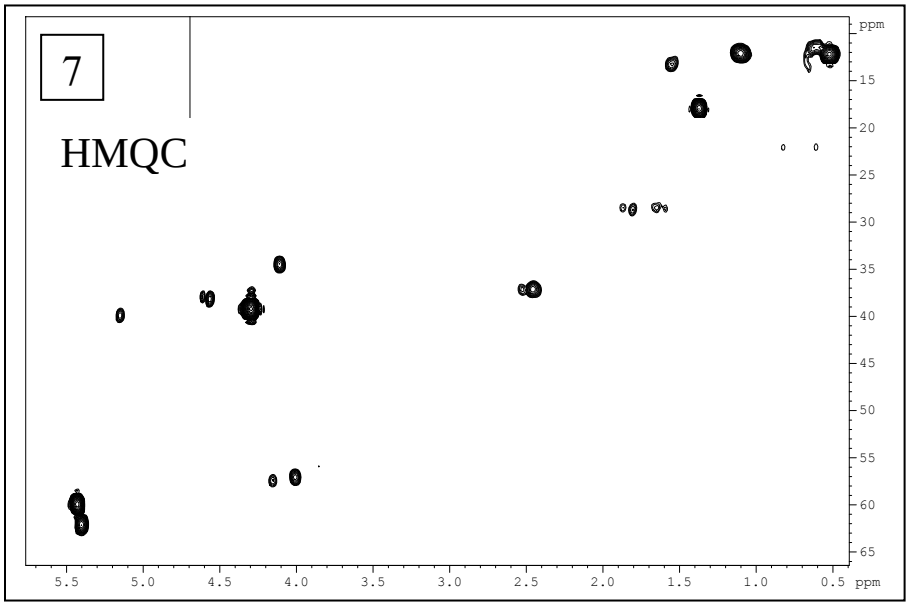

Figure S11. HMQC spectrum of 7 in pyridine (enlarged)

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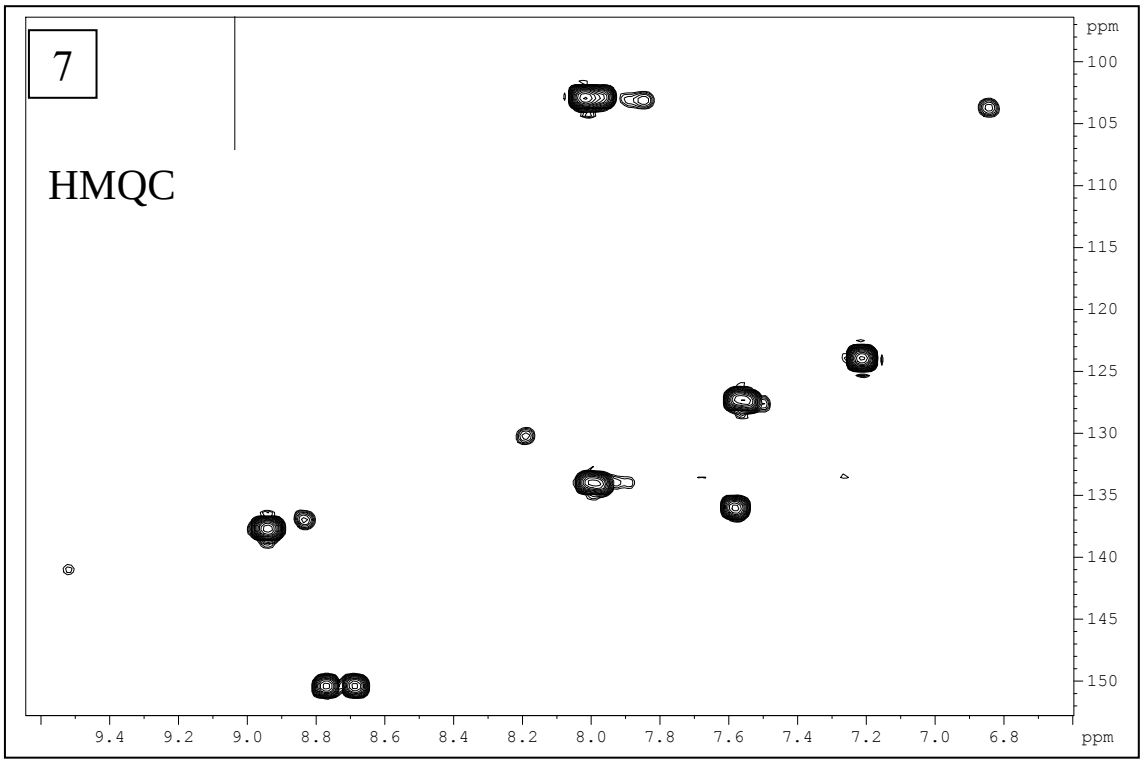

Figure S12. HMQC spectrum of 7 in pyridine (enlarged)

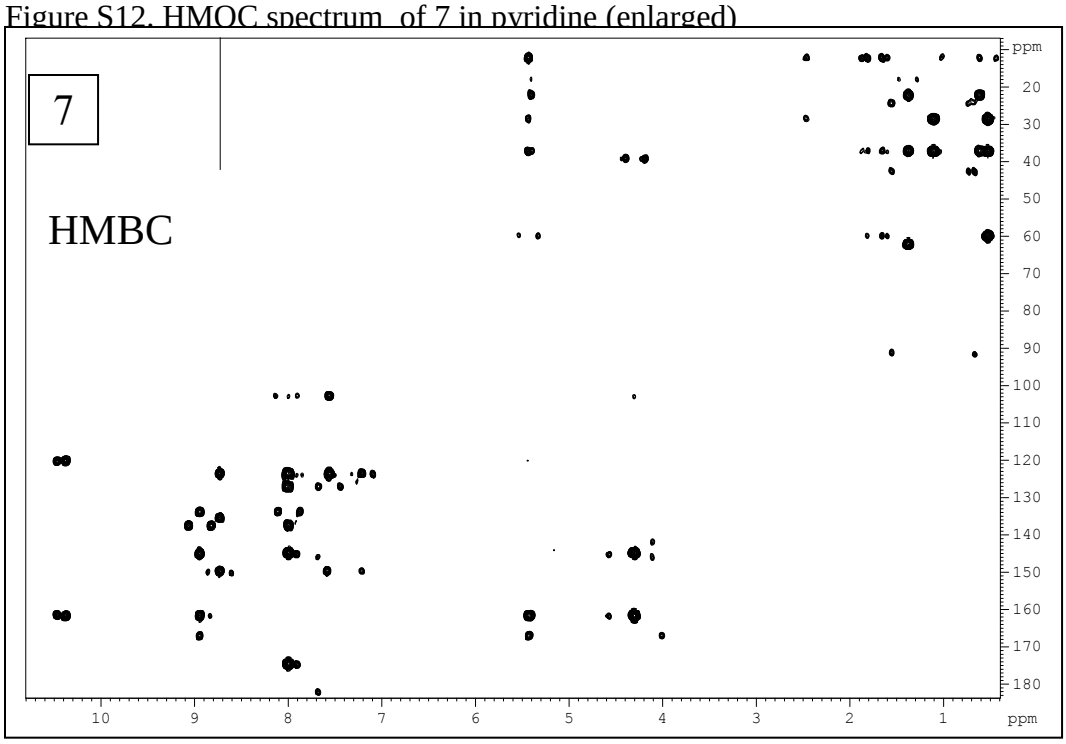

Figure S13. HMBC spectrum of 7 in pyridine

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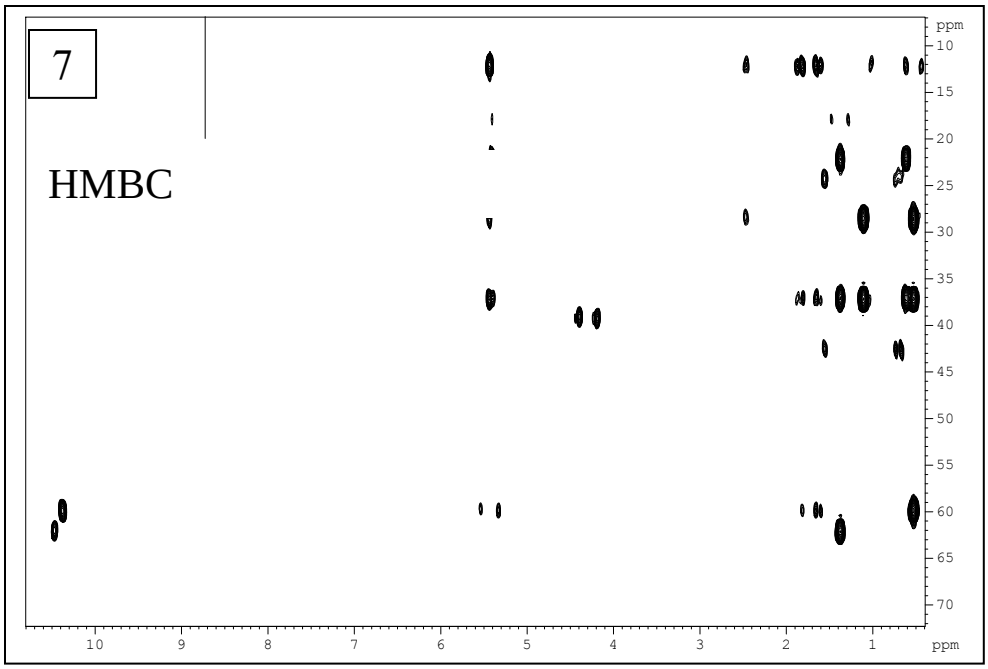

Figure S14. HMBC spectrum of 7 in pyridine (enlarged)

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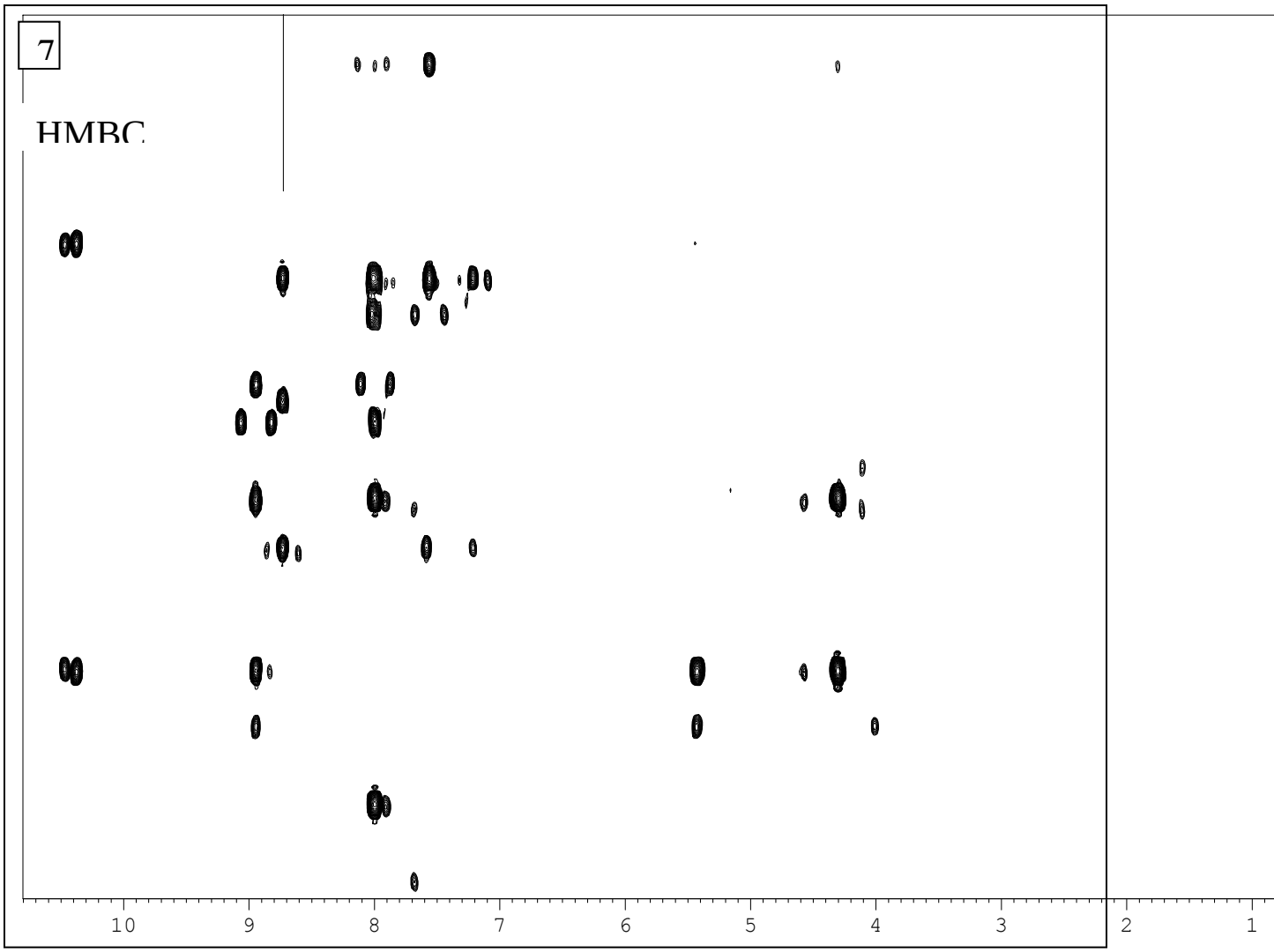

Figure S15. HMBC spectrum of 7 in pyridine (enlarged)

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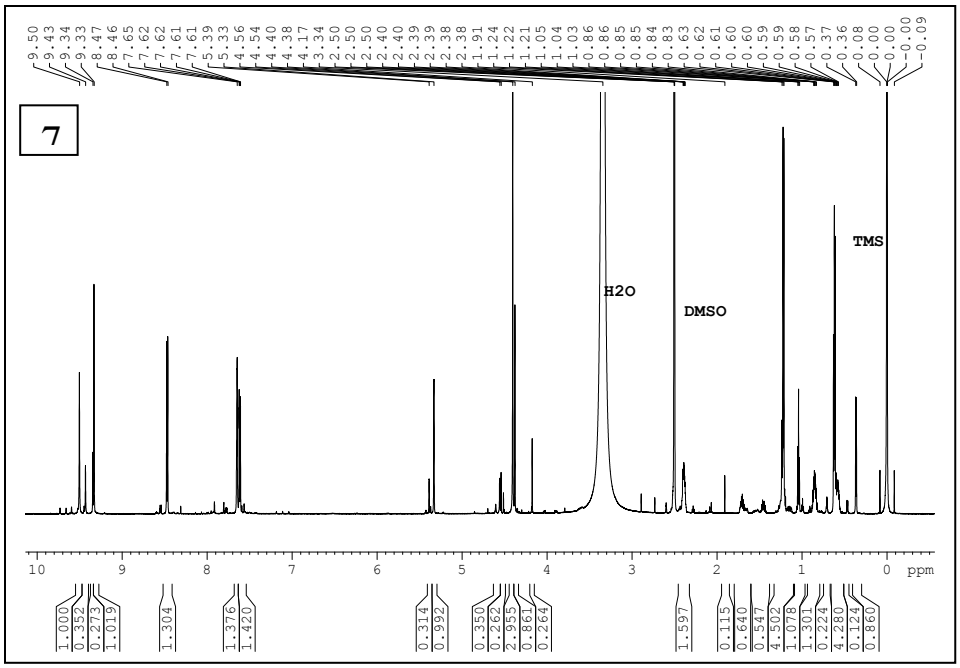

Figure S16. H-NMR of 7 in DMSO

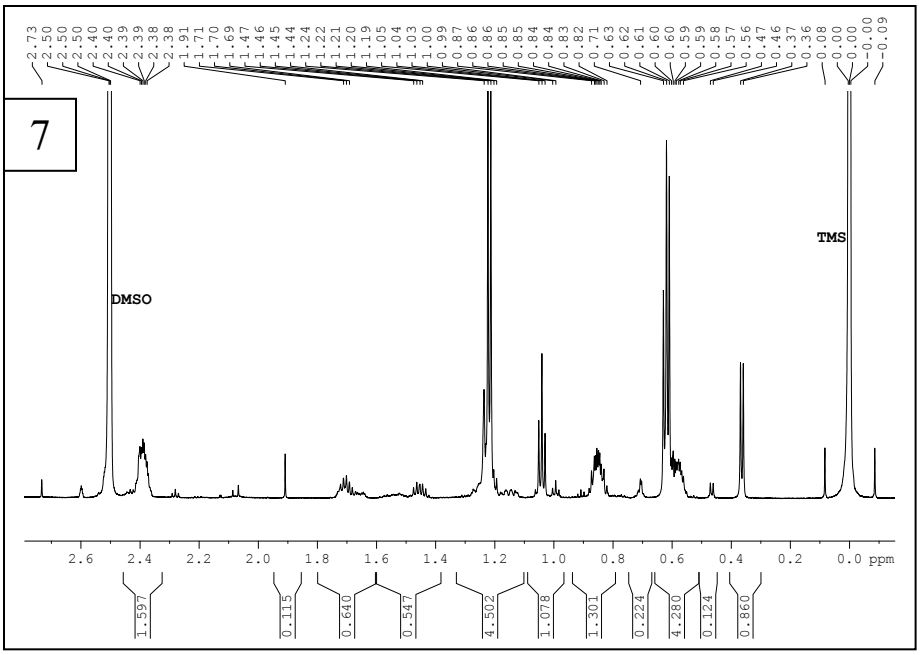

Figure S17. H-NMR of 7 in DMSO (enlarged)

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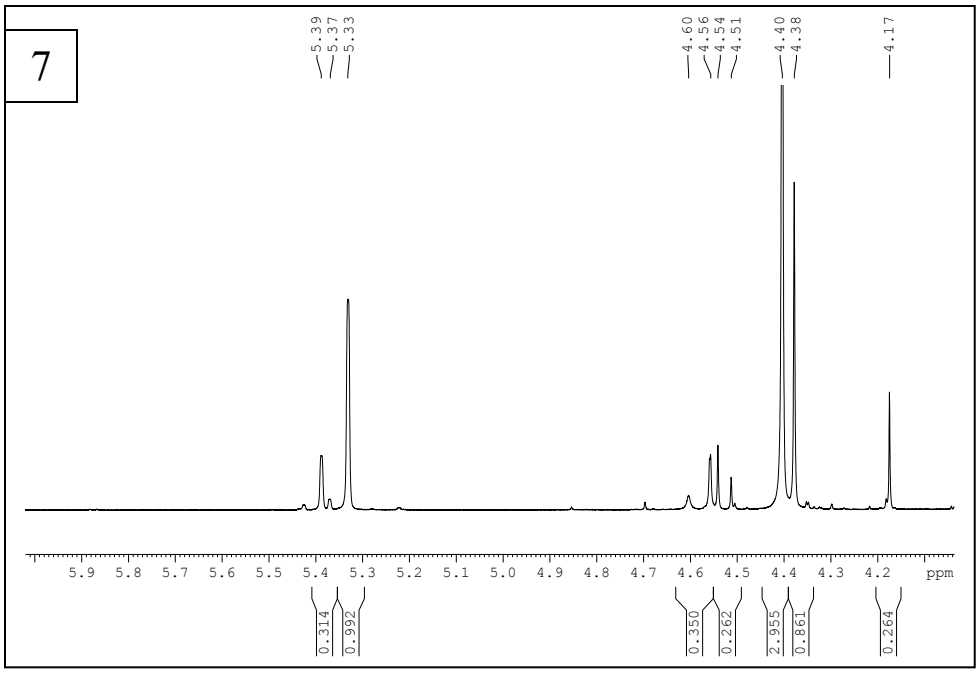

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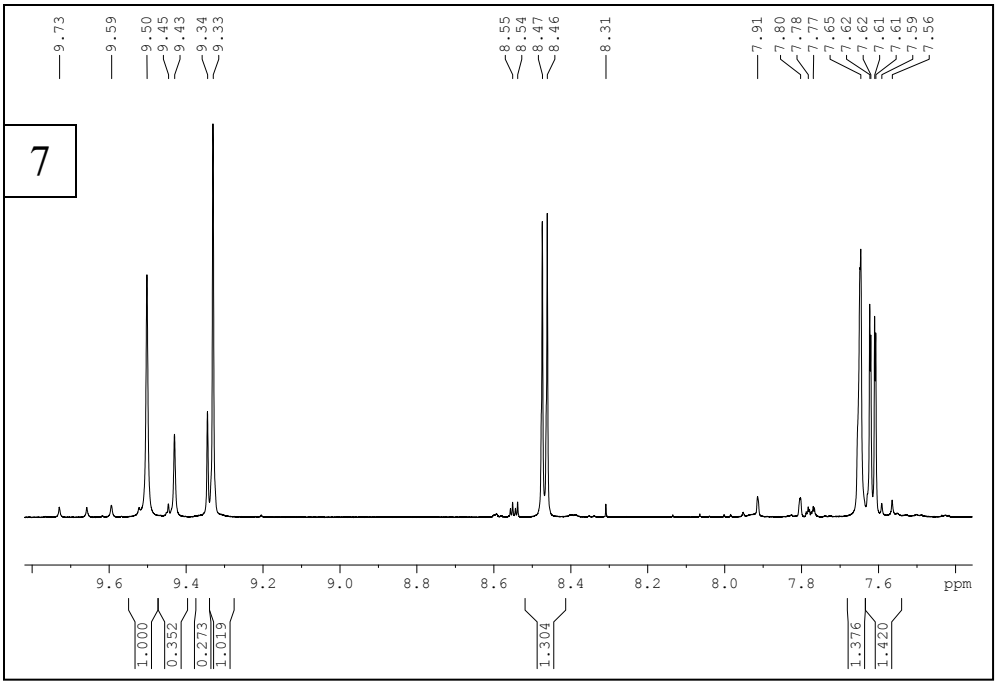

Figure S19. H-NMR of 7 in DMSO (enlarged)

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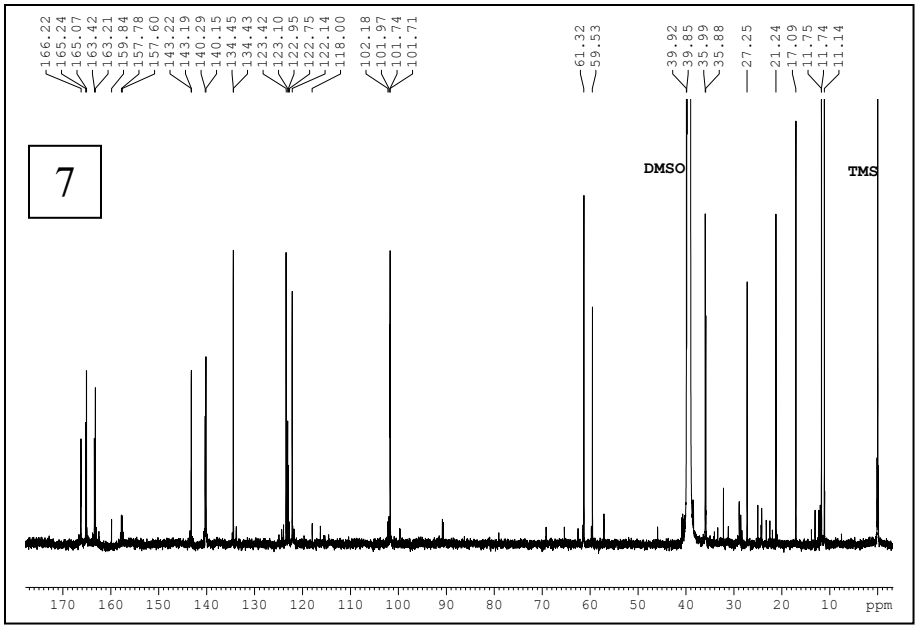

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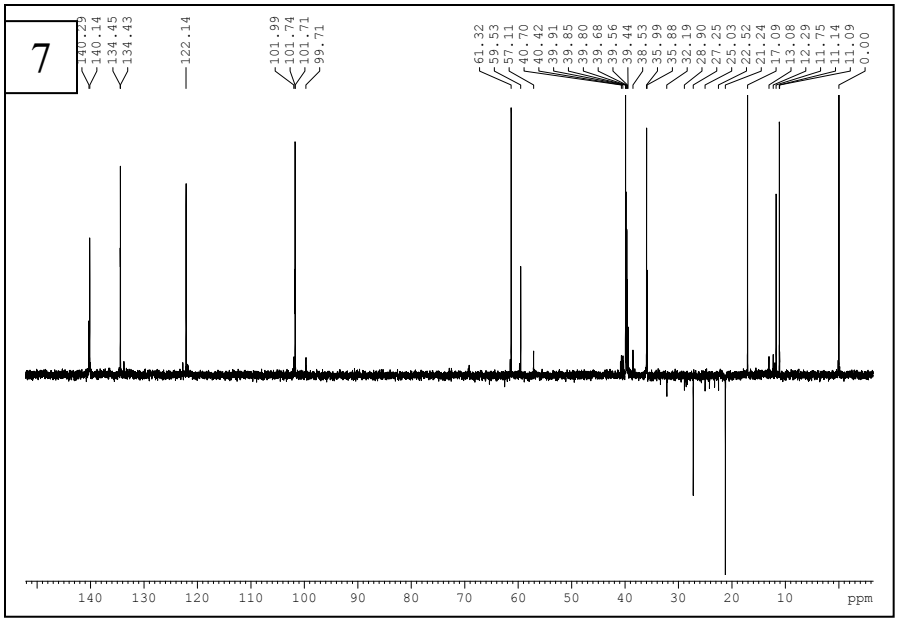

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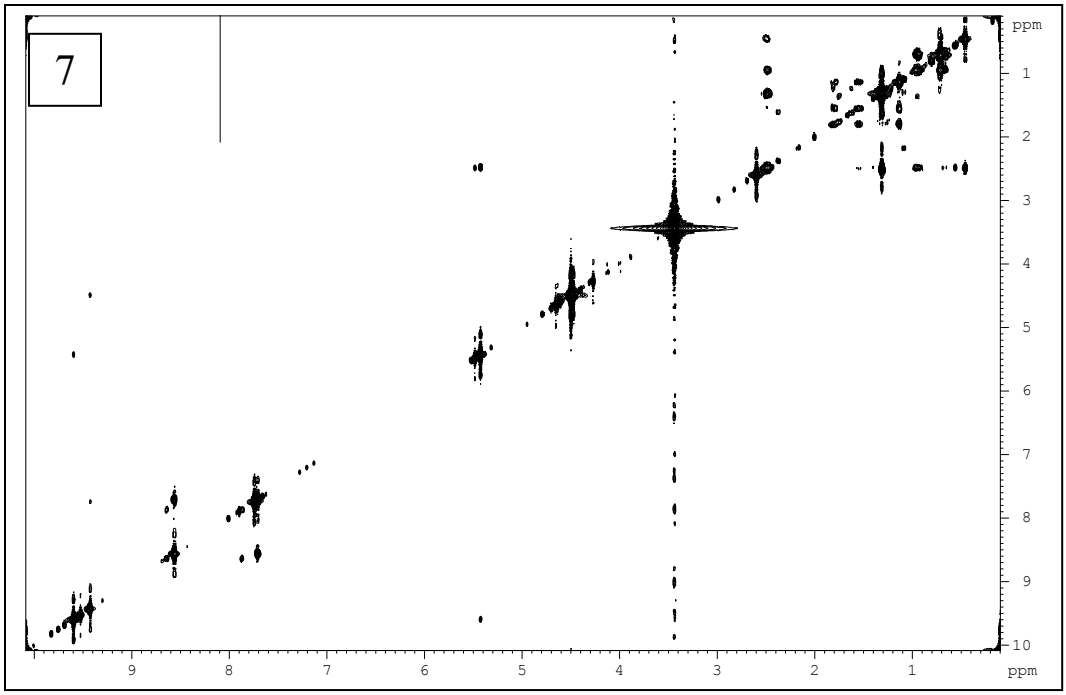

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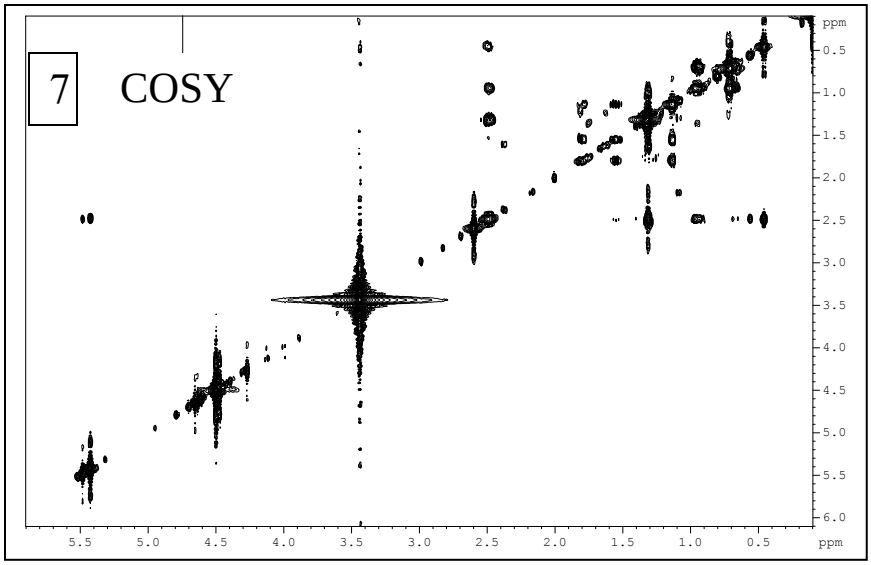

Figure S23. COSY spectrum of 7 in DMSO (enlarged)

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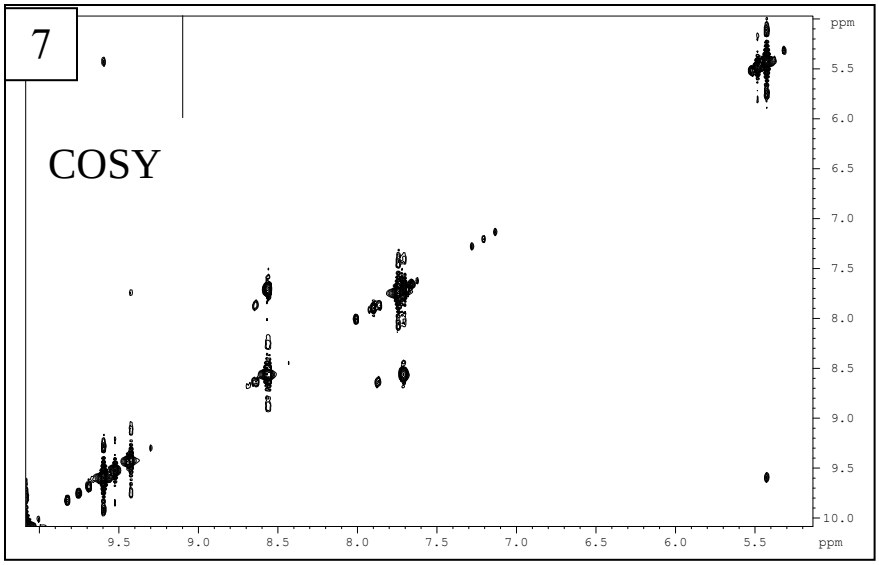

Figure S24. COSY spectrum of 7 in DMSO (enlarged)

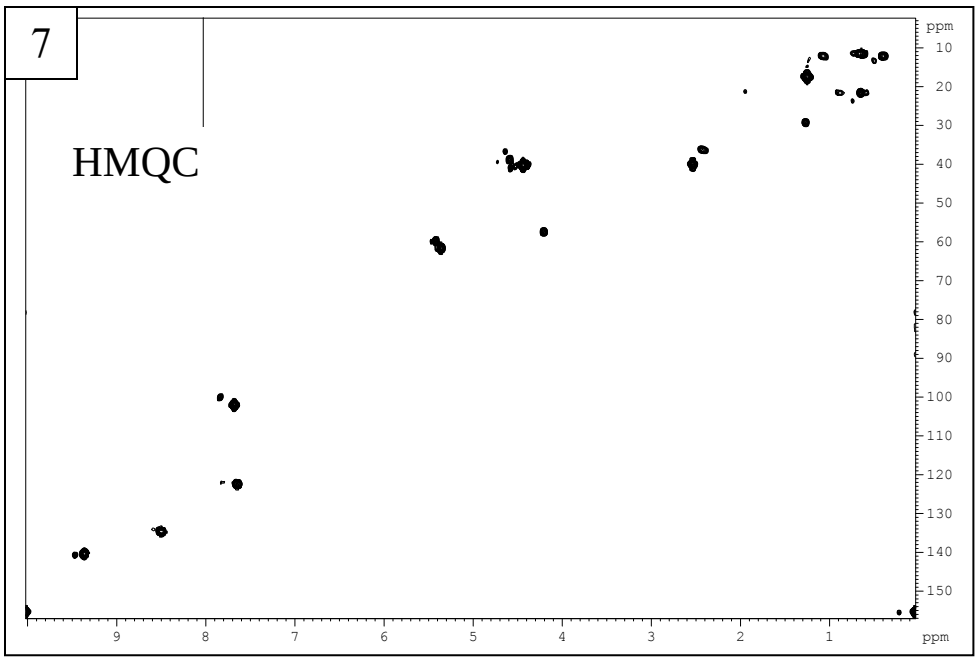

Figure S25. HMQC spectrum of 7 in DMSO (enlarged)

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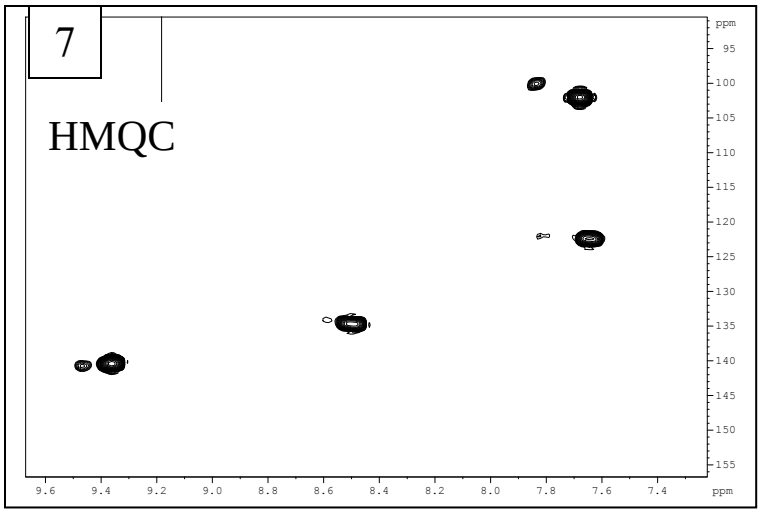

Figure S26. HMQC spectrum of 7 in DMSO (enlarged)

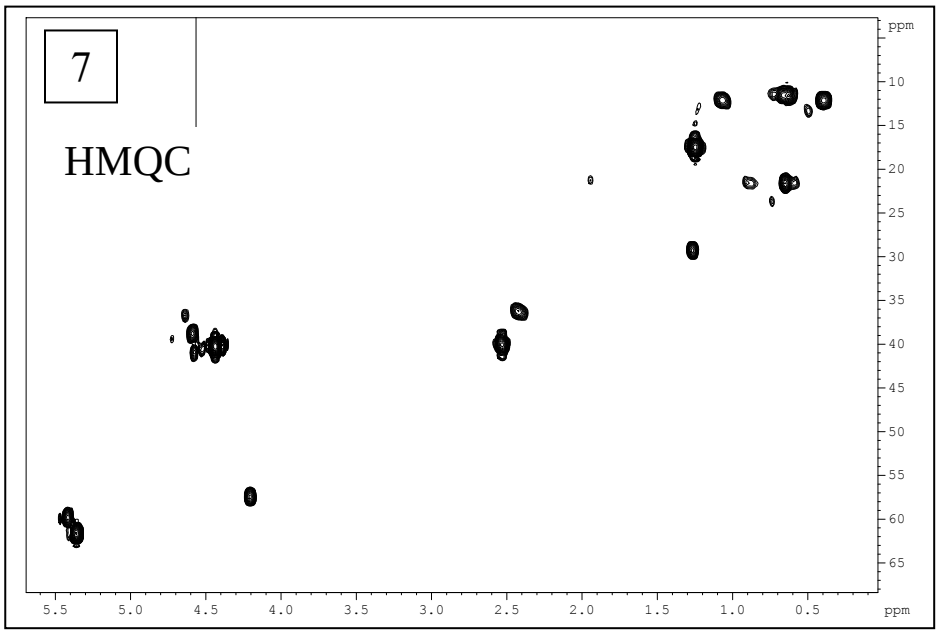

Figure S27. HMQC spectrum of 7 in DMSO (enlarged)

