Supporting Information

For

New Panx-1 blockers: synthesis, biological evaluation and molecular dynamic studies

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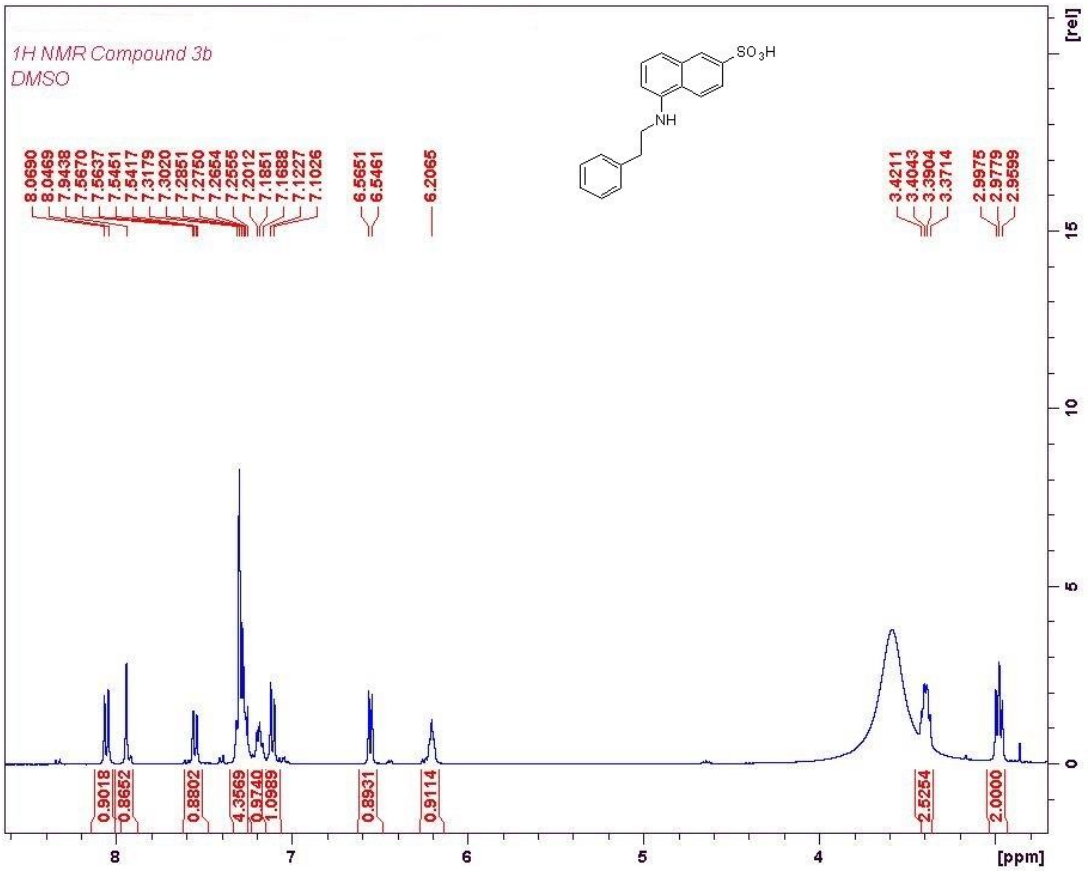
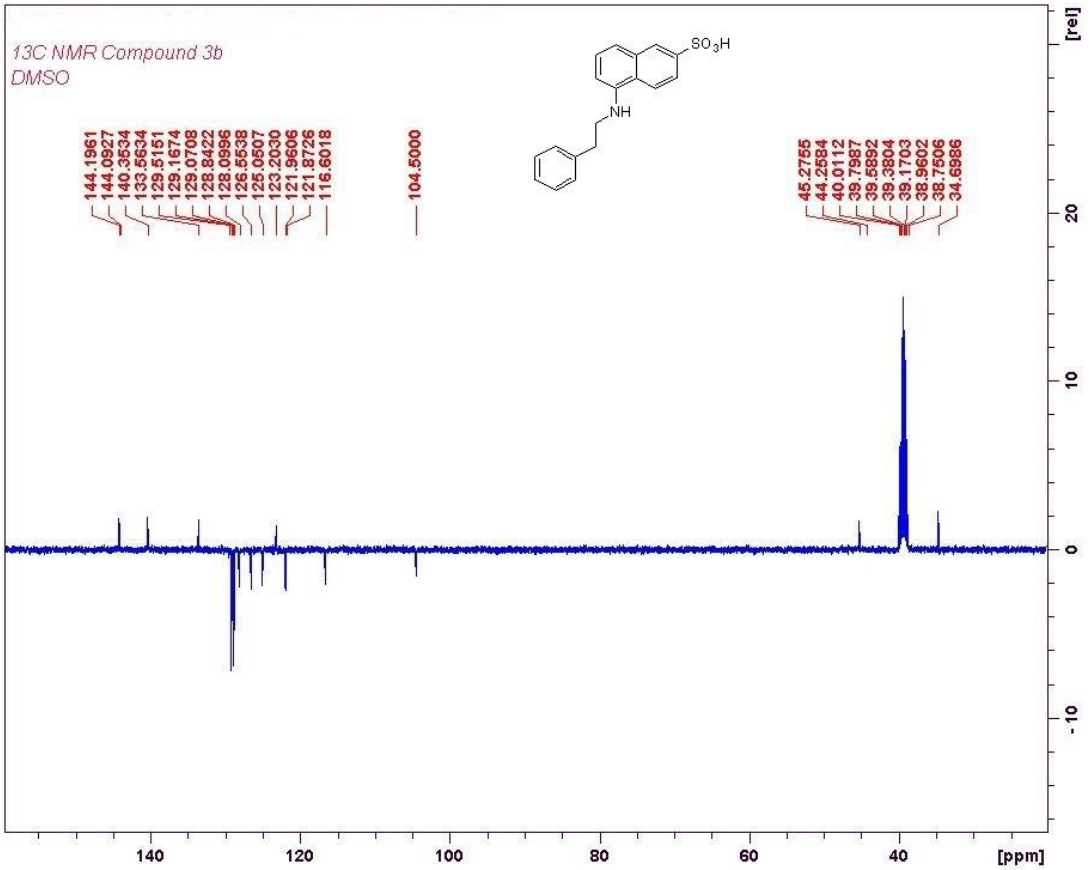
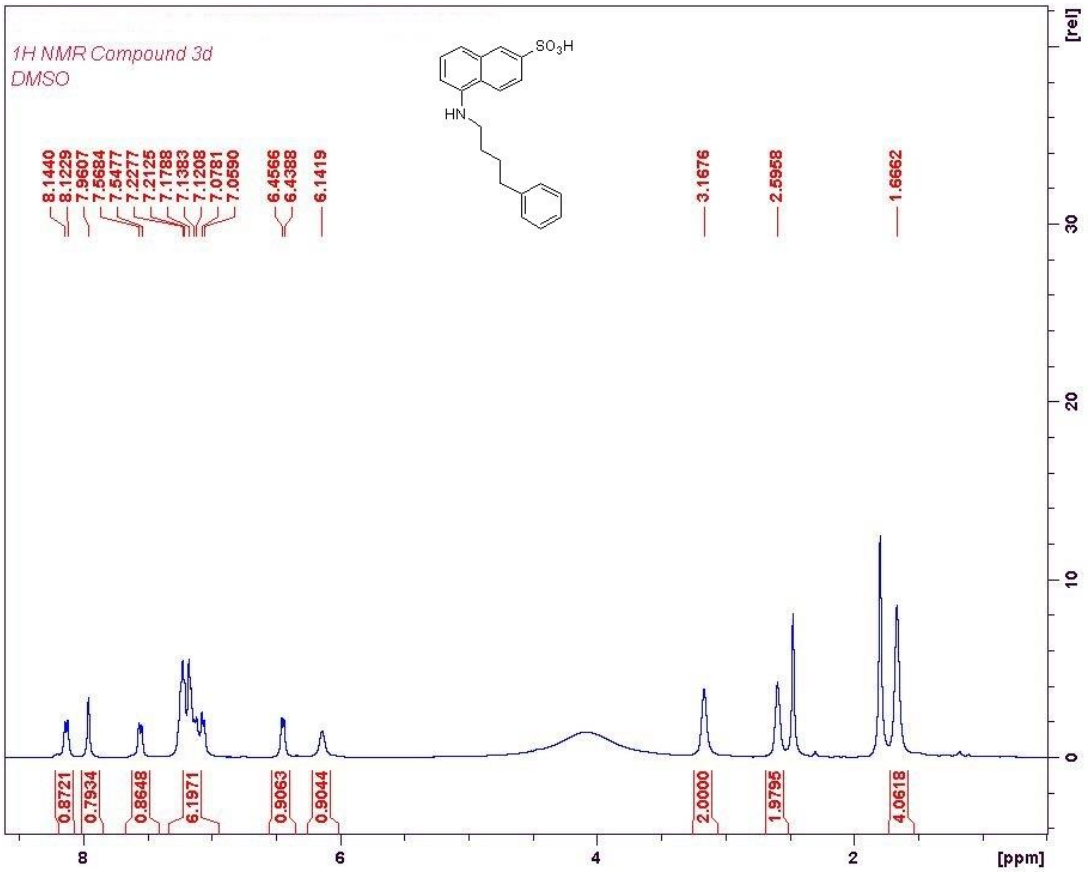
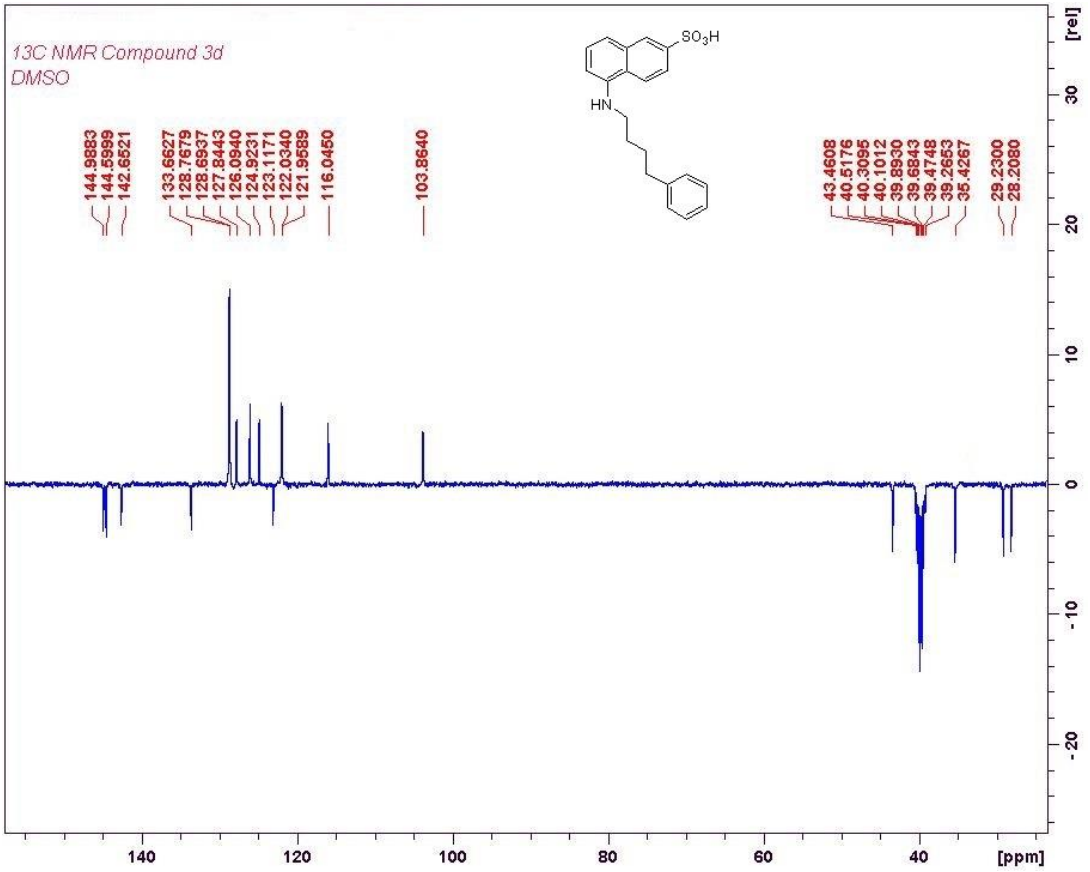


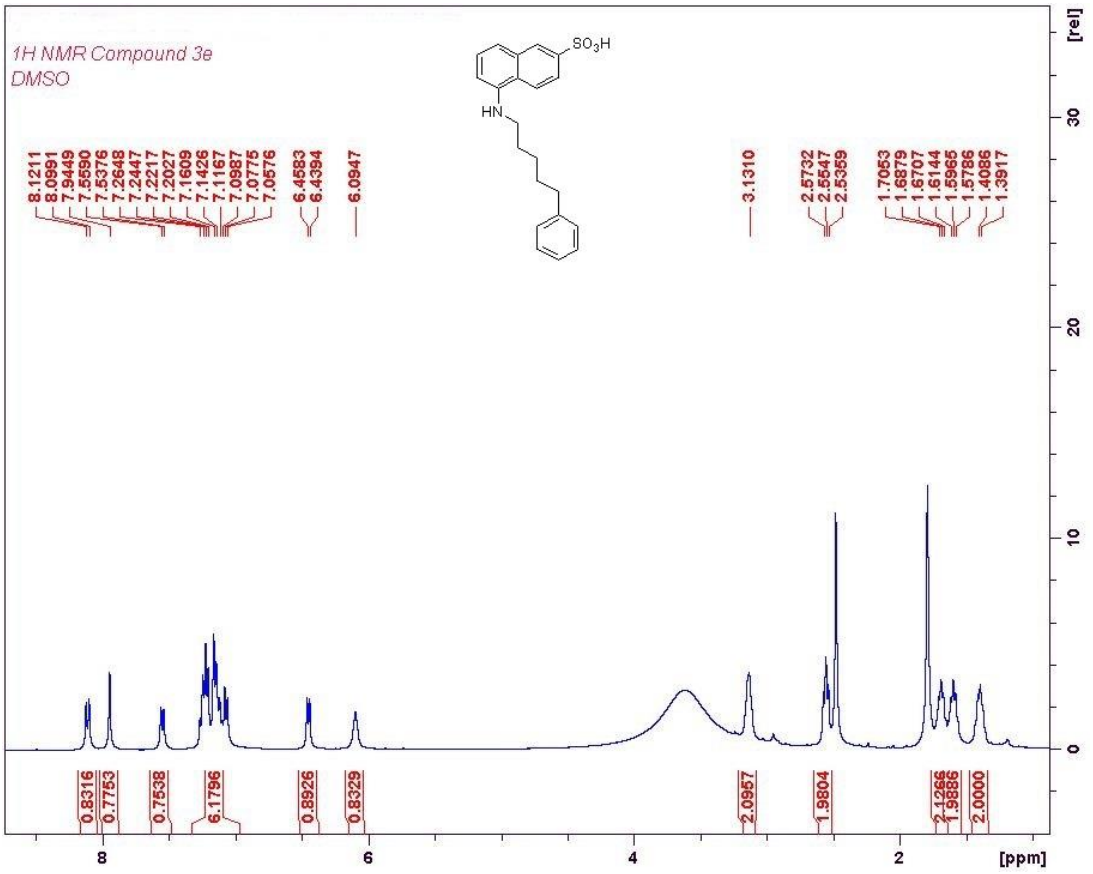


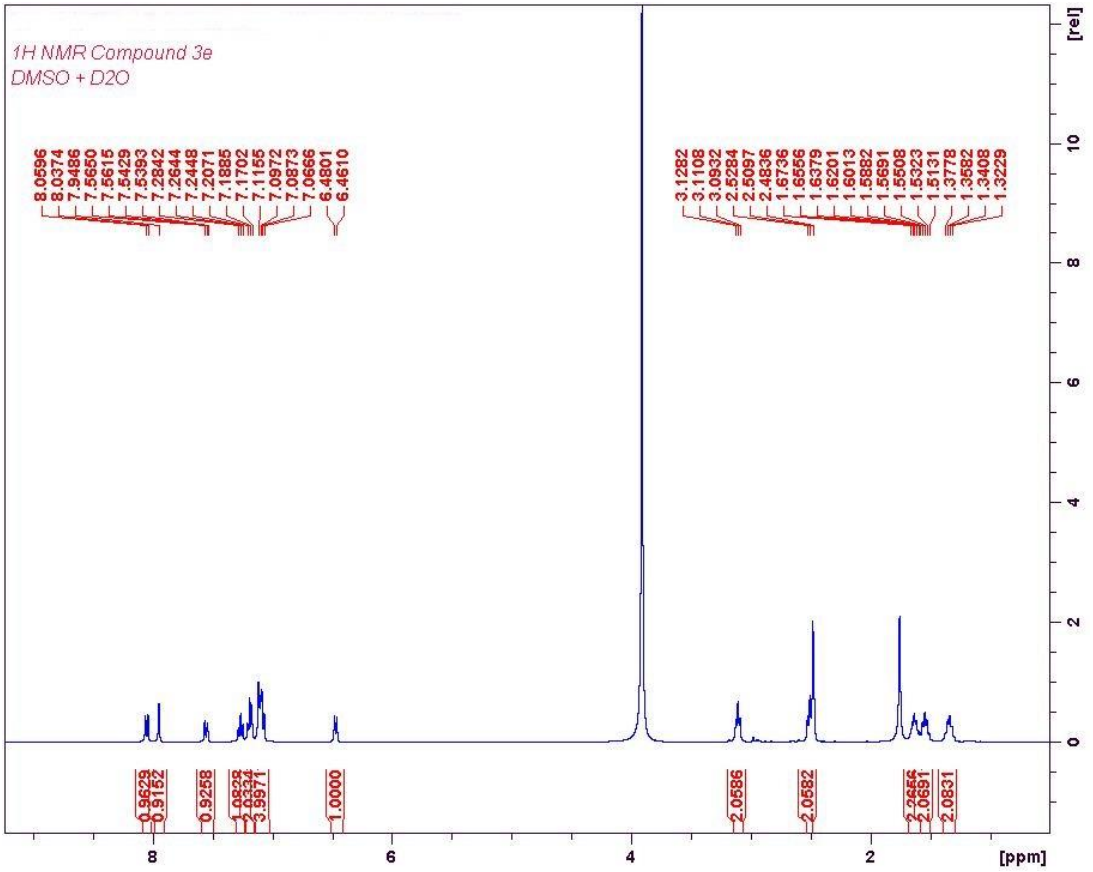
^{1}H-NMR and ^{13}C-NMR spectra of compound **3d**

