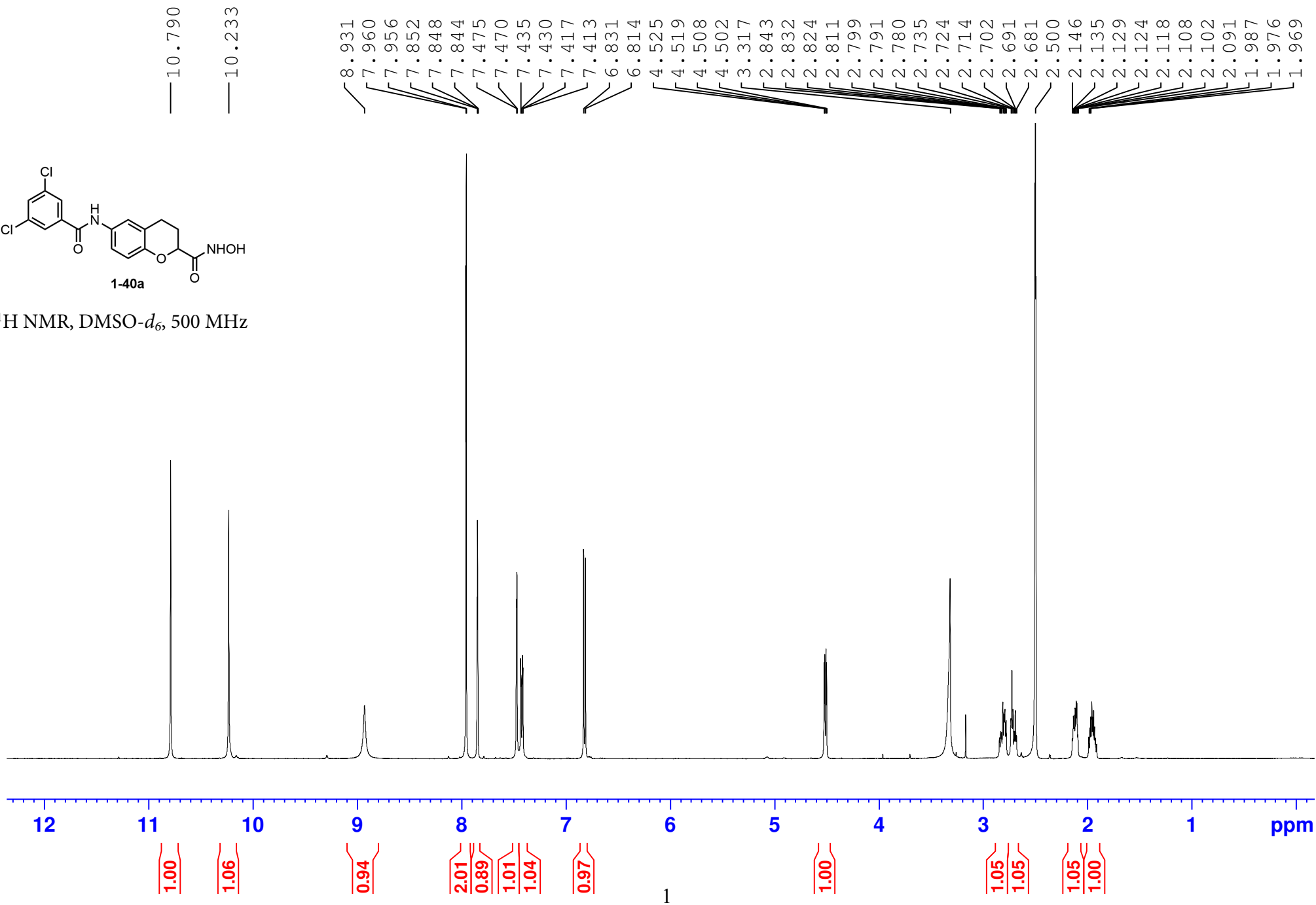
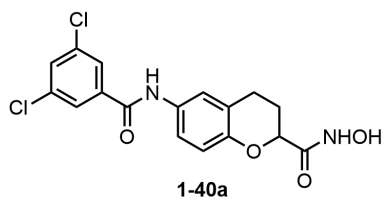
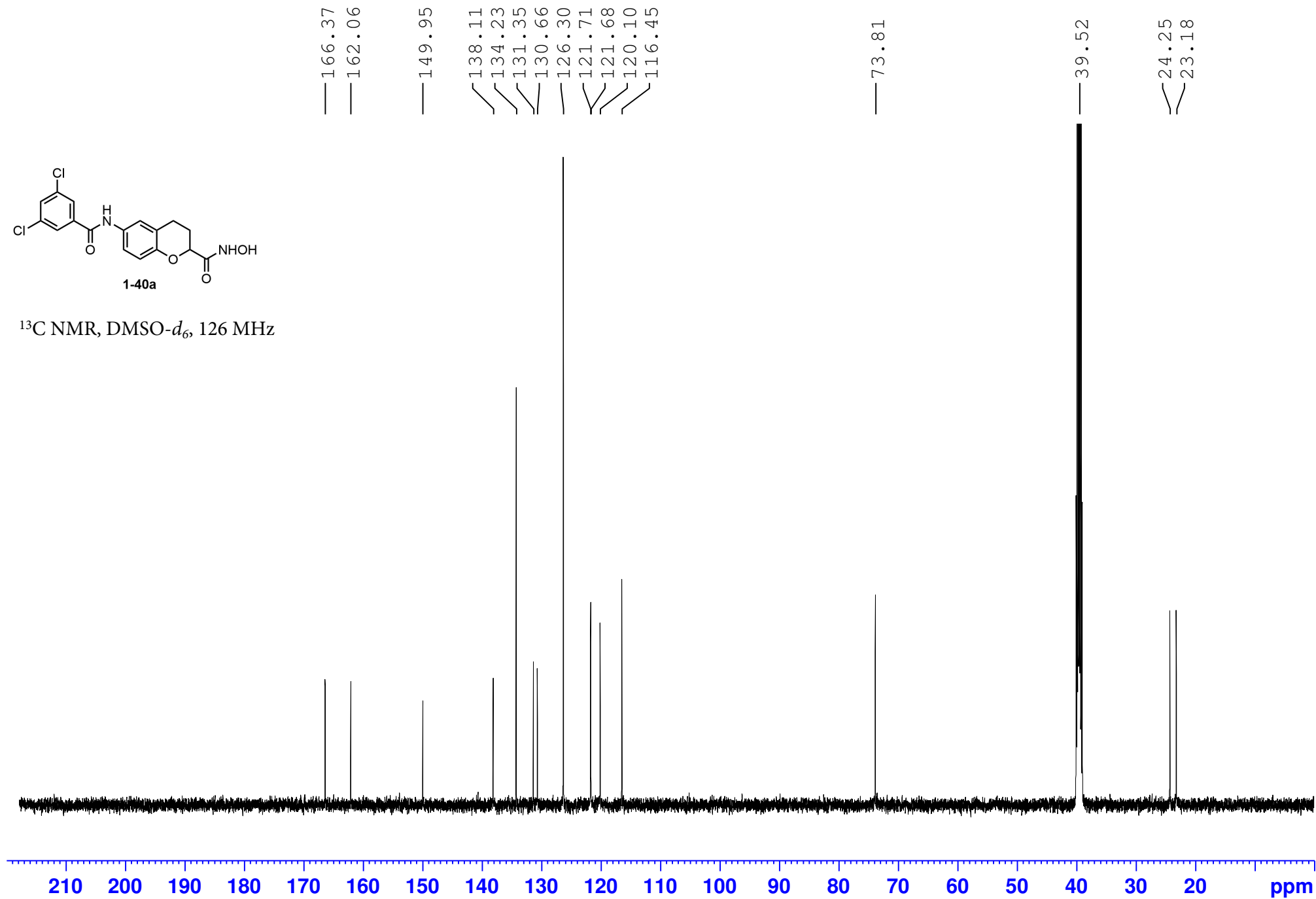


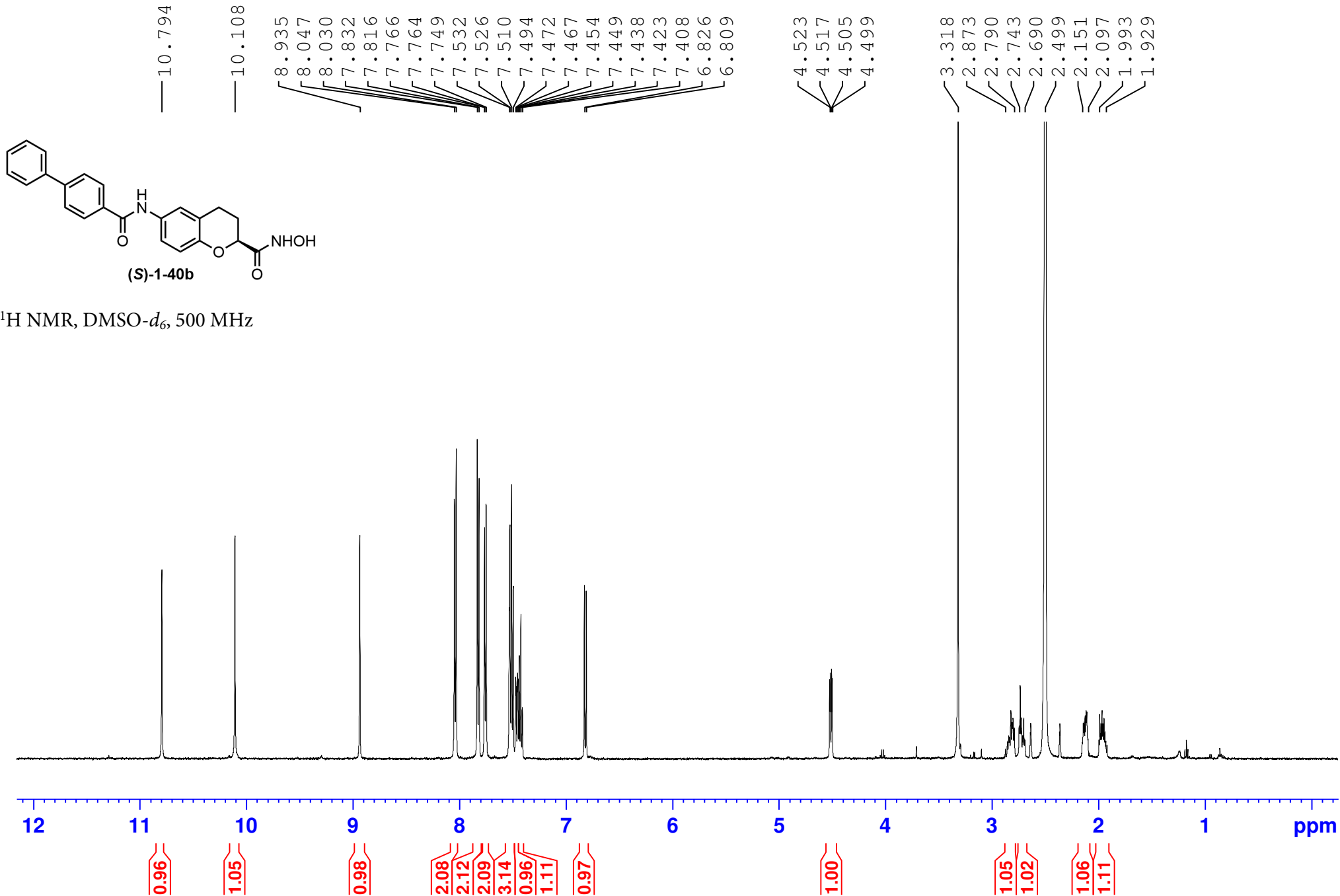
$^1\text{H NMR}$, $\text{DMSO-}d_6$, 500 MHz

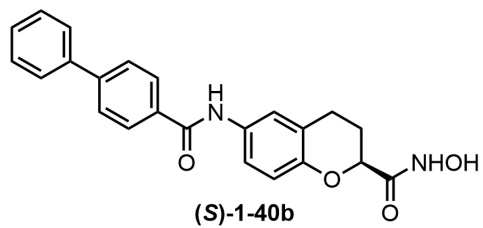




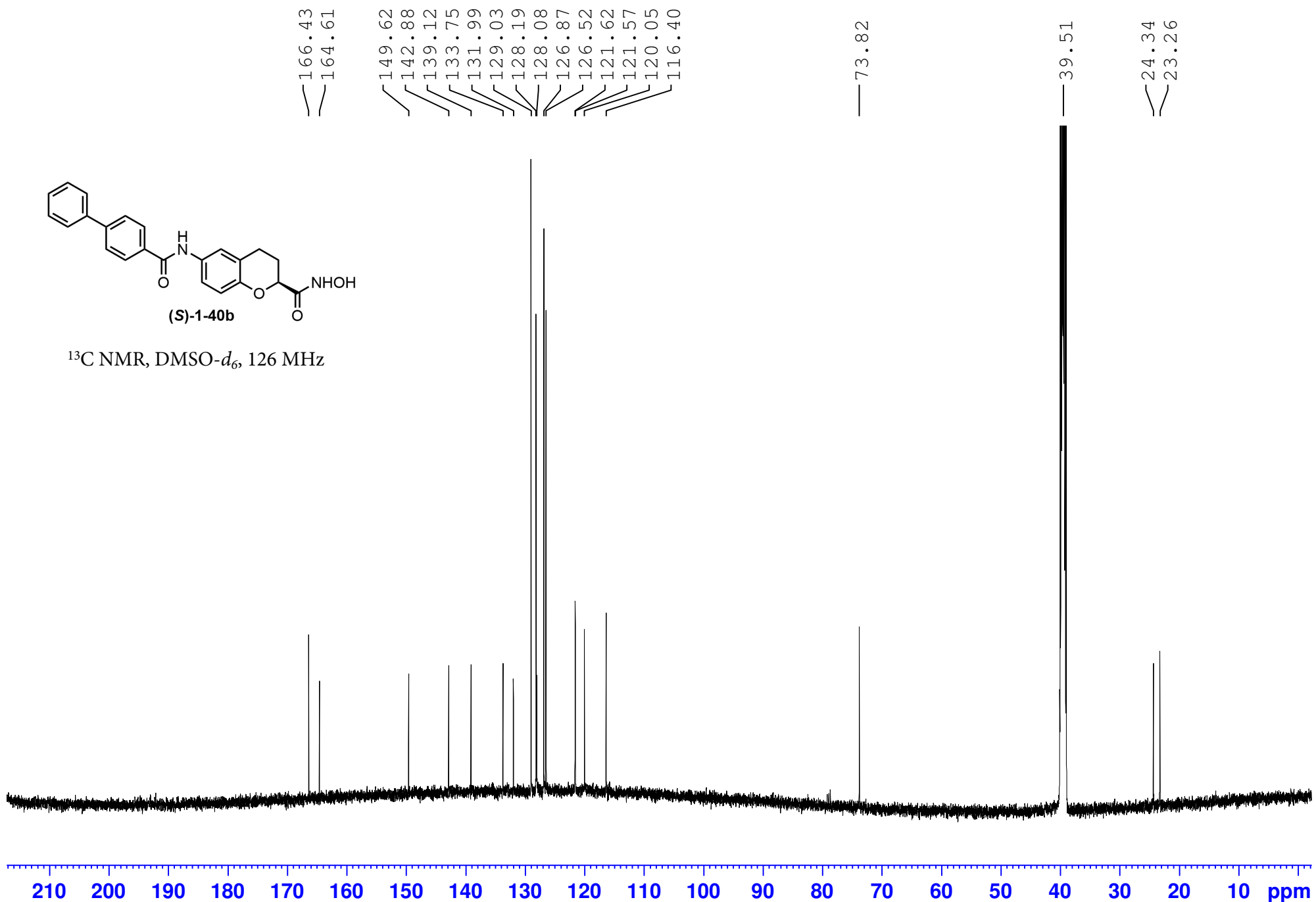
^{13}C NMR, DMSO- d_6 , 126 MHz

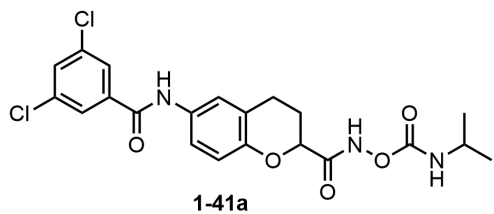




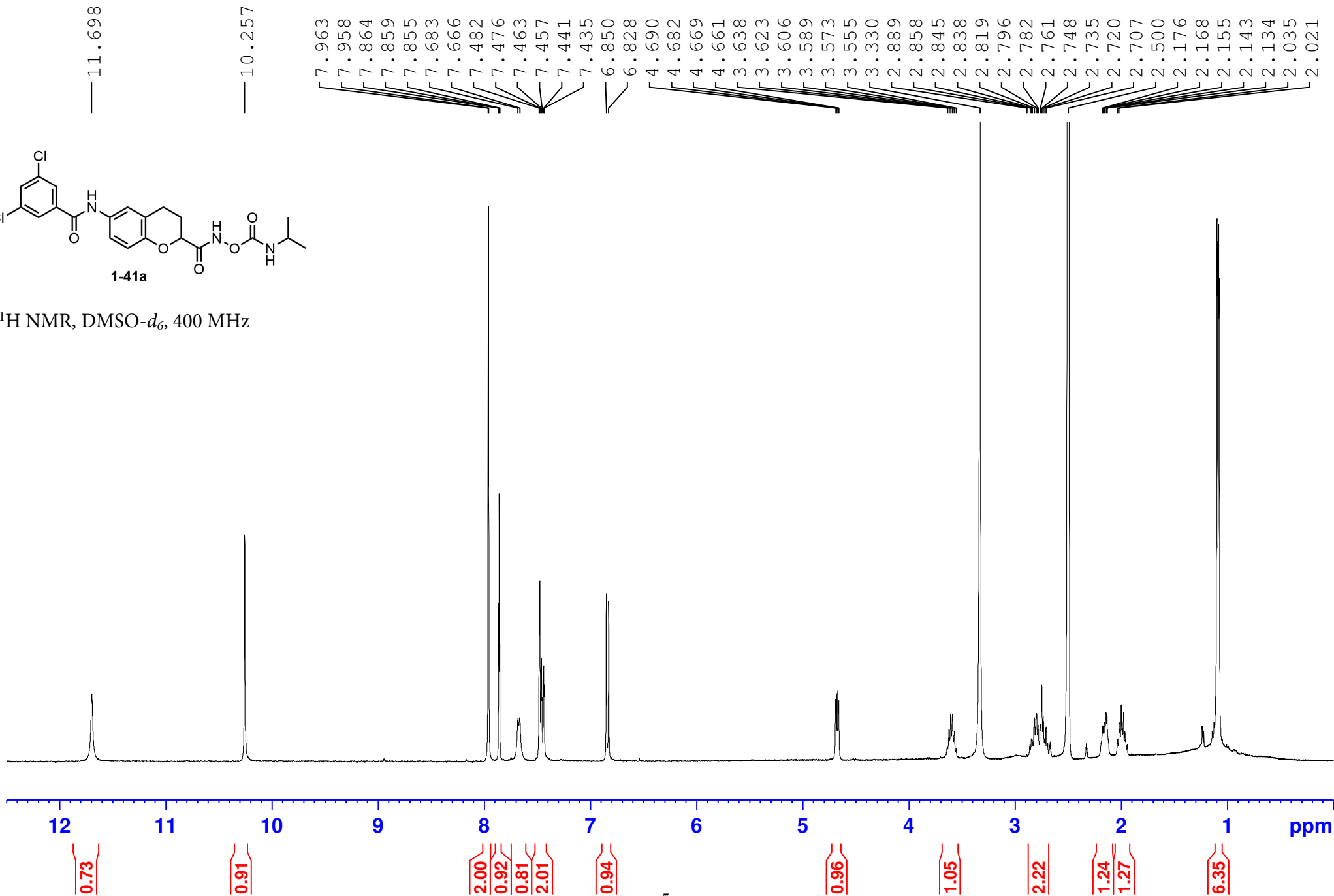


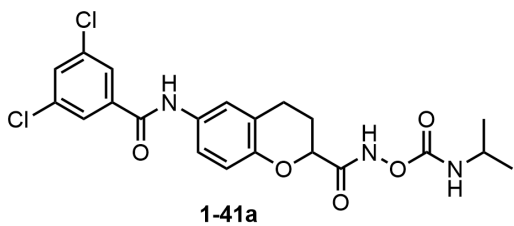
^{13}C NMR, DMSO- d_6 , 126 MHz



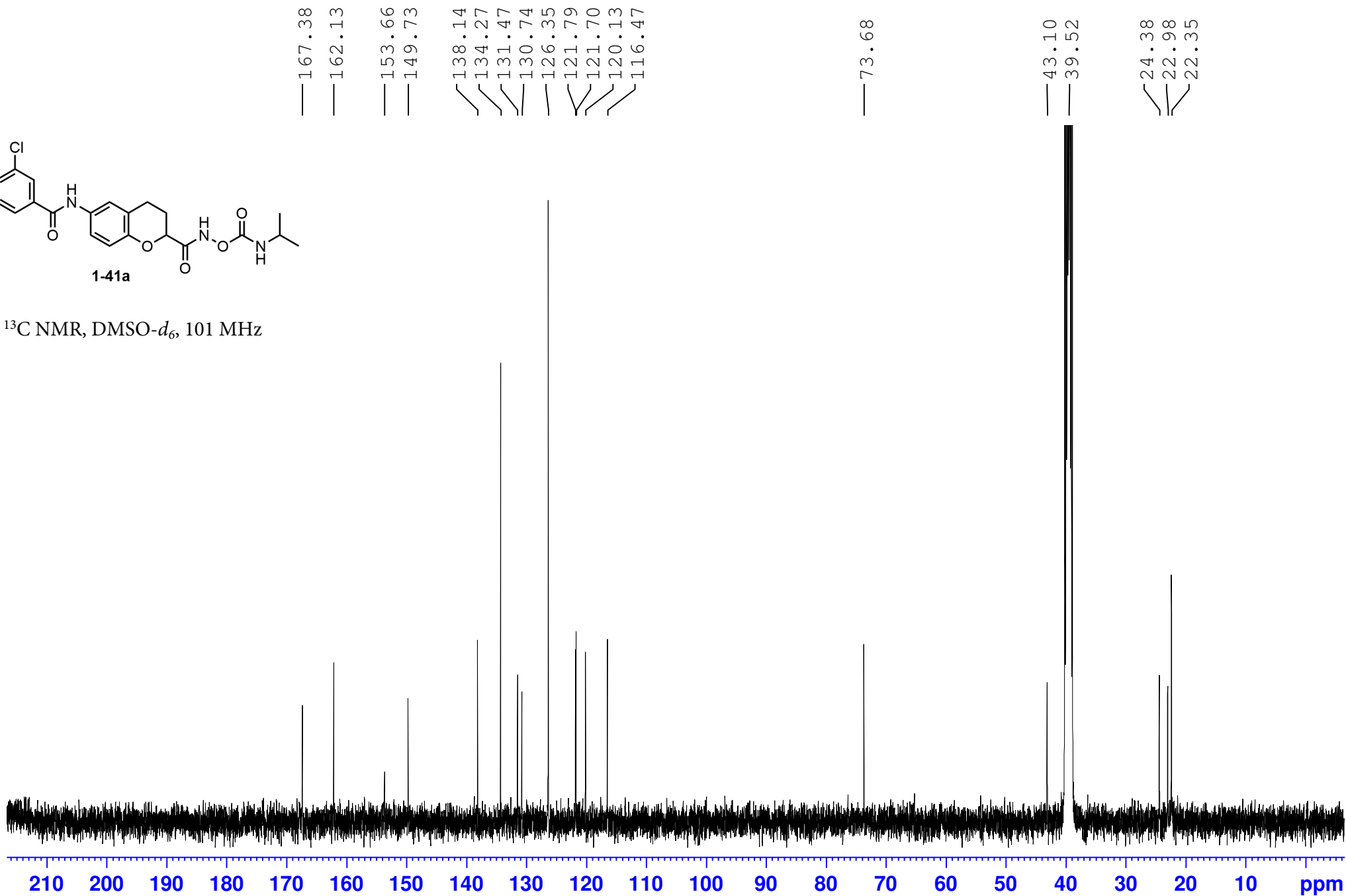


¹H NMR, DMSO-*d*₆, 400 MHz

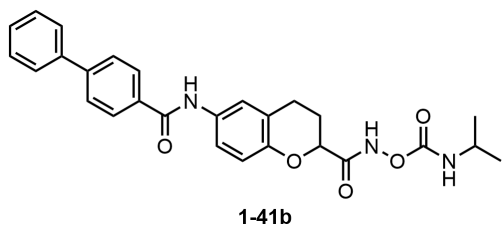




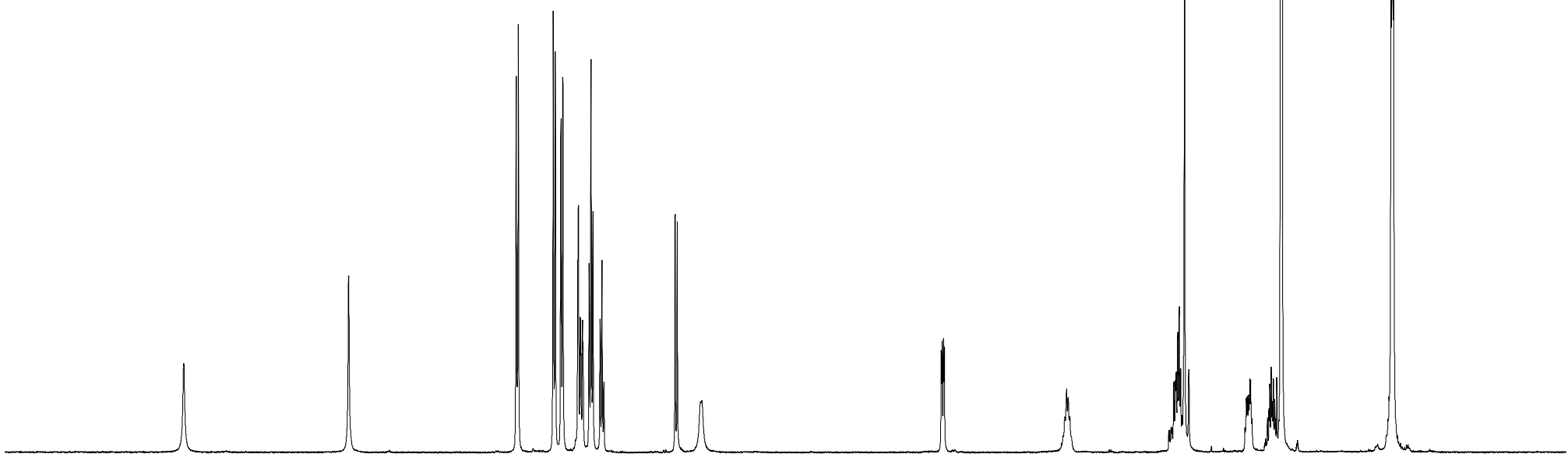
^{13}C NMR, $\text{DMSO-}d_6$, 101 MHz



10.720
 9.417
 8.093
 8.077
 7.802
 7.785
 7.740
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 7.602
 7.587
 7.583
 7.570
 7.565
 7.517
 7.503
 7.487
 7.430
 7.416
 7.401
 6.838
 6.821
 6.638
 6.626
 4.735
 4.729
 4.718
 4.712
 3.760
 3.745
 3.734
 3.721
 2.899
 2.887
 2.880
 2.867
 2.856
 2.845
 2.815
 2.326
 2.319
 2.314
 2.309
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 2.147
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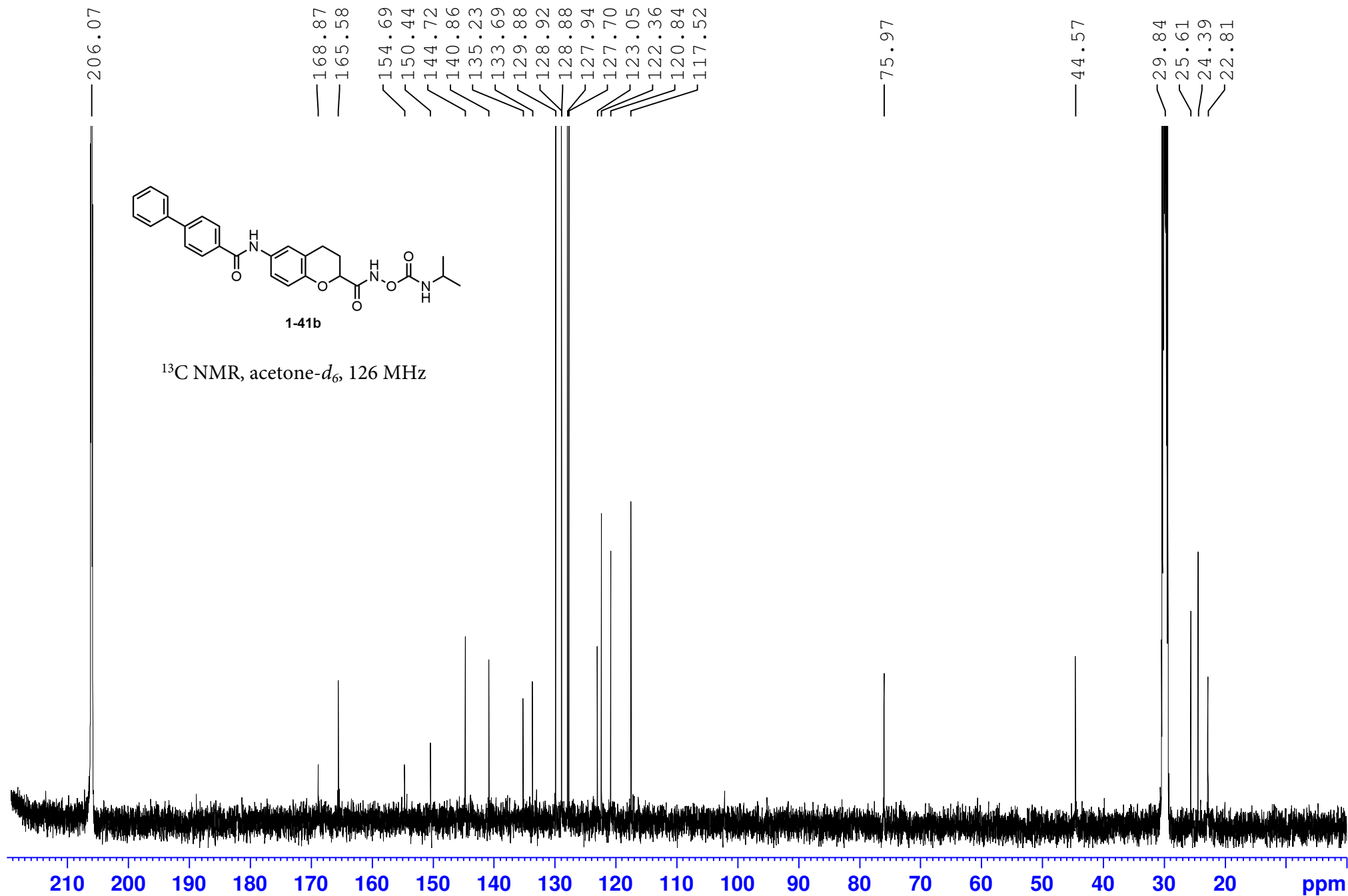