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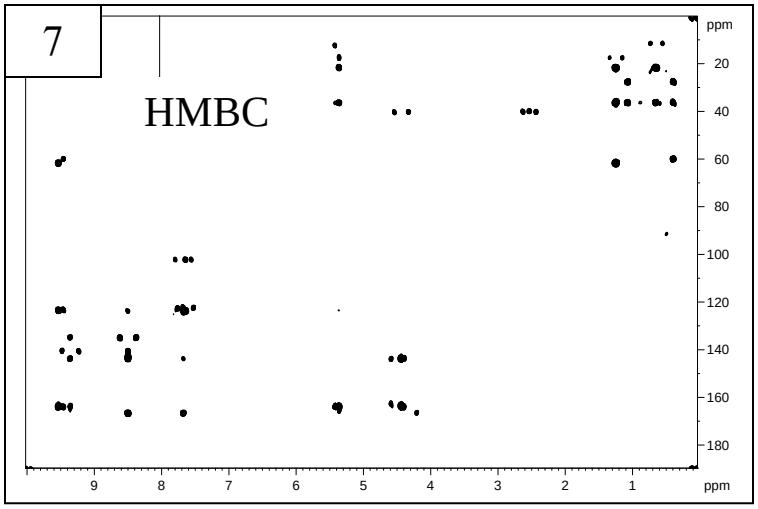

Figure S28. HMBC spectrum of 7 in DMSO

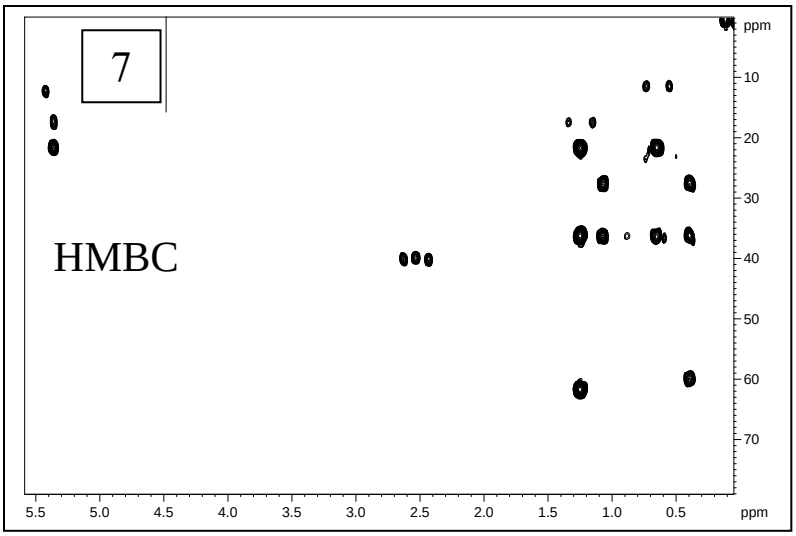

Figure S29. HMBC spectrum of 7 in DMSO (enlarged)

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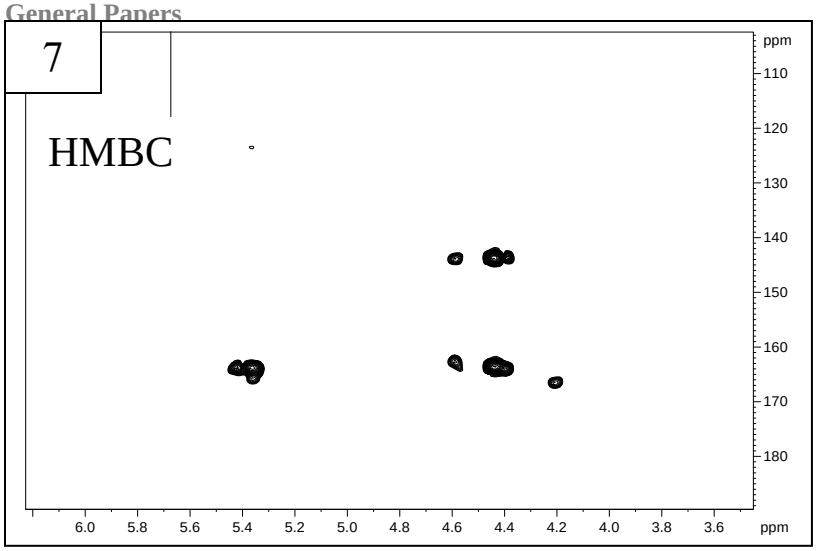

Figure S30. HMBC spectrum of 7 in DMSO (enlarged)

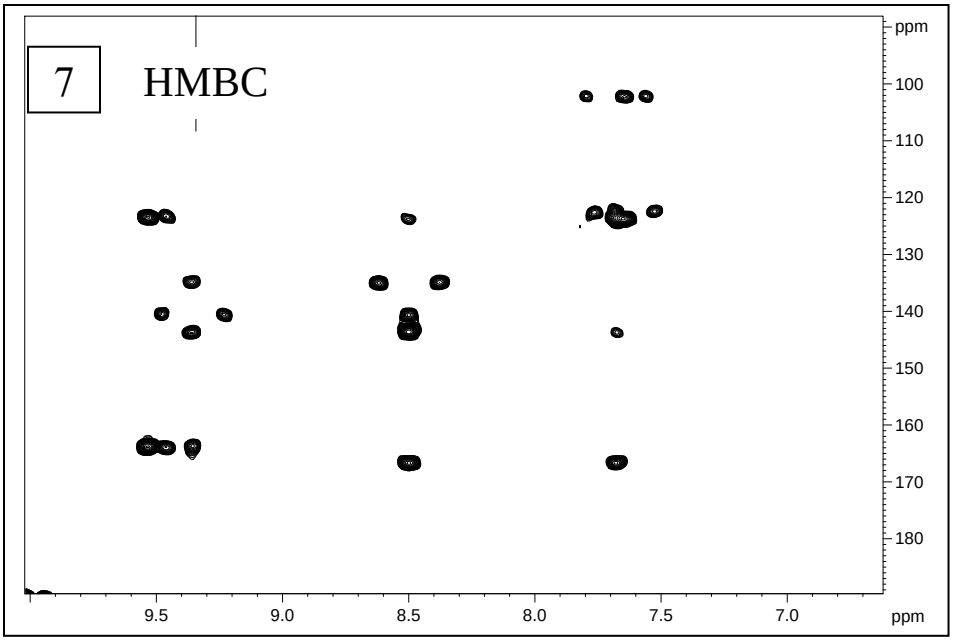

Figure S31. HMBC spectrum of 7 in DMSO (enlarged)

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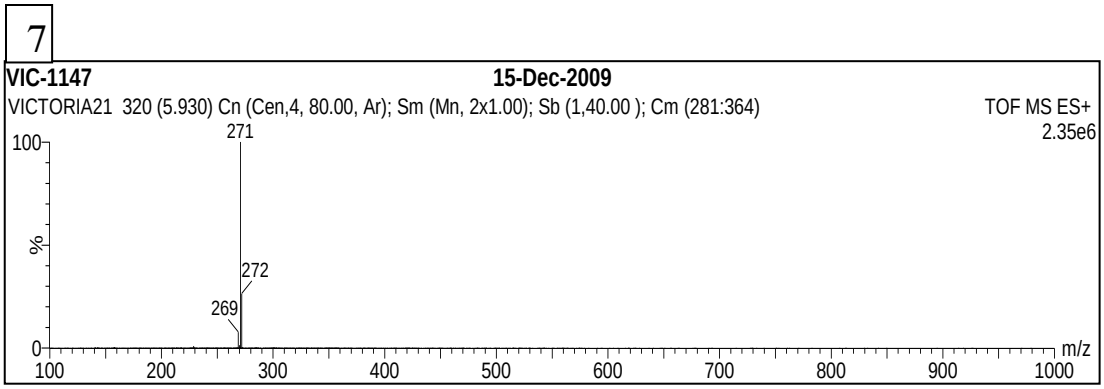


Figure S32. QTOF-MS of 7

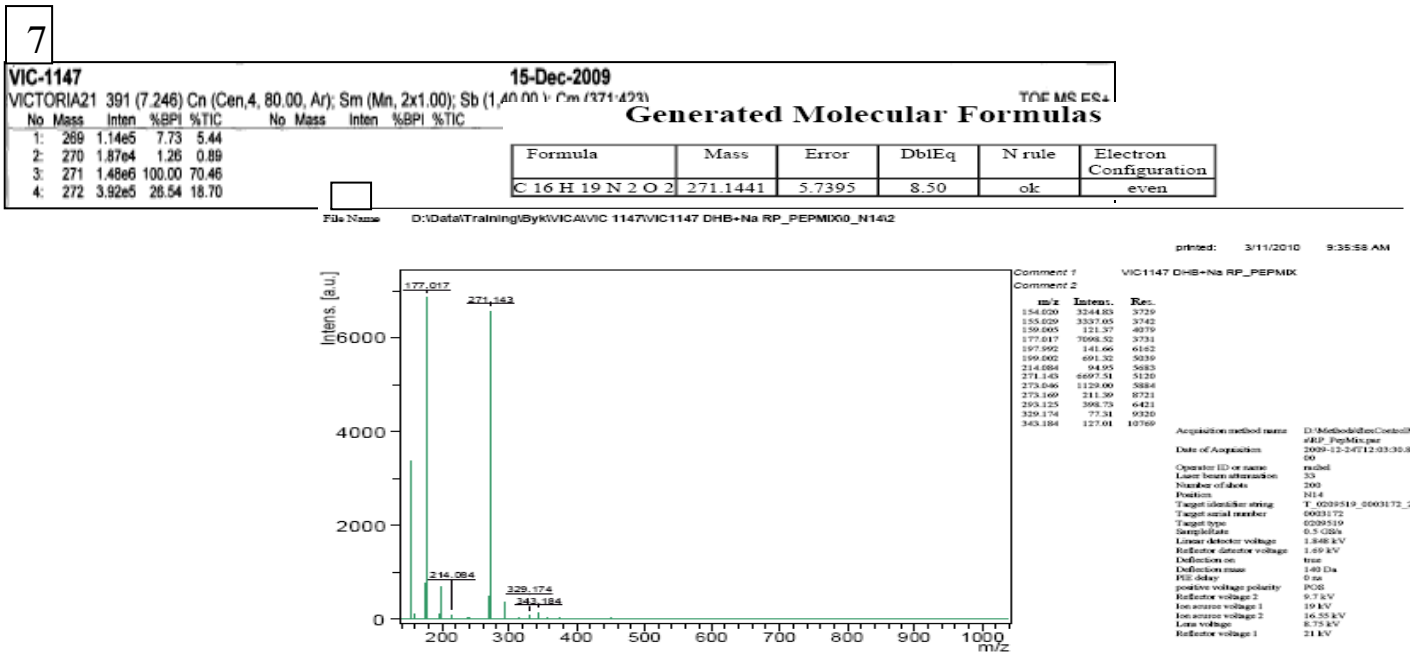
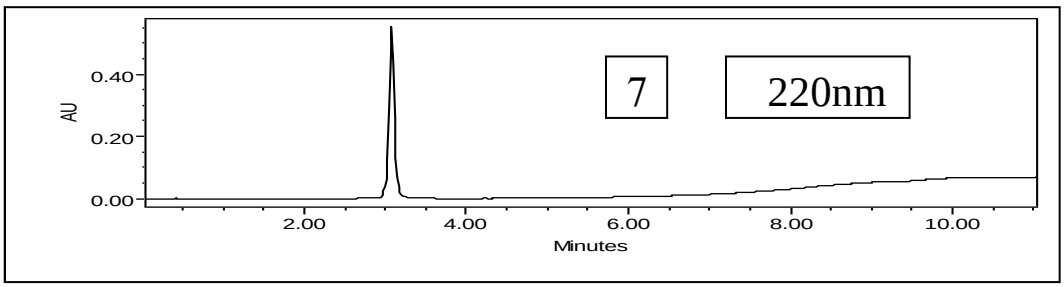


Figure S33. HR-MALDI-TOF MS of compound 7



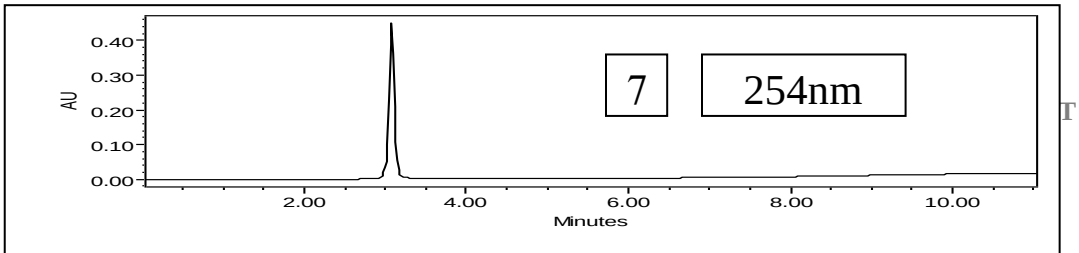


Figure S34. HPLC of compound 7

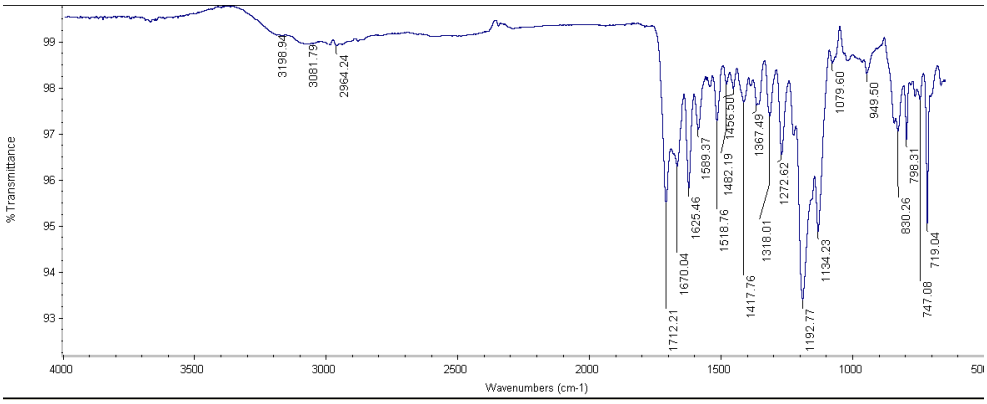


Figure S35. IR spectrum of compound 7

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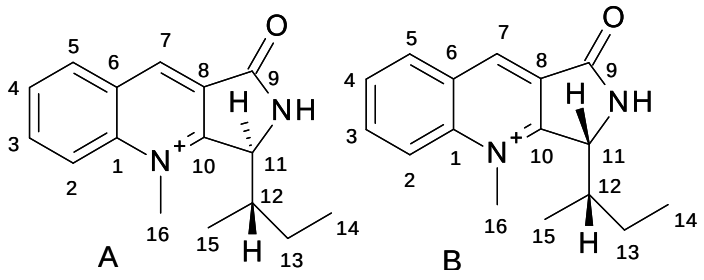


Figure S36. Arbitrary atom numbering of compound 6b for NMR assignments.

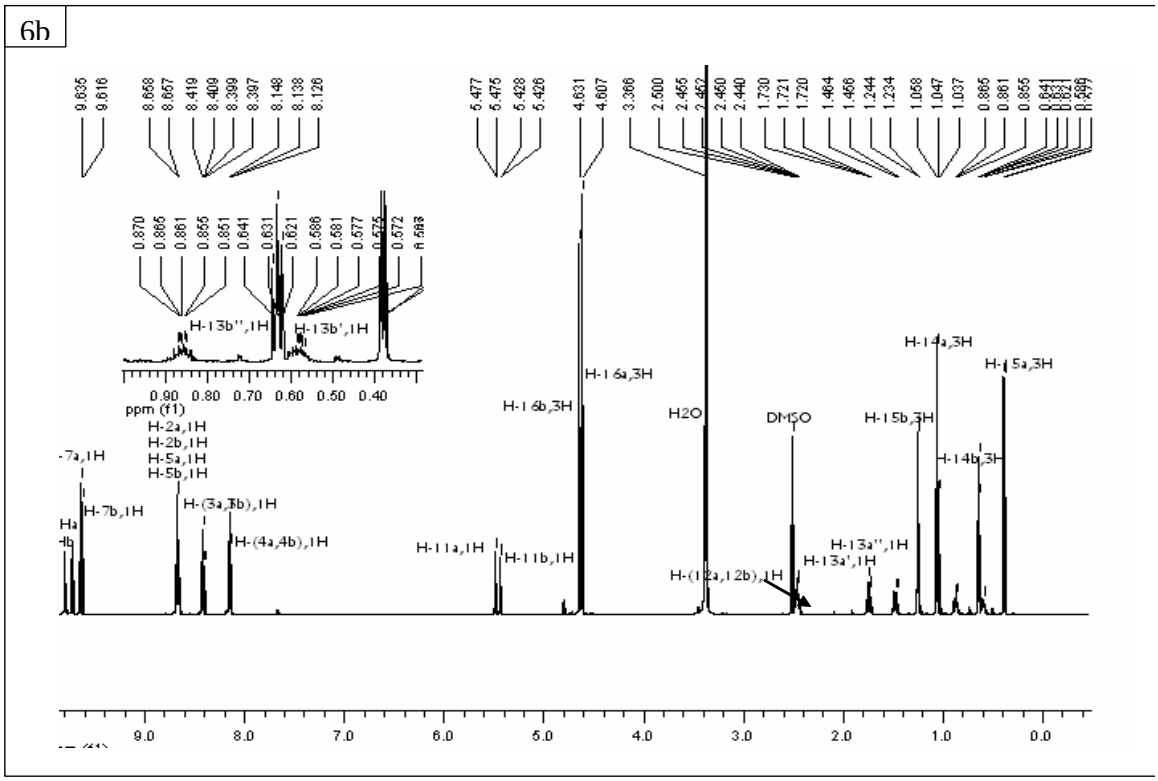


Figure S37. H NMR of compound 6b in DMSO

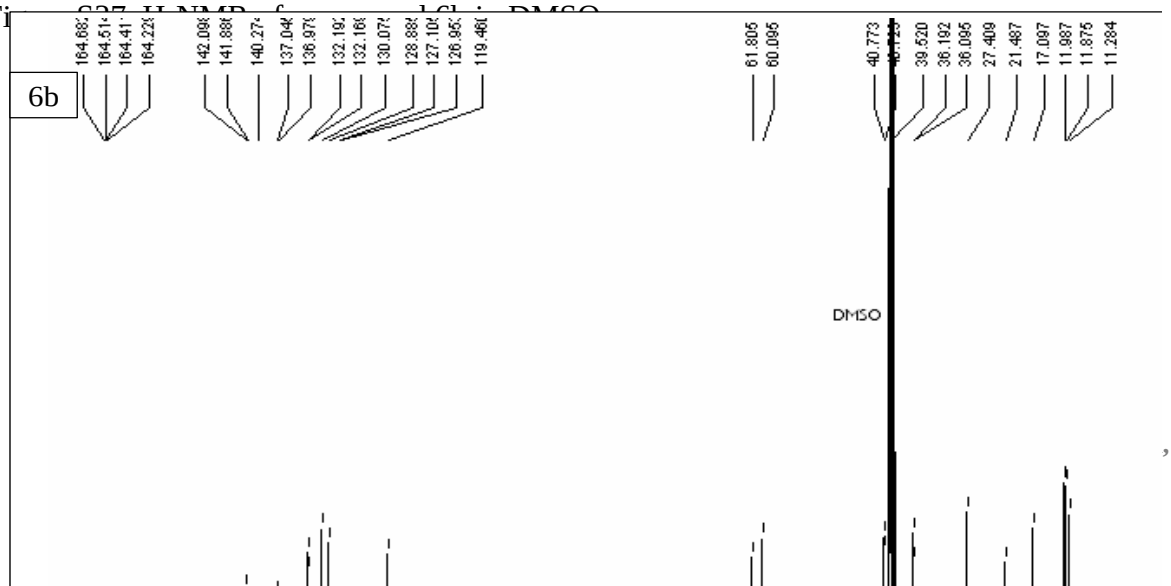
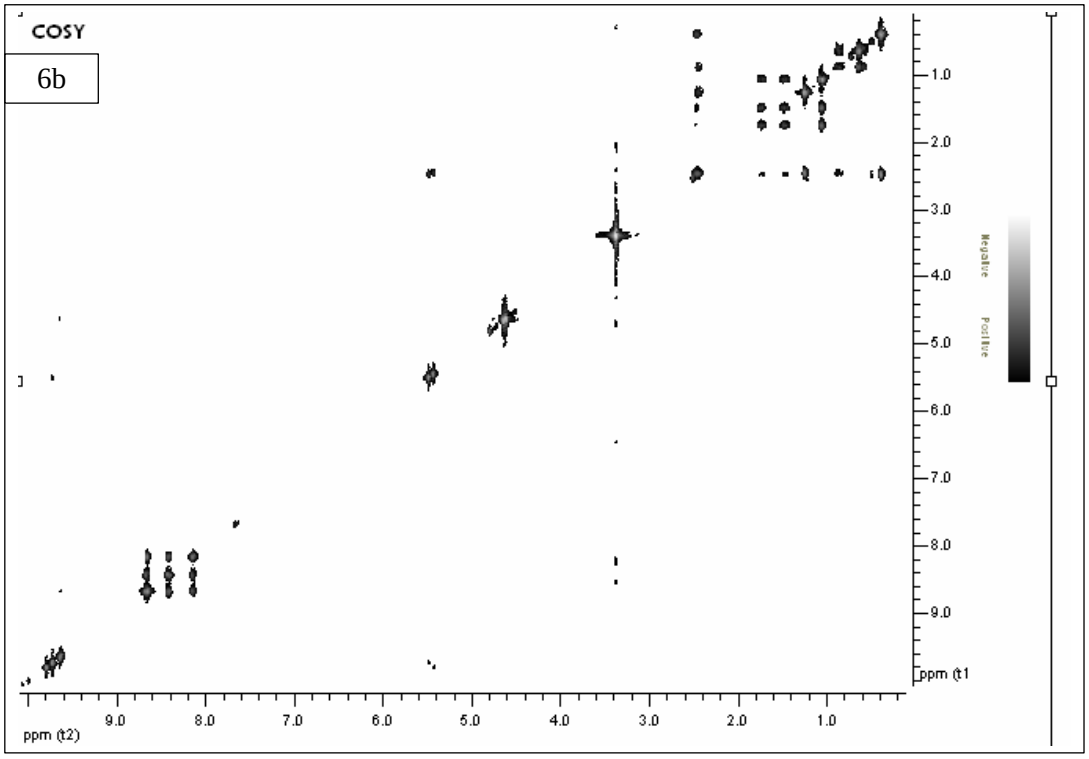


Figure S38. C-NMR of compound 6b in DMSO



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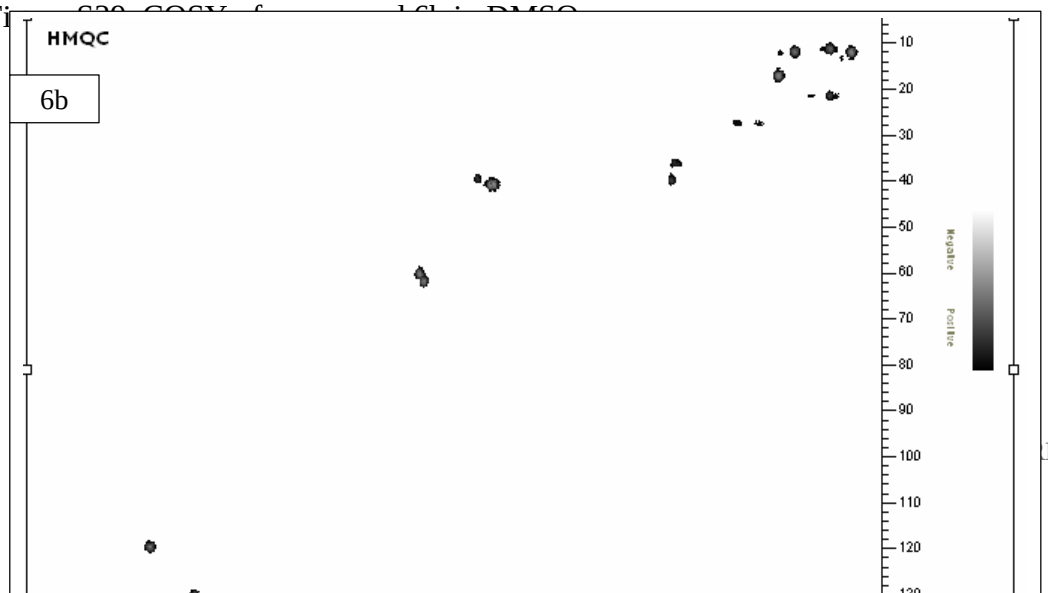


Figure S40. HMQC of compound 6b in DMSO

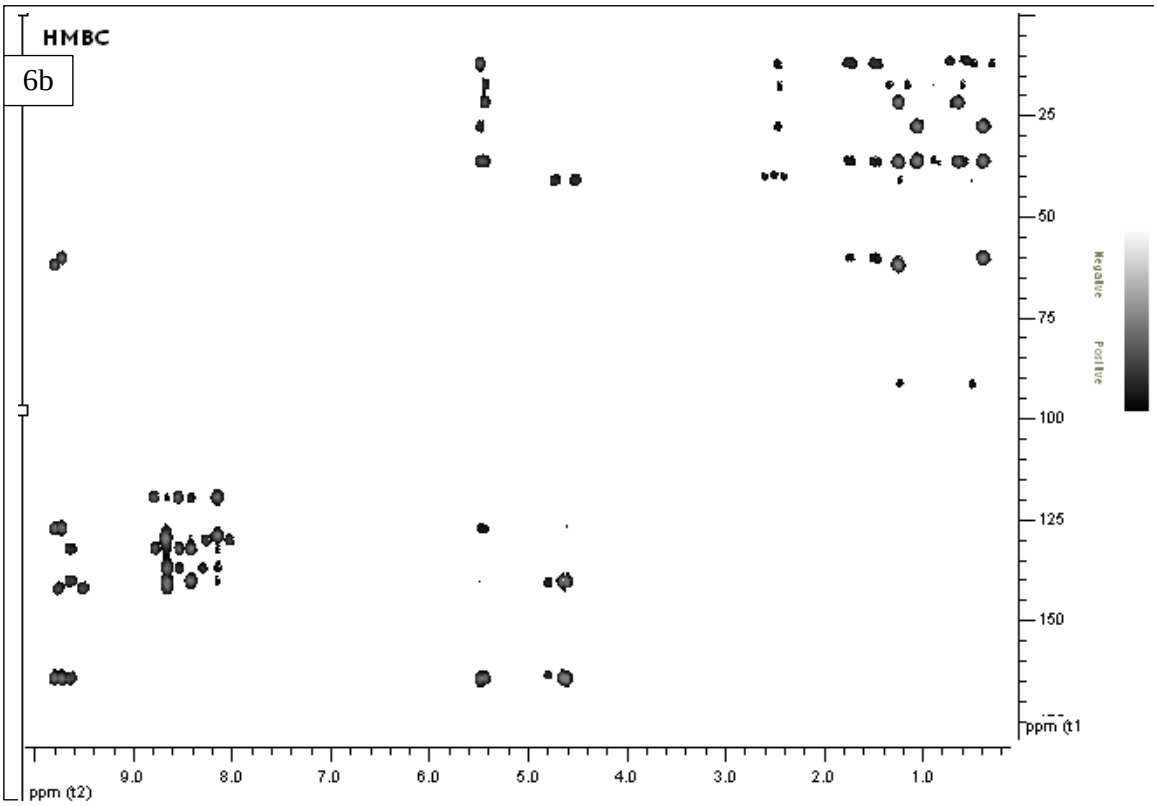
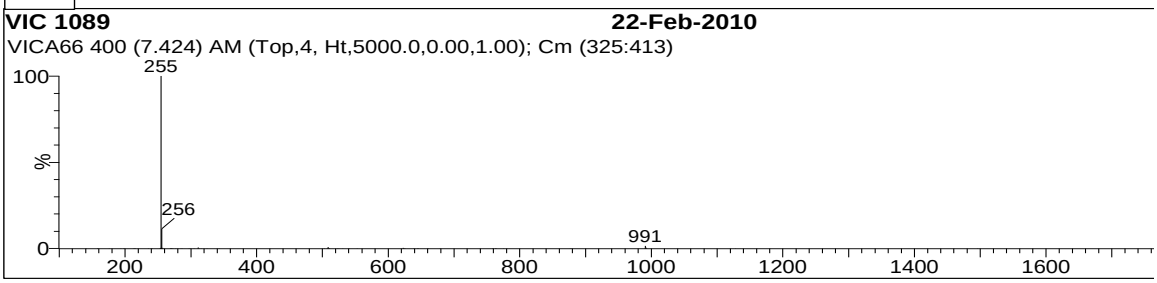


Figure S41. HMBC of compound 6b in DMSO

6b



6b

VIC 1089 22-Feb-2010

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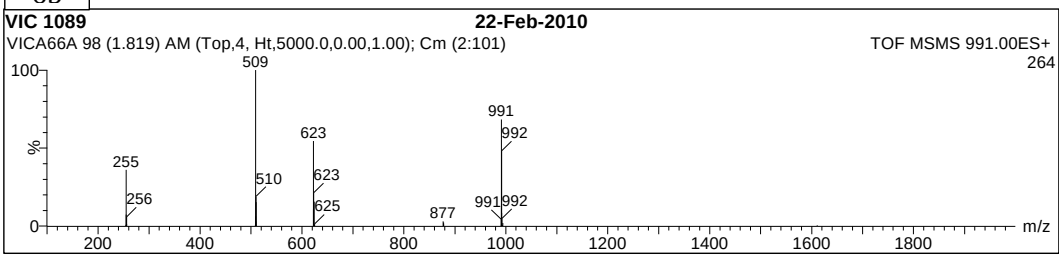
2:	255	1.98e2	0.20	0.17															
3:	255	2.76e2	0.28	0.24															
4:	255	9.84e4	100.00	85.32															
5:	255	1.74e2	0.18	0.15															
6:	256	1.11e4	11.28	9.63															
7:	257	2.09e2	0.21	0.18															
8:	311	5.10e2	0.52	0.44															
9:	509	7.45e2	0.76	0.65															

Figure S42. QTOF-MS of compound 6b

6b



6b

VIC 1089 22-Feb-2010

VICA66A 98 (1.819) AM (Top,4, Ht,5000.0,0.00,1.00); Cm (2:101) TOF MSMS 991.00ES+

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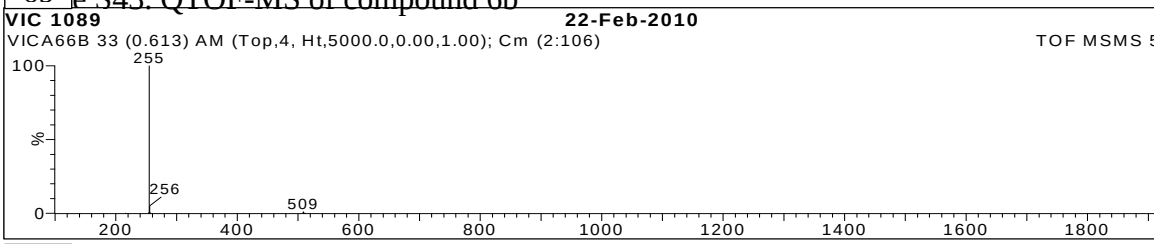
2:	255	9.50e1	35.98	7.84																		
3:	255	1.90e1	7.20	1.57																		
4:	256	1.50e1	5.68	1.24																		
5:	256	3.00e0	1.14	0.25																		
6:	509	2.00e0	0.76	0.17																		
7:	509	1.60e1	6.06	1.32																		
8:	509	2.64e2	100.00	21.80																		
9:	509	7.00e0	2.65	0.58																		
10:	510	8.00e0	3.03	0.66																		
11:	510	4.00e1	15.15	3.30																		
12:	510	5.00e1	18.94	4.13																		
13:	623	2.80e1	10.61	2.31																		
14:	623	1.44e2	54.55	11.89																		
15:	623	5.60e1	21.21	4.62																		
16:	623	7.00e0	2.65	0.58																		
17:	624	4.10e1	15.53	3.39																		
18:	625	3.00e0	1.14	0.25																		
19:	877	8.00e0	3.03	0.66																		
20:	878	3.00e0	1.14	0.25																		
21:	878	6.00e0	2.27	0.50																		
22:	991	1.10e1	4.17	0.91																		
23:	991	1.80e2	68.18	14.86																		
24:	991	3.20e1	12.12	2.64																		
25:	991	2.00e0	0.76	0.17																		
26:	992	2.20e1	8.33	1.82																		
27:	992	1.27e2	48.11	10.49																		
28:	992	1.20e1	4.55	0.99																		
29:	993	2.00e0	0.76	0.17																		
30:	994	5.00e0	1.89	0.41																		
31:	1611	1.00e0	0.38	0.08																		

6b

e S43. QTOF-MS of compound 6b



6b

VIC 1089 22-Feb-2010

VICA66B 33 (0.613) AM (Top,4, Ht,5000.0,0.00,1.00); Cm (2:106) TOF MSM

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No
1:	215	1.00e0	0.02	0.02																
2:	254	3.00e0	0.06	0.06																
3:	254	2.00e0	0.04	0.04																
4:	254	2.00e0	0.04	0.04																
5:	254	4.00e0	0.08	0.07																
6:	254	3.00e0	0.06	0.06																
7:	254	8.00e0	0.16	0.15																
8:	254	4.00e0	0.08	0.07																
9:	255	1.20e1	0.24	0.22																
10:	255	4.90e3	100.00	91.07																
11:	255	3.60e1	0.73	0.67																
12:	255	6.00e0	0.12	0.11																
13:	255	3.00e0	0.06	0.06																
14:	256	2.00e0	0.04	0.04																
15:	256	2.40e2	4.90	4.46																
16:	257	5.00e0	0.10	0.09																
17:	257	1.70e1	0.35	0.32																
18:	509	5.10e1	1.04	0.95																
19:	509	5.20e1	1.06	0.97																