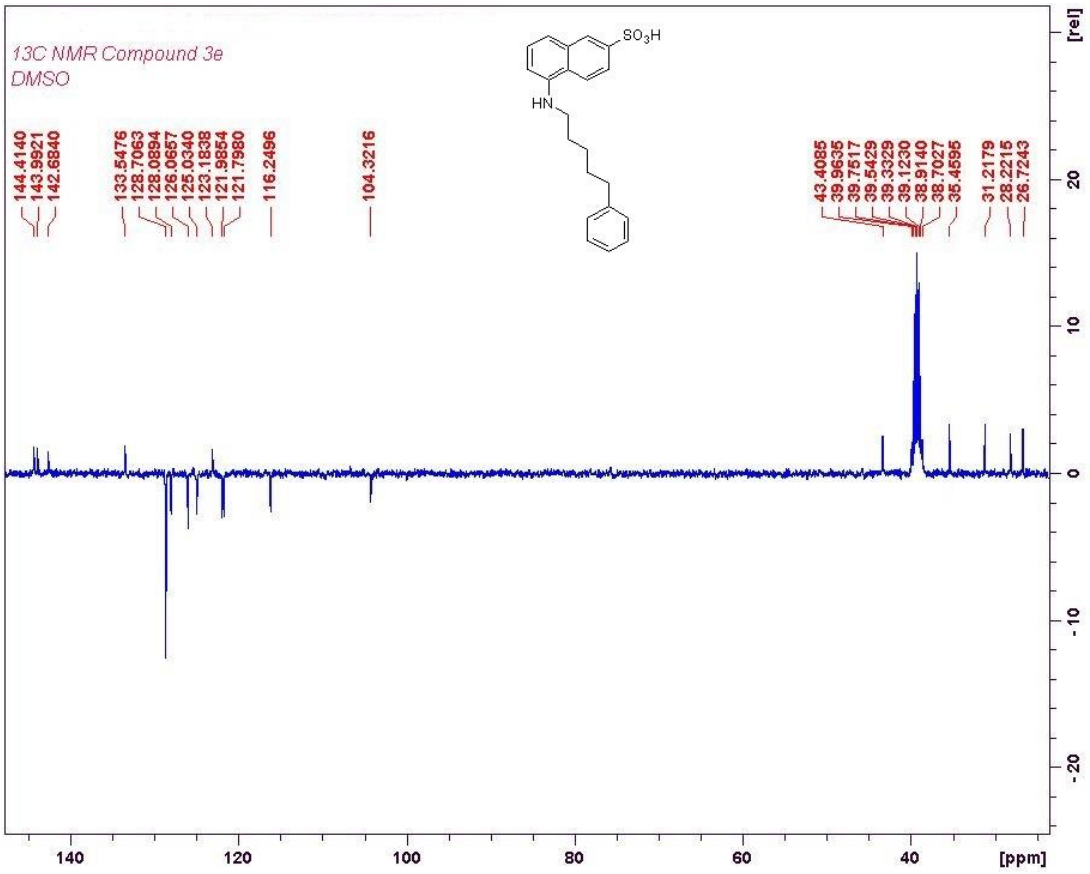




^{1}H-NMR and ^{13}C-NMR spectra of compound **3e**






13C NMR Compound 3e
DMSO
SO3H
HN
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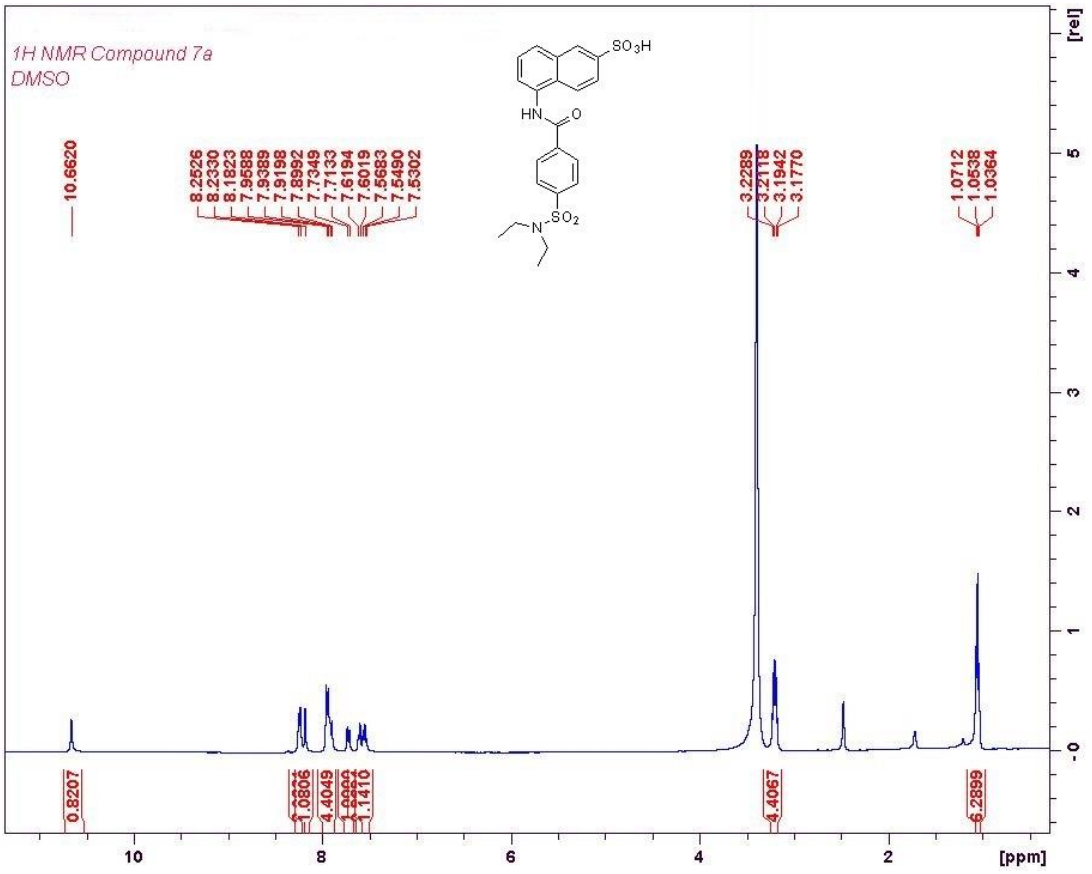
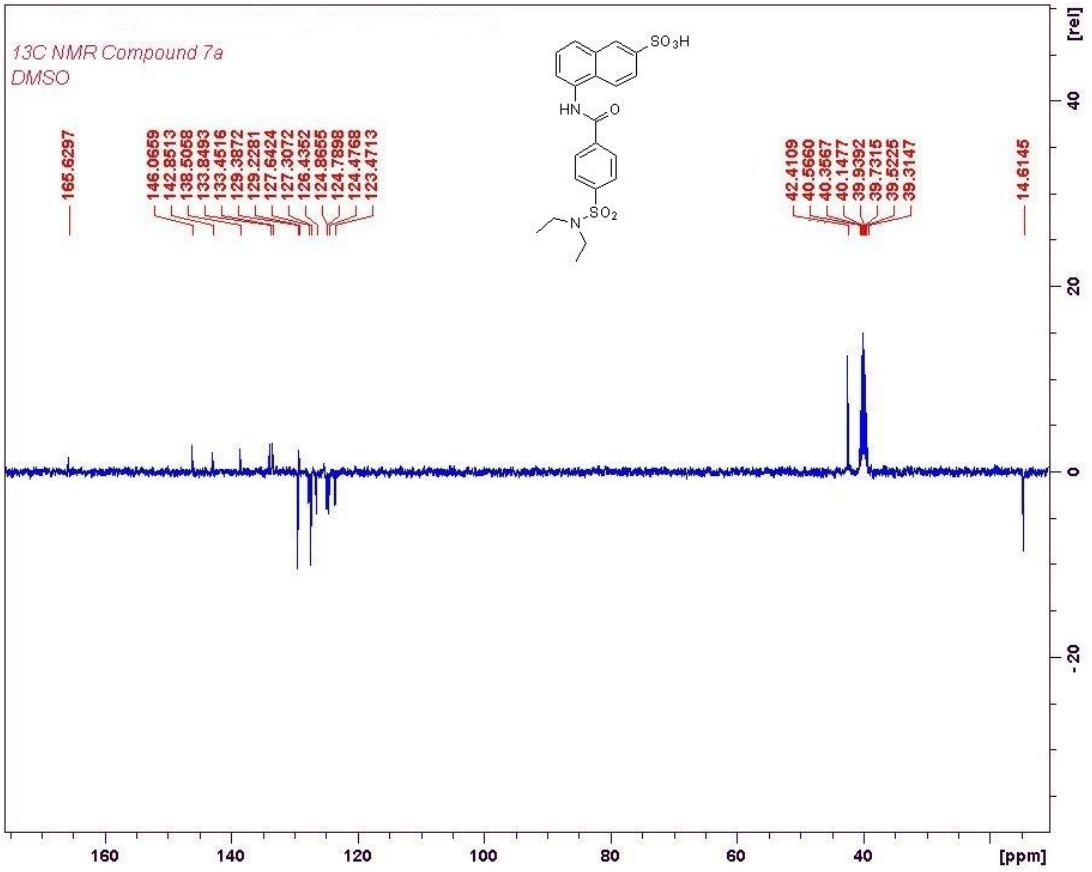
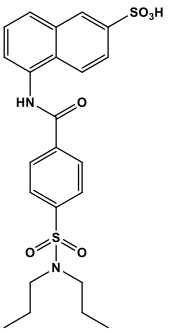
143.9921
142.6840
133.5476
128.7063
128.0894
126.0657
125.0340
123.1838
121.9854
121.7980
116.2496
104.3216
43.4085
39.9635
39.7517
39.5429
39.3329
39.1230
38.9140
38.7027
35.4595
31.2179
28.2215
26.7243
[rel]
20
10
0
-10
-20
140
120
100
80
60
40
[ppm]

^{1}H-NMR and ^{13}C-NMR spectra of compound **7a**

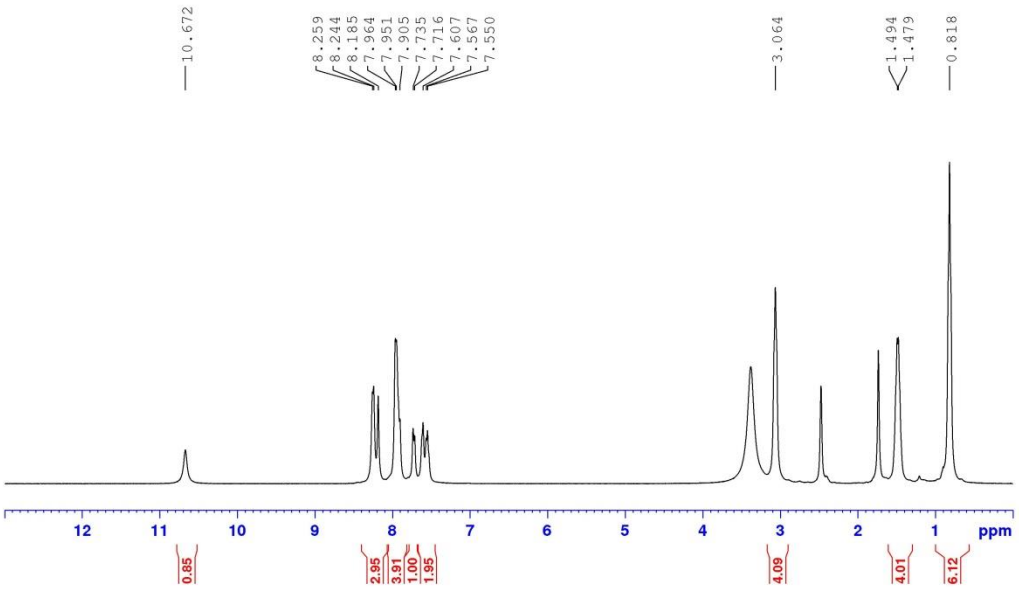




^{1}H-NMR and ^{13}C-NMR spectra of compound **7b**



1H NMR Compound 7b
DMSO



13C NMR Compound 7b
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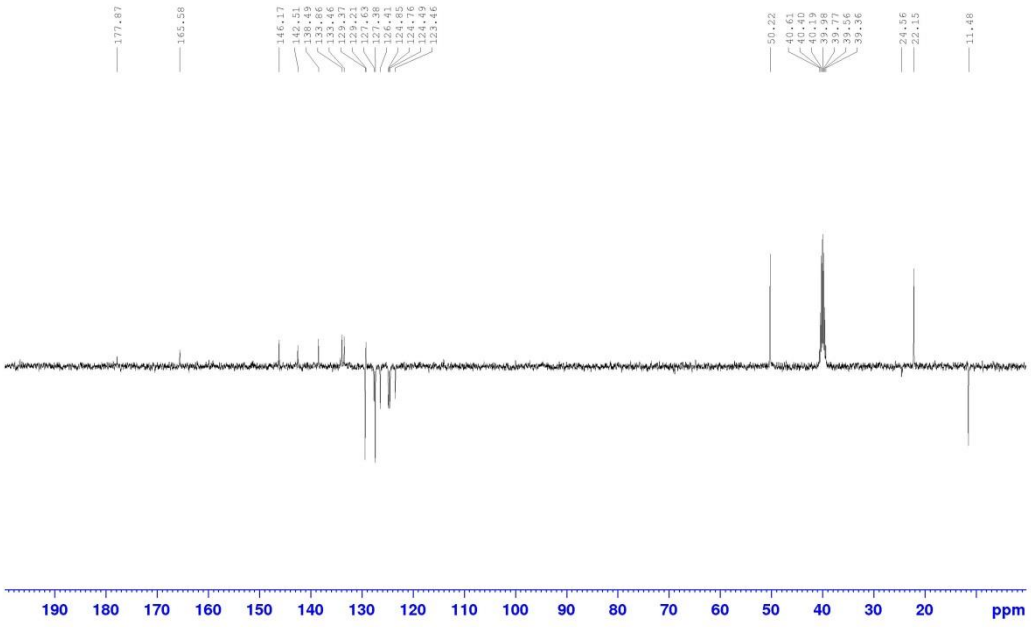
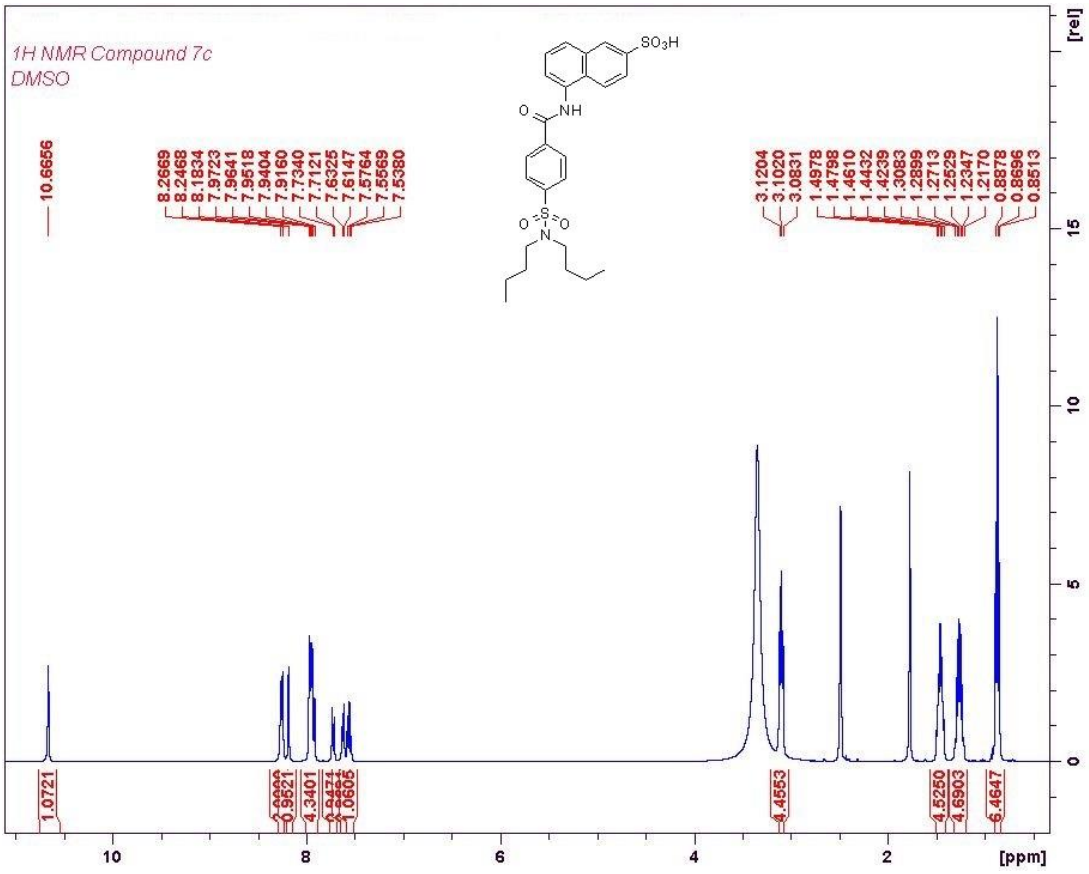
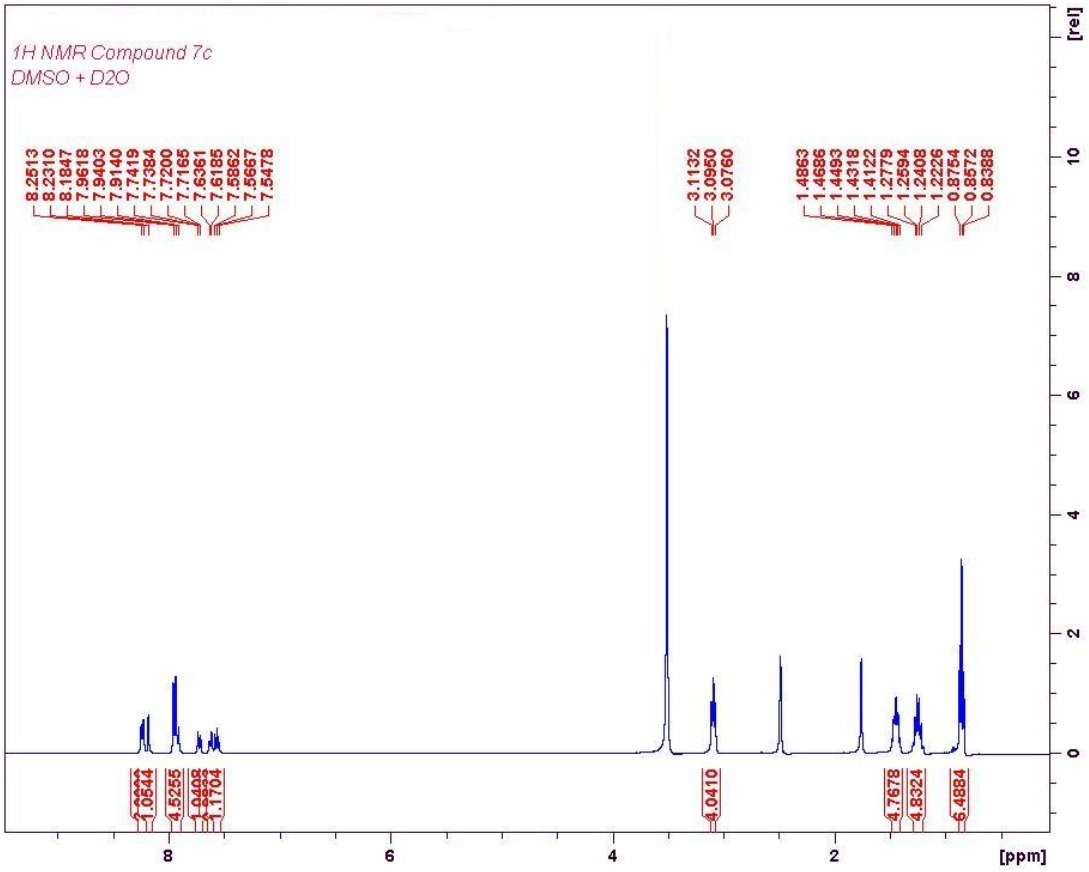
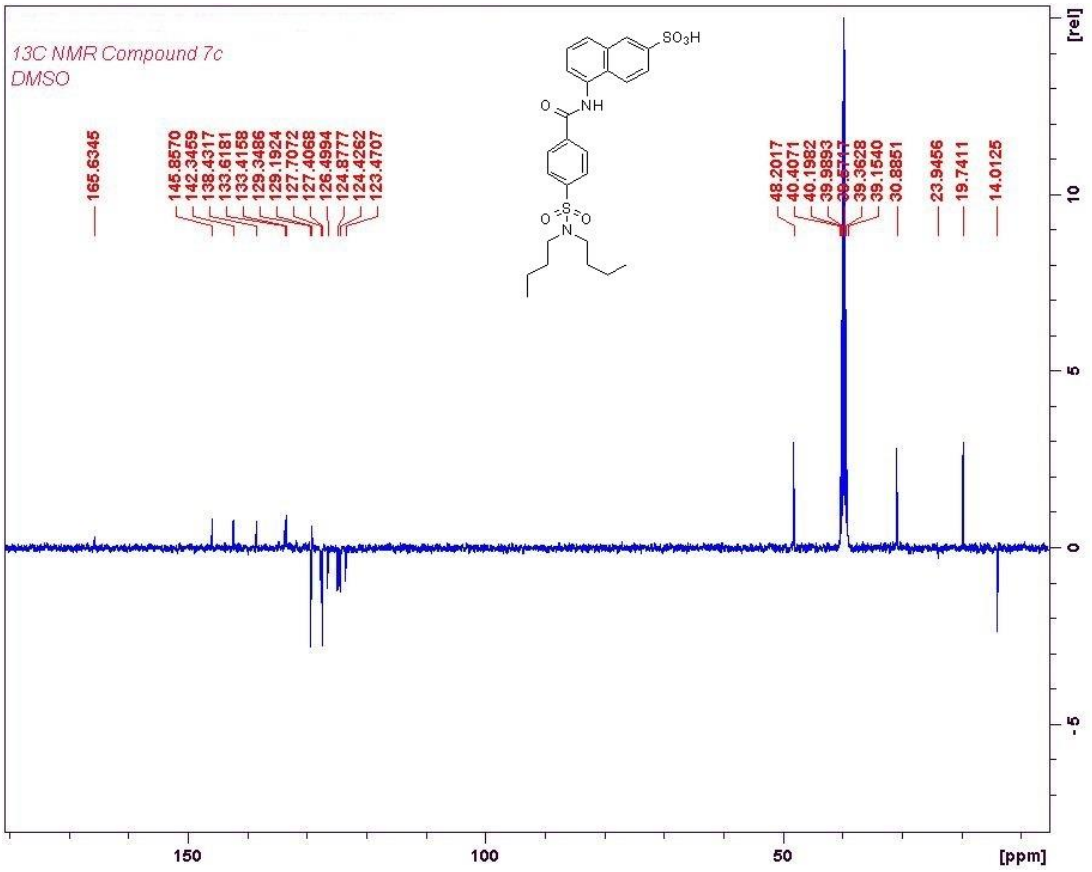


