SUPPORTING INFORMATION

Orally Bioavailable 6-Chloro-7-methoxy-4(1*H*)-quinolones Efficacious against Multiple Stages of *Plasmodium*

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[‡]These authors contributed equally.

Table S1. Physicochemical Properties

Compound	Human Liver Microsomal CL_{int} (µL/min/mg protein)	Kinetic Solubility pH 7.4[a] (µM)	Pe pH 7.4[b] (10^{-6} cm/s)	Log *D* pH 7.4[c]
3	56	6-12	57	2.4
4	17	2-6	48	1.7
12	25	6-12	191	2.5
13	21	< 2	< 5	2.8
14	N.D. [e]	< 2	549	3.0
15	N.D.	2-6	406	3.3
16	N.D.	2-6	443	2.9
17	34	< 2	N.D.	3.6
18	N.D.	< 2	< 5	3.8
19	N.D.	N.D.	38	N.D.
20	11	≥20	10	4.1
21	15	6-12	< 5	1.8
22	N.D.	≥ 20	11	N.D.
23	20	6-12	137	1.9
24	34	≥ 20	< 5	1.9
25	59	N.D.	< 5	2.1
26	93	N.D.	67	2.0
27	< 7 [d]	≥ 20	24	1.8
28	N.D.	N.D.	256	N.D.
29	29	< 2	73	3.2
30	N.D.	< 2	241	3.5
31	N.D.	< 2	178	2.4
32	N.D.	< 2	46	3.5
33	< 7 [d]	< 2	97	2.4
34	8	< 2	427	3.3
35	N.D.	< 2	107	2.2
36	11	< 2	< 5	2.3
37	N.D.	N.D.	< 5	N.D.
38	N.D.	N.D.	198	N.D.
39	15	2-6	238	2.6
40	17	< 2	119	2.2
41	< 7 [d]	N.D.	8	1.8
42	N.D.	12-20	19	1.8
43	< 7 [d]	N.D.	9	3.5
44	< 7 [d]	N.D.	< 5	1.8
45	14	< 2	< 5	3.7
46	19	< 2	41	3.7
47	N.D.	< 2	< 5	3.5
48	22	2-6	< 5	3.7
49	31	2-6	65	2.6
50	9	2-6	315	2.6
51	N.D.	N.D.	151	2.1
52	< 7 [d]	< 2	< 5	2.4
53	N.D.	< 2	< 5	4.0
54	N.D.	N.D.	688	N.D.
55	N.D.	< 2	145	2.9
56	N.D.	N.D.	275	2.7
57	N.D.	N.D.	411	3.0
58	< 7 [d]	< 2	6	3.4

[a]Standards for the solubility assay include carbamazepine and albendazole. Solubility for carbamazepine at pH 7.4, 4.0, and 2.0 was 95 μM, 100 μM, and 100 μM, respectively. Solubility for albendazole at pH 7.4, 4.0, and 2.0 was 6.1 μM, 12 μM, and 100 μM respectively.

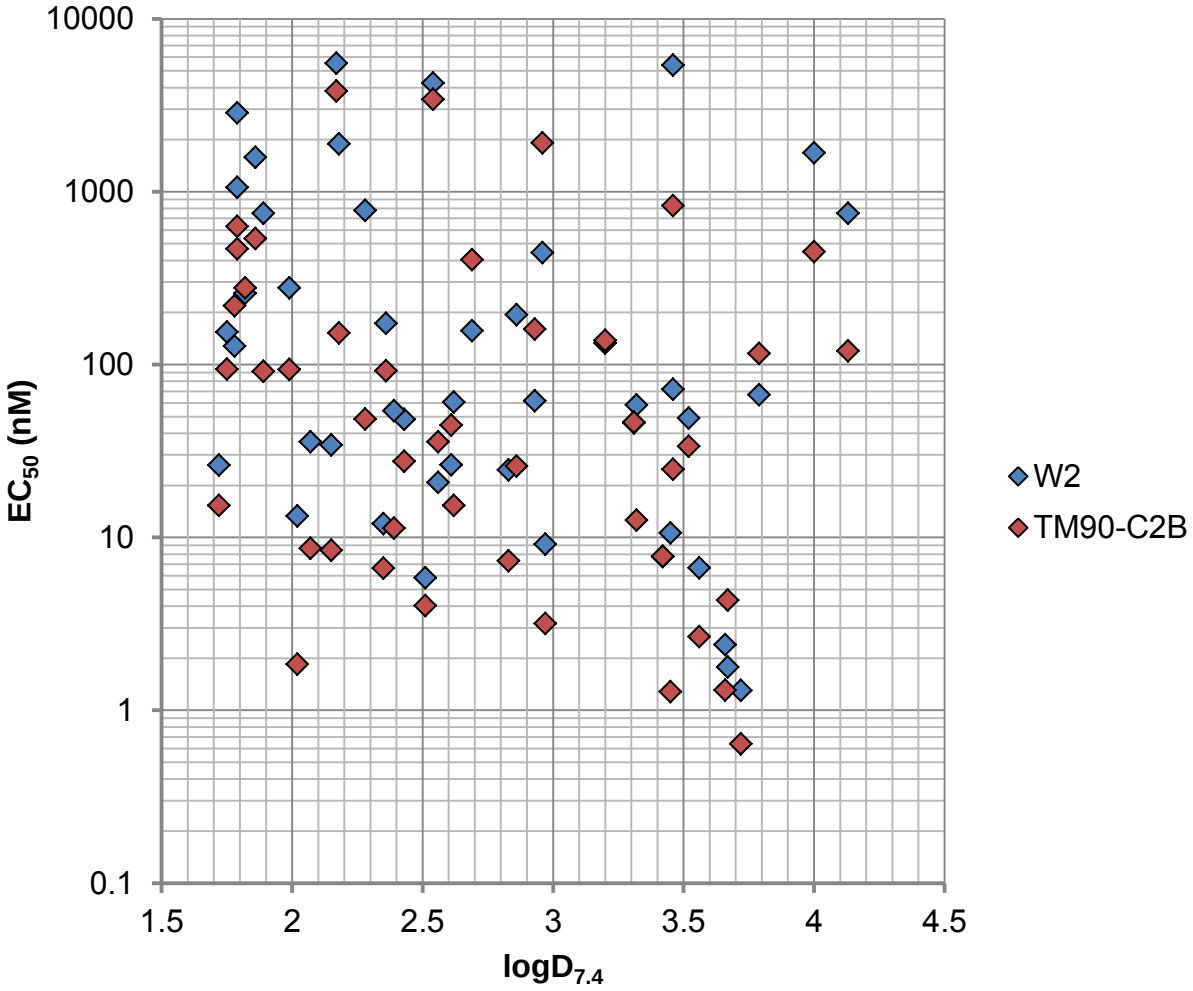
[b]Standards for the permeability assay include verapamil HCl (P_e = 1405 x10^{-6} cm/s at pH=7.4 and 39 x10^{-6} cm/s at pH=4.0), carbamazepine (P_e = 112 x10^{-6} cm/s at pH=7.4 and 108 x10^{-6} cm/s at pH=4.0), and ranitidine HCl (P_e = 0.5 x10^{-6} cm/s at pH=7.4 and 0 x10^{-6} cm/s at pH=4.0).

[c]Standards for the log $D_{7.4}$ assay include cinnarizine (log $D_{7.4}$ 5.68), hydrocortisone-21-acetate (log $D_{7.4}$ 2.19), ketoconazole (log $D_{7.4}$ 3.83), metronidazole (log $D_{7.4}$ -0.02), nadolol (log $D_{7.4}$ 0.68), pyrene (log $D_{7.4}$ 4.88), theophyline (log $D_{7.4}$ -0.05), and tolnaftate (log $D_{7.4}$ 5.40).

[d]These compounds displayed little to no observable degradation throughout the assay duration (typically 250 min).

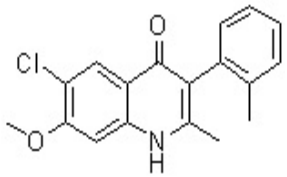
[e]N.D. Not determined

Figure S1. Plot of in vitro efficacy versus distribution coefficient log $D_{7.4}$.



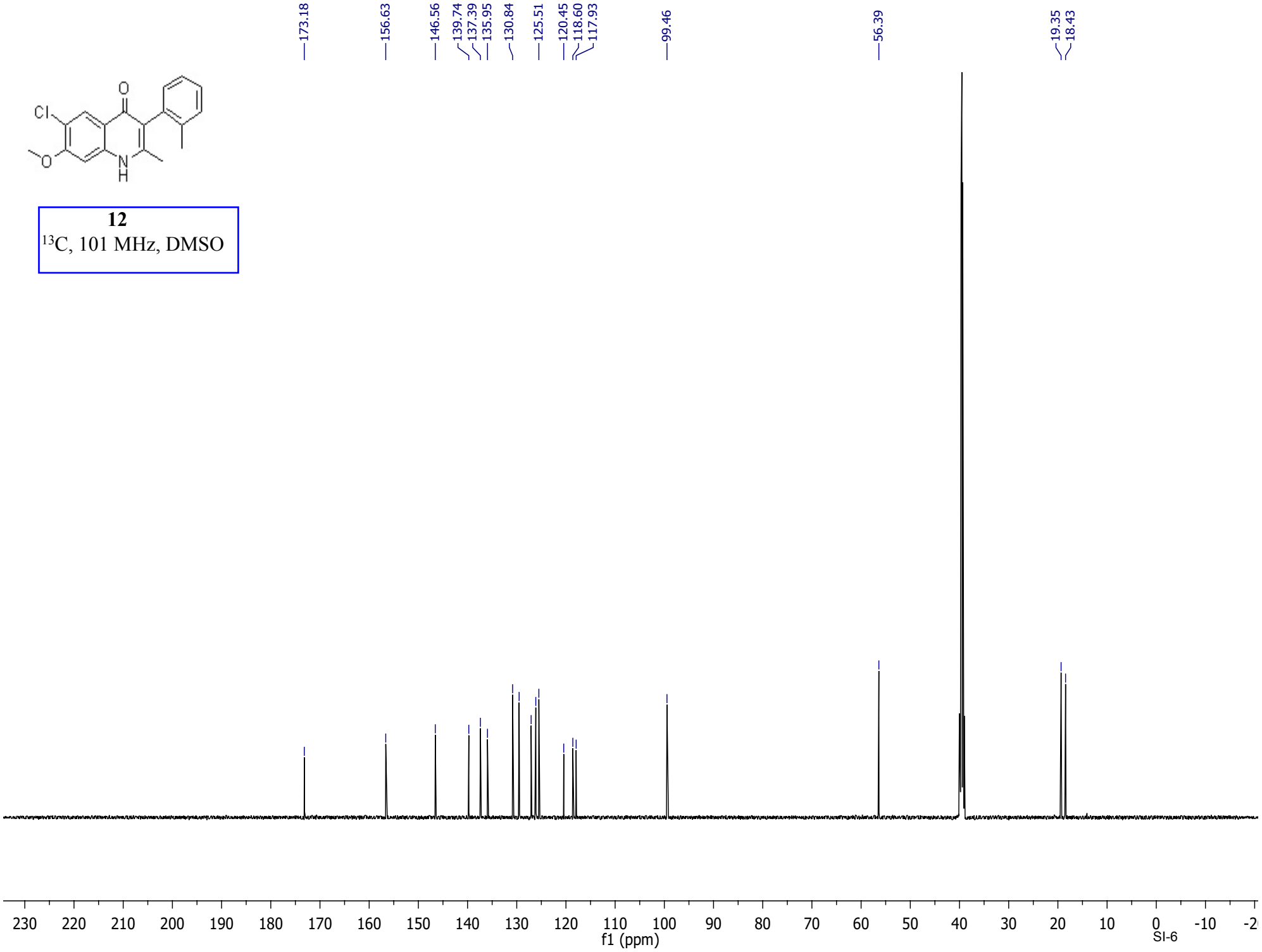
X-ray Crystallography

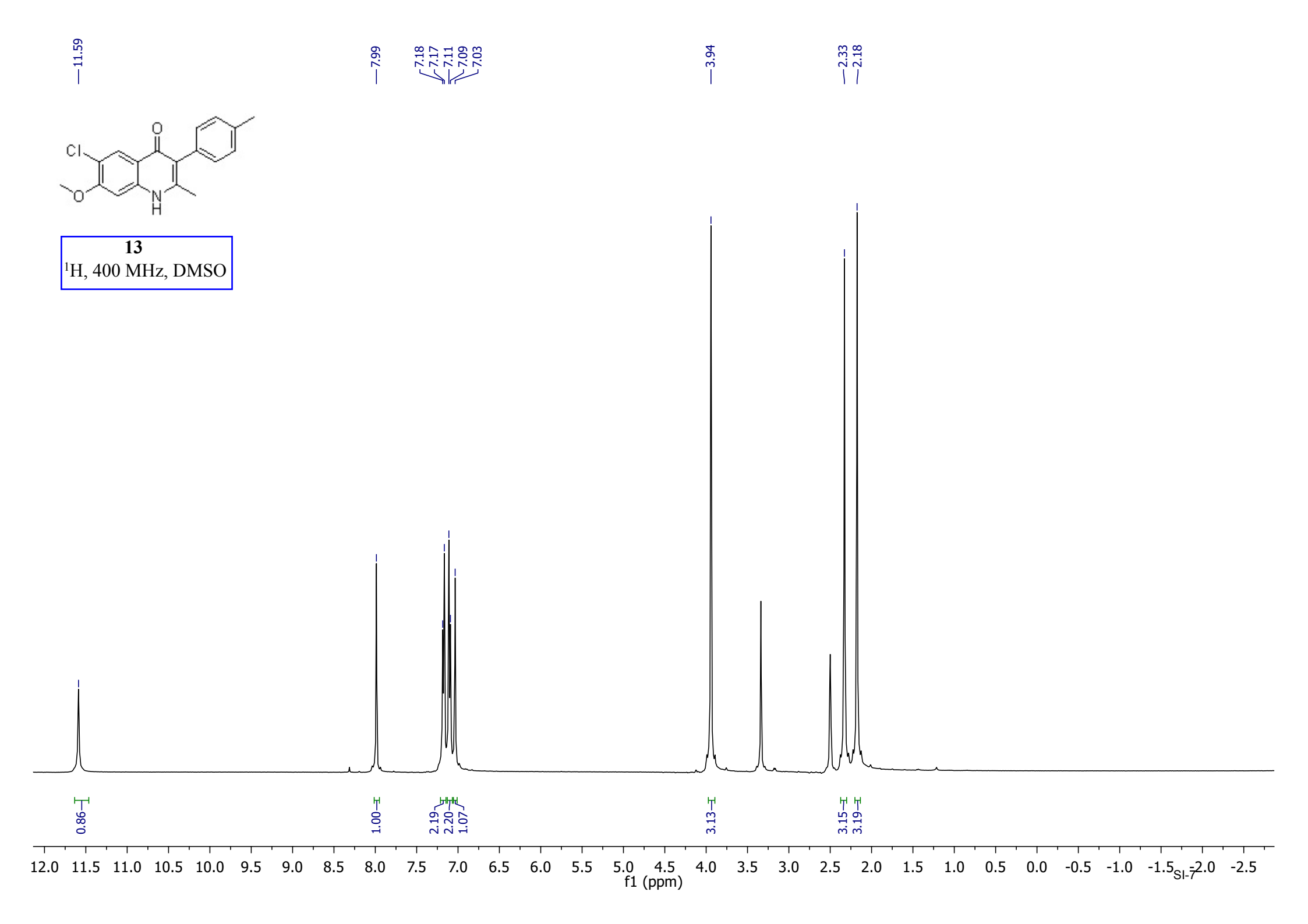
Crystal Data: **4**, $C_{17}H_{14}ClNO_2$, FW=299.74, monoclinic $P2_1/c$, a=22.483(2), b=5.7461(5), c=11.0799(10) Å, β=104.036(5)°, T=100K, Z=4, R=0.030, GOF=1.025, CCDC 1023754; **12**, $C_{18}H_{16}ClNO_2$, FW=313.77, monoclinic $P2_1/c$, a=23.770(2), b=9.7135(10), c=13.4414(15) Å, β=92.364(5)°, T=100K, Z=8, R=0.047, GOF=1.040, CCDC 1023753.



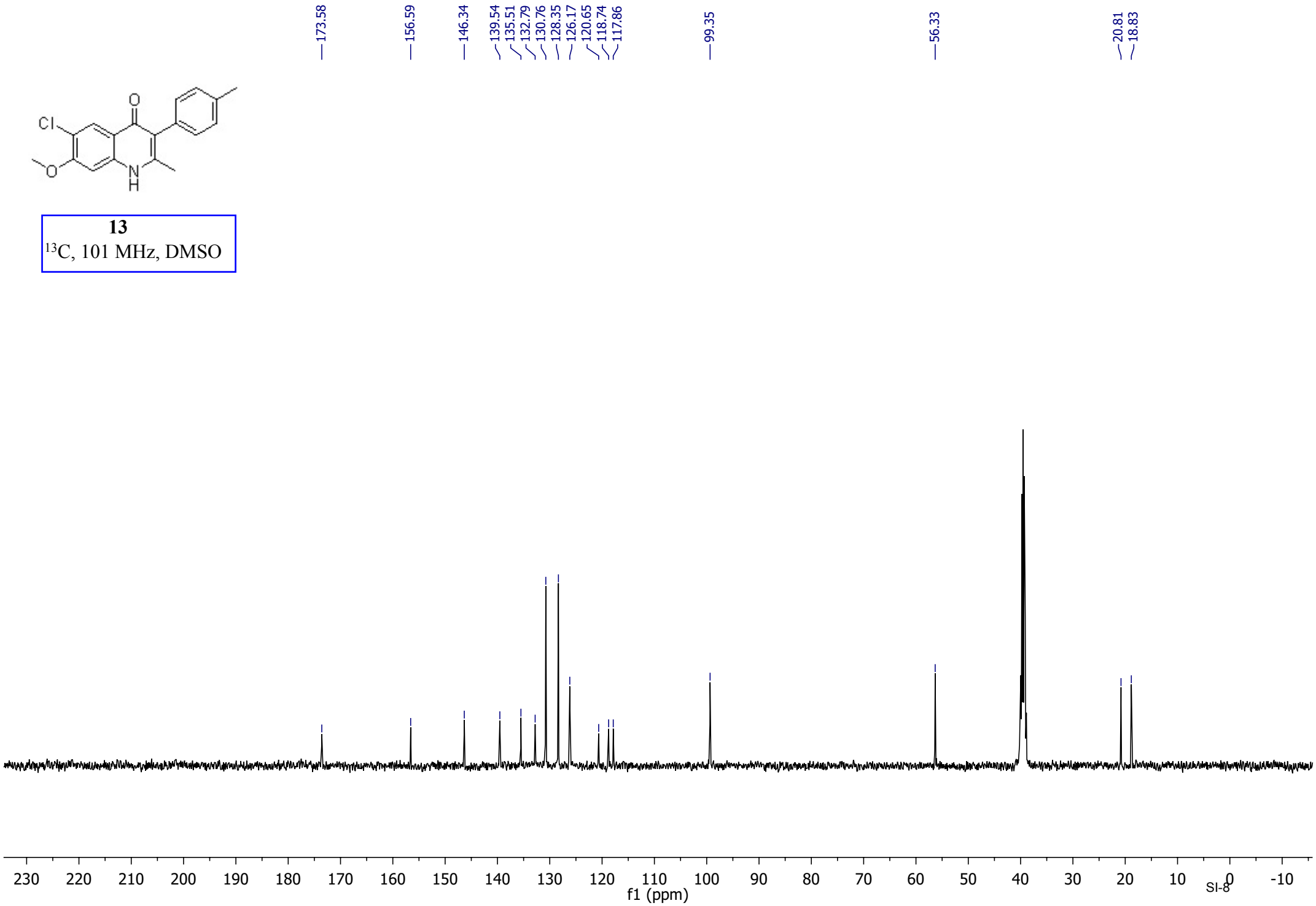
12
^{1}H, 400 MHz, DMSO

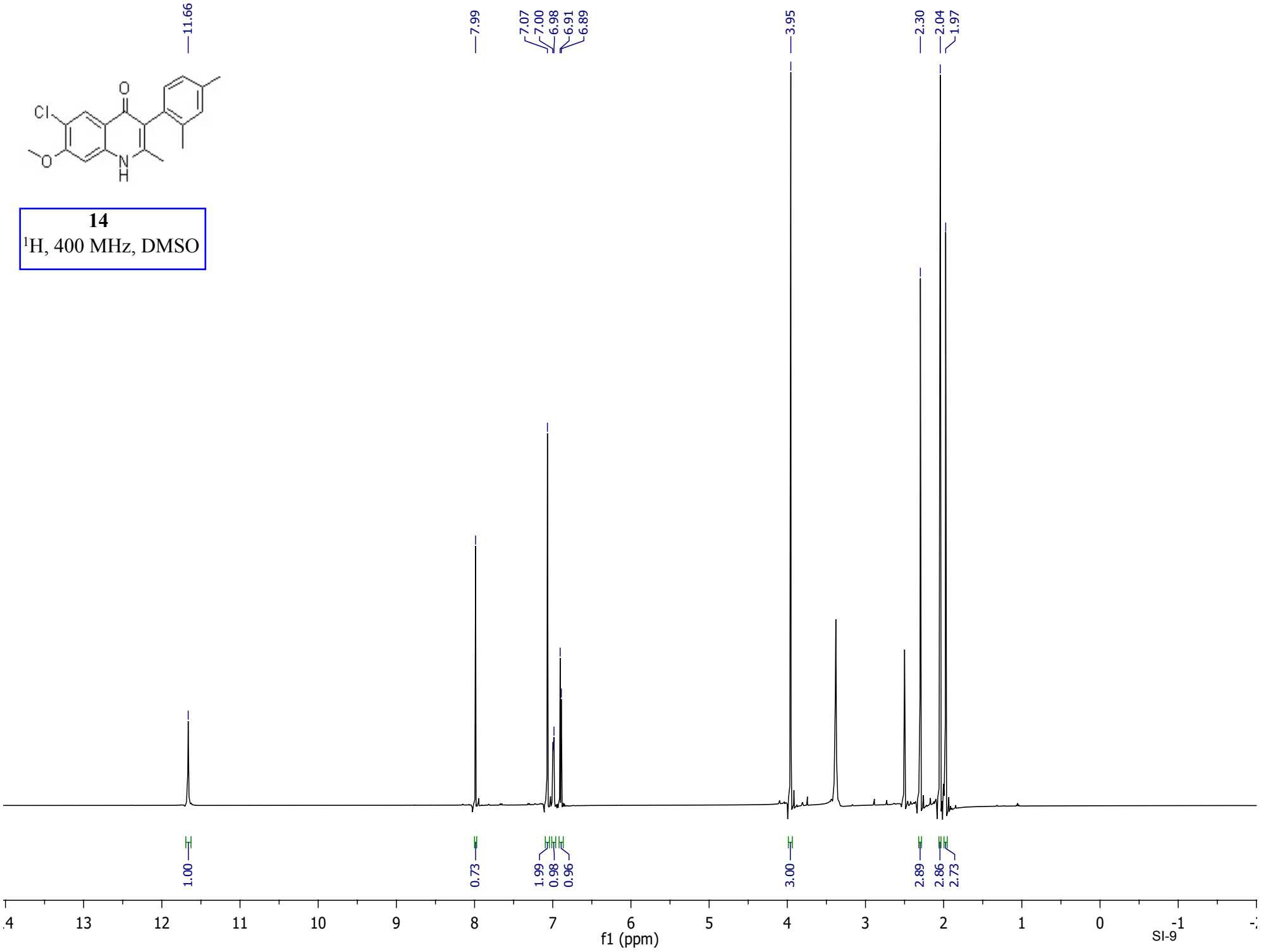
12
^{13}C, 101 MHz, DMSO




11.59
7.99
7.18
7.17
7.11
7.09
7.03
3.94
2.33
2.18
Cl
O
O
N
H
13
1H, 400 MHz, DMSO
0.86
1.00
2.19
2.20
1.07
3.13
3.15
3.19
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5
f1 (ppm)
SI-7

13
^{13}C, 101 MHz, DMSO

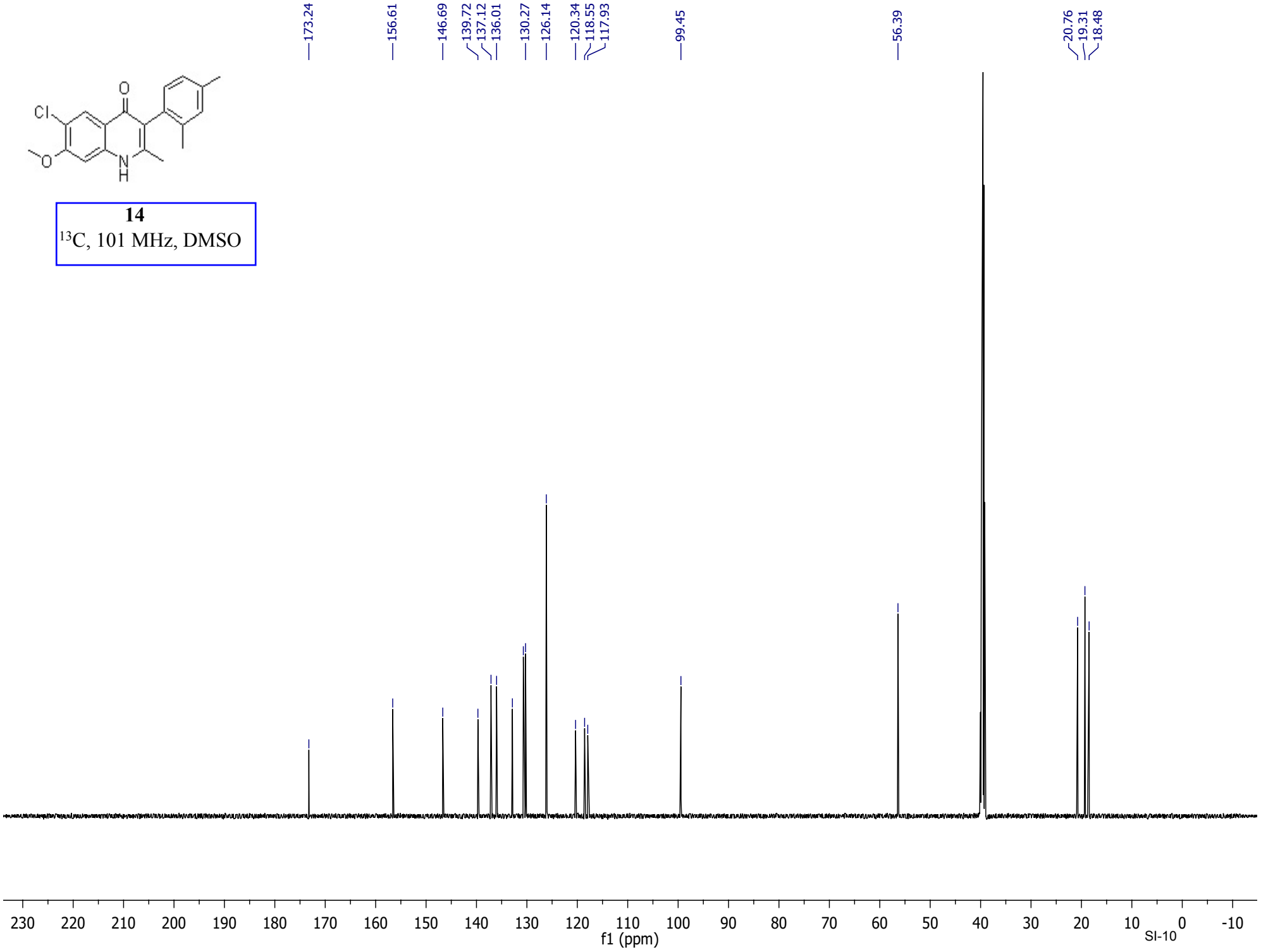




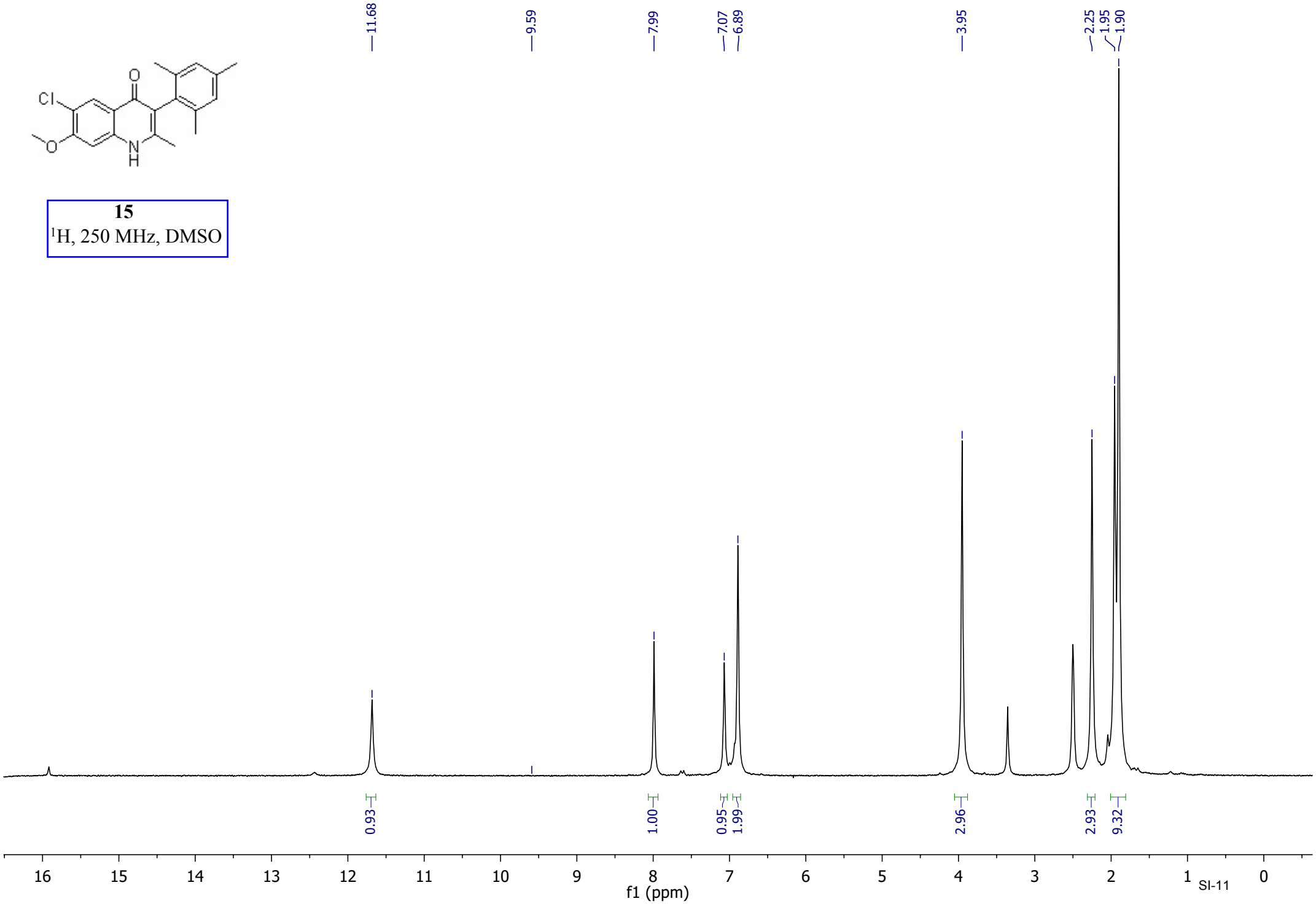
14
^{1}H, 400 MHz, DMSO

14

^{13}C, 101 MHz, DMSO

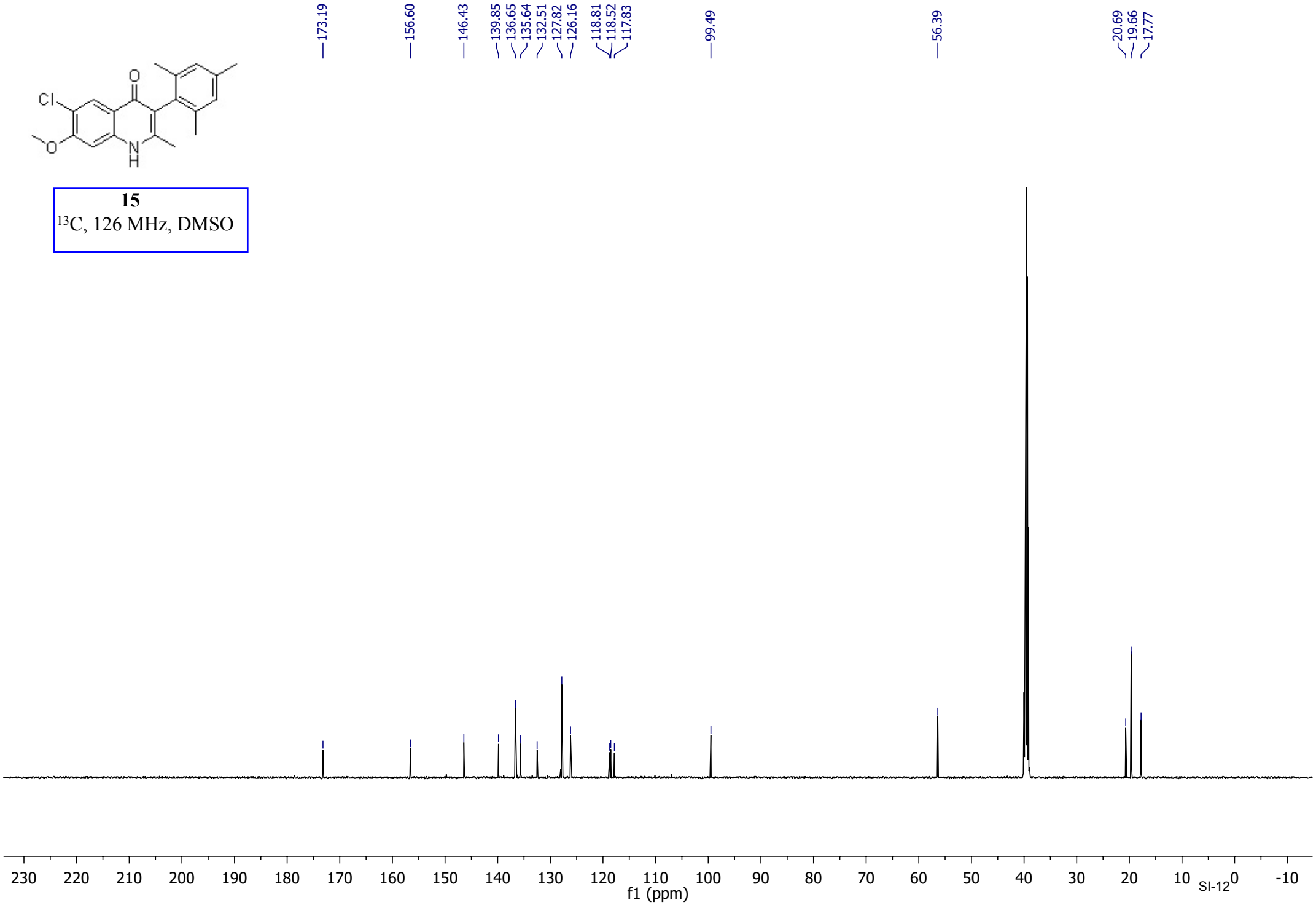


15
^{1}H, 250 MHz, DMSO

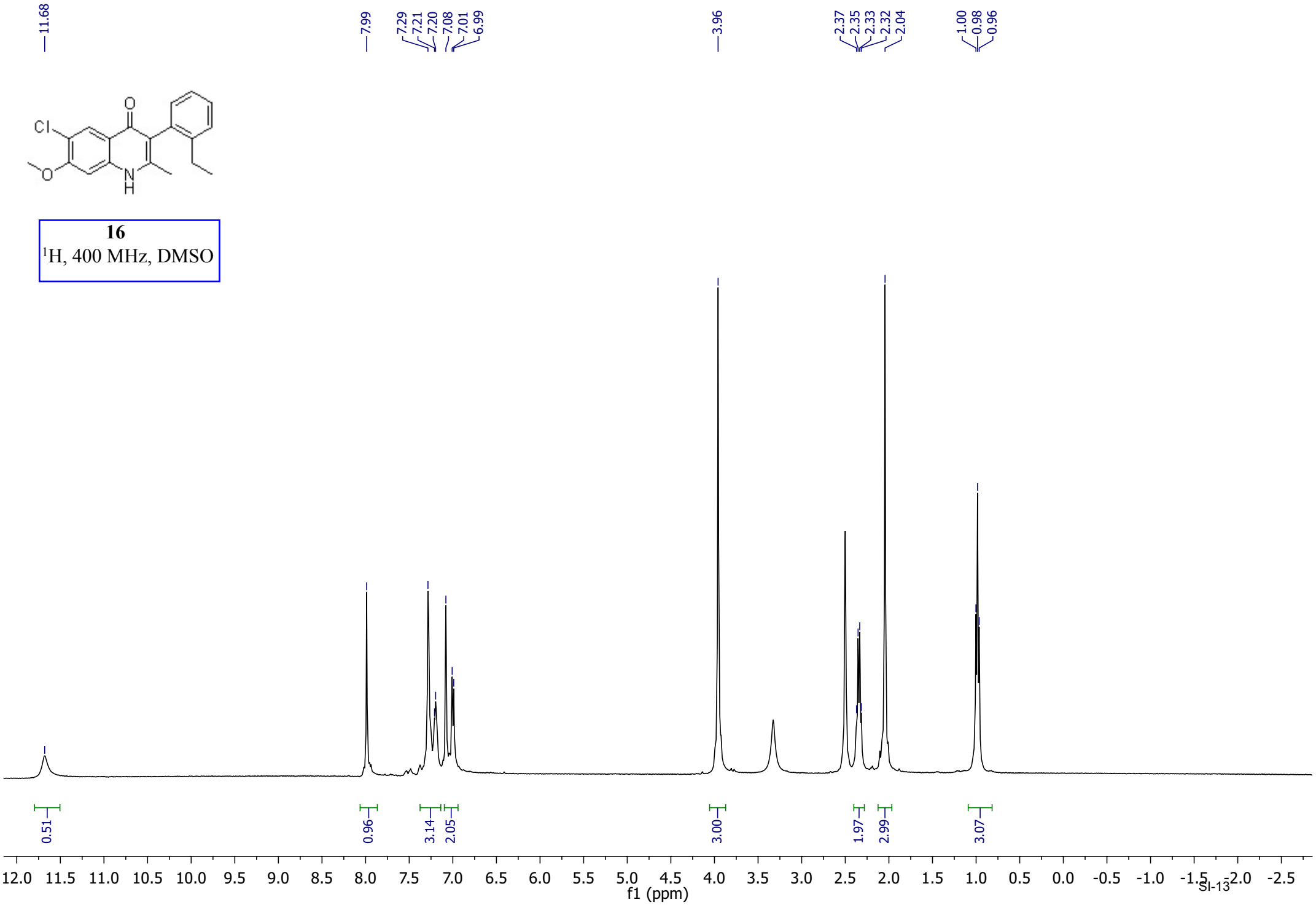


15

^{13}C, 126 MHz, DMSO

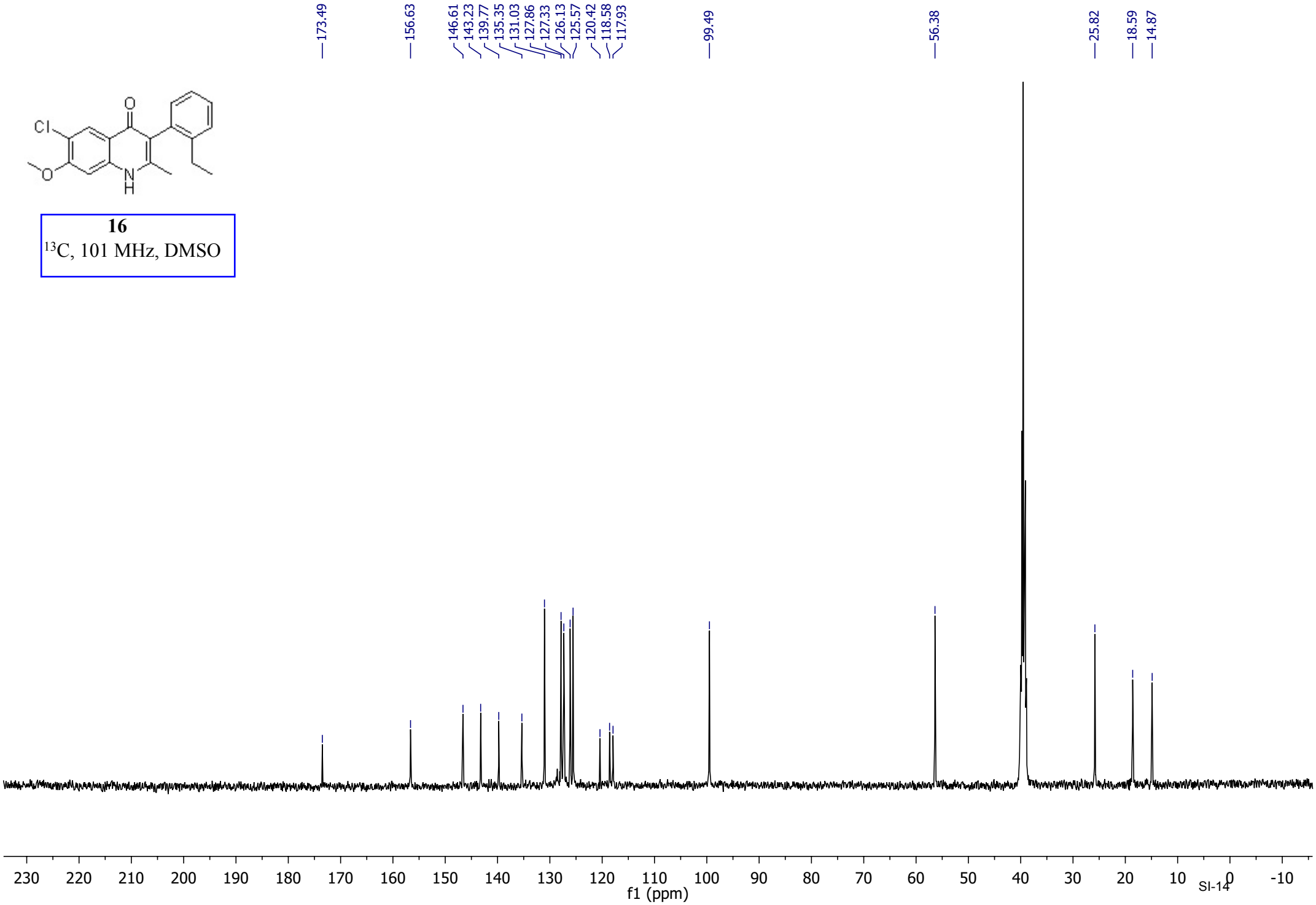


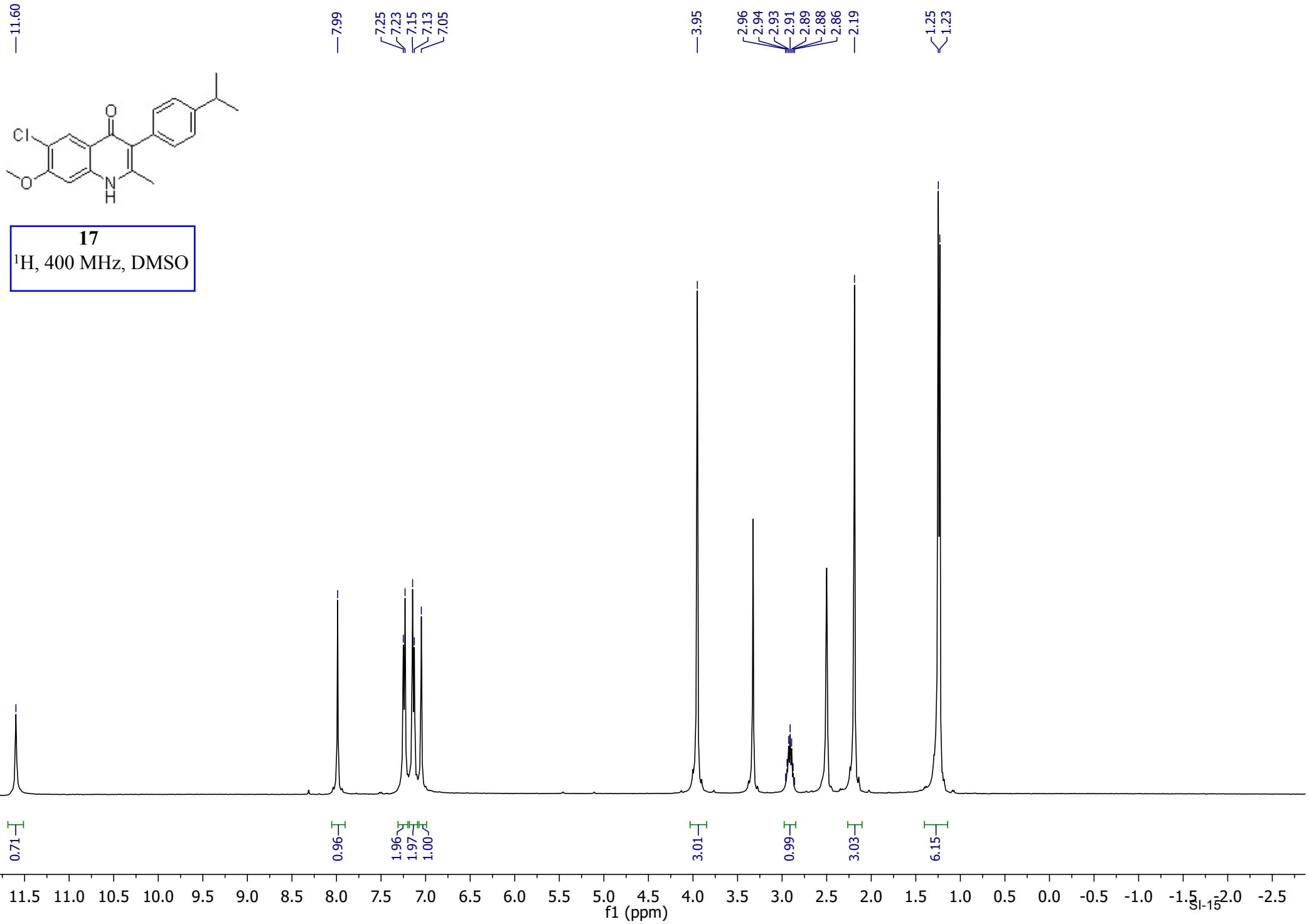
16
^{1}H, 400 MHz, DMSO

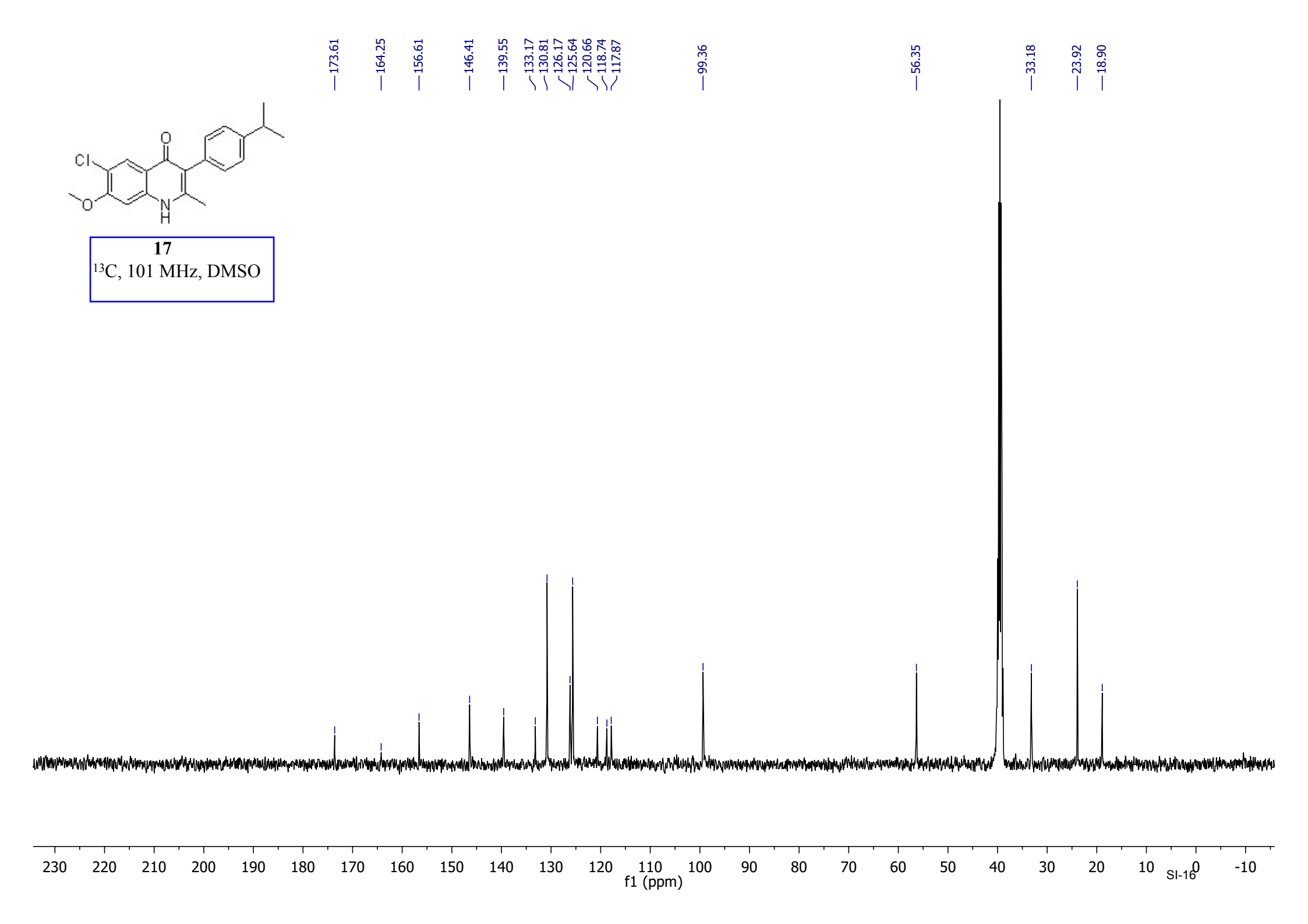


16

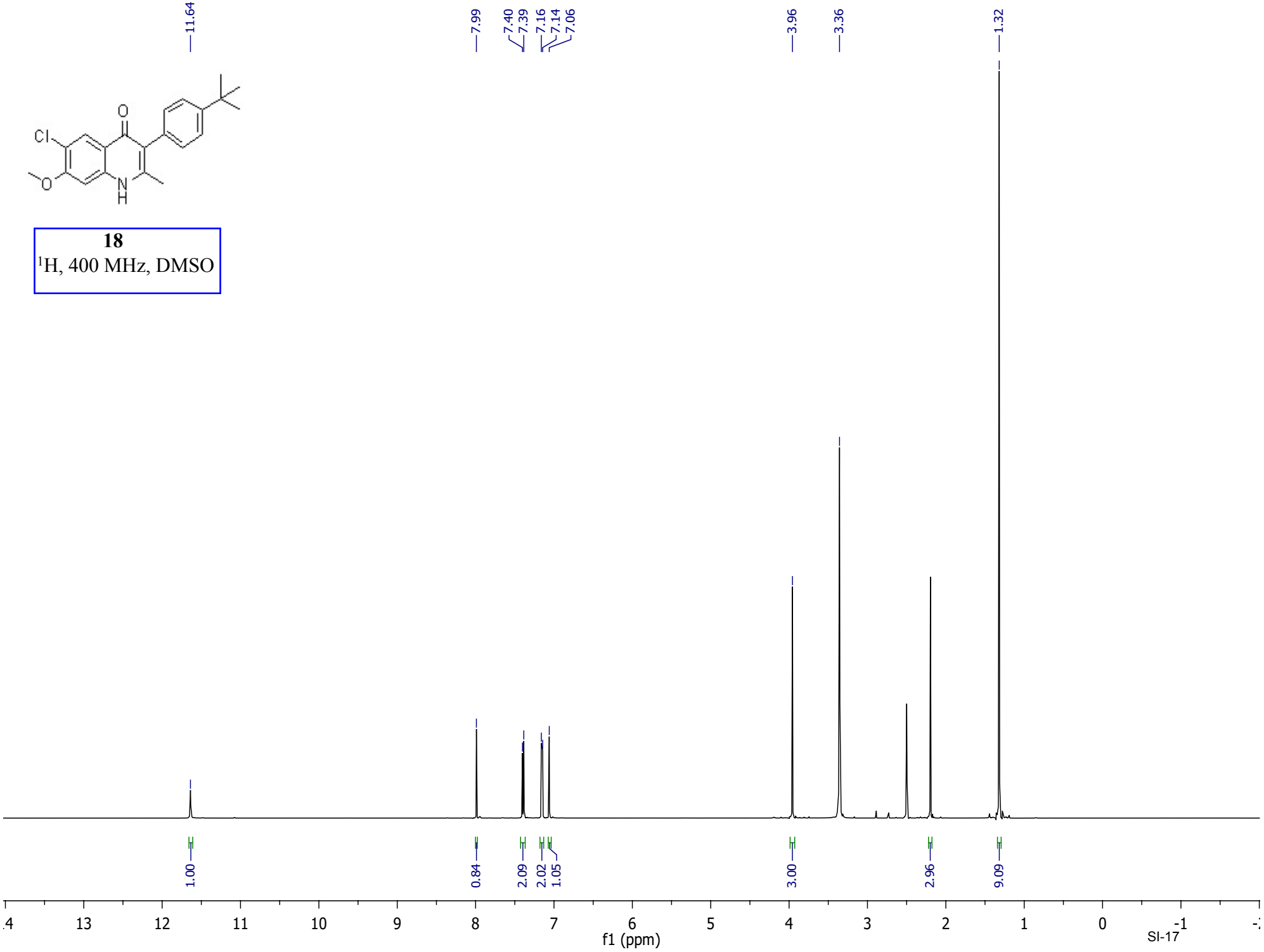
^{13}C, 101 MHz, DMSO




11.60
7.99
7.25
7.23
7.15
7.13
7.05
3.95
2.96
2.94
2.93
2.91
2.89
2.88
2.86
2.19
1.25
1.23
Cl
O
O
N
H
17
1H, 400 MHz, DMSO
0.71
0.96
1.96
1.97
1.00
3.01
0.99
3.03
6.15
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5
f1 (ppm)

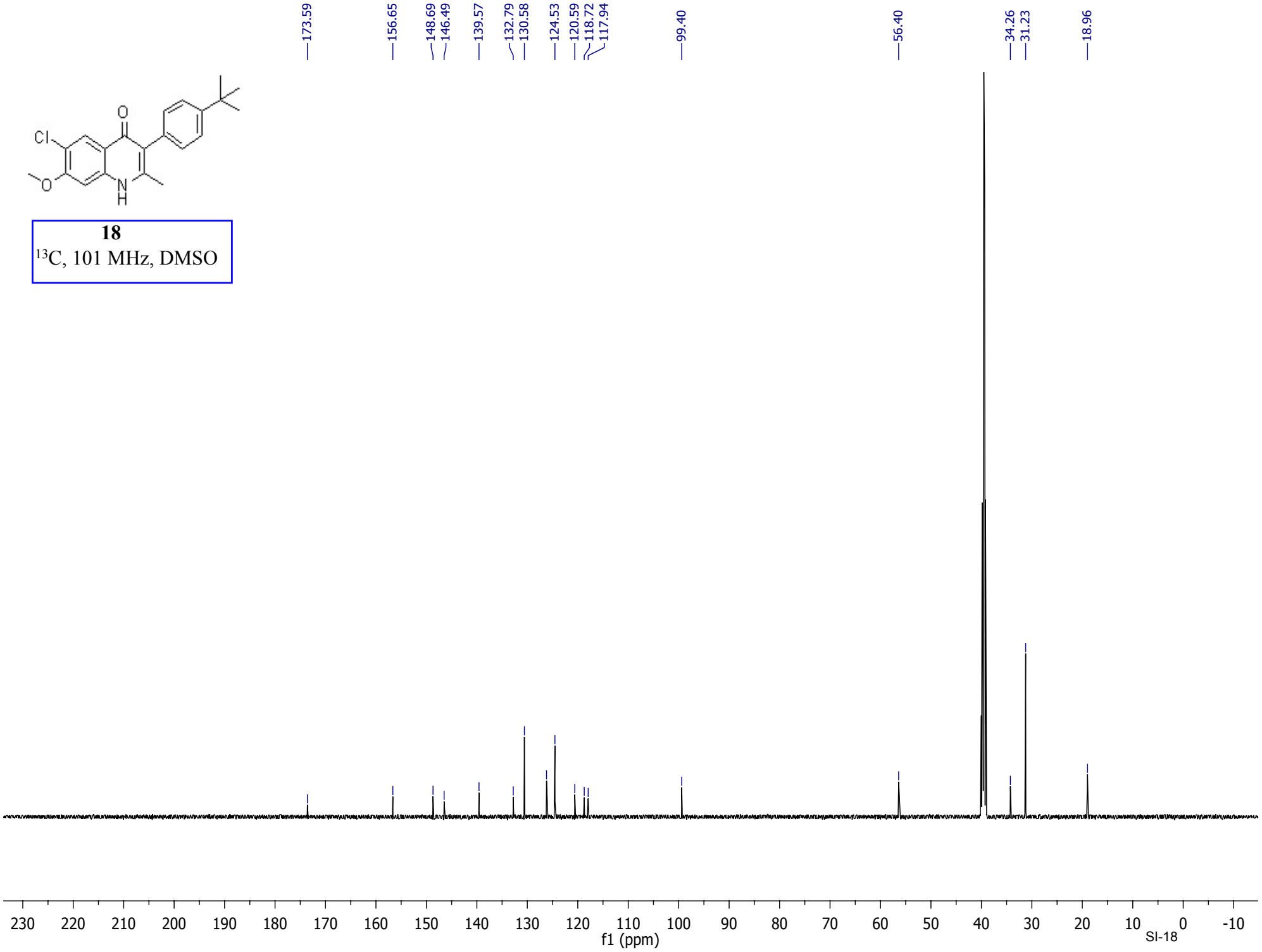

173.61
164.25
156.61
146.41
139.55
133.17
130.81
126.17
125.64
120.66
118.74
117.87
99.36
56.35
33.18
23.92
18.90
Cl
O
O
N
H
17
13C, 101 MHz, DMSO
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