Figure S44. QTOF-MS of compound 6b

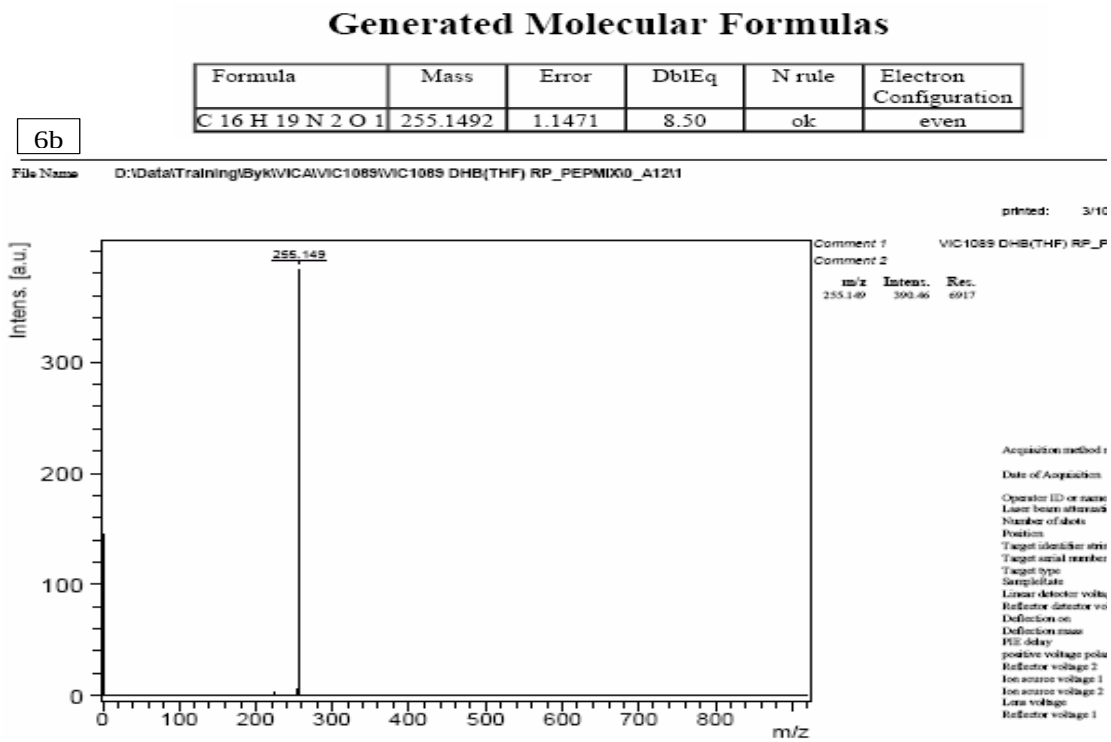
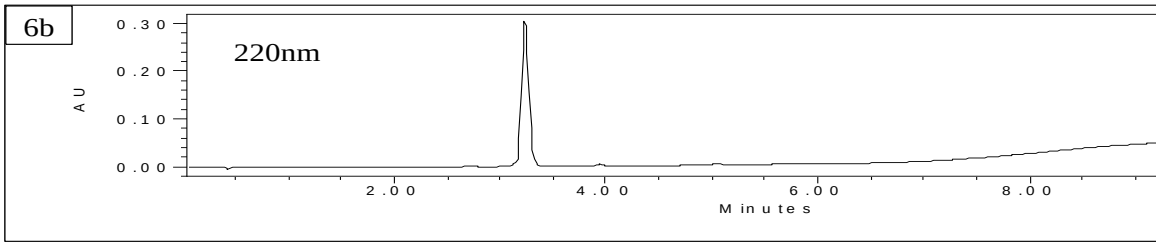


Figure S45. MALDI-TOF MS of compound 6b



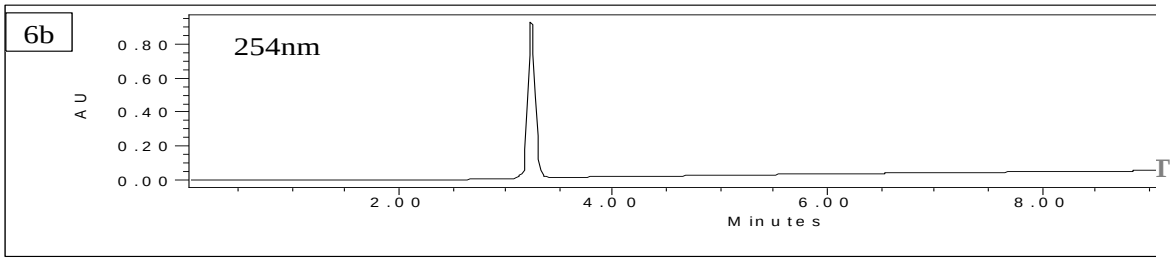


Figure S46. HPLC of compound 6b

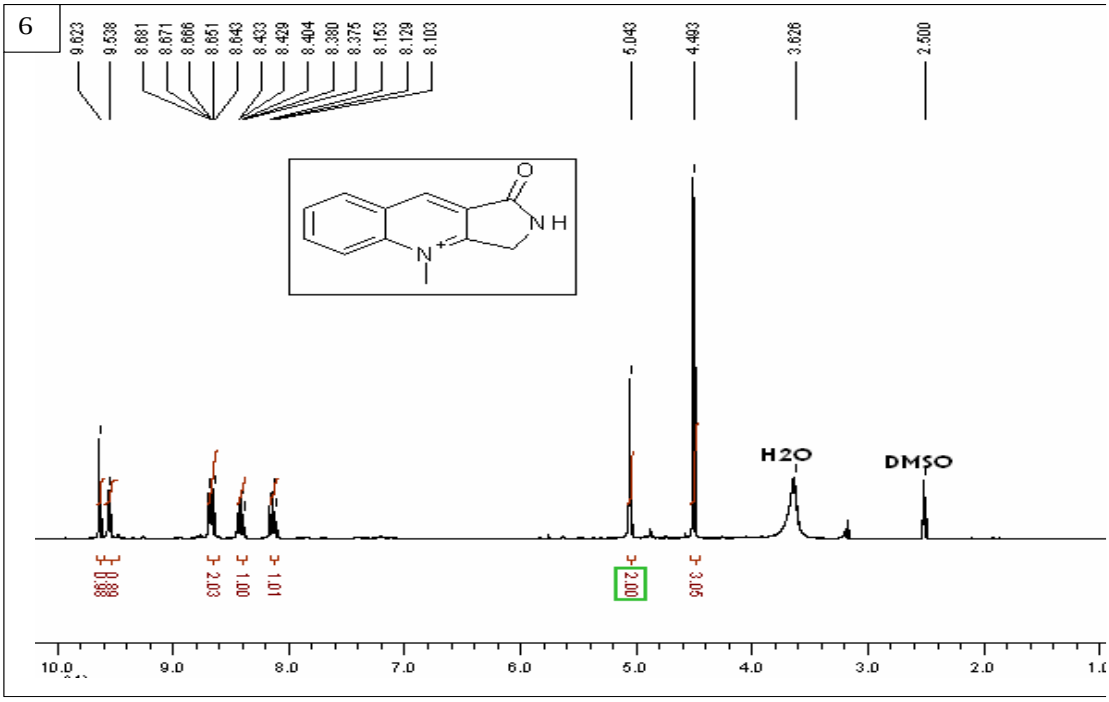


Figure S47. H-NMR of compound 6a in DMSO

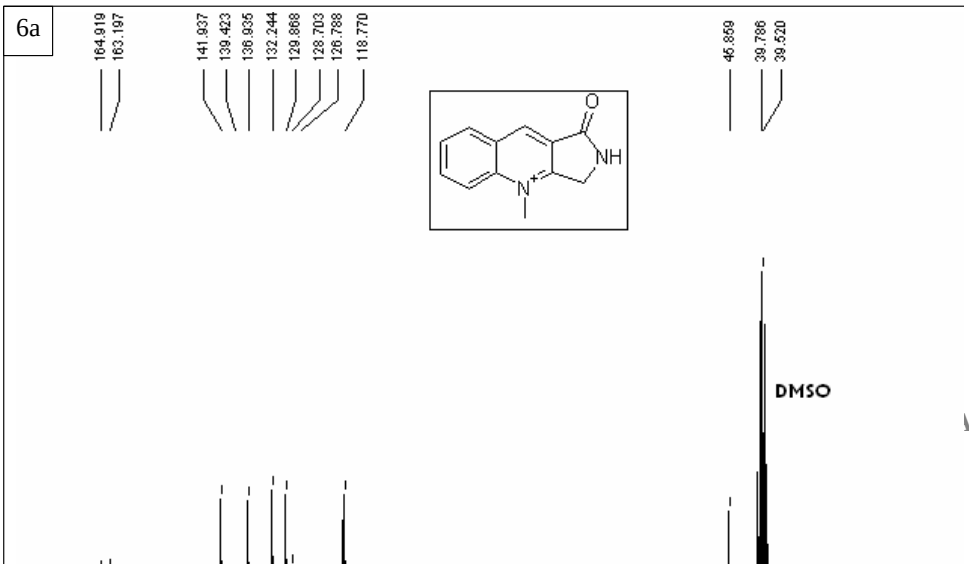
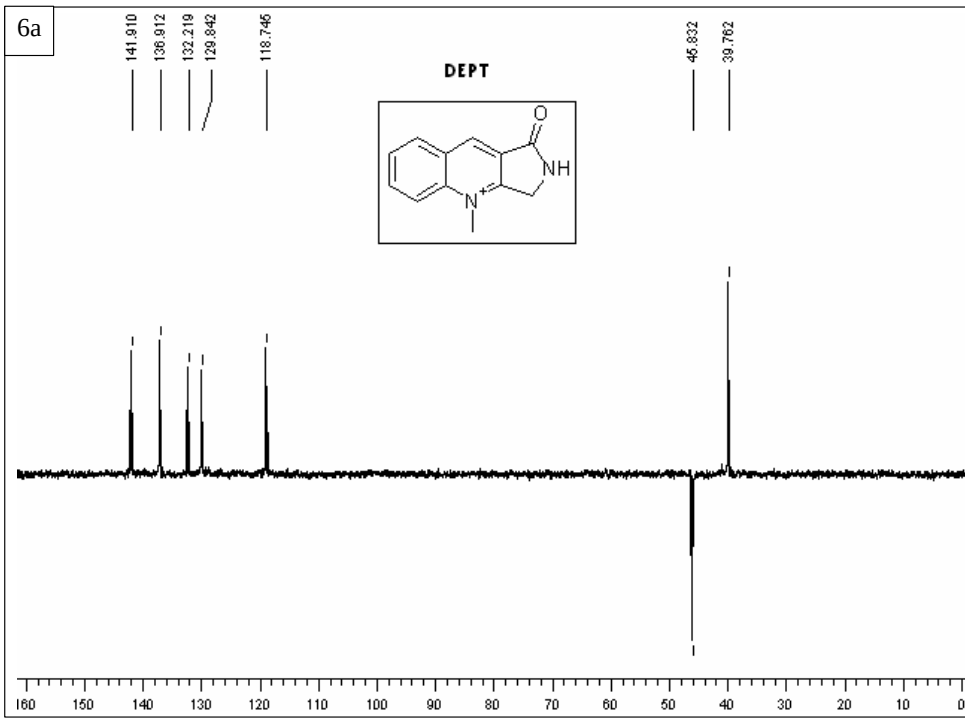
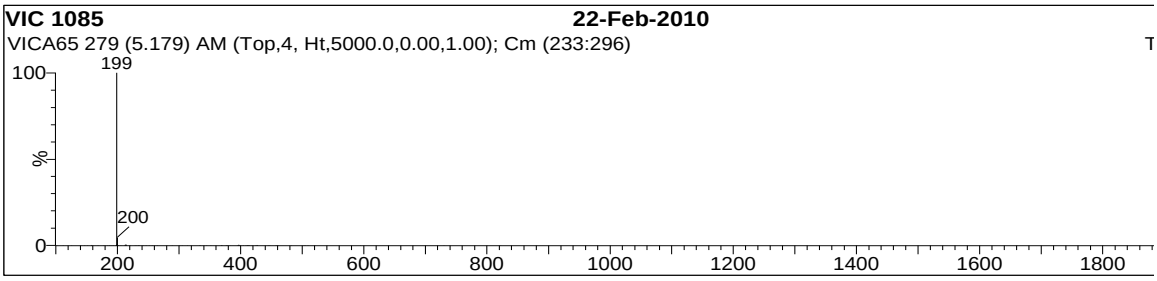


Figure S48. C-NMR of compound 6a in DMSO

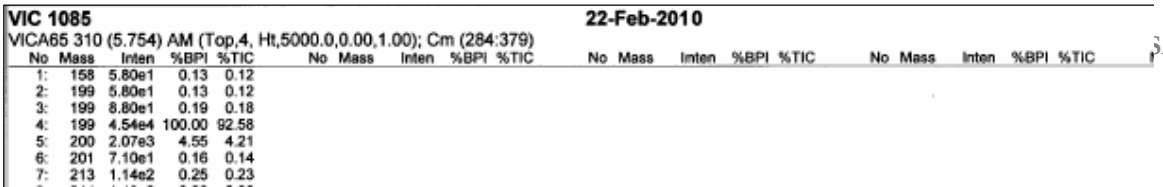


6a

Figure S49. DEPT of compound 6a in DMSO



6a



No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	158	5.80e1	0.13	0.12															
2:	199	5.80e1	0.13	0.12															
3:	199	8.80e1	0.19	0.18															
4:	199	4.54e4	100.00	92.58															
5:	200	2.07e3	4.55	4.21															
6:	201	7.10e1	0.16	0.14															
7:	213	1.14e2	0.25	0.23															

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Figure S50. QTOF-MS of compound 6a

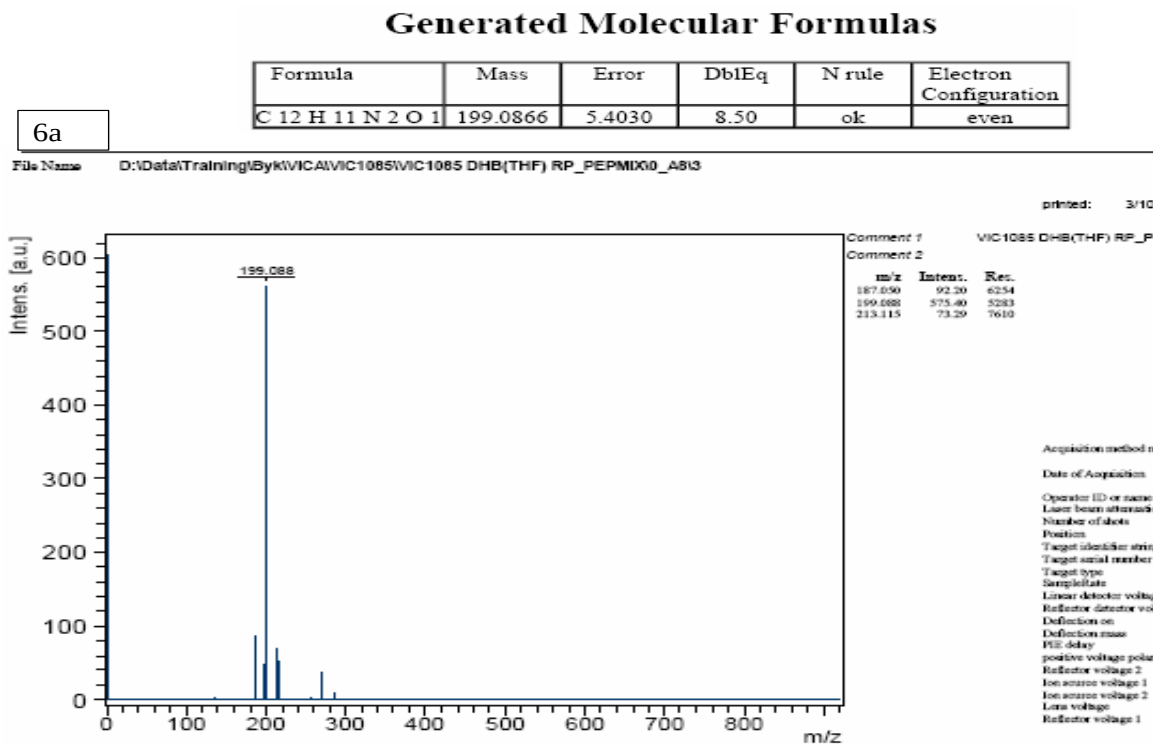


Figure S51. HR-MALDI-TOF MS of compound 6a

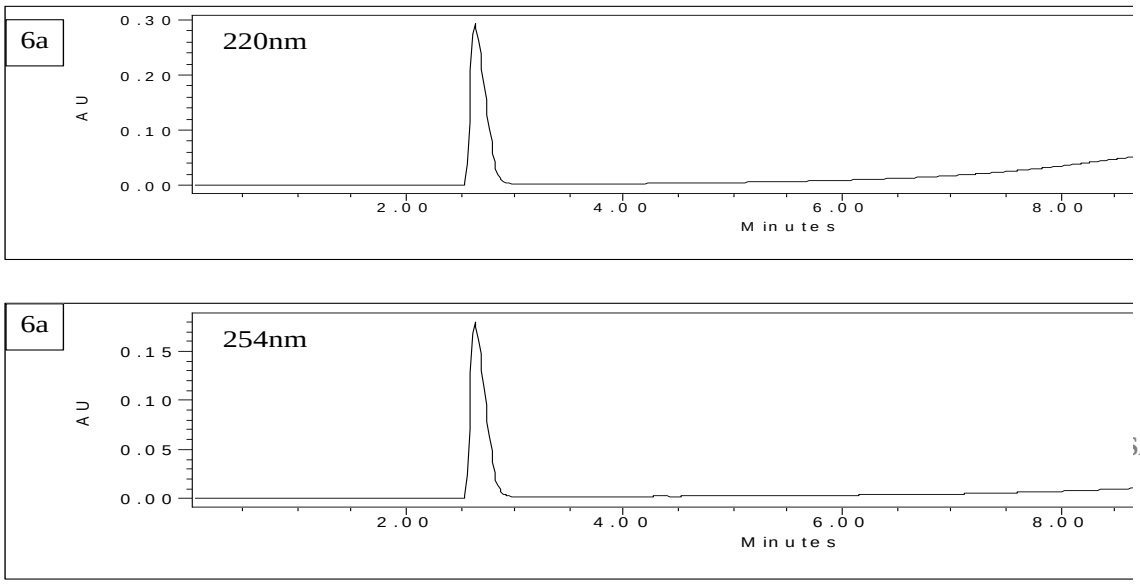


Figure S52. HPLC of compound 6a

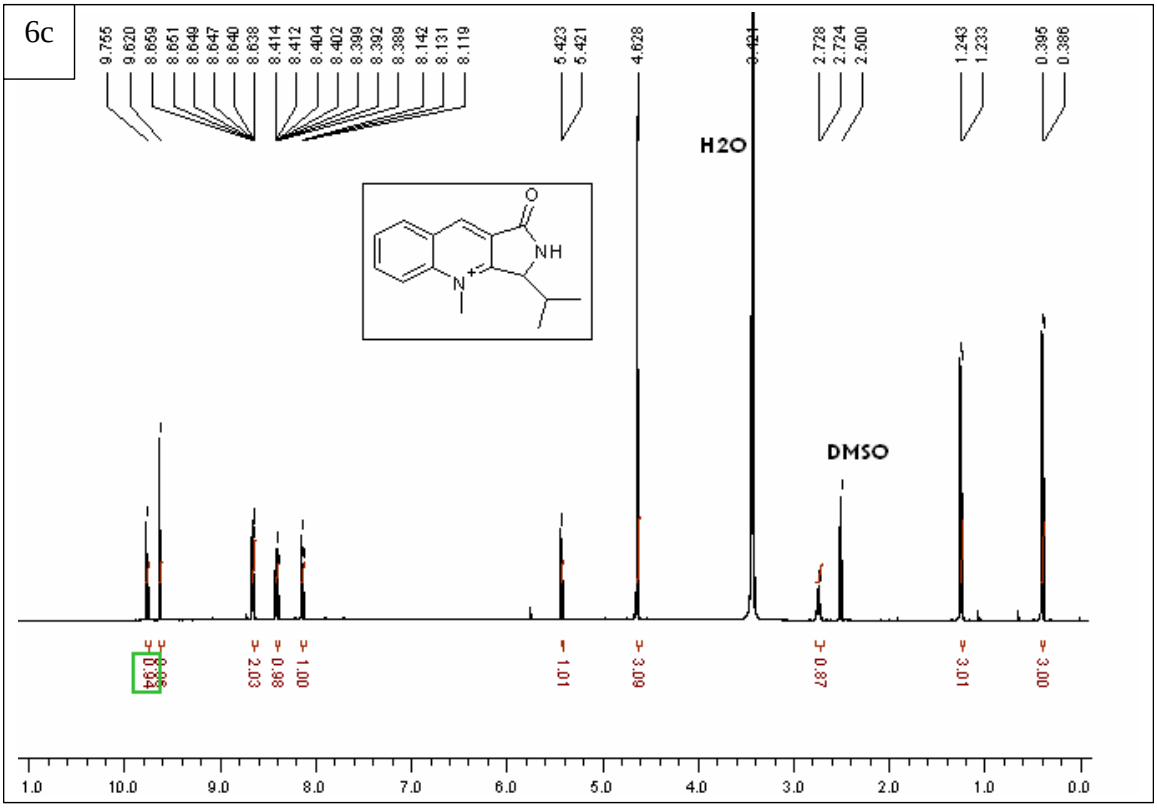


Figure S53. H-NMR of compound 6c in DMSO

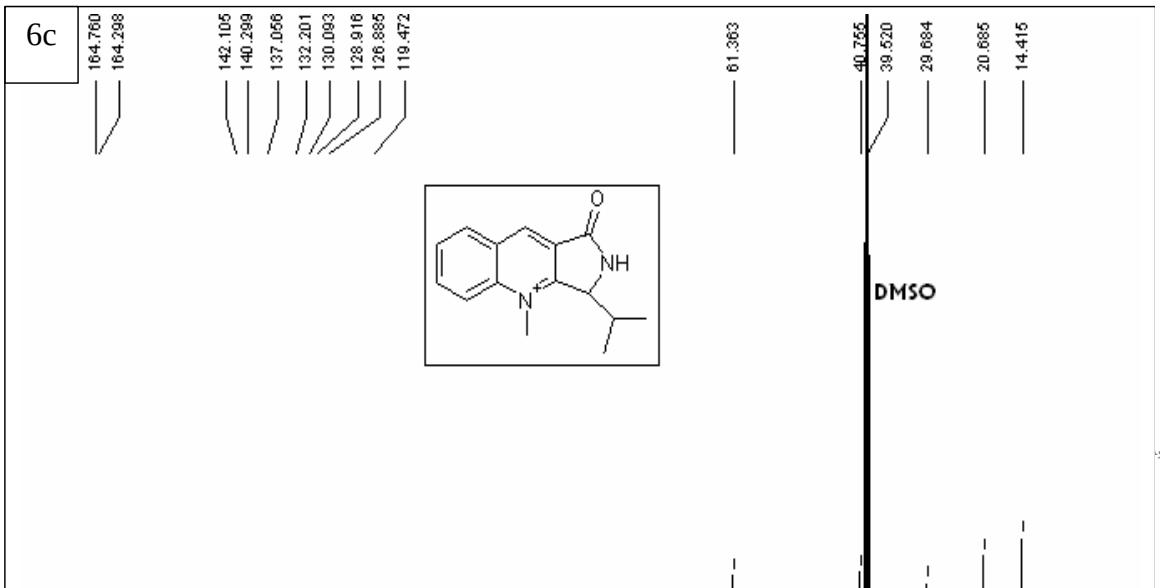
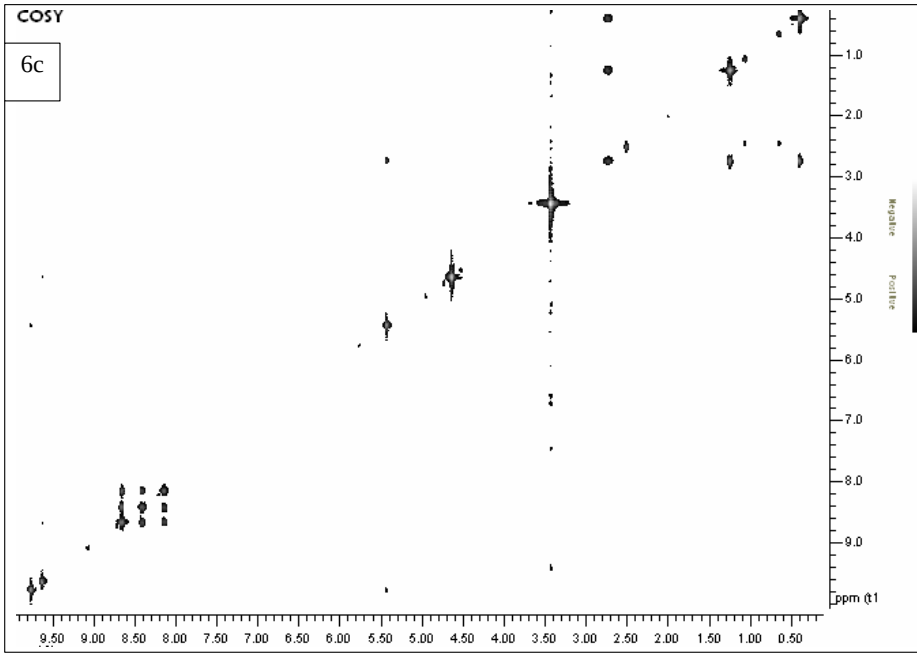


Figure S54. C-NMR of compound 6c in DMSO



Fi

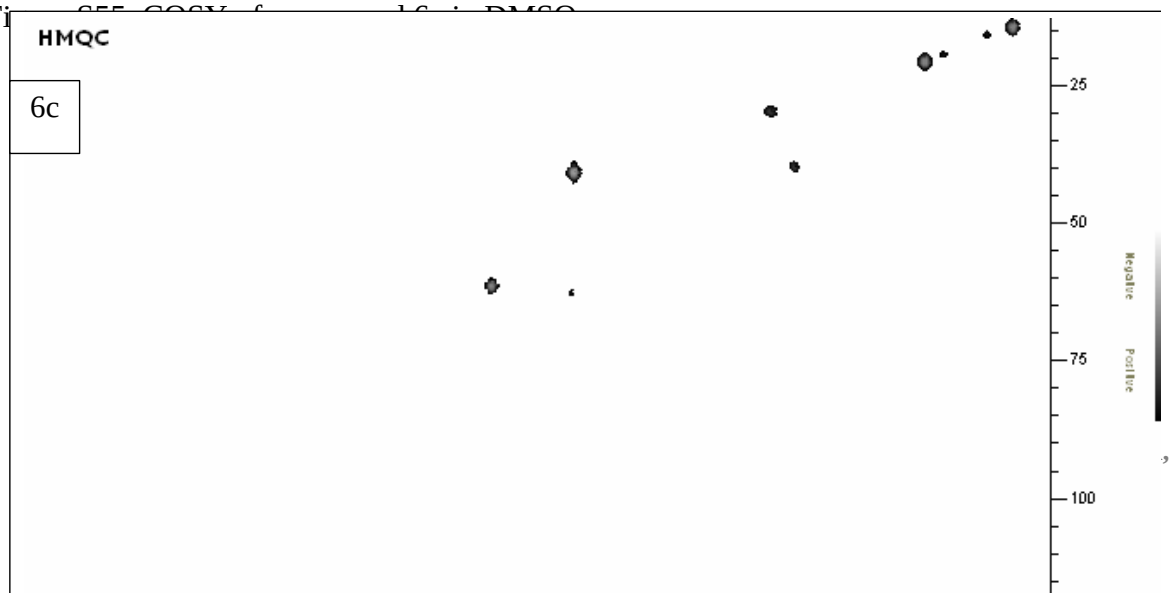


Figure S56. HMQC of compound 6c in DMSO

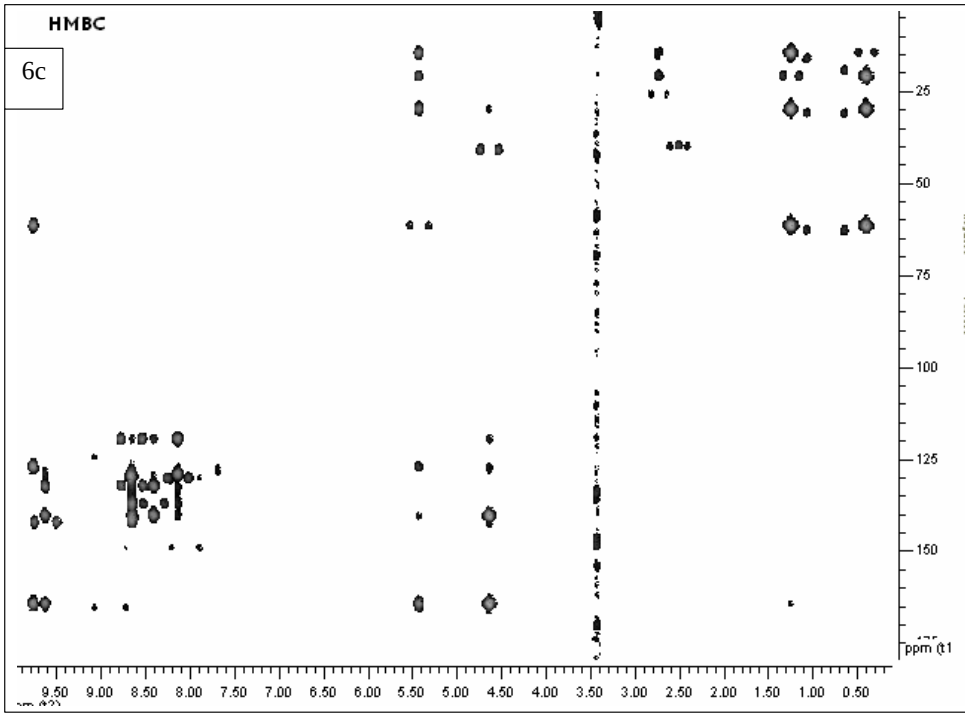


Figure S57. HMBC of compound 6c in DMSO

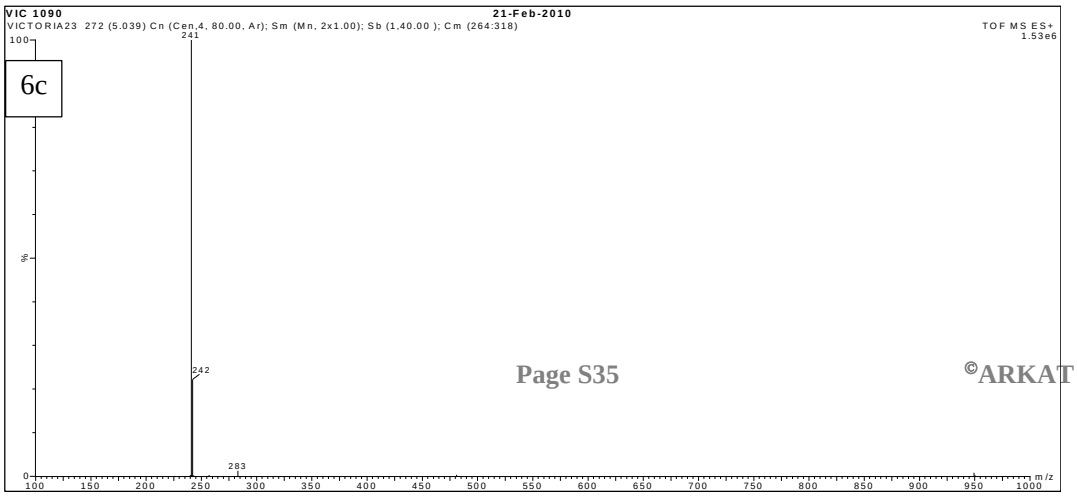


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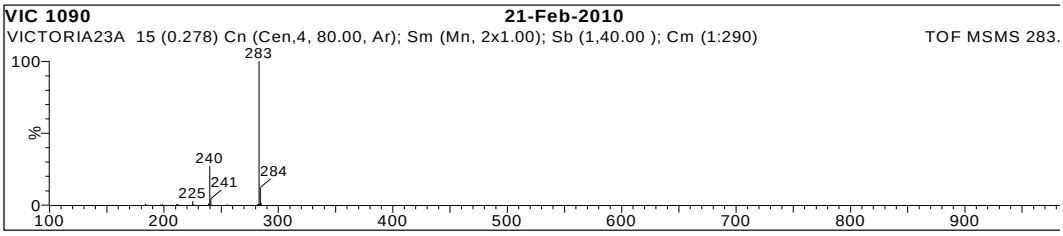
Figure S58. QTOF-MS of compound 6c

6c



No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten
1:	143	1.50e1	0.25	0.08	49:	239	9.89e0	0.16	0.05								
2:	156	3.53e1	0.59	0.18	50:	239	2.44e1	0.41	0.13								
3:	157	9.60e1	1.60	0.49	51:	240	3.84e1	0.64	0.20								
4:	168	7.33e0	0.12	0.04	52:	240	2.92e1	0.49	0.15								
5:	168	2.29e1	0.38	0.12	53:	240	4.81e1	0.80	0.25								
6:	169	4.80e1	0.80	0.25	54:	240	1.52e2	2.53	0.78								
7:	170	2.10e2	3.49	1.08	55:	240	5.26e3	87.56	27.03								
8:	171	1.41e1	0.23	0.07	56:	240	1.38e1	0.23	0.07								
9:	180	1.87e1	0.31	0.10	57:	241	8.16e2	13.57	4.19								
10:	181	8.56e0	0.14	0.04	58:	242	9.67e0	0.16	0.05								
11:	182	1.80e1	0.30	0.09	59:	242	3.13e1	0.52	0.16								
12:	183	2.14e1	0.36	0.11	60:	255	8.04e1	1.34	0.41								
13:	183	7.11e1	1.18	0.37	61:	281	9.33e0	0.16	0.05								
14:	184	4.89e2	8.14	2.51	62:	281	8.22e0	0.14	0.04								
15:	185	1.25e2	2.09	0.64	63:	281	6.33e0	0.11	0.03								
16:	192	2.02e1	0.34	0.10	64:	281	6.78e0	0.11	0.03								
17:	196	1.22e1	0.20	0.06	65:	282	1.74e1	0.29	0.09								
18:	196	4.03e1	0.67	0.21	66:	282	1.30e1	0.22	0.07								
19:	197	5.09e2	8.48	2.62	67:	282	8.22e0	0.14	0.04								
20:	198	1.18e2	1.97	0.61	68:	282	1.38e1	0.23	0.07								
21:	199	2.93e2	4.88	1.50	69:	282	1.88e1	0.31	0.10								
22:	200	1.71e1	0.28	0.09	70:	282	1.24e1	0.21	0.06								
23:	207	9.78e0	0.16	0.05	71:	282	1.07e1	0.18	0.05								
24:	210	3.46e1	0.58	0.18	72:	282	1.04e1	0.17	0.05								
25:	211	3.93e2	6.55	2.02	73:	282	2.60e1	0.43	0.13								
26:	212	3.09e2	5.14	1.59	74:	282	1.40e1	0.23	0.07								
27:	213	3.88e1	0.65	0.20	75:	282	3.23e1	0.54	0.17								
28:	213	9.22e0	0.15	0.05	76:	283	9.67e0	0.16	0.05								
29:	223	7.01e1	1.17	0.36	77:	283	2.86e1	0.48	0.15								
30:	224	6.51e1	1.08	0.33	78:	283	1.22e1	0.20	0.06								
31:	224	3.26e1	0.54	0.17	79:	283	6.93e1	1.15	0.36								
32:	225	9.89e0	0.16	0.05	80:	283	4.28e1	0.71	0.22								
33:	225	7.00e0	0.12	0.04	81:	283	6.01e3	100.00	30.85								
34:	225	1.30e3	21.62	6.67	82:	283	1.41e1	0.23	0.07								
35:	226	2.07e2	3.44	1.06	83:	284	1.90e1	0.32	0.10								
36:	227	7.00e0	0.12	0.04	84:	284	8.30e2	13.82	4.26								
37:	238	6.67e0	0.11	0.03	85:	285	3.06e1	0.51	0.16								
38:	238	1.49e1	0.25	0.08	86:	285	3.41e1	0.57	0.18								
39:	238	2.53e1	0.42	0.13													
40:	238	6.56e0	0.11	0.03													
41:	239	5.31e1	0.88	0.27													
42:	239	2.22e1	0.37	0.11													
43:	239	1.42e1	0.24	0.07													
44:	239	4.29e2	7.14	2.20													
45:	239	3.52e1	0.59	0.18													
46:	239	1.06e1	0.18	0.05													
47:	239	1.33e1	0.22	0.07													
48:	239	1.70e1	0.28	0.09													