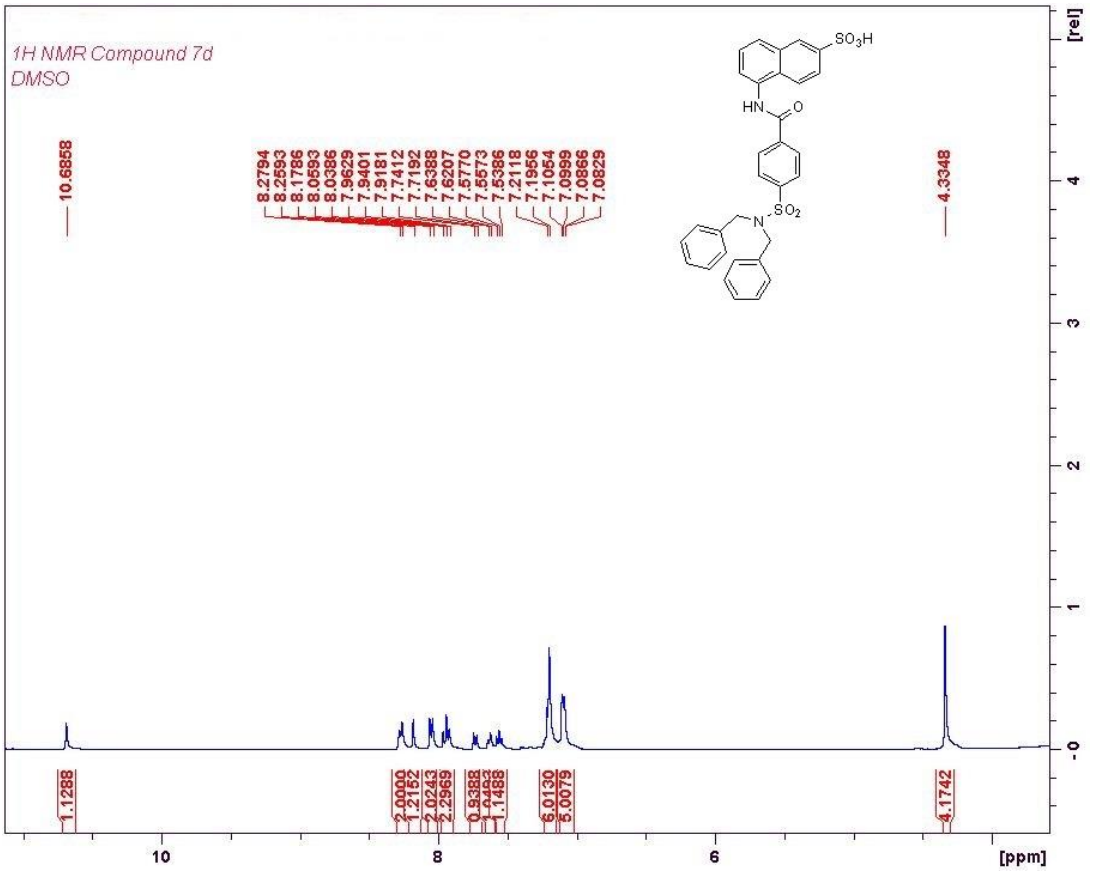
^{1}H-NMR and ^{13}C-NMR spectra of compound **7c**

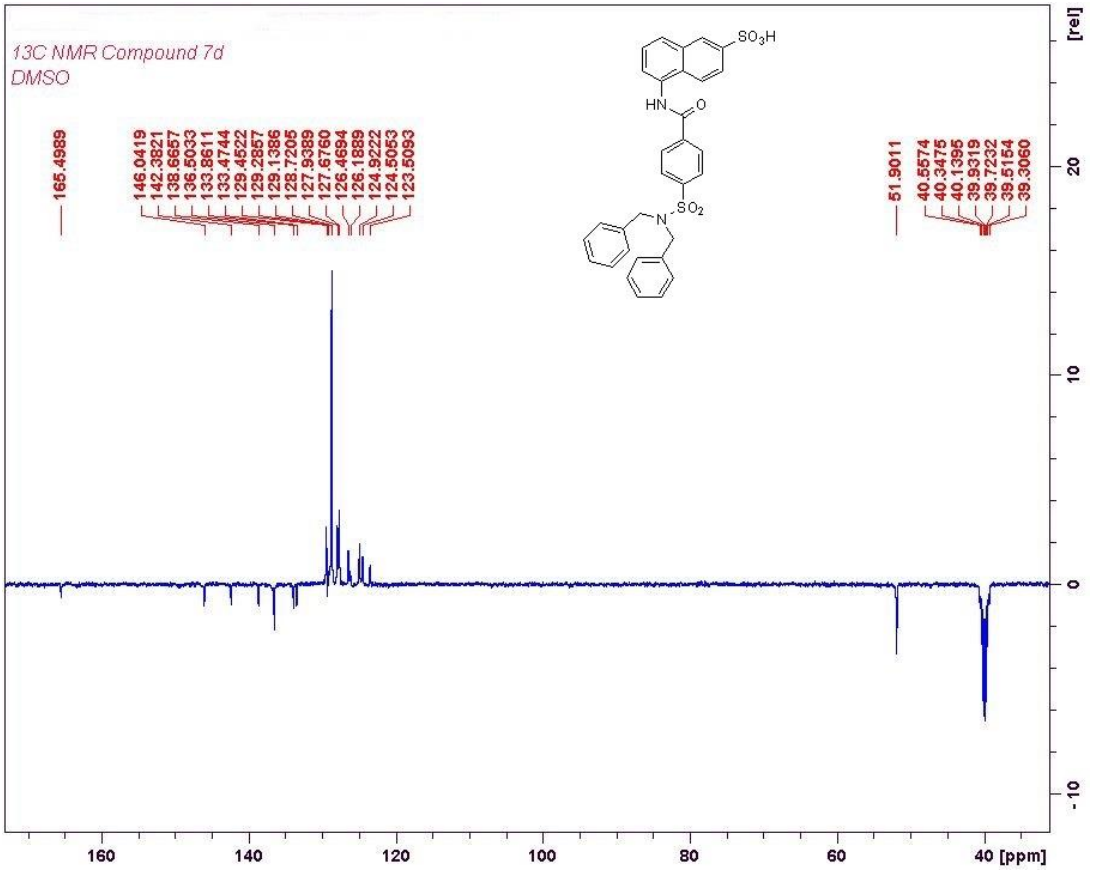




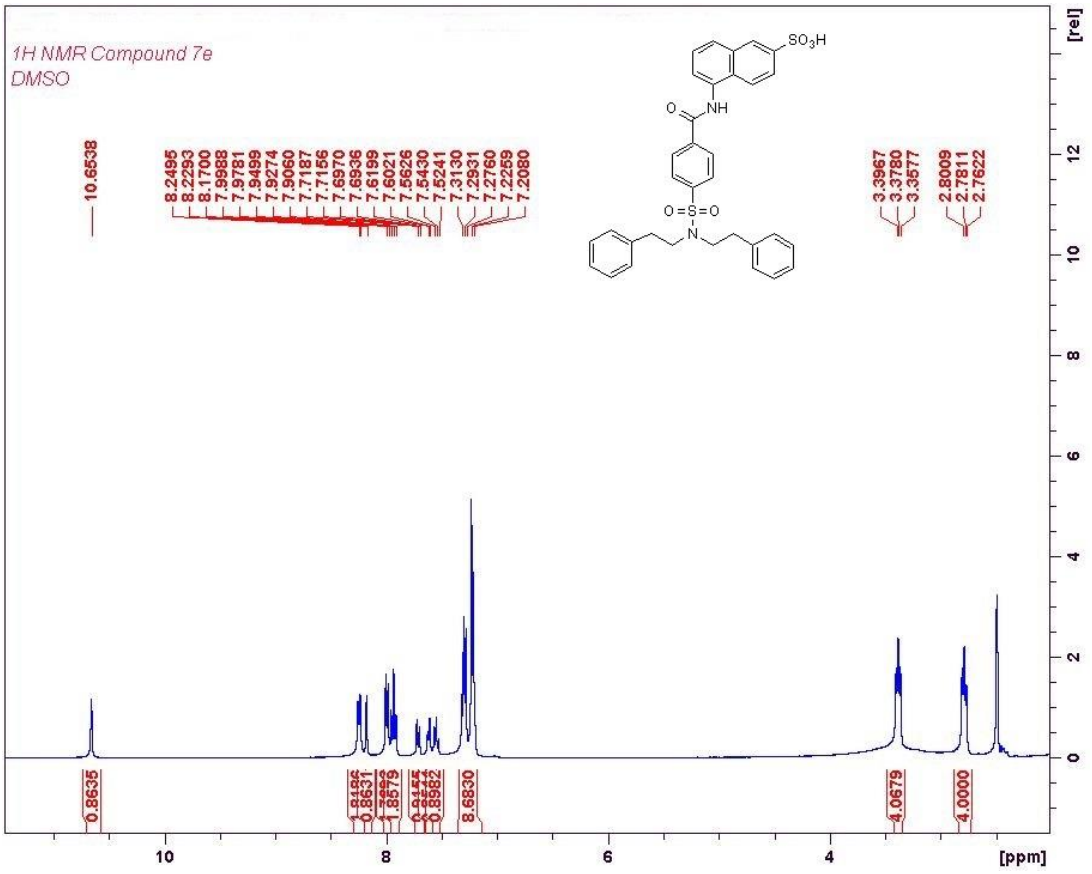

13C NMR Compound 7c
DMSO
165.6345
145.8570
142.3459
138.4317
133.6181
133.4158
129.3486
129.1924
127.7072
127.4068
126.4994
124.8777
124.4262
123.4707
48.2017
40.4071
40.1982
39.9893
39.3628
39.1540
30.8851
23.9456
19.7411
14.0125
SO3H
NH
O
S
N
[rel]
10
5
0
-5
150
100
50
[ppm]

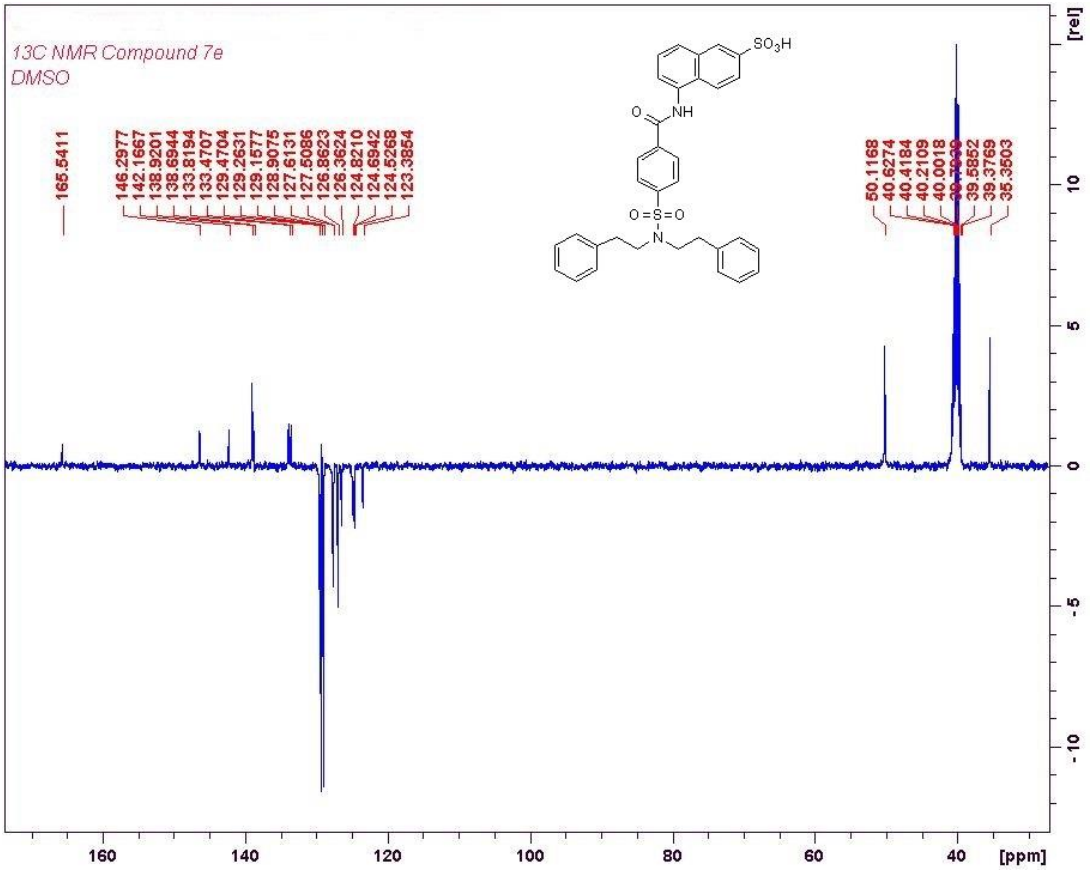
^{1}H-NMR and ^{13}C-NMR spectra of compound **7d**



