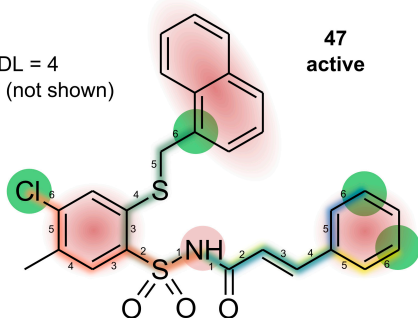


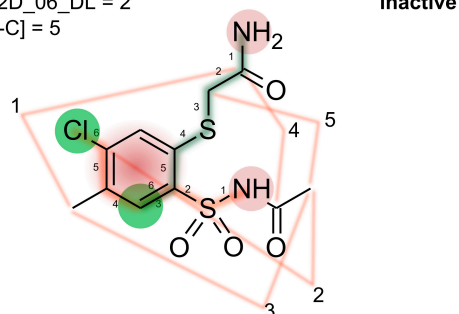
# Supplementary Materials

**A**

NRS = 3  
CATS2D\_06\_DL = 4  
F07[C-C] = 26 (not shown)

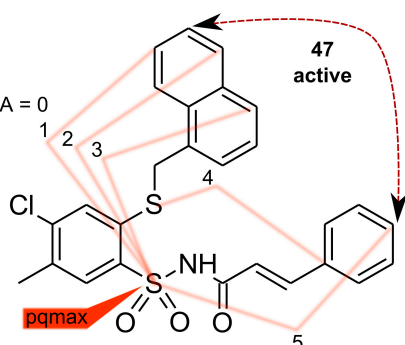


NRS = 1  
CATS2D\_06\_DL = 2  
F07[C-C] = 5

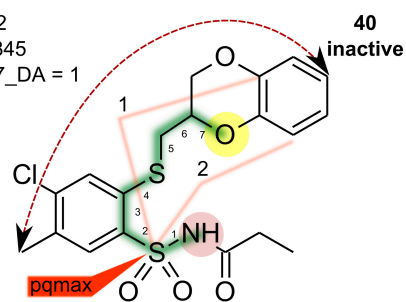


**B**

F08[C-S] = 5  
qpmax = 2.848  
CATS2D\_07\_DA = 0  
ECC = 442

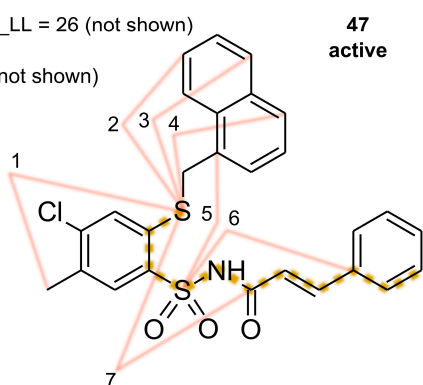


F08[C-S] = 2  
qpmax = 2.845  
CATS2D\_07\_DA = 1  
ECC = 305

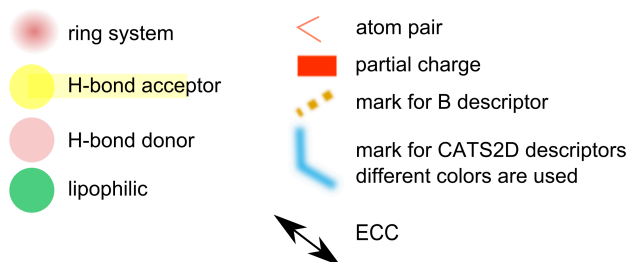
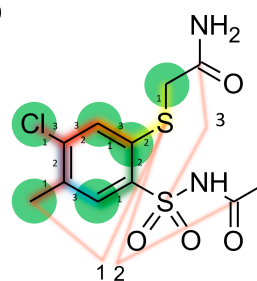


**C**

CATS2D\_03\_LL = 26 (not shown)  
F05[C-S] = 7  
C-024 = 14 (not shown)  
B10[C-S] = 1



CATS2D\_03\_LL = 5  
F05[C-S] = 3  
C-024 = 2  
B10[C-S] = 0



**Figure S1.** Visualization of molecular descriptors values incorporated in QSAR models for MCF-7 (A); HeLa (B); HCT-116 (C) cell lines.

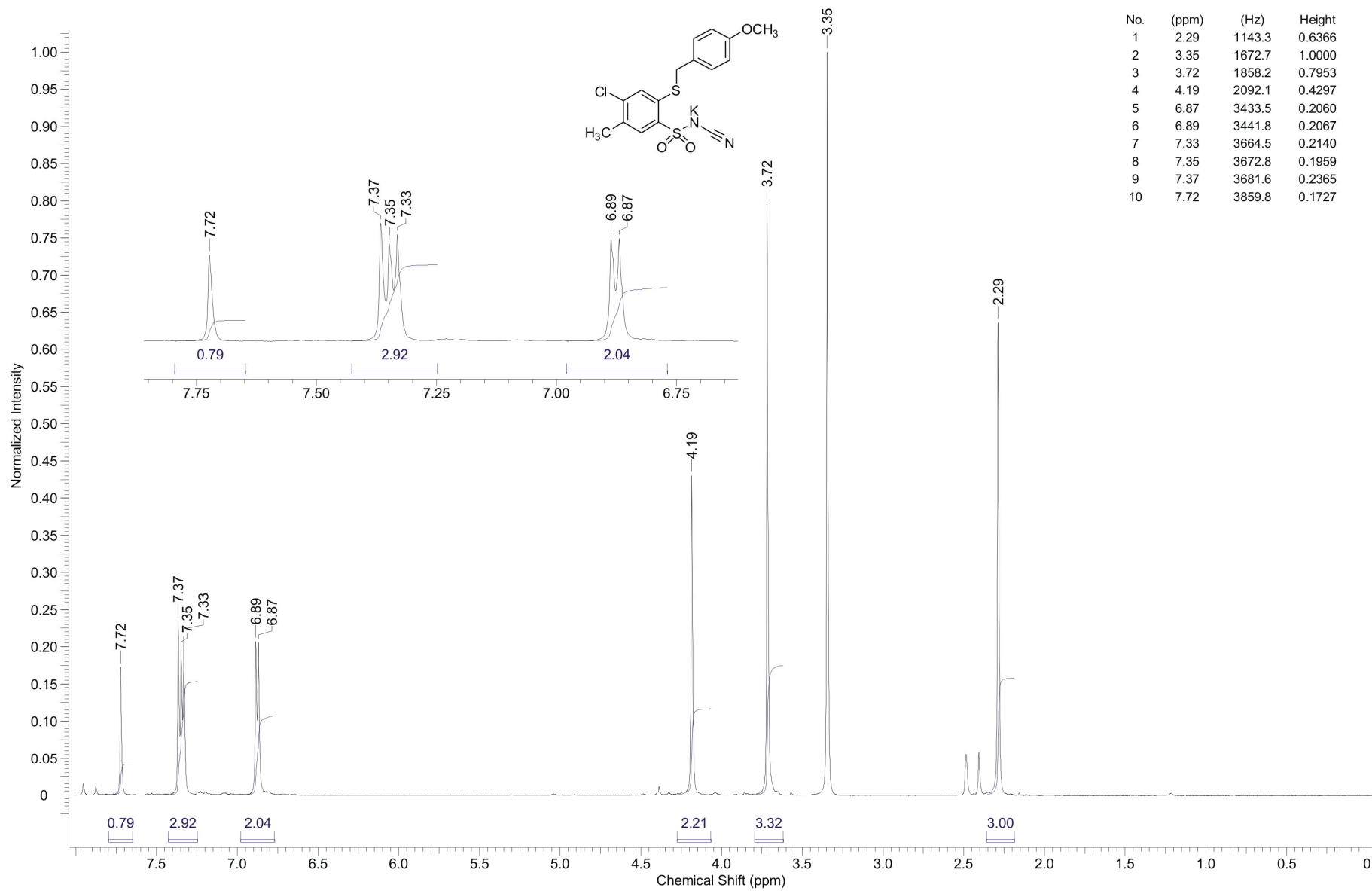


Figure S2.  $^1\text{H-NMR}$  of compound 10 (500 MHz,  $\text{DMSO-}d_6$ ).

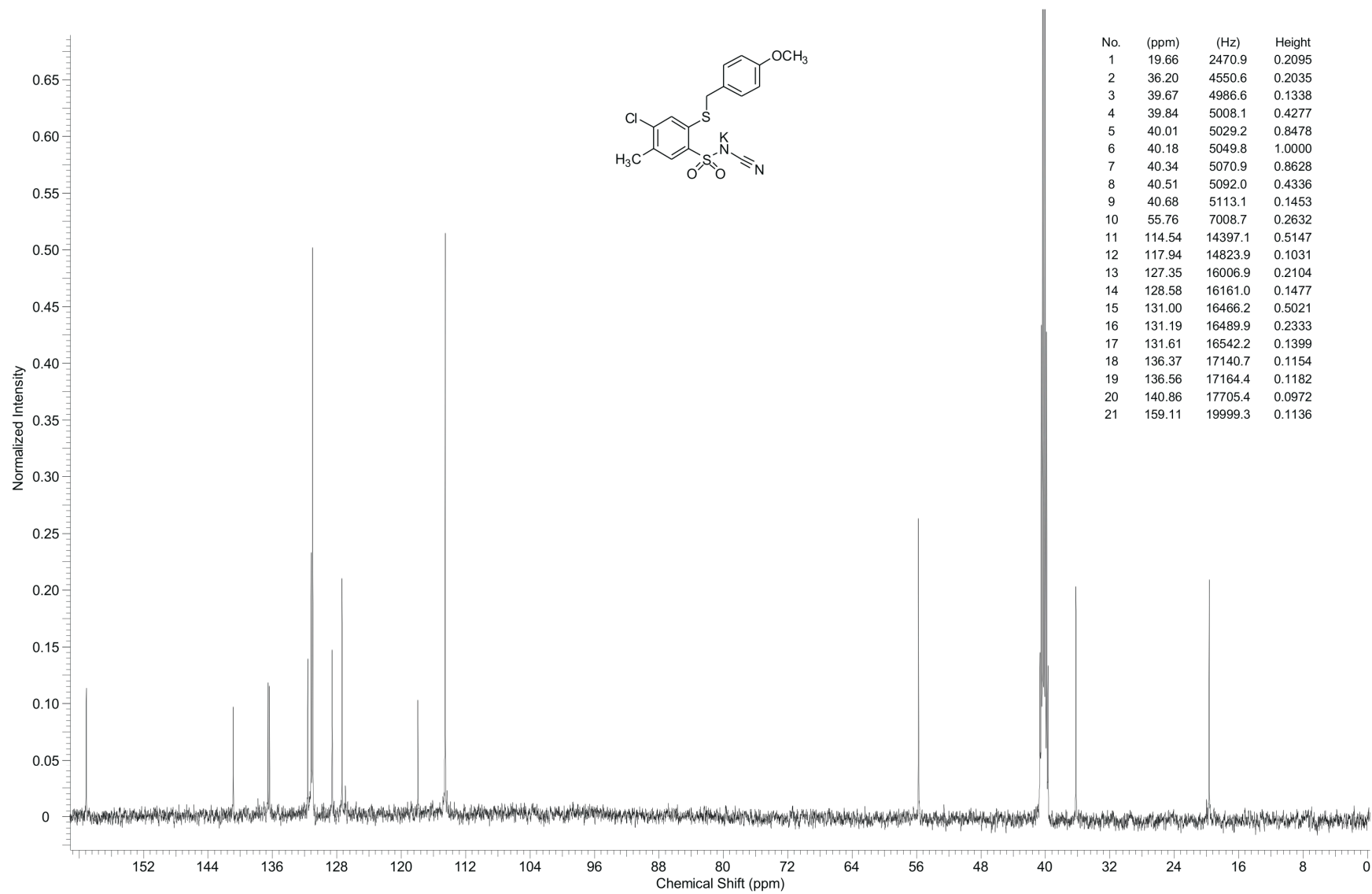


Figure S3.  $^{13}\text{C}$ -NMR of compound 10 (125 MHz,  $\text{DMSO-}d_6$ ).

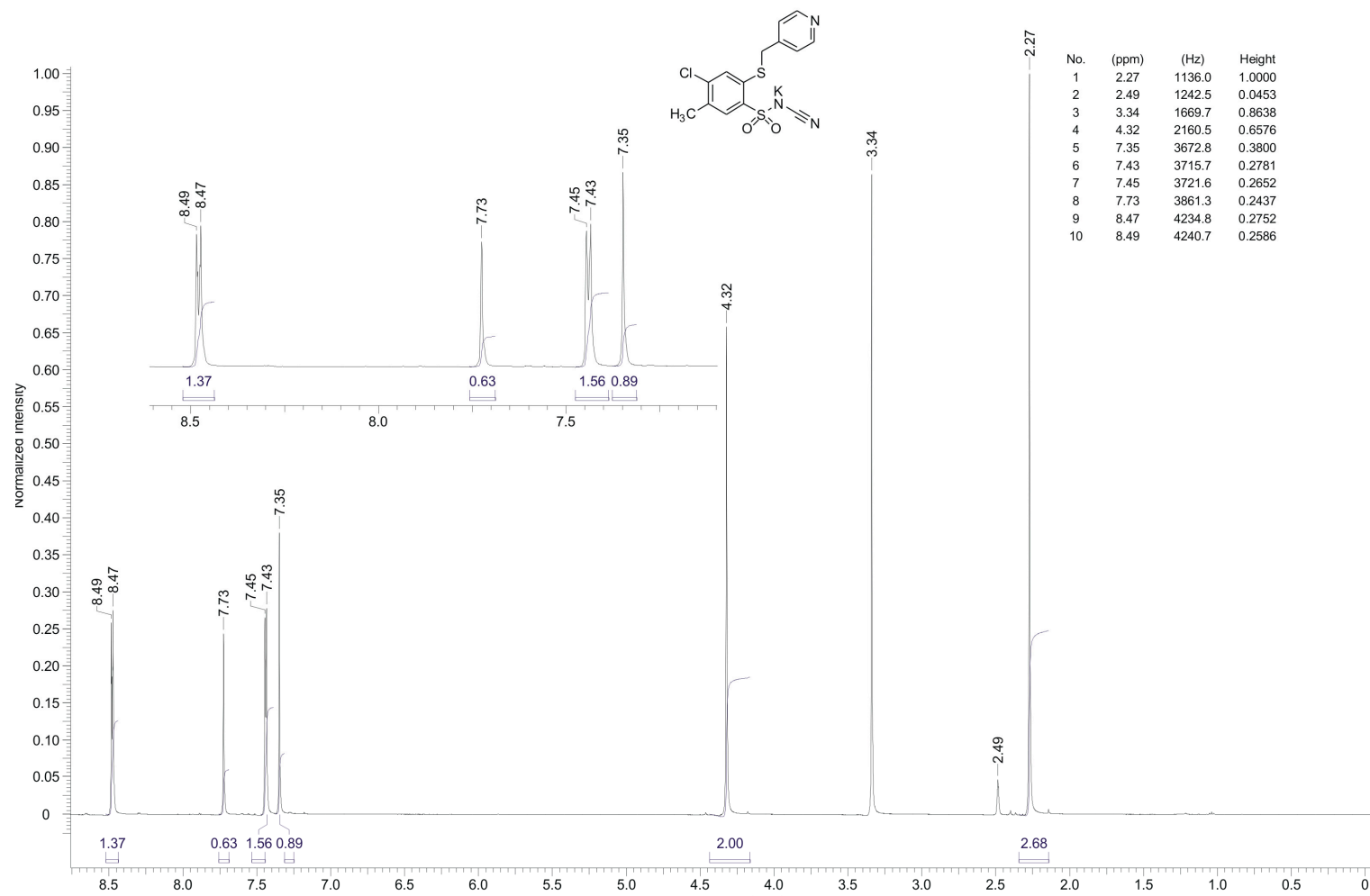


Figure S4.  $^1\text{H-NMR}$  of compound 11 (500 MHz,  $\text{DMSO-}d_6$ ).

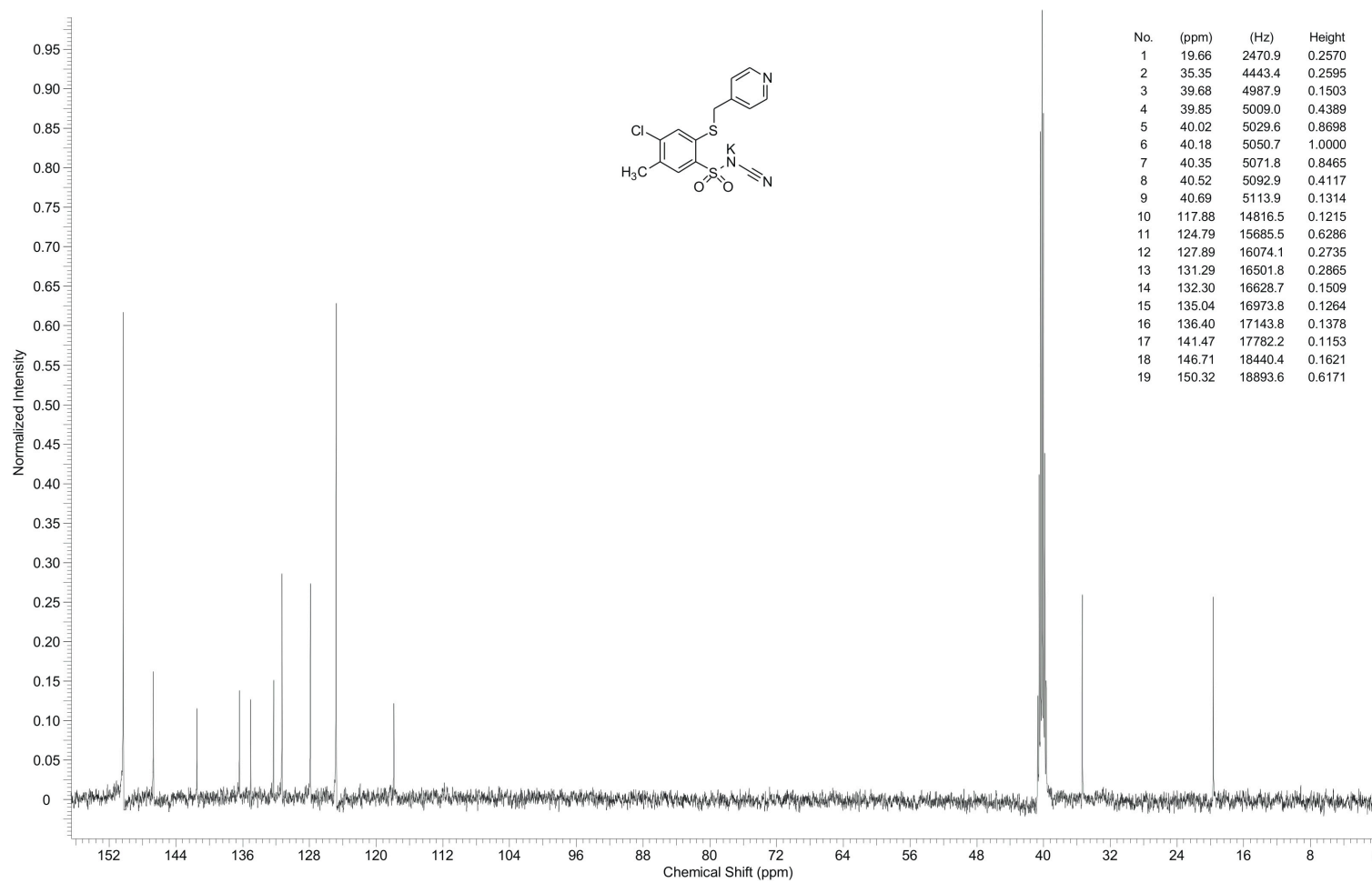


Figure S5.  $^{13}\text{C}$ -NMR of compound 11 (125 MHz DMSO- $d_6$ ).