Figure S59. QTOF-M

Generated Molecular Formulas

Formula	Mass	Error	DblEq	N rule	Electron Configuration
C 15 H 17 N 2 O 1	241.1335	1.4888	8.50	ok	even

6c

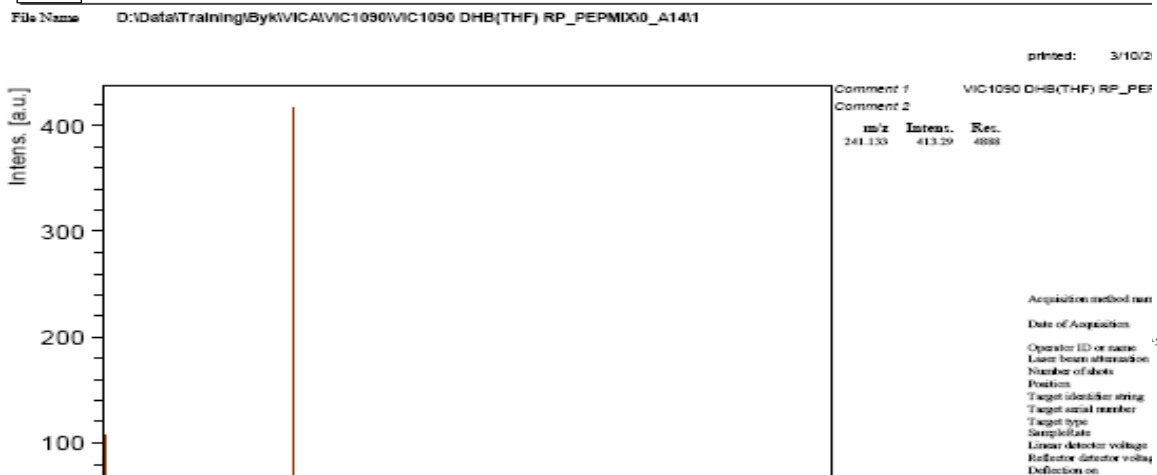


Figure S60. MALDI-TOF MS of compound 6c

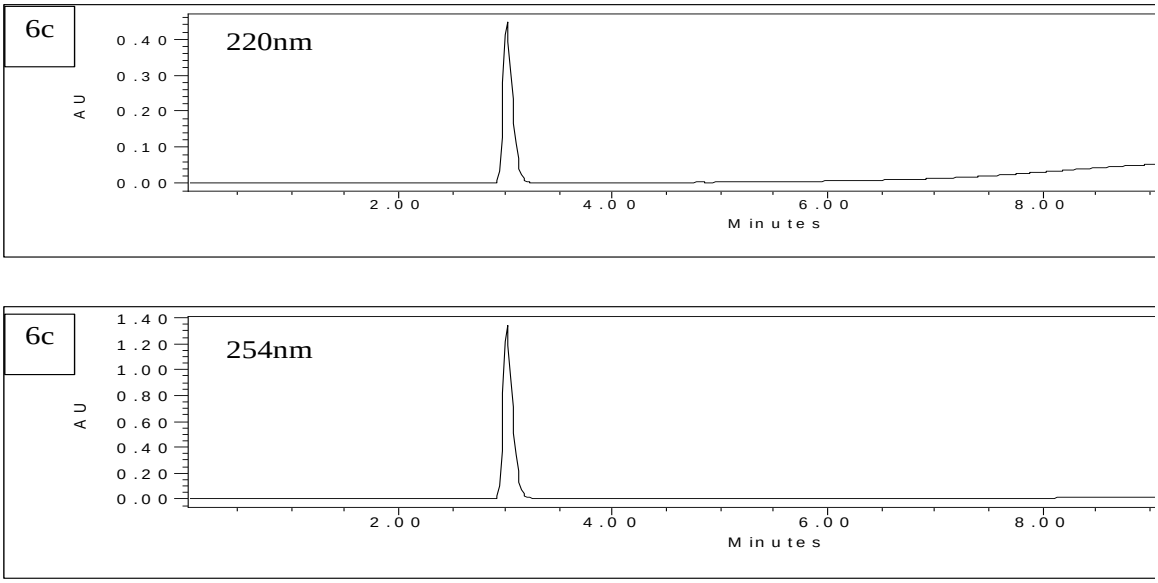


Figure S61. HPLC of compound 6c

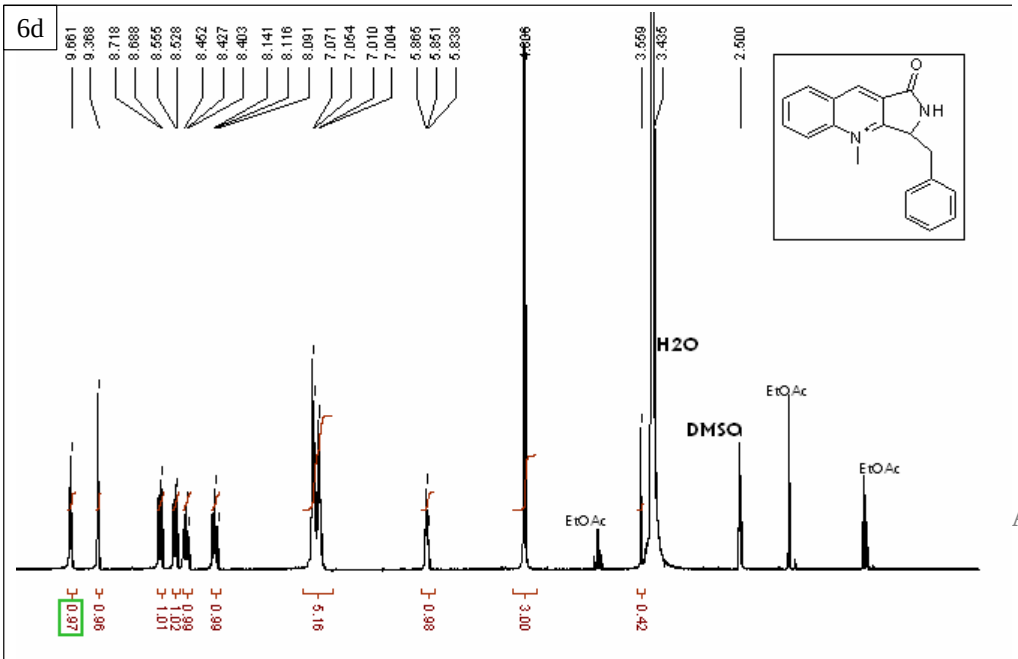


Figure S62. H-NMR of compound 6d in DMSO

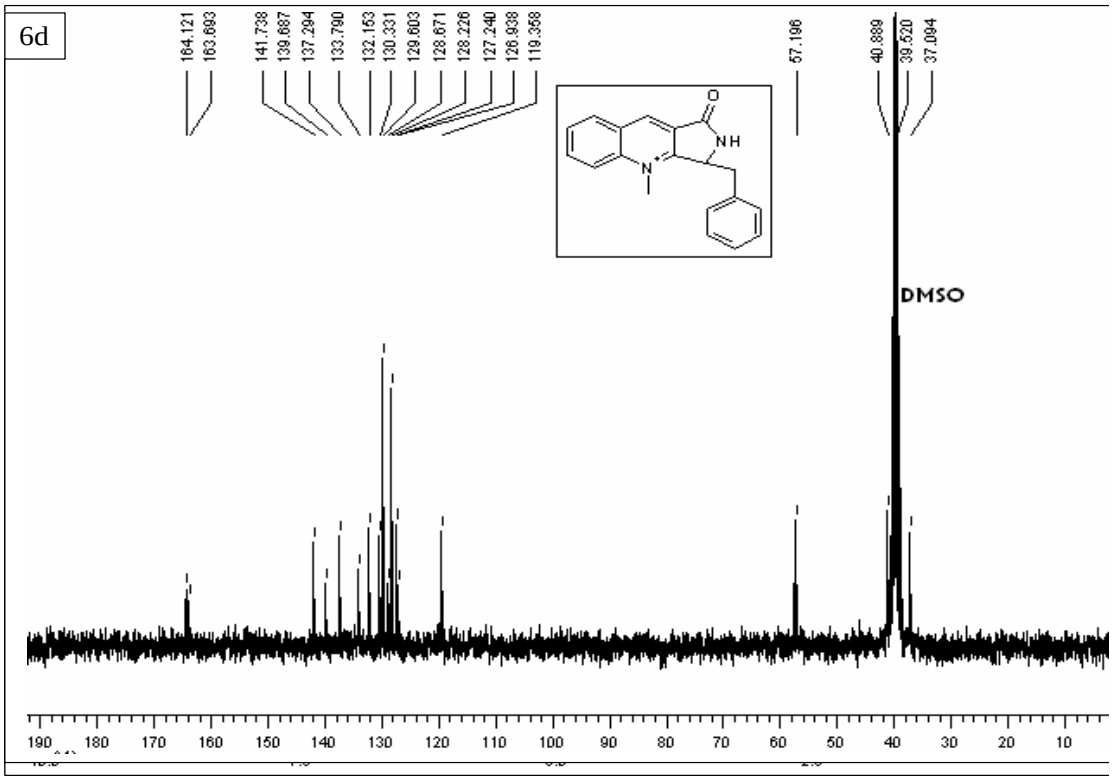
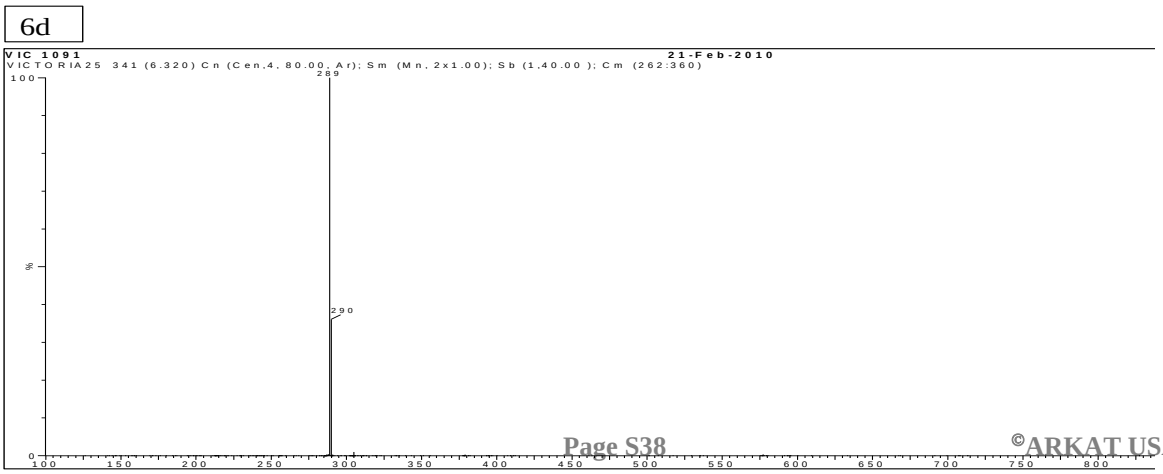


Figure S63. C-NMR of compound 6d in DMSO



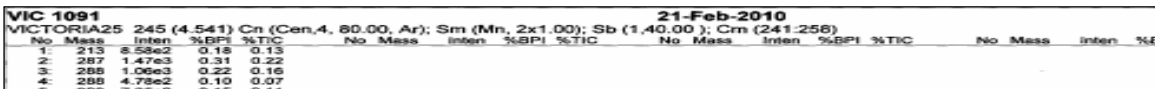


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Figure S64. QTOF-MS of compound 6d

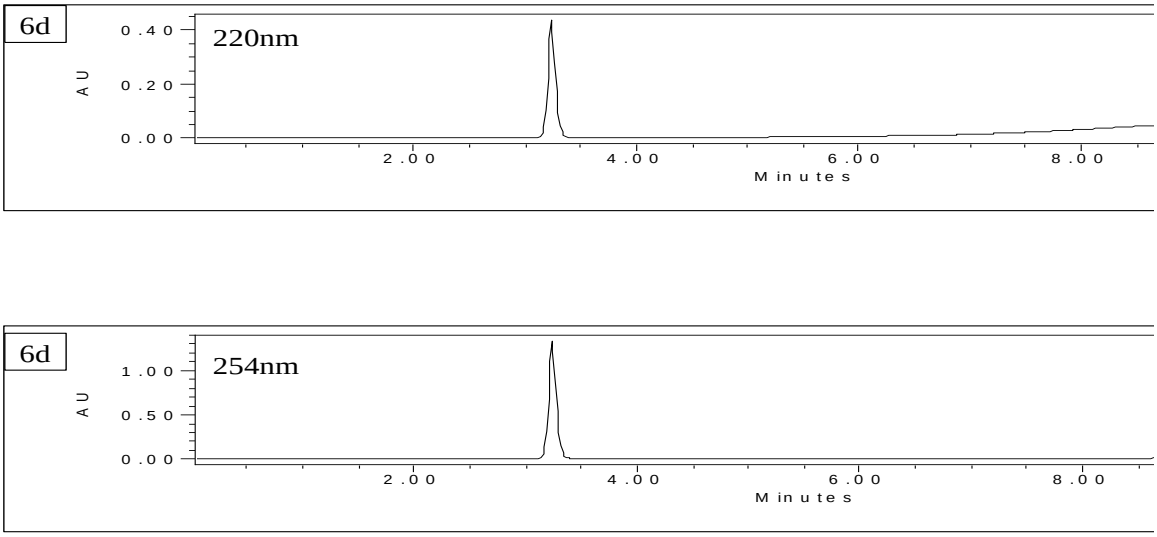


Figure S65. HPLC of compound 6d

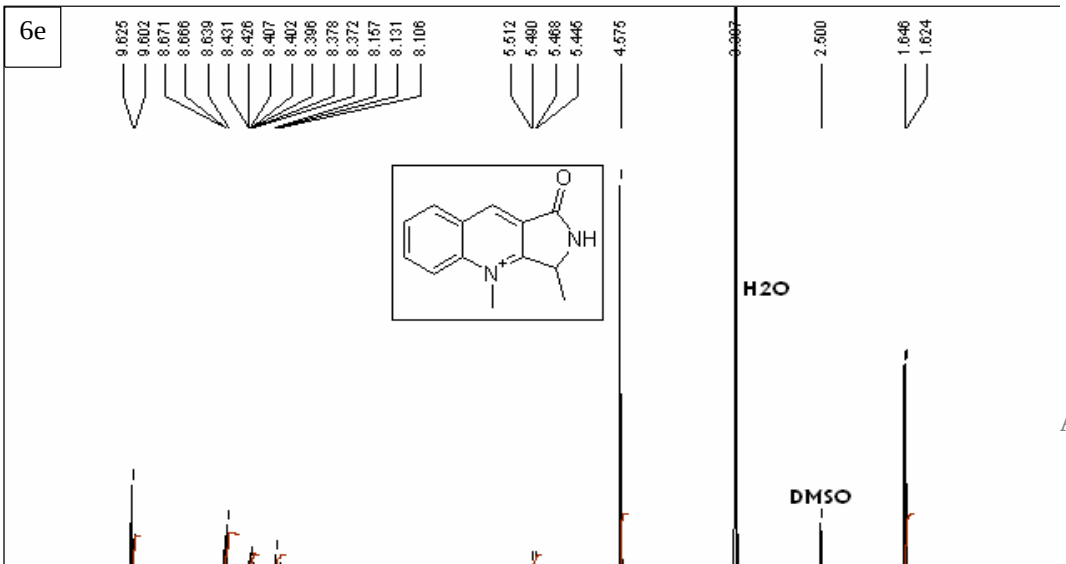


Figure S66. H-NMR of compound 6e in DMSO

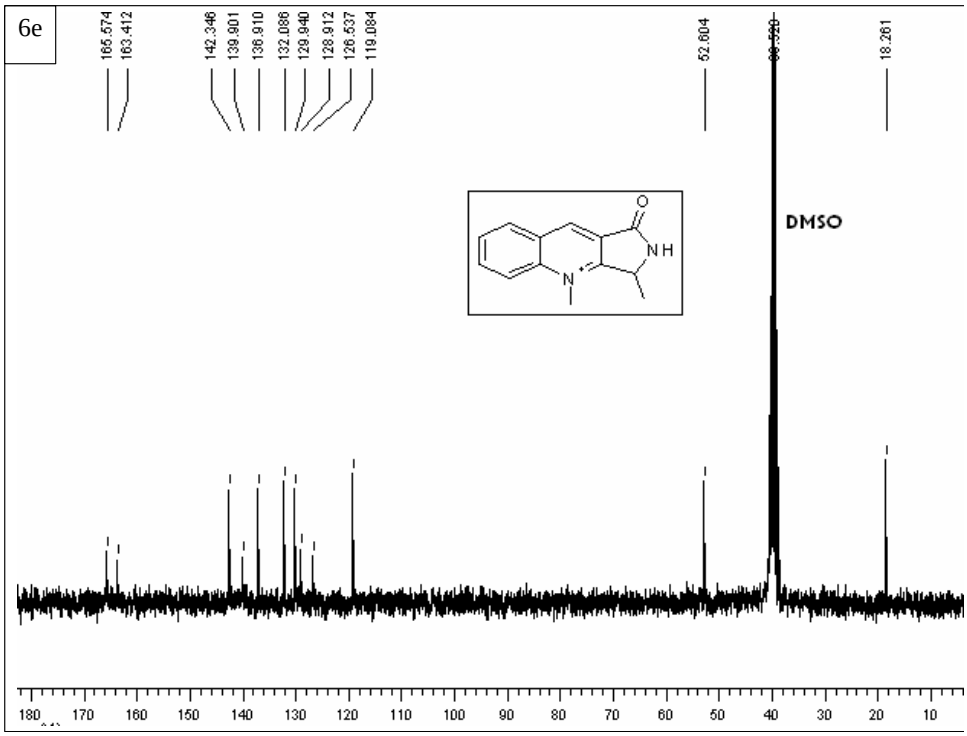


Figure S67. C-NMR of compound 6e in DMSO

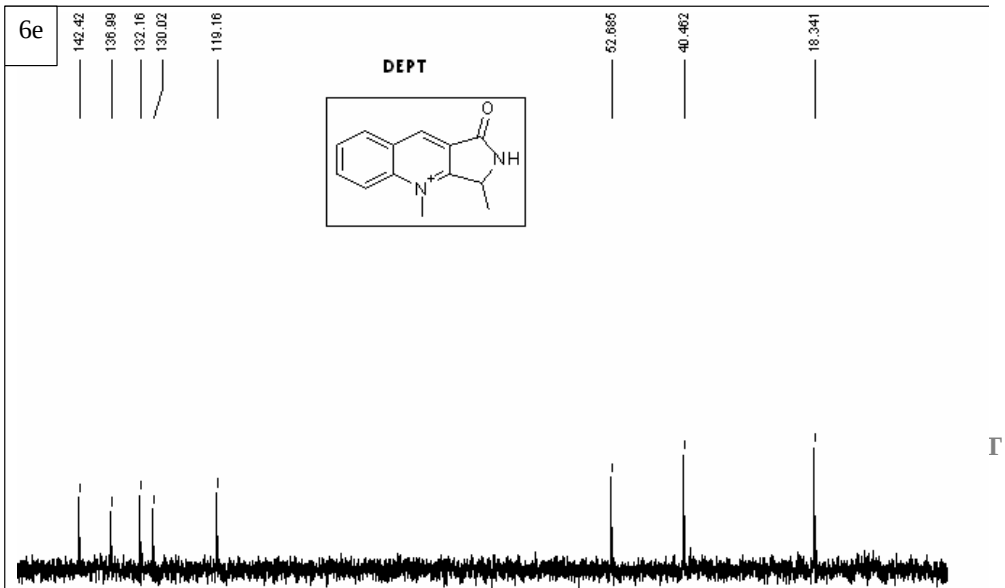
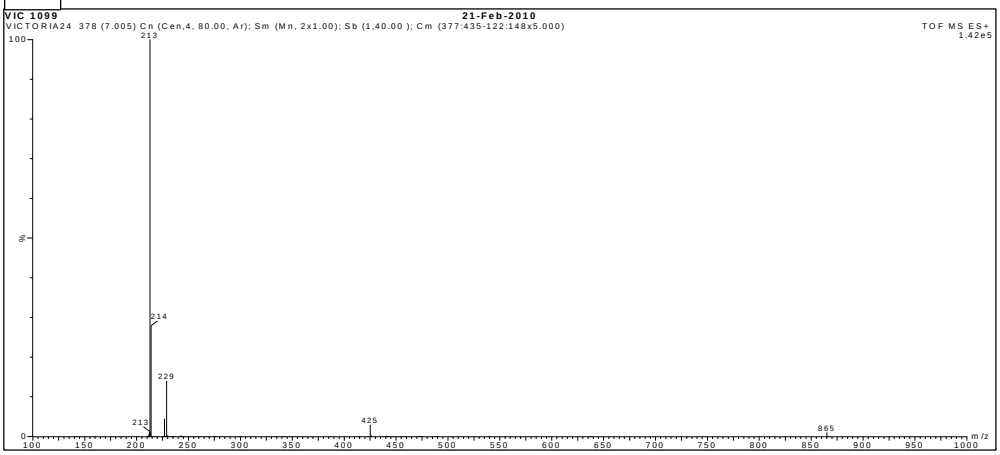


Figure S68. DEPT of compound 6e in DMSO

6e



VIC 1099 21-Feb-2010

VICTORIA24 262 (4.856) Cn (Cen,4, 80.00, Ar); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (262:326-121:137x5.000) TOF MS ES+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten
1:	212	1.76e3	0.25	0.18													
2:	212	9.33e2	0.13	0.09													
3:	212	7.34e2	0.10	0.07													
4:	212	1.76e3	0.25	0.18													
5:	212	1.57e3	0.22	0.16													
6:	213	1.90e3	0.26	0.19													
7:	213	7.17e5	100.00	72.91													
8:	213	2.34e3	0.33	0.24													
9:	214	1.75e5	24.37	17.77													
10:	215	1.63e3	0.23	0.17													
11:	227	1.29e4	1.81	1.32													
12:	229	4.29e4	5.98	4.36													
13:	230	1.40e3	0.20	0.14													
14:	243	2.72e3	0.38	0.28													
15:	425	5.91e3	0.83	0.60													
16:	865	1.71e3	0.24	0.17													

Figure S69. QTOF-MS of compound 6e

6e

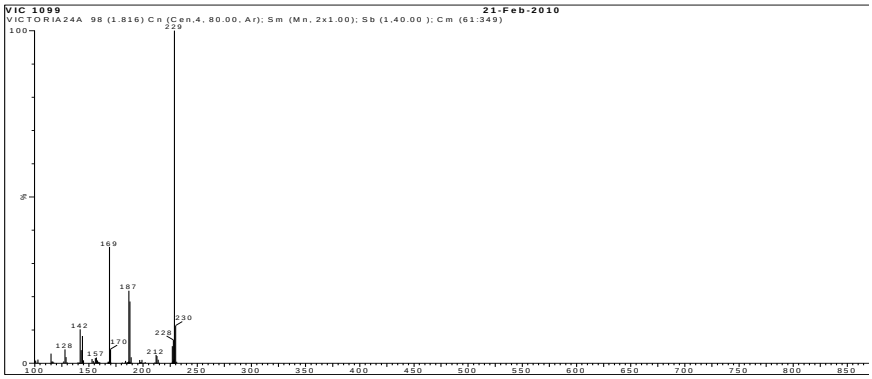


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Figure S70. QTOF-MS of compound 6e

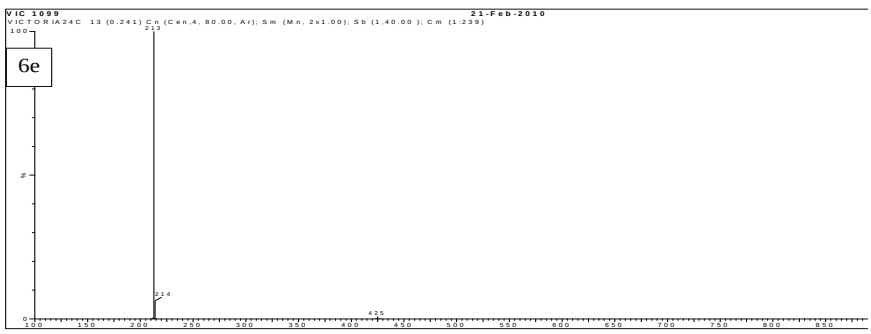
6e

VIC 1099 **21-Feb-2010**

VICTORIA24A 98 (1.816) Cn (Cen,4, 80.00, Ar); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (58:354)

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TI
1:	101	9.20e1	0.77	0.28	49:	229	5.94e1	0.50	0.18					
2:	103	1.27e2	1.06	0.39	50:	229	8.47e1	0.71	0.26					
3:	115	3.40e2	2.84	1.04	51:	229	1.33e2	1.11	0.41					
4:	116	1.04e2	0.87	0.32	52:	229	1.20e4	100.00	36.54					
5:	117	5.10e1	0.43	0.16	53:	230	1.36e3	11.39	4.16					
6:	127	5.70e1	0.48	0.17	54:	231	4.93e1	0.41	0.15					
7:	128	4.88e2	4.07	1.49										
8:	129	2.13e2	1.78	0.65										
9:	142	1.19e3	9.95	3.64										
10:	143	4.67e2	3.90	1.42										
11:	144	9.50e2	7.94	2.90										
12:	145	9.81e1	0.82	0.30										
13:	153	1.48e2	1.24	0.45										
14:	154	8.30e1	0.69	0.25										
15:	156	1.77e2	1.48	0.54										
16:	157	1.94e2	1.62	0.59										
17:	158	9.40e1	0.79	0.29										
18:	158	7.73e1	0.65	0.24										
19:	160	3.60e1	0.30	0.11										
20:	168	5.52e1	0.46	0.17										
21:	168	3.76e1	0.31	0.11										
22:	169	4.01e1	0.34	0.12										
23:	169	4.06e3	33.95	12.40										
24:	170	4.86e2	4.06	1.48										
25:	184	7.90e1	0.66	0.24										
26:	187	4.66e1	0.39	0.14										
27:	187	2.52e3	21.09	7.71										
28:	188	4.49e1	0.38	0.14										
29:	188	2.17e3	18.11	6.62										
30:	189	2.06e2	1.72	0.63										
31:	197	1.11e2	0.93	0.34										
32:	199	1.12e2	0.94	0.34										
33:	212	2.90e2	2.43	0.89										
34:	213	2.44e2	2.04	0.75										
35:	214	1.22e2	1.02	0.37										
36:	227	6.07e2	5.07	1.85										
37:	228	3.87e1	0.32	0.12										
38:	228	3.71e1	0.31	0.11										
39:	228	6.79e1	0.57	0.21										
40:	228	4.69e1	0.39	0.14										
41:	228	5.73e1	0.48	0.18										
42:	228	8.18e2	6.83	2.50										
43:	228	4.50e1	0.38	0.14										
44:	228	5.32e1	0.44	0.16										
45:	228	4.43e1	0.37	0.14										
46:	228	3.61e1	0.30	0.11										
47:	229	5.11e1	0.43	0.16										
48:	229	1.27e2	1.06	0.39										

Figure S71. QTOF-MS of compound 6e



6e

VIC 1099 **21-Feb-2010**

VICTORIA24C 13 (0.241) Cn (Cen,4, 80.00, Ar); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (1:243)

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	211	2.15e2	0.29	0.27										
2:	212	2.56e2	0.35	0.32										
3:	213	8.39e1	0.11	0.10										
4:	213	7.78e1	0.11	0.10										
5:	213	1.89e2	0.26	0.23										
6:	213	1.12e2	0.15	0.14										
7:	213	1.84e2	0.25	0.23										
8:	213	7.38e4	100.00	91.31										
9:	214	4.62e3	6.26	5.72										
10:	215	2.03e2	0.27	0.25										
11:	425	5.94e2	0.80	0.73										

Figure S72. QTOF-MS of compound 6e

Generated Molecular Formulas

6e

Formula	Mass	Error	DblEq	N rule	Electron Configuration
C 13 H 13 N 2 O 1	213.1022	0.9076	8.50	ok	even

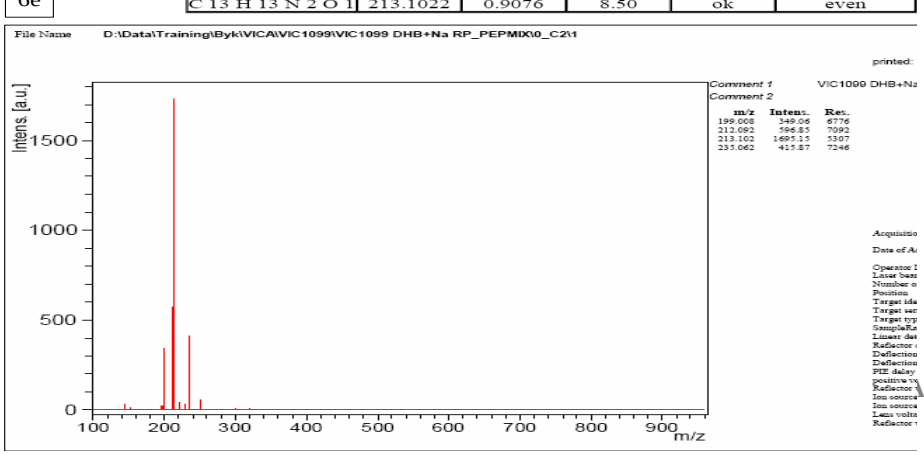


Figure S73. MALDI-TOF MS of compound 6e

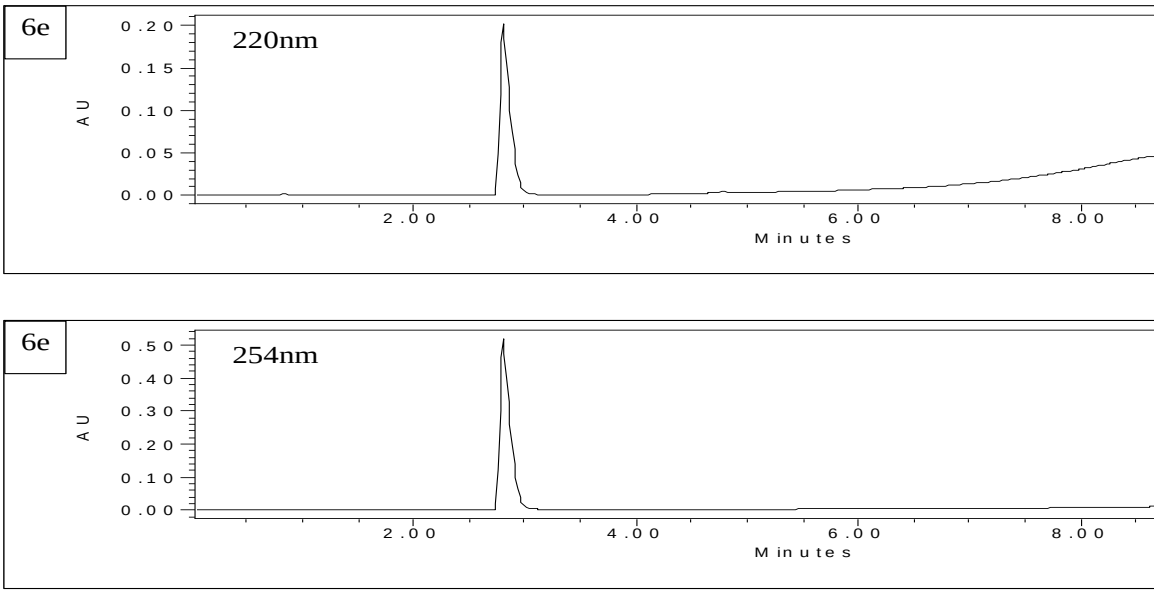


Figure S74. HPLC of compound 6e

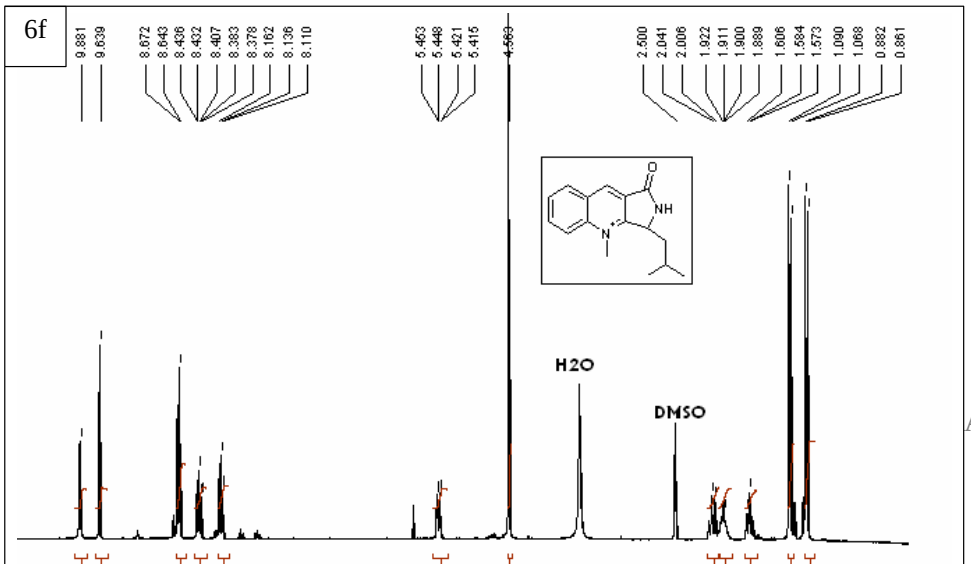


Figure S75. H-NMR of compound 6f in DMSO

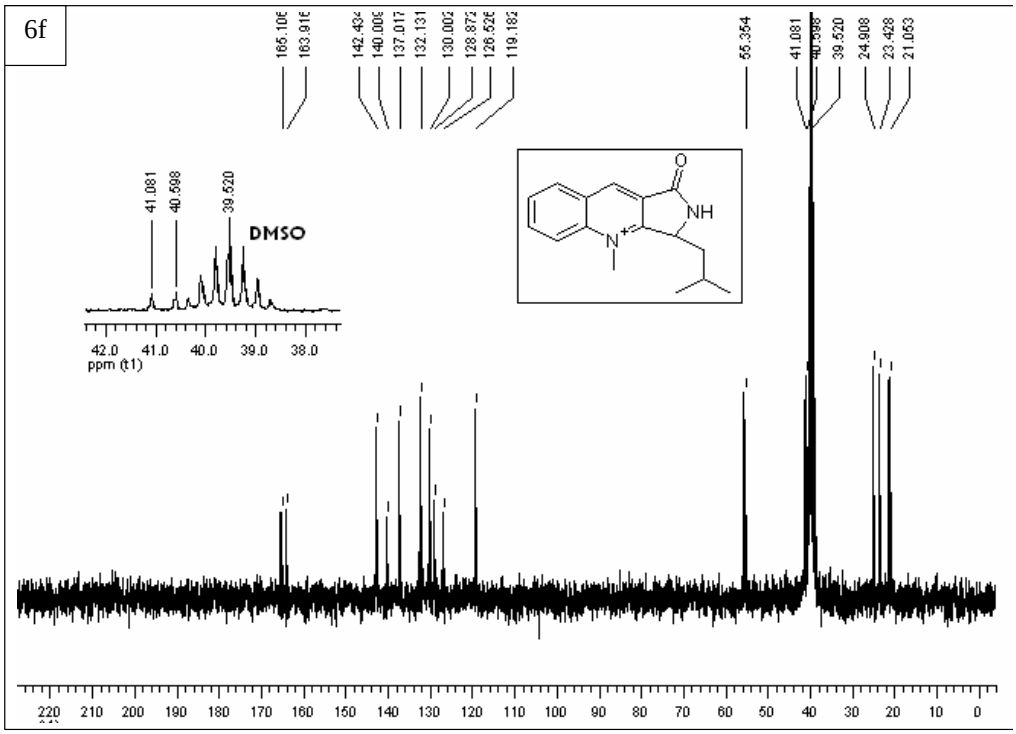
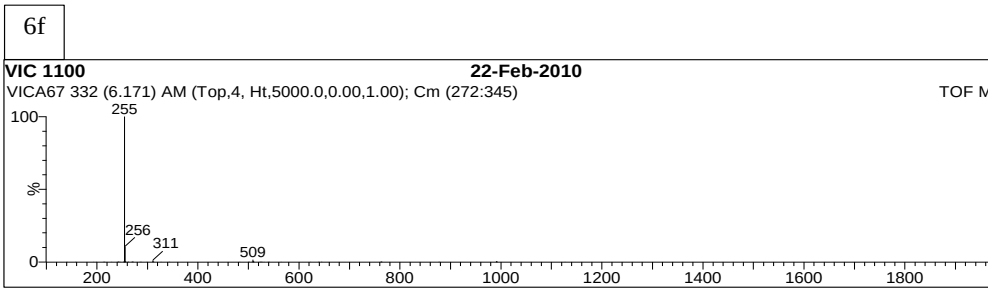
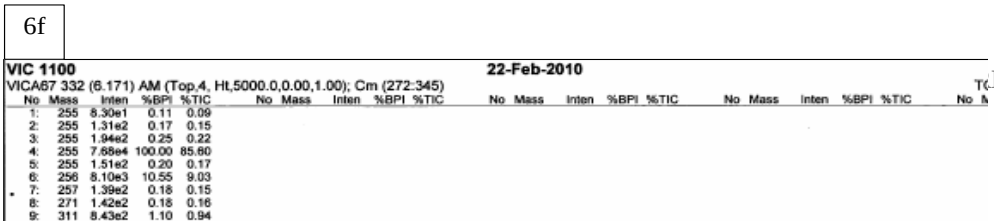