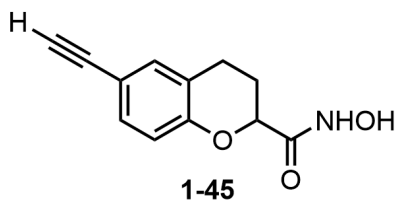
¹H NMR, acetone-*d*₆, 500 MHz



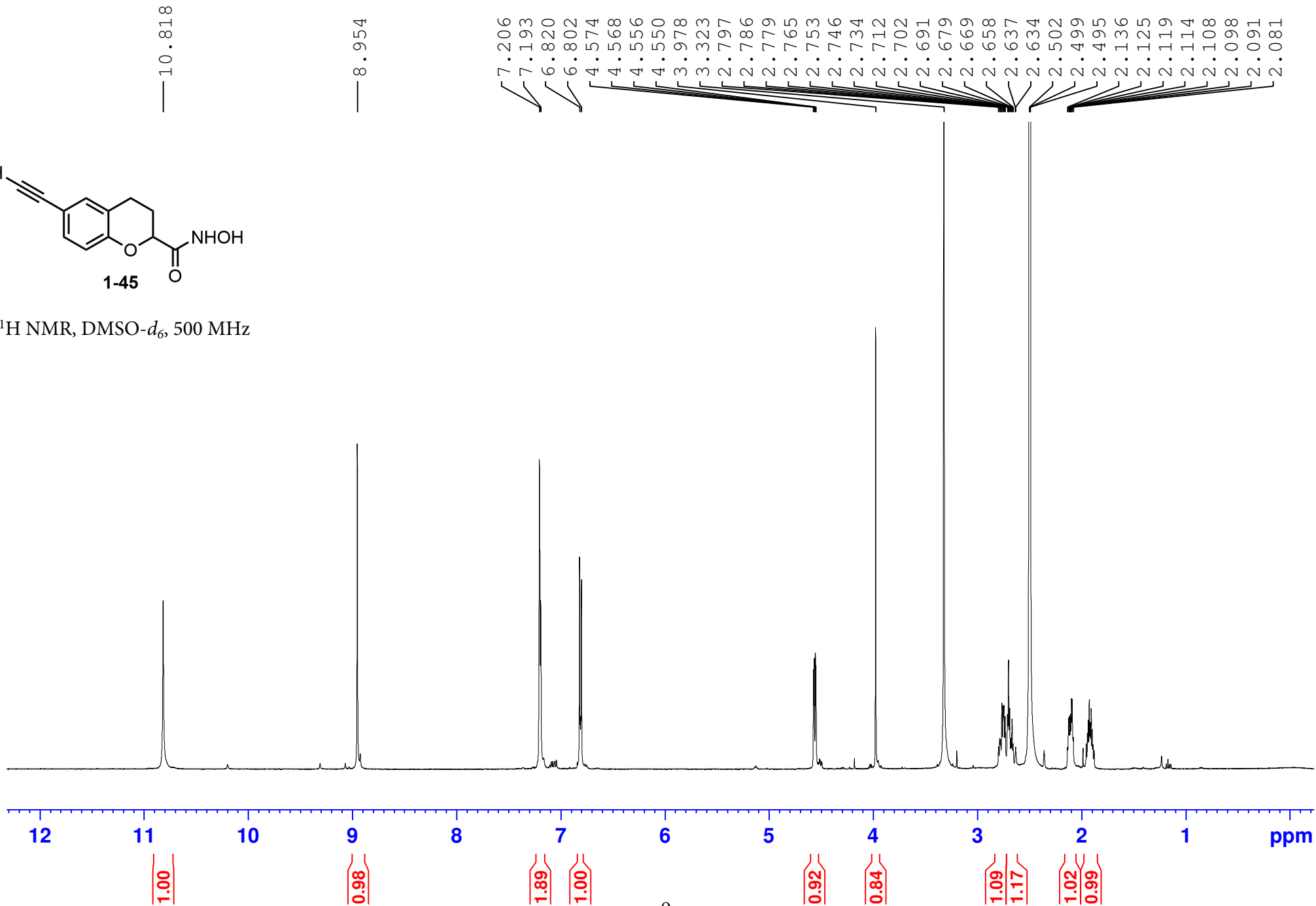
12 11 10 9 8 7 6 5 4 3 2 1 ppm

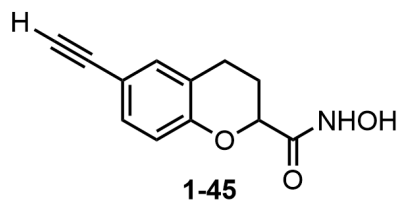
0.86
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 2.13
 2.17
 2.13
 2.17
 1.04
 1.04
 0.88
 1.00
 1.03
 1.97
 1.05
 1.19
 6.40



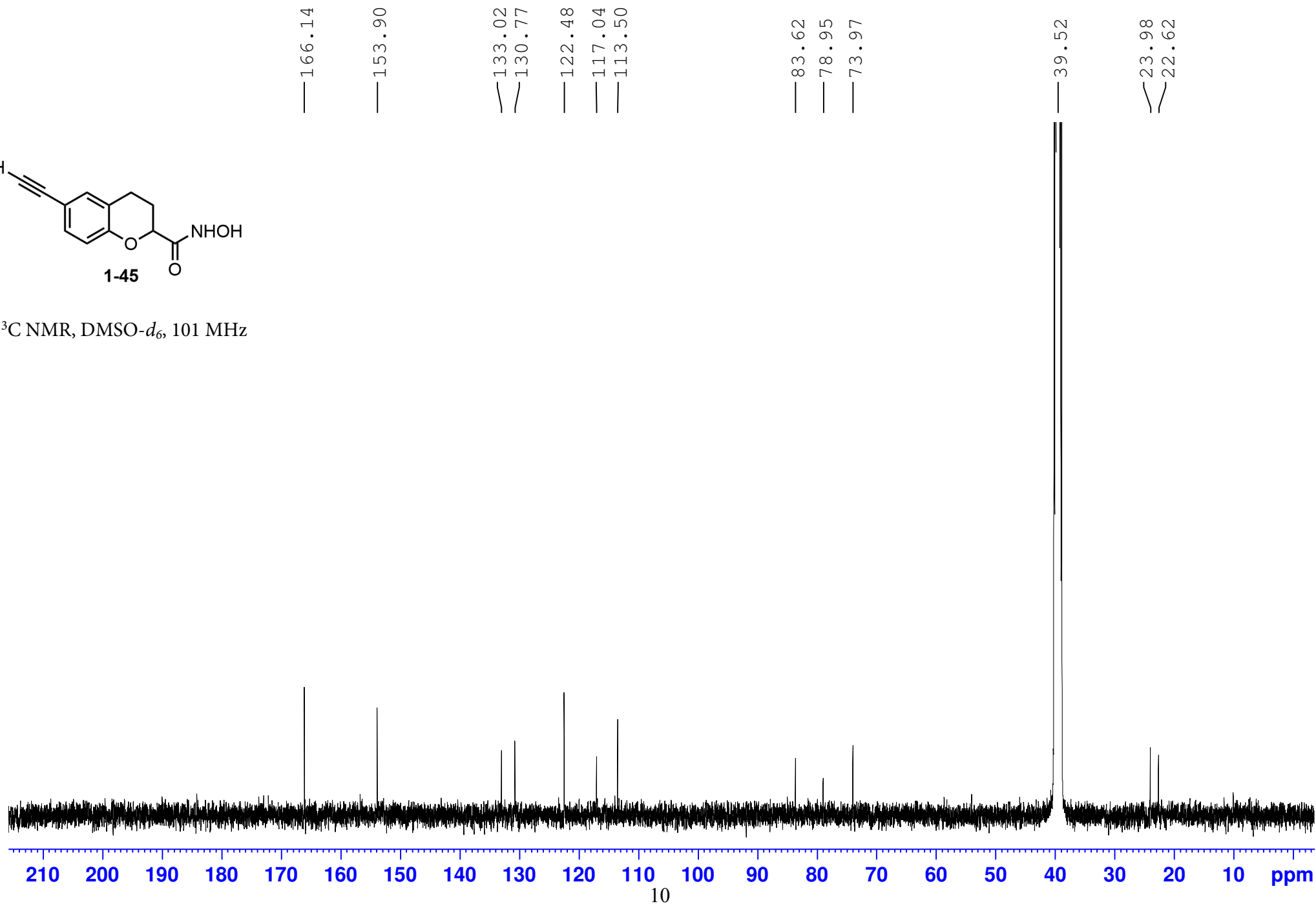


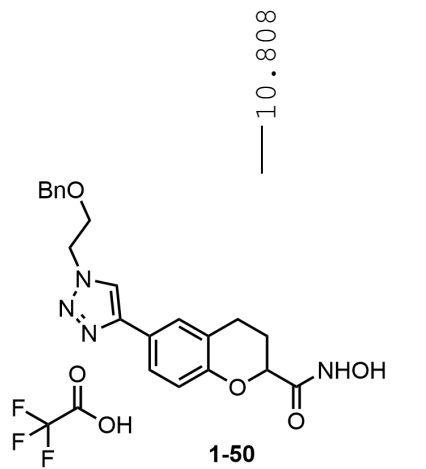
¹H NMR, DMSO-*d*₆, 500 MHz



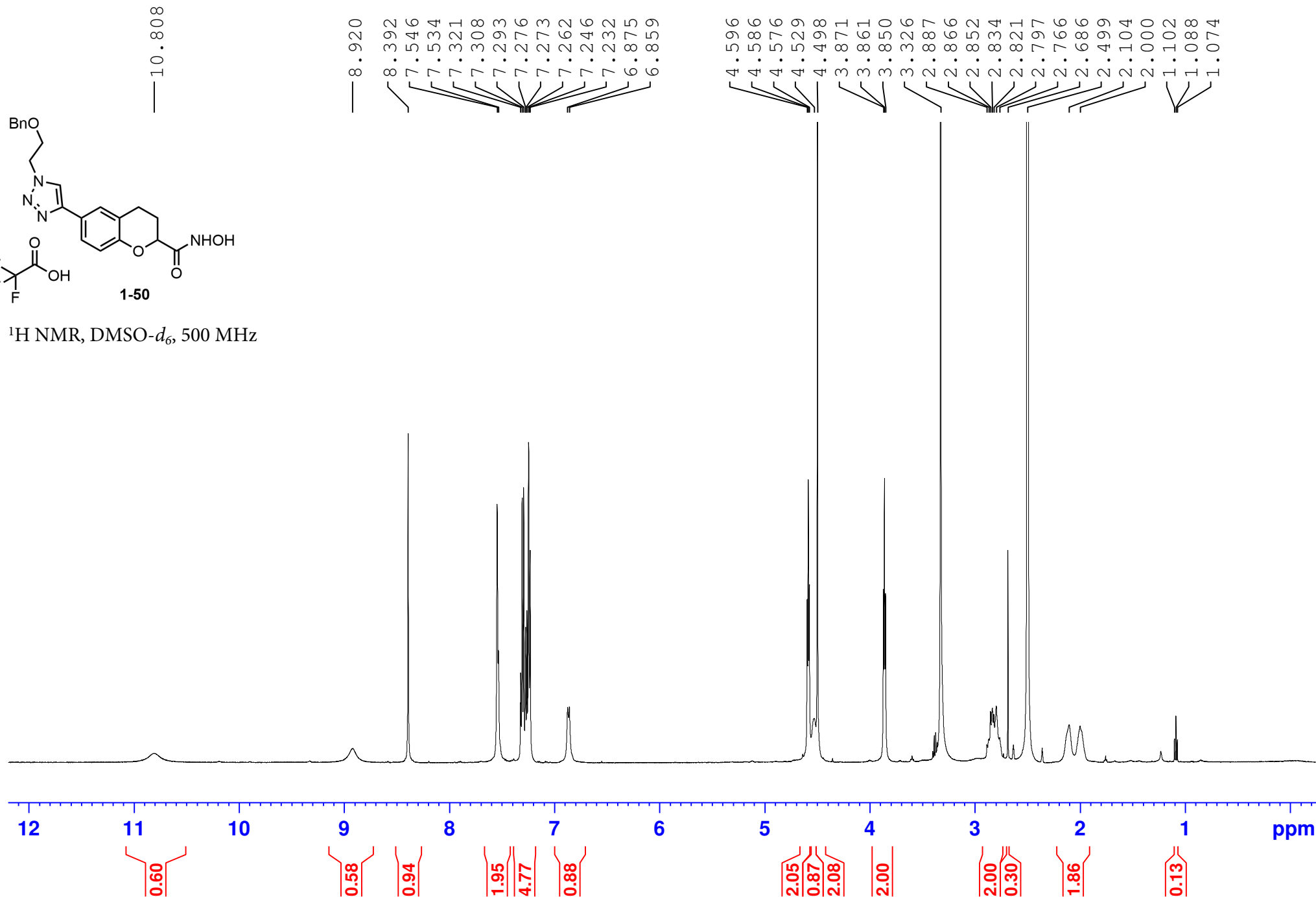


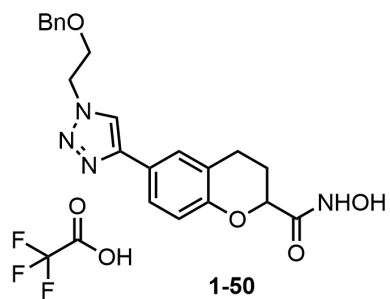
¹³C NMR, DMSO-*d*₆, 101 MHz



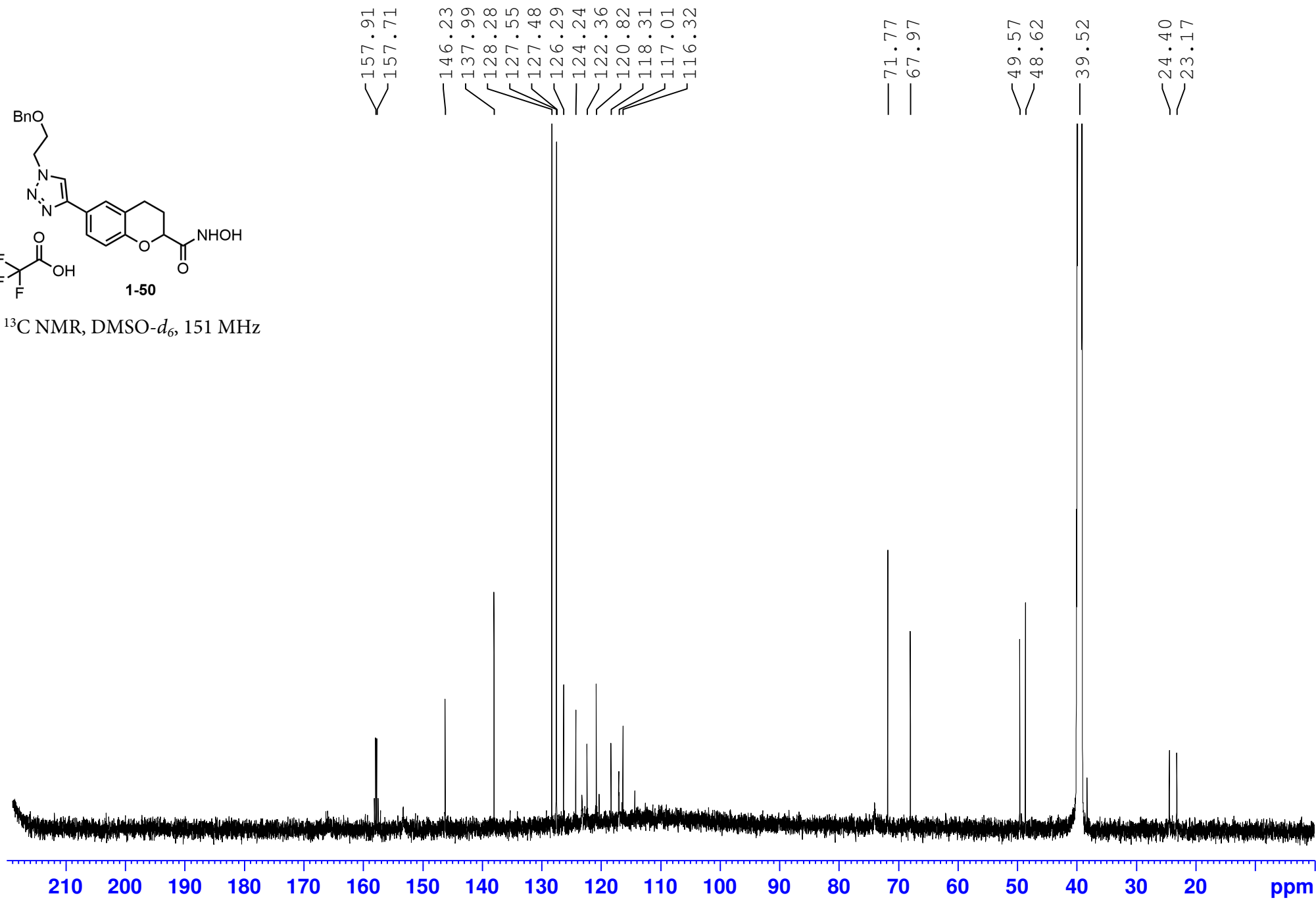


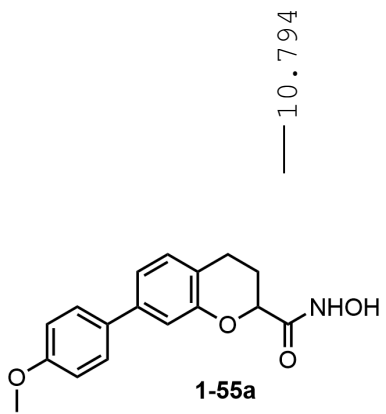
$^1\text{H NMR}$, $\text{DMSO-}d_6$, 500 MHz