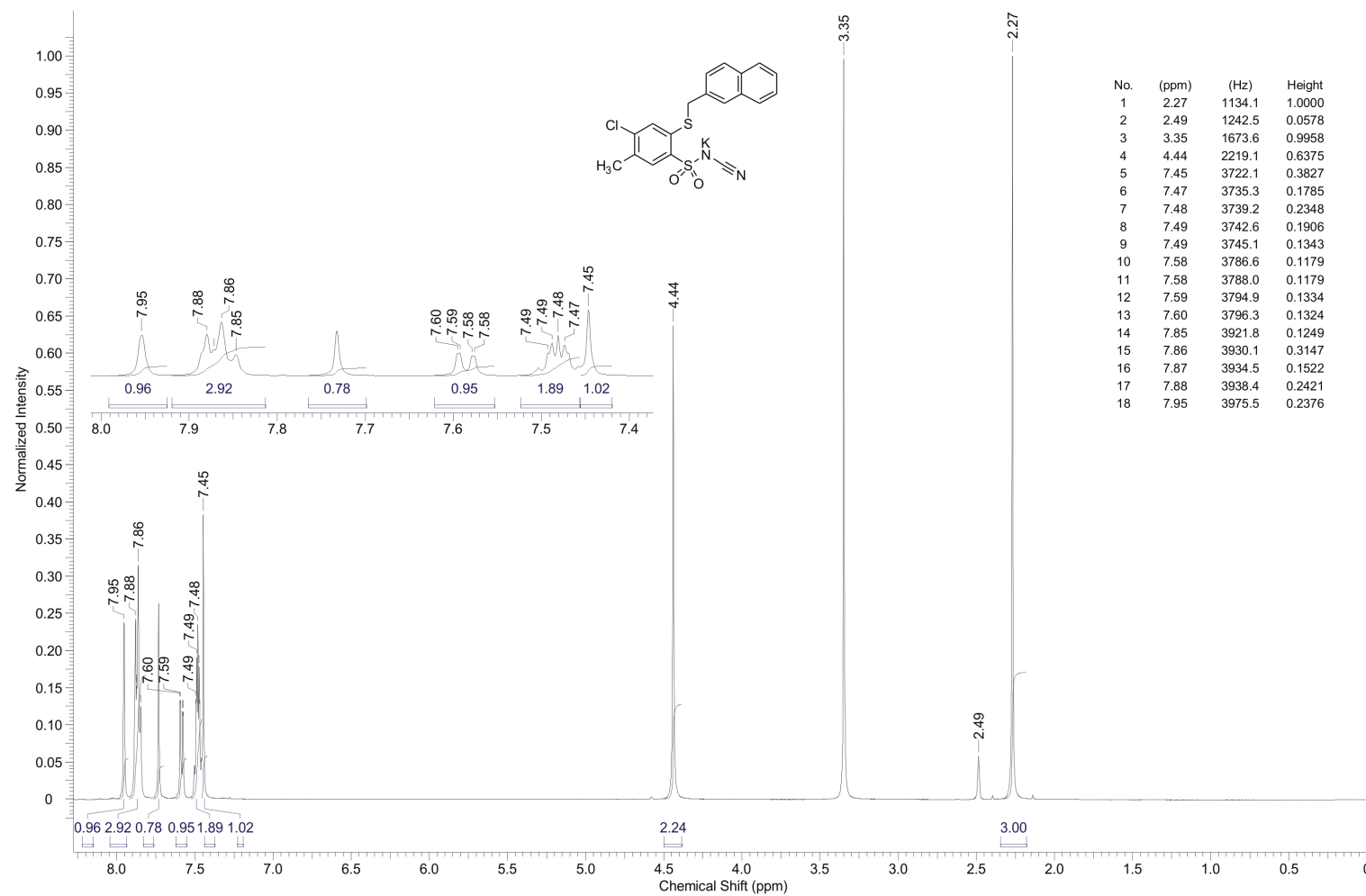


Figure S6.  $^1\text{H-NMR}$  of compound 13 (500 MHz,  $\text{DMSO-}d_6$ ).

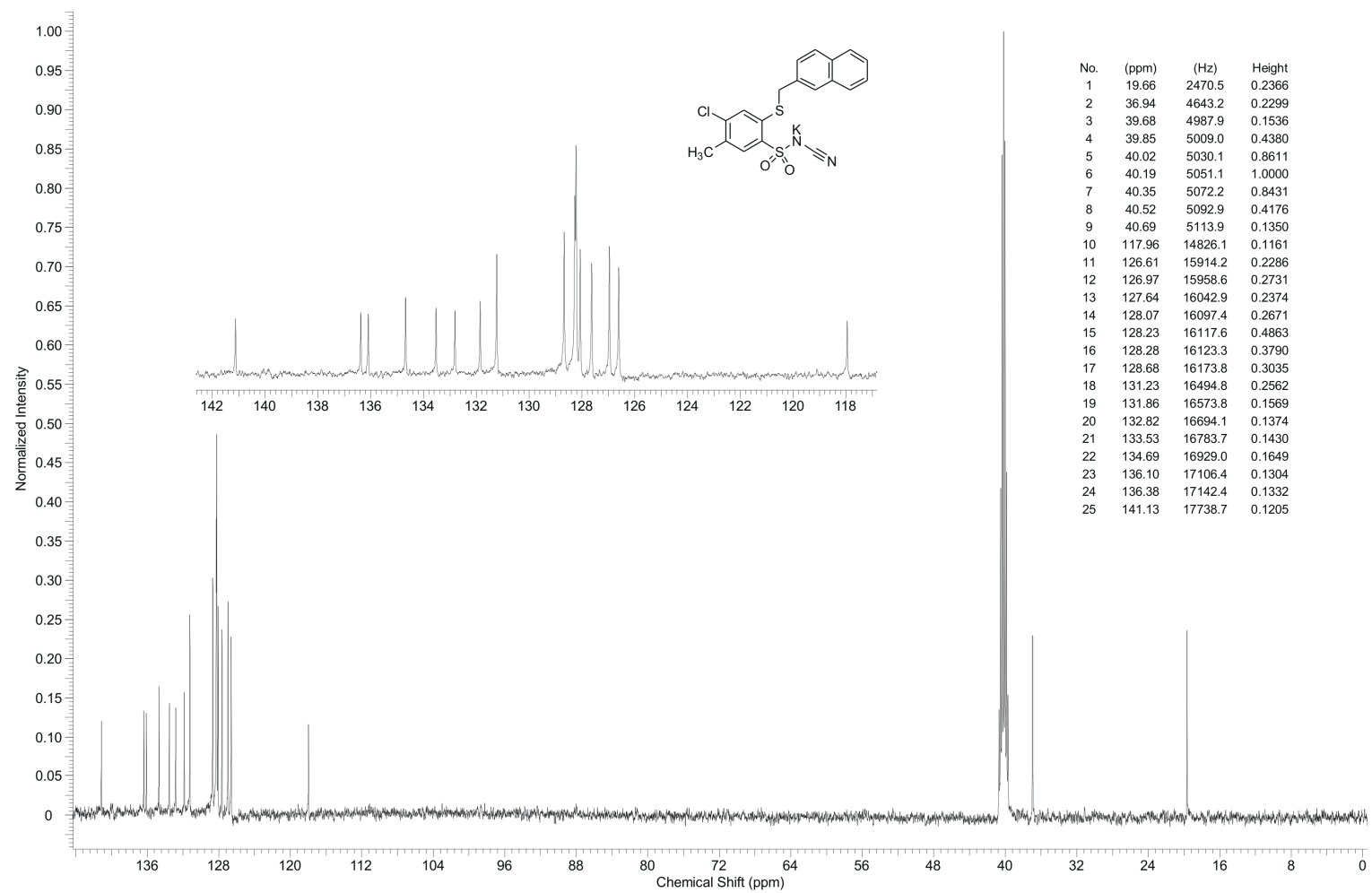


Figure S7.  $^{13}\text{C}$ -NMR of compound 13 (125 MHz,  $\text{DMSO-}d_6$ ).

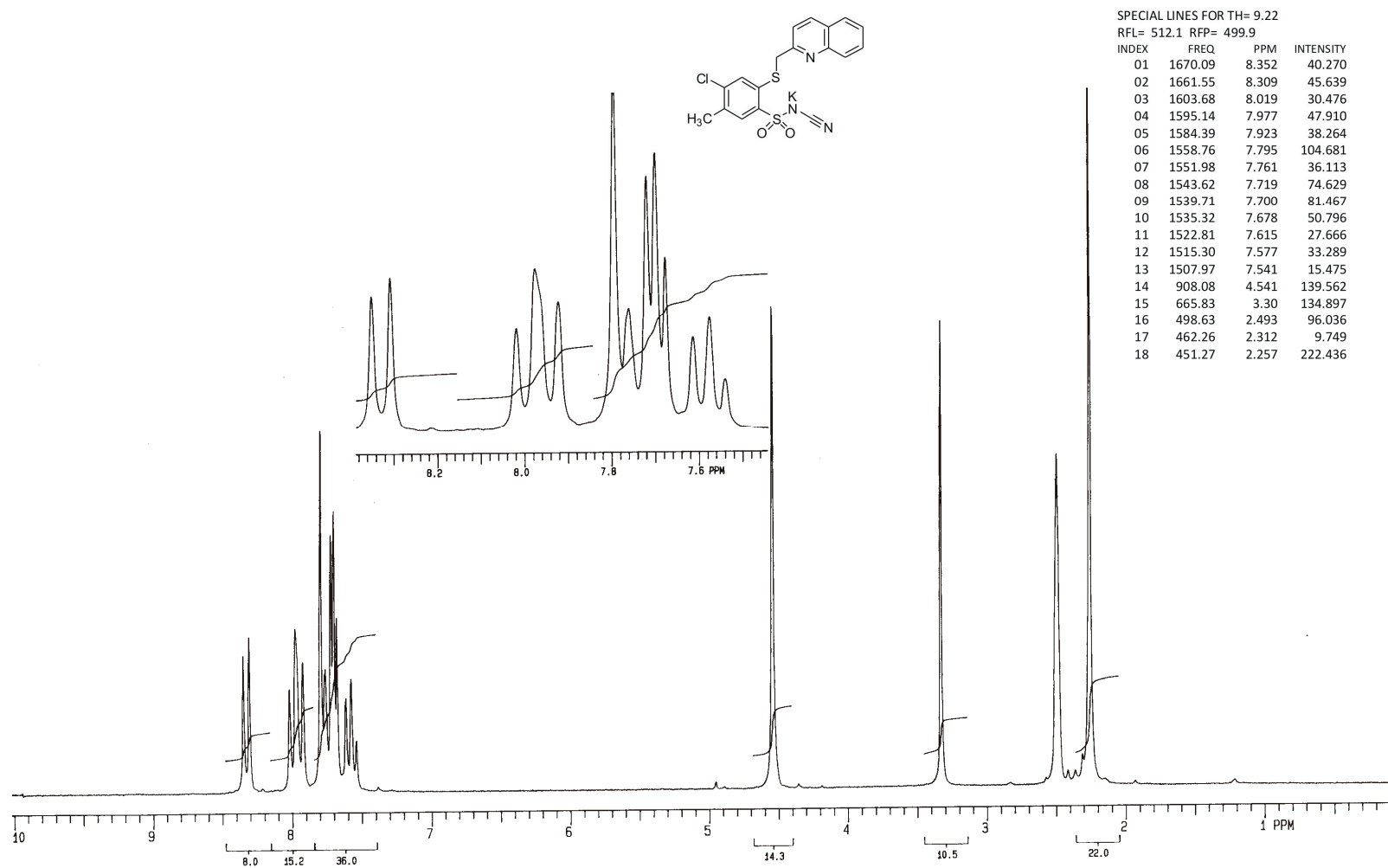


Figure S8.  $^1\text{H-NMR}$  of compound 14 (200 MHz,  $\text{DMSO-}d_6$ ).



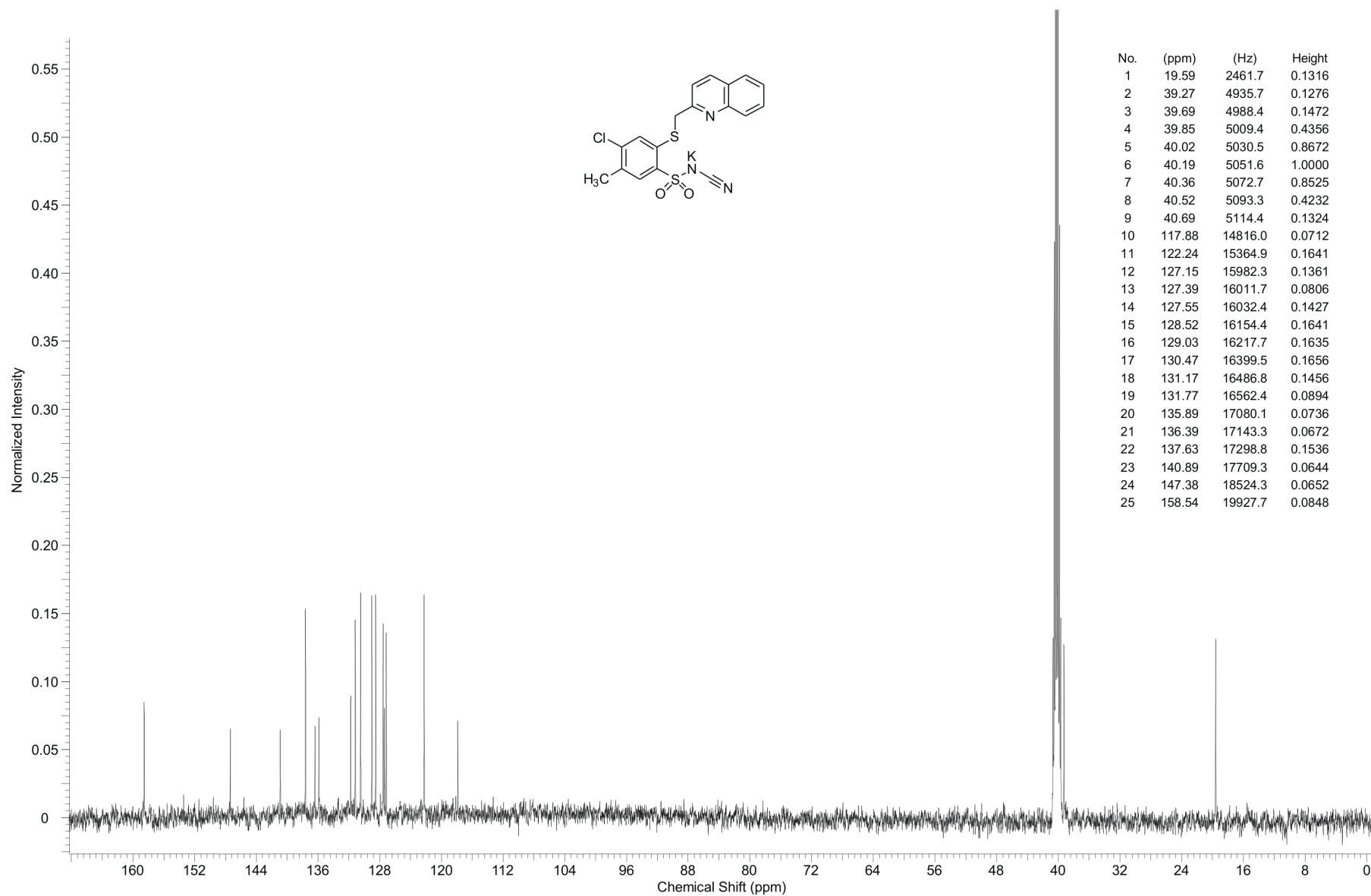


Figure S9.  $^{13}\text{C}$ -NMR of compound 14 (125 MHz,  $\text{DMSO-}d_6$ ).

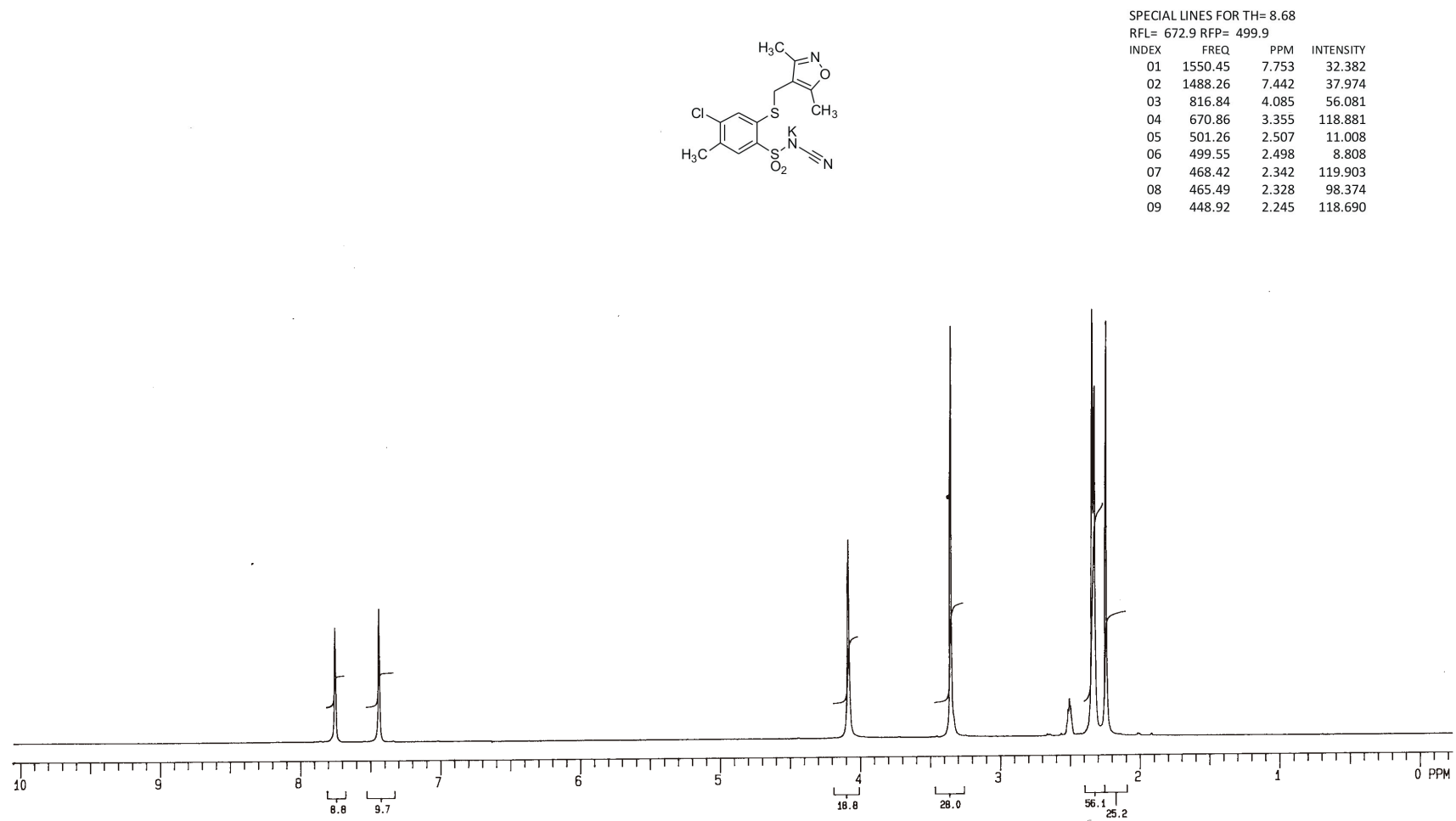


Figure S10.  $^1\text{H-NMR}$  of compound 17 (200 MHz,  $\text{DMSO-}d_6$ ).