Figure S76. C-NMR of compound 6f in DMSO

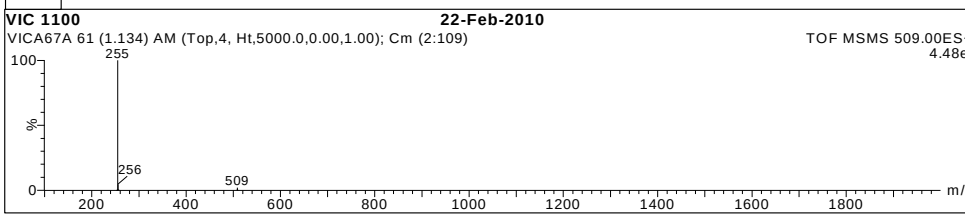




No	Mass	Inten	%BPI	%TIC
1:	255	8.30e1	0.11	0.09
2:	255	1.31e2	0.17	0.15
3:	255	1.94e2	0.25	0.22
4:	255	7.68e4	100.00	85.60
5:	255	1.51e2	0.20	0.17
6:	256	8.10e3	10.55	9.03
* 7:	257	1.39e2	0.18	0.15
8:	271	1.42e2	0.18	0.16
9:	311	8.43e2	1.10	0.94

Figure S77. QTOF-MS of compound 6f

6f



6f

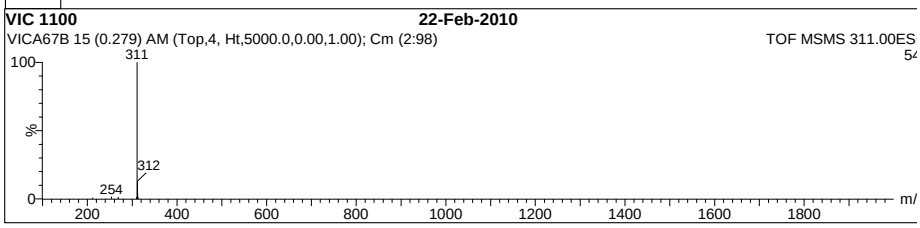
VIC 1100 22-Feb-2010

VICA67A 61 (1.134) AM (Top,4, Ht,5000.0,0.00,1.00); Cm (2:109) TOF MSMS 509.00E

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Int
1:	253	3.00e0	0.07	0.06													
2:	254	2.00e0	0.04	0.04													
3:	254	4.00e0	0.09	0.08													
4:	254	3.00e0	0.07	0.06													
5:	254	2.00e0	0.04	0.04													
6:	254	3.00e0	0.07	0.06													
7:	254	5.00e0	0.11	0.10													
8:	254	4.00e0	0.09	0.08													
9:	254	4.00e0	0.09	0.08													
10:	254	3.00e0	0.07	0.06													
11:	255	6.00e0	0.13	0.12													
12:	255	1.00e1	0.22	0.20													
13:	255	4.48e3	100.00	90.59													
14:	255	9.00e0	0.20	0.18													
15:	255	4.00e0	0.09	0.08													
16:	255	2.00e0	0.04	0.04													
17:	255	2.00e0	0.04	0.04													
18:	256	2.00e0	0.04	0.04													
19:	256	1.00e0	0.02	0.02													
20:	256	2.03e2	4.53	4.11													
21:	256	1.00e1	0.22	0.20													
22:	257	1.50e1	0.33	0.30													
23:	509	3.50e1	0.78	0.71													
24:	509	8.40e1	1.88	1.70													
25:	509	4.50e1	1.00	0.91													
26:	511	4.00e0	0.09	0.08													

Figure S78. QTOF-MS of compound 6f

6f



6f

VIC 1100 22-Feb-2010

VICA67B 15 (0.279) AM (Top,4, Ht,5000.0,0.00,1.00); Cm (2:98) TOF MSMS 311.00E

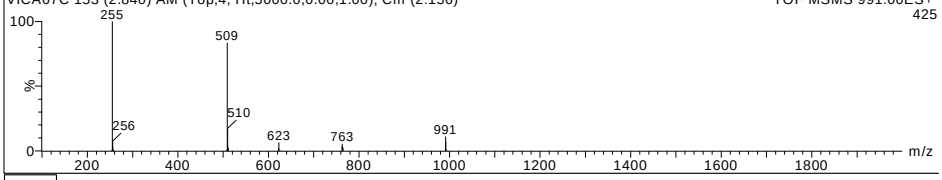
No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Int
1:	212	5.00e0	0.93	0.68													
2:	254	9.00e0	1.67	1.23													
3:	269	5.00e0	0.93	0.68													
4:	269	6.00e0	1.11	0.82													
5:	310	3.00e0	0.56	0.41													
6:	310	2.00e0	0.37	0.27													
7:	310	3.00e0	0.56	0.41													
8:	310	3.00e0	0.56	0.41													
9:	310	4.00e0	0.74	0.55													
10:	310	3.00e0	0.56	0.41													
11:	311	5.00e0	0.93	0.68													
12:	311	8.00e0	1.48	1.09													
13:	311	5.40e2	100.00	73.67													
14:	311	6.00e0	1.11	0.82													
15:	311	2.00e0	0.37	0.27													
16:	312	2.00e1	3.70	2.73													
17:	312	6.90e1	12.78	9.41													
18:	312	2.50e1	4.63	3.41													
19:	312	8.00e0	1.48	1.09													
20:	313	7.00e0	1.30	0.95													

Figure S79. QTOF-MS of compound 6f

6f

VIC 1100 **22-Feb-2010**

VICA67C 153 (2.840) AM (Top,4, Ht,5000.0,0.00,1.00); Cm (2:156) TOF MSMS 991.00ES+



6f

VIC 1100 **22-Feb-2010**

VICA67C 153 (2.840) AM (Top,4, Ht,5000.0,0.00,1.00); Cm (2:156) TOF MSMS 991.00ES+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten
1:	254	2.00e0	0.47	0.17													
2:	255	3.00e0	0.71	0.26													
3:	255	4.25e2	100.00	36.57													
4:	256	1.40e1	3.29	1.20													
5:	256	3.20e1	7.53	2.75													
6:	256	6.00e0	1.41	0.52													
7:	257	4.00e0	0.94	0.34													
8:	257	3.00e0	0.71	0.26													
9:	507	2.00e0	0.47	0.17													
10:	509	5.00e0	1.18	0.43													
11:	509	3.55e2	83.53	30.55													
12:	510	1.10e1	2.59	0.95													
13:	510	7.40e1	17.41	6.37													
14:	510	1.90e1	4.47	1.64													
15:	511	5.00e0	1.18	0.43													
16:	511	9.00e0	2.12	0.77													
17:	623	9.00e0	2.12	0.77													
18:	623	2.70e1	6.35	2.32													
19:	625	2.00e0	0.47	0.17													
20:	763	1.50e1	3.53	1.29													
21:	763	2.20e1	5.18	1.89													
22:	764	9.00e0	2.12	0.77													
23:	764	1.20e1	2.82	1.03													
24:	764	3.00e0	0.71	0.26													
25:	991	5.00e0	1.18	0.43													
26:	991	4.70e1	11.06	4.04													
27:	991	4.00e0	0.94	0.34													
28:	992	3.10e1	7.29	2.67													
29:	993	3.00e0	0.71	0.26													
30:	993	2.00e0	0.47	0.17													
31:	993	2.00e0	0.47	0.17													

Figure S80. QTOF-MS of compound 6f

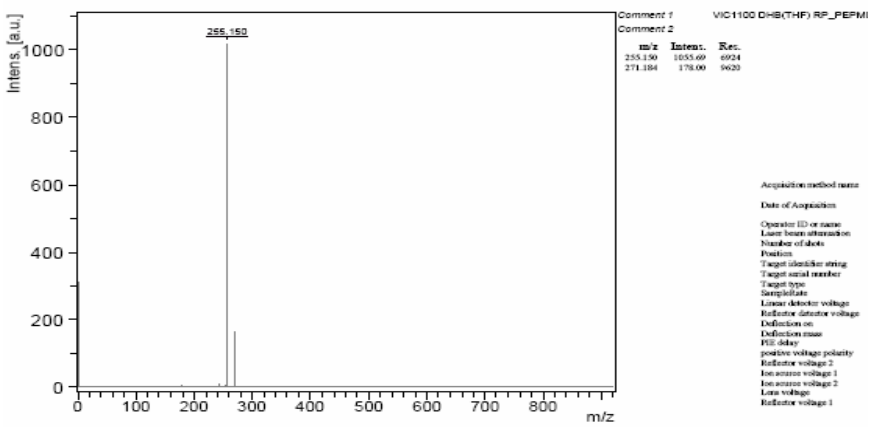
Generated Molecular Formulas

6f

Formula	Mass	Error	DblEq	N rule	Electron Configuration
C 16 H 19 N 2 O 1	255.1492	5.0317	8.50	ok	even

File Name D:\Data\Training\Byk\VICA\VIC1100A\VIC1100 DHB(THF) RP_PEPMIX\0_A20\2

printed: 3/10/2010



Comment 1 VIC1100 DHB(THF) RP_PEPMI
Comment 2

m/z	Intens.	Res.
255.150	1055.69	6924
271.184	178.00	9620

Acquisition method name
Date of Acquisition
Operator ID or name
Laser beam attenuation
Number of shots
Position
Target identifier string
Target serial number
Target type
Sampleplate
Linear detector voltage
Reflector detector voltage
Deflection on
Deflection mass
PIE delay
positive voltage polarity
Reflector voltage 2
Ion source voltage 1
Ion source voltage 2
Lens voltage
Reflector voltage 1

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Figure S81. MALDI-TOF MS of compound 6f

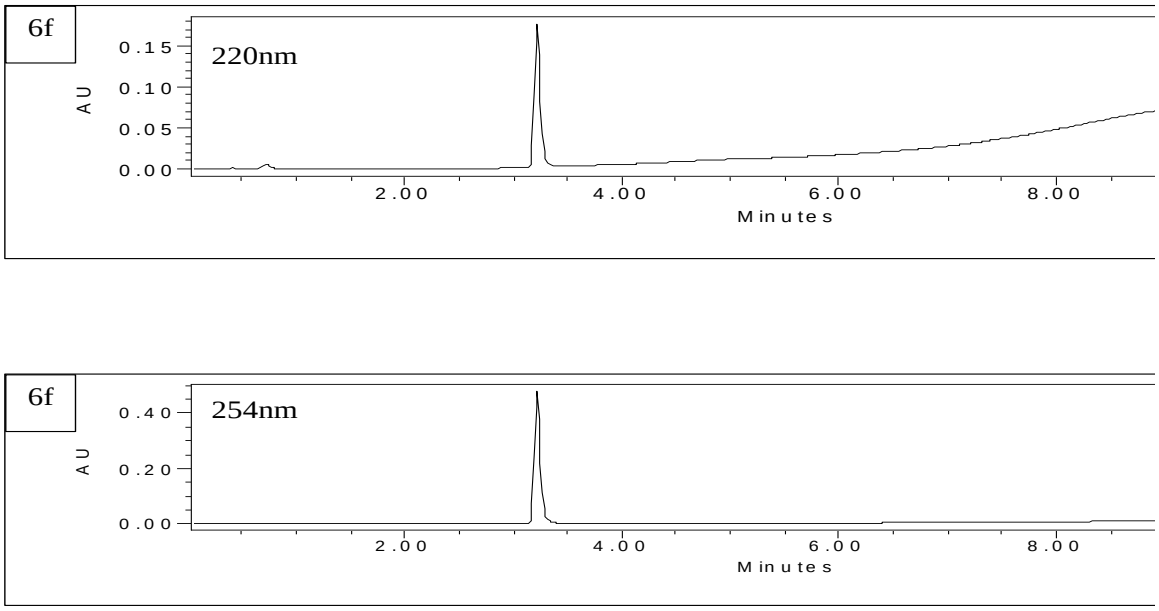


Figure S82. HPLC of compound 6f

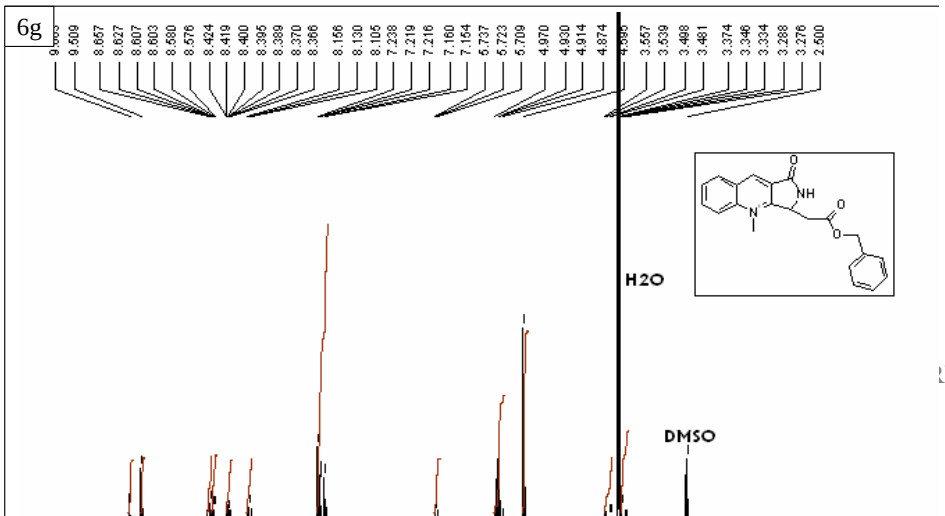


Figure S83. H-NMR of compound 6g in DMSO

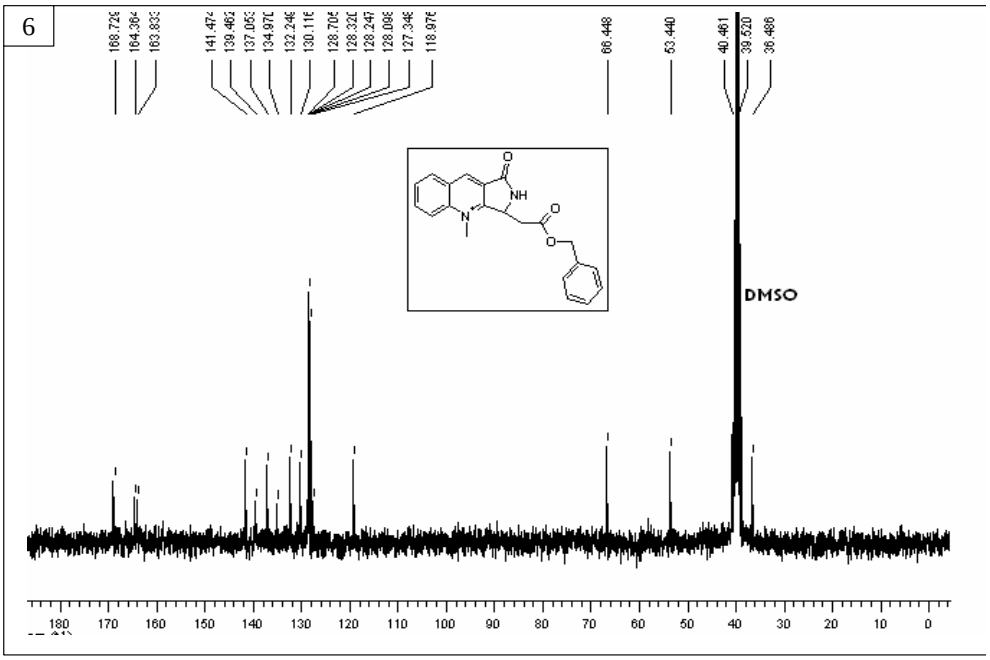
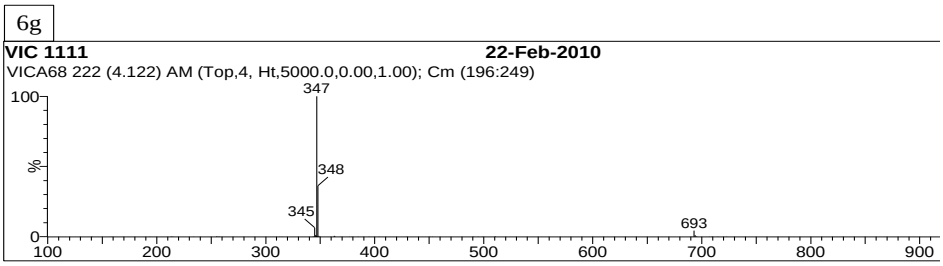


Figure S84. C-NMR of compound 6g in DMSO



6g

VIC 1111 **22-Feb-2010**

VICA68 222 (4.122) AM (Top,4, Ht,5000.0,0.00,1.00); Cm (196:249)

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	345	4.09e3	6.25	4.09															
2:	346	7.30e1	0.11	0.07															
3:	346	5.31e2	0.81	0.53															
4:	346	3.06e2	0.47	0.31															
5:	346	1.50e2	0.23	0.15															
6:	347	3.05e2	0.47	0.30															
7:	347	6.55e4	100.00	65.51															
8:	347	1.25e2	0.19	0.12															
9:	348	2.36e4	36.06	23.62															
10:	349	3.54e2	0.54	0.35															
11:	363	3.24e2	0.49	0.32															

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Figure S85. QTOF-MS of compound 6g

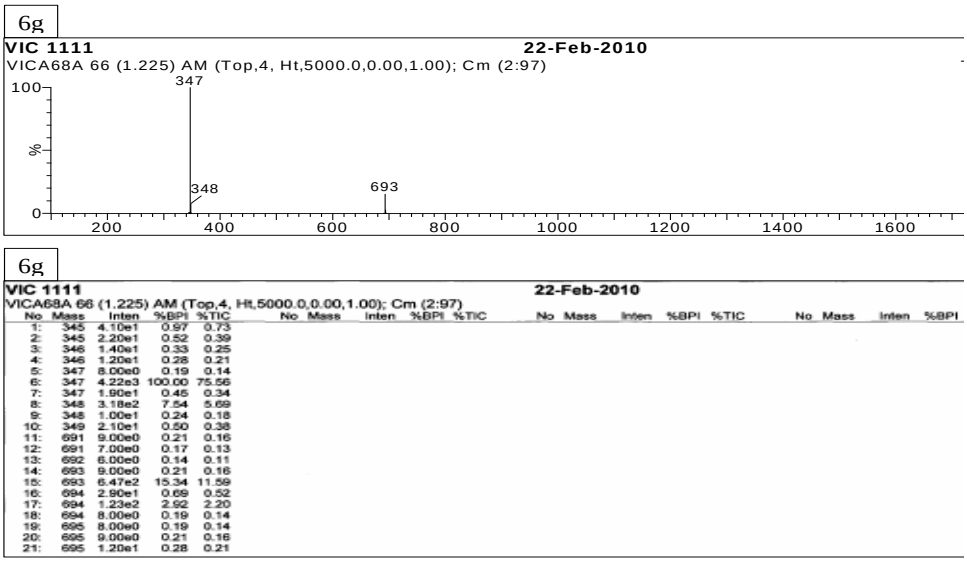


Figure S86. QTOF-MS of compound 6g

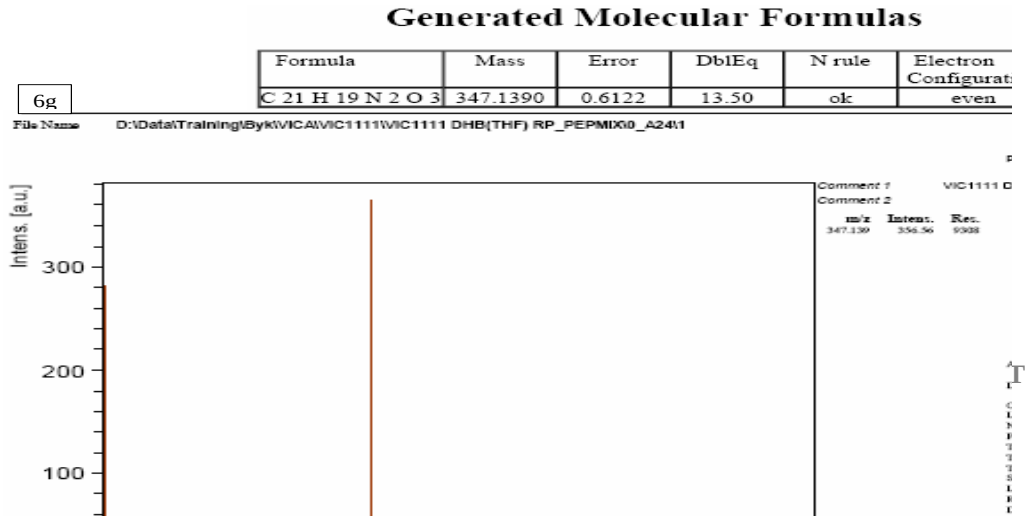


Figure S87. MALDI-TOF MS of compound 6f

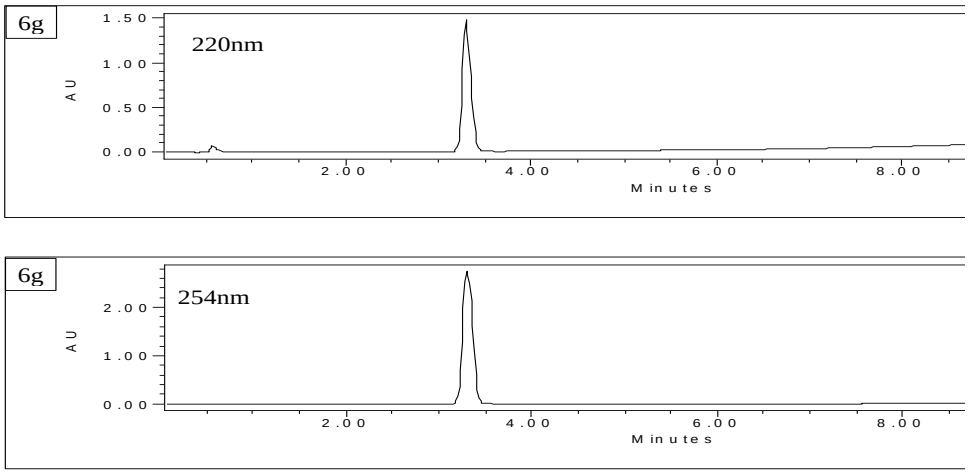
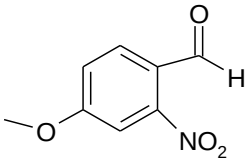


Figure S88. HPLC of compound 6g

4-methoxy-2-nitrobenzaldehyde



^{1}HNMR: (300 MHz, DMSO-d_6), $\delta_{H(ppm)}$: 3.94 (s,3H), 7.42 (dd,1H,J=8.7Hz, J=2.4Hz), 7.62(d,1H, J=2.4Hz),7.96 (s,3H, J=8.7Hz), 10.04 (s,1H).

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^{13}CNMR: (75 MHz, DMSO-d_6), $\delta_{C\ (ppm)}$:56.72, 109.8, 118.58, 122.05, 132.61, 151, 163.54, 188.22. (yield 11%)**MS:** MW=181 g/mol, MH^+ =182. **HPLC:** t_R =2.974 min**.**

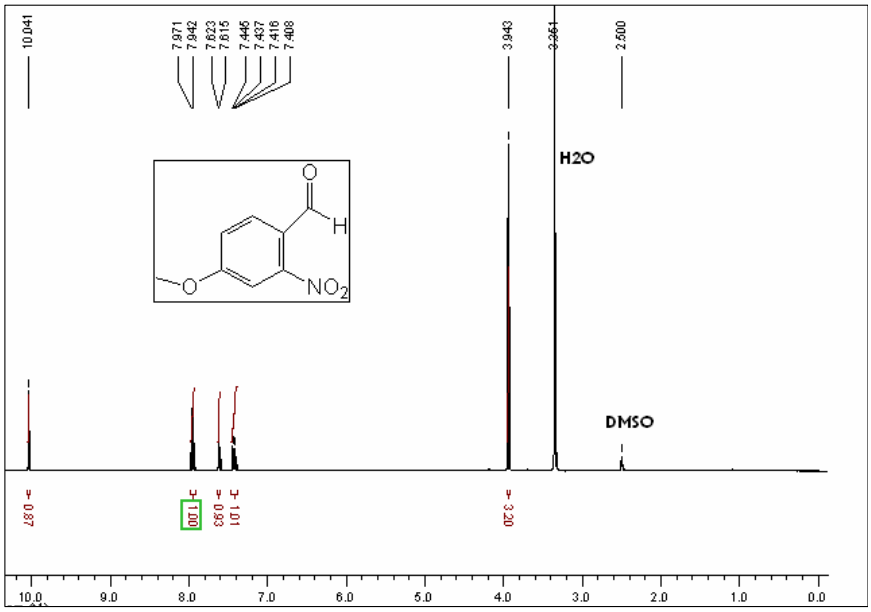

Figure S89. H-NMR of 4-methoxy-2-nitrobenzaldehyde in DMSO**.**

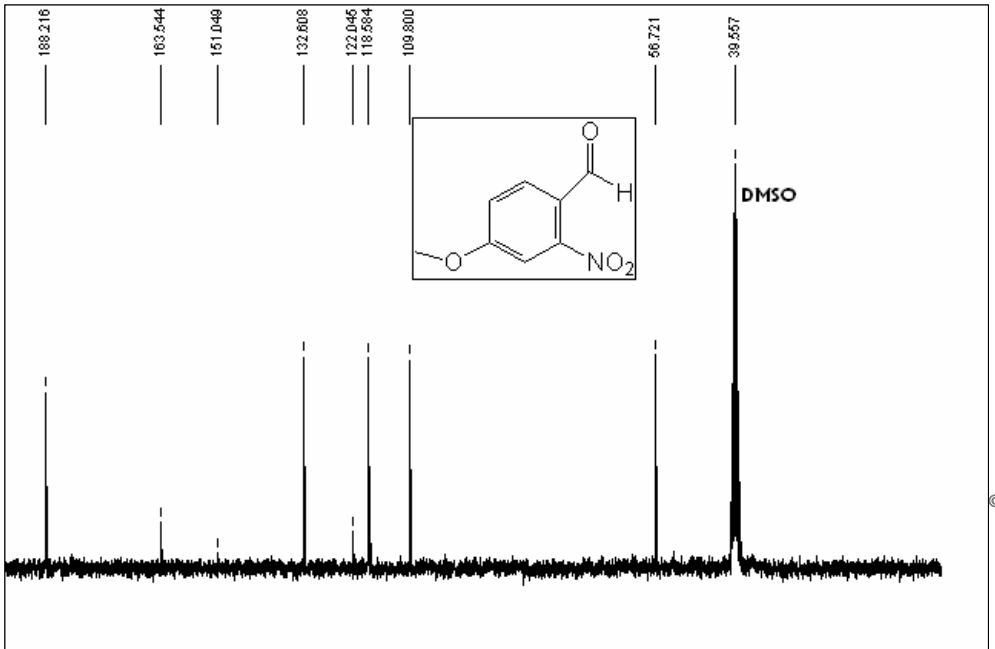

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Figure S90. C-NMR of 4-methoxy-2-nitrobenzaldehyde in DMSO

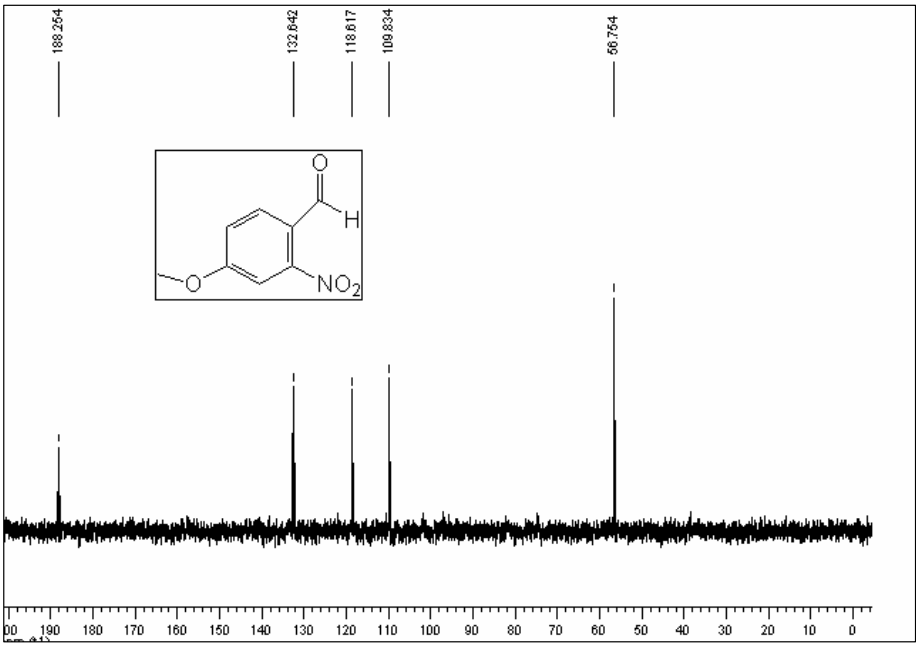


Figure S91. DEPT of 4-methoxy-2-nitrobenzaldehyde in DMSO

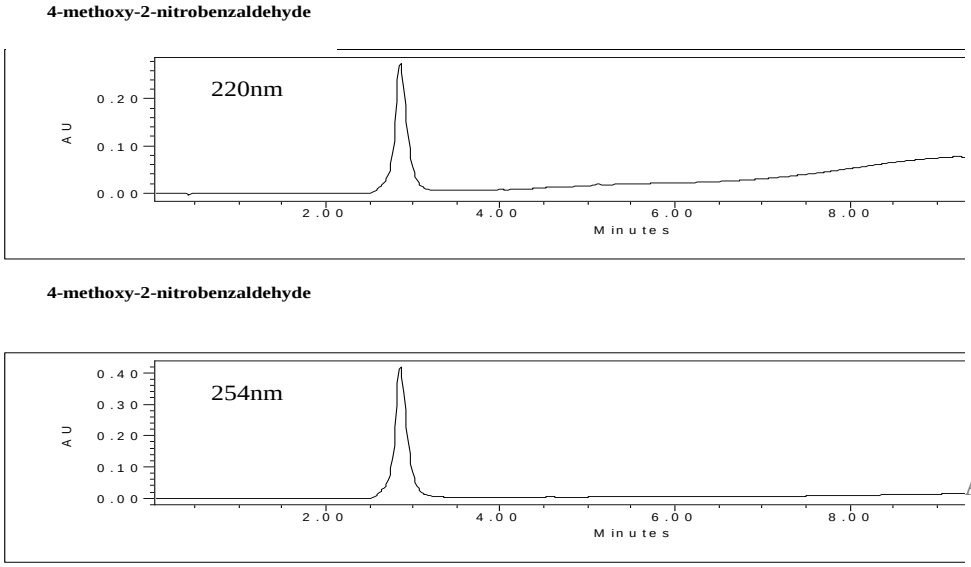
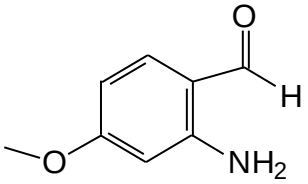


Figure S92. HPLC of 4-methoxy-2-nitrobenzaldehyde

2-amino-4-methoxybenzaldehyde



^{1}HNMR: (300 MHz, DMSO-d_6), $\delta_{H(ppm)}$: 3.75 (s,3H), 6.23 (m,2H), 7.19 (bs, NH), 7.42 (d,1H, J=9.3Hz), 9.63 (s,1H).

