

SUPPORTING INFORMATION

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

R. Matthew Cross,^{§, ‡} *David L. Flanigan*,^{§, ‡} *Andrii Monastyrskyi*,[§] *Alexis N. LaCruce*,[‡] *Fabián E. Sáenz*,^{‡, †} *Jordany R. Maignan*,[§] *Tina S. Mutka*,[‡] *Karen L. White*,[£] *David M. Shackleford*,[£] *Ian Bathurst*,^{€J} *Frank R Fronczek*,[#] *Lukasz Wojtas*,[§] *Wayne C. Guida*,[§] *Susan A. Charman*,[£] *Jeremy N. Burrows*,[€] *Dennis E. Kyle*,[‡] and *Roman Manetsch*^{*,§}

[§]Department of Chemistry, University of South Florida, CHE 205, 4202 E. Fowler Ave, Tampa, Florida 33620, USA; [‡]Department of Global Health, College of Public Health, University of South Florida, 3720 Spectrum Blvd, Suite 304, Tampa, Florida 33612, USA; [£]Centre for Drug Candidate Optimisation, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, Victoria 3052, Australia; [#]Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803, USA; [€]Medicines for Malaria Venture, 20, rte de Pré-Bois, P.O. Box 1826, 1215 Geneva 15, Switzerland.

[‡]These authors contributed equally.

Table S1. Physicochemical Properties

Compound	Human Liver Microsomal CL _{int} ($\mu\text{L}/\text{min}/\text{mg}$ 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

^aStandards 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.

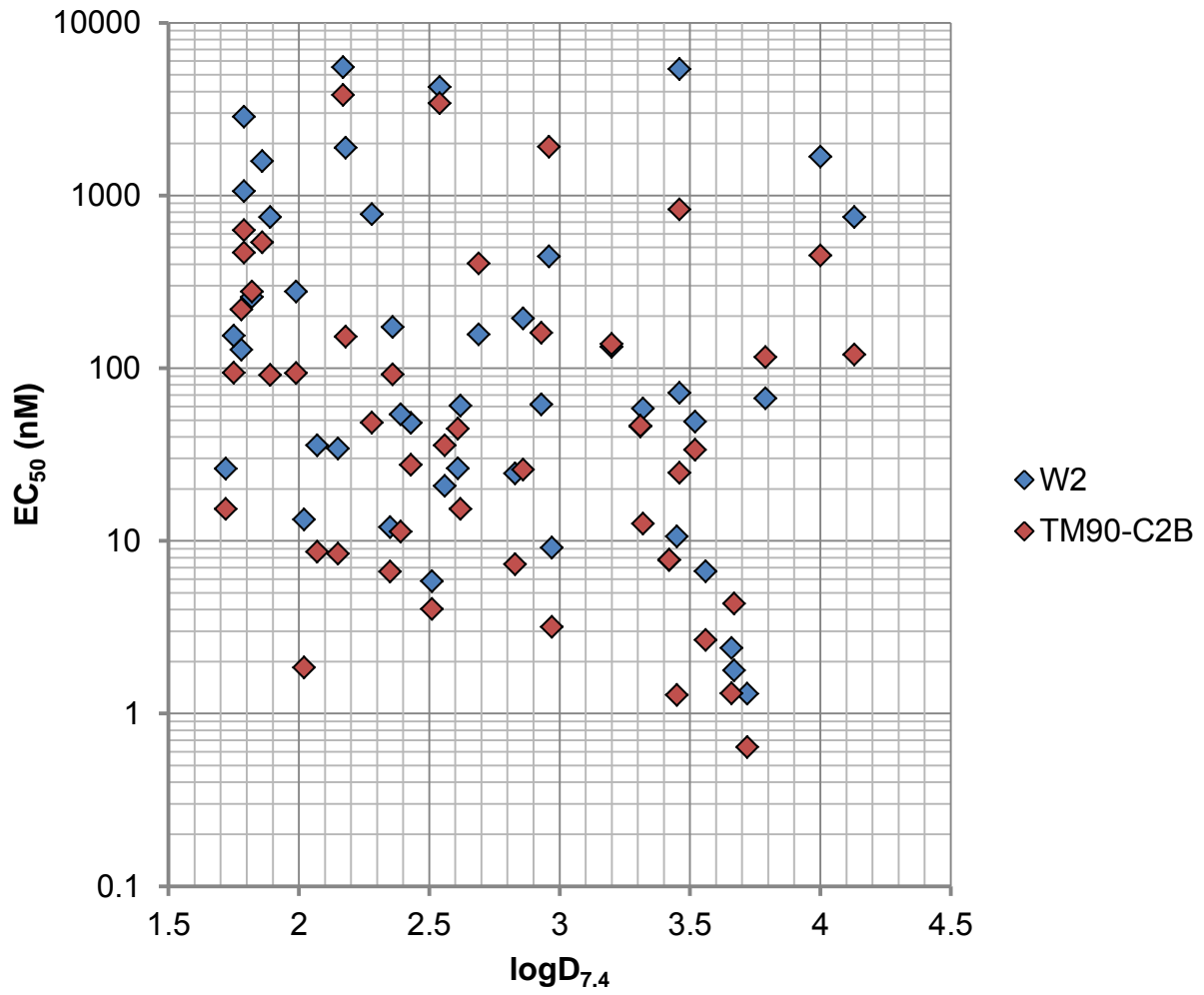
^bStandards for the permeability assay include verapamil HCl ($P_e = 1405 \times 10^{-6}$ cm/s at pH=7.4 and 39×10^{-6} cm/s at pH=4.0), carbamazepine ($P_e = 112 \times 10^{-6}$ cm/s at pH=7.4 and 108×10^{-6} cm/s at pH=4.0), and ranitidine HCl ($P_e = 0.5 \times 10^{-6}$ cm/s at pH=7.4 and 0×10^{-6} cm/s at pH=4.0).

^cStandards 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), theophylline ($\log D_{7.4}$ -0.05), and tolnaftate ($\log D_{7.4}$ 5.40).

^dThese compounds displayed little to no observable degradation throughout the assay duration (typically 250 min).

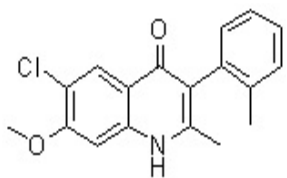
^eN.D. Not determined

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

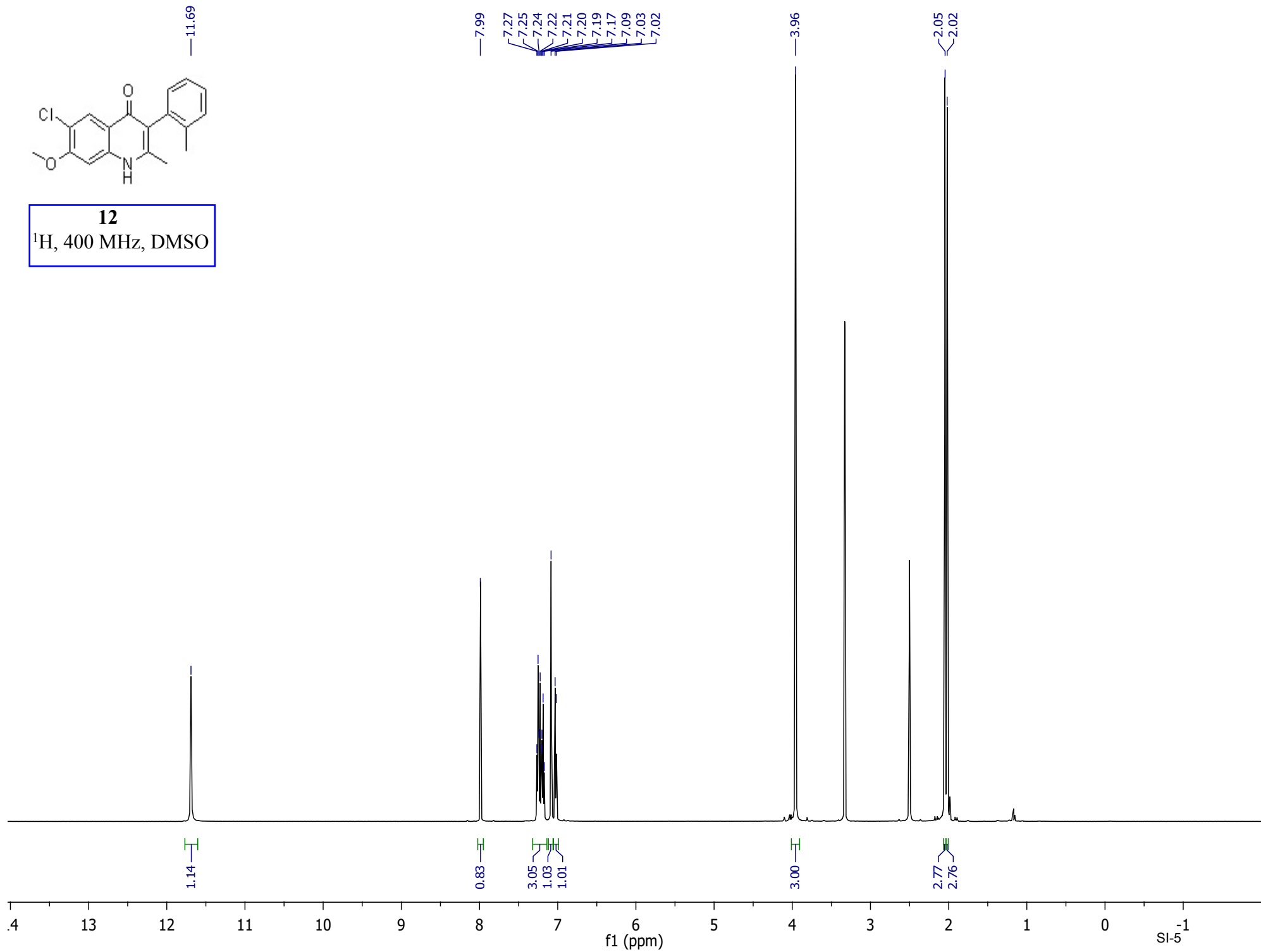


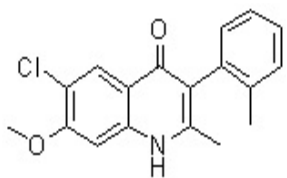
X-ray Crystallography

Crystal Data: **4**, C₁₇H₁₄ClNO₂, FW=299.74, monoclinic P2₁/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**, C₁₈H₁₆ClNO₂, FW=313.77, monoclinic P2₁/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
¹H, 400 MHz, DMSO





12

^{13}C , 101 MHz, DMSO

—173.18

—156.63

—146.56

—139.74

—137.39

—135.95

—130.84

—125.51

—120.45

—118.60

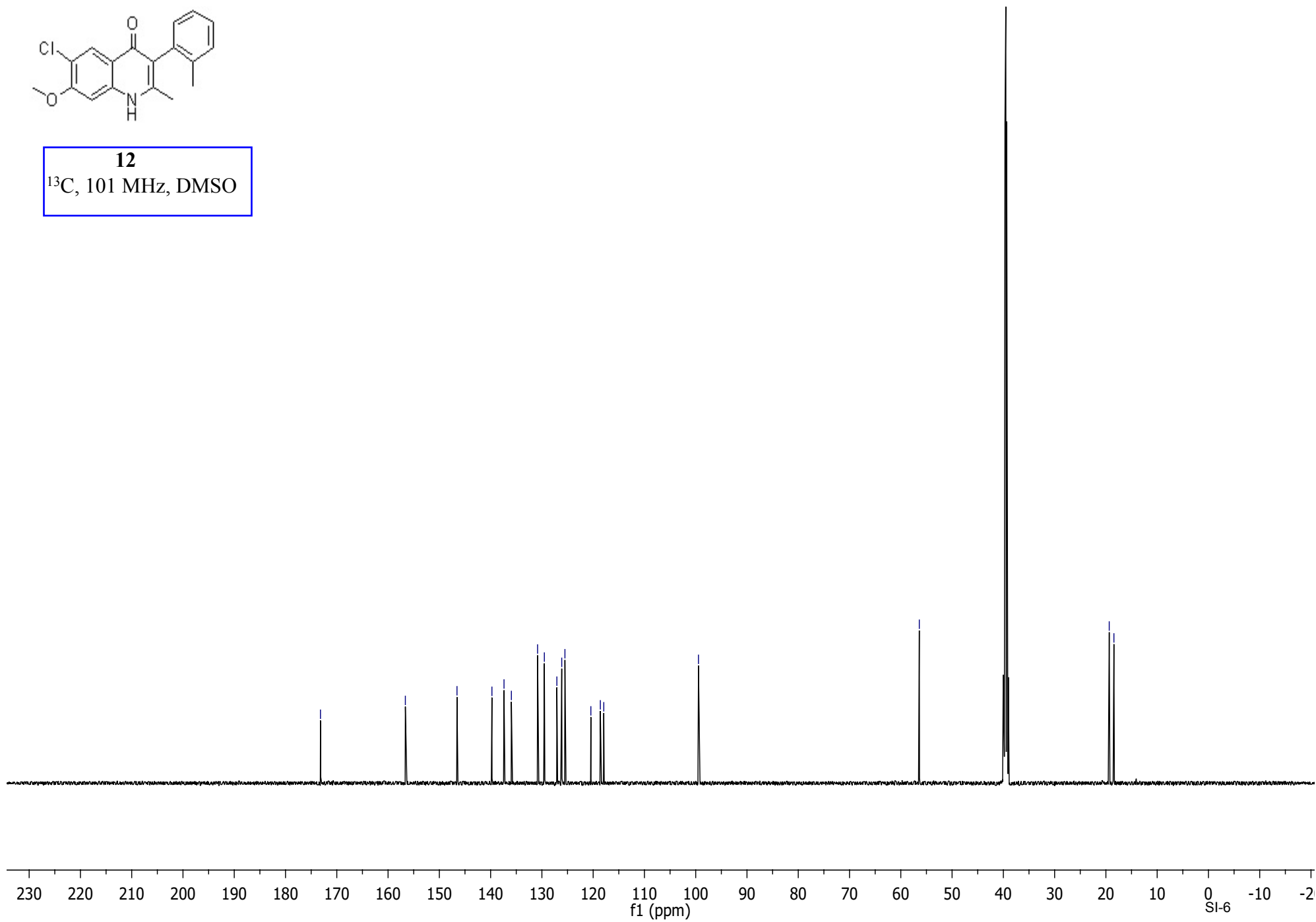
—117.93

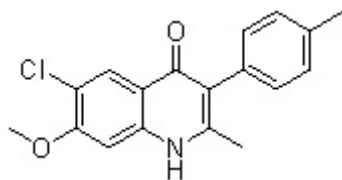
—99.46

—56.39

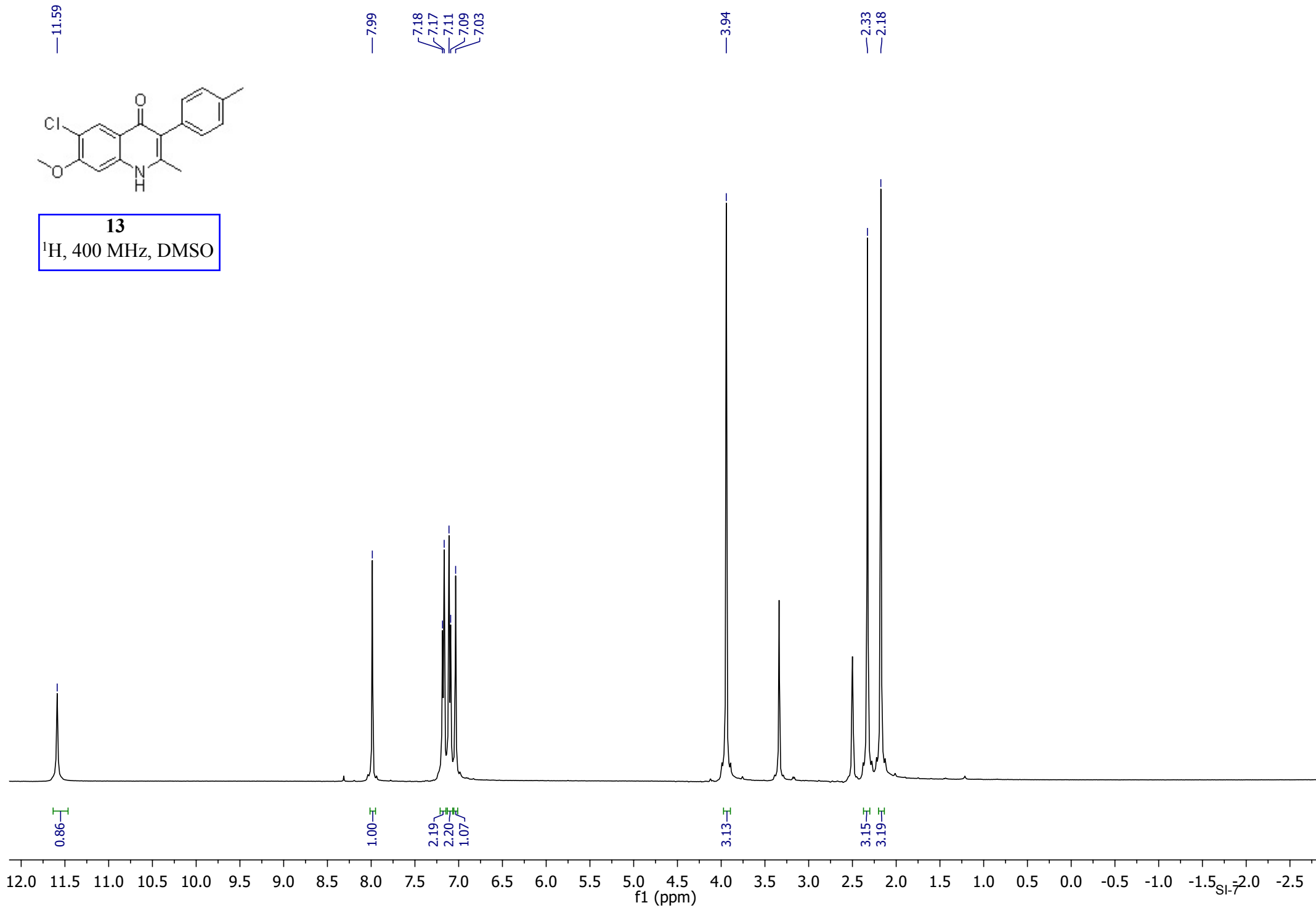
—19.35

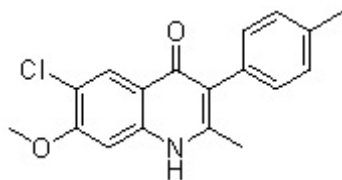
—18.43





13
¹H, 400 MHz, DMSO





13

¹³C, 101 MHz, DMSO

—173.58

—156.59

—146.34

—139.54

—135.51

—132.79

—130.76

—128.35

—126.17

—120.65

—118.74

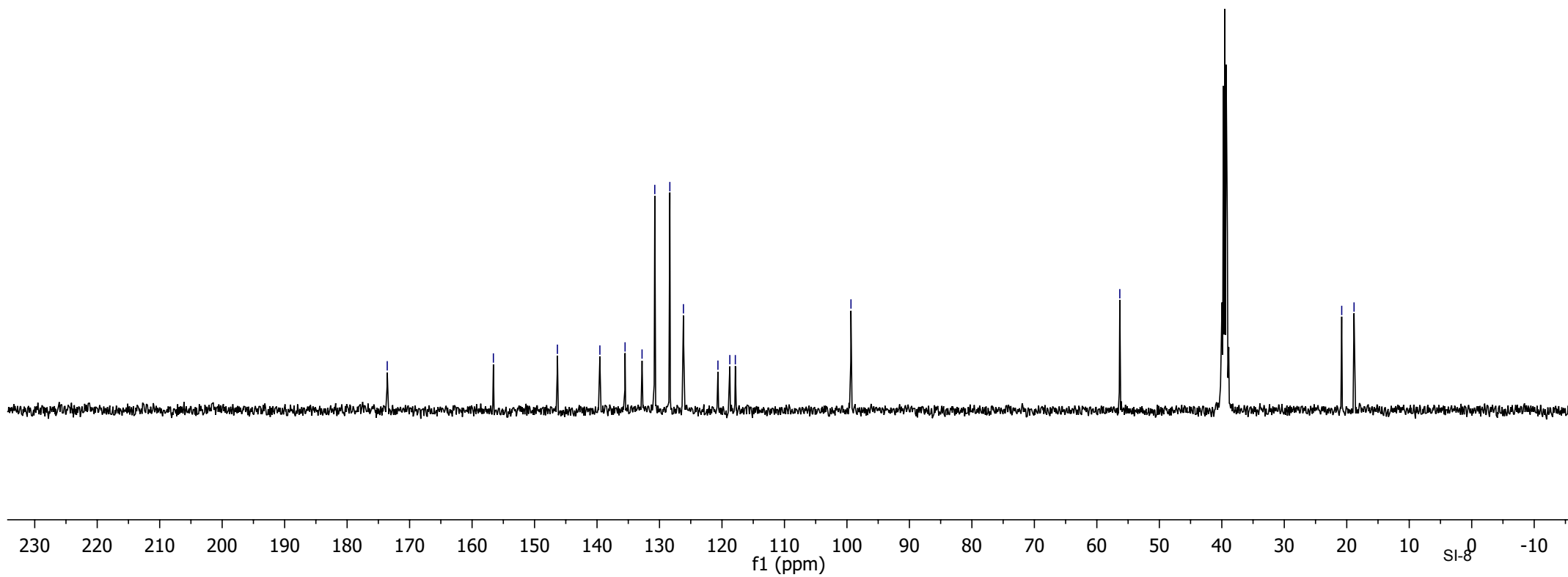
—117.86

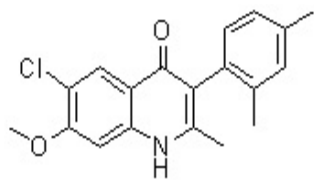
—99.35

—56.33

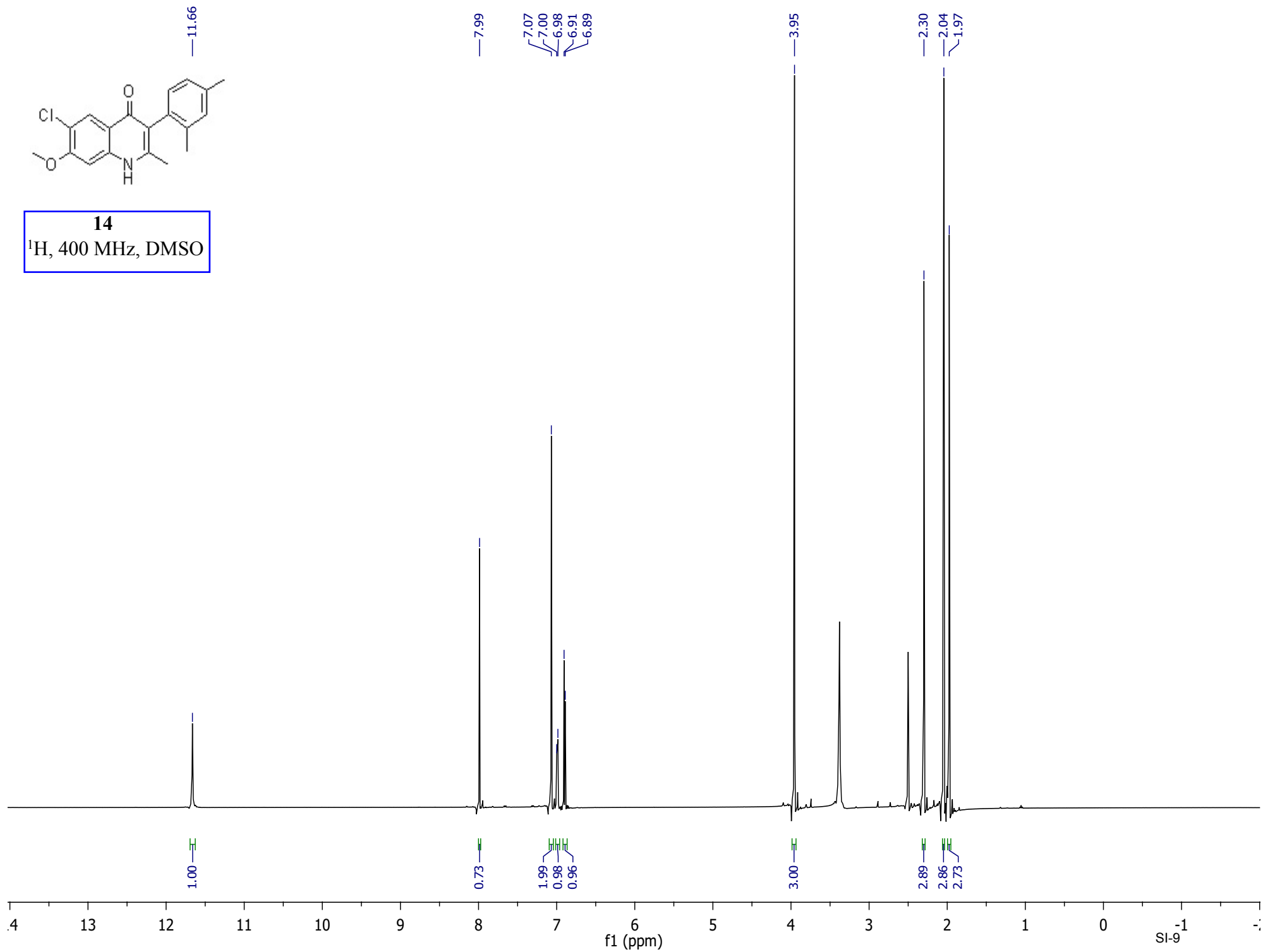
—20.81

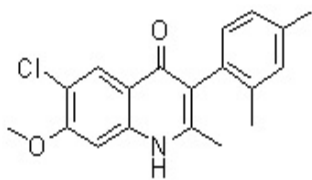
—18.83





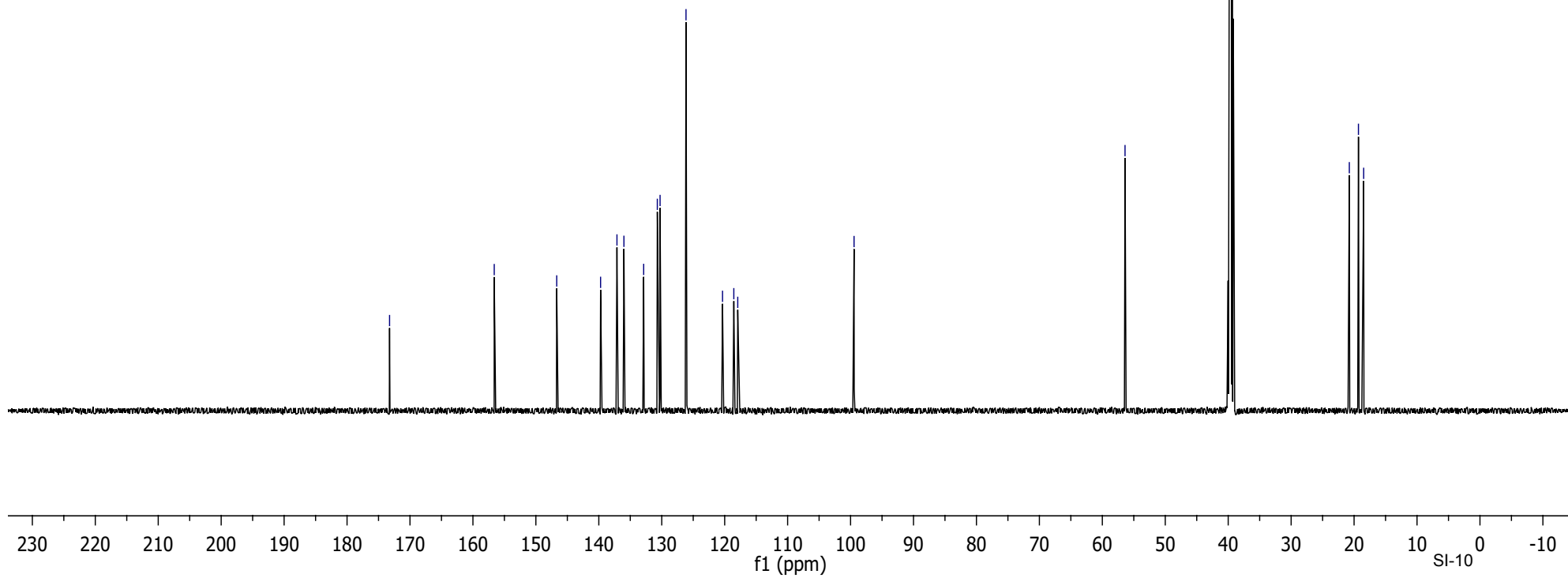
14
¹H, 400 MHz, DMSO

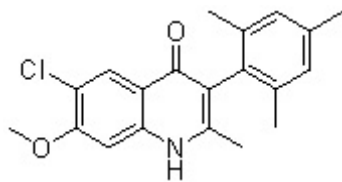




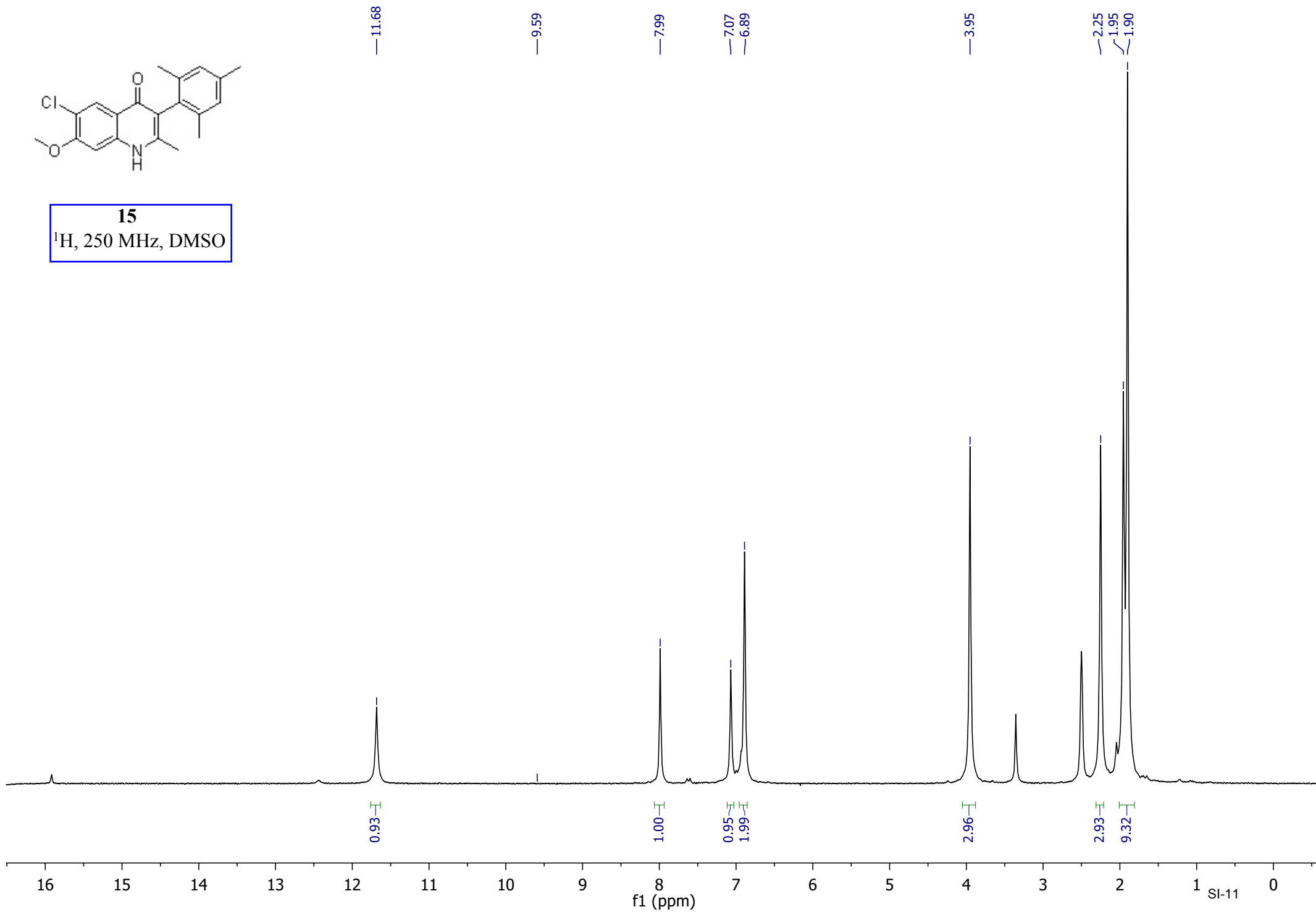
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 ^{13}C , 101 MHz, DMSO

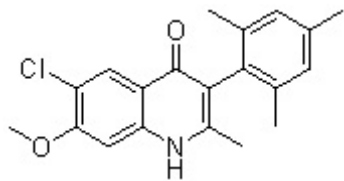
—173.24
—156.61
—146.69
—139.72
—137.12
—136.01
—130.27
—126.14
—120.34
—118.55
—117.93
—99.45
—56.39
—20.76
—19.31
—18.48





15
¹H, 250 MHz, DMSO





15

^{13}C , 126 MHz, DMSO

—173.19

—156.60

—146.43

—139.85

—136.65

—135.64

—132.51

—127.82

—126.16

—118.81

—118.52

—117.83

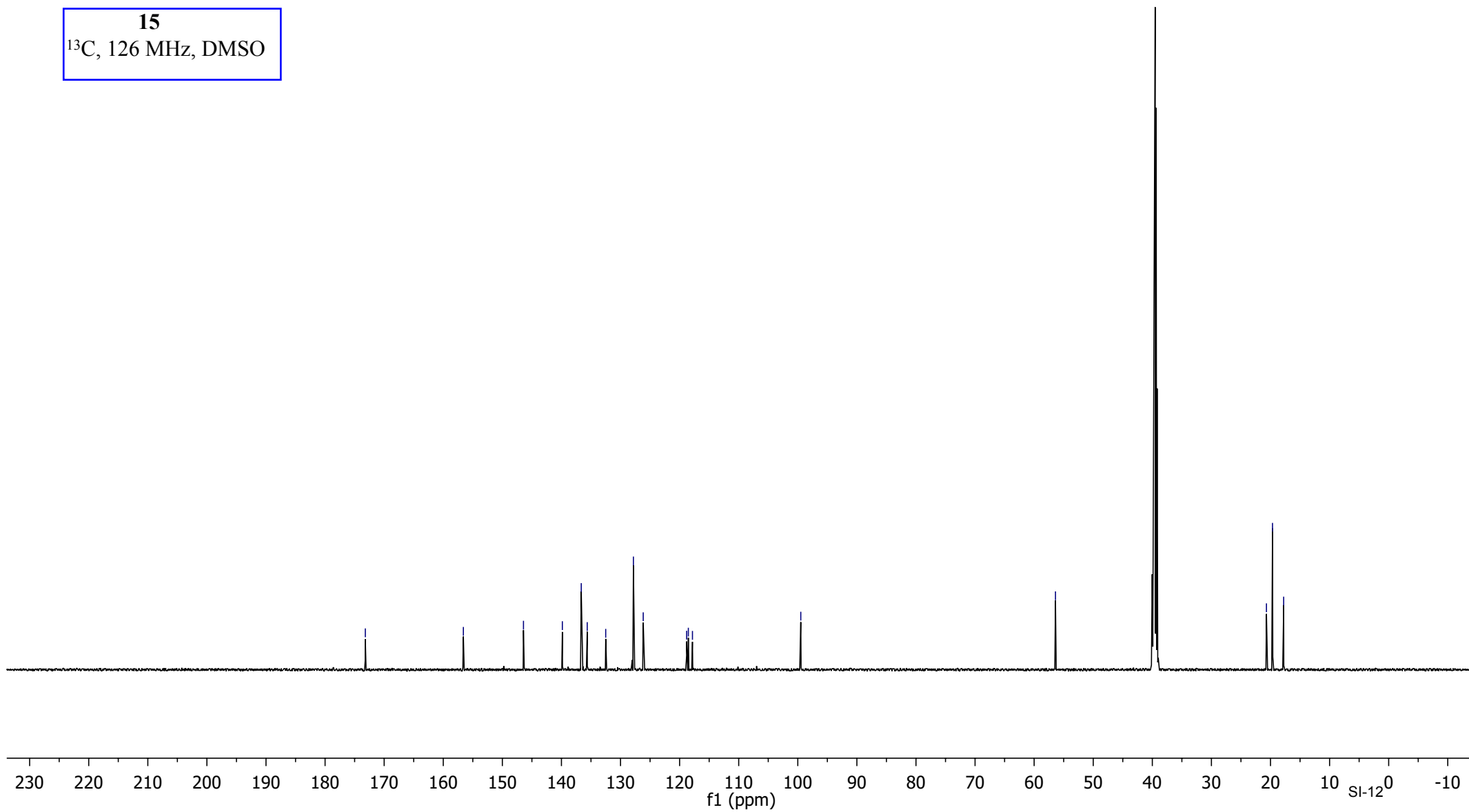
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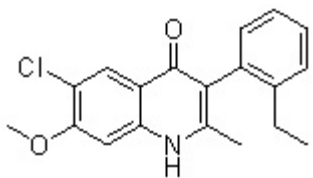
—56.39

—20.69

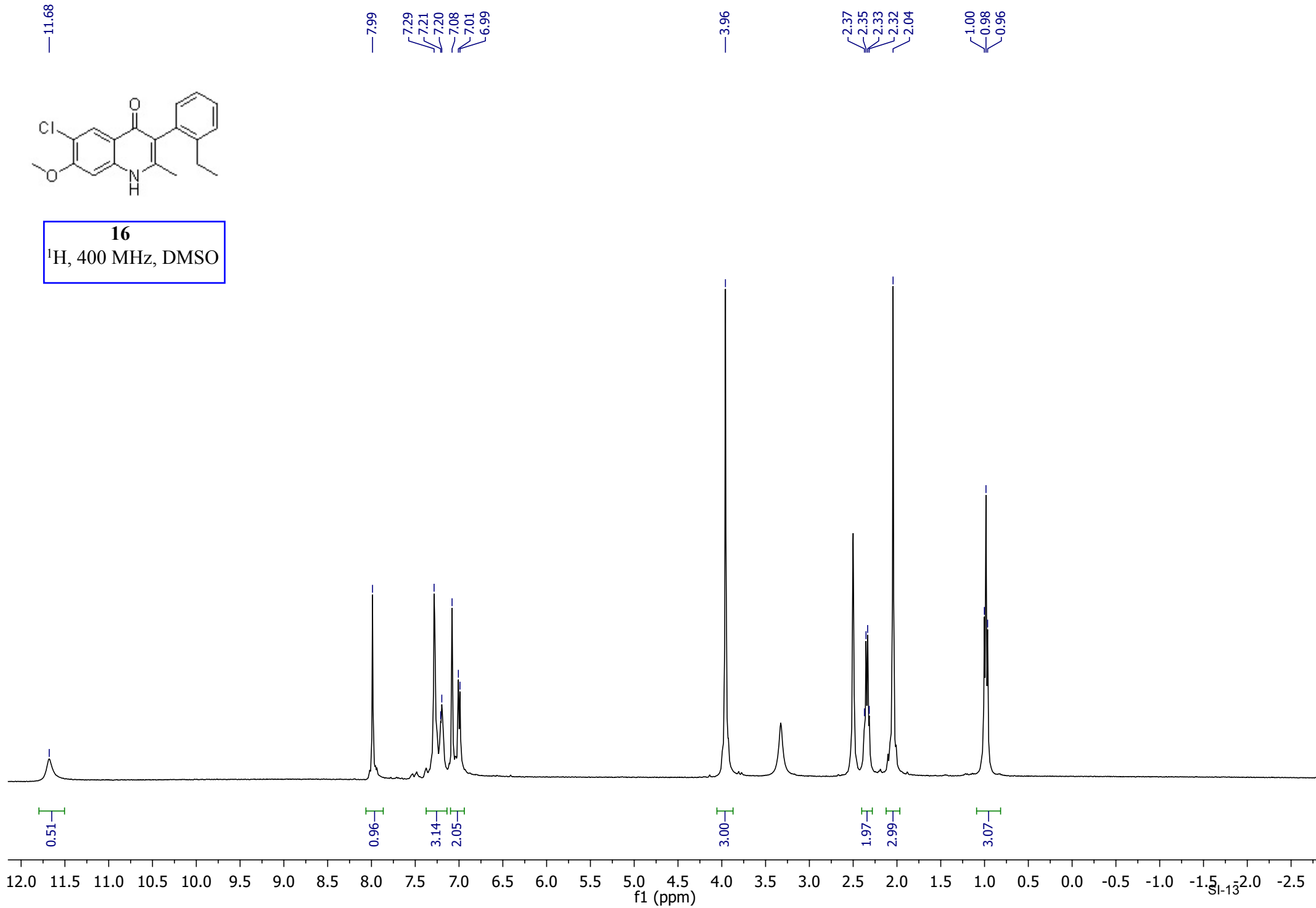
—19.66

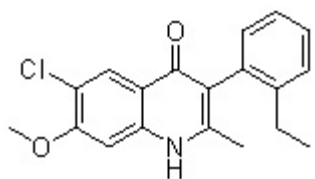
—17.77





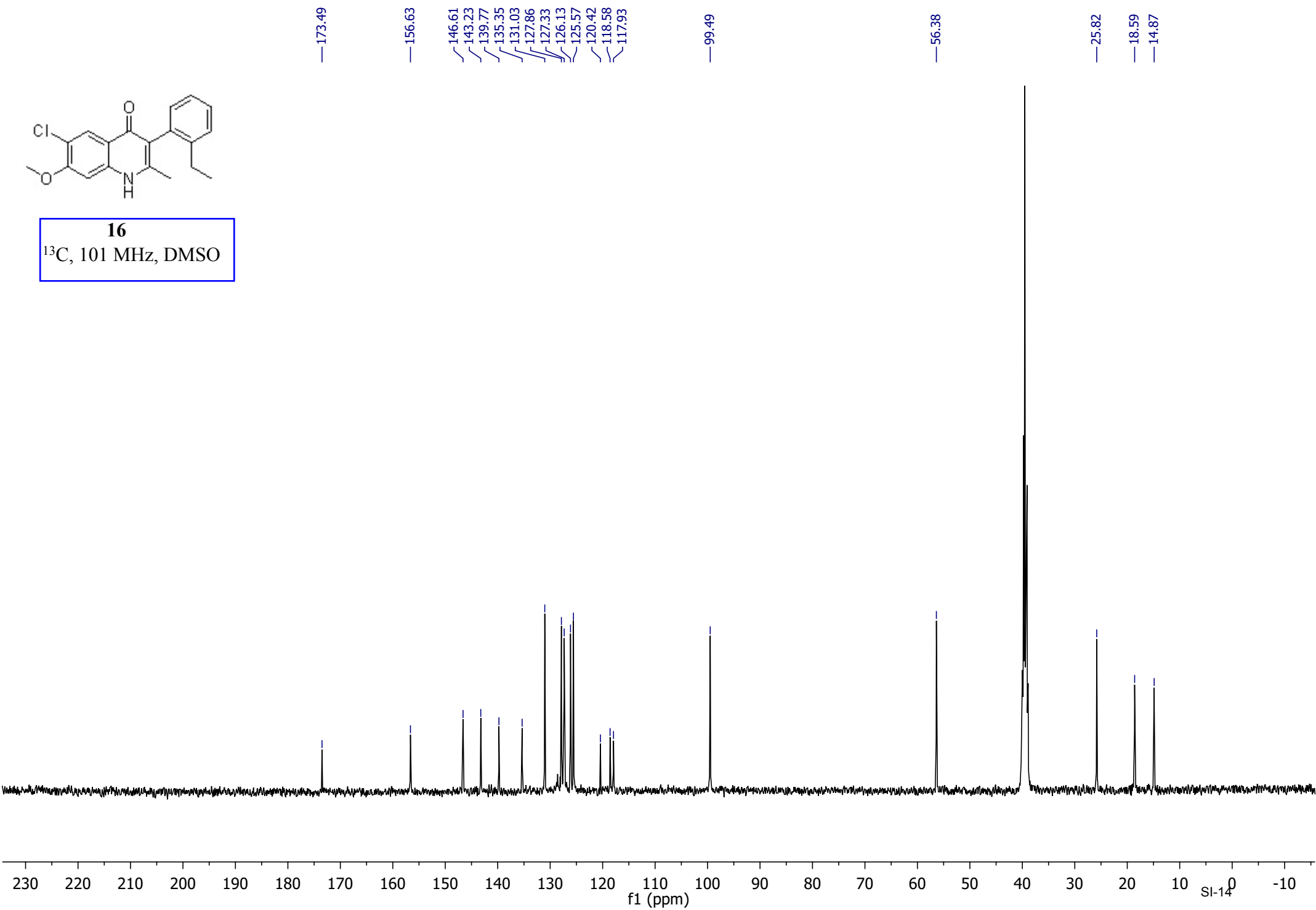
16
¹H, 400 MHz, DMSO

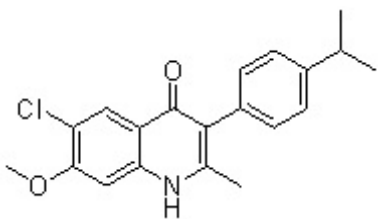




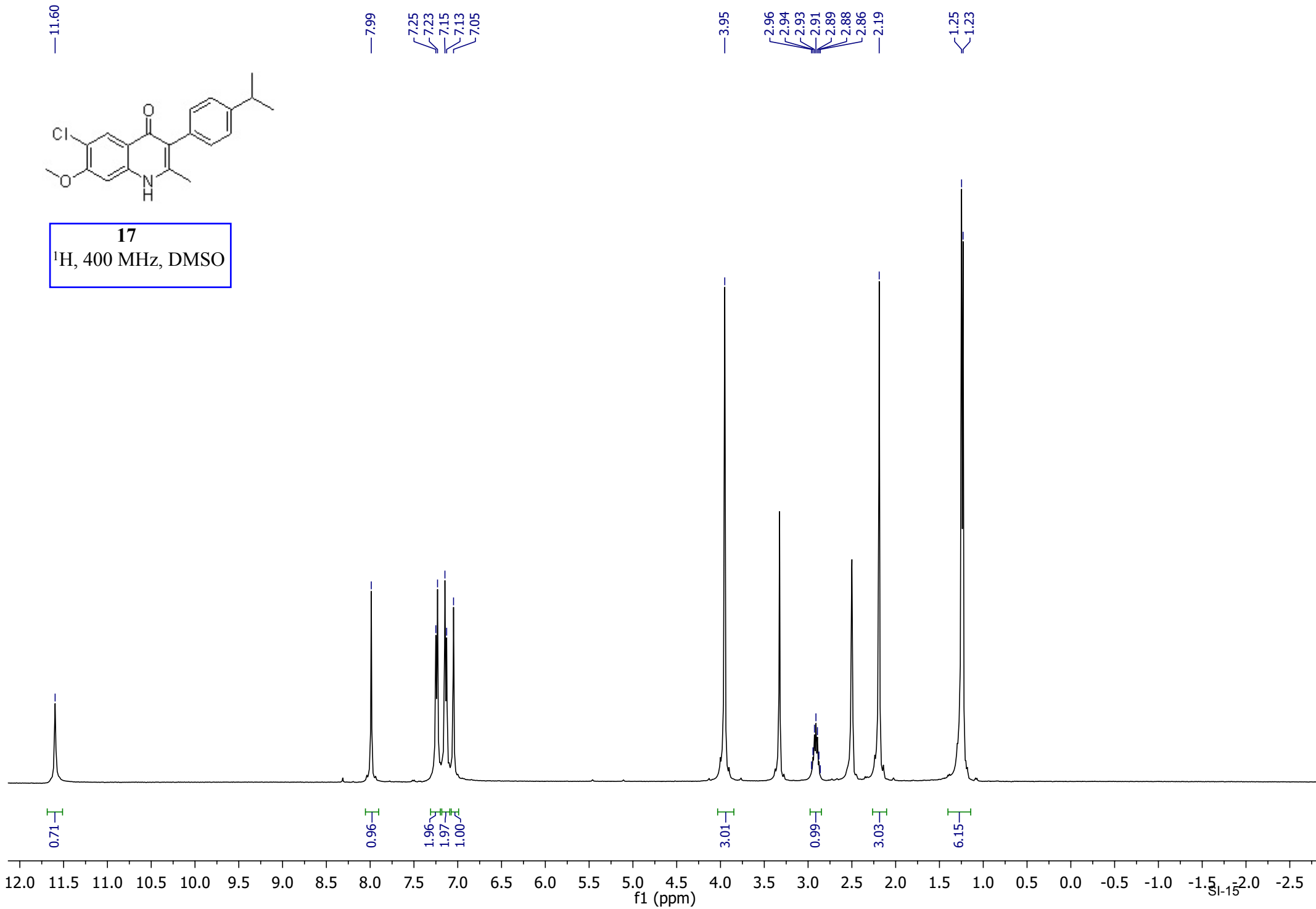
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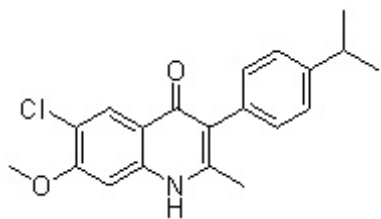
^{13}C , 101 MHz, DMSO





17
¹H, 400 MHz, DMSO

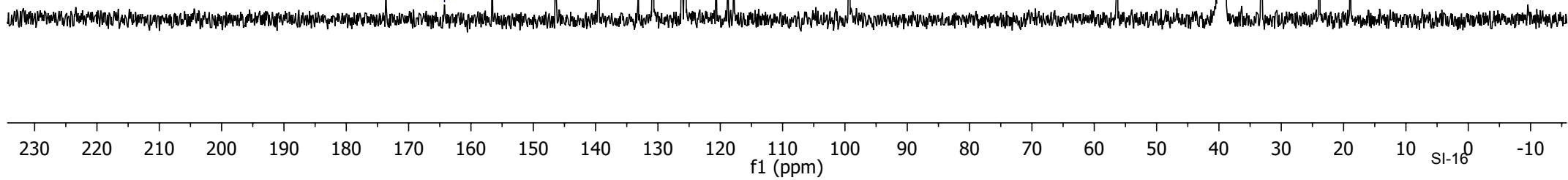


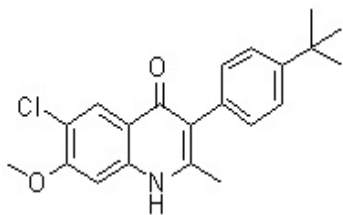


17

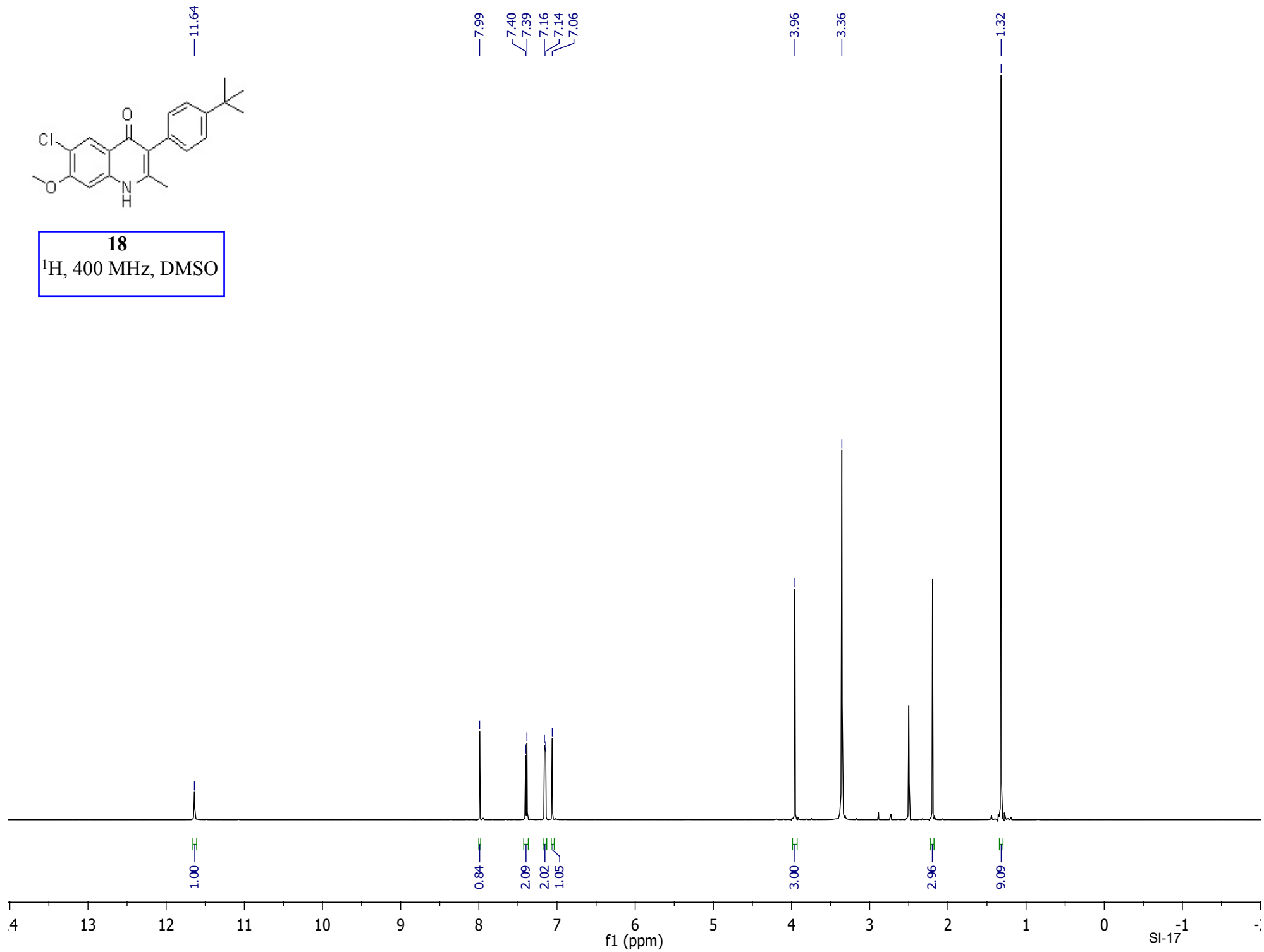
¹³C, 101 MHz, DMSO

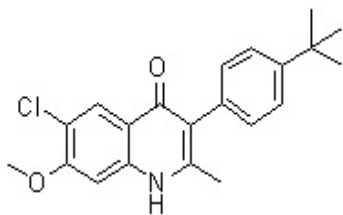
—173.61 —164.25 —156.61 —146.41 —139.55 —133.17 —130.81 —126.17 —125.64 —120.66 —118.74 —117.87 —99.36 —56.35 —33.18 —23.92 —18.90