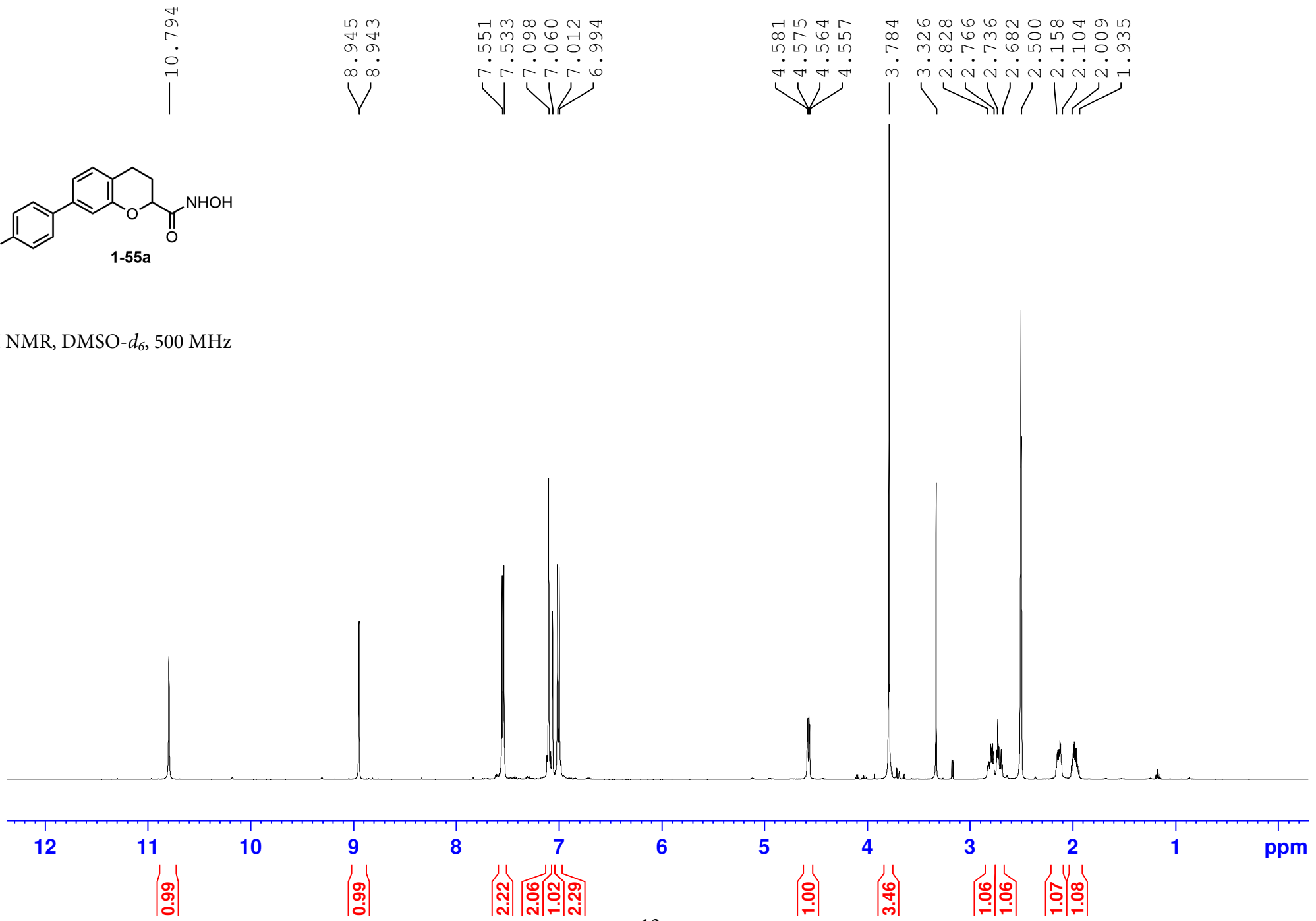


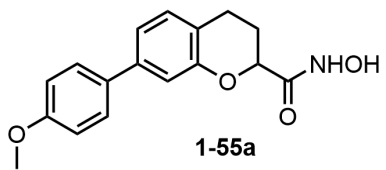
^{13}C NMR, DMSO- d_6 , 151 MHz



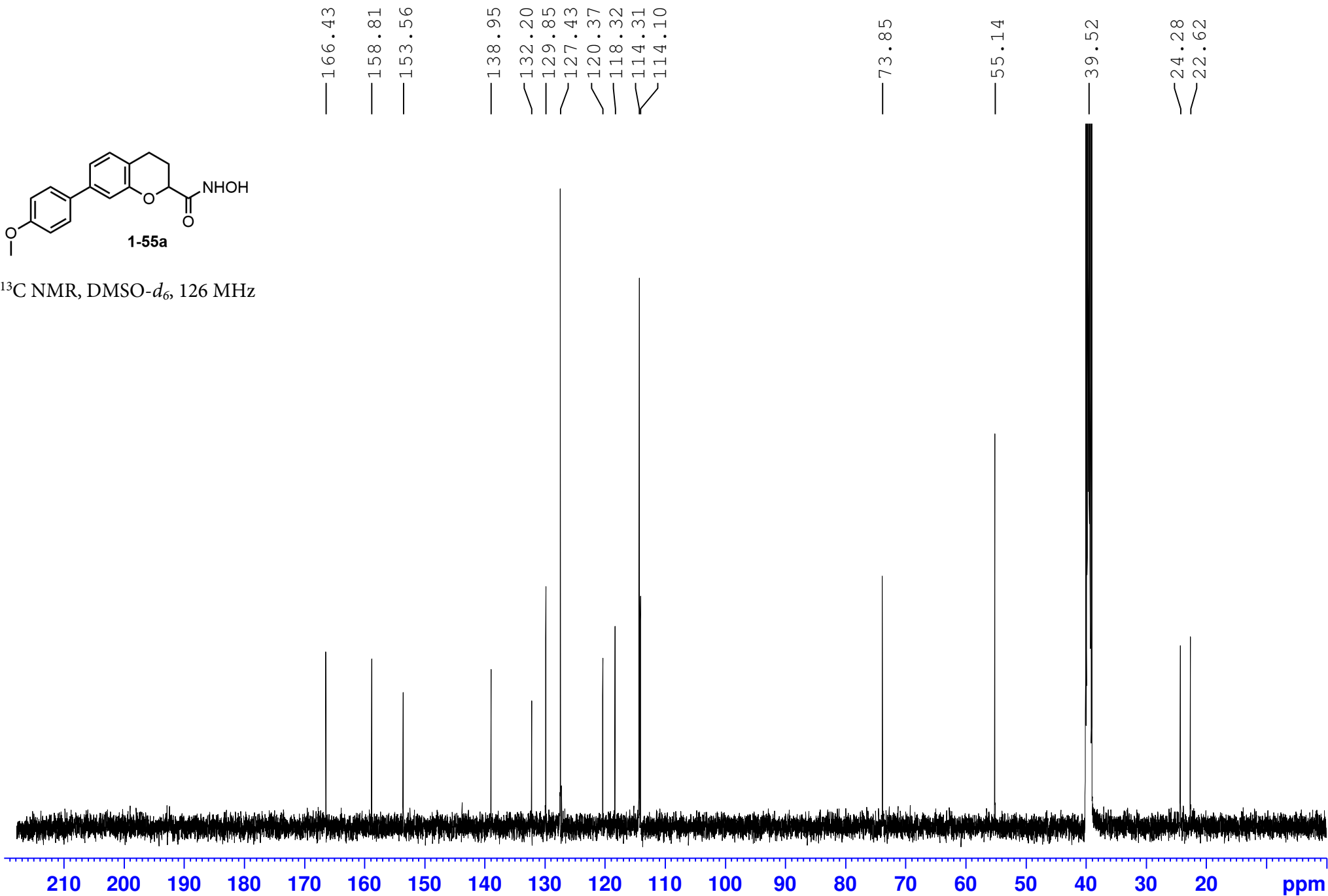


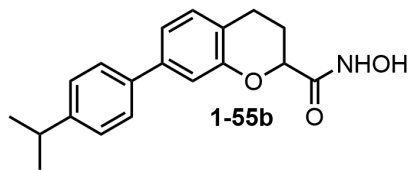
¹H NMR, DMSO-*d*₆, 500 MHz



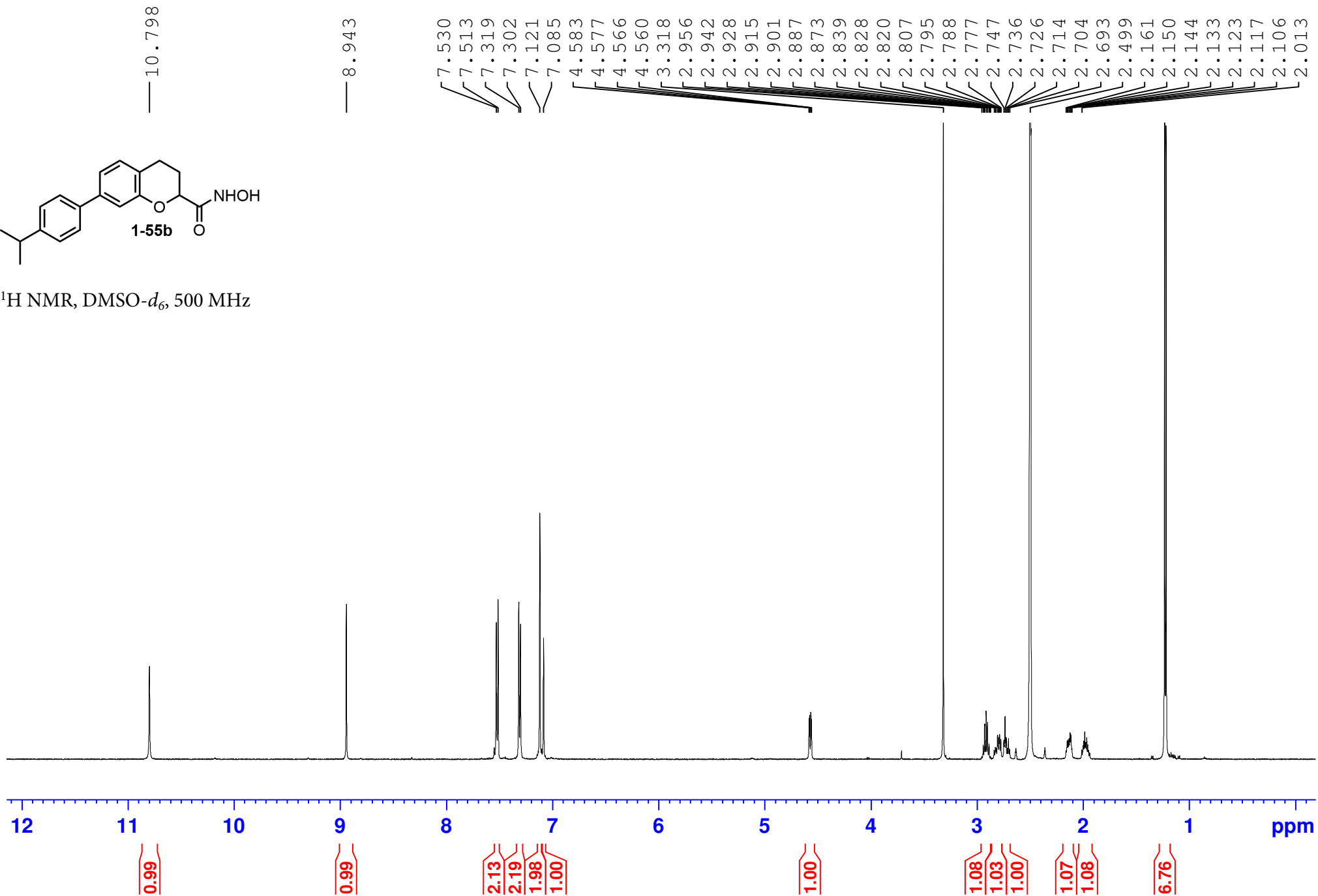


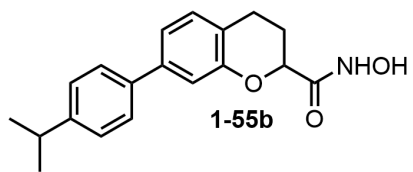
^{13}C NMR, DMSO- d_6 , 126 MHz





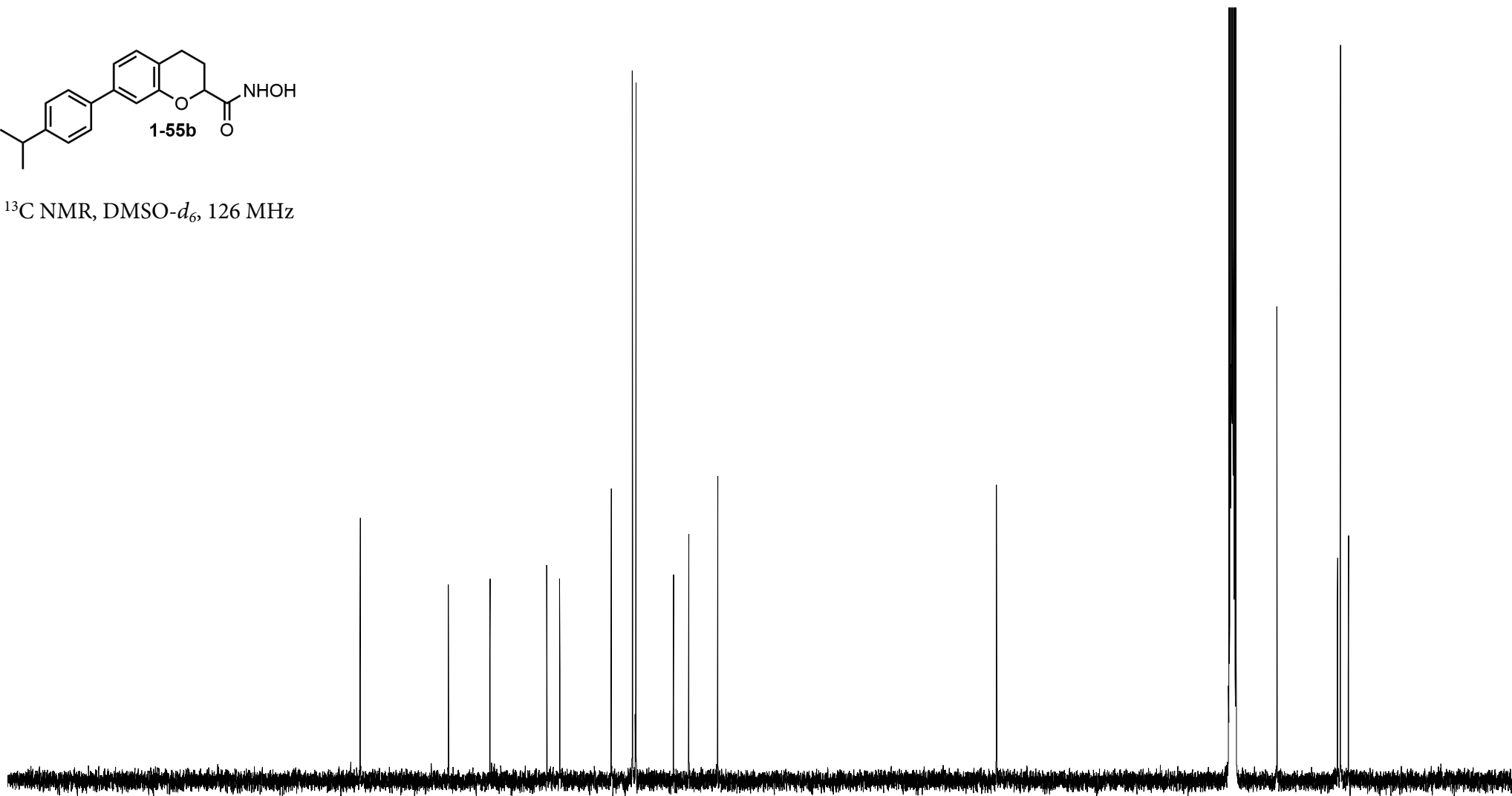
^1H NMR, DMSO- d_6 , 500 MHz



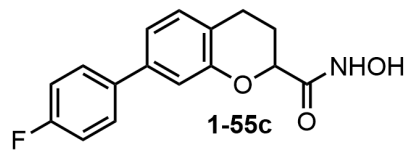


^{13}C NMR, DMSO- d_6 , 126 MHz

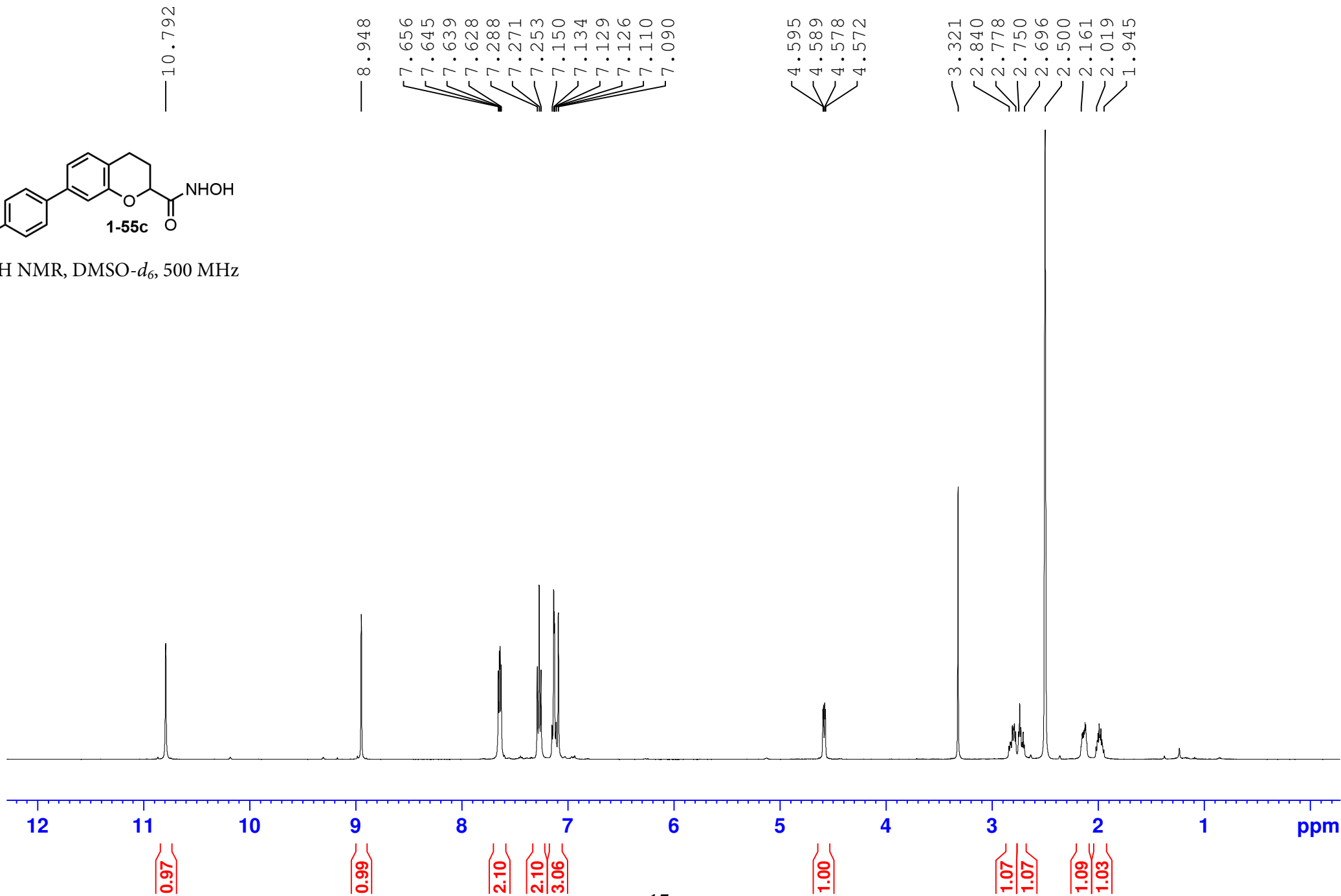
- 166.41
- 153.58
- 147.53
- 139.25
- 137.38
- 129.87
- 126.80
- 126.29
- 120.84
- 118.60
- 114.39
- 73.85
- 39.51
- 33.05
- 24.25
- 23.82
- 22.65