^{13}CNMR: (75 MHz, DMSO-d_6), $\delta_{C\ (ppm)}$: 55.17, 97.66, 104.30, 112.92, 137.61, 153.02, 164.71, 191.62. (yield 83%)**. MS:** MW=151.16 g/mol, MH^+ =152. **HPLC:** t_R =2.51 min**.**

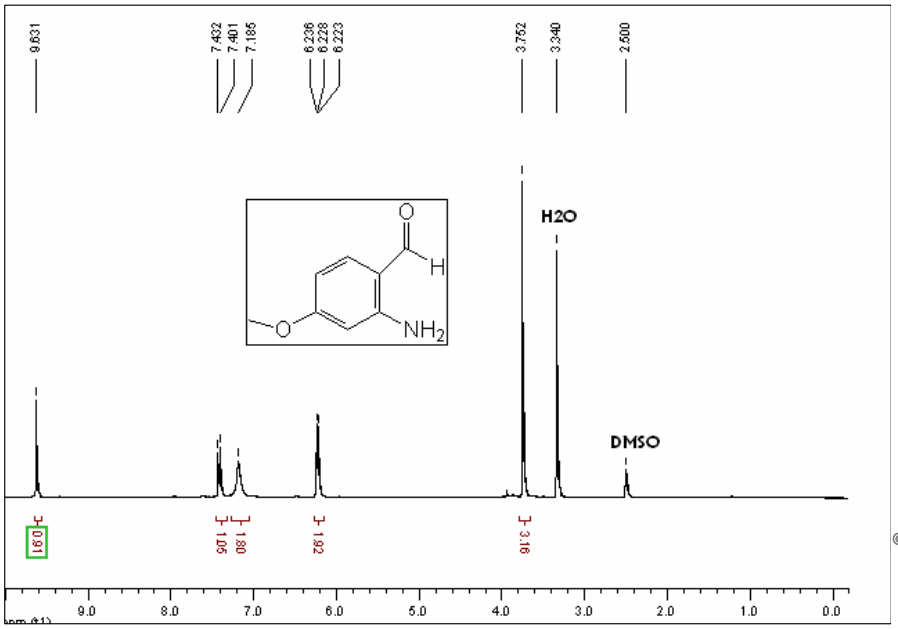


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Figure S93. H-NMR of 4-methoxy-2-nitrobenzaldehyde in DMSO

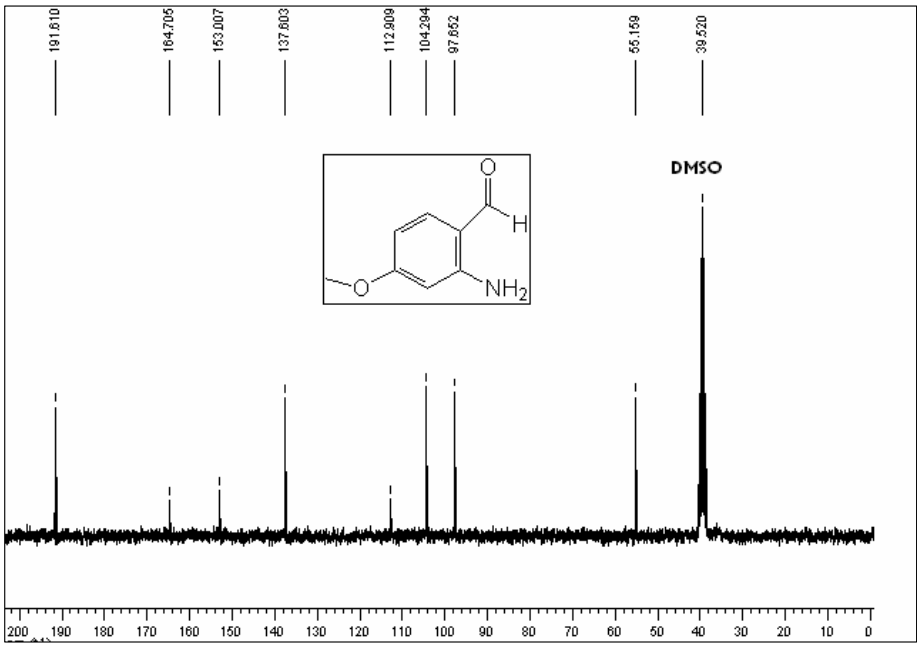

Figure S94. C-NMR of 4-methoxy-2-nitrobenzaldehyde in DMSO

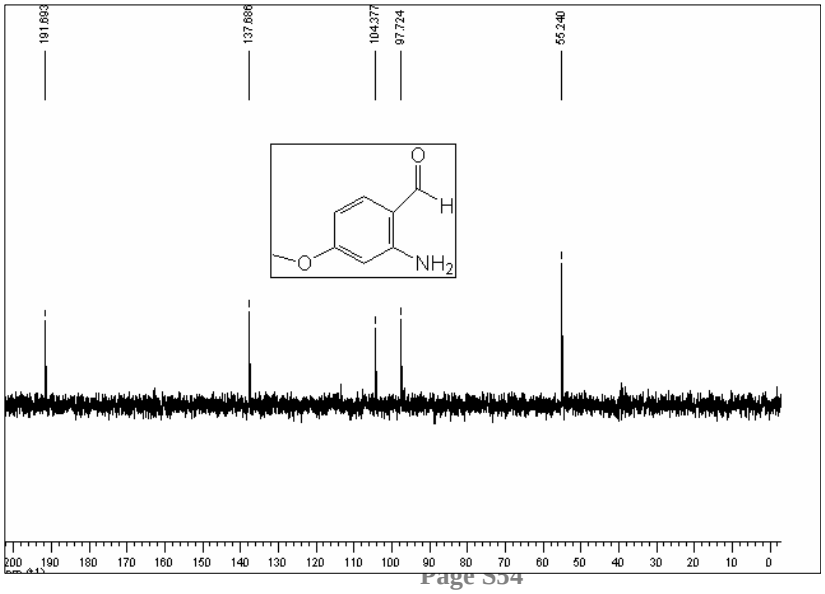

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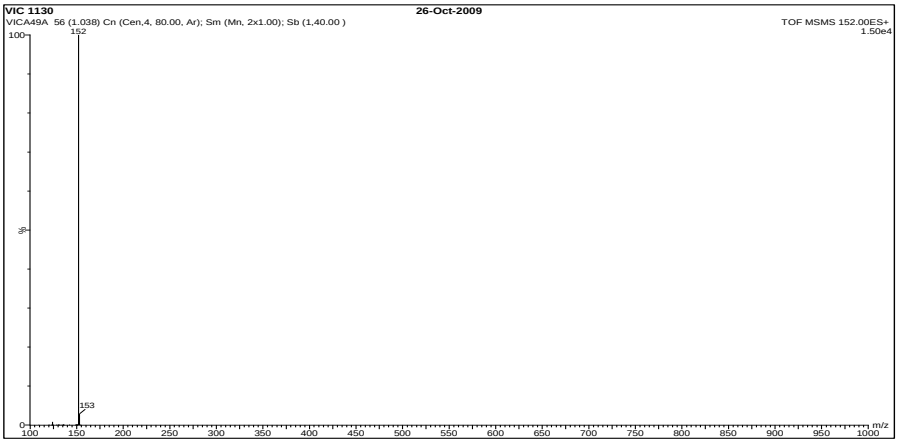
Figure S95. DEPT of 4-methoxy-2-aminobenzaldehyde in DMSO



VIC 1130 **26-Oct-2009**

VICA49A 56 (1.038) Cn (Cen,4, 80.00, Ar); Sm (Mn, 2x1.00); Sb (1,40.00)

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%I
1:	124	1.20e2	0.80	0.77														
2:	150	3.07e1	0.20	0.20														
3:	152	1.50e4	100.00	96.20														
4:	153	4.19e2	2.79	2.69														

Figure S96. QTOF-MS of 4-methoxy-2-aminobenzaldehyde

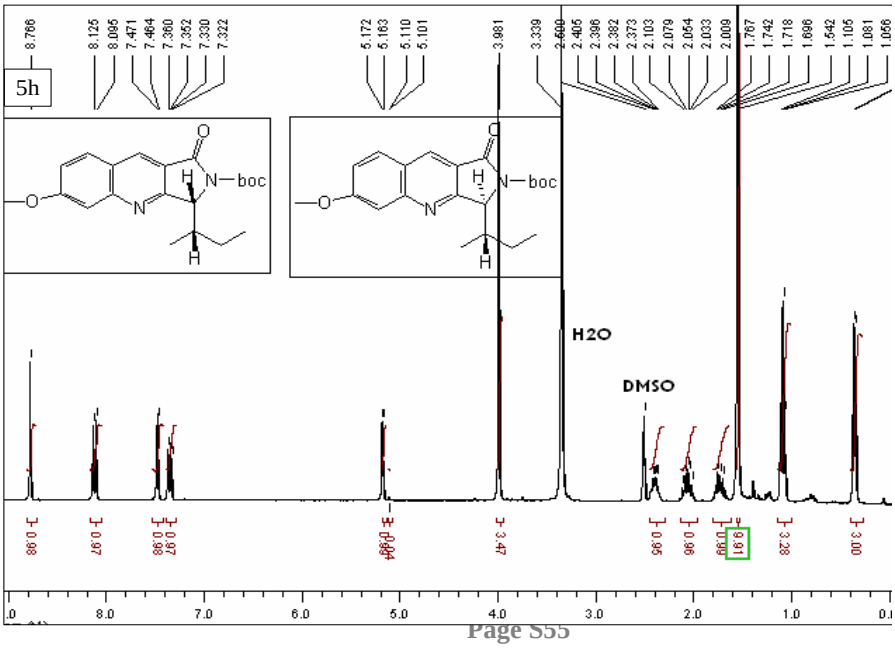


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Figure S97. H-NMR of compound 5h in DMSO

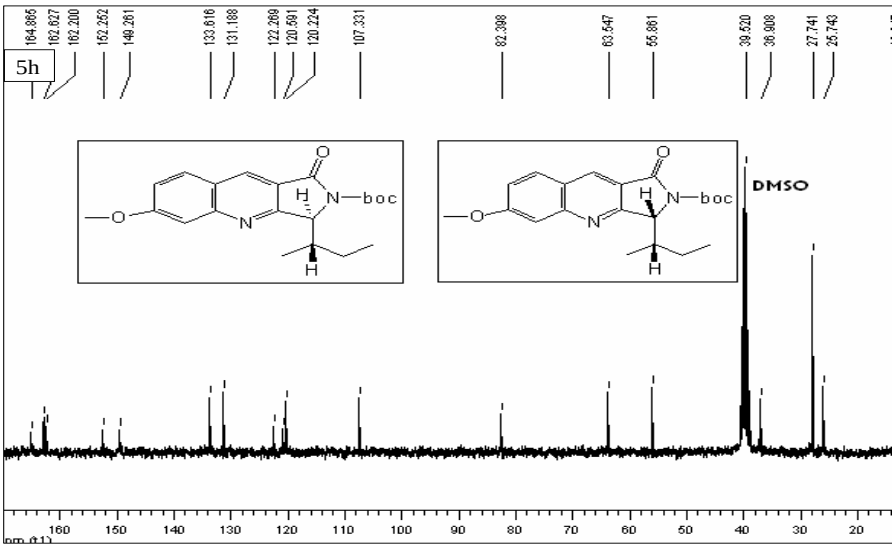


Figure S98. C-NMR of compound 5h in DMSO

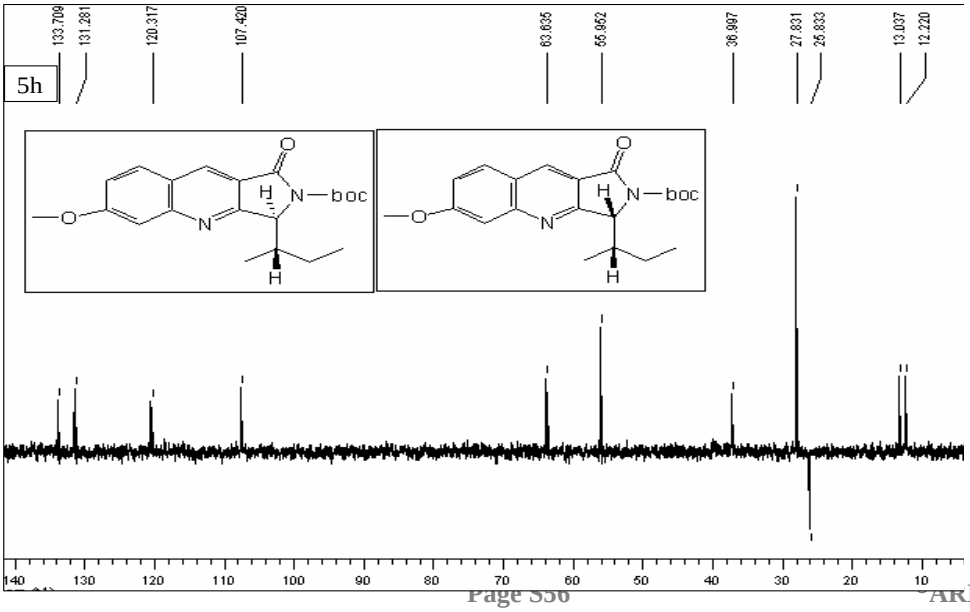


Figure S99. DEPT of compound 5h in DMSO

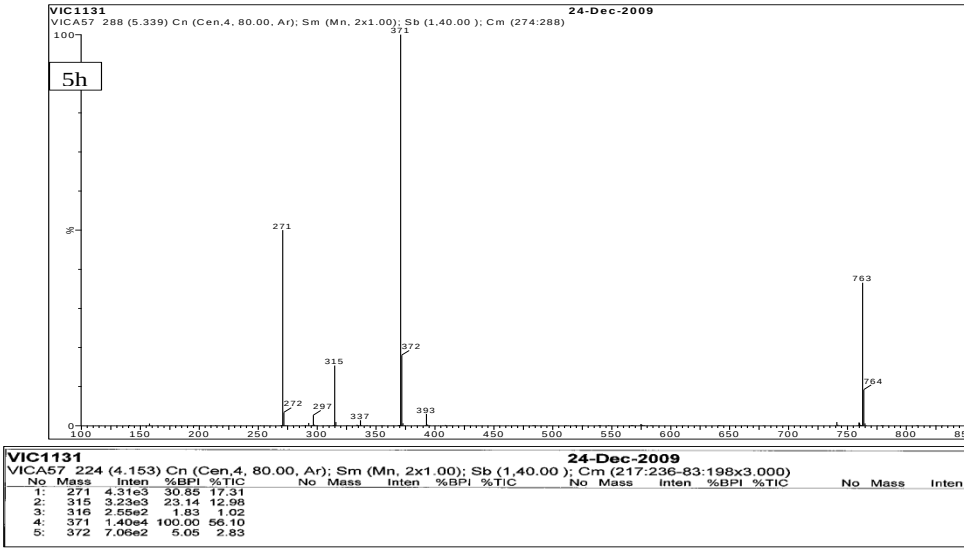
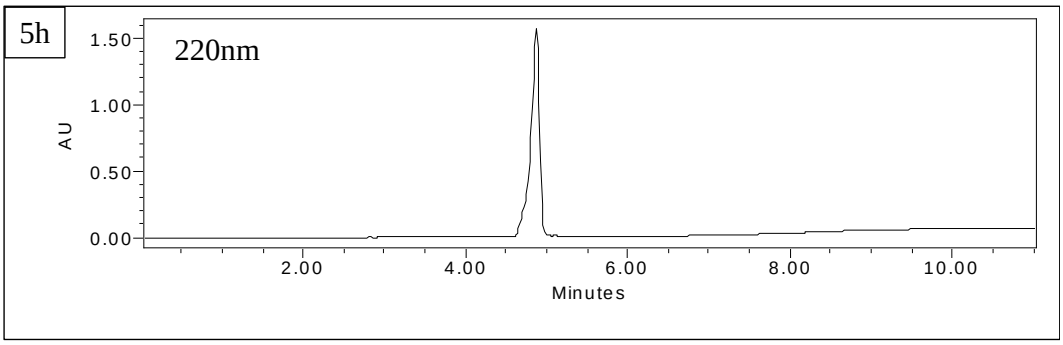


Figure S100. QTOF-MS of compound 5h



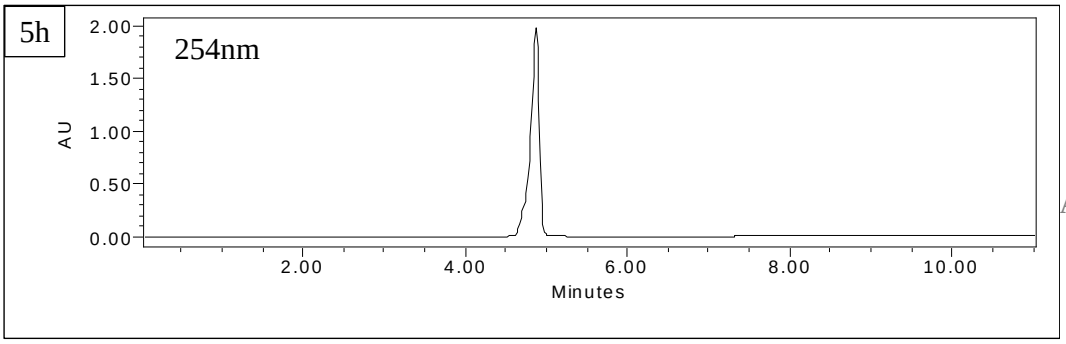


Figure S101. HPLC of compound 5h

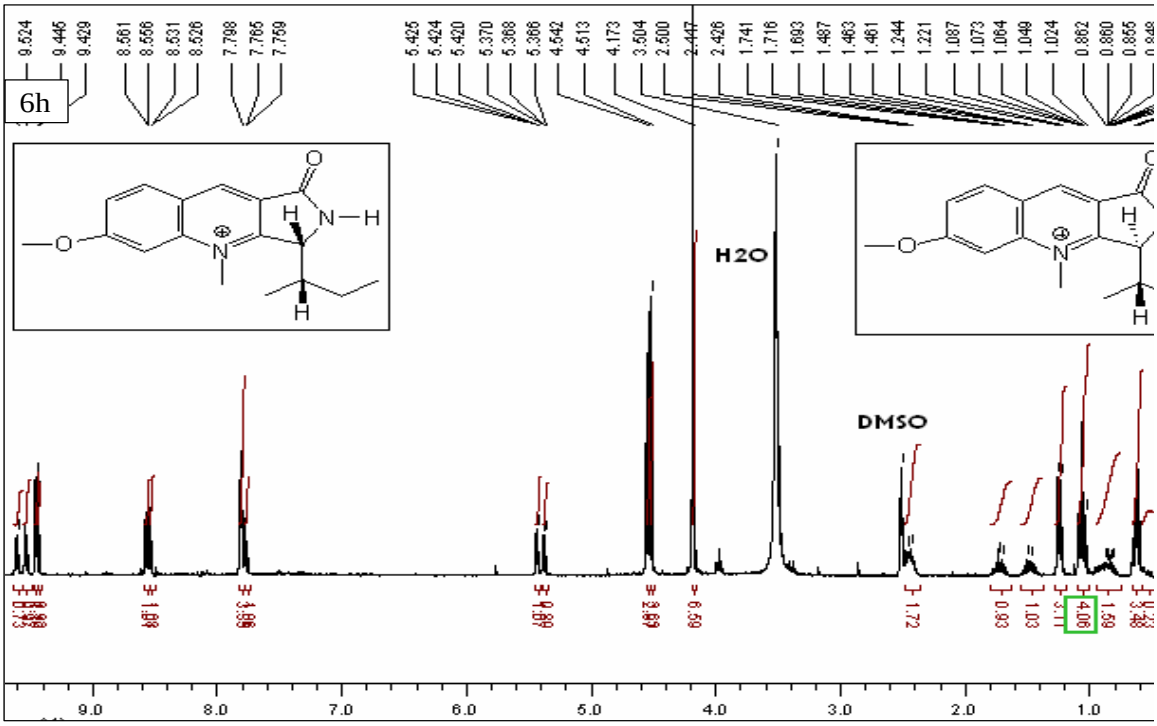


Figure S102. H-NMR of compound 6h in DMSO

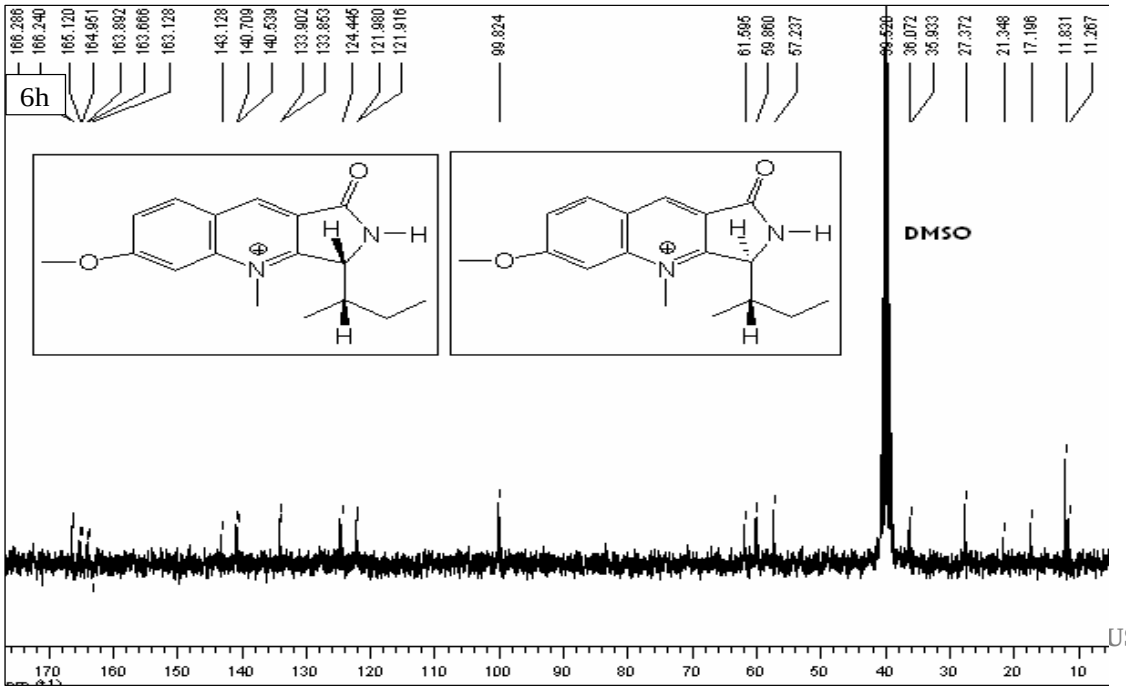


Figure S103. C-NMR of compound 6h in DMSO

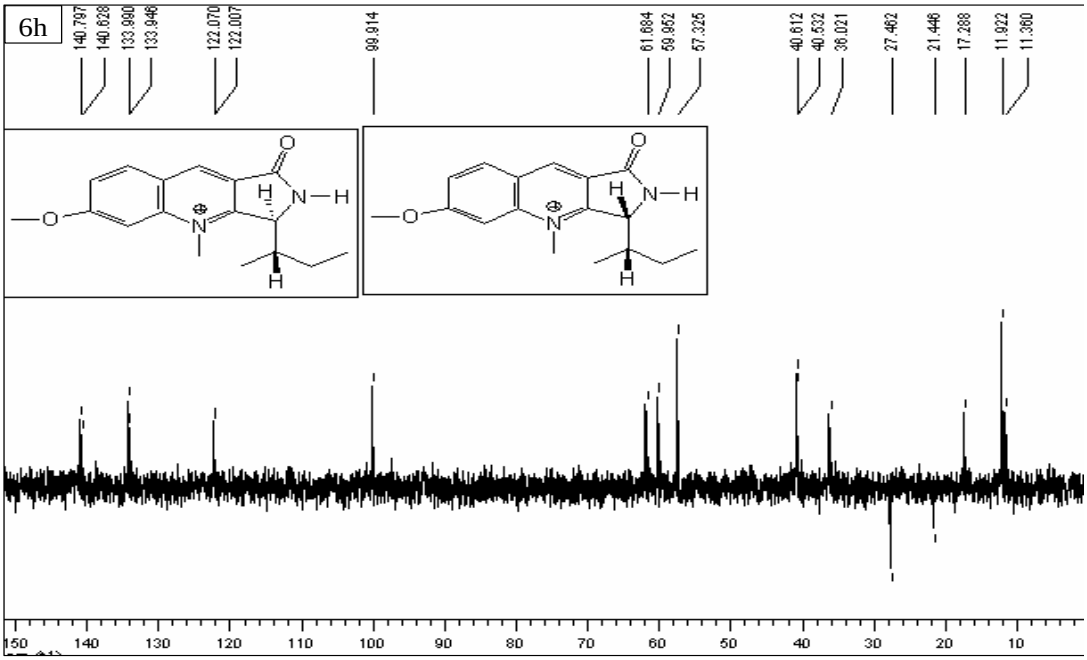


Figure S104. DEPT of compound 6h in DMSO

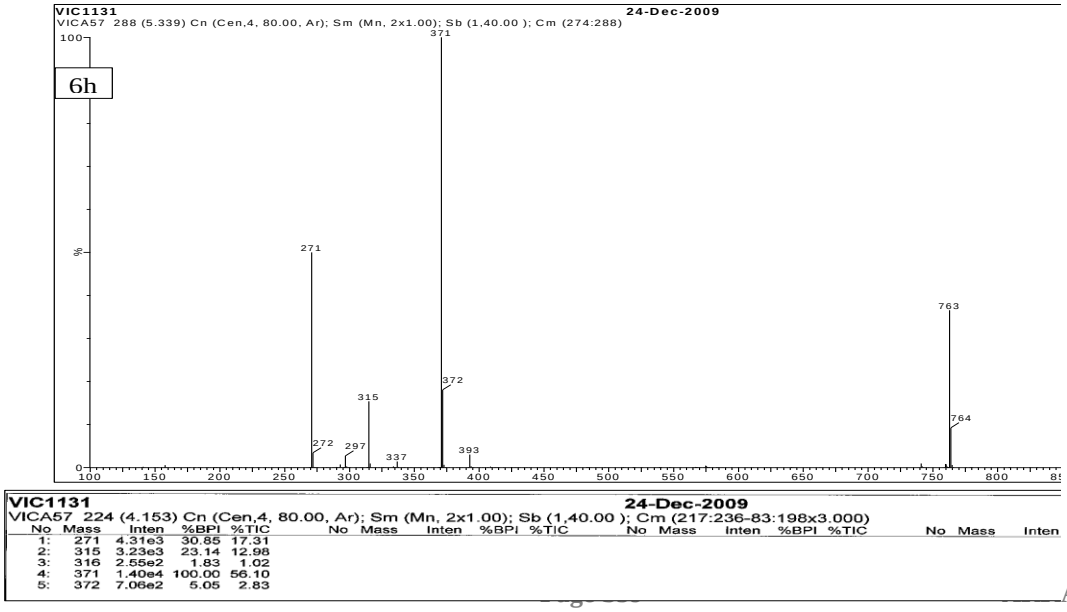
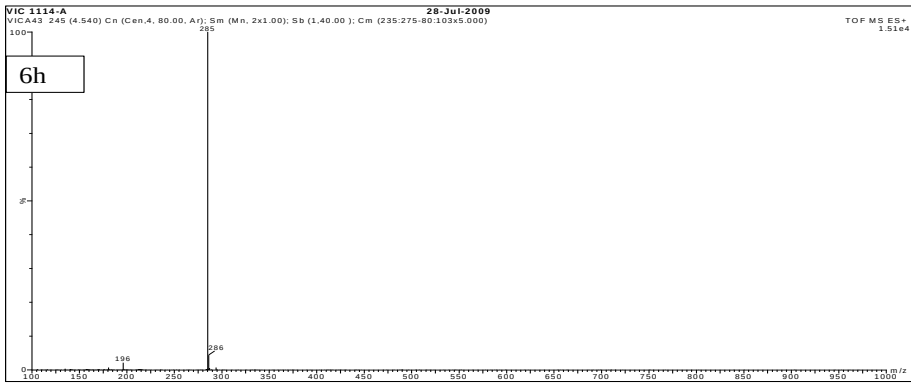


Figure S105. QTOF-MS of compound 6h



VIC 1114-A 28-Jul-2009

VICA43 184 (3.409) Cn (Cen,4, 80.00, Ar); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (184:251-58:126)

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TI
1:	141	3.19e3	11.00	4.51															
2:	158	1.12e4	38.80	15.93															
3:	159	6.61e2	2.28	0.94															
4:	160	4.52e2	1.56	0.64															
5:	196	7.24e2	2.50	1.02															
6:	214	1.33e4	45.90	18.84															
7:	215	1.24e3	4.26	1.75															
8:	216	5.77e2	1.99	0.82															
9:	236	5.20e2	1.79	0.74															
10:	285	2.90e4	100.00	41.04															
11:	286	3.39e3	11.71	4.80															
12:	287	4.04e2	1.39	0.57															

Figure S106. QTOF-MS of compound 6h

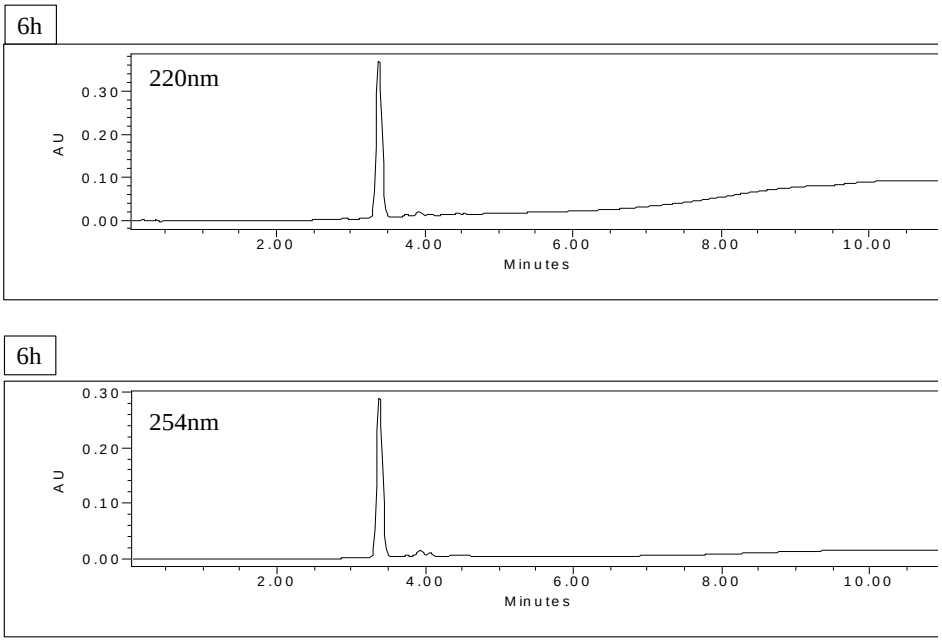


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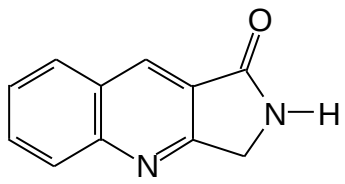
Figure S107. HPLC of compound 6h

5a



^{1}HNMR: (300 MHz, DMSO-d_6), $\delta_{H(ppm)}$: 4.56 (s,2H), 7.68 (t,1H,J=6.9Hz), 7.89 (t,1H,J=6.9Hz), 8.10 (d,1H,J=8.7Hz), 8.21 (d,1H,J=8.7Hz), 8.76 (s,1H), 8.94(bs,N-H) . **^{13}CNMR:** (75 MHz, DMSO-d_6, $\delta_{C(ppm)}$: 46.68, 124.08, 126.62, 127.02, 128.50, 129.87, 131.37, 132.24, 149.12, 163.14, 167.81.(yield 89%) **MS:** MW=184 g/mol, MH^+ =185. **HPLC:** t_R = 3.26min**.**

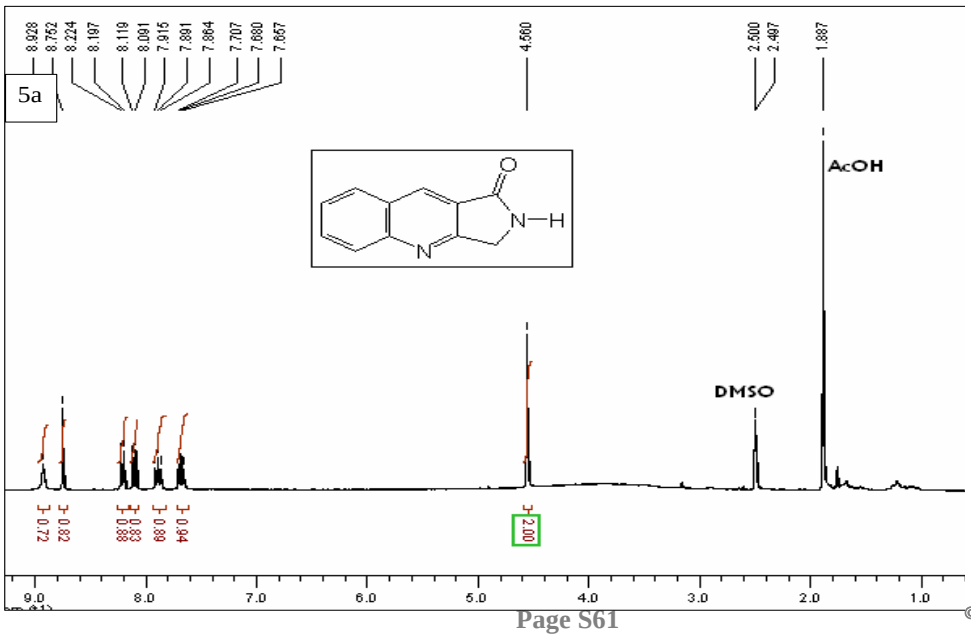


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Figure S108. H-NMR of compound 5a in DMSO

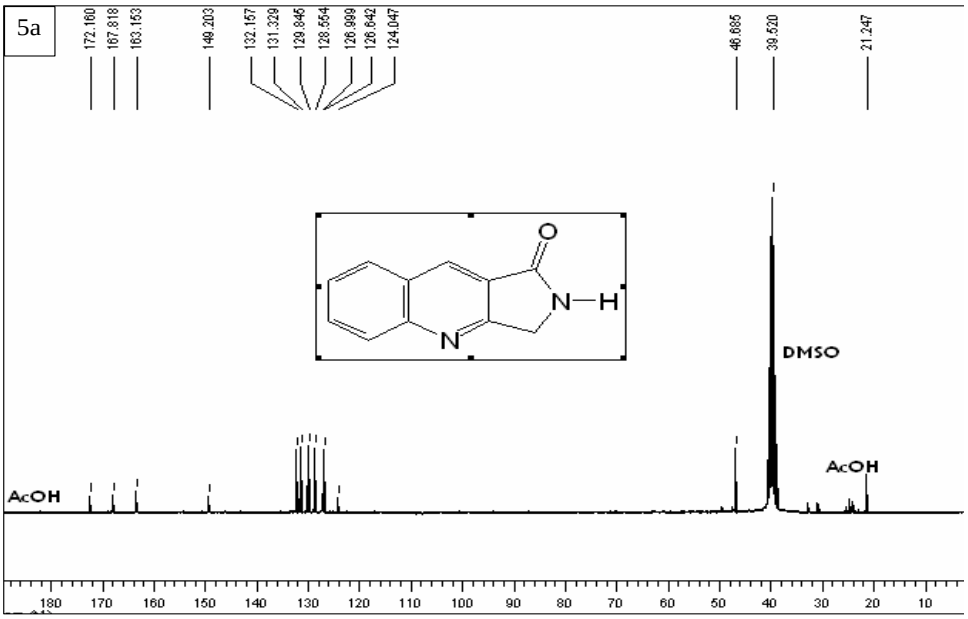

Figure S109. C-NMR of compound 5a in DMSO

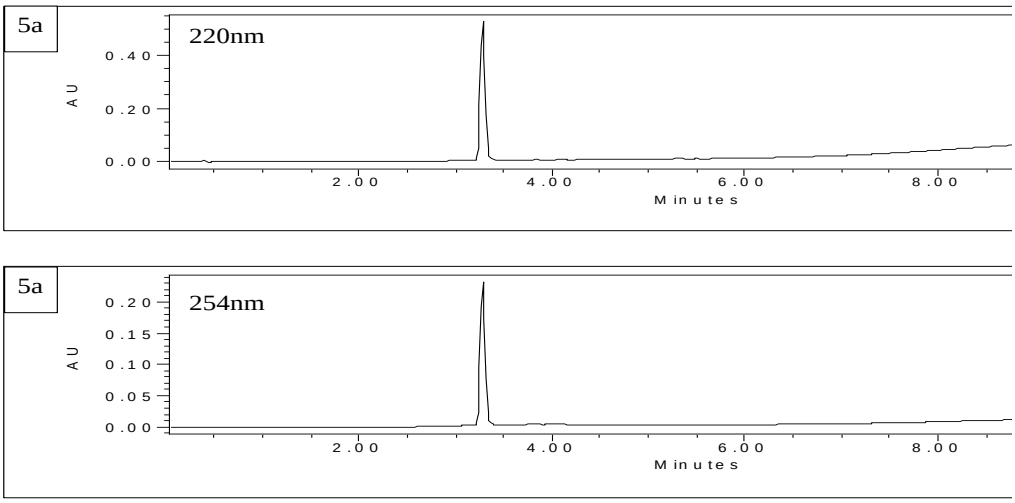

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Figure S110. HPLC of compound 5a