18
¹H, 400 MHz, DMSO

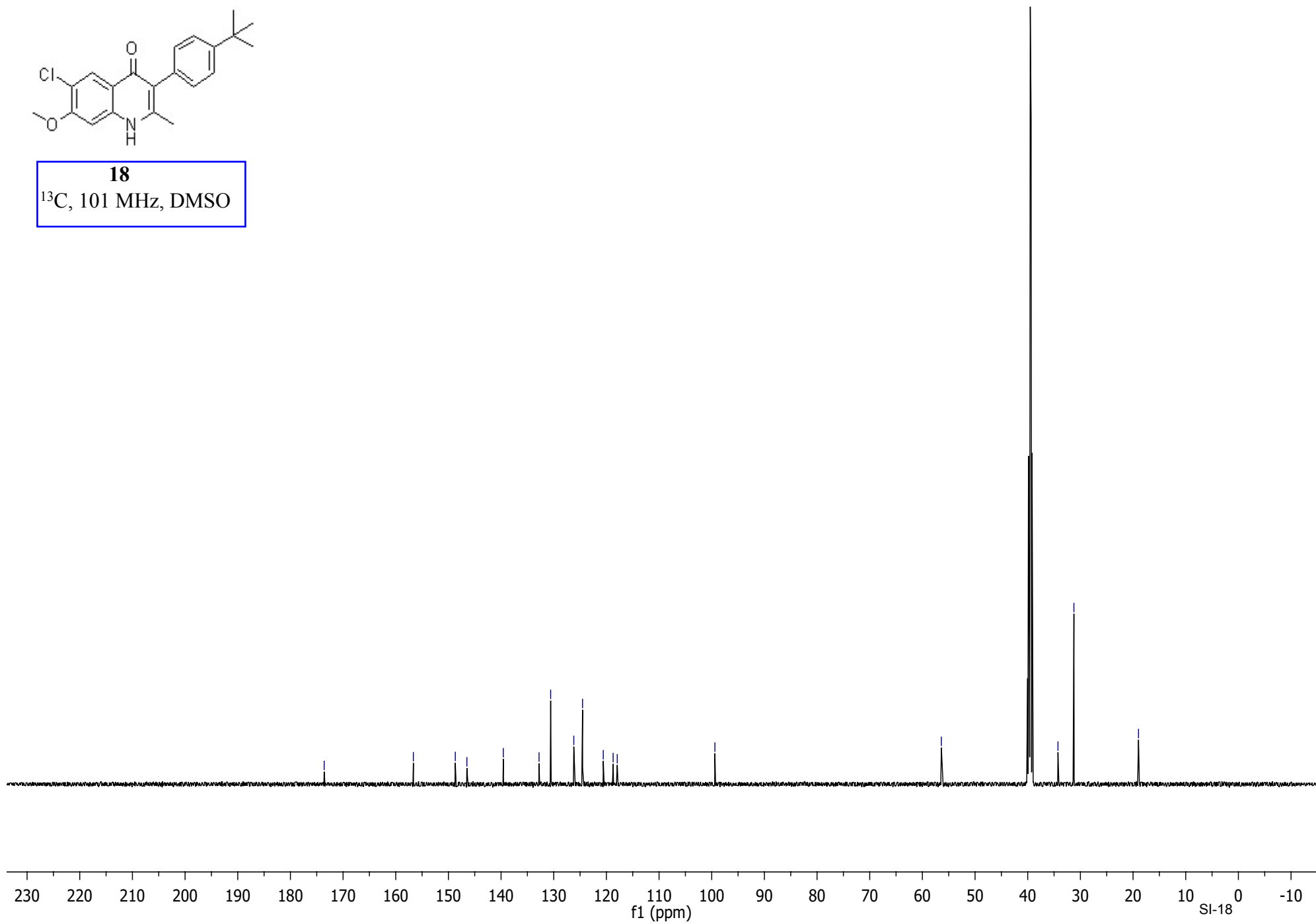


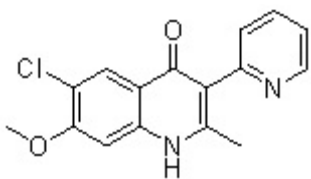


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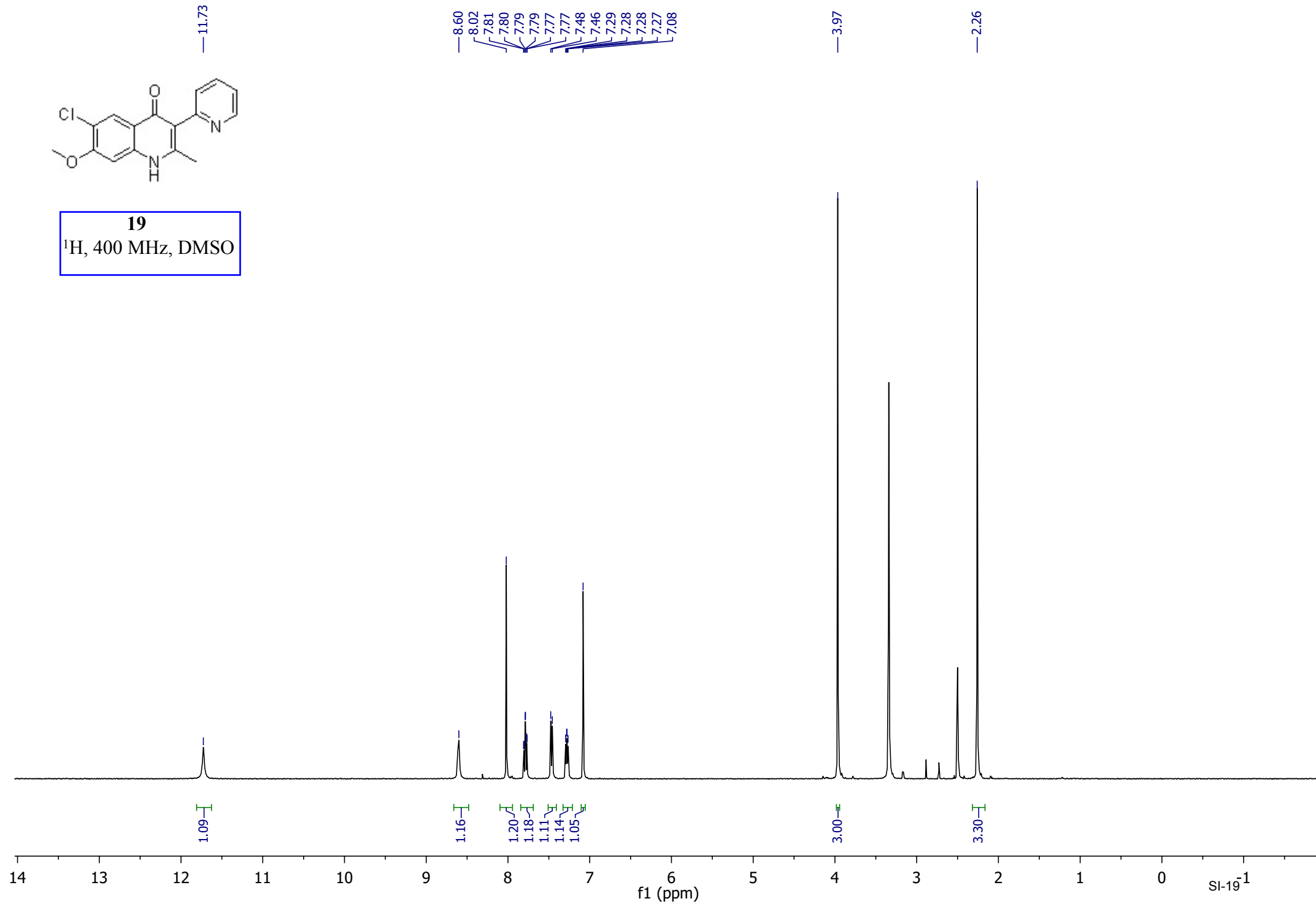
^{13}C , 101 MHz, DMSO

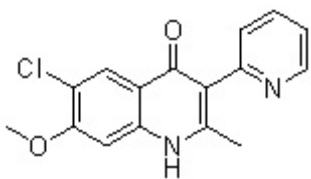
—173.59
—156.65
—148.69
—146.49
—139.57
—132.79
—130.58
—124.53
—120.59
—118.72
—117.94
—99.40
—56.40
—34.26
—31.23
—18.96





19
¹H, 400 MHz, DMSO





19

^{13}C , 101 MHz, DMSO

— 173.30

— 156.78

— 155.00

— 148.65

— 148.10

— 139.53

— 135.44

— 126.84

— 126.10

— 121.59

— 120.09

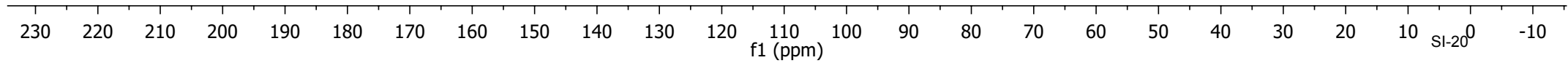
— 119.06

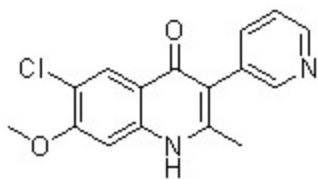
— 118.24

— 99.60

— 56.39

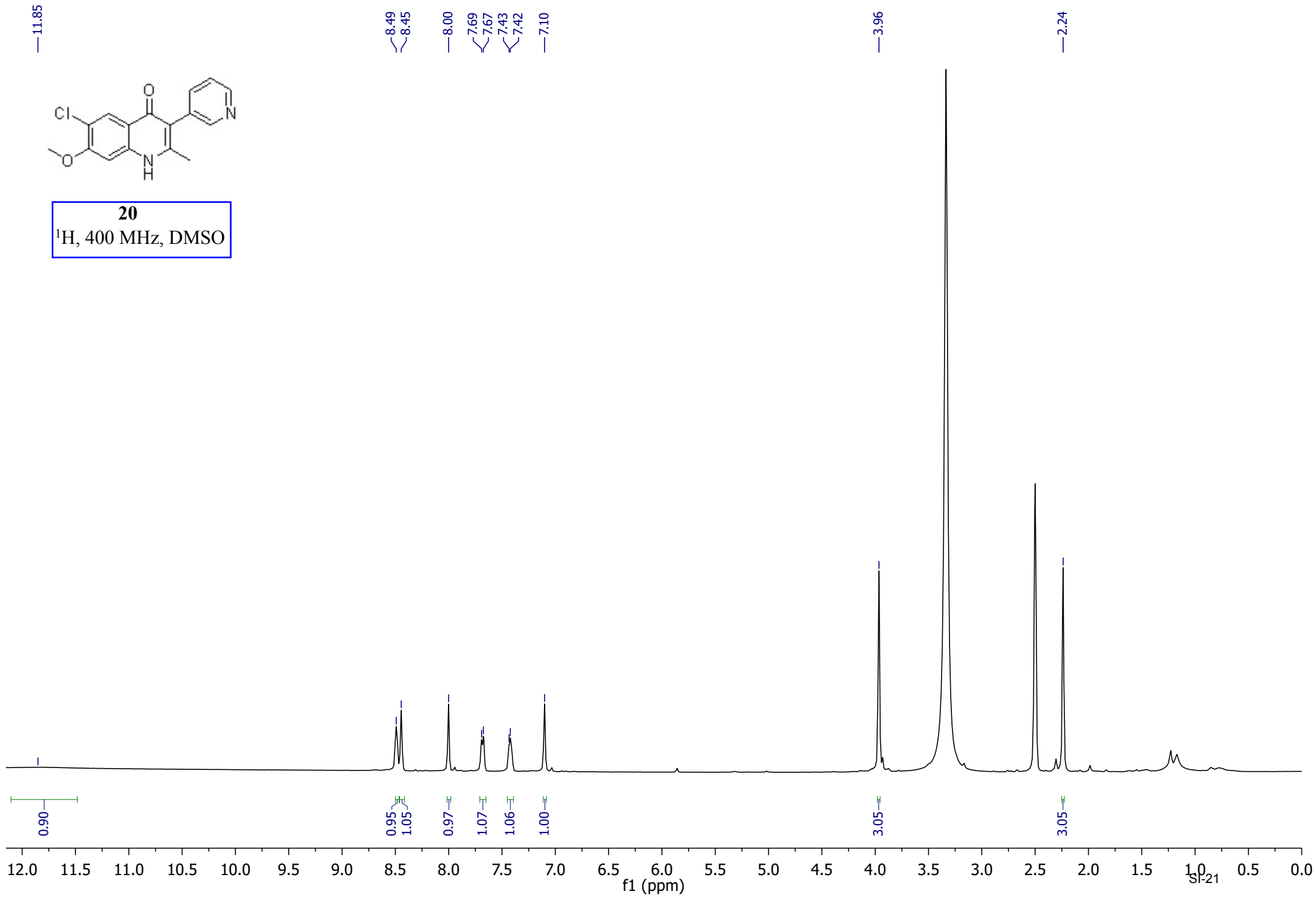
— 18.59

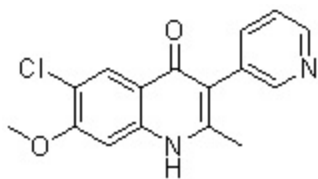




20

^1H , 400 MHz, DMSO





20

¹³C, 101 MHz, DMSO

— 173.40

— 156.83

— 151.34

— 147.48

— 147.24

— 139.72

— 138.44

— 131.58

— 126.10

— 122.96

— 118.62

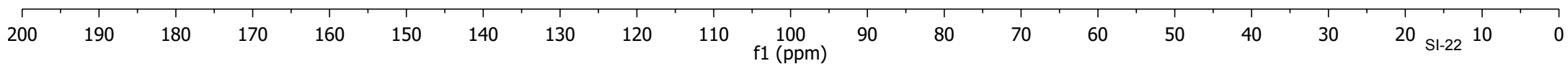
— 118.23

— 117.24

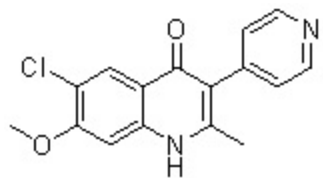
— 99.60

— 56.42

— 18.85



11.80



21
¹H, 400 MHz, DMSO

8.58
8.57

8.00

7.31
7.30
7.29
7.07

3.96

2.25

0.85

2.04

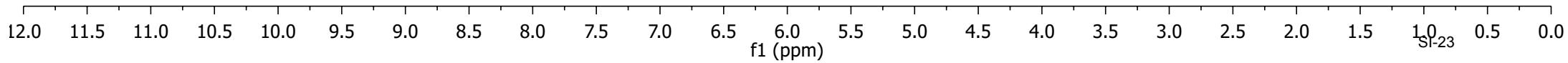
0.75

2.12

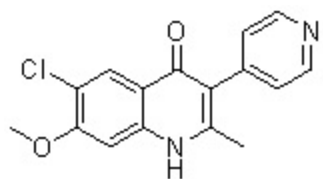
1.00

3.21

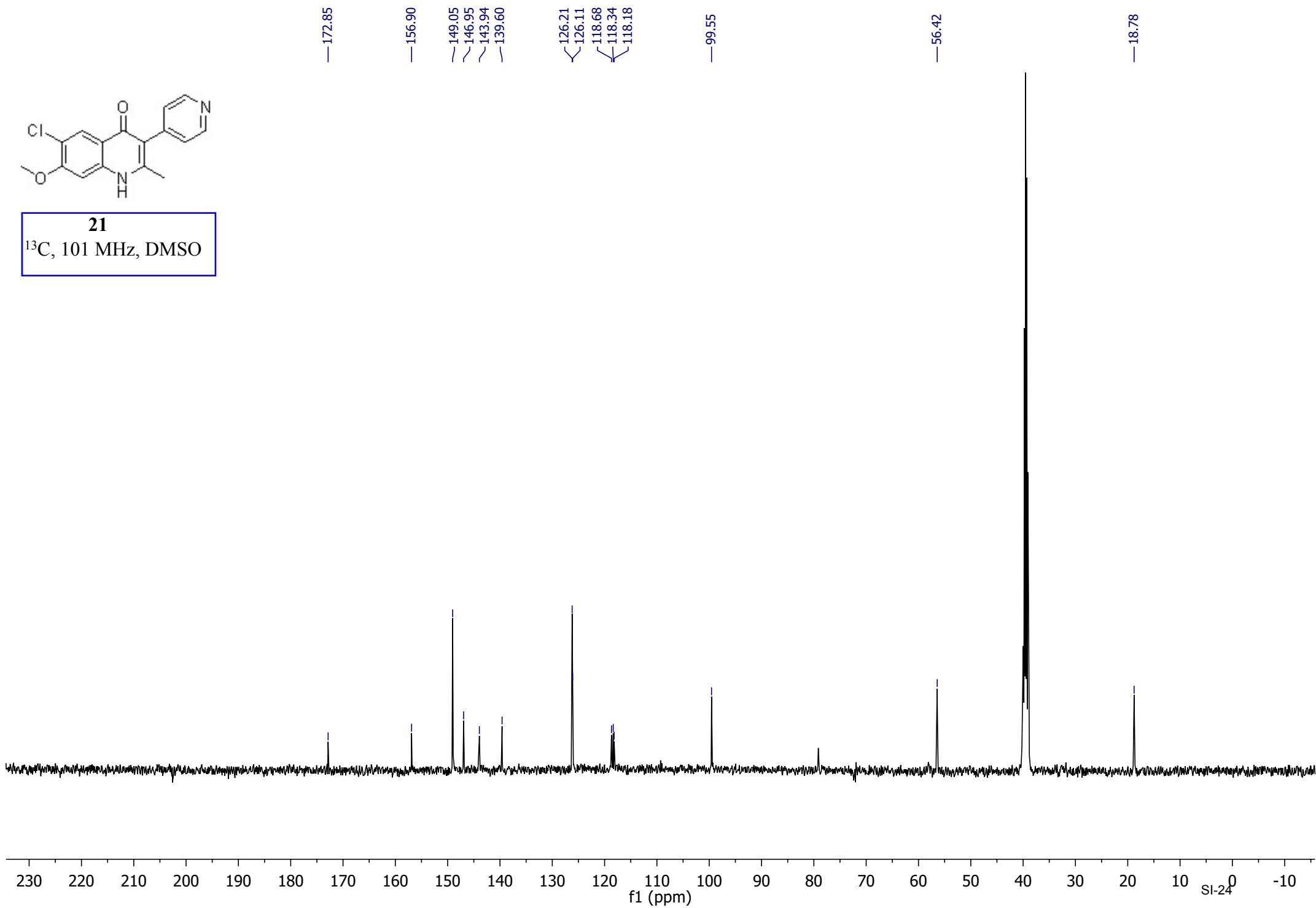
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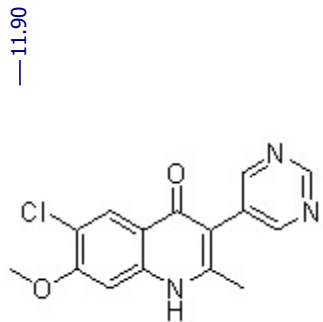


SF-23

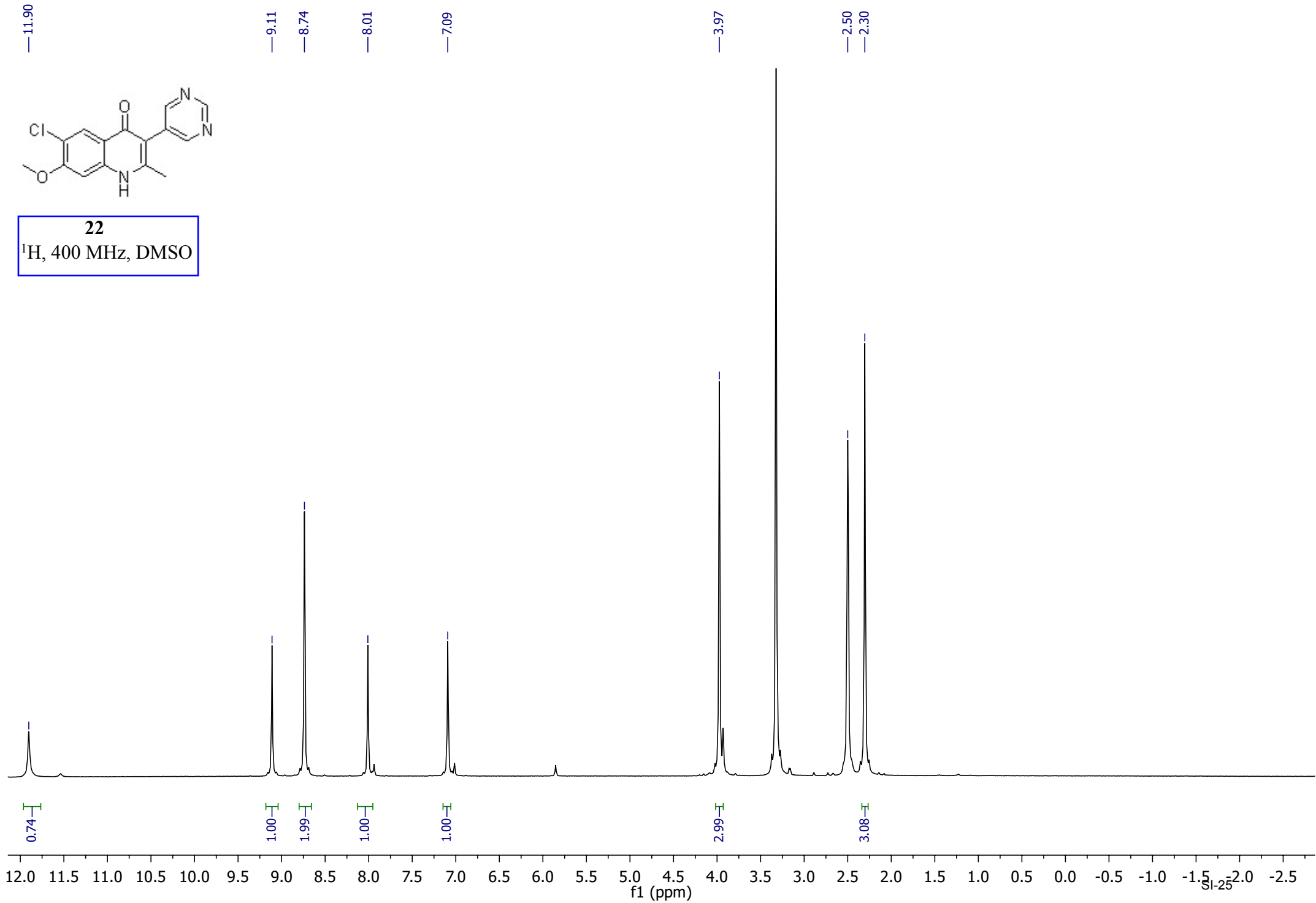


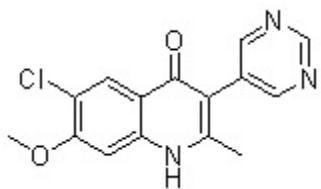
21
¹³C, 101 MHz, DMSO





22
¹H, 400 MHz, DMSO





22

^{13}C , 101 MHz, DMSO

—173.88

—159.05

—157.73

—157.12

—148.56

—140.37

—130.39

—126.76

—119.27

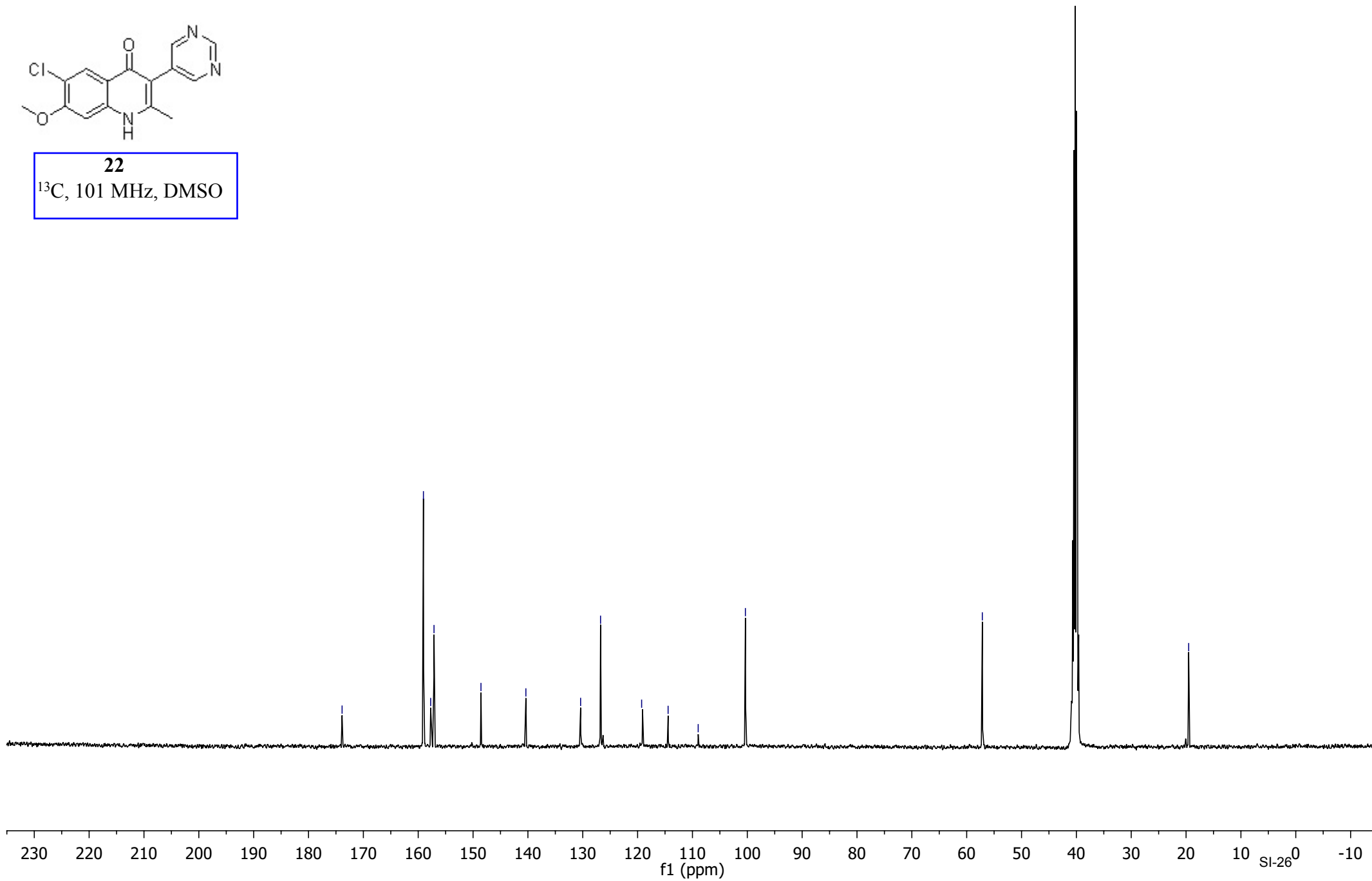
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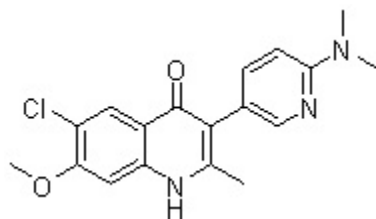
—108.95

—100.35

—57.15

—19.52





23

¹H, 400 MHz, DMSO

11.61

7.98
7.94
7.94
7.40
7.40
7.38
7.38
7.03
6.66
6.63

3.95

3.04

2.24

0.98

1.06

1.06

1.00

1.08

0.99

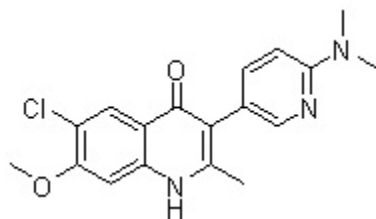
2.97

6.06

3.10

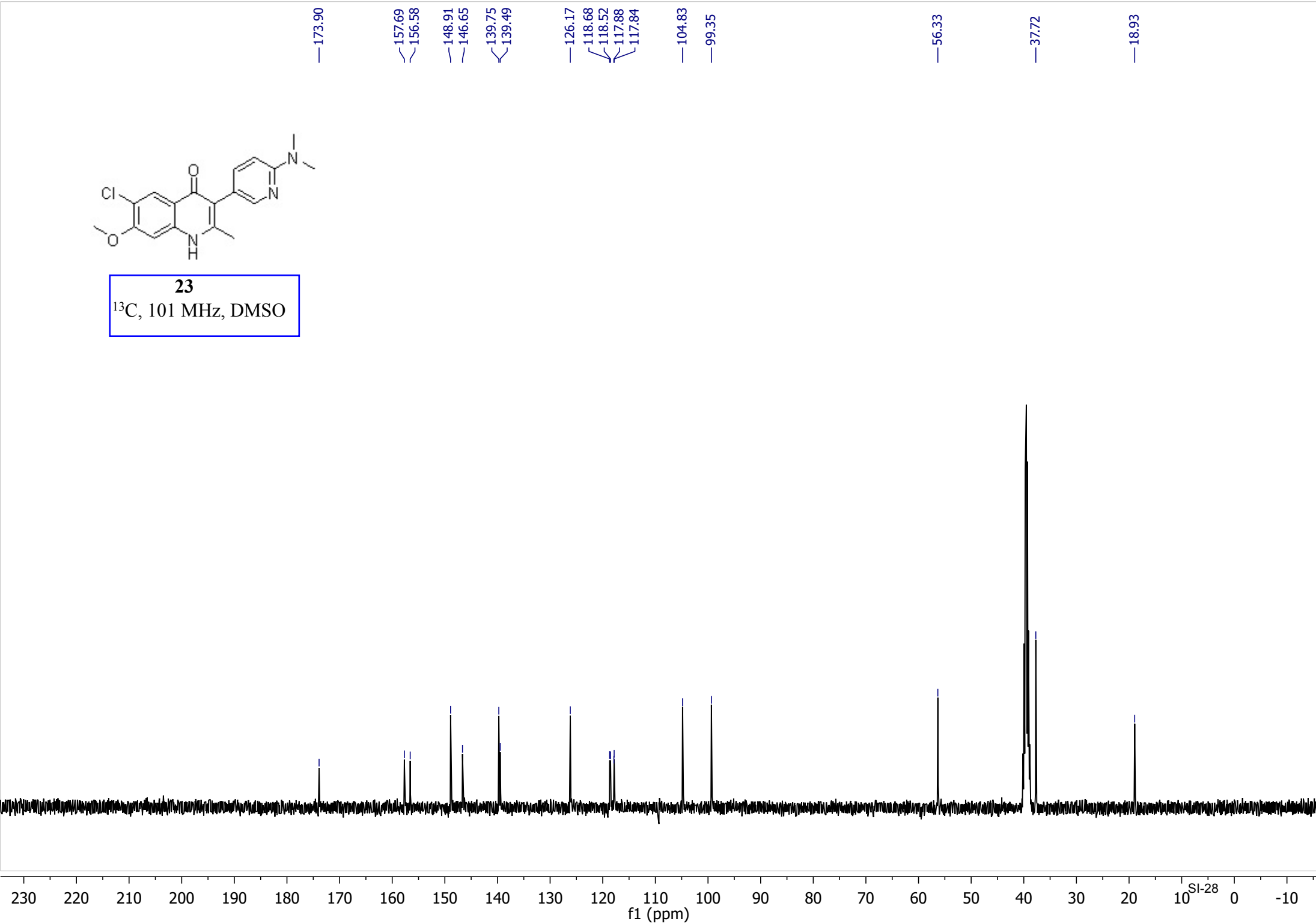
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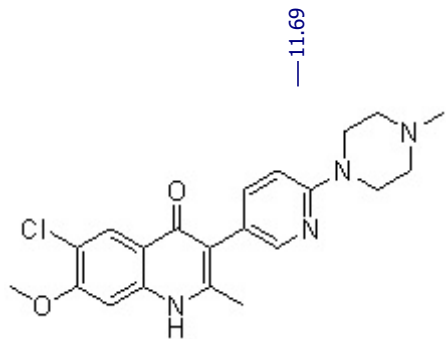
f1 (ppm)



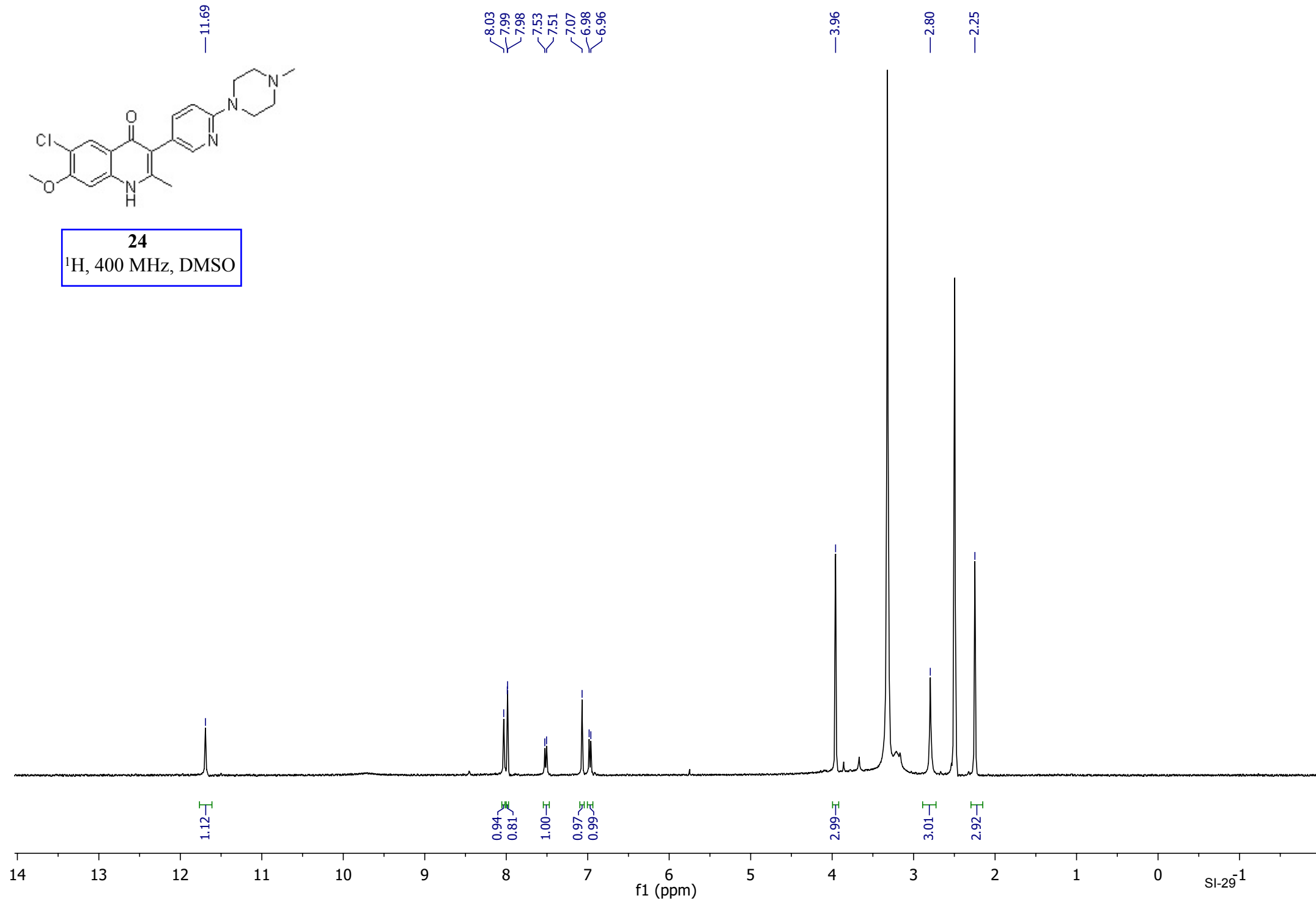
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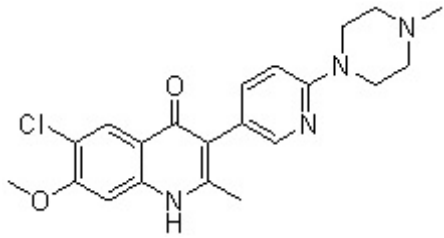
^{13}C , 101 MHz, DMSO





24
¹H, 400 MHz, DMSO





24
¹³C, 101 MHz, DMSO

—173.77

156.69
156.49

149.03
146.93

140.49
139.55

126.14

121.62

118.51

118.04

117.30

—106.76

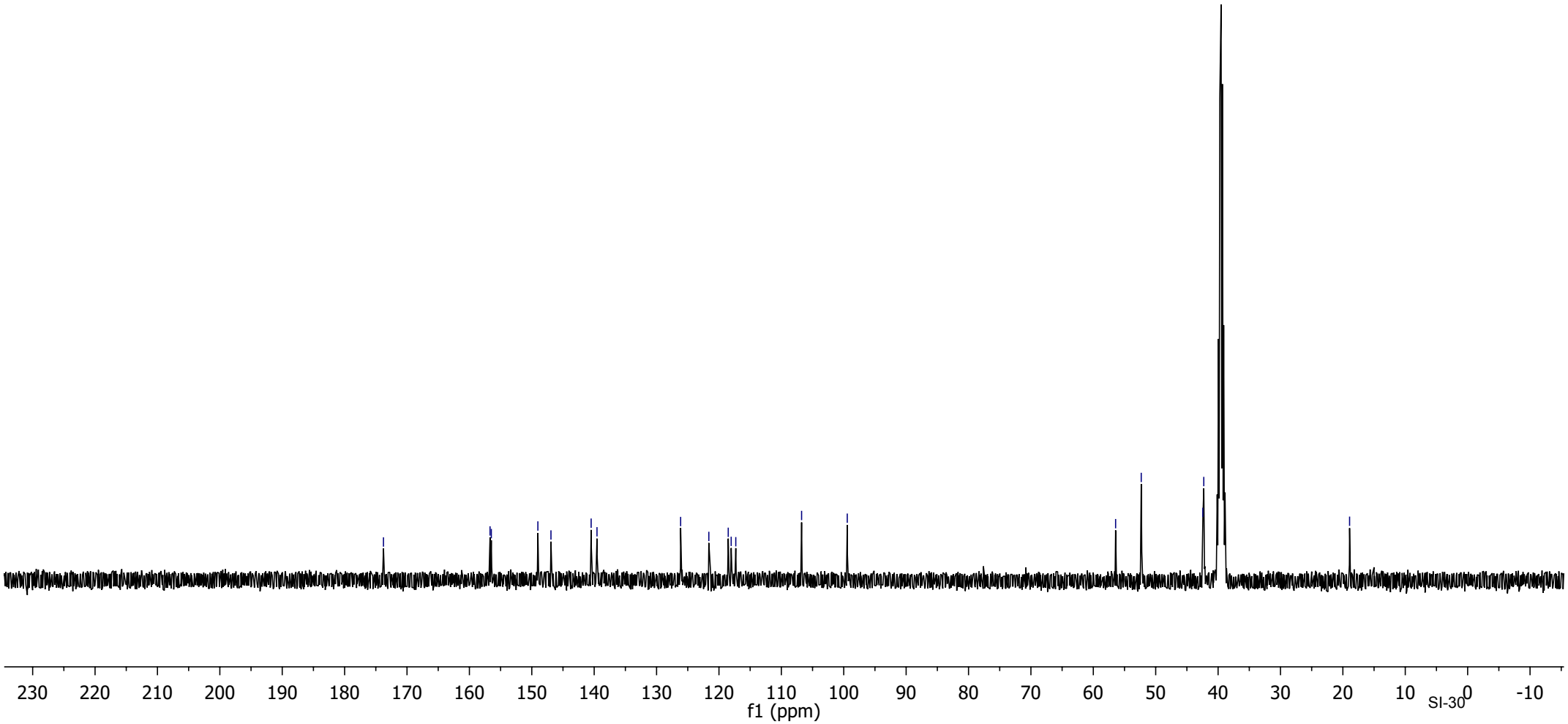
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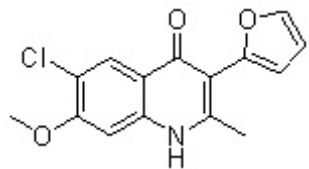
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—52.32

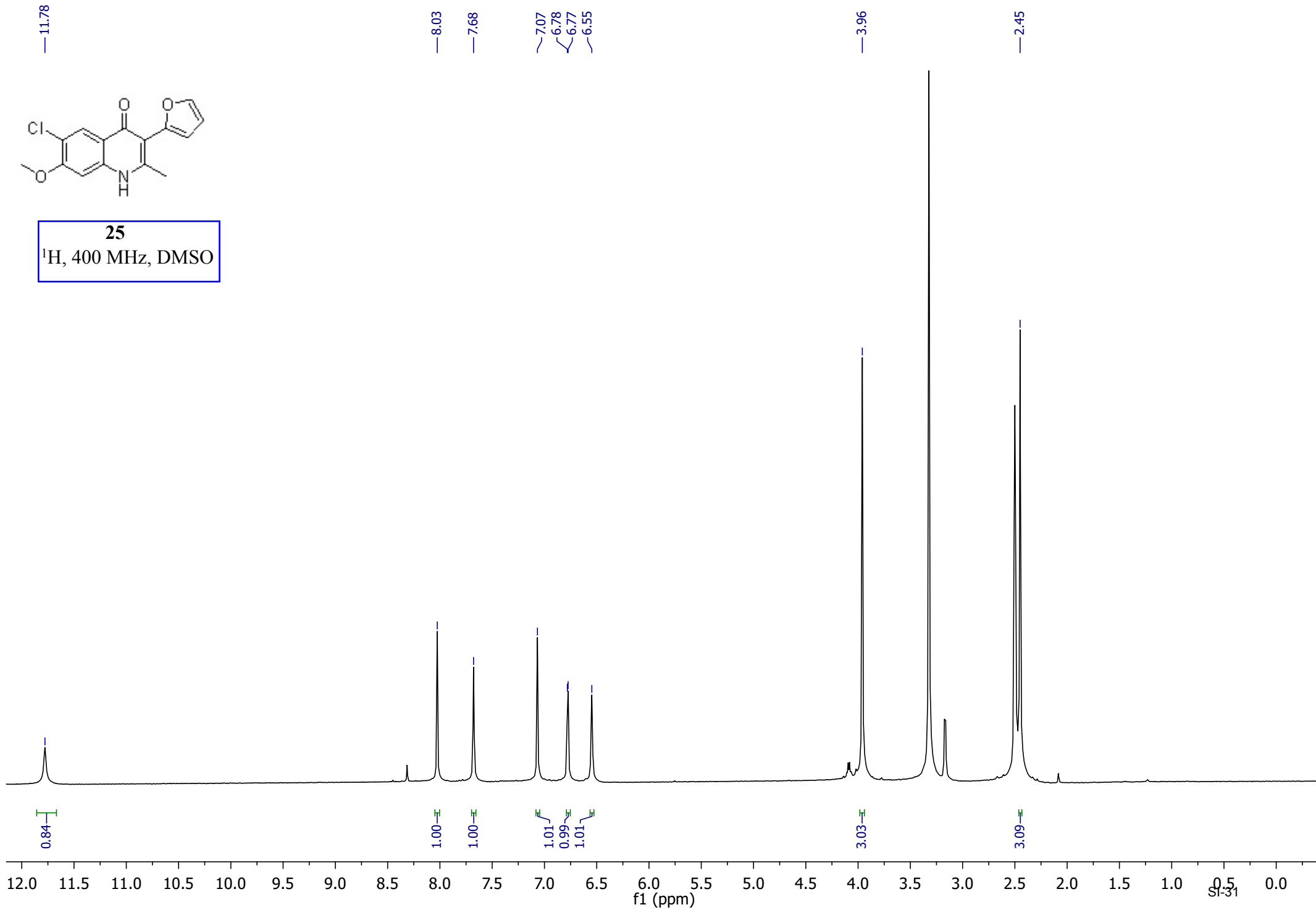
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42.29

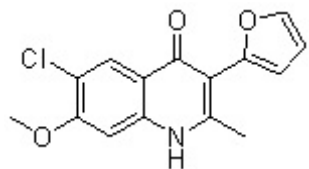
—18.92





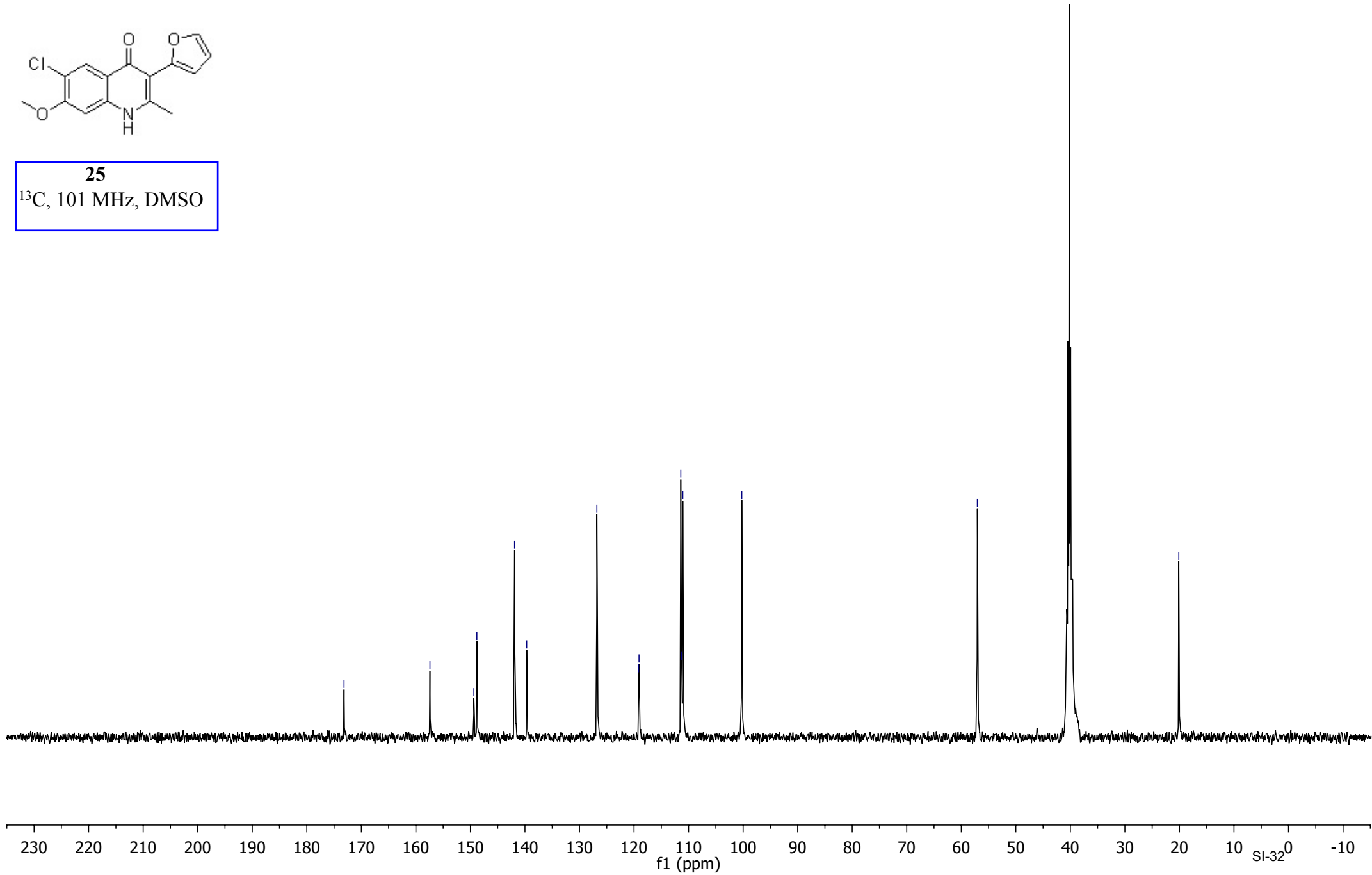
25
¹H, 400 MHz, DMSO

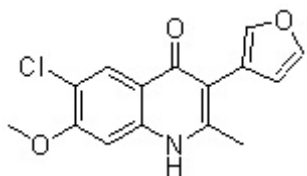




25
¹³C, 101 MHz, DMSO

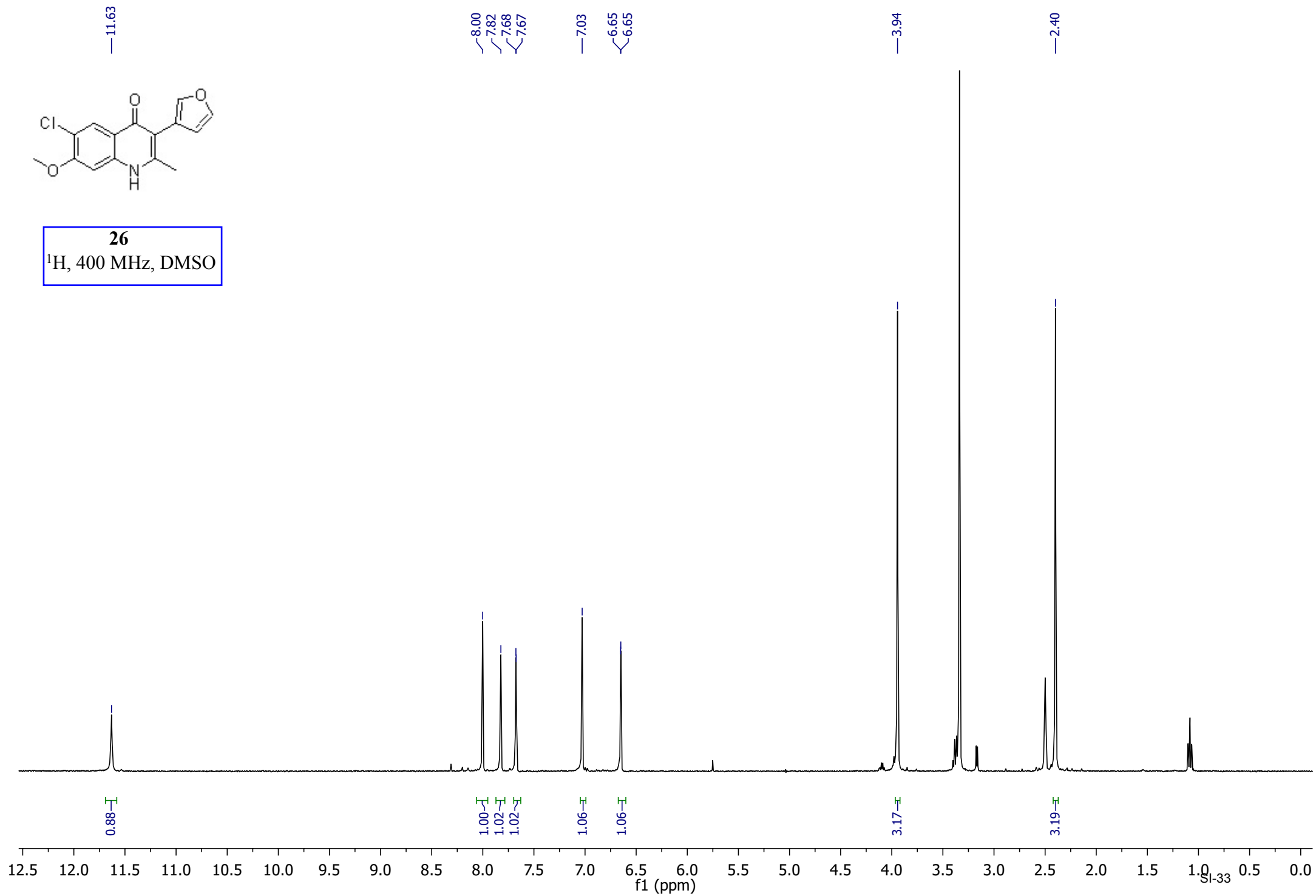
—173.17
—157.42
—149.37
—148.82
—141.91
—139.68
—126.81
—119.17
—119.09
—111.42
—111.27
—111.06
—100.24
—57.06
—20.11