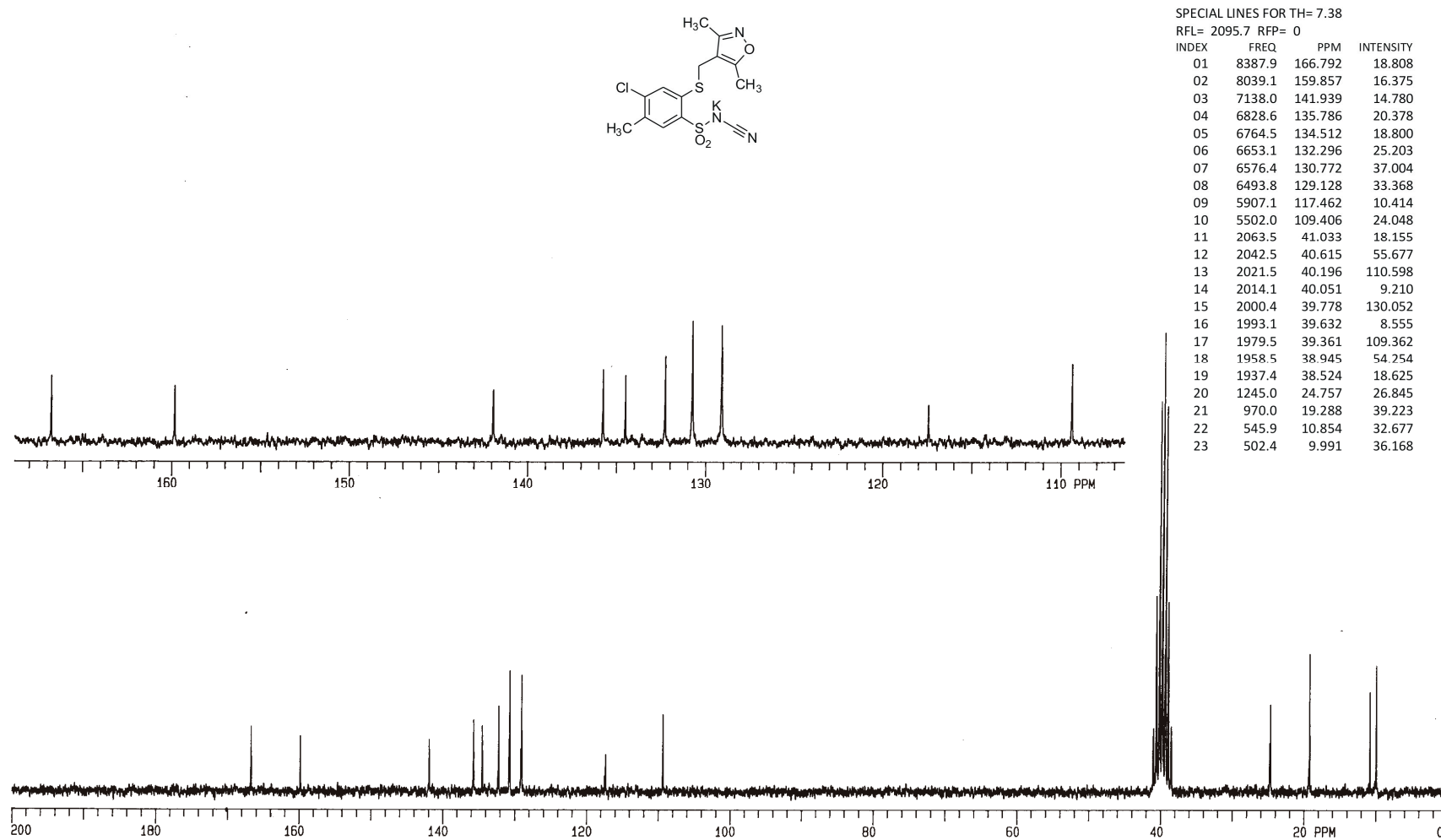


Figure S11.  $^{13}\text{C}$ -NMR of compound 17 (50 MHz,  $\text{DMSO-}d_6$ ).

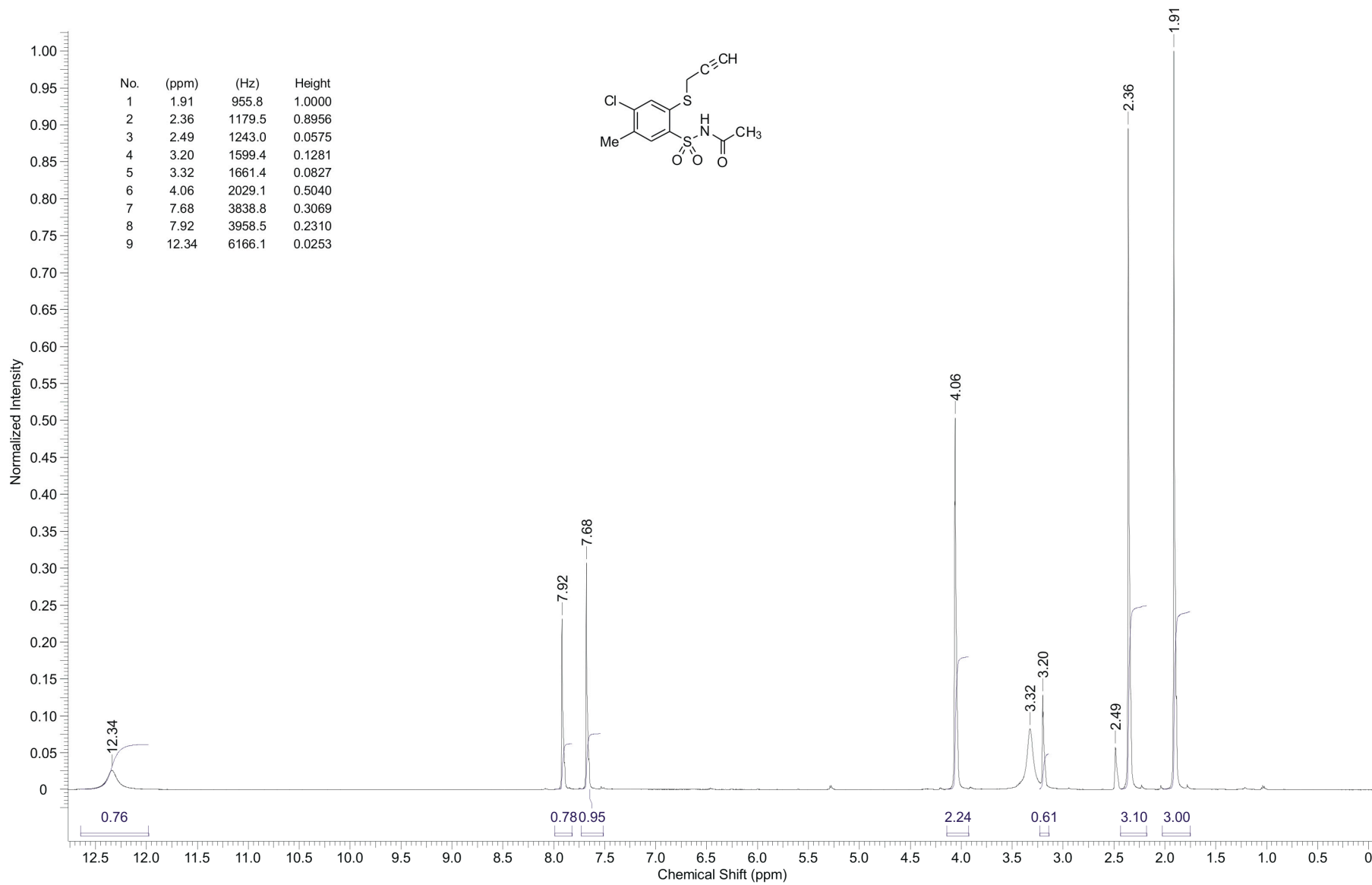


Figure S12.  $^1\text{H}$ -NMR of compound 19 (500 MHz,  $\text{DMSO-}d_6$ ).

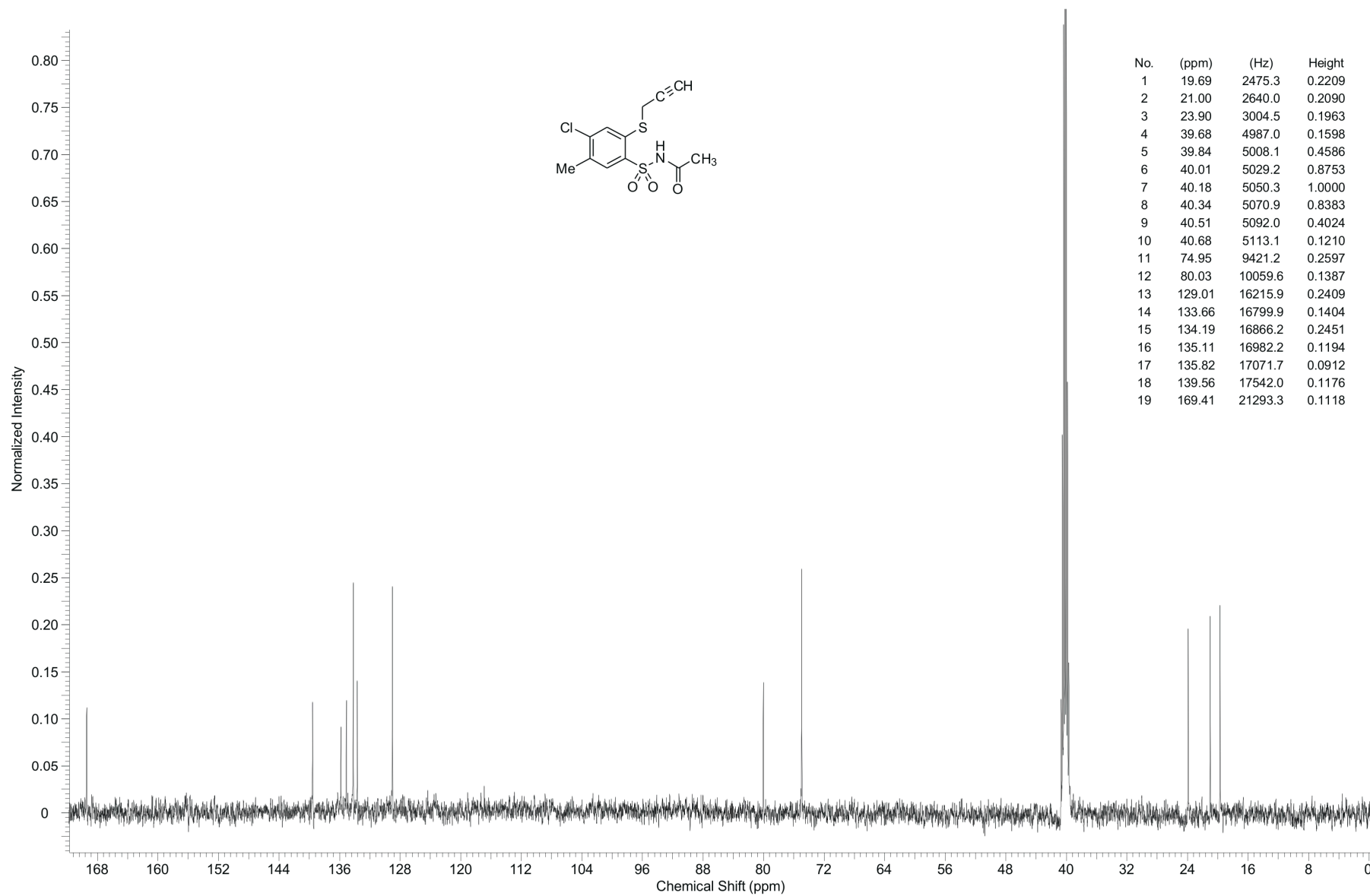
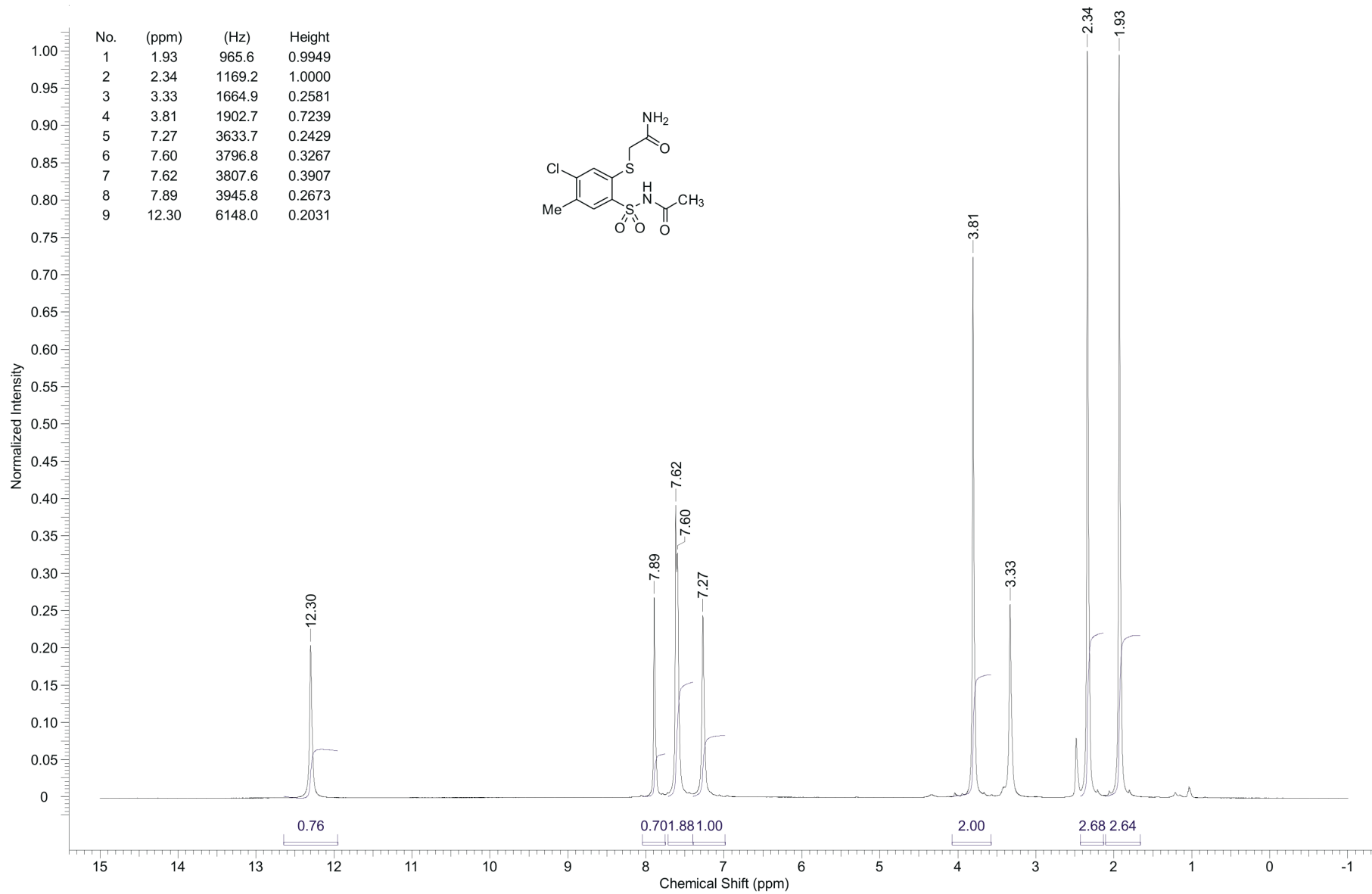
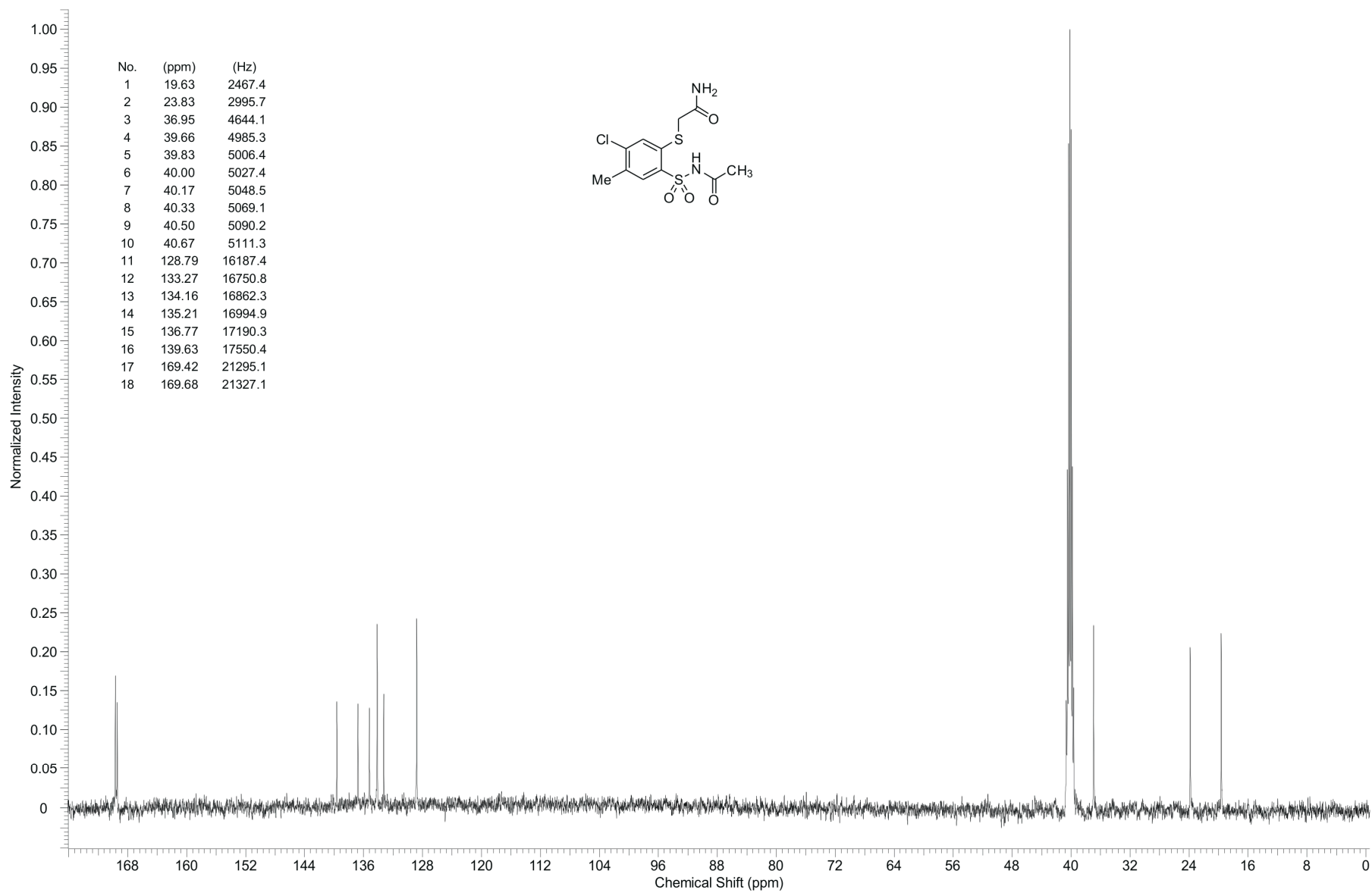


Figure S13.  $^{13}\text{C}$ -NMR of compound 19 (125 MHz,  $\text{DMSO-}d_6$ ).