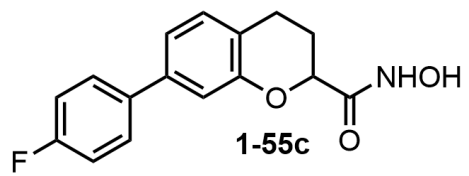


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

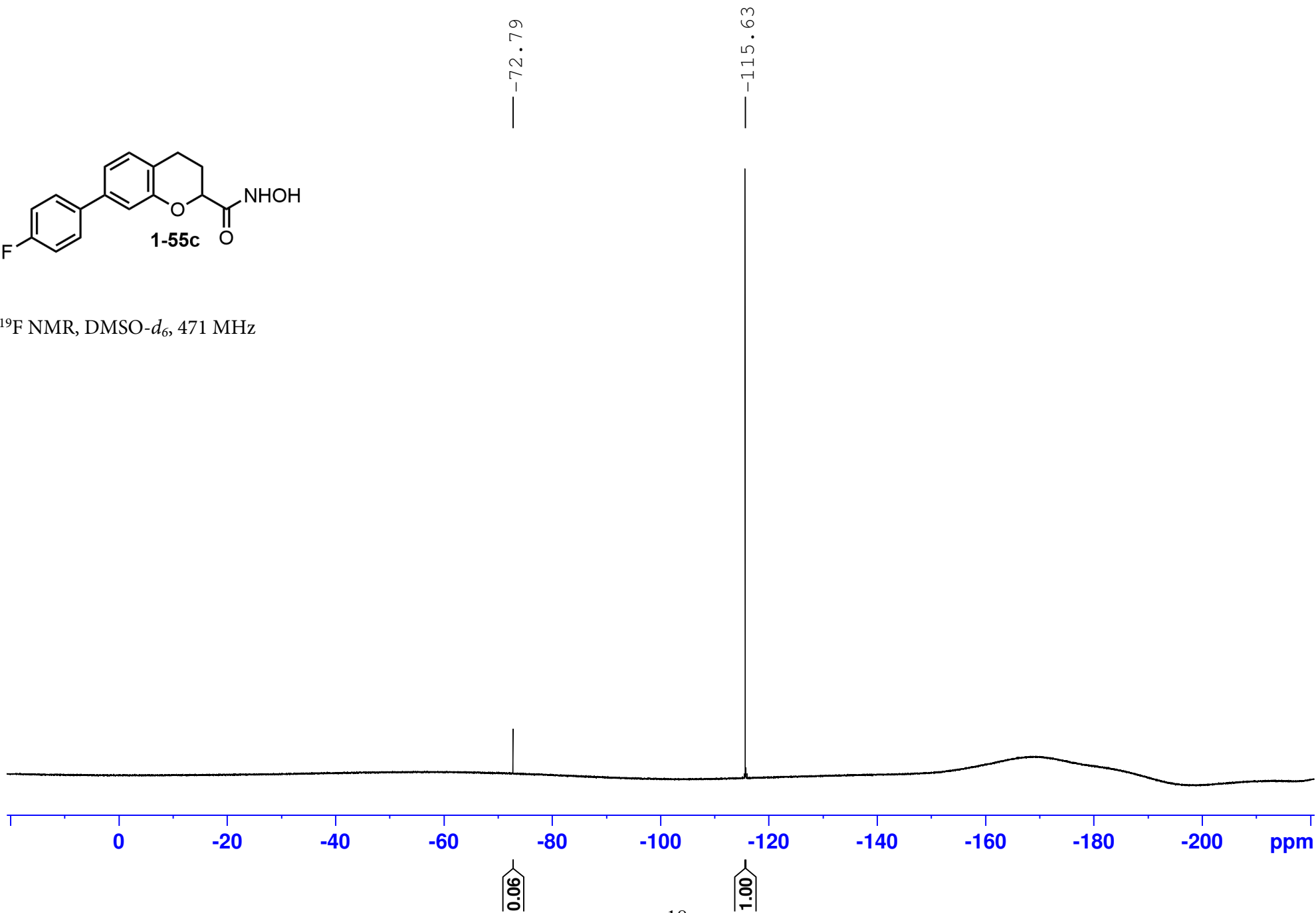


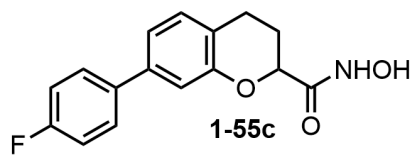
^1H NMR, DMSO- d_6 , 500 MHz



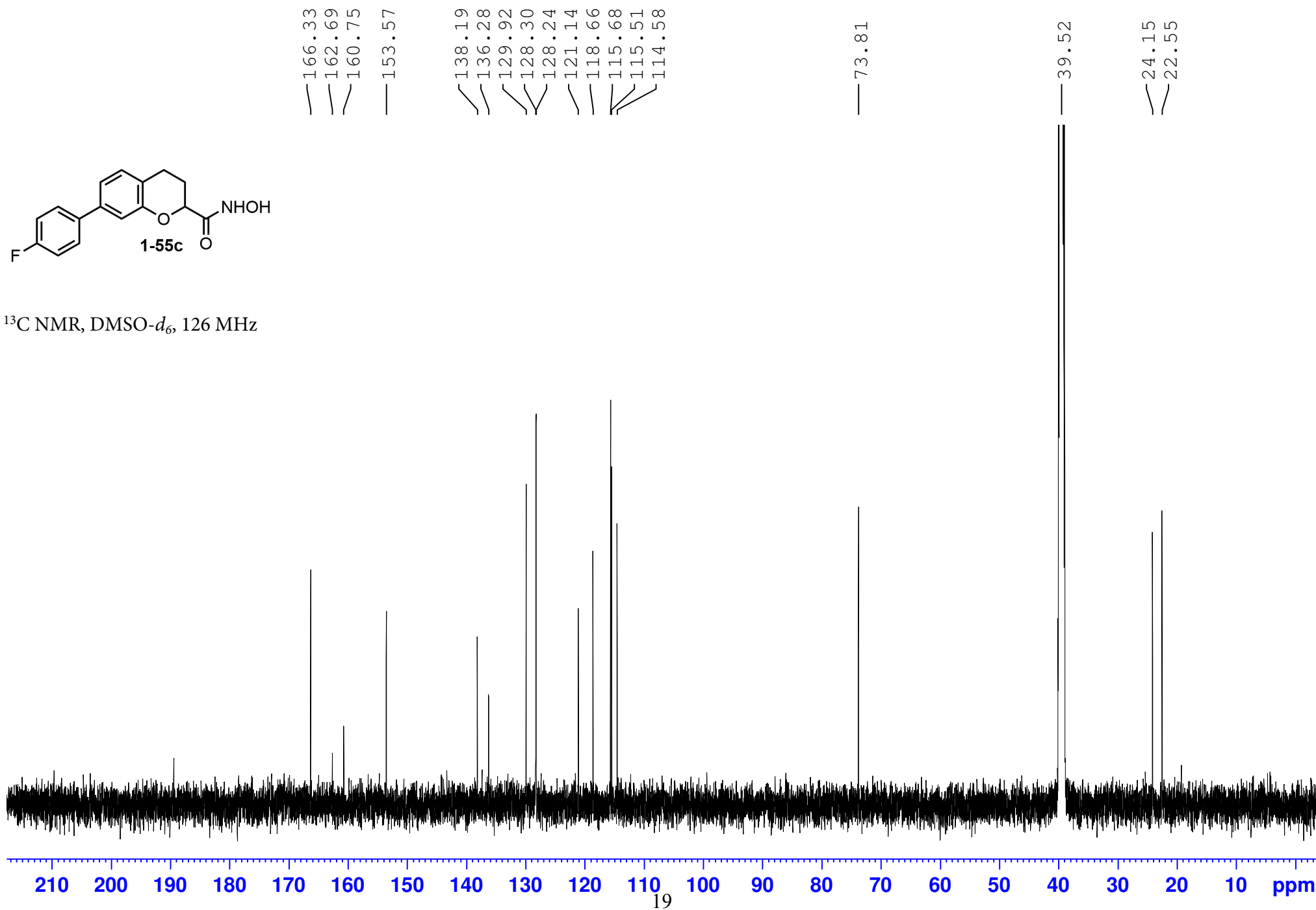


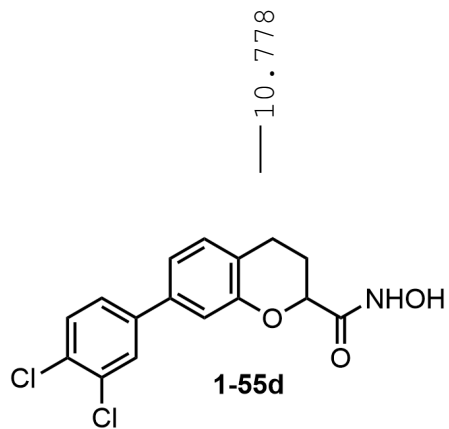
^{19}F NMR, DMSO- d_6 , 471 MHz



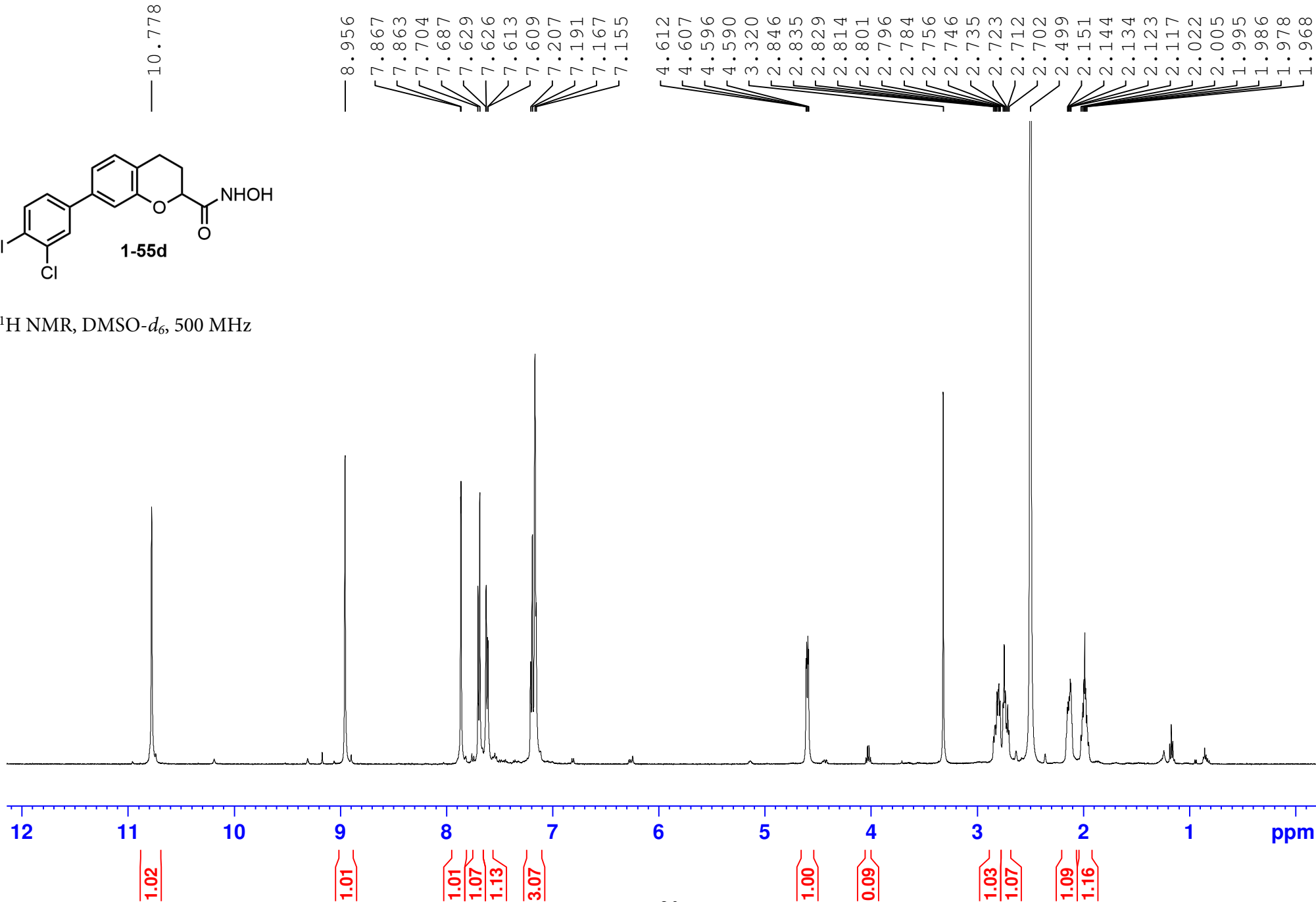


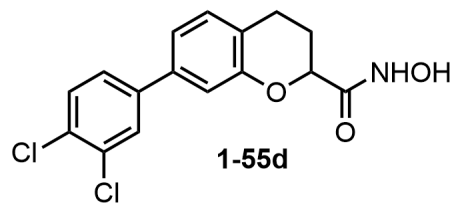
^{13}C NMR, $\text{DMSO-}d_6$, 126 MHz



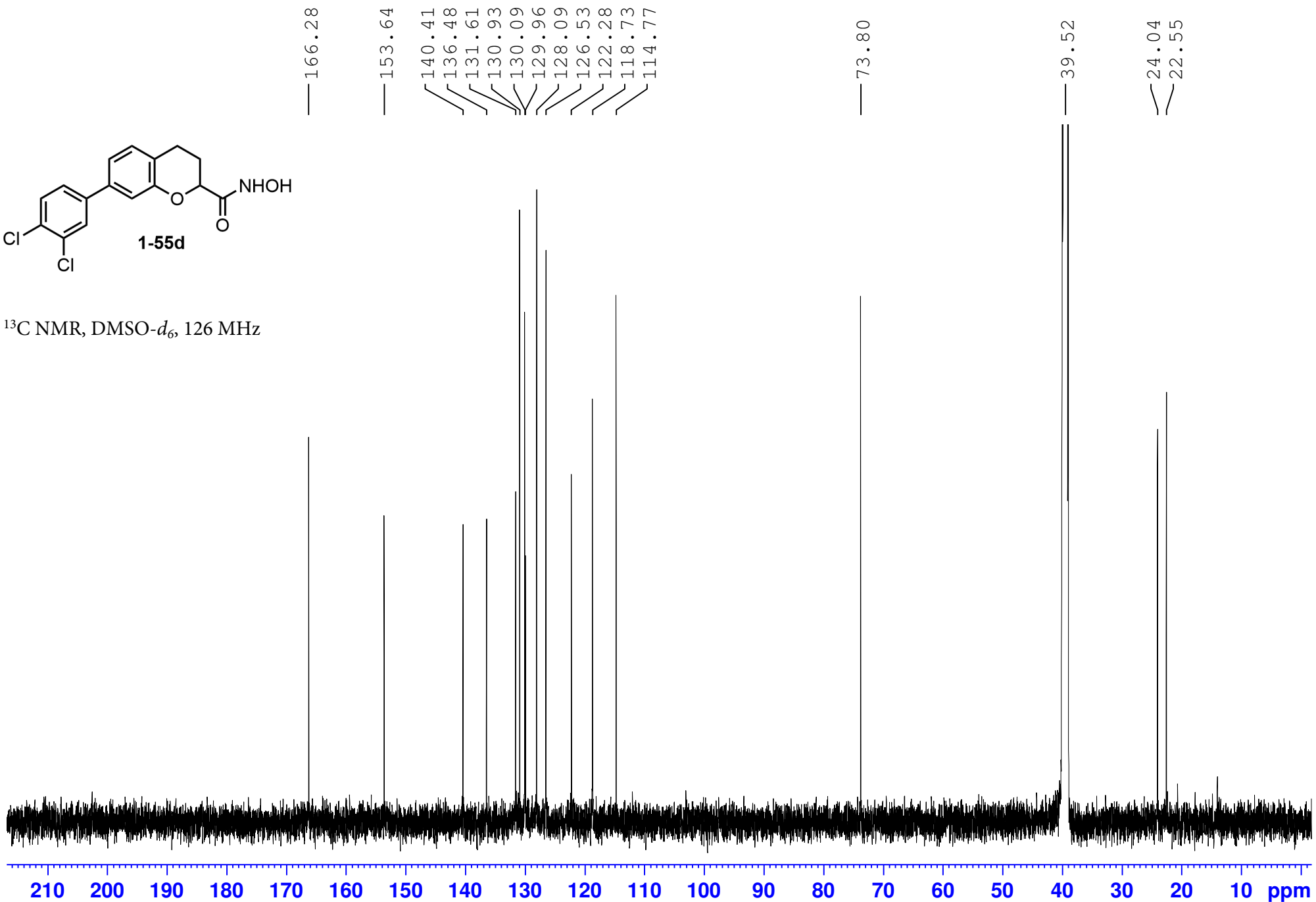


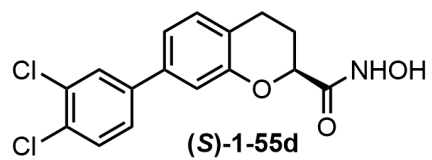
^1H NMR, DMSO- d_6 , 500 MHz



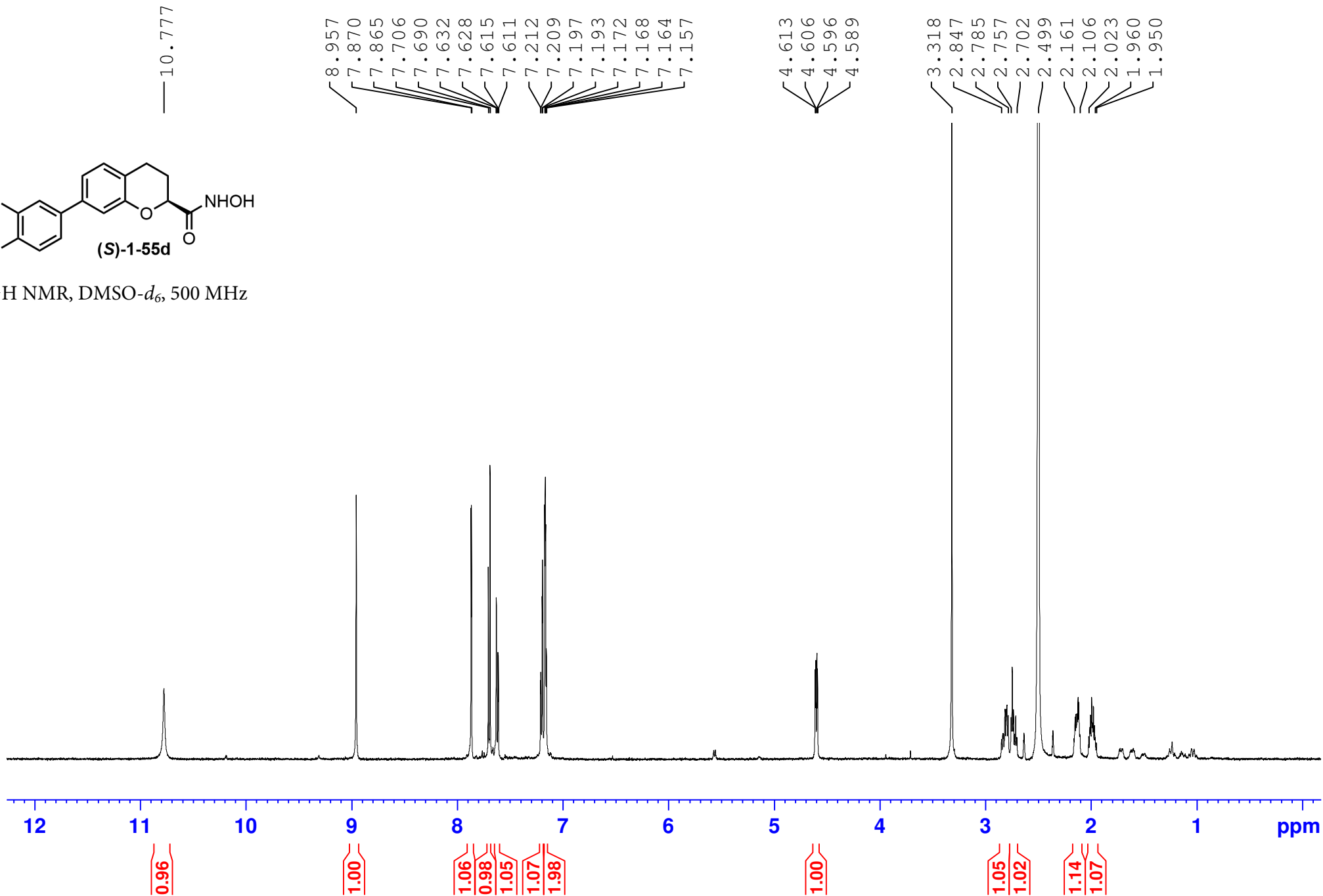


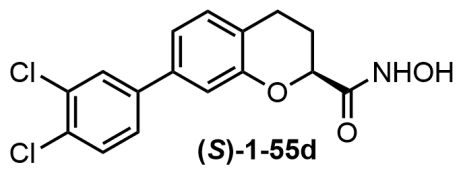
^{13}C NMR, DMSO- d_6 , 126 MHz



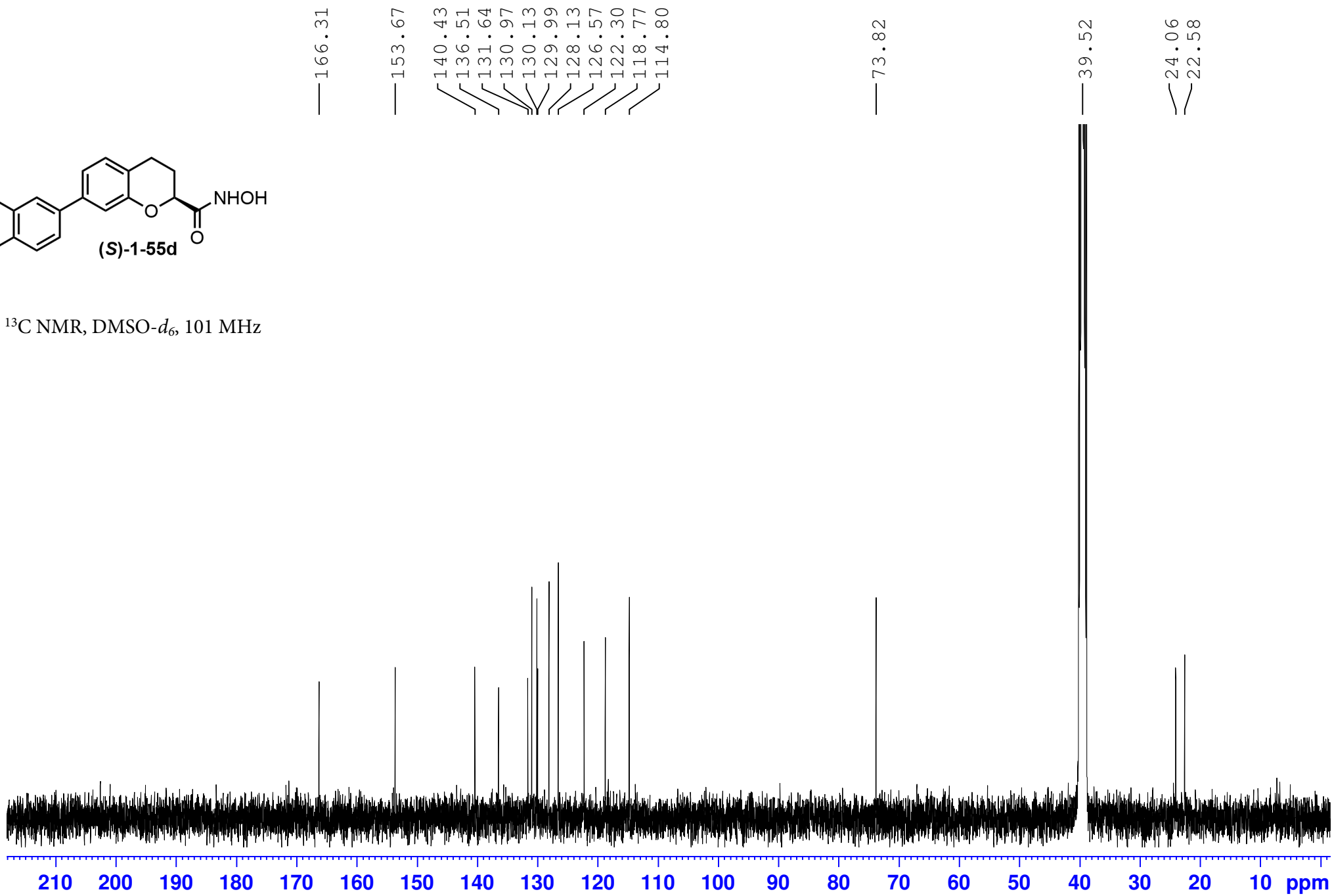


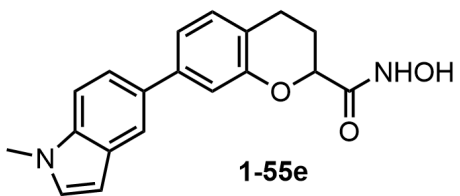
^1H NMR, DMSO- d_6 , 500 MHz



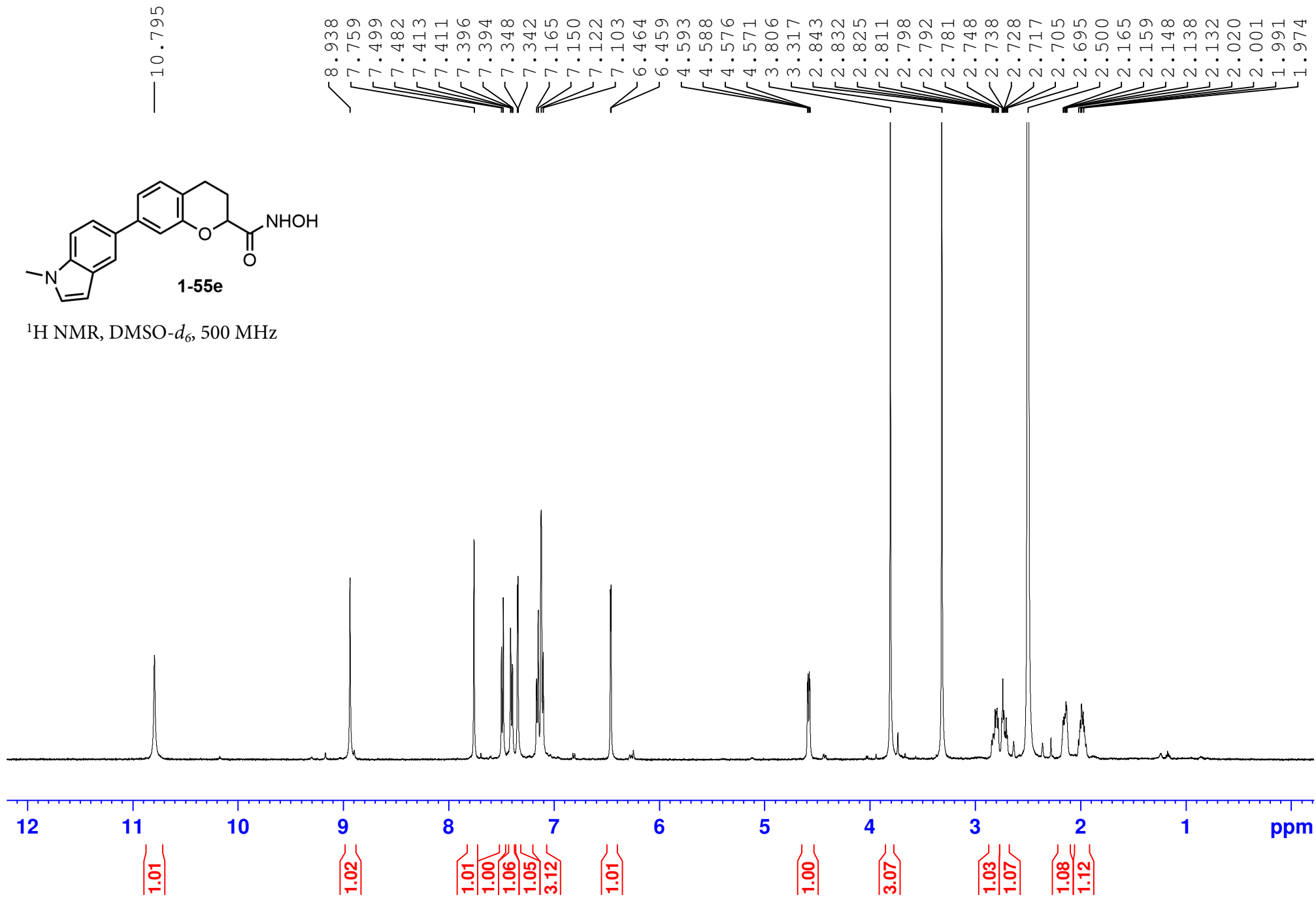


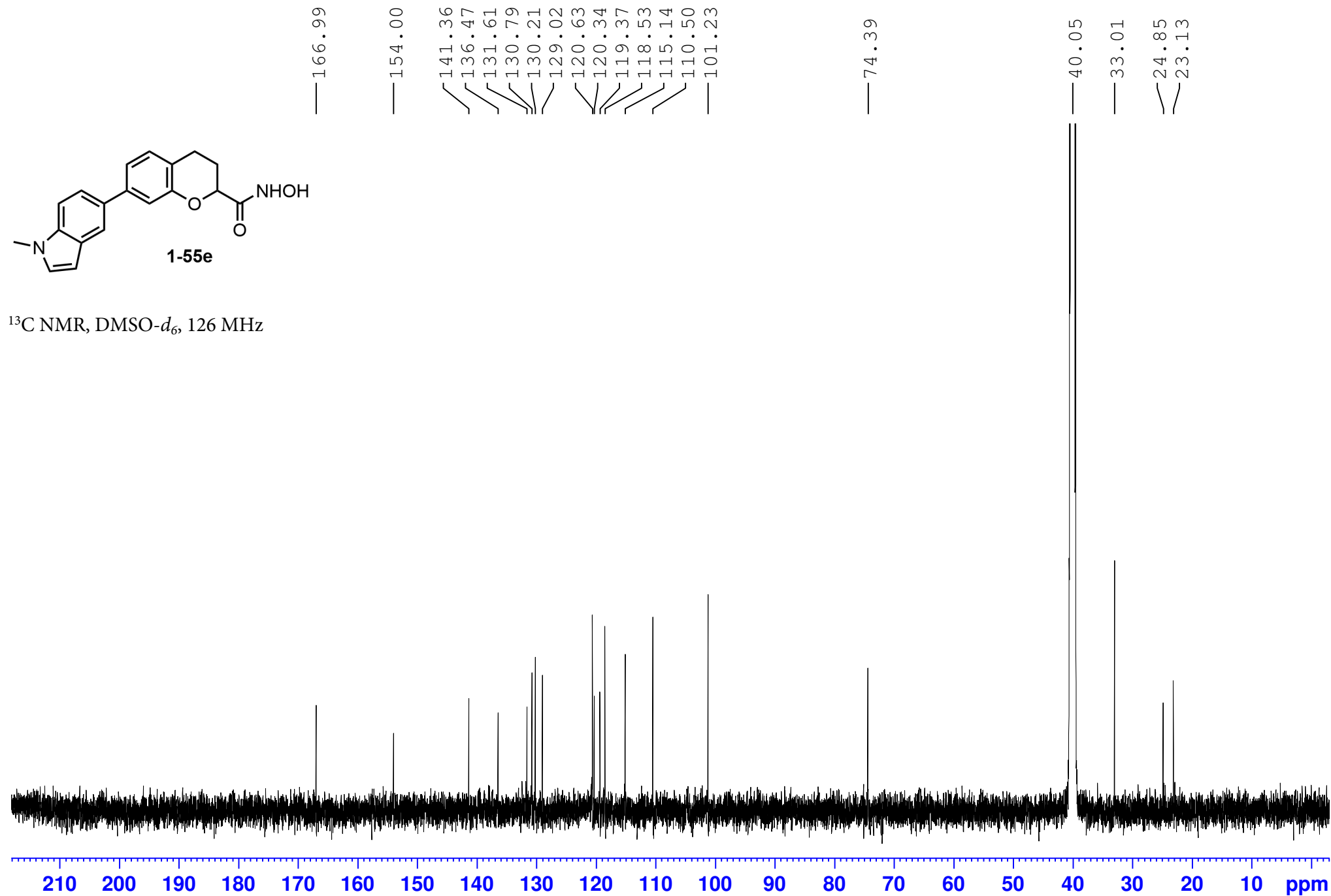
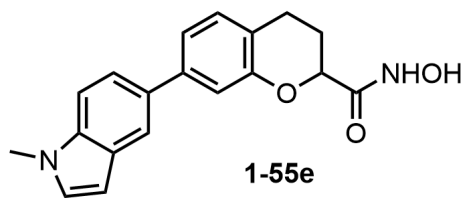
^{13}C NMR, DMSO- d_6 , 101 MHz

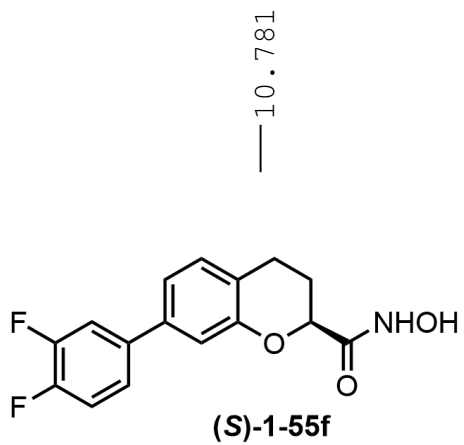




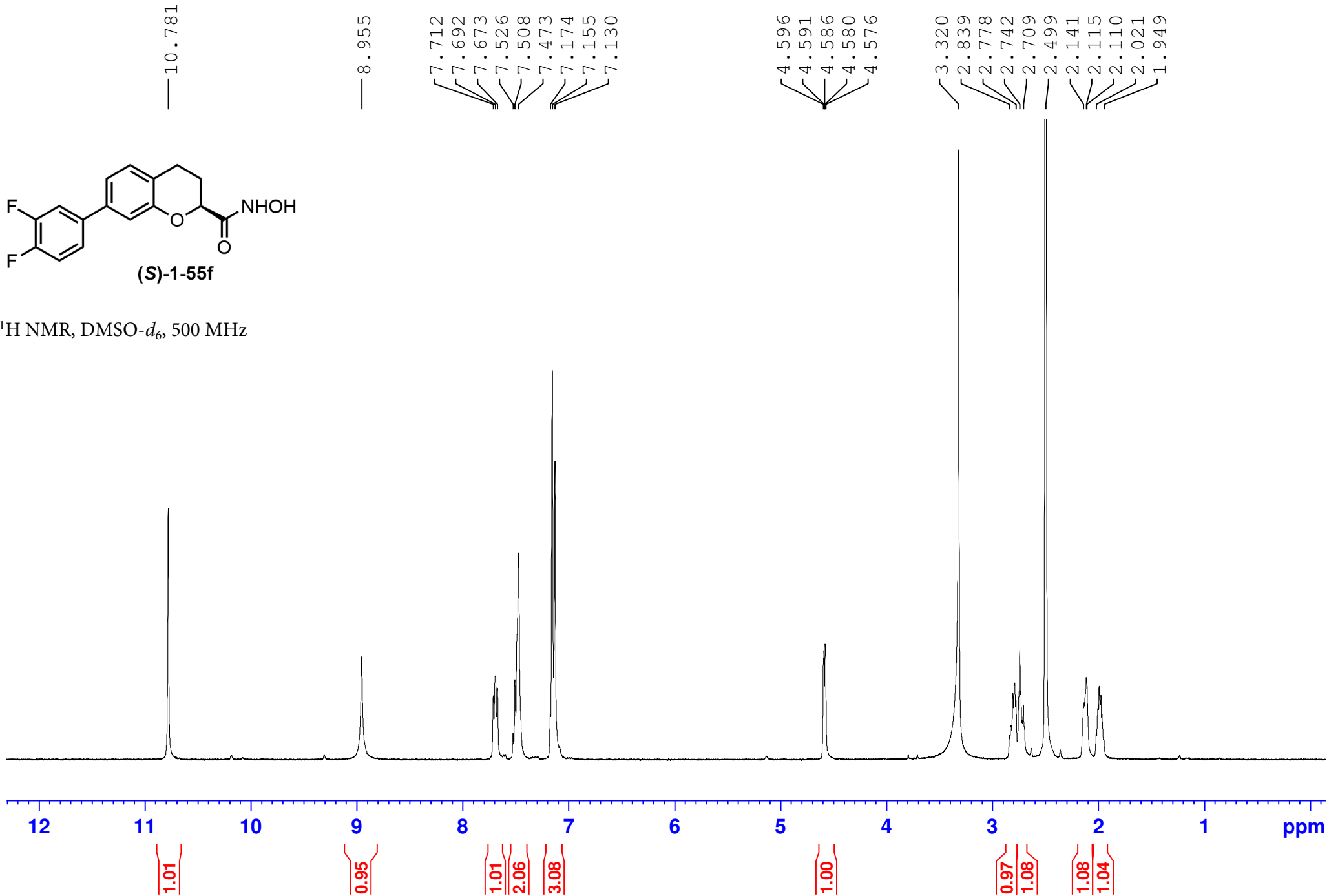
$^1\text{H NMR}$, $\text{DMSO-}d_6$, 500 MHz