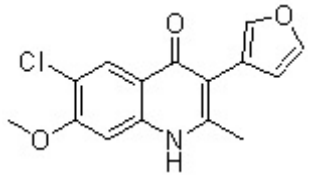




26

¹H, 400 MHz, DMSO





26

¹³C, 101 MHz, DMSO

—173.41

—156.74

~147.03

~142.01

~141.82

~139.25

—126.28

~118.37

~118.33

~118.23

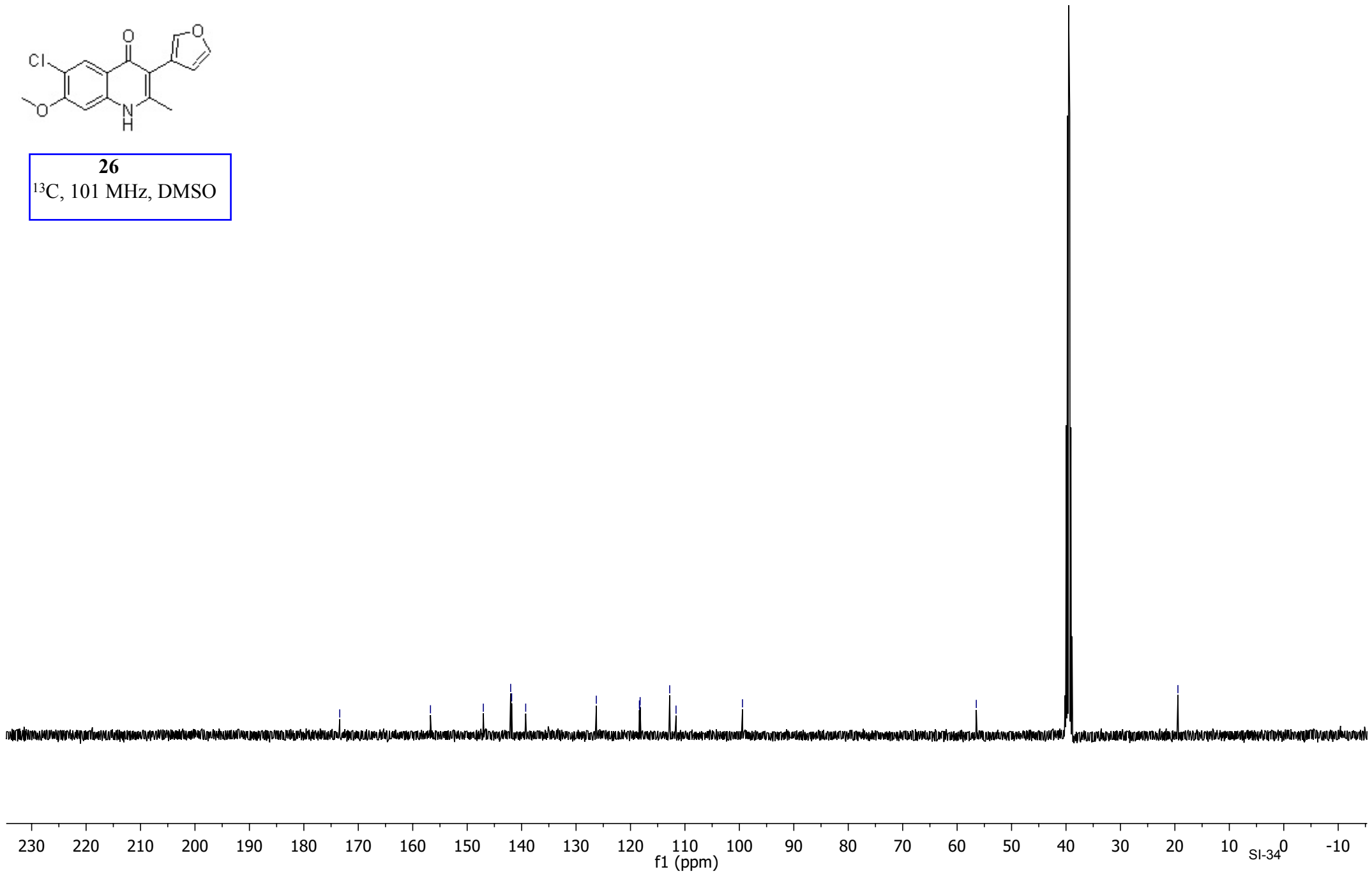
~112.80

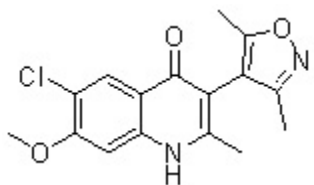
~111.63

—99.42

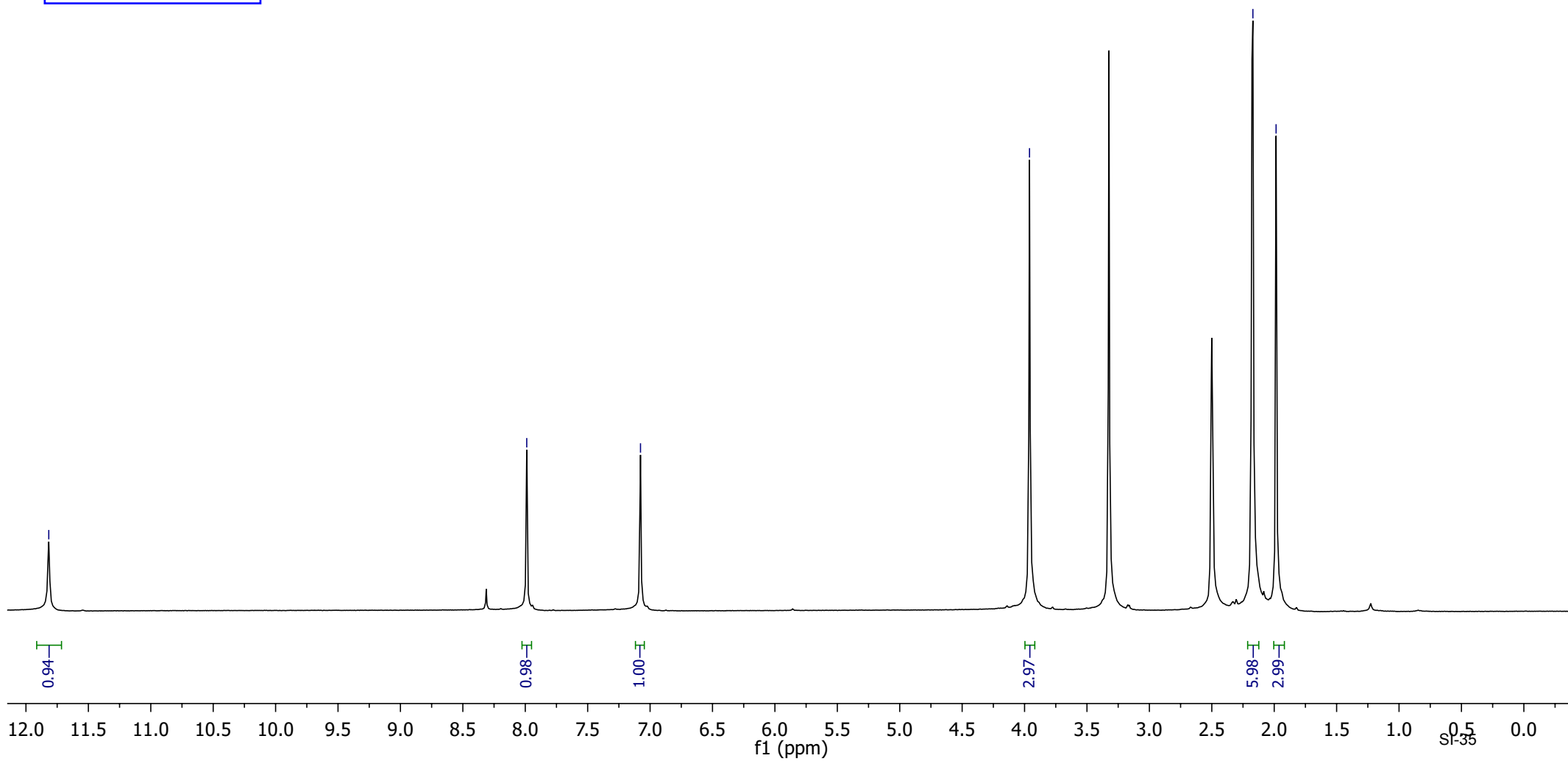
—56.48

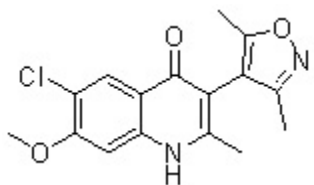
—19.44





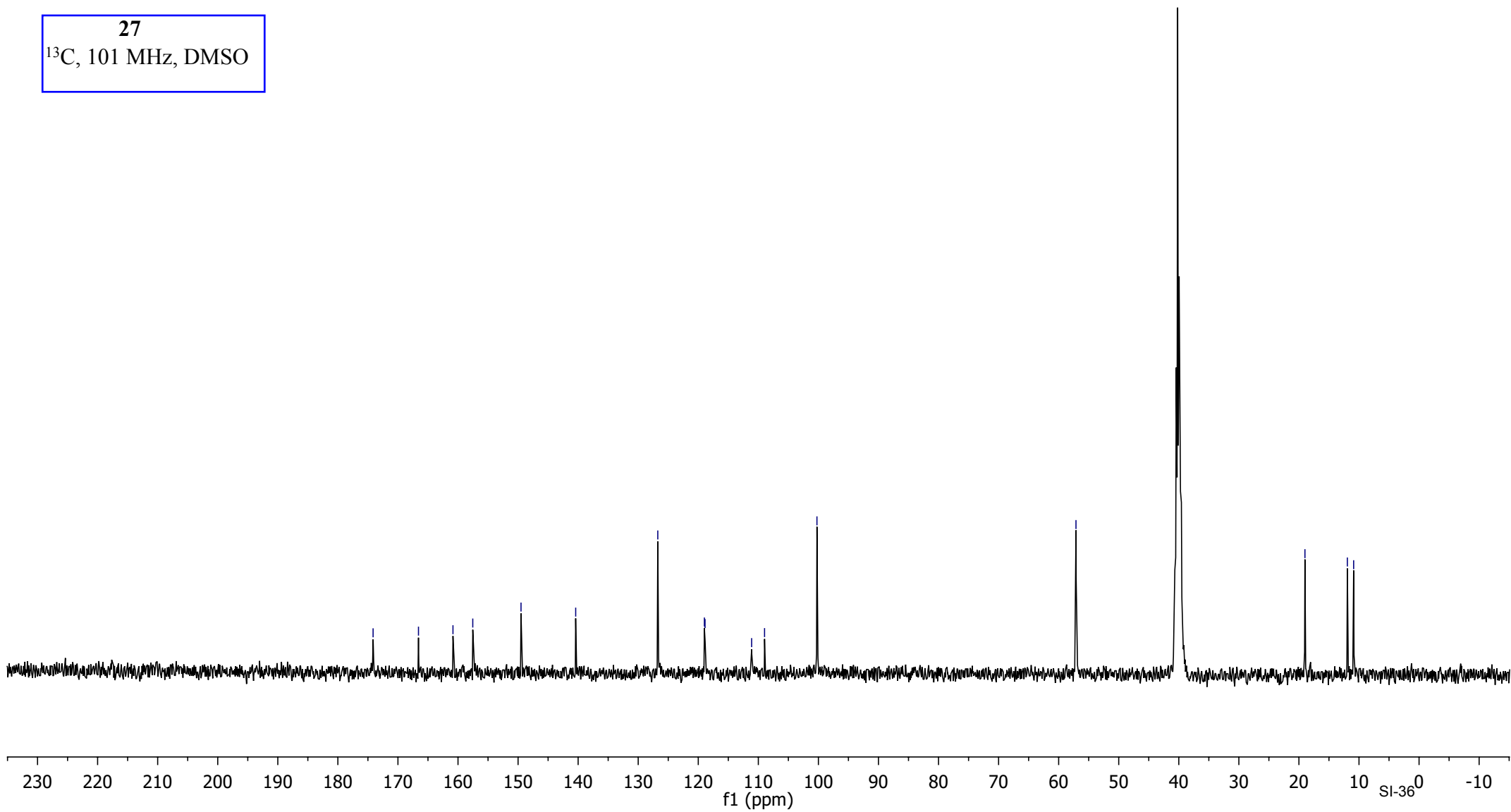
27
¹H, 400 MHz, DMSO

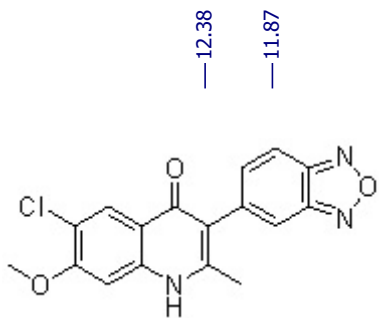




27
¹³C, 101 MHz, DMSO

—174.14
—166.58
—160.84
—157.54
—149.51
—140.41
—126.74
—118.98
—118.87
—111.11
—108.96
—100.24
—57.12
—19.00
—11.94
—10.89





28
 ^1H , 400 MHz, DMSO

12.38

11.87

8.01

8.00

7.97

7.90

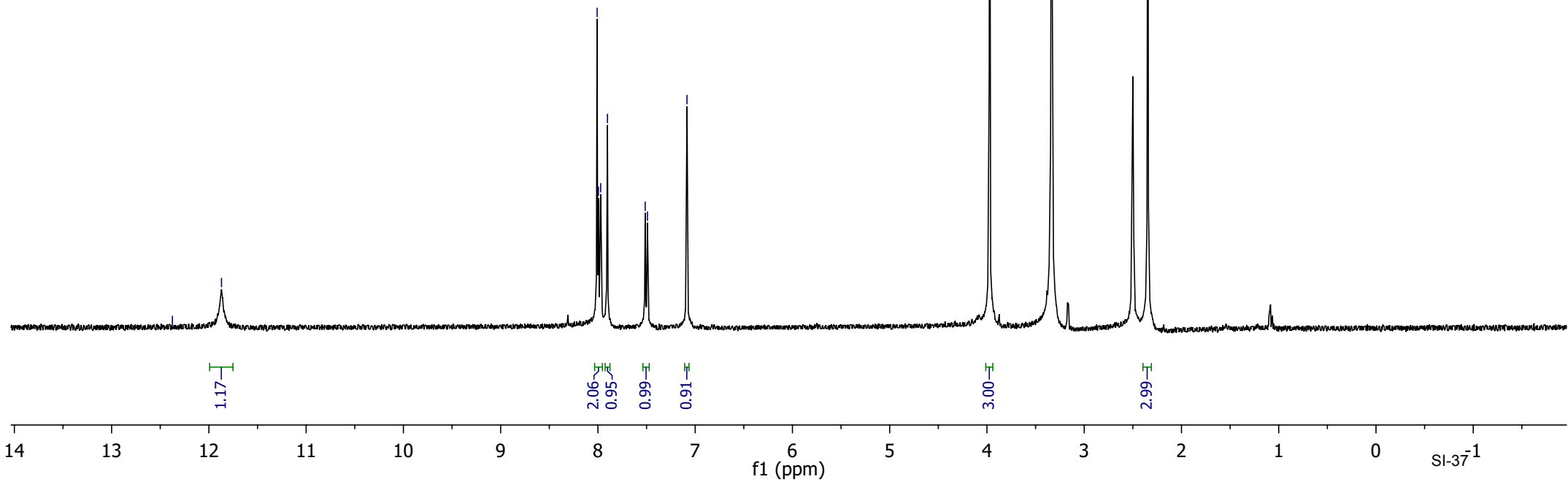
7.51

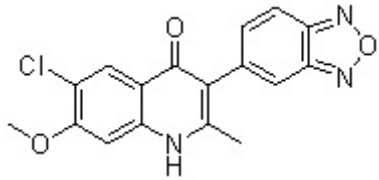
7.49

7.08

3.97

2.35





28

^{13}C , 101 MHz, DMSO

— 173.29

— 156.99

— 149.19

— 148.10

— 147.73

— 140.84

— 139.64

— 137.44

— 132.57

— 125.99

— 118.63

— 118.52

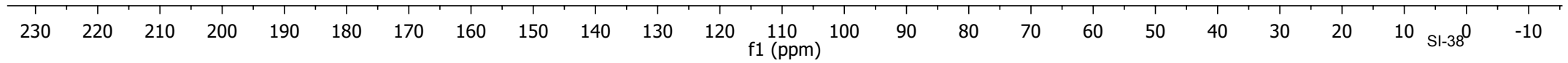
— 116.11

— 114.31

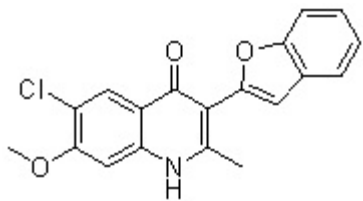
— 99.61

— 56.48

— 18.87



11.94



29

¹H, 400 MHz, DMSO

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

0.73

0.85

0.95

1.00

2.94

1.00

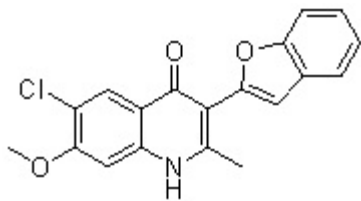
3.00

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)

SI-39



29

¹³C, 101 MHz, DMSO

—172.67

—156.95

—153.40

—151.64

—149.42

—139.08

—128.58

—126.15

—123.60

—122.59

—120.60

—118.73

—118.50

—110.67

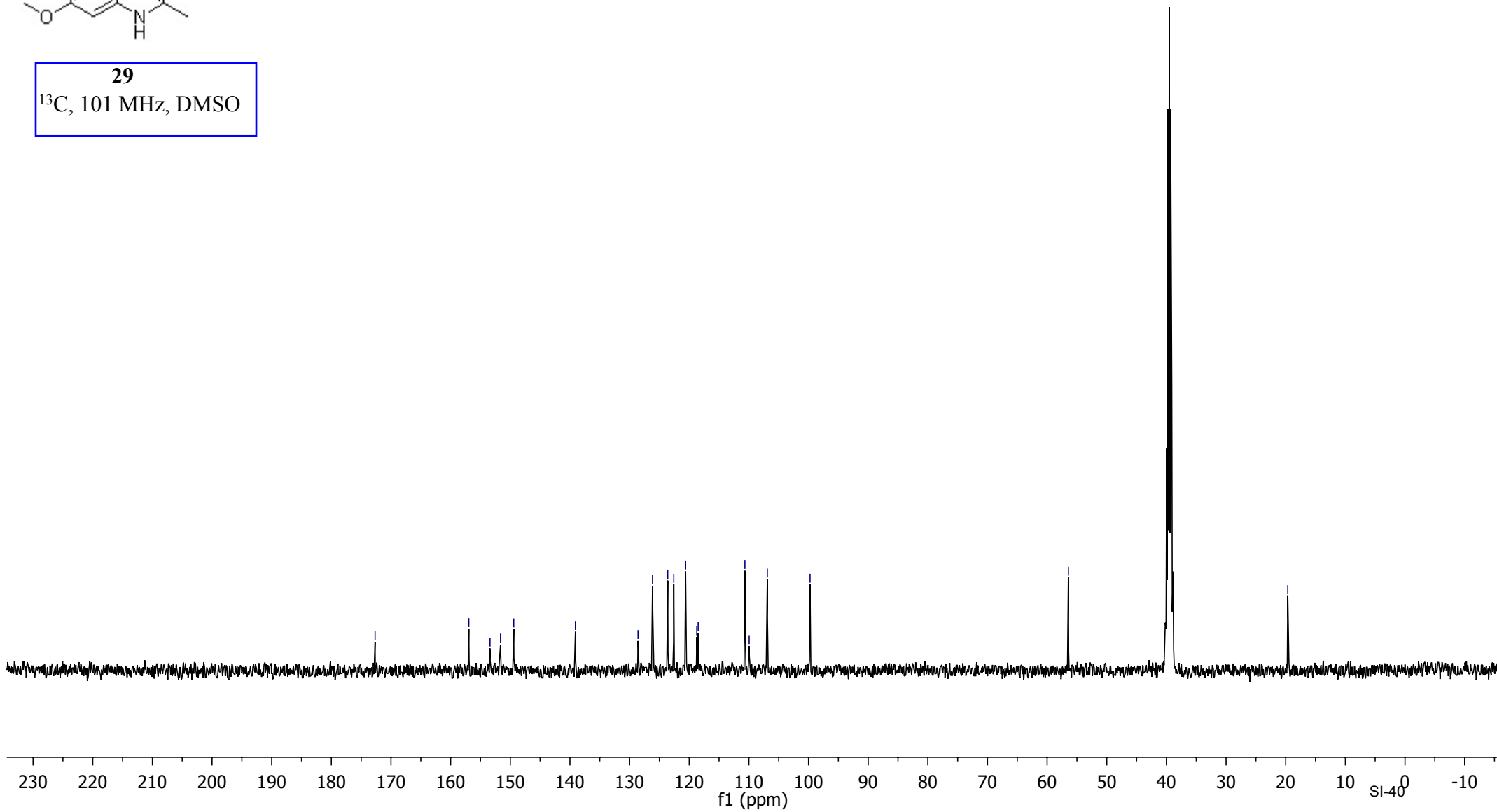
—109.95

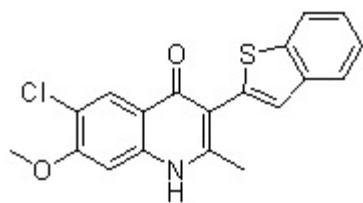
—106.91

—99.74

—56.44

—19.66





30

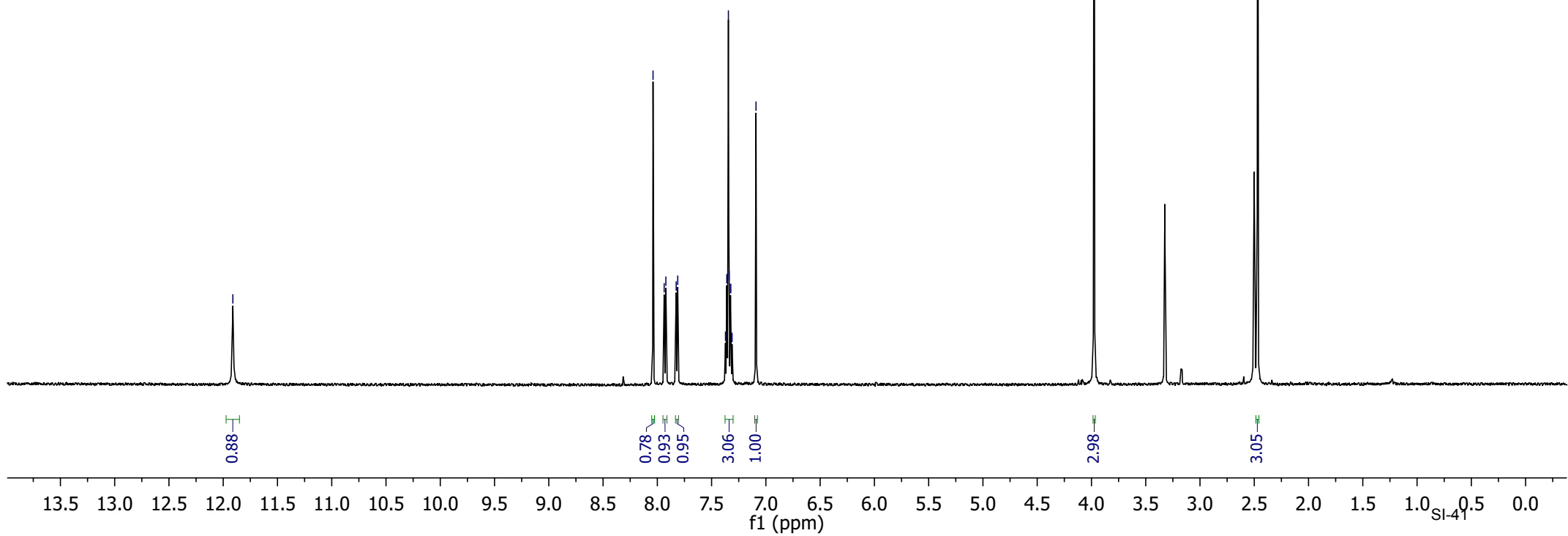
¹H, 500 MHz, DMSO

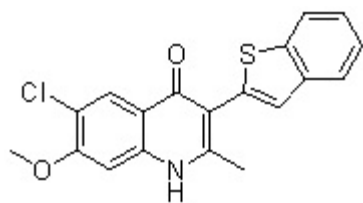
11.91

8.04
7.94
7.92
7.83
7.81
7.37
7.36
7.35
7.34
7.33
7.32
7.31
7.09

3.98

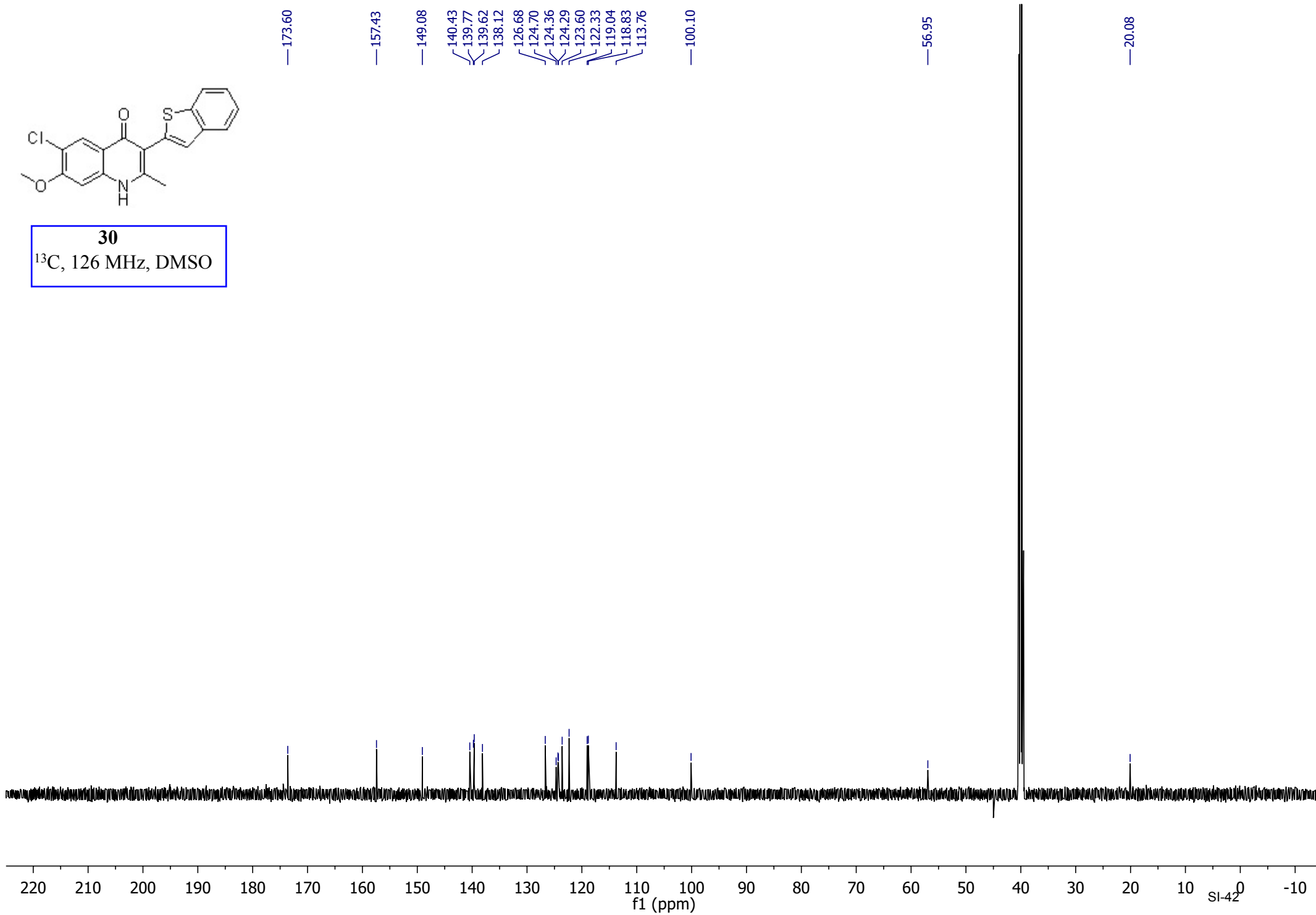
2.47

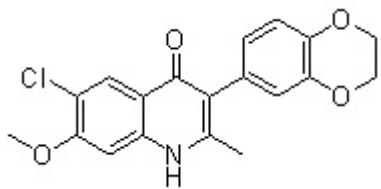




30

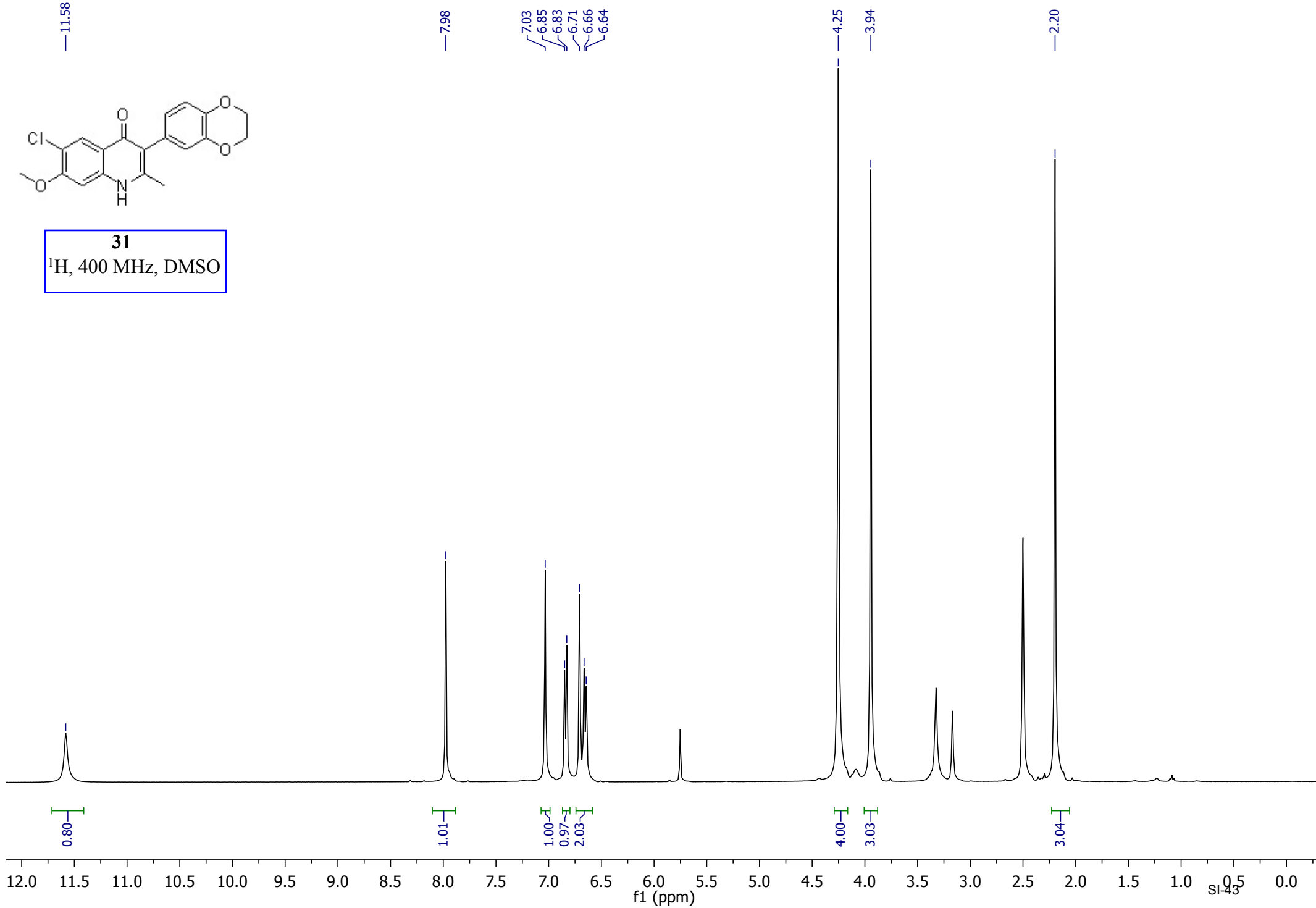
¹³C, 126 MHz, DMSO

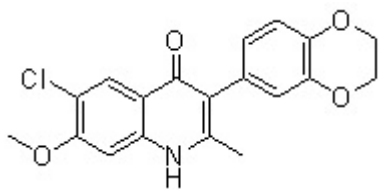




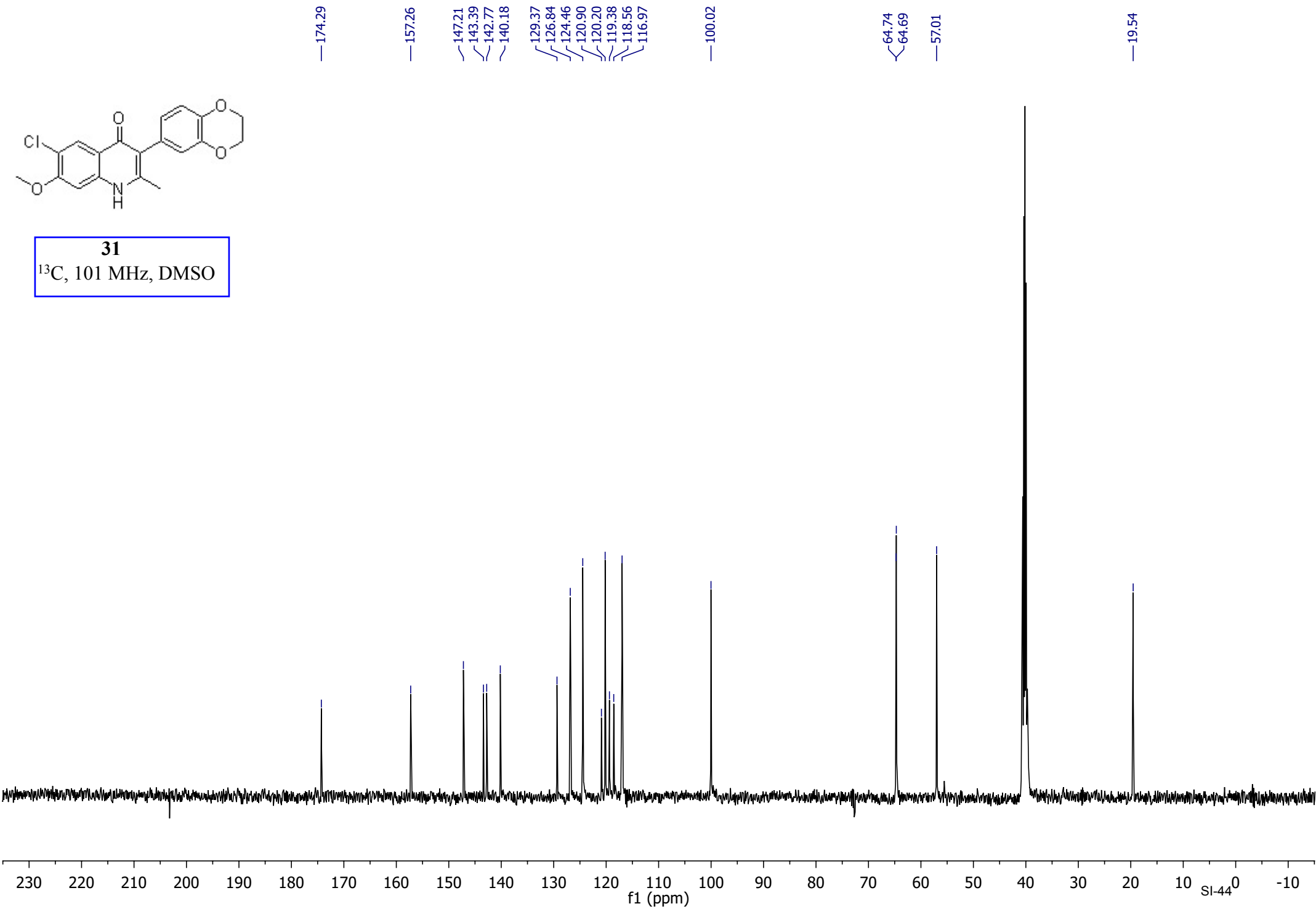
31

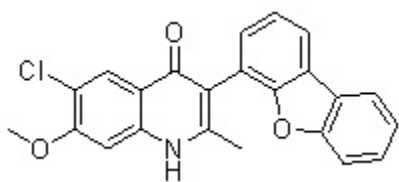
¹H, 400 MHz, DMSO



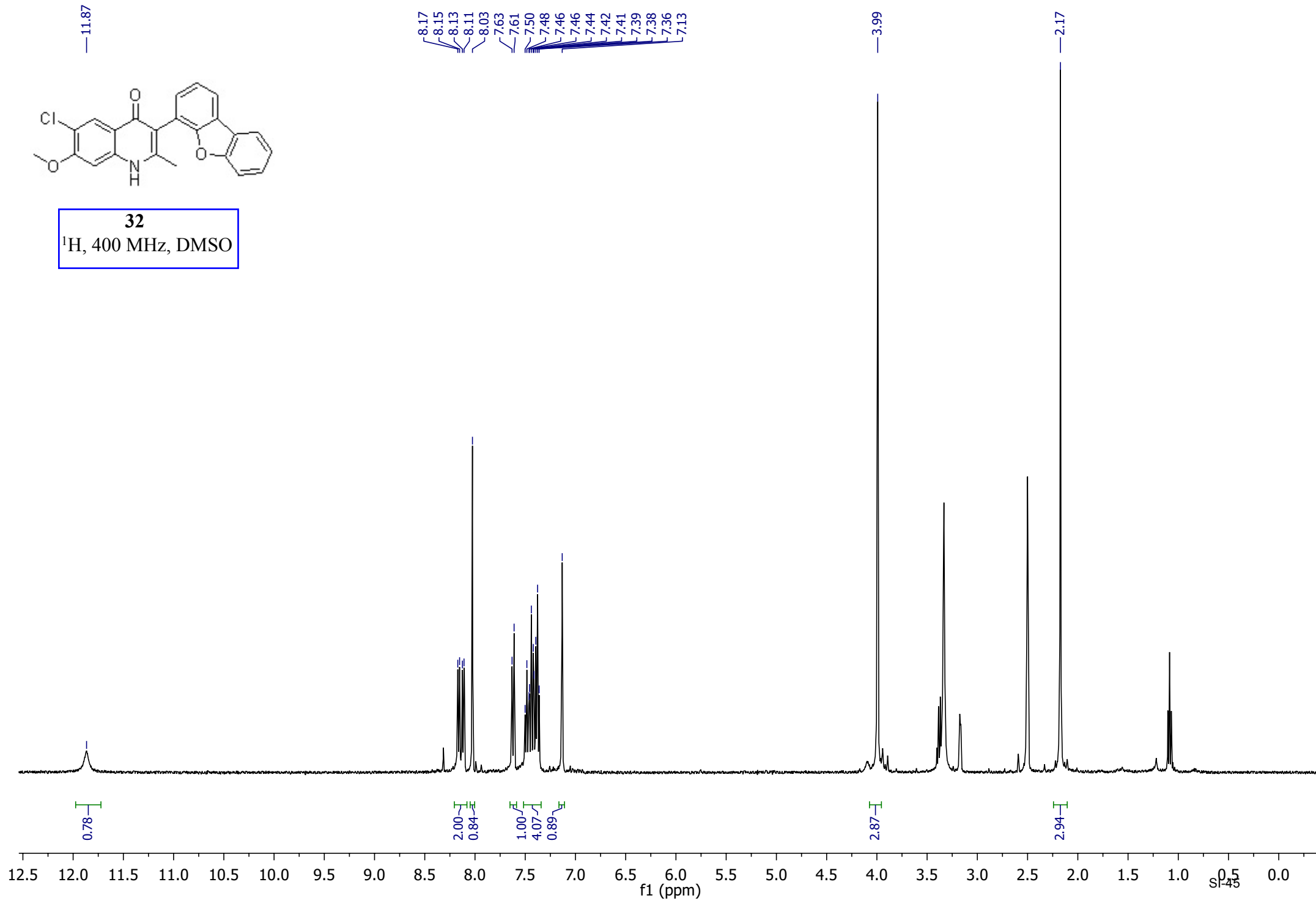


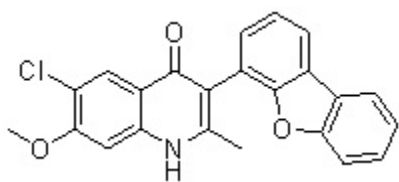
31
¹³C, 101 MHz, DMSO





32
¹H, 400 MHz, DMSO





32

^{13}C , 101 MHz, DMSO

— 173.27

— 156.84

— 155.22

— 154.07

— 147.61

— 139.81

— 130.28

— 127.35

— 126.15

— 123.86

— 123.45

— 122.95

— 122.81

— 121.04

— 120.42

— 119.95

— 118.60

— 118.25

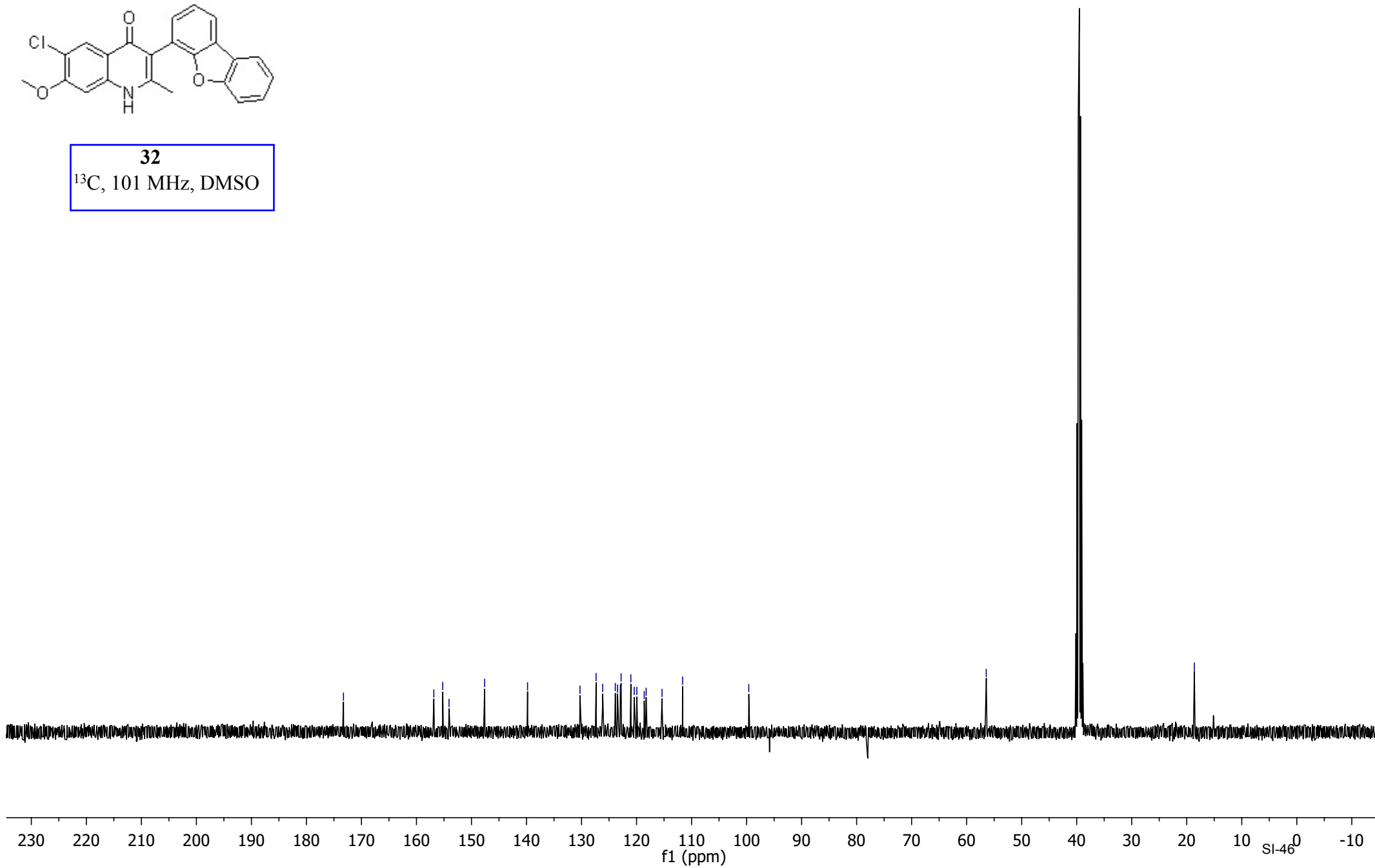
— 115.37

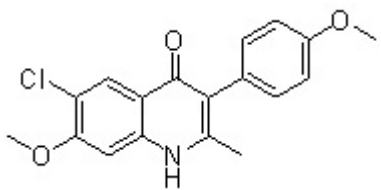
— 111.63

— 99.60

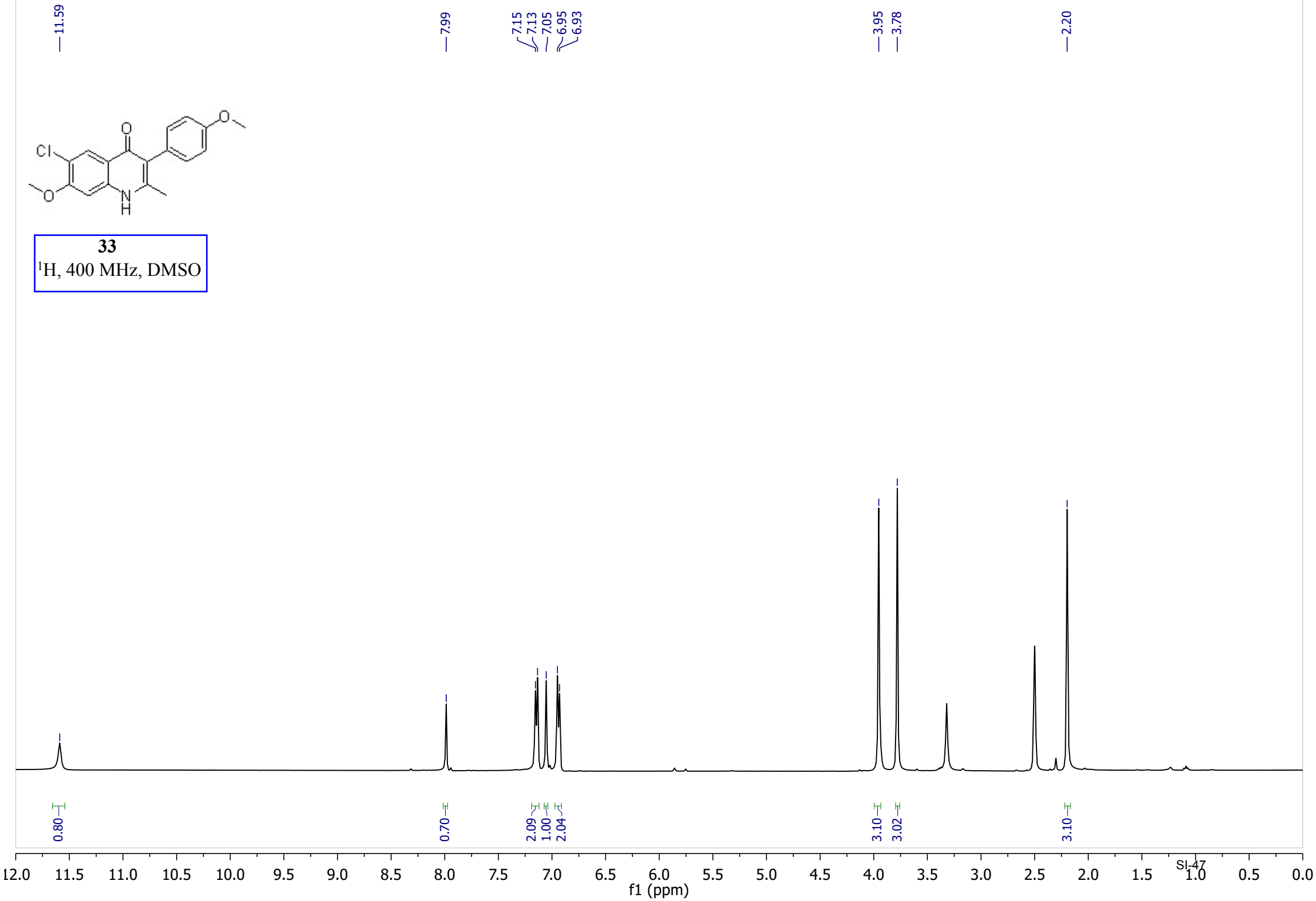
— 56.44

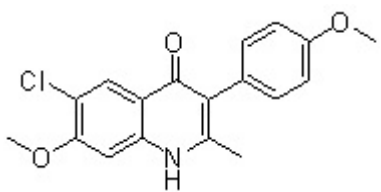
— 18.62





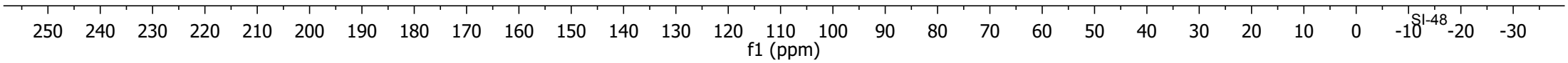
33
¹H, 400 MHz, DMSO

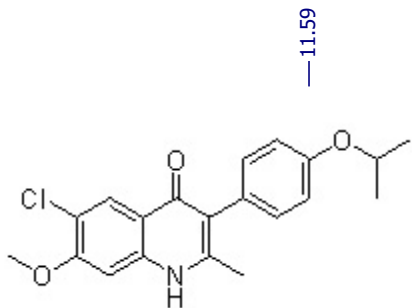




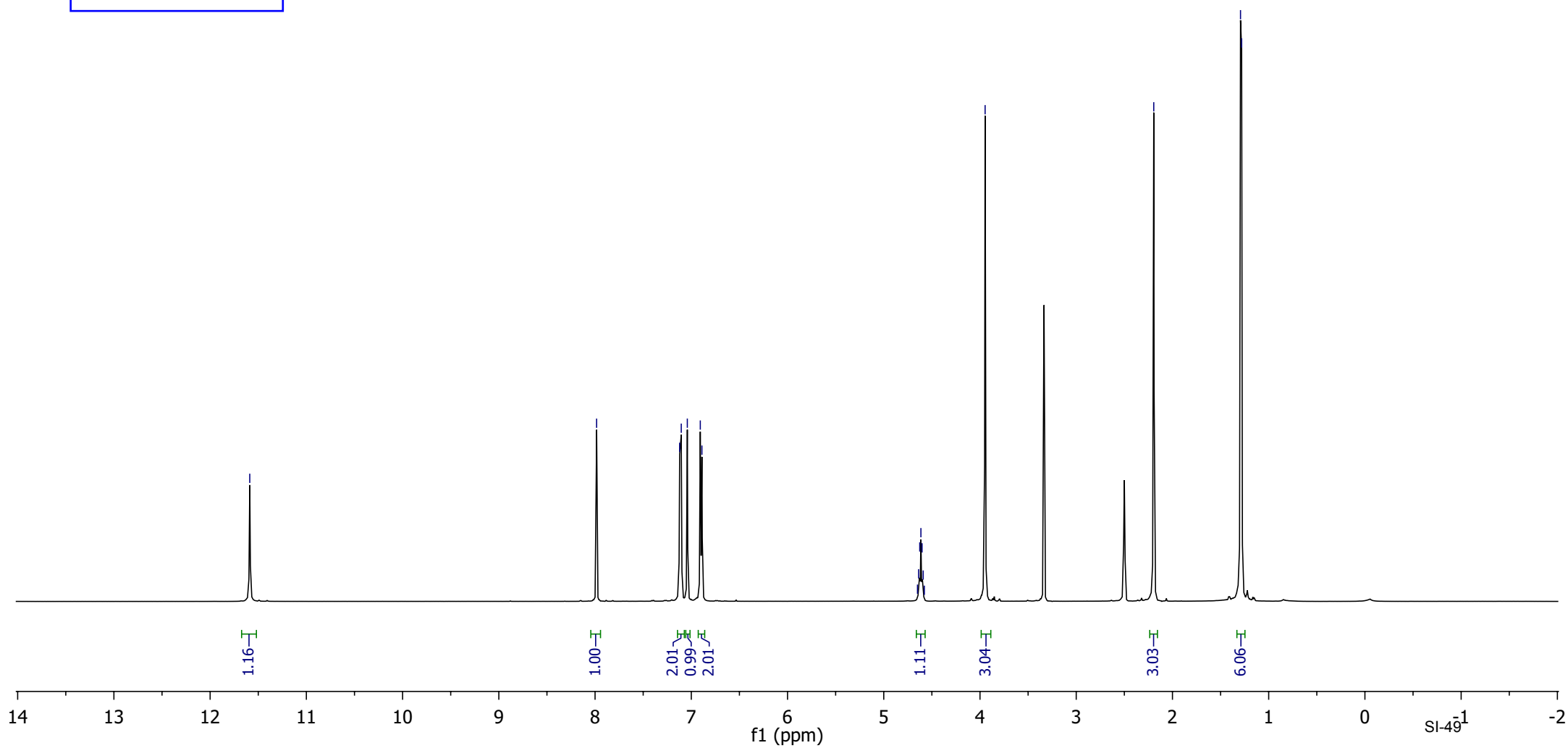
33
 ^{13}C , 101 MHz, DMSO

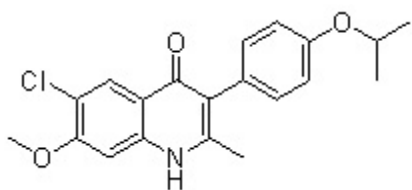
— 173.73
~ 157.92
~ 156.61
— 146.46
— 139.55
~ 131.99
~ 127.82
~ 126.21
~ 120.39
~ 118.74
~ 117.88
~ 113.25
— 99.38
~ 56.37
~ 55.01
— 18.90





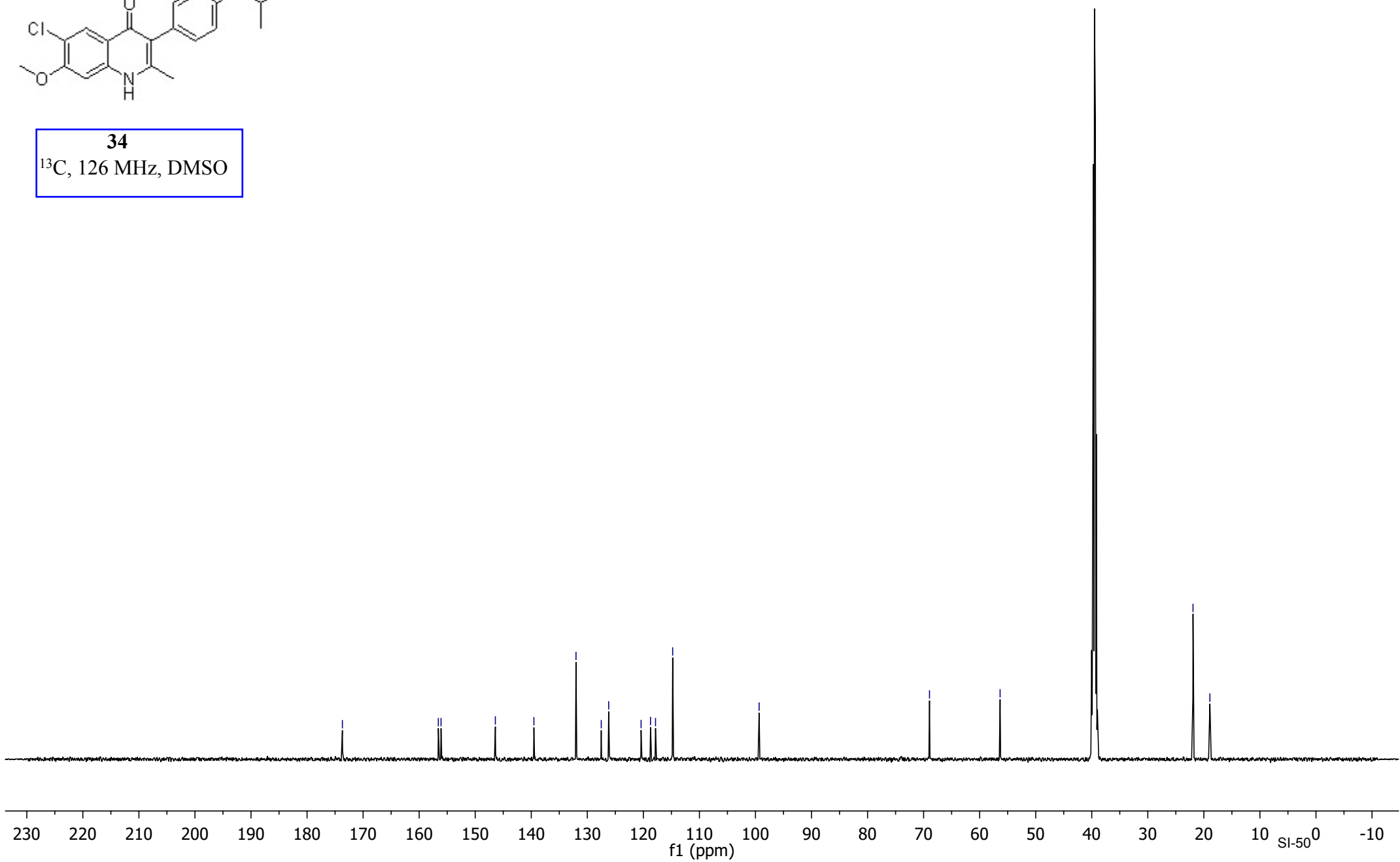
34
¹H, 500 MHz, DMSO

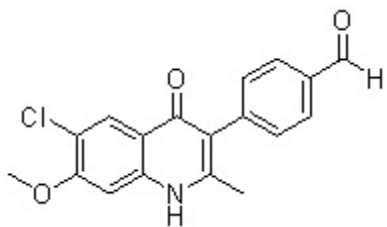




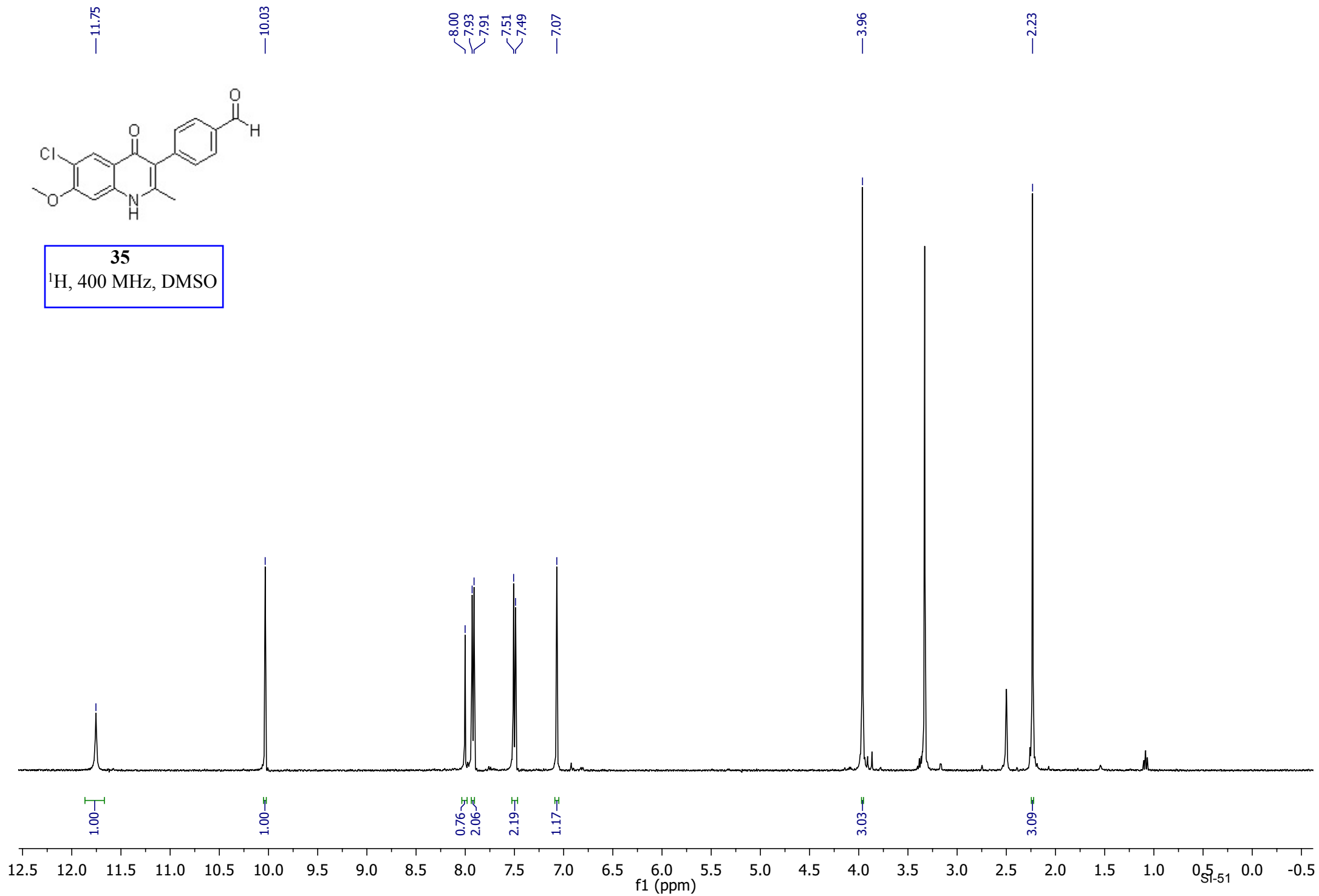
34
¹³C, 126 MHz, DMSO

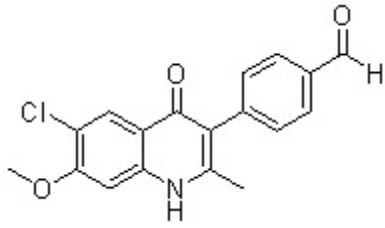
- 173.70
- 156.58
- 156.10
- 146.41
- 139.53
- 132.02
- 127.51
- 126.19
- 120.41
- 118.72
- 117.83
- 114.77
- 99.35
- 68.95
- 56.35
- 21.94
- 18.92