18
^{1}H, 400 MHz, DMSO

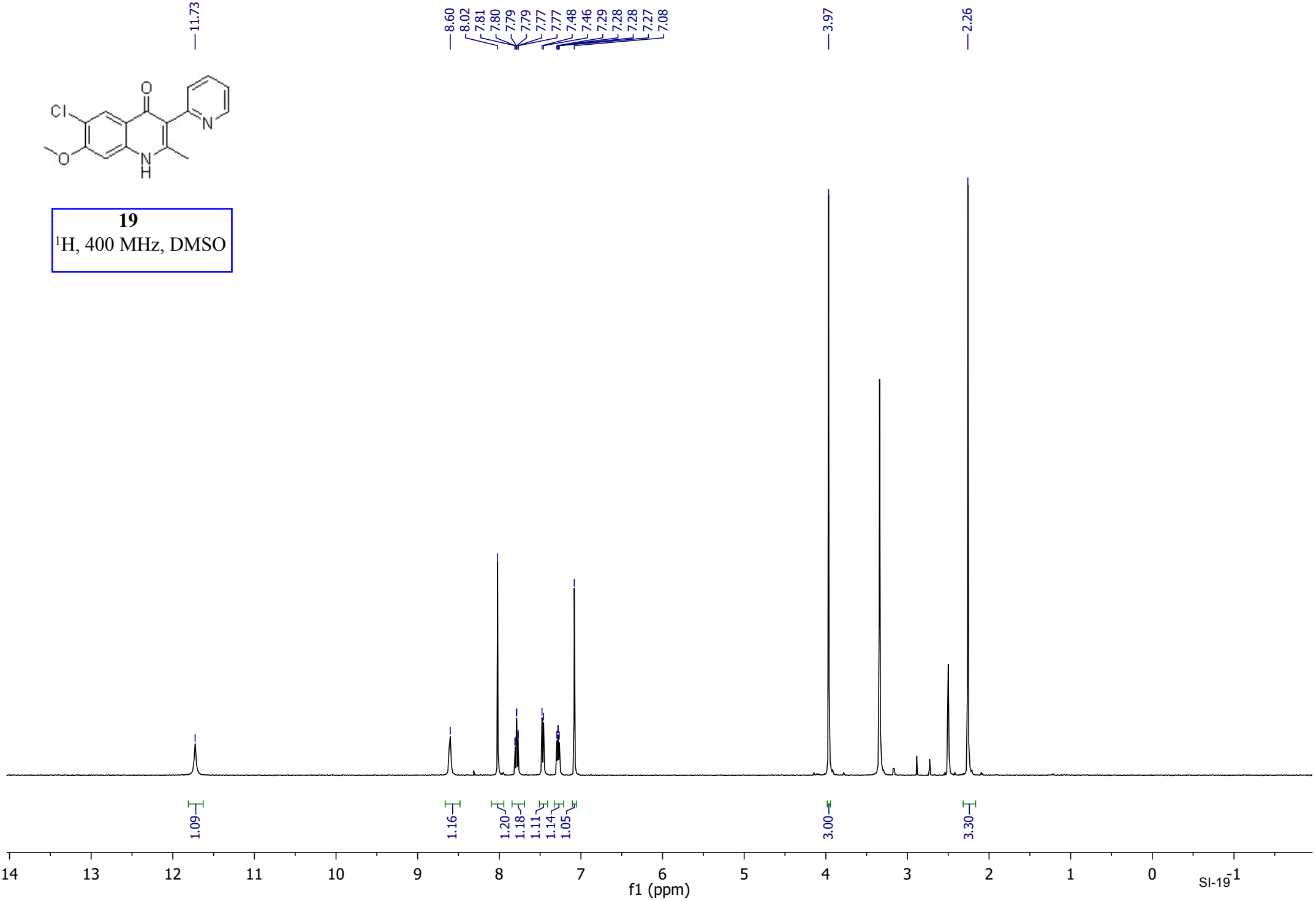


18

^{13}C, 101 MHz, DMSO

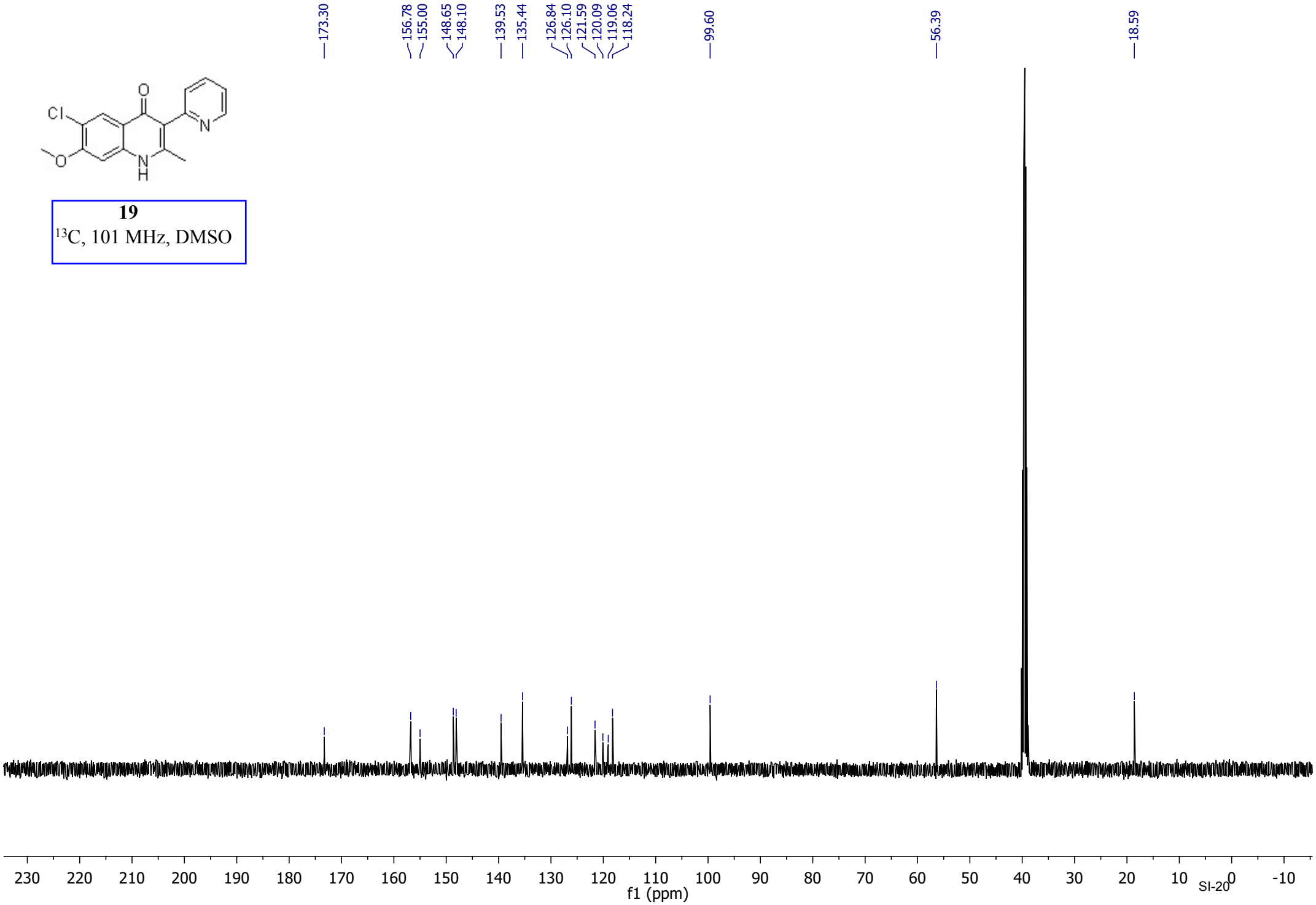


19
^{1}H, 400 MHz, DMSO

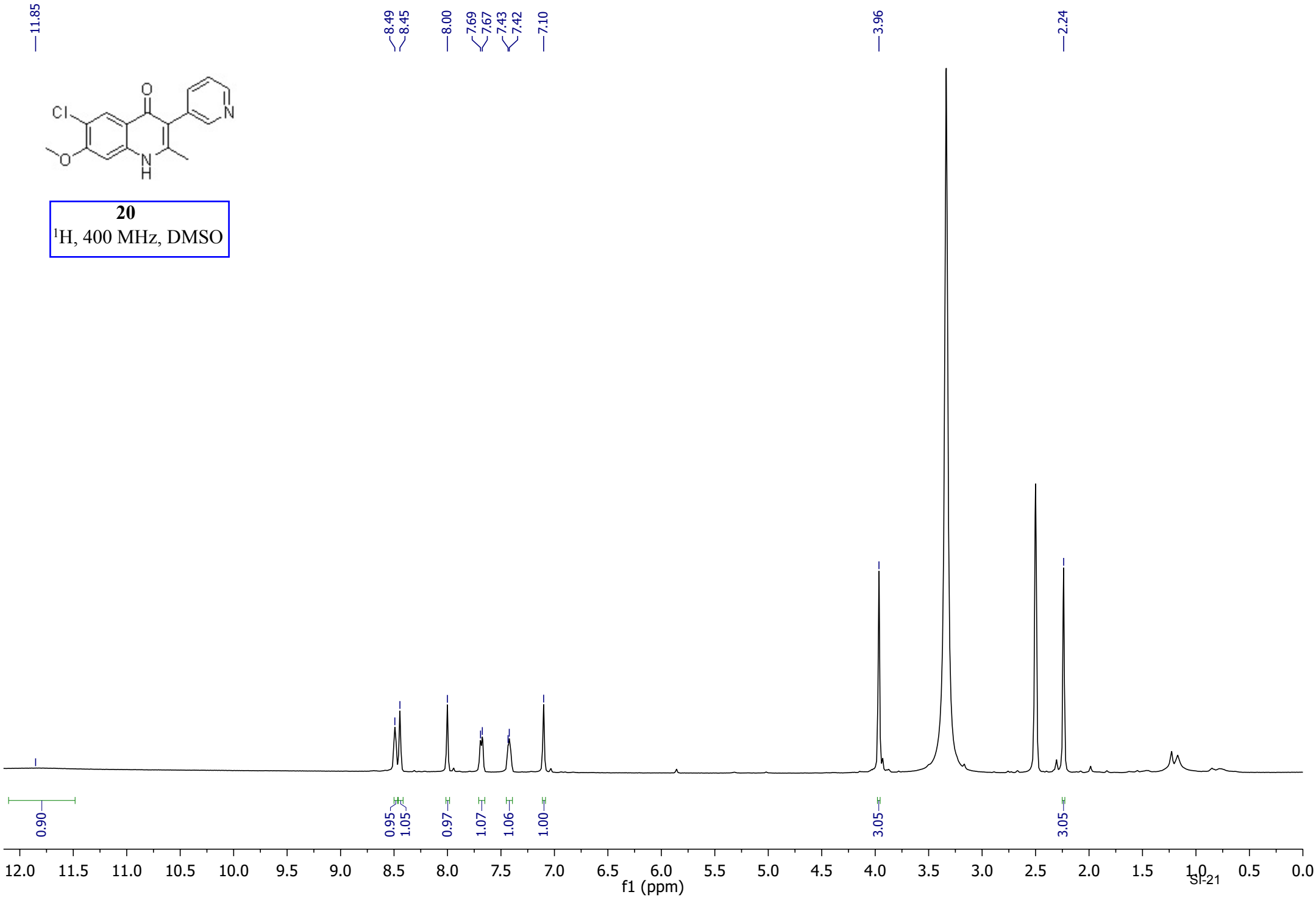


19

^{13}C, 101 MHz, DMSO

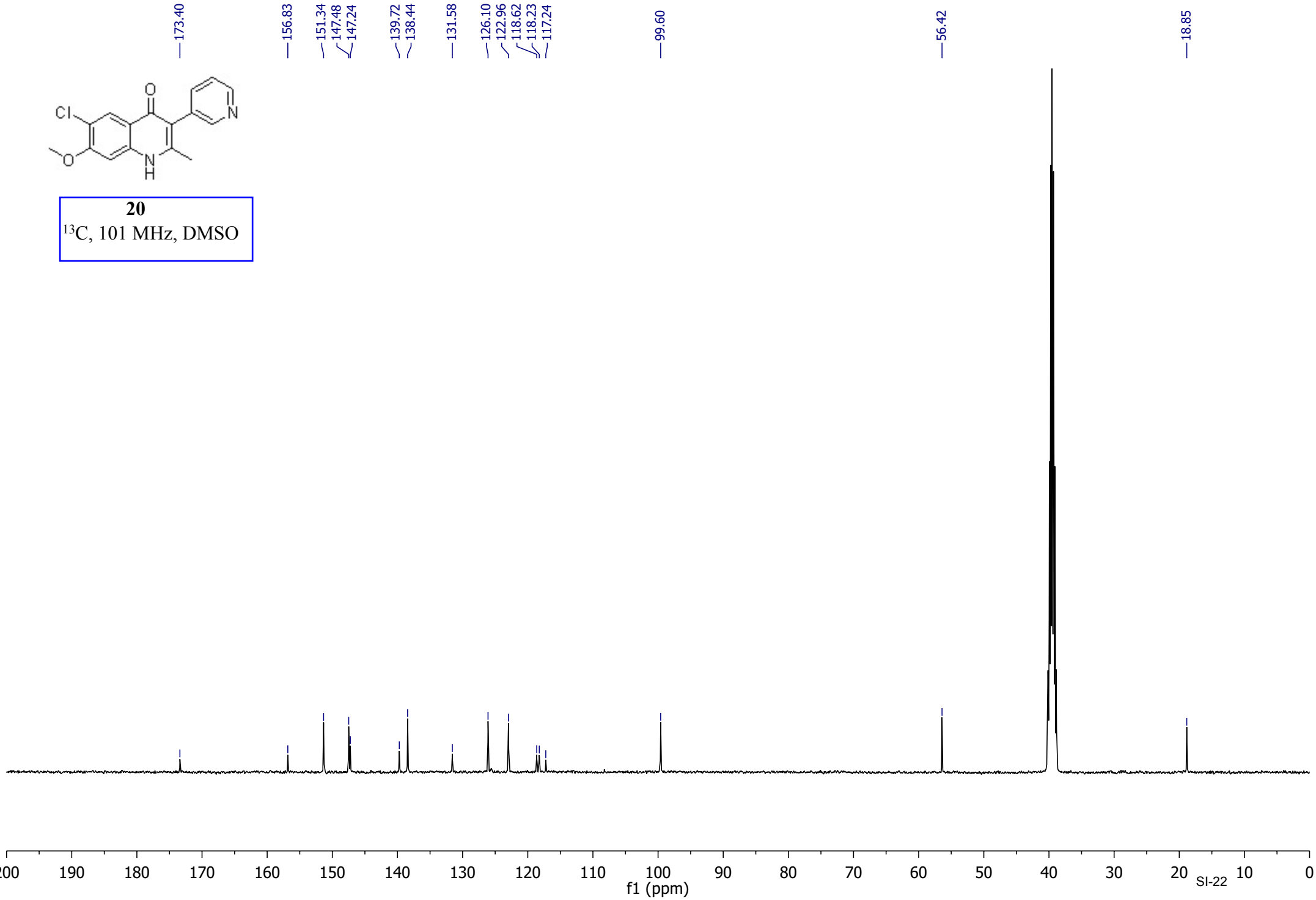


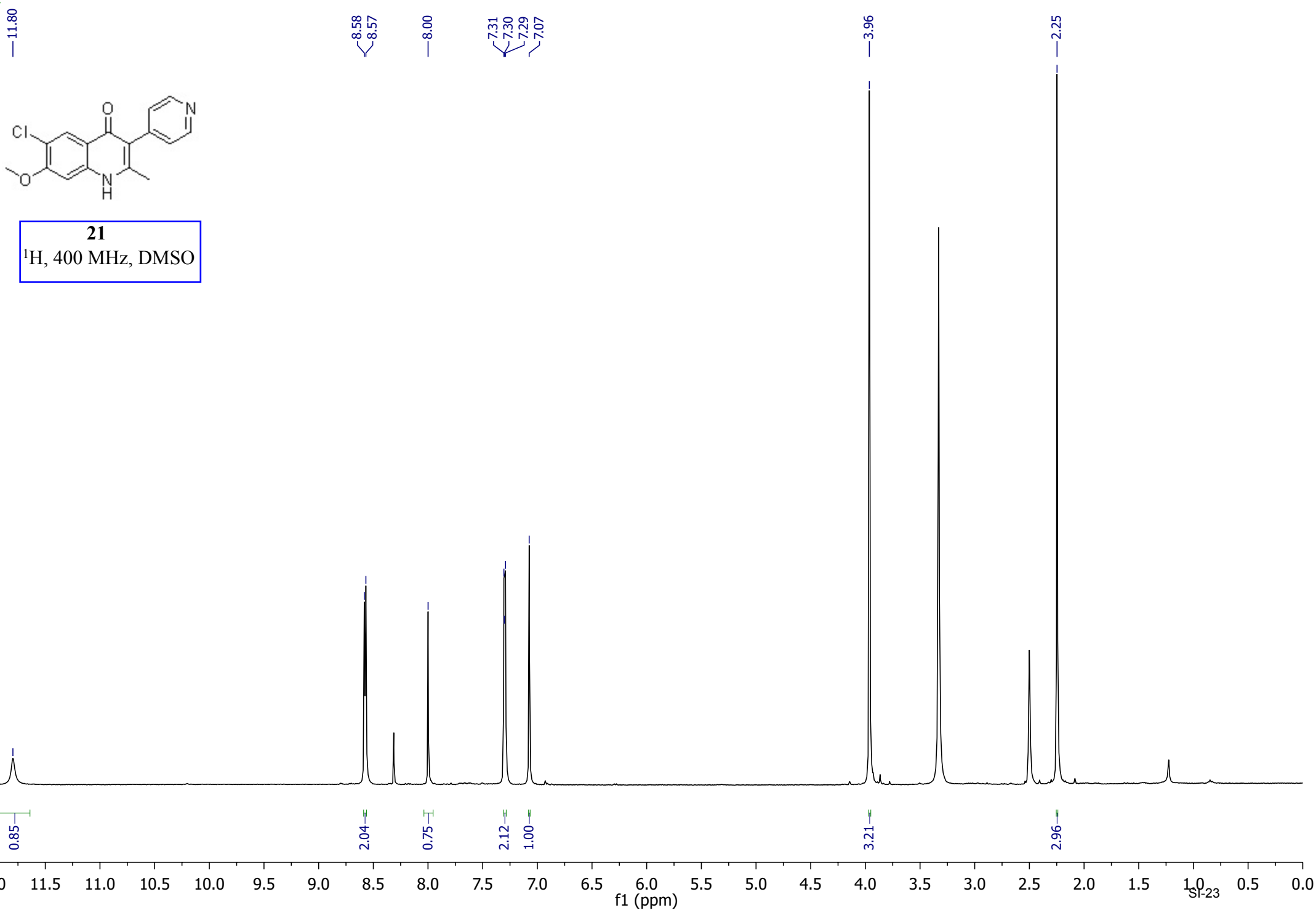
20
^{1}H, 400 MHz, DMSO

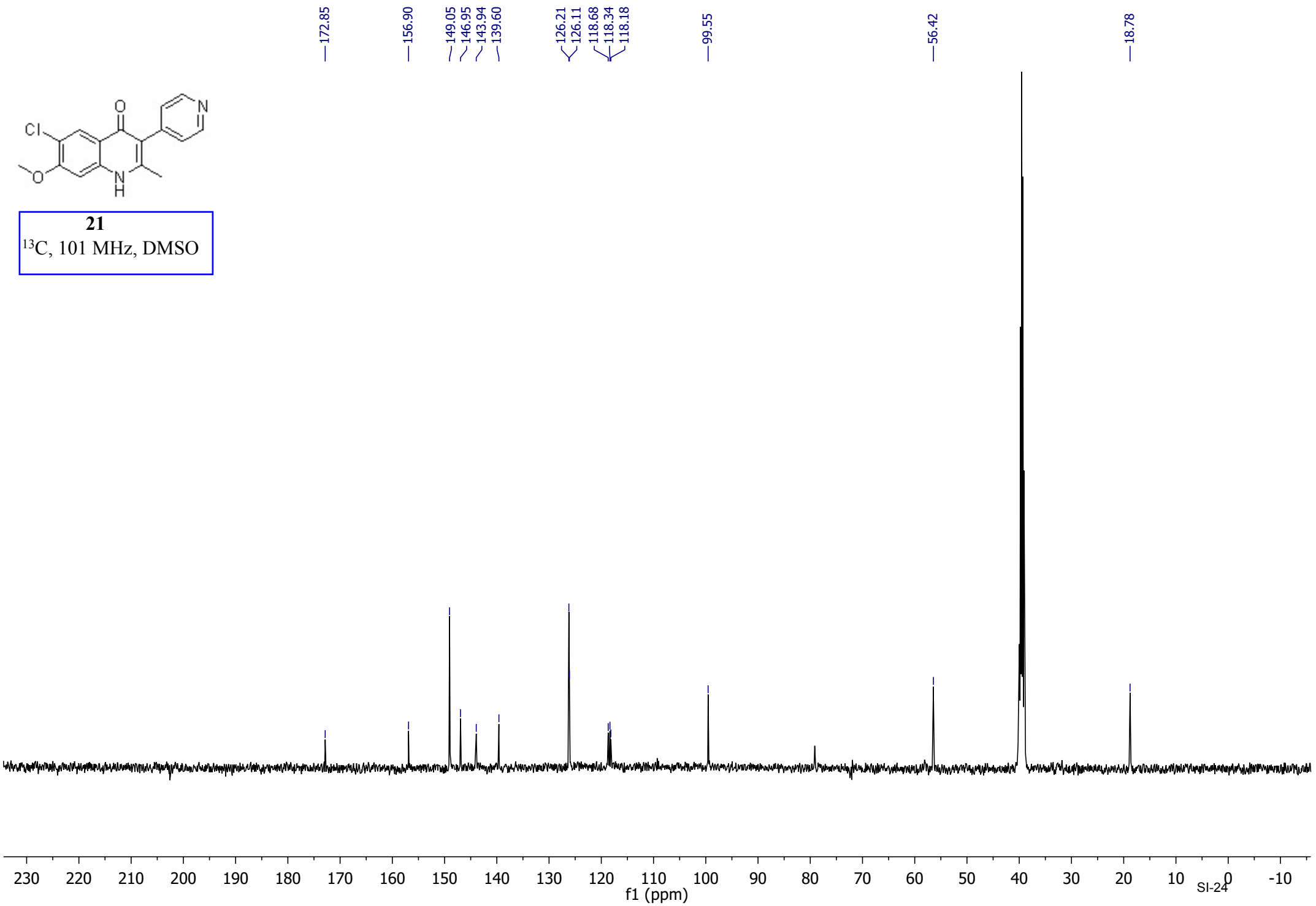


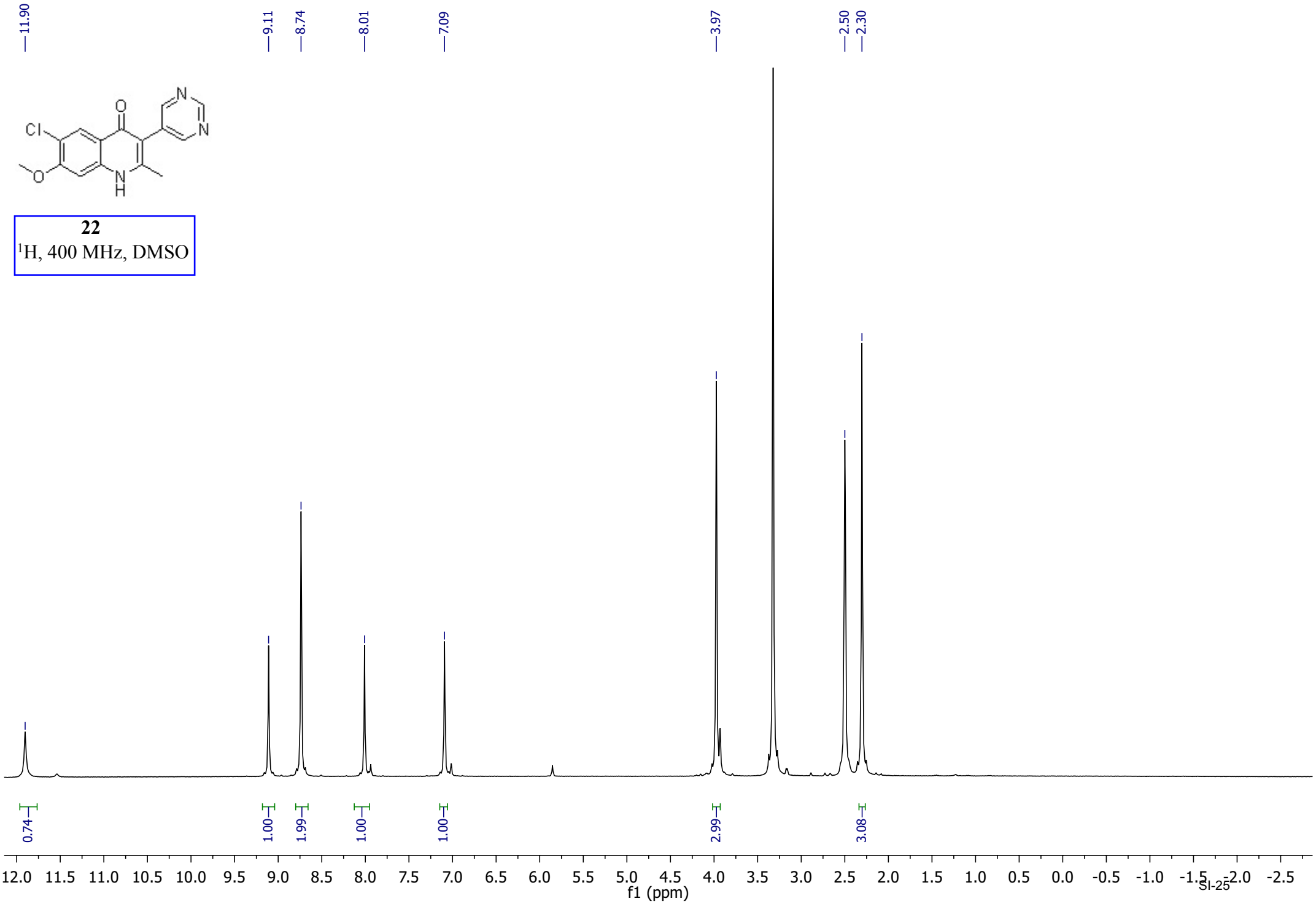
20

^{13}C, 101 MHz, DMSO



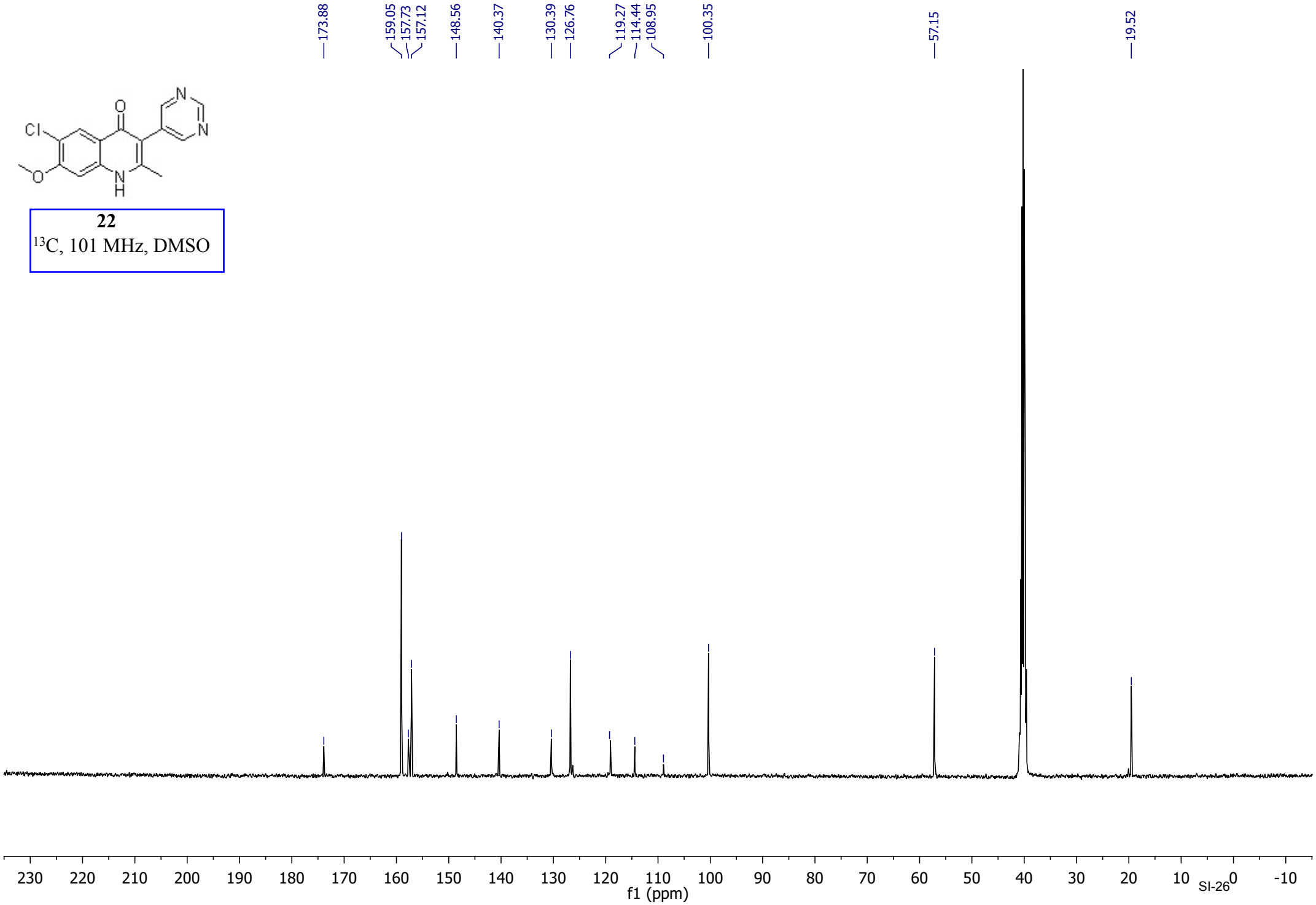

11.80
8.58
8.57
8.00
7.31
7.30
7.29
7.07
3.96
2.25
Cl
O
N
O
N
H
21
1H, 400 MHz, DMSO
0.85
2.04
0.75
2.12
1.00
3.21
2.96
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

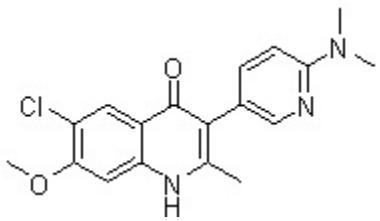

172.85
156.90
149.05
146.95
143.94
139.60
126.21
126.11
118.68
118.34
118.18
99.55
56.42
18.78
Cl
O
N
O
N
H
21
13C, 101 MHz, DMSO
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


11.90
9.11
8.74
8.01
7.09
3.97
2.50
2.30
Cl
O
N
N
O
N
H
22
1H, 400 MHz, DMSO
0.74
1.00
1.99
1.00
1.00
2.99
3.08
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5
f1 (ppm)

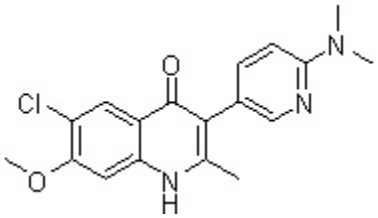
22

^{13}C, 101 MHz, DMSO



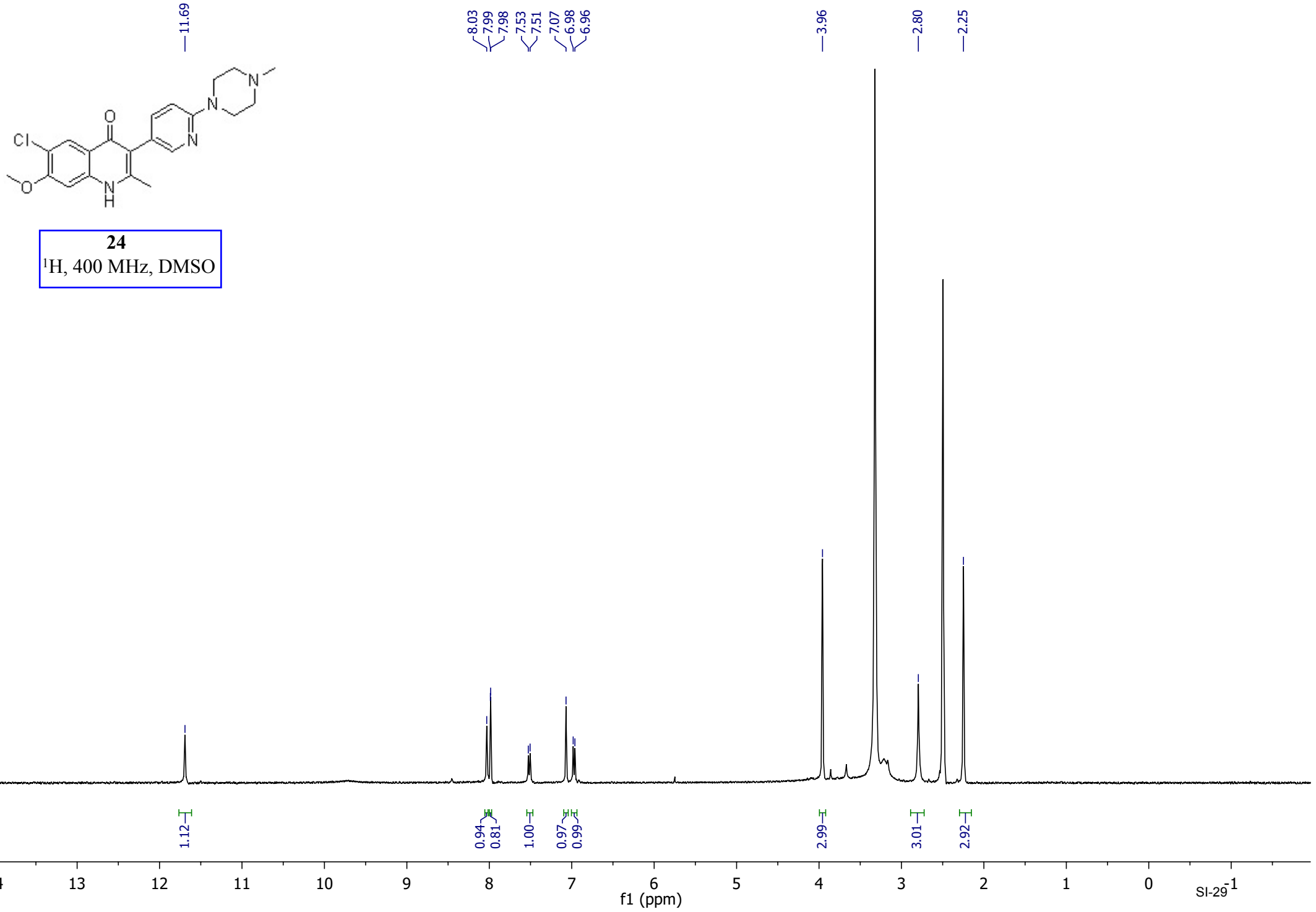


23
^{1}H, 400 MHz, DMSO



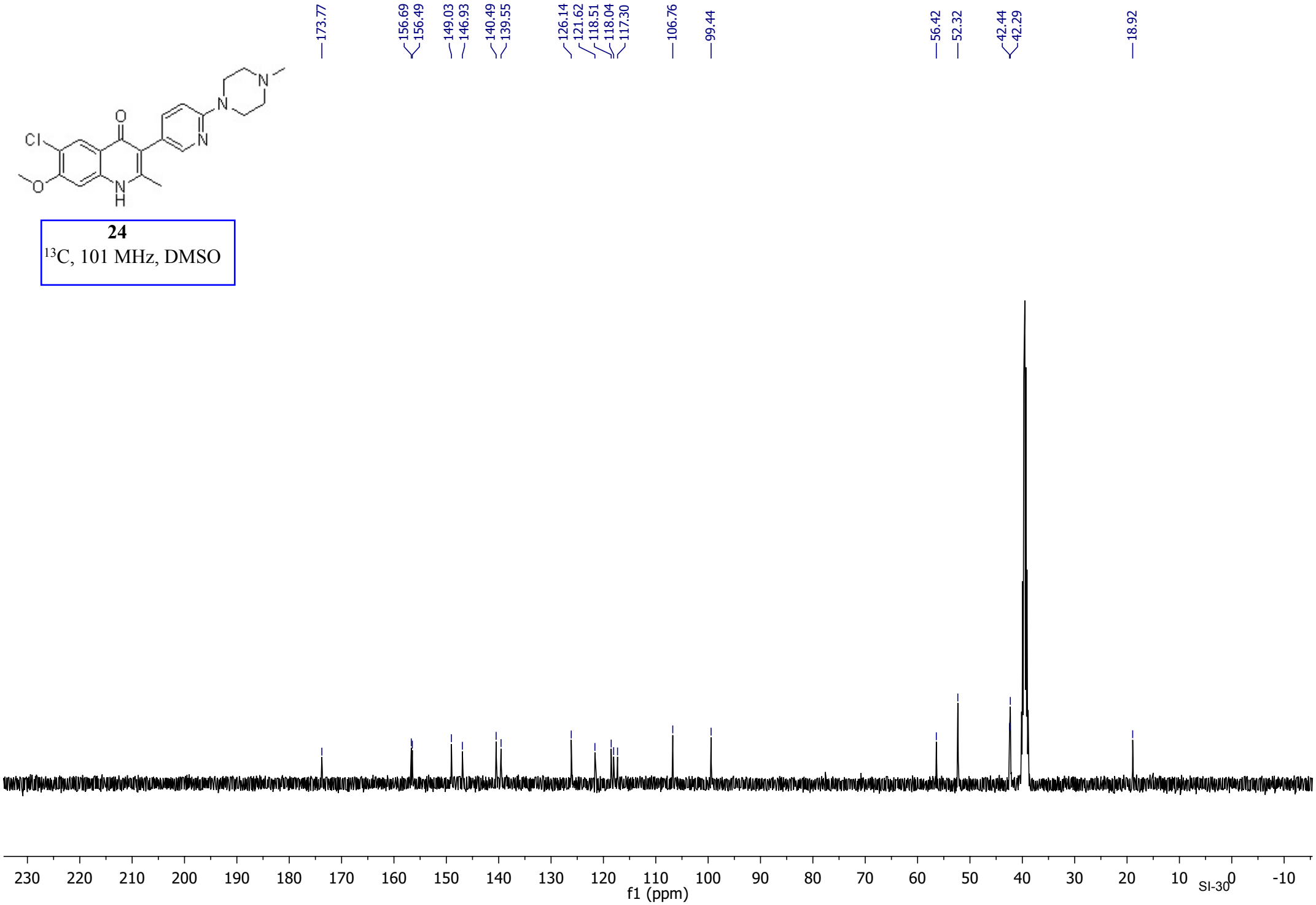
23

^{13}C, 101 MHz, DMSO

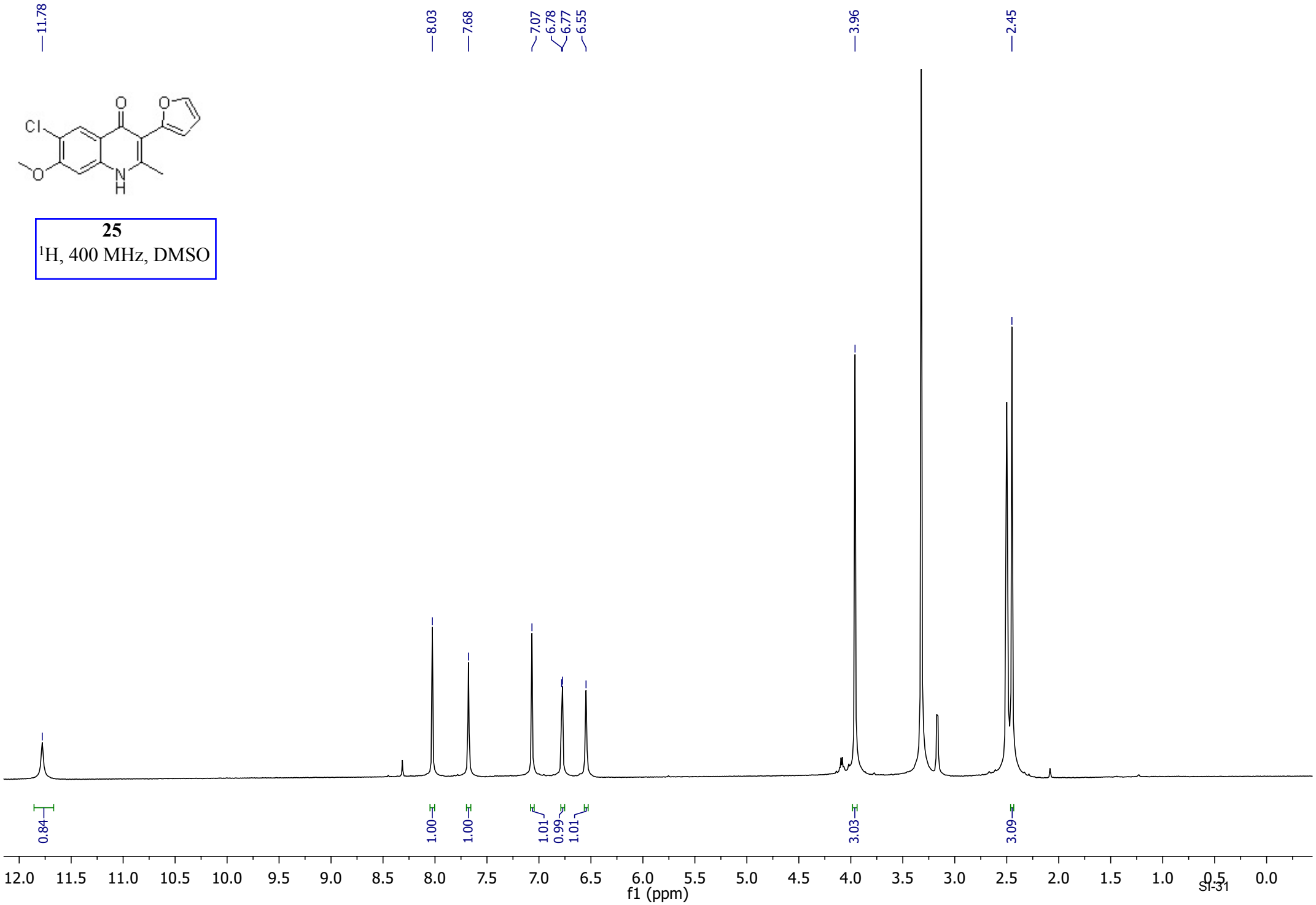

11.69
8.03
7.99
7.98
7.53
7.51
7.07
6.98
6.96
3.96
2.80
2.25
Cl
O
N
N
O
N
H
24
1H, 400 MHz, DMSO
1.12
0.94
0.81
1.00
0.97
0.99
2.99
3.01
2.92
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)
SI-29

24

^{13}C, 101 MHz, DMSO

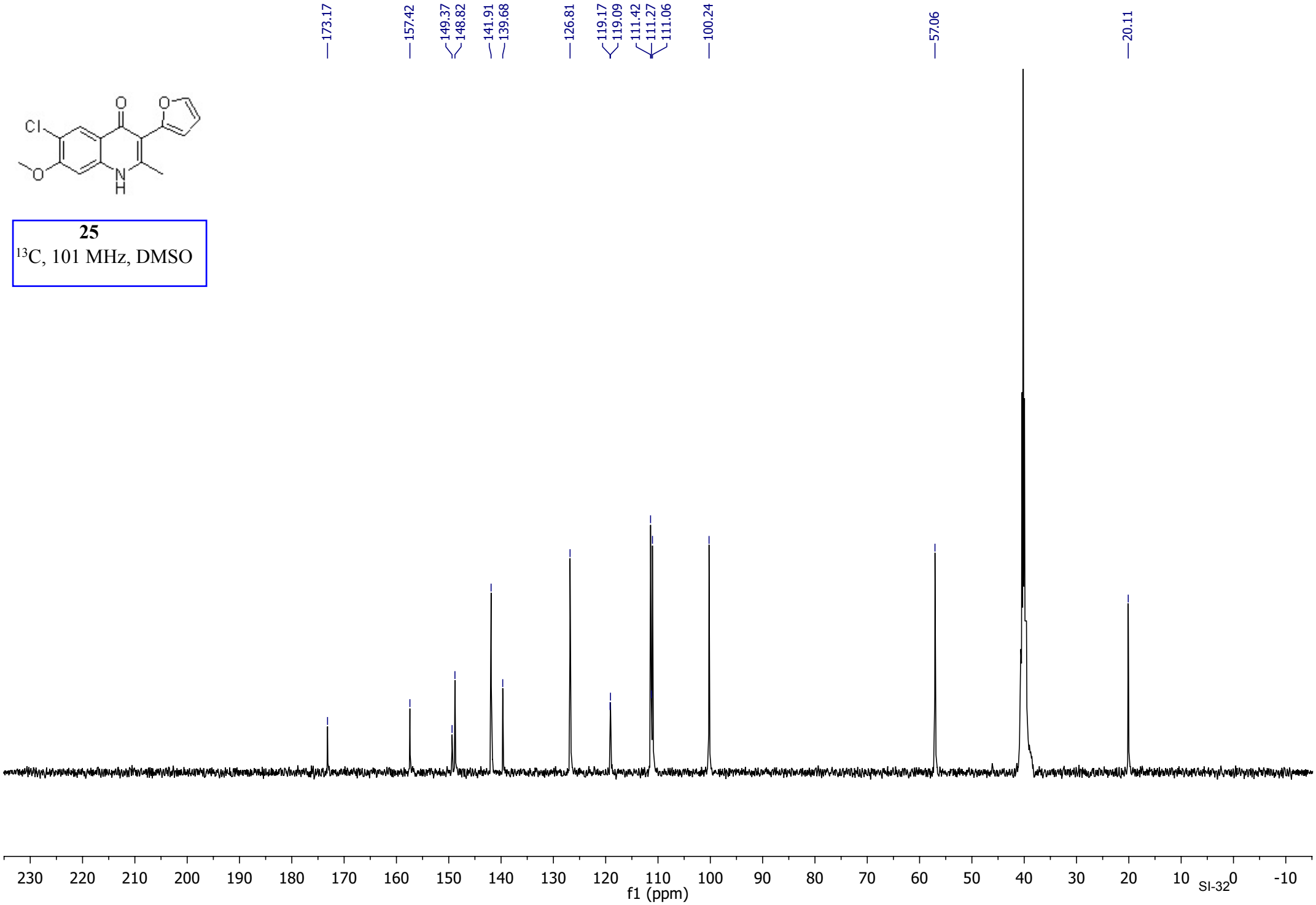


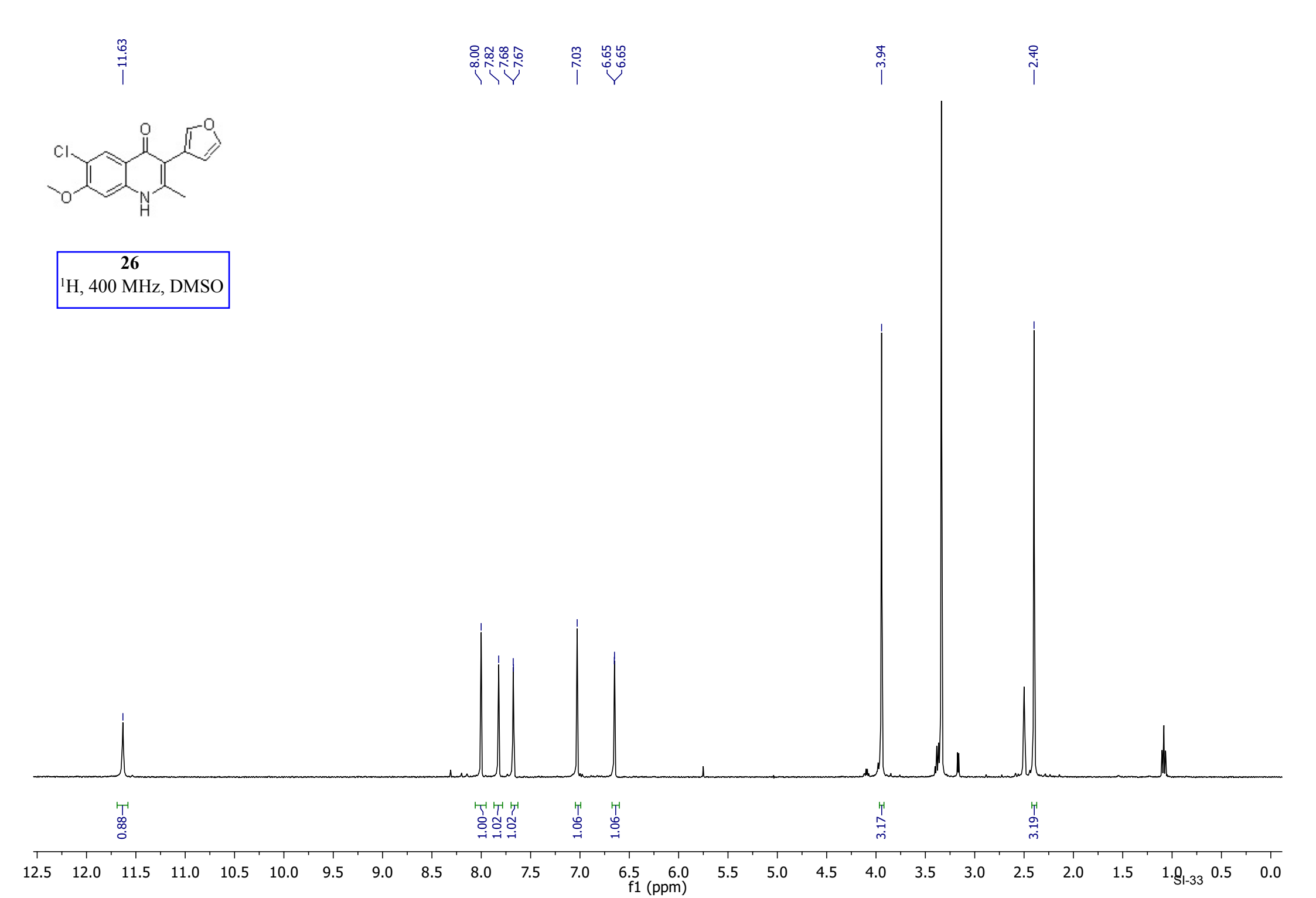
25
^{1}H, 400 MHz, DMSO



25

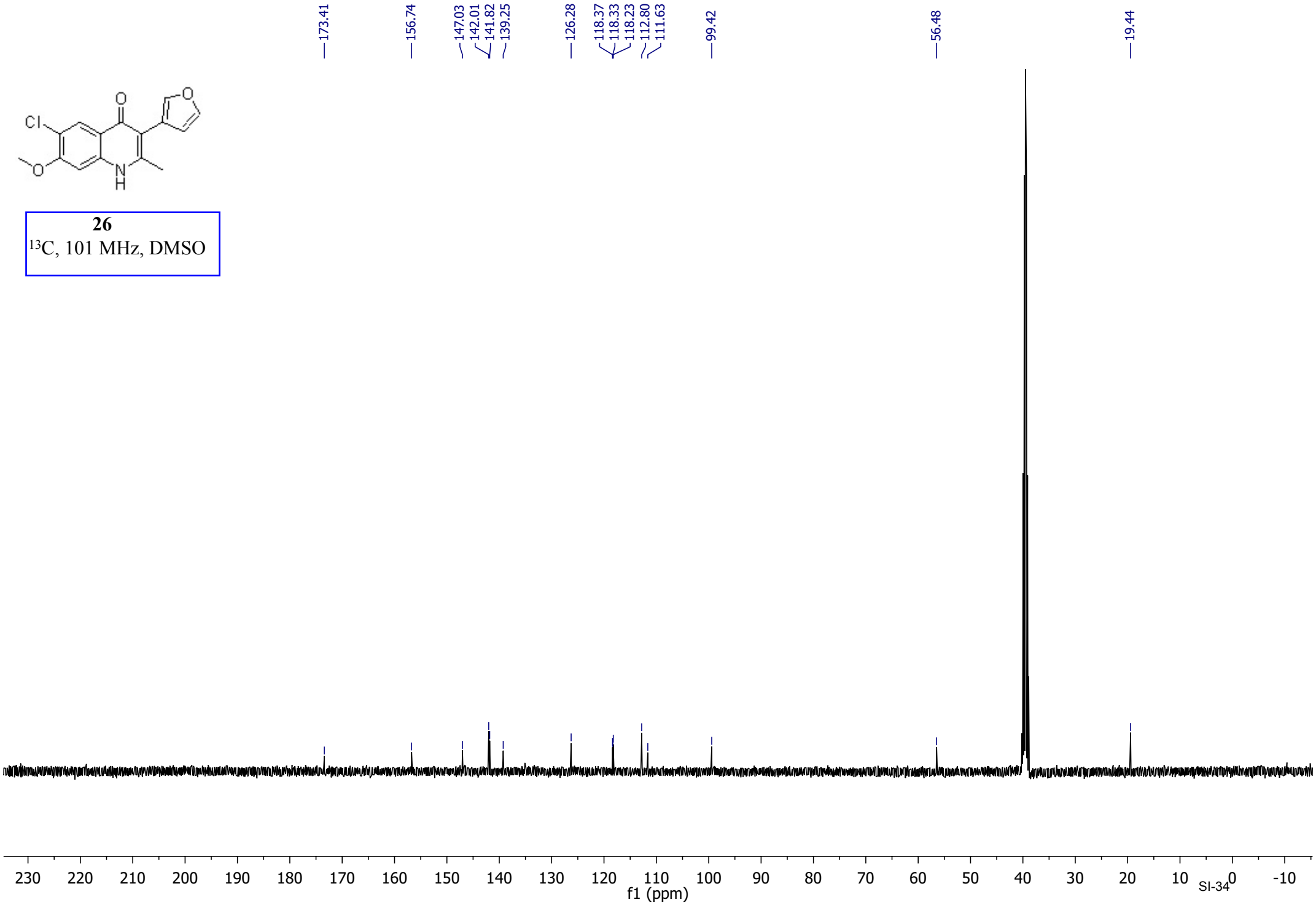
^{13}C, 101 MHz, DMSO



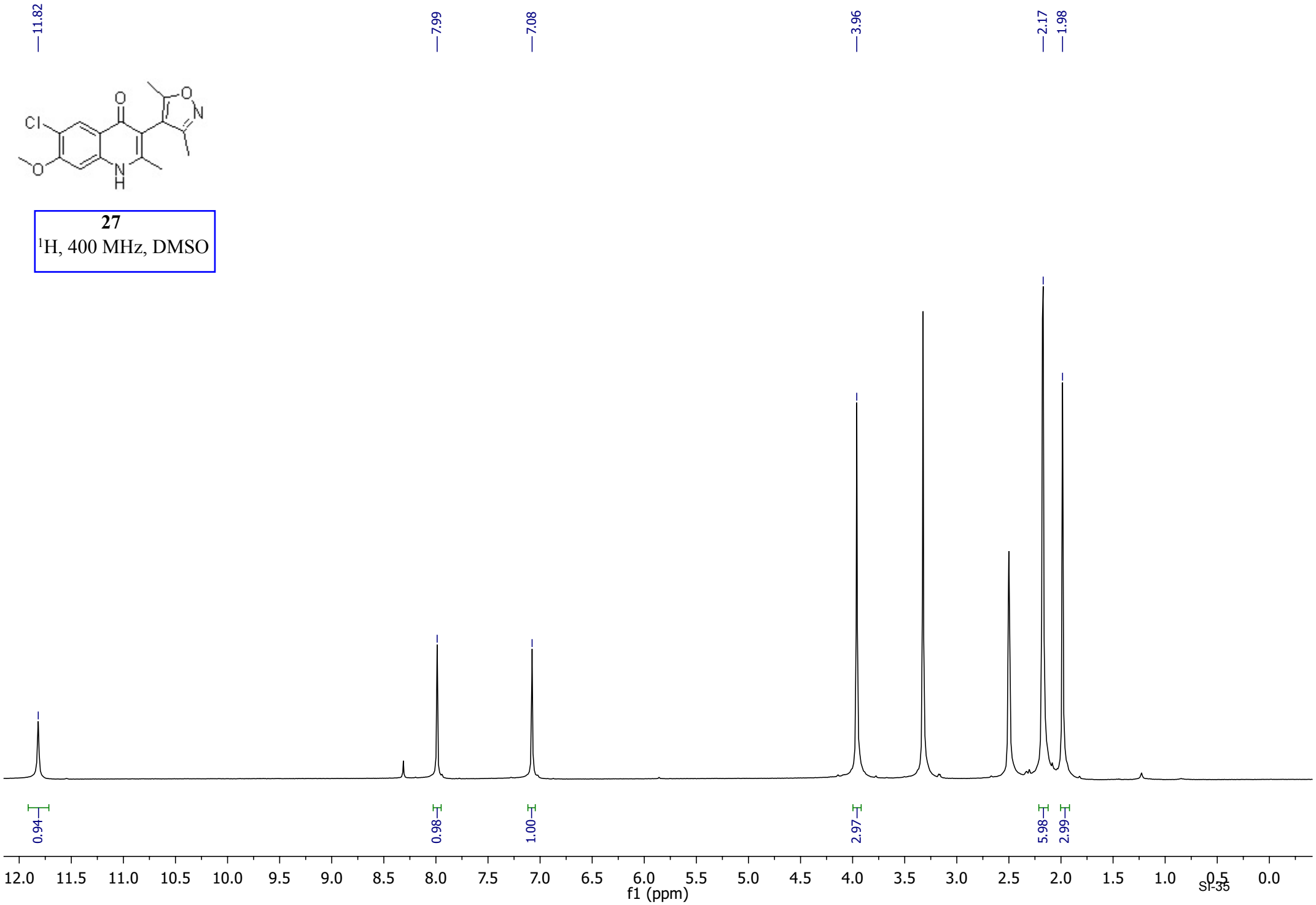

11.63
8.00
7.82
7.68
7.67
7.03
6.65
6.65
3.94
2.40
Cl
O
O
O
N
H
26
1H, 400 MHz, DMSO
0.88
1.00
1.02
1.02
1.06
1.06
3.17
3.19
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