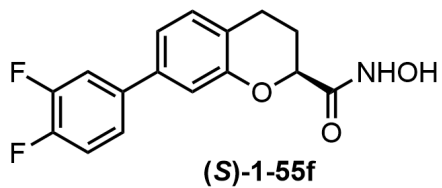




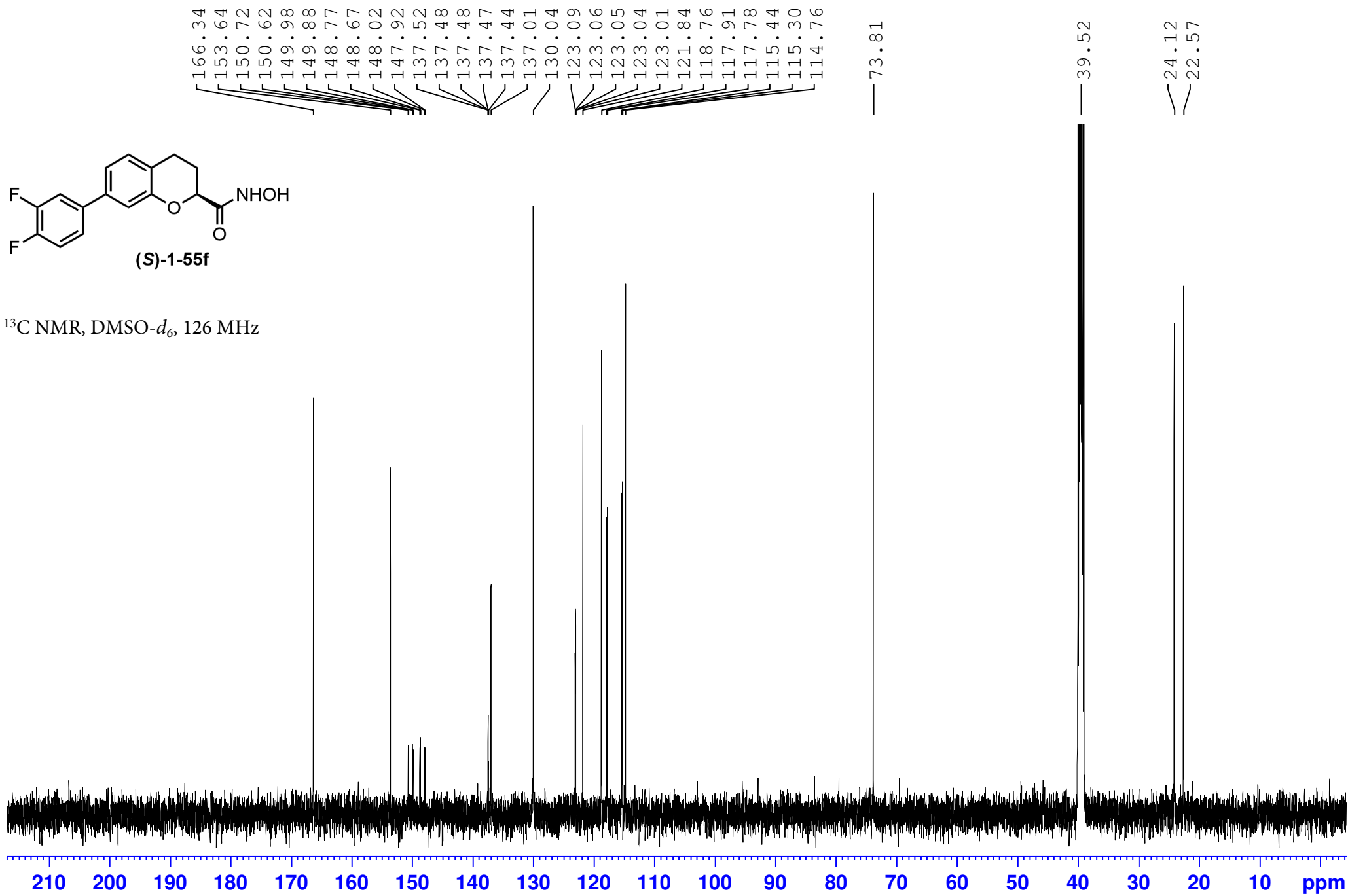


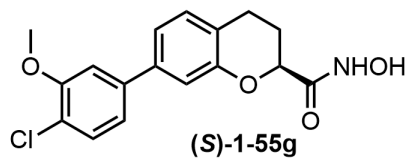
^1H NMR, DMSO- d_6 , 500 MHz





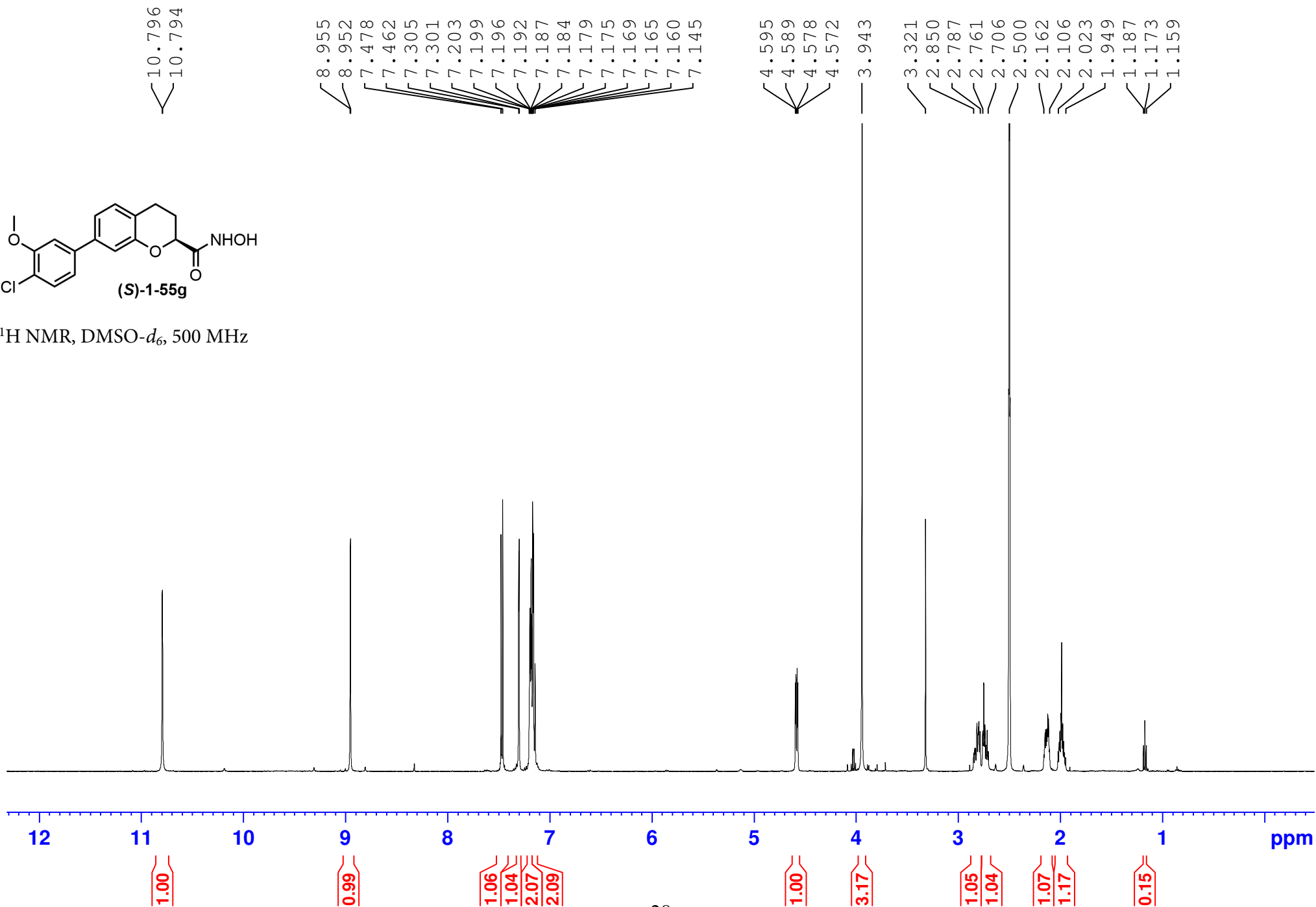
^{13}C NMR, $\text{DMSO-}d_6$, 126 MHz

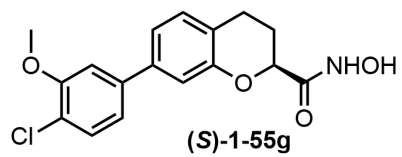




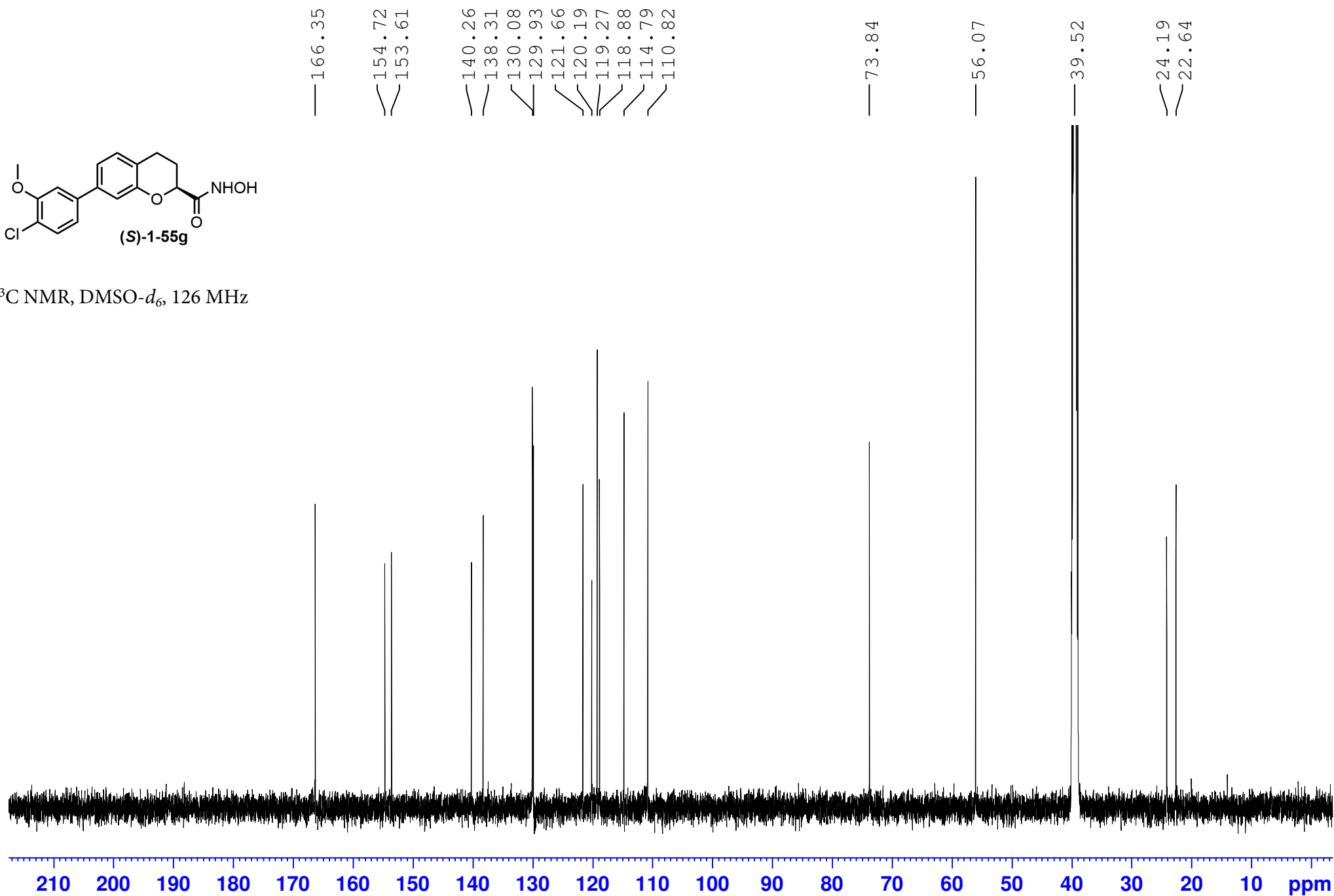
(S)-1-55g

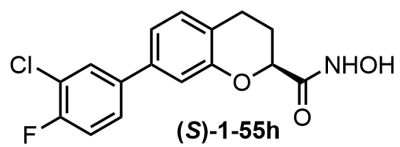
^1H NMR, DMSO- d_6 , 500 MHz



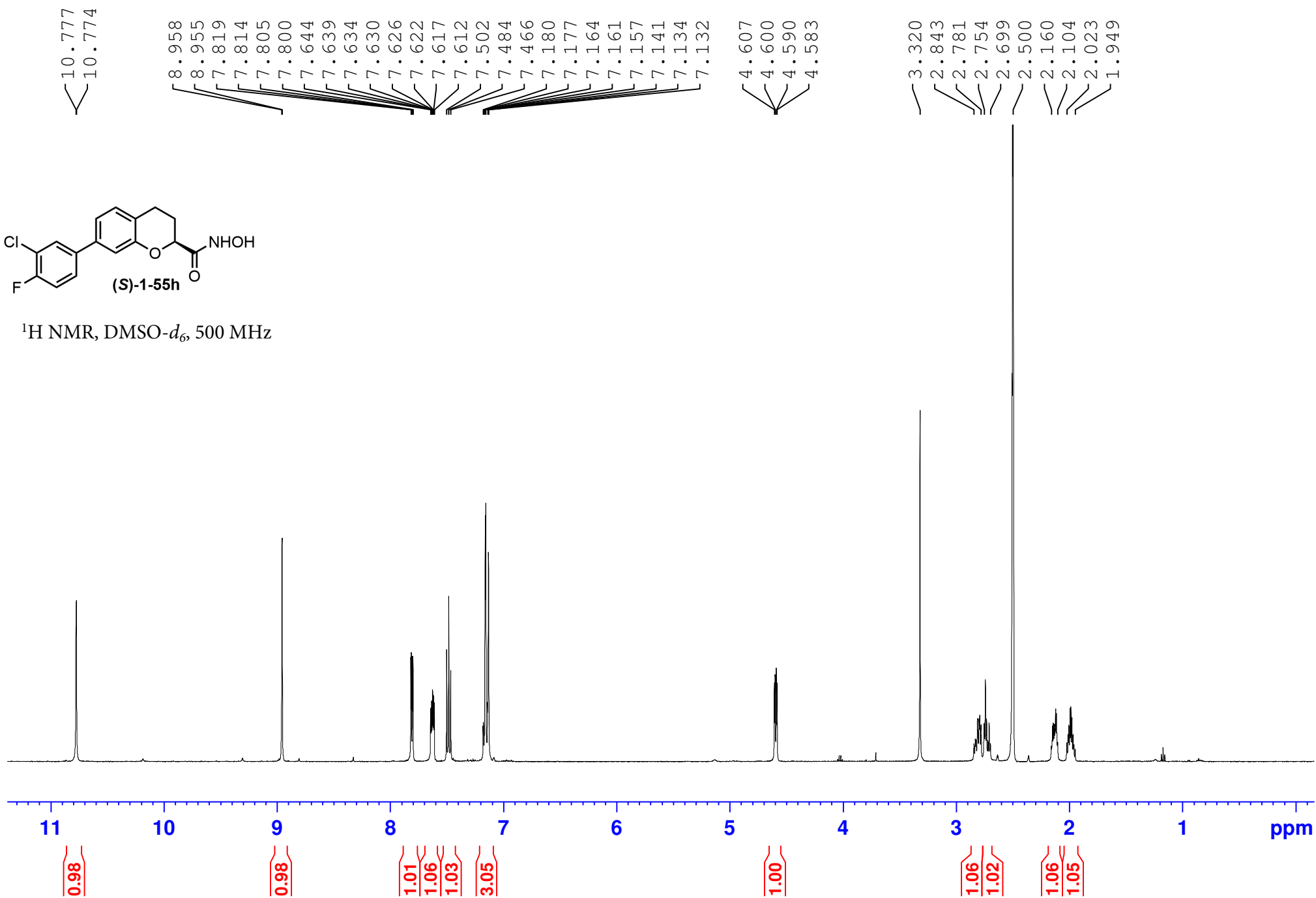


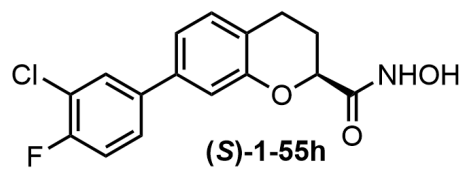
^{13}C NMR, DMSO- d_6 , 126 MHz



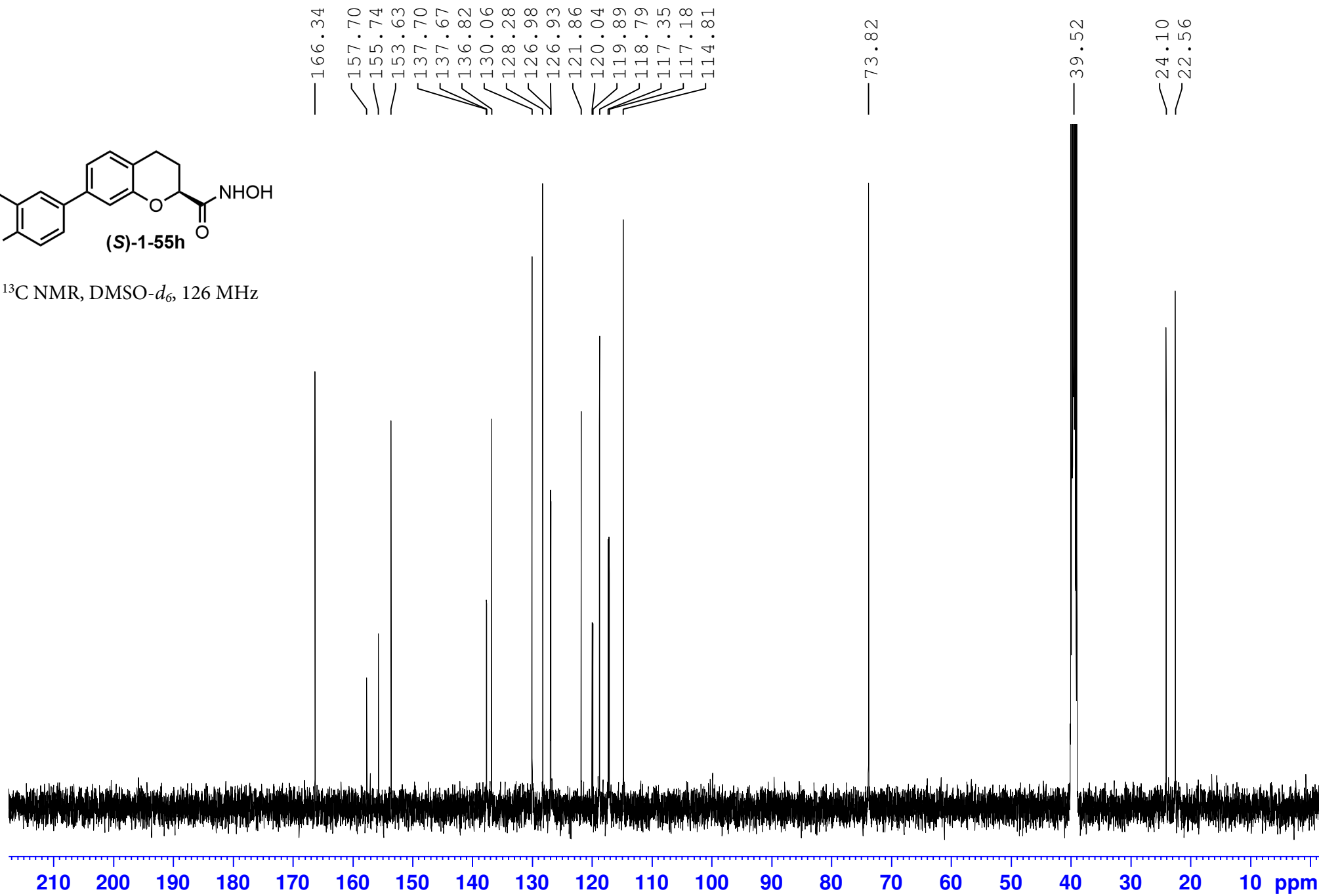


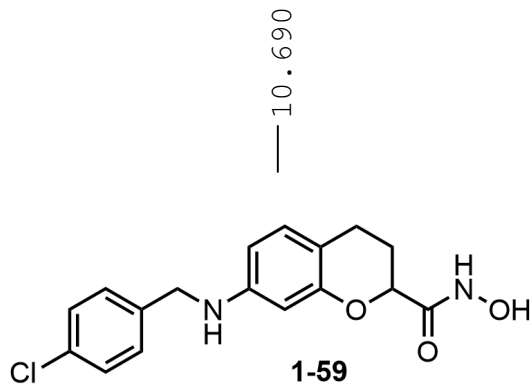
$^1\text{H NMR}$, $\text{DMSO-}d_6$, 500 MHz



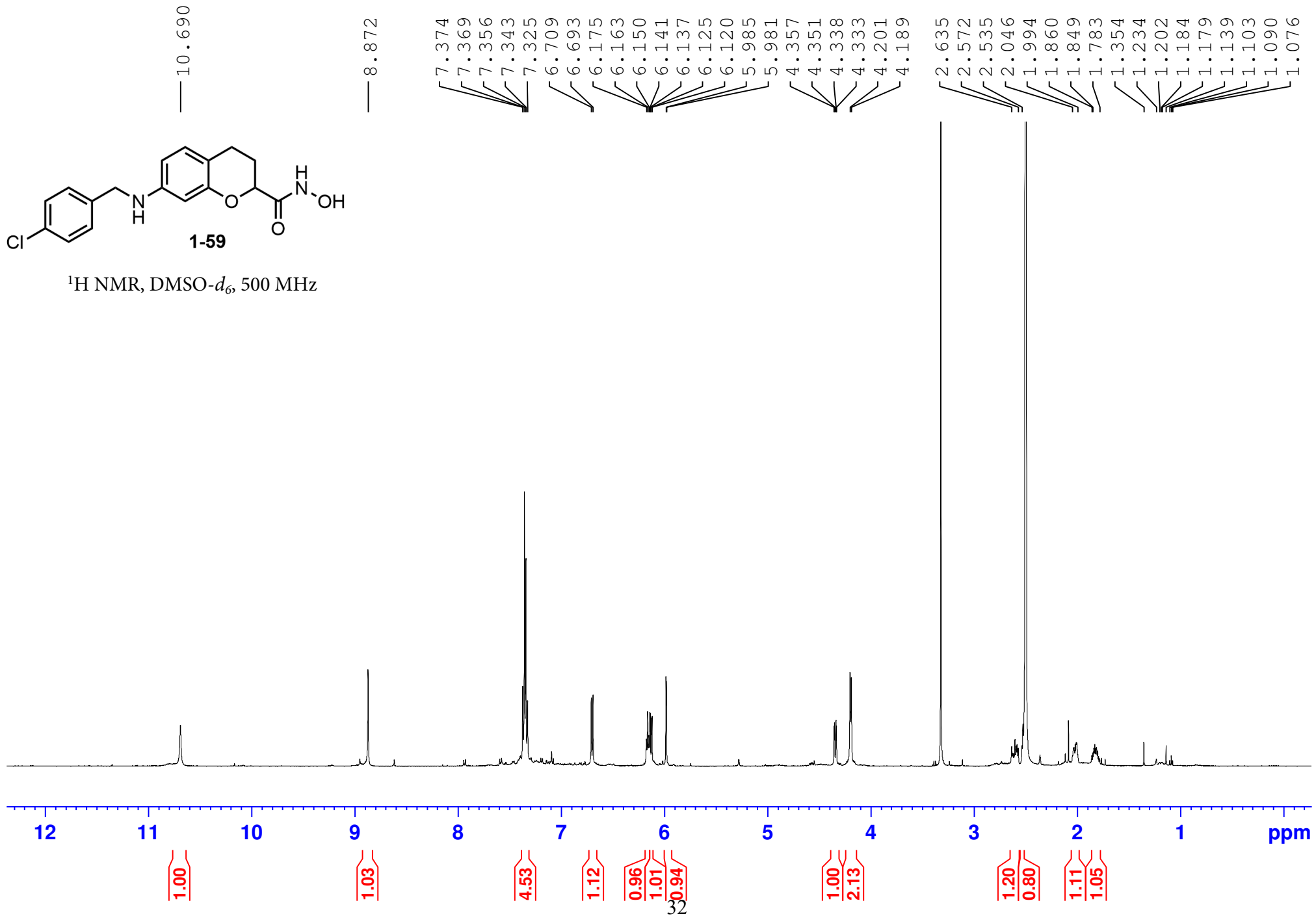


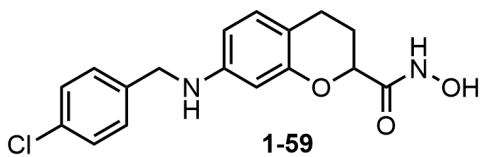
^{13}C NMR, DMSO- d_6 , 126 MHz



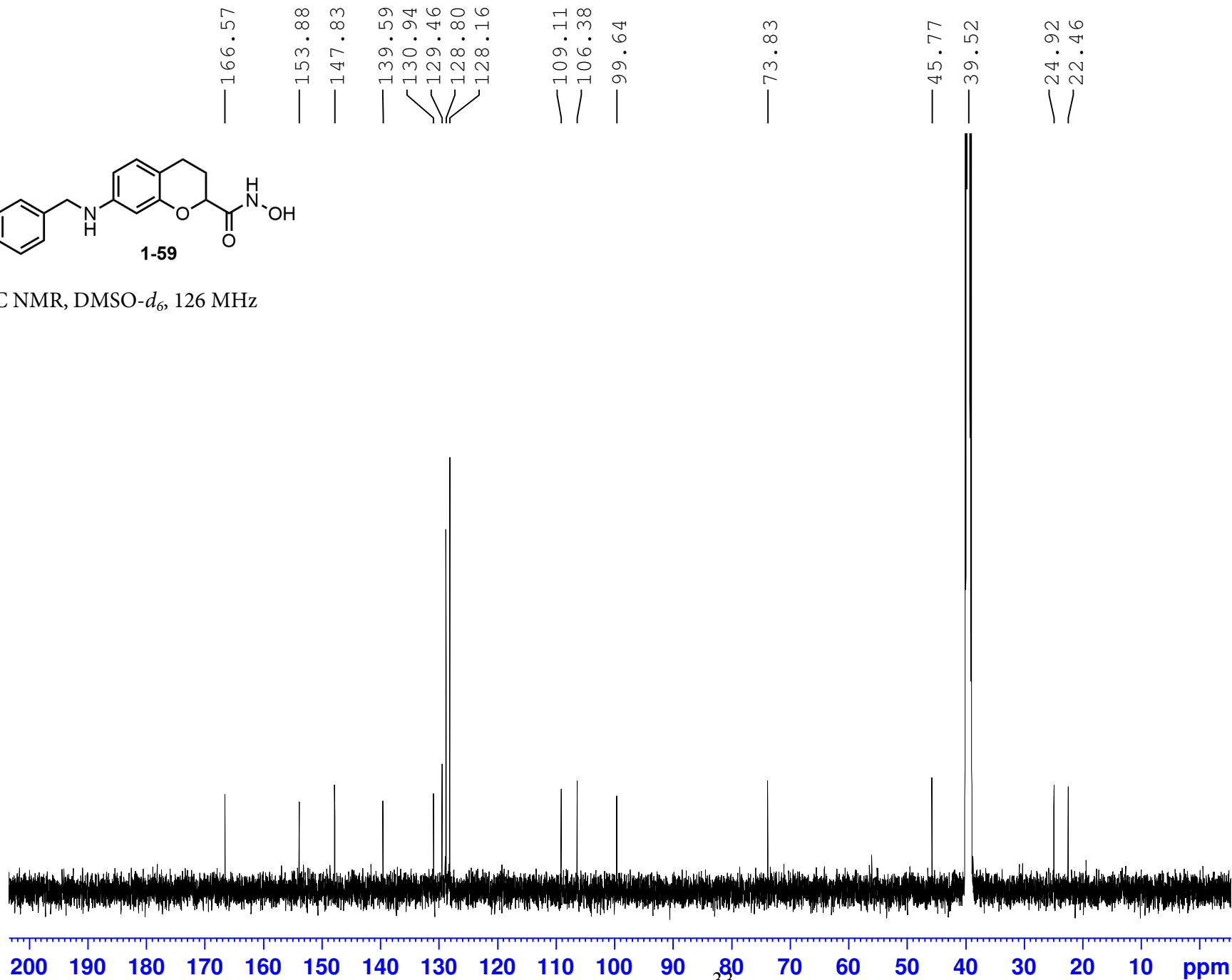


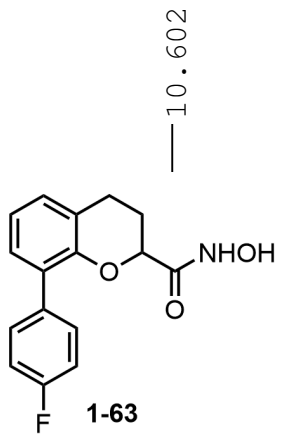
¹H NMR, DMSO-*d*₆, 500 MHz





^{13}C NMR, $\text{DMSO-}d_6$, 126 MHz

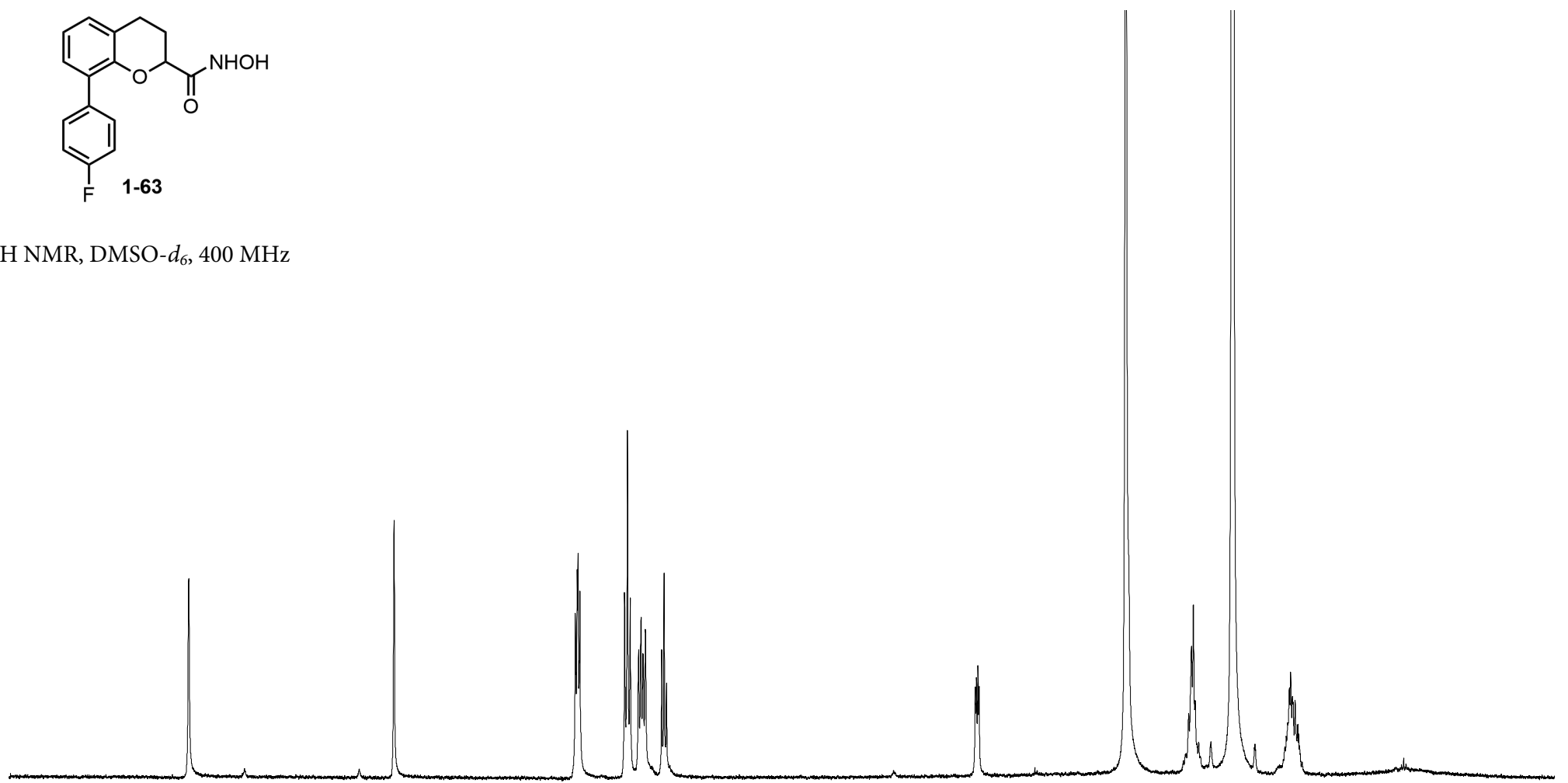


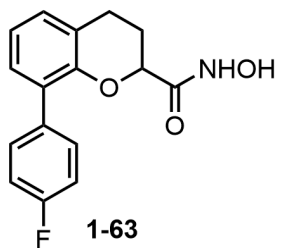


— 10.602

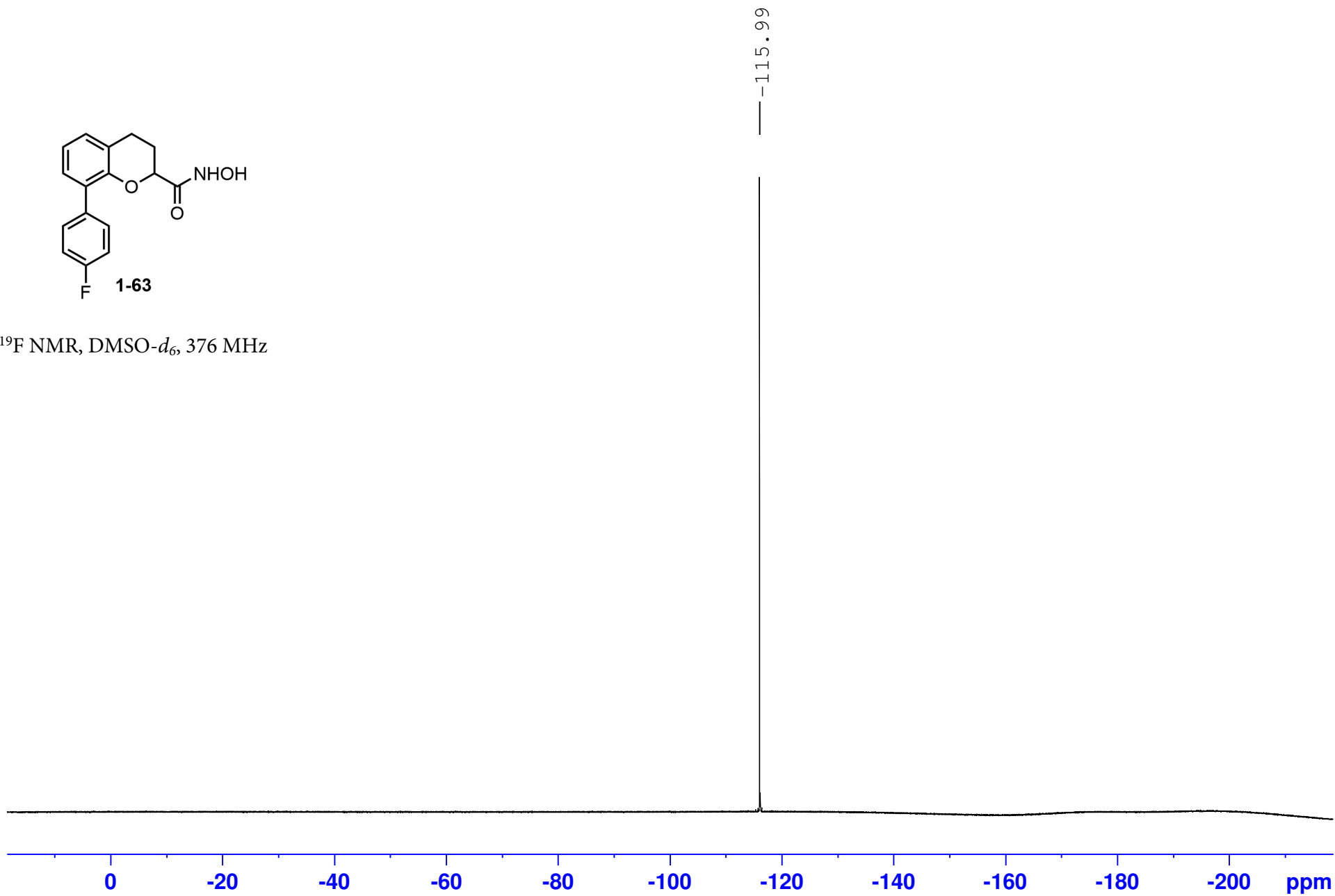
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 7.077
 7.058
 6.932
 6.913
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 4.477
 4.468
 3.328
 2.882
 2.861
 2.763
 2.500
 2.137
 1.960