35
¹H, 400 MHz, DMSO





35
¹³C, 101 MHz, DMSO

—192.77

—173.12

—156.84

—146.81

—142.61

—139.59

—134.54

—131.82

—128.89

—126.14

—119.67

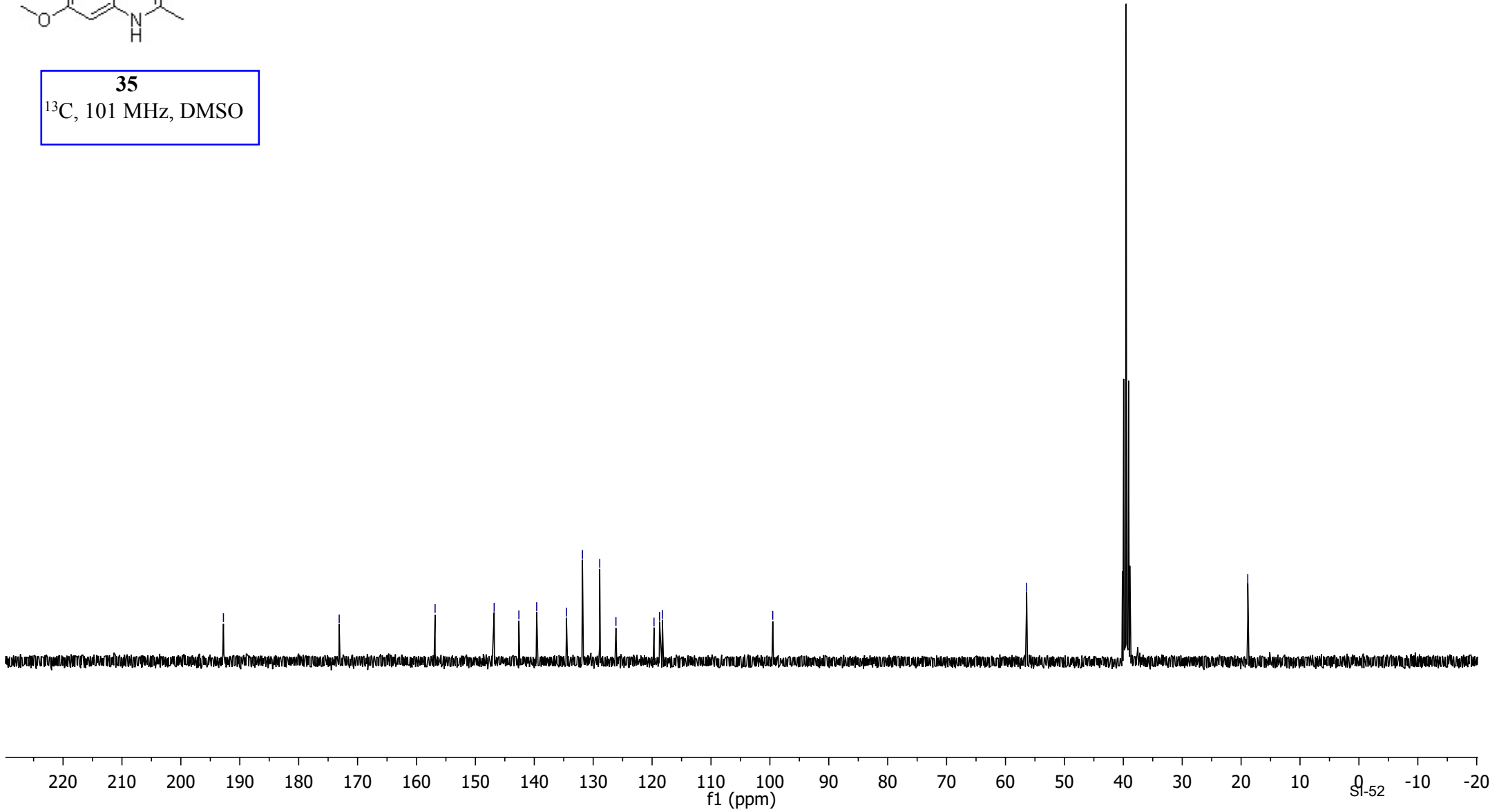
—118.73

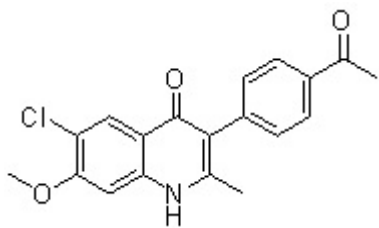
—118.25

—99.52

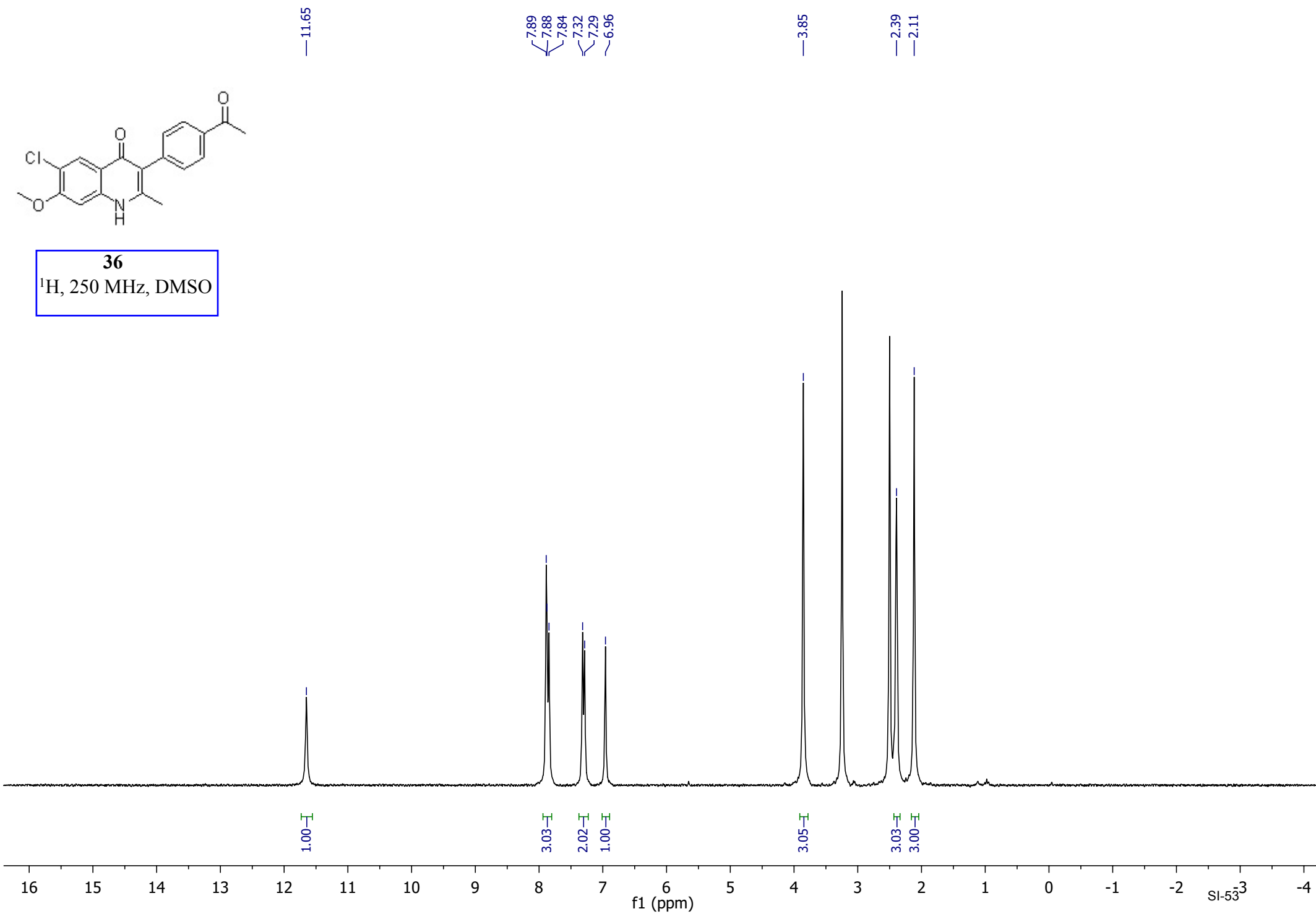
—56.41

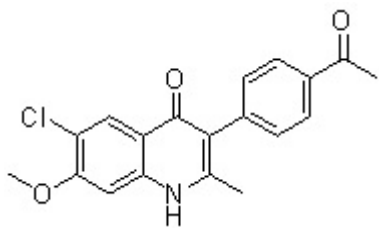
—18.87



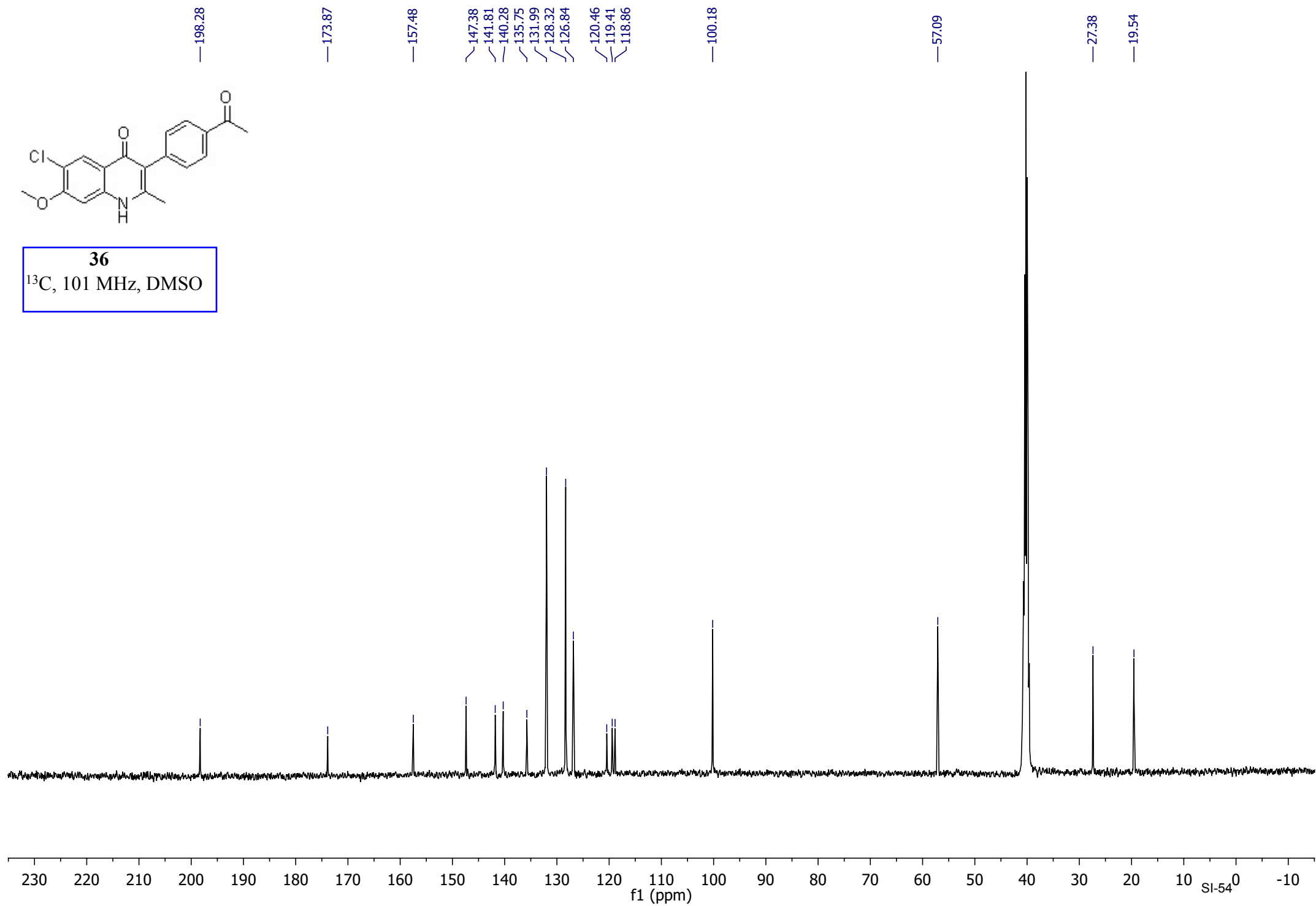


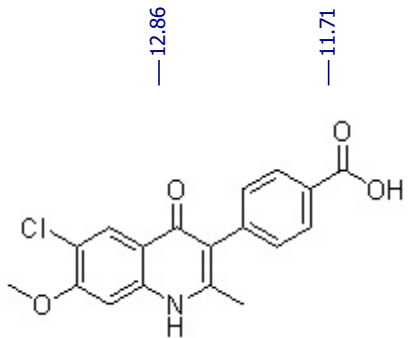
36
¹H, 250 MHz, DMSO



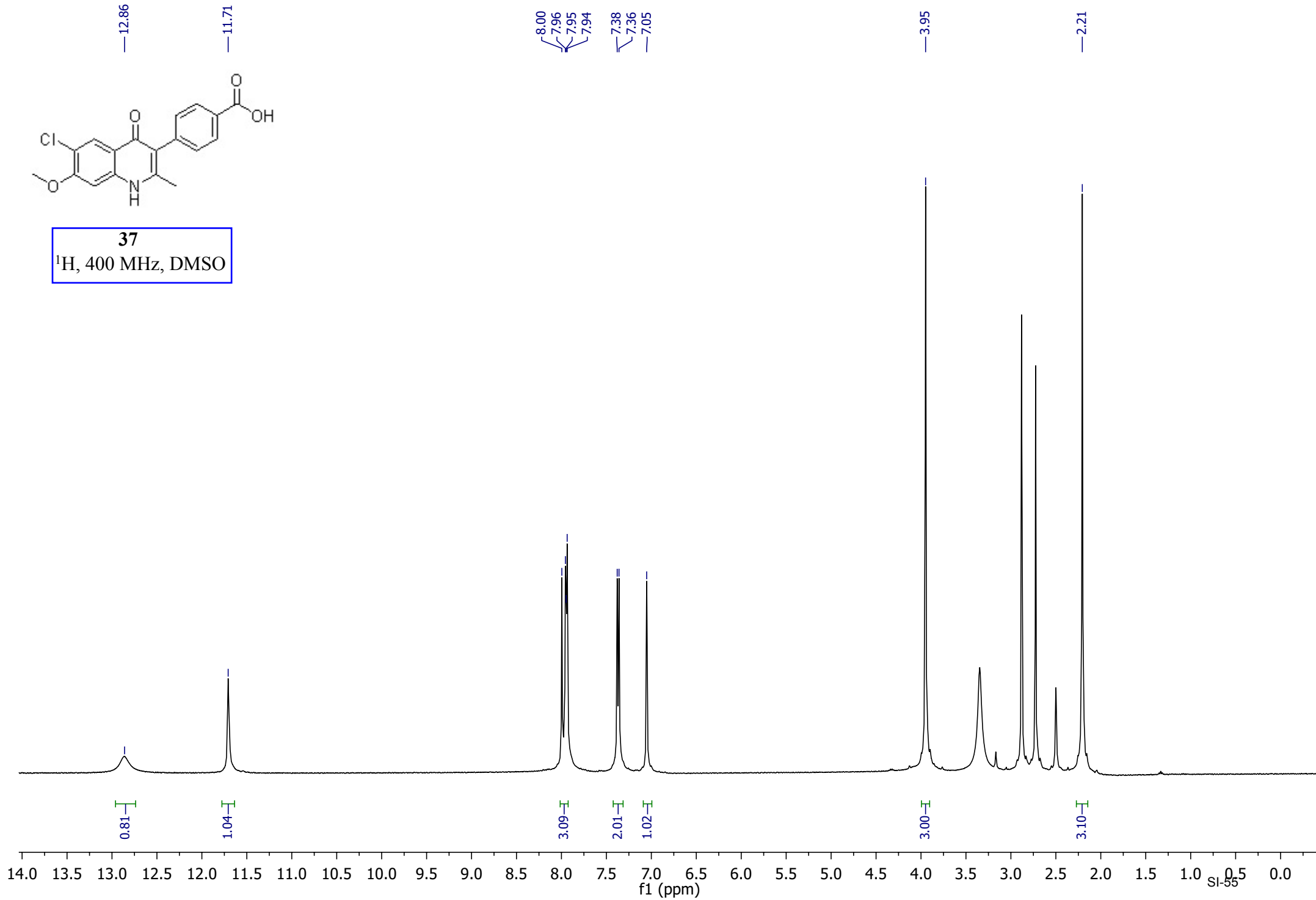


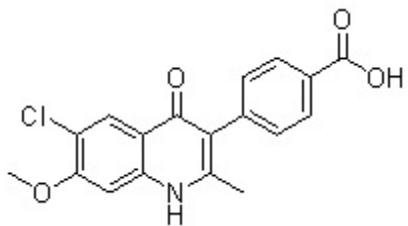
36
¹³C, 101 MHz, DMSO





37
¹H, 400 MHz, DMSO





37

^{13}C , 101 MHz, DMSO

—173.23

—167.32

—156.79

—146.70

—140.76

—139.60

—131.22

—128.92

—128.73

—126.15

—119.85

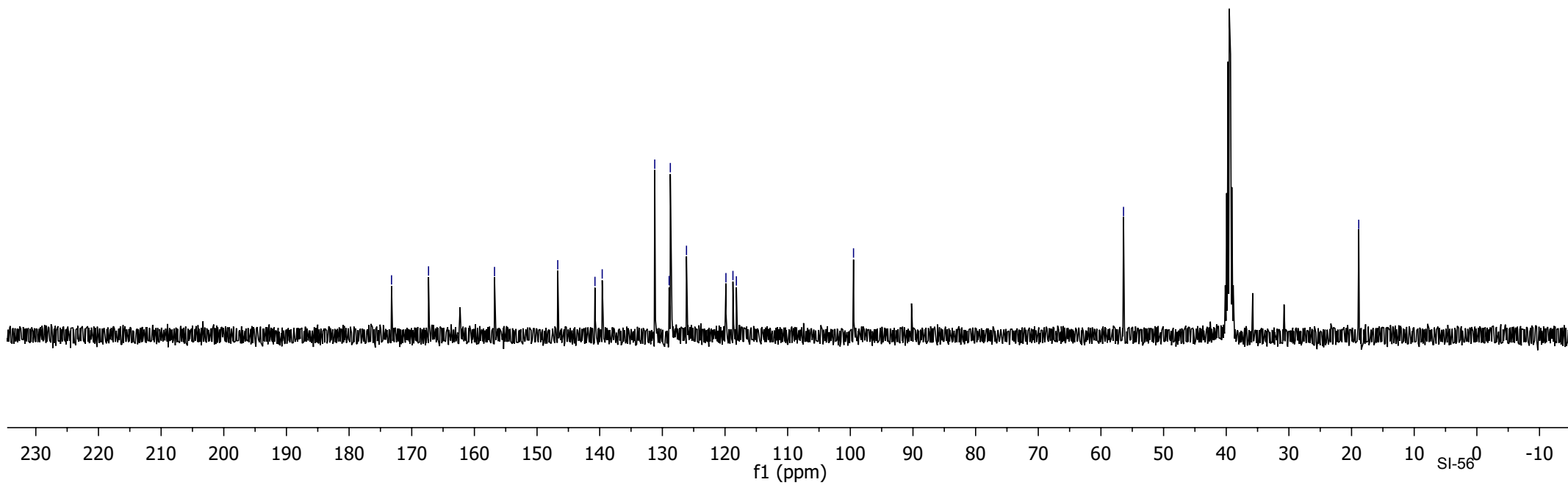
—118.73

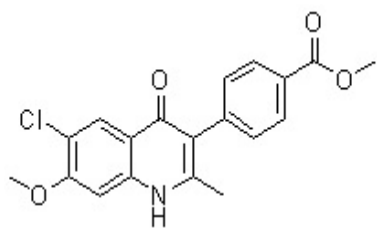
—118.19

—99.49

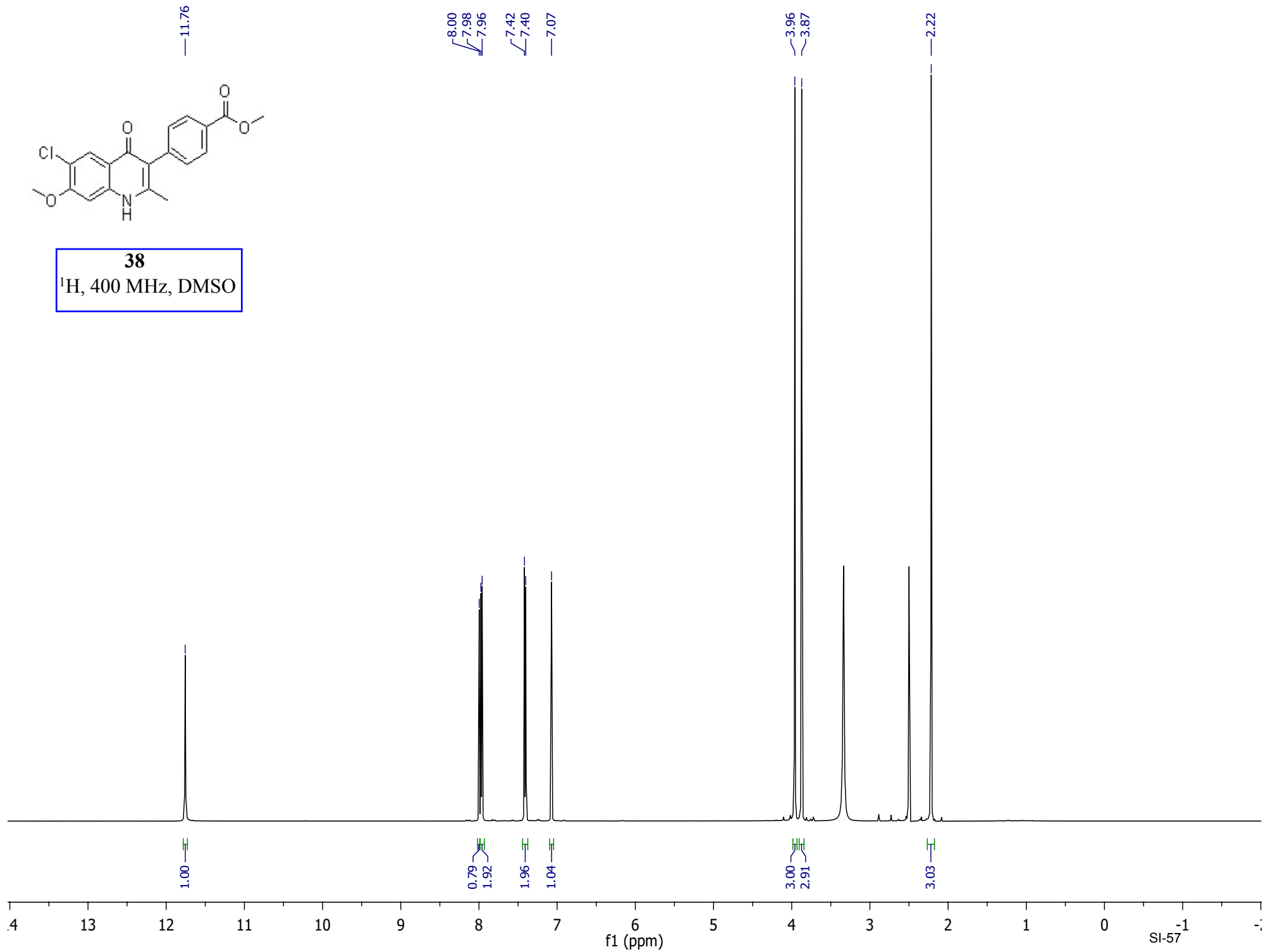
—56.39

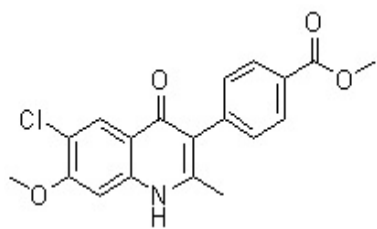
—18.85





38
¹H, 400 MHz, DMSO





38

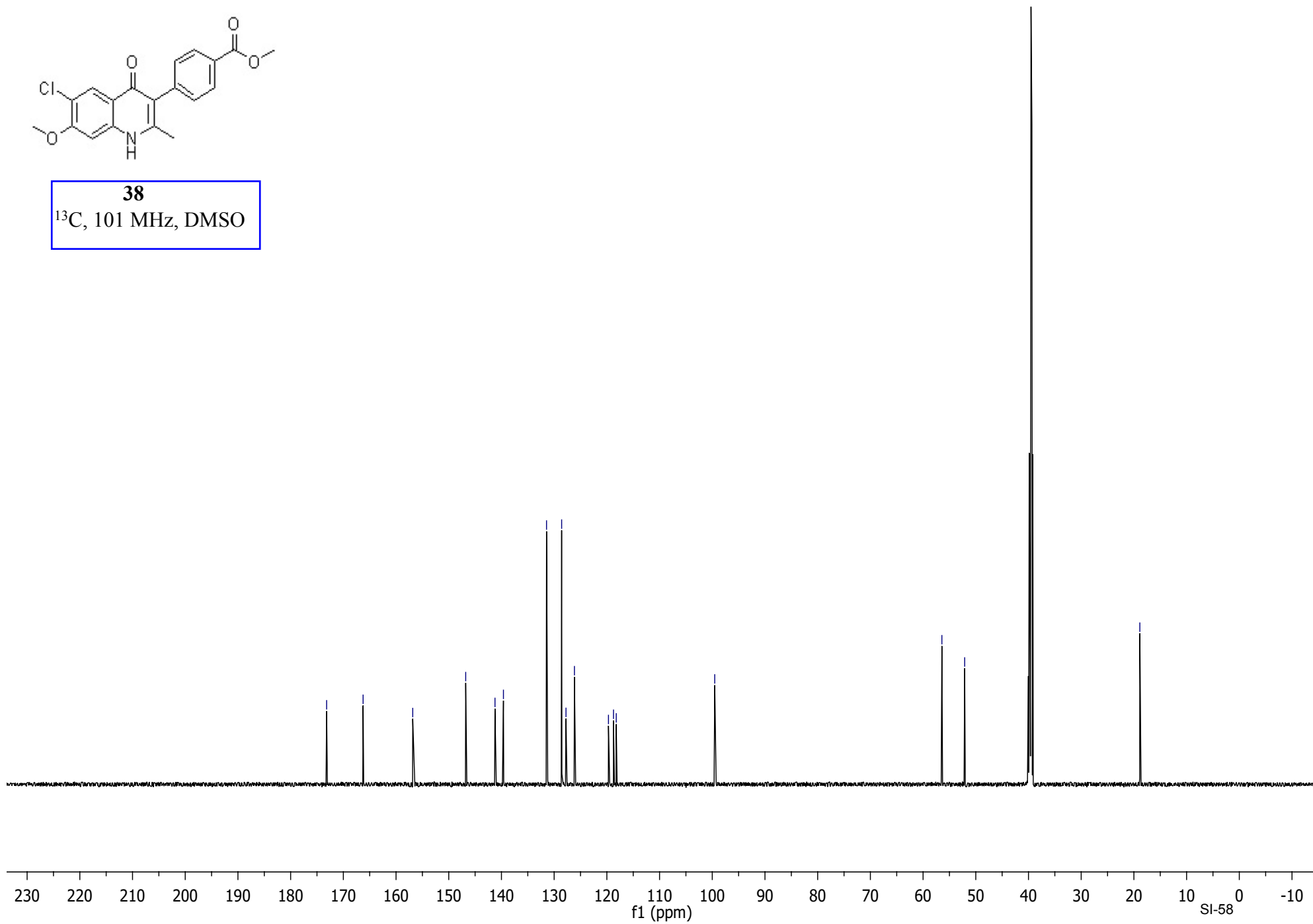
^{13}C , 101 MHz, DMSO

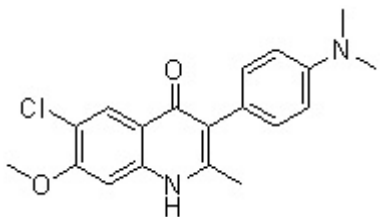
—173.17
—166.25
—156.83
—146.78
—139.62
—131.44
—128.58
—127.75
—126.15
—119.70
—118.74
—118.22

—99.53

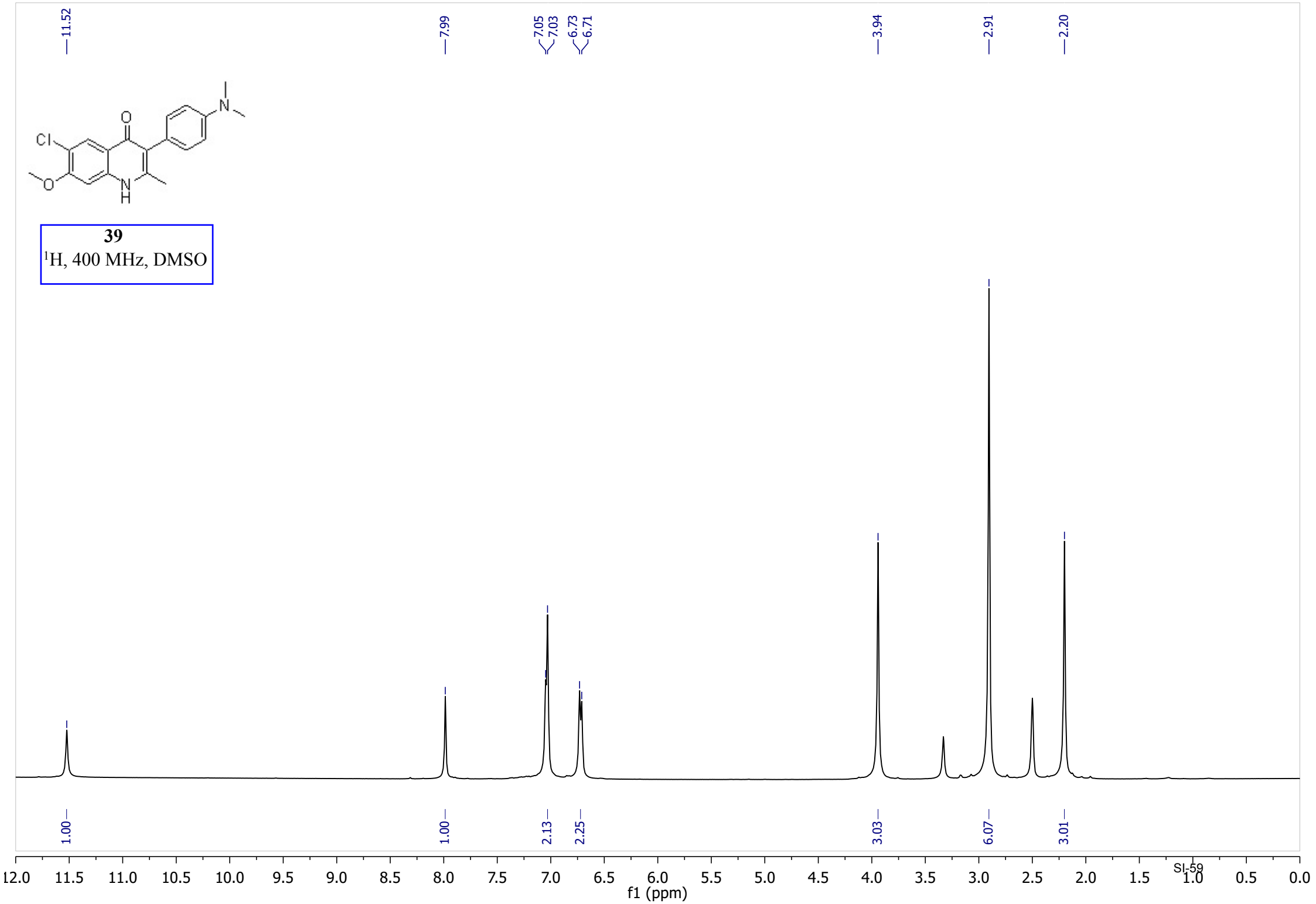
—56.43
—52.11

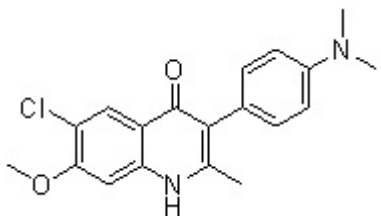
—18.87





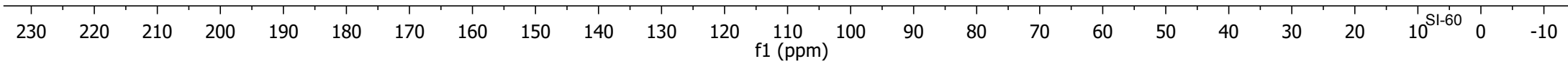
39
¹H, 400 MHz, DMSO

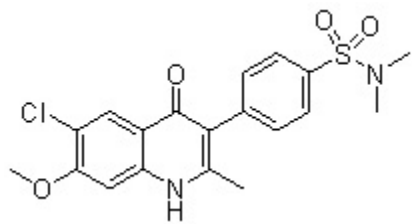




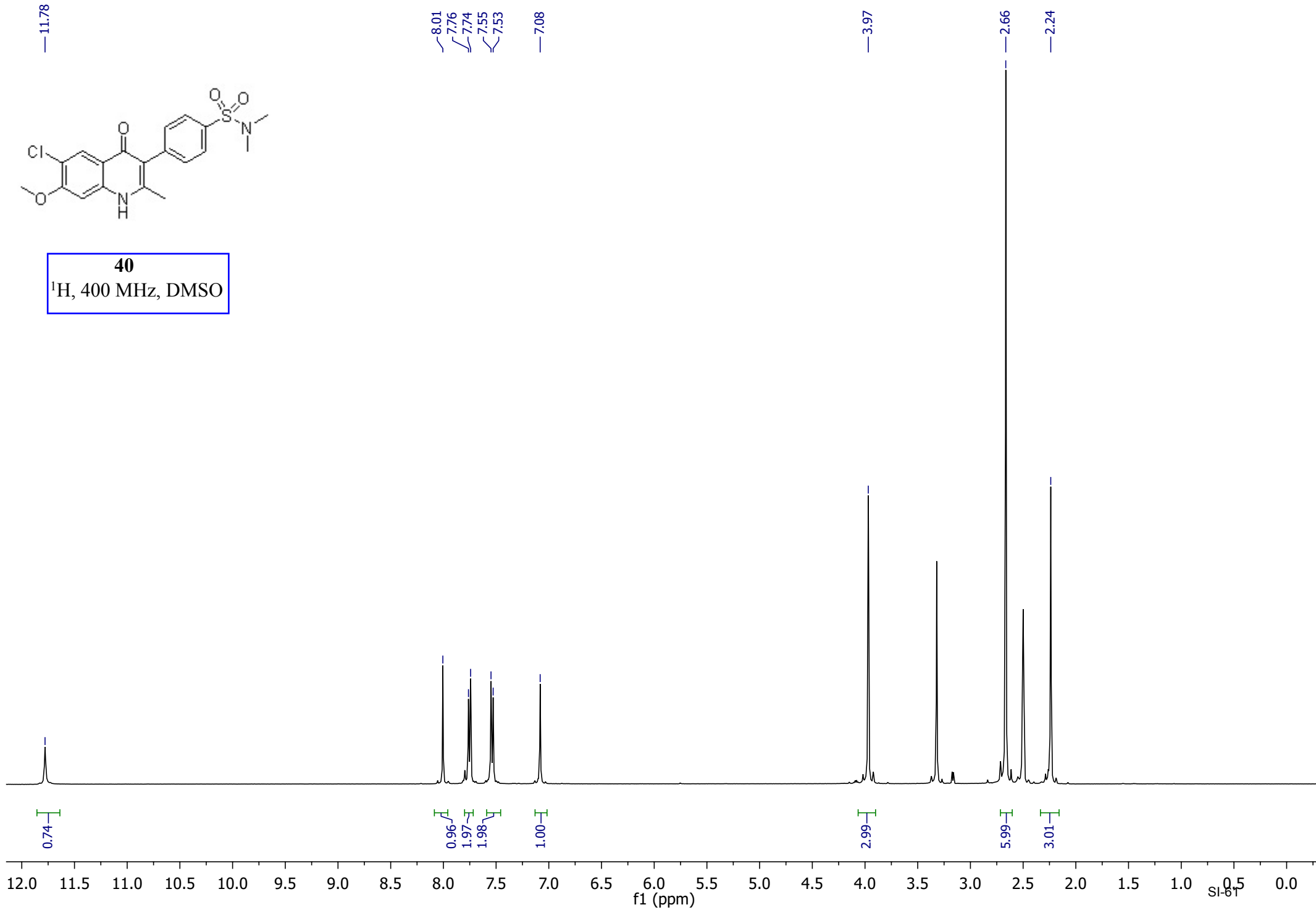
39
¹³C, 101 MHz, DMSO

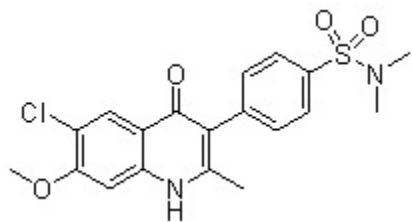
—173.86 —156.46 —149.07 —146.14 —139.45 —131.36 —126.21 —123.29 —120.83 —118.72 —117.65 —111.81 —99.29 —56.30 —40.19 —18.92





40
¹H, 400 MHz, DMSO





40
¹³C, 101 MHz, DMSO

—173.06

—156.87

—146.98

—140.84

—139.60

—132.84

—131.88

—126.92

—126.09

—119.14

—118.69

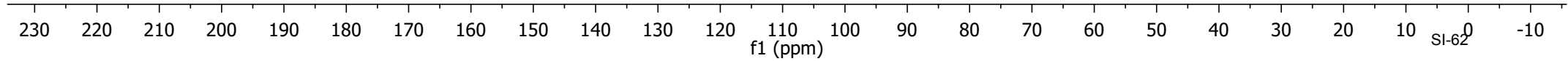
—118.28

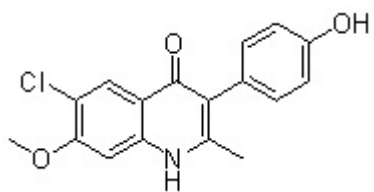
—99.54

—56.42

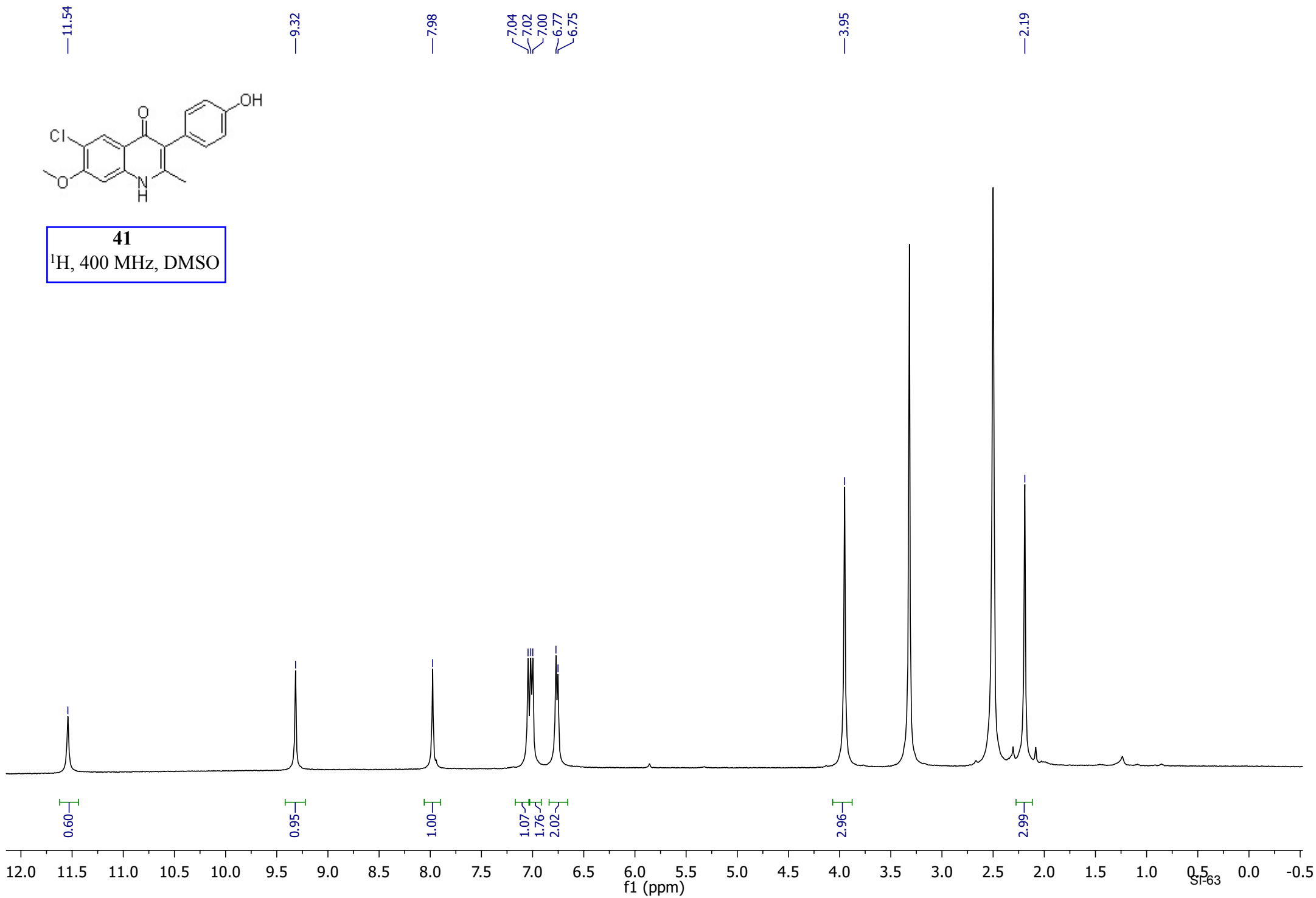
—37.60

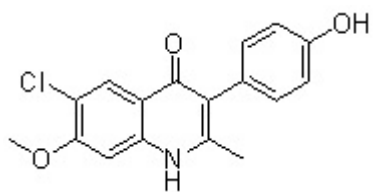
—18.87





41
¹H, 400 MHz, DMSO





41
¹³C, 101 MHz, DMSO

—174.44

—157.22
—156.64

—146.98

—140.18

—132.55

—126.87

—126.74

—121.40

—119.40

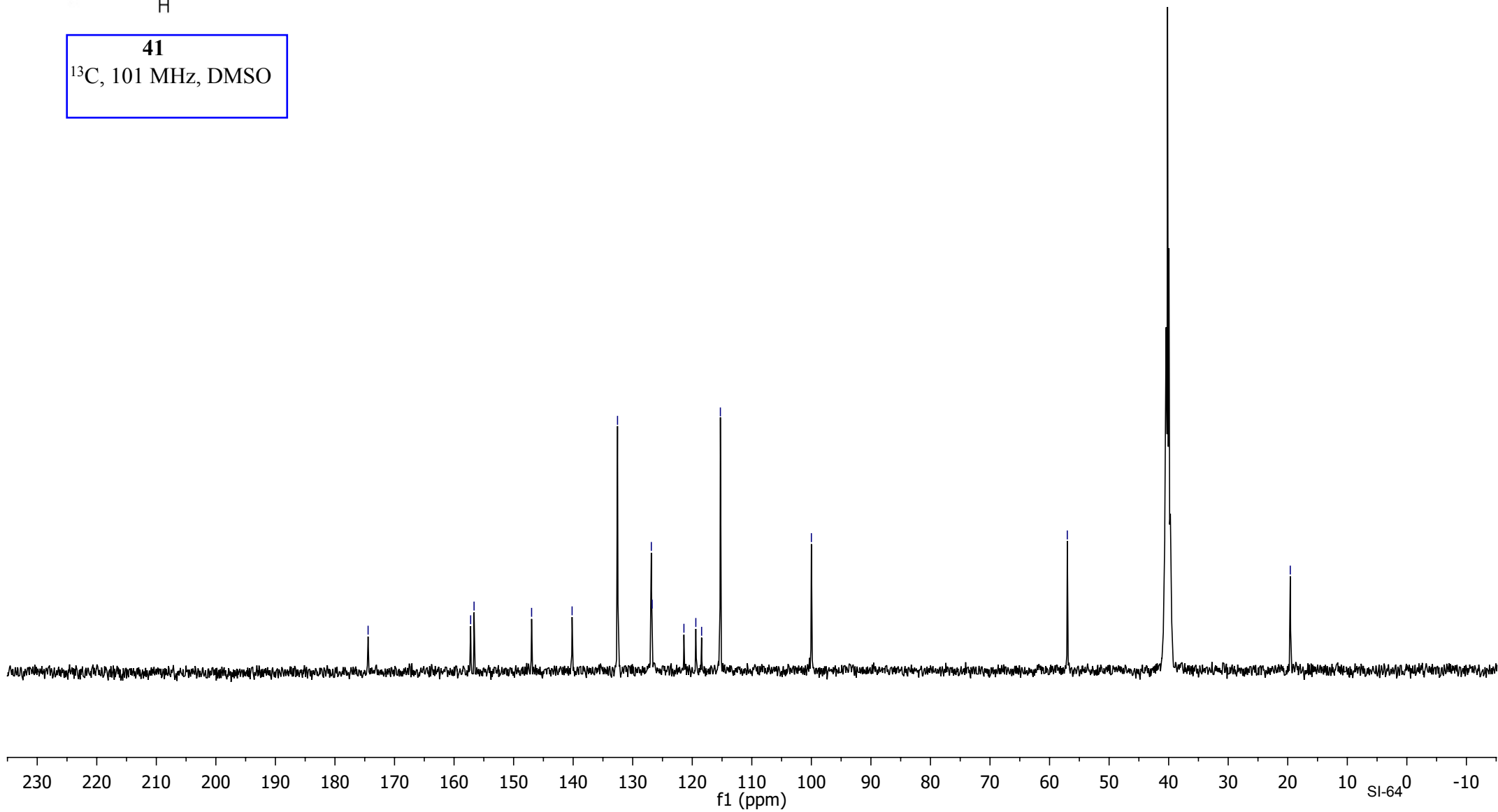
—118.43

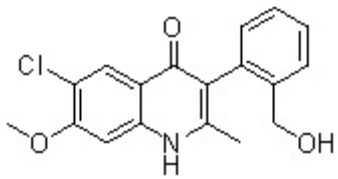
—115.28

—100.00

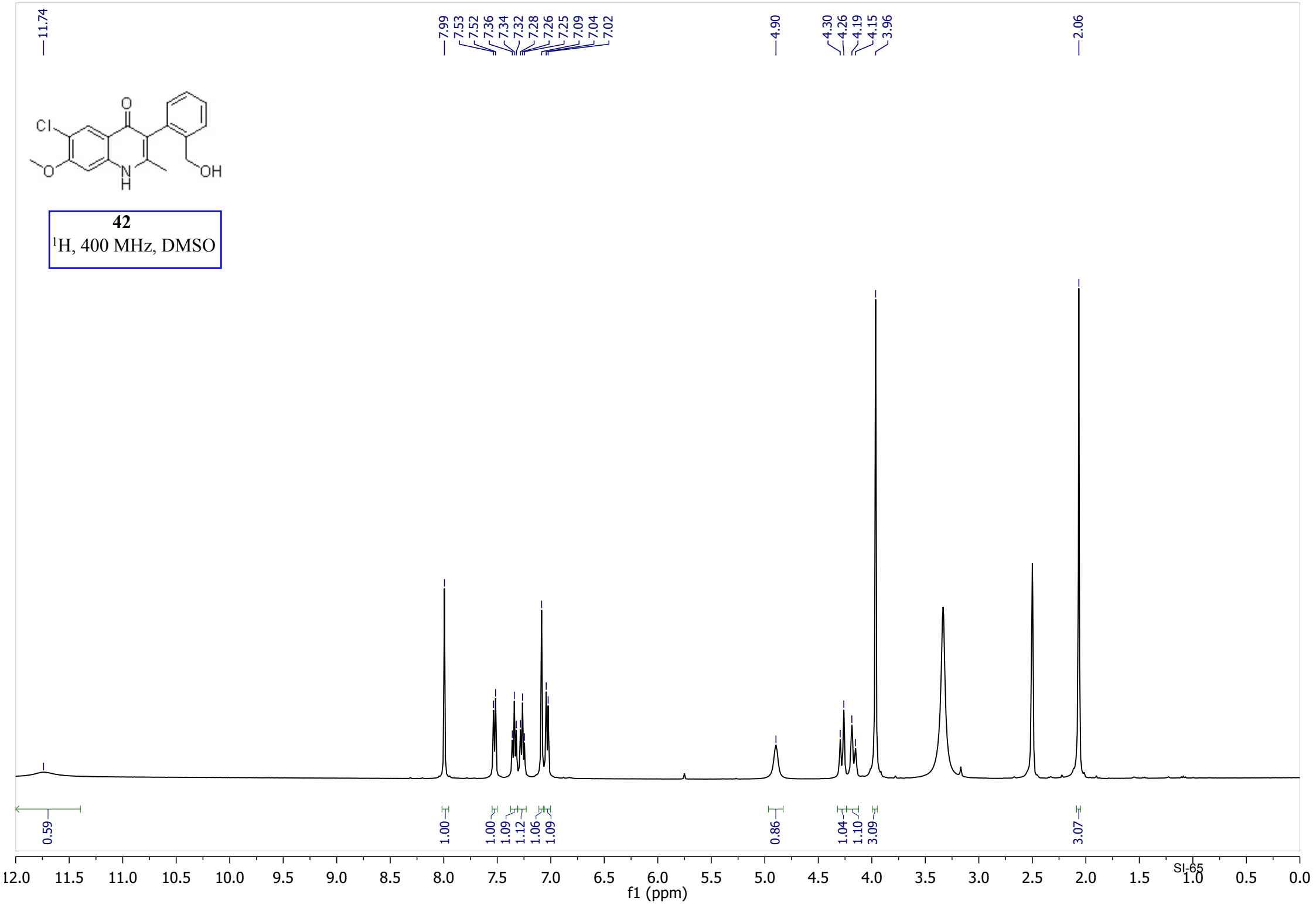
—57.02

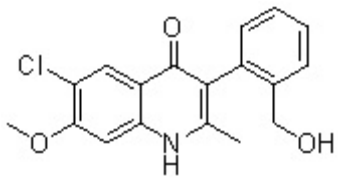
—19.58





42
¹H, 400 MHz, DMSO





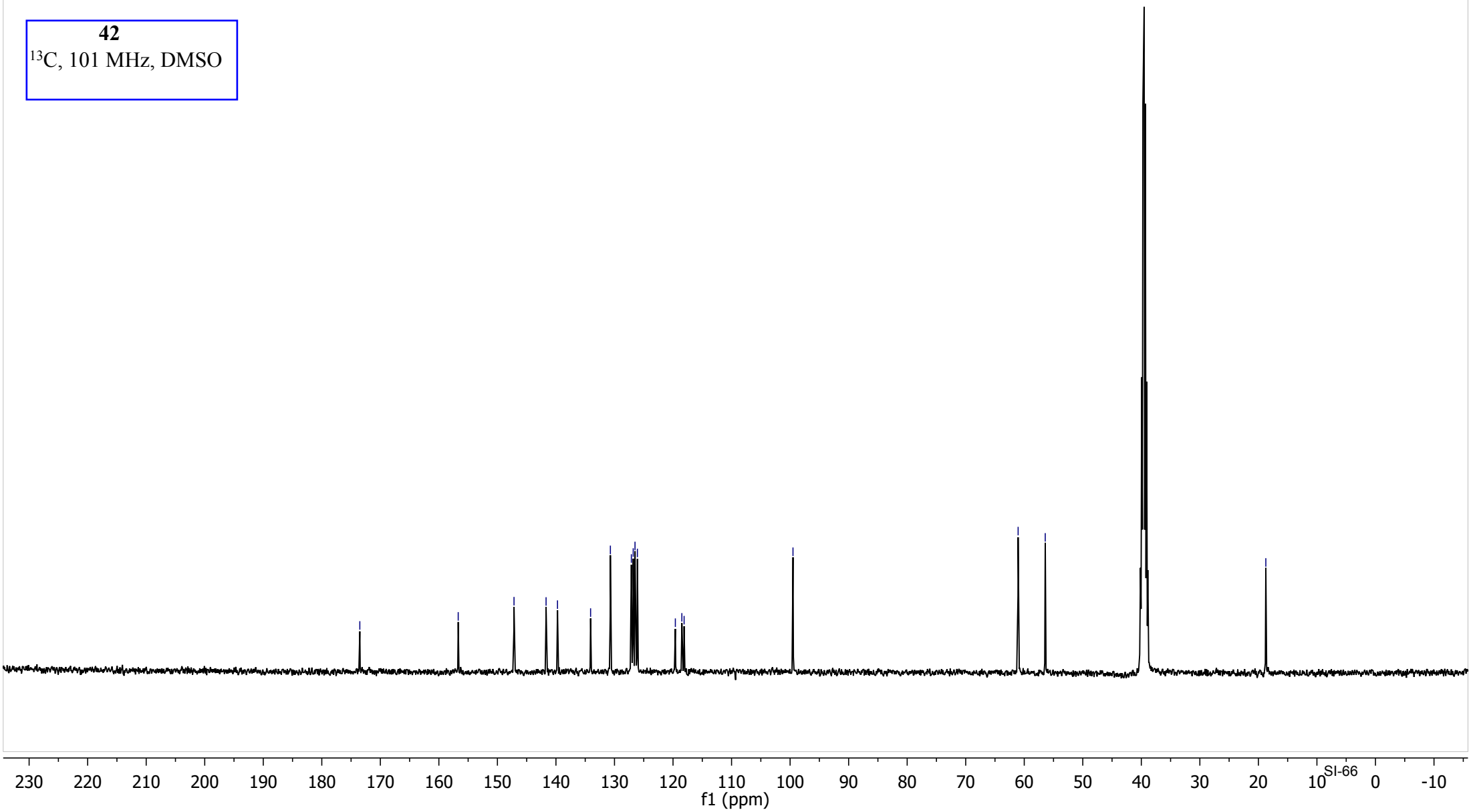
42
¹³C, 101 MHz, DMSO

—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

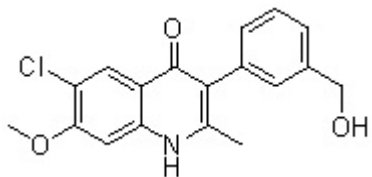
—61.05
—56.41

—18.73

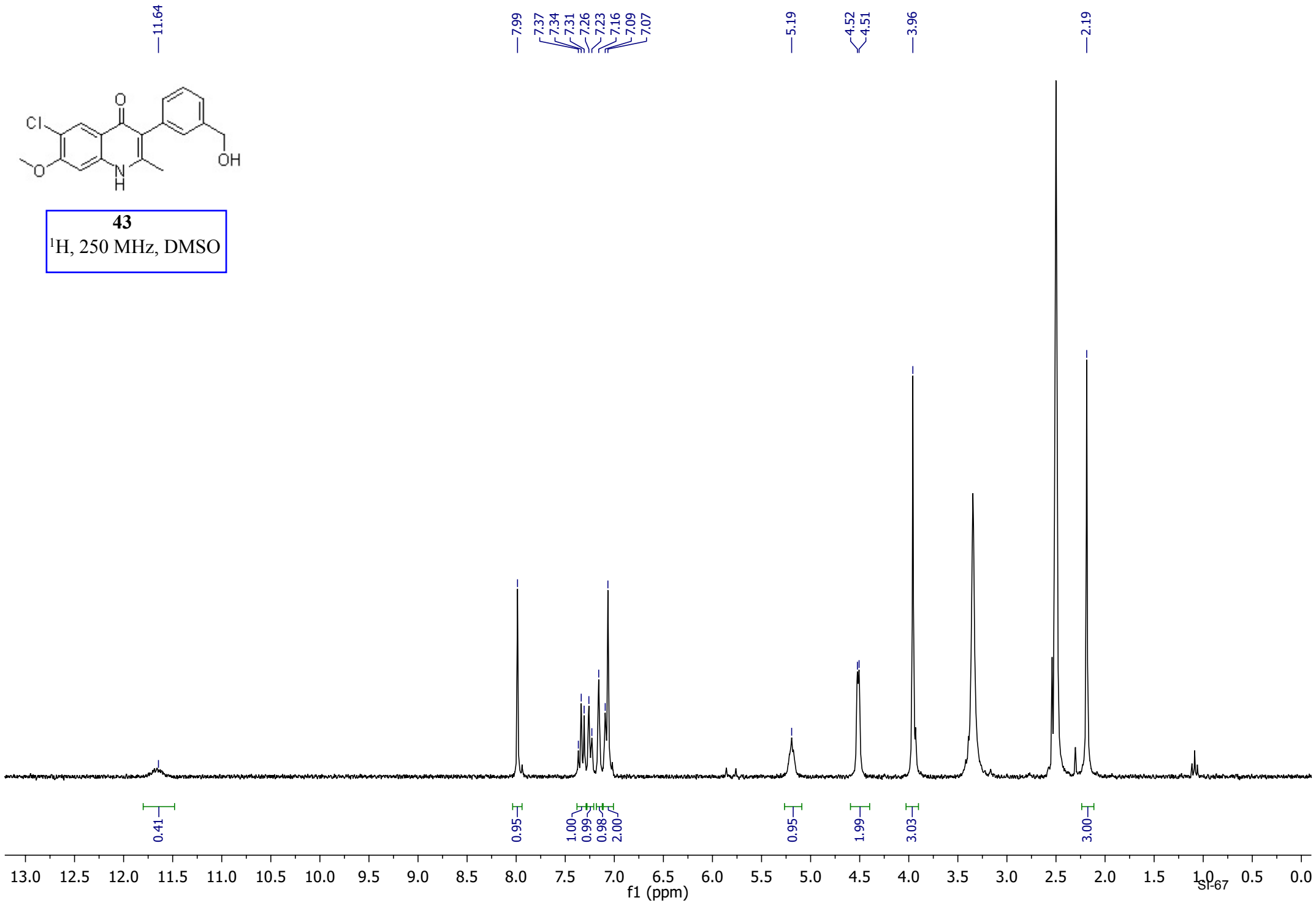


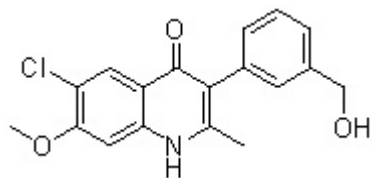
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10^{SI-66} 0 -10

f1 (ppm)