**Figure S15.** <sup>13</sup>C-NMR of compound **20** (125 MHz, DMSO-*d*<sub>6</sub>).

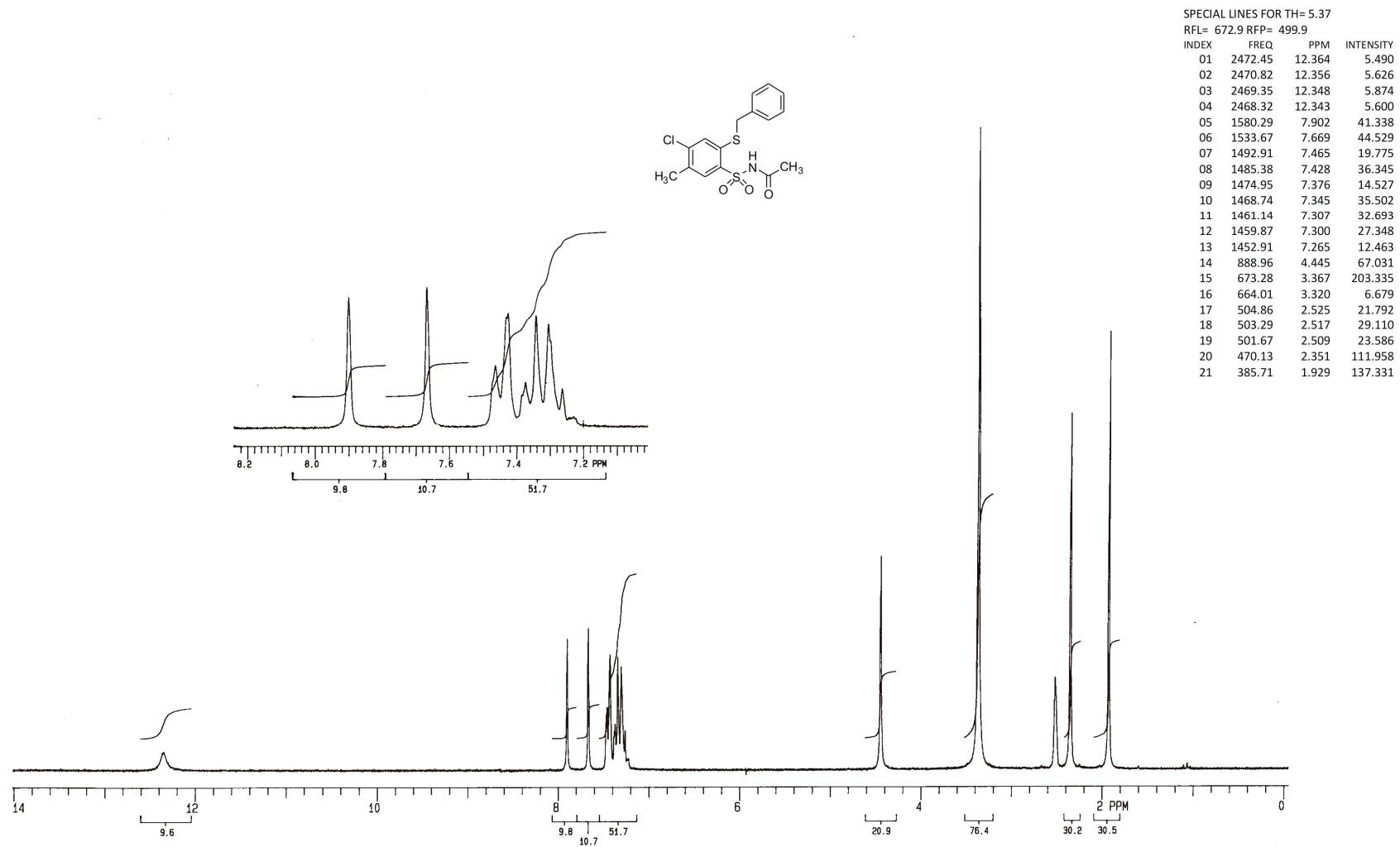


Figure S16.  $^1\text{H-NMR}$  of compound **21** (200 MHz,  $\text{DMSO-}d_6$ ).



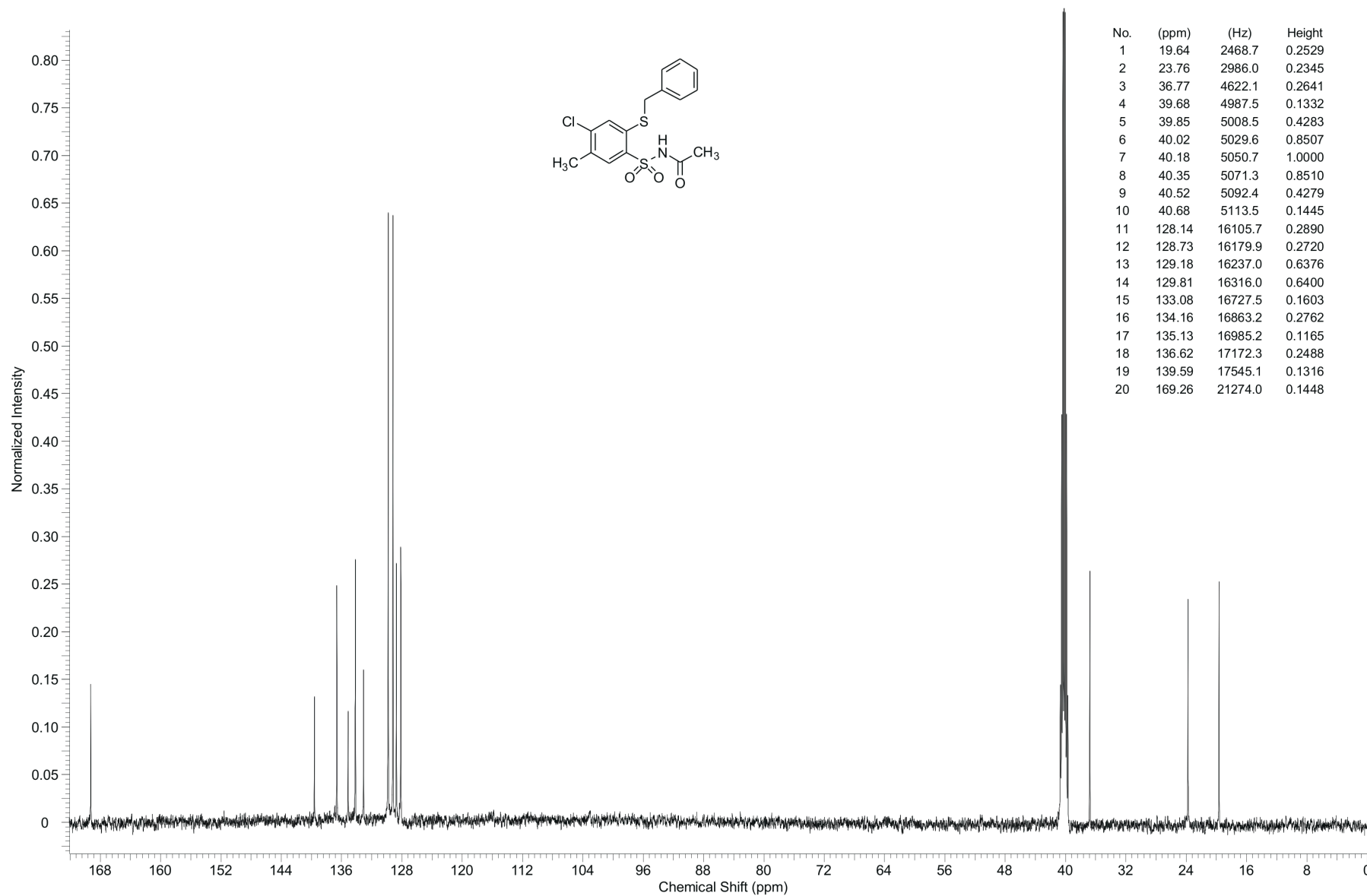


Figure S17.  $^{13}\text{C}$ -NMR of compound **21** (125 MHz,  $\text{DMSO-}d_6$ ).

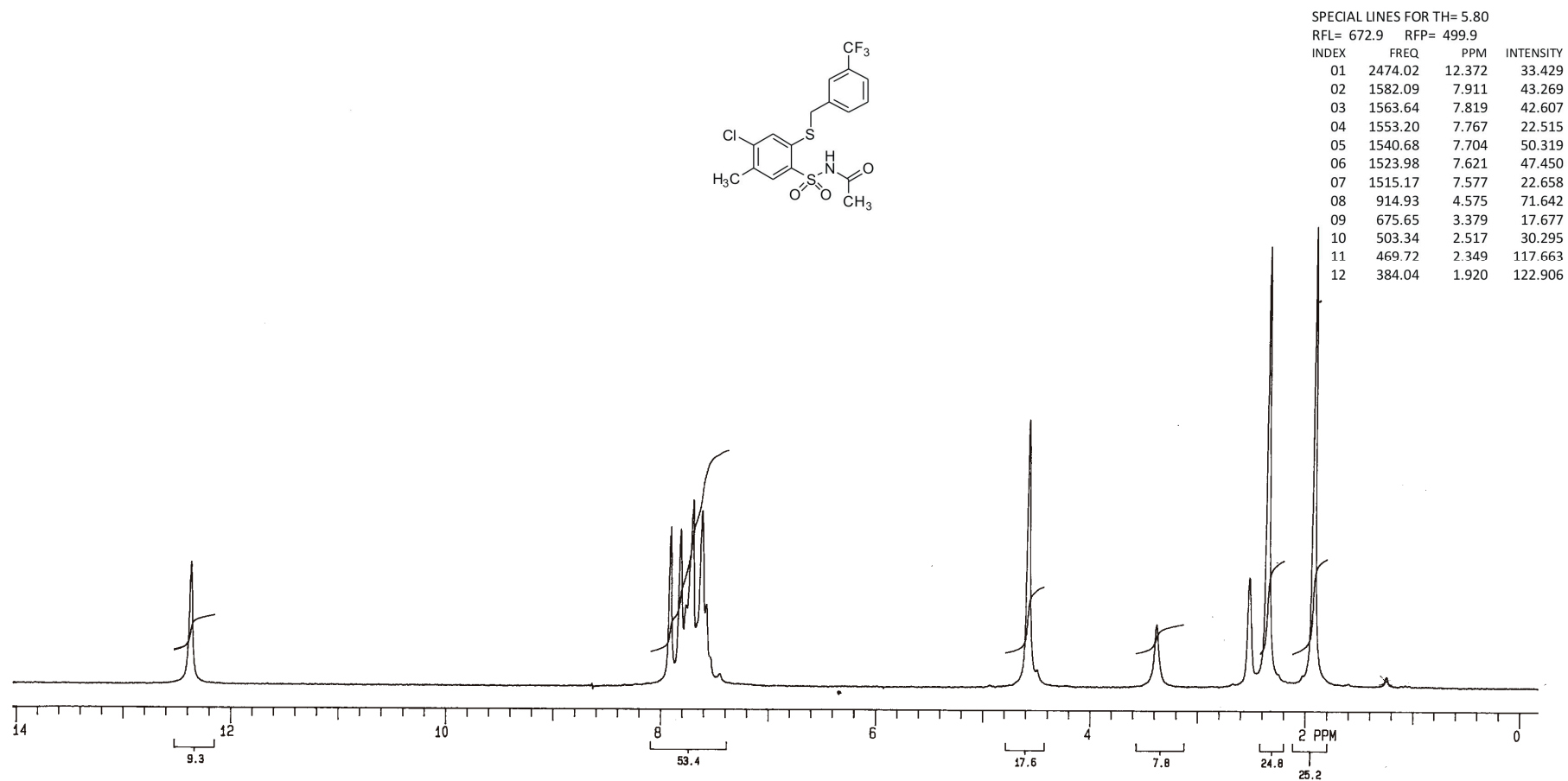


Figure S18.  $^1\text{H-NMR}$  of compound **22** (200 MHz,  $\text{DMSO-}d_6$ ).

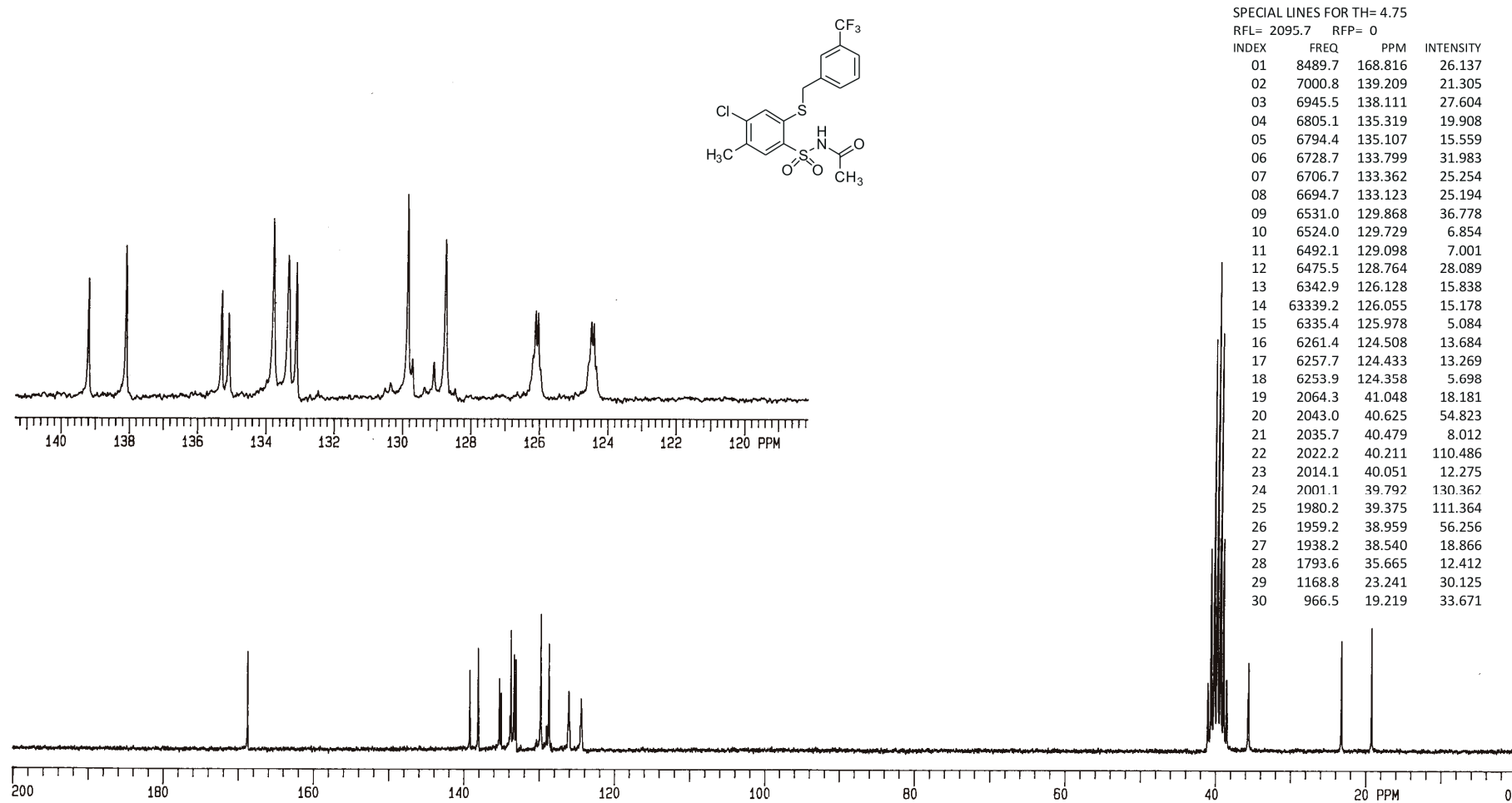


Figure S19.  $^{13}\text{C}$ -NMR of compound **22** (50 MHz,  $\text{DMSO-}d_6$ ).

SPECIAL LINES FOR TH= 9.35

RFL= 672.9 RFP= 499.9

INDEX	FREQ	PPM	INTENSITY
01	2468.32	12.346	26.951
02	1581.45	7.808	51.920
03	1535.20	7.676	54.794
04	1496.50	7.489	29.862
05	1488.22	7.442	108.825
06	1484.33	7.423	95.347
07	1477.83	7.390	17.035
08	1475.93	7.381	19.267
09	891.51	4.458	85.462
10	671.94	3.360	67.694
11	504.40	2.522	30.415
12	502.88	2.515	31.683
13	470.77	2.354	139.716
14	385.25	1.923	159.619

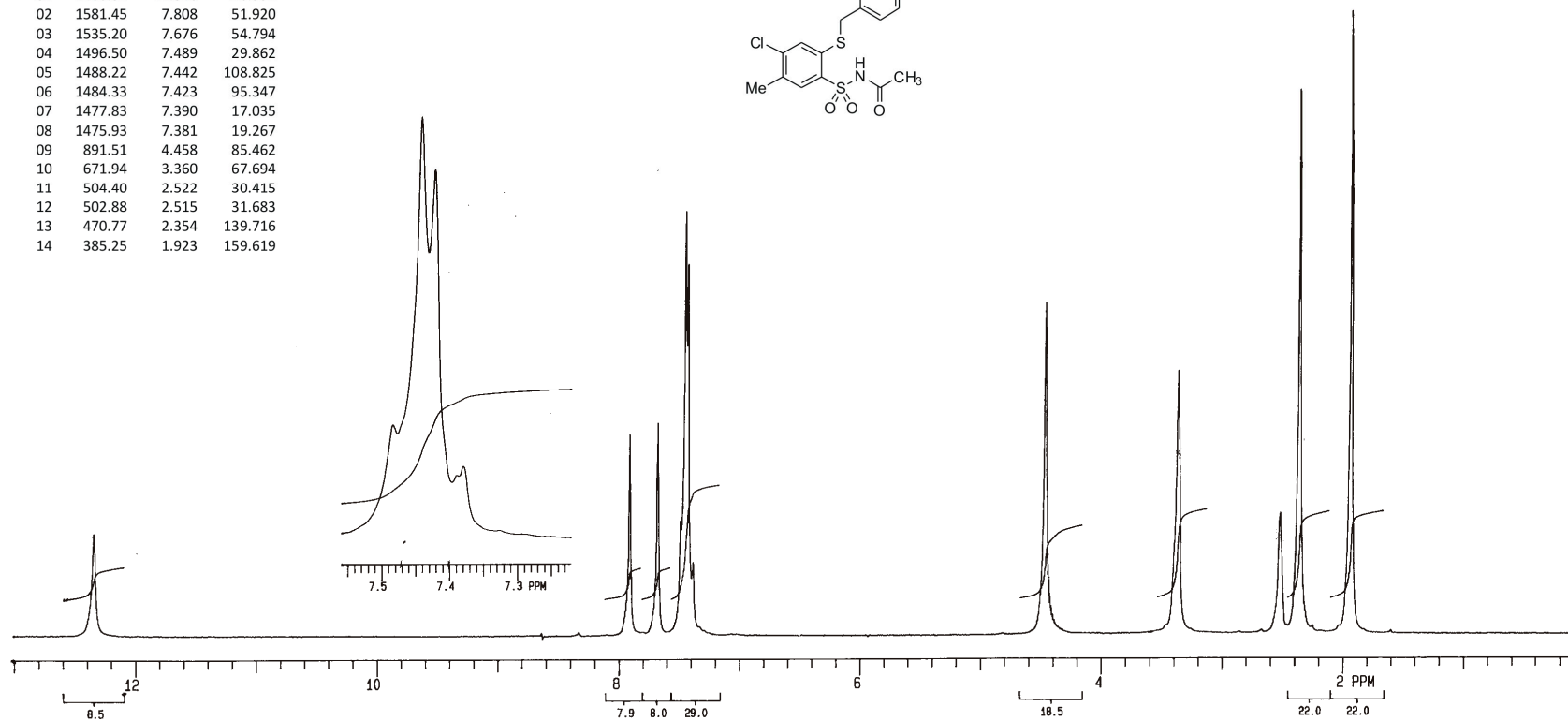
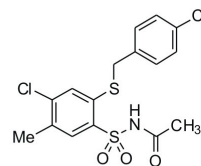


Figure S20.  $^1\text{H-NMR}$  of compound **24** (200 MHz,  $\text{DMSO-}d_6$ ).