26

^{13}C, 101 MHz, DMSO

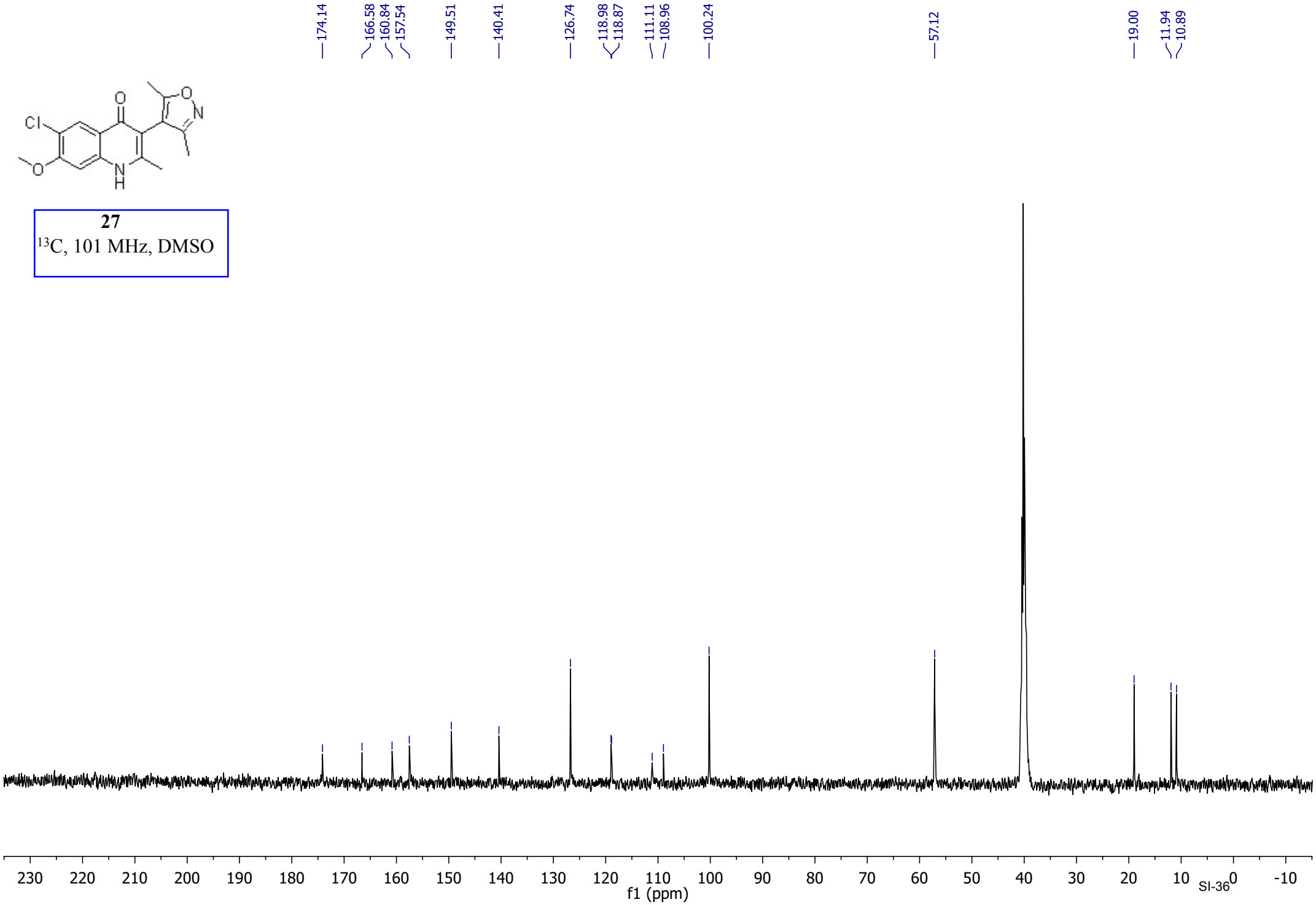


27
^{1}H, 400 MHz, DMSO

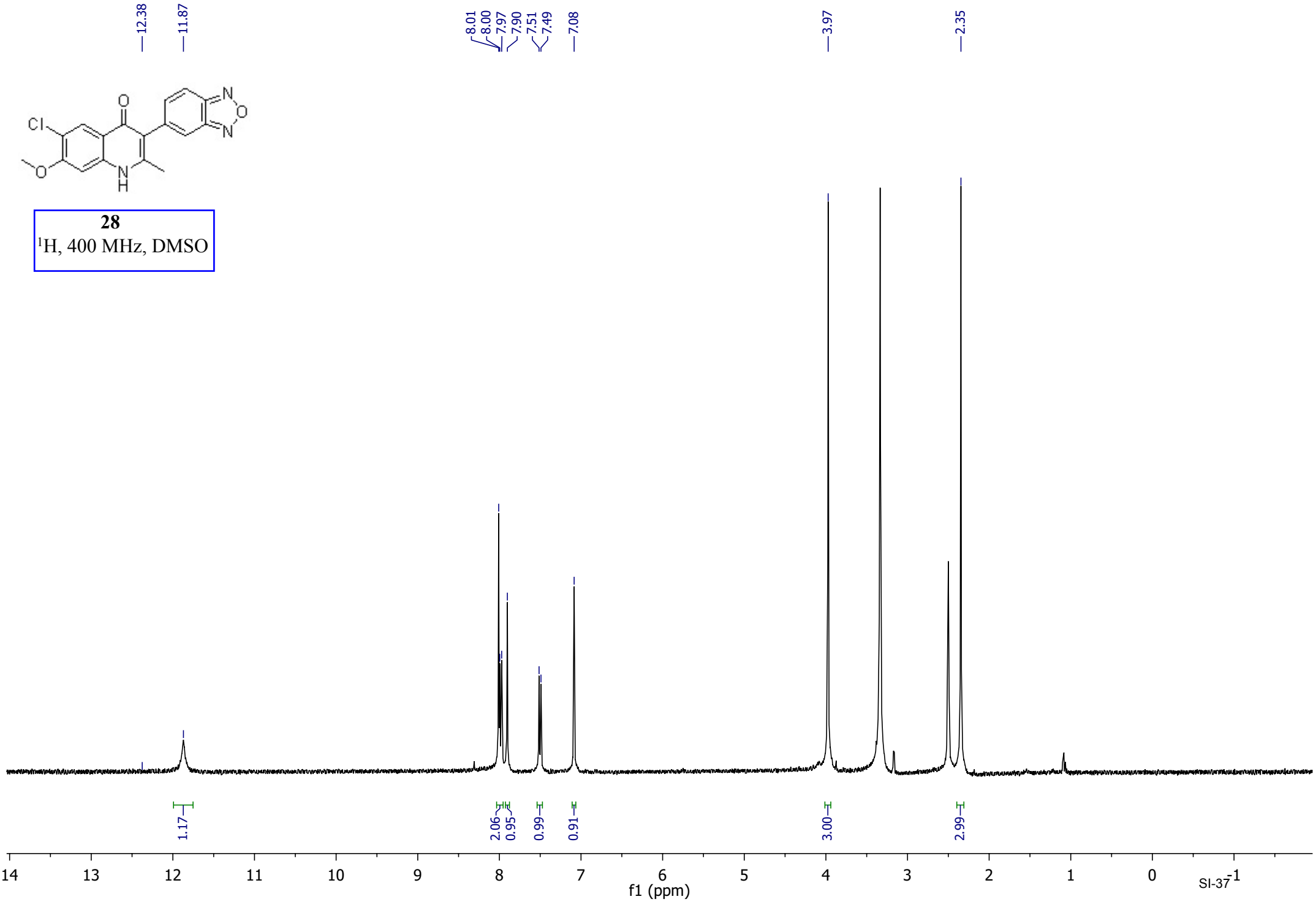


27

^{13}C, 101 MHz, DMSO

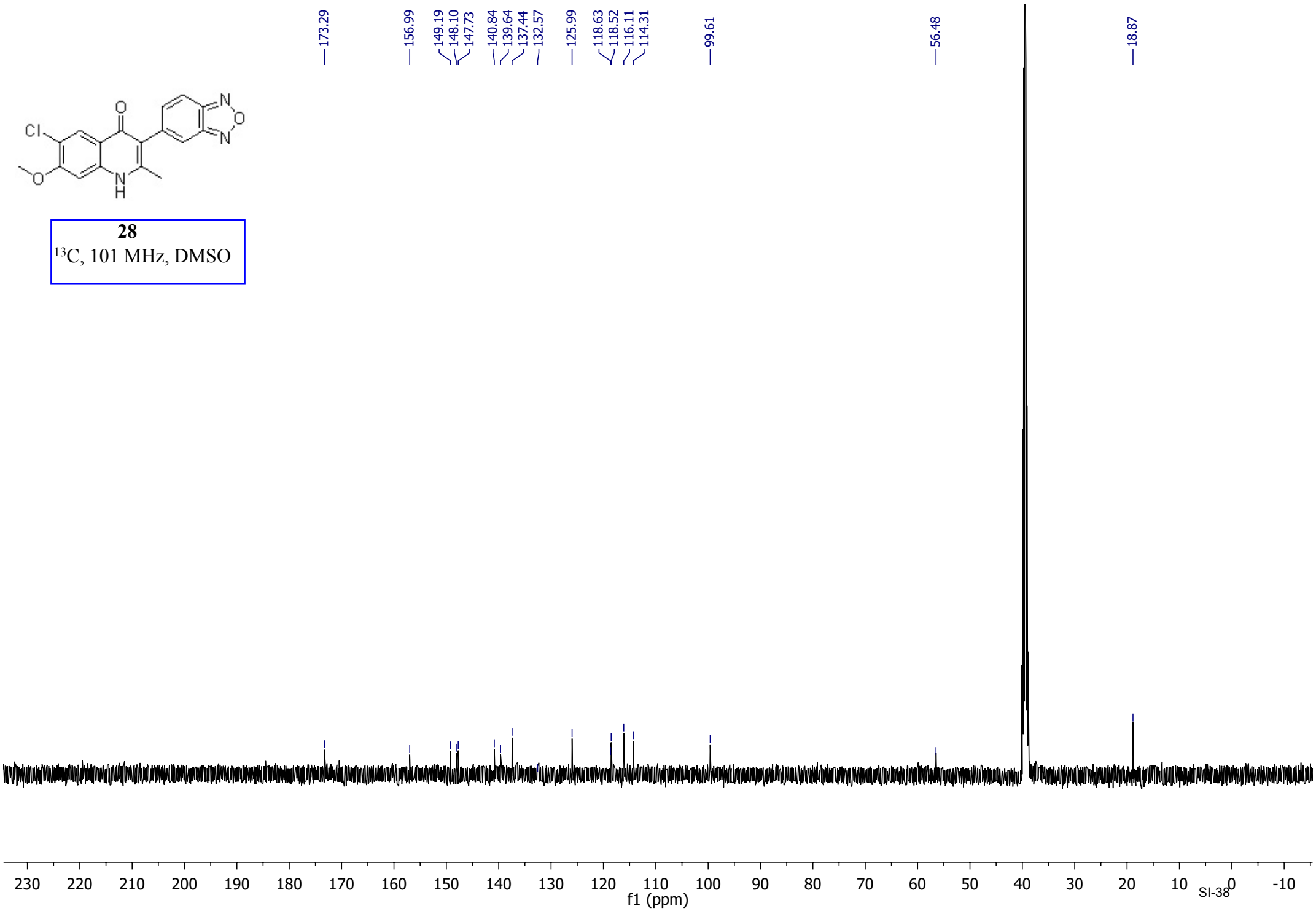


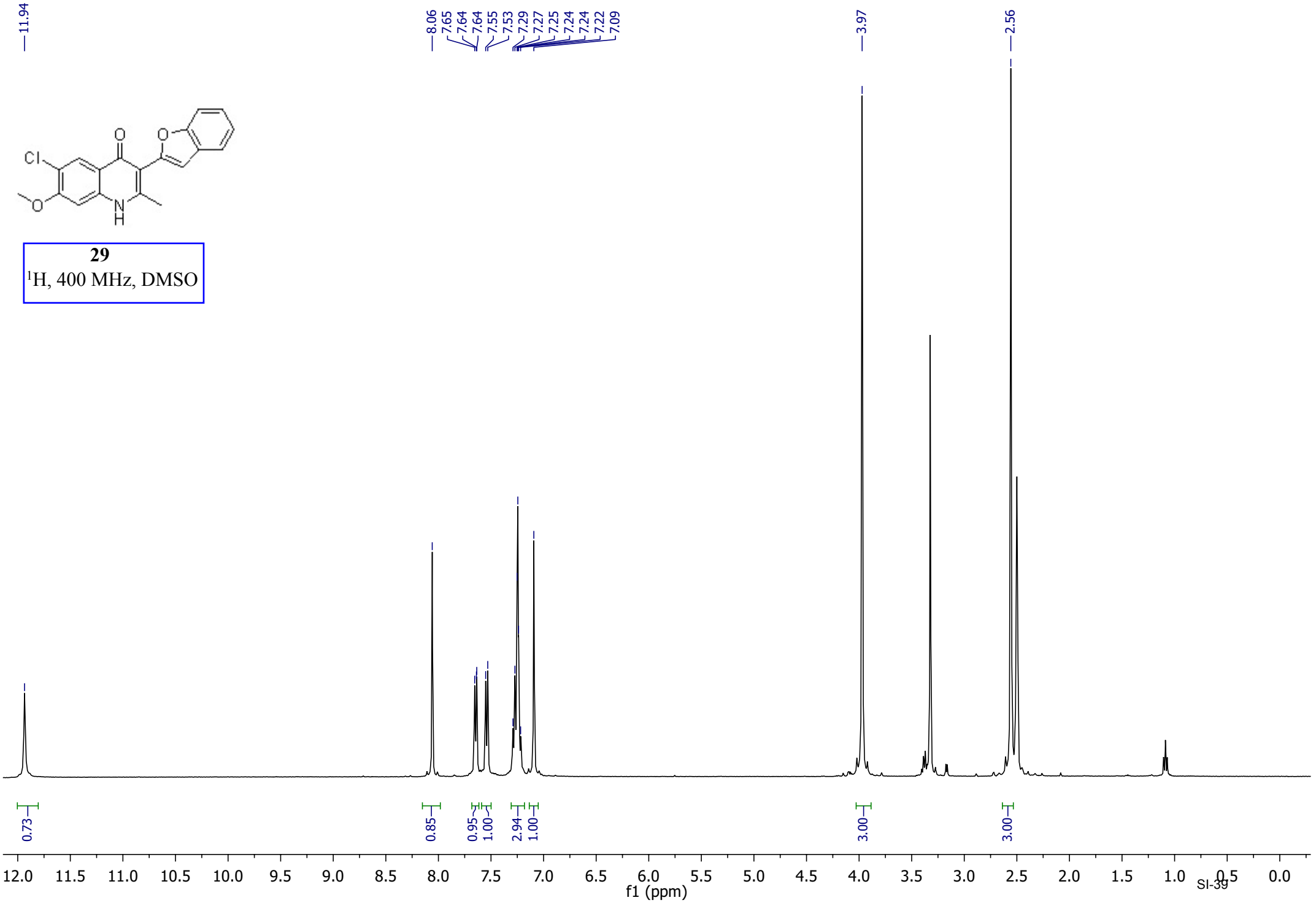
28
^{1}H, 400 MHz, DMSO



28

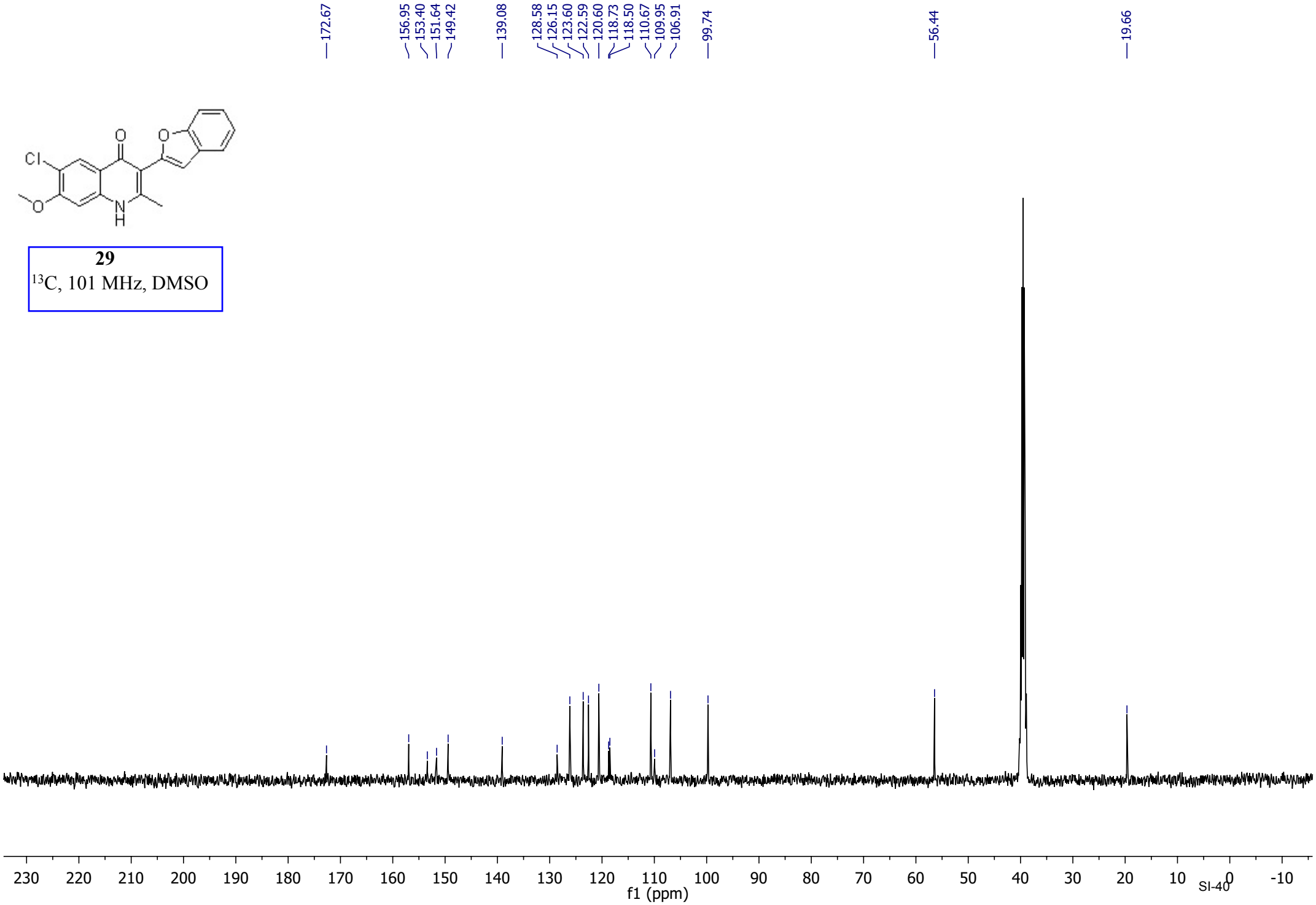
^{13}C, 101 MHz, DMSO



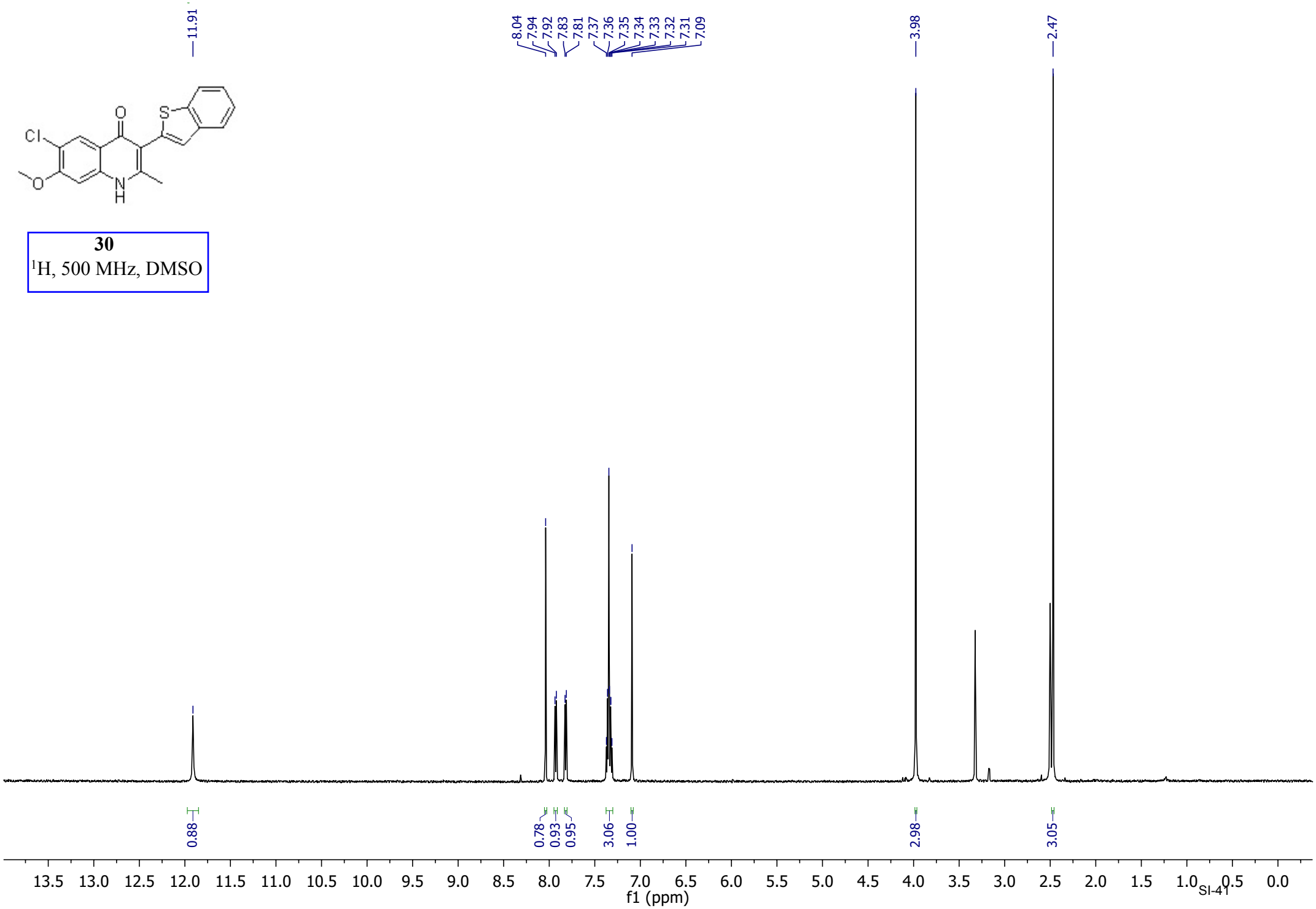

11.94
8.06
7.65
7.64
7.64
7.55
7.53
7.29
7.27
7.25
7.24
7.24
7.22
7.09
3.97
2.56
Cl
O
O
O
N
H
29
1H, 400 MHz, DMSO
0.73
0.85
0.95
1.00
2.94
1.00
3.00
3.00
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

29

^{13}C, 101 MHz, DMSO

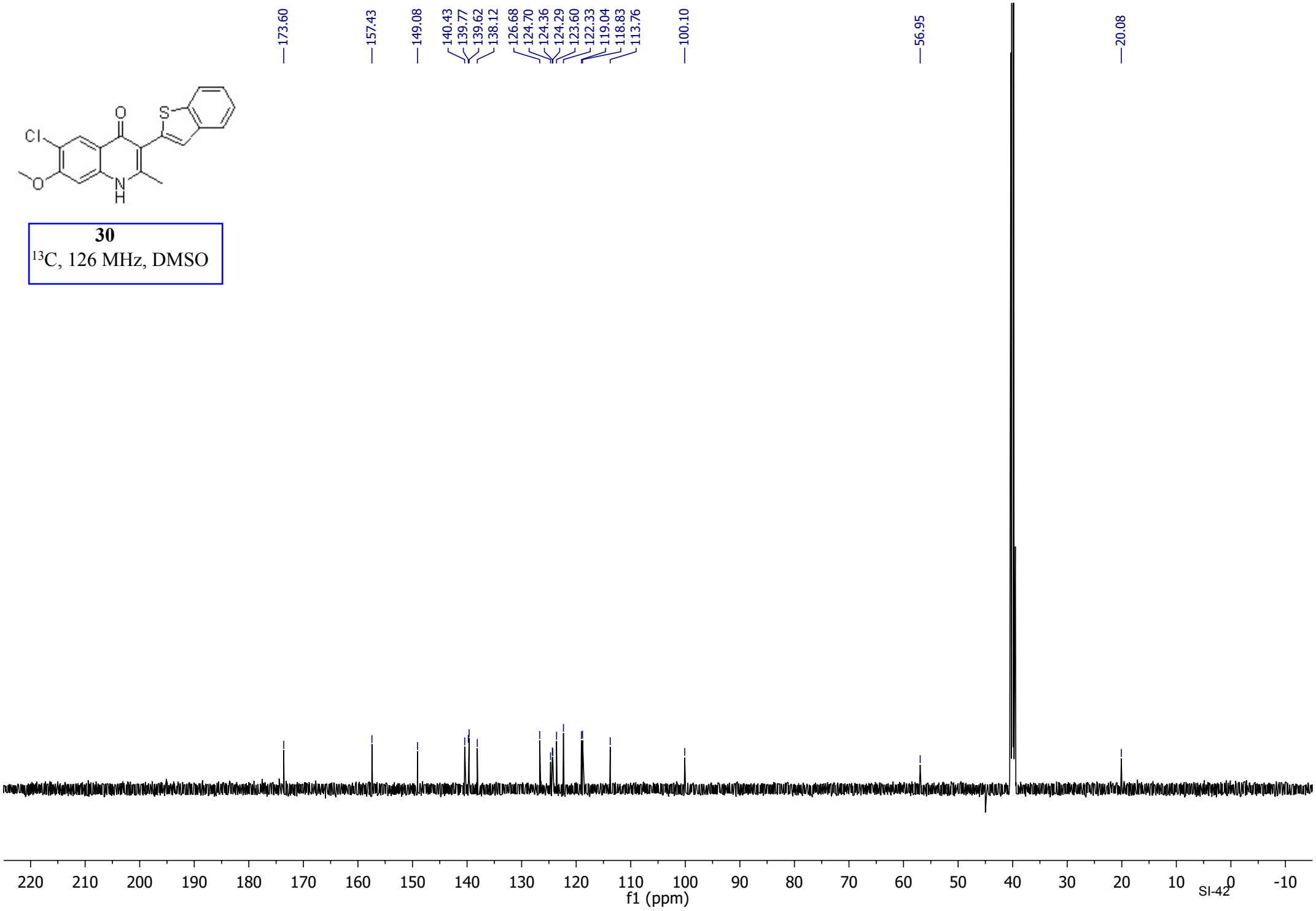


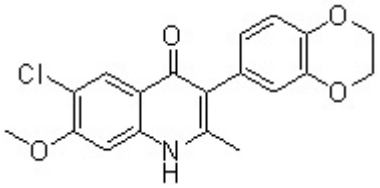
30
^{1}H, 500 MHz, DMSO



30

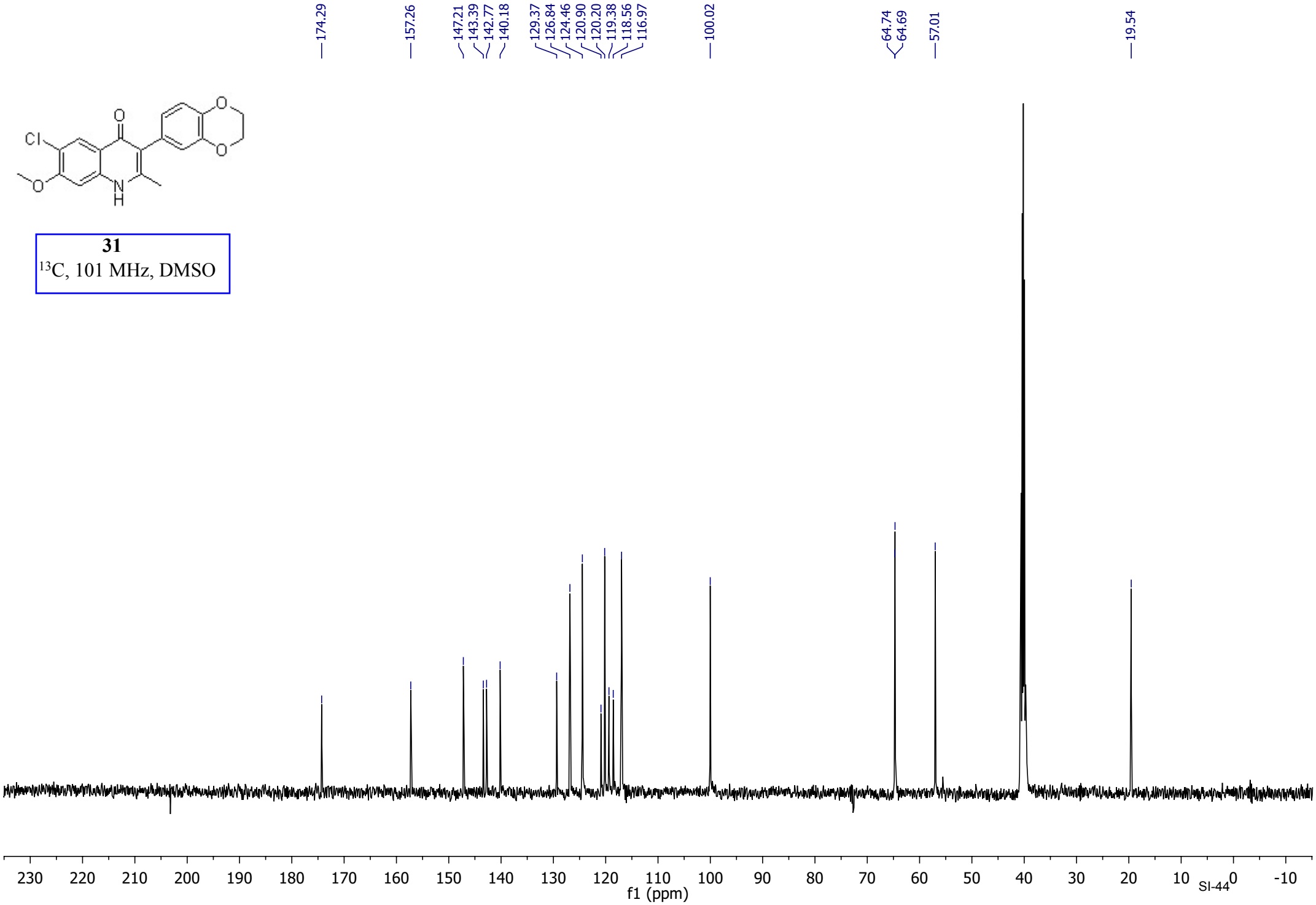
^{13}C, 126 MHz, DMSO



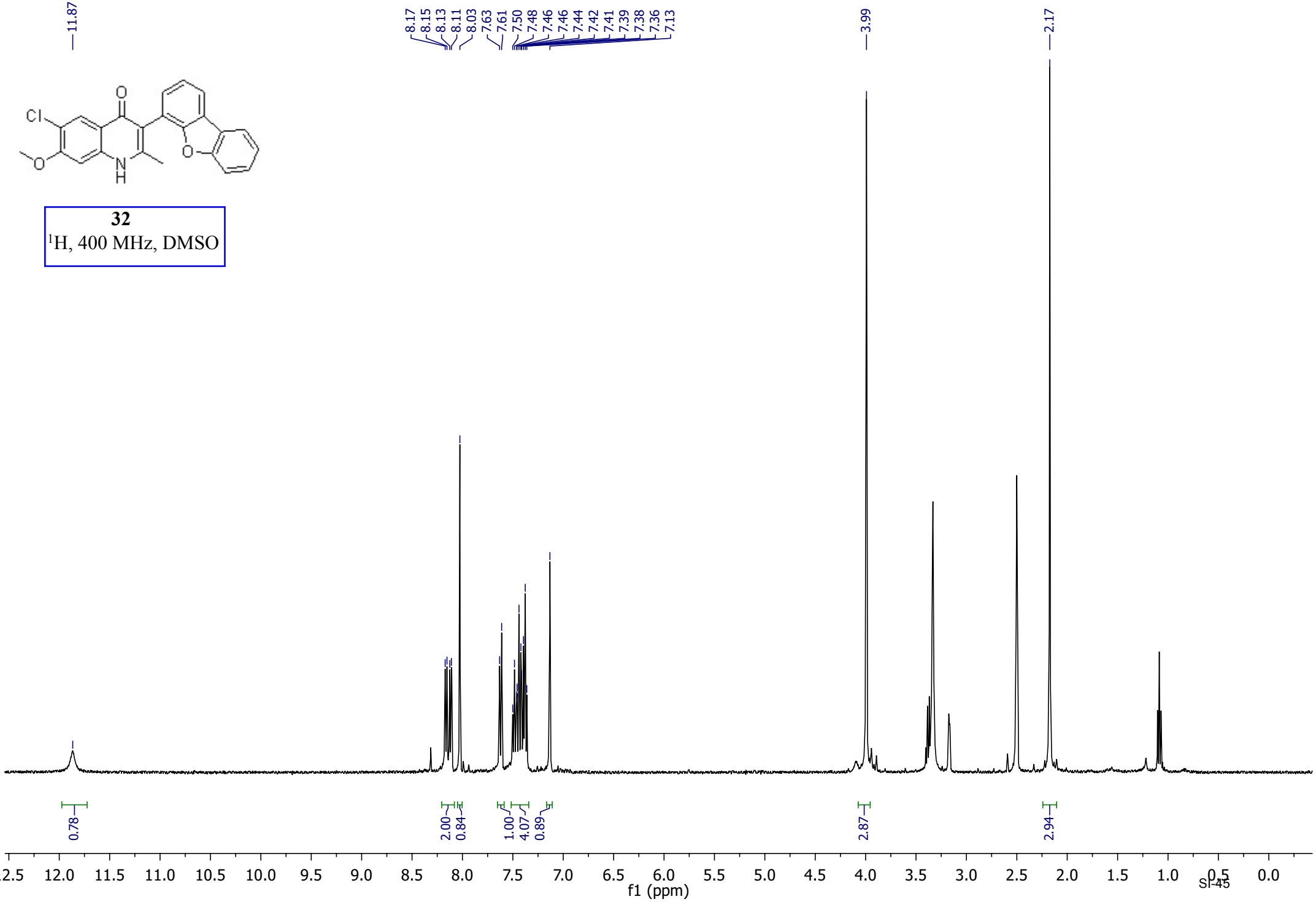


31
^{1}H, 400 MHz, DMSO

31
^{13}C, 101 MHz, DMSO

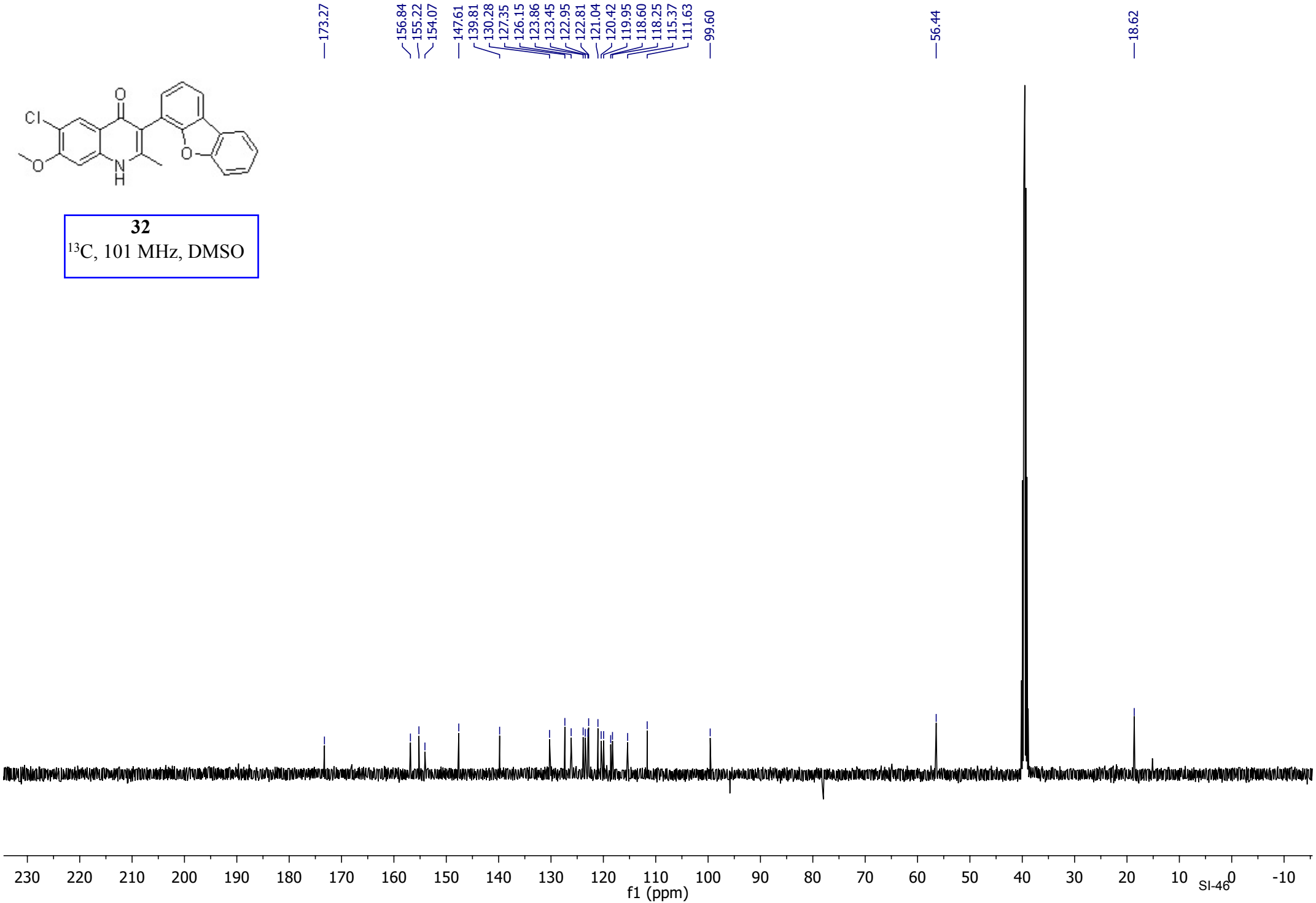


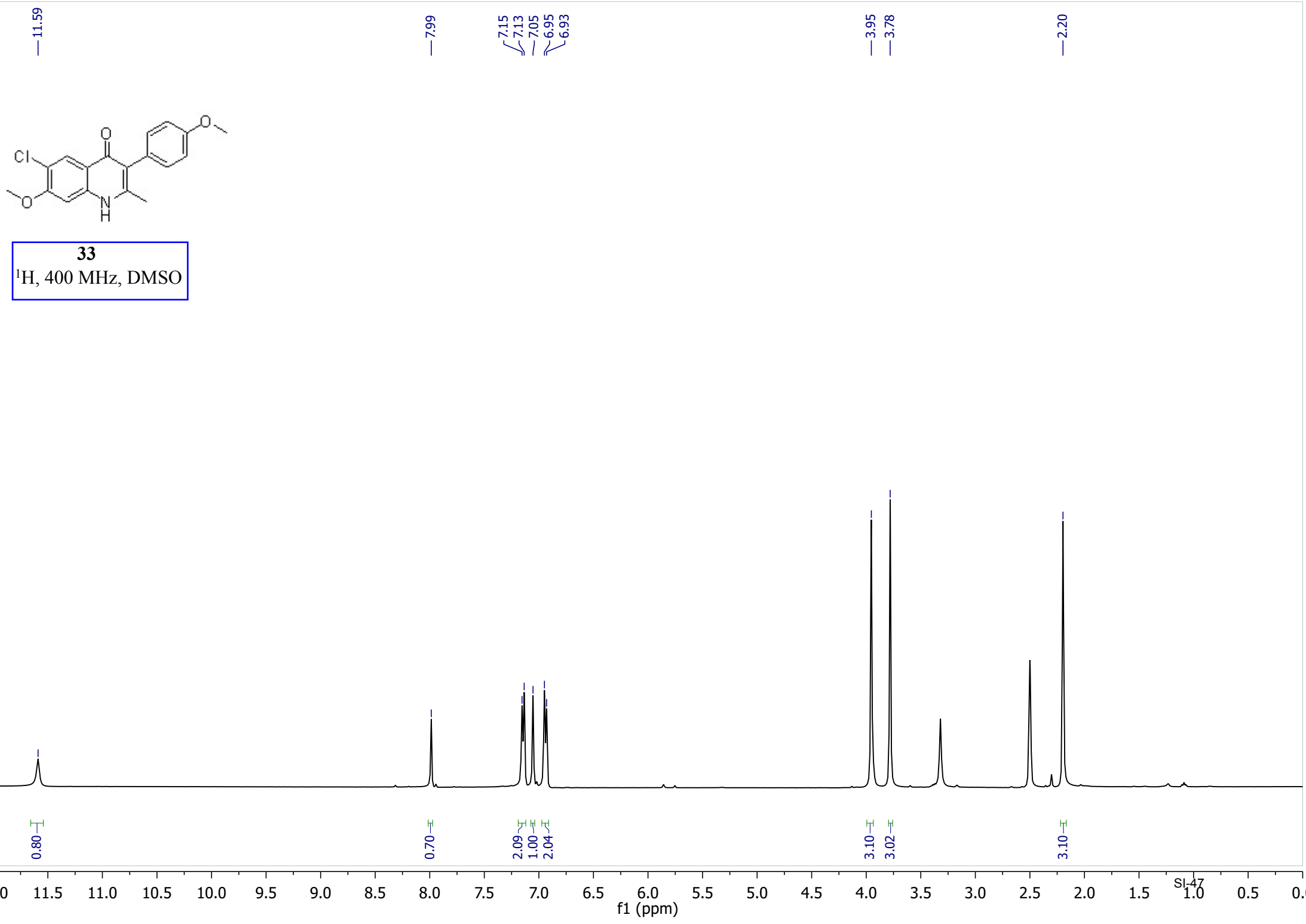
32
^{1}H, 400 MHz, DMSO



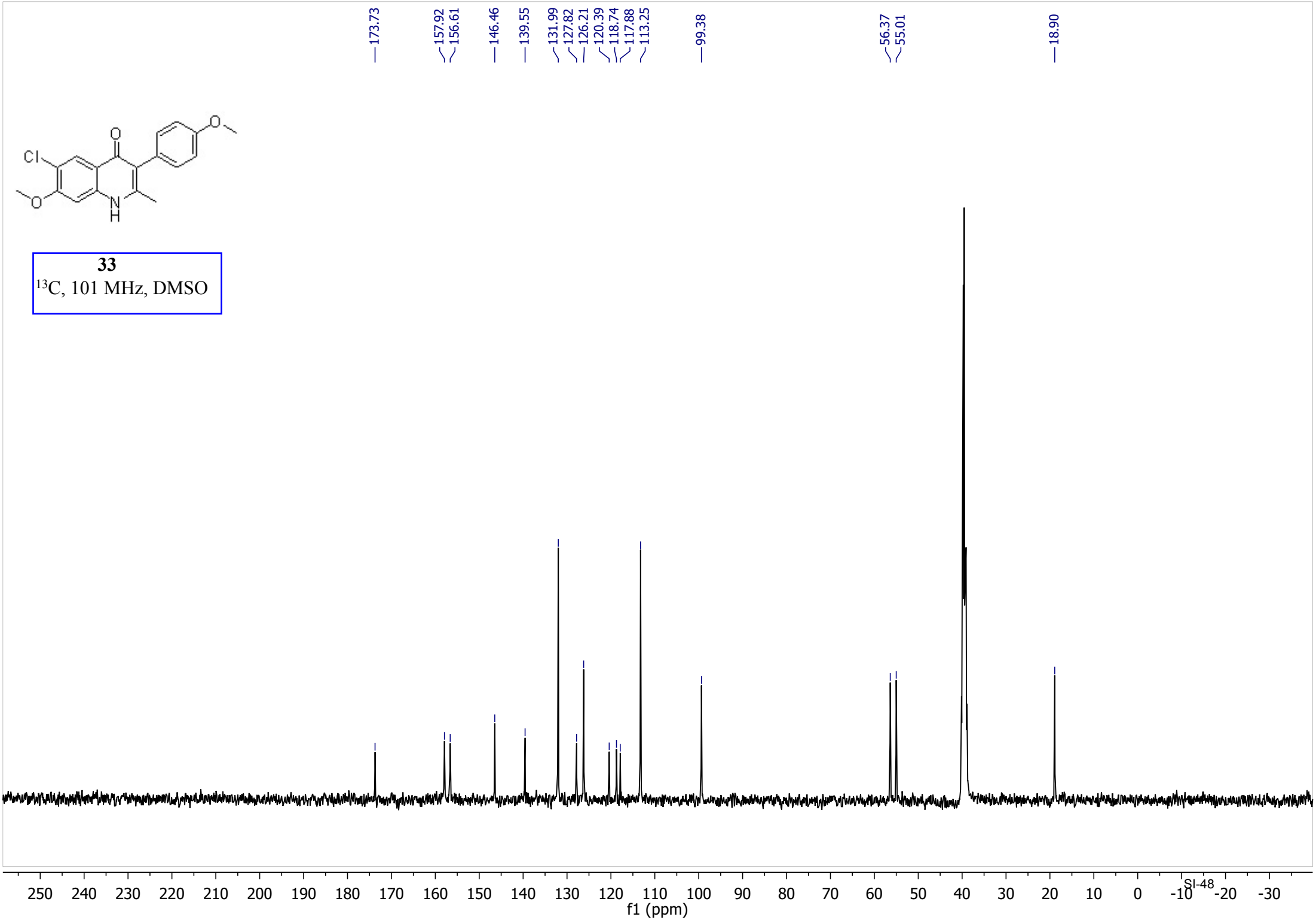
32

^{13}C, 101 MHz, DMSO

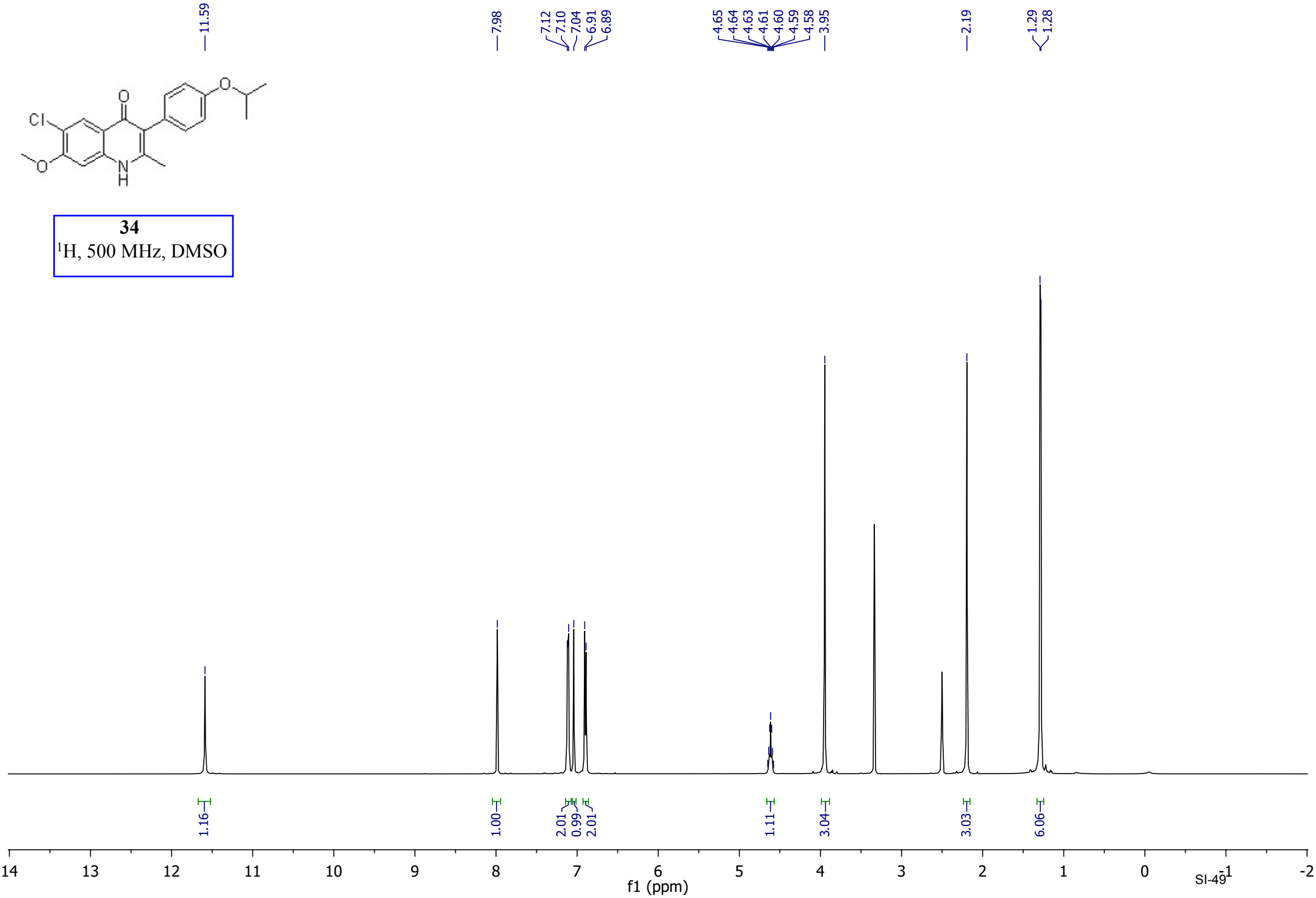




33
^{1}H, 400 MHz, DMSO

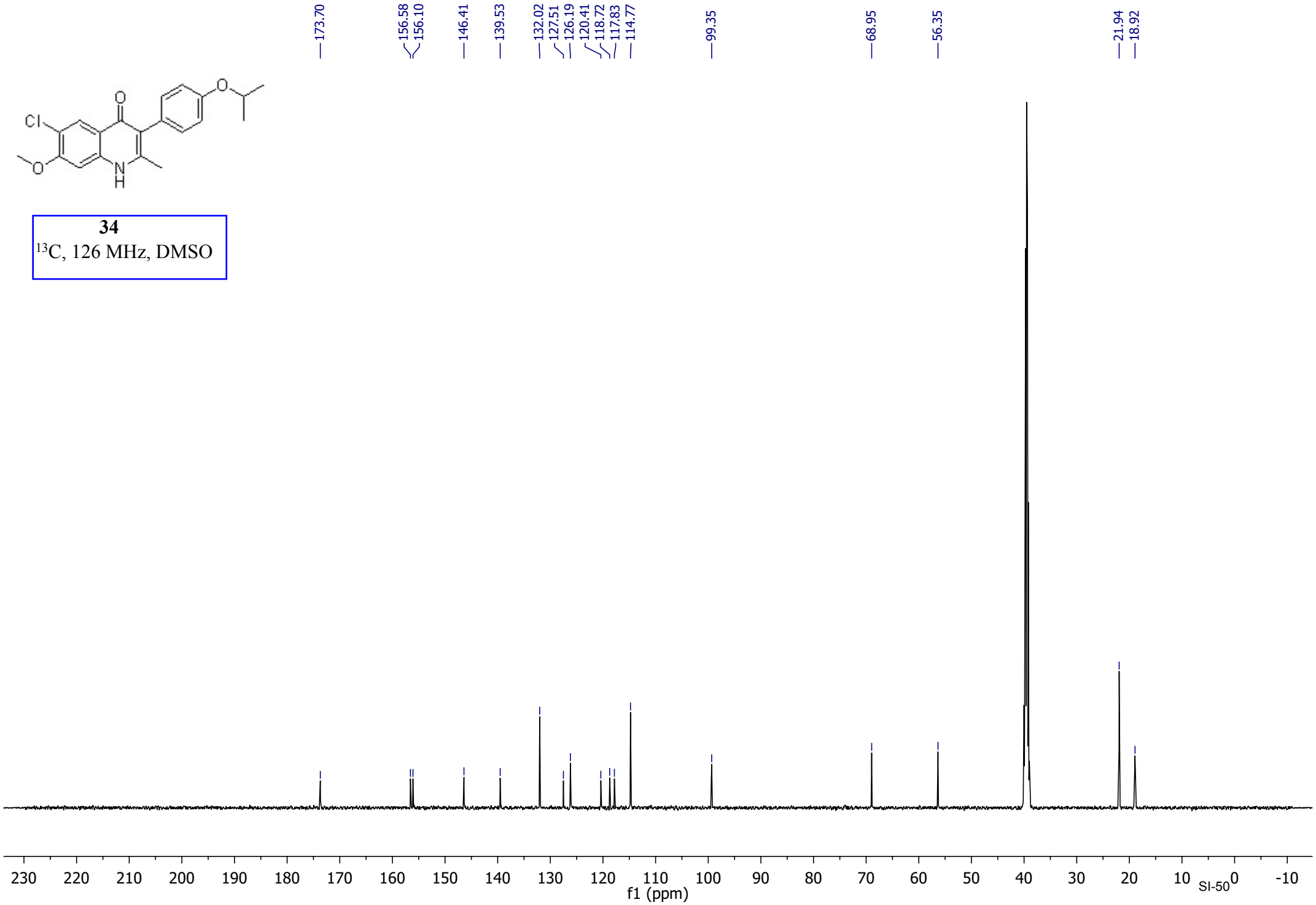

173.73
157.92
156.61
146.46
139.55
131.99
127.82
126.21
120.39
118.74
117.88
113.25
99.38
56.37
55.01
18.90
Cl
O
O
O
N
H
33
13C, 101 MHz, DMSO
250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30
f1 (ppm)