43
¹H, 250 MHz, DMSO





43

¹³C, 101 MHz, DMSO

—174.19

—157.30

—147.08

—142.64

—140.29

—136.30

—129.90

—129.69

—128.18

—126.83

—125.41

—121.60

—119.46

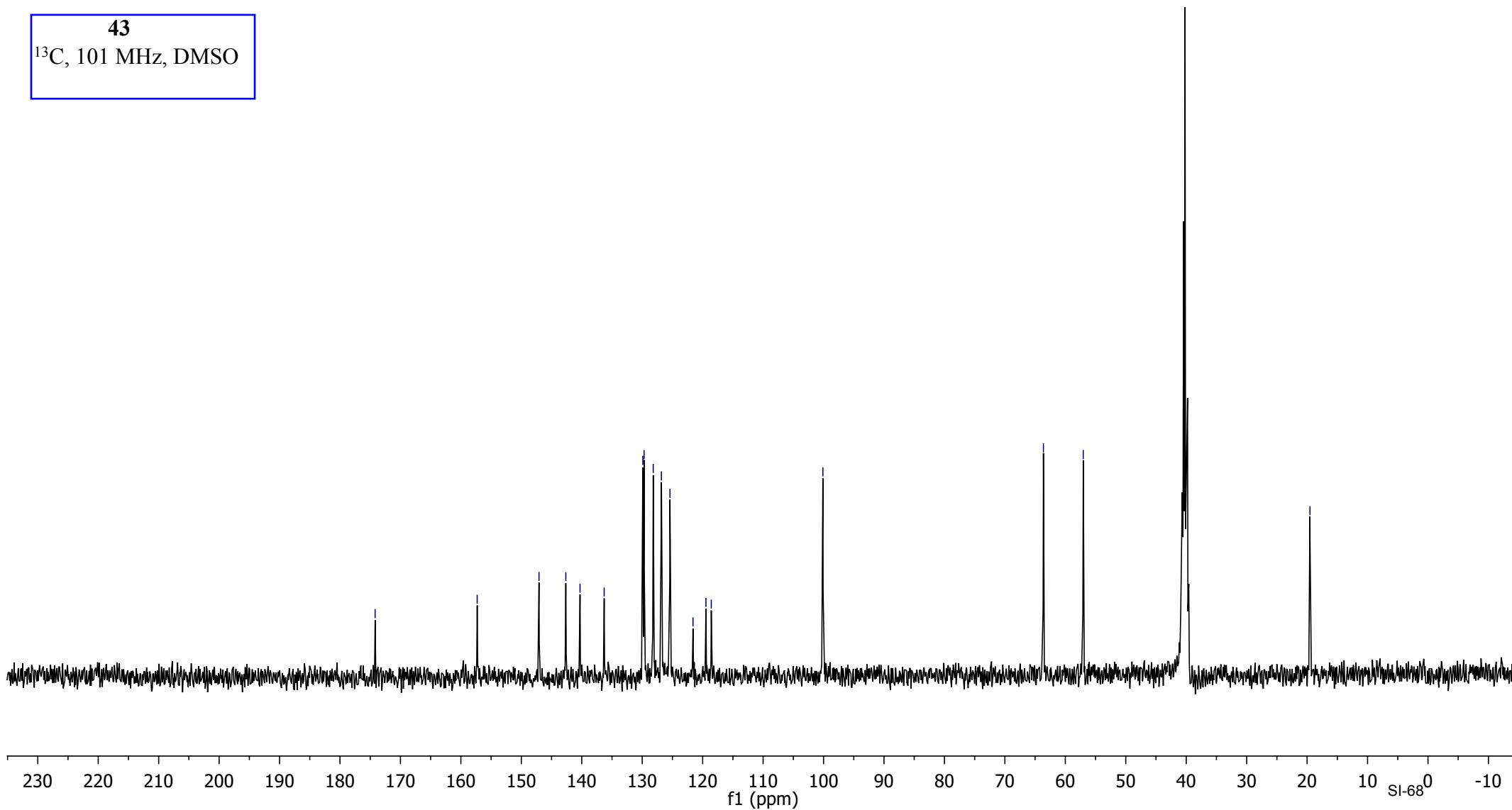
—118.57

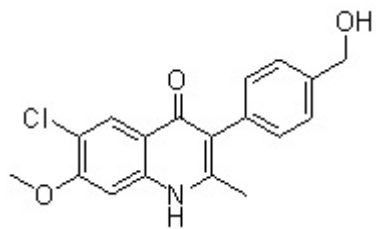
—100.11

—63.62

—57.03

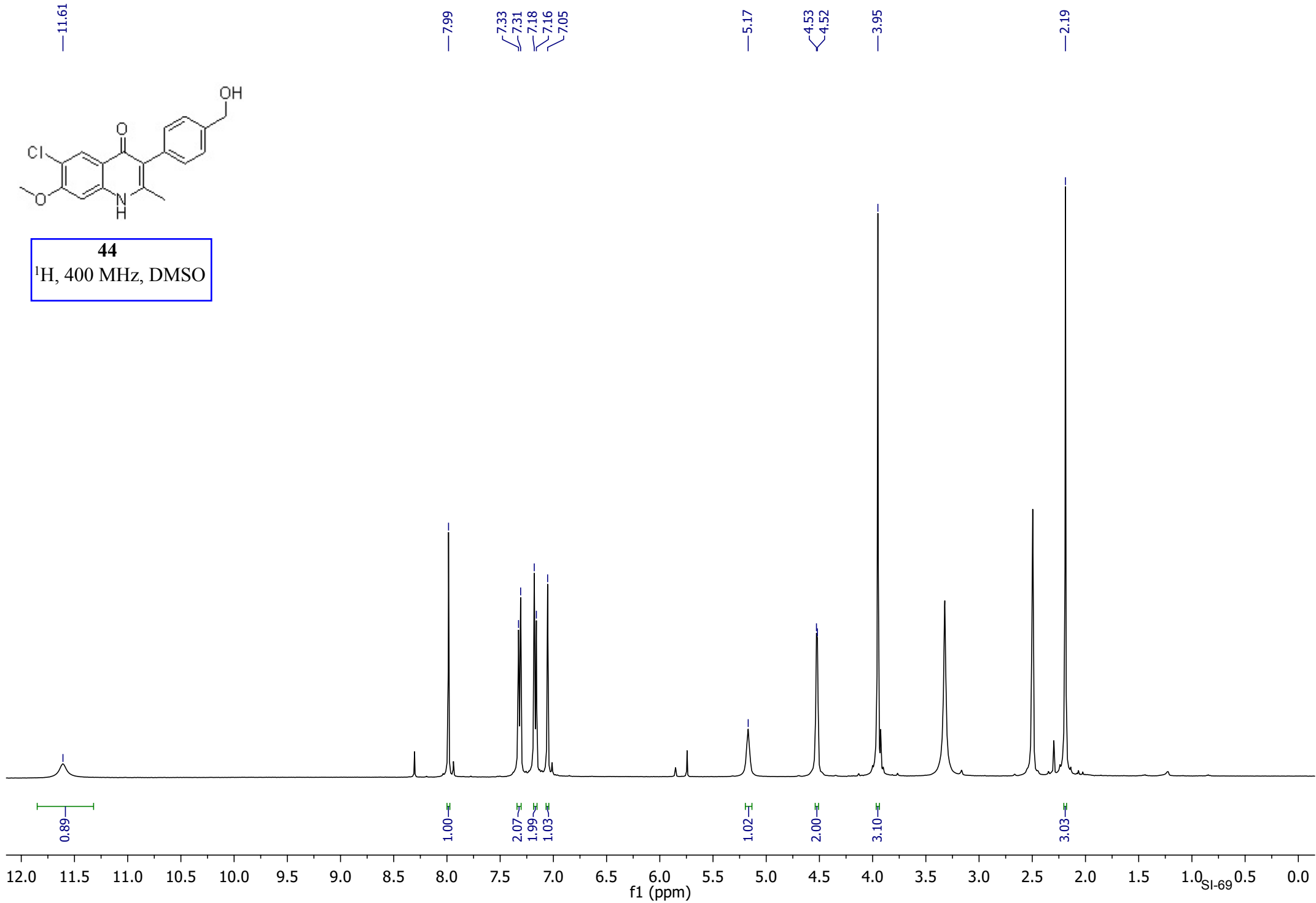
—19.53

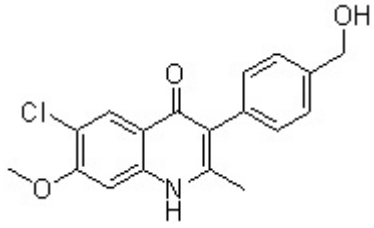




44

^1H , 400 MHz, DMSO





44
¹³C, 101 MHz, DMSO

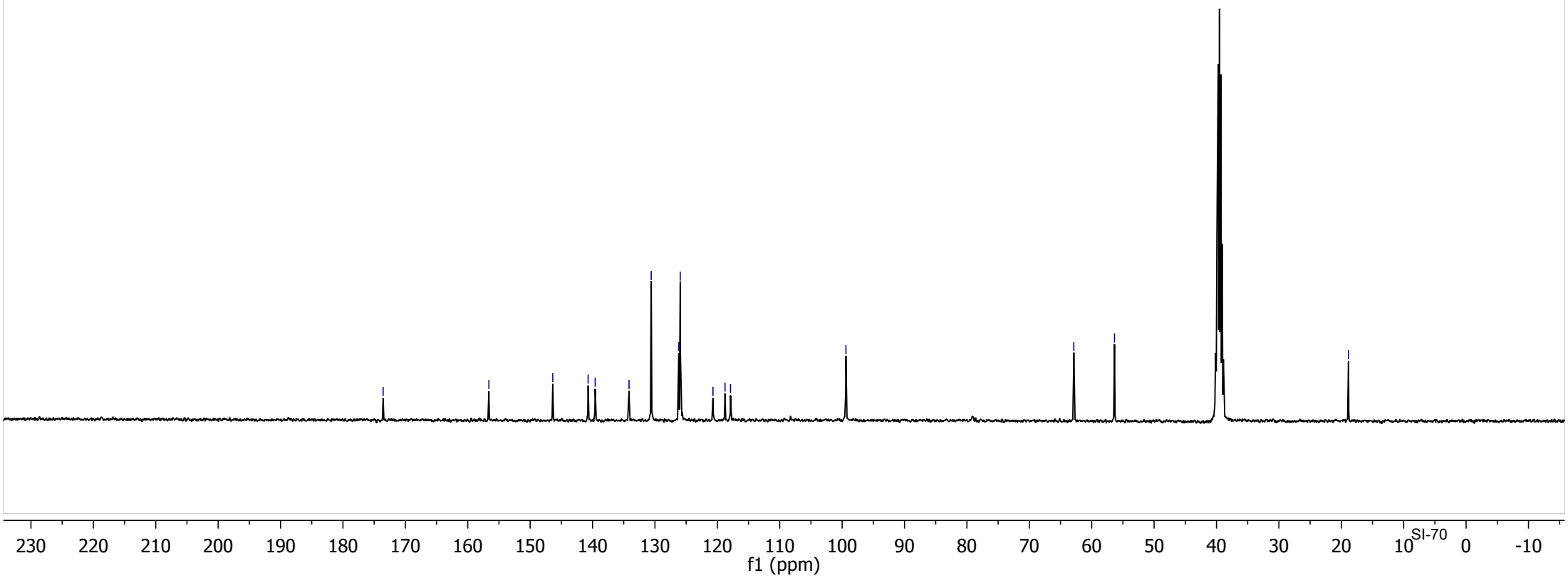
—173.56
—156.62
~146.37
~140.71
~139.58
~134.15
~130.60
~126.17
~125.94
~120.70
~118.77
~117.89

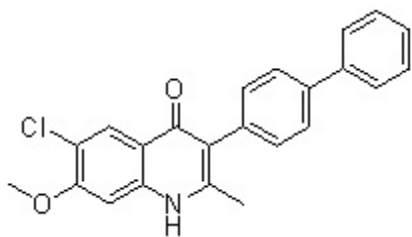
—99.39

—62.87

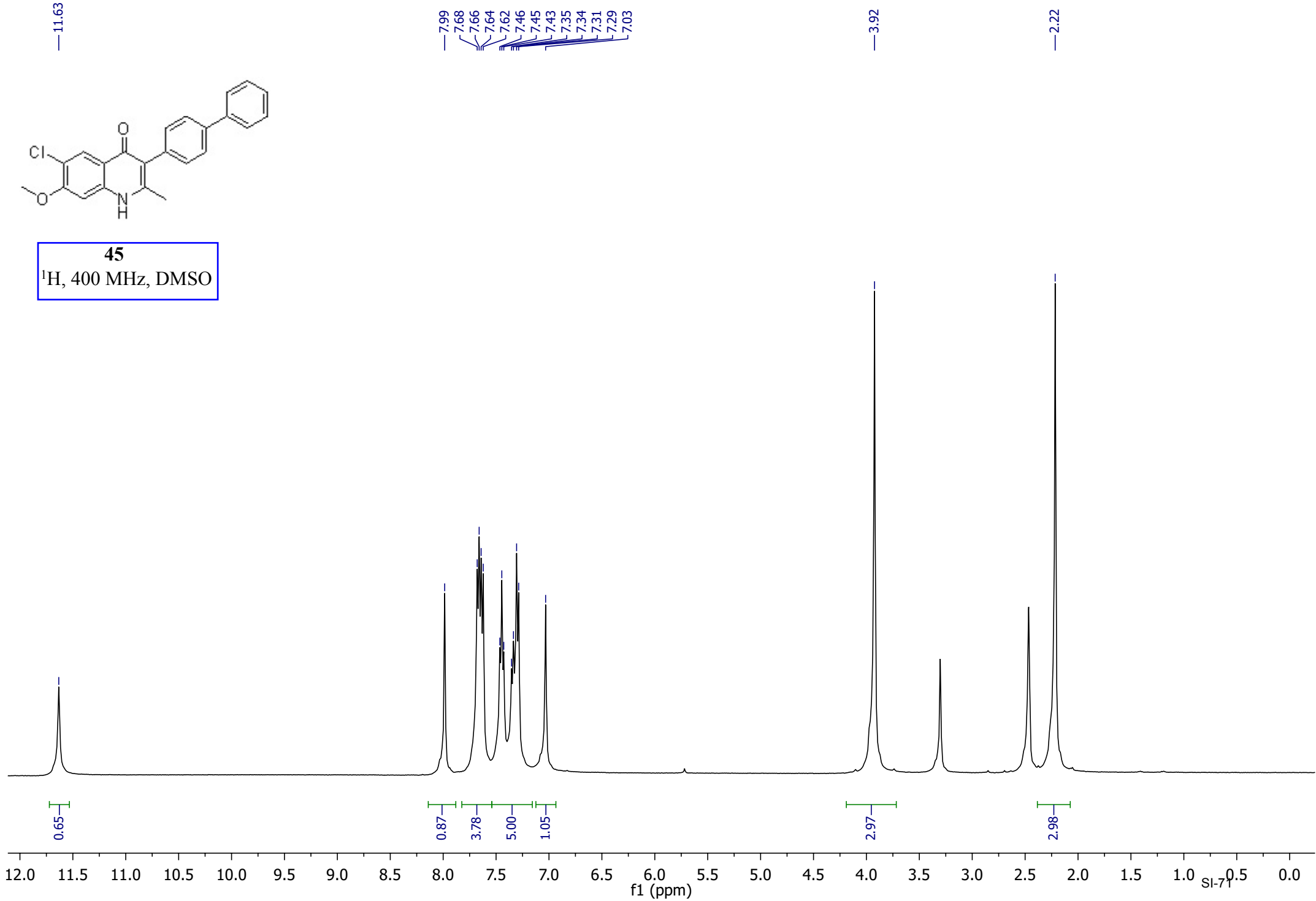
—56.34

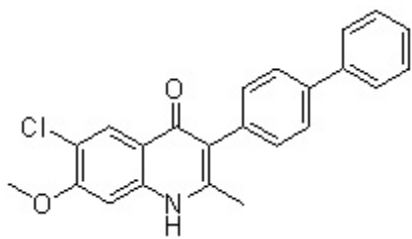
—18.85





45
¹H, 400 MHz, DMSO





45
¹³C, 101 MHz, DMSO

—174.21

—157.36

—147.21

—140.75

—140.26

—138.98

—135.73

—132.22

—129.61

—127.97

—127.23

—126.87

—126.70

—120.95

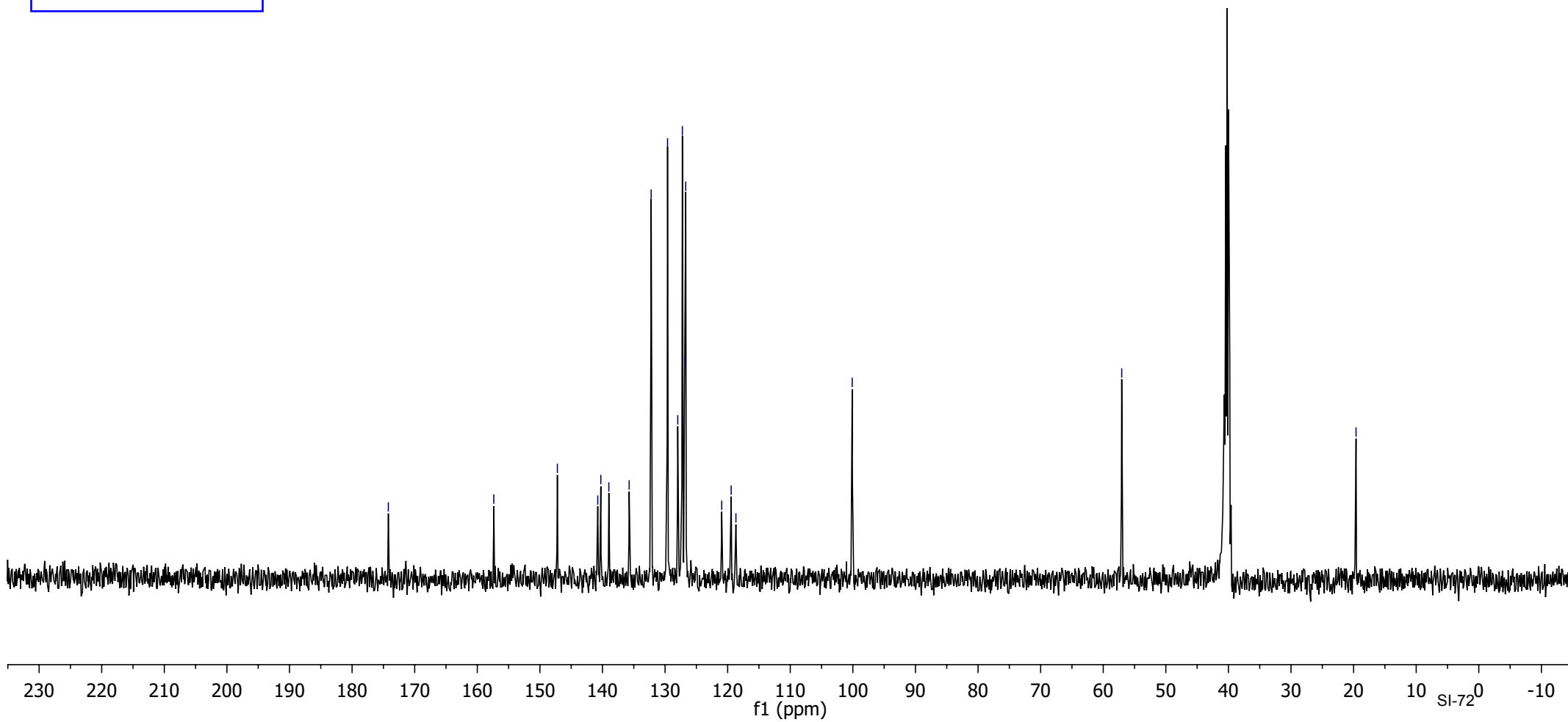
—119.44

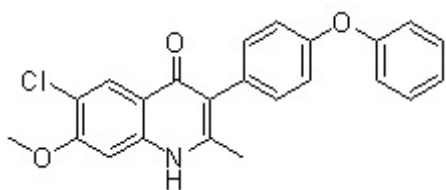
—118.68

—100.10

—57.05

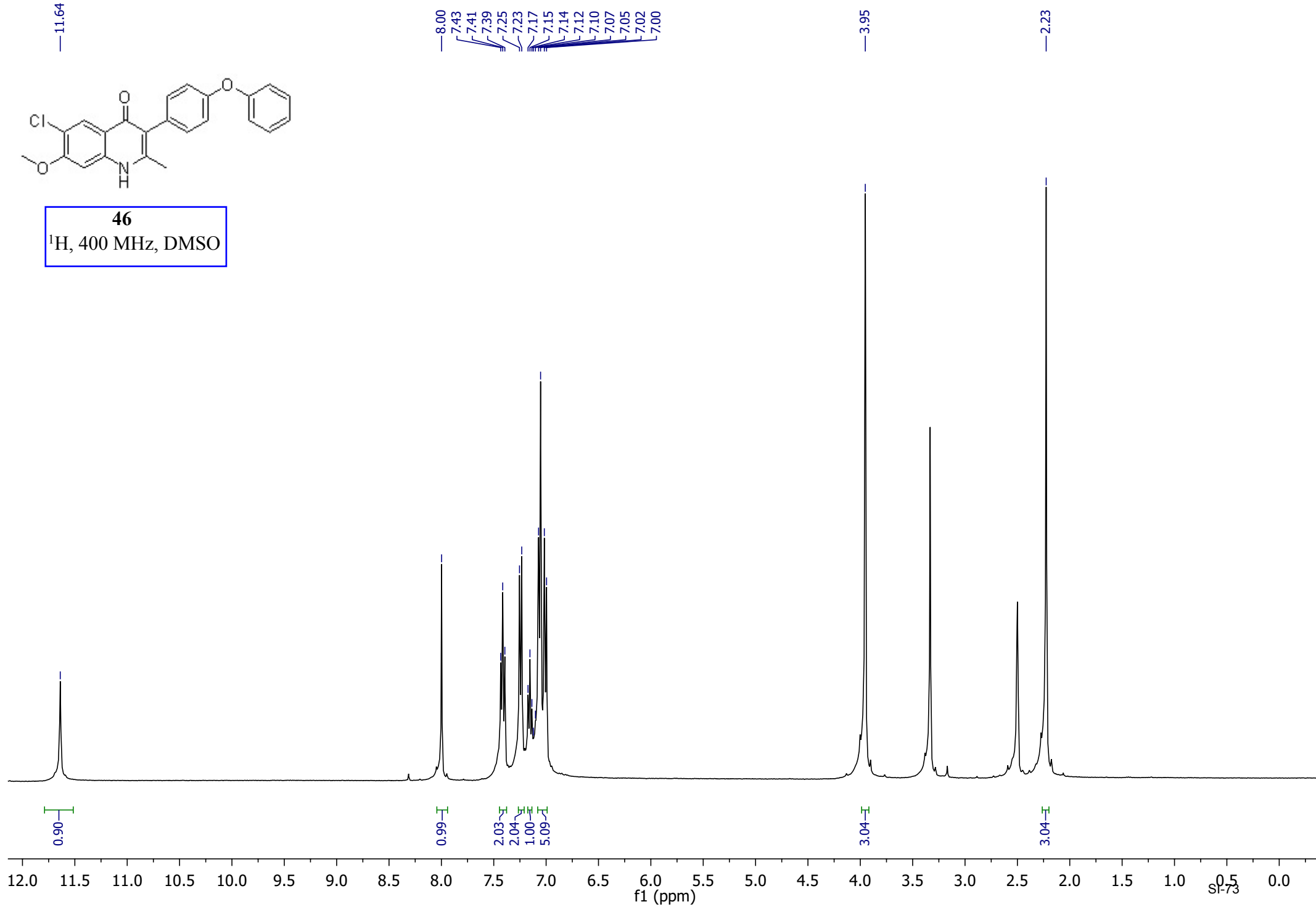
—19.61

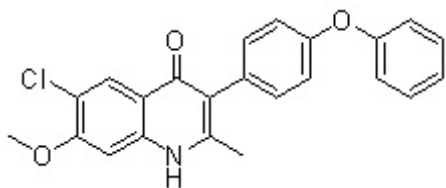




46

¹H, 400 MHz, DMSO





46
¹³C, 101 MHz, DMSO

—173.53

—156.64
—155.31

—146.54

—139.55

—132.52

—130.80

—130.02

—126.15

—123.43

—120.00

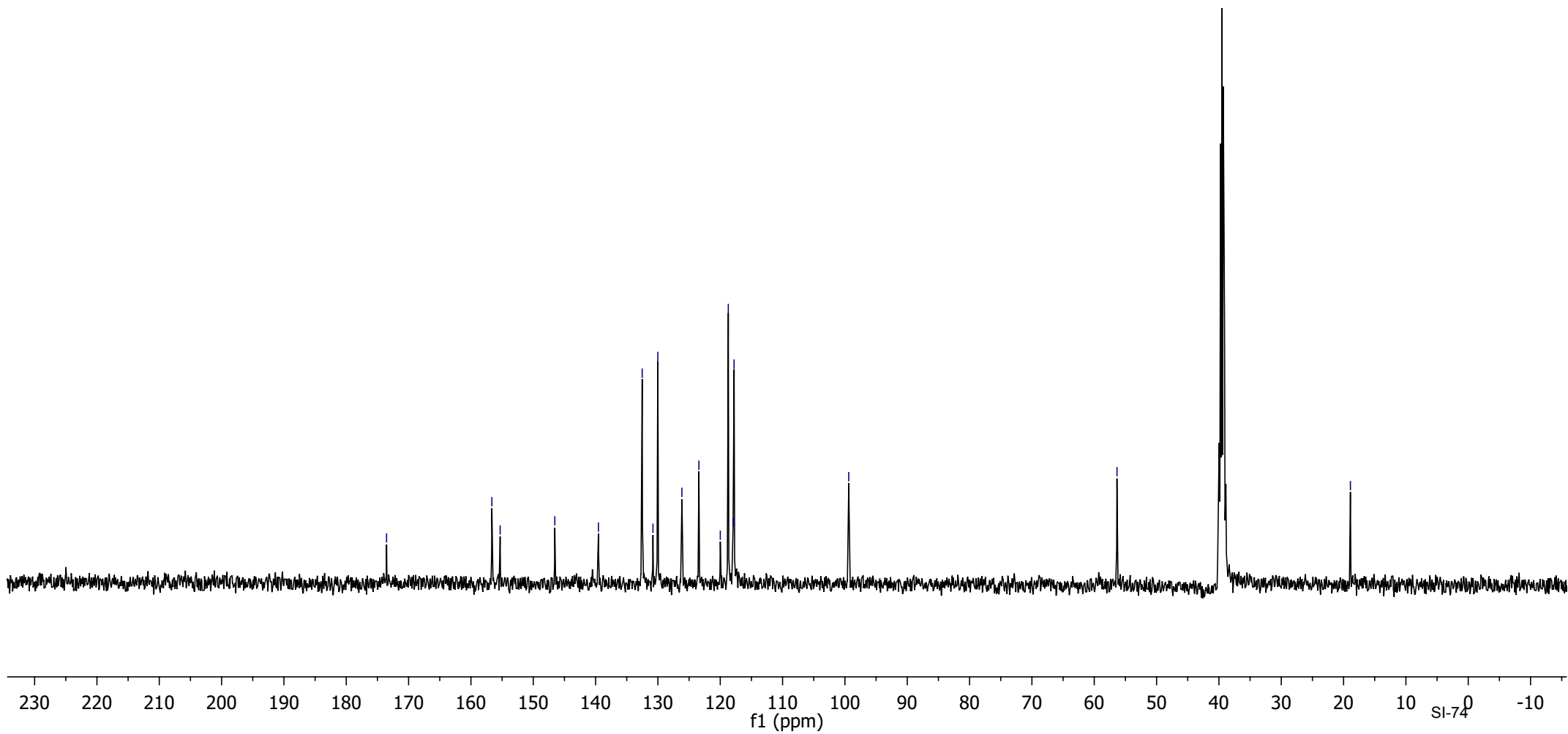
—118.71

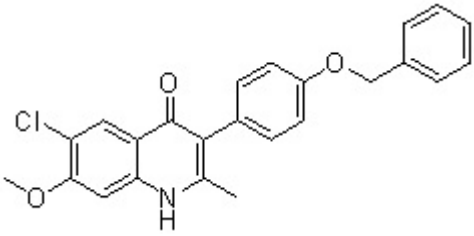
—117.94

—99.38

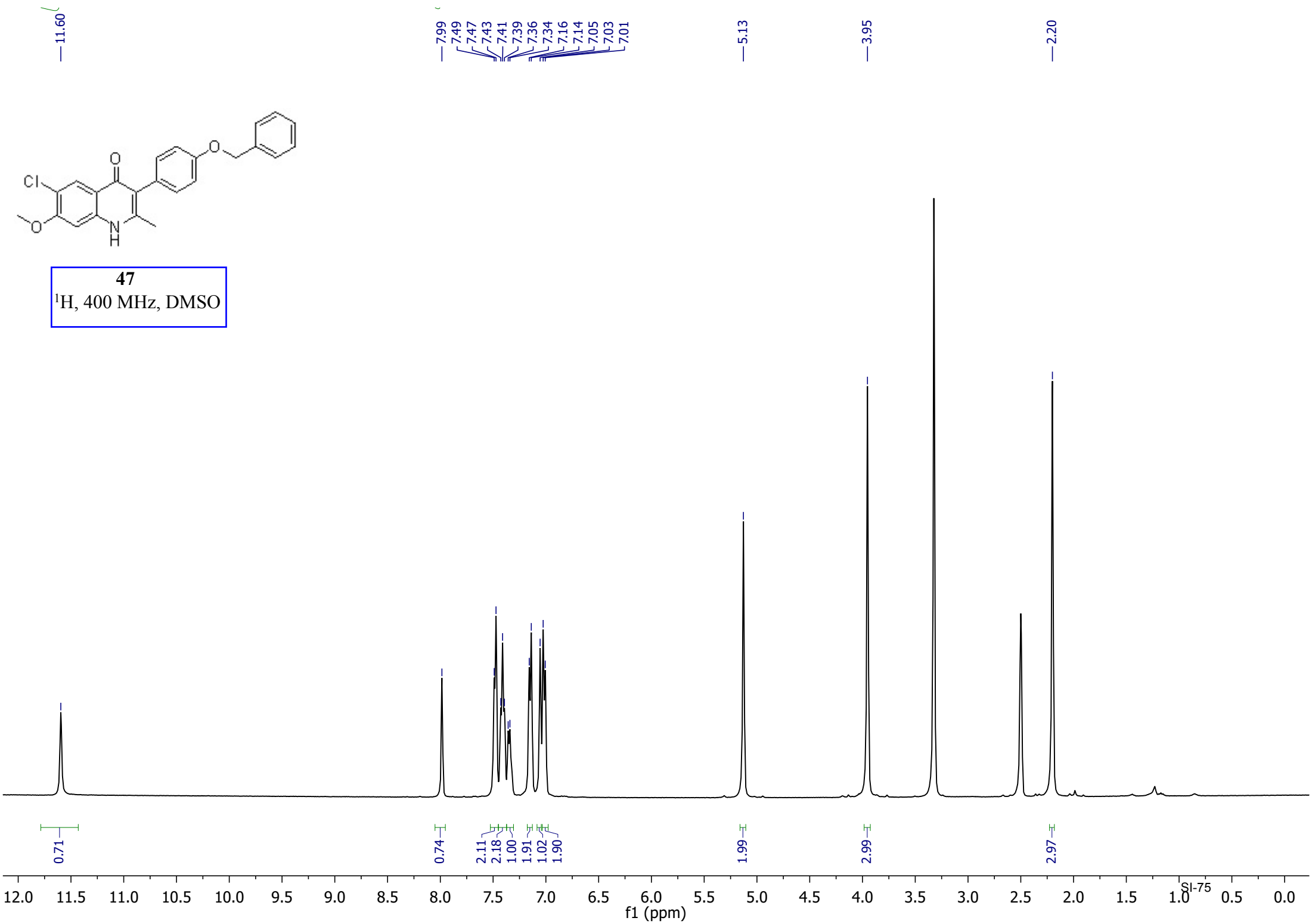
—56.35

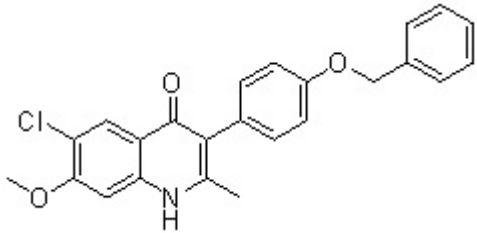
—18.90





47
¹H, 400 MHz, DMSO





47
¹³C, 101 MHz, DMSO

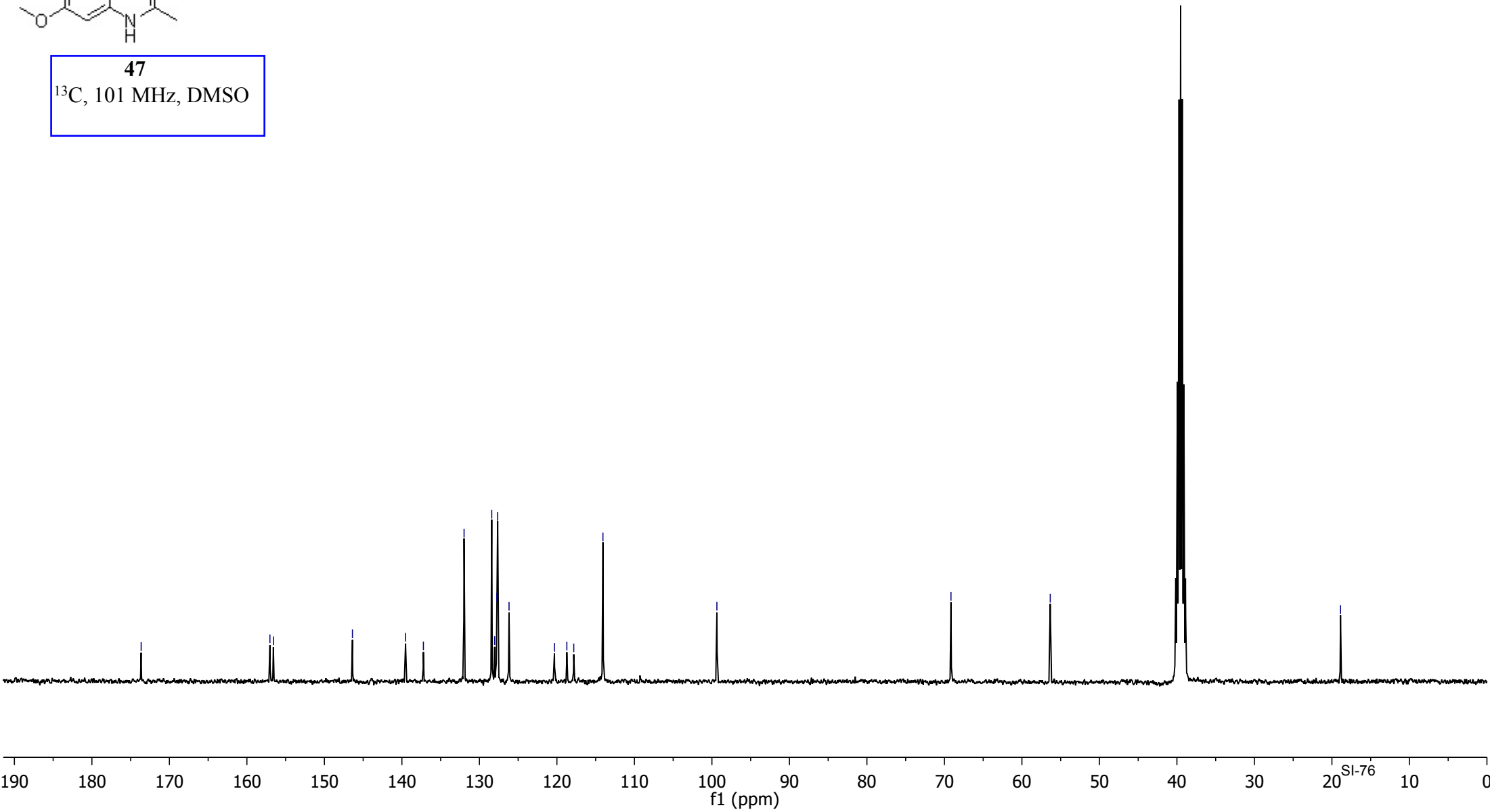
—173.64
—157.03
—156.59
—146.38
—139.53
—137.23
—131.98
—128.41
—128.04
—127.76
—127.64
—126.18
—120.32
—118.72
—117.83
—114.06

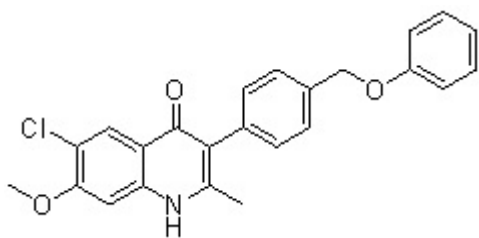
—99.36

—69.15

—56.35

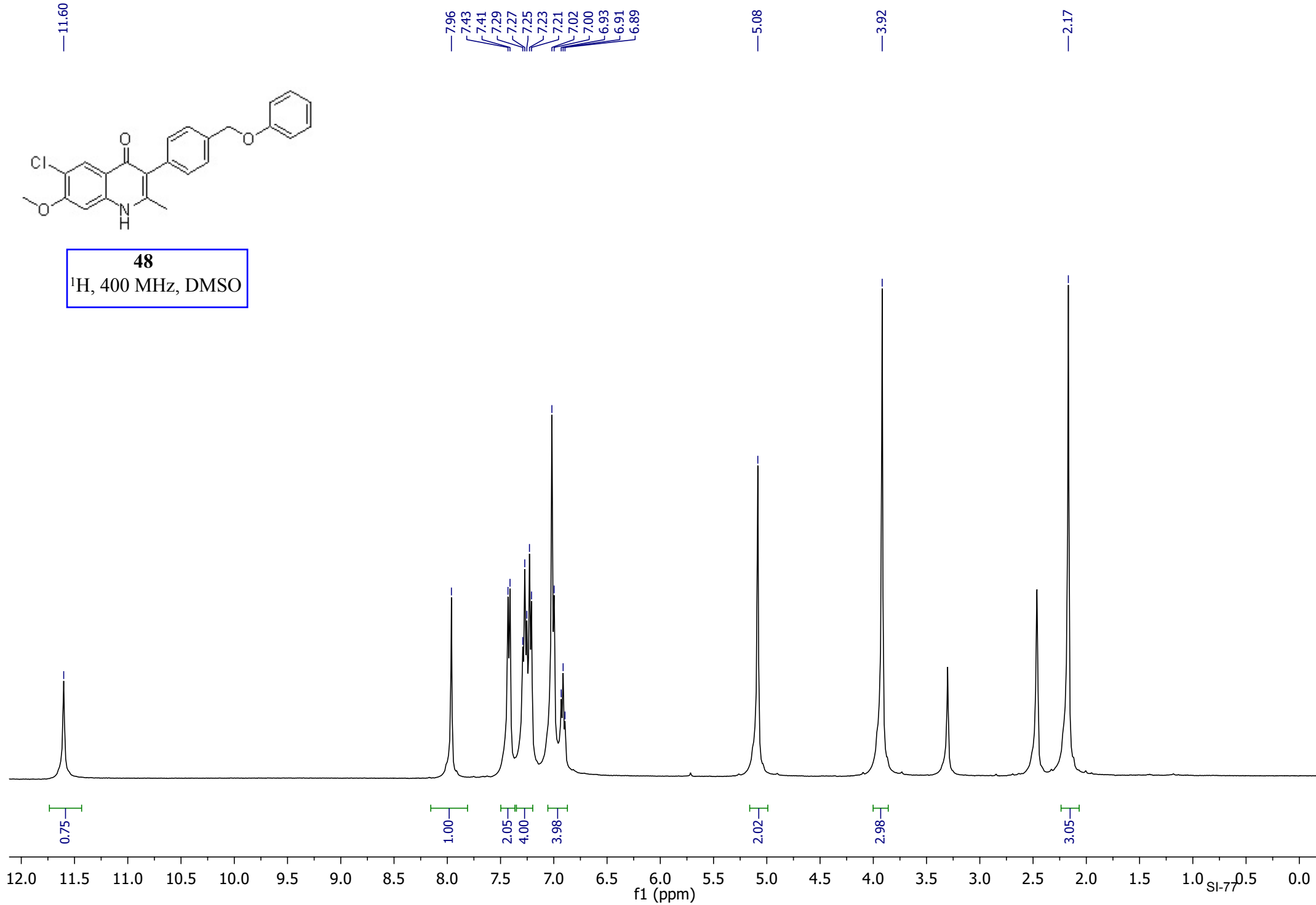
—18.89

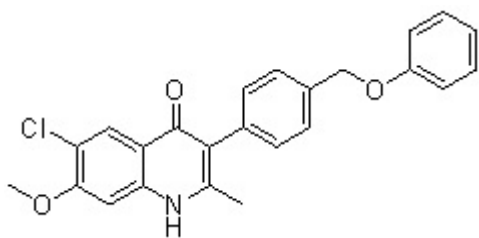




48

^1H , 400 MHz, DMSO





48
¹³C, 101 MHz, DMSO

—174.17

—159.11
—157.35

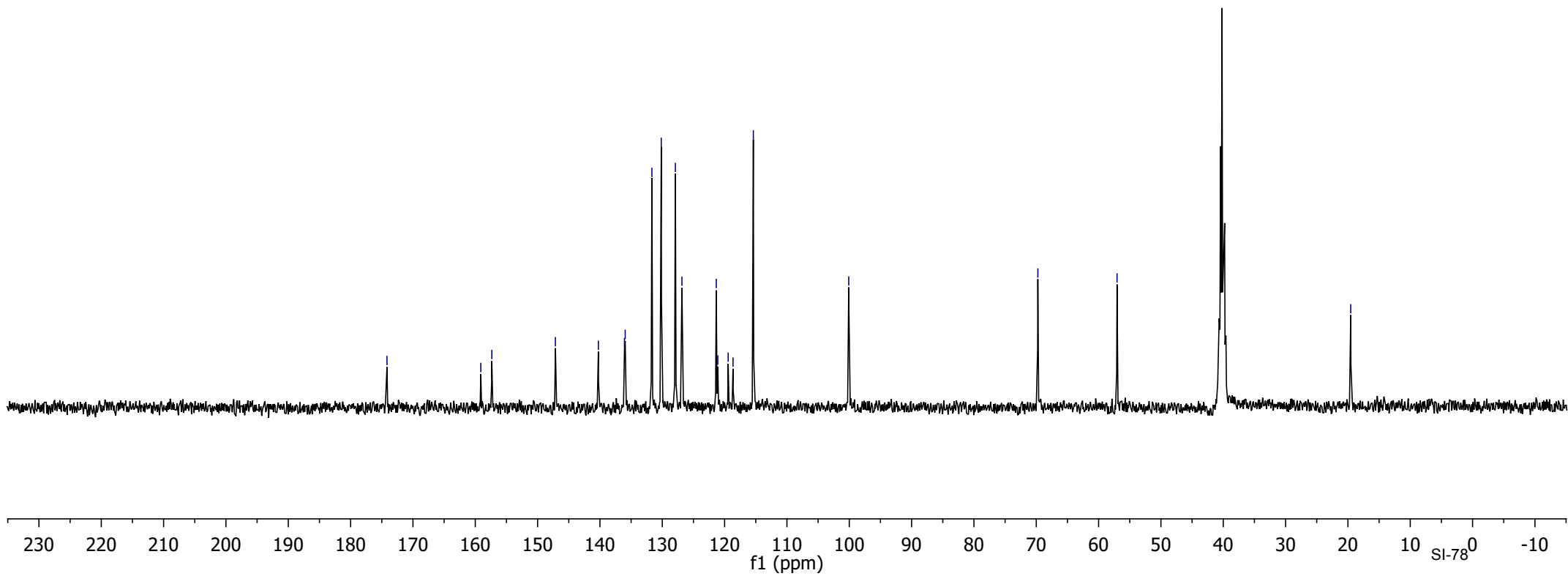
—147.15
—140.25
—136.07
—135.95
—131.67
—130.16
—127.90
—126.85
—121.34
—121.09
—119.43
—118.65
—115.39