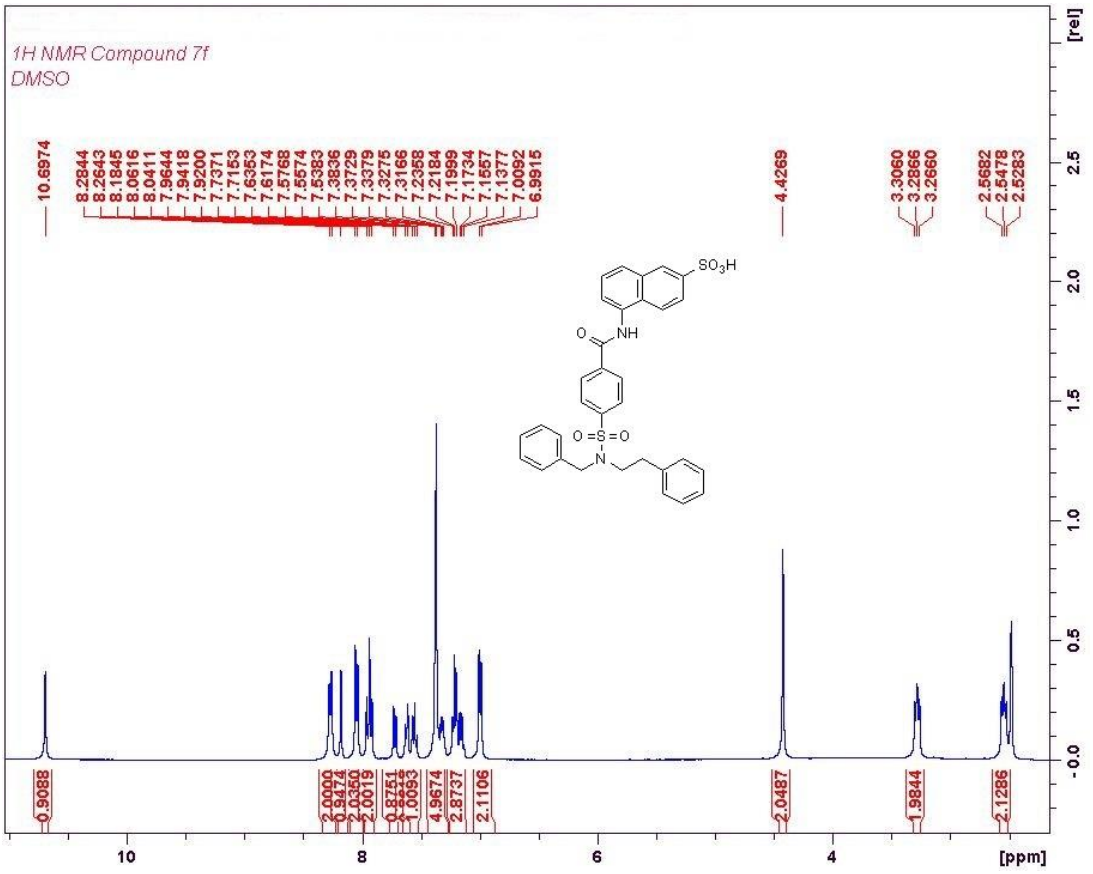


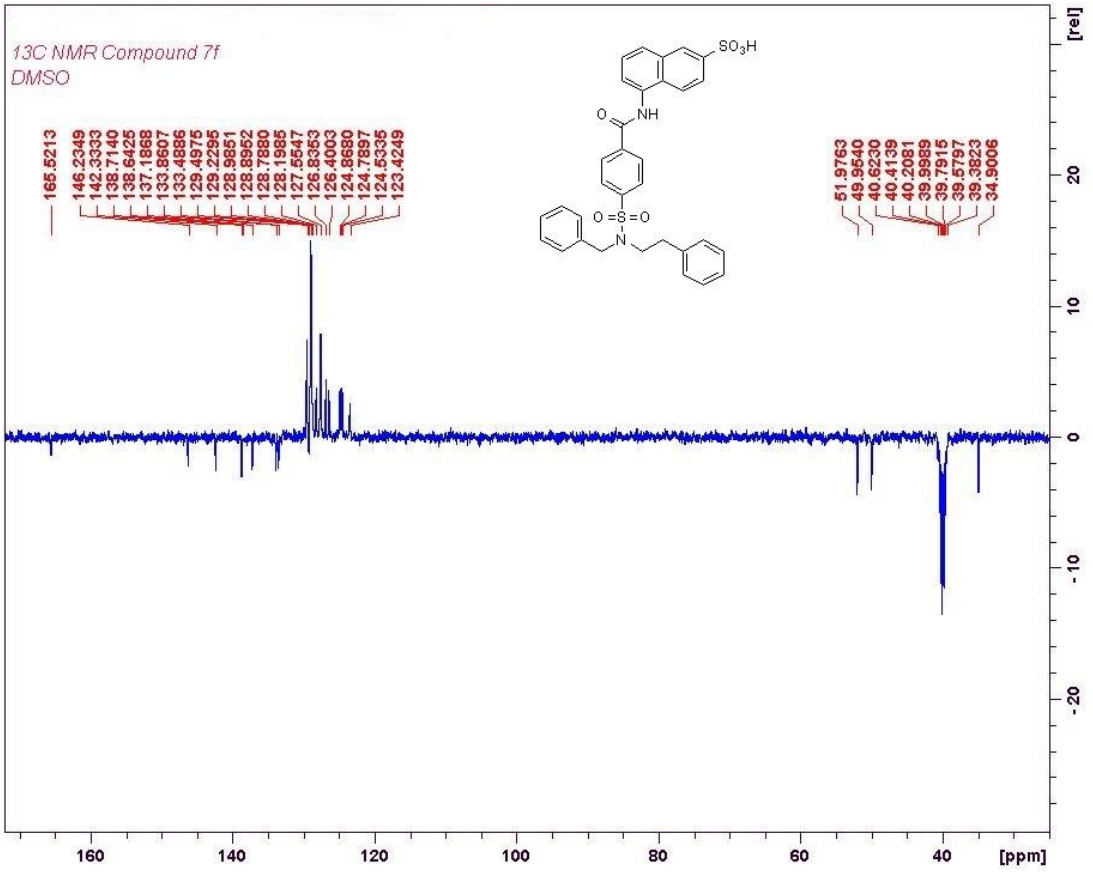
^{1}H-NMR and ^{13}C-NMR spectra of compound **7e**



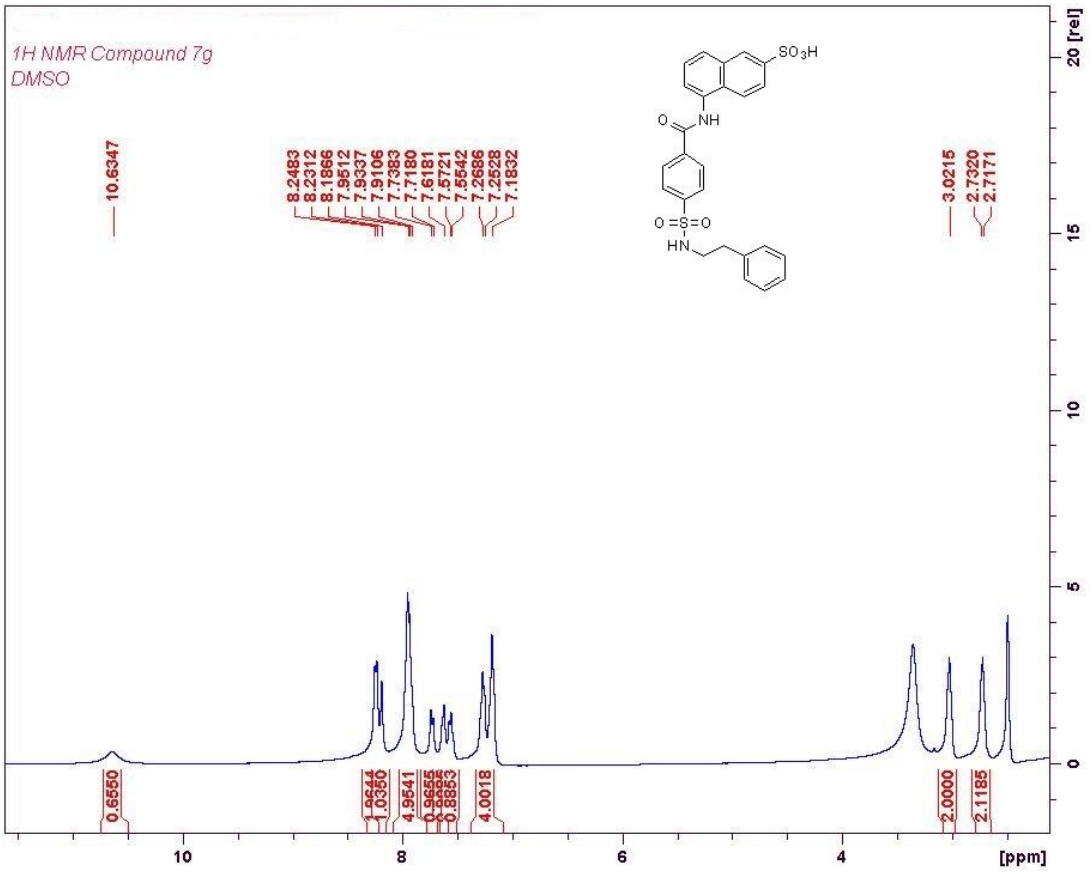


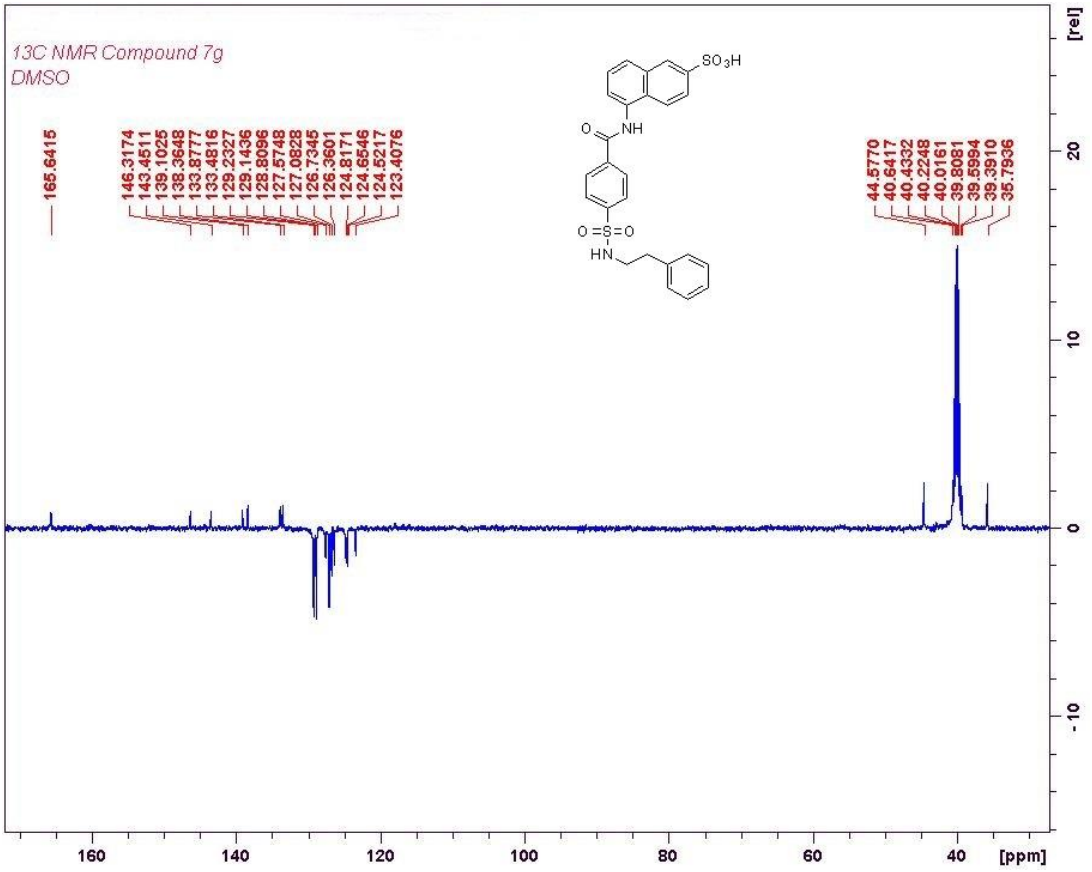
^{1}H-NMR and ^{13}C-NMR spectra of compound **7f**



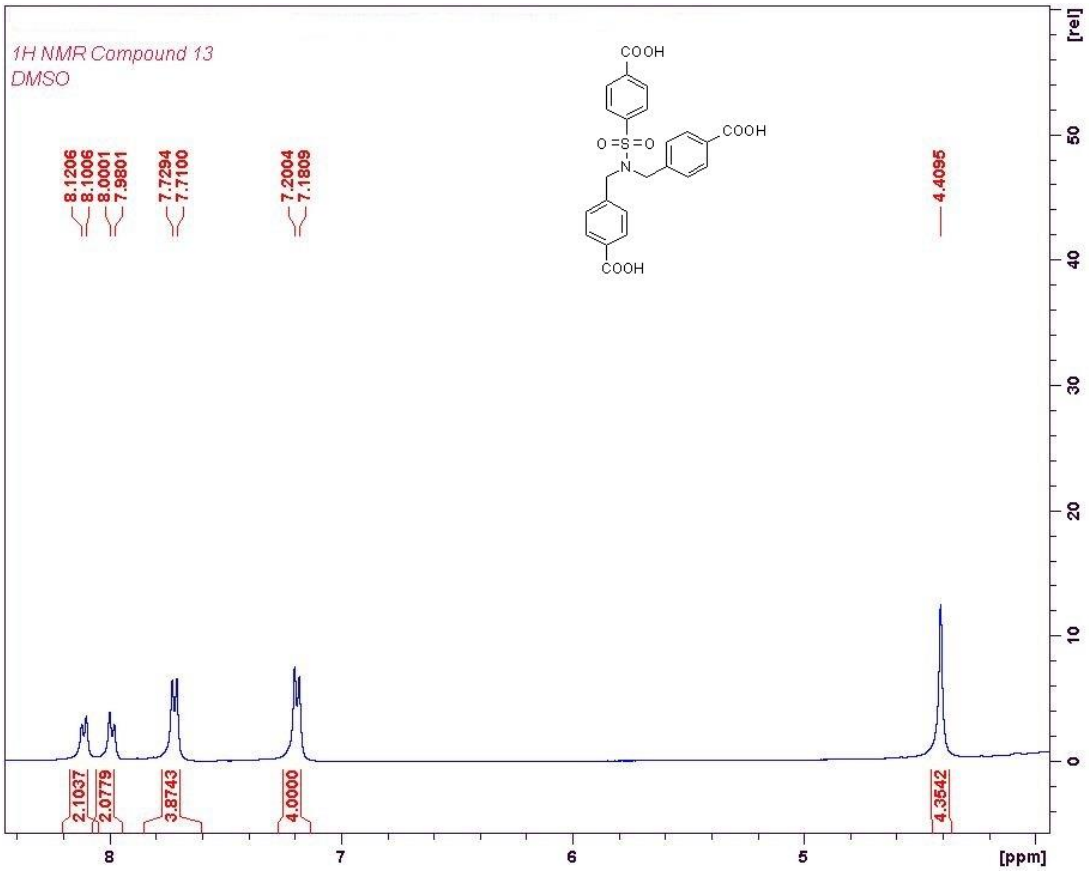


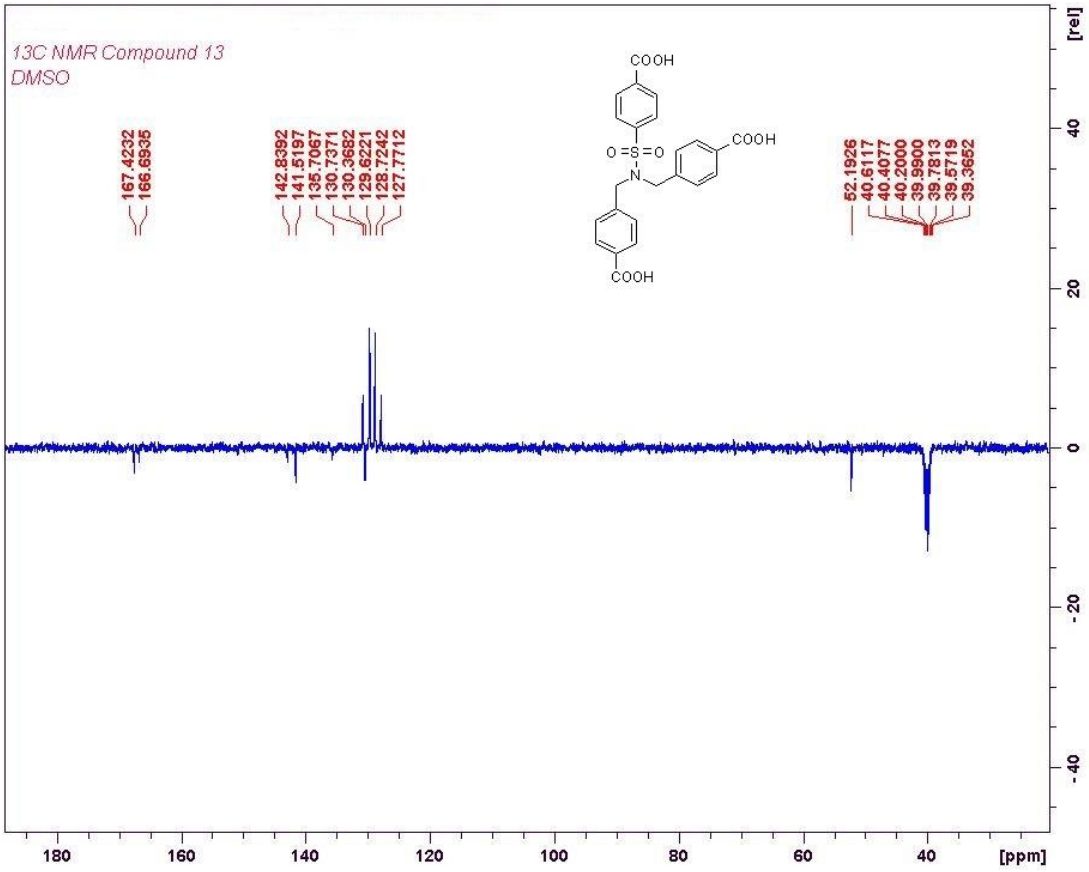
^{1}H-NMR and ^{13}C-NMR spectra of compound **7g**