34
^{1}H, 500 MHz, DMSO



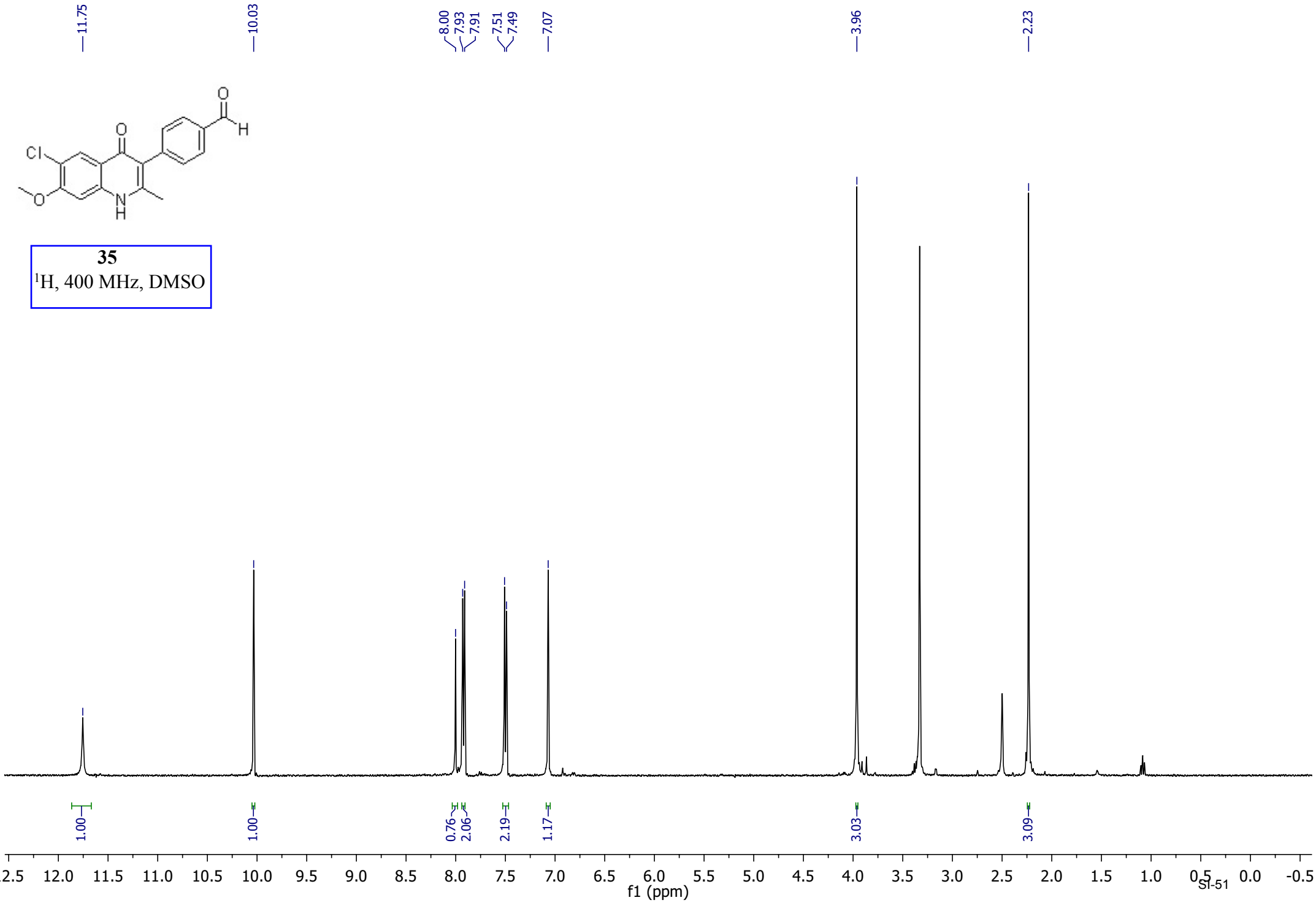
34

^{13}C, 126 MHz, DMSO



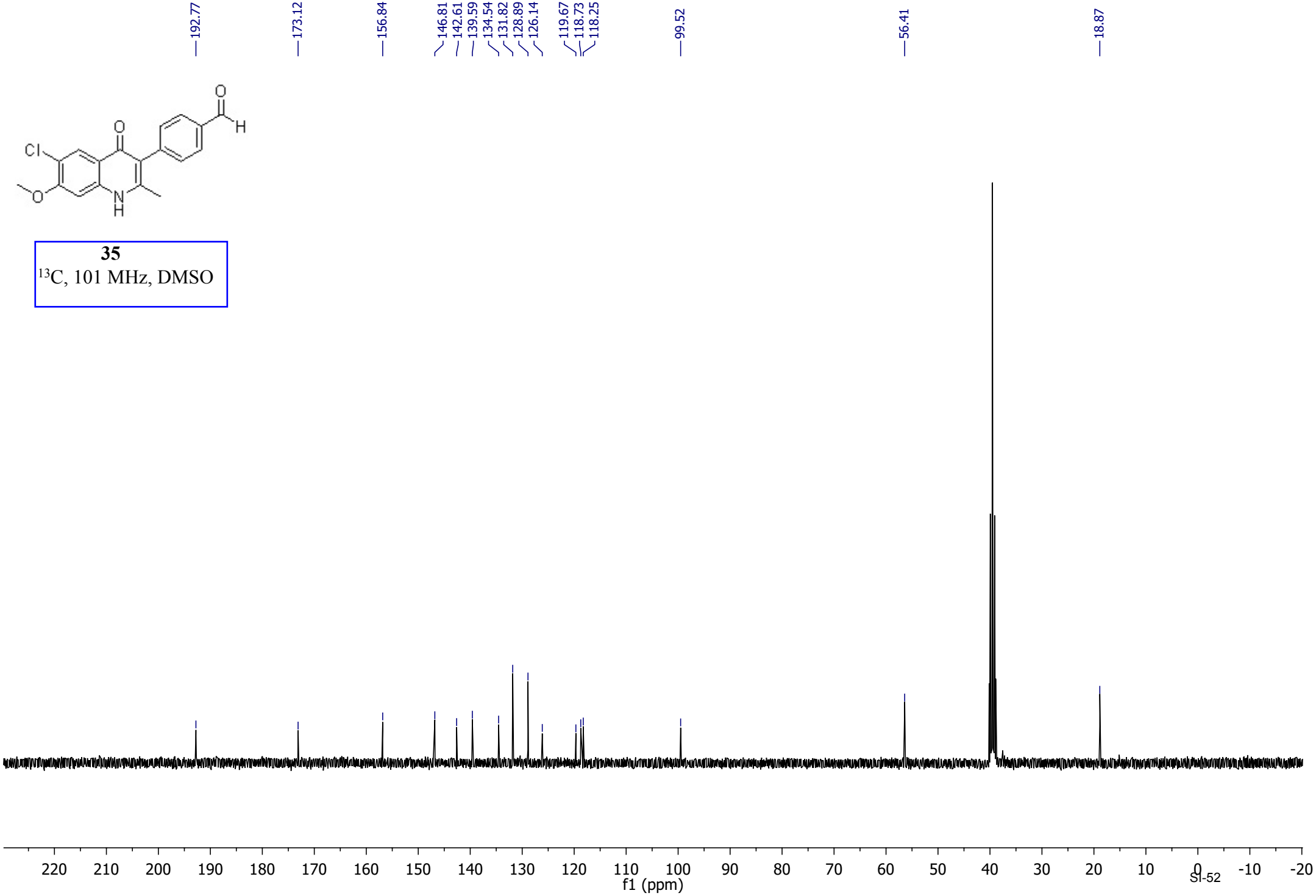
35

^{1}H, 400 MHz, DMSO

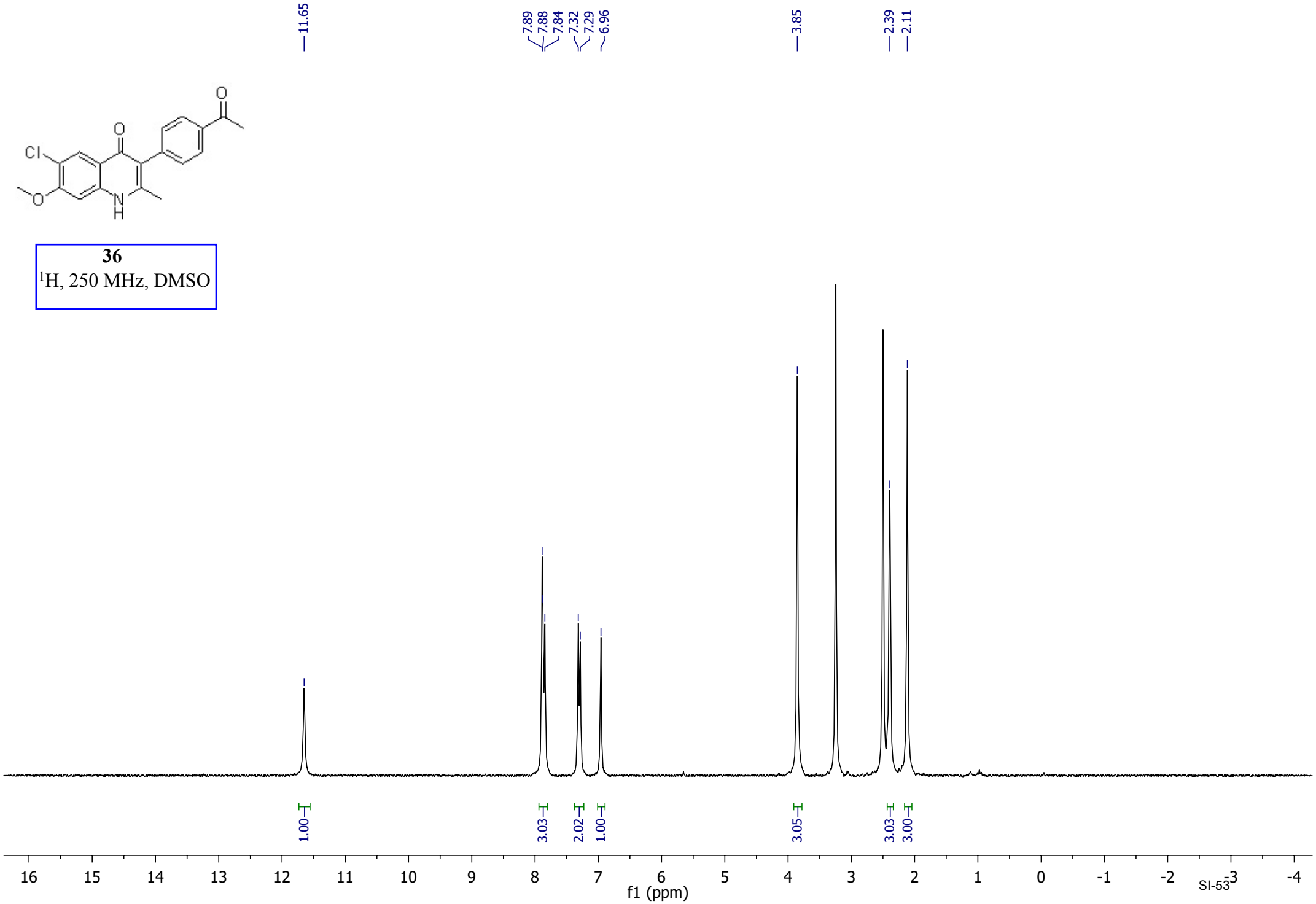


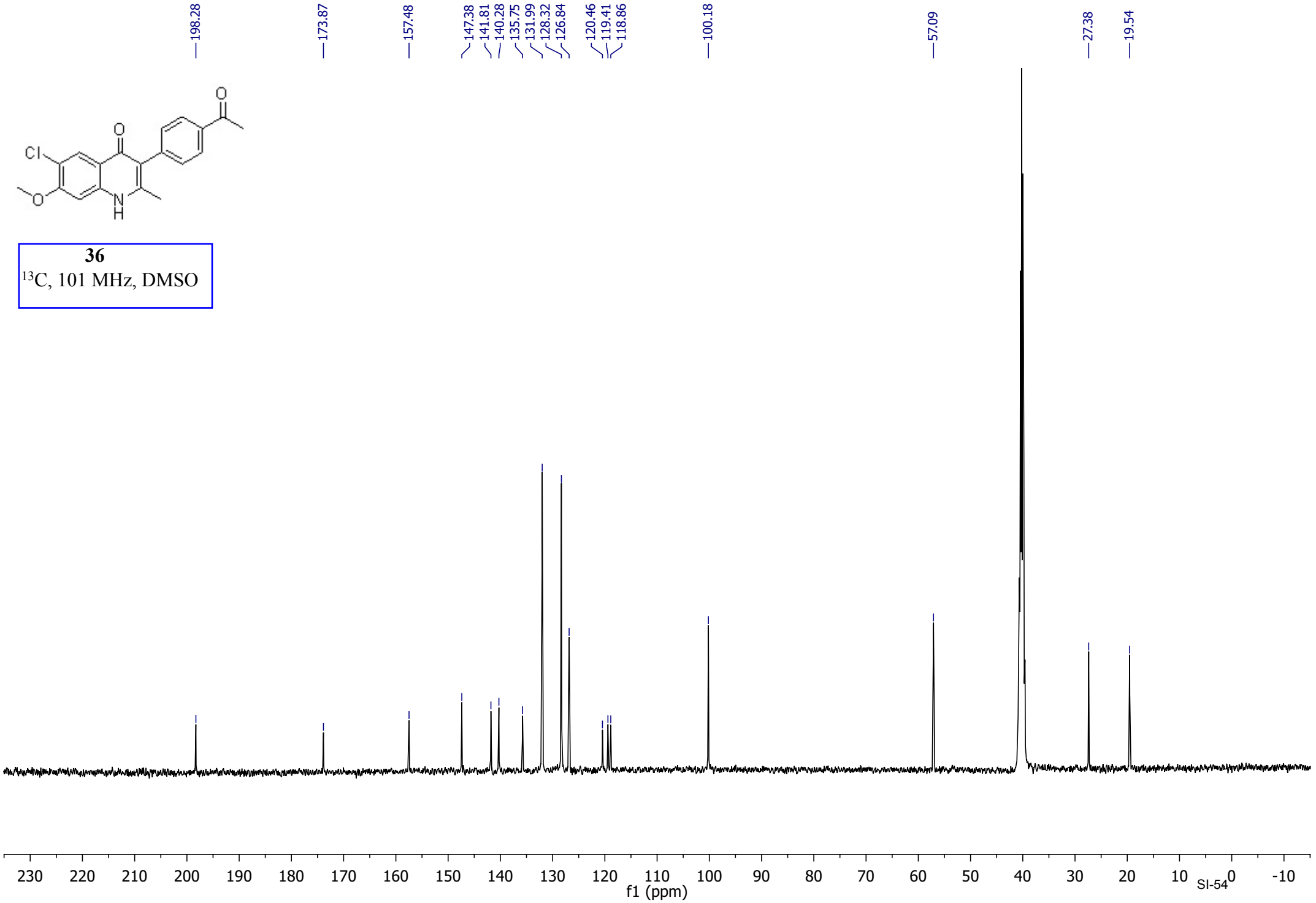
35

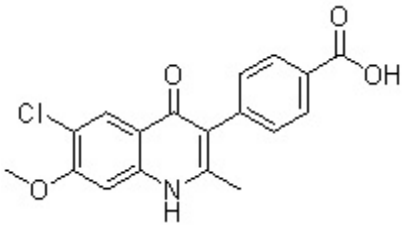
^{13}C, 101 MHz, DMSO



36
^{1}H, 250 MHz, DMSO



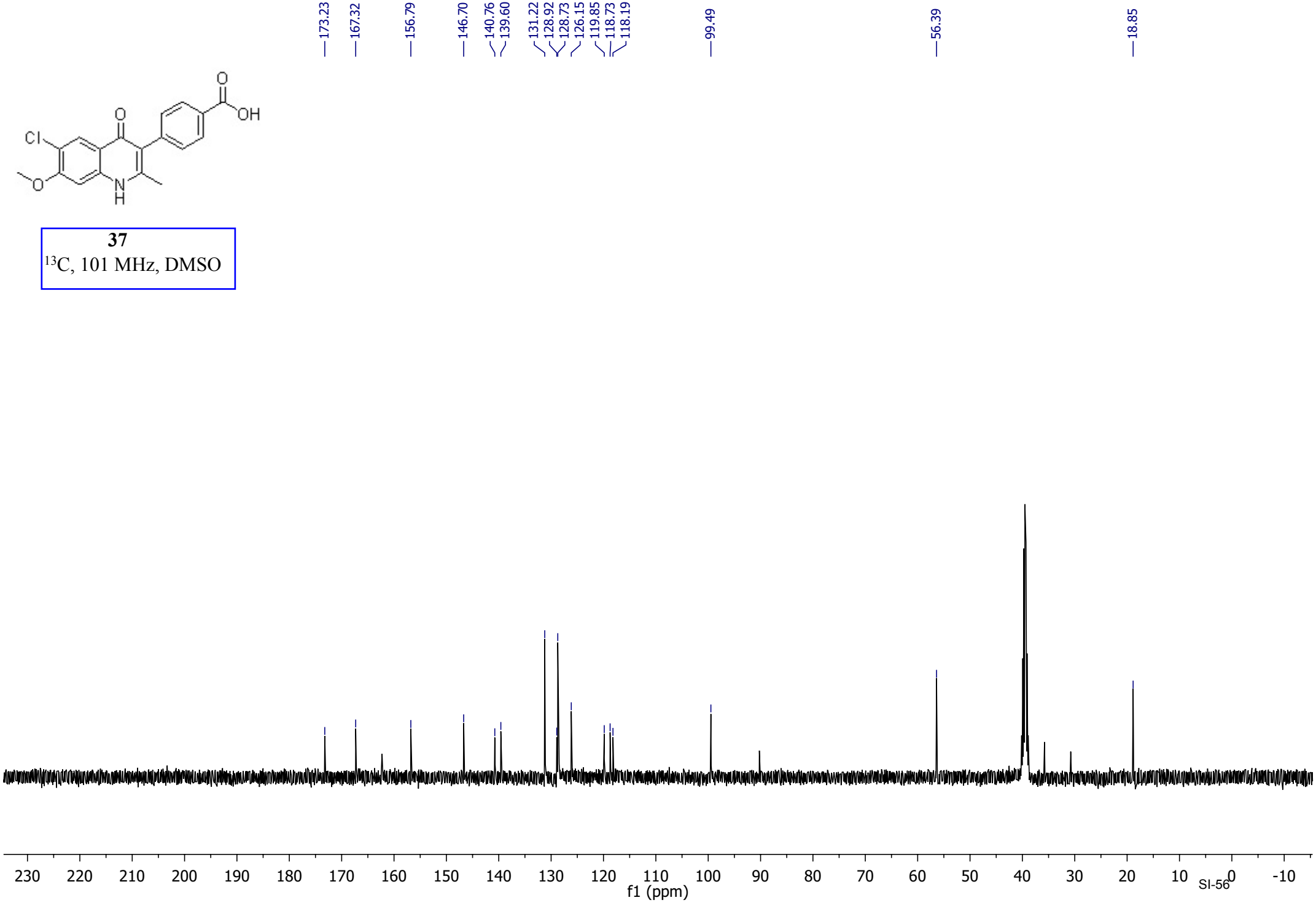

198.28
173.87
157.48
147.38
141.81
140.28
135.75
131.99
128.32
126.84
120.46
119.41
118.86
100.18
57.09
27.38
19.54
Cl
O
O
O
N
H
36
13C, 101 MHz, DMSO
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
SI-54



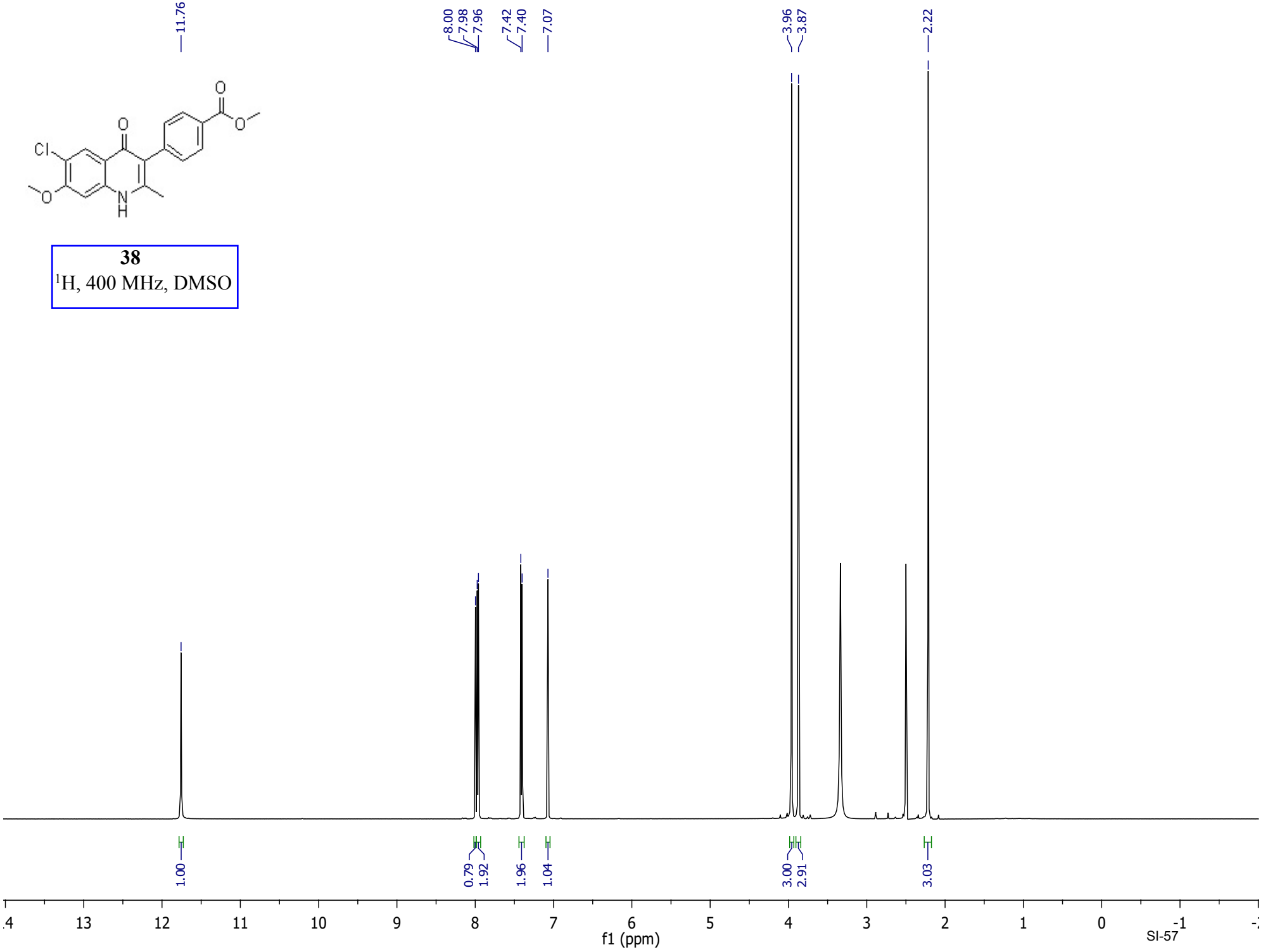
37
^{1}H, 400 MHz, DMSO

37

^{13}C, 101 MHz, DMSO

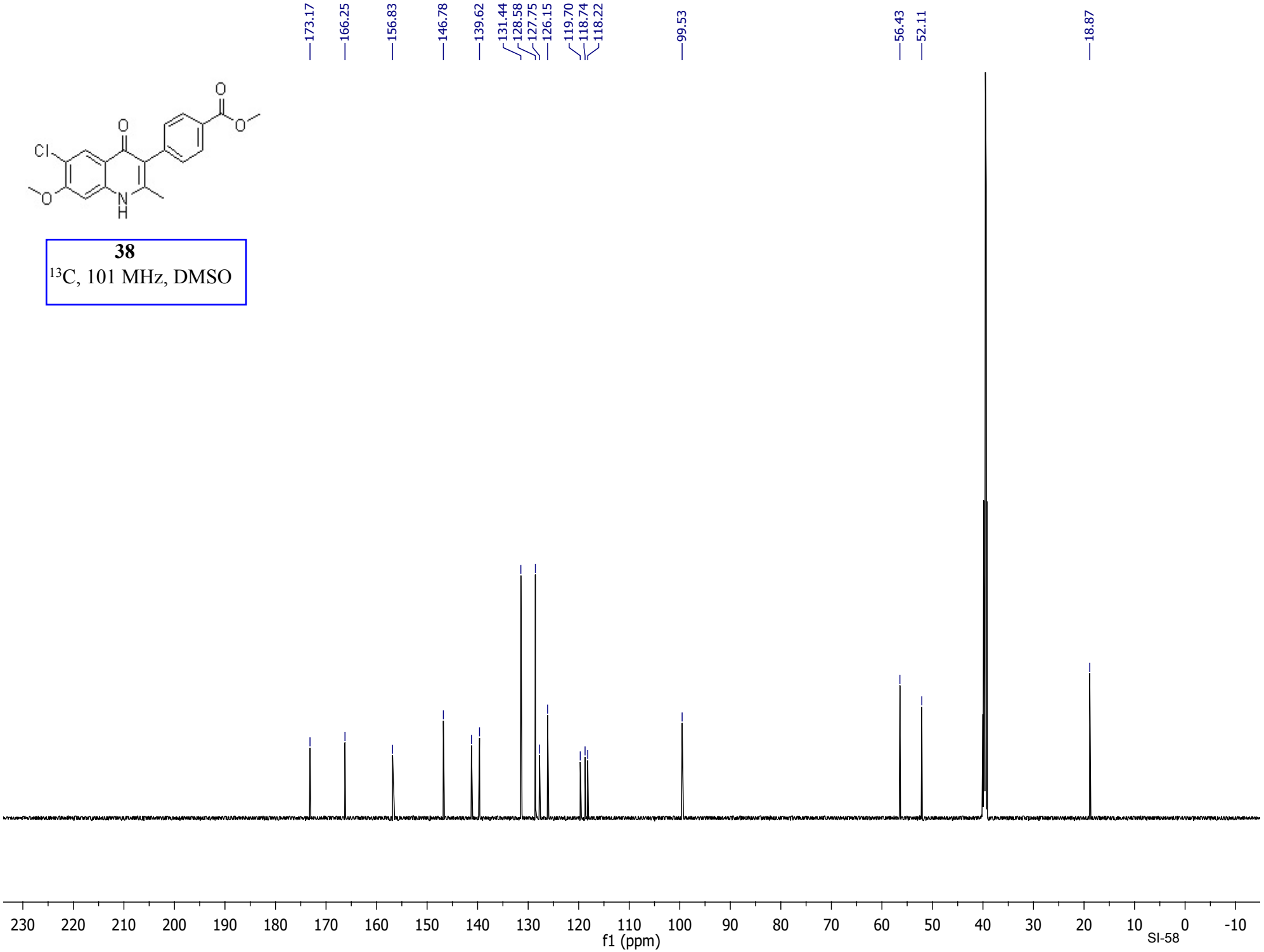


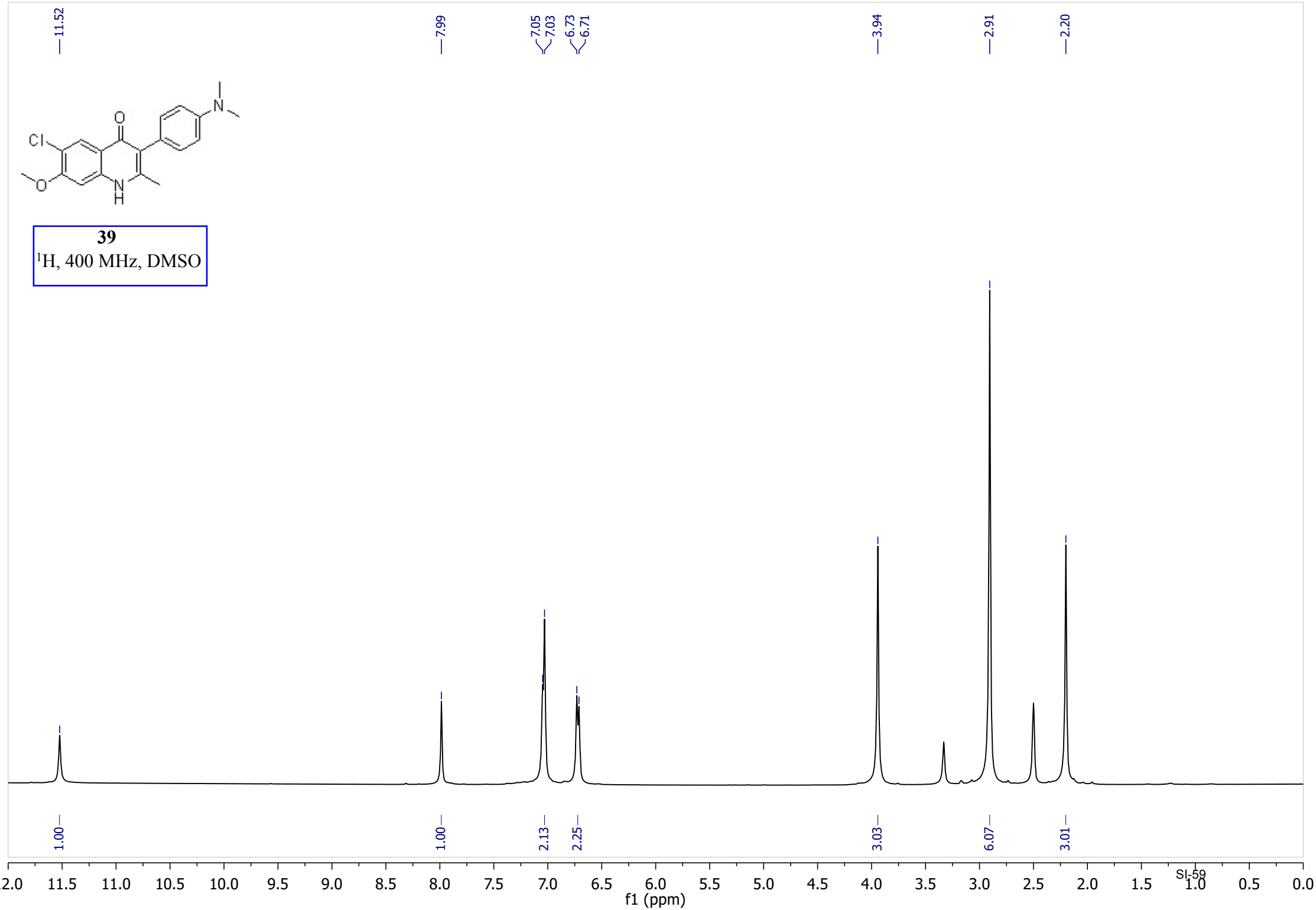
38
^{1}H, 400 MHz, DMSO

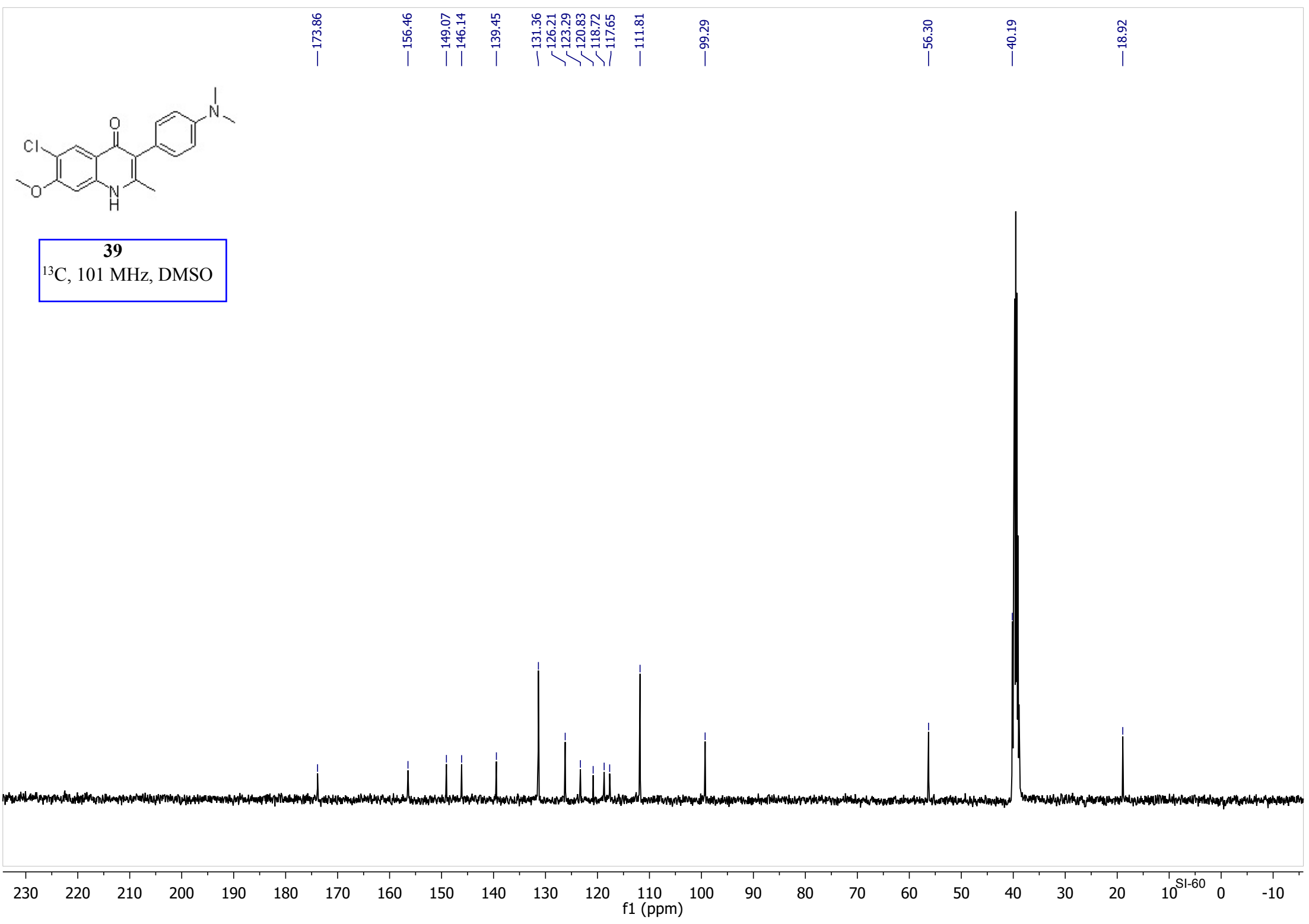


38

^{13}C, 101 MHz, DMSO

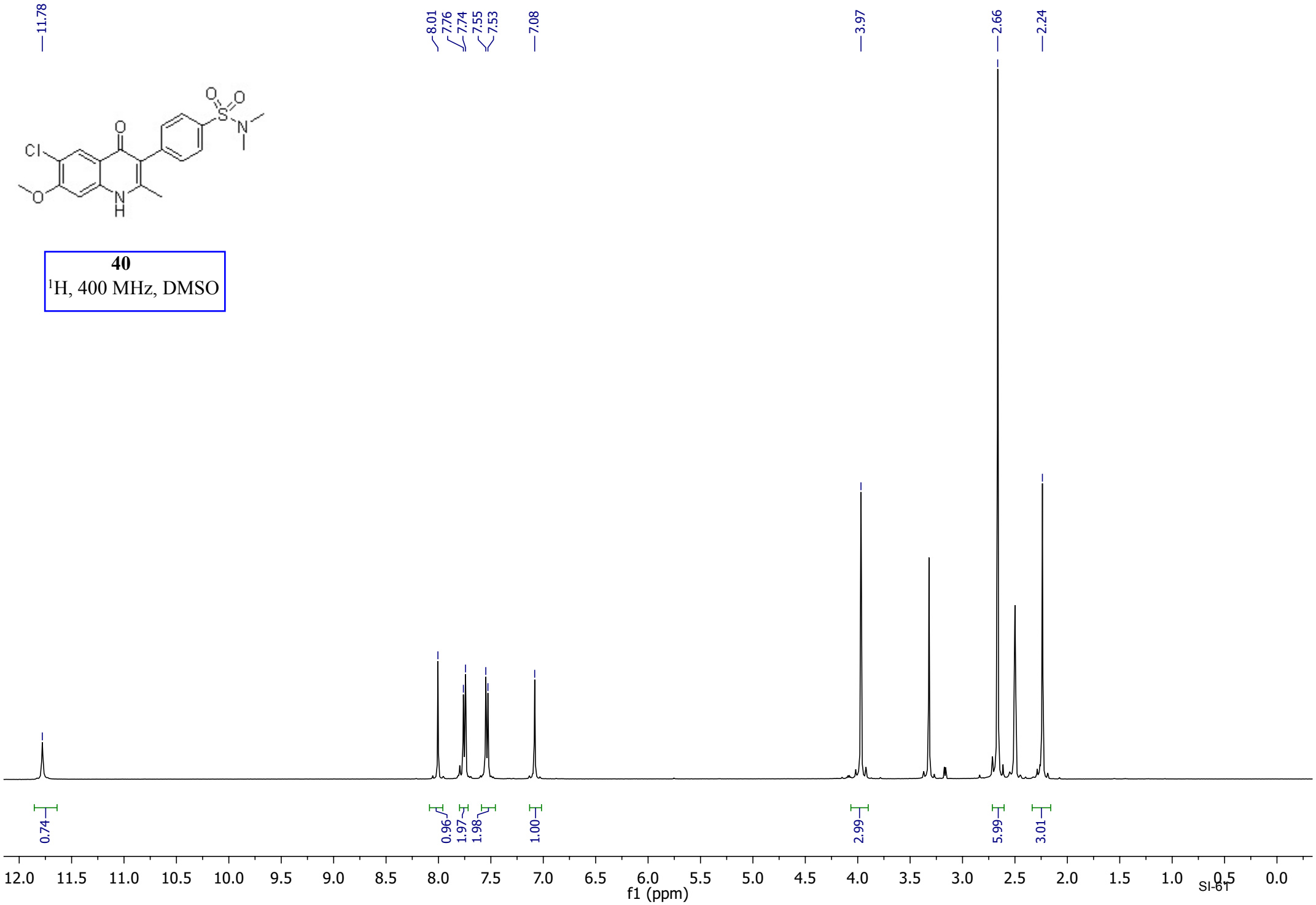



11.52
7.99
7.05
7.03
6.73
6.71
3.94
2.91
2.20
Cl
O
N
O
N
H
39
1H, 400 MHz, DMSO
1.00
1.00
2.13
2.25
3.03
6.07
3.01
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


173.86
156.46
149.07
146.14
139.45
131.36
126.21
123.29
120.83
118.72
117.65
111.81
99.29
56.30
40.19
18.92
Cl
O
N
O
N
H
39
13C, 101 MHz, DMSO
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
SI-60

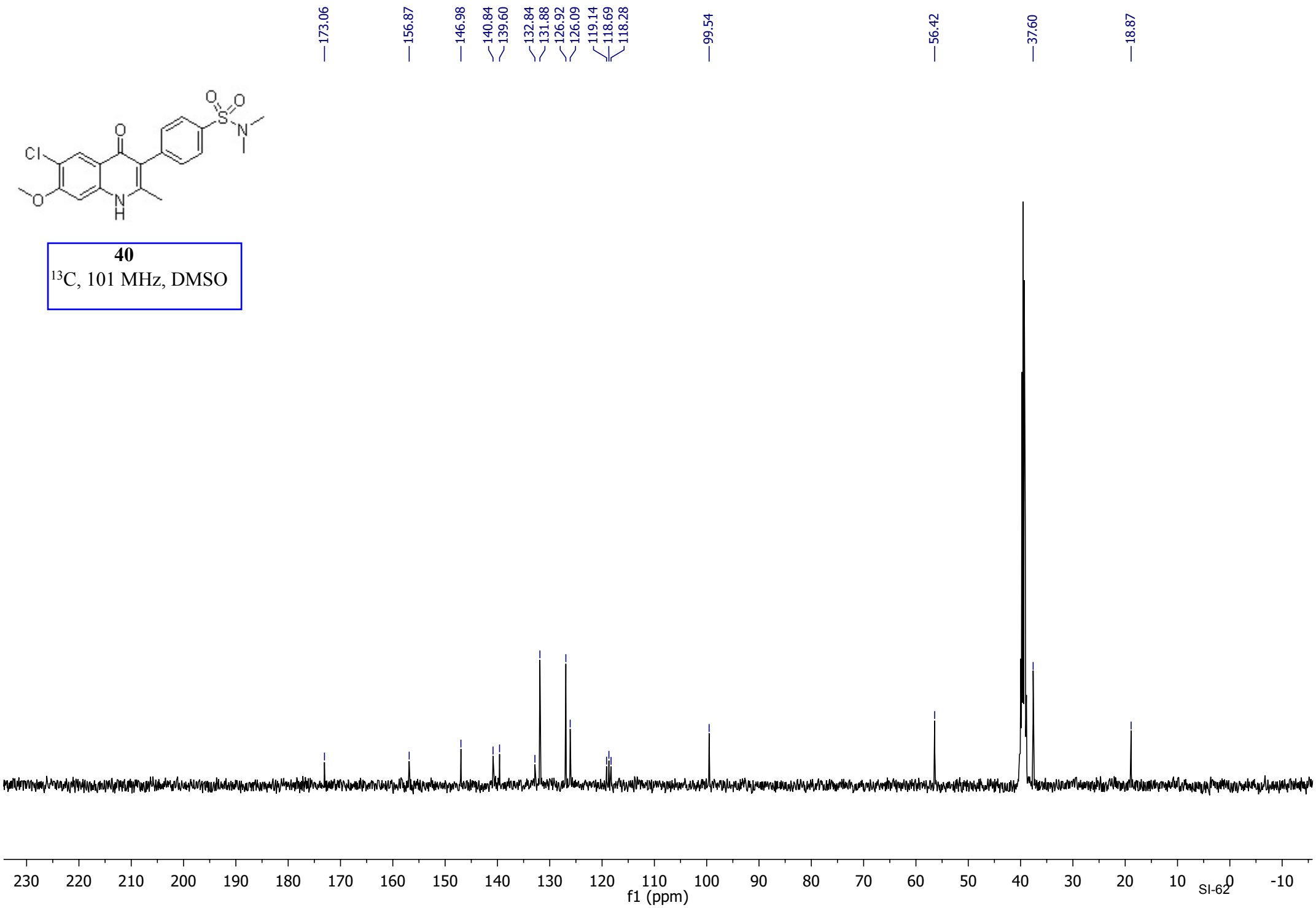
40

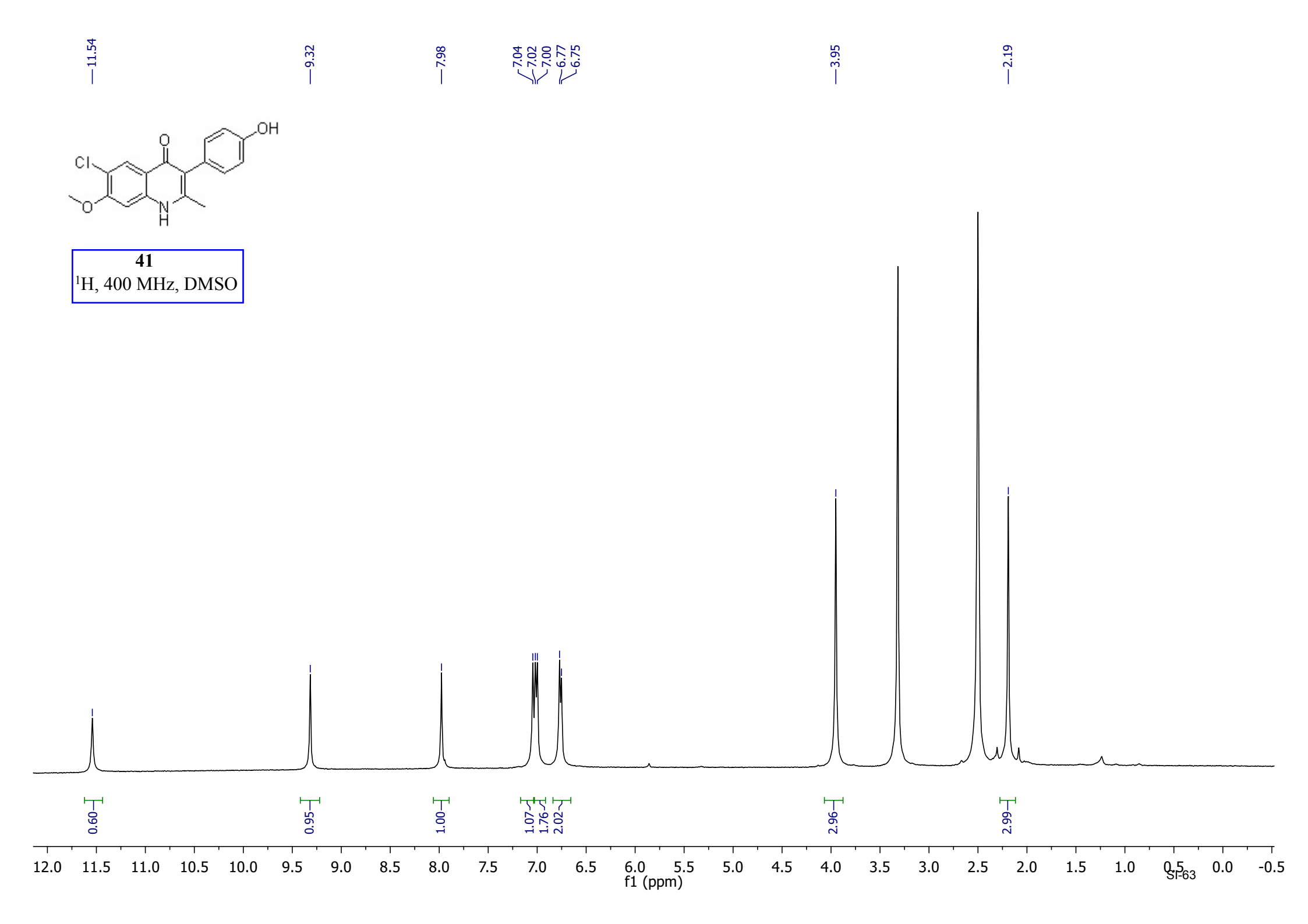
^{1}H, 400 MHz, DMSO



40

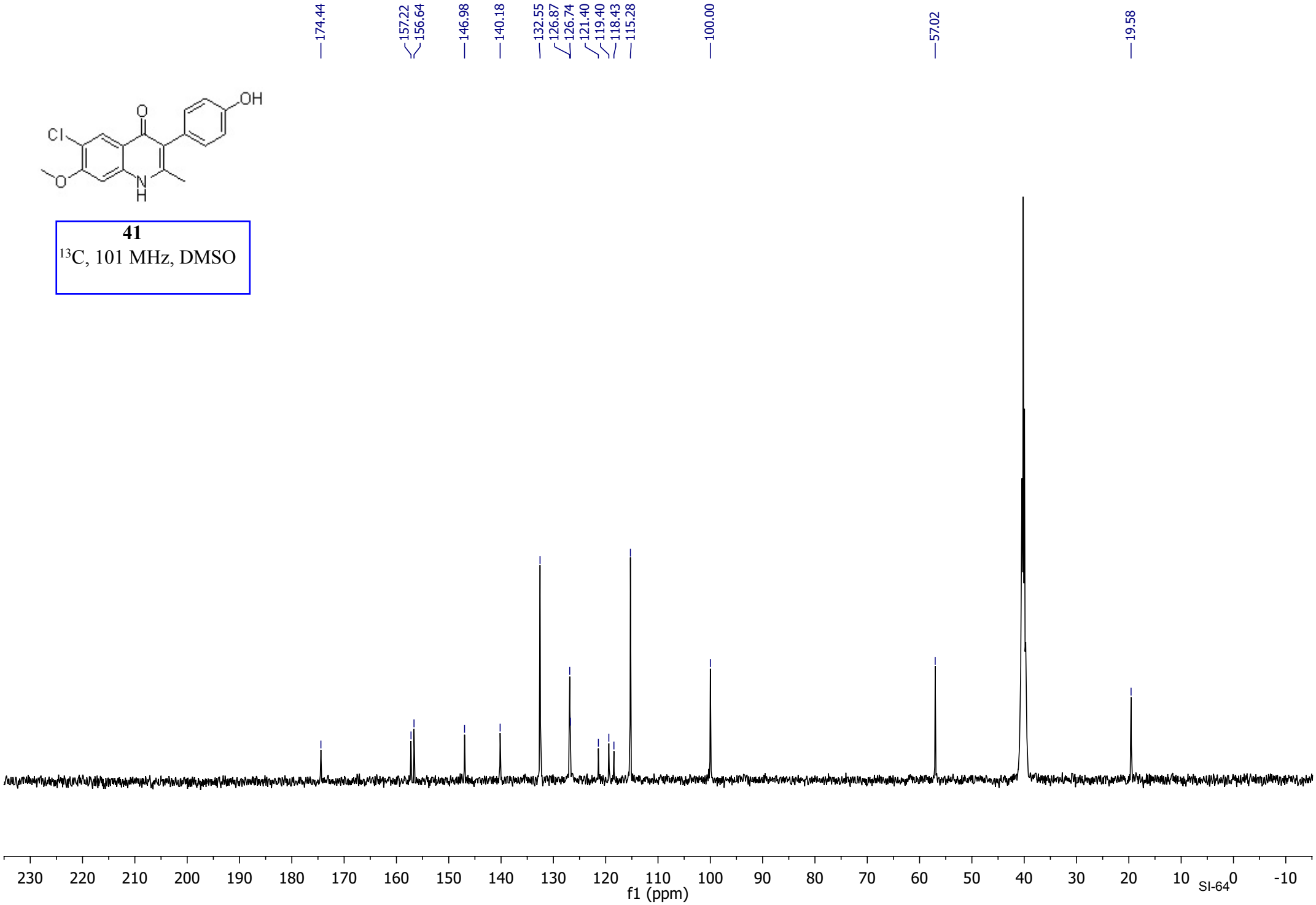
^{13}C, 101 MHz, DMSO

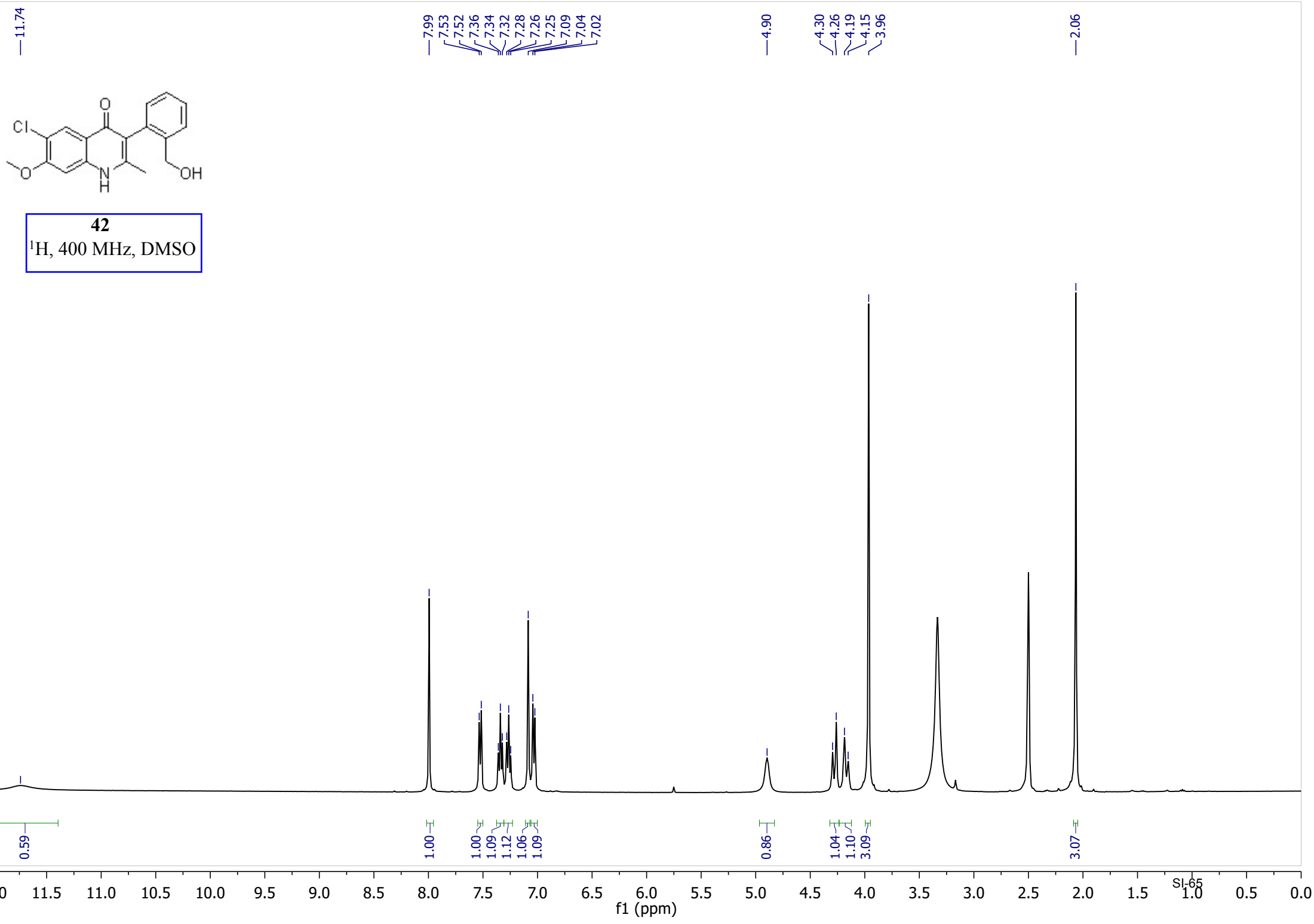


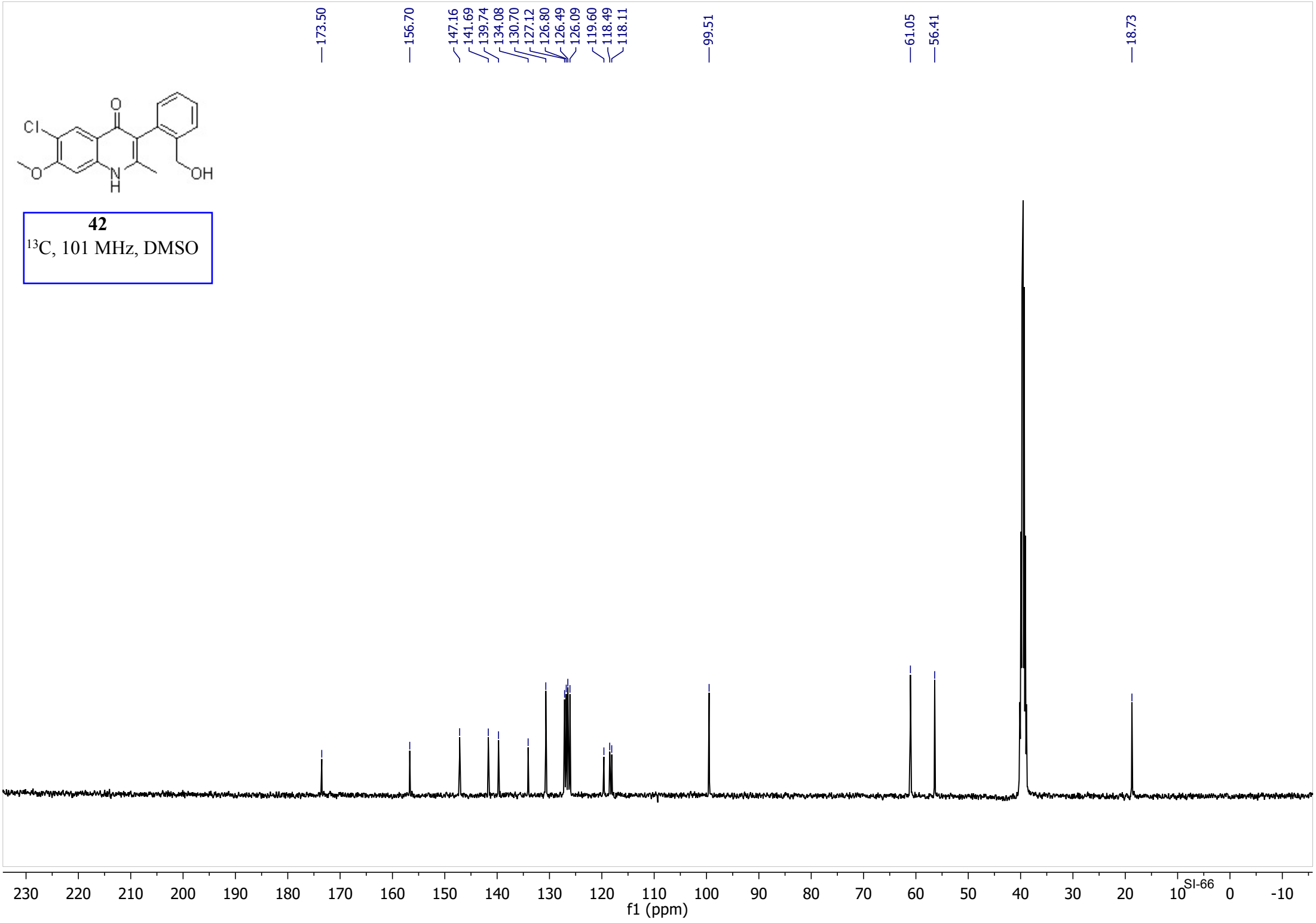

11.54
9.32
7.98
7.04
7.02
7.00
6.77
6.75
3.95
2.19
OH
O
Cl
O
N
H
41
1H, 400 MHz, DMSO
0.60
0.95
1.00
1.07
1.76
2.02
2.96
2.99
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
SI-63

41

^{13}C, 101 MHz, DMSO

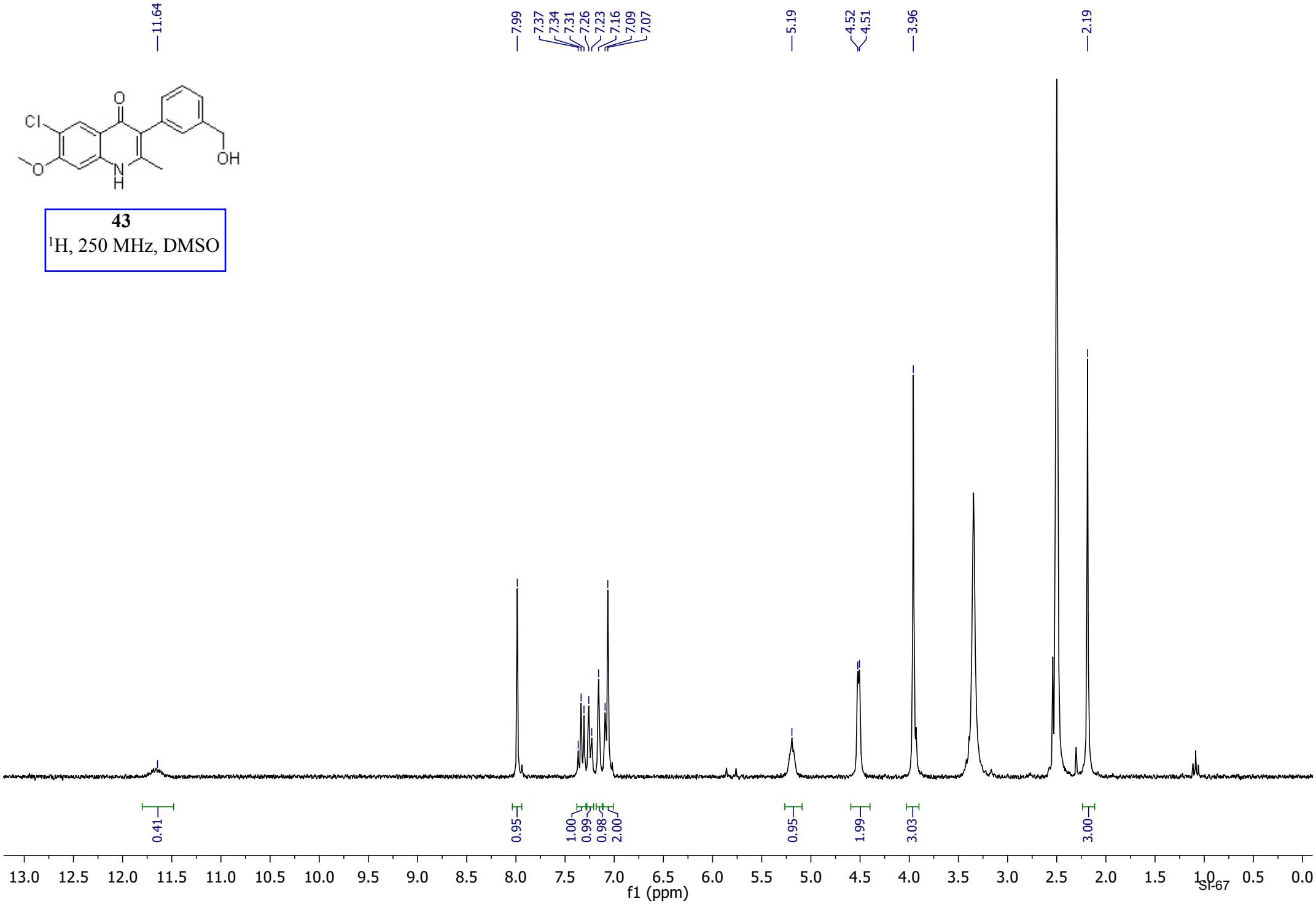



11.74
7.99
7.53
7.52
7.36
7.34
7.32
7.28
7.26
7.25
7.09
7.04
7.02
4.90
4.30
4.26
4.19
4.15
3.96
2.06
Cl
O
N
H
OH
42
1H, 400 MHz, DMSO
0.59
1.00
1.00
1.09
1.12
1.06
1.09
0.86
1.04
1.10
3.09
3.07
f1 (ppm)
SI-65


173.50
156.70
147.16
141.69
139.74
134.08
130.70
127.12
126.80
126.49
126.09
119.60
118.49
118.11
99.51
61.05
56.41
18.73
Cl
O
N
H
OH
42
13C, 101 MHz, DMSO
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