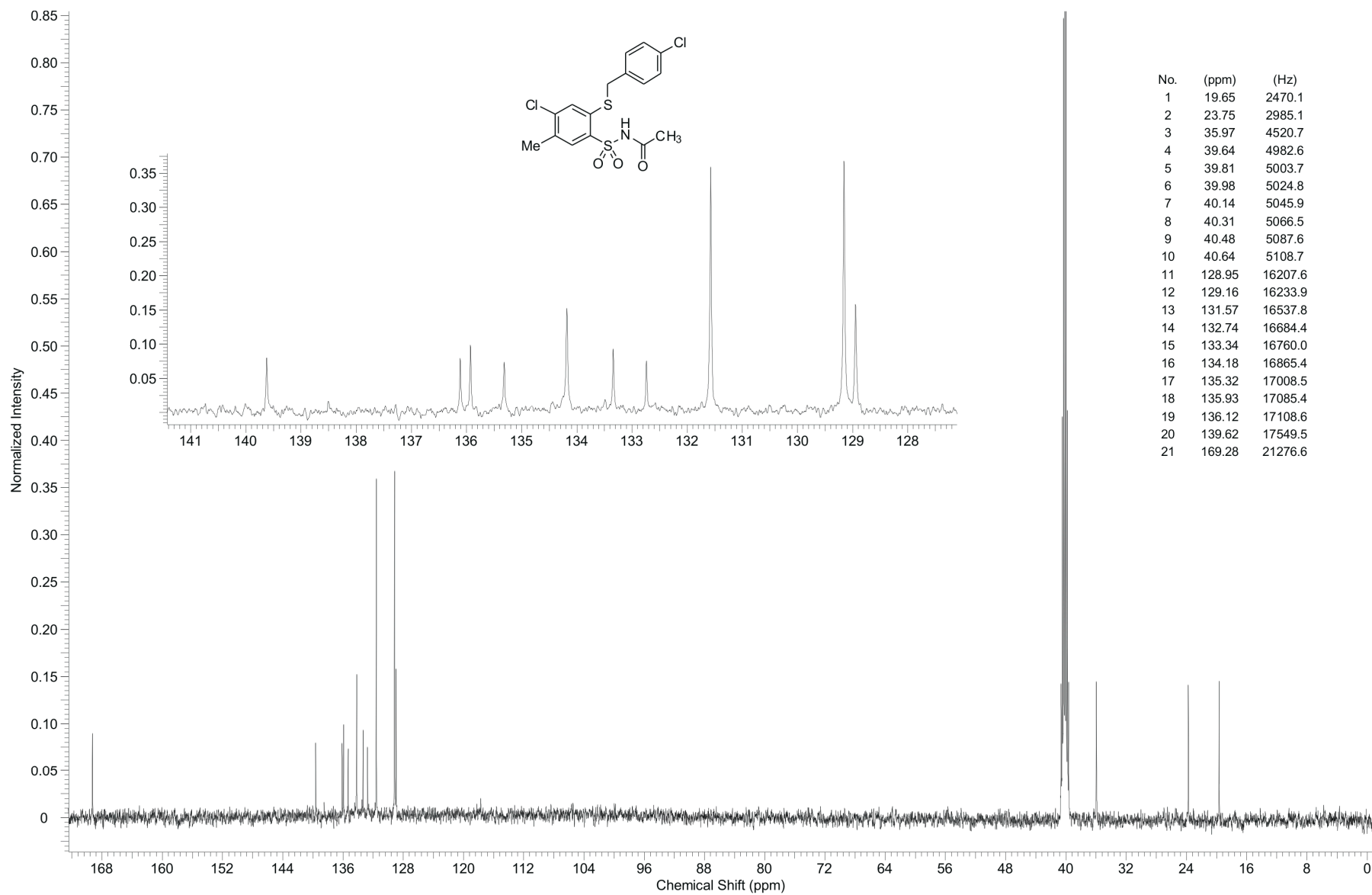


Figure S21.  $^{13}\text{C}$ -NMR of compound 24 (125 MHz,  $\text{DMSO-}d_6$ ).

SPECIAL LINES FOR TH= 4.04

RFL= 672.9 RFP= 499.9

INDEX	FREQ	PPM	INTENSITY
01	2461.78	12.310	25.620
02	1582.84	7.915	36.722
03	1533.90	7.670	39.035
04	1490.59	7.454	21.193
05	1483.99	7.421	37.685
06	1473.37	7.368	16.889
07	1467.40	7.338	36.040
08	1459.92	7.301	38.603
09	1452.97	7.266	13.257
10	1447.92	7.240	5.441
11	888.55	4.443	61.971
12	672.36	3.362	38.196
13	503.34	2.517	36.909
14	471.52	2.358	100.658
15	457.84	2.289	12.276
16	450.42	2.252	30.265
17	443.00	2.215	30.772
18	435.57	2.178	11.754
19	400.79	2.004	6.583
20	249.63	1.248	4.221
21	237.52	1.188	4.107
22	185.57	0.928	32.100
23	178.21	0.891	60.336
24	170.78	0.854	28.544

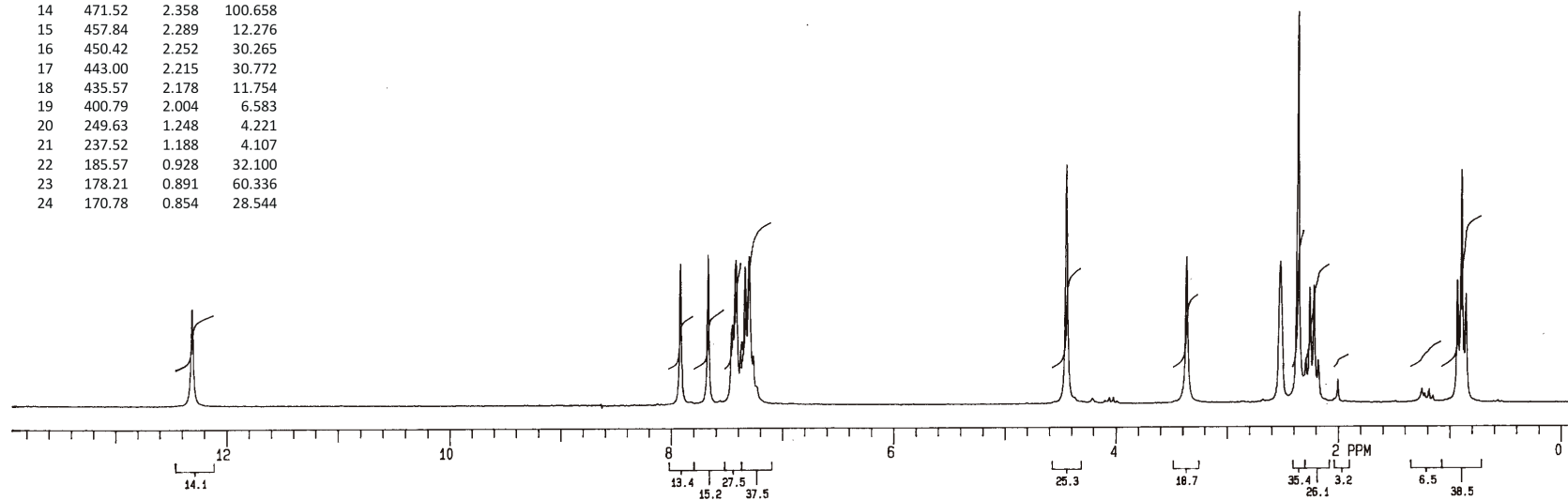
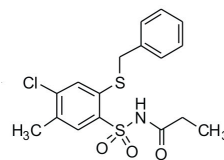


Figure S22.  $^1\text{H-NMR}$  of compound **33** (200 MHz,  $\text{DMSO-}d_6$ ).

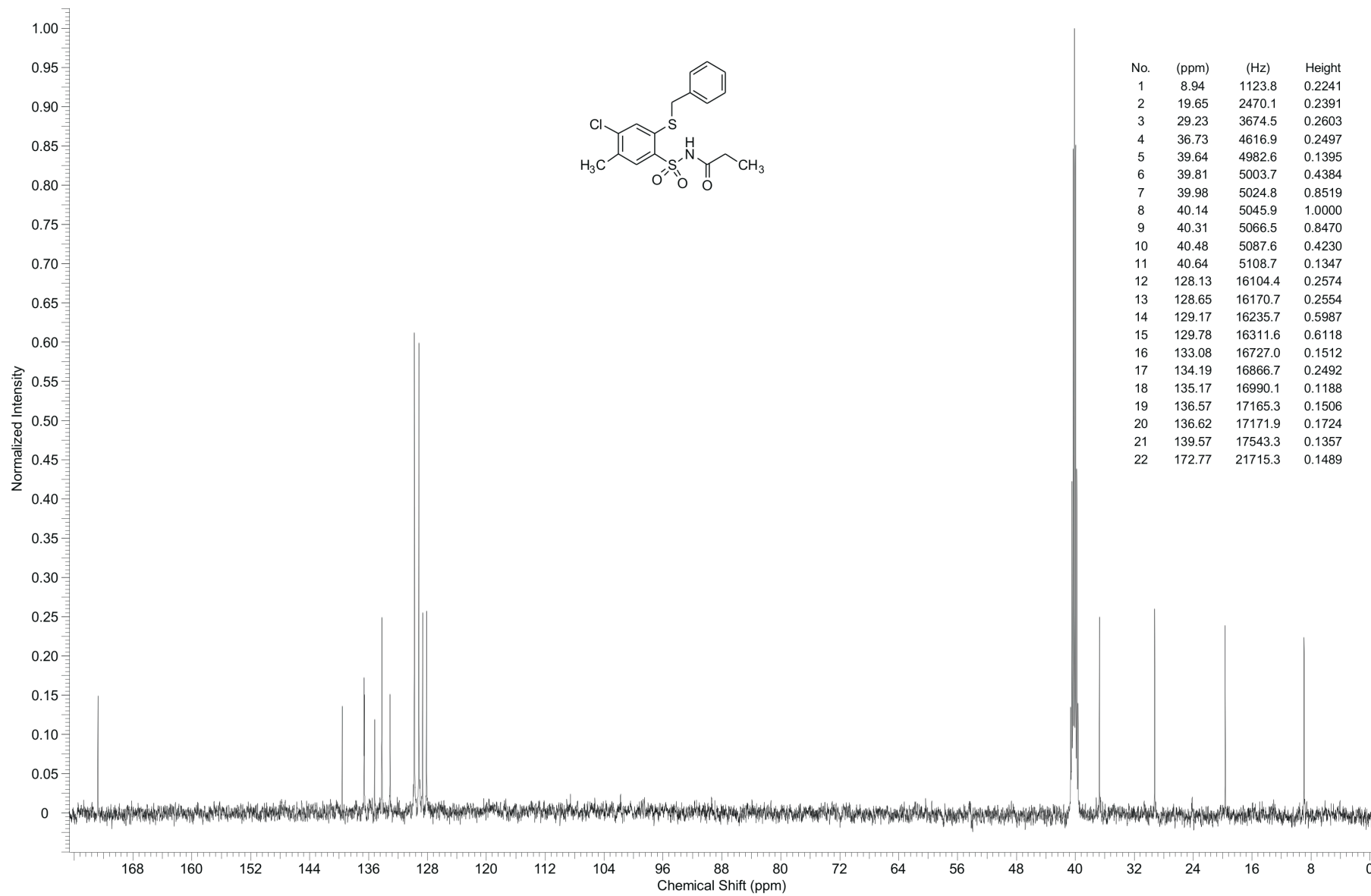


Figure S23.  $^{13}\text{C}$ -NMR of compound 33 (125 MHz,  $\text{DMSO-}d_6$ ).

SPECIAL LINES FOR TH= 4.04  
RFL= 672.9 RFP= 499.9

INDEX	FREQ	PPM	INTENSITY
01	2453.94	12.271	37.393
02	1581.16	7.907	43.672
03	1531.30	7.657	44.954
04	1473.79	7.359	50.301
05	1464.74	7.325	57.055
06	1380.89	6.905	51.189
07	1373.65	6.869	46.027
08	873.71	4.369	76.249
09	746.28	3.732	139.120
10	670.68	3.351	88.837
11	501.49	2.508	77.017
12	471.11	2.356	124.565
13	455.47	2.278	23.265
14	448.51	2.243	41.904
15	441.32	2.207	42.421
16	434.47	2.173	21.431
17	183.31	0.917	44.163
18	176.94	0.885	73.982
19	169.99	0.850	42.362

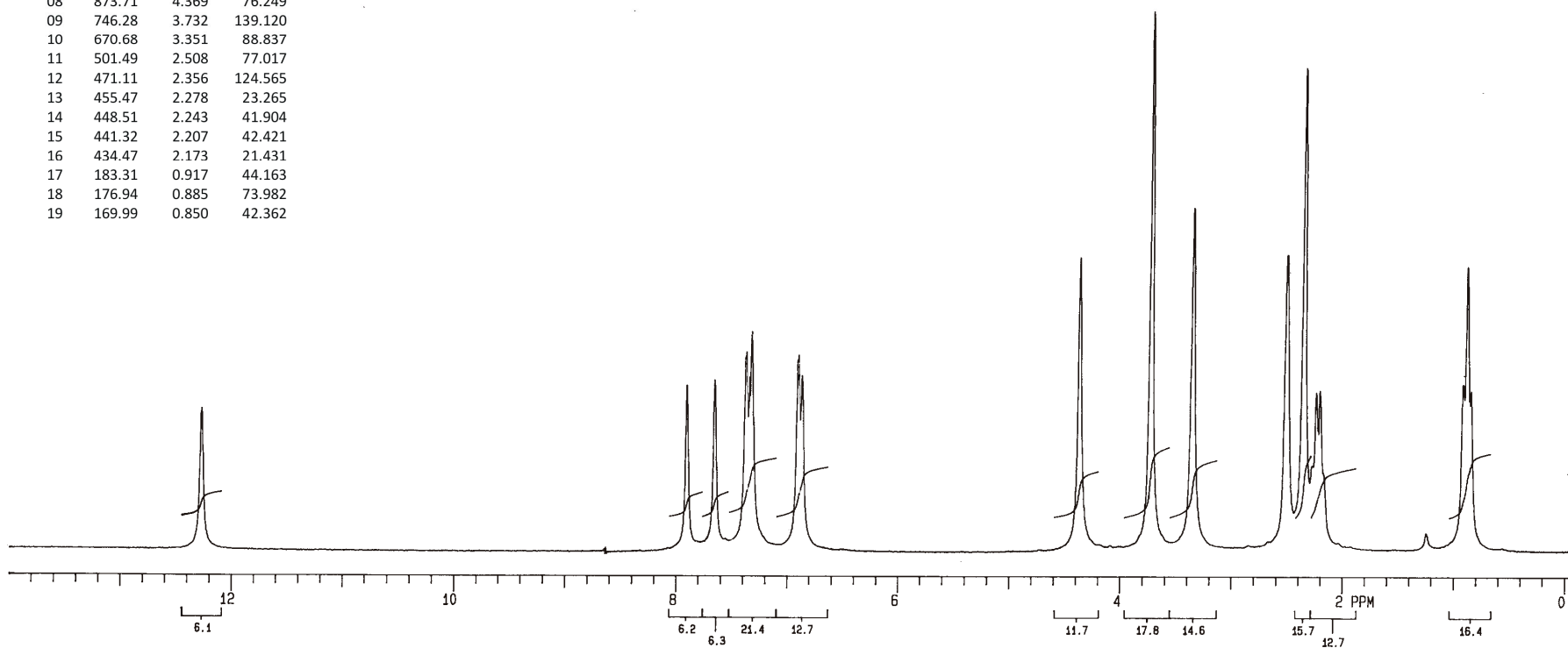
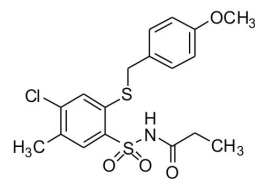


Figure S24.  $^1\text{H-NMR}$  of compound **37** (200 MHz,  $\text{DMSO-}d_6$ ).