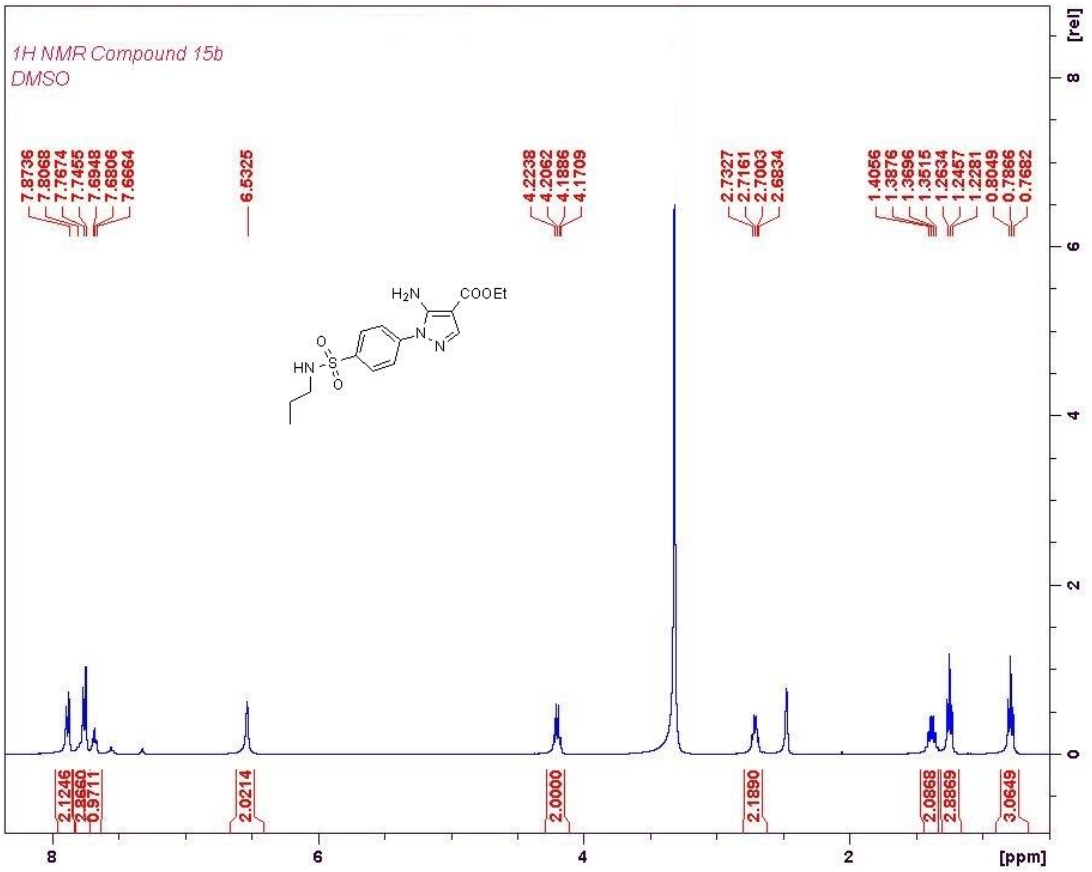


^{1}H-NMR and ^{13}C-NMR spectra of compound **13**

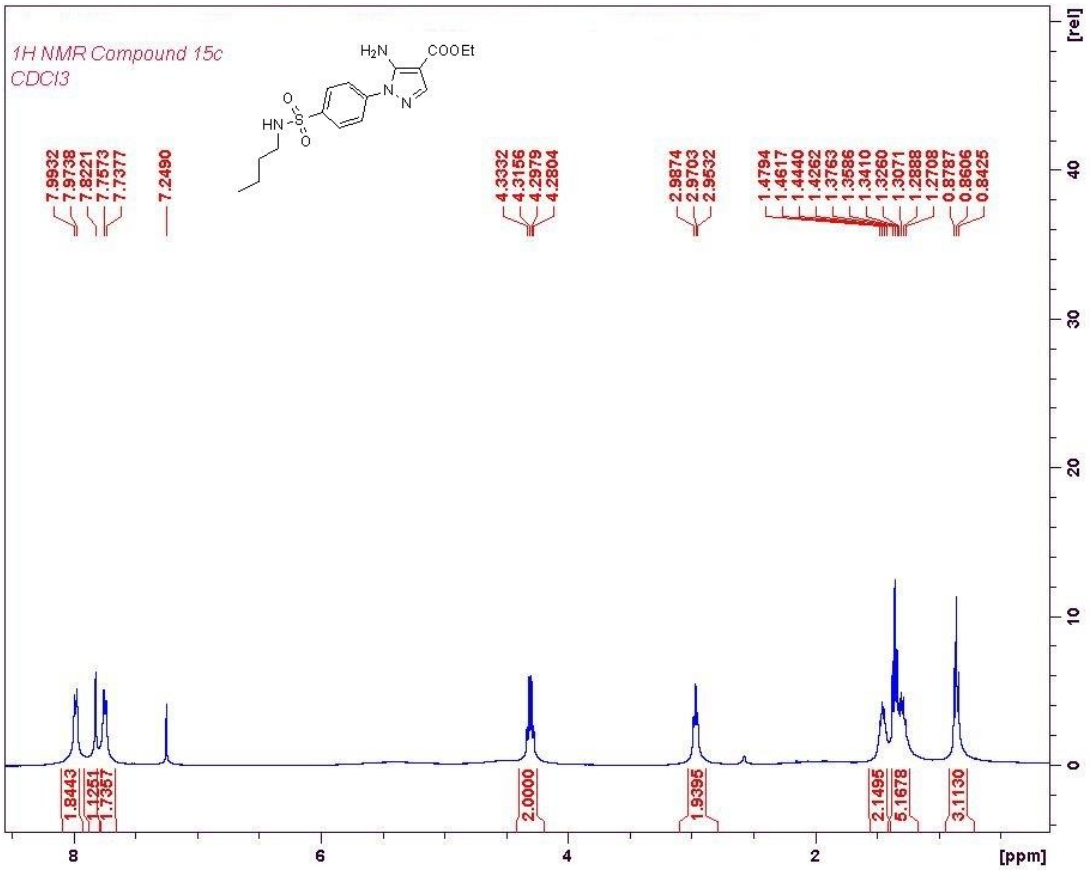




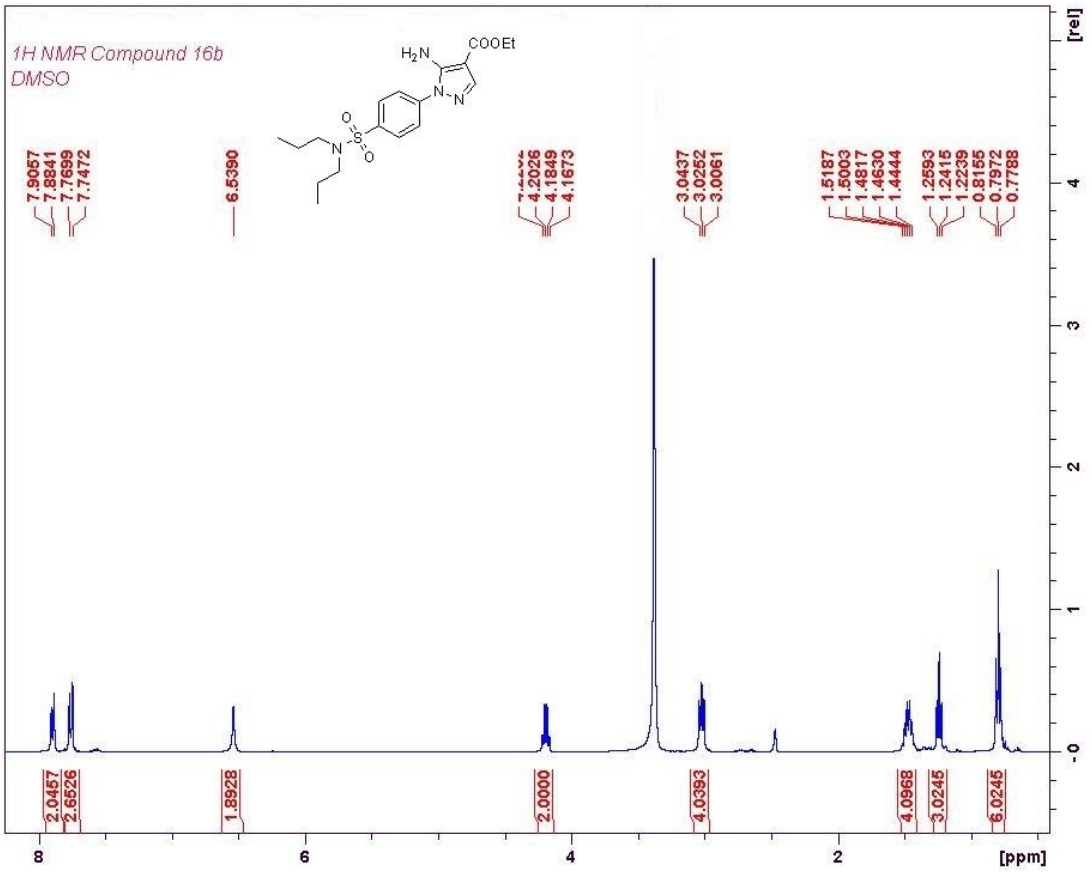
^{1}H-NMR spectrum of intermediate **15b**



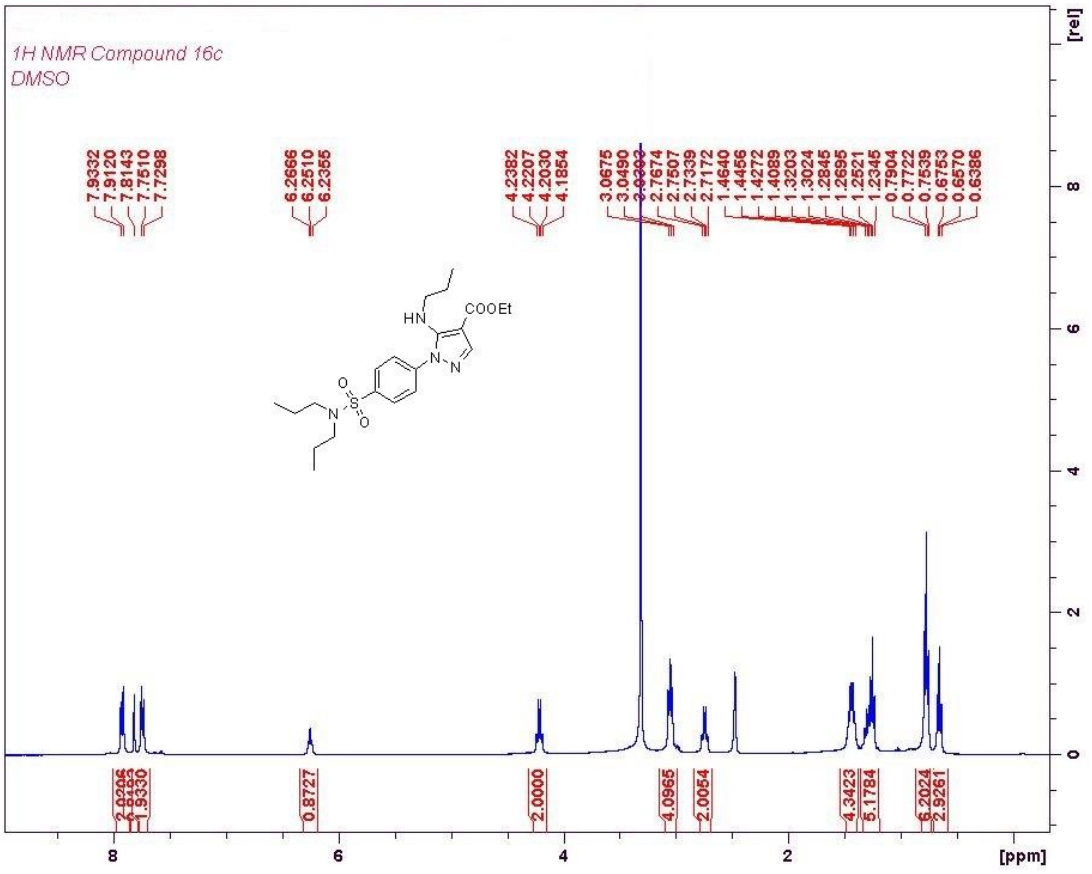
^{1}H-NMR spectrum of intermediate **15c**



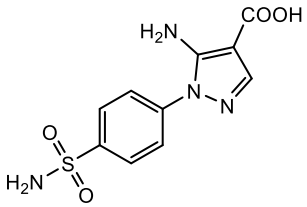
^{1}H-NMR spectrum of intermediate **16b**



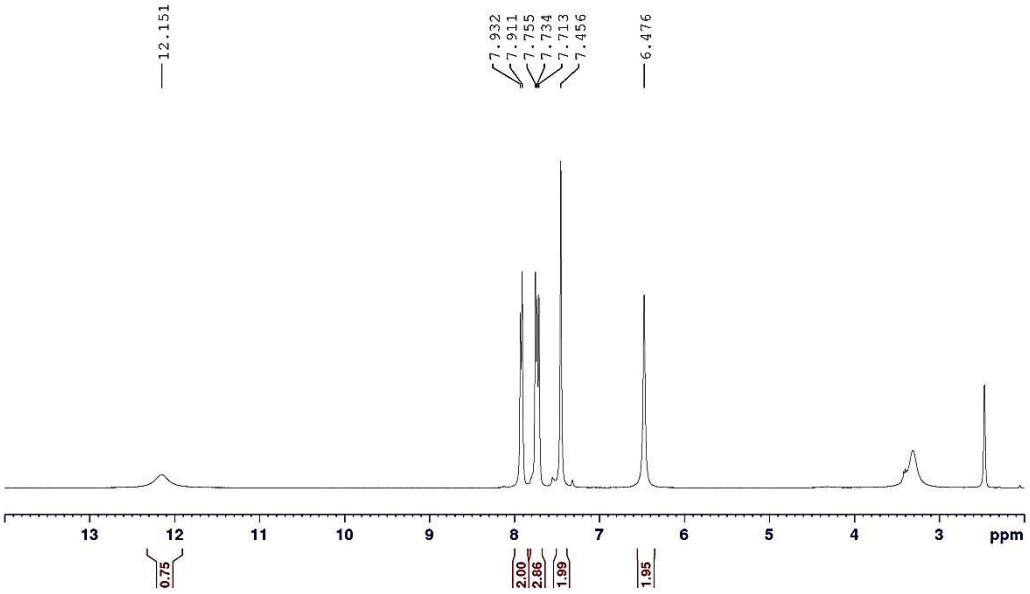
^{1}H-NMR spectrum of intermediate **16c**



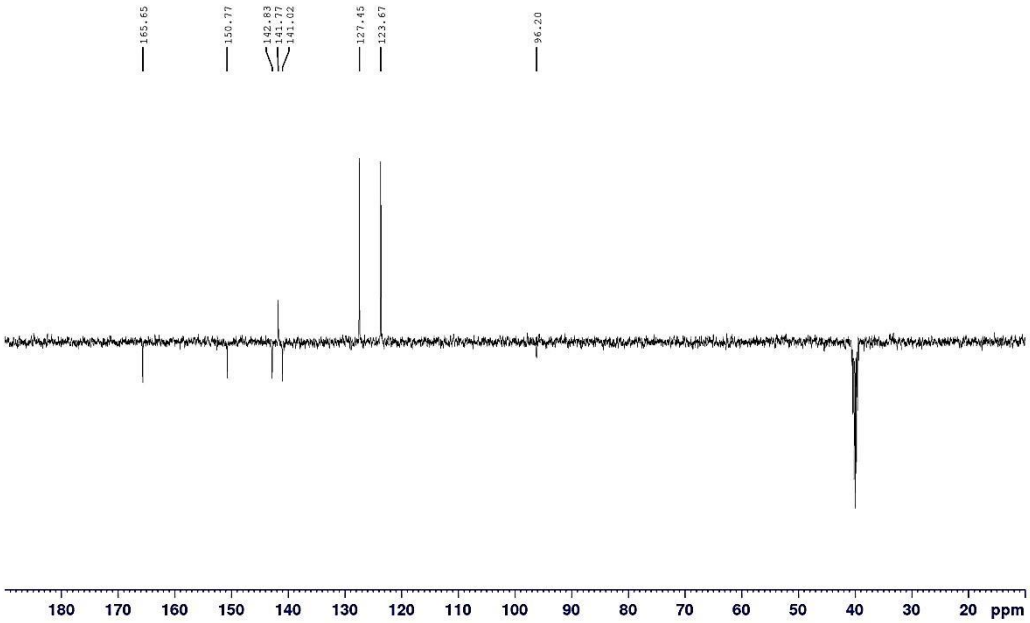
^{1}H-NMR and ^{13}C-NMR spectra of compound **17**