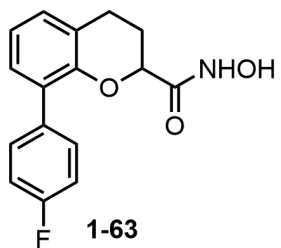
¹H NMR, DMSO-*d*₆, 400 MHz





^{19}F NMR, $\text{DMSO-}d_6$, 376 MHz





— 166.64
— 162.42
— 160.00

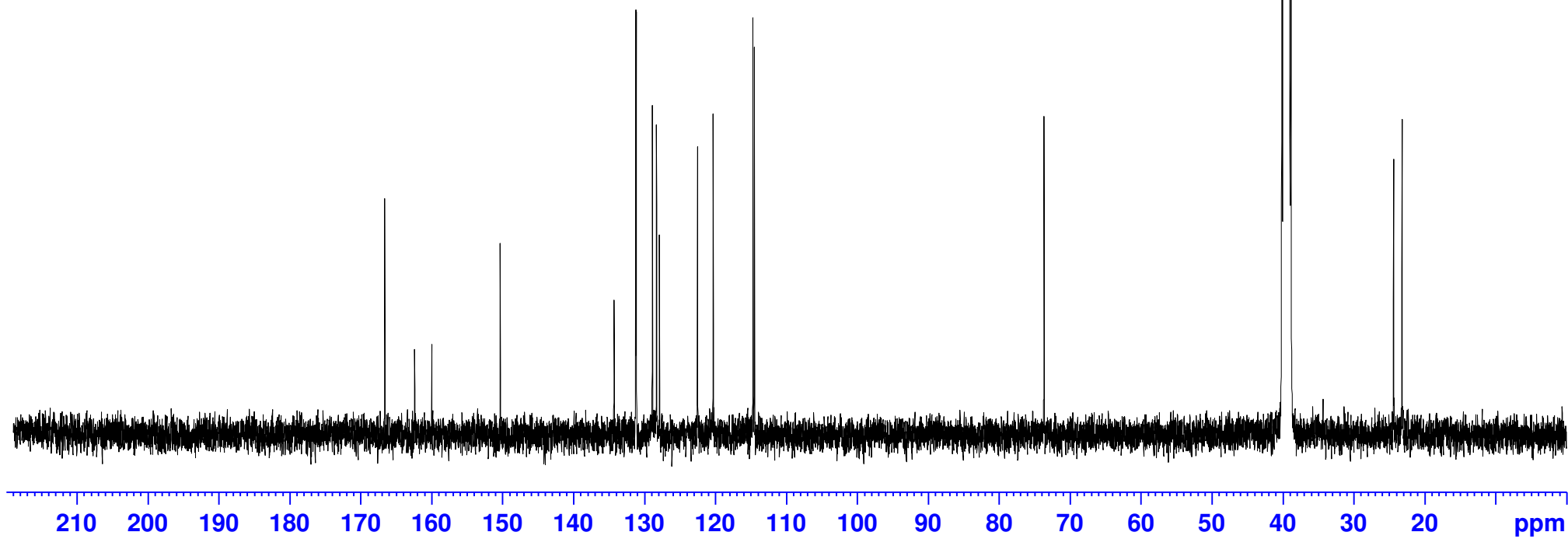
— 150.36
— 134.33
— 134.29
— 131.24
— 131.16
— 128.91
— 128.33
— 127.91
— 122.54
— 120.34
— 114.73
— 114.53