5a

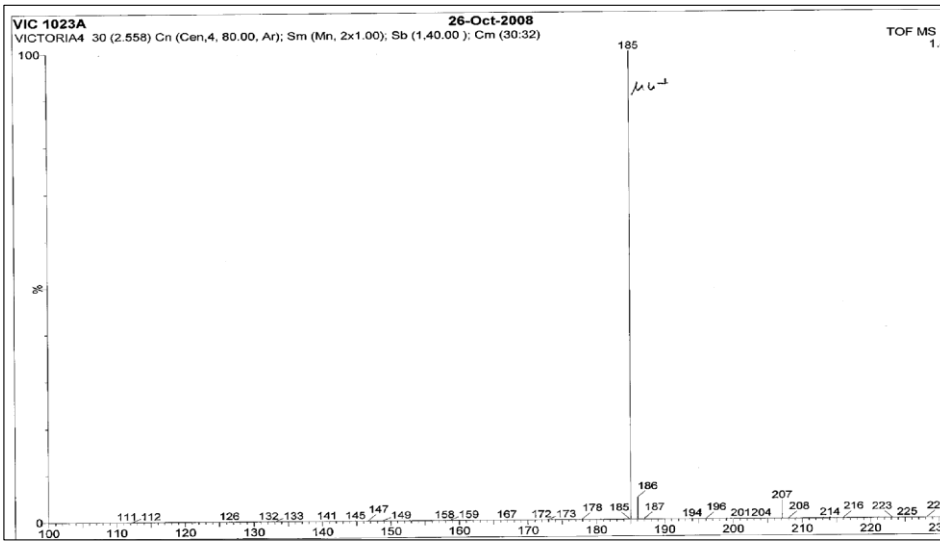


Figure S111. QTOF-MS of compound 5a

5a

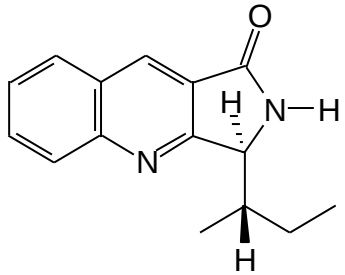
VIC 1023A 26-Oct-2008

VICTORIA4 30 (2.558) Cn (Cen,4, 80.00, Ar); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (30:32) TOF M

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass
1:	111	1.00e0	0.00	0.00	49:	186	8.61e3	4.65	4.11												
2:	112	1.00e0	0.00	0.00	50:	187	1.25e2	0.07	0.06												
3:	126	1.00e0	0.00	0.00	51:	188	1.00e0	0.00	0.00												
4:	132	8.00e0	0.00	0.00	52:	190	7.00e0	0.00	0.00												
5:	132	1.00e0	0.00	0.00	53:	194	3.30e1	0.02	0.02												
6:	133	1.00e0	0.00	0.00	54:	195	1.00e0	0.00	0.00												
7:	136	1.00e0	0.00	0.00	55:	196	2.00e0	0.00	0.00												
8:	140	1.00e0	0.00	0.00	56:	199	1.00e0	0.00	0.00												
9:	141	7.00e0	0.00	0.00	57:	199	1.00e0	0.00	0.00												
10:	141	3.00e0	0.00	0.00	58:	201	1.10e1	0.01	0.01												
11:	145	2.00e0	0.00	0.00	59:	203	1.00e0	0.00	0.00												
12:	145	3.00e0	0.00	0.00	60:	204	2.20e1	0.01	0.01												
13:	147	1.00e0	0.00	0.00	61:	207	7.14e3	3.86	3.41												
14:	149	1.00e0	0.00	0.00	62:	208	1.63e2	0.09	0.08												
15:	153	1.00e0	0.00	0.00	63:	209	7.00e0	0.00	0.00												
16:	156	1.00e0	0.00	0.00	64:	212	7.00e0	0.00	0.00												
17:	158	5.10e1	0.03	0.02	65:	213	1.00e0	0.00	0.00												
18:	159	3.00e1	0.02	0.01	66:	214	8.89e-1	0.00	0.00												
19:	160	1.00e0	0.00	0.00	67:	214	2.06e2	0.11	0.10												
20:	161	1.00e0	0.00	0.00	68:	214	6.43e1	0.03	0.03												
21:	167	1.00e0	0.00	0.00	69:	215	3.00e0	0.00	0.00												
22:	172	4.00e0	0.00	0.00	70:	216	1.68e2	0.09	0.08												
23:	173	1.00e0	0.00	0.00	71:	216	2.00e0	0.00	0.00												
24:	173	2.00e0	0.00	0.00	72:	217	3.00e0	0.00	0.00												
25:	174	1.00e0	0.00	0.00	73:	217	2.00e0	0.00	0.00												
26:	178	2.00e0	0.00	0.00	74:	217	1.00e0	0.00	0.00												
27:	183	2.00e0	0.00	0.00	75:	219	1.00e0	0.00	0.00												
28:	184	1.22e0	0.00	0.00	76:	221	1.00e0	0.00	0.00												
29:	184	7.22e0	0.00	0.00	77:	222	1.00e0	0.00	0.00												
30:	184	4.00e0	0.00	0.00	78:	223	7.00e0	0.00	0.00												
31:	184	7.11e0	0.00	0.00	79:	224	1.00e0	0.00	0.00												
32:	184	2.00e0	0.00	0.00	80:	225	5.00e0	0.00	0.00												
33:	184	6.22e0	0.00	0.00	81:	225	2.00e0	0.00	0.00												
34:	184	5.67e0	0.00	0.00	82:	225	8.89e-1	0.00	0.00												
35:	184	3.78e0	0.00	0.00	83:	225	5.43e1	0.03	0.03												
36:	184	2.89e0	0.00	0.00	84:	226	1.01e1	0.01	0.00												
37:	184	1.69e1	0.01	0.01	85:	226	8.89e-1	0.00	0.00												
38:	184	3.78e0	0.00	0.00	86:	226	2.00e0	0.00	0.00												
39:	185	1.17e1	0.01	0.01	87:	227	1.30e1	0.01	0.01												
40:	185	2.33e1	0.01	0.01	88:	228	2.47e1	0.01	0.01												
41:	185	2.04e1	0.01	0.01	89:	228	2.62e1	0.01	0.01												
42:	185	1.20e1	0.01	0.01	90:	229	5.00e0	0.00	0.00												
43:	185	5.64e1	0.03	0.03	91:	229	1.00e0	0.00	0.00												
44:	185	3.53e1	0.02	0.02																	
45:	185	1.85e5	100.00	88.47																	
46:	185	1.00e0	0.00	0.00																	
47:	186	1.00e0	0.00	0.00																	
48:	186	1.00e0	0.00	0.00																	

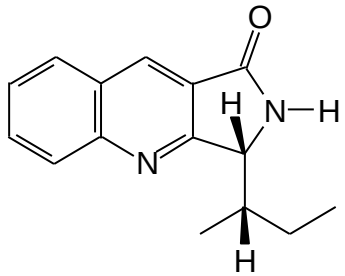
Figure S112. QTOF-MS of compound 5a

5b(major SS)



^{1}HNMR: (300 MHz, DMSO-d_6, $\delta_{H(ppm)}$: 0.49 (d,3H,J=6.6Hz), 0.98 (t,3H, J=7.5Hz), 1.33 (m,1H), 1.60 (m,1H), , 2.24 (m,1H), 4.76 (d,1H,J=2.1Hz), 7.67 (m,1H), 7.87 (m,1H), 8.11 (d,1H,J=8.1Hz), 8.19 (d,1H,J=8.1Hz), 8.71 (s,1H), 9.01 (bs,1H). **^{13}CNMR:** (75 MHz, DMSO-d_6, $\delta_{C(ppm)}$: 11.98, 12.64, 15.42, 26.35, 37.32, 60.82, 83.73, 124.45, 126.63, 128.69, 129.79, 131.28, 131.91, 149.19, 165.49, 167.80. (yield 50.8%) **MS:** MW=240 g/mol, MH^+ =241. **HPLC:** t_R = 3.88min**.**

5b(minor RS)



^{1}HNMR: (300 MHz, DMSO-d_6, $\delta_{H(ppm)}$: 0.77 (t,3H, J=7.5Hz), 0.93 (d,3H,J=7.2Hz), 0.92 (m,1H), 1.17 (m,1H), 2.16 (m,1H), 4.69 (d,1H,J=2.7Hz), 7.67 (m,1H), 7.87 (m,1H), 8.11

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(d,1H,J=8.1Hz), 8.19 (d,1H,J=8.1Hz), 8.70 (s,1H), 9.04 (bs,1H). **^{13}CNMR:** (75 MHz, DMSO-d_6, $\delta_{C(ppm)}$: 11.79, 12.64, 15.42, 23.37, 37.55, 62.01, 83.73, 124.62, 127.09, 128.79, 129.79, 131.28, 131.84, 149.06, 165.09, 167.49. (yield 43.2%) **MS:** MW=240 g/mol, MH^+ =241. **HPLC:** t_R =3.88 min**.**

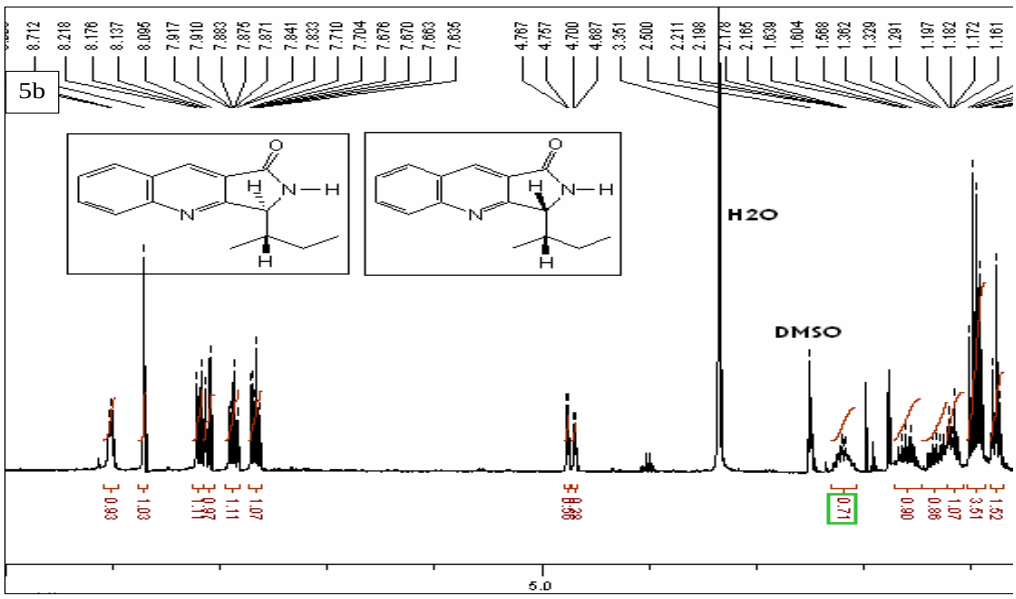


Figure S113. H-NMR of compound 5b in DMSO

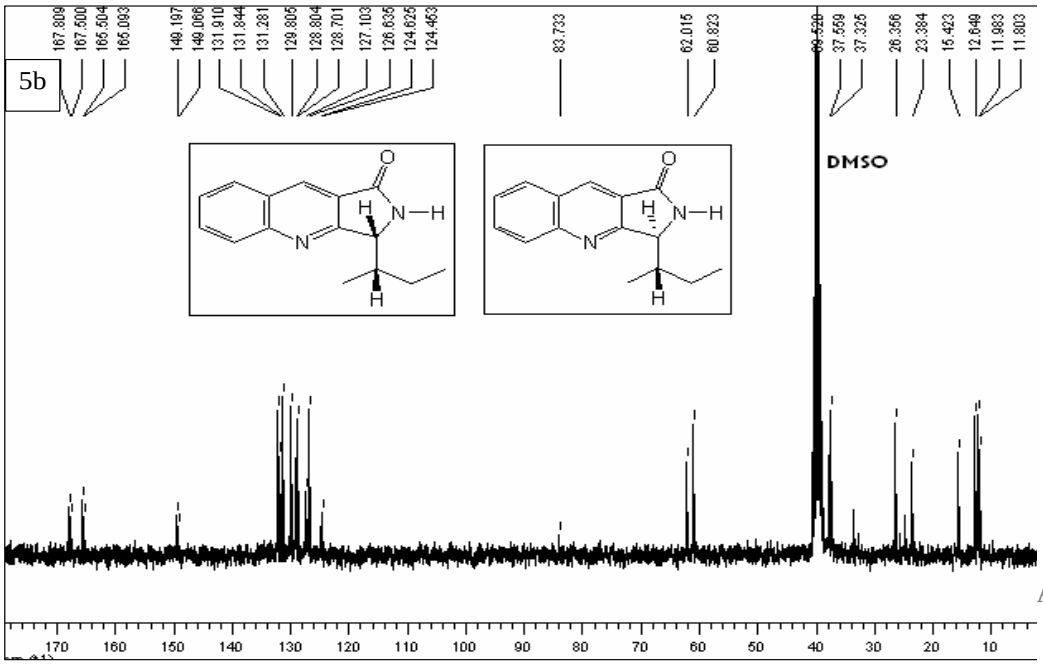


Figure S114. C-NMR of compound 5b in DMSO

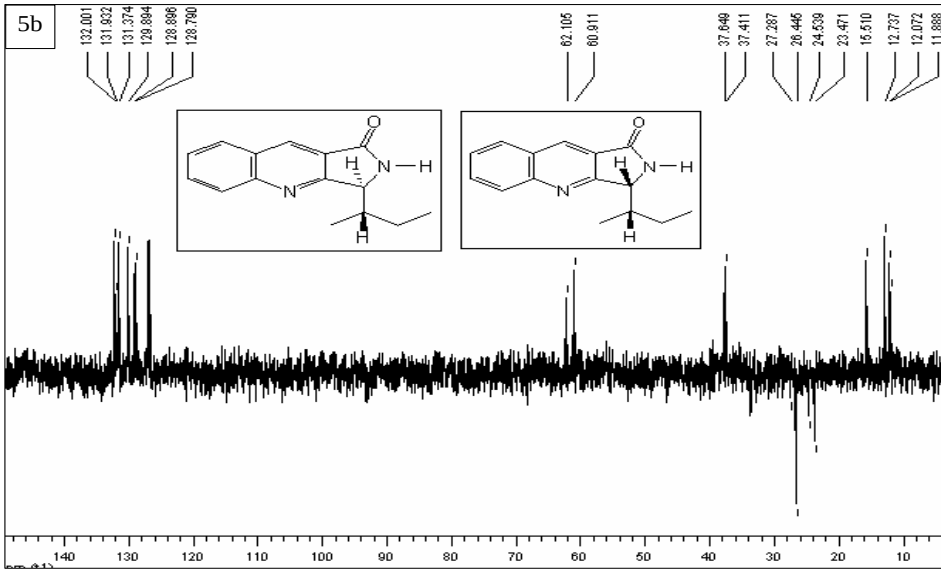
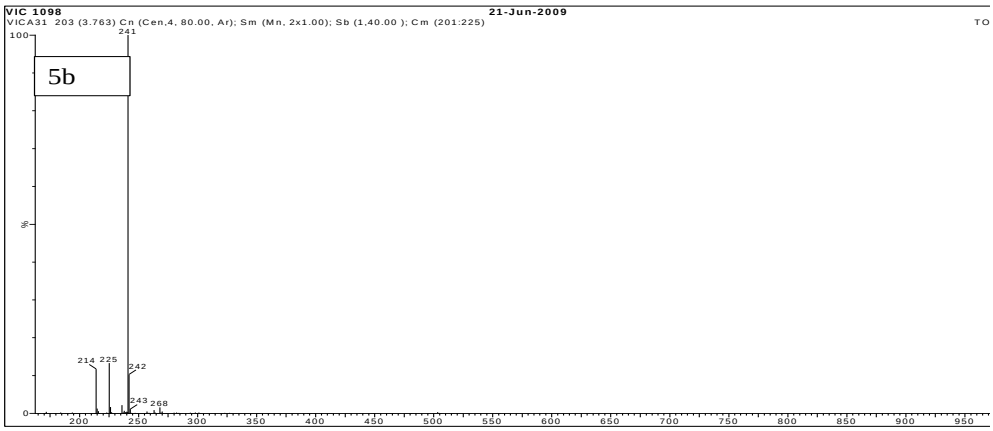


Figure S115. DEPT of compound 5b in DMSO



VIC 1098 21-Jun-2009
VICA31 185 (3.429) Cn (Cen,4, 80.00, Ar); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (173:186-43:56)

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI
1:	158	6.60e2	1.30	0.94									
2:	214	8.89e2	1.75	1.27									
3:	225	6.23e3	12.24	8.90									
4:	226	8.02e2	1.57	1.14									
5:	241	5.09e4	100.00	72.69									
6:	242	5.17e3	10.15	7.38									
7:	243	5.49e2	1.08	0.78									

Figure S116. QTOF-MS of compound 5b

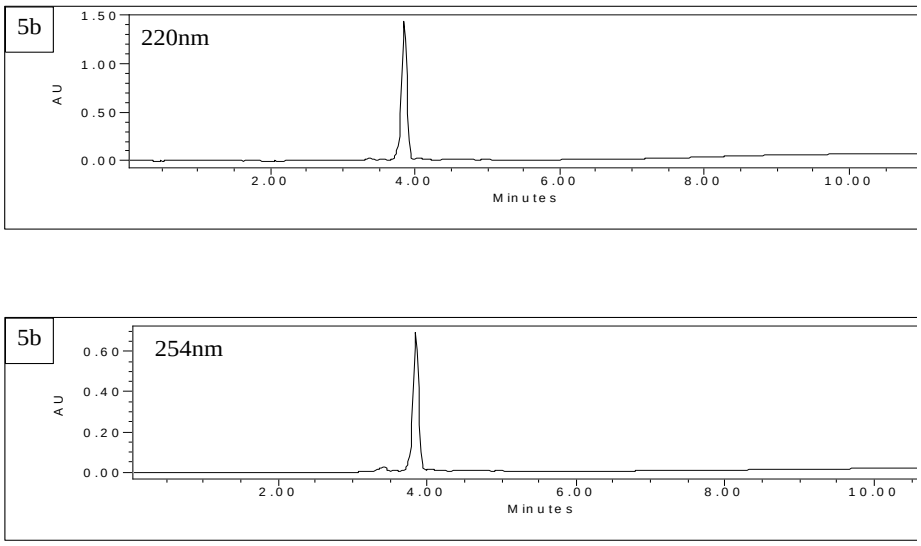
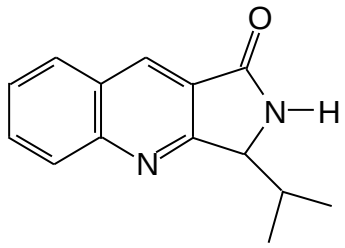


Figure S117. HPLC of compound 5b

5c



^{1}HNMR: (300 MHz, DMSO-d_6), $\delta_{H(ppm)}$: 0.65 (d,3H, J=6.9Hz), 1.06 (d,3H,J=6.9Hz), 2.43 (m,1H), 4.65 (d,1H,J=3.3Hz), 7.67 (m,1H), 7.87 (m,1H), 8.11 (d,1H,J=8.4Hz), 8.19

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(d,1H,J=8.1Hz), 8.72 (s,1H), 9.04 (bs,1H). **^{13}CNMR:** (75 MHz, DMSO-d$_6$, $\delta_{C(ppm)}$: 15.75, 19.21, 30.77, 62.48, 124.39, 126.65, 127.09, 128.76, 129.78, 131.26, 131.90, 149.12, 165.15, 167.68. (yield 63%) **MS:** MW=226 g/mol, MH$^+$ =227. **HPLC:** t$_R$ =3.67 min**.**

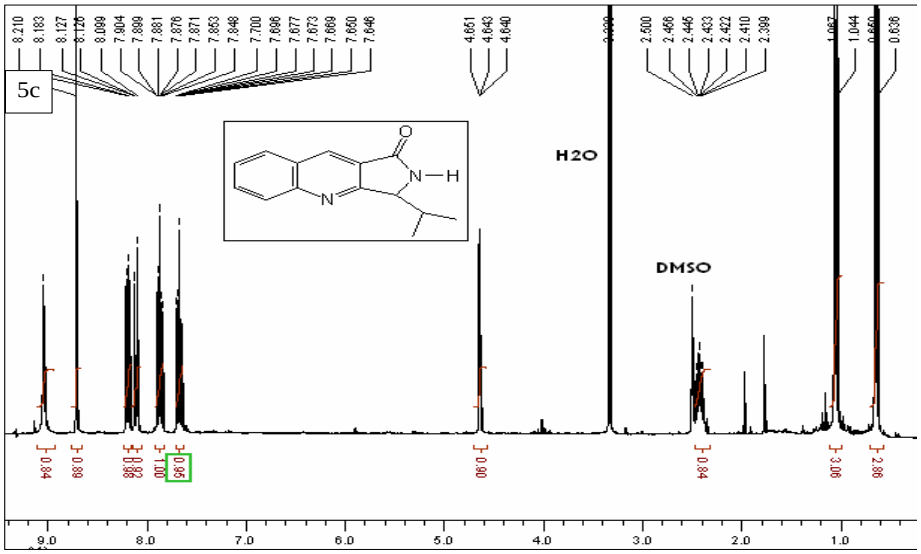

Figure S118. H-NMR of compound 5c in DMSO

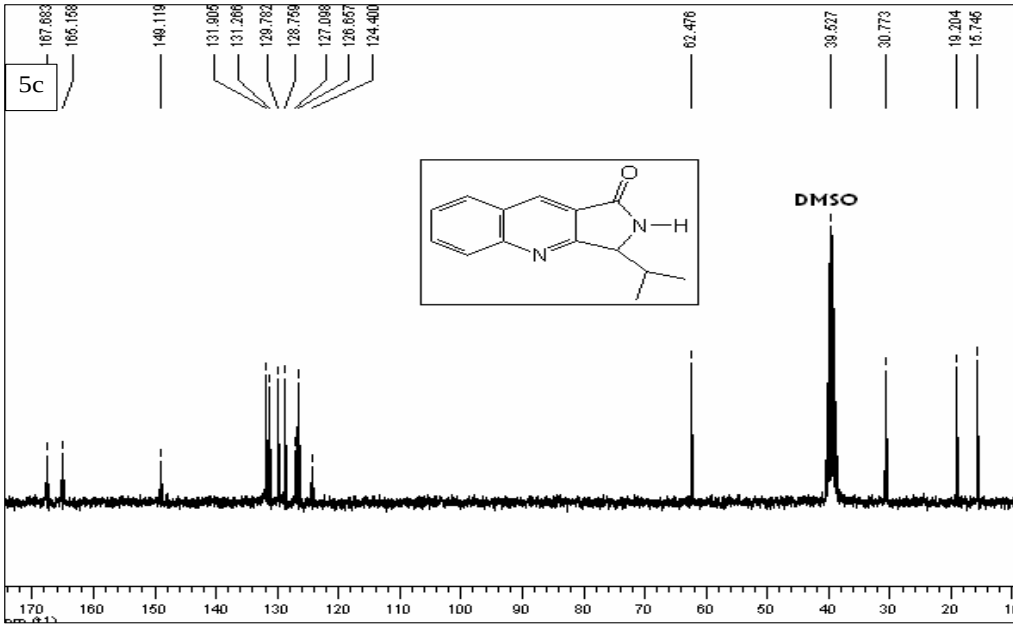

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Figure S119. C-NMR of compound 5c in DMSO

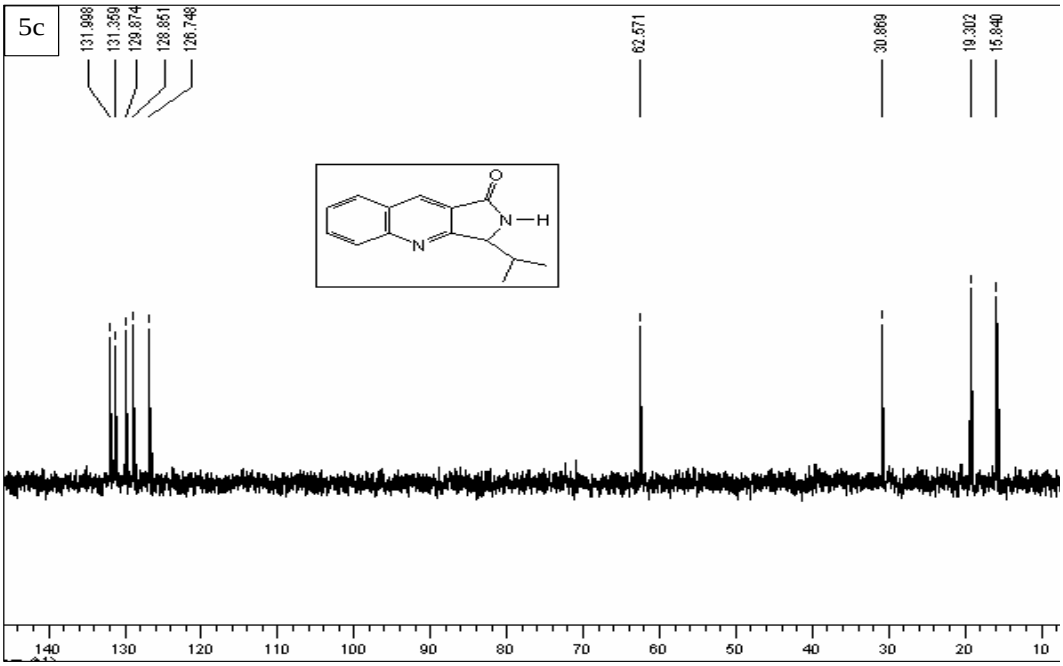
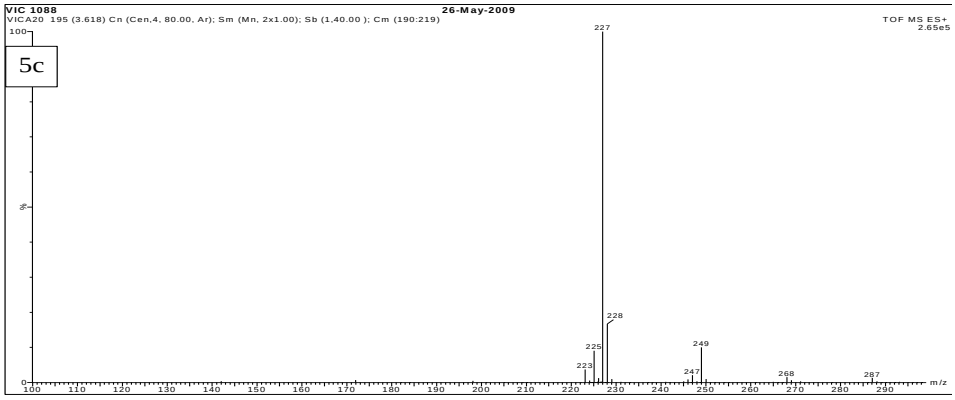


Figure S120. DEPT of compound 5c in DMSO



VIC 1088 26-May-2009

VICA20 157 (2.913) Cn (Cen,4, 80.00, Ar); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (154:180-15:53)

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%B
1:	223	7.74e3	2.97	1.66														
2:	225	1.87e4	7.19	4.02														
3:	227	2.60e5	100.00	55.99														
4:	228	4.34e4	16.68	9.34														
5:	247	4.83e3	1.86	1.04														
6:	249	2.08e4	7.98	4.47														

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Figure S121. QTOF-MS of compound 5c

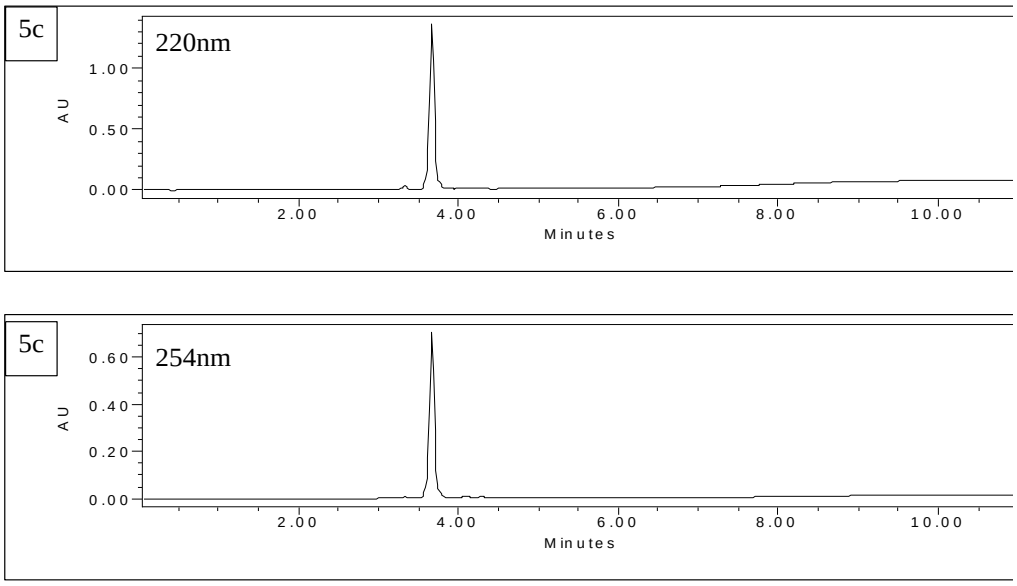
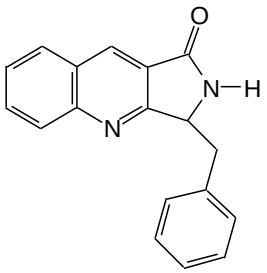


Figure S122. HPLC of compound 5c

5d



^{1}HNMR: (300 MHz, DMSO-d_6), $\delta_{H(ppm)}$: 3.25 (m,2H), 5.09 (t,1H,J=4.8Hz), 7.05 (m,5H),7.67 (m,1H), 7.92 (m,1H), 8.15 (d,1H,J=8.7Hz), 8.19 (m,1H,J=8.1Hz), 8.56 (s.1H), 9.01 (NH, bs) . **^{13}CNMR:** (75 MHz, DMSO-d_6, $\delta_{C(ppm)}$:38.07, 57.94, 124.21, 126.26,

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126.71, 127.00, 127.72, 128.69, 129.76, 131.32, 131.88, 135.81, 149.04, 164.88, 166.96. (yield 88.7%)**MS:** MW=274 g/mol, MH^+ =275.

HPLC: t_R = 3.97 min**.**

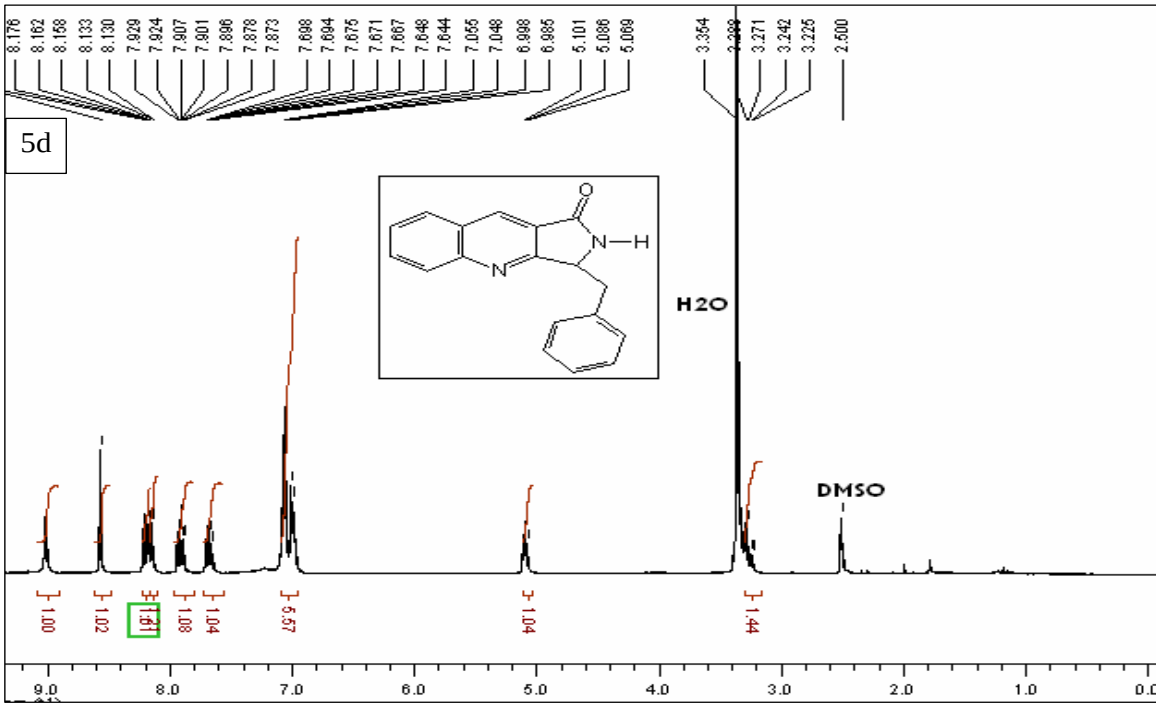

Figure S123. H-NMR of compound 5d in DMSO

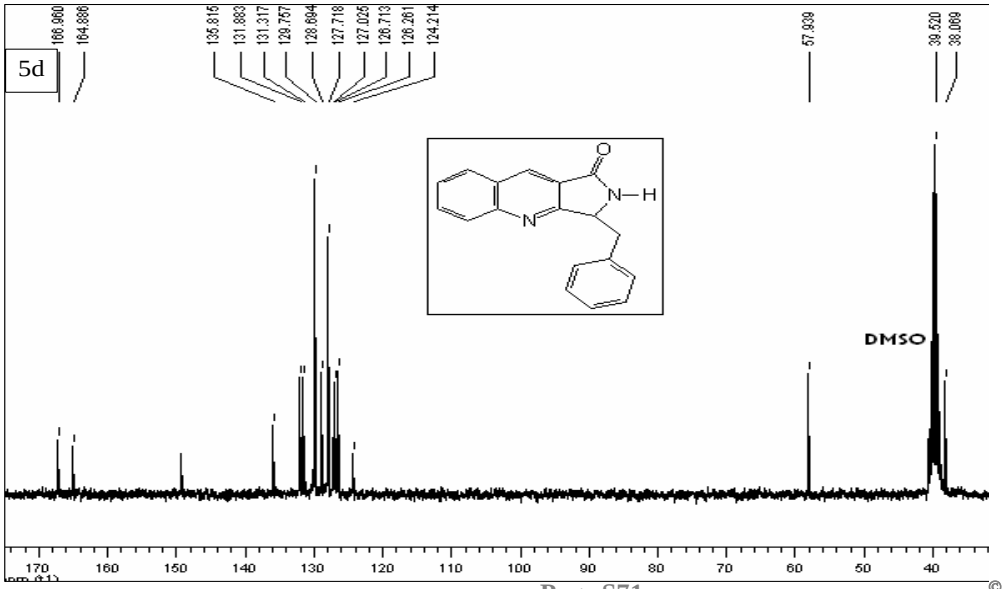

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Figure S124. C-NMR of compound 5d in DMSO

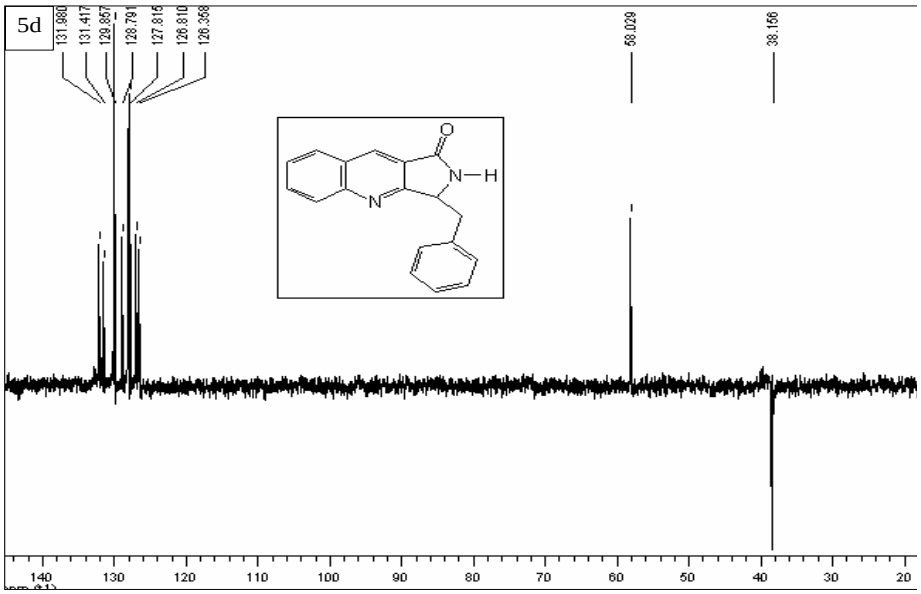
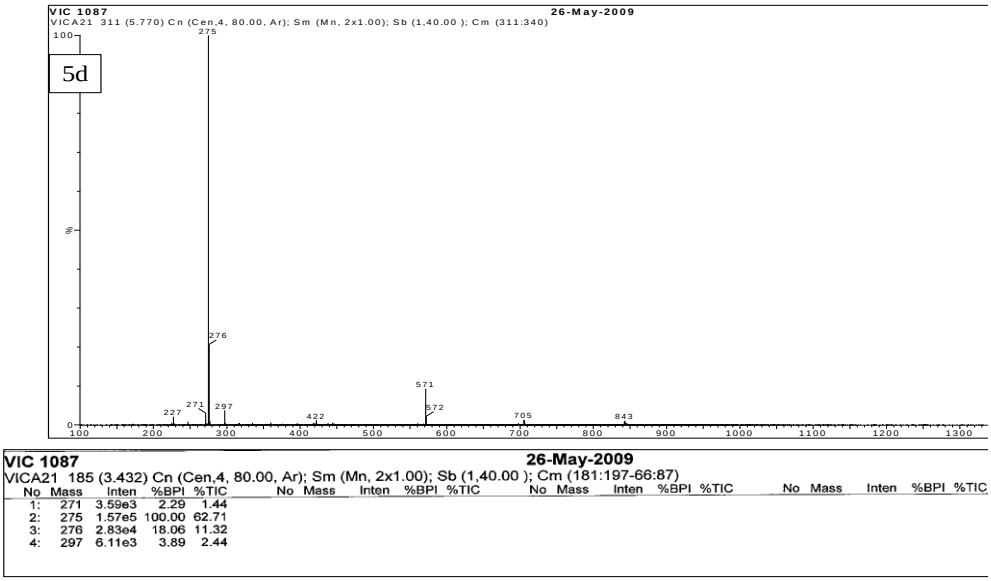


Figure S125. DEPT of compound 5d in DMSO



 ©ARKAT USA, Inc.