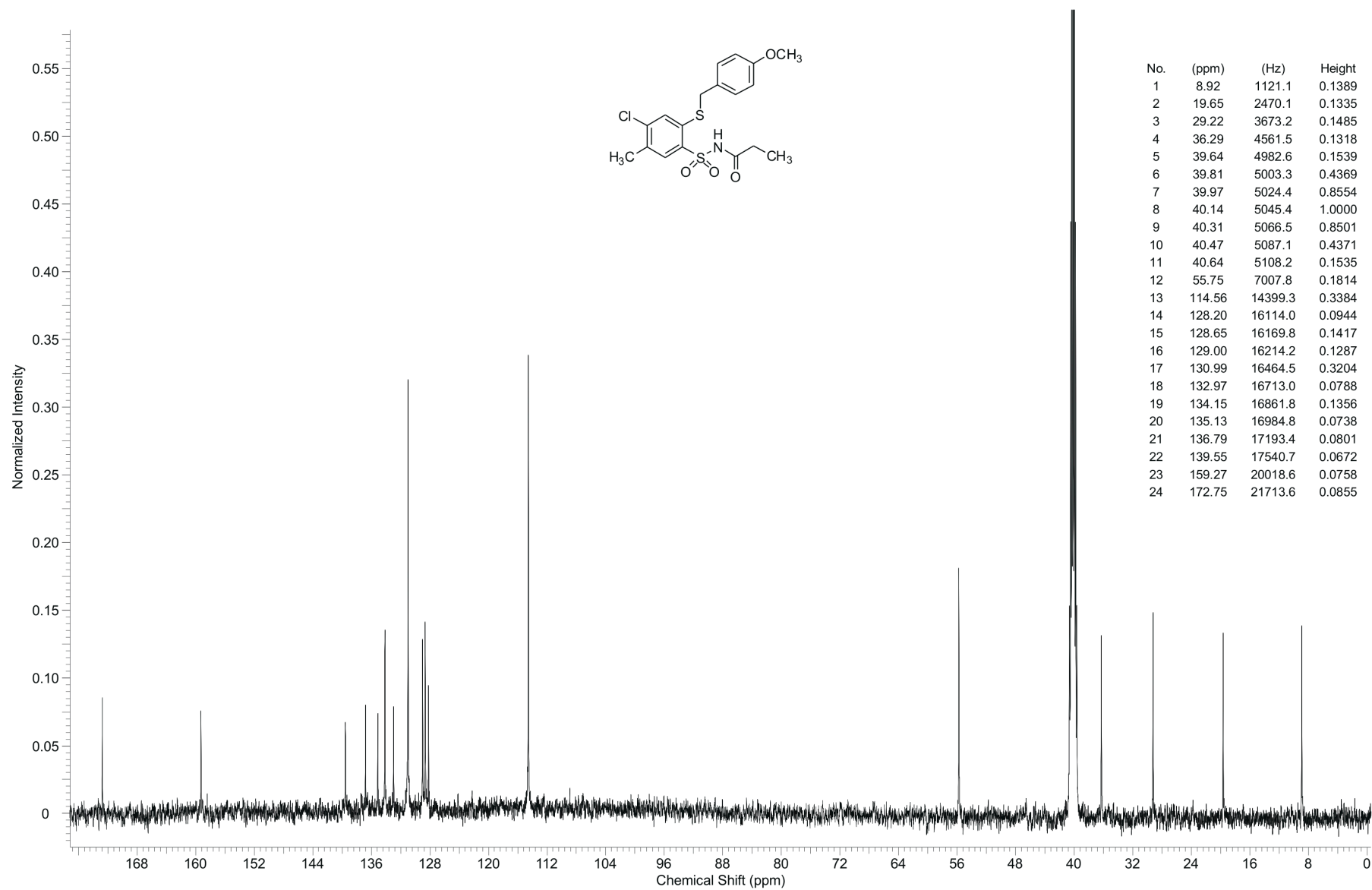
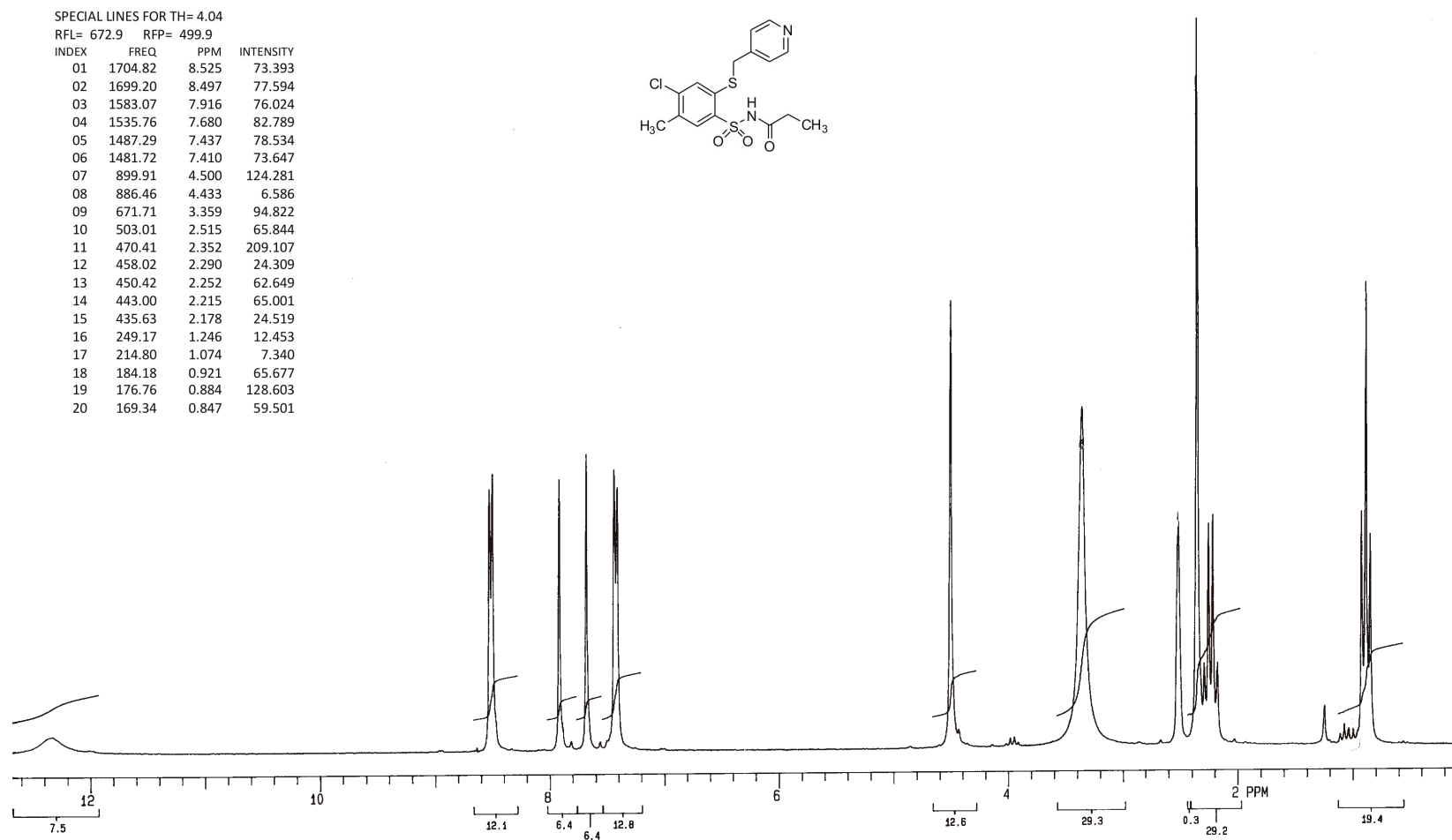
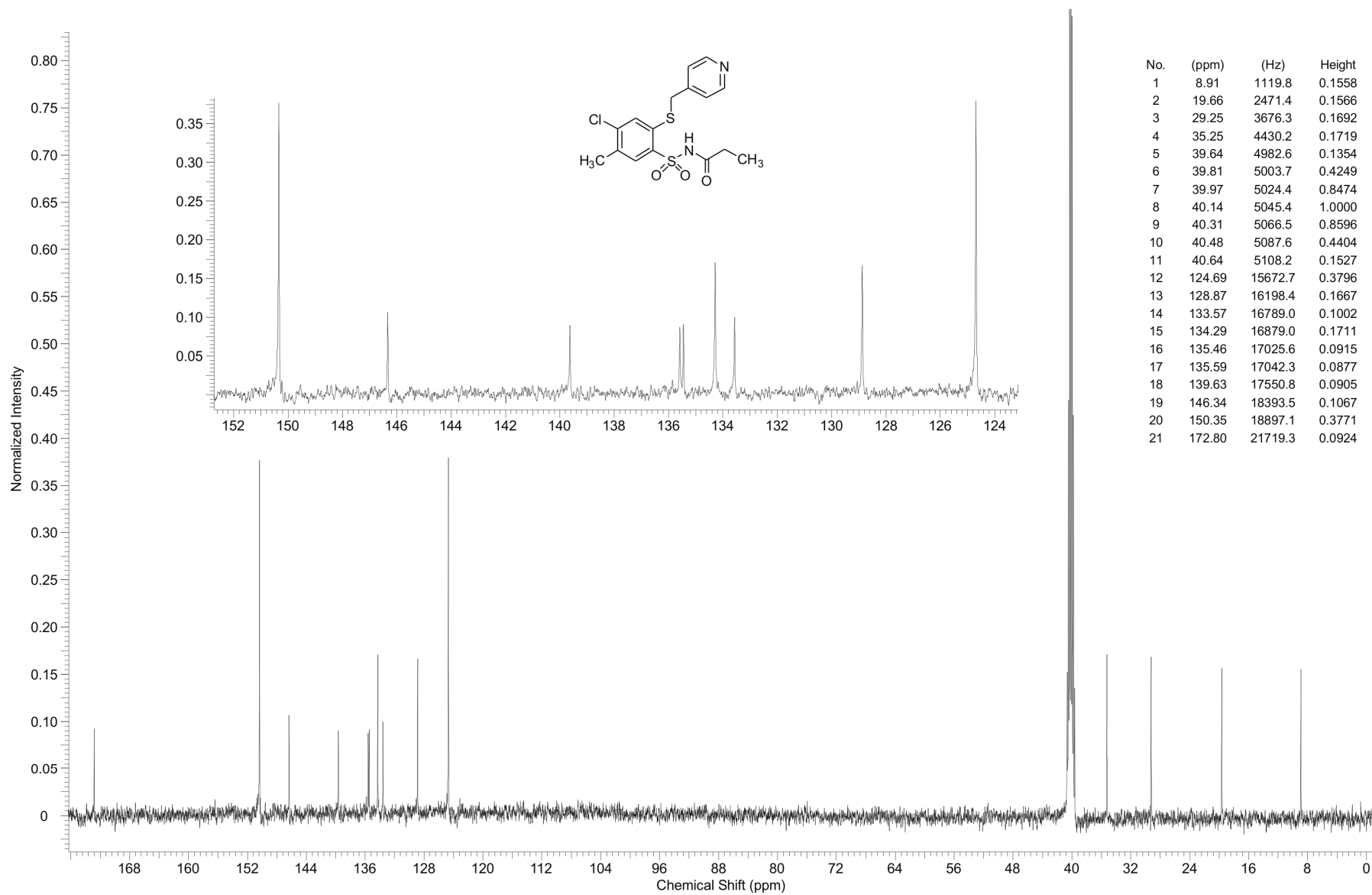
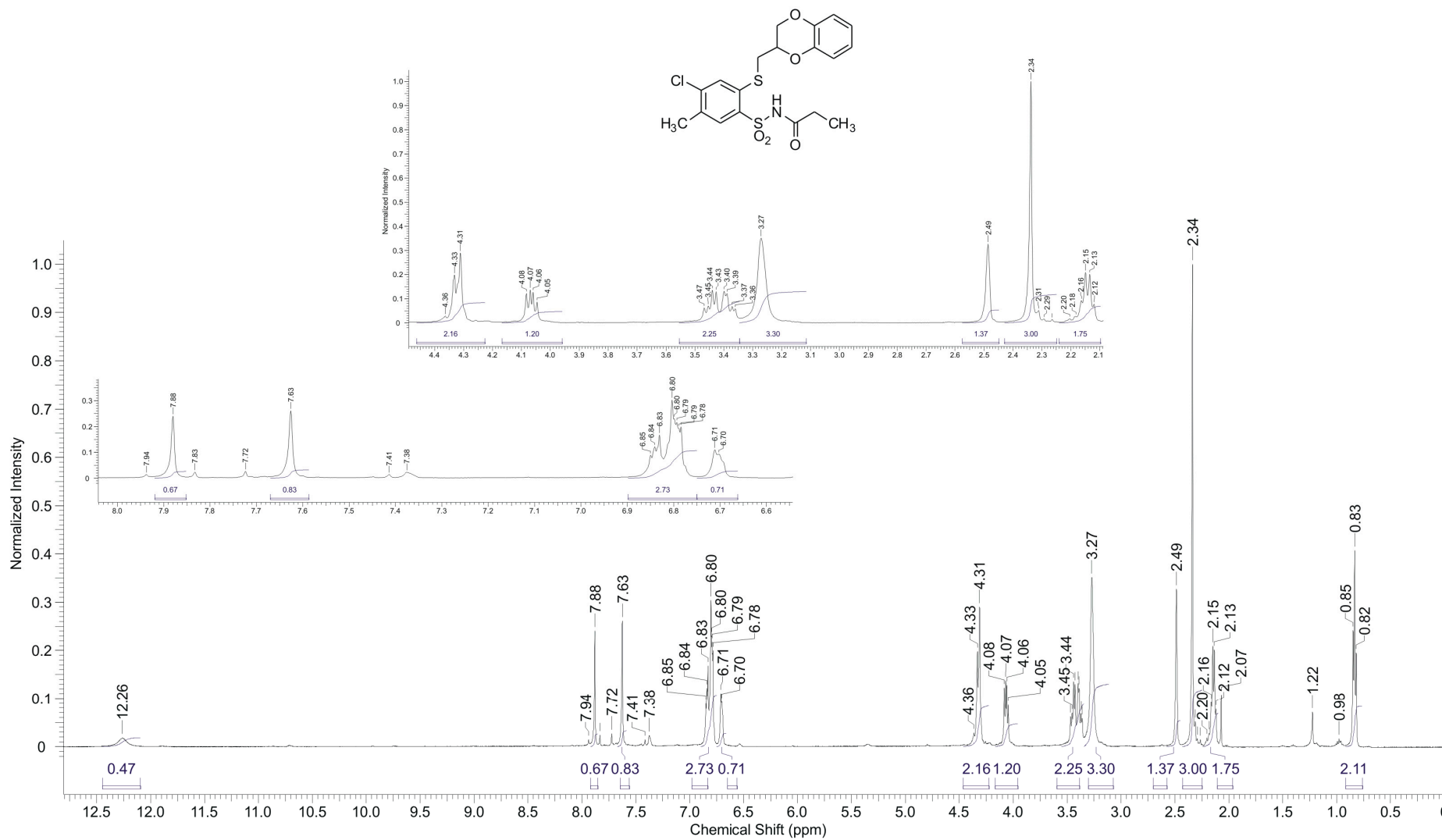


Figure S25.  $^{13}\text{C}$ -NMR of compound 37 (125 MHz,  $\text{DMSO}-d_6$ ).





**Figure S27.**  $^{13}\text{C}$ -NMR of compound **38** (125 MHz,  $\text{DMSO-}d_6$ ).



**Figure S28.** <sup>1</sup>H-NMR of compound **40** (500 MHz, DMSO-*d*<sub>6</sub>).

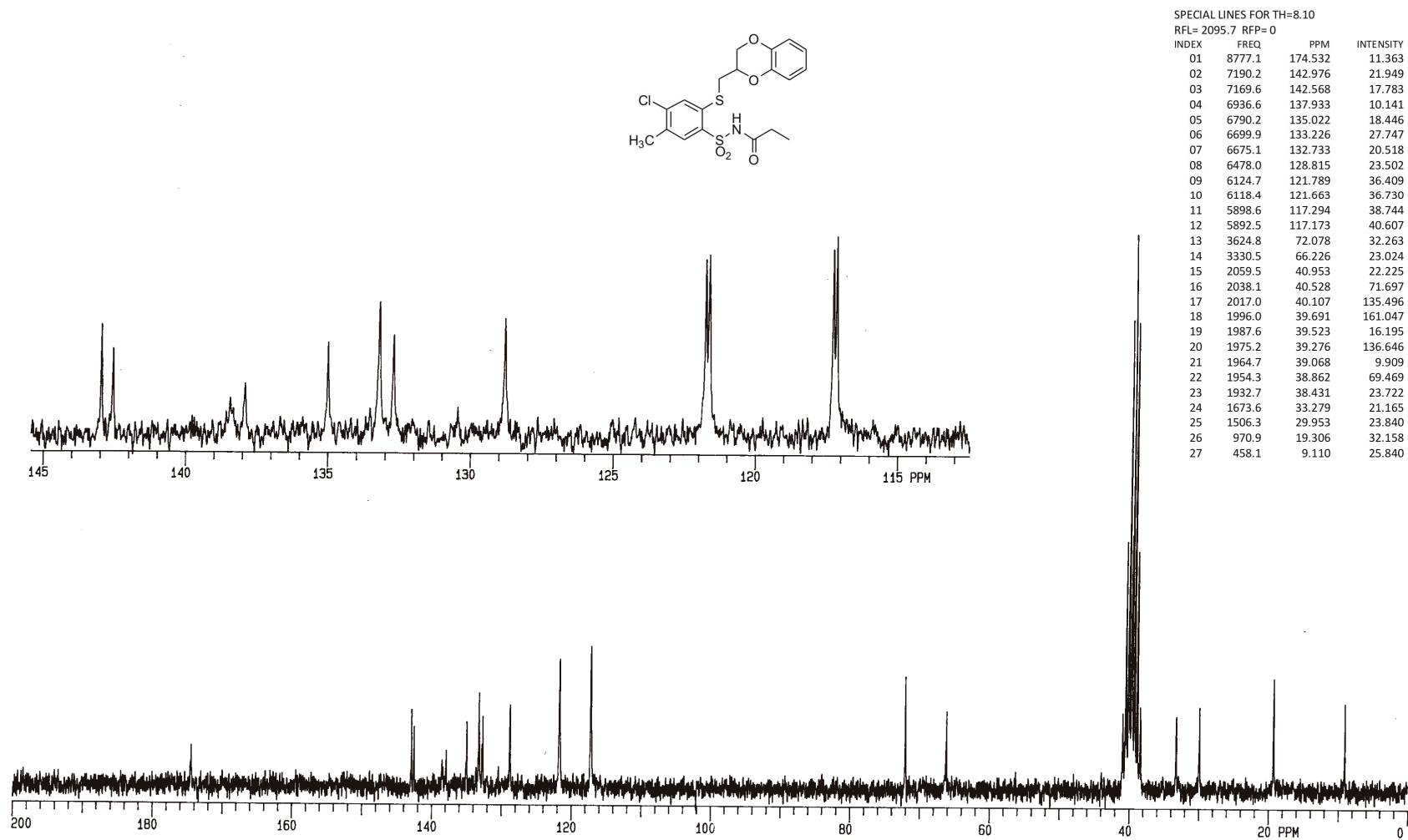


Figure S29.  $^{13}\text{C}$ -NMR of compound **40** (50 MHz,  $\text{DMSO-}d_6$ ).

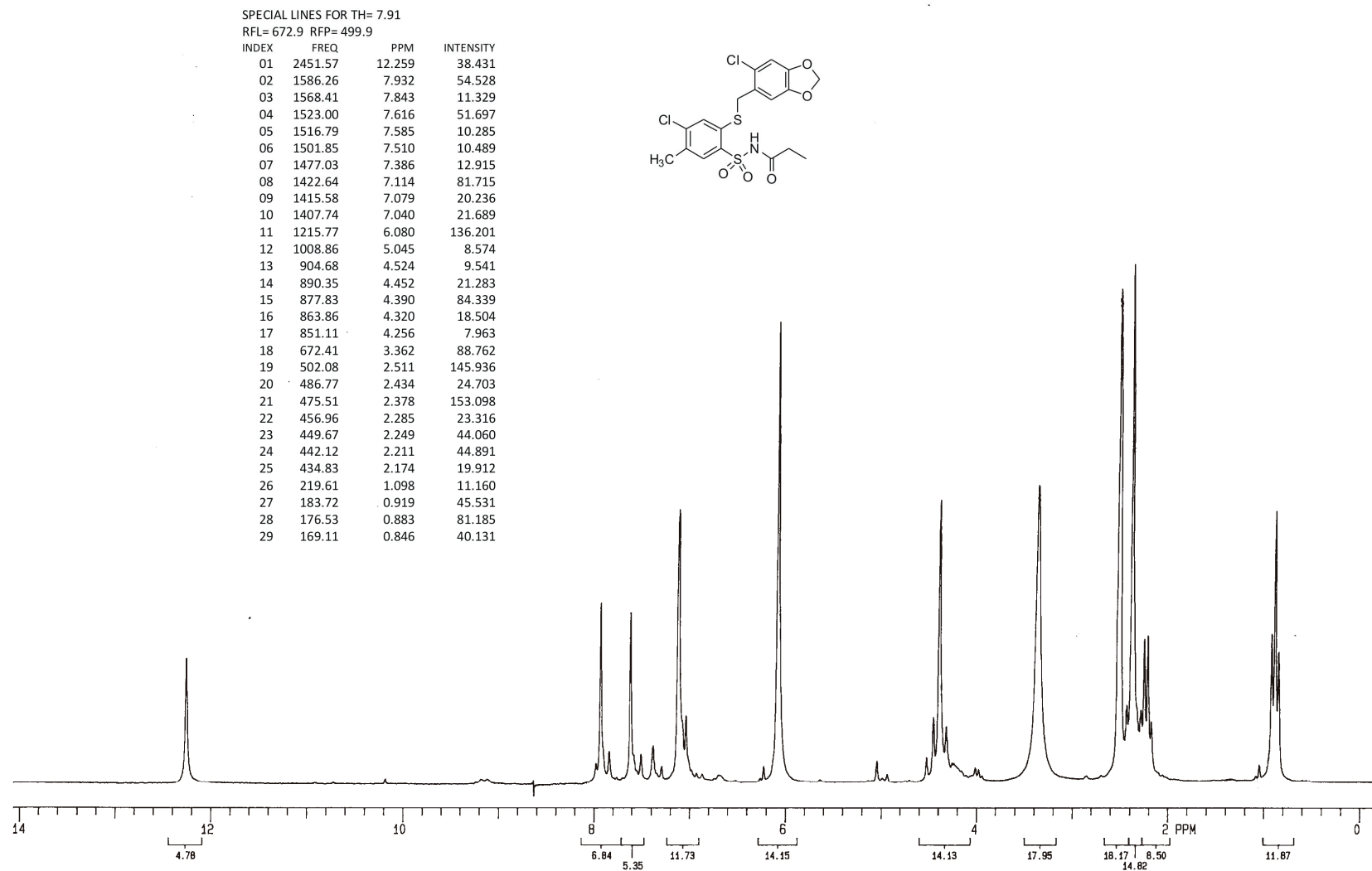
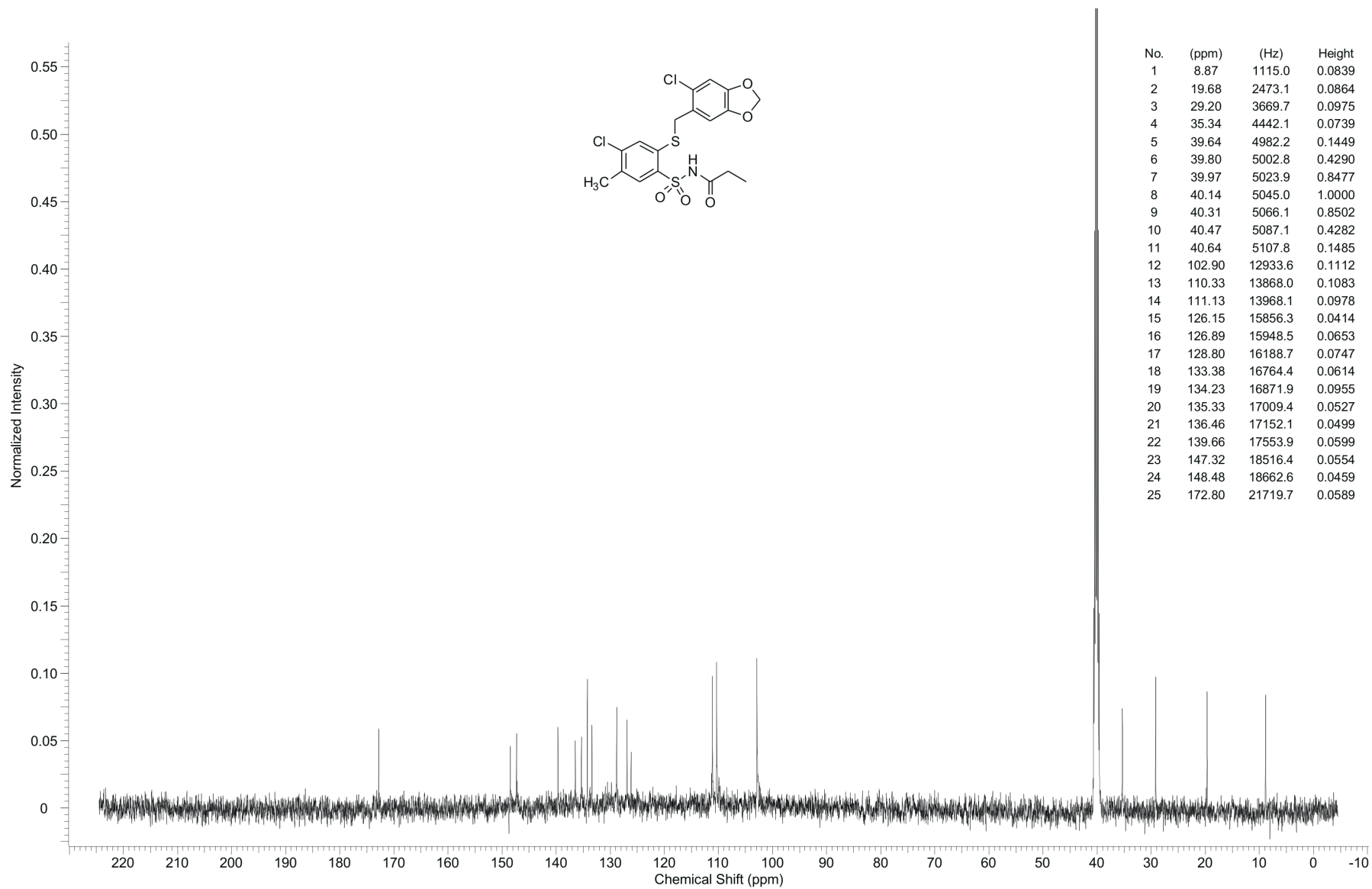


Figure S30.  $^1\text{H-NMR}$  of compound **41** (200 MHz,  $\text{DMSO-}d_6$ ).