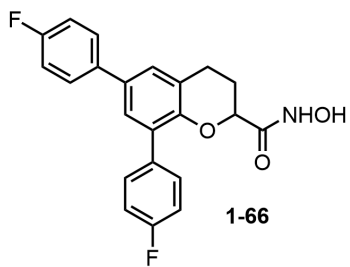
— 73.69

— 39.52

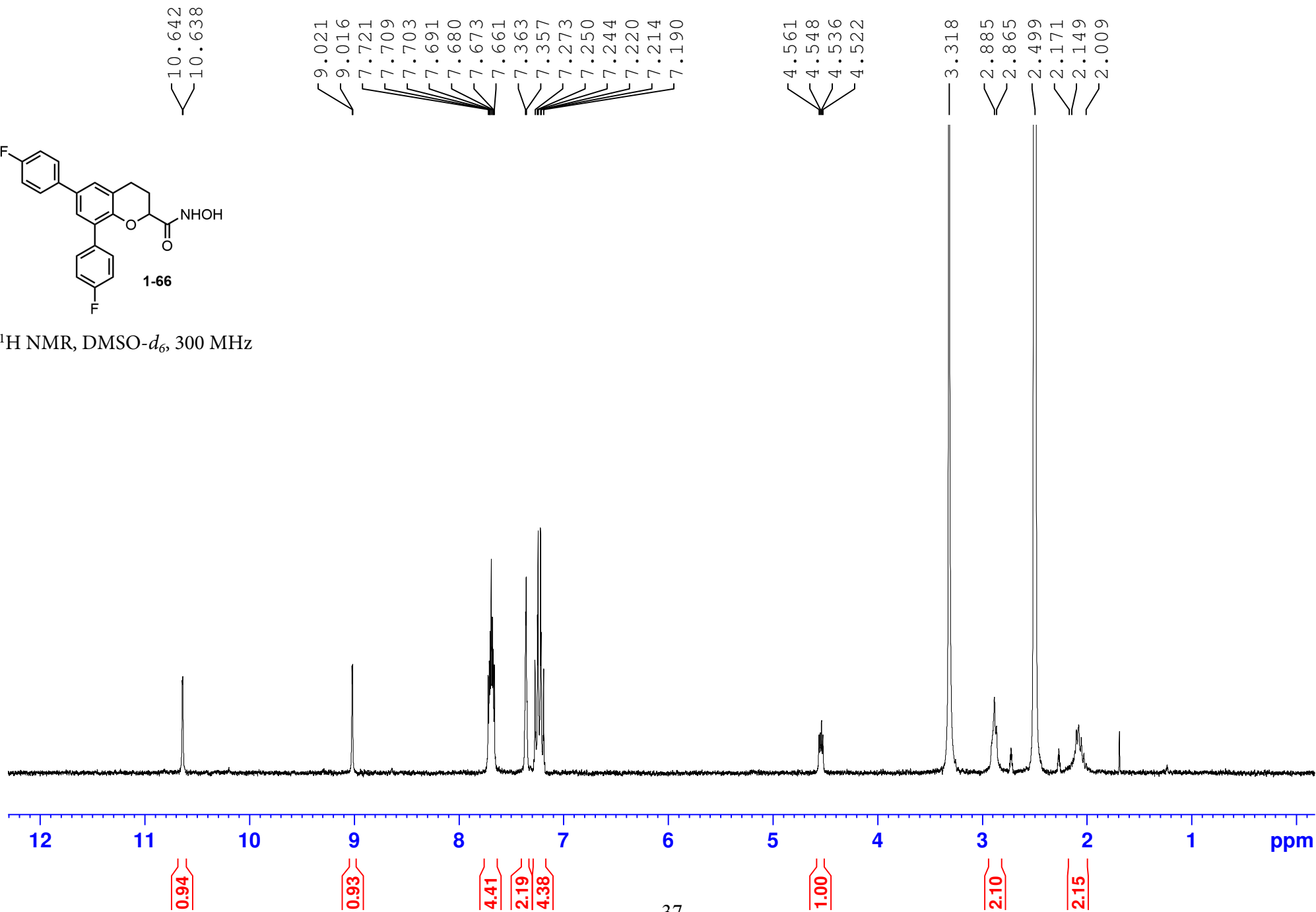
— 24.40
— 23.21

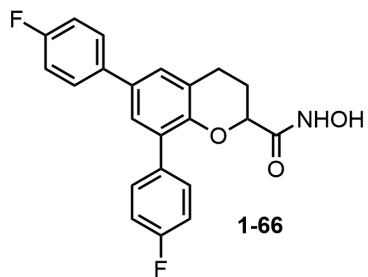
^{13}C NMR, DMSO- d_6 , 101 MHz



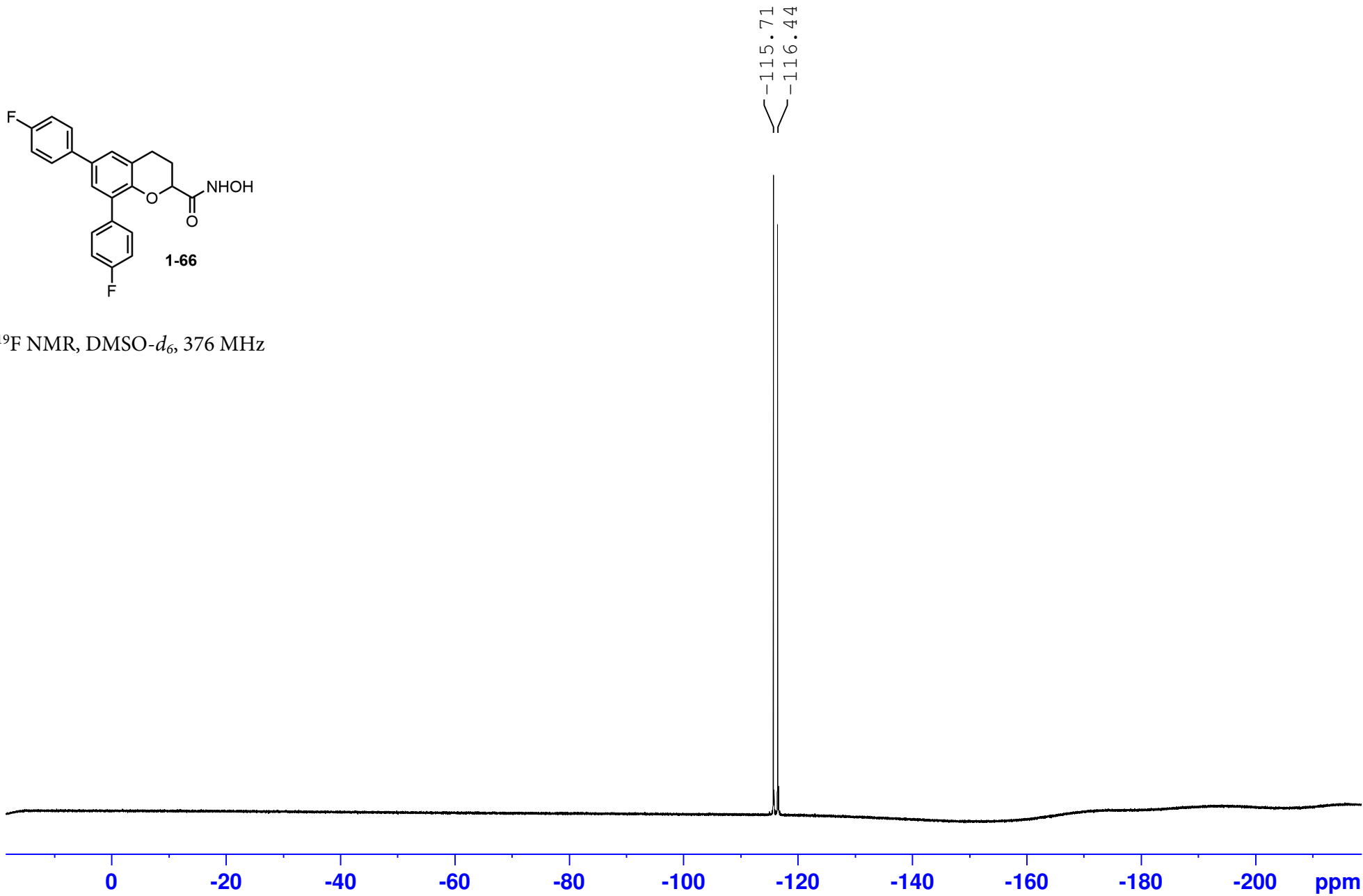


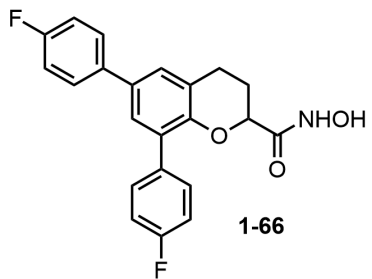
^1H NMR, DMSO- d_6 , 300 MHz



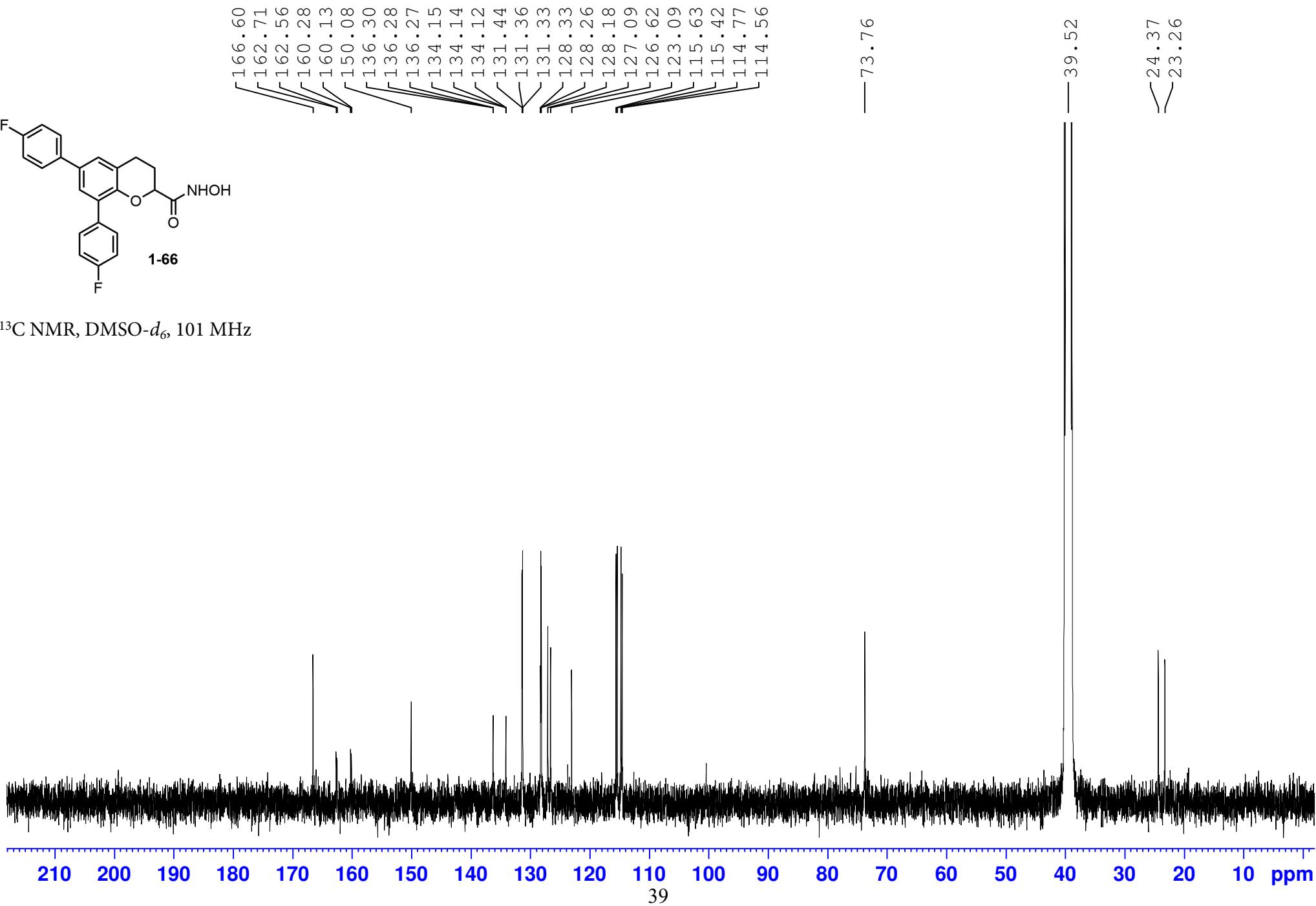


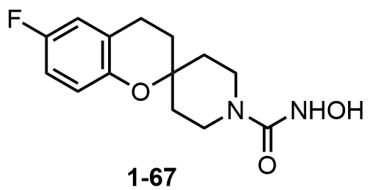
^{19}F NMR, $\text{DMSO-}d_6$, 376 MHz



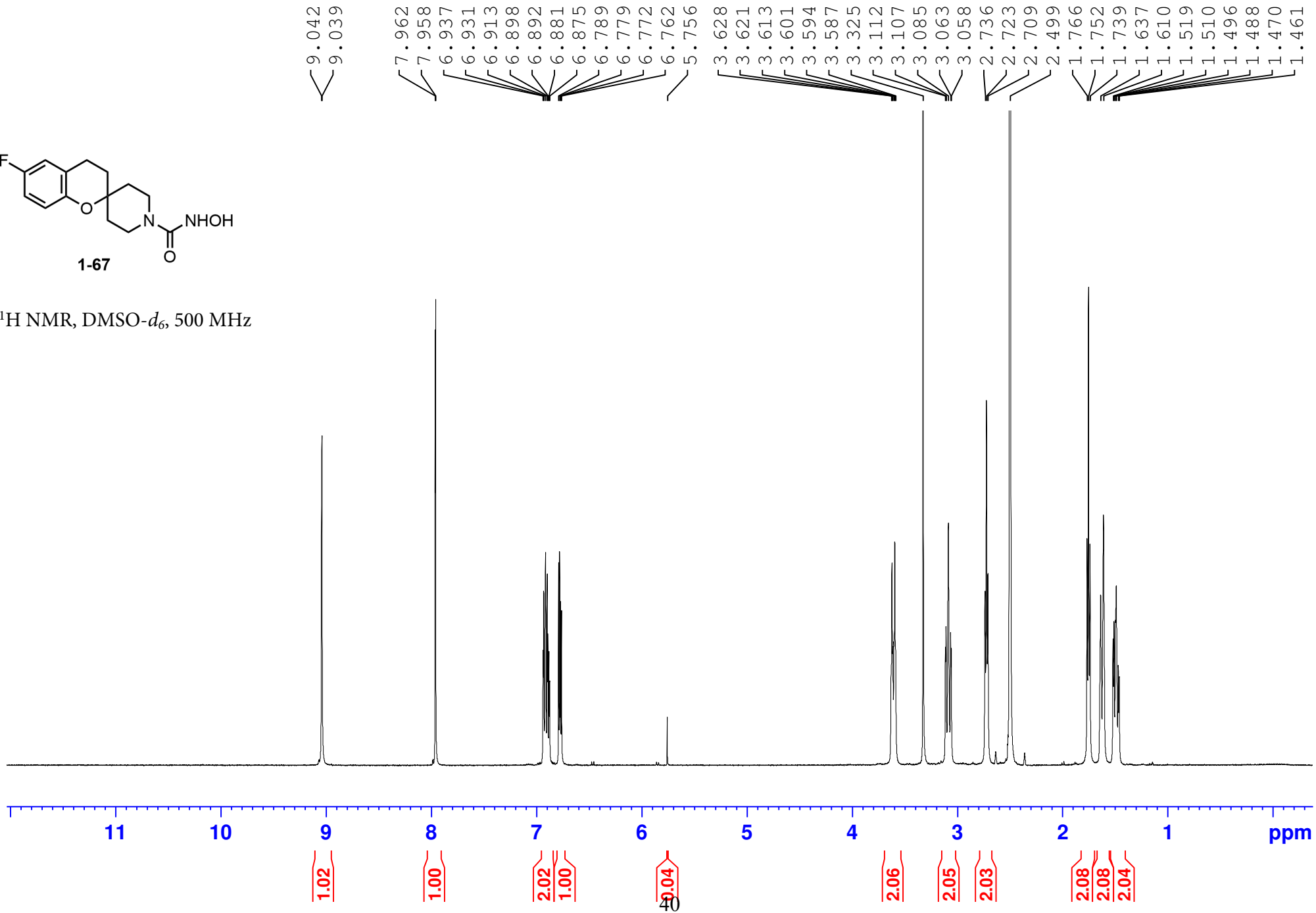


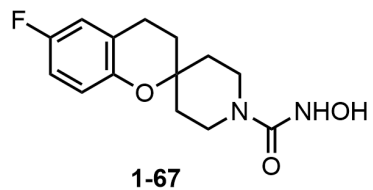
^{13}C NMR, DMSO- d_6 , 101 MHz



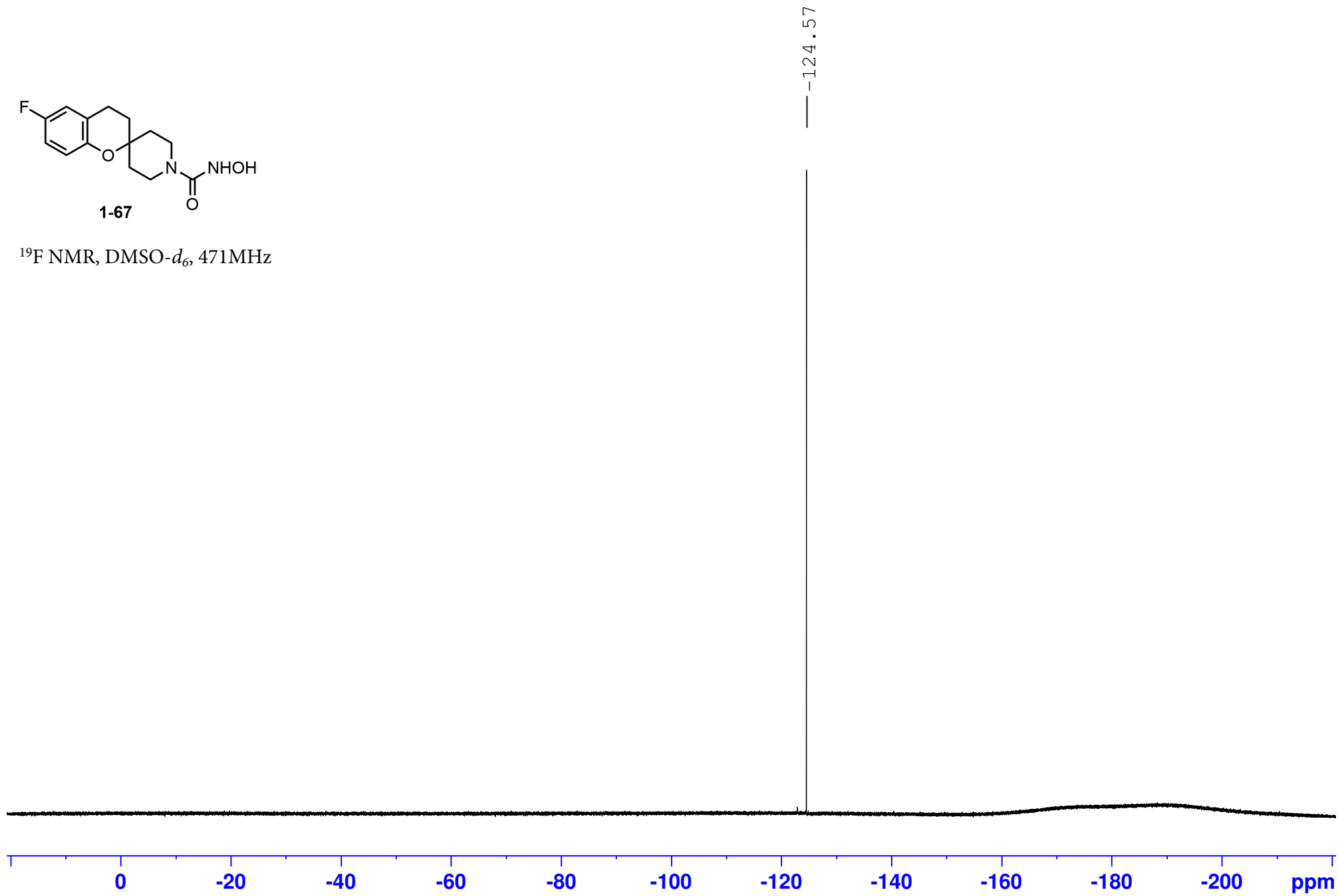


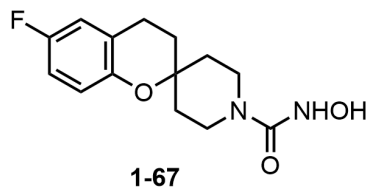
^1H NMR, DMSO- d_6 , 500 MHz





^{19}F NMR, $\text{DMSO-}d_6$, 471MHz





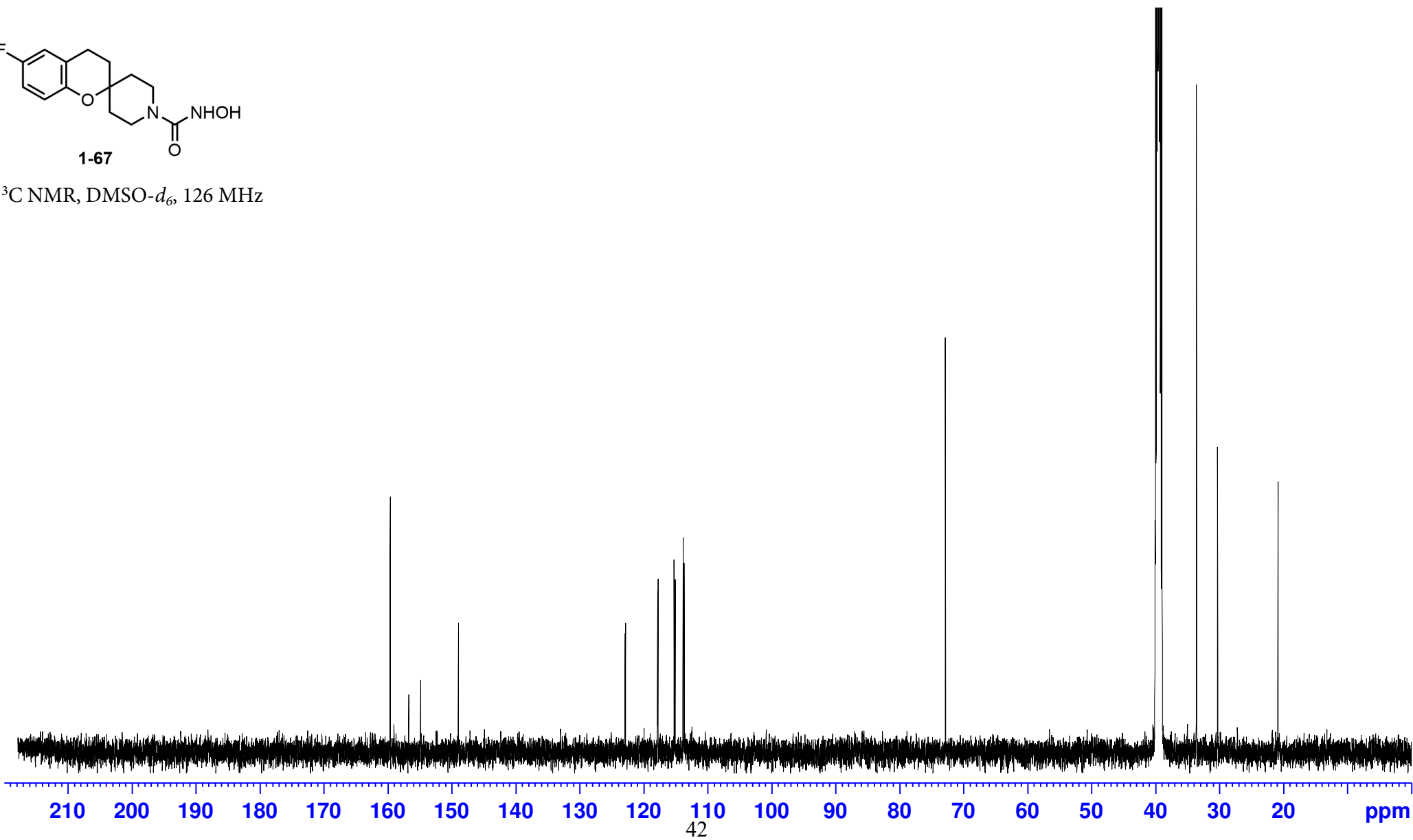
^{13}C NMR, $\text{DMSO-}d_6$, 126 MHz

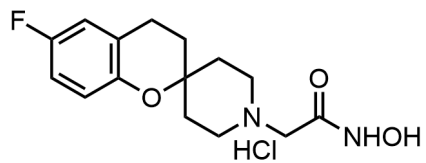
159.66
156.76
154.88
148.98

122.94
122.88
117.86
117.79
115.28
115.10
113.87
113.69

72.86

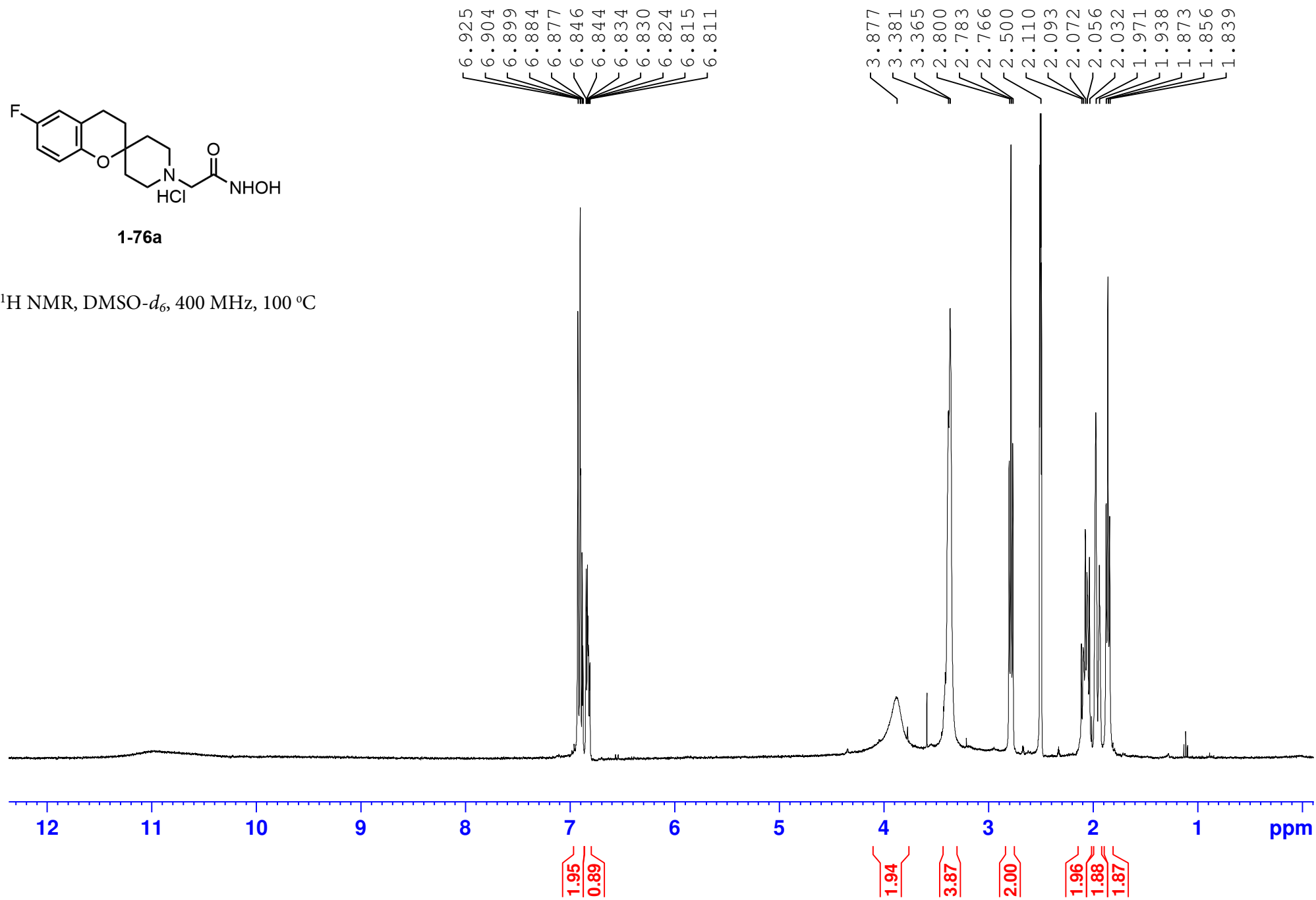
39.52
33.62
30.32
20.87

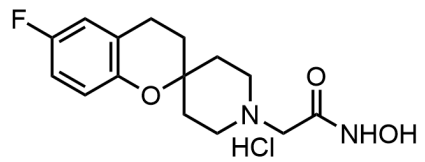




1-76a

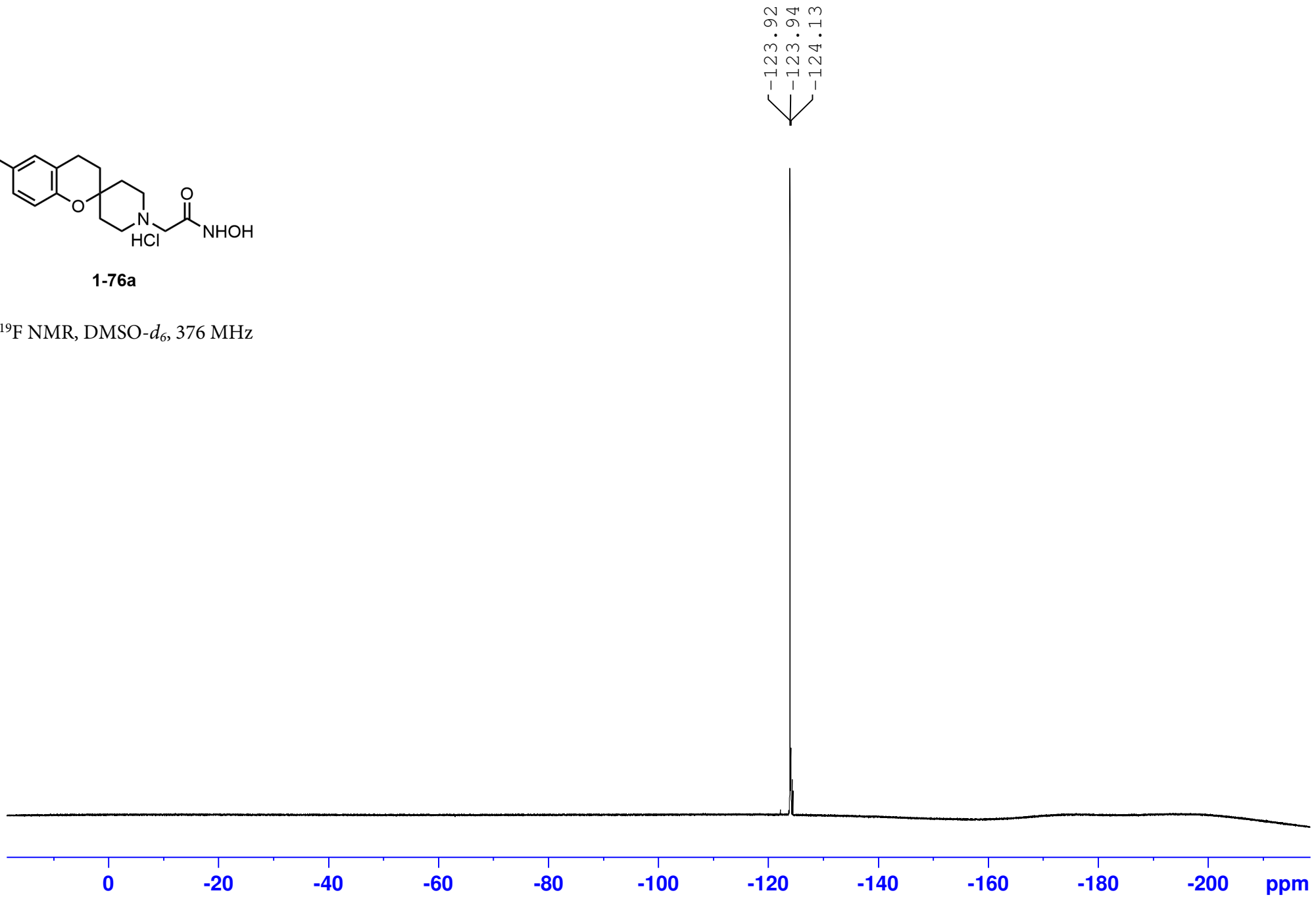
^1H NMR, DMSO- d_6 , 400 MHz, 100 °C

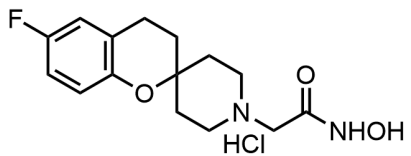




1-76a

¹⁹F NMR, DMSO-*d*₆, 376 MHz





1-76a

^{13}C NMR, DMSO- d_6 , 101 MHz

— 166.76
— 160.71
— 157.30
— 154.96
— 148.33

122.90
122.83
118.08
118.00
115.49
115.26
114.10
113.87

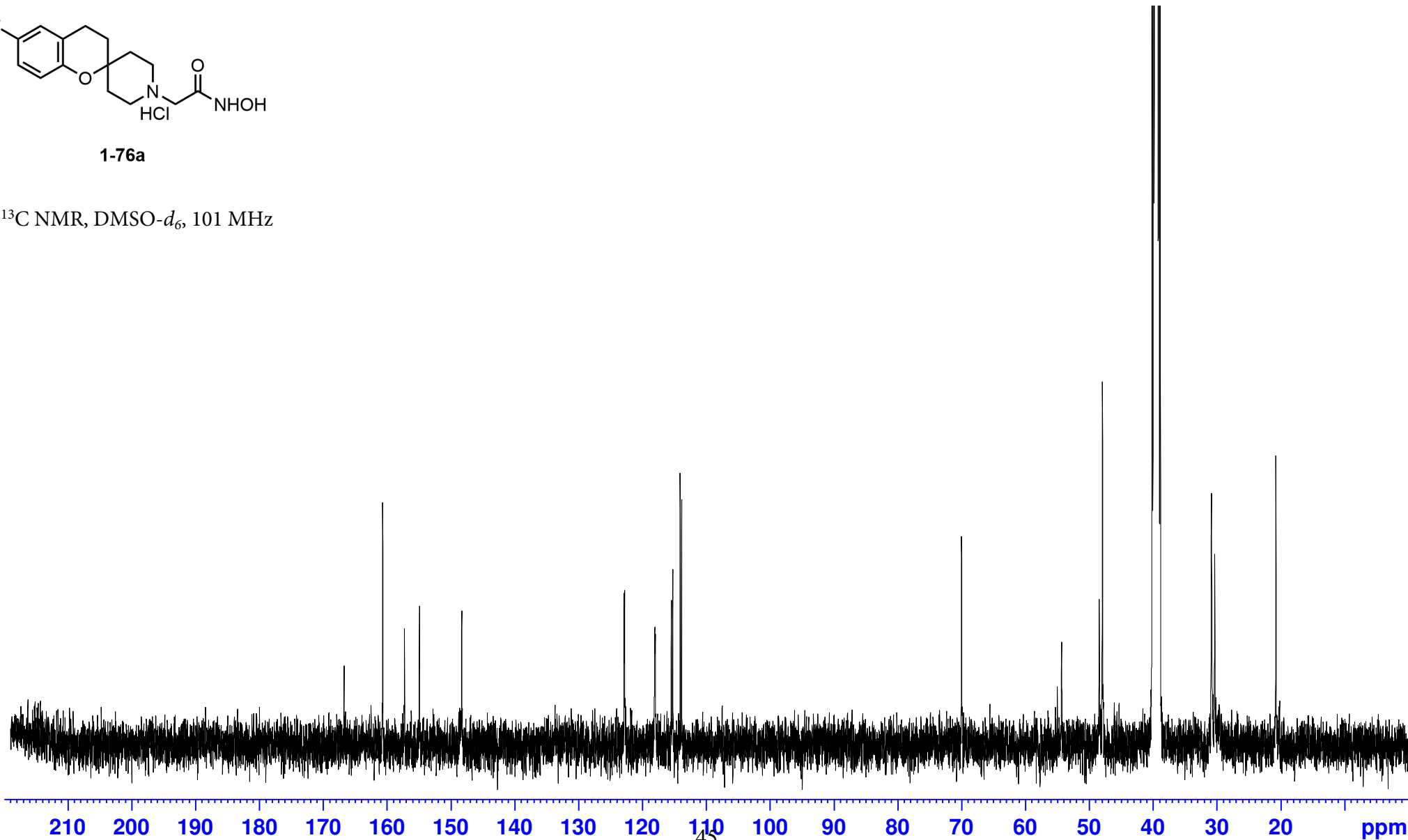
— 70.01

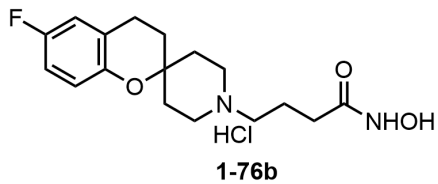
— 54.33
— 48.45
— 47.94

— 39.52

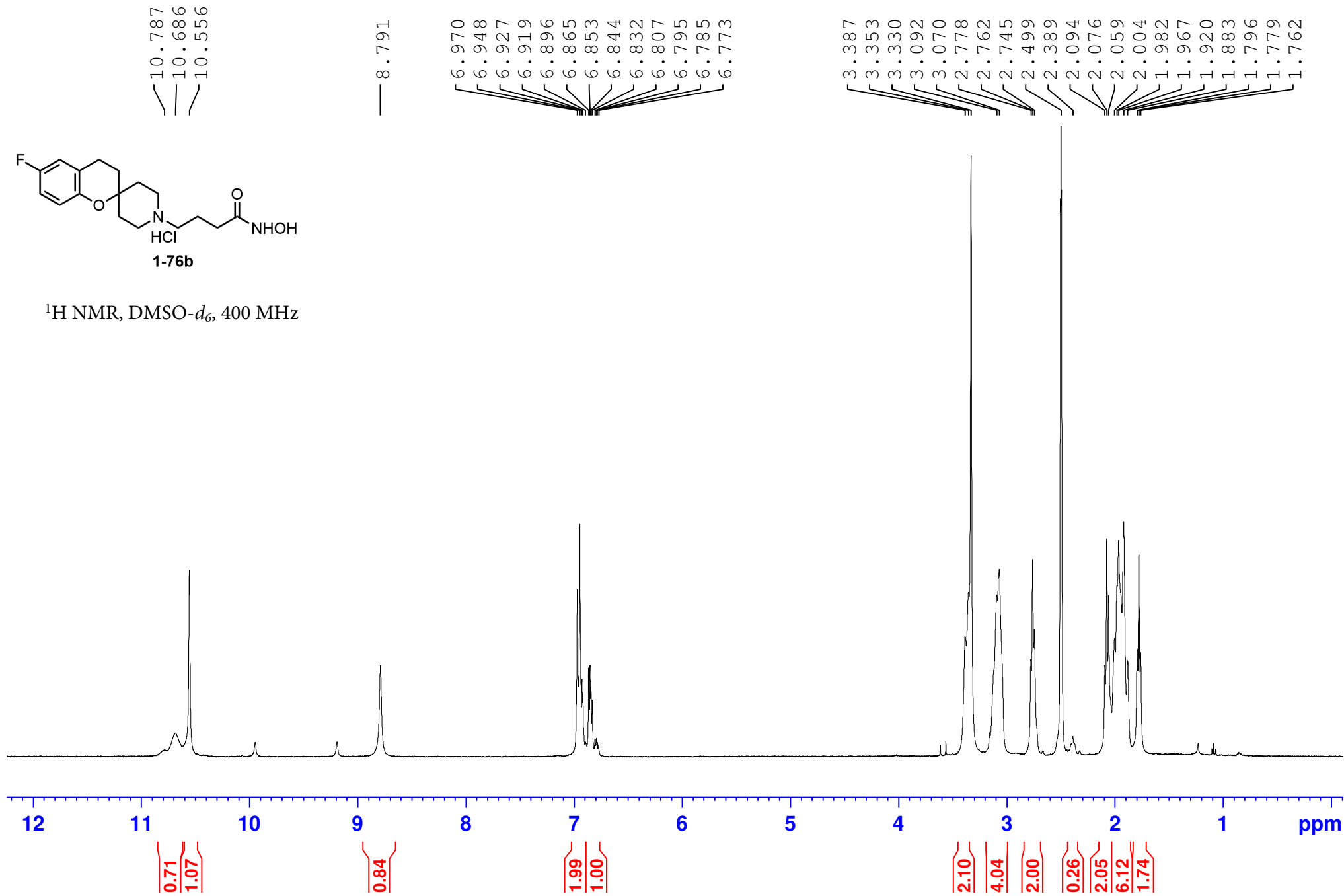
— 30.85
— 30.36

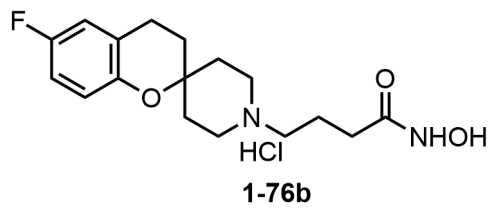
— 20.77



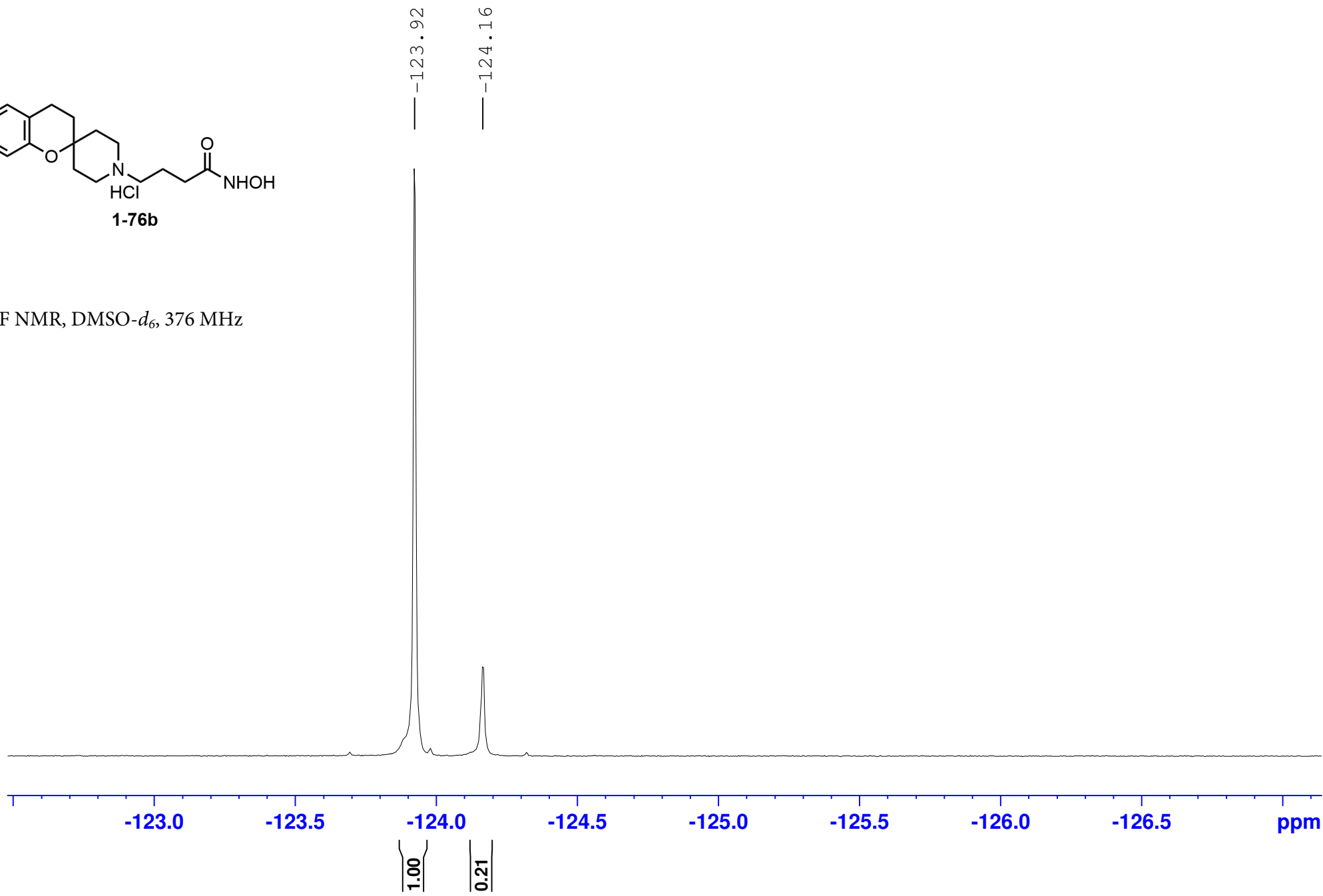


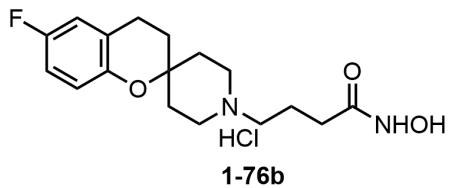
¹H NMR, DMSO-*d*₆, 400 MHz





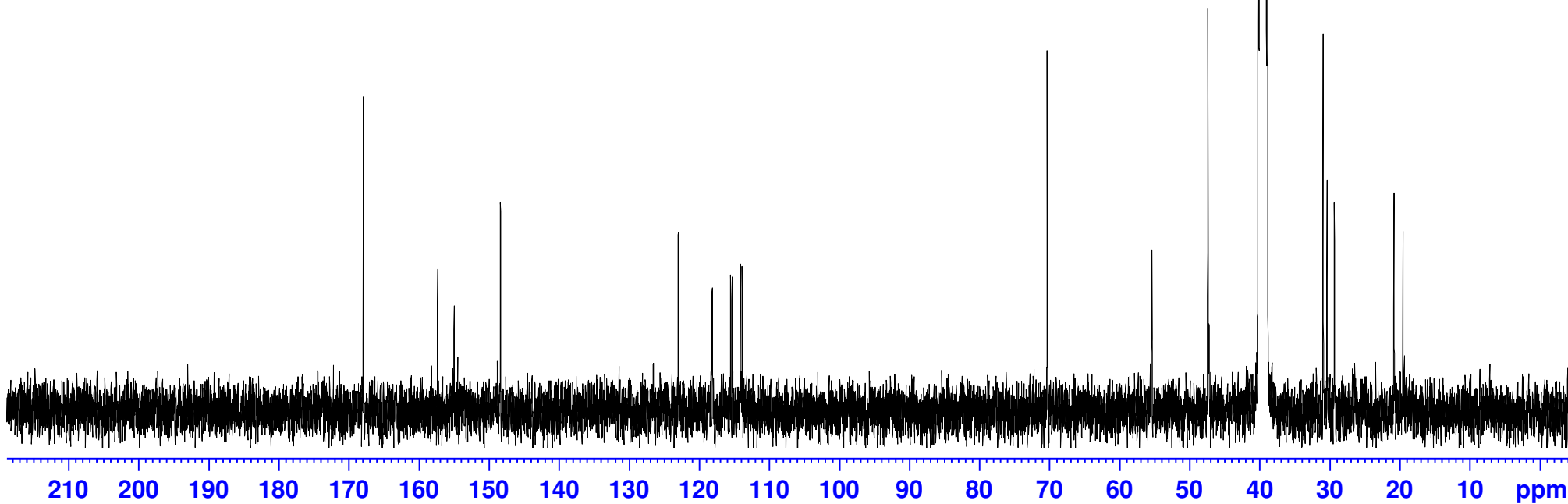
^{19}F NMR, DMSO- d_6 , 376 MHz

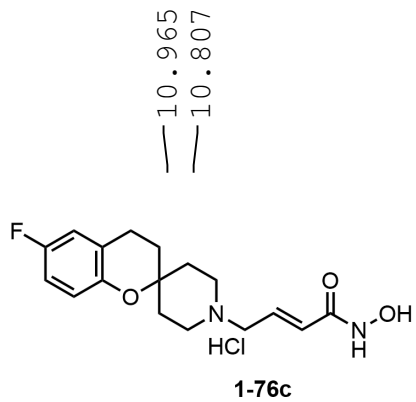




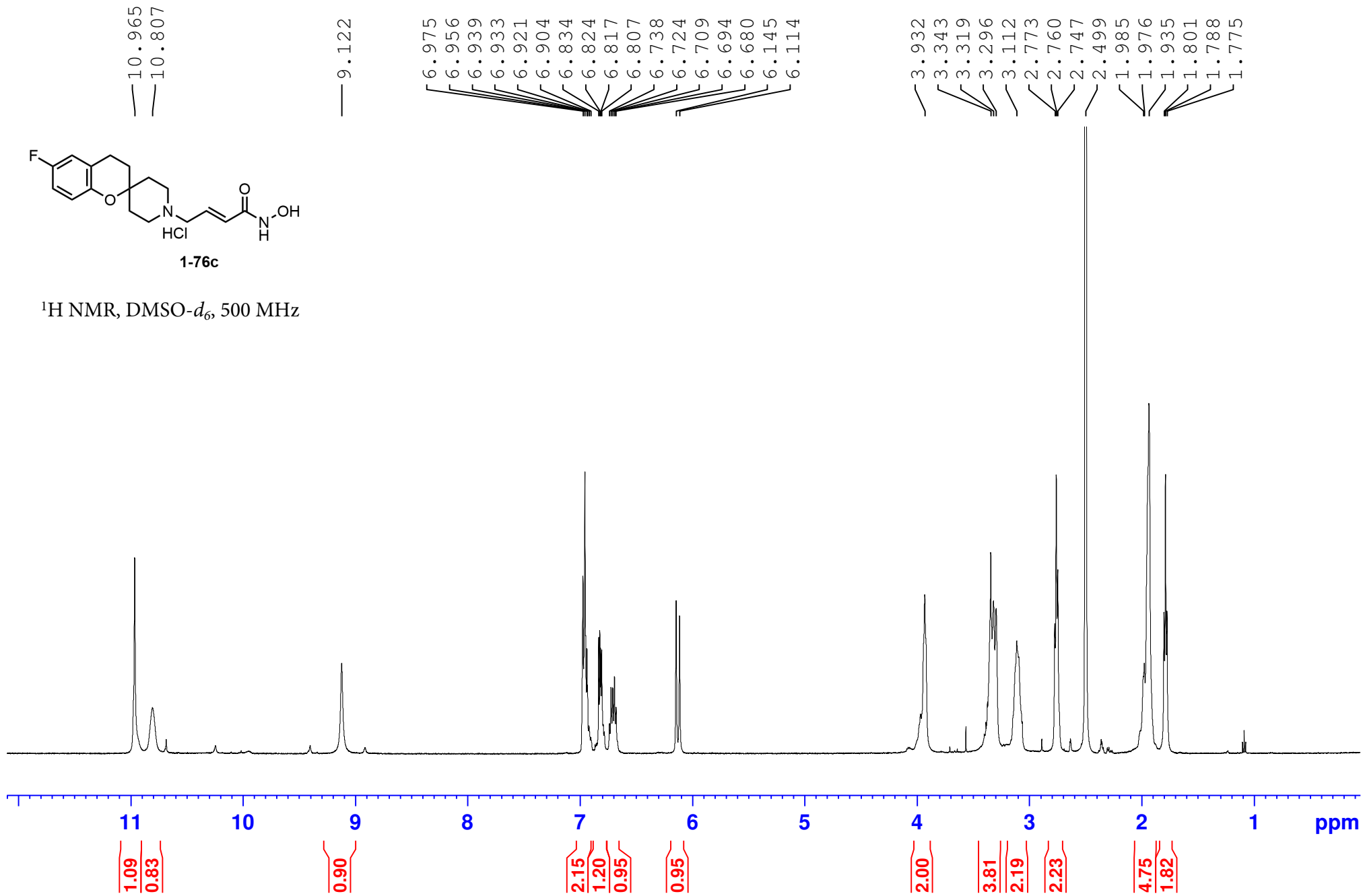
— 167.92
— 157.32
— 154.97
— 148.35
122.97
122.89
118.16
118.07
115.49
115.26
114.08
113.85
— 70.32
— 55.35
— 47.37
— 39.52
30.91
30.36
29.31
20.80
19.50