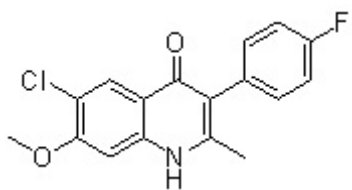
—100.09

—69.74

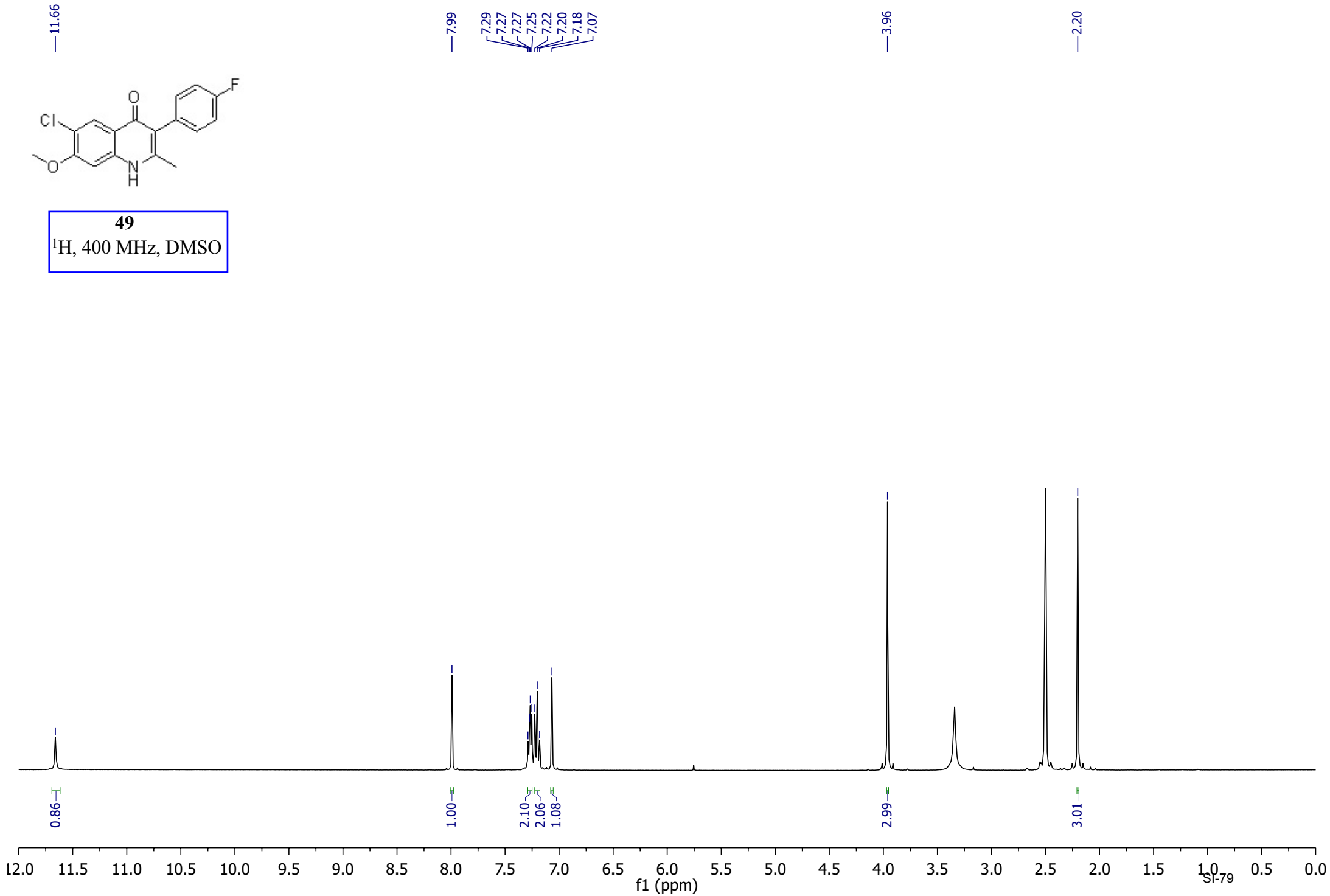
—57.04

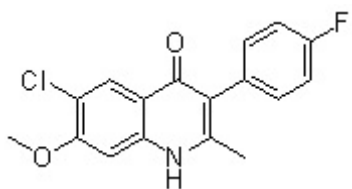
—19.55



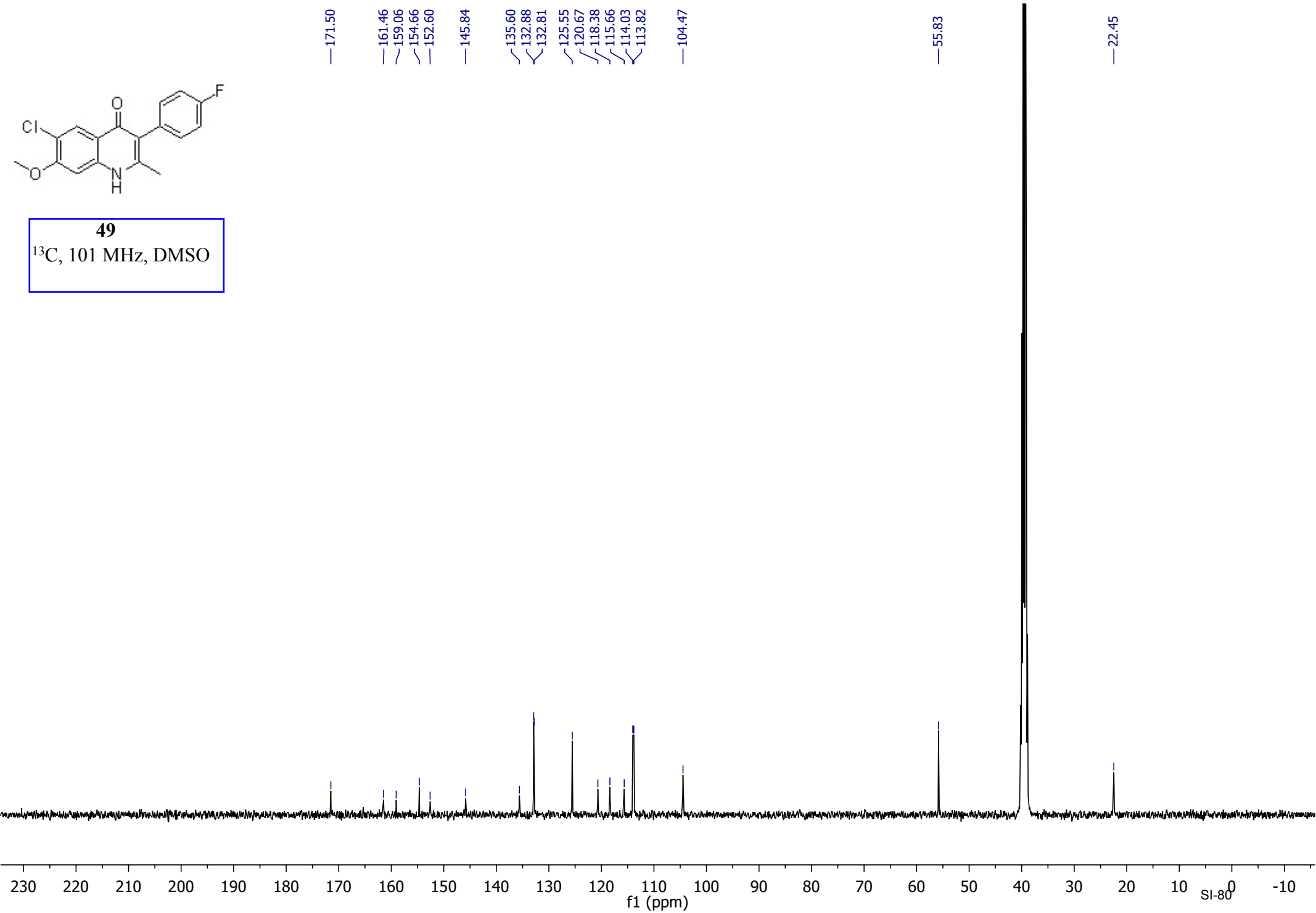


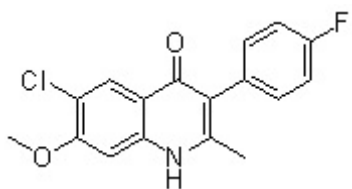
49
¹H, 400 MHz, DMSO





49
 ^{13}C , 101 MHz, DMSO

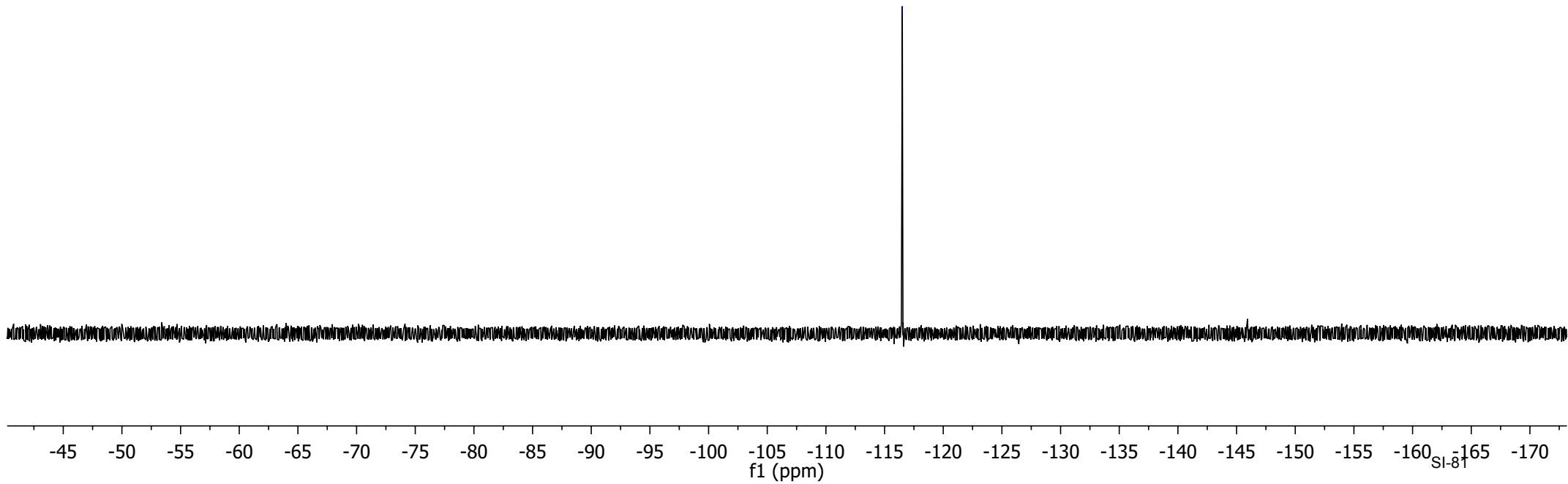


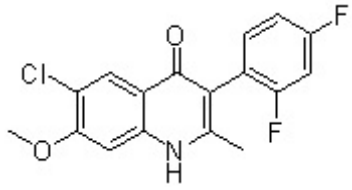


49

^{19}F , 376 MHz, DMSO

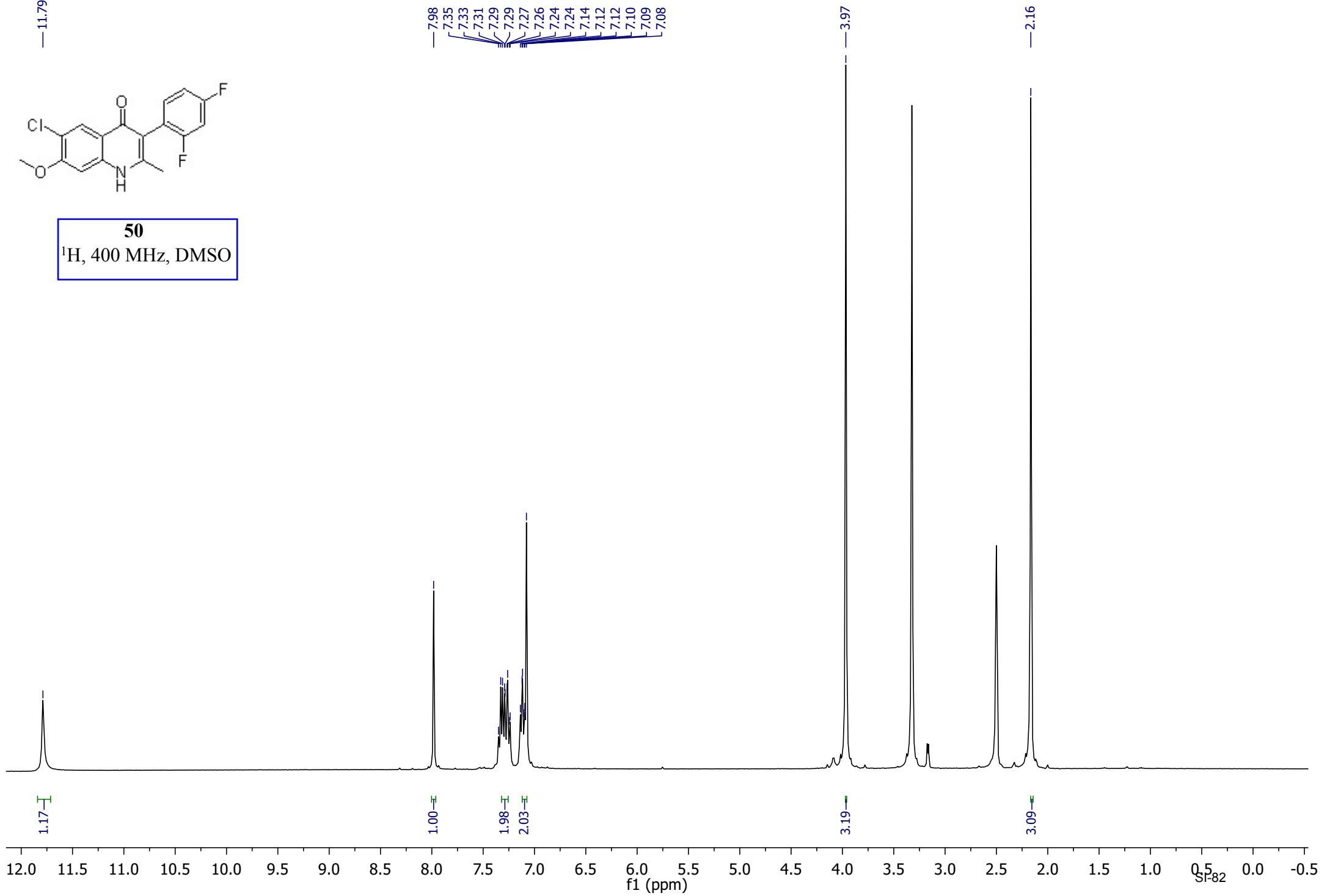
— -116.51

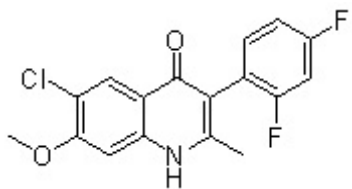




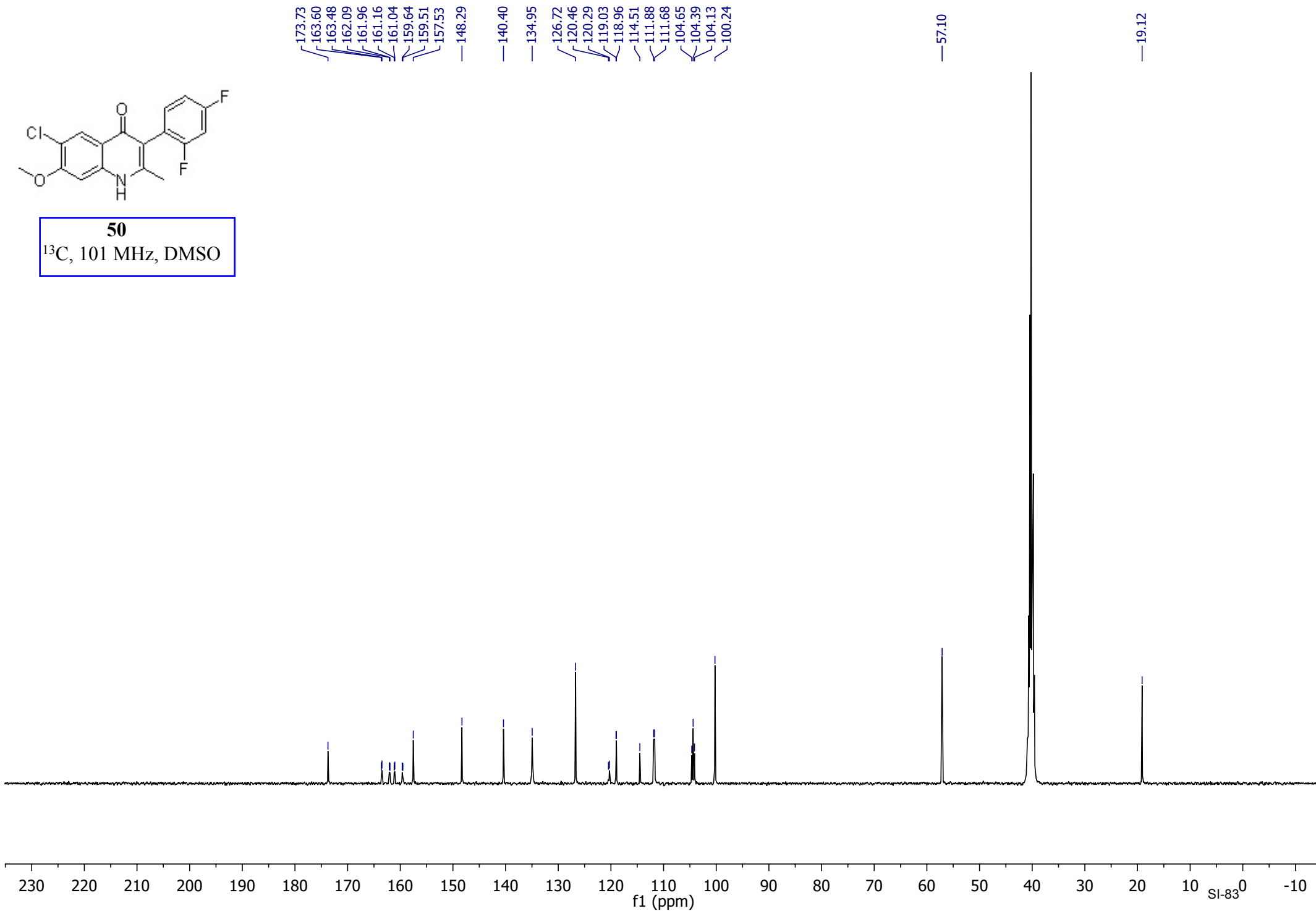
50

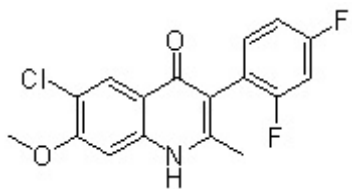
¹H, 400 MHz, DMSO





50
¹³C, 101 MHz, DMSO

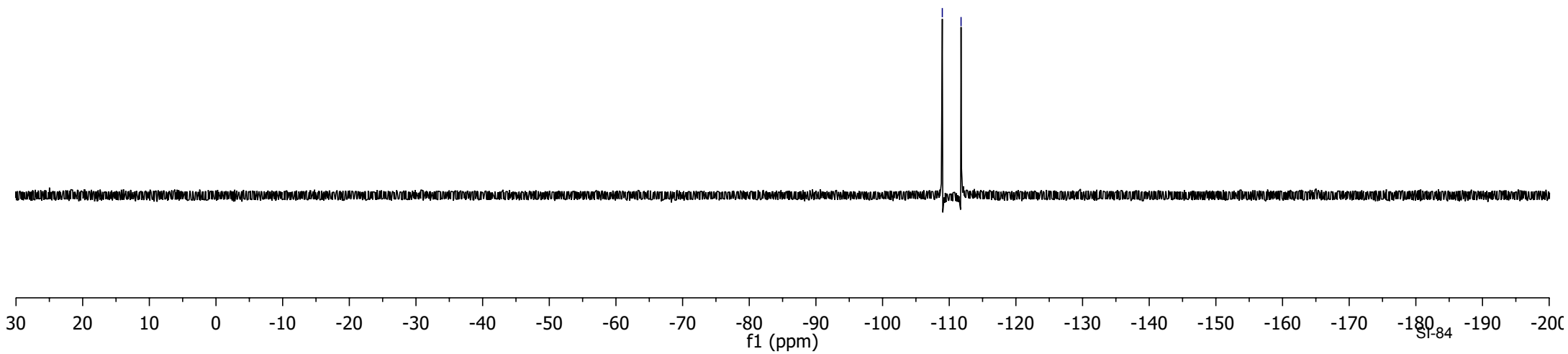


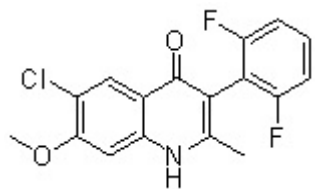


50

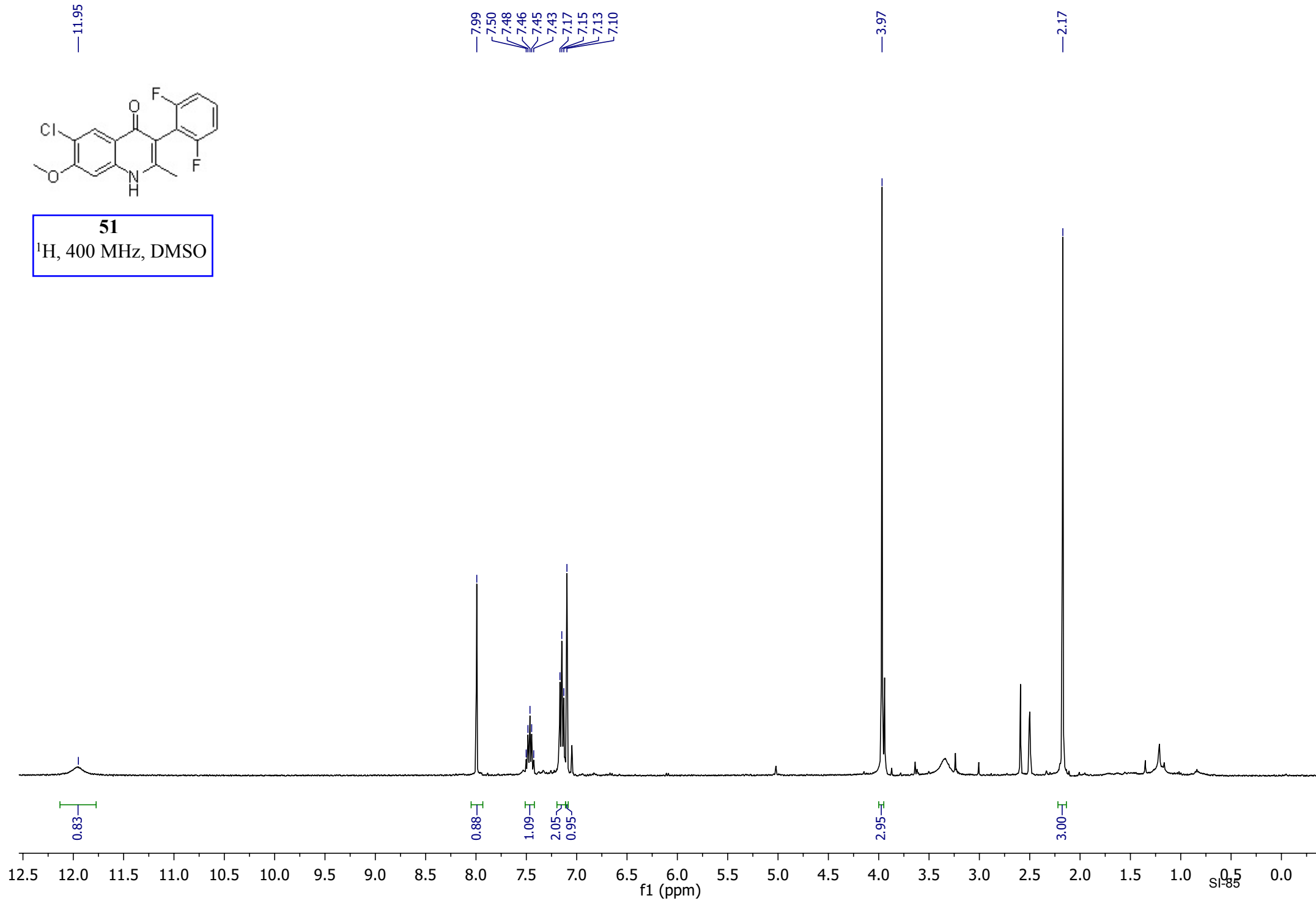
¹⁹F, 376 MHz, DMSO

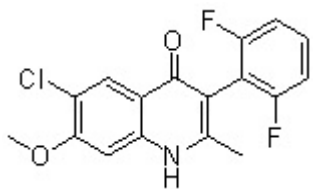
— -108.96
— -111.77





51
¹H, 400 MHz, DMSO

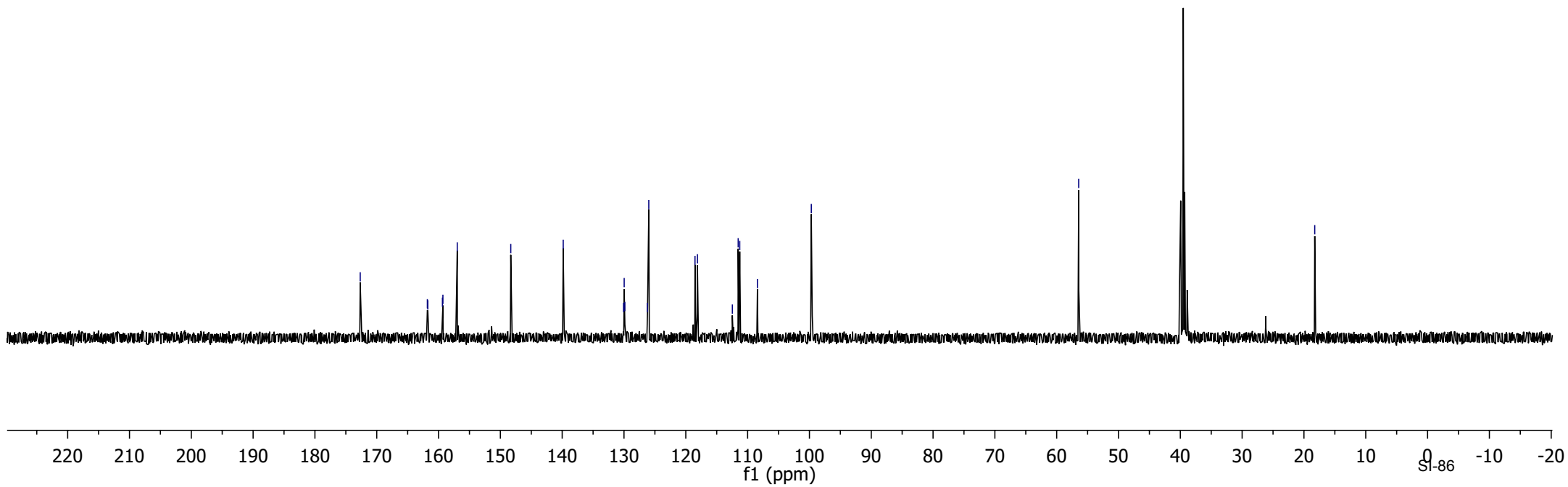


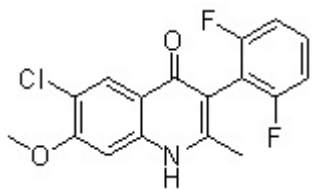


51

^{13}C , 101 MHz, DMSO

—172.67
161.81
161.73
159.37
159.30
156.98
—148.32
—139.83
130.07
129.97
129.87
126.20
125.99
118.51
118.12
112.47
111.53
111.27
108.41
—99.70
—56.44
—18.25

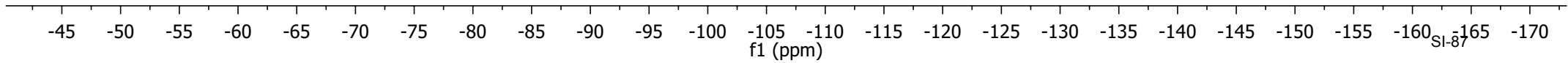


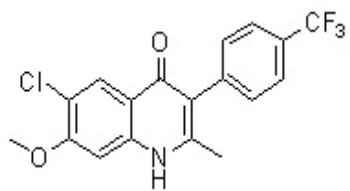


51

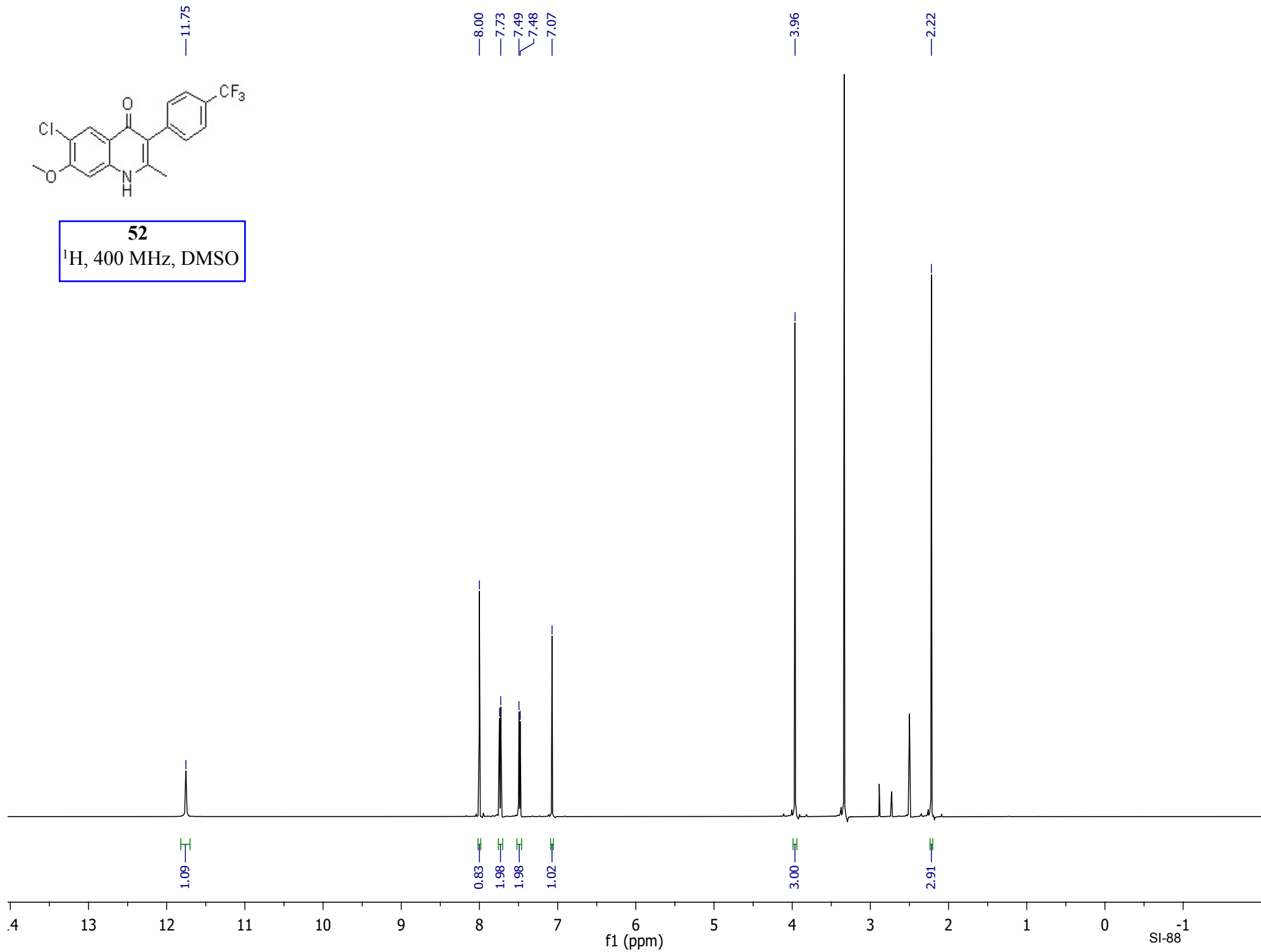
¹⁹F, 376 MHz, DMSO

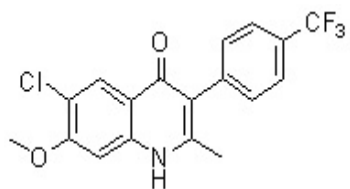
-111.50





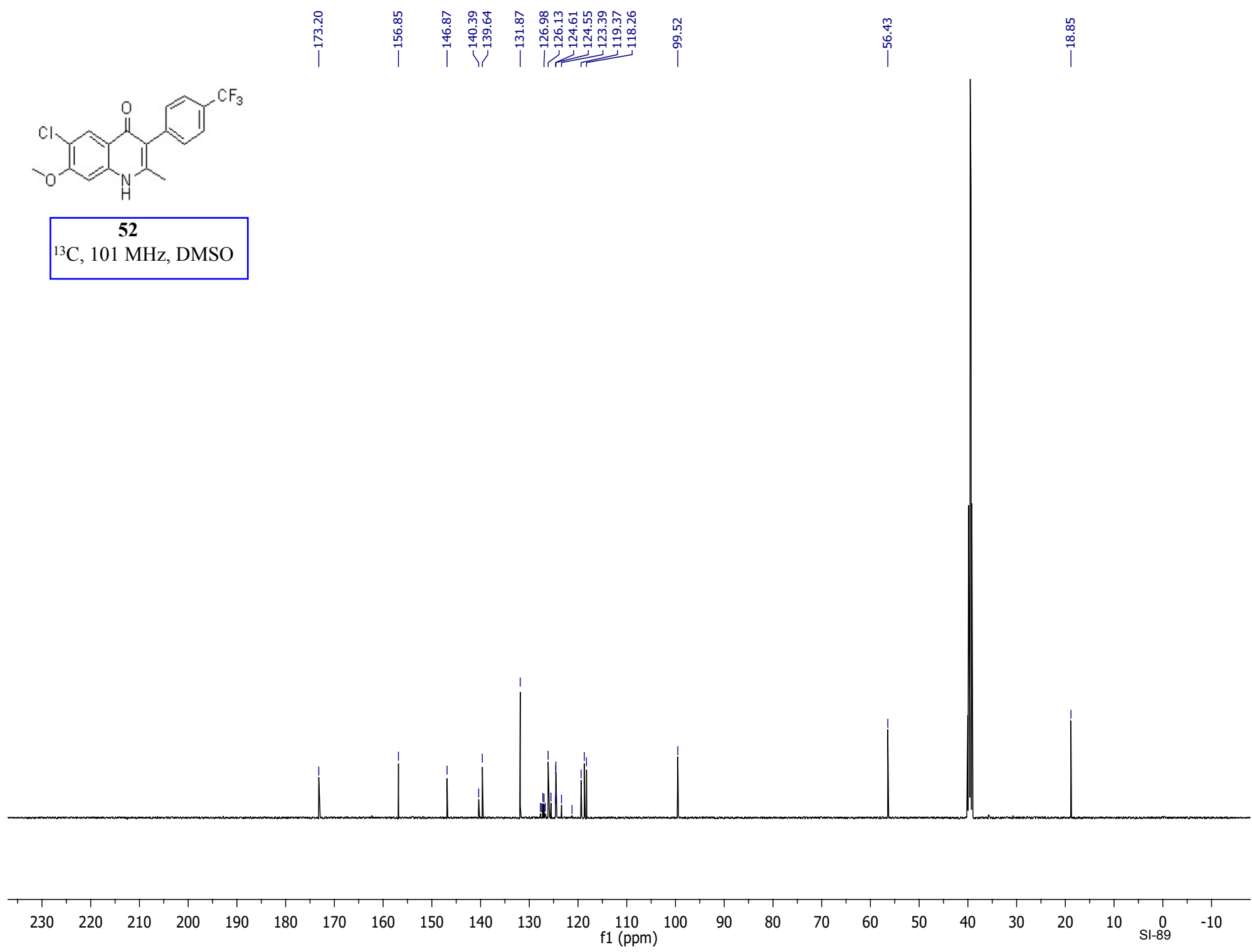
52
¹H, 400 MHz, DMSO

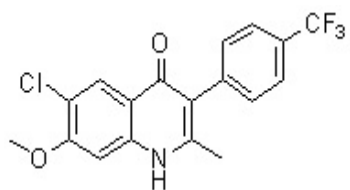




52

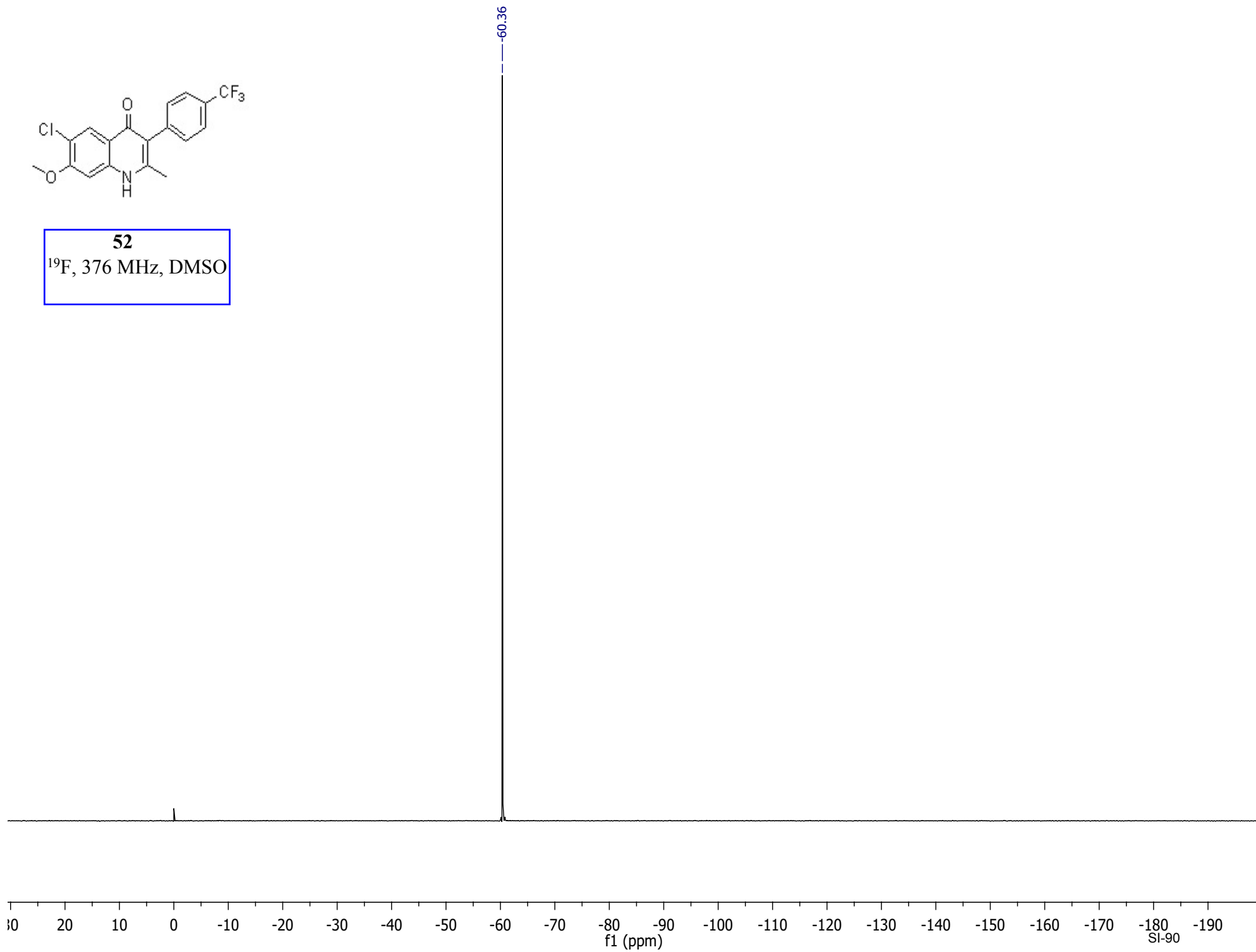
¹³C, 101 MHz, DMSO



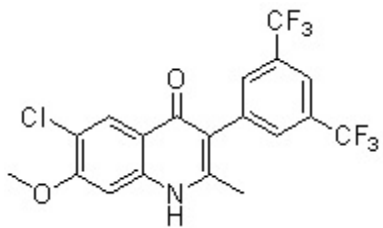


52

^{19}F , 376 MHz, DMSO



—11.88



53

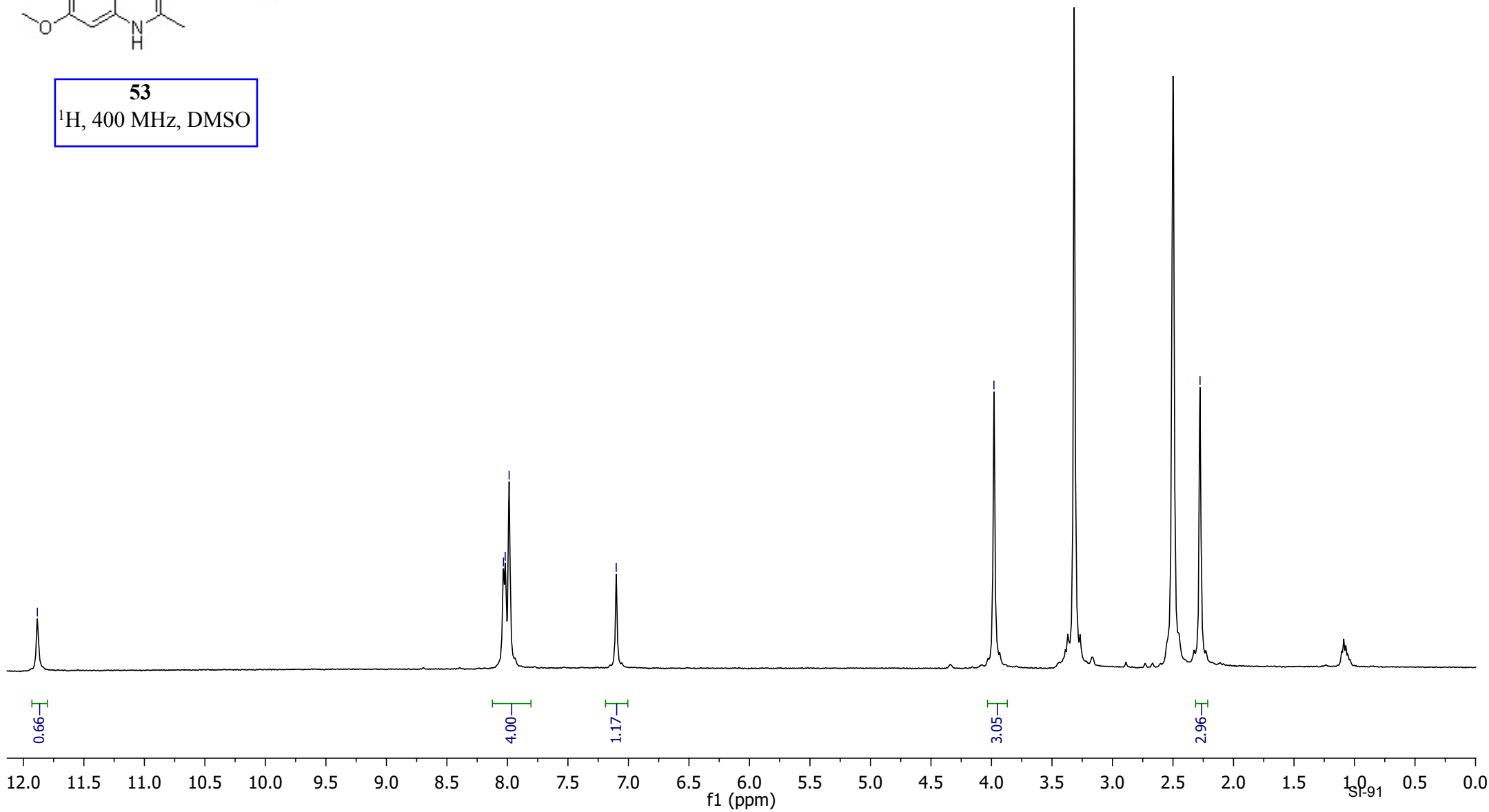
¹H, 400 MHz, DMSO

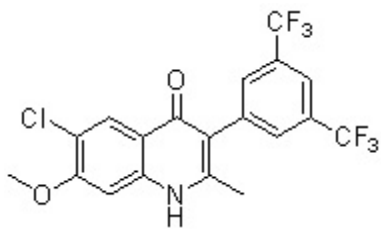
8.03
8.02
7.99

—7.10

—3.98

—2.28





53

^{13}C , 101 MHz, DMSO

—172.99

—156.99

—147.62

139.63

138.52

131.83

130.21

129.89

129.57

129.24

127.54

126.08

124.84

122.13

120.24

119.44

118.60

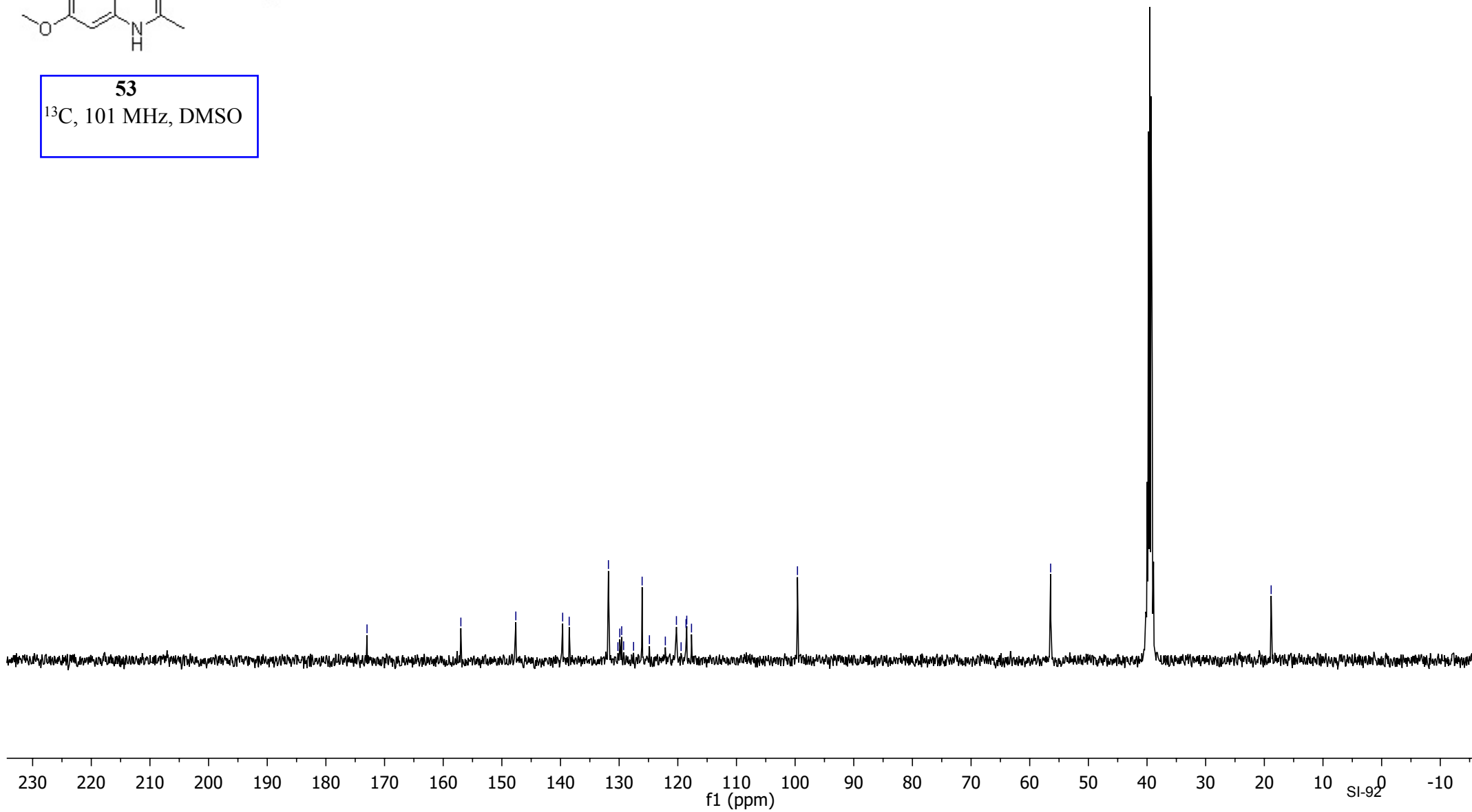
118.48

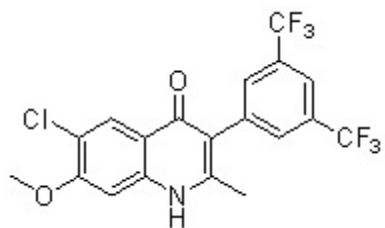
117.67

99.60

—56.43

—18.84



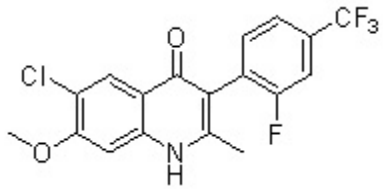


53

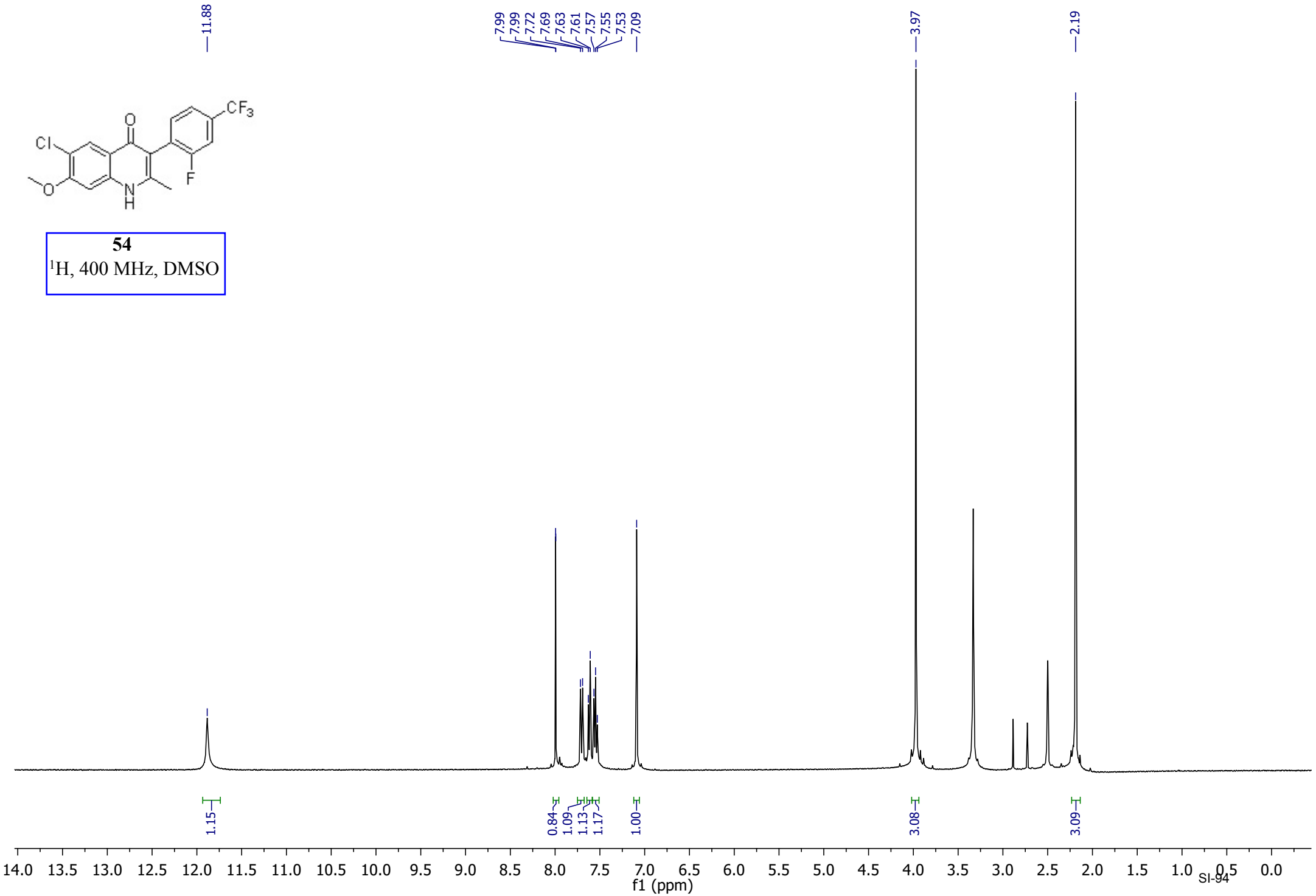
^{19}F , 376 MHz, DMSO

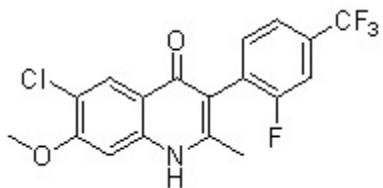
-61.54

-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) SI-93



54
¹H, 400 MHz, DMSO

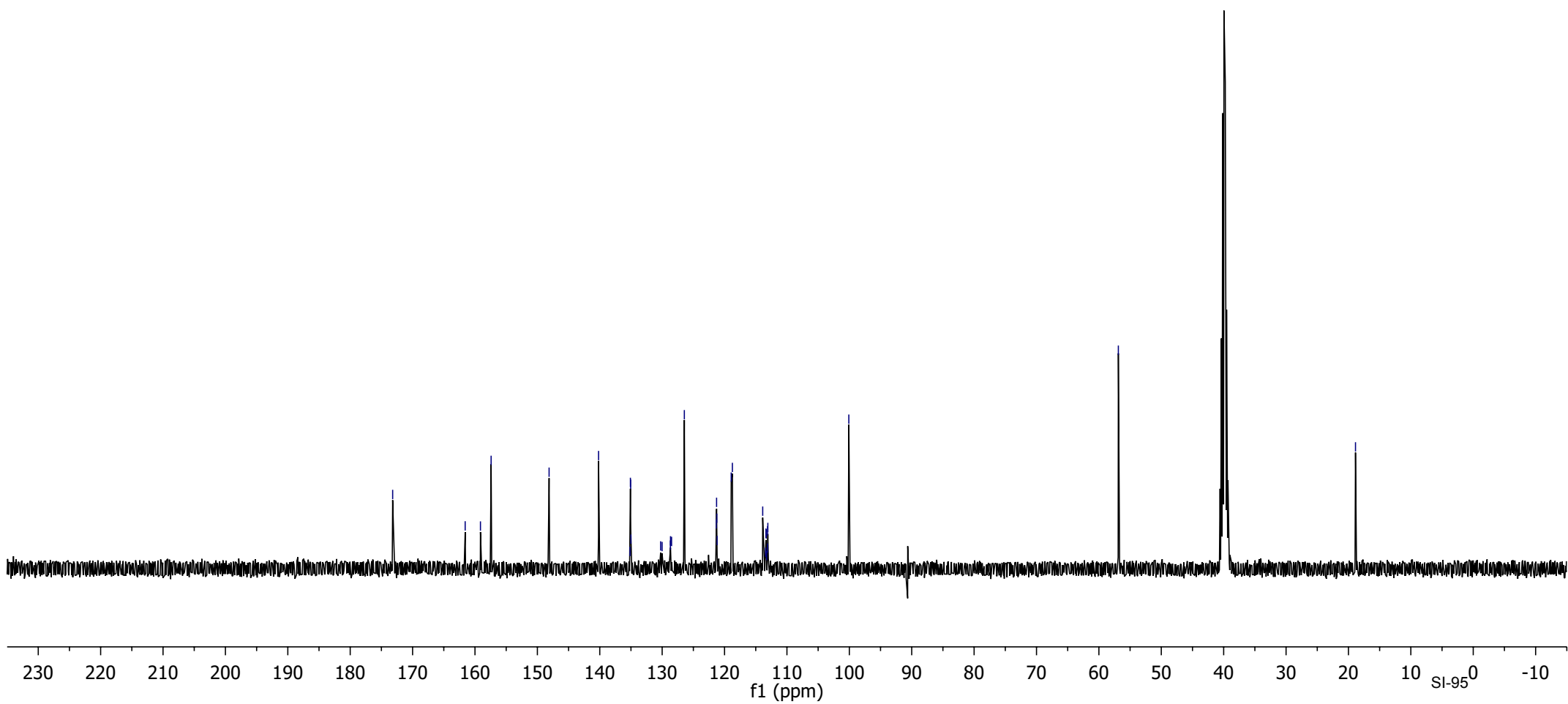


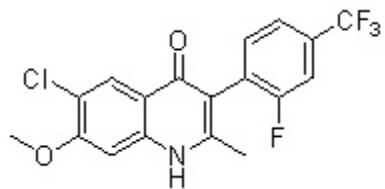


54

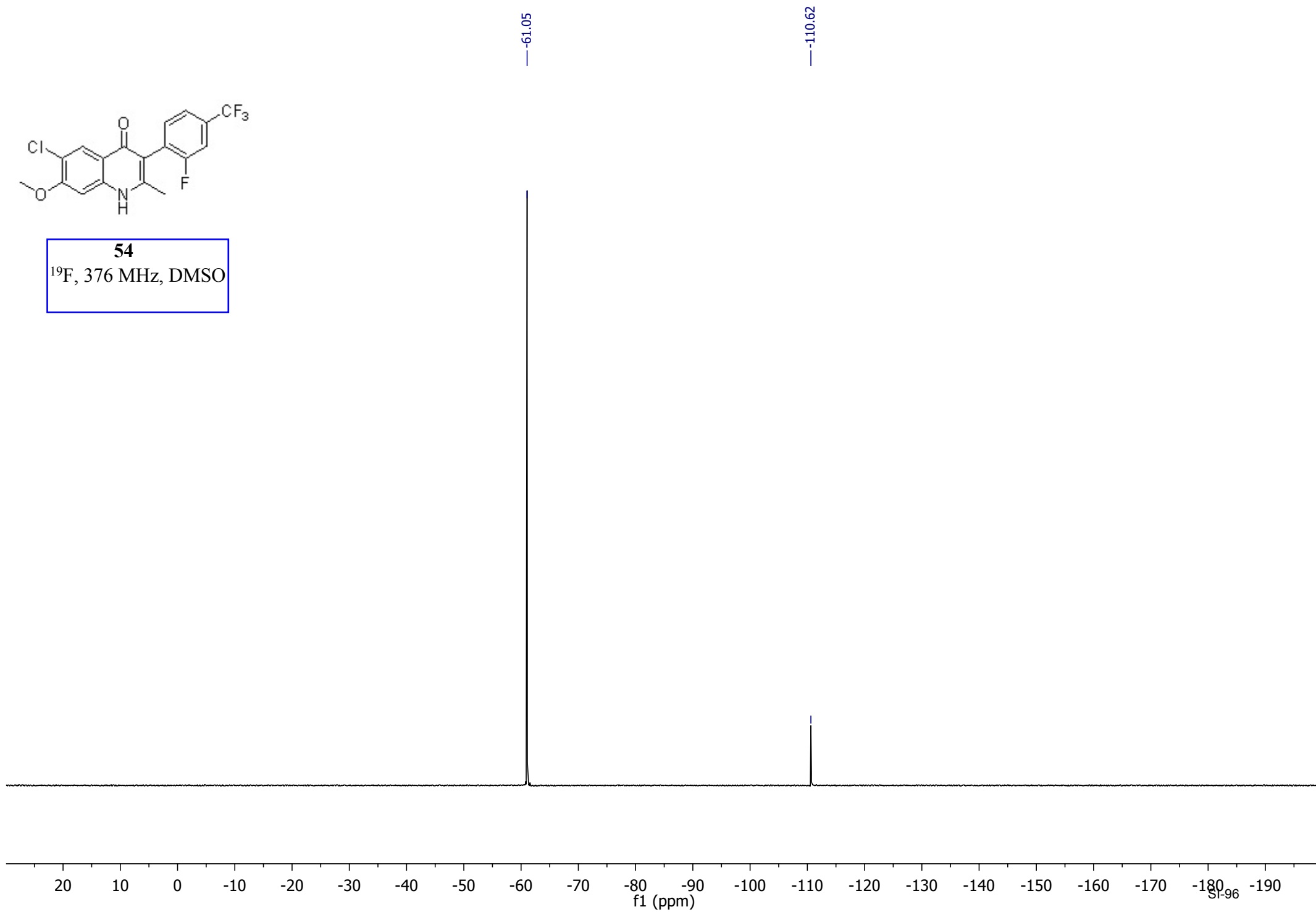
^{13}C , 101 MHz, DMSO

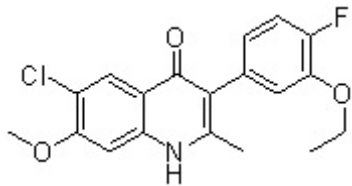
- 173.20
- 161.57
- 159.12
- 157.41
- 148.12
- 140.19
- 135.15
- 135.09
- 135.05
- 135.01
- 130.25
- 130.01
- 128.68
- 128.66
- 128.49
- 126.44
- 121.31
- 121.28
- 121.24
- 121.20
- 118.93
- 118.74
- 113.88
- 113.41
- 113.36
- 113.33
- 113.24
- 113.13
- 113.10
- 113.06
- 100.08
- 56.88
- 18.87