Figure S126. QTOF-MS of compound 5d

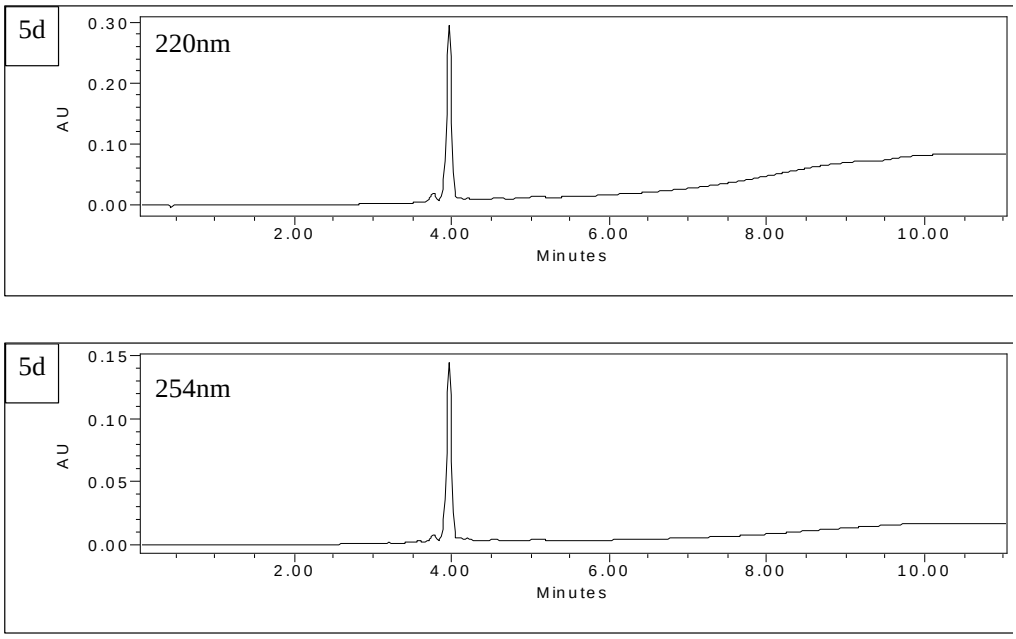
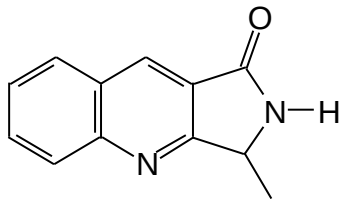


Figure S127. HPLC of compound 5d

5e



^{1}HNMR: (300 MHz, DMSO-d_6), $\delta_{H(ppm)}$: 1.49 (d,3H, J=6.6Hz), 4.78 (q,1H, J=6.6Hz), 7.67 (m,1H), 7.88 (m,1H), 8.12 (d, 1H,J=8.1Hz), 8.19 (d, 1H,J=8.1Hz), 8.73 (s, 1H), 9.02 (bs,1H).

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^{13}CNMR: (75 MHz, DMSO-d$_6$, δ $_{C\ (ppm)}$:19.25, 53.35, 123.46, 126.67, 127.15, 128.64, 129.79, 131.29, 132.33, 149.16, 166.72. (yield 54.7%)**MS:** MW=198 g/mol, MH$^+$ =199. **HPLC:** t$_R$ = 3.29 min**.**

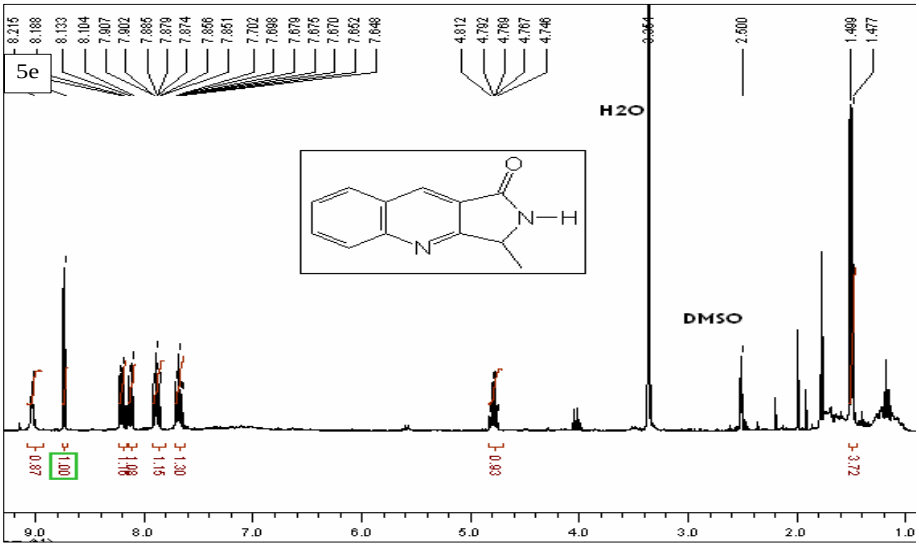


Figure S128. H-NMR of compound 5e in DMSO

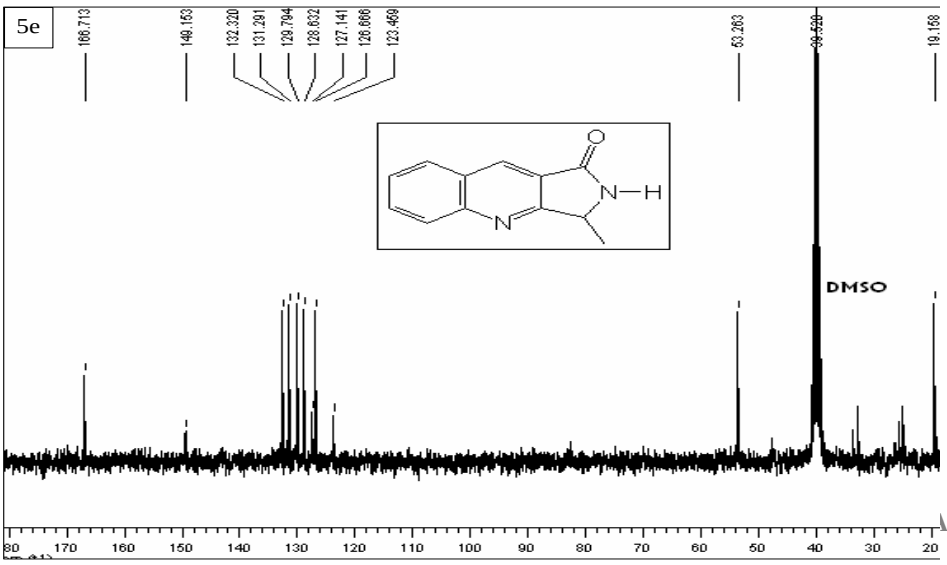


Figure S129. C-NMR of compound 5e in DMSO

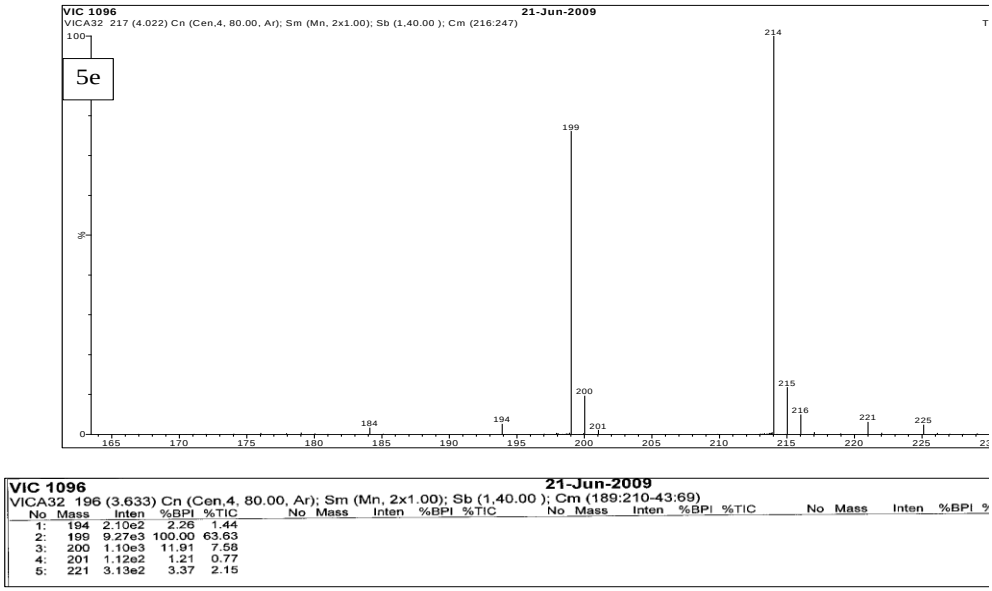


Figure S130. QTOF-MS of compound 5e

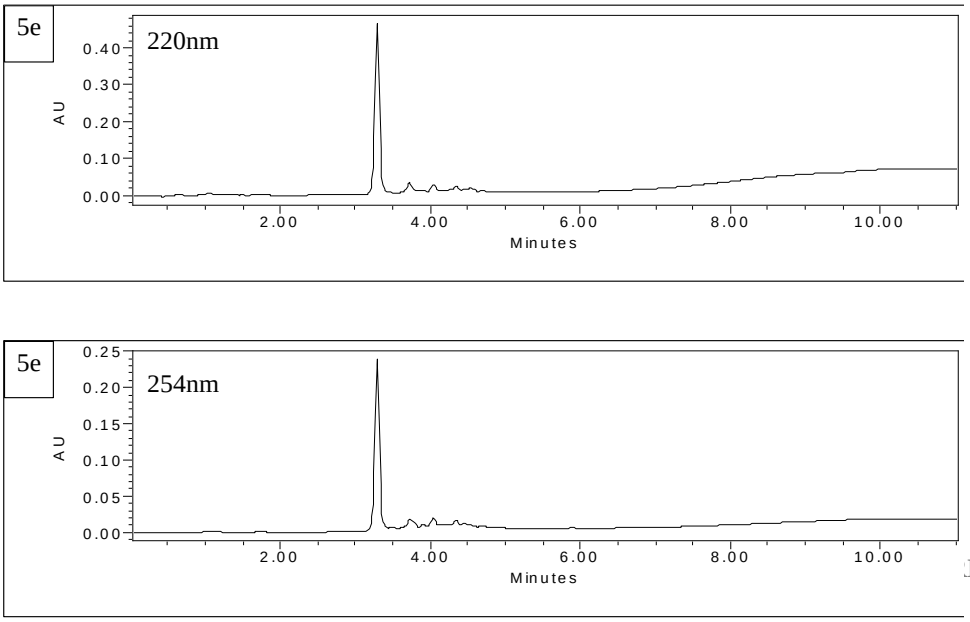
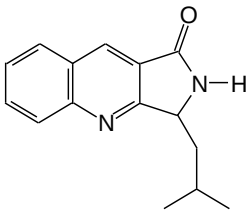


Figure S131. HPLC of compound 5e

5f



^{1}HNMR: (300 MHz, DMSO-d$_6$), $\delta_{H(ppm)}$: 0.89 (d,3H,J=6.6Hz), 1.01 (d,3H, J=6.6Hz), 1.46 (m,1H), 1.88 (m,1H), 2.20 (m,1H), 4.73 (dd,1H, J=8.7Hz,J=3.9Hz), 7.67(m,1H), 7.87 (m, 1H), 8.12 (d,1H,J=8.1Hz), 8.19 (d,1H,J=8.1Hz), 8.72 (s,1H), 9.16 (bs,1H, NH). **^{13}CNMR:** (75 MHz, DMSO-d$_6$, $\delta_{C(ppm)}$:21.81, 23.47, 24.53, 39.55, 43.10, 55.90, 123.69, 126.65, 127.17, 128.69, 129.80, 131.29, 132.25, 149.16, 166.37, 167.19. (yield 95.8%) **MS:** MW=240 g/mol, MH$^+$ =241. **HPLC:** t_R = 3.91 min**.**

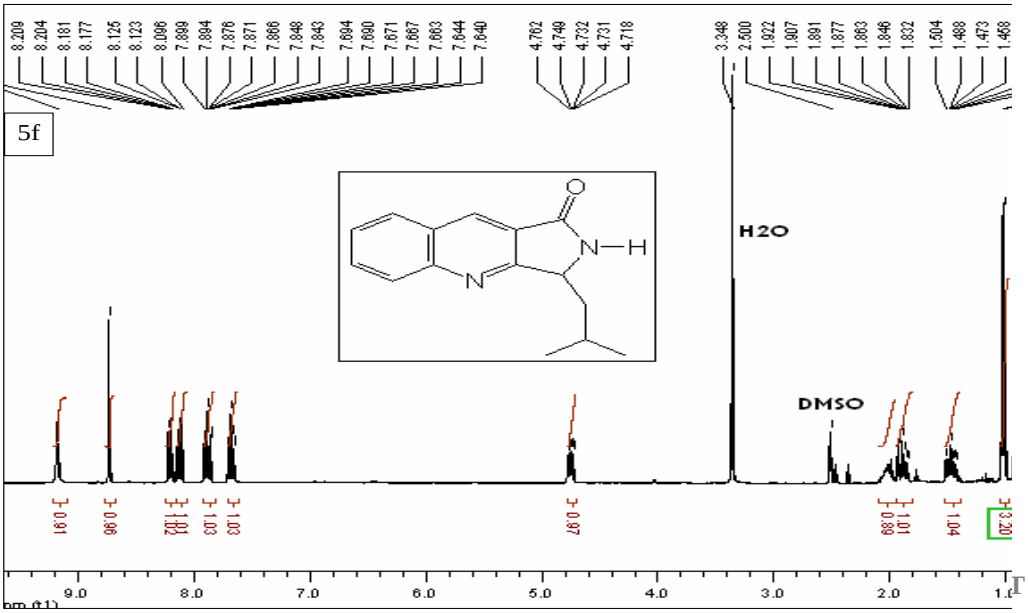


Figure S132. H-NMR of compound 5f in DMSO

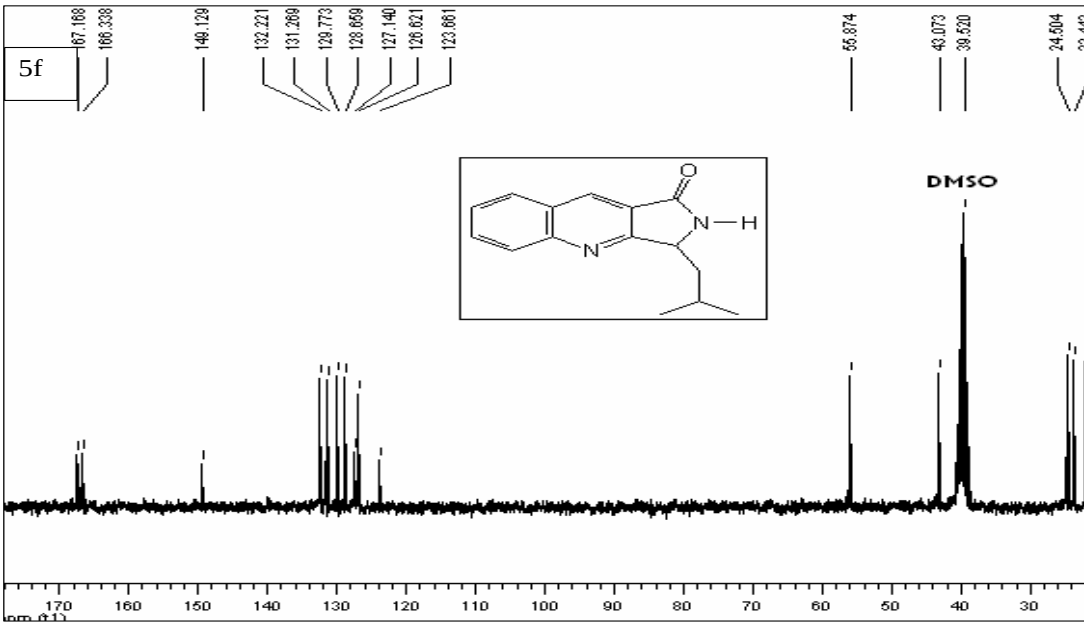


Figure S133. C-NMR of compound 5f in DMSO

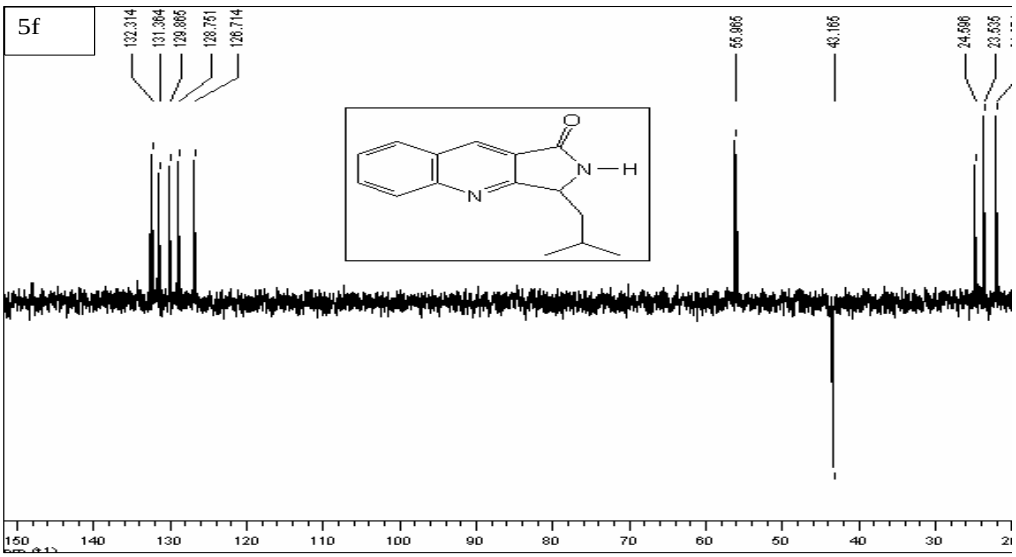


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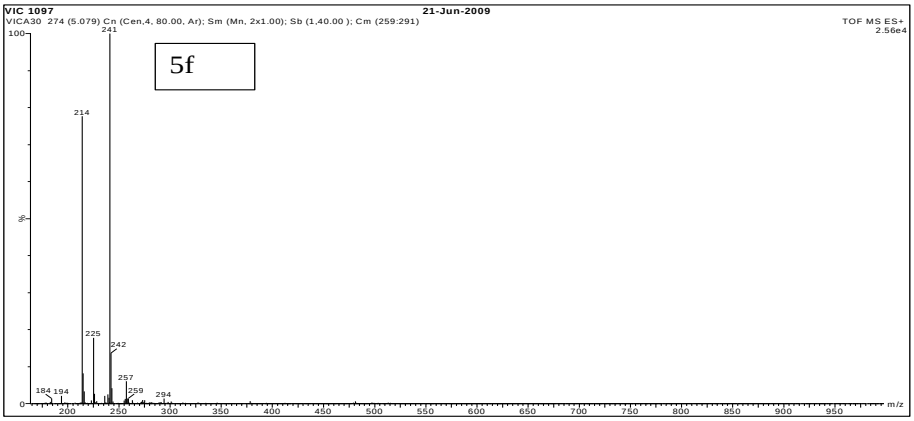
Figure S134. DEPT of compound 5f in DMSO

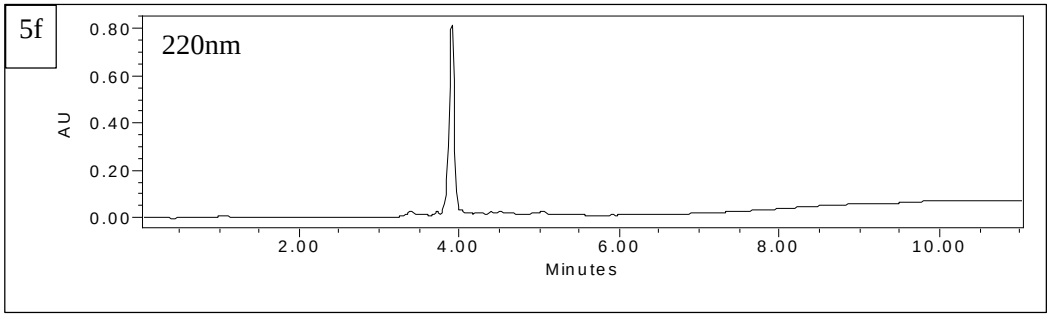


VIC 1097 21-Jun-2009

VICA30 274 (5.079) Cn (Cen,4, 80.00, Ar); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (233:298-32:76)

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TI
1:	141	6.17e3	12.98	5.42															
2:	158	2.05e4	43.11	18.01															
3:	159	1.35e3	2.84	1.19															
4:	160	9.53e2	2.00	0.84															
5:	214	1.12e4	23.44	9.79															
6:	215	1.49e3	3.13	1.31															
7:	216	8.59e2	1.81	0.75															
8:	225	1.73e3	3.65	1.52															
9:	236	5.94e2	1.25	0.52															
10:	239	6.21e2	1.31	0.55															
11:	241	4.76e4	100.00	41.78															
12:	242	6.08e3	12.79	5.34															
13:	243	1.43e3	3.00	1.25															
14:	257	2.64e3	5.55	2.32															
15:	294	6.93e2	1.46	0.61															

Figure S135. QTOF-MS of compound 5f



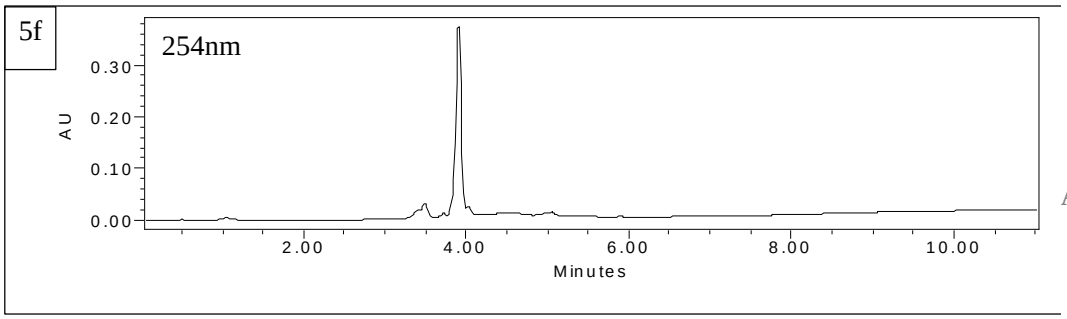
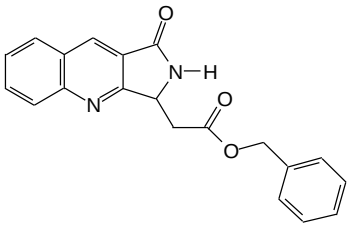


Figure S136. HPLC of compound 5f

5g



^{1}HNMR: (300 MHz, DMSO-d_6), $\delta_{H(ppm)}$: 3.00 (dd,1H,J=6.6Hz, J=16.2Hz), 3.13 (dd,1H,J=5.1Hz, J=16.2Hz), 5.04 (d, 2H, J=1.8Hz), 5.08 (d,1H, J=5.7Hz), 7.26 (m,5H), 7.69 (m,1H), 7.89 (m, 1H), 8.09 (d,1H, J=8.4Hz), 8.20 (dd,1H, J=1.5Hz, J=8.4Hz), 8.71 (s,1H), 9.06 (bs, NH). **^{13}CNMR:** (75 MHz, DMSO-d_6), $\delta_{C(ppm)}$:37.35, 54.15, 65.73, 123.91, 126.73, 127.21, 127.81, 127.90, 128.25, 128.59, 129.82, 131.31, 132.18, 135.73, 149.04, 164.74, 167.19, 169.55. (yield 66%) **MS:** MW=332 g/mol, MH^+ =332. **HPLC:** t_R = 4.25 min.

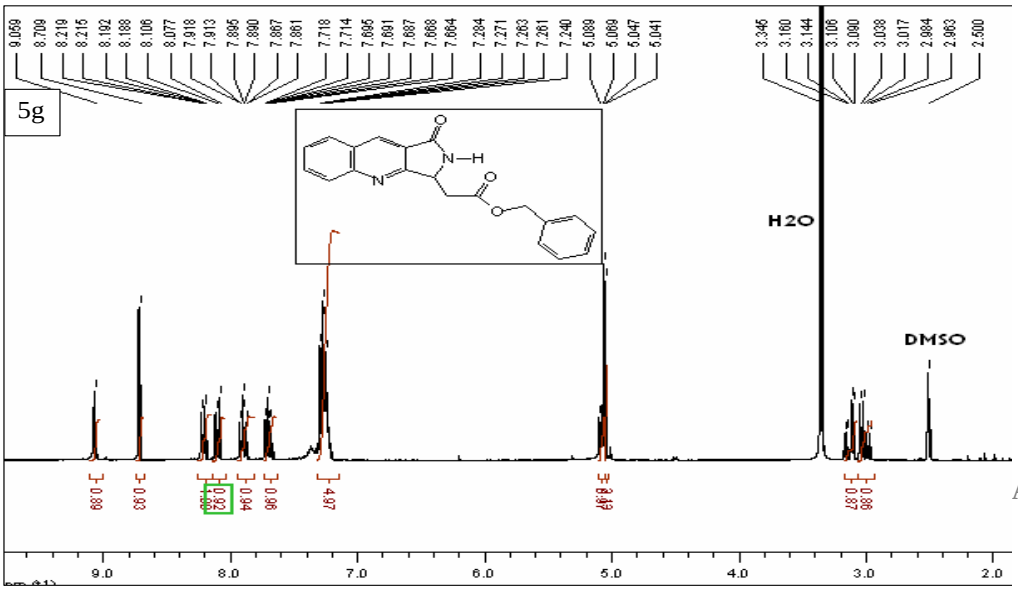


Figure S137. H-NMR of compound 5g in DMSO

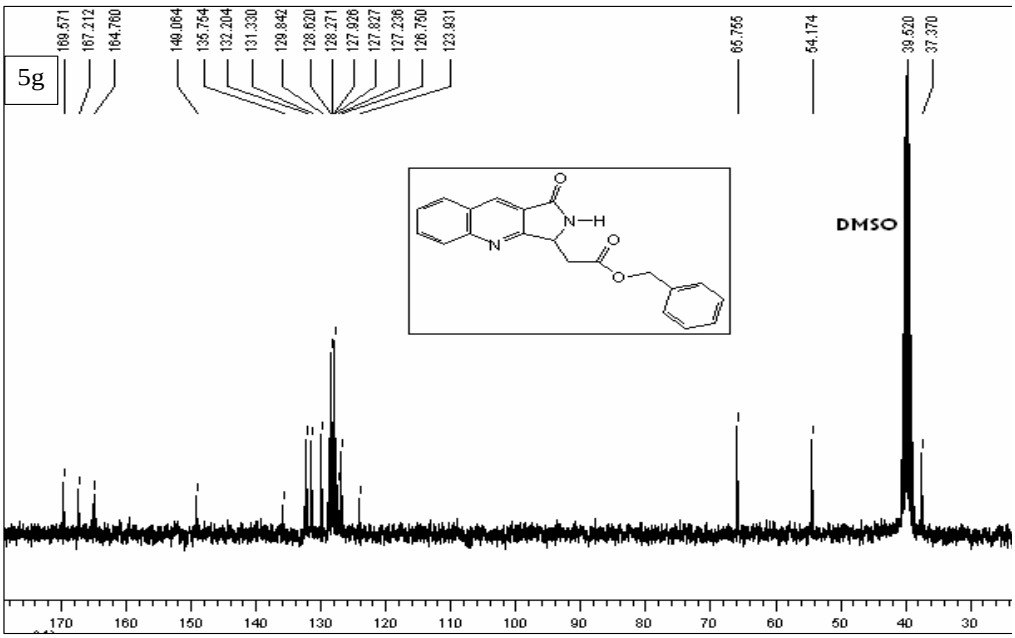


Figure S138. C-NMR of compound 5g in DMSO

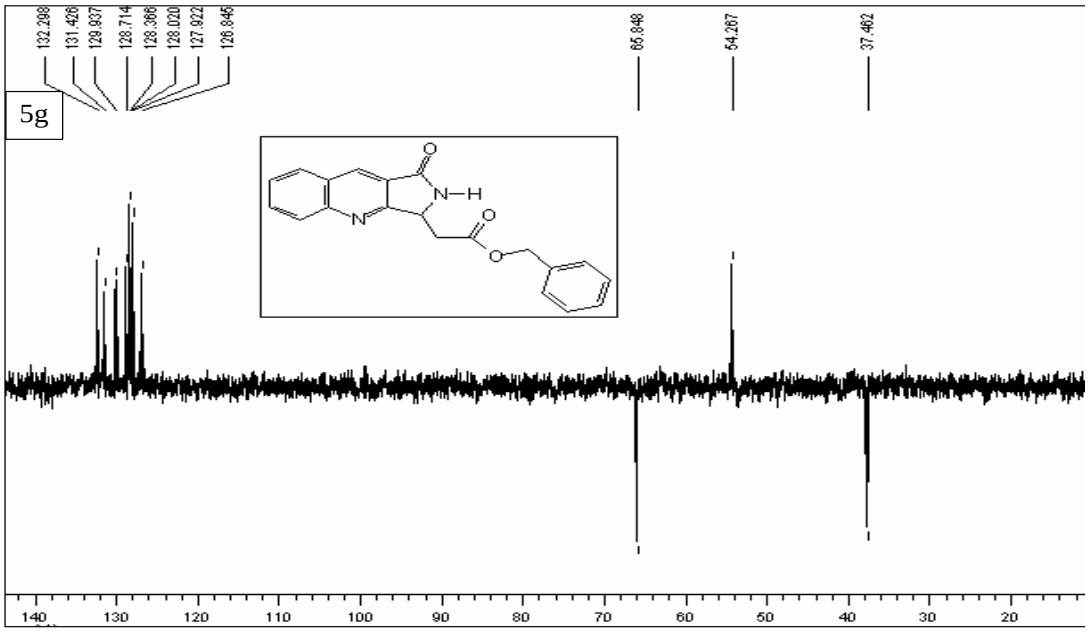


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Figure S139. DEPT of compound 5g in DMSO

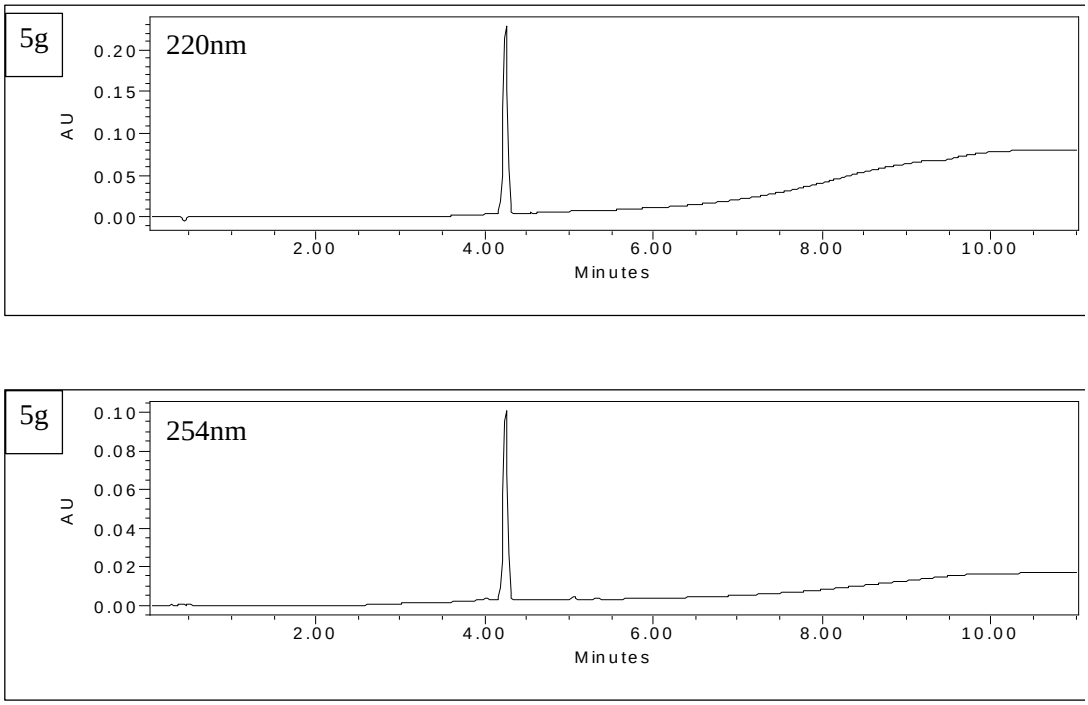

Figure S140. HPLC of compound 5g

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