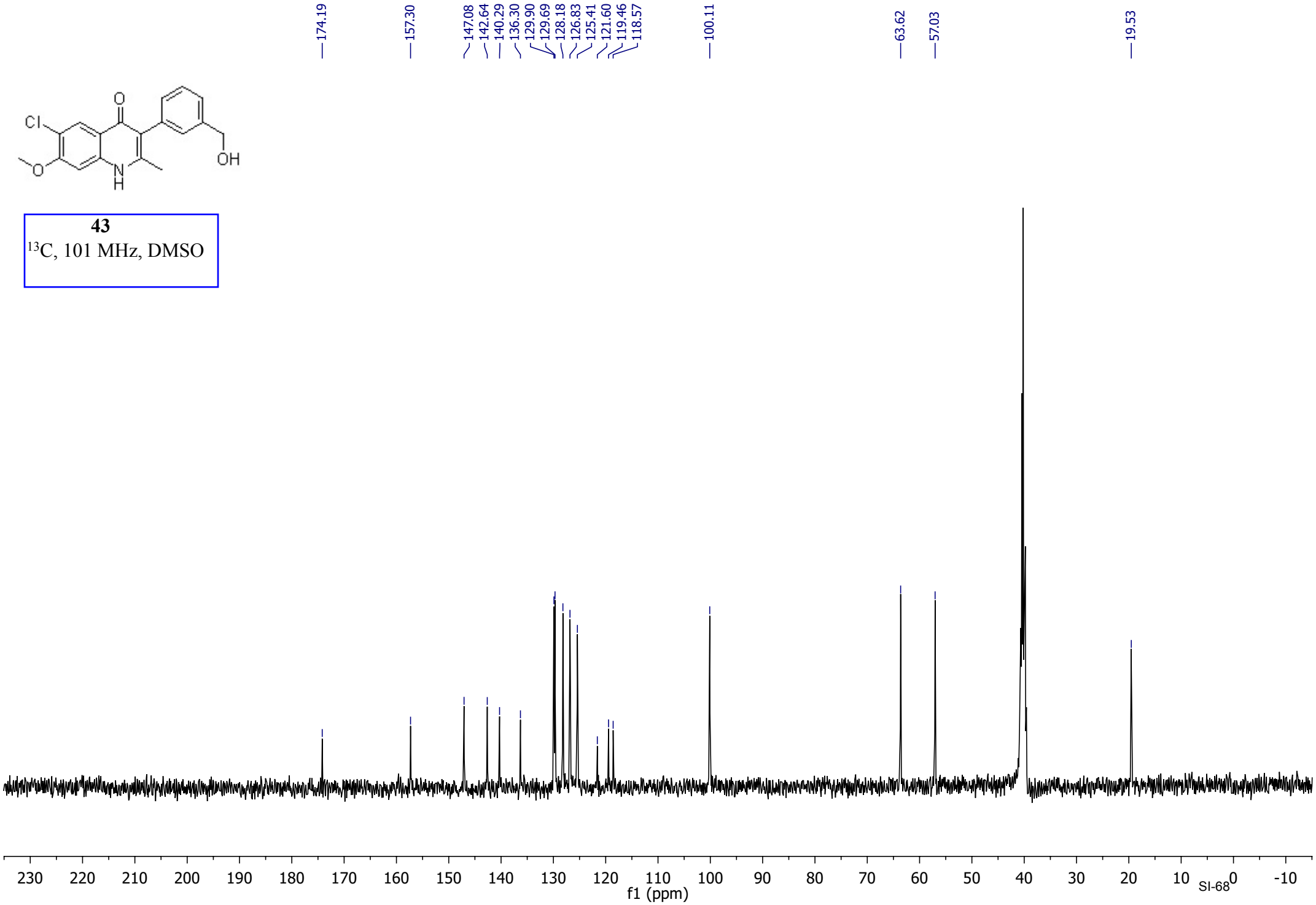
43

^{1}H, 250 MHz, DMSO



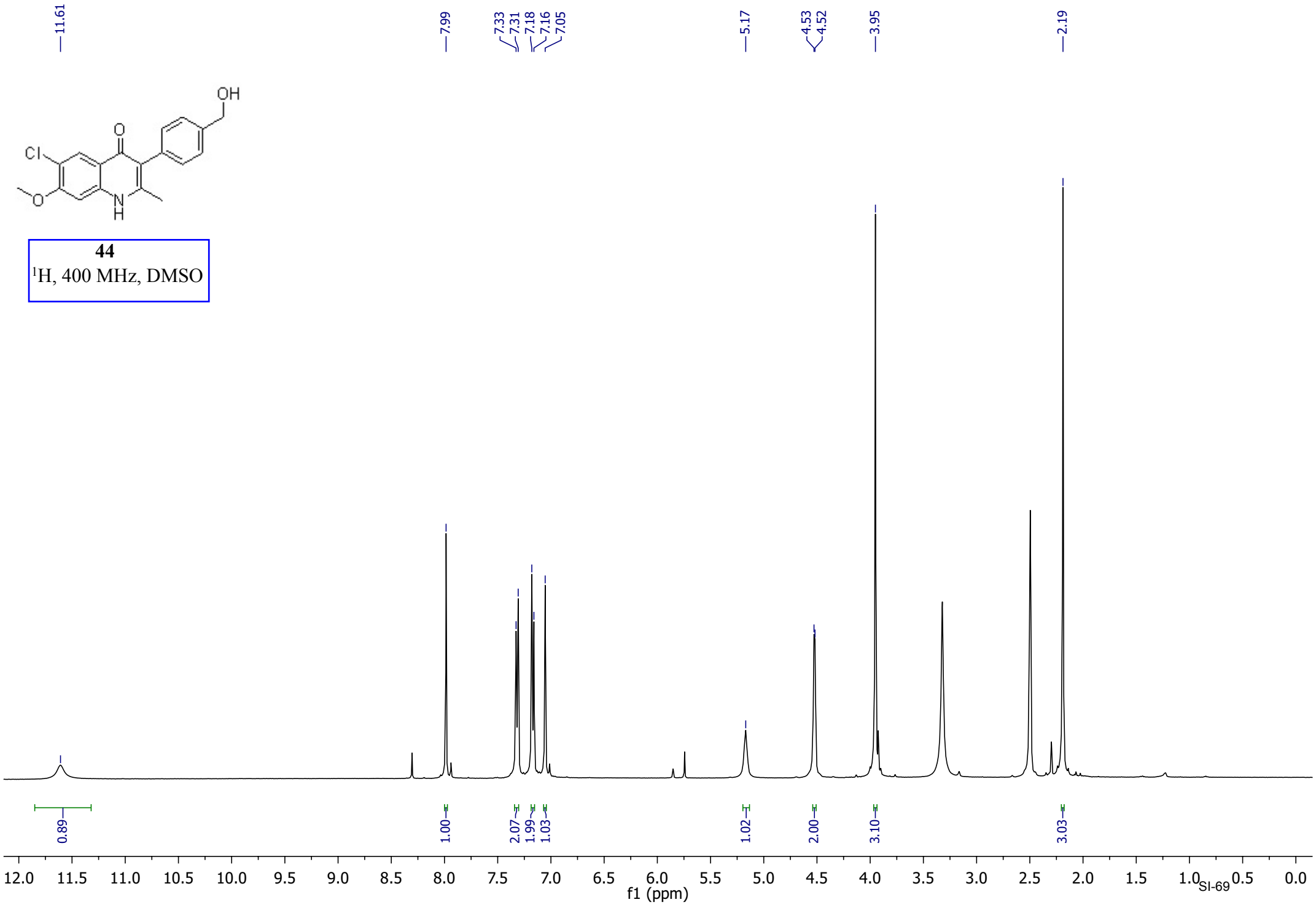
43

^{13}C, 101 MHz, DMSO



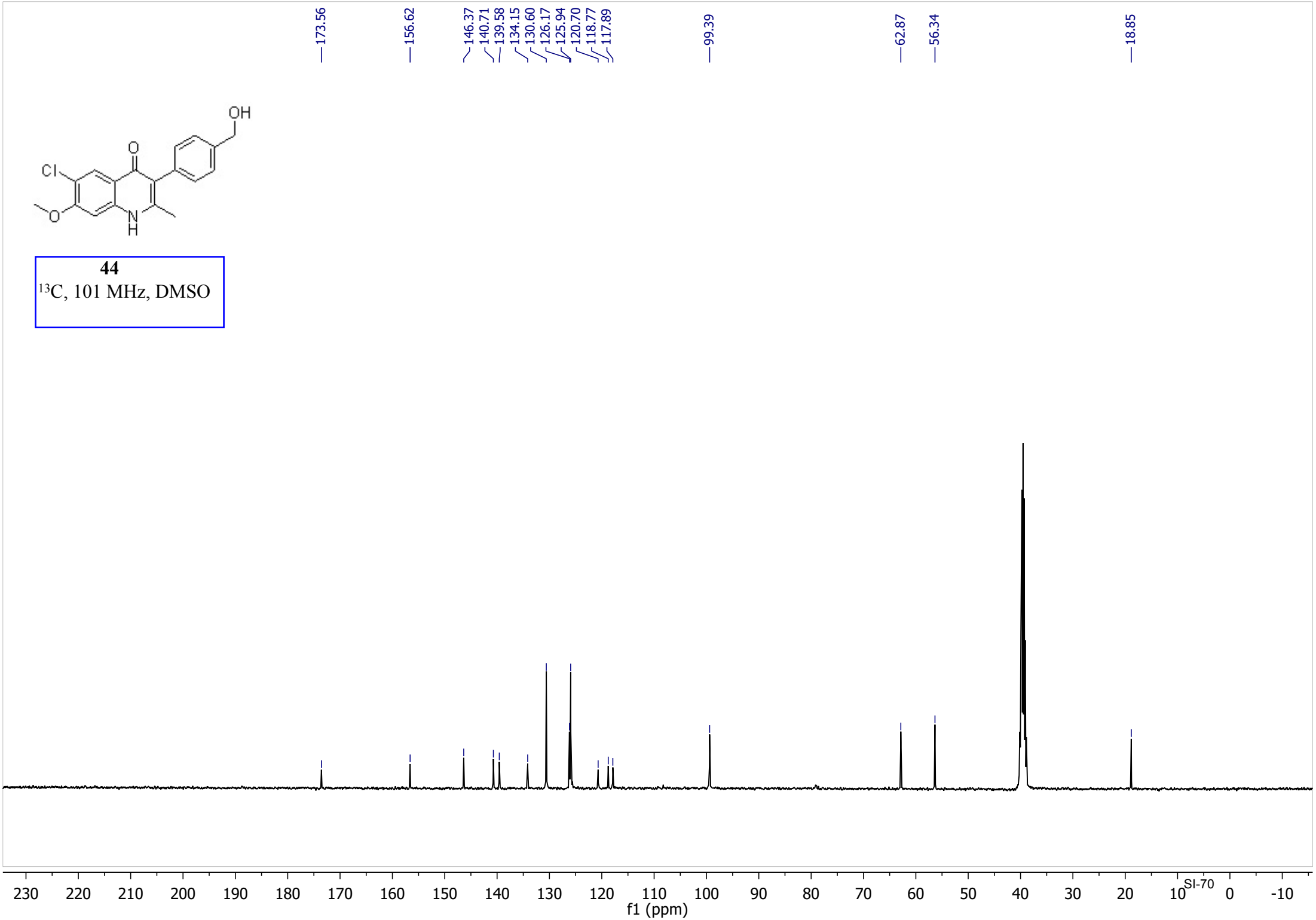
44

^{1}H, 400 MHz, DMSO



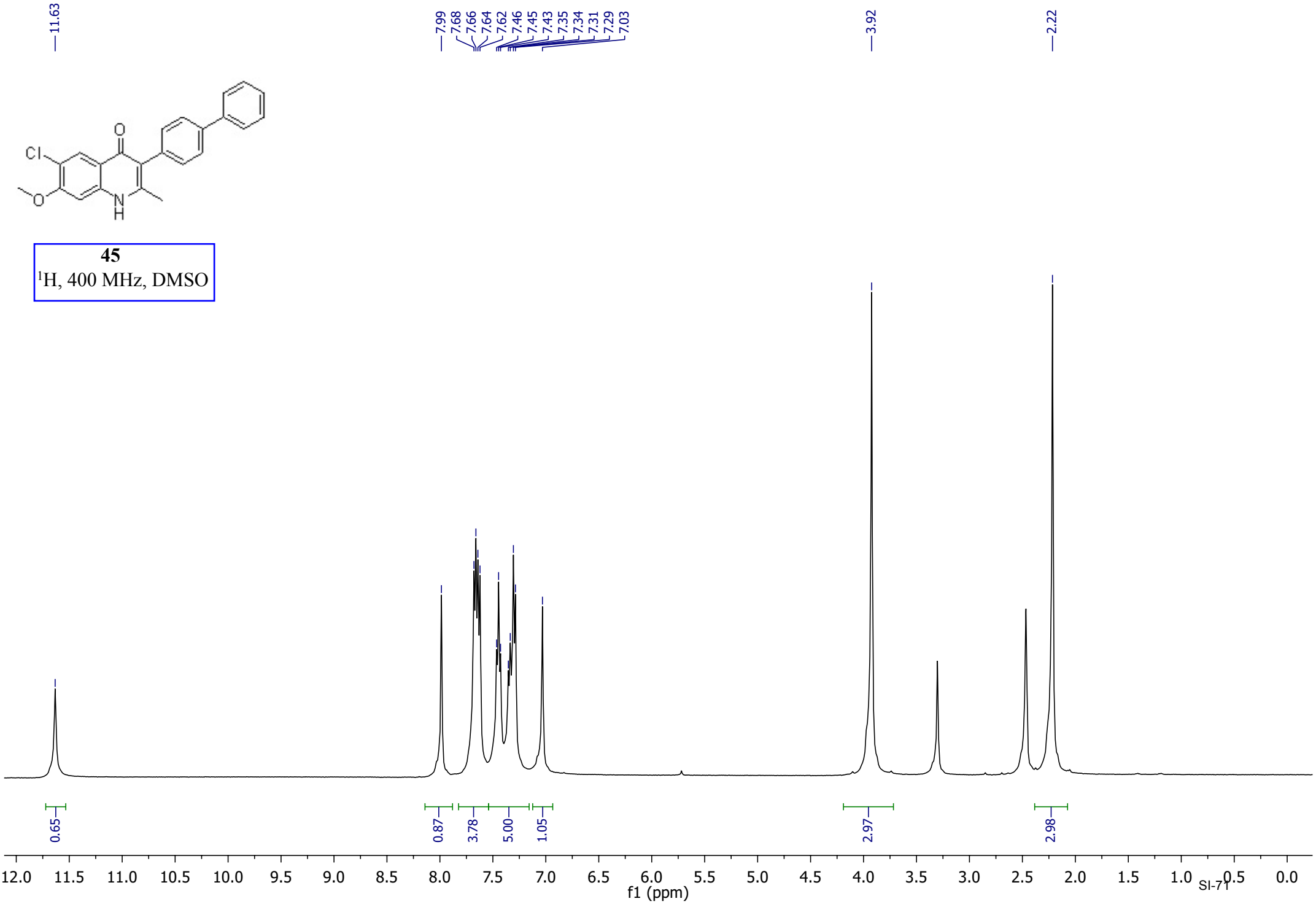
44

^{13}C, 101 MHz, DMSO



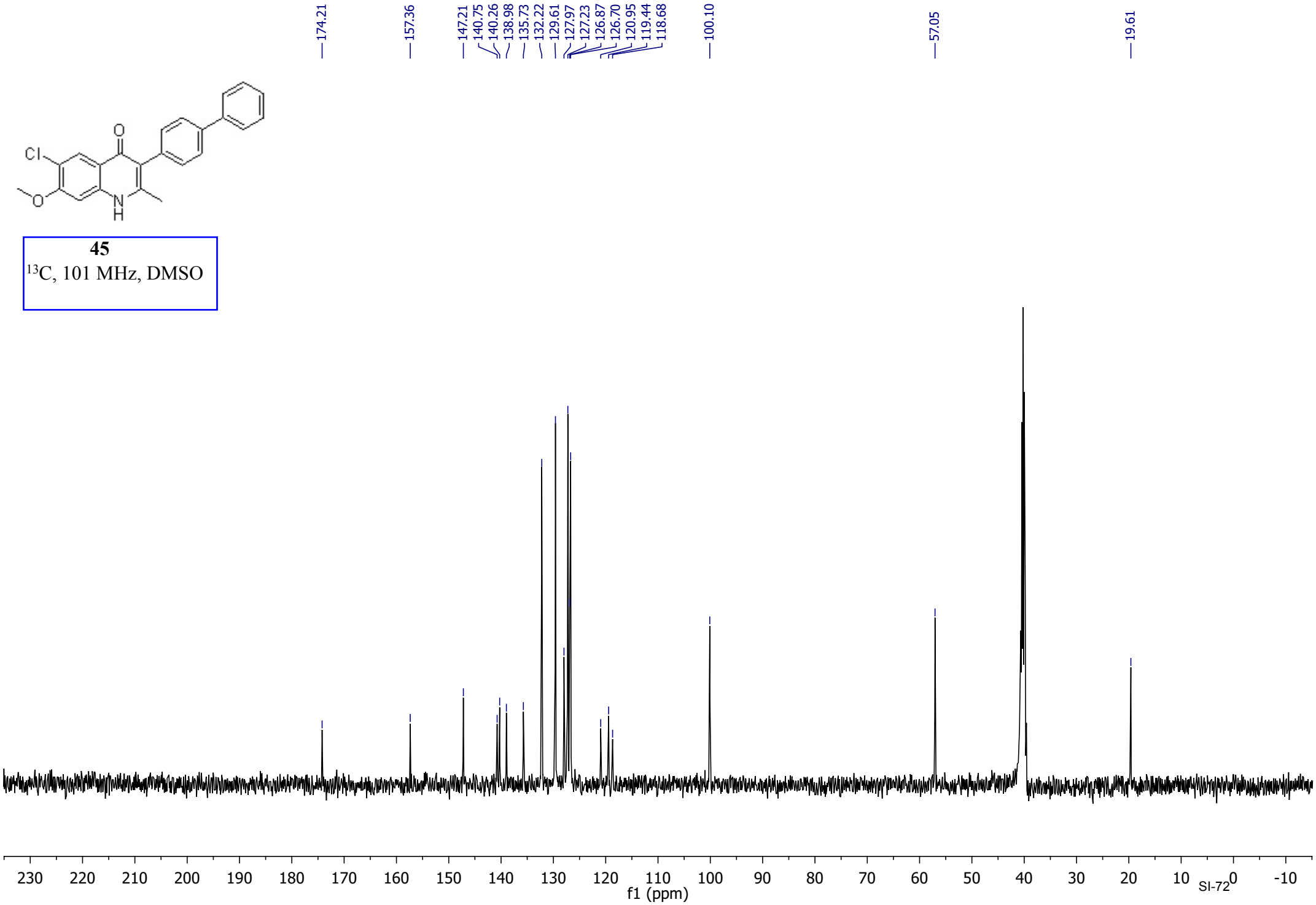
45

^{1}H, 400 MHz, DMSO

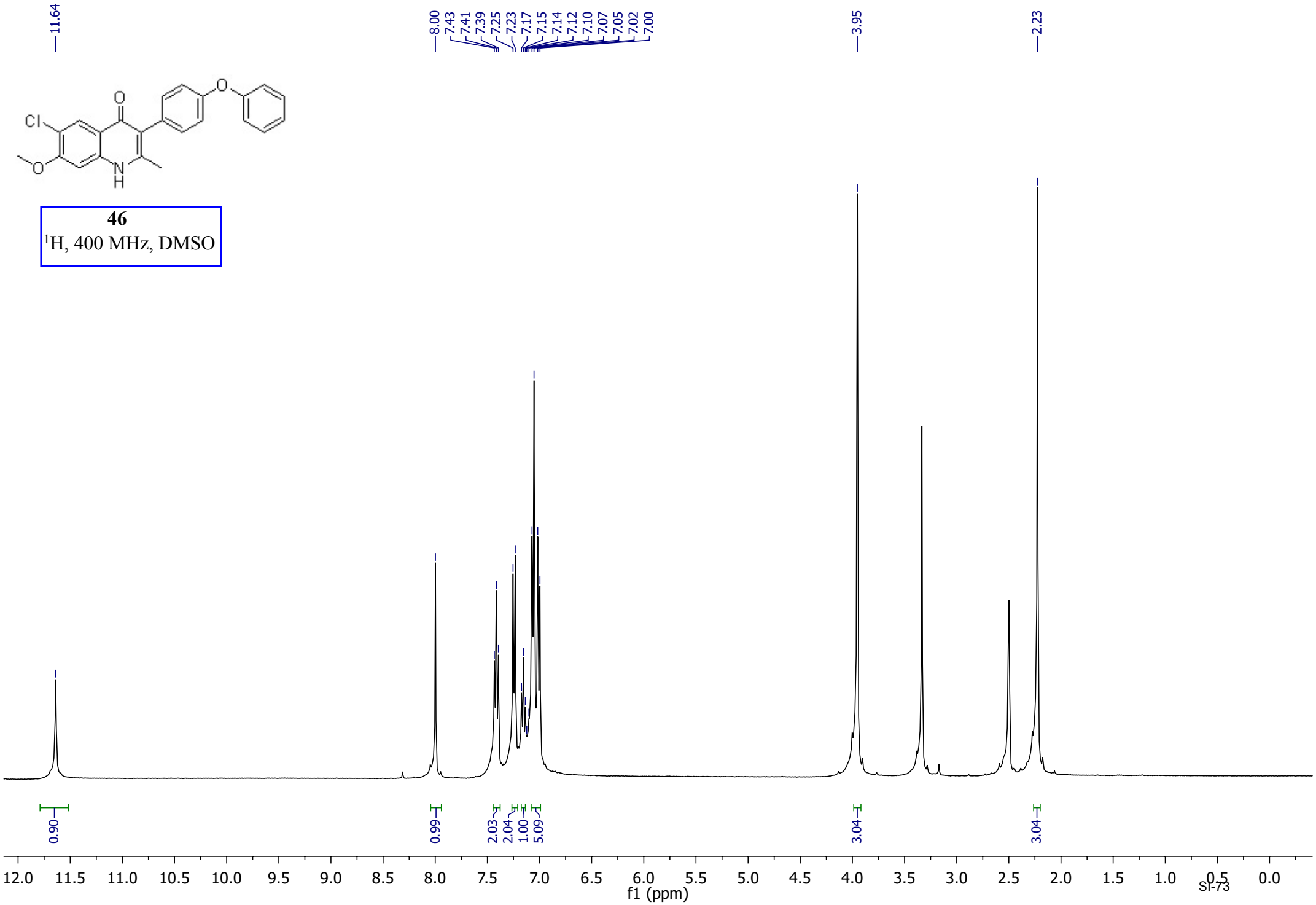


45

^{13}C, 101 MHz, DMSO

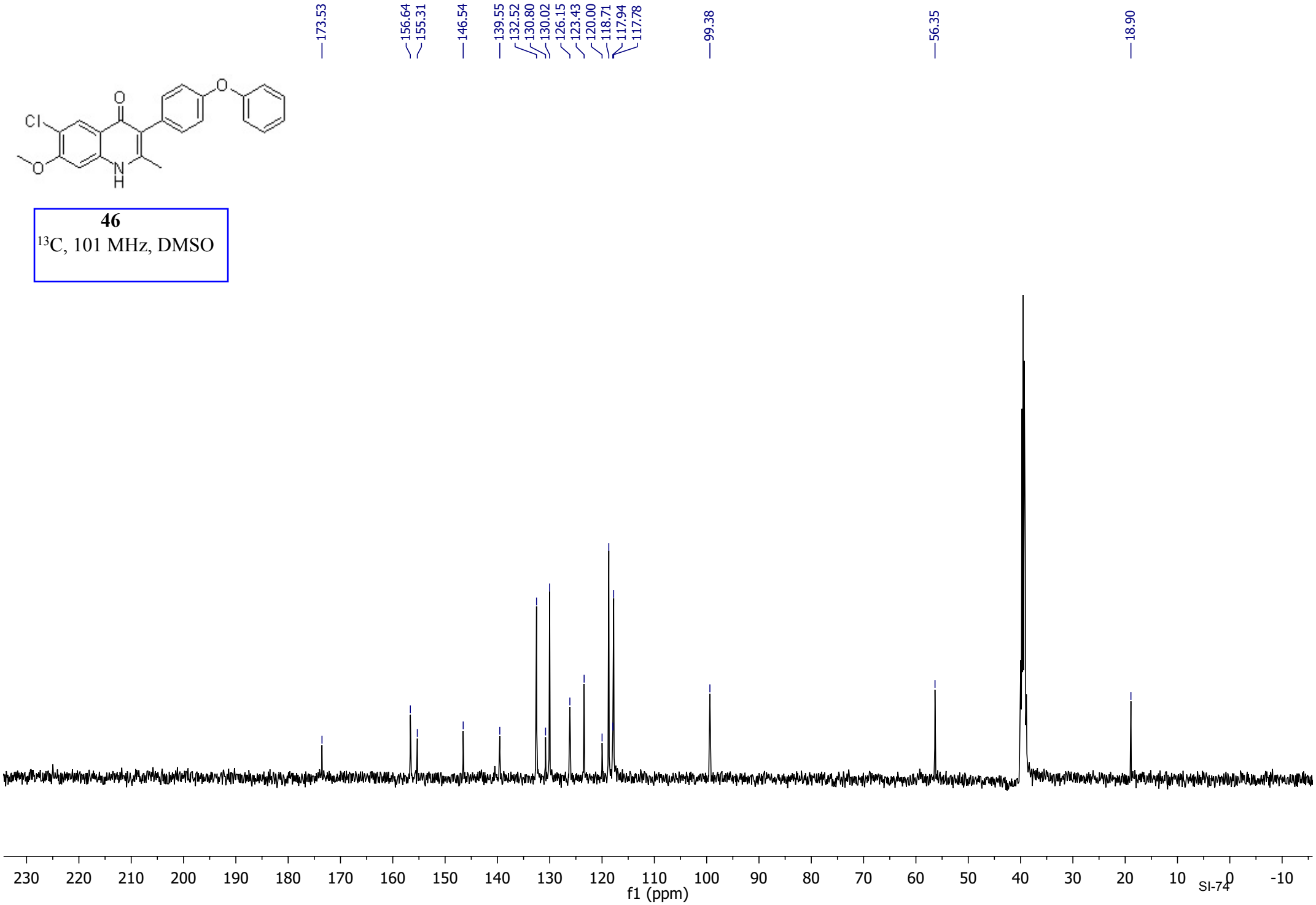


46
^{1}H, 400 MHz, DMSO

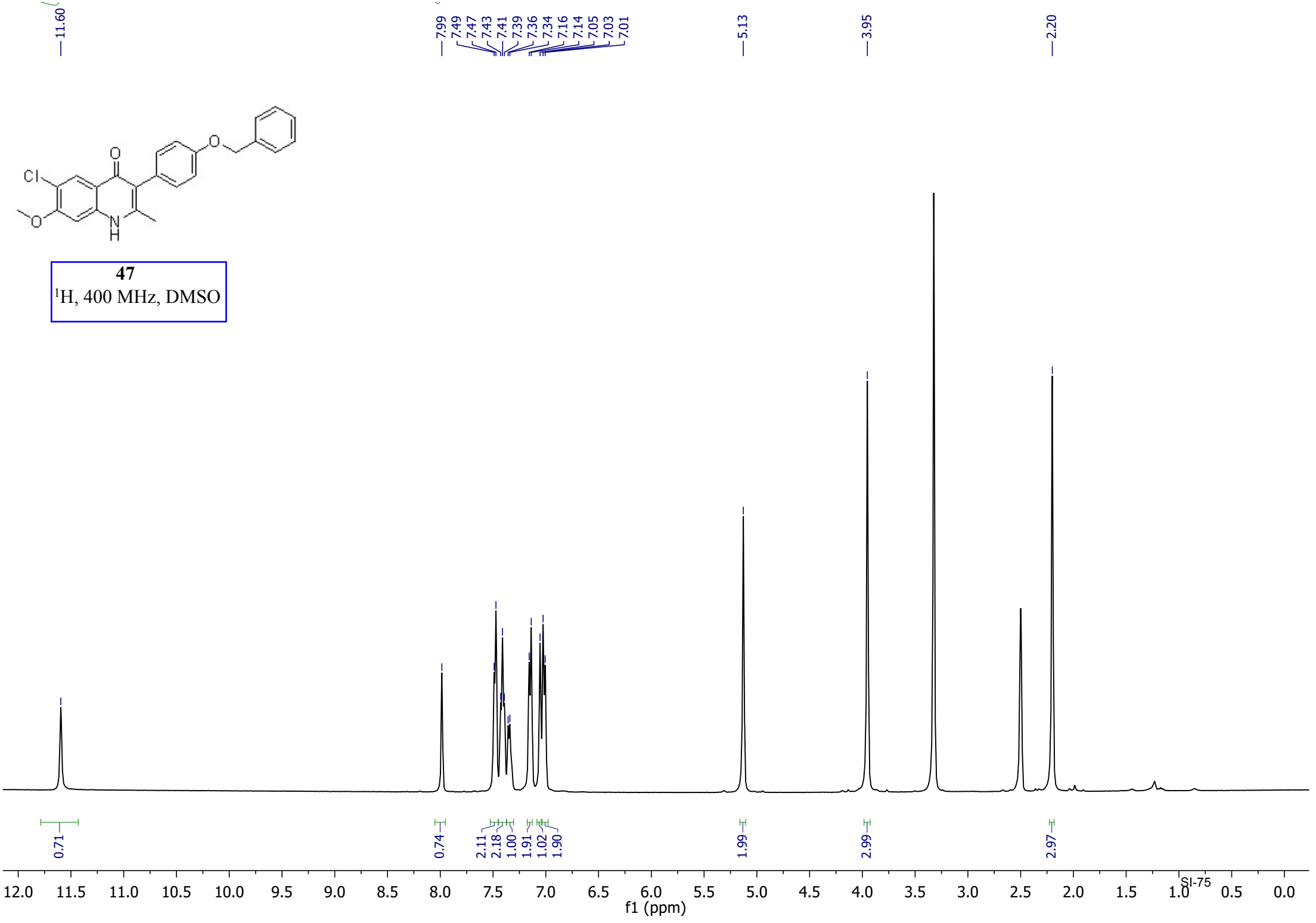


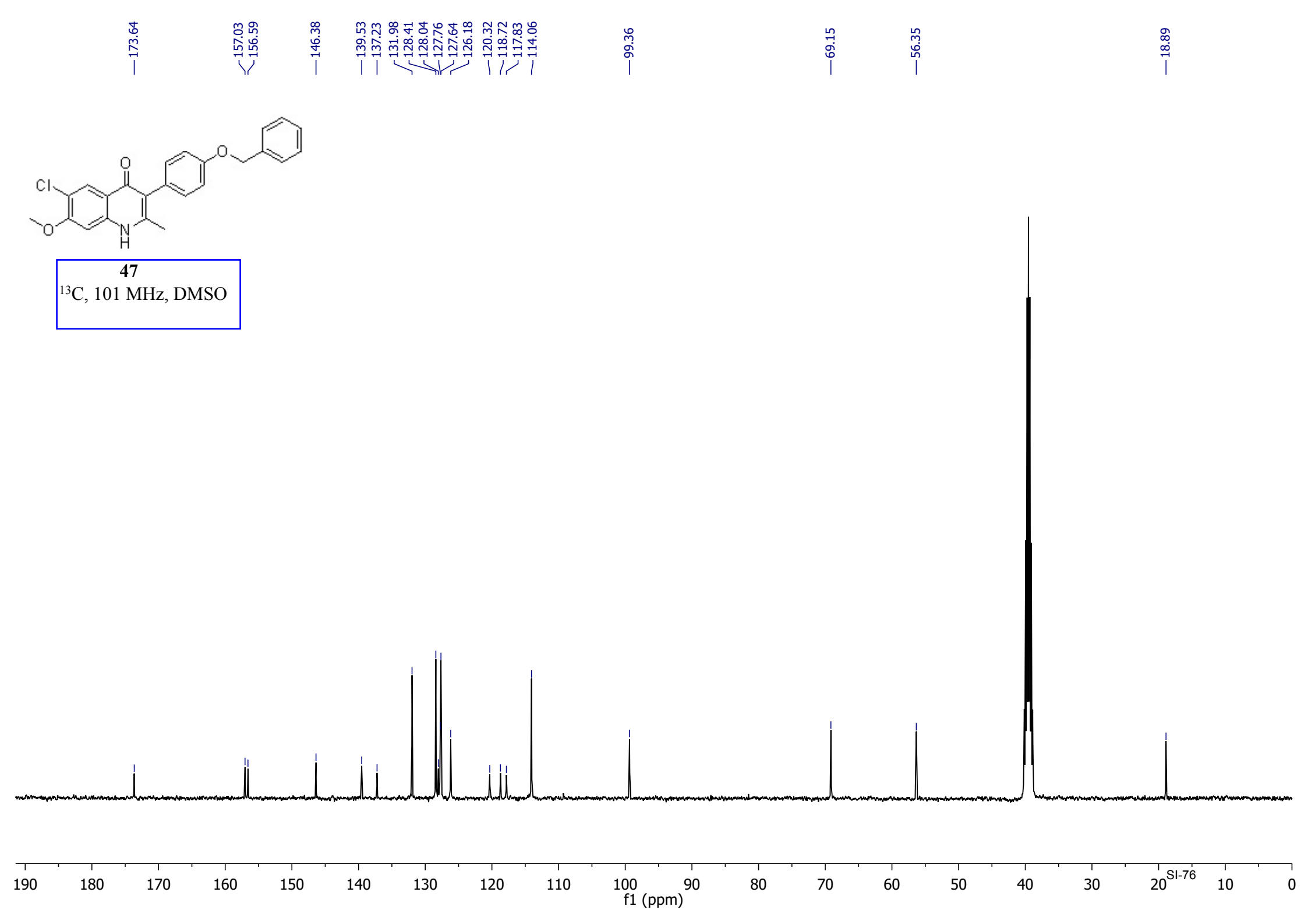
46

^{13}C, 101 MHz, DMSO

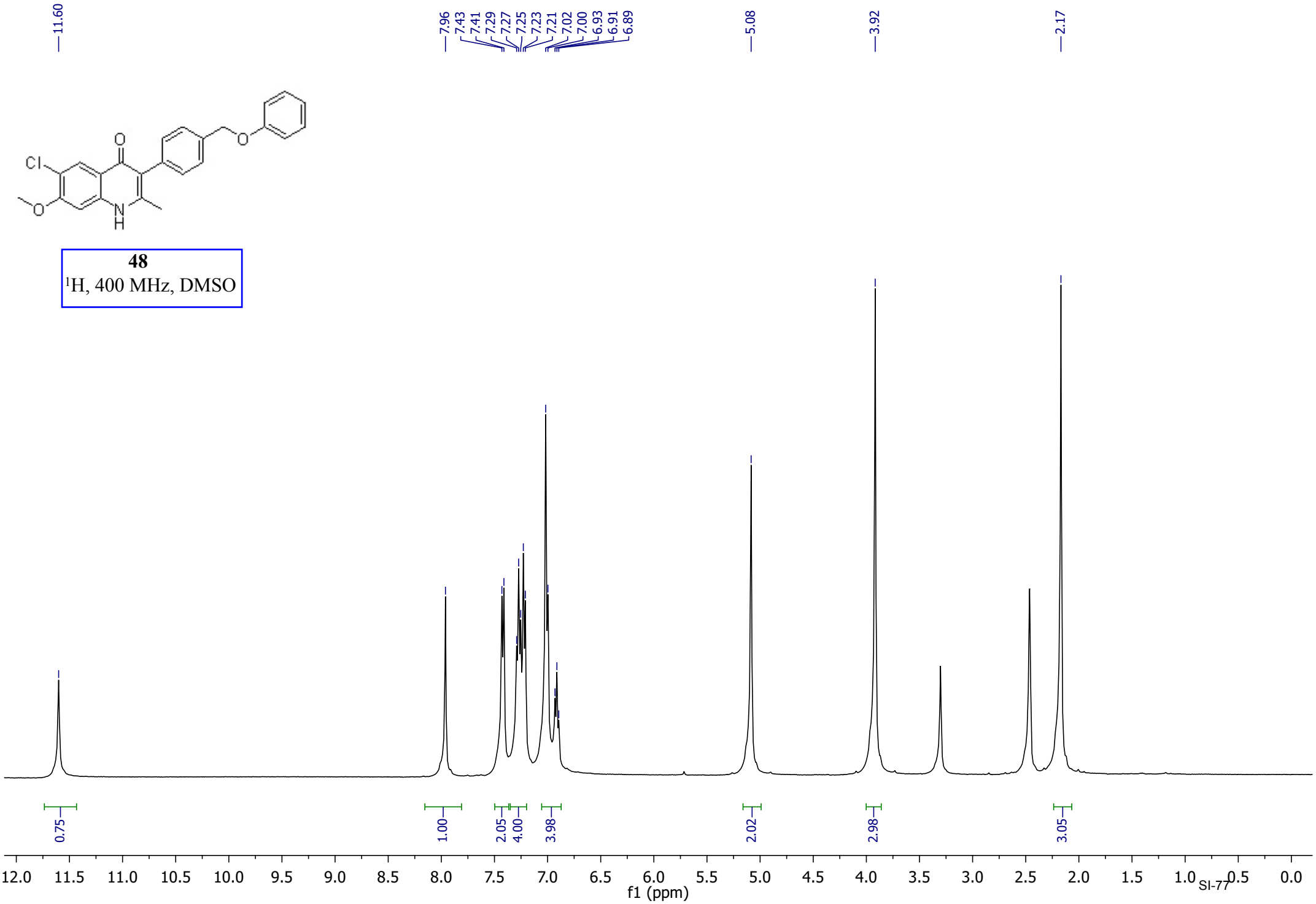


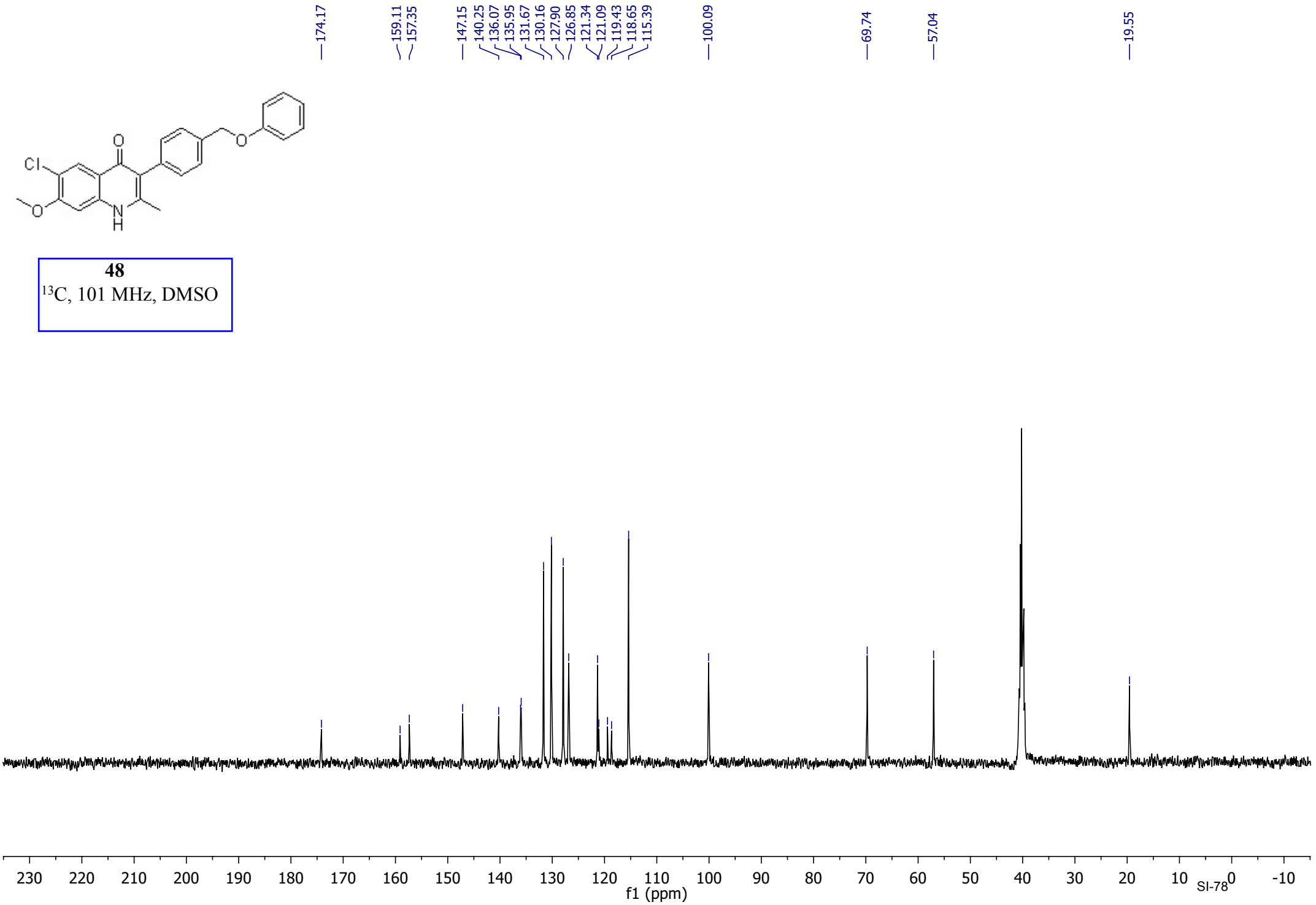
47
^{1}H, 400 MHz, DMSO



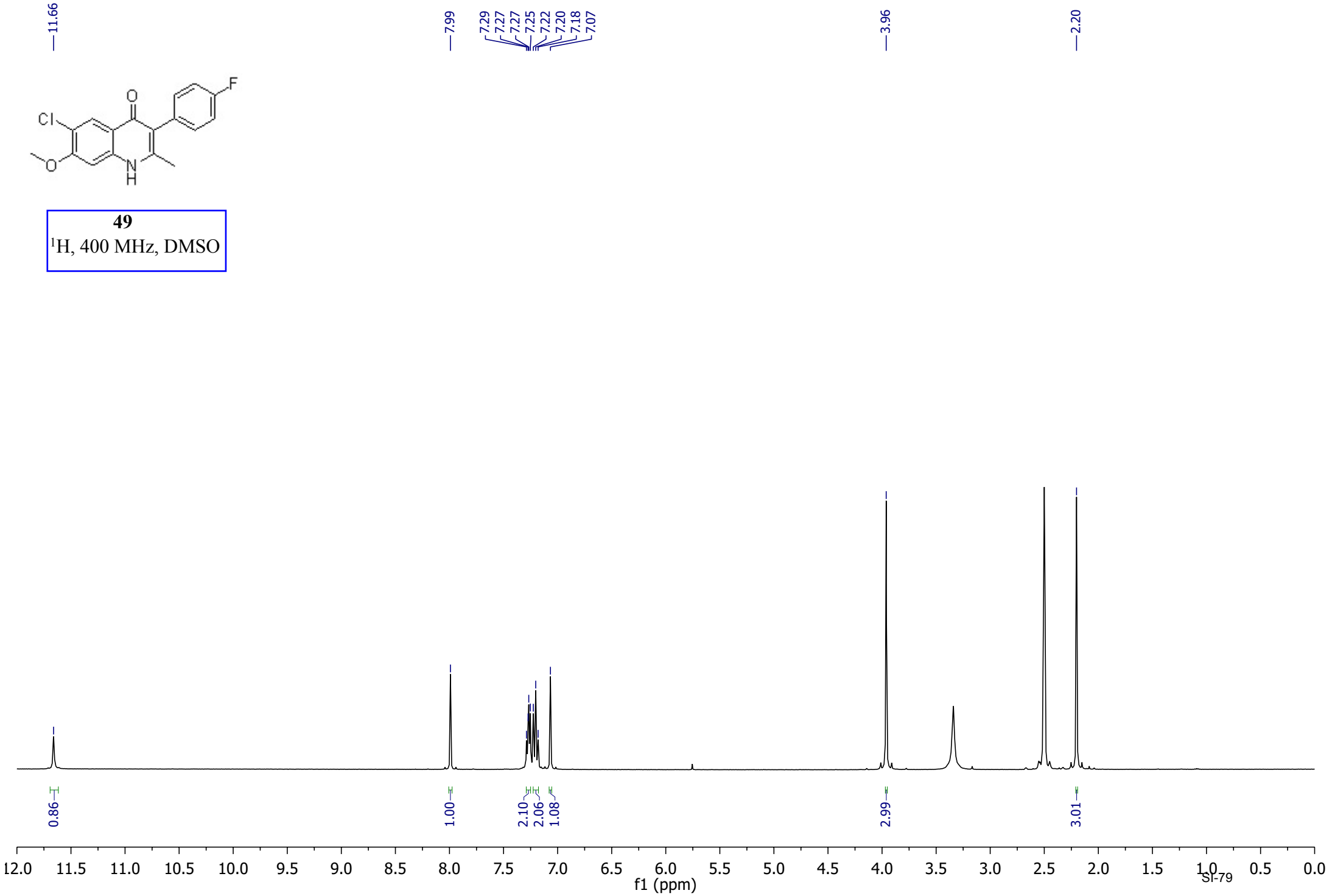

173.64
157.03
156.59
146.38
139.53
137.23
131.98
128.41
128.04
127.76
127.64
126.18
120.32
118.72
117.83
114.06
99.36
69.15
56.35
18.89
Cl
O
O
O
N
H
47
13C, 101 MHz, DMSO
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

48
^{1}H, 400 MHz, DMSO



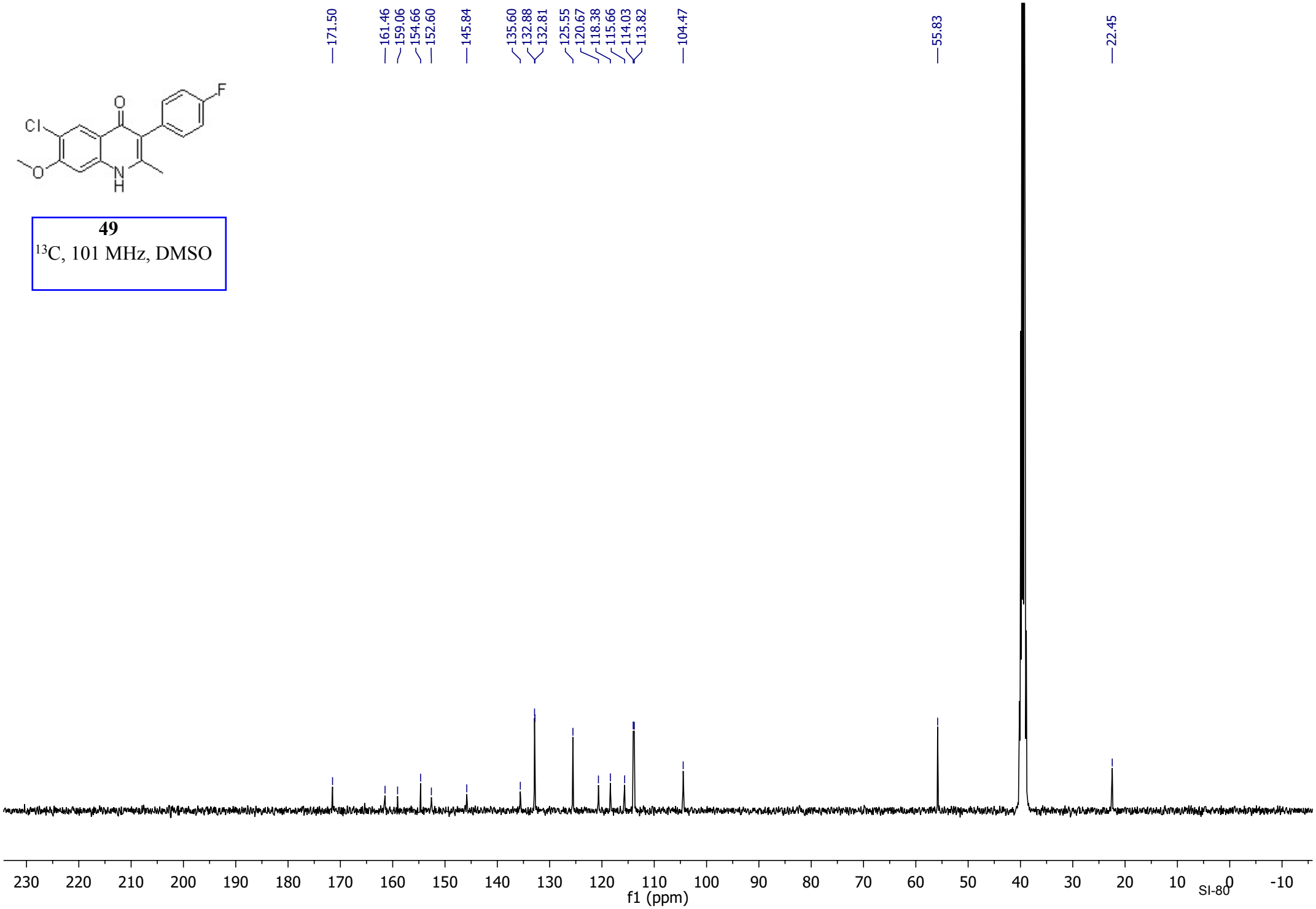

174.17
159.11
157.35
147.15
140.25
136.07
135.95
131.67
130.16
127.90
126.85
121.34
121.09
119.43
118.65
115.39
100.09
69.74
57.04
19.55
Cl
O
O
O
N
H
48
13C, 101 MHz, DMSO
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
SI-78