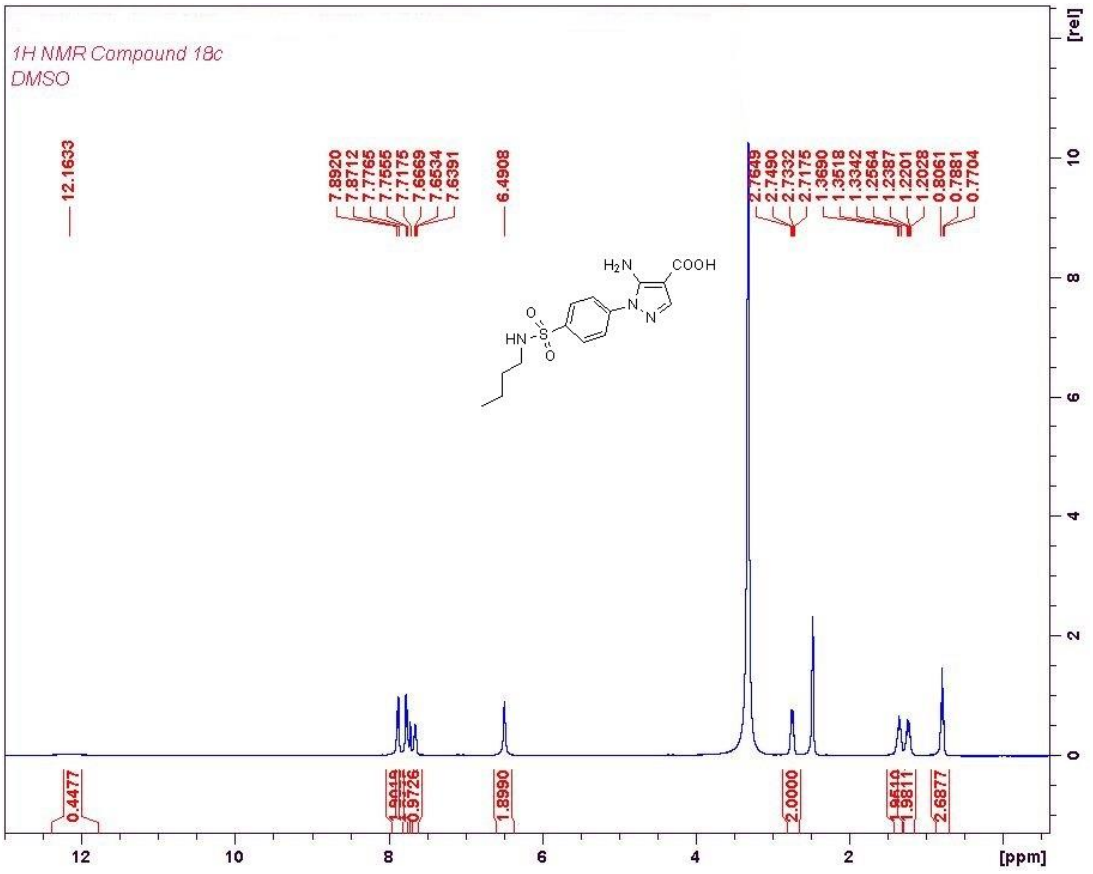
1H NMR Compound 17
DMSO

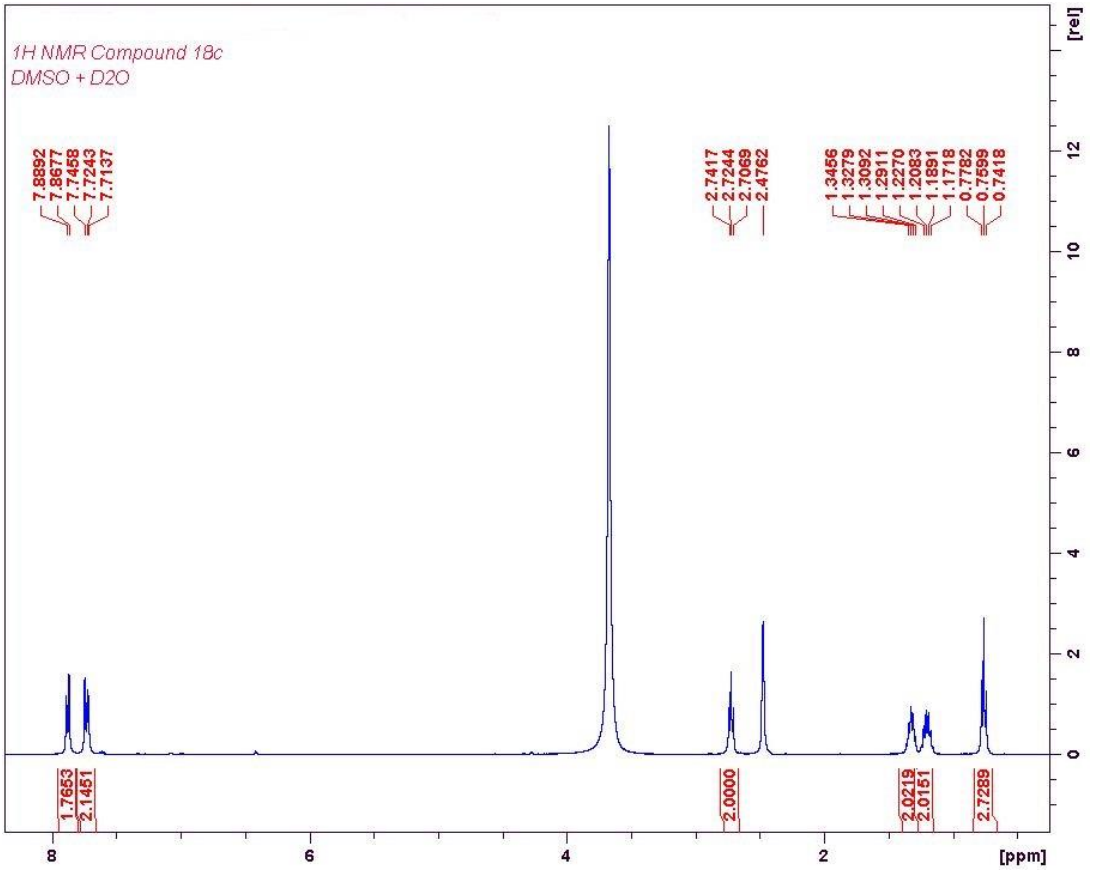


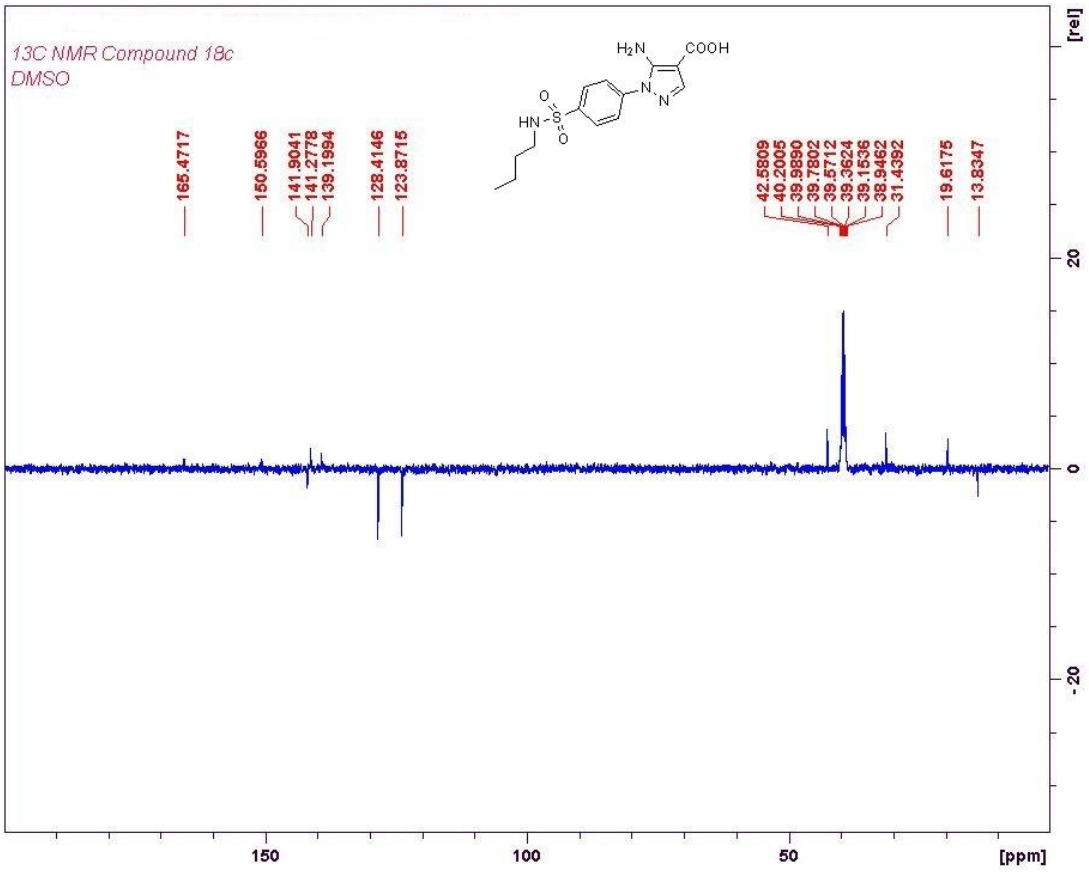
13C NMR Compound 17
DMSO



^{1}H-NMR and ^{13}C-NMR spectra of compound **18c**






13C NMR Compound 18c
DMSO
H2N
COOH
HN
O
S
O
N
N
165.4717
150.5966
141.9041
141.2778
139.1994
128.4146
123.8715
42.5809
40.2005
39.9890
39.7802
39.5712
39.3624
39.1536
38.9462
31.4392
19.6175
13.8347
[rel]
20
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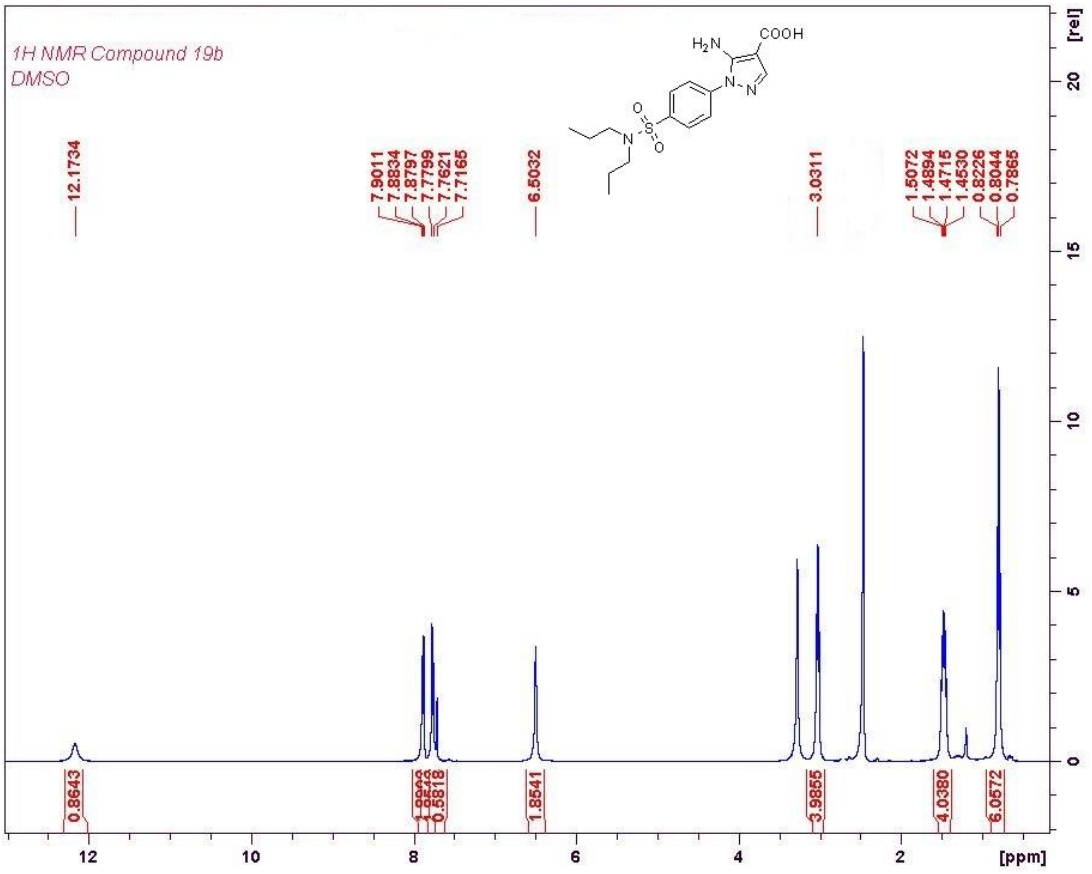
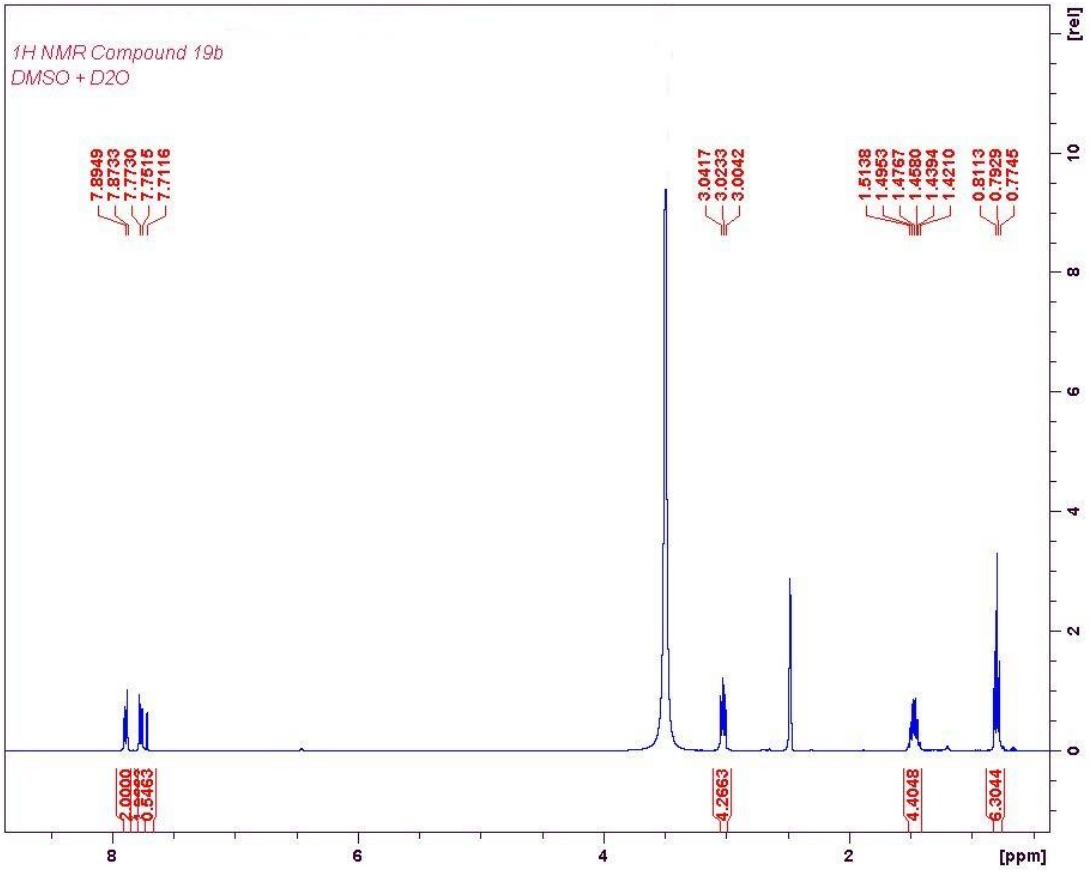
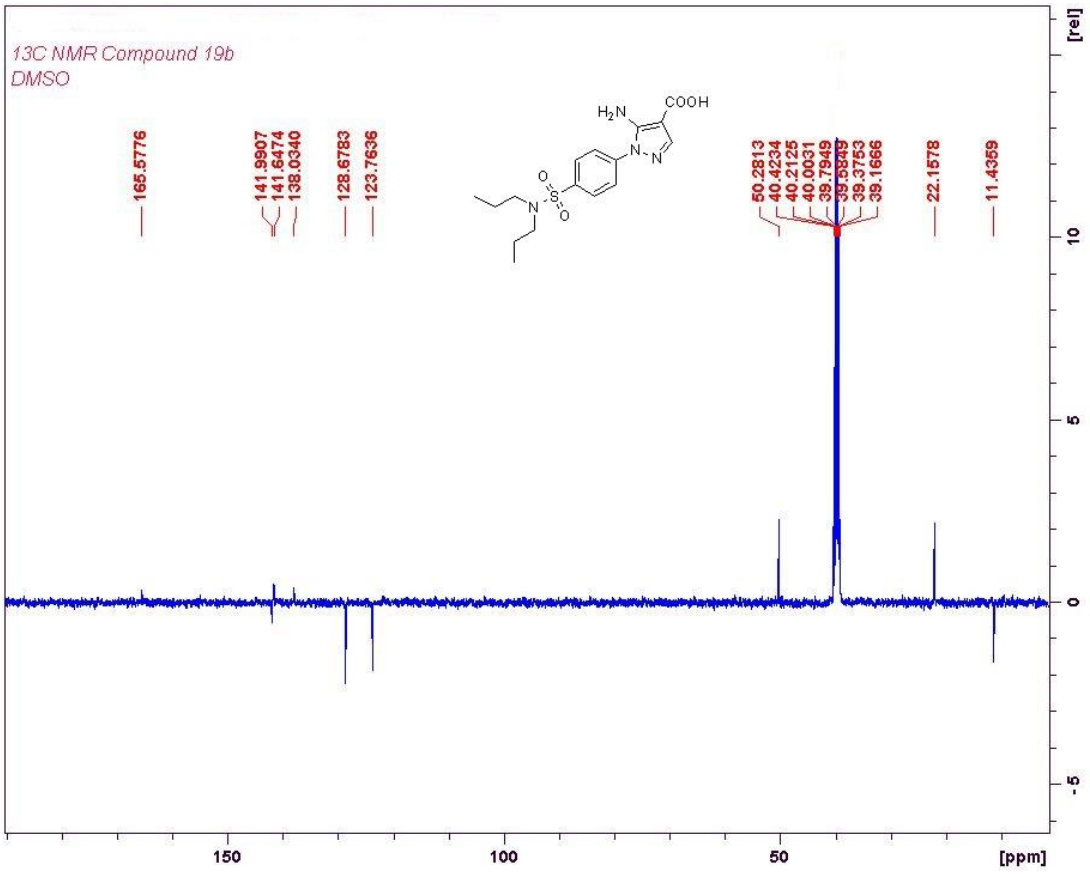
150
100
50
[ppm]