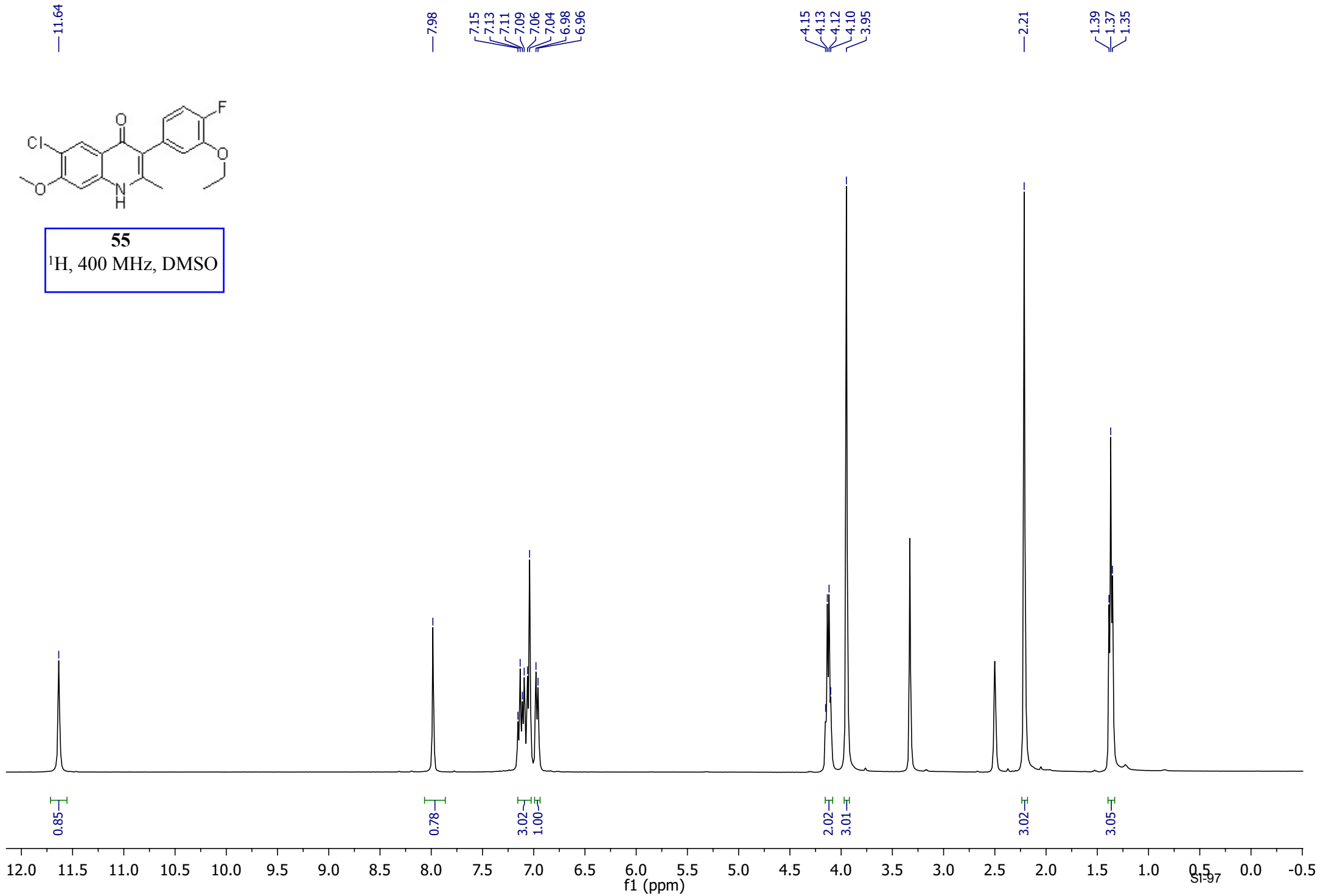


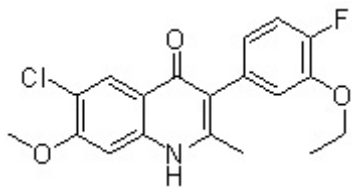
54
¹⁹F, 376 MHz, DMSO





55
 ^1H , 400 MHz, DMSO





55

^{13}C , 101 MHz, DMSO

—174.12

—157.34

—152.96

—150.55

—147.38

—145.67

—145.56

—140.19

—129.15

—127.81

—126.82

—120.04

—119.36

—119.21

—119.03

—118.66

—114.75

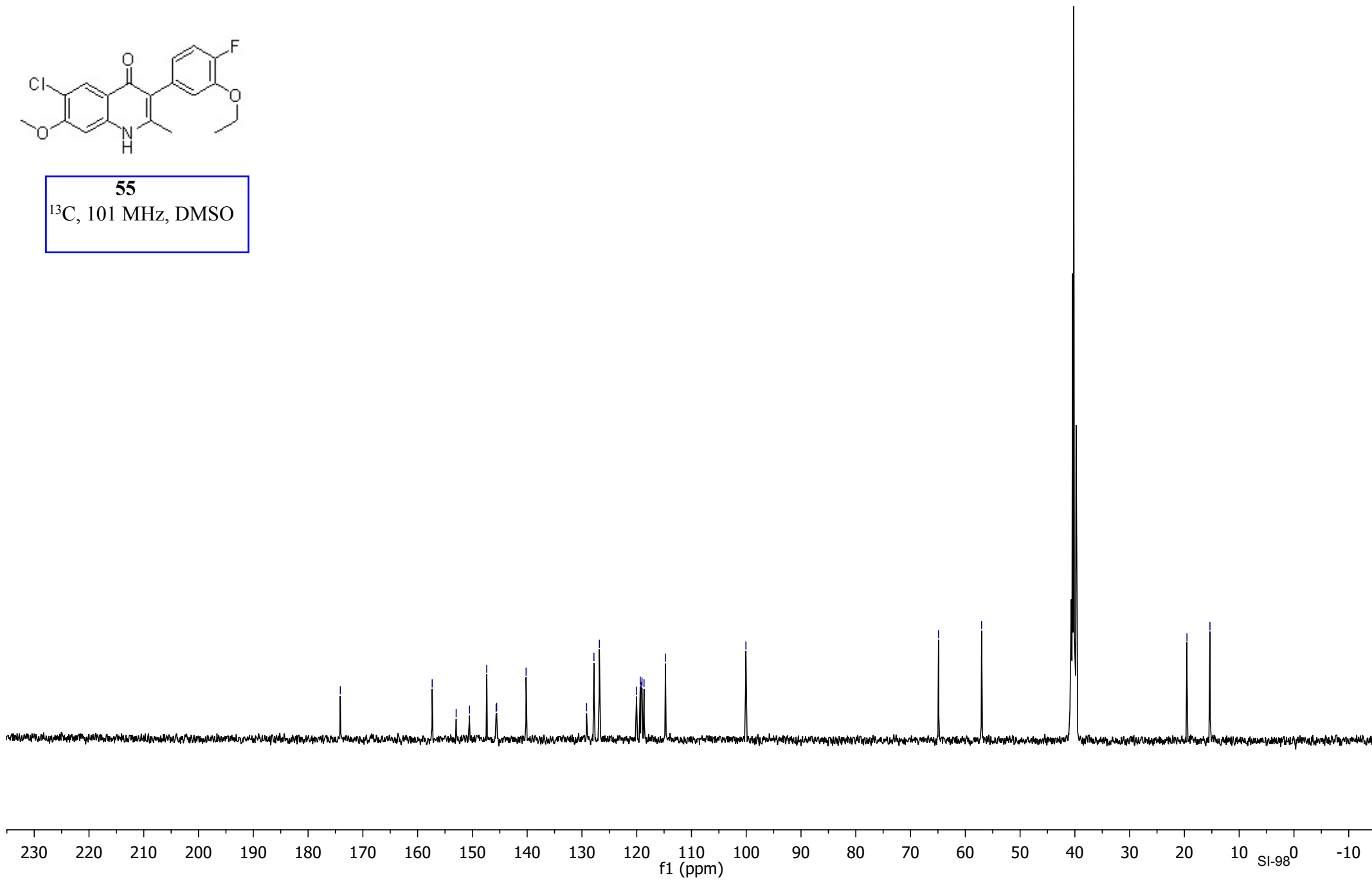
—100.06

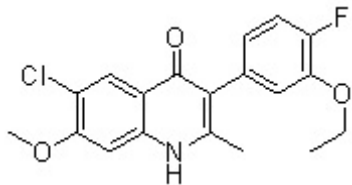
—64.90

—57.03

—19.54

—15.33

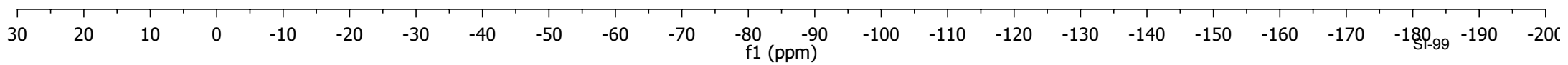


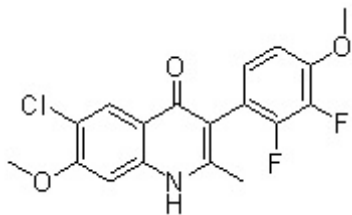


55

¹⁹F, 376 MHz, DMSO

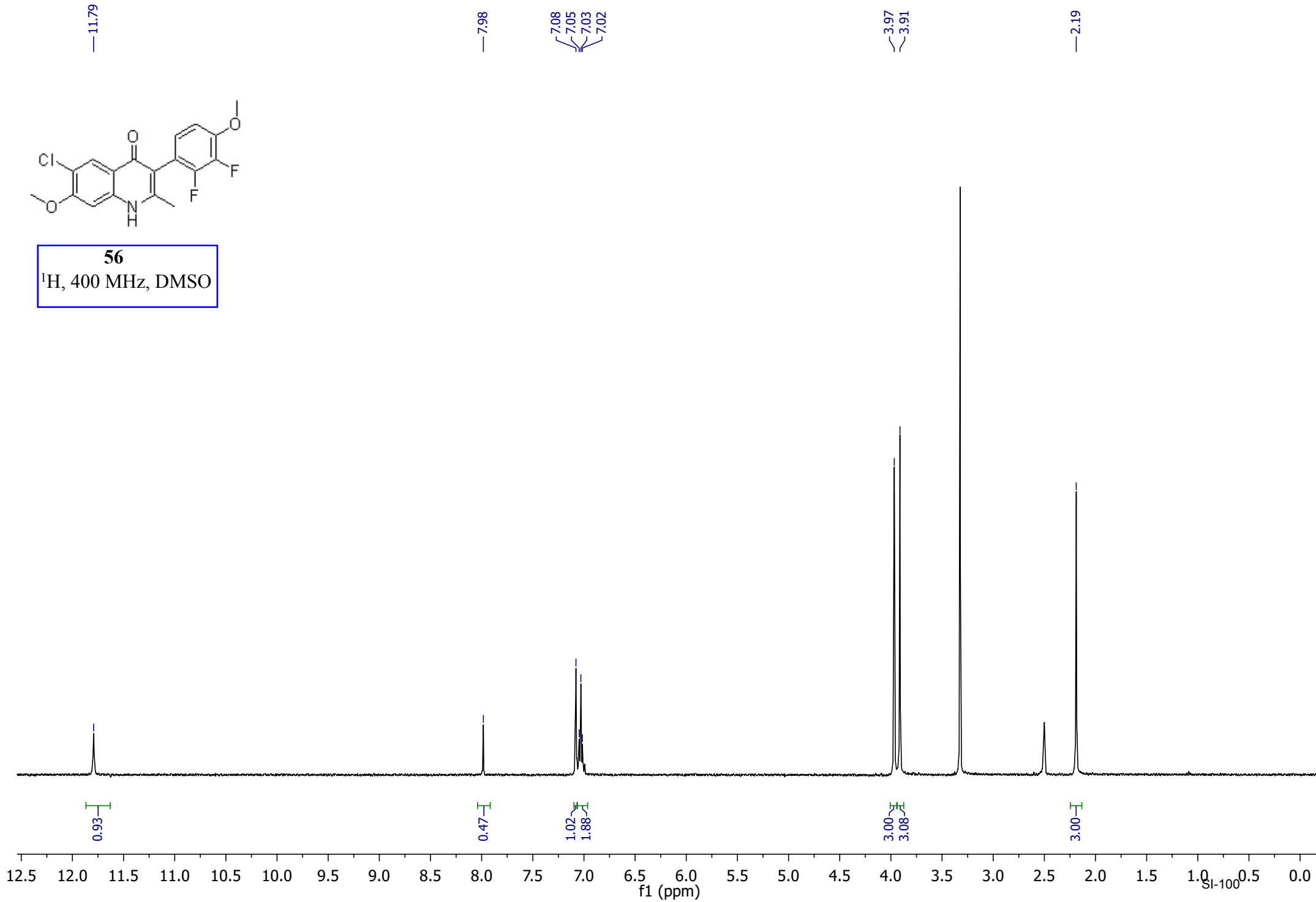
— -136.21

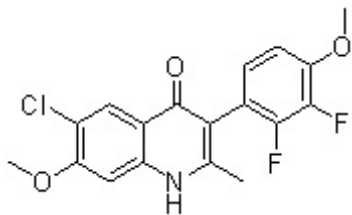




56

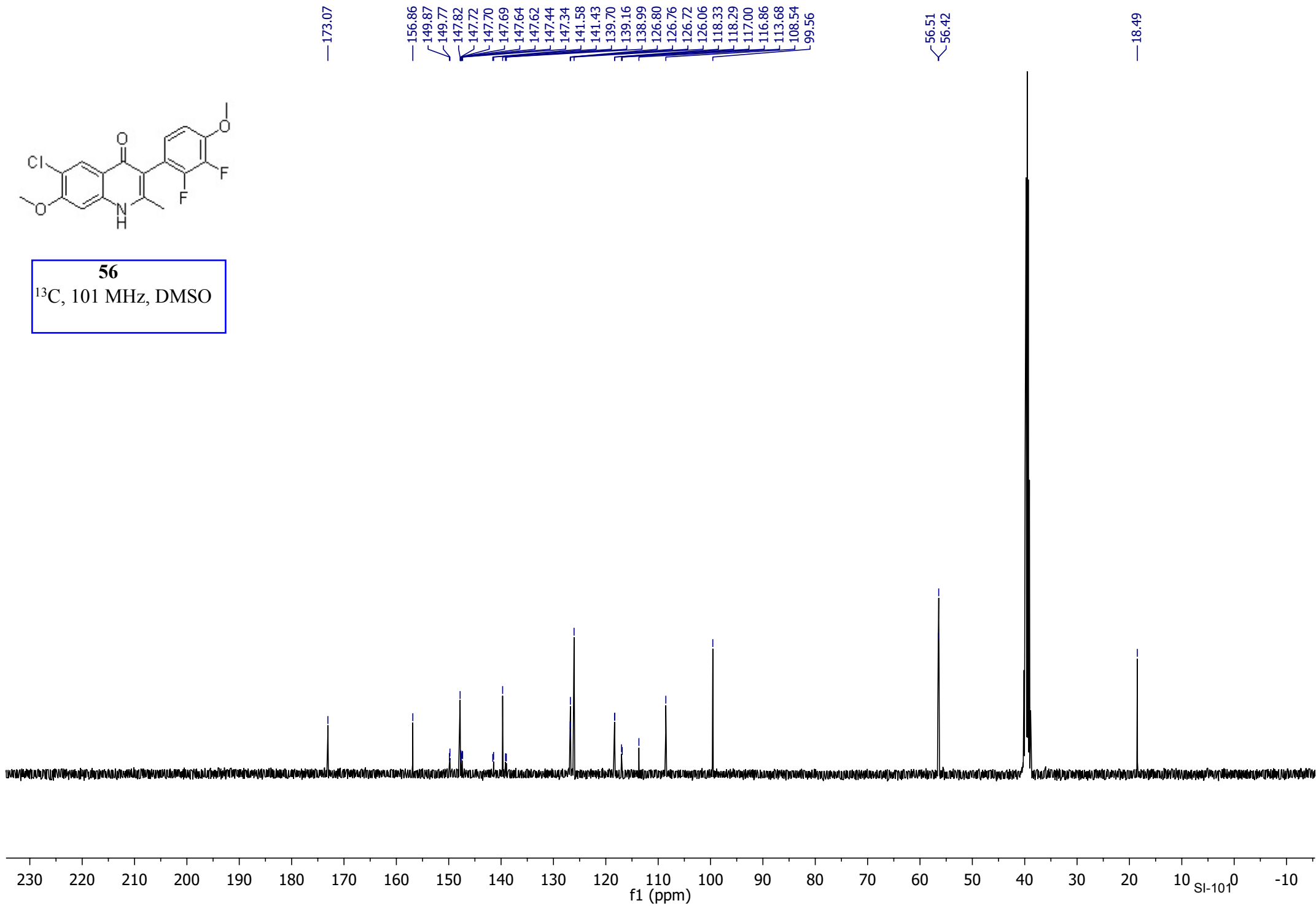
¹H, 400 MHz, DMSO

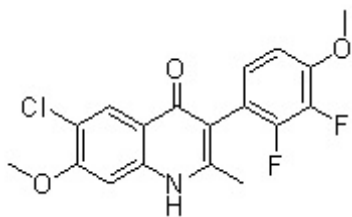




56

^{13}C , 101 MHz, DMSO





56

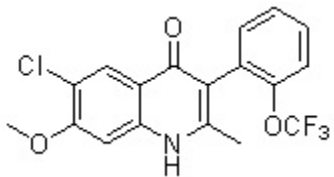
¹⁹F, 376 MHz, DMSO

— -137.32

— -161.39



20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm) St-102



57

¹H, 400 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

1.03

1.00

4.02

1.07

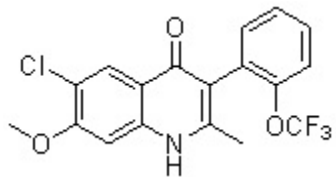
1.17

3.15

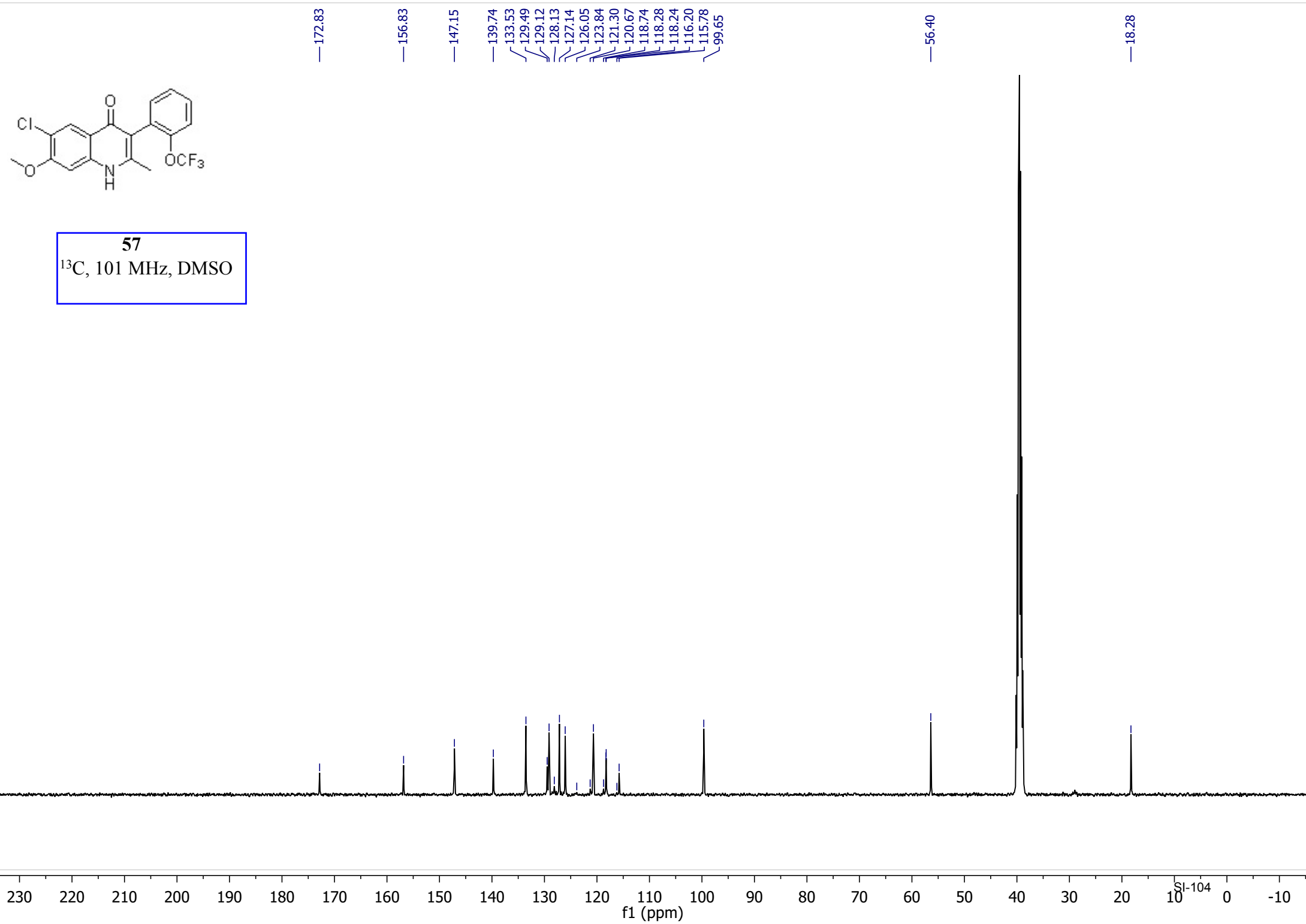
3.01

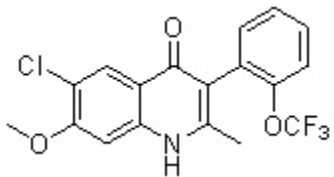
SI-103

f1 (ppm)



57
¹³C, 101 MHz, DMSO

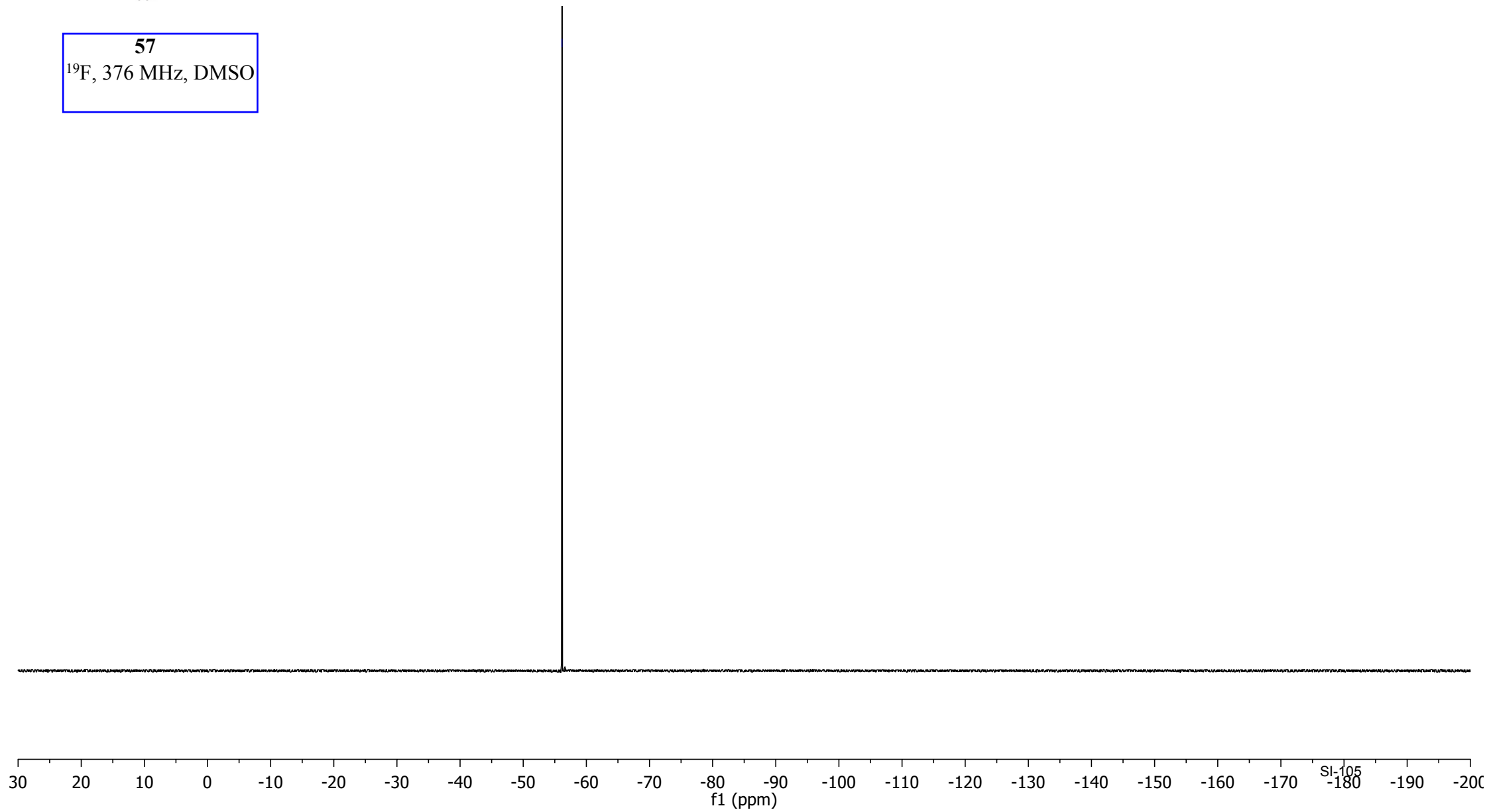


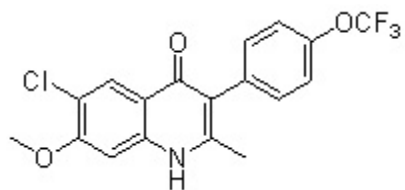


57

^{19}F , 376 MHz, DMSO

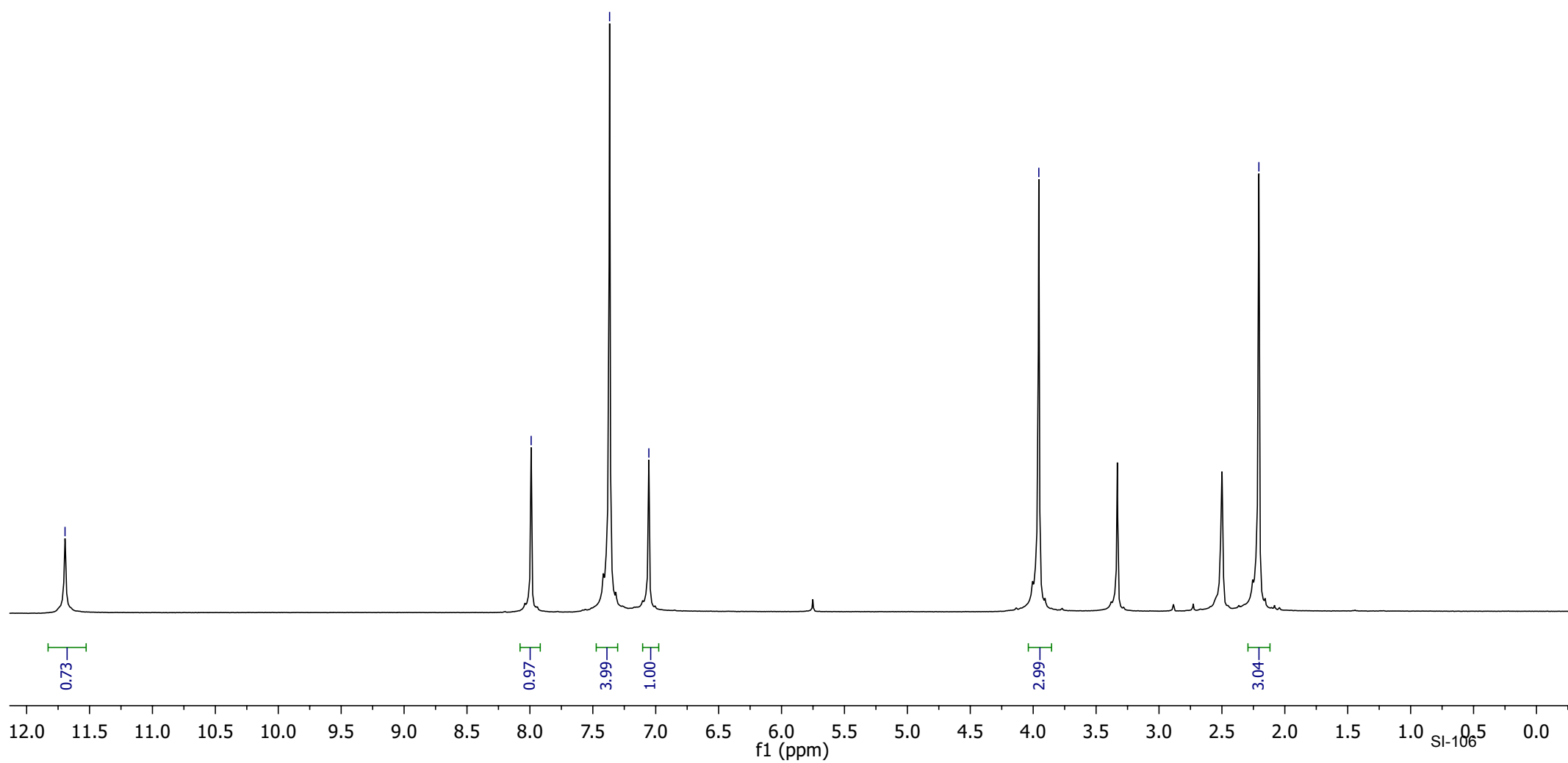
—56.14

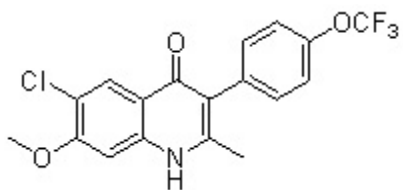




58

¹H, 400 MHz, DMSO





58
 ^{13}C , 101 MHz, DMSO

—173.31

—156.75

146.97
146.71

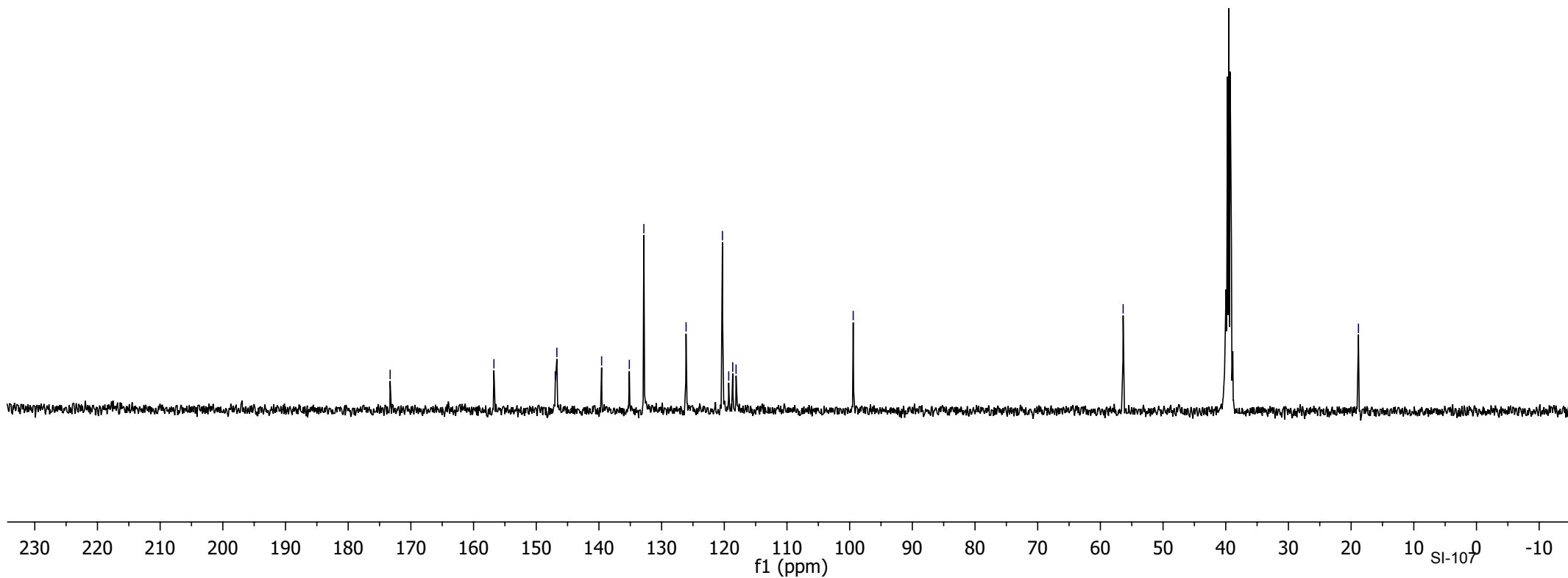
139.57
135.15
132.83

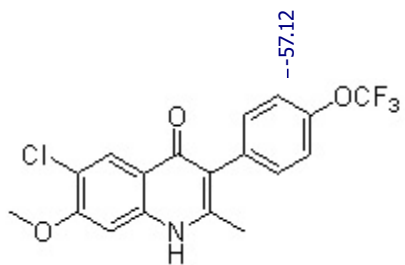
126.10
120.30
119.29
118.65
118.12

—99.43

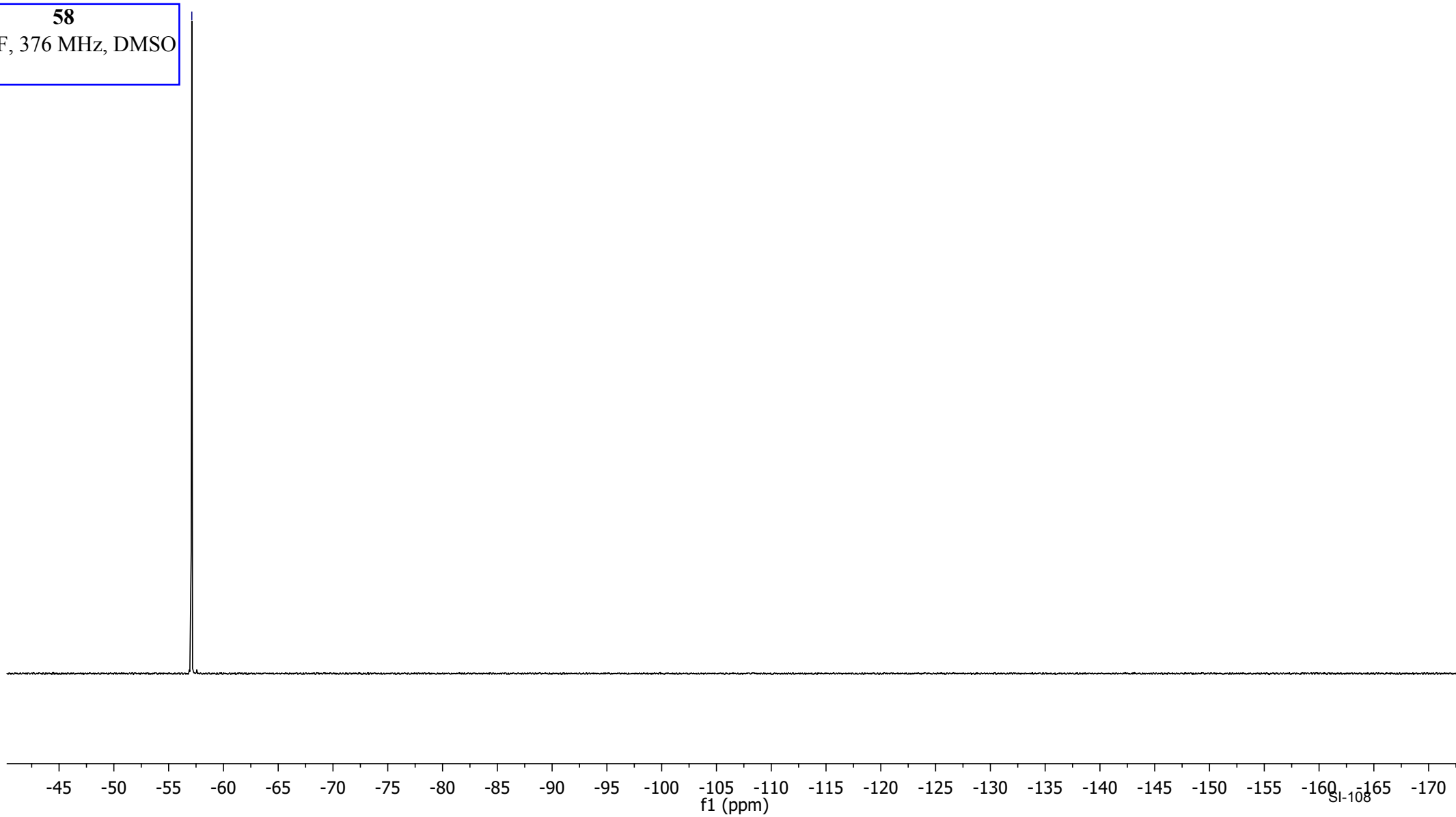
—56.37

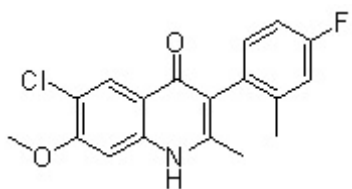
—18.83





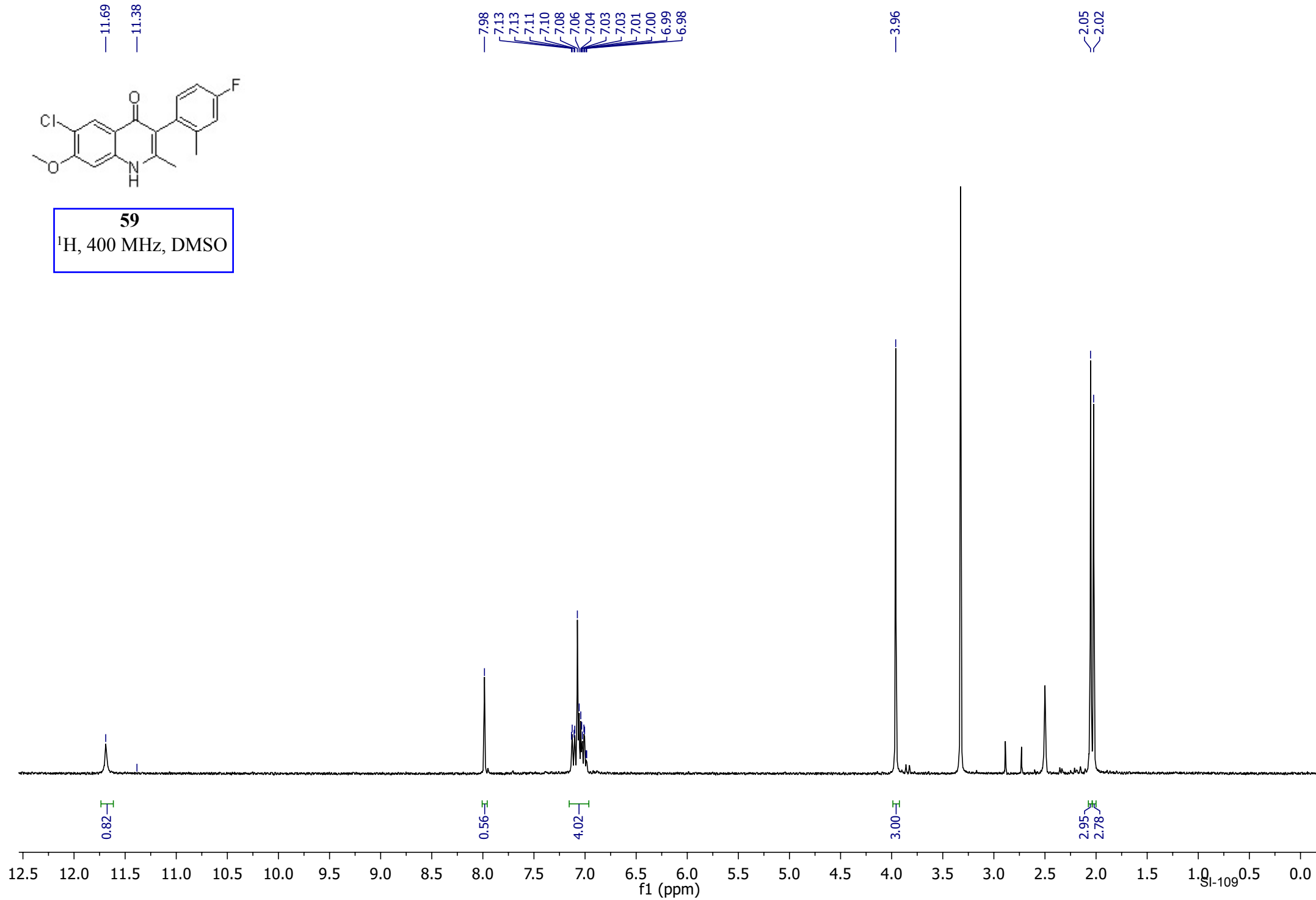
58
 ^{19}F , 376 MHz, DMSO

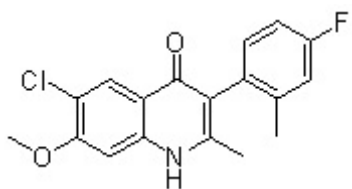




59

¹H, 400 MHz, DMSO



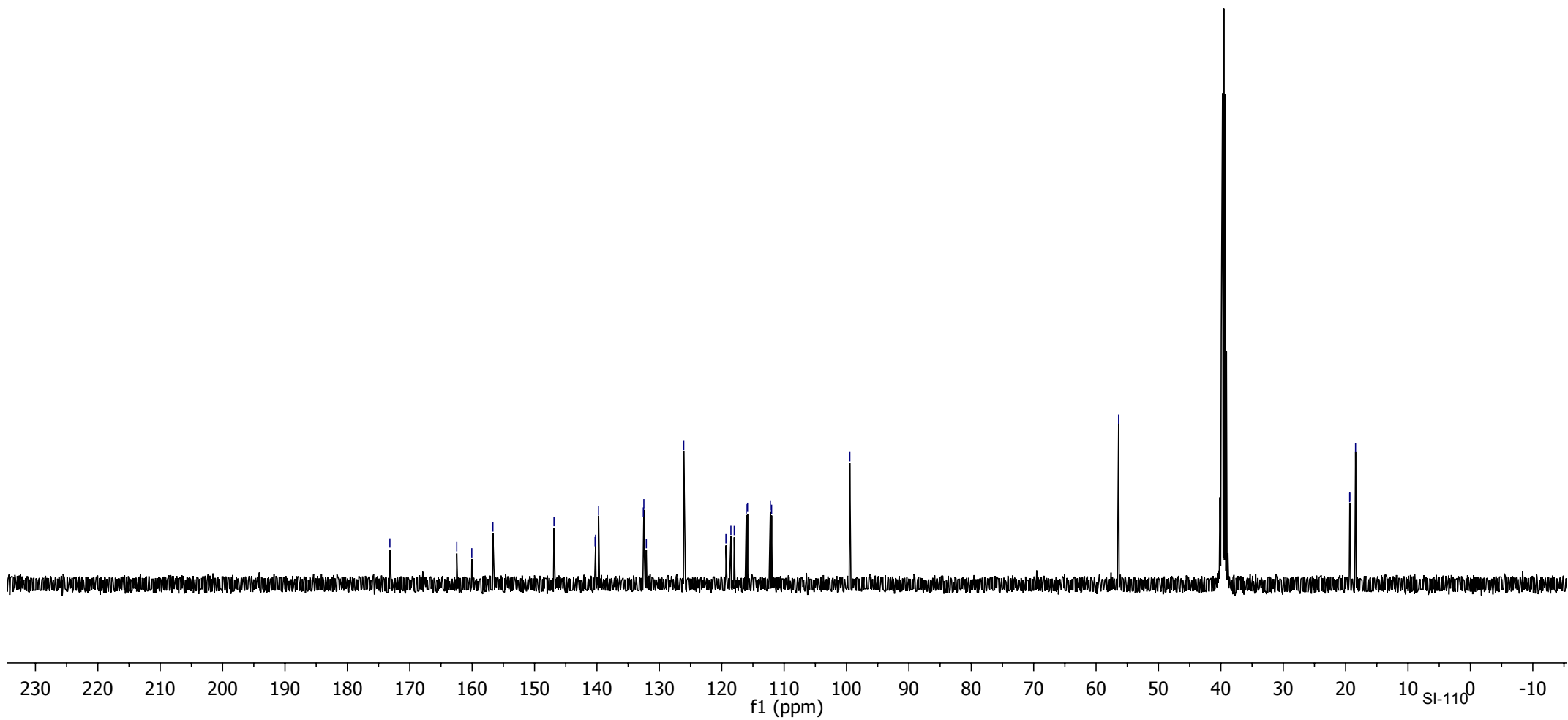


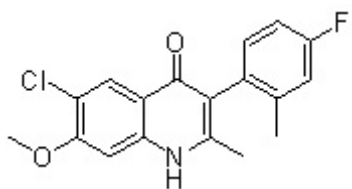
59
¹³C, 101 MHz, DMSO

- 173.19
- 162.47
- 160.06
- 156.67
- 146.88
- 140.30
- 140.22
- 139.73
- 132.56
- 132.48
- 132.09
- 126.09
- 119.33
- 118.53
- 118.00
- 116.07
- 115.86
- 112.21
- 112.00
- 99.47

56.38

- 19.35
- 19.33
- 18.41

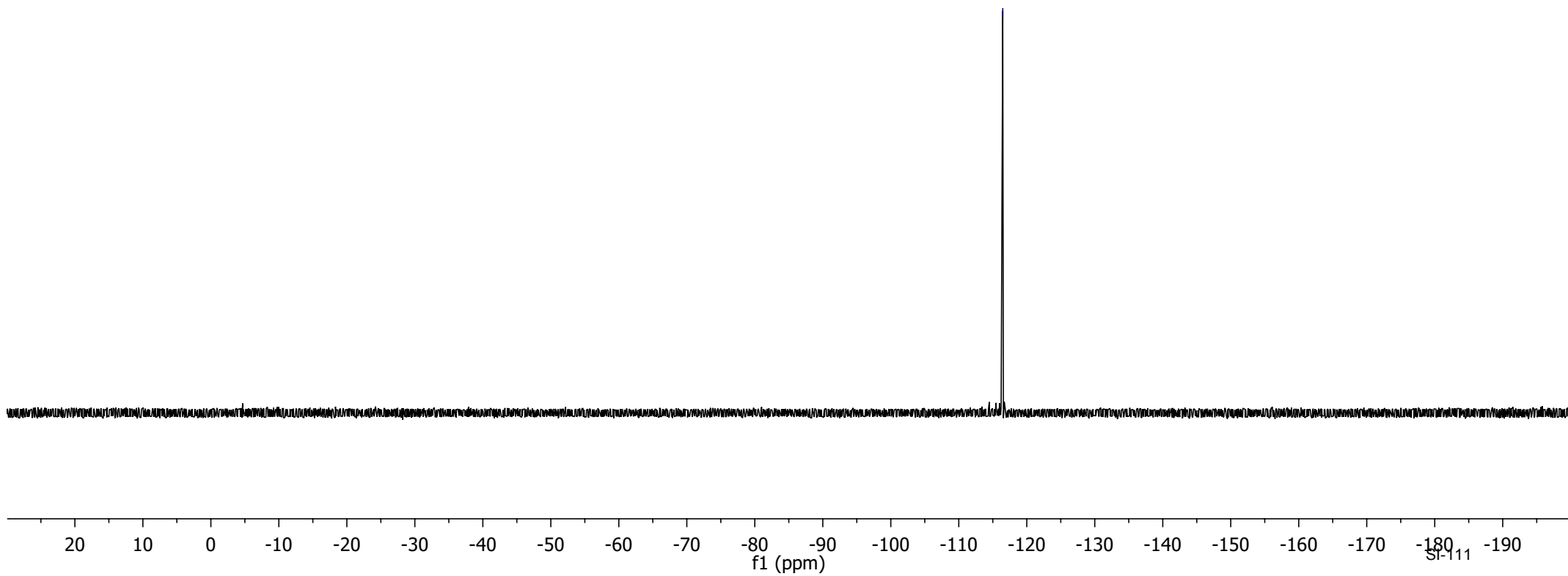


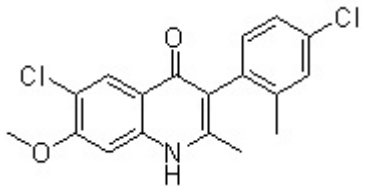


59

^{19}F , 376 MHz, DMSO

— -116.47





60
¹H, 400 MHz, DMSO

11.71

7.98

7.35

7.26

7.24

7.08

7.05

3.96

2.06

2.02

1.00

1.03

0.95

2.14

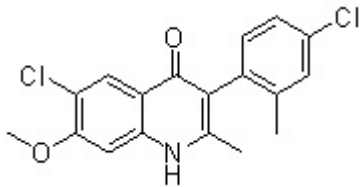
2.02

3.32

6.13

SI-112

f1 (ppm)