49
^{1}H, 400 MHz, DMSO



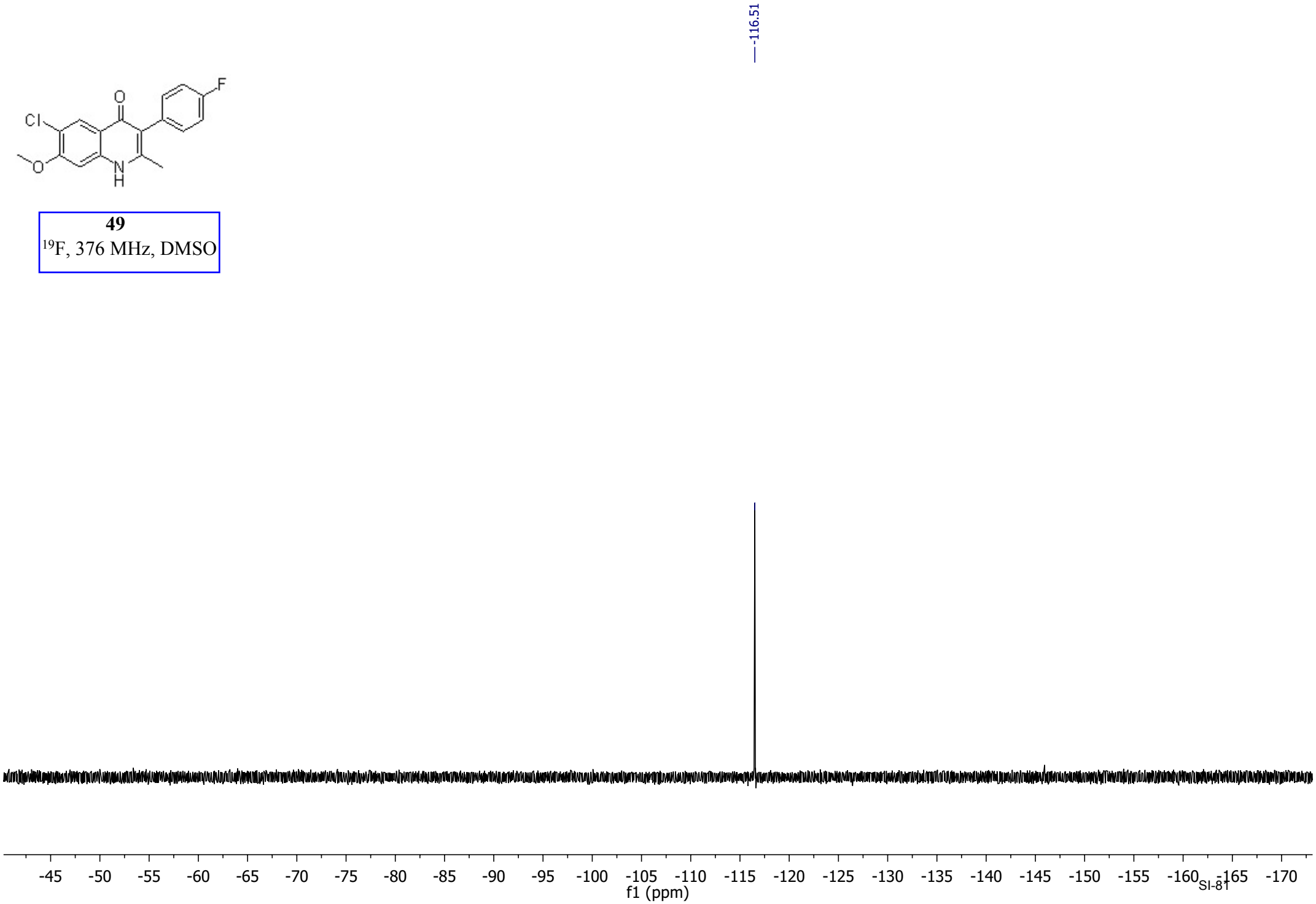
49

^{13}C, 101 MHz, DMSO

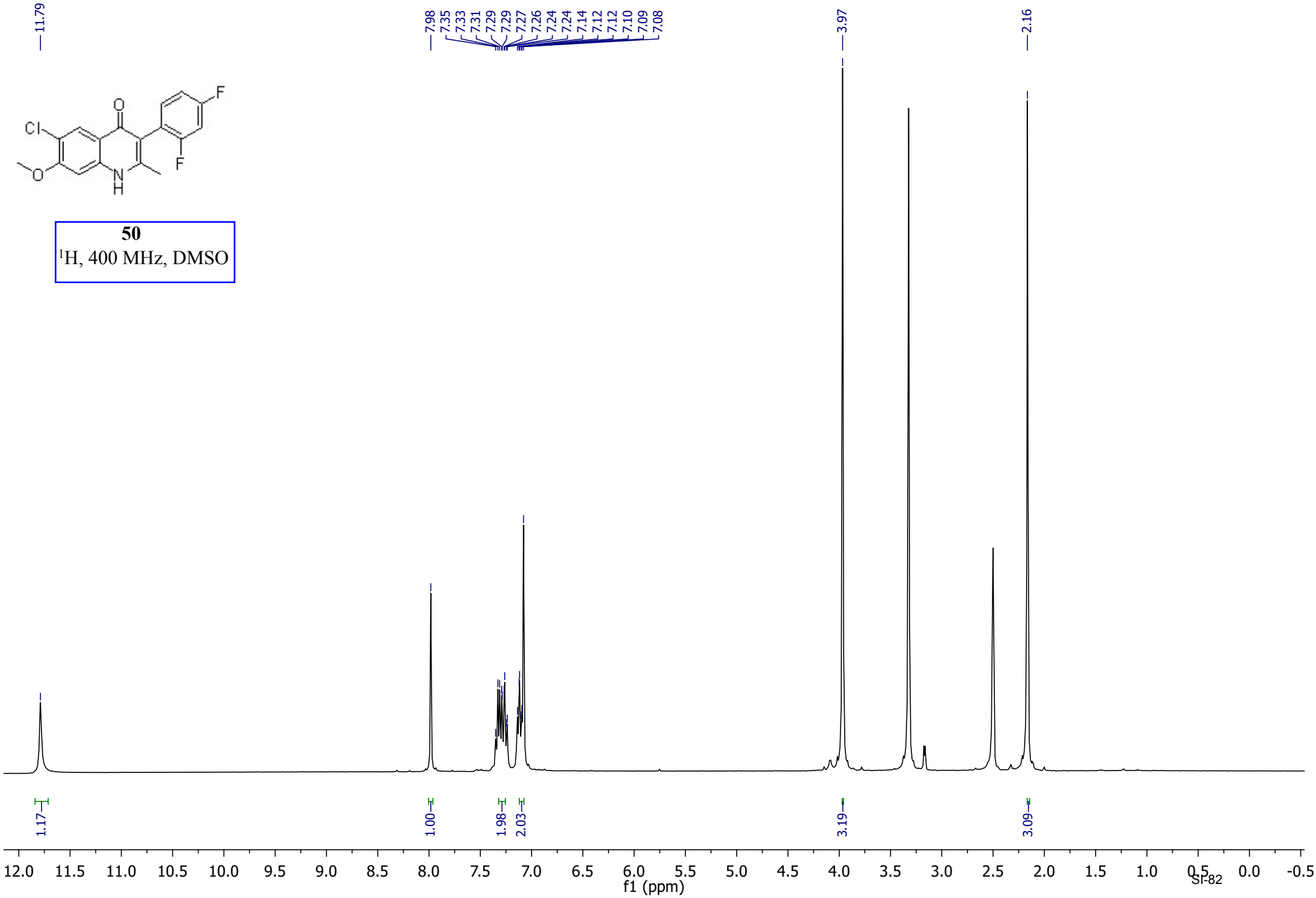


49

^{19}F, 376 MHz, DMSO

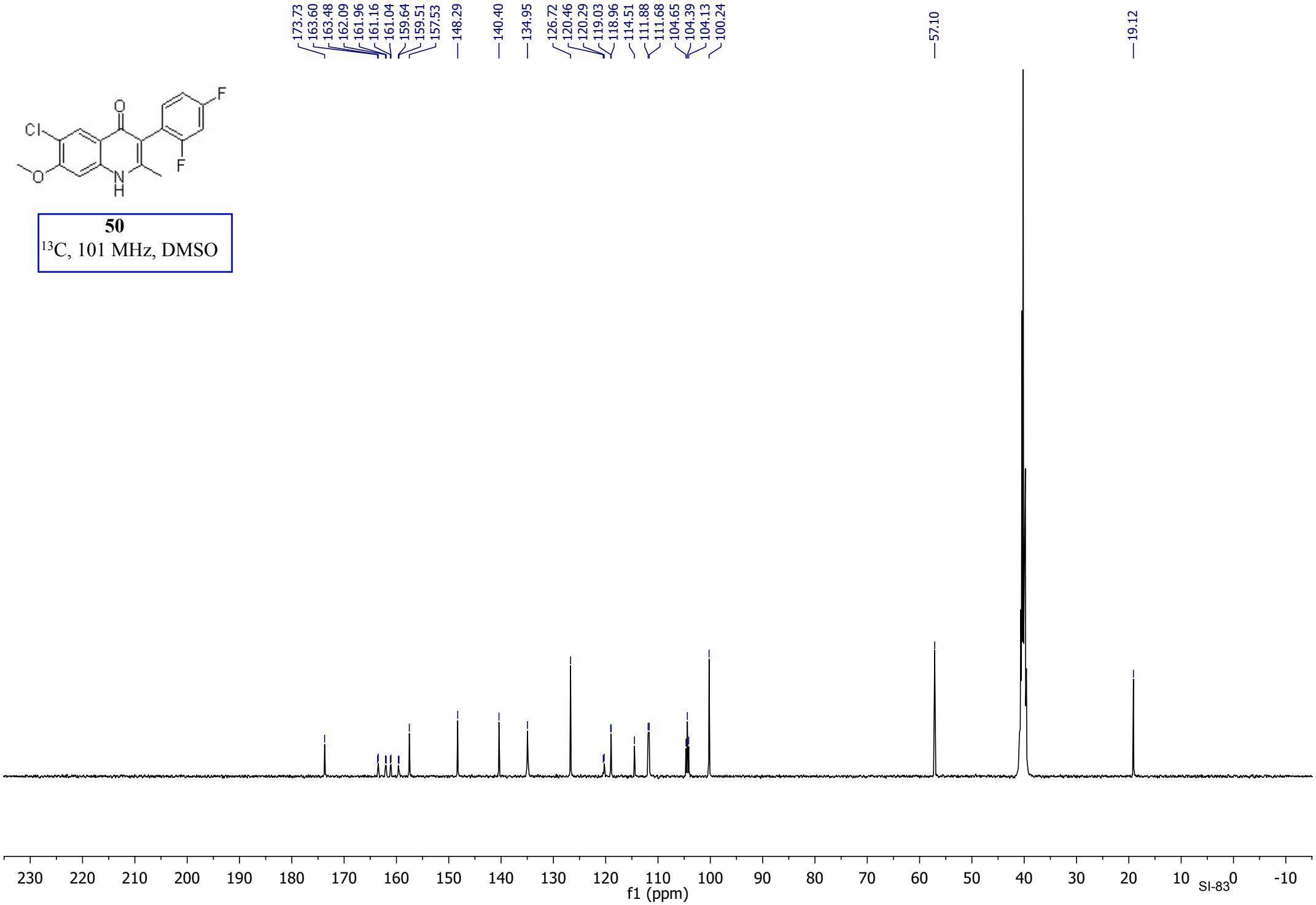


50
^{1}H, 400 MHz, DMSO



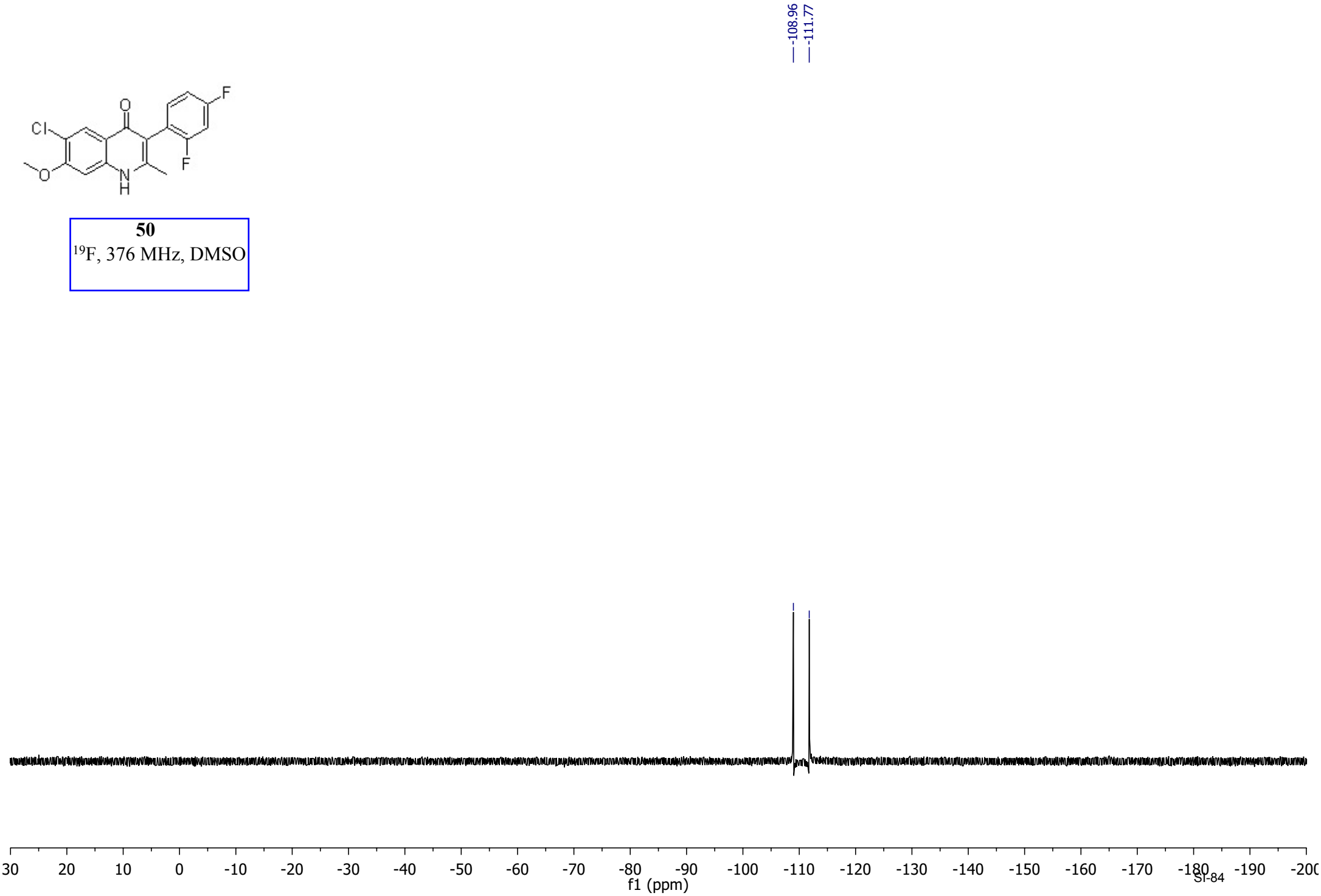
50

^{13}C, 101 MHz, DMSO

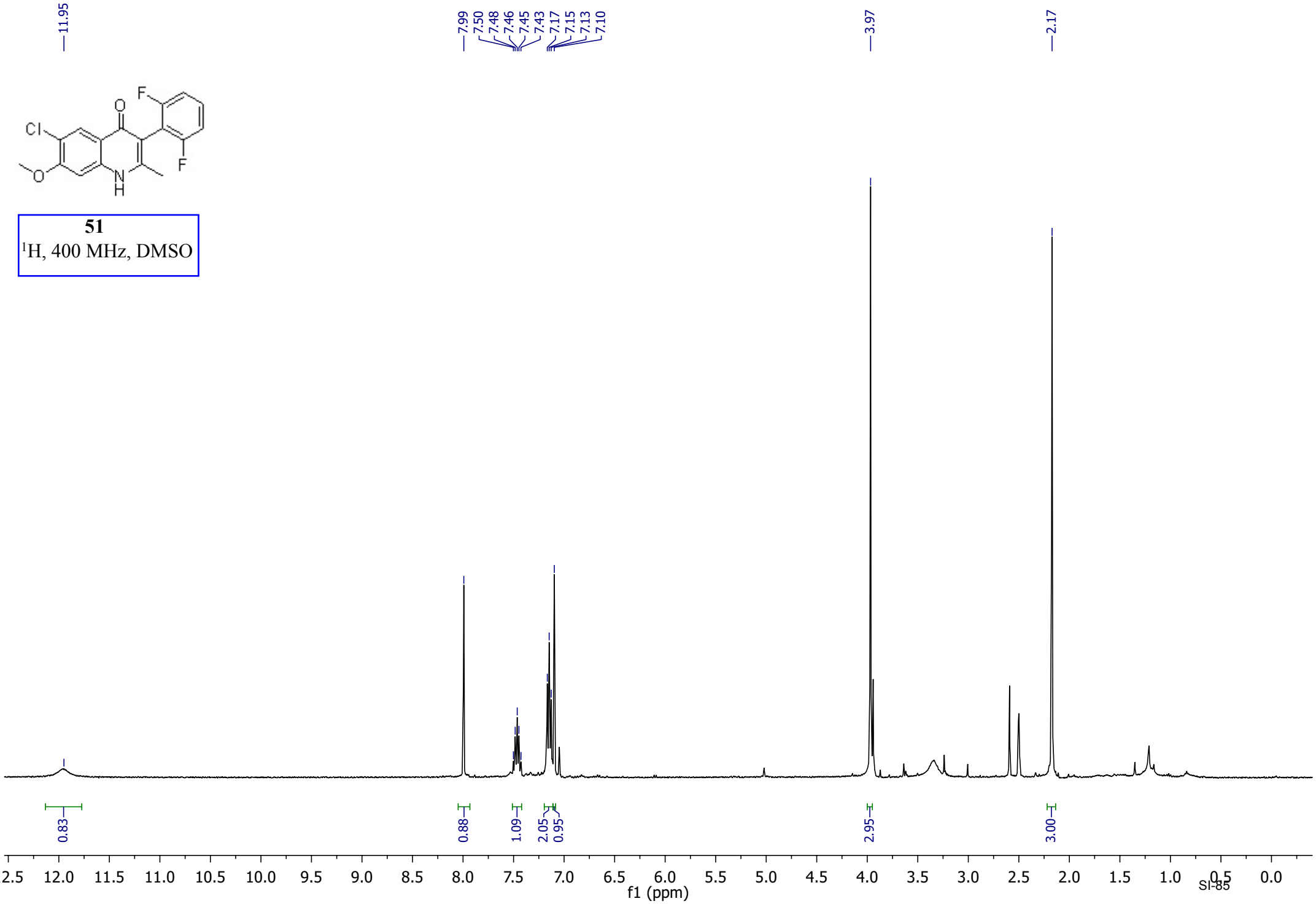


50

^{19}F, 376 MHz, DMSO

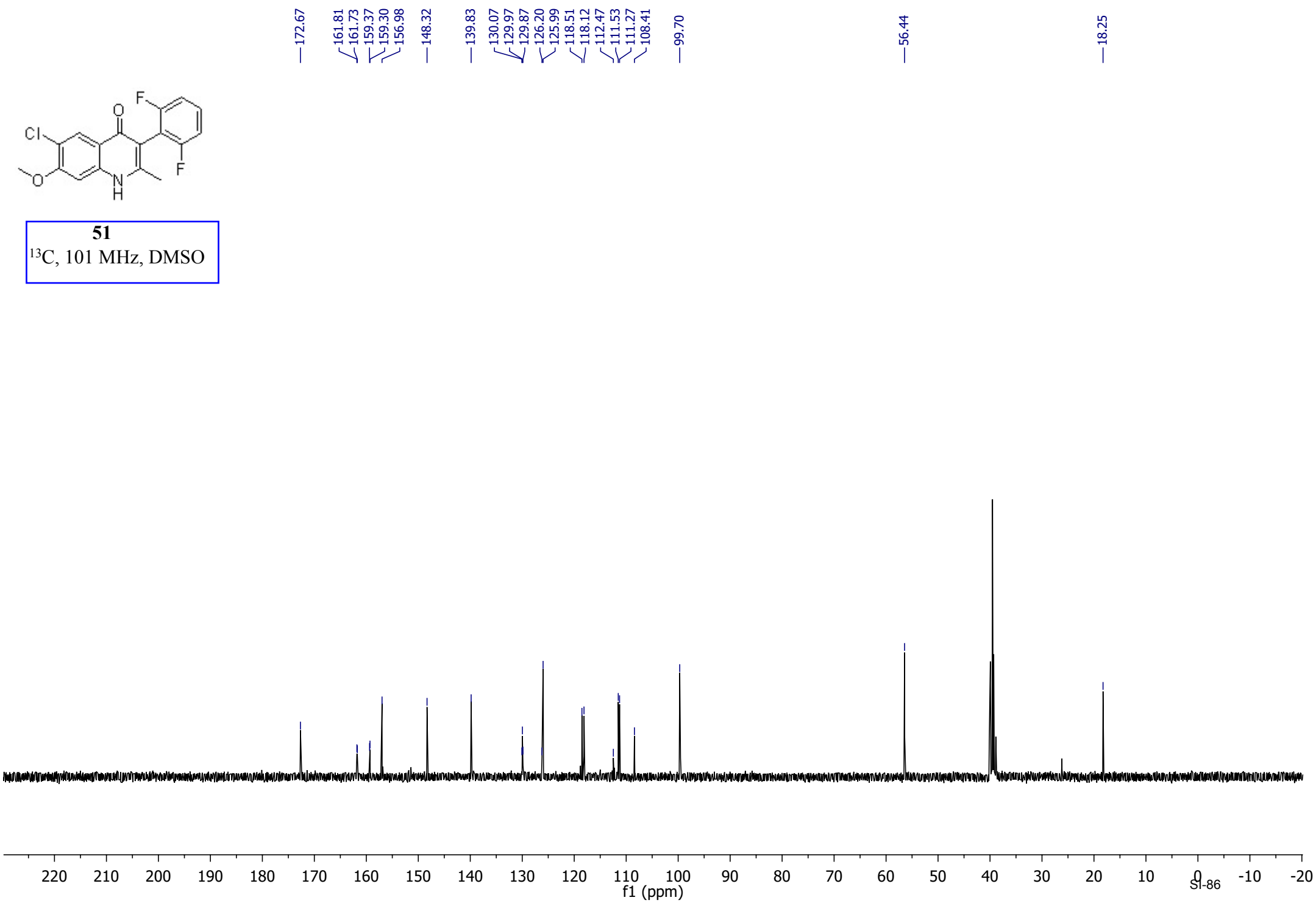


51
^{1}H, 400 MHz, DMSO

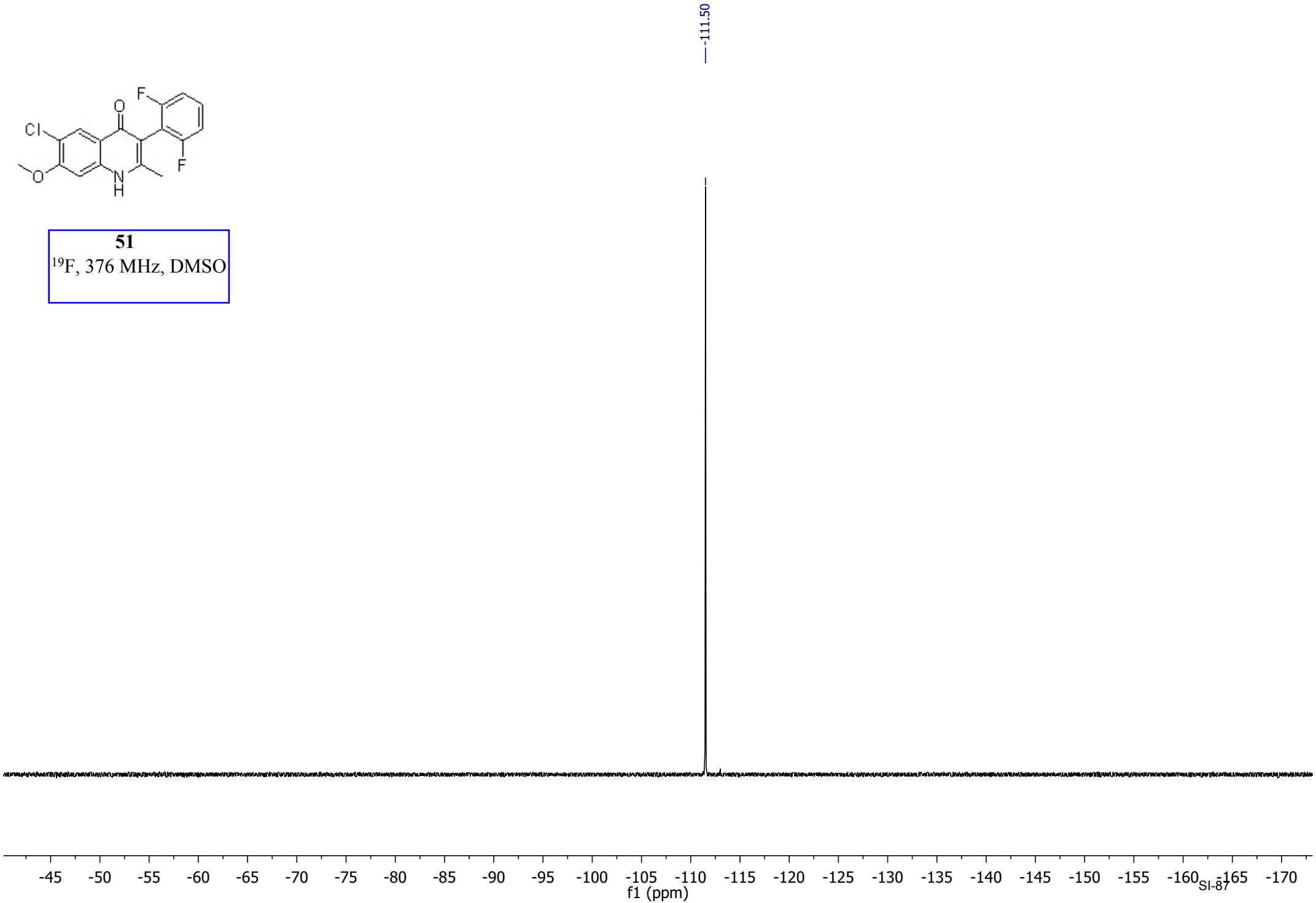


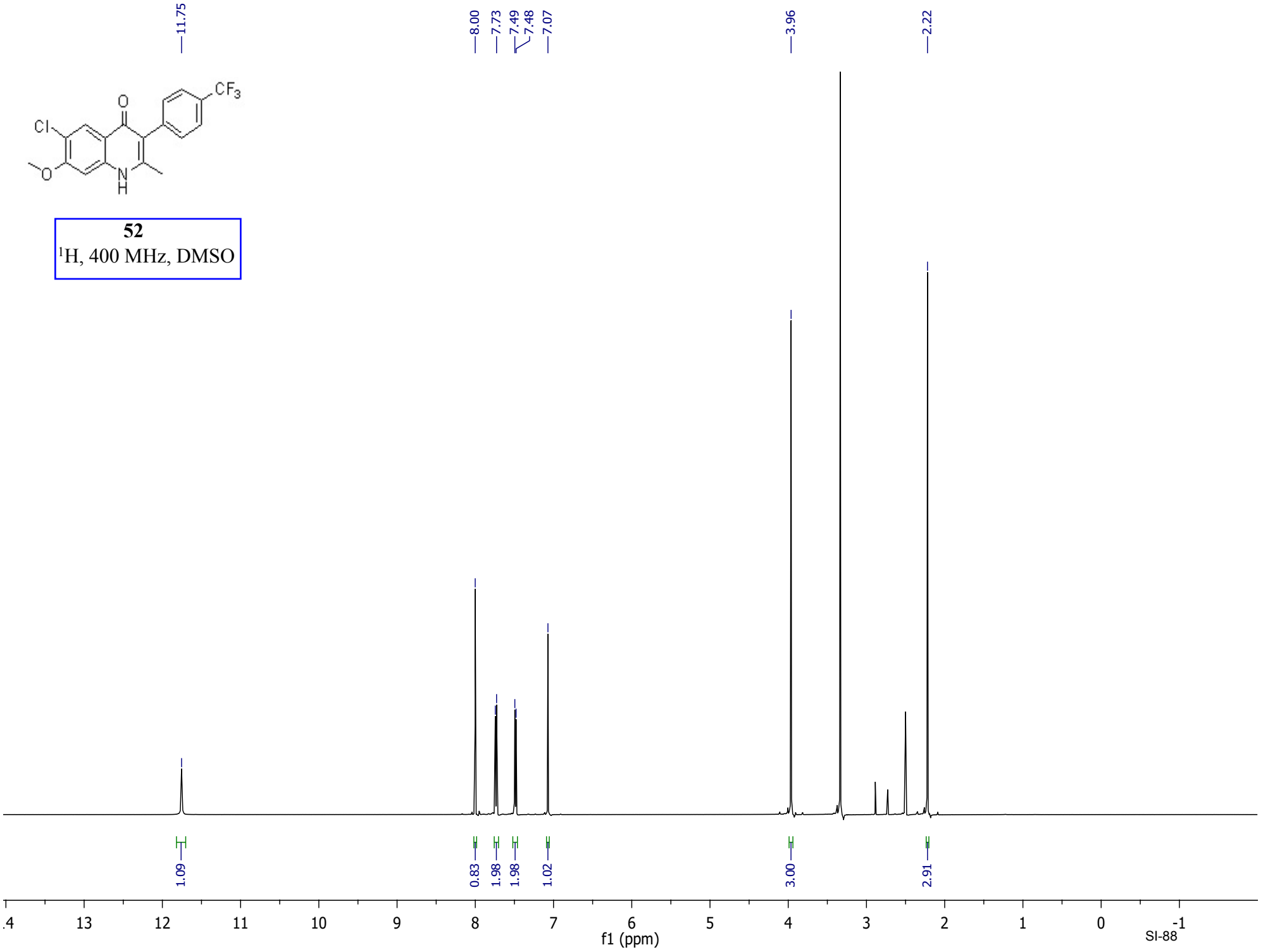
51

^{13}C, 101 MHz, DMSO



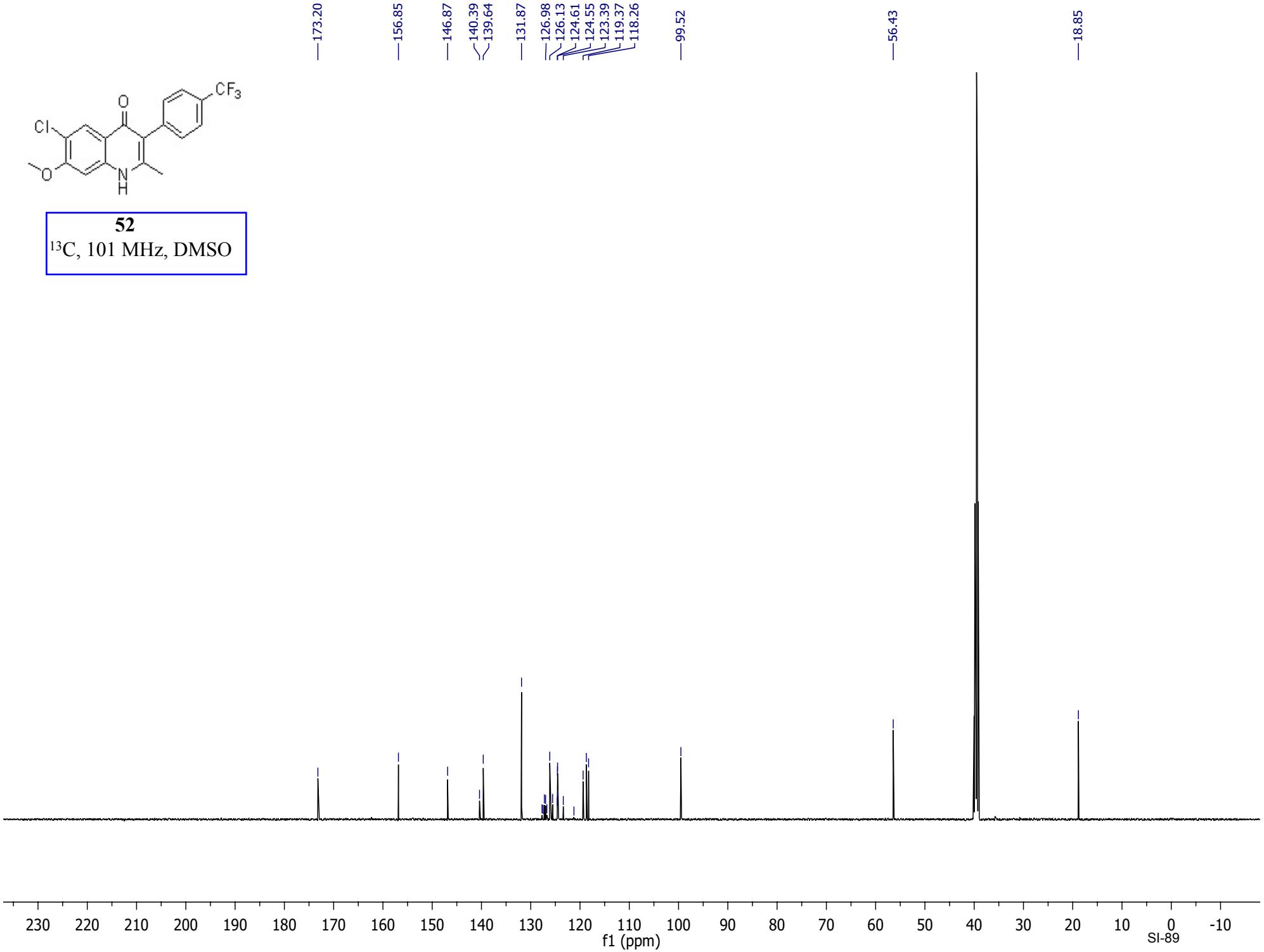
51
^{19}F, 376 MHz, DMSO




11.75
8.00
7.73
7.49
7.48
7.07
3.96
2.22
Cl
O
CF3
O
N
H
52
1H, 400 MHz, DMSO
1.09
0.83
1.98
1.98
1.02
3.00
2.91
f1 (ppm)
SI-88