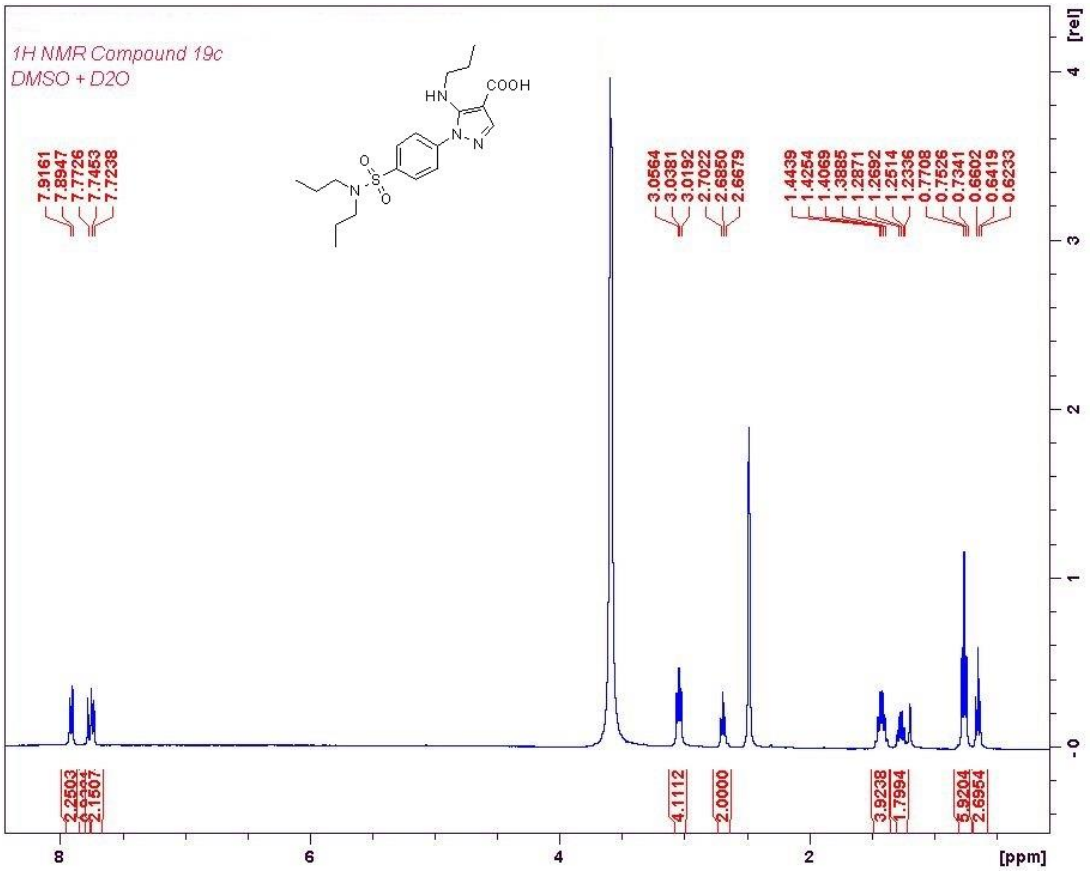
^{1}H-NMR and ^{13}C-NMR spectra of compound **19b**

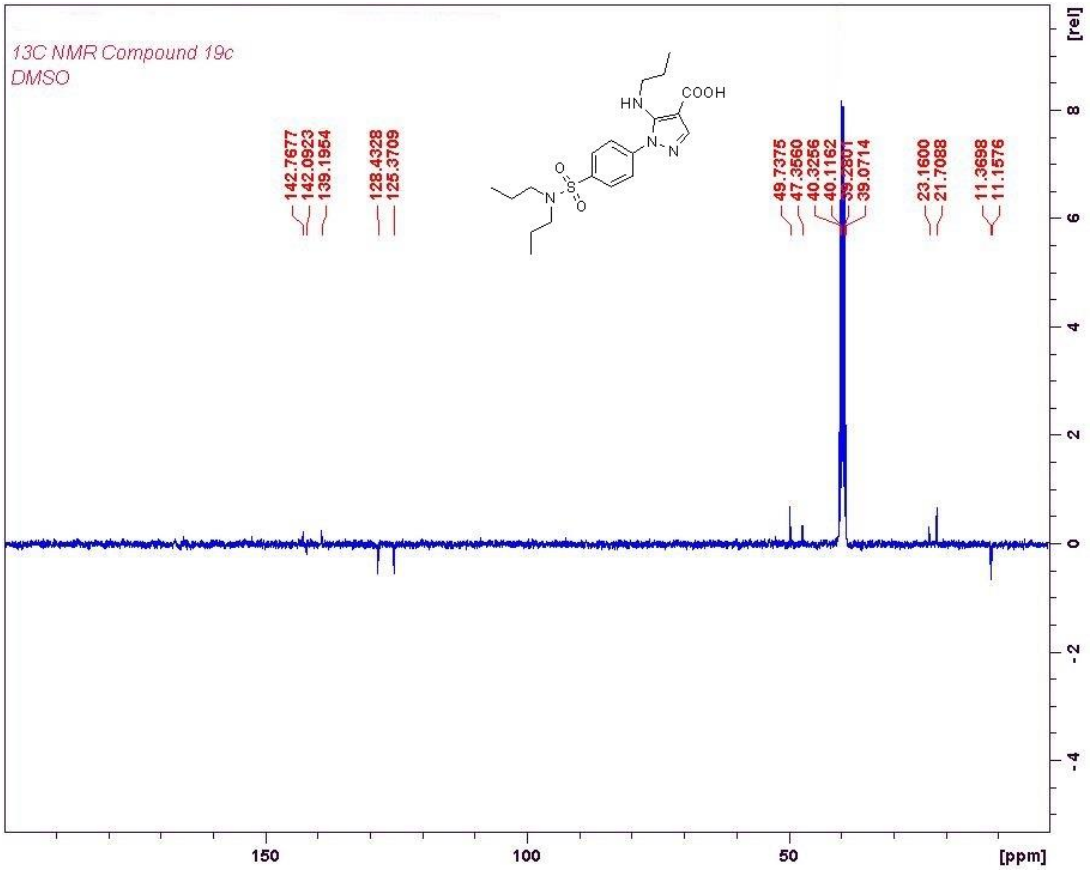




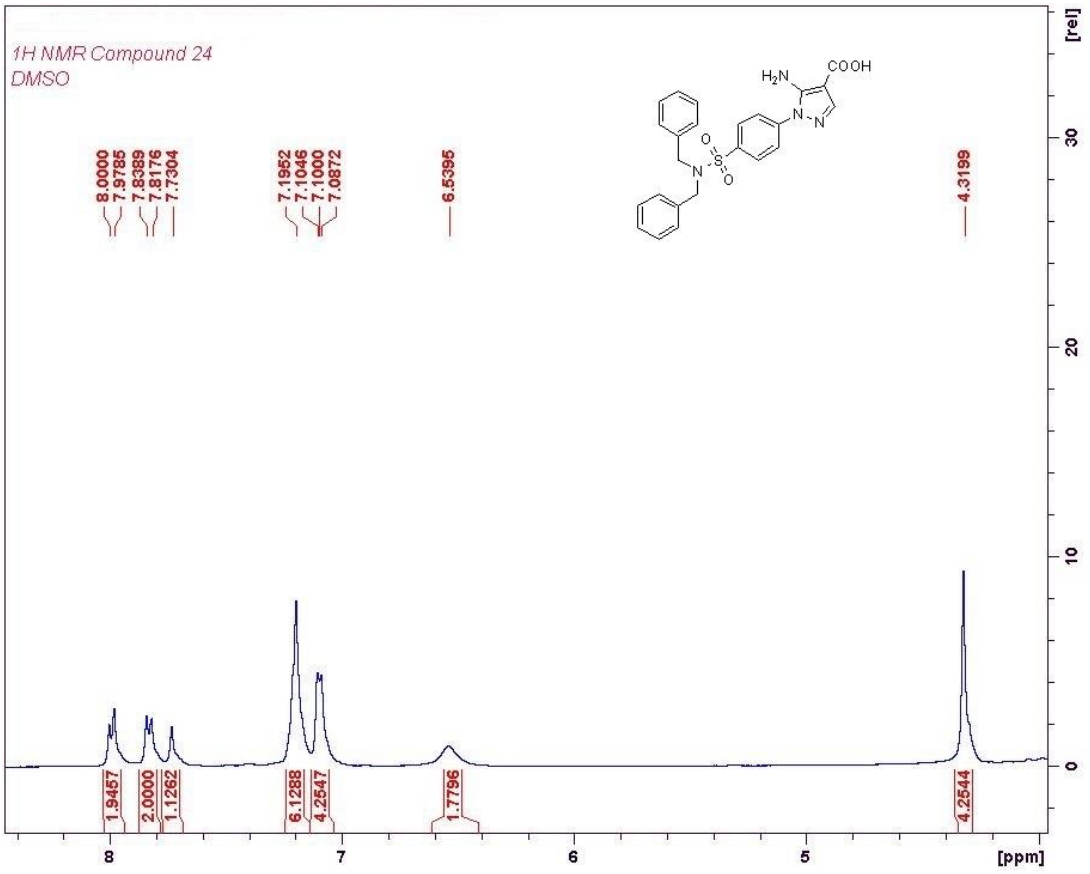

13C NMR Compound 19b
DMSO
165.5776
141.9907
141.6474
138.0340
128.6783
123.7636
50.2813
40.4234
40.2125
40.0031
39.7949
39.5849
39.3753
39.1666
22.1578
11.4359
COOH
H_2N
N
N
O
S
O
150
100
50
[ppm]
10
5
0
-5
[rel]

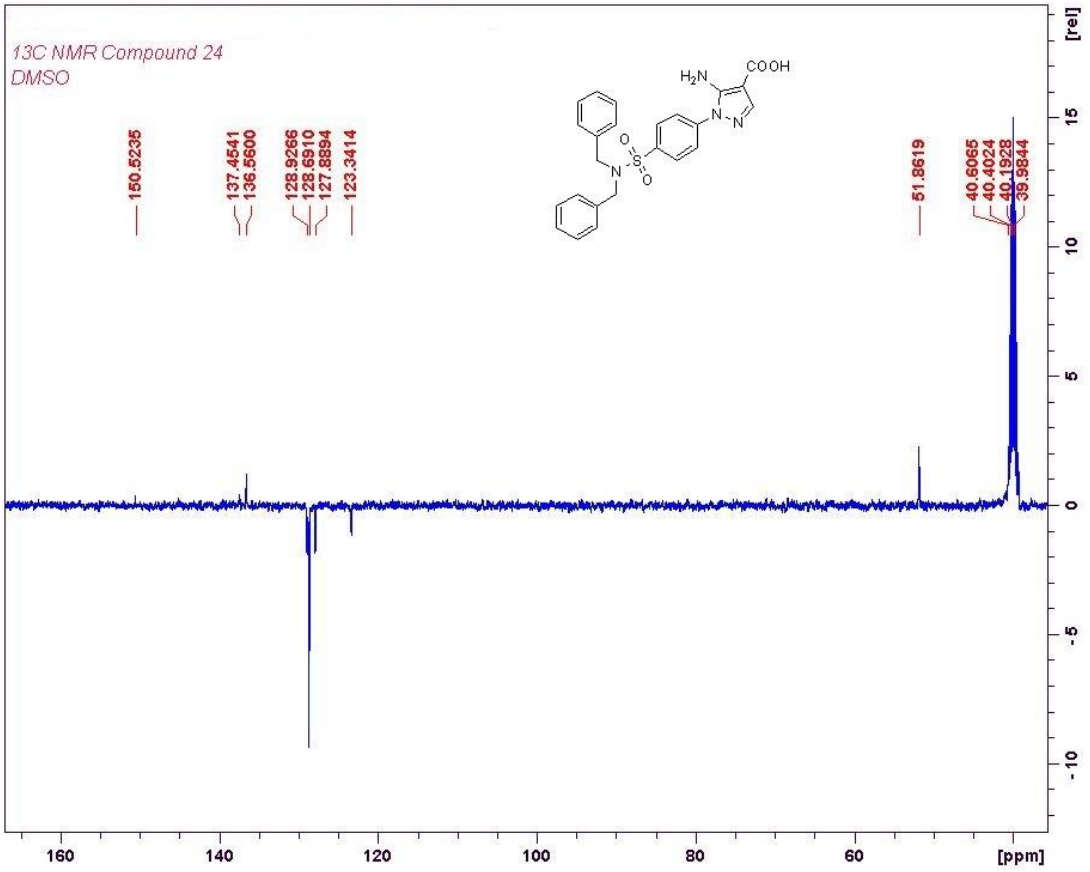
^{1}H-NMR and ^{13}C-NMR spectra of compound **19c**