60
¹³C, 101 MHz, DMSO

—173.71

—157.40

—147.46

140.82

140.42

135.62

133.30

132.18

129.84

126.76

126.09

119.83

119.19

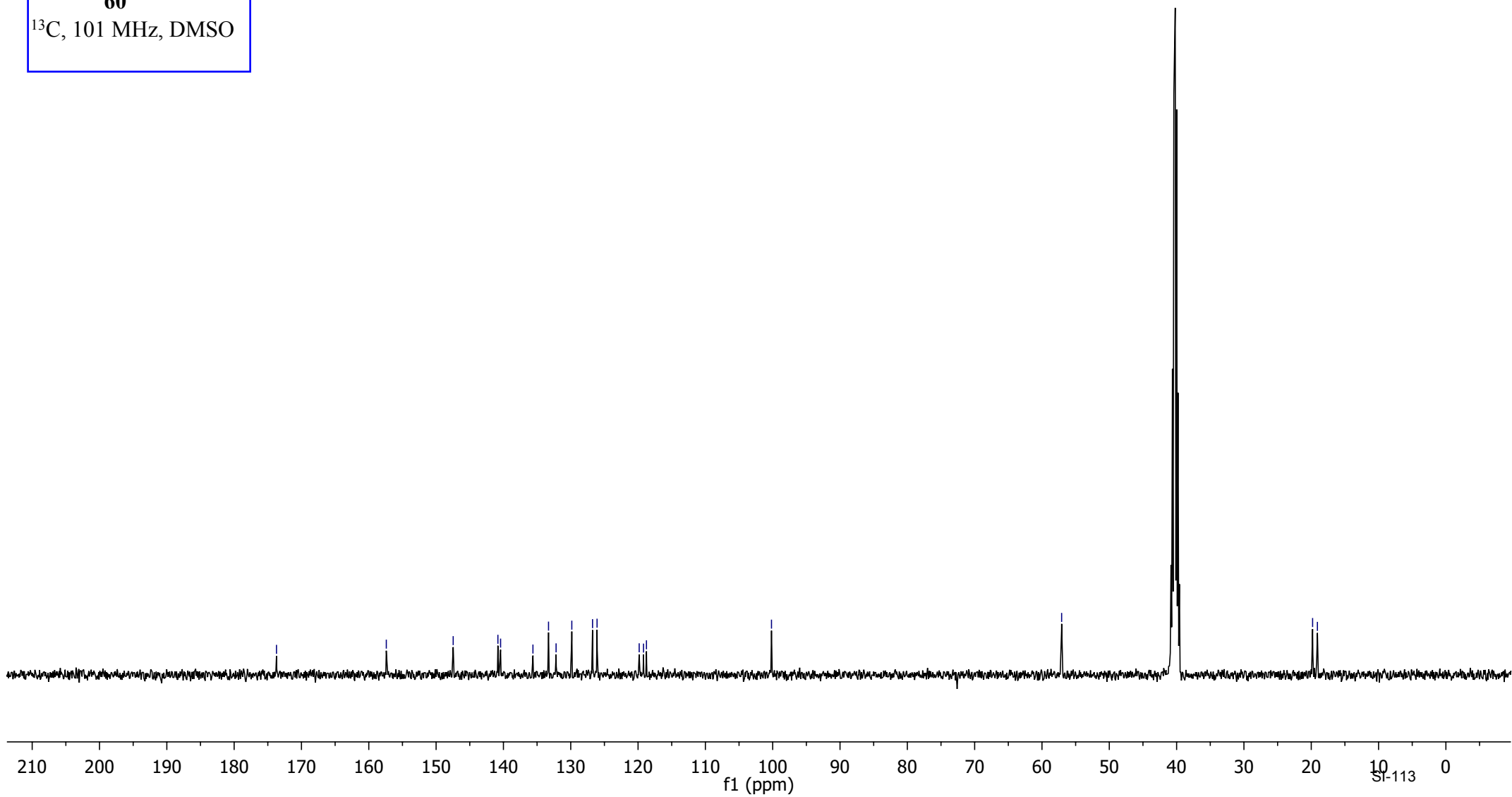
118.75

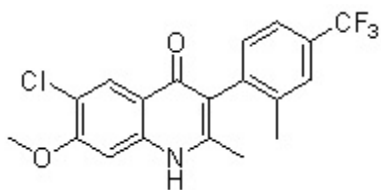
—100.18

—57.08

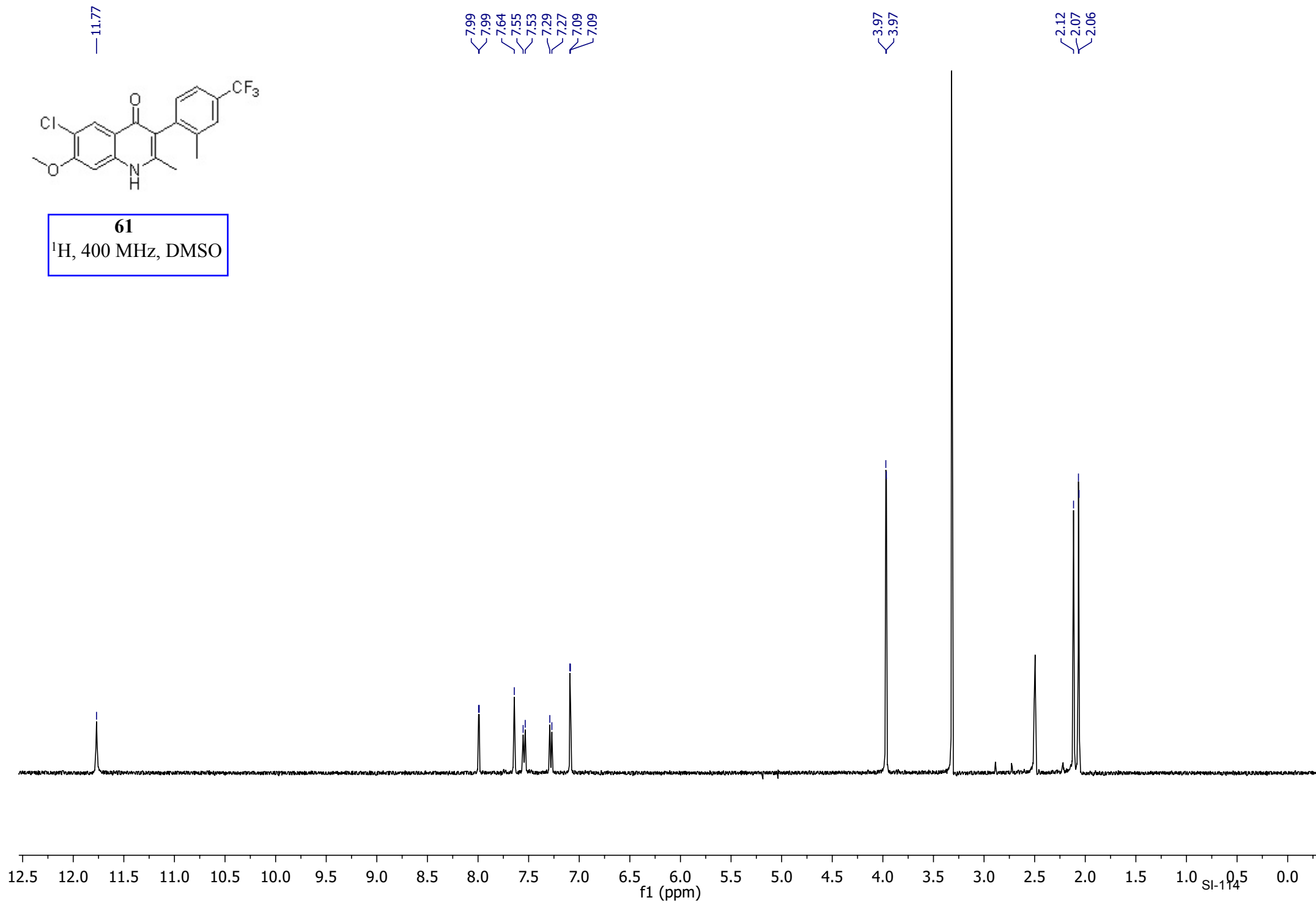
19.80

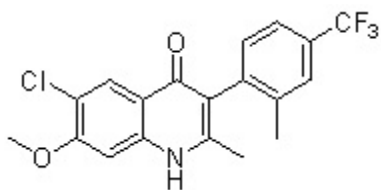
19.08



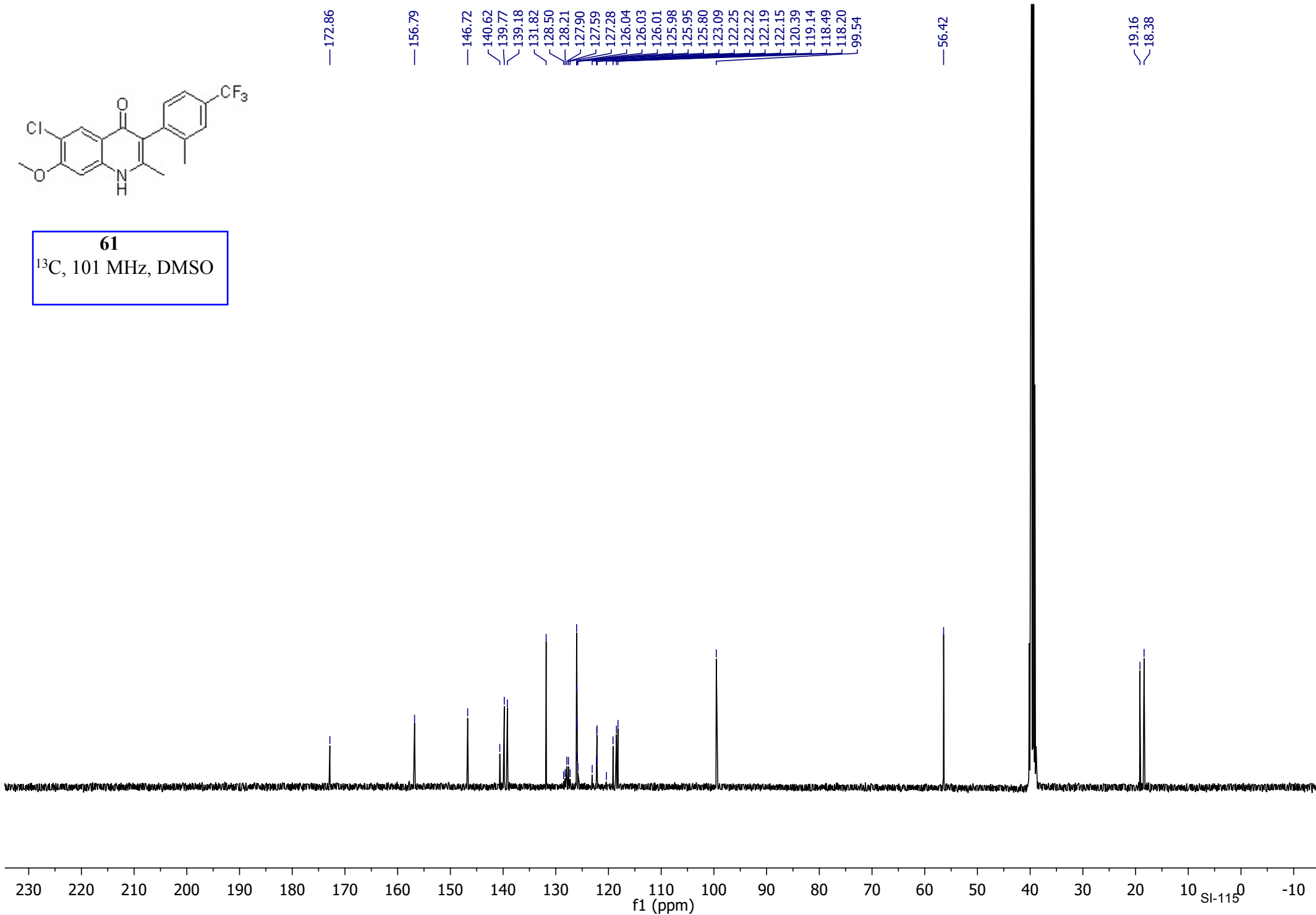


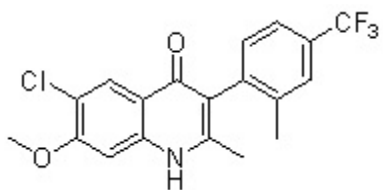
61
¹H, 400 MHz, DMSO





61
 ^{13}C , 101 MHz, DMSO

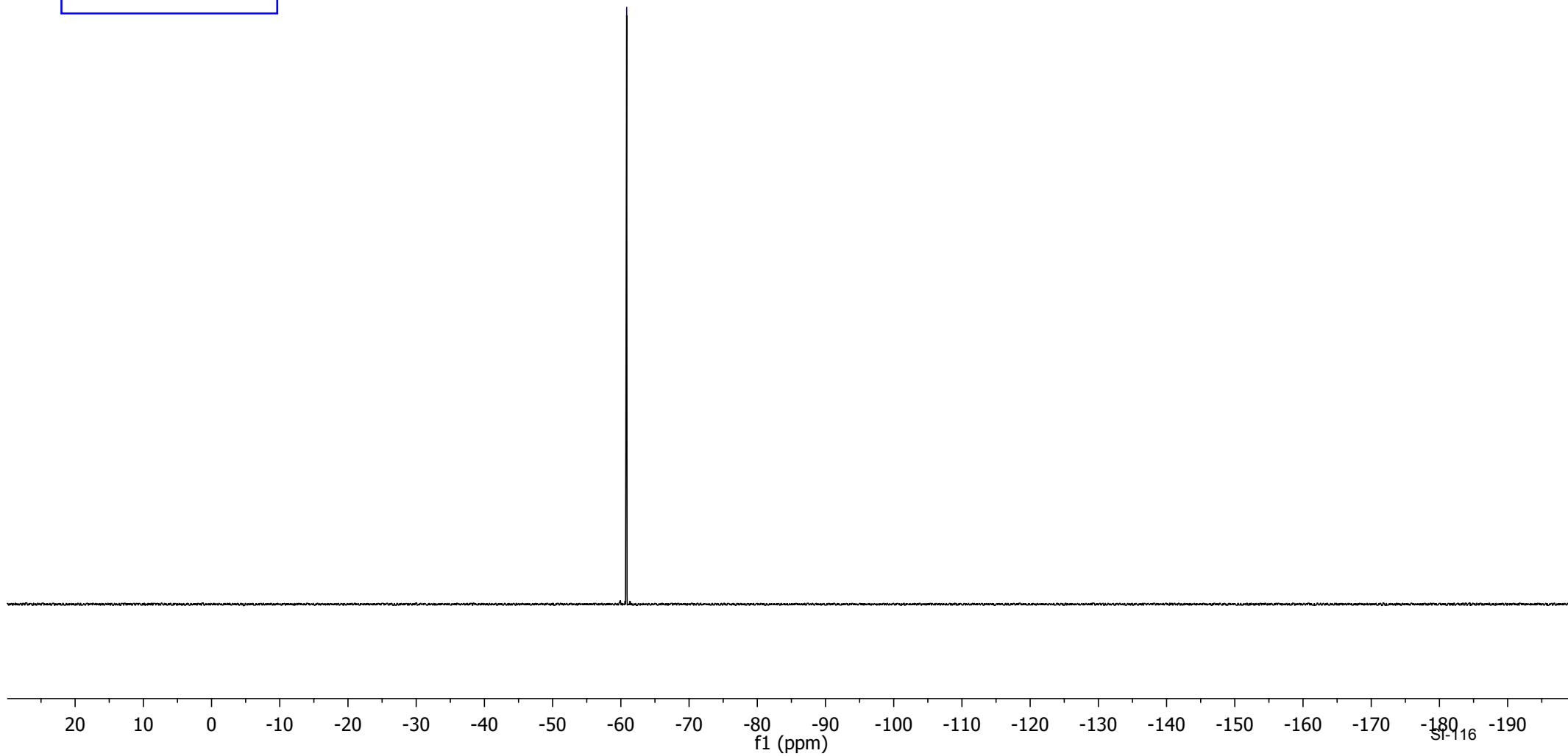


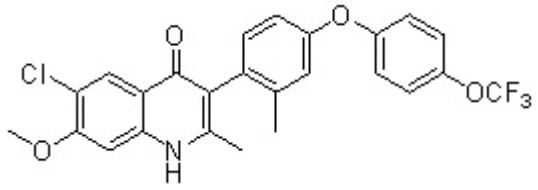


61

¹⁹F, 376 MHz, DMSO

—60.86





62

¹H, 400 MHz, DMSO

11.68

7.99
7.42
7.39
7.15
7.13
7.08
7.06
6.99
6.88
6.87

3.96

2.09
2.01

0.91

0.71

1.78

1.87

1.85

0.87

0.91

3.00

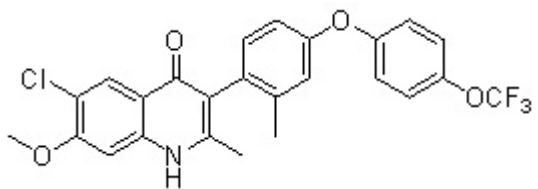
2.97

2.99

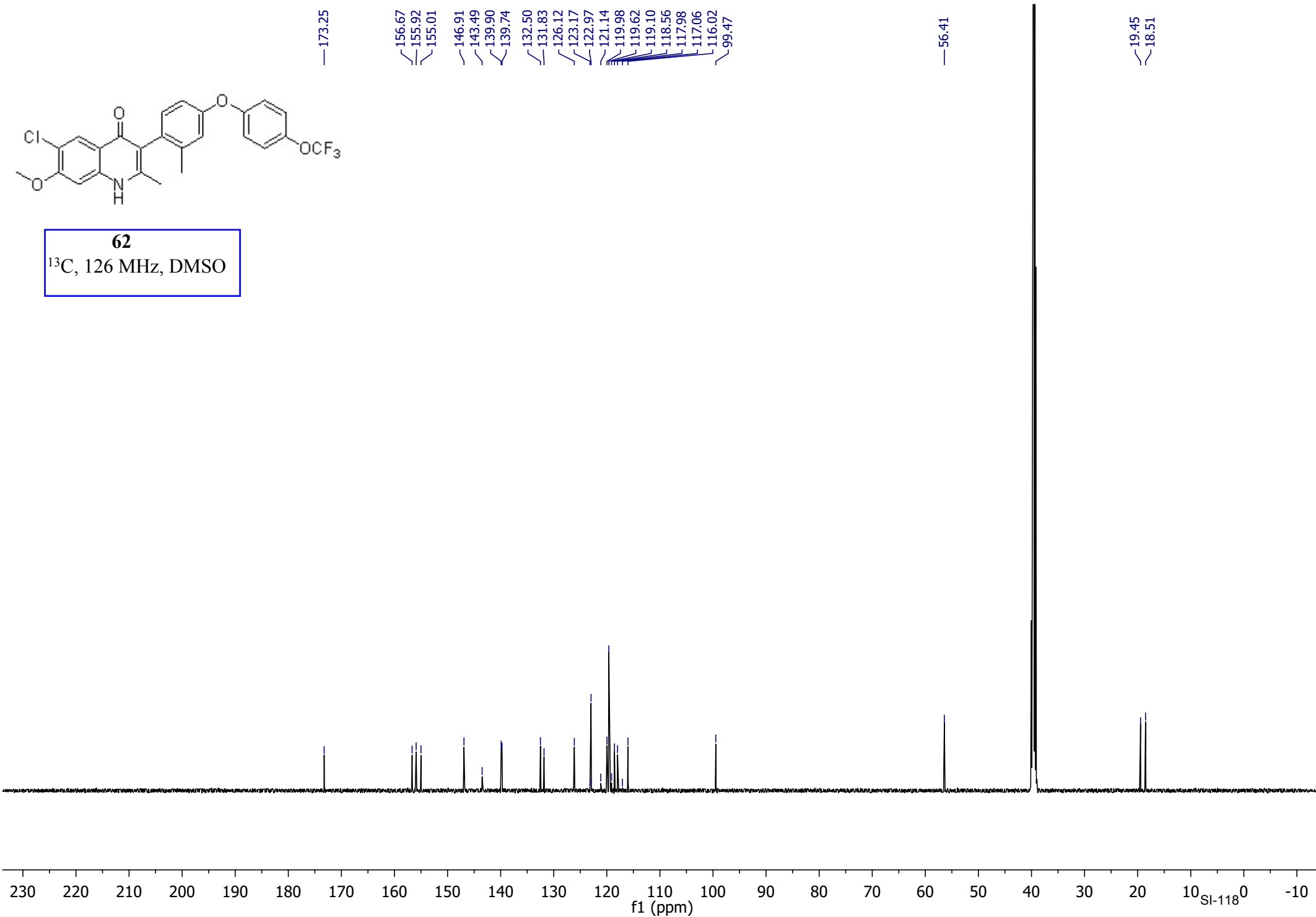
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

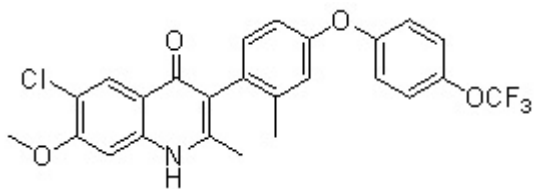
f1 (ppm)

SI-117



62
¹³C, 126 MHz, DMSO

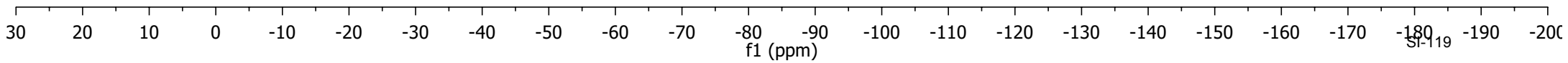


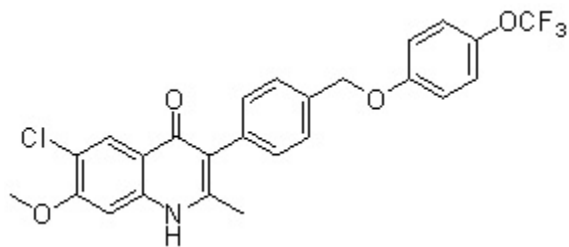


62

^{19}F , 376 MHz, DMSO

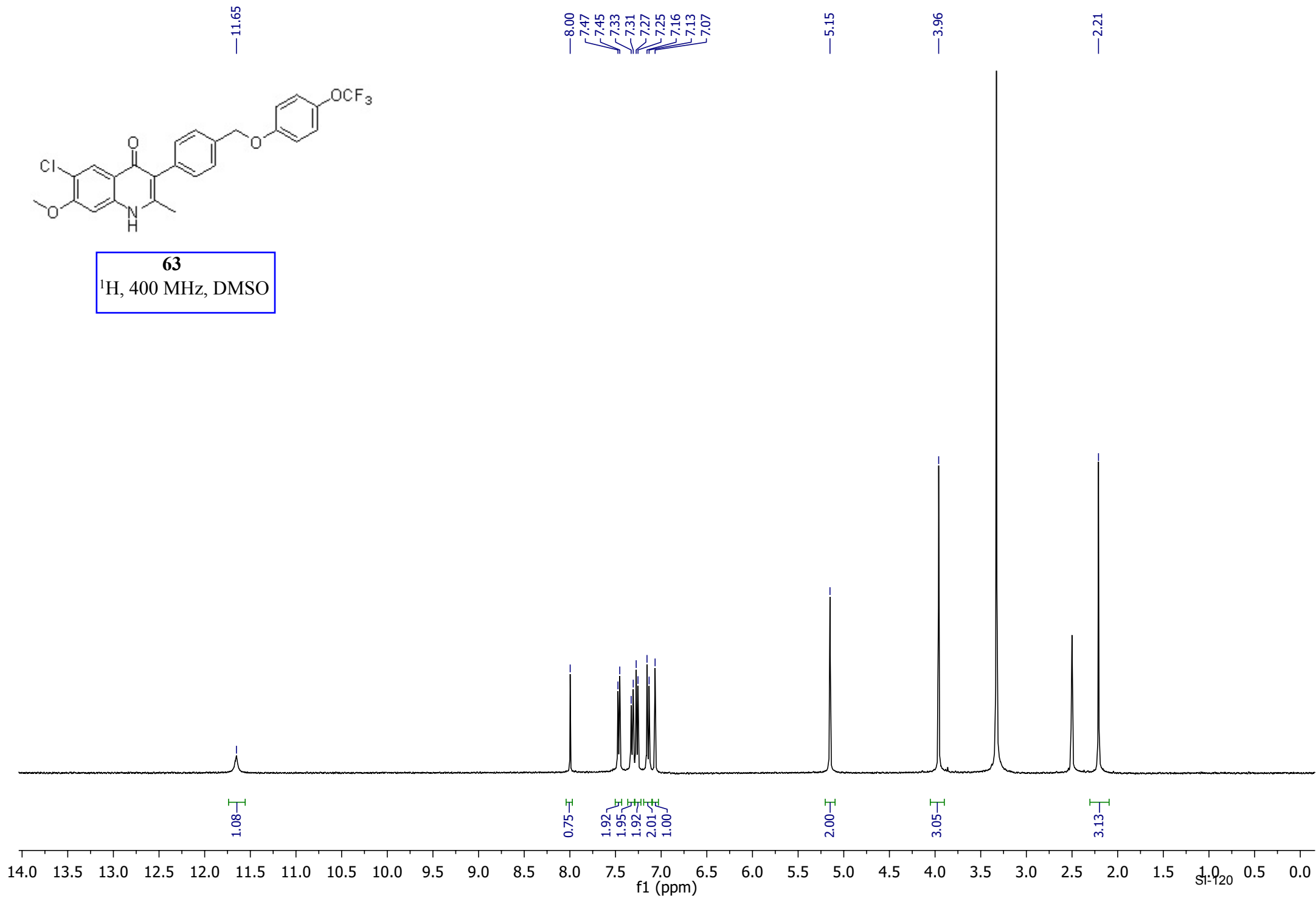
—57.20

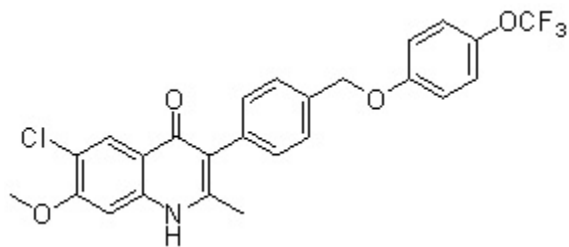




63

¹H, 400 MHz, DMSO





63

¹³C, 126 MHz, DMSO

—173.48

157.33

156.69

146.54

141.81

139.63

135.59

134.81

131.06

127.36

126.18

123.23

122.56

121.20

120.38

119.17

118.77

117.98

117.14

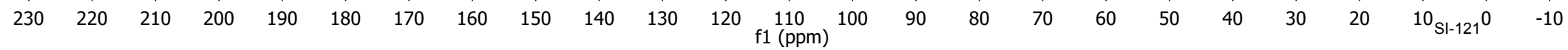
115.95

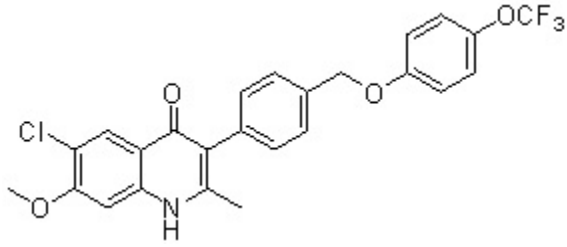
—99.46

—69.71

—56.39

—18.91

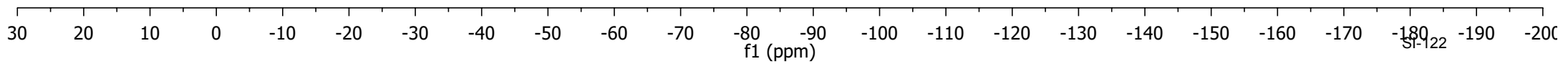


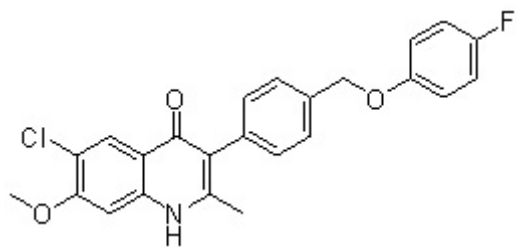


63

^{19}F , 376 MHz, DMSO

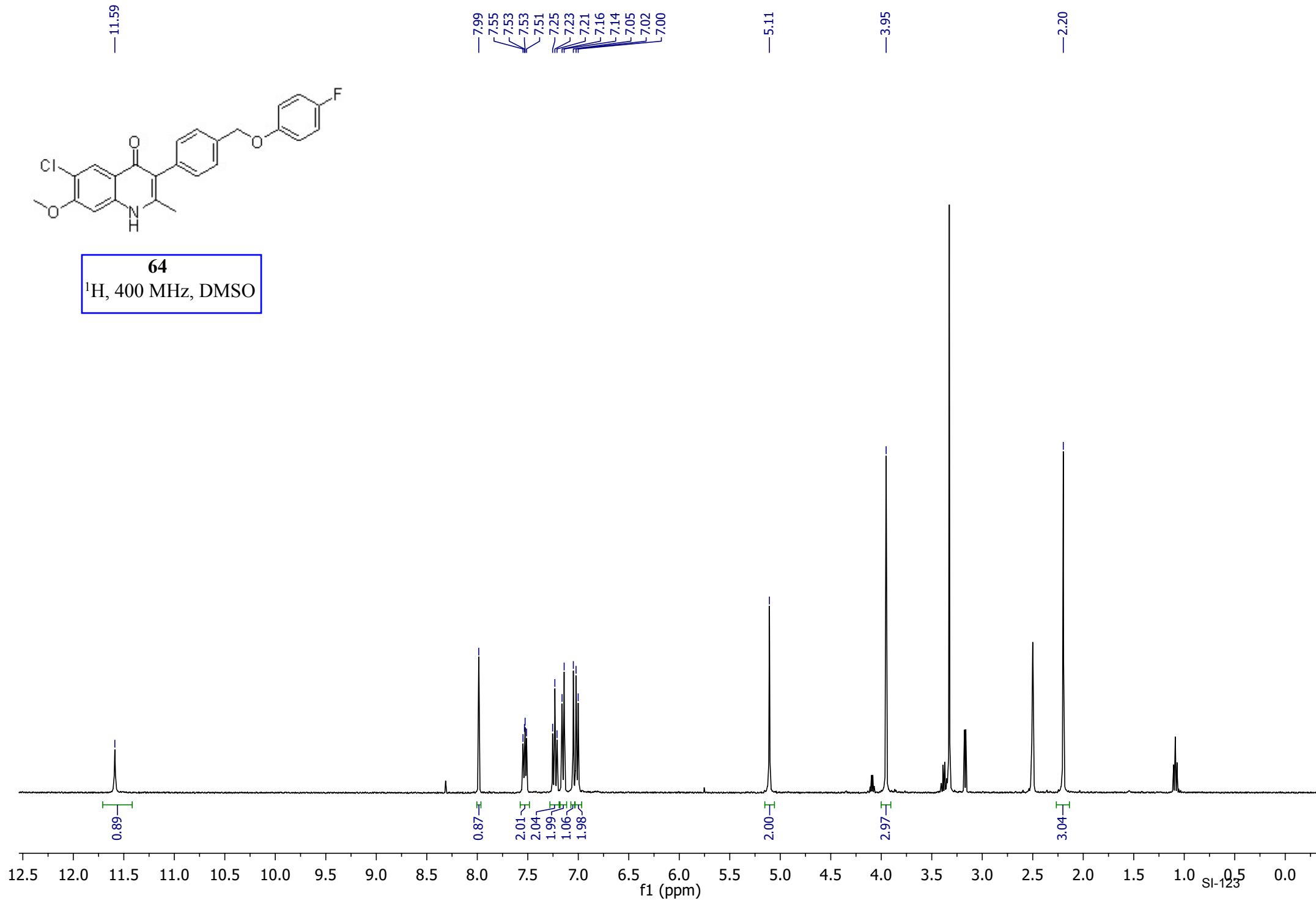
—57.30

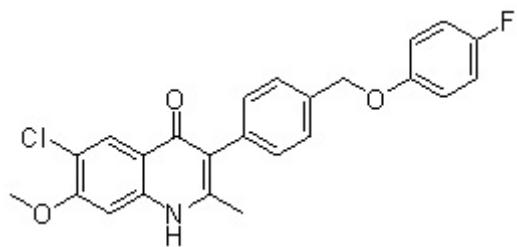




64

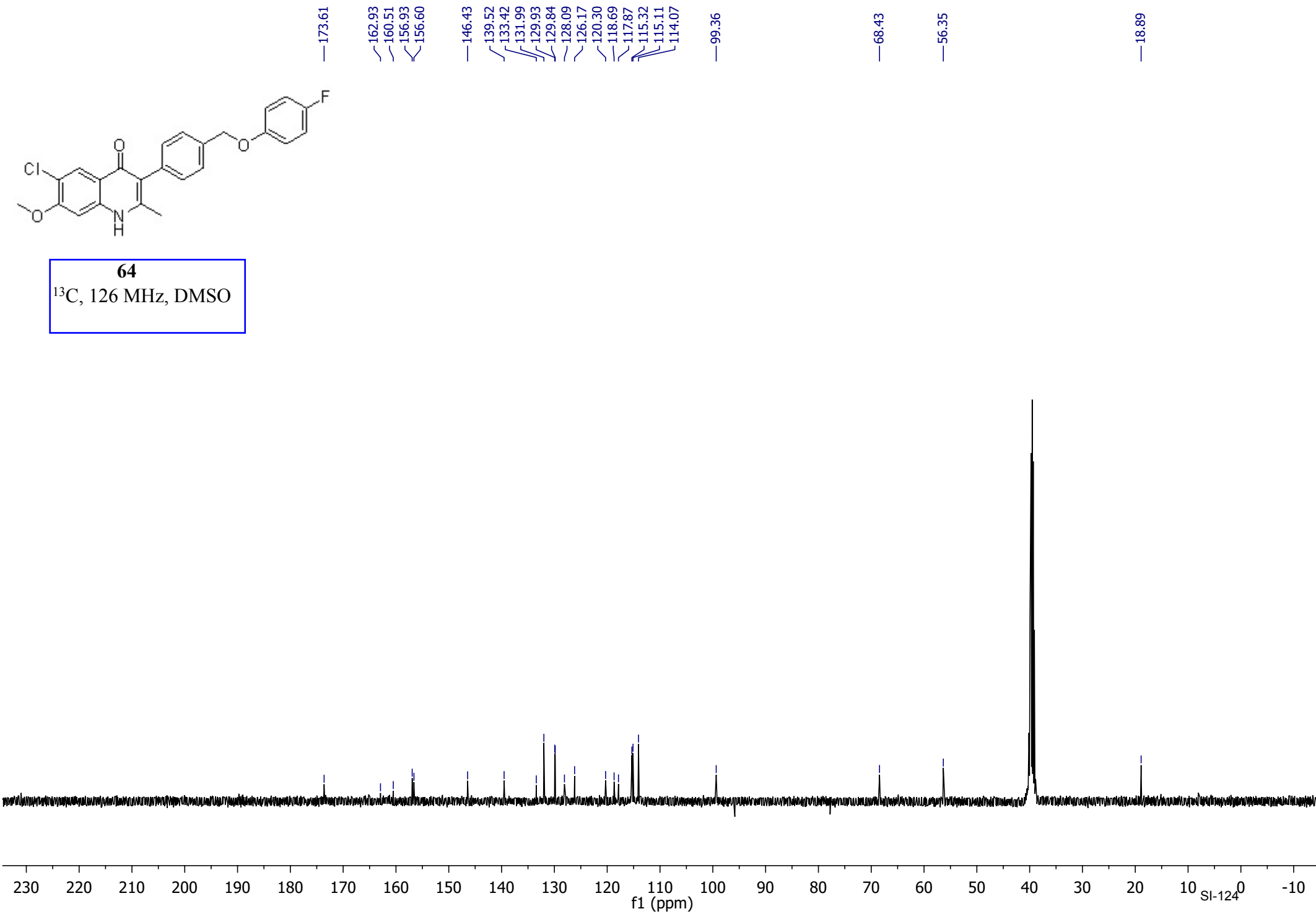
¹H, 400 MHz, DMSO

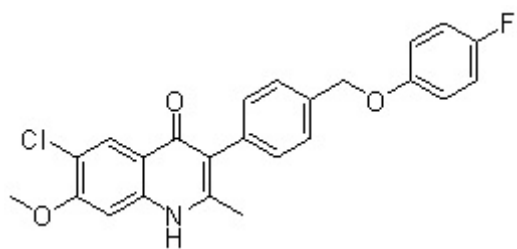




64

^{13}C , 126 MHz, DMSO

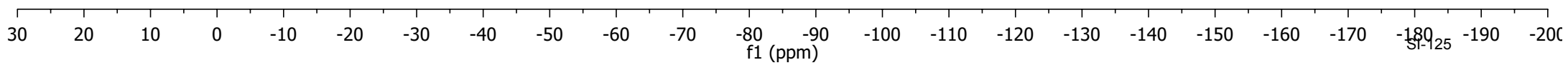


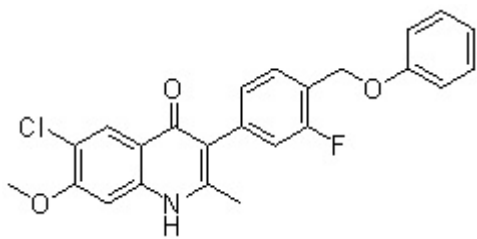


64

^{19}F , 376 MHz, DMSO

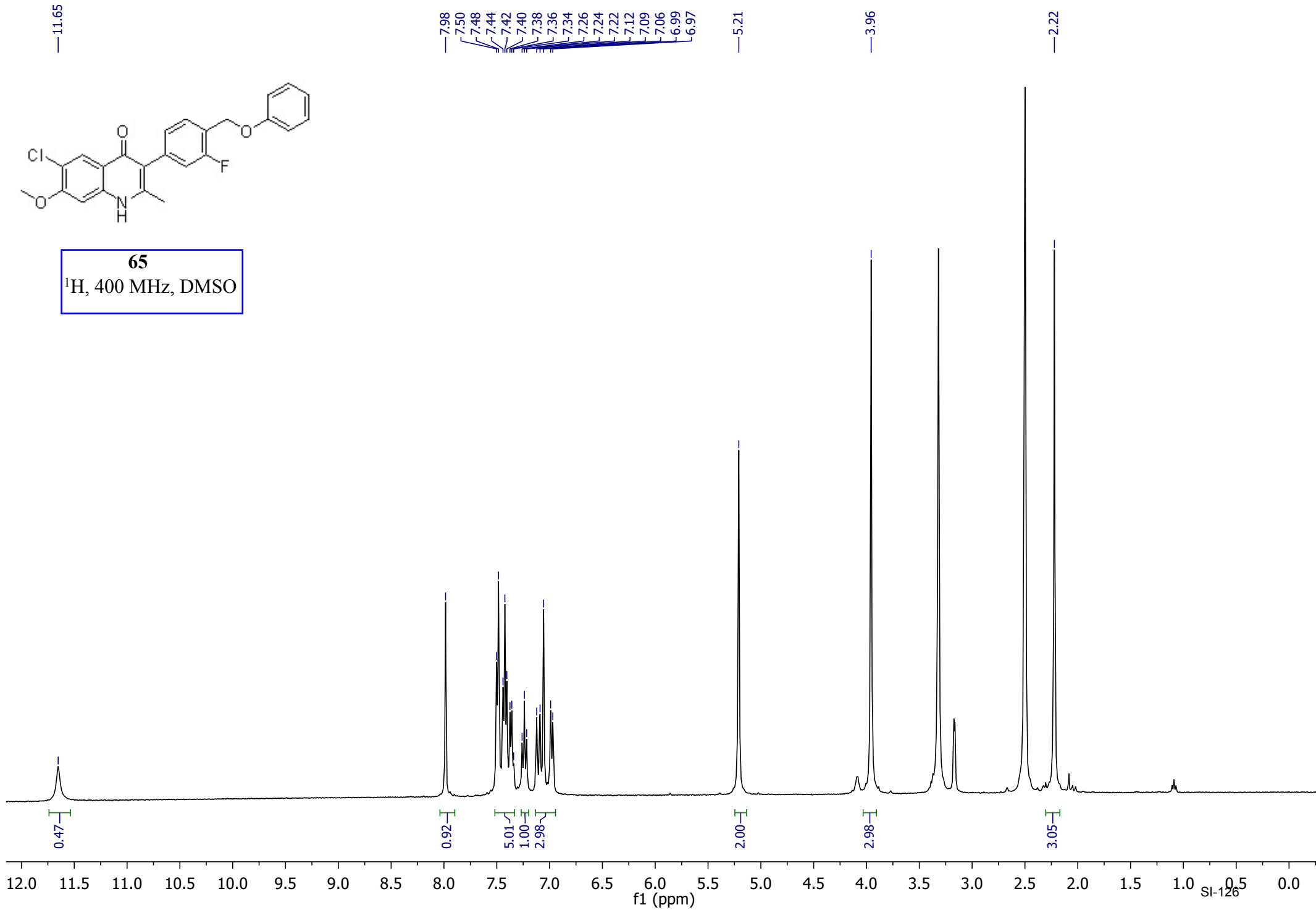
— -114,58

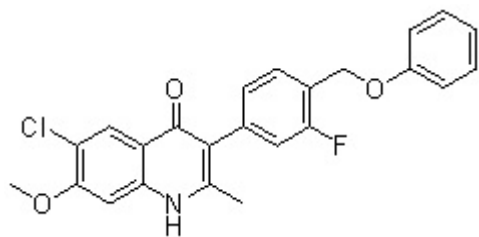




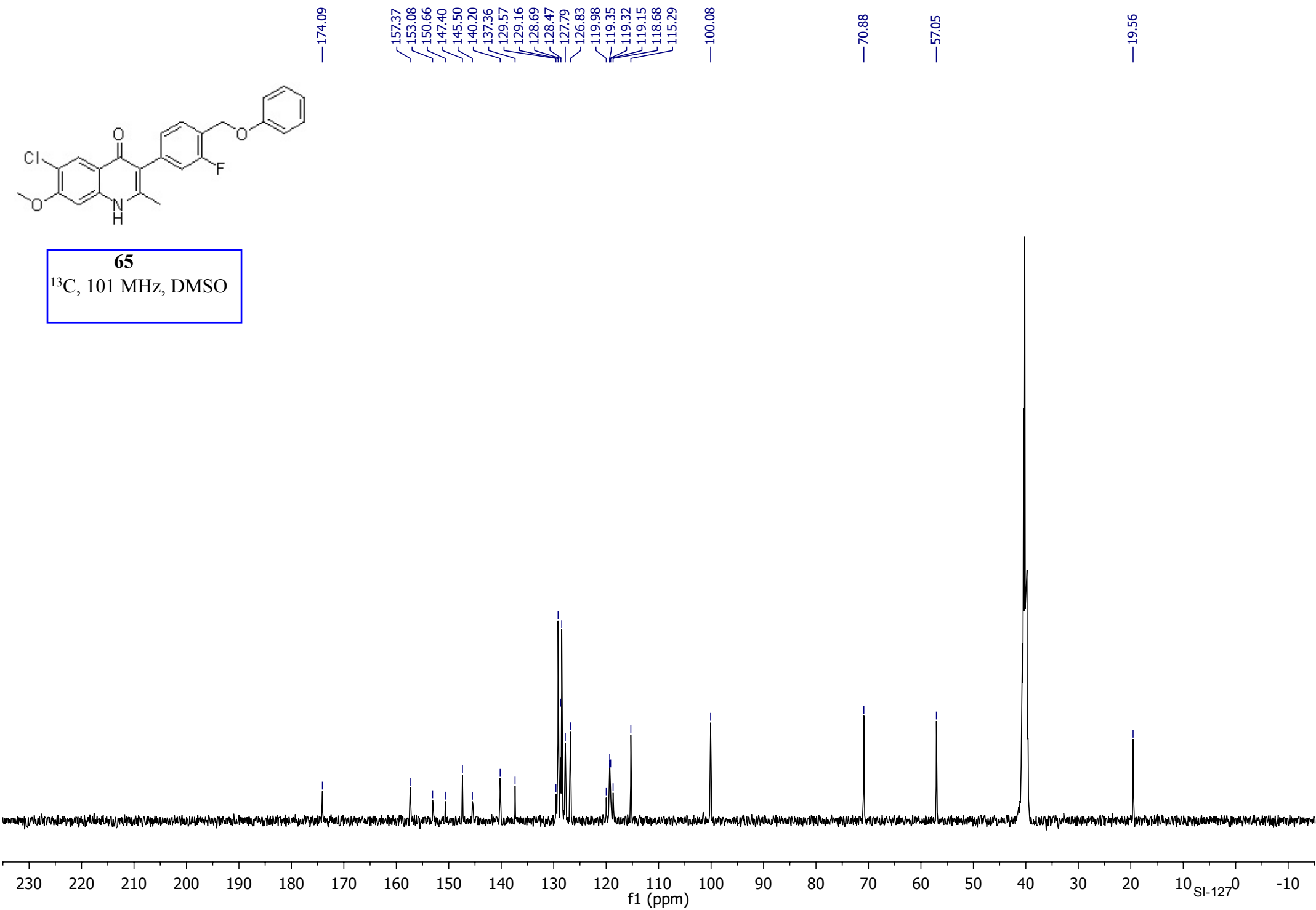
65

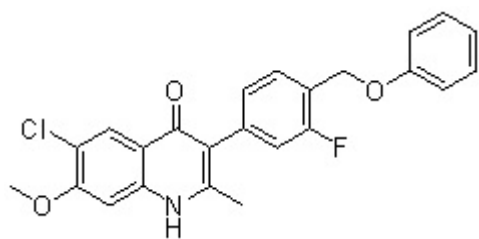
¹H, 400 MHz, DMSO





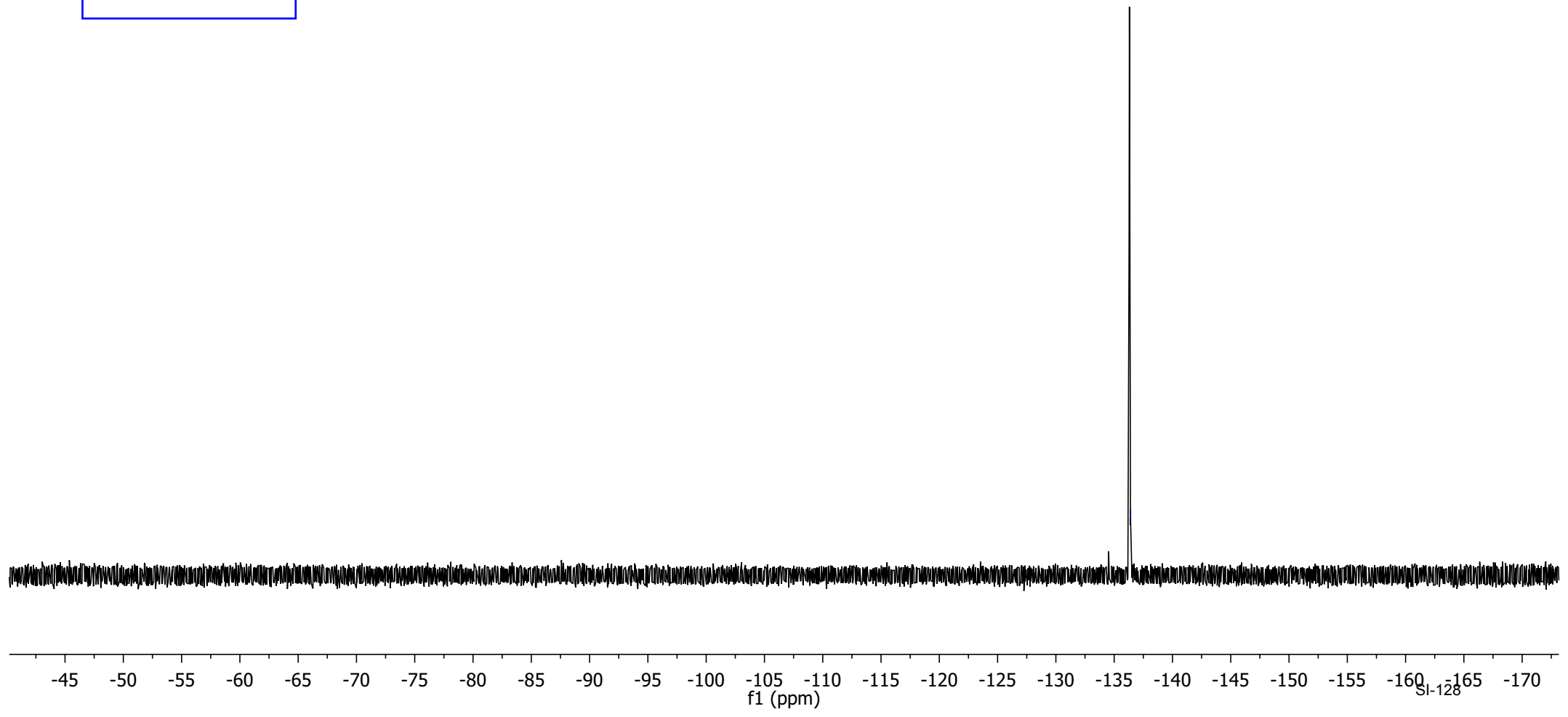
65
¹³C, 101 MHz, DMSO

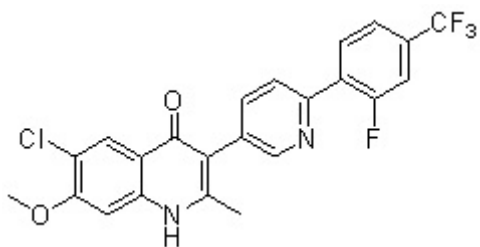




65
¹⁹F, 376 MHz, DMSO

— -136.41





66

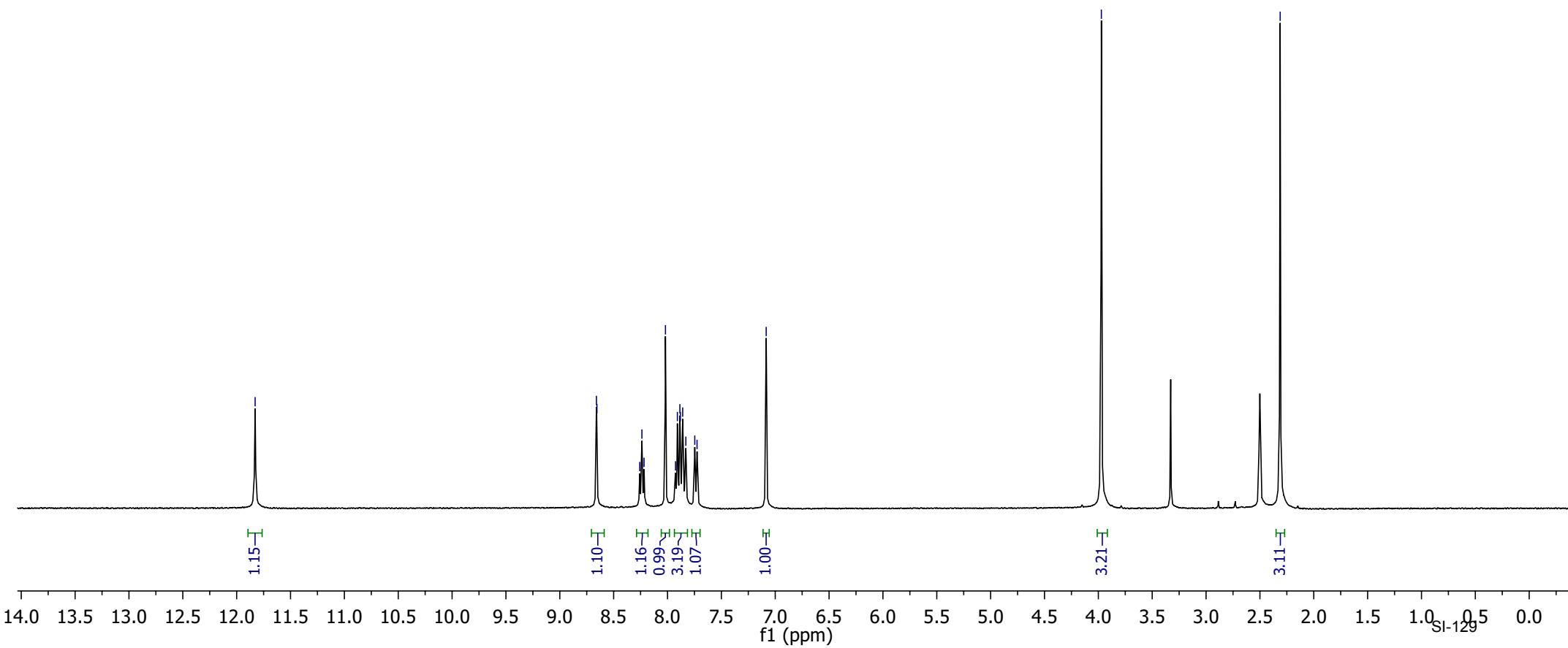
¹H, 400 MHz, DMSO

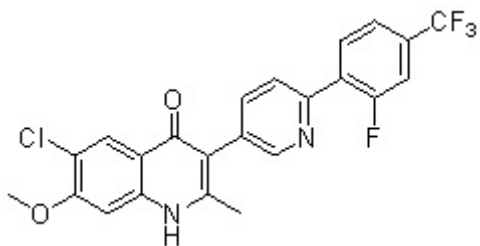
—11.83

8.66
8.66
8.26
8.24
8.22
8.02
7.93
7.91
7.89
7.88
7.86
7.83
7.75
7.73
—7.08

—3.97

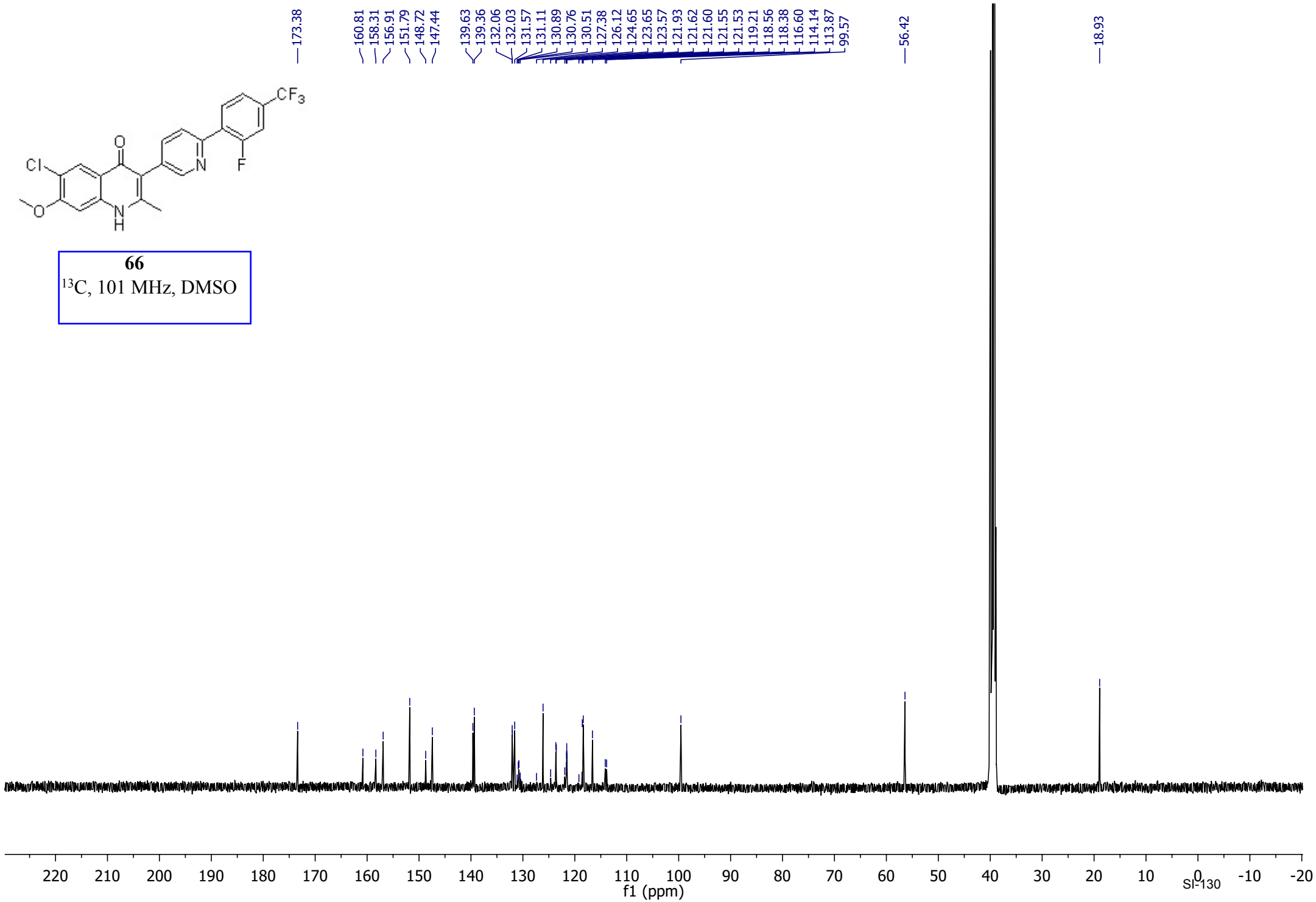
—2.31

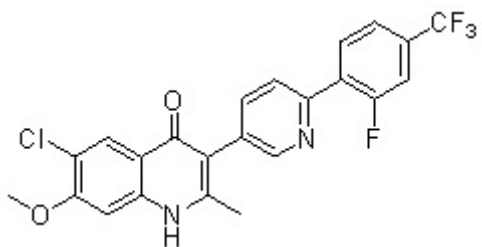




66

¹³C, 101 MHz, DMSO





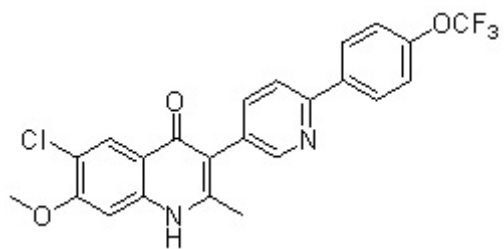
66

^{19}F , 376 MHz, DMSO

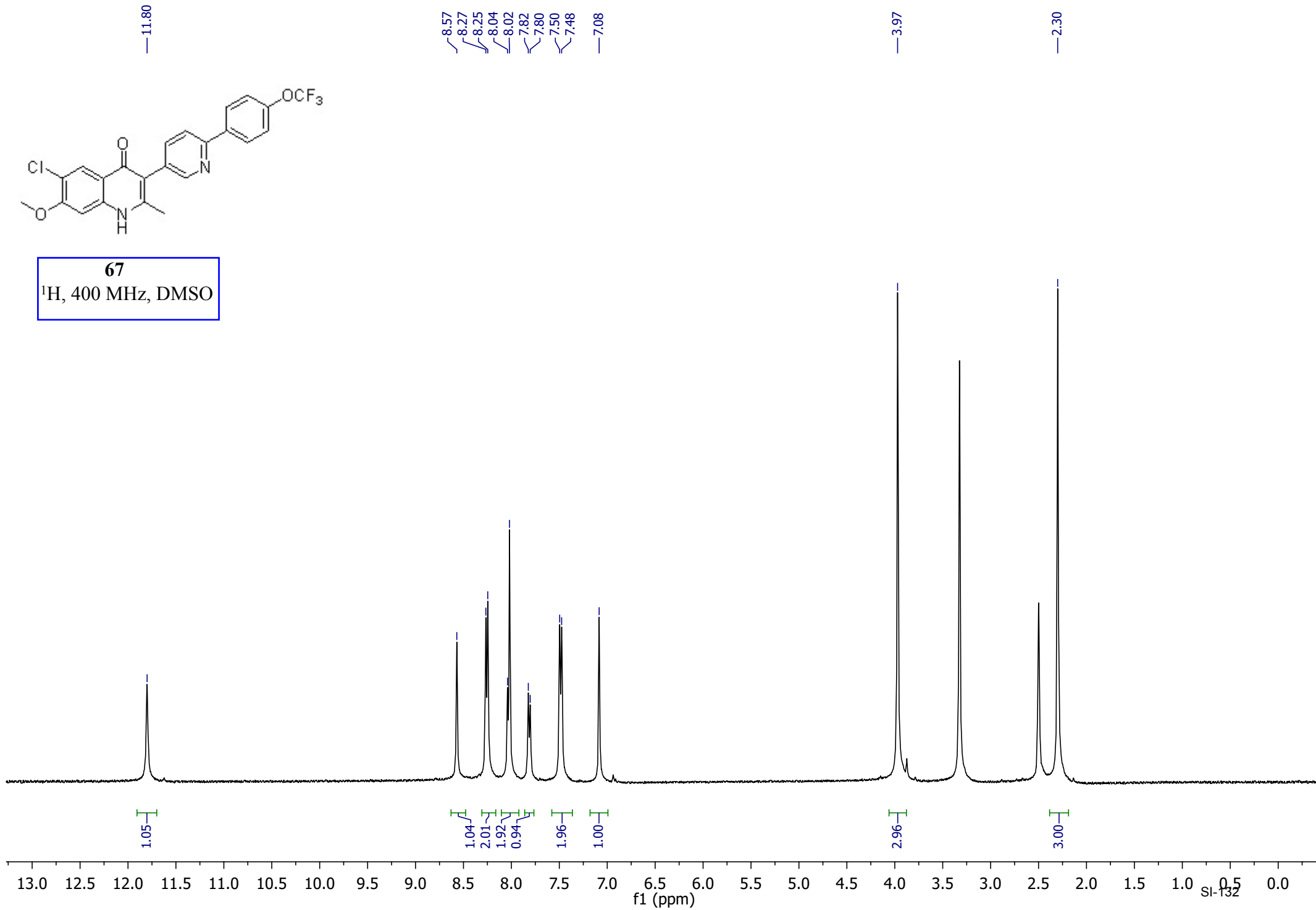
— -61.22

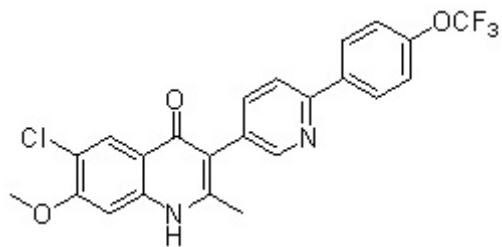
— -114.52

20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm) SI-131

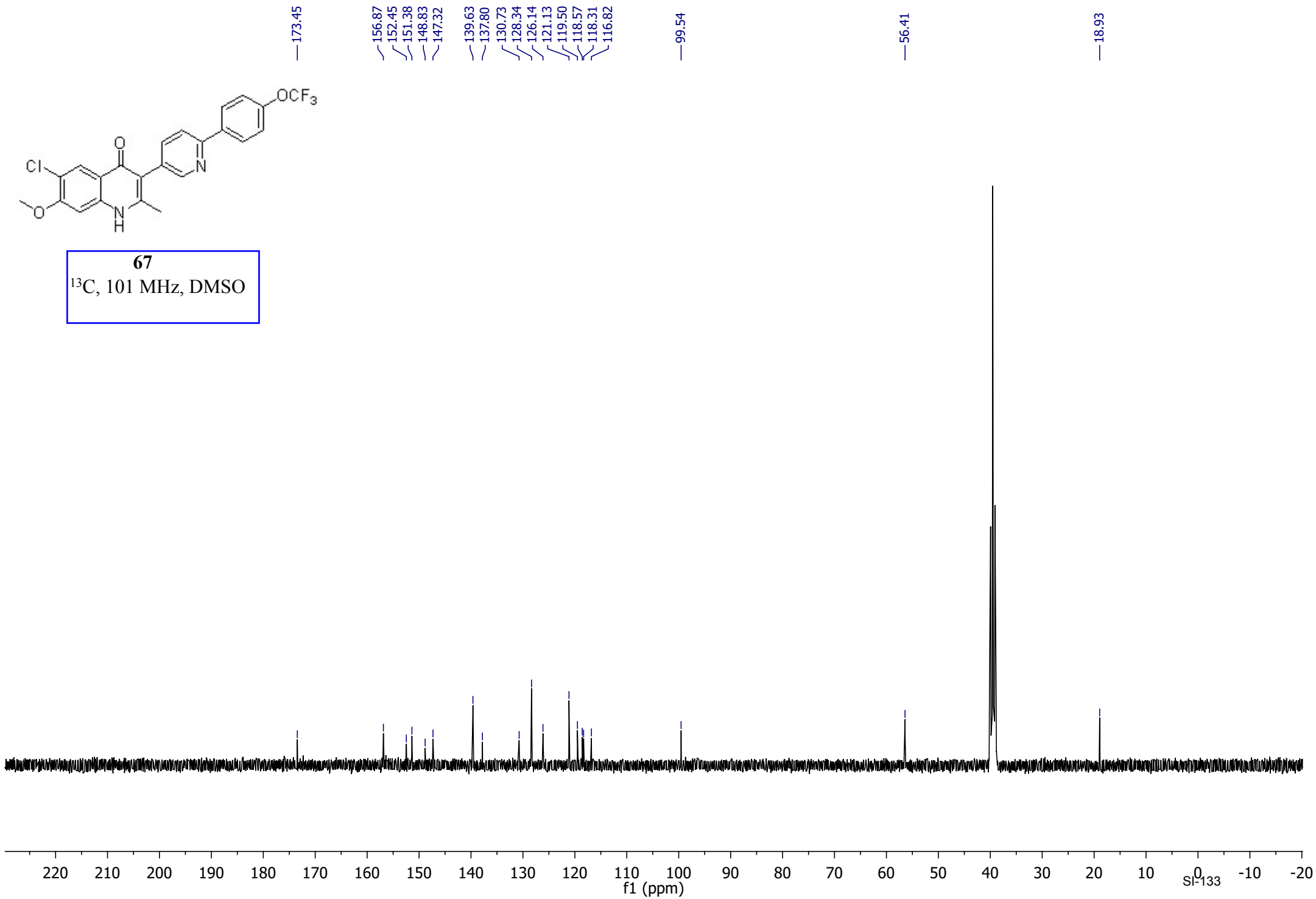


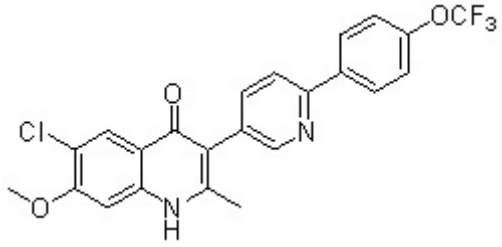
67
¹H, 400 MHz, DMSO





67
 ^{13}C , 101 MHz, DMSO





67

^{19}F , 376 MHz, DMSO

-56.70