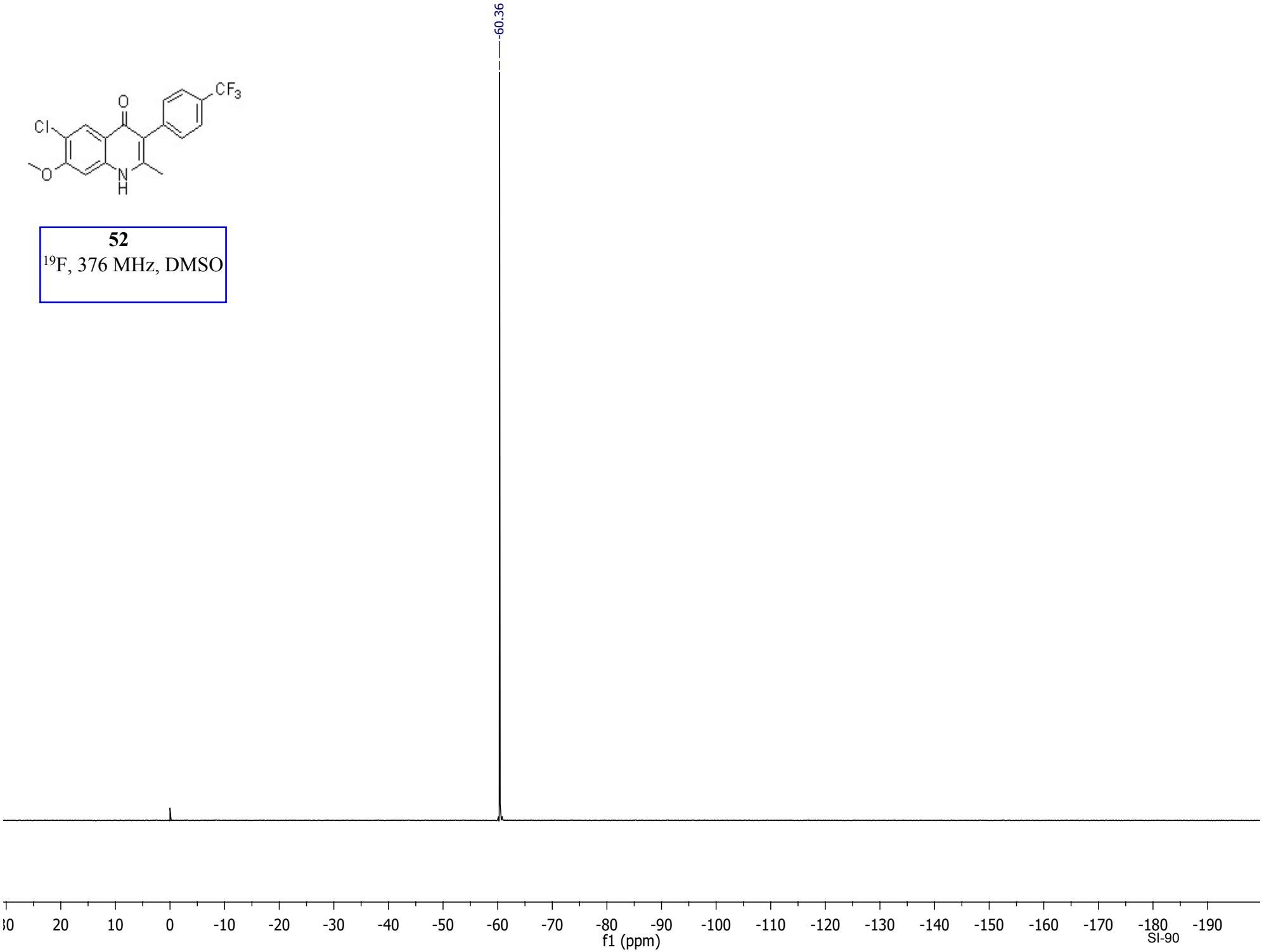
52

^{13}C, 101 MHz, DMSO

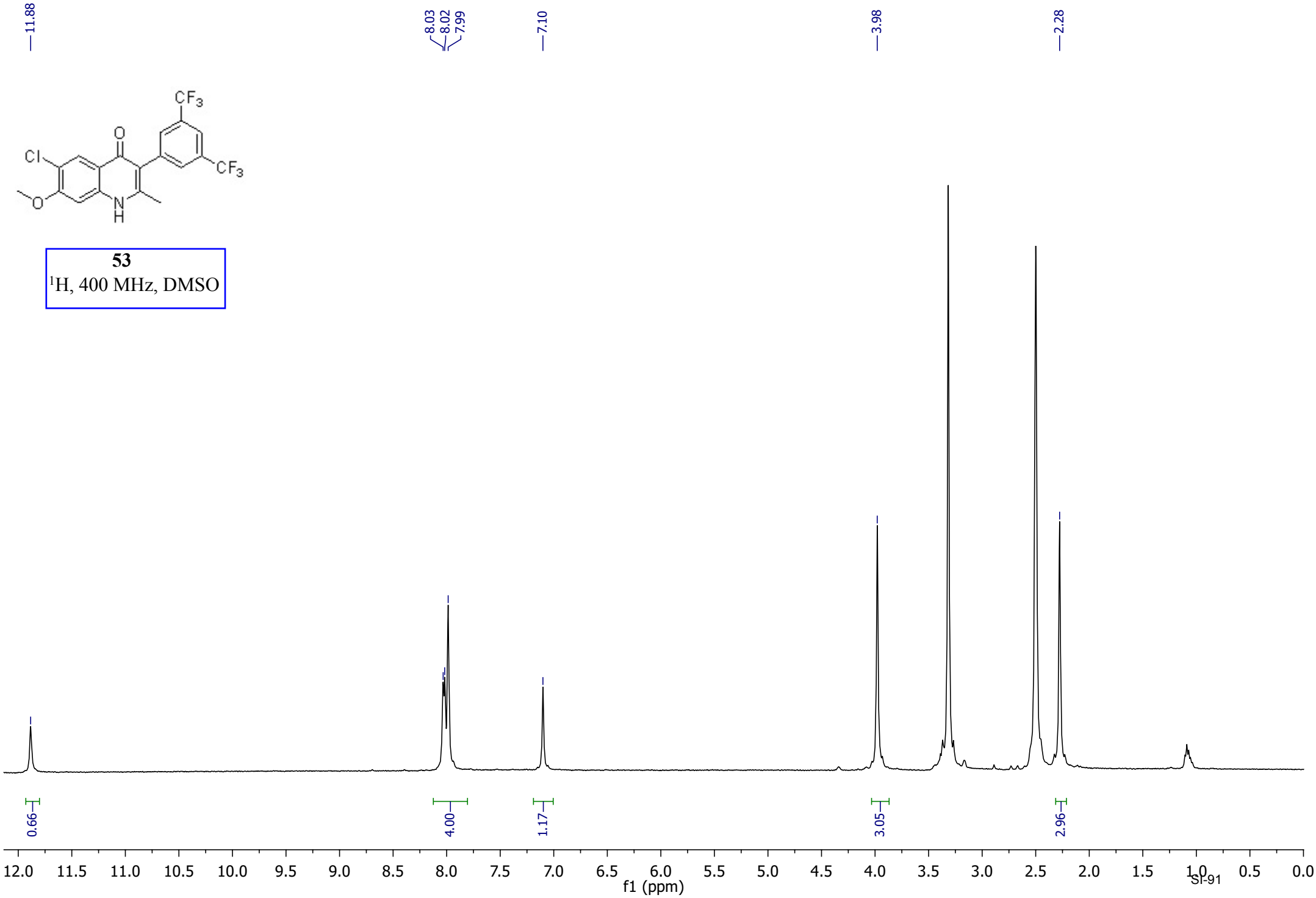


52

^{19}F, 376 MHz, DMSO

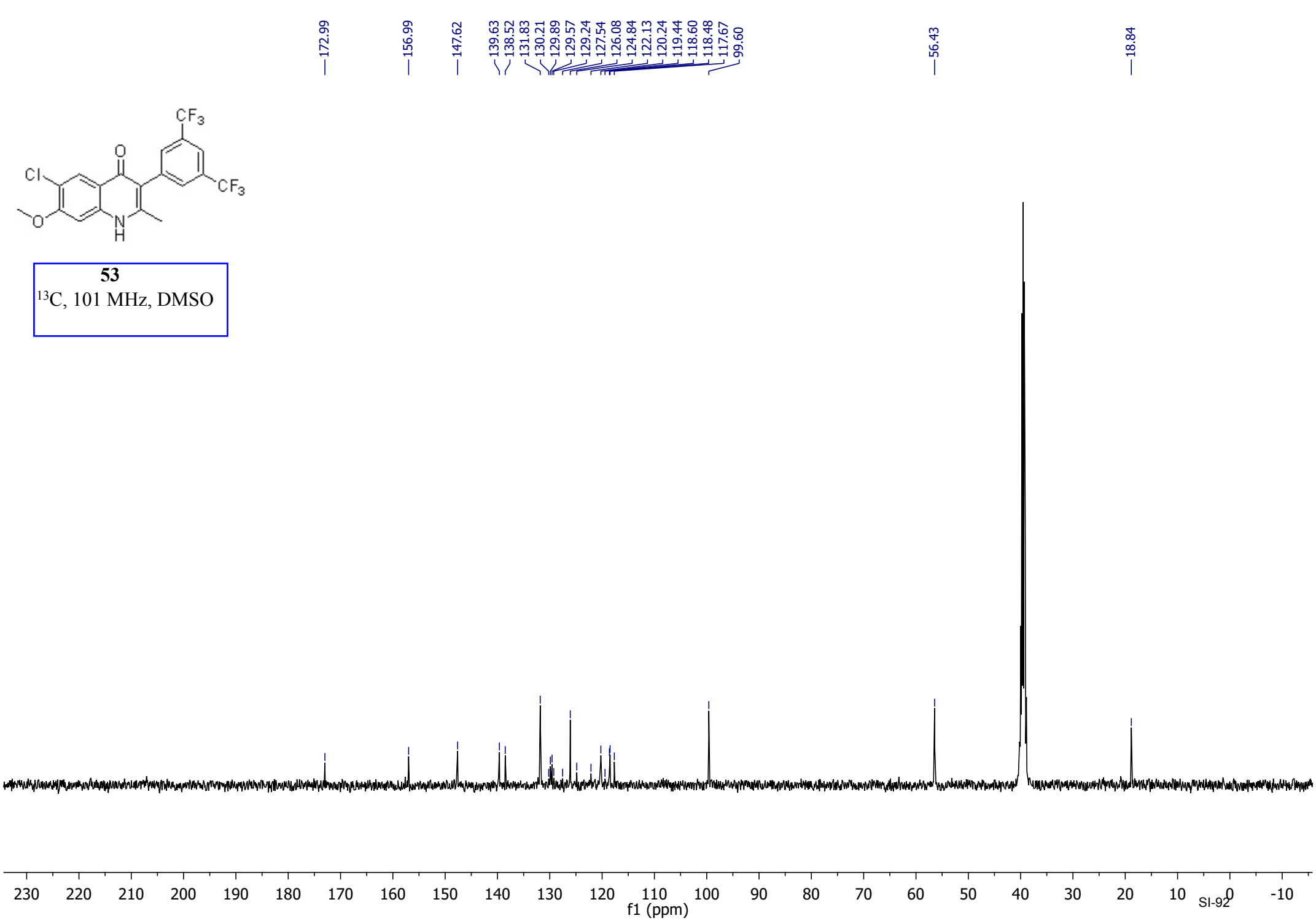


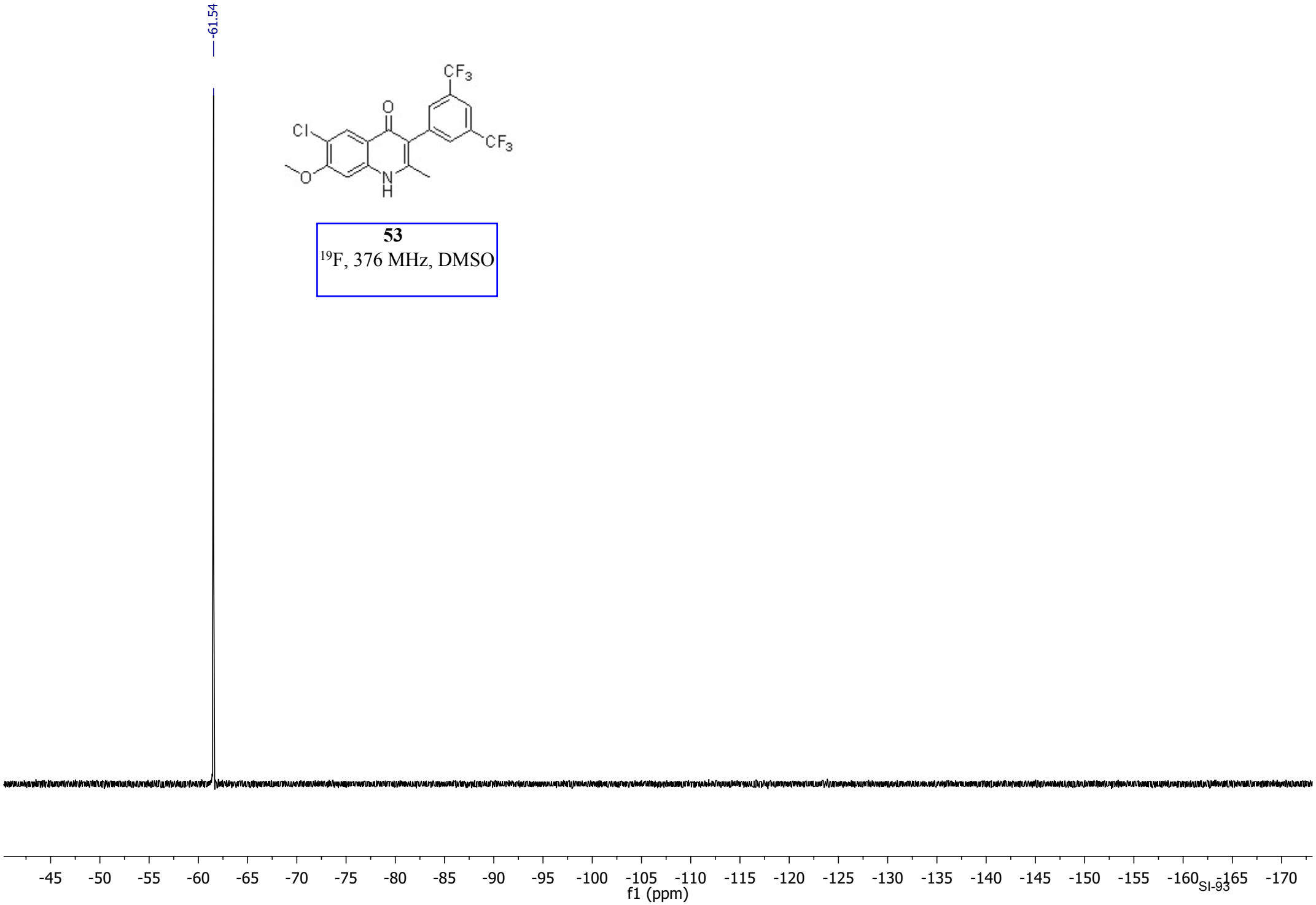
53
^{1}H, 400 MHz, DMSO



53

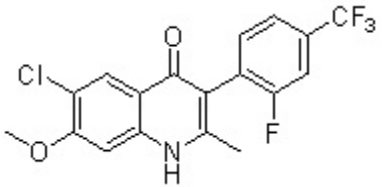
^{13}C, 101 MHz, DMSO





53

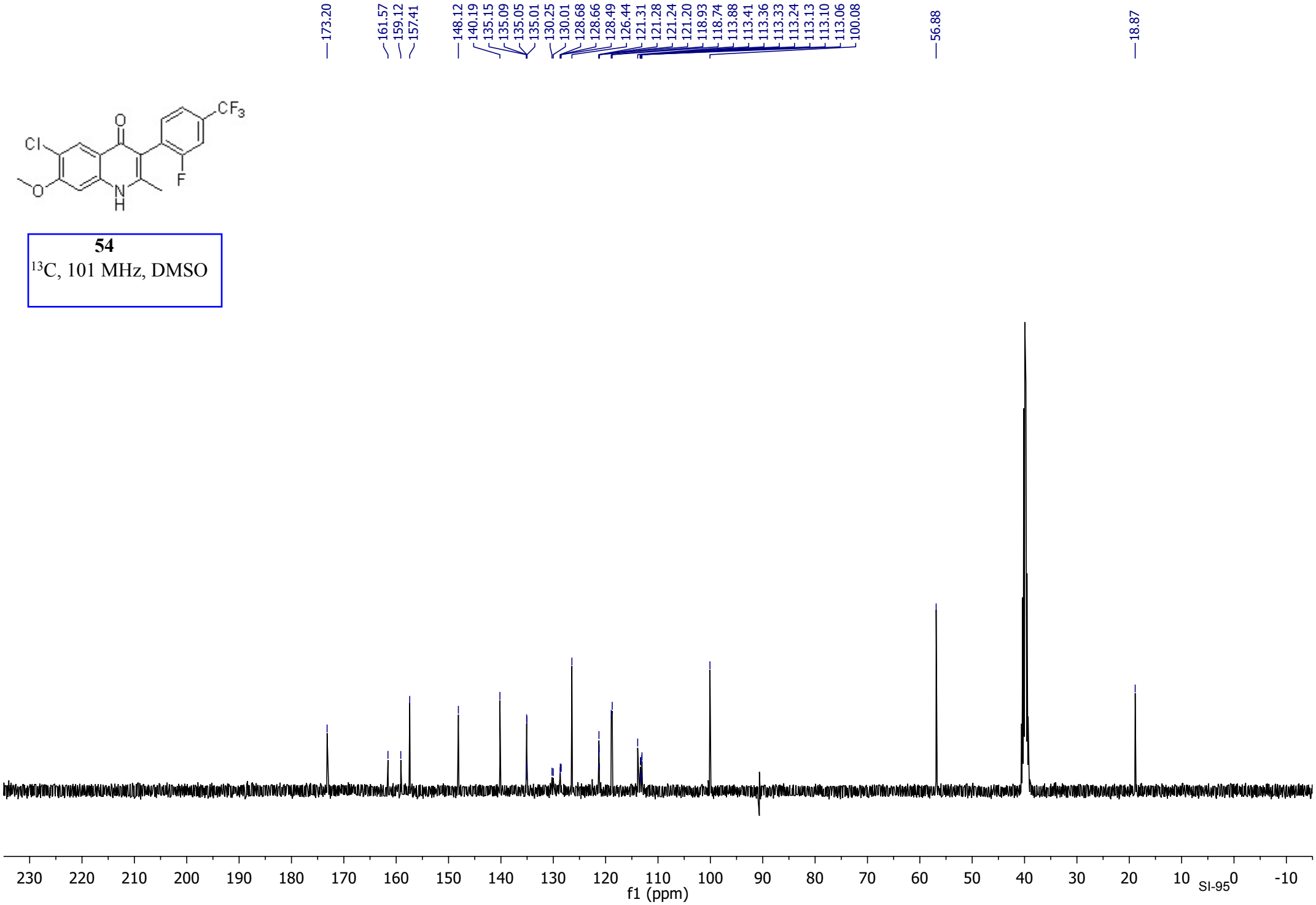
^{19}F, 376 MHz, DMSO



54
^{1}H, 400 MHz, DMSO

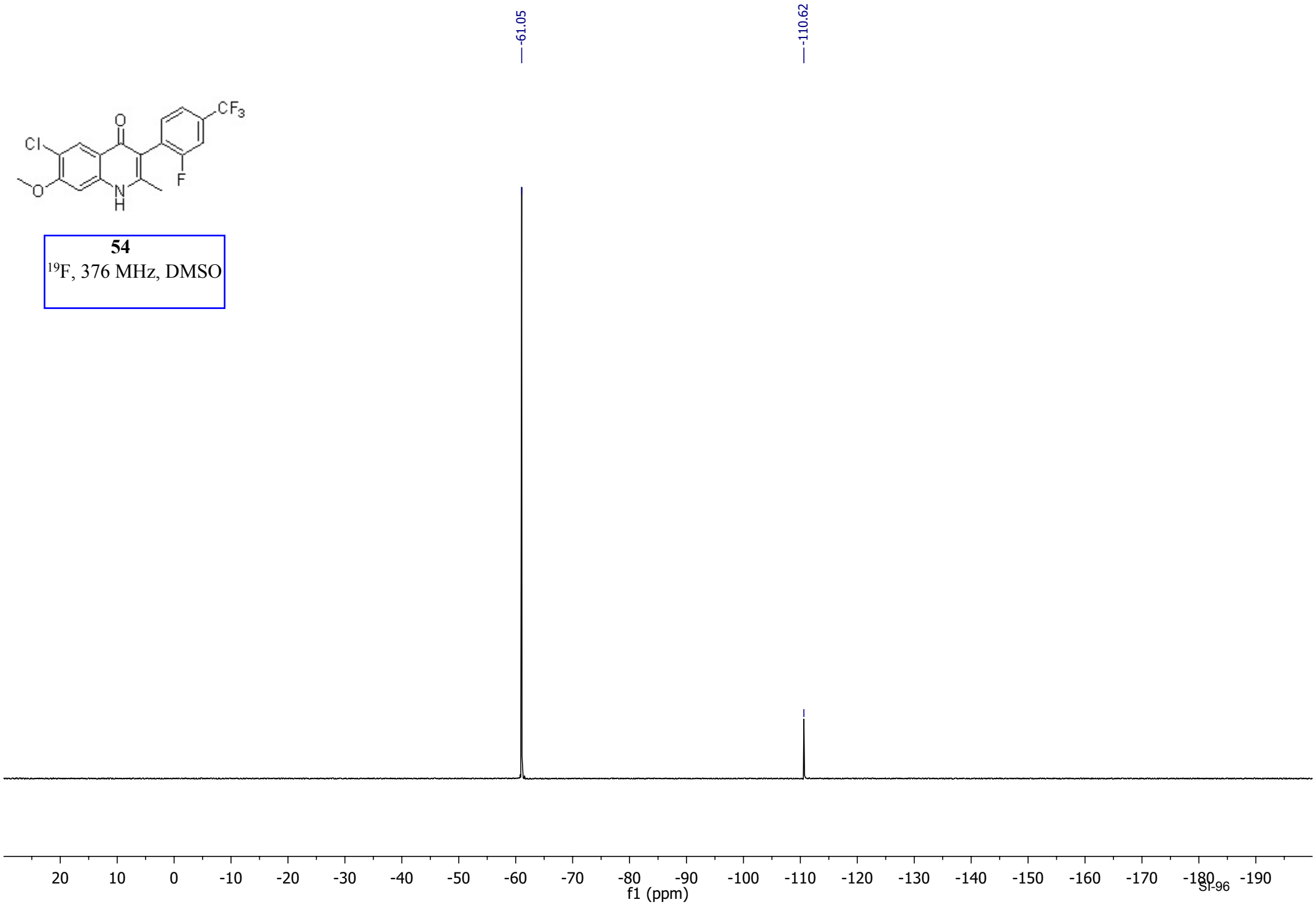
54

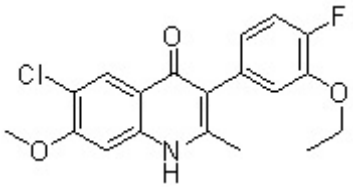
^{13}C, 101 MHz, DMSO



54

^{19}F, 376 MHz, DMSO

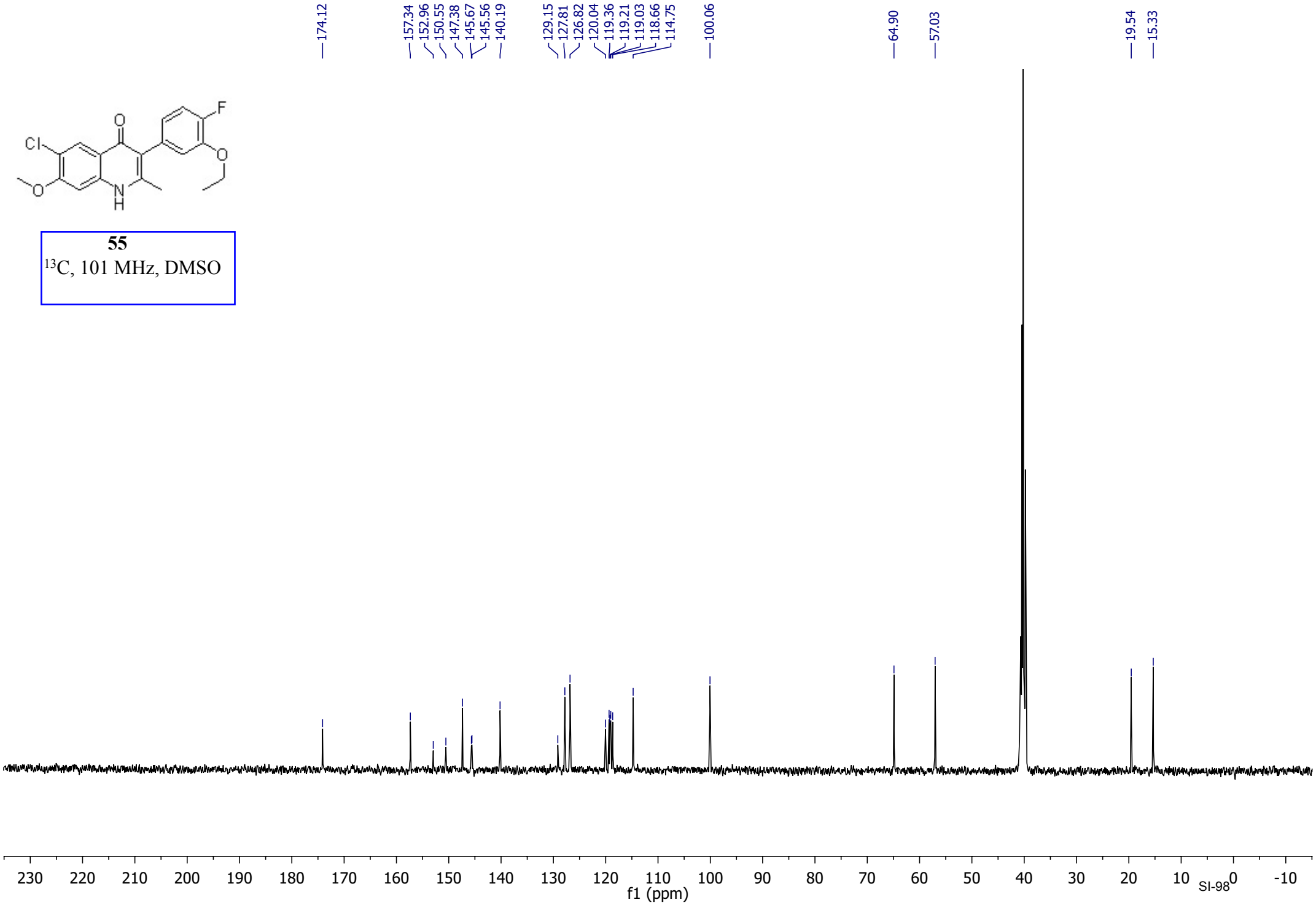




55
^{1}H, 400 MHz, DMSO

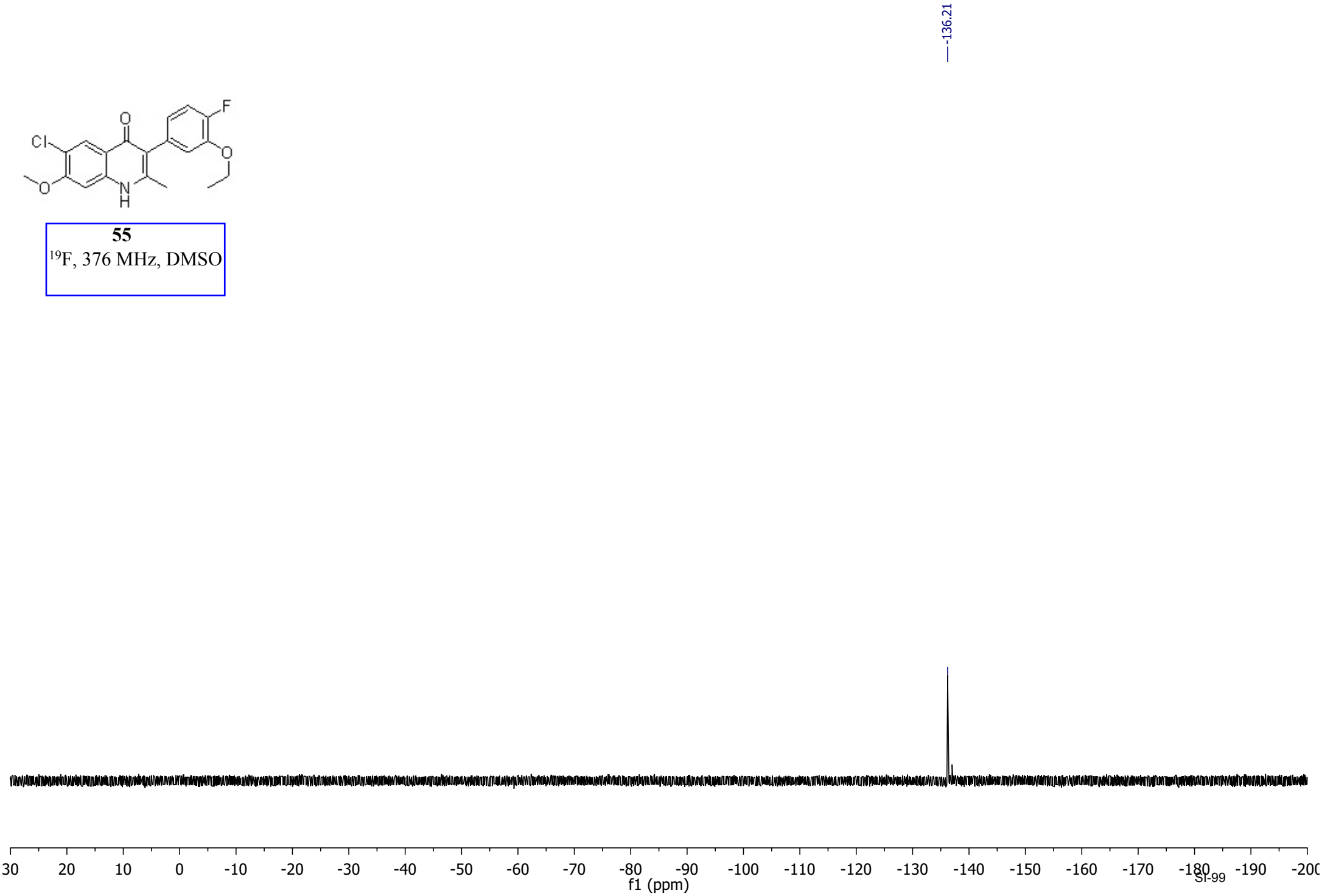
55

^{13}C, 101 MHz, DMSO

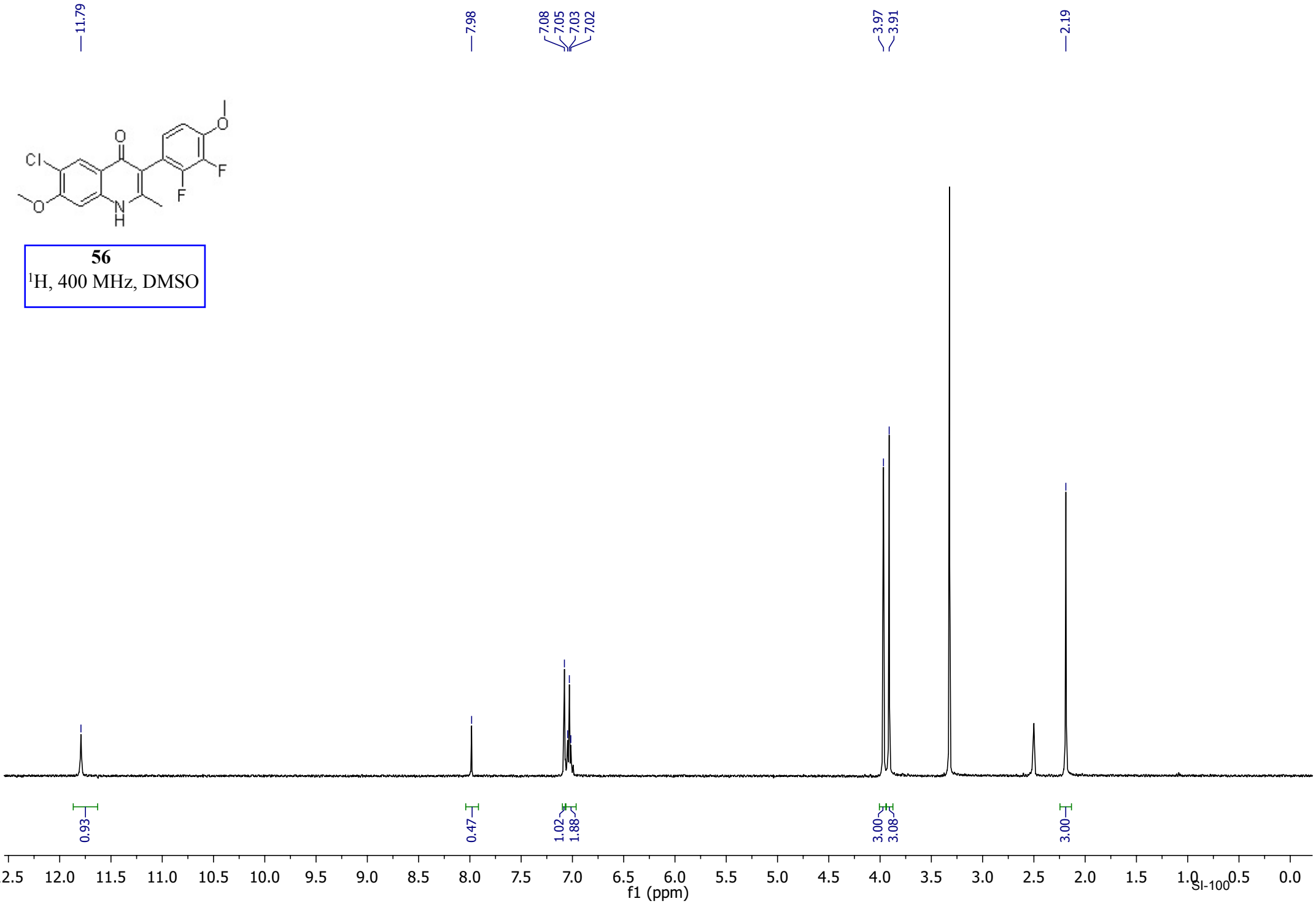


55

^{19}F, 376 MHz, DMSO

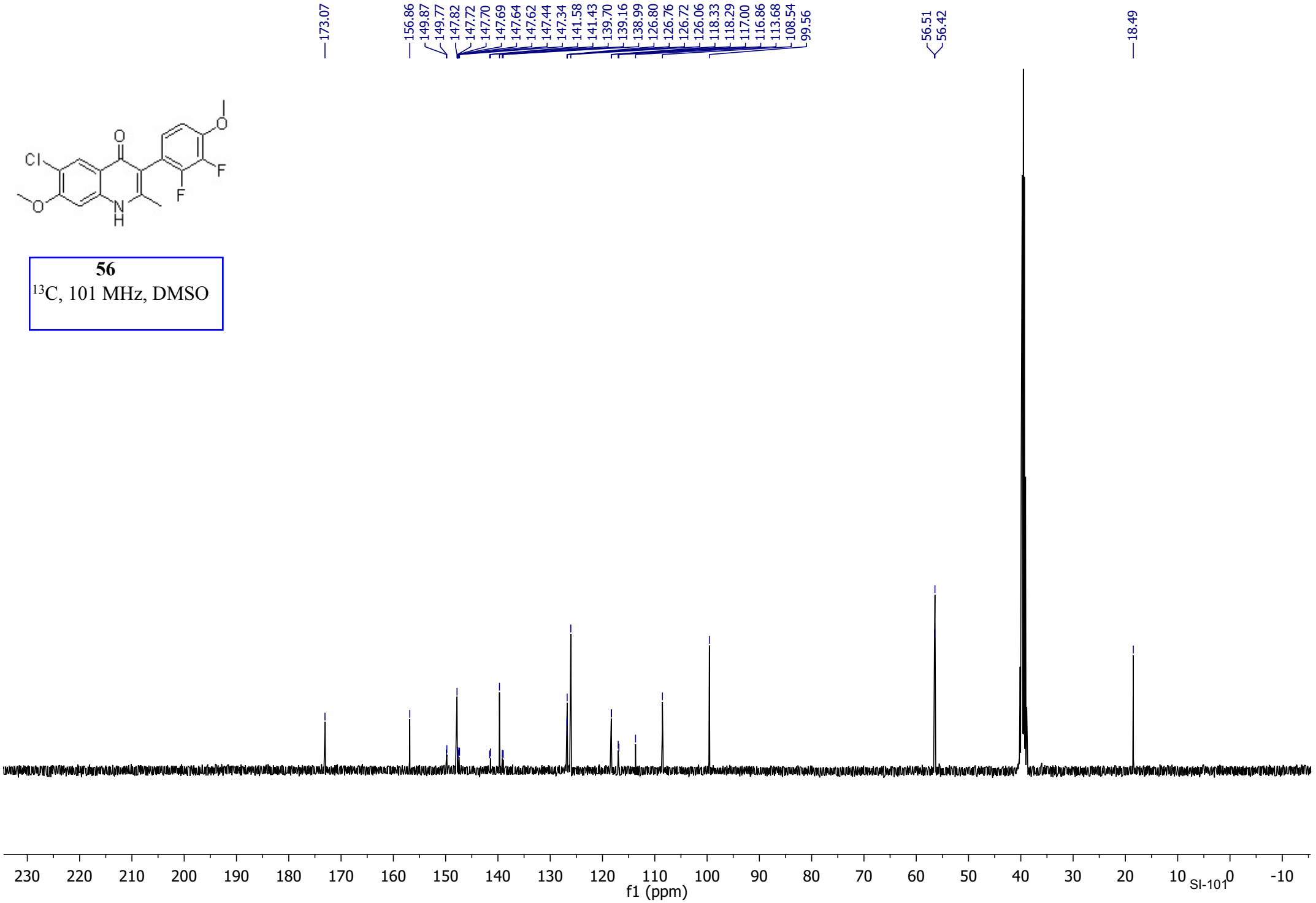


56
^{1}H, 400 MHz, DMSO



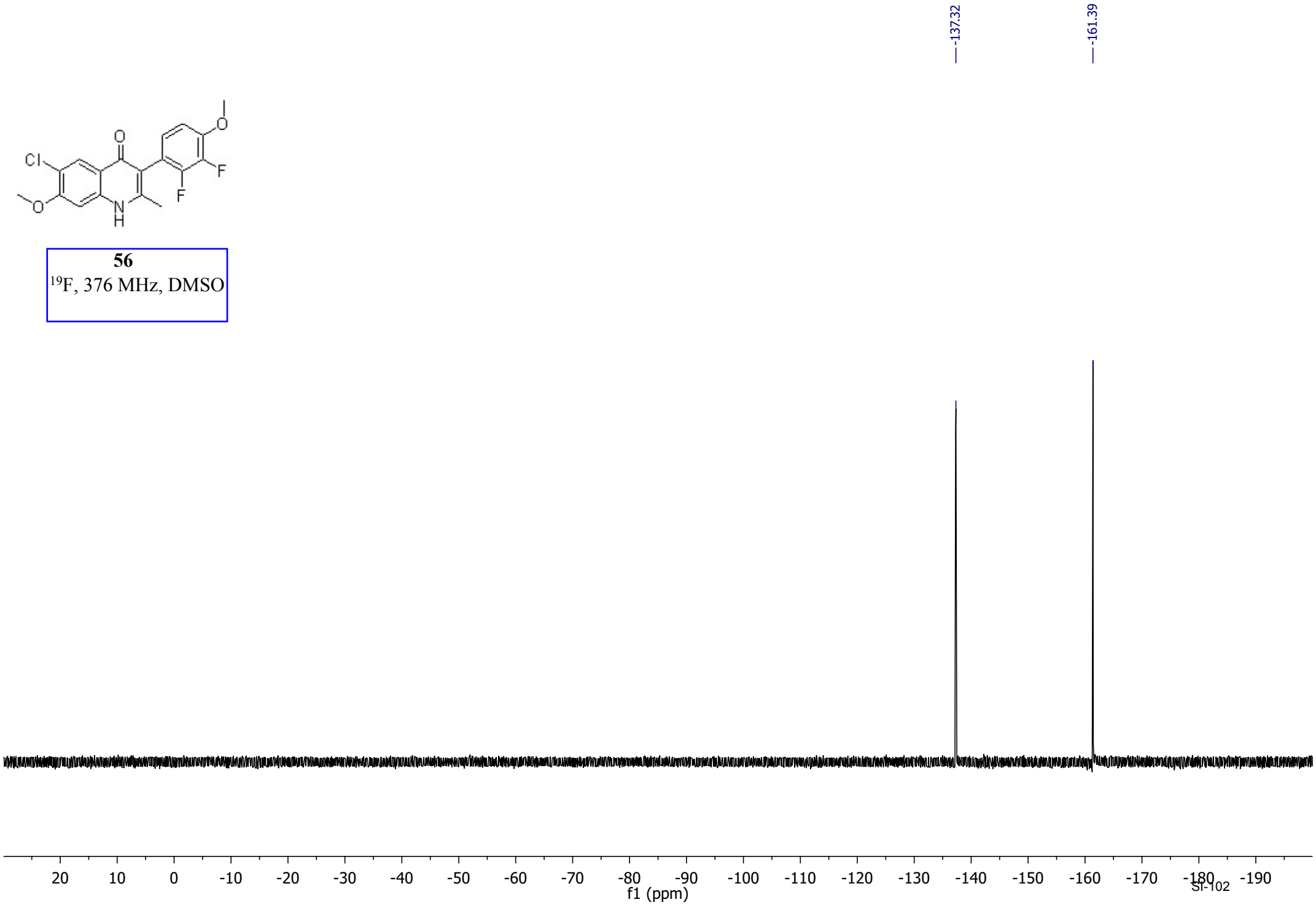
56

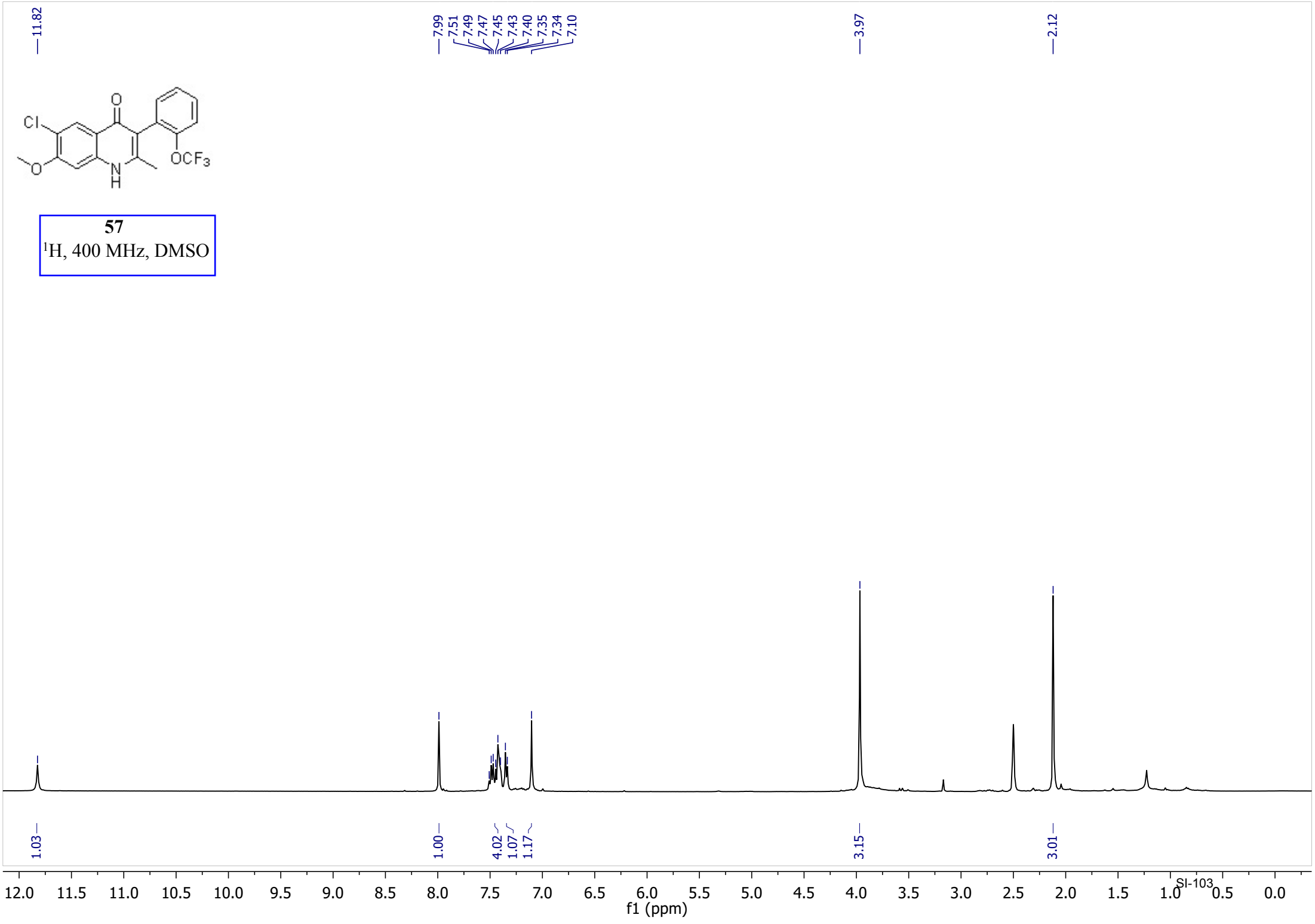
^{13}C, 101 MHz, DMSO

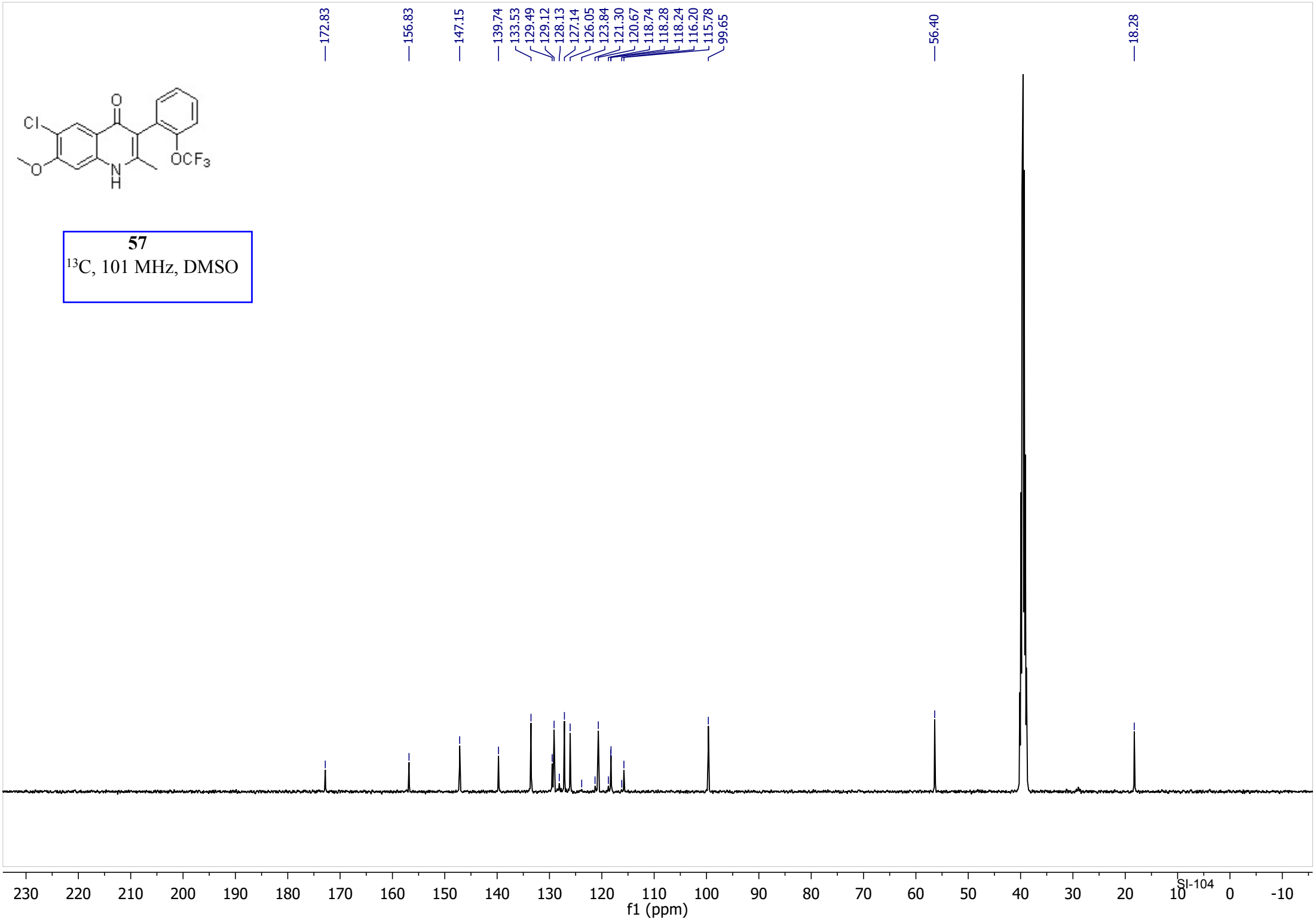


56

^{19}F, 376 MHz, DMSO

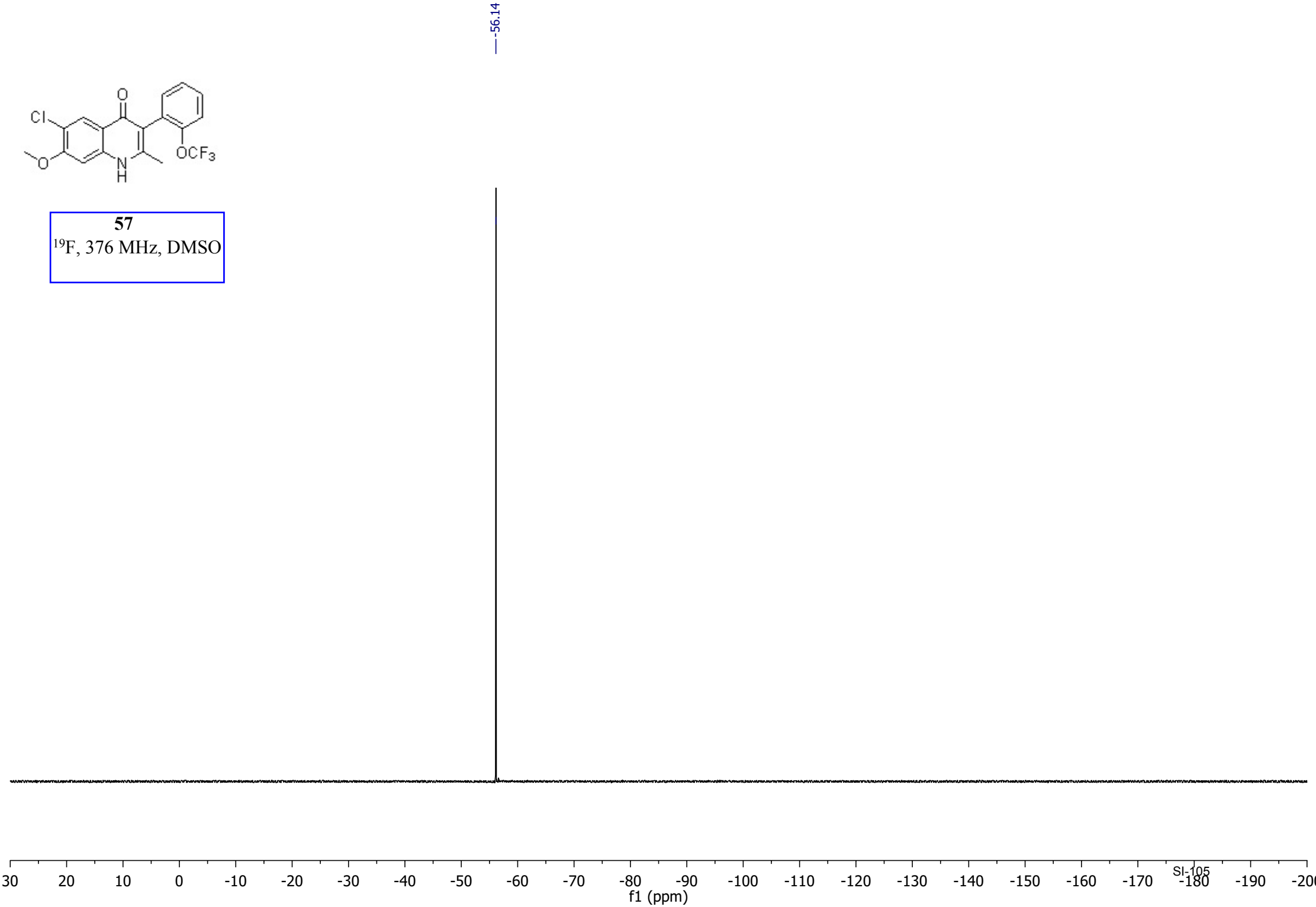



11.82
7.99
7.51
7.49
7.47
7.45
7.43
7.40
7.35
7.34
7.10
3.97
2.12
Cl
O
N
H
OCF3
57
1H, 400 MHz, DMSO
1.03
1.00
4.02
1.07
1.17
3.15
3.01
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
SI-103


172.83
156.83
147.15
139.74
133.53
129.49
129.12
128.13
127.14
126.05
123.84
121.30
120.67
118.74
118.28
118.24
116.20
115.78
99.65
56.40
18.28
Cl
O
N
H
OCF3
57
13C, 101 MHz, DMSO
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
SI-104

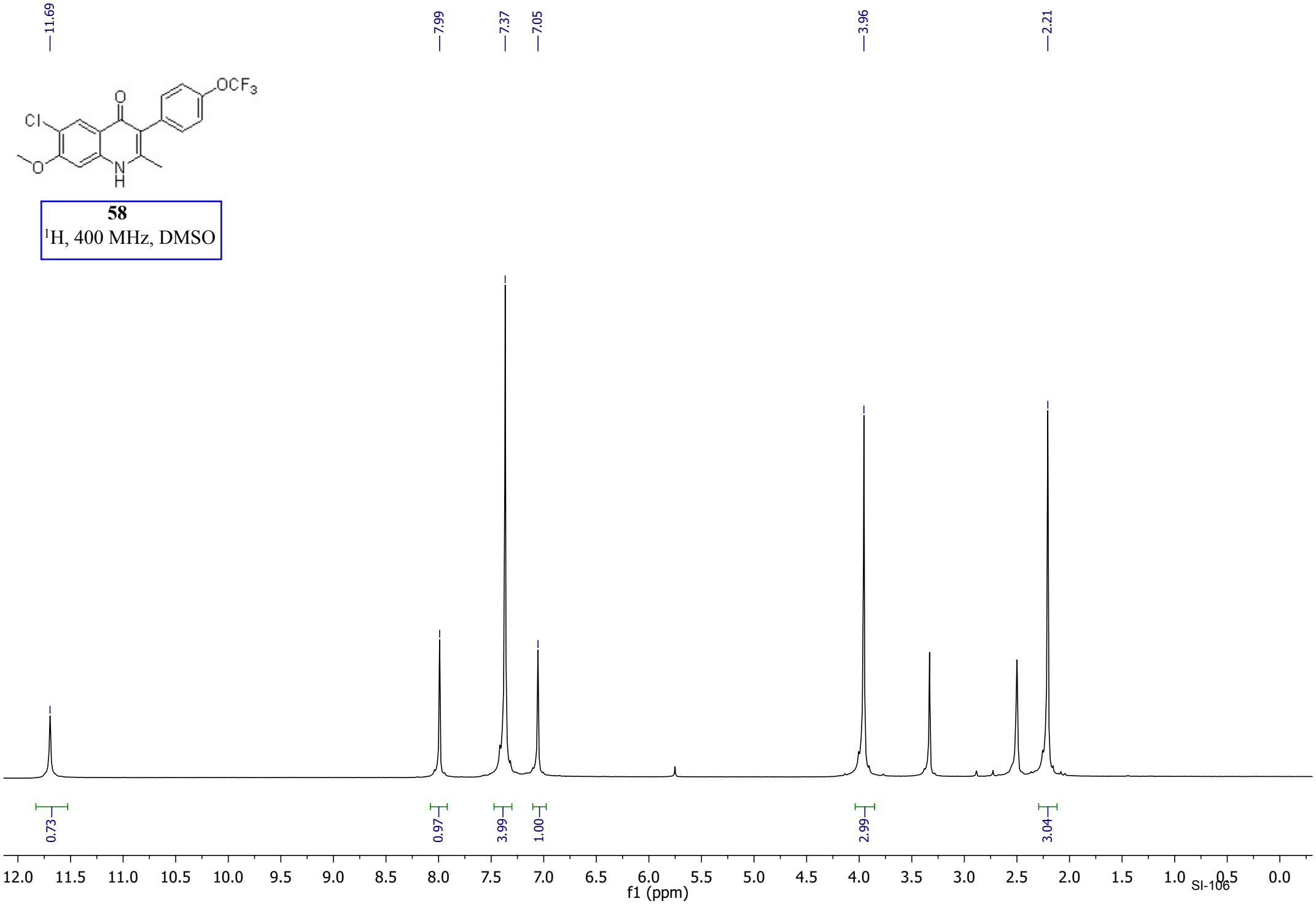
57

^{19}F, 376 MHz, DMSO



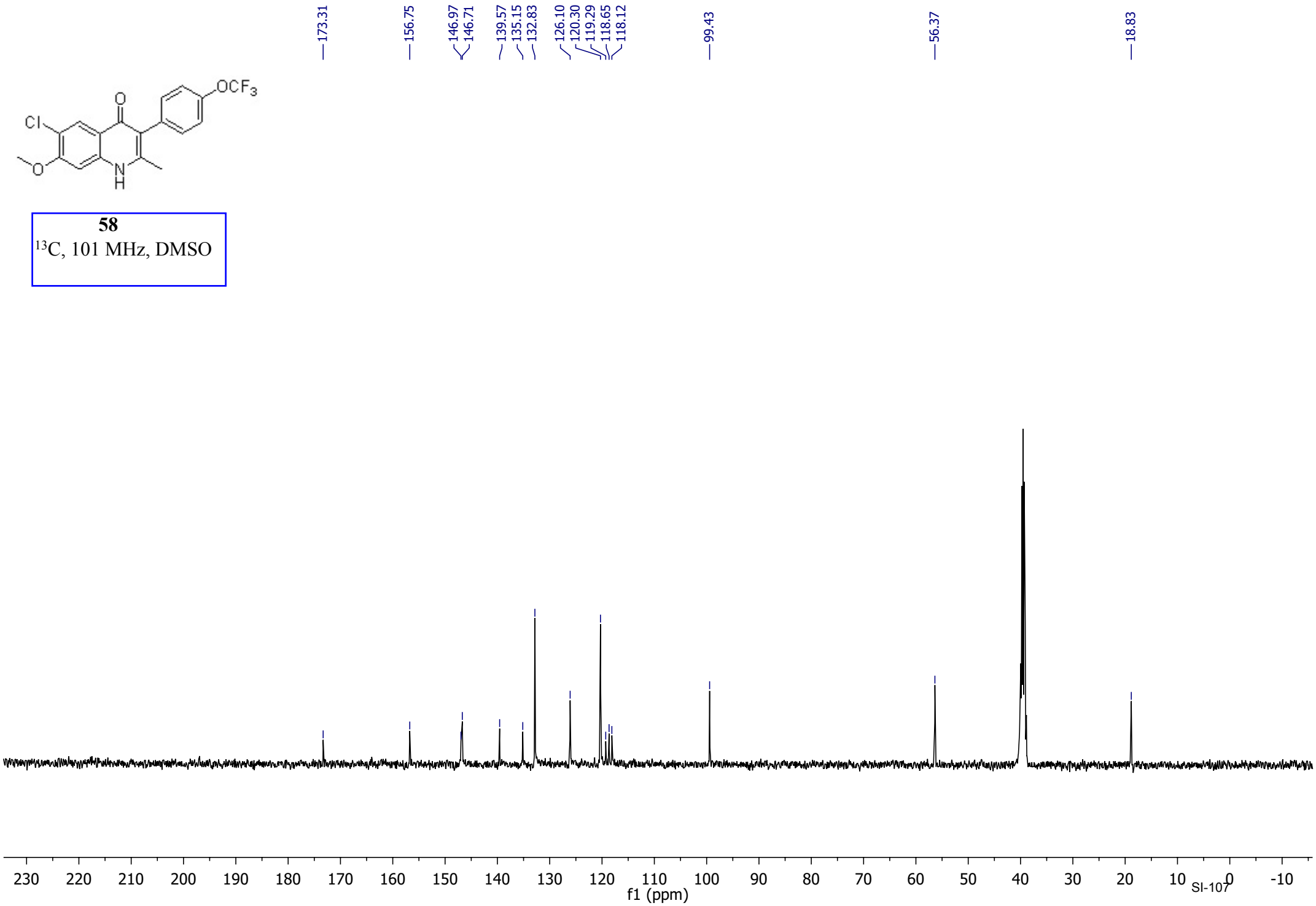
58

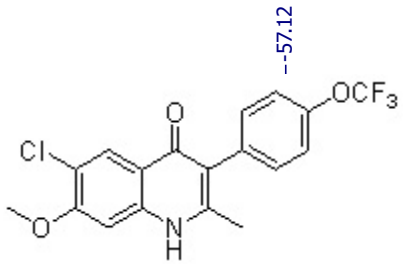
^{1}H, 400 MHz, DMSO



58

^{13}C, 101 MHz, DMSO





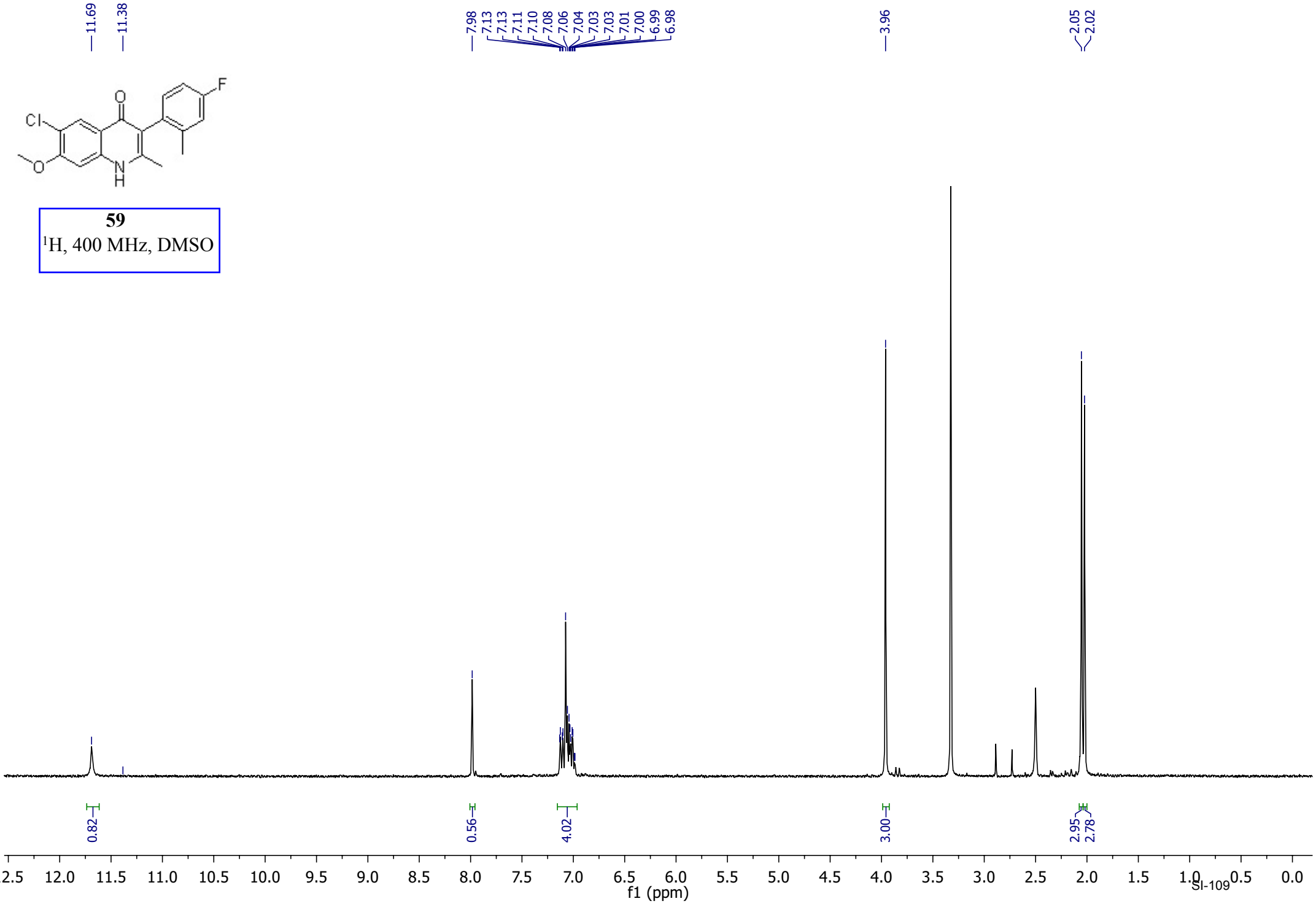
58

^{19}F, 376 MHz, DMSO

-45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155 -160 -165 -170

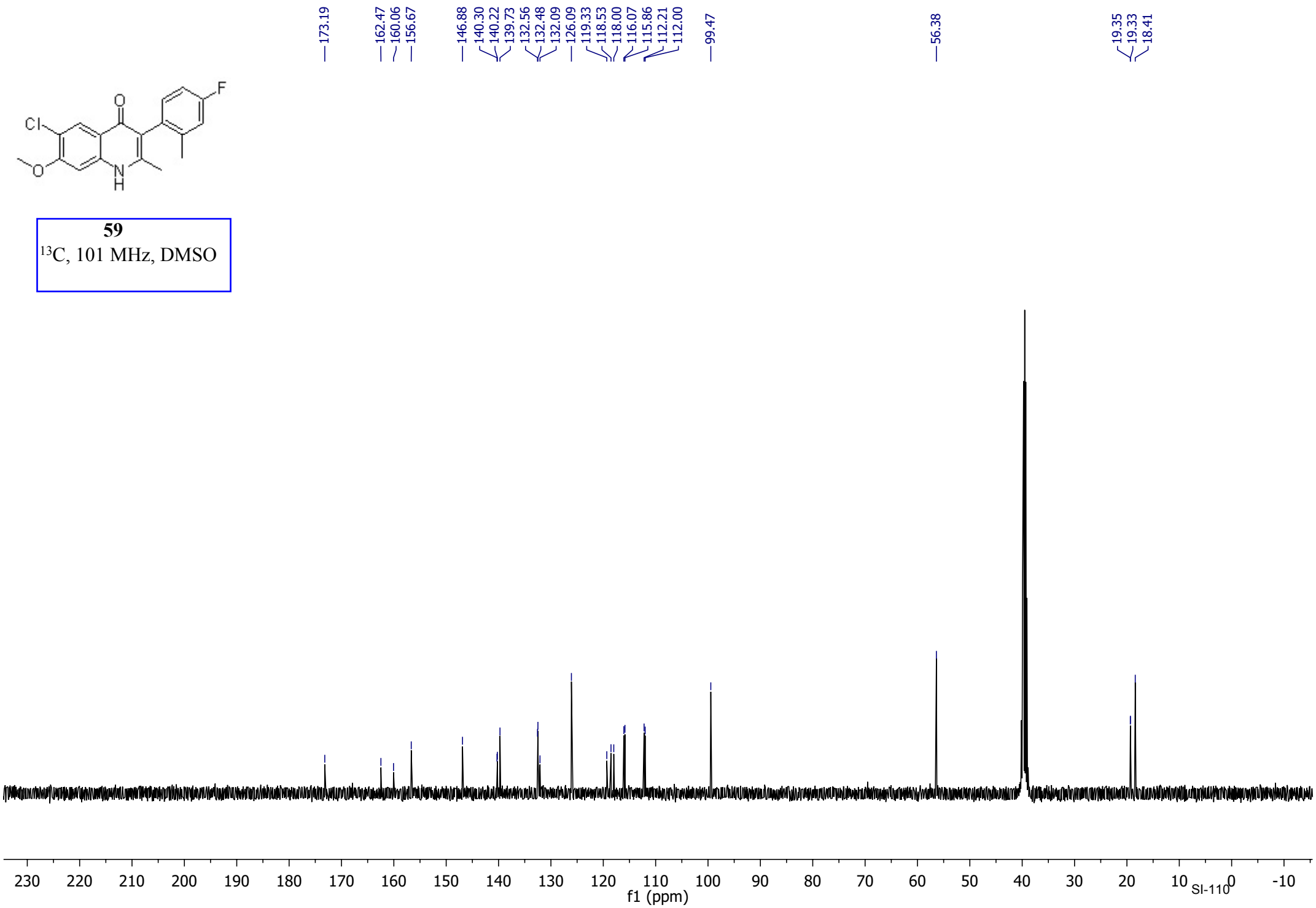
f1 (ppm)

59
^{1}H, 400 MHz, DMSO

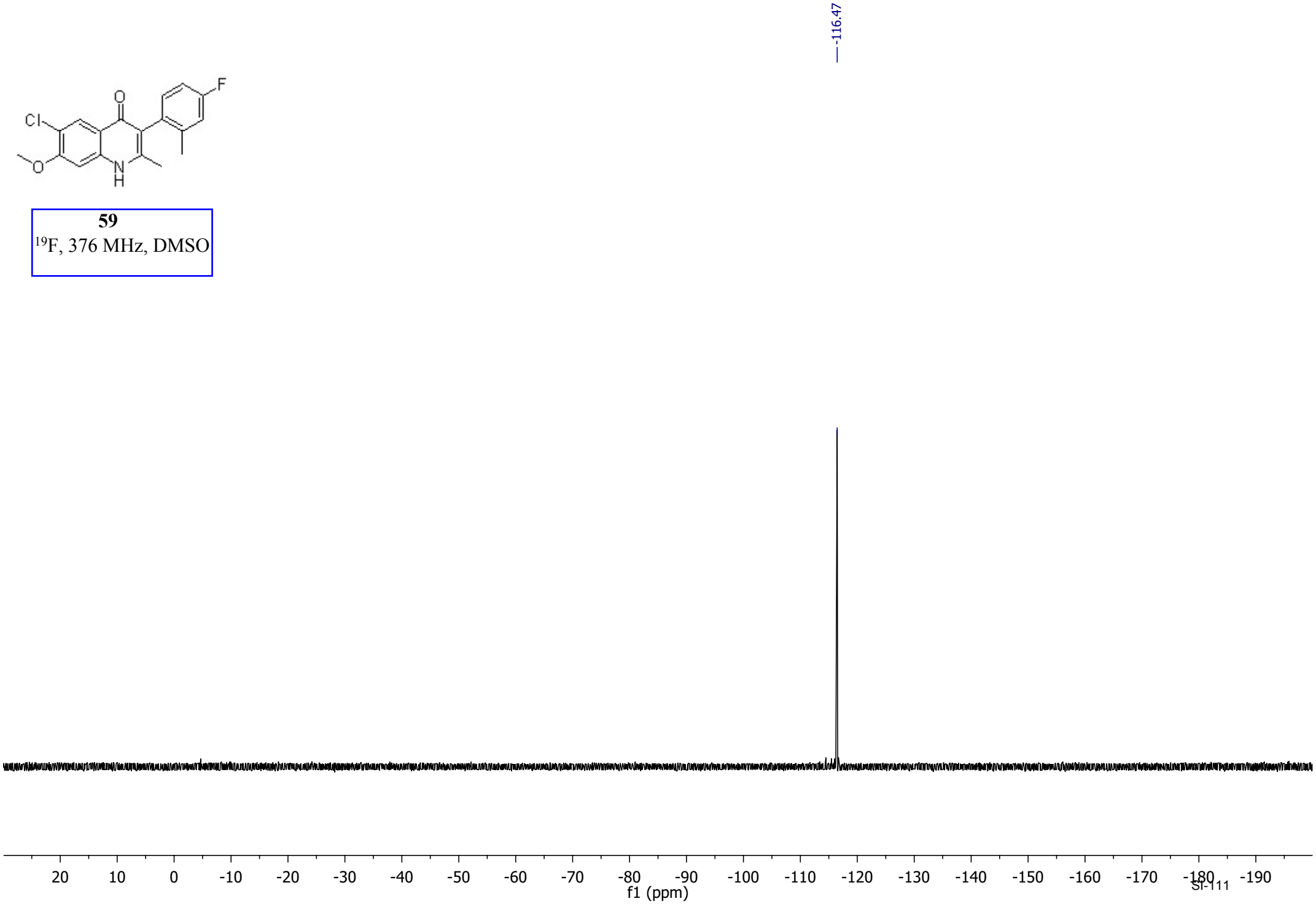


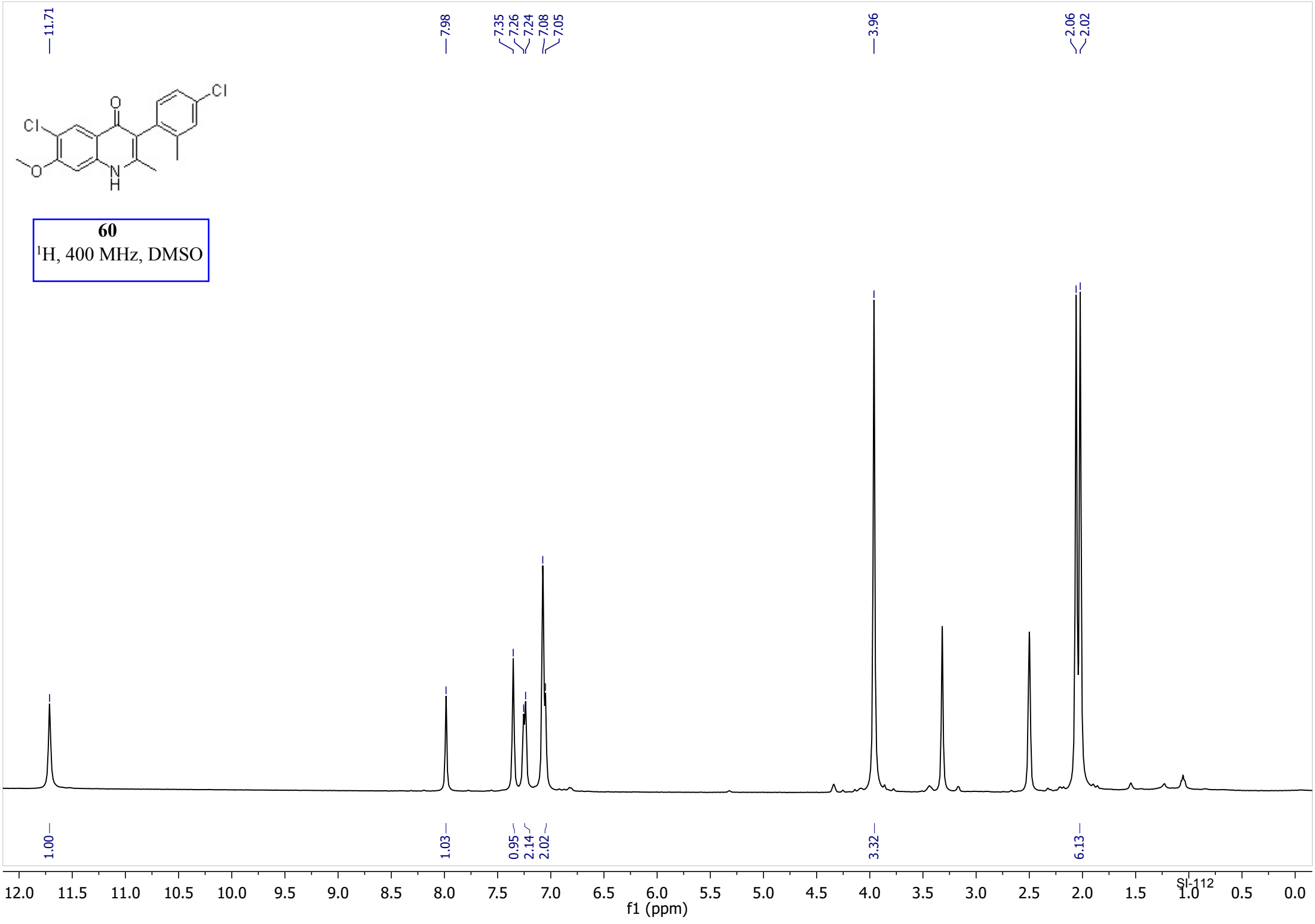
59

^{13}C, 101 MHz, DMSO



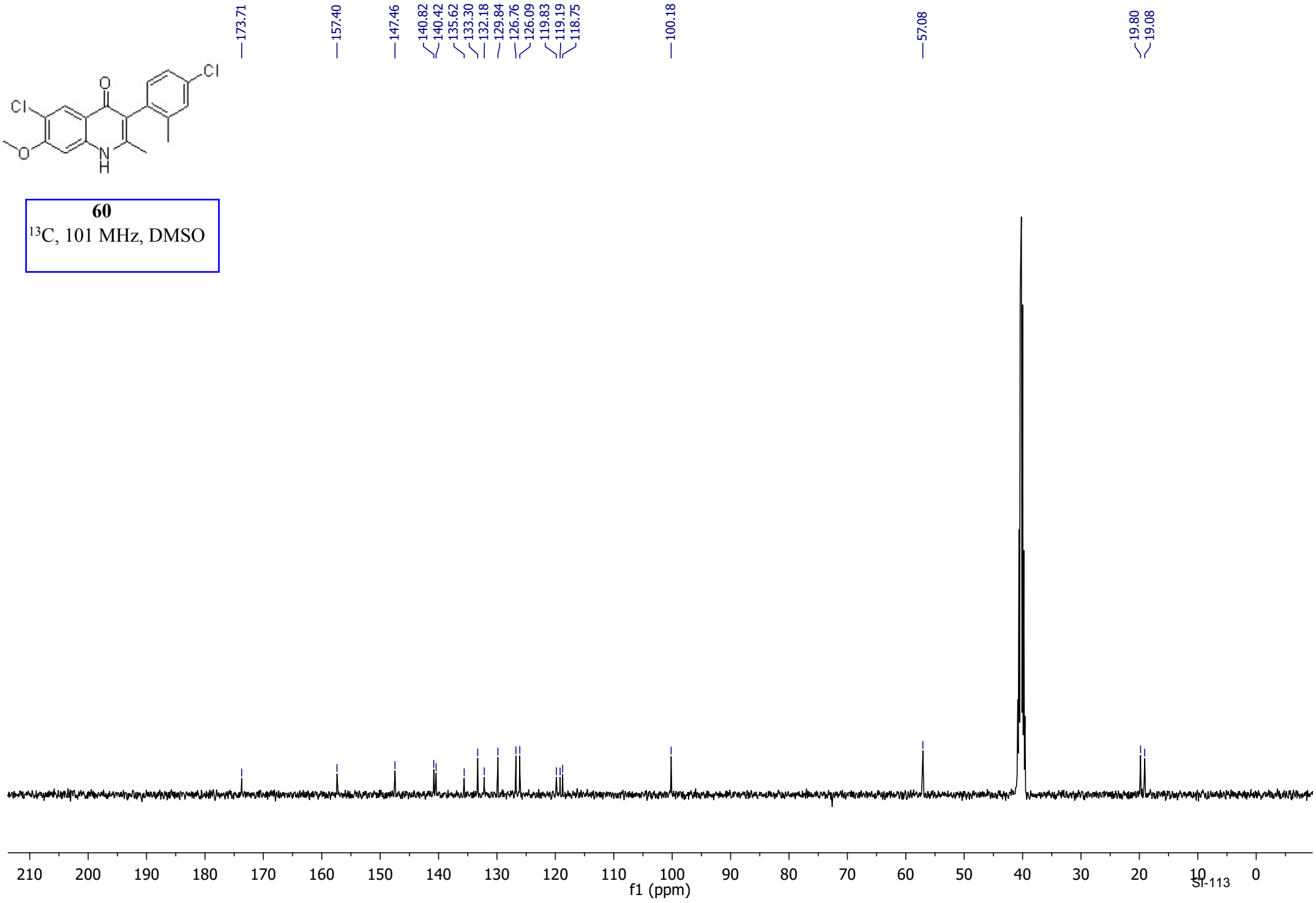
59
^{19}F, 376 MHz, DMSO



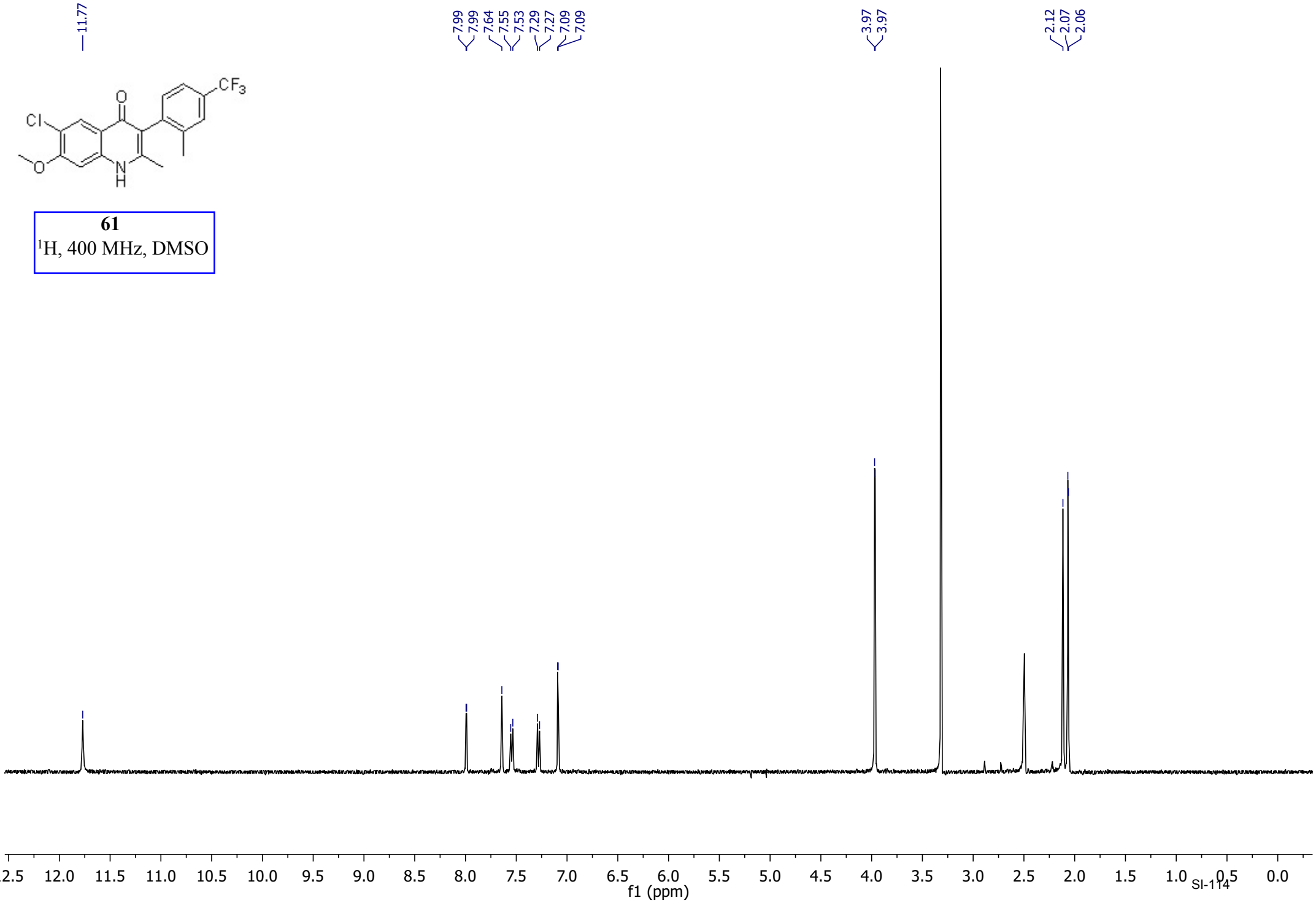

11.71
7.98
7.35
7.26
7.24
7.08
7.05
3.96
2.06
2.02
Cl
Cl
O
O
N
H
60
[1]H, 400 MHz, DMSO
1.00
1.03
0.95
2.14
2.02
3.32
6.13
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
SI-112