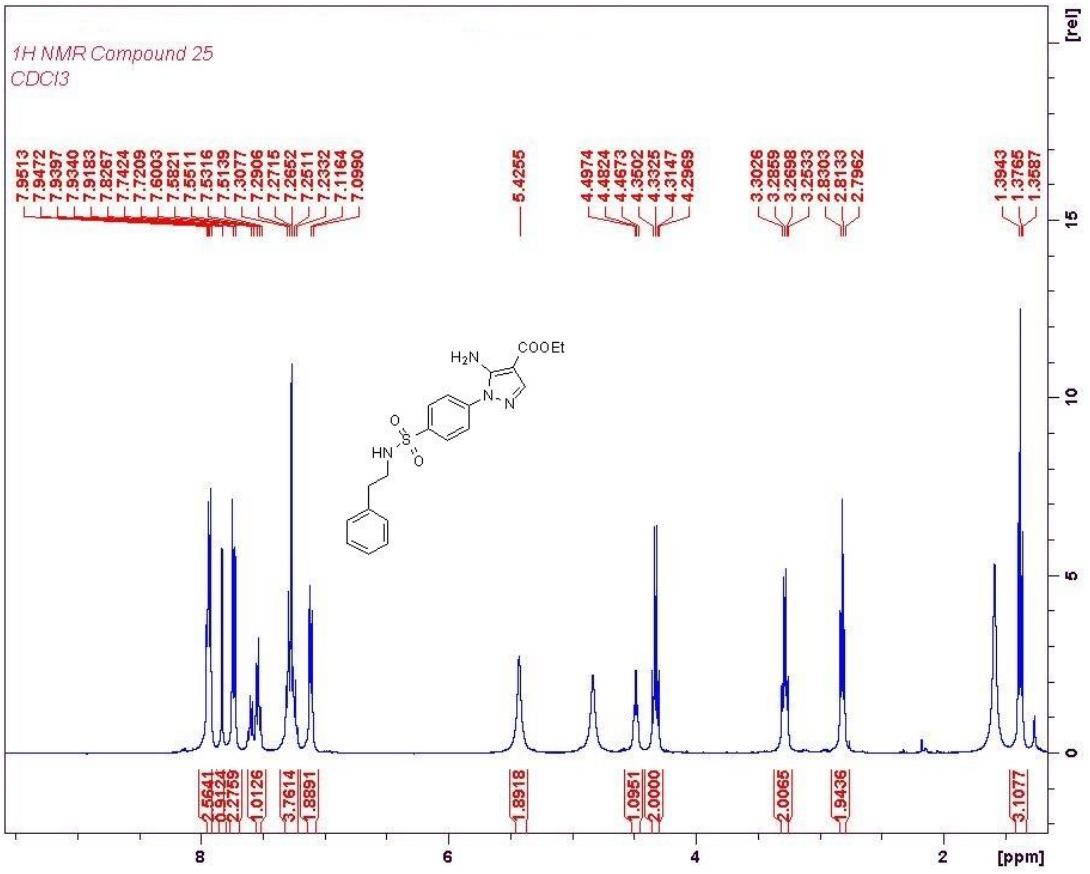


^{1}H-NMR and ^{13}C-NMR spectra of compound **24**

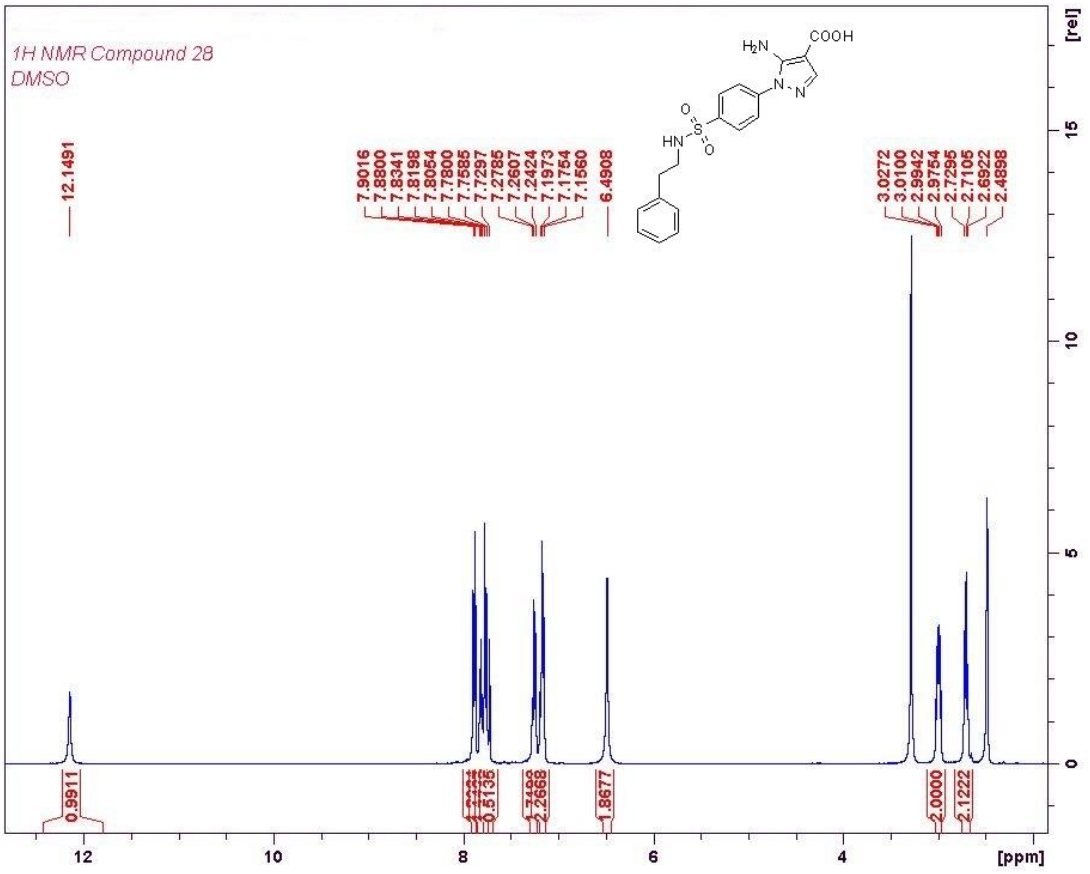


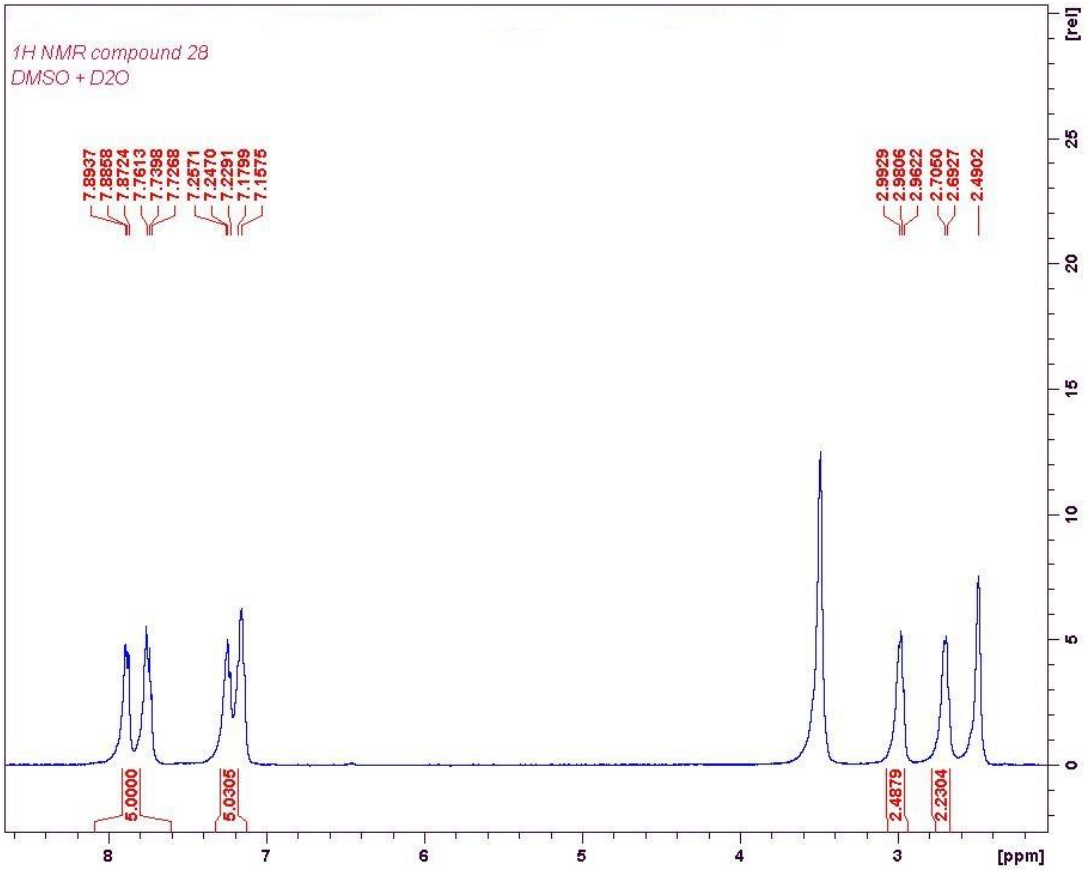


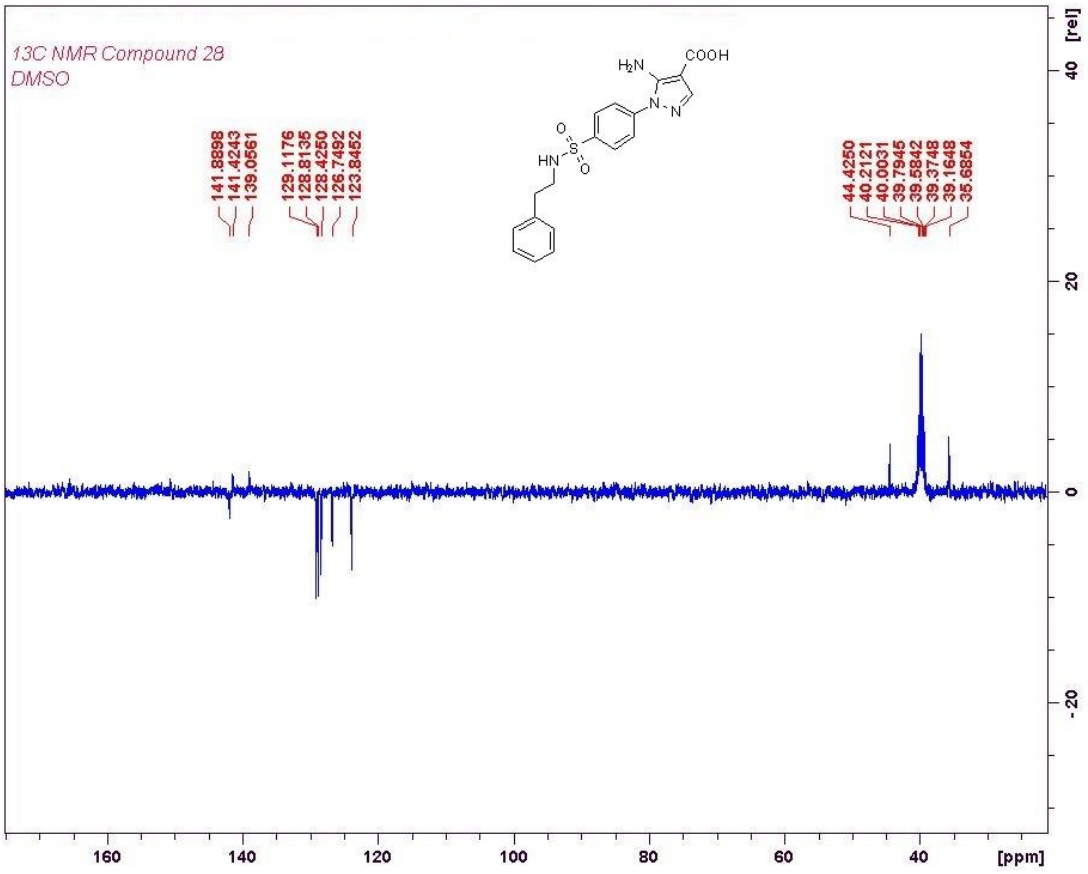
^{1}H-NMR spectrum of intermediate **25**



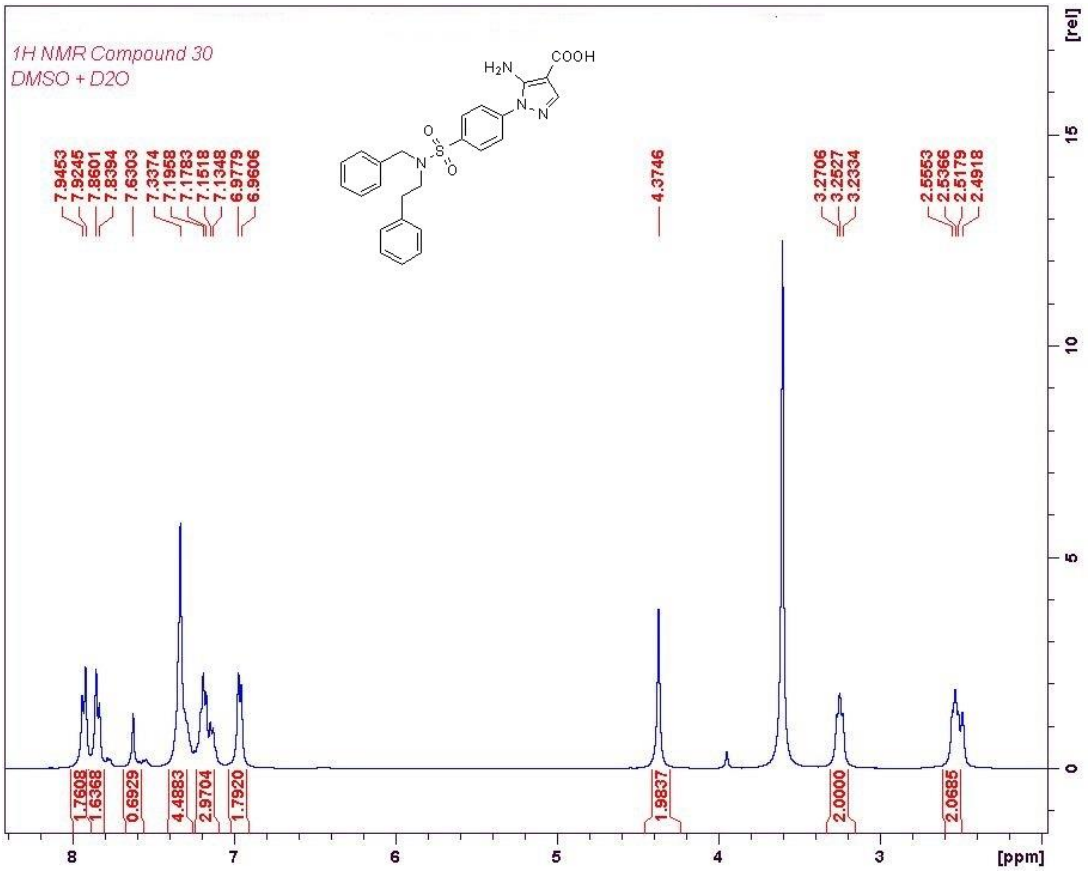
^{1}H-NMR and ^{13}C-NMR spectra of compound **28**






13C NMR Compound 28
DMSO
141.8898
141.4243
139.0561
129.1176
128.8135
128.4250
126.7492
123.8452
44.4250
40.2121
40.0031
39.7945
39.5842
39.3748
39.1648
35.6854
H2N
COOH
HN
O
S
O
N
N
40
20
0
-20
[rel]
160
140
120
100
80
60
40
[ppm]

^{1}H-NMR and ^{13}C-NMR spectra of compound **30**



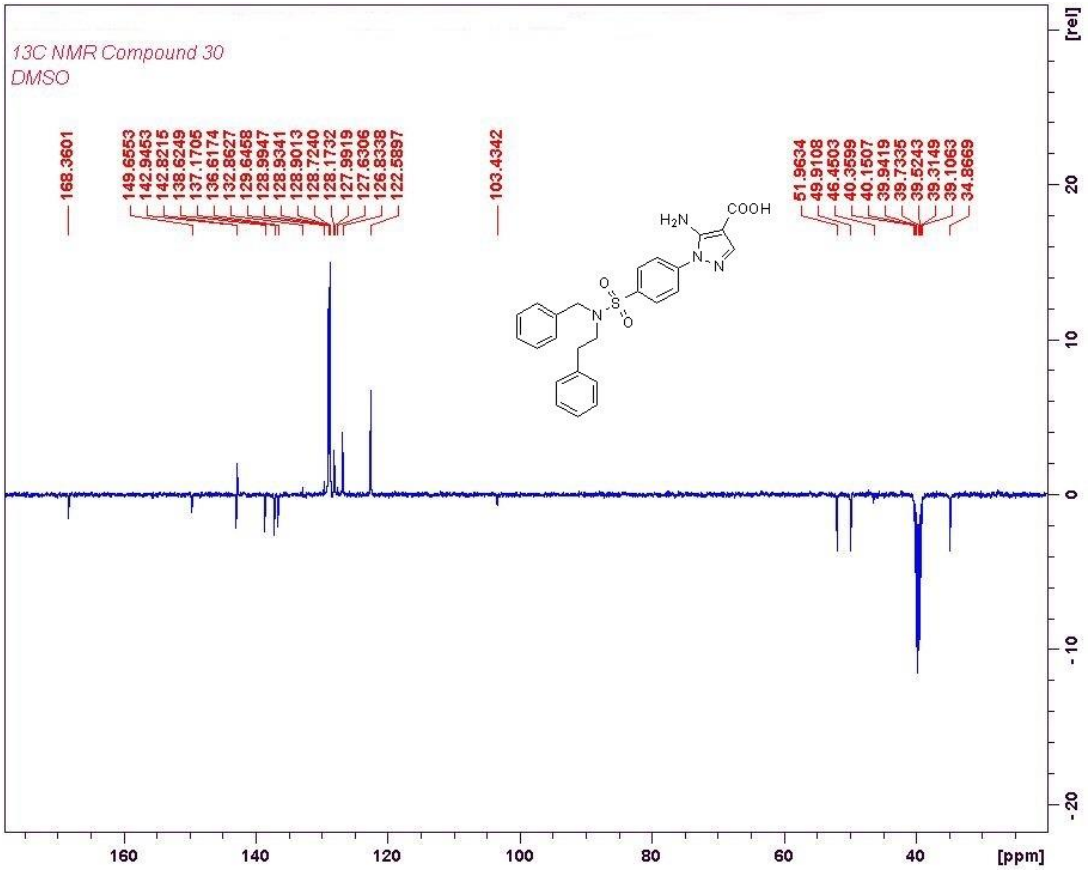


Table S1. Elemental analysis

Comp.	Formula (MW)	Anal. Calcd.				Anal. Found		
		C	H	N		C	H	N
3a	$C_{17}H_{15}NO_3S$ (313.37)	65.16	4.82	4.47		65.42	4.84	4.49
3b	$C_{18}H_{17}NO_3S$ (327.40)	66.04	5.23	4.28		66.30	5.25	4.30
3c	$C_{19}H_{19}NO_3S$ (341.43)	66.84	5.61	4.10		66.57	5.59	4.08
3d	$C_{20}H_{21}NO_3S$ (355.45)	67.58	5.96	3.94		67.30	5.94	3.92
3e	$C_{21}H_{23}NO_3S$ (369.48)	68.27	6.27	3.79		68.54	6.29	3.80
4	$C_{18}H_{15}NO_5S$ (357.38)	60.50	4.23	3.92		60.74	4.25	3.93
5	$C_{18}H_{17}NO_3S$ (327.40)	66.04	5.23	4.28		66.30	5.25	4.30
7a	$C_{21}H_{22}N_2O_6S_2$ (462.54)	54.53	4.79	6.06		54.31	4.77	6.03
7b	$C_{23}H_{26}N_2O_6S_2$ (490.59)	56.31	5.34	5.71		56.08	5.32	5.69
7c	$C_{25}H_{30}N_2O_6S_2$ (518.64)	57.90	5.83	5.40		57.67	5.80	5.38
7d	$C_{31}H_{26}N_2O_6S_2$ (586.68)	63.47	4.47	4.78		63.72	4.49	4.80
7e	$C_{33}H_{30}N_2O_6S_2$ (614.73)	64.48	4.92	4.56		64.22	4.90	4.54
7f	$C_{32}H_{28}N_2O_6S_2$ (600.70)	63.98	4.70	4.66		63.72	4.68	4.64
7g	$C_{25}H_{22}N_2O_6S_2$ (510.58)	58.81	4.34	5.49		58.57	4.32	5.47
8	$C_{17}H_{13}NO_4S$ (327.35)	62.37	4.00	4.28		62.62	4.01	4.30
9	$C_{25}H_{29}N_2NaO_6S_2$ (540.62)	55.54	5.41	5.18		55.76	5.43	5.20
13	$C_{23}H_{19}NO_8S$ (469.46)	58.84	4.08	2.98		59.07	4.10	2.99
17	$C_{10}H_{10}N_4O_4S$ (282.27)	42.55	3.57	19.85		42.72	3.58	19.92
18a	$C_{12}H_{14}N_4O_4S$ (310.33)	46.45	4.55	18.05		46.36	4.53	17.98
18b	$C_{13}H_{16}N_4O_4S$ (324.36)	48.14	4.97	17.27		48.33	4.99	17.33
18c	$C_{14}H_{18}N_4O_4S$ (338.38)	49.69	5.36	16.56		49.49	5.34	16.49
19a	$C_{14}H_{18}N_4O_4S$ (338.38)	49.69	5.36	16.56		49.49	5.34	16.49
19b	$C_{16}H_{22}N_4O_4S$(366.44)	52.44	6.05	15.29		59.28	3.97	5.53
19c	$C_{19}H_{28}N_4O_4S$ (408.52)	55.86	6.91	13.71		55.64	6.88	16.65
23	$C_{17}H_{16}N_4O_4S$ (372.40)	54.83	4.33	15.05		54.61	4.31	14.99
24	$C_{24}H_{22}N_4O_4S$ (462.52)	62.32	4.79	12.11		62.56	4.80	12.16
28	$C_{18}H_{18}N_4O_4S$ (386.43)	55.95	4.70	14.50		55.72	4.68	14.44
29	$C_{26}H_{26}N_4O_4S$ (490.58)	63.66	5.34	11.42		63.91	5.36	11.46
30	$C_{25}H_{24}N_4O_4S$ (476.55)	63.01	5.08	11.76		63.26	5.10	11.80

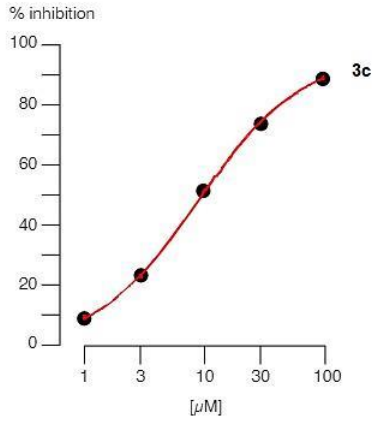


Figure S1. Quantitative analysis of the % inhibition of Panx1-mediated membrane currents in oocytes for compound **3c**.

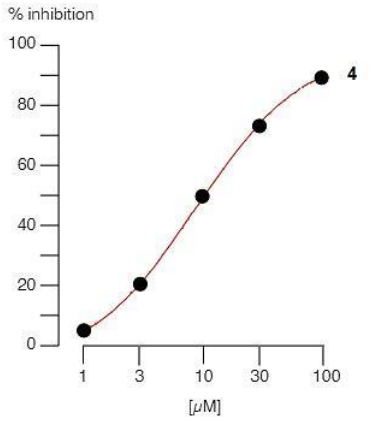


Figure S2. Quantitative analysis of the % inhibition of Panx1-mediated membrane currents in oocytes for compound **4**.

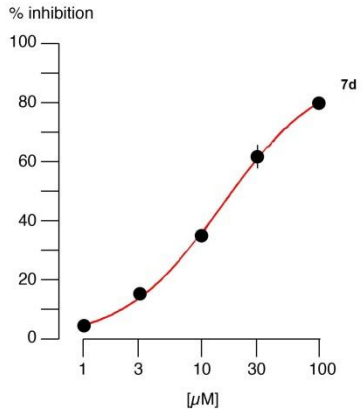


Figure S3. Quantitative analysis of the % inhibition of Panx1-mediated membrane currents in oocytes for compound **7d**.