**Figure S31.** <sup>13</sup>C-NMR of compound **41** (125 MHz, DMSO-*d*<sub>6</sub>).

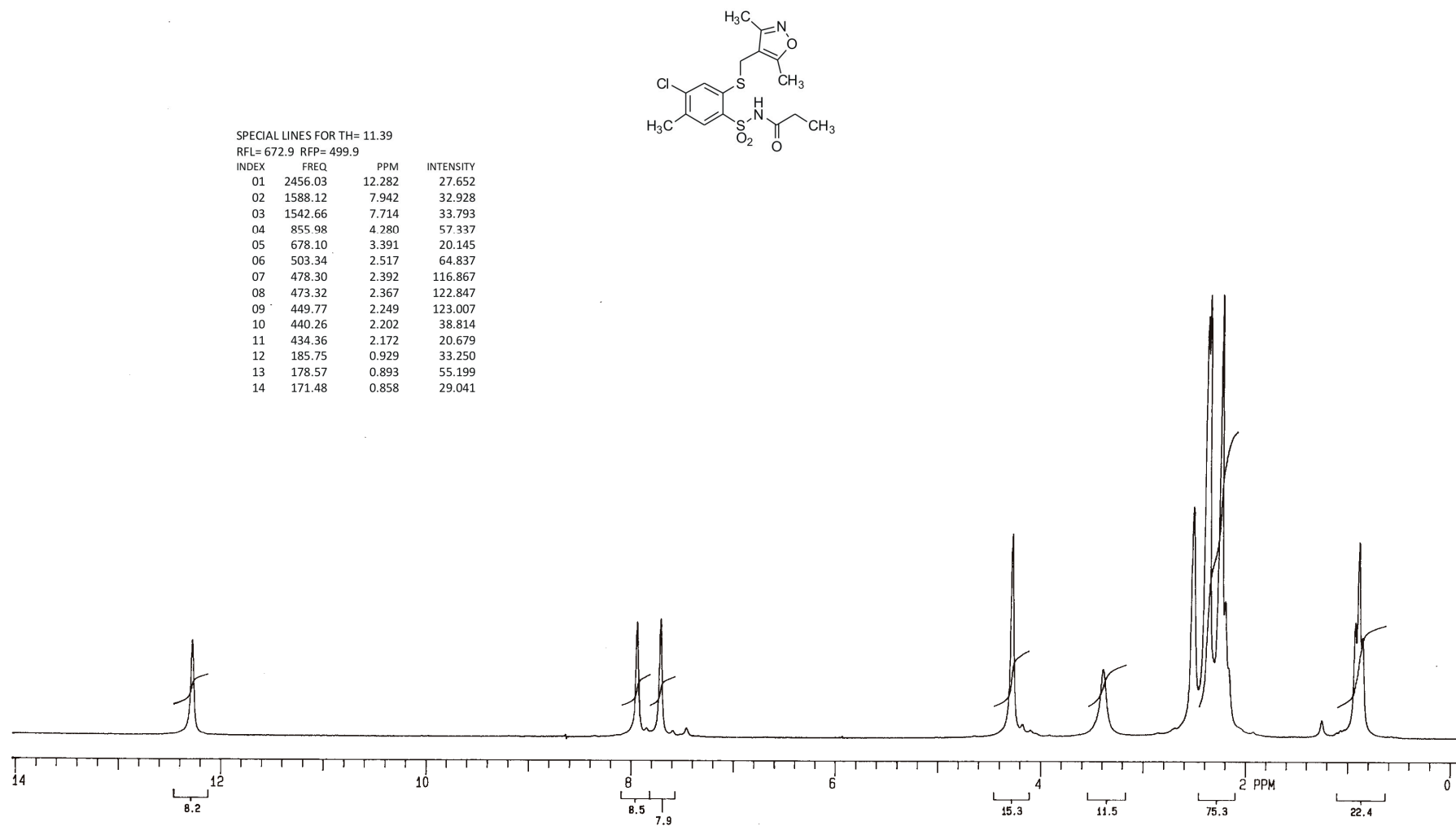


Figure S32.  $^1\text{H-NMR}$  of compound **42** (200 MHz,  $\text{DMSO-}d_6$ ).



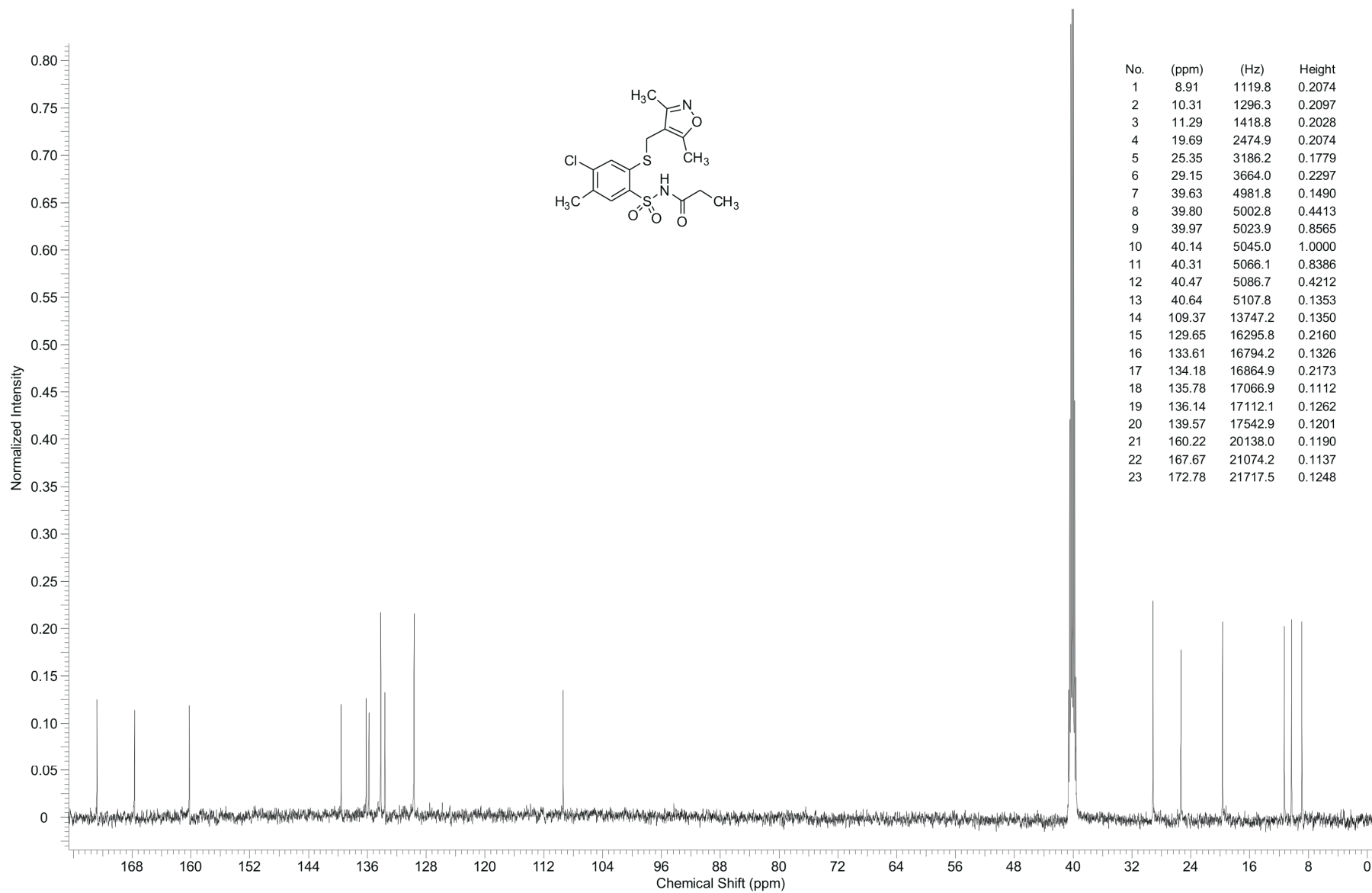


Figure S33.  $^{13}\text{C}$ -NMR of compound 42 (125 MHz,  $\text{DMSO-}d_6$ ).

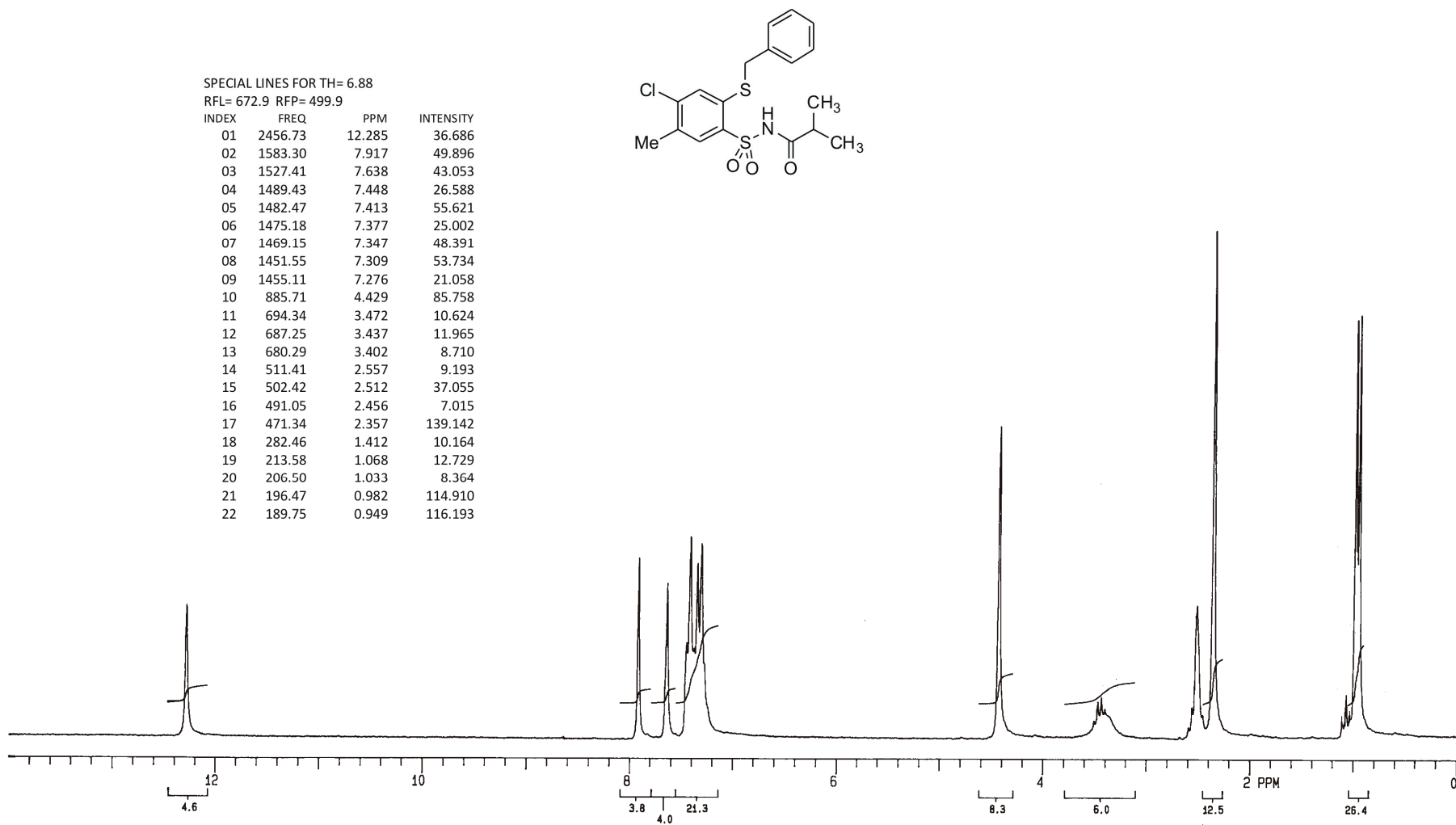


Figure S34.  $^1\text{H-NMR}$  of compound **43** (200 MHz,  $\text{DMSO-}d_6$ ).

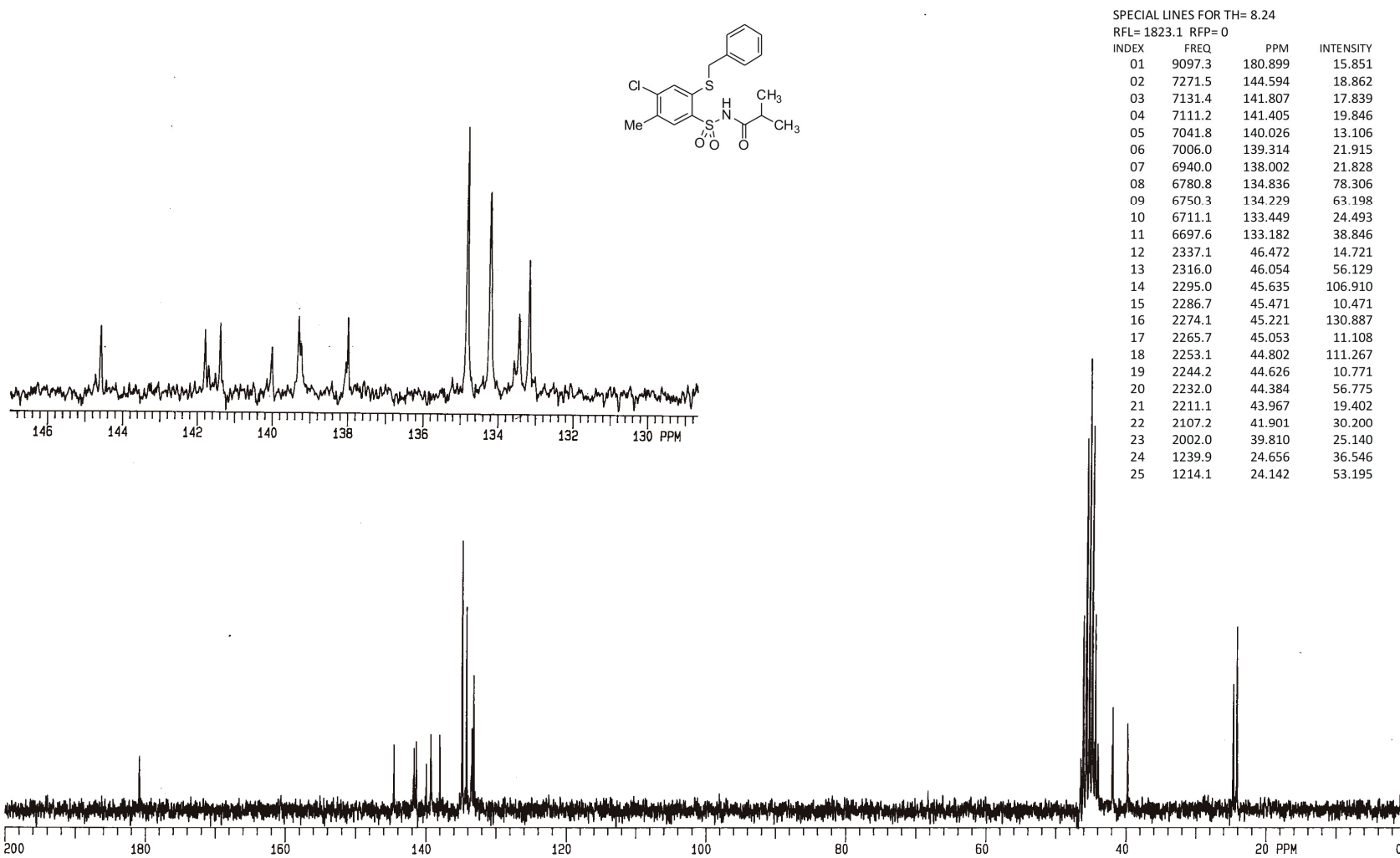


Figure S35.  $^{13}\text{C}$ -NMR of compound **43** (50 MHz,  $\text{DMSO-}d_6$ ).

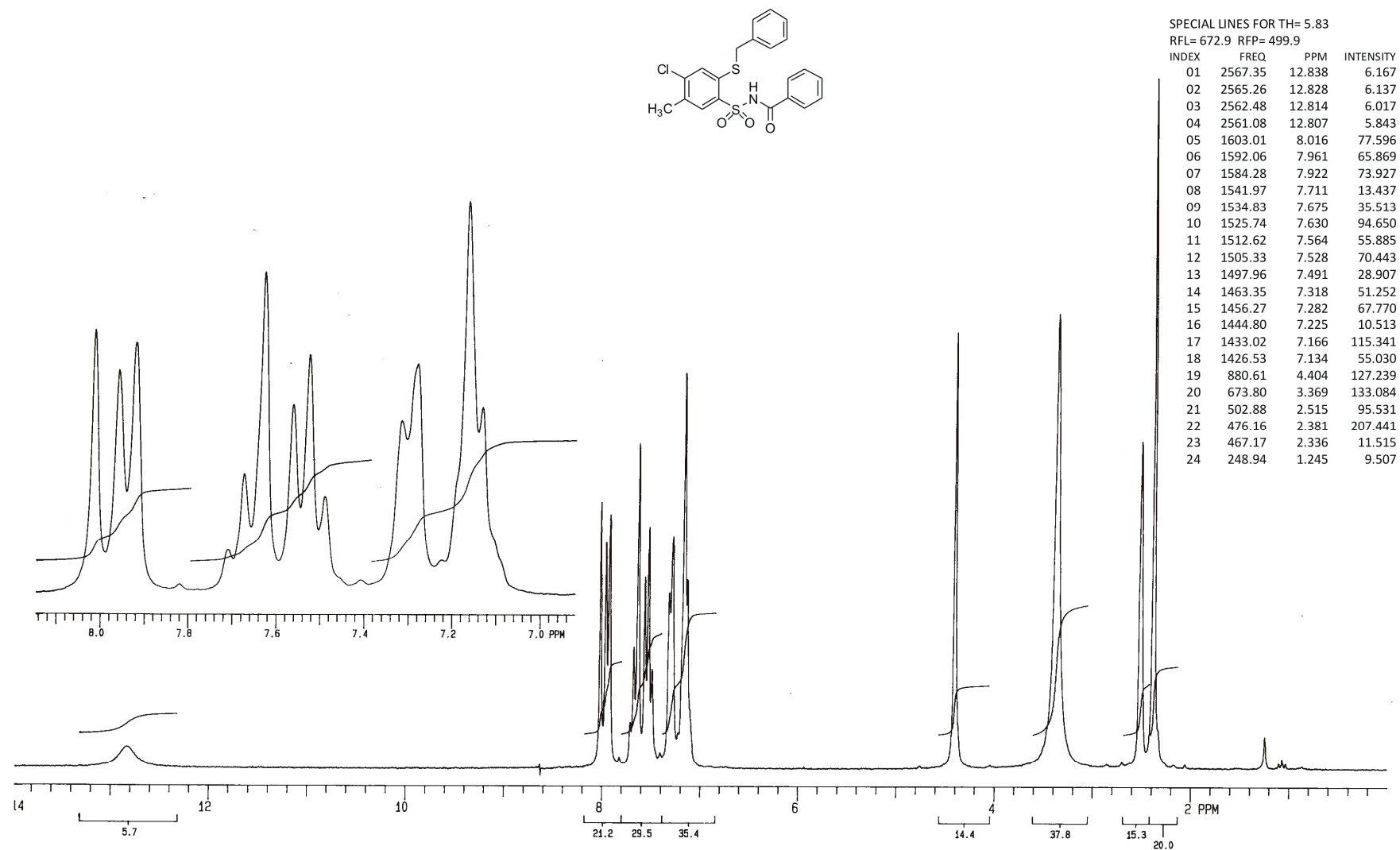


Figure S36. <sup>1</sup>H-NMR of compound 45 (200 MHz, DMSO-*d*<sub>6</sub>).