60

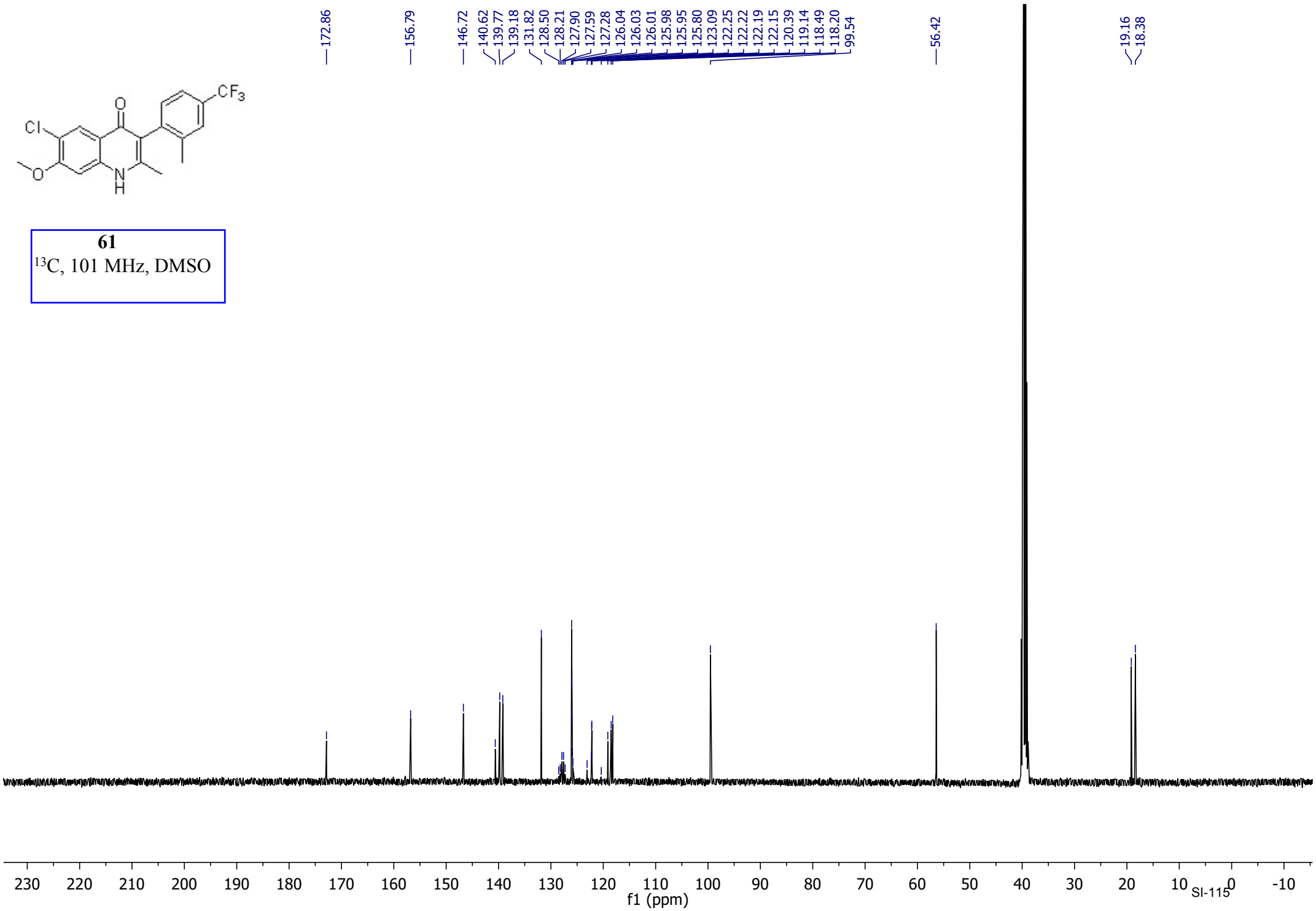
^{13}C, 101 MHz, DMSO



61
^{1}H, 400 MHz, DMSO

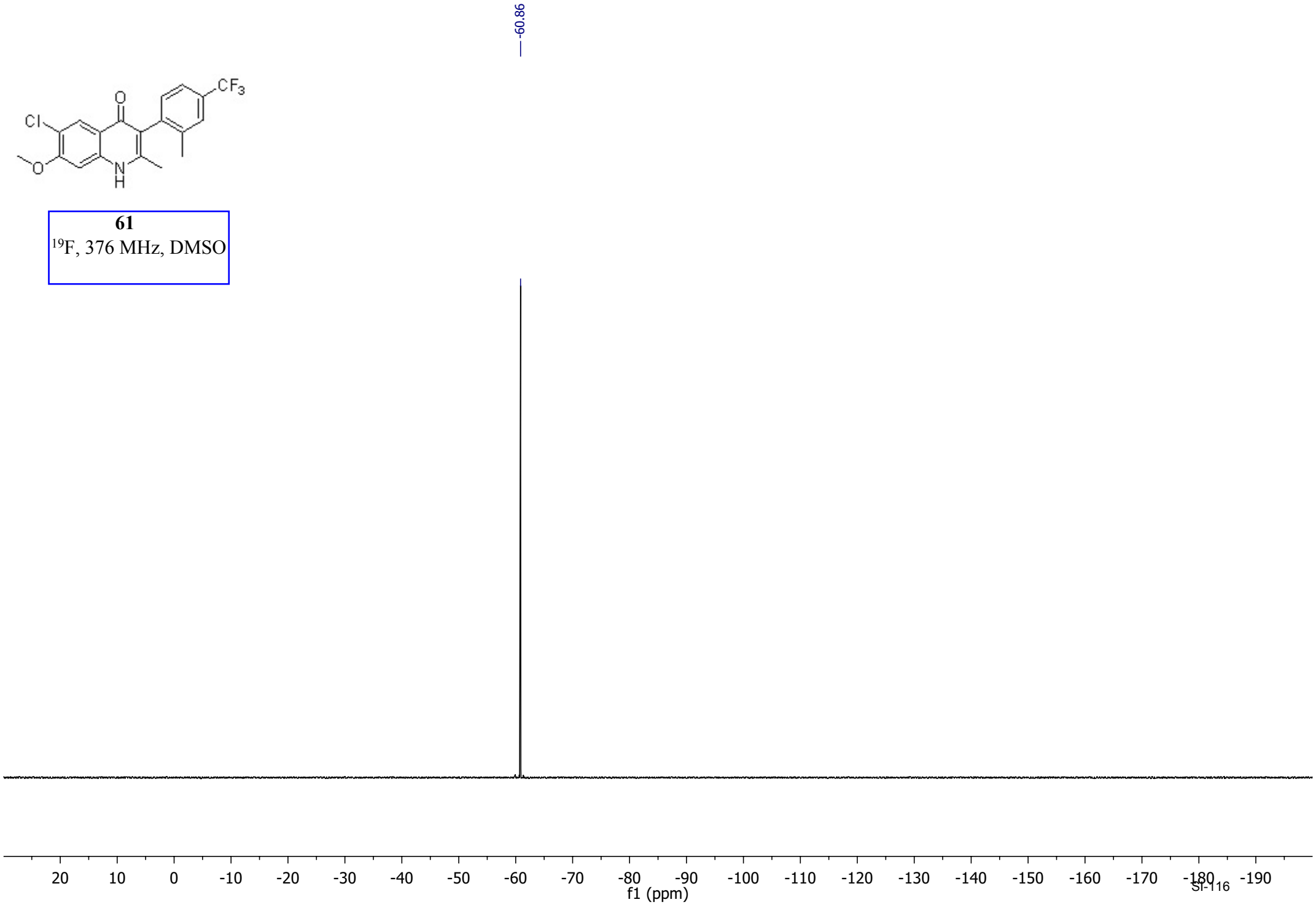


61
^{13}C, 101 MHz, DMSO

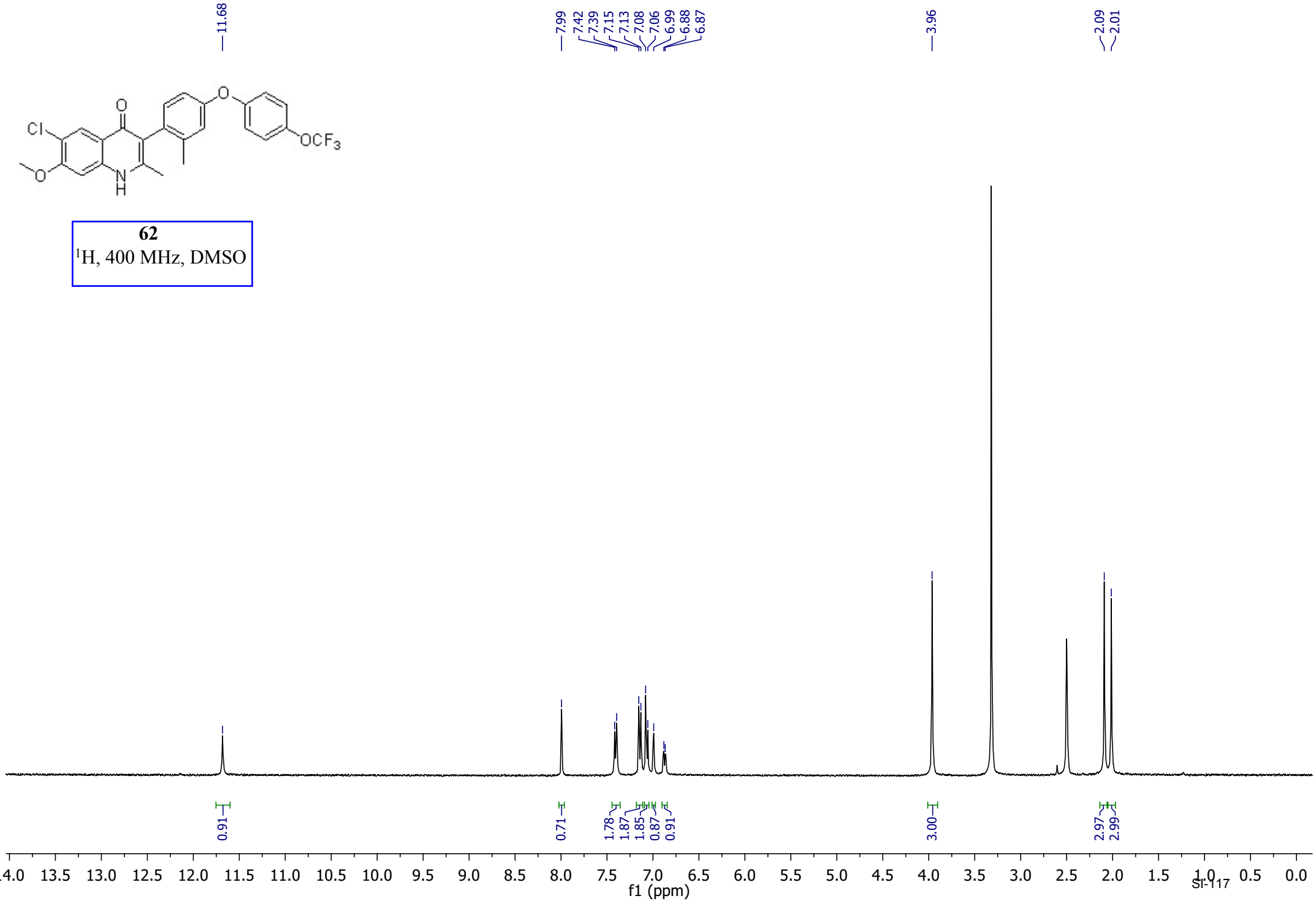


61

^{19}F, 376 MHz, DMSO

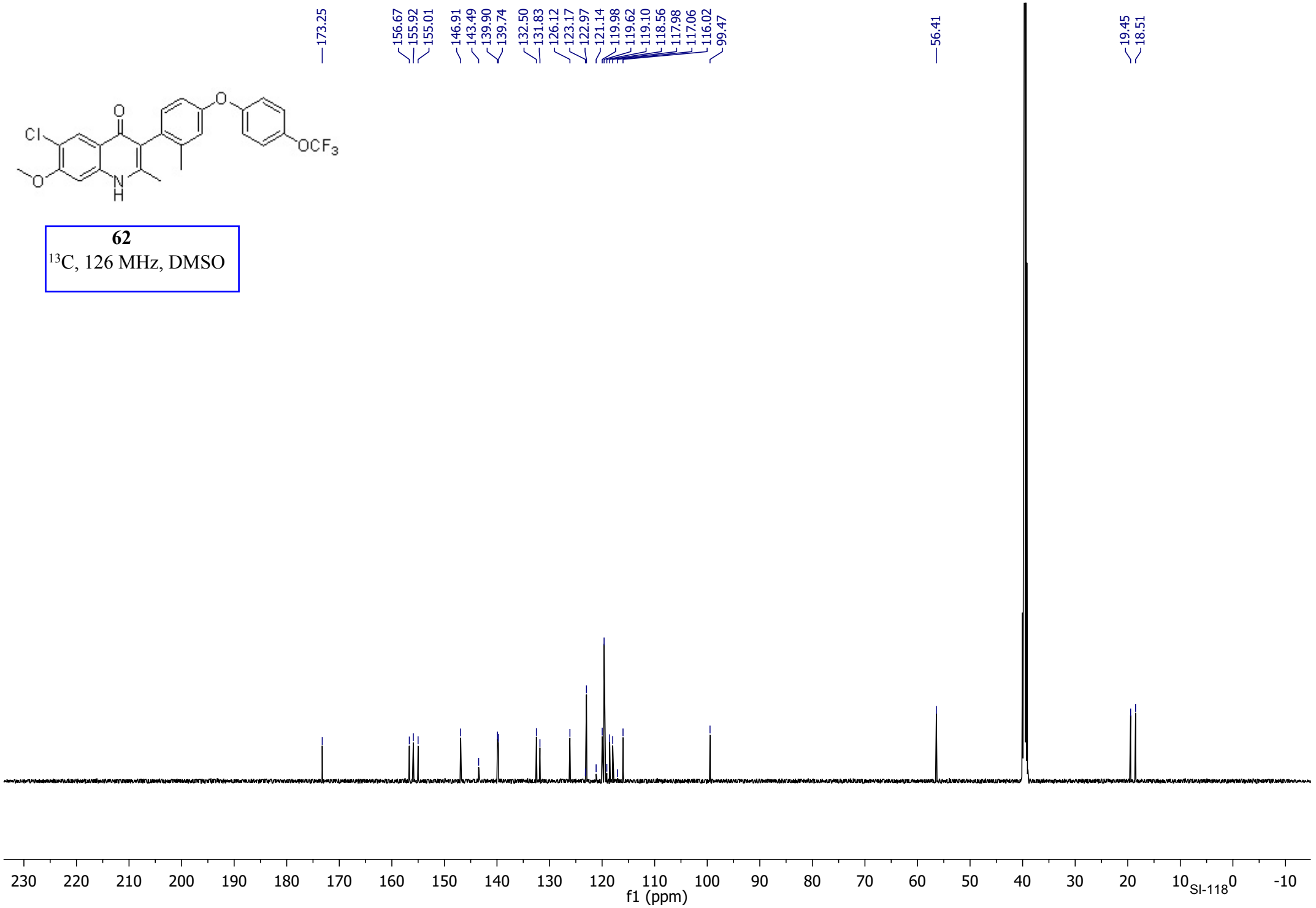


62
^{1}H, 400 MHz, DMSO

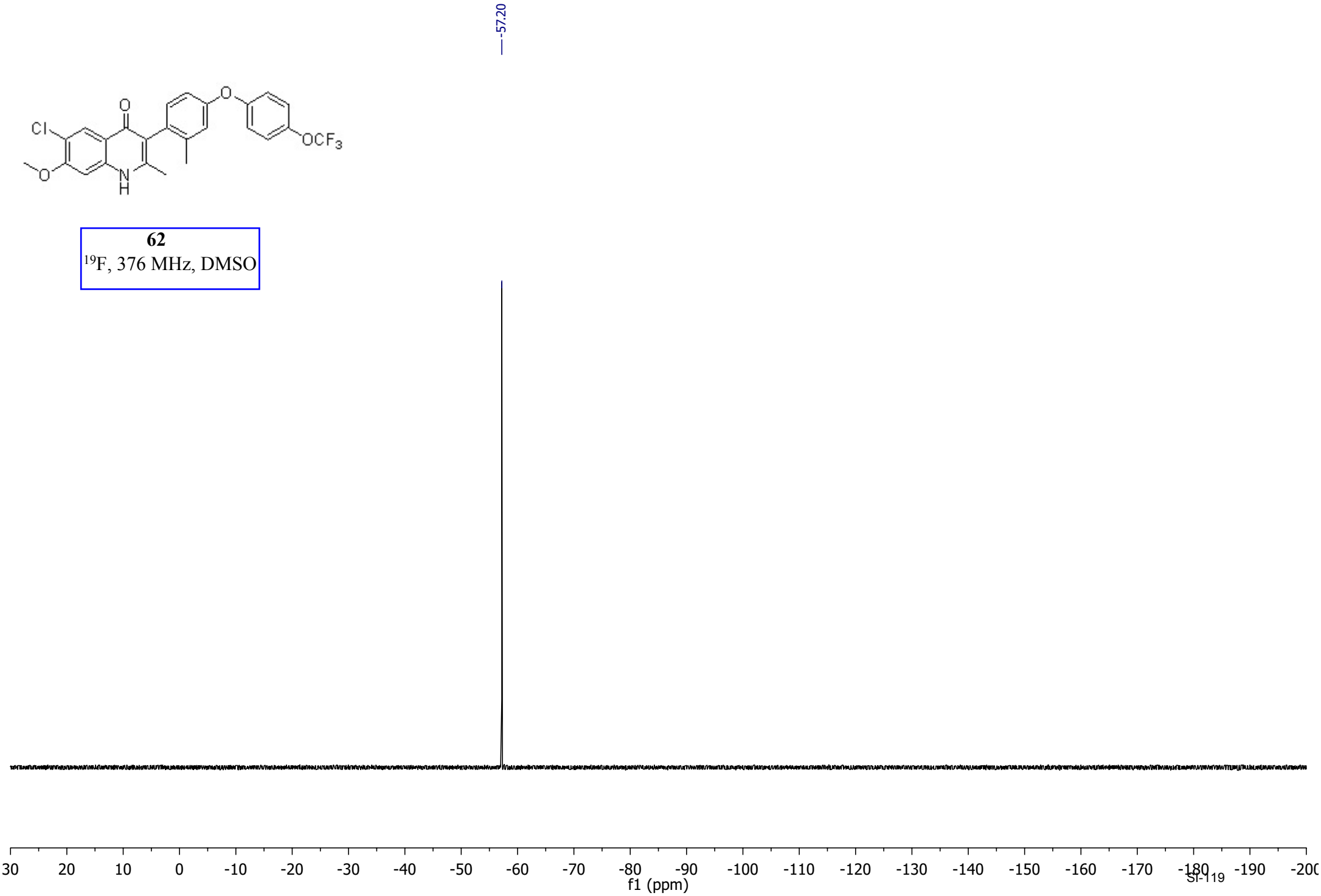


62

^{13}C, 126 MHz, DMSO

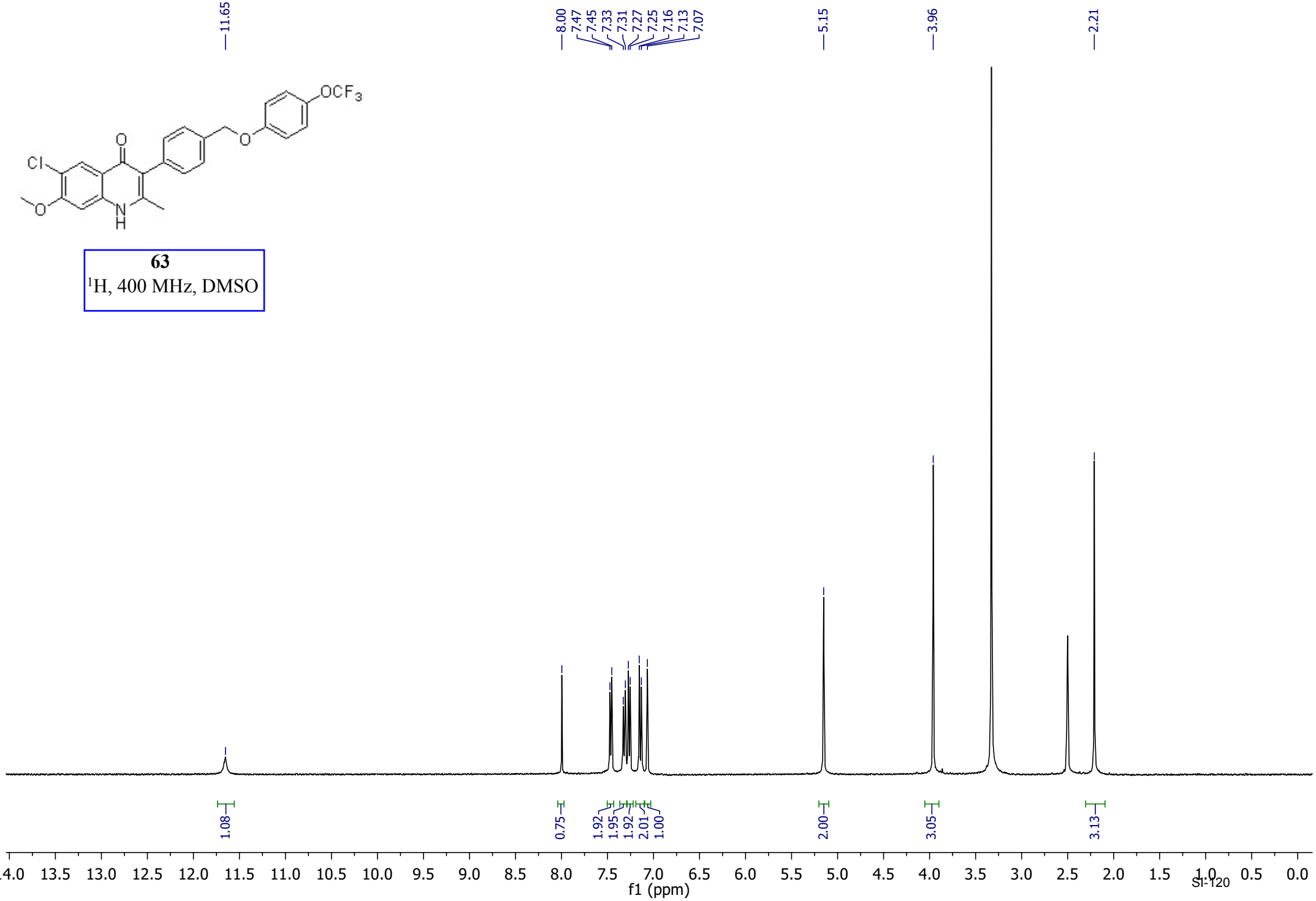


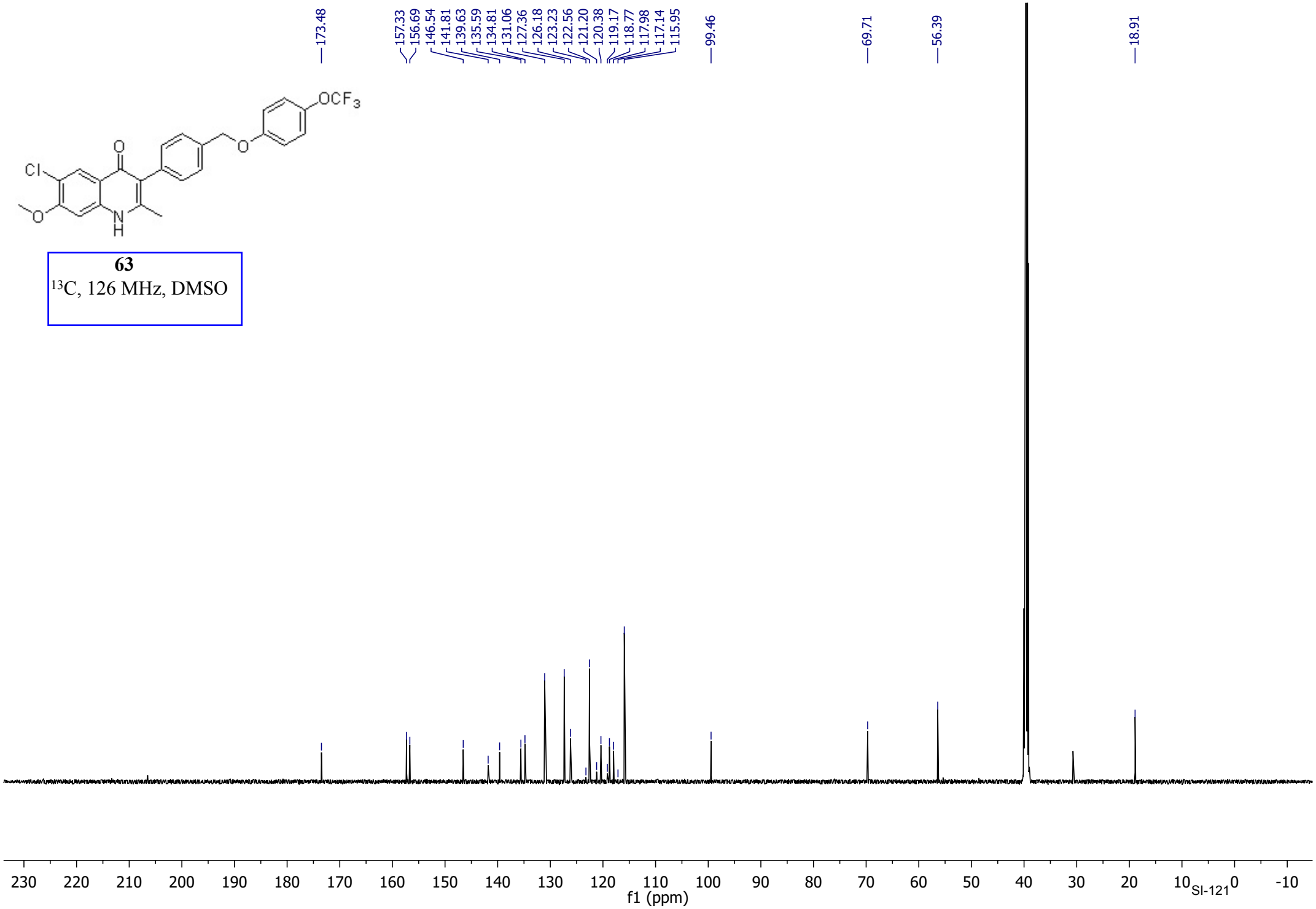
62
^{19}F, 376 MHz, DMSO



63

^{1}H, 400 MHz, DMSO



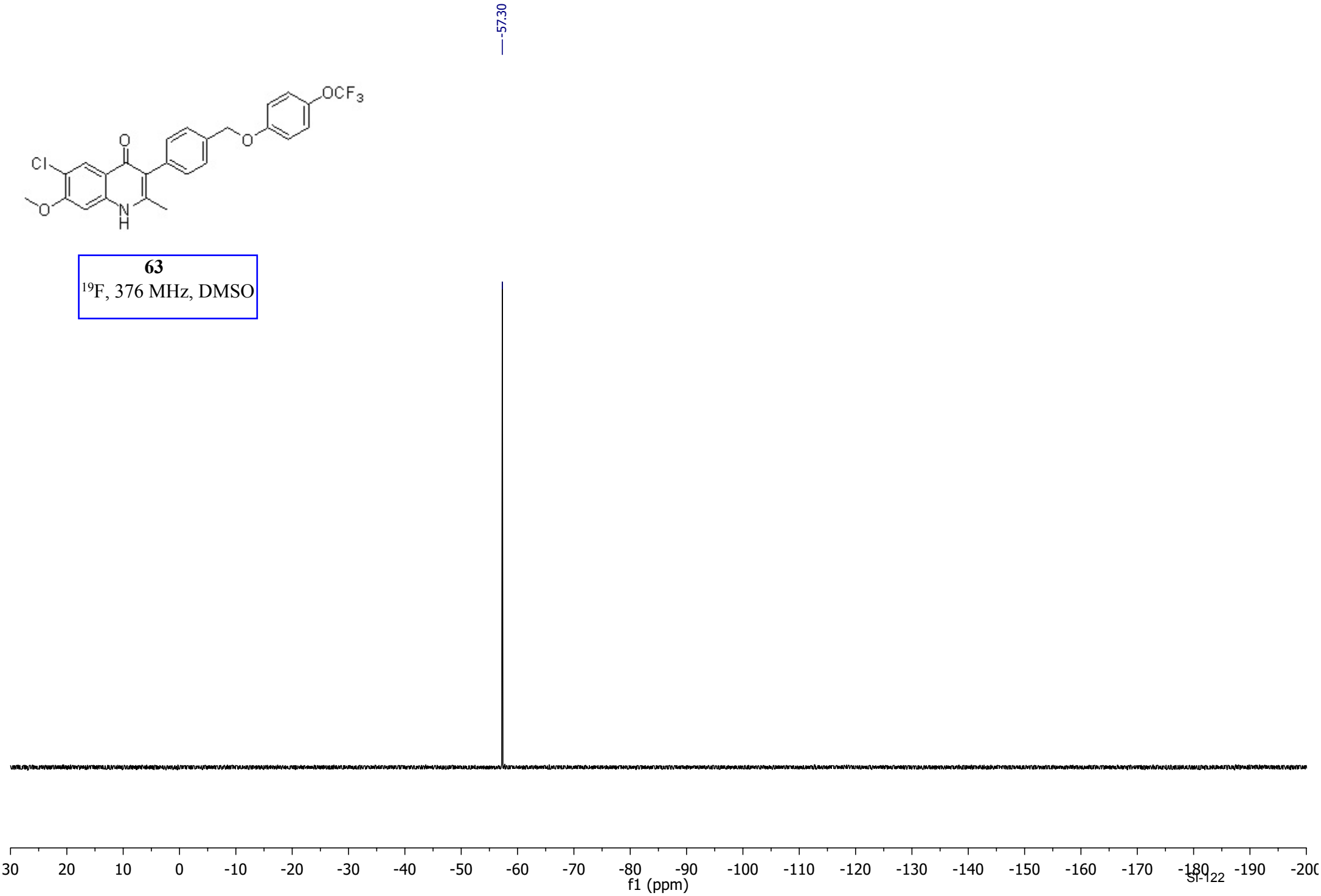


63

^{13}C, 126 MHz, DMSO

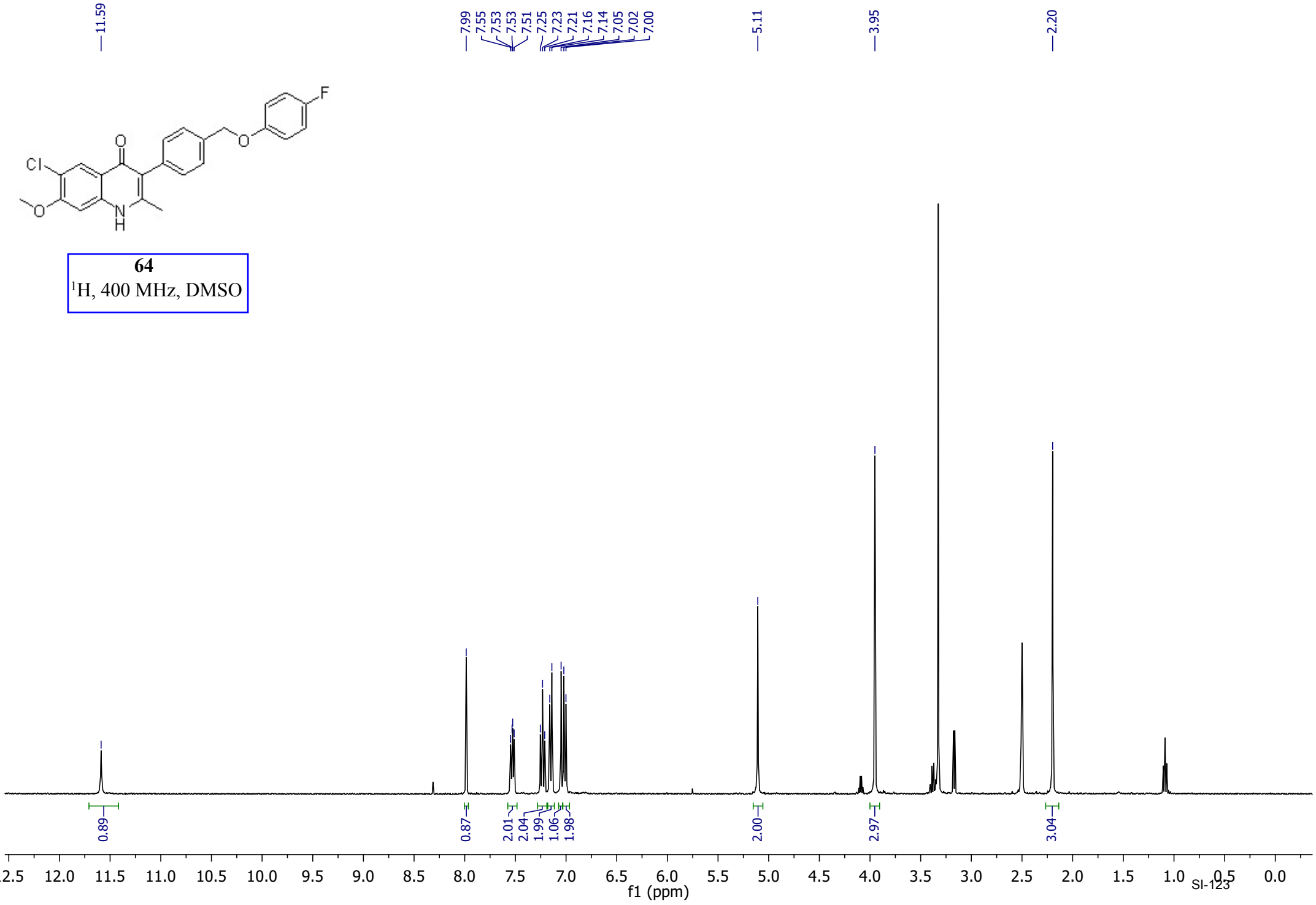
63

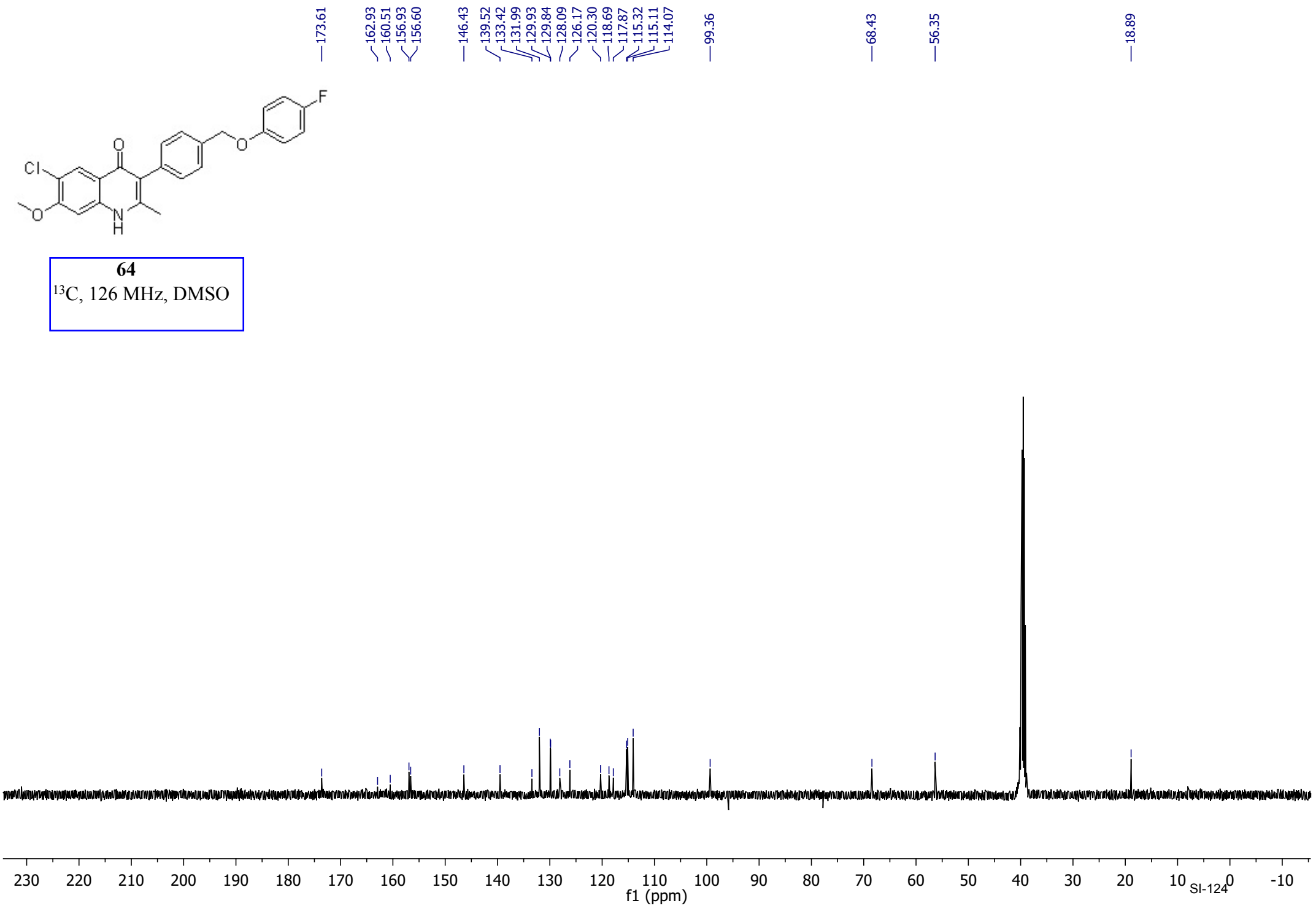
^{19}F, 376 MHz, DMSO



64

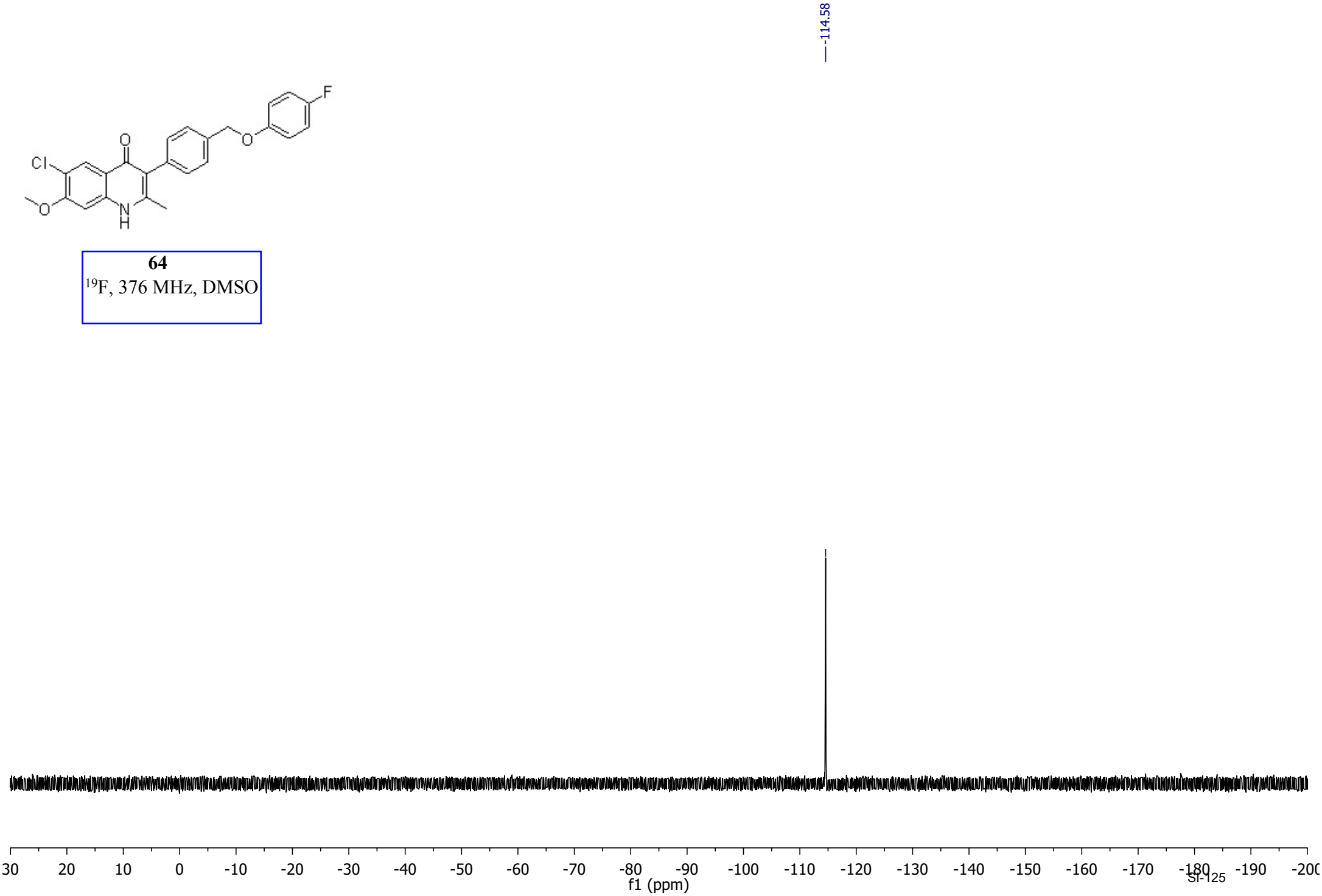
^{1}H, 400 MHz, DMSO



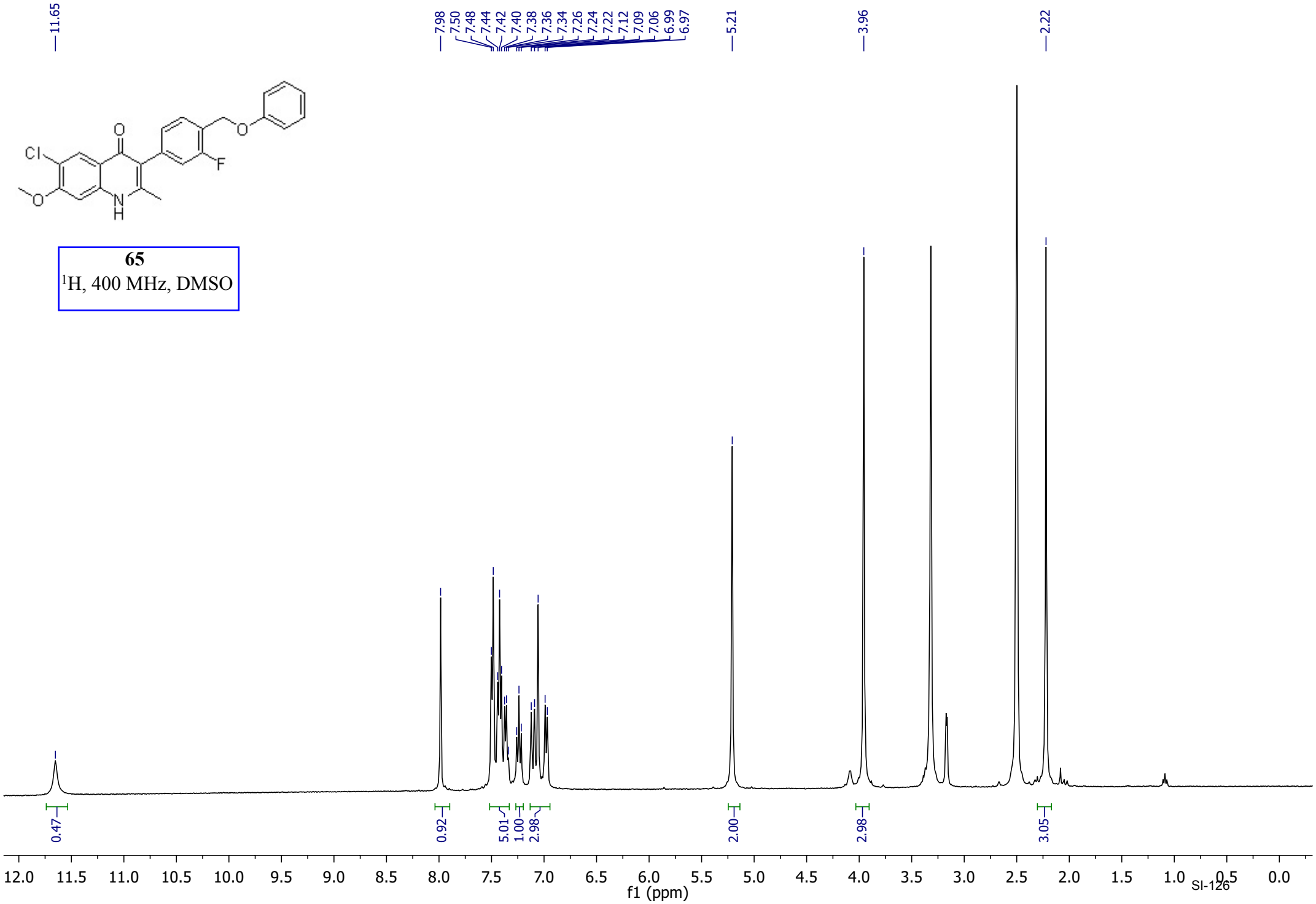

173.61
162.93
160.51
156.93
156.60
146.43
139.52
133.42
131.99
129.93
129.84
128.09
126.17
120.30
118.69
117.87
115.32
115.11
114.07
99.36
68.43
56.35
18.89
F
O
O
Cl
O
N
H
64
13C, 126 MHz, DMSO
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
Sl-124

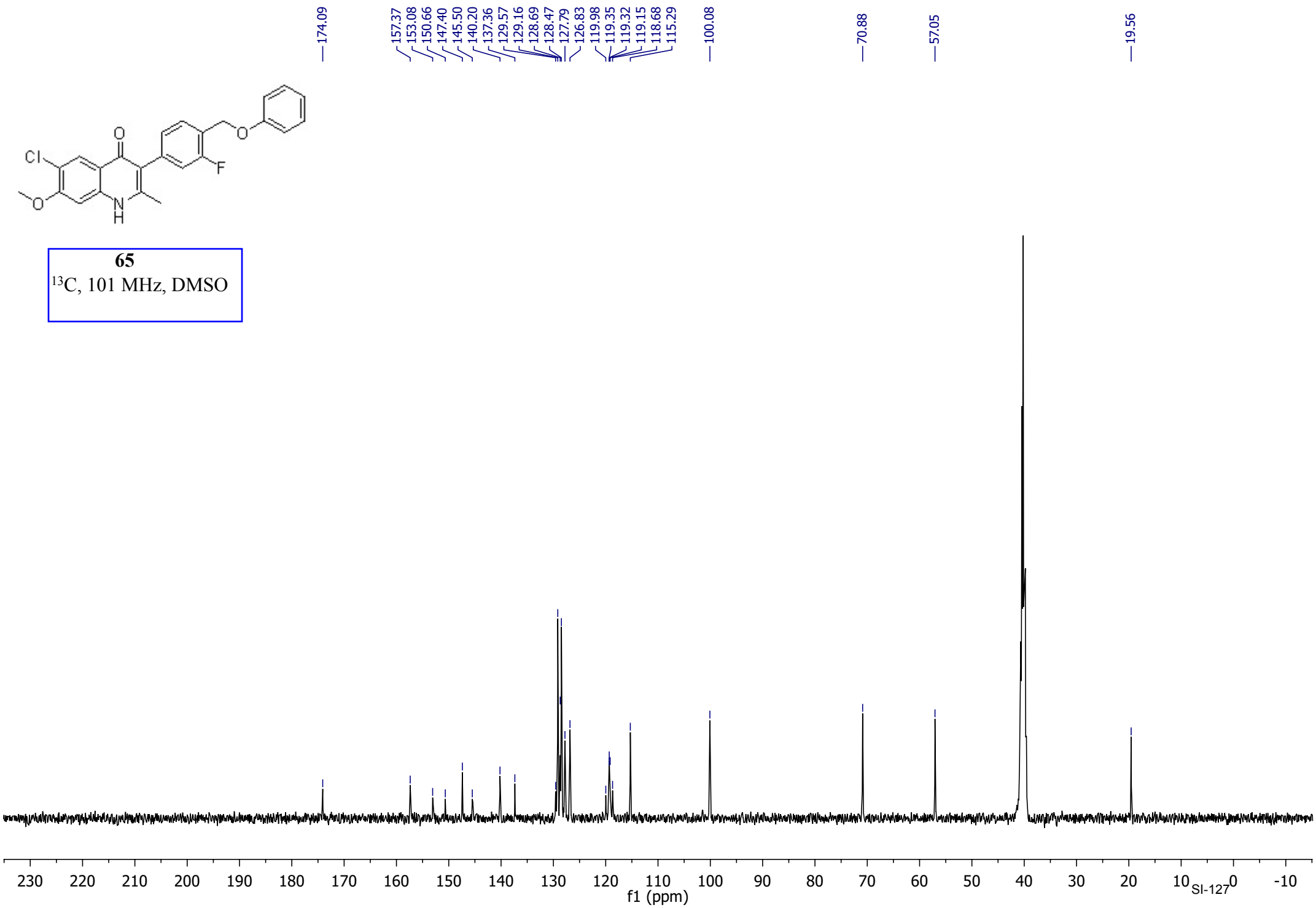
64

^{19}F, 376 MHz, DMSO



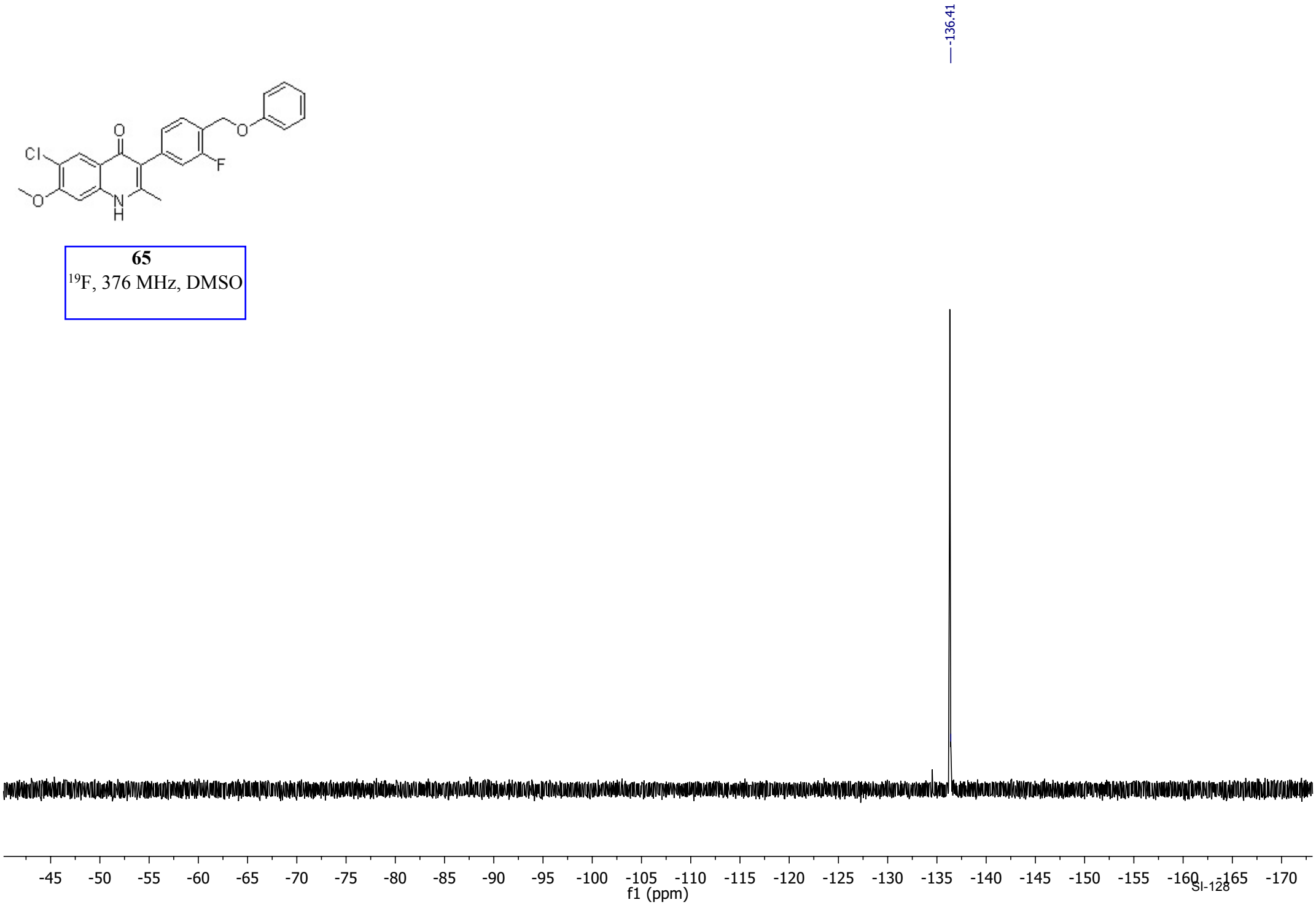
65
^{1}H, 400 MHz, DMSO




174.09
157.37
153.08
150.66
147.40
145.50
140.20
137.36
129.57
129.16
128.69
128.47
127.79
126.83
119.98
119.35
119.32
119.15
118.68
115.29
100.08
70.88
57.05
19.56
Cl
O
O
F
O
N
H
65
13C, 101 MHz, DMSO
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
Sl-127

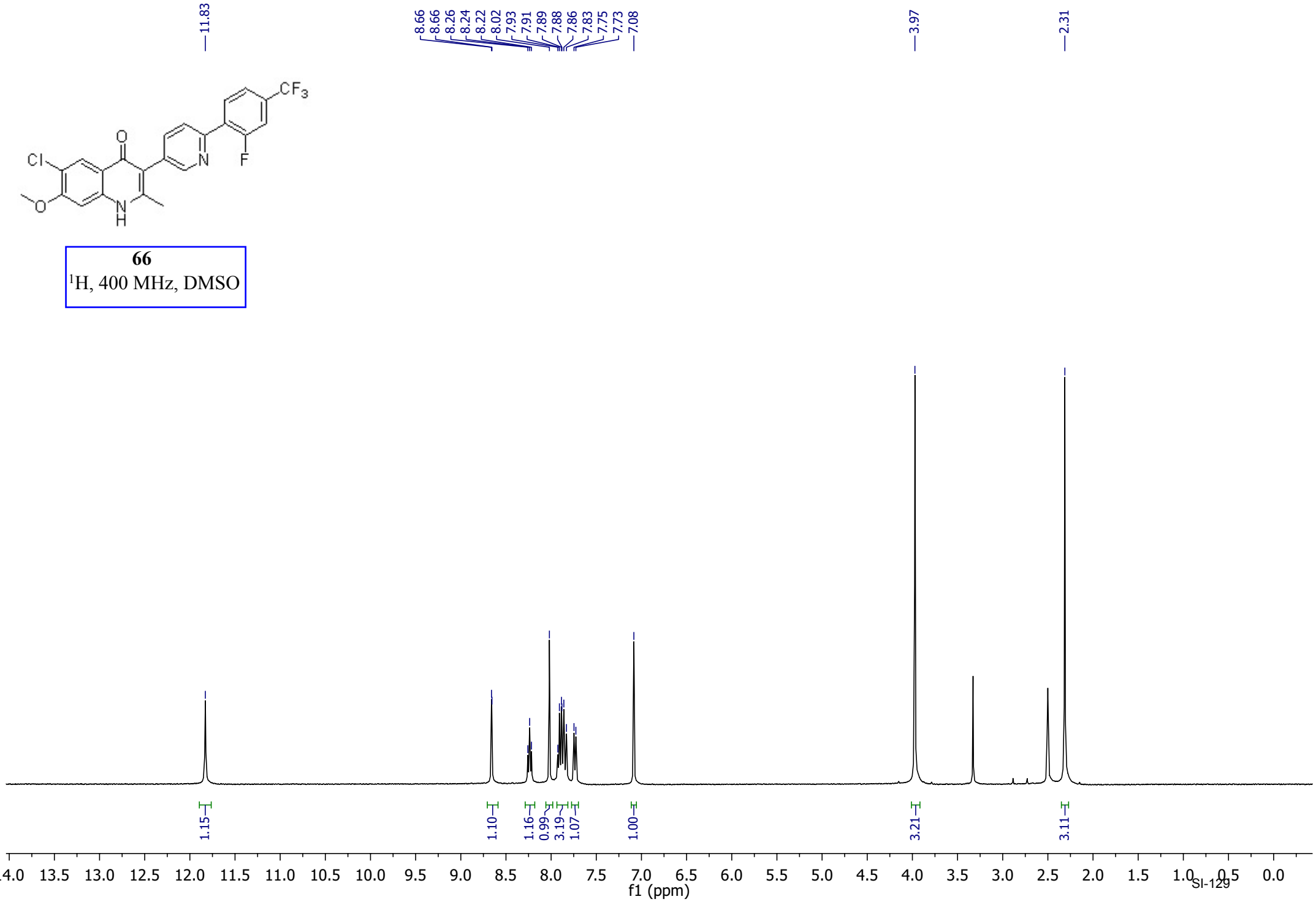
65

^{19}F, 376 MHz, DMSO



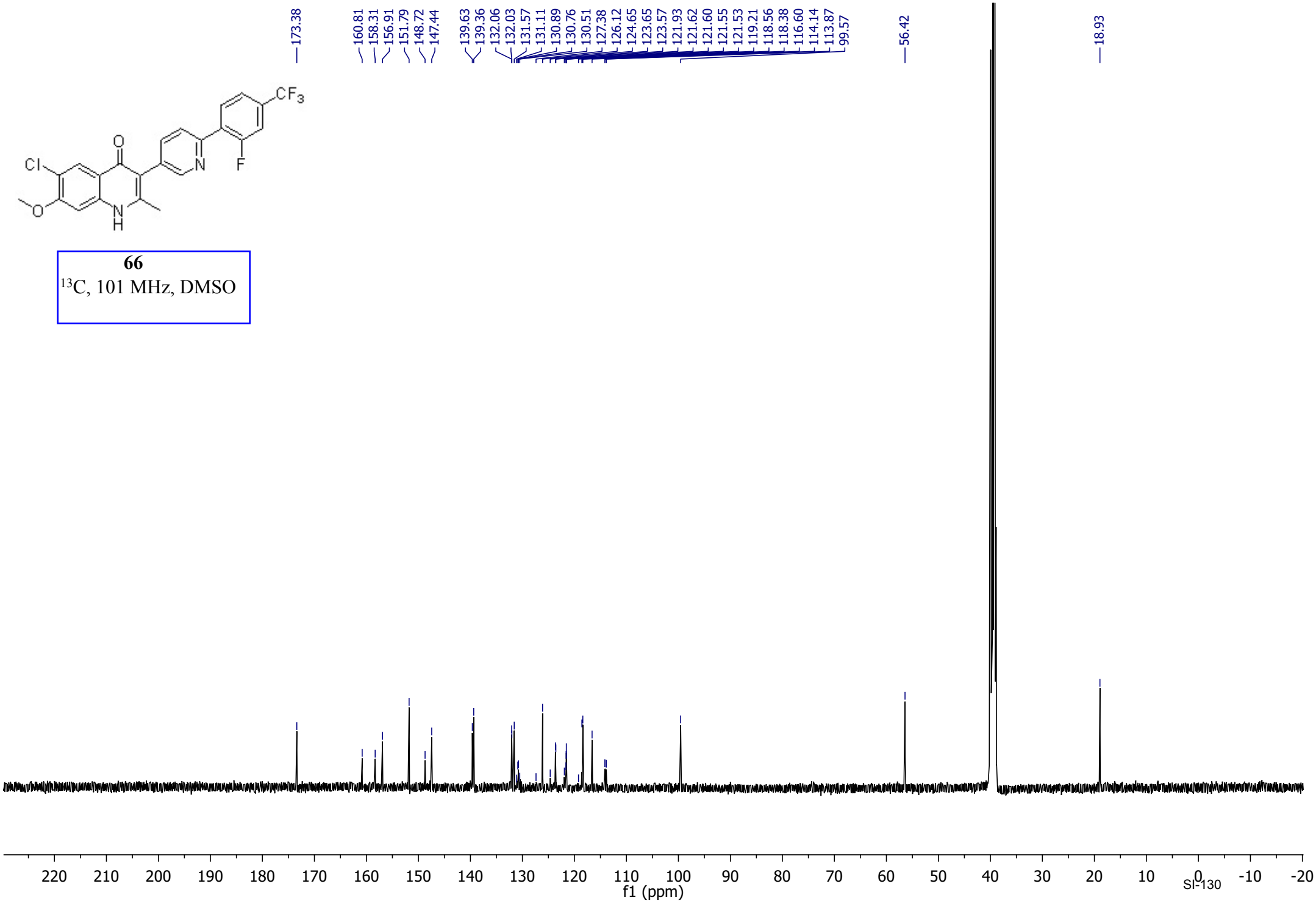
66

^{1}H, 400 MHz, DMSO



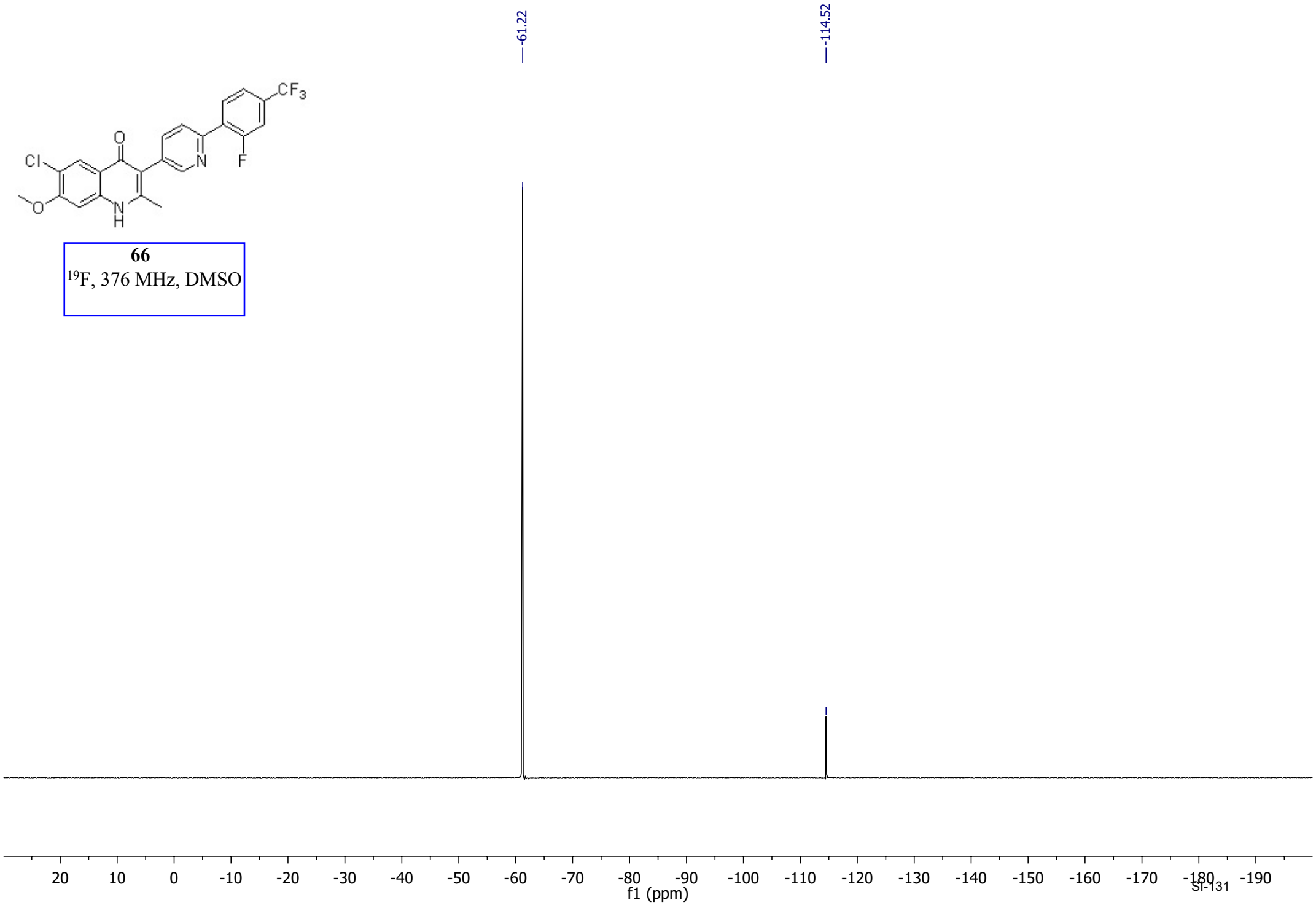
66

^{13}C, 101 MHz, DMSO

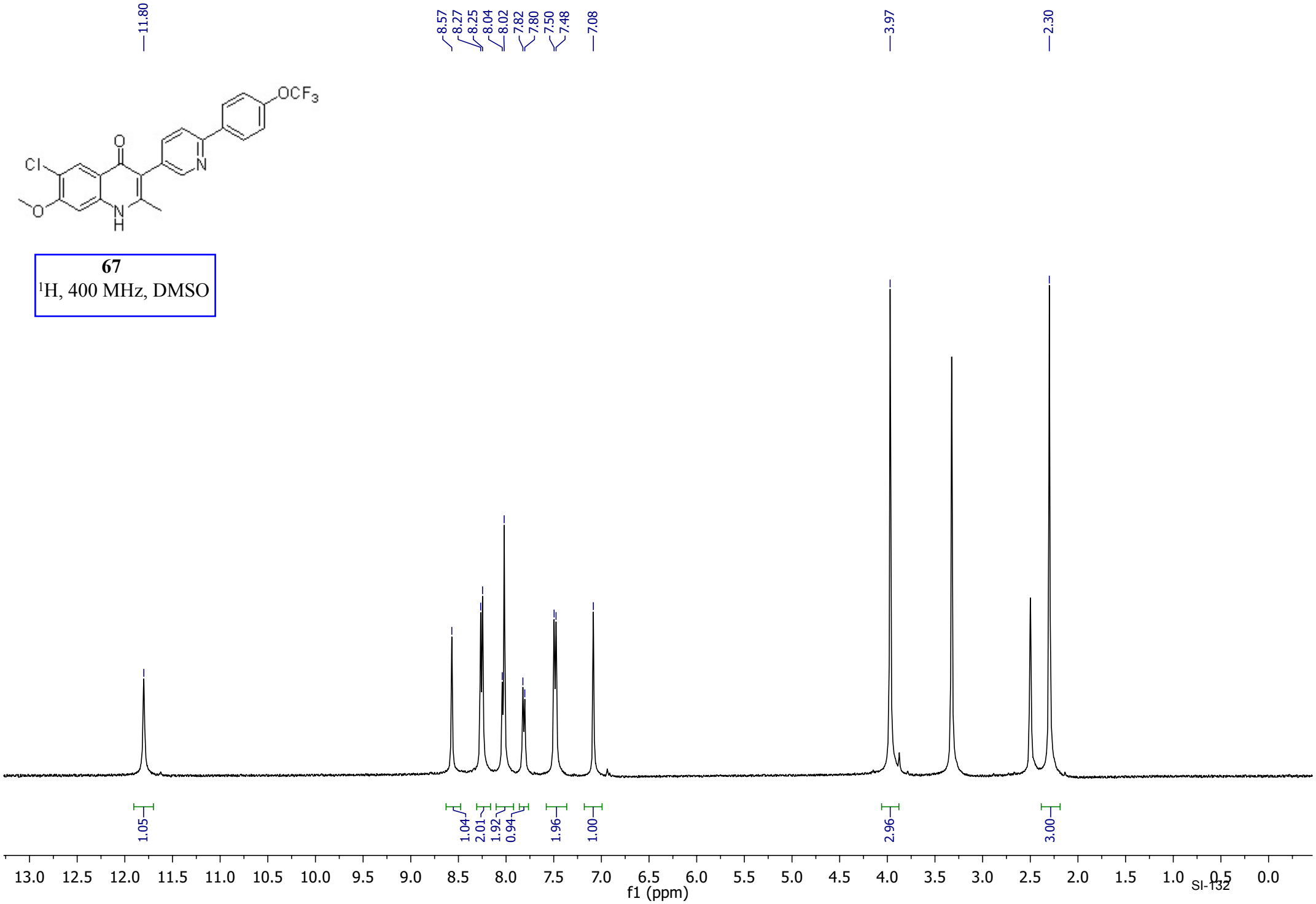


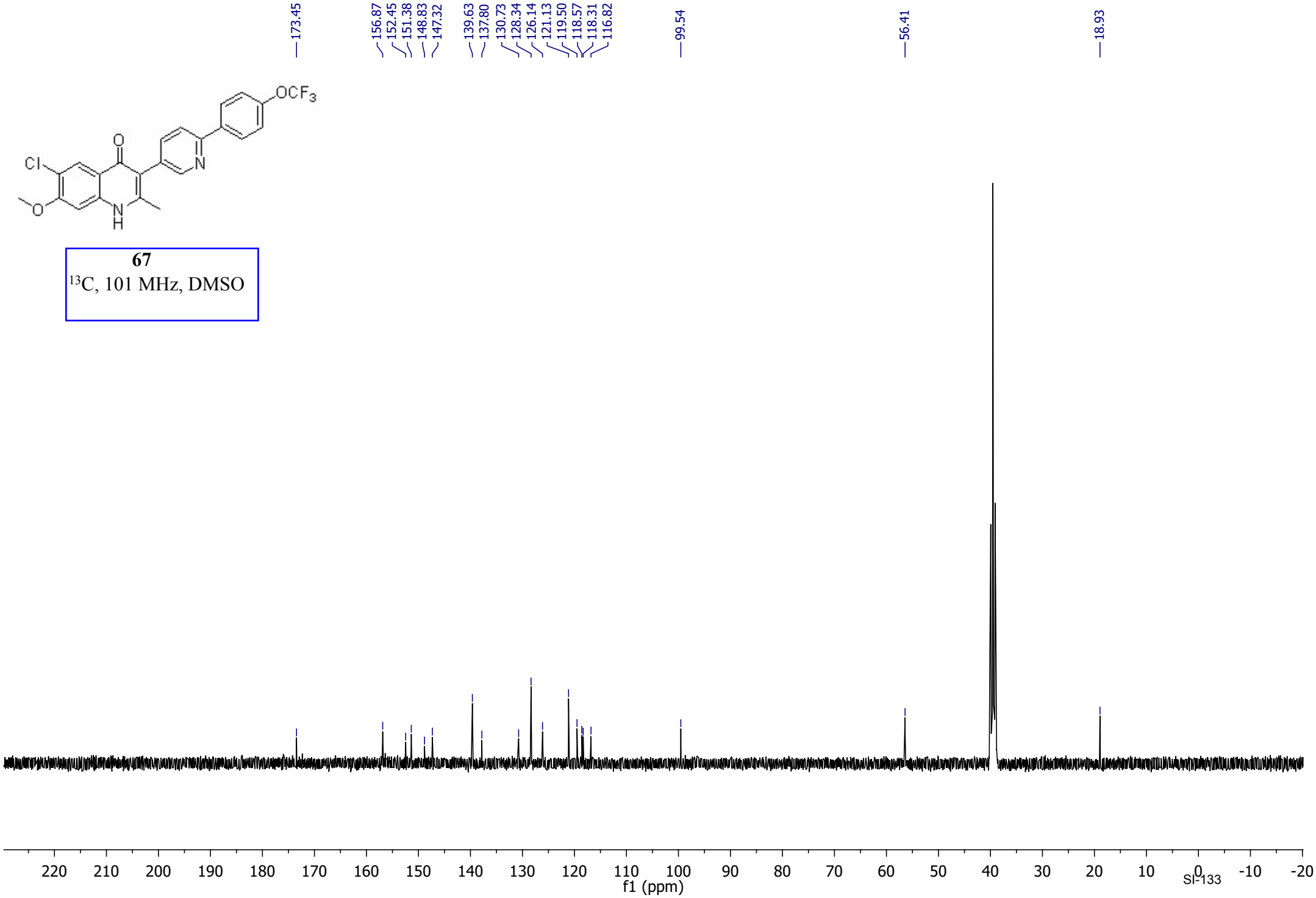
66

^{19}F, 376 MHz, DMSO



67
^{1}H, 400 MHz, DMSO





67

^{13}C, 101 MHz, DMSO

67

^{19}F, 376 MHz, DMSO