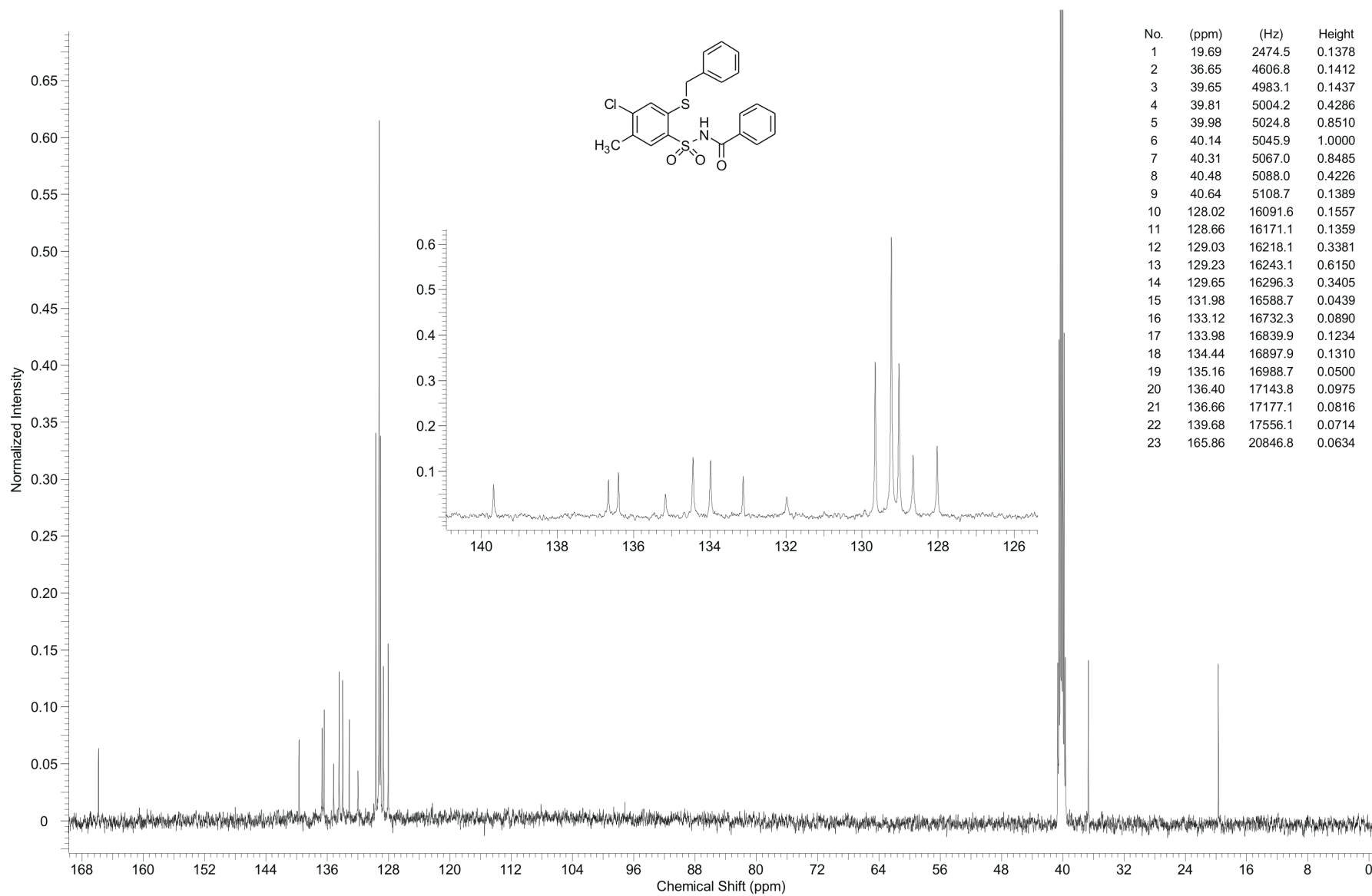


Figure S37.  $^{13}\text{C}$ -NMR of compound 45 (125 MHz,  $\text{DMSO-}d_6$ ).

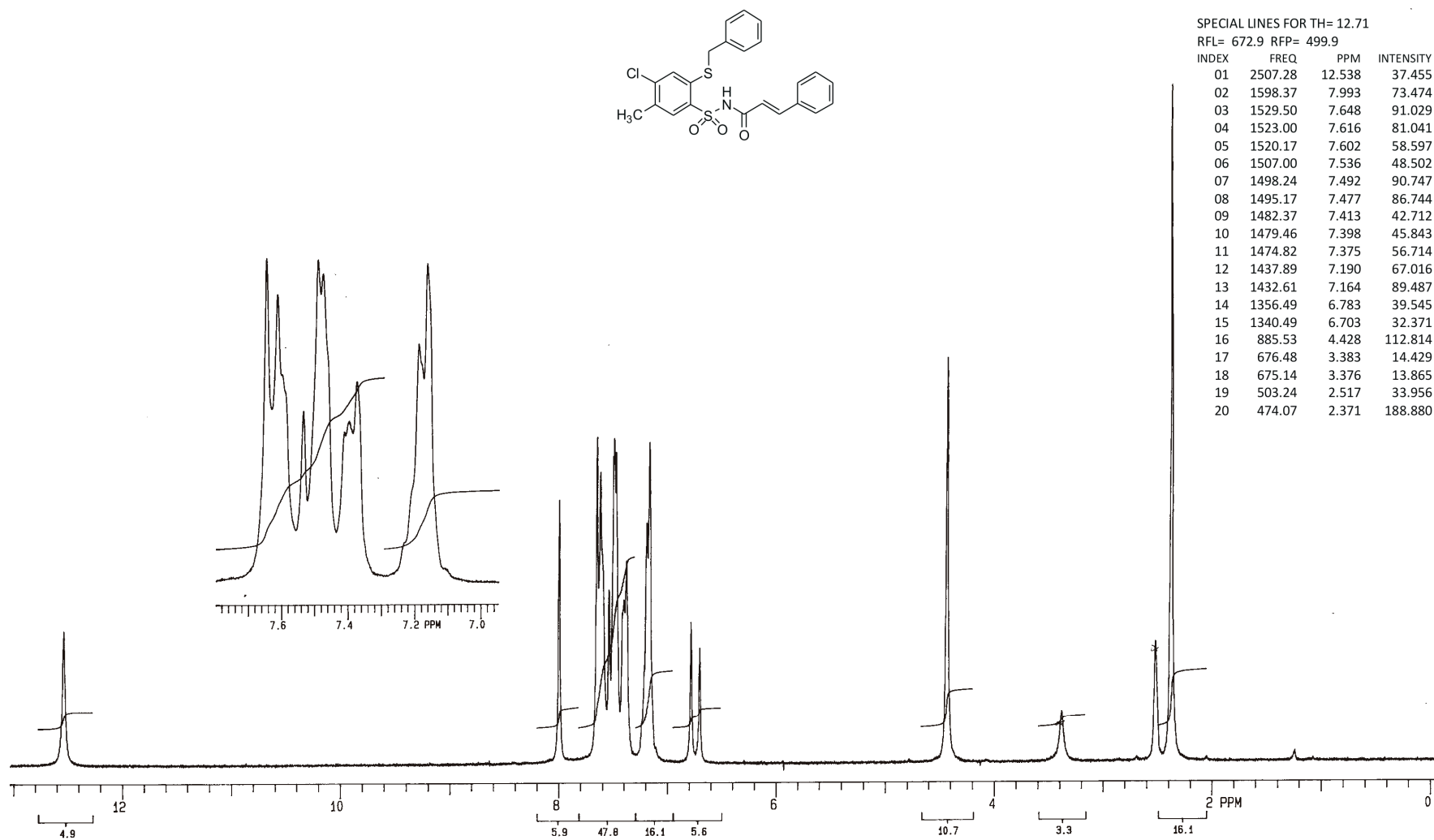


Figure S38.  $^1\text{H-NMR}$  of compound **46** (200 MHz,  $\text{DMSO-}d_6$ ).

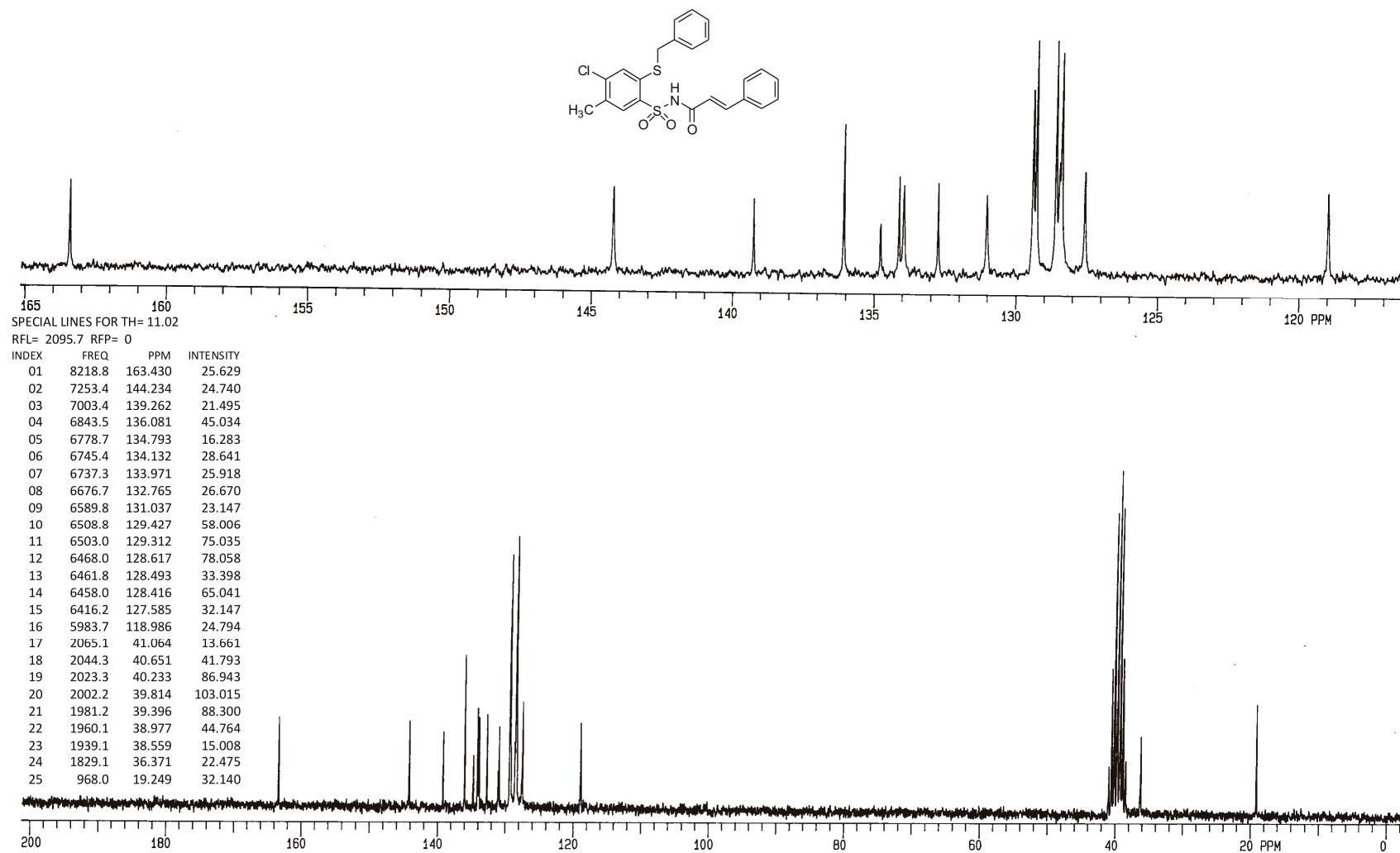


Figure S39.  $^{13}\text{C}$ -NMR of compound **46** (50 MHz,  $\text{DMSO-}d_6$ ).

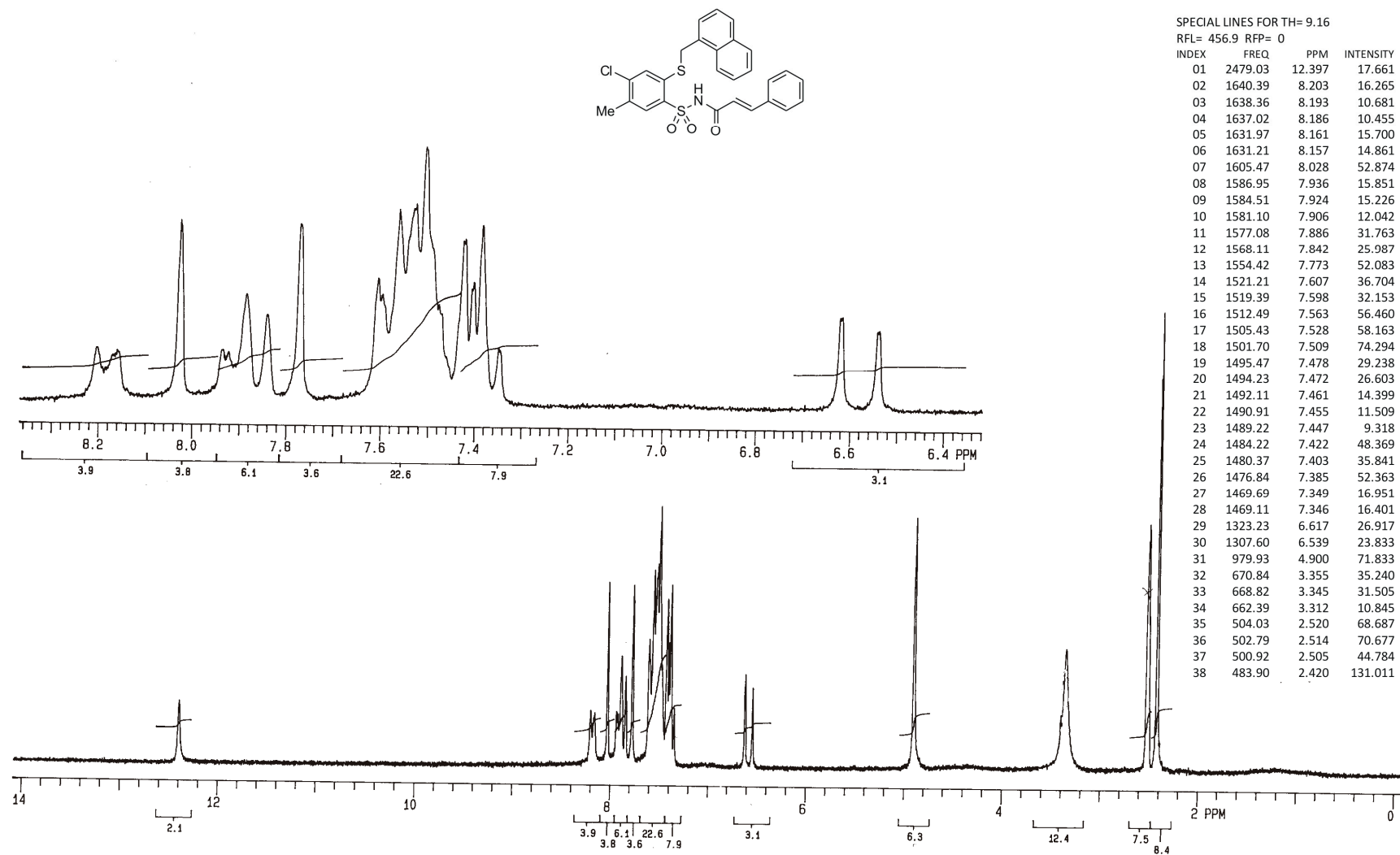


Figure S40.  $^1\text{H-NMR}$  of compound 47 (200 MHz,  $\text{DMSO-}d_6$ ).



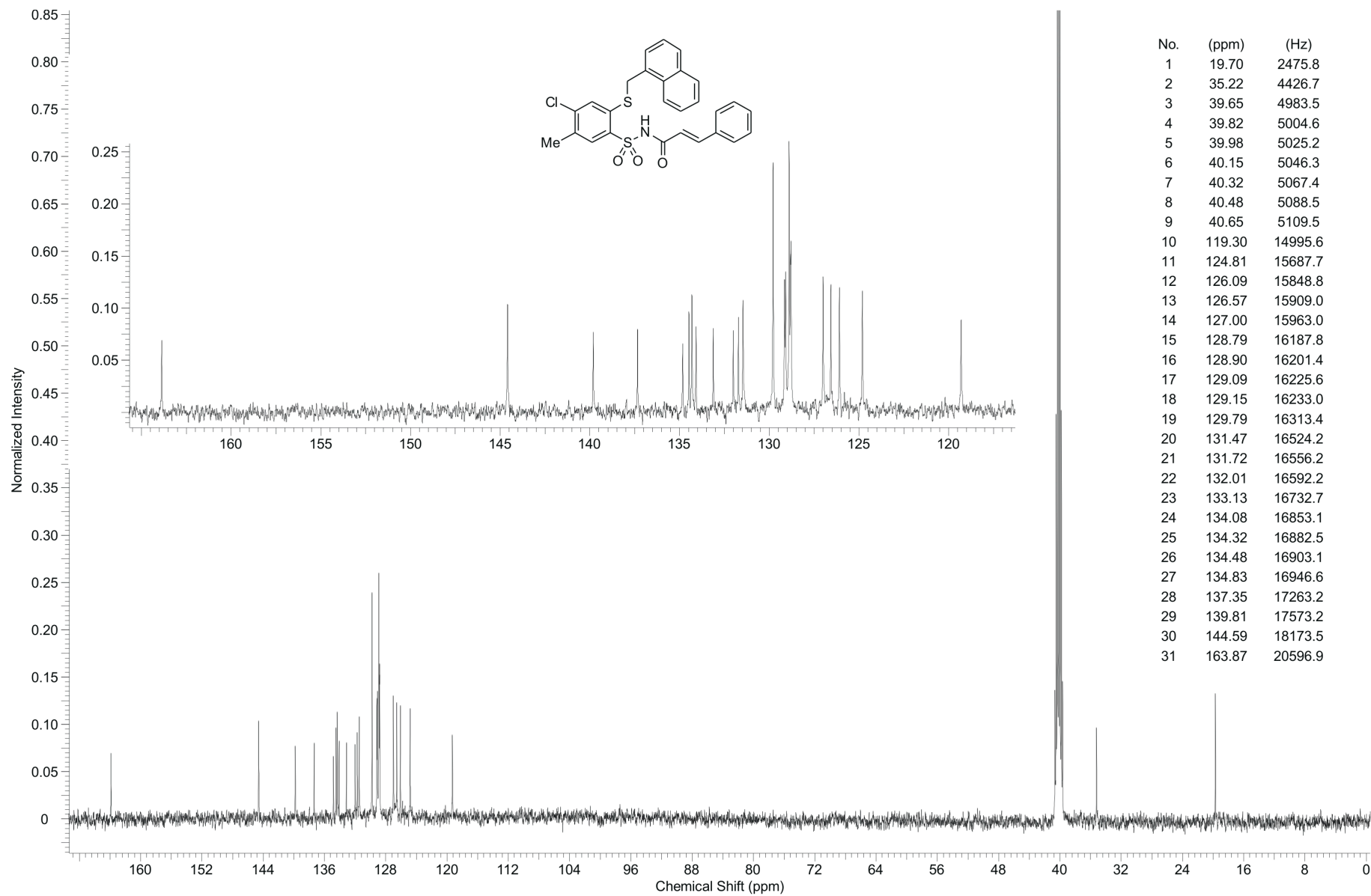


Figure S41.  $^{13}\text{C}$ -NMR of compound 47 (125 MHz,  $\text{DMSO-}d_6$ )