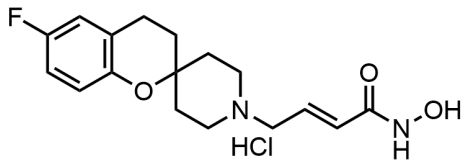
^{13}C NMR, DMSO- d_6 , 101 MHz





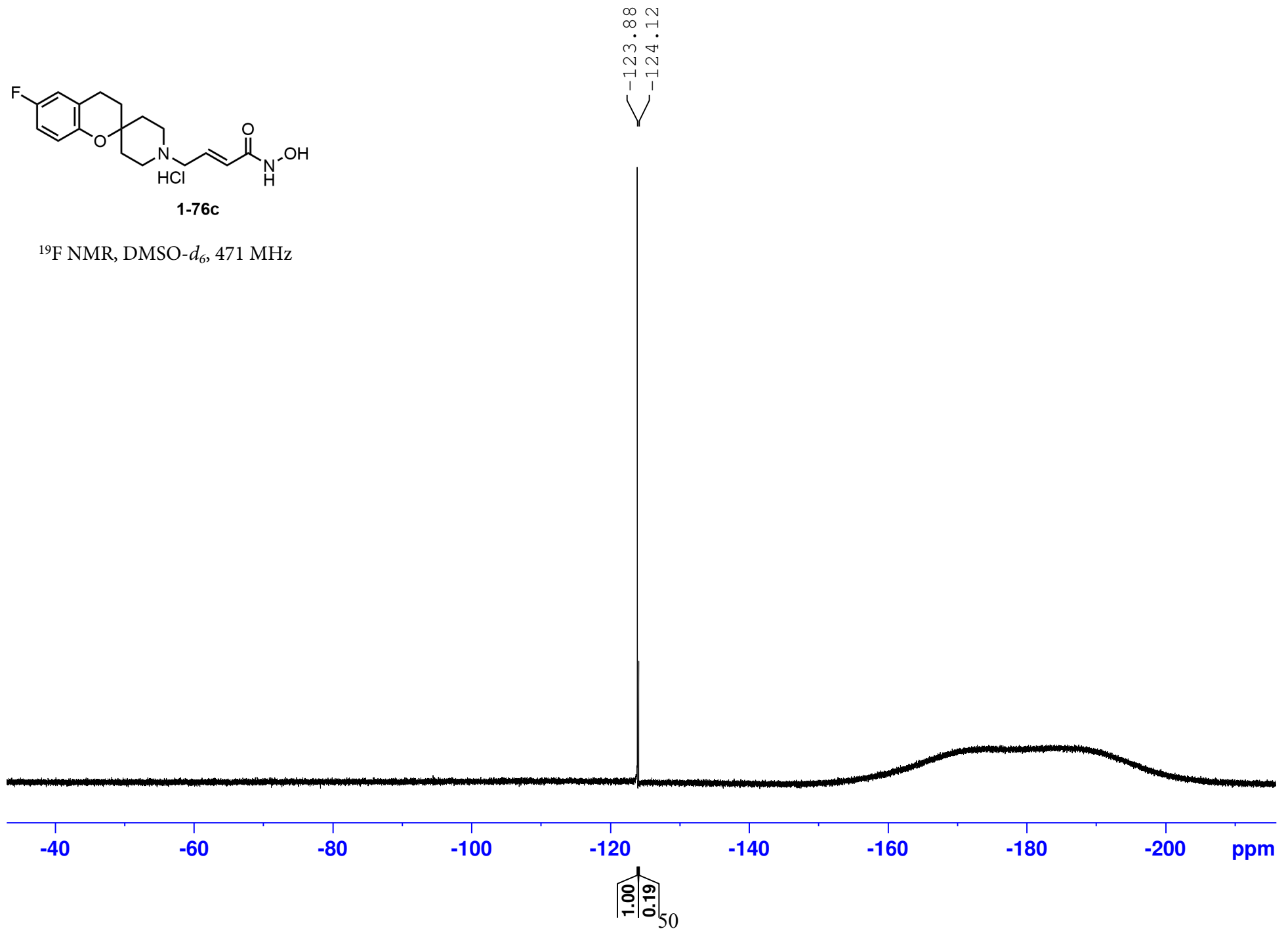
$^1\text{H NMR}$, $\text{DMSO-}d_6$, 500 MHz

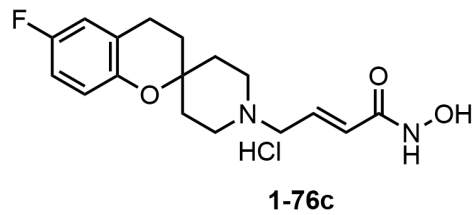




1-76c

^{19}F NMR, DMSO- d_6 , 471 MHz





160.84
 157.31
 154.97
 148.32

129.70
 129.12
 122.97
 122.89
 118.06
 117.97
 115.53
 115.31
 114.10
 113.87

70.27

55.80

47.21

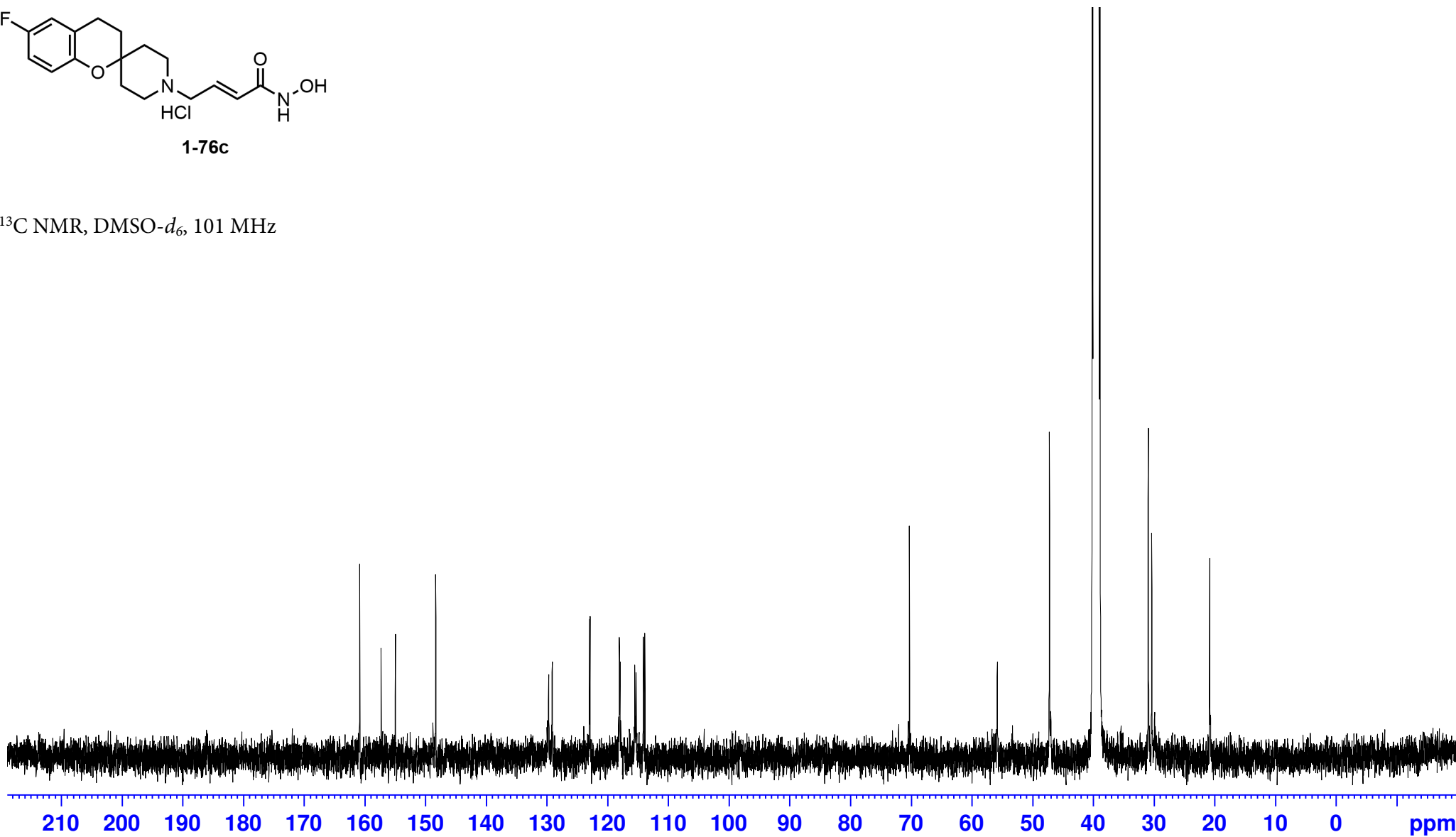
39.52

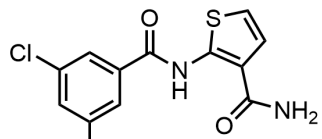
30.93

30.35

20.80

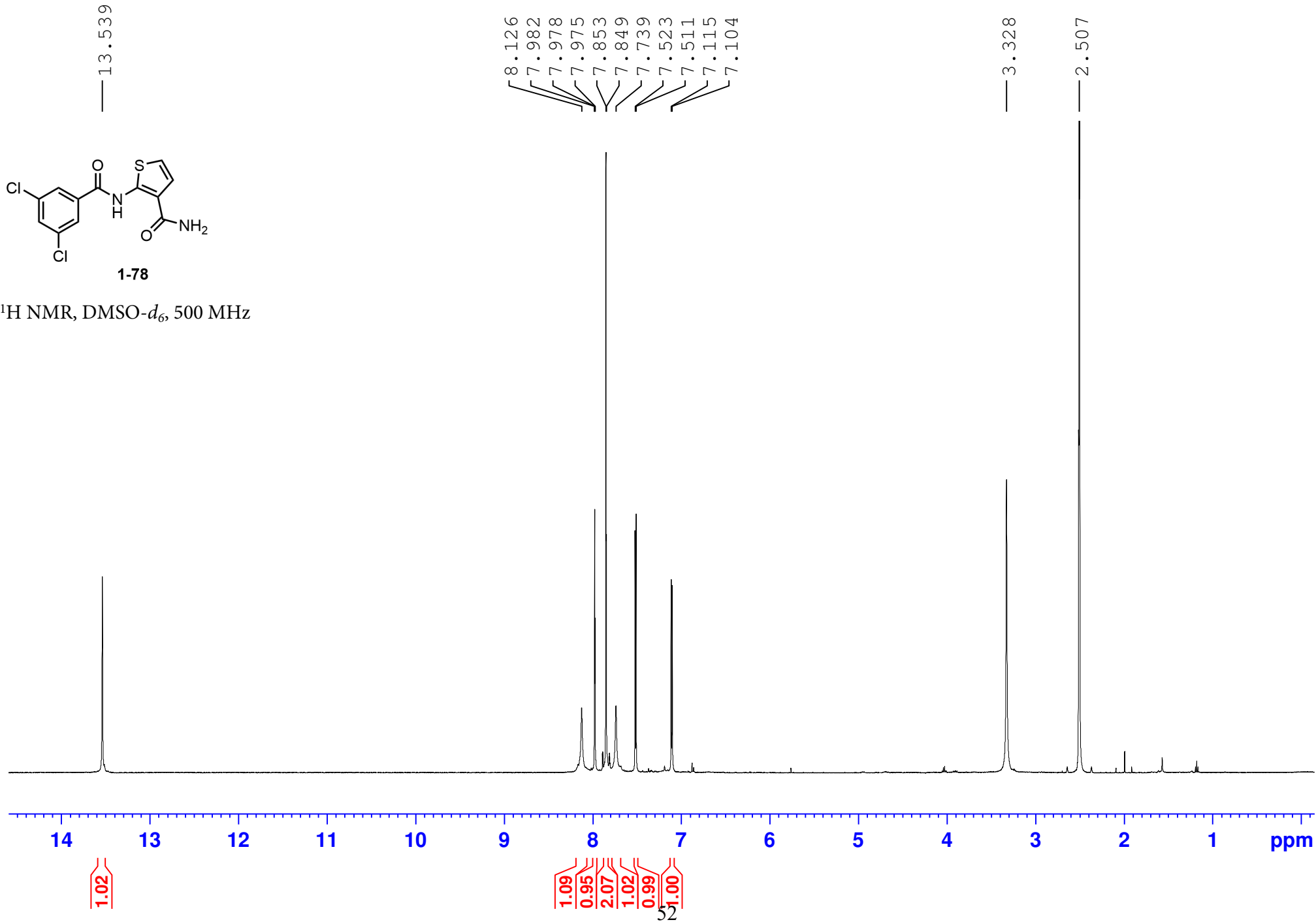
¹³C NMR, DMSO-*d*₆, 101 MHz

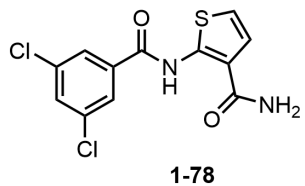




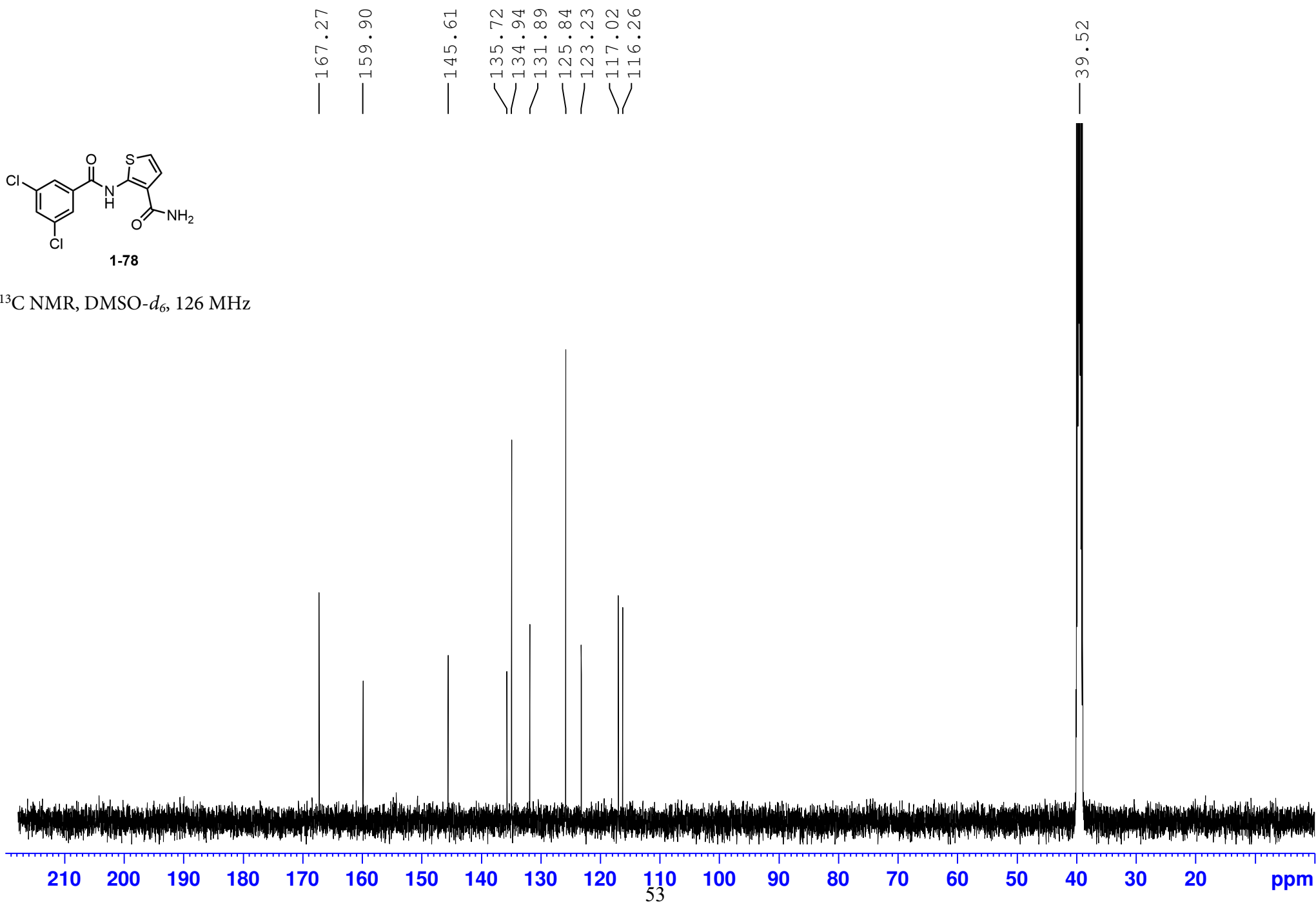
1-78

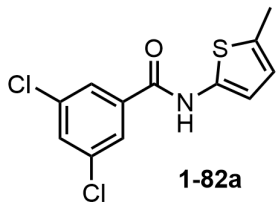
¹H NMR, DMSO-*d*₆, 500 MHz



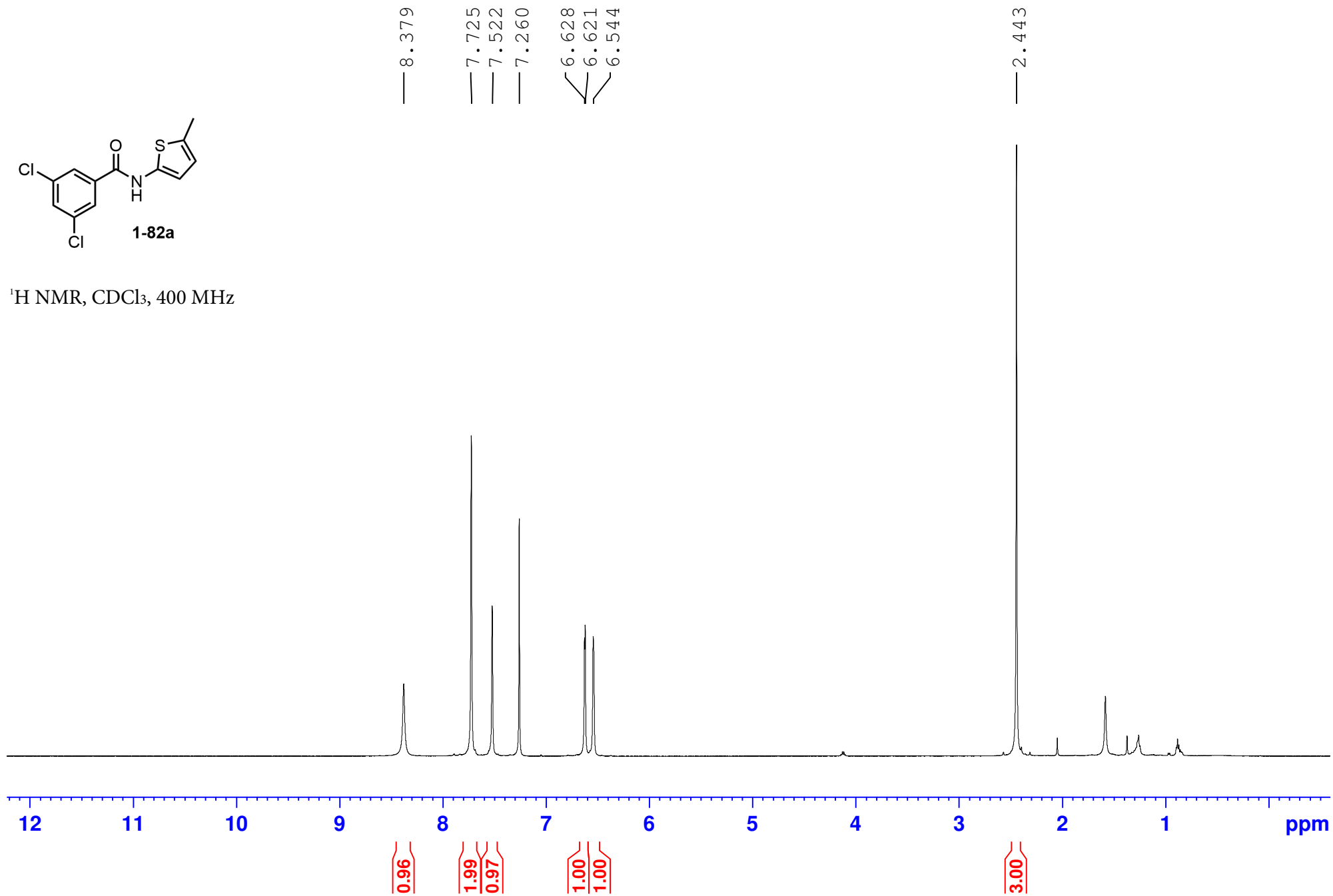


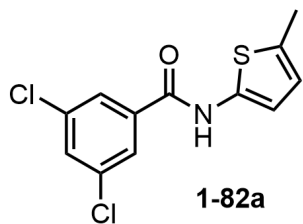
^{13}C NMR, $\text{DMSO-}d_6$, 126 MHz



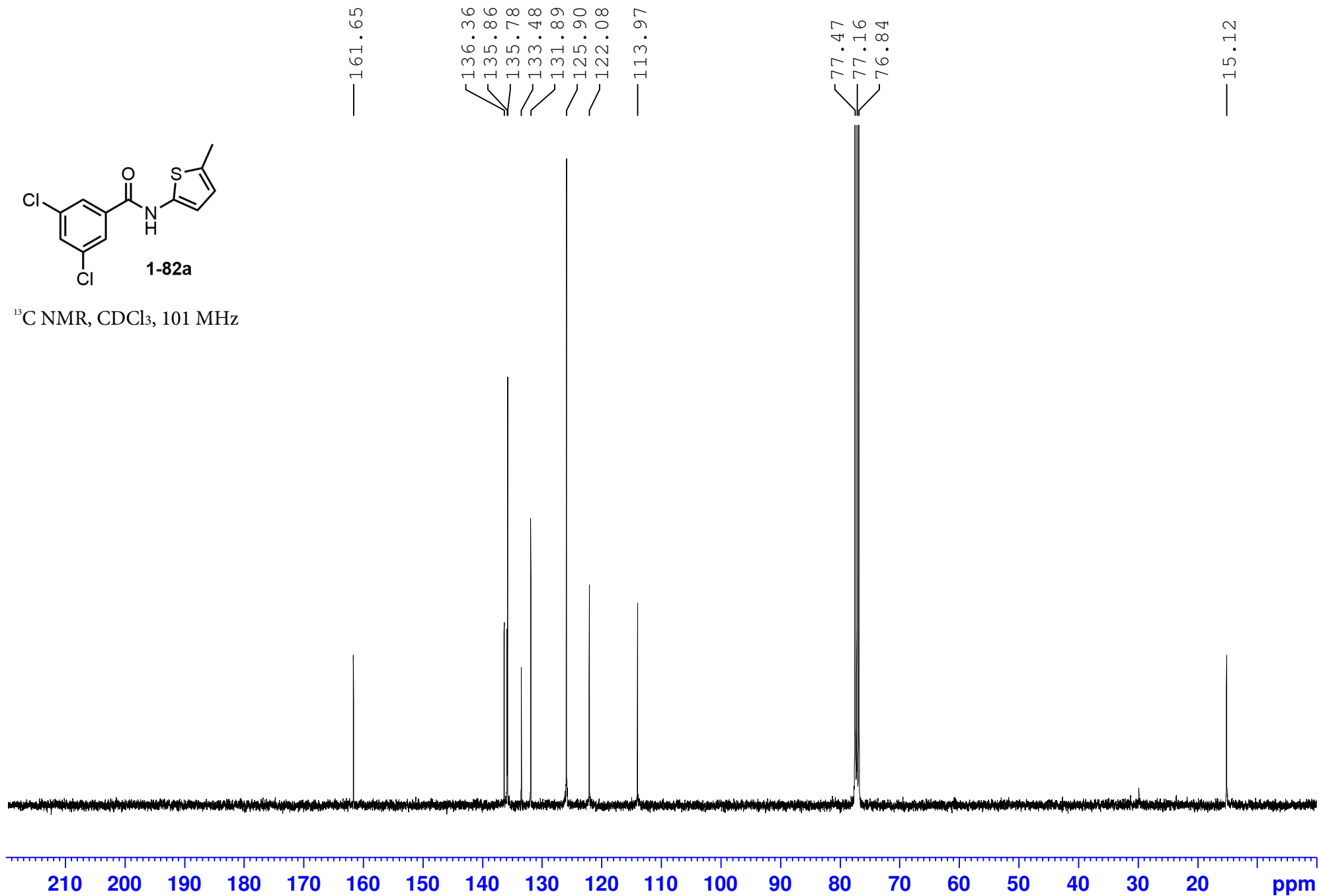


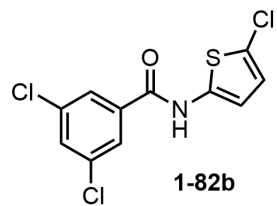
¹H NMR, CDCl₃, 400 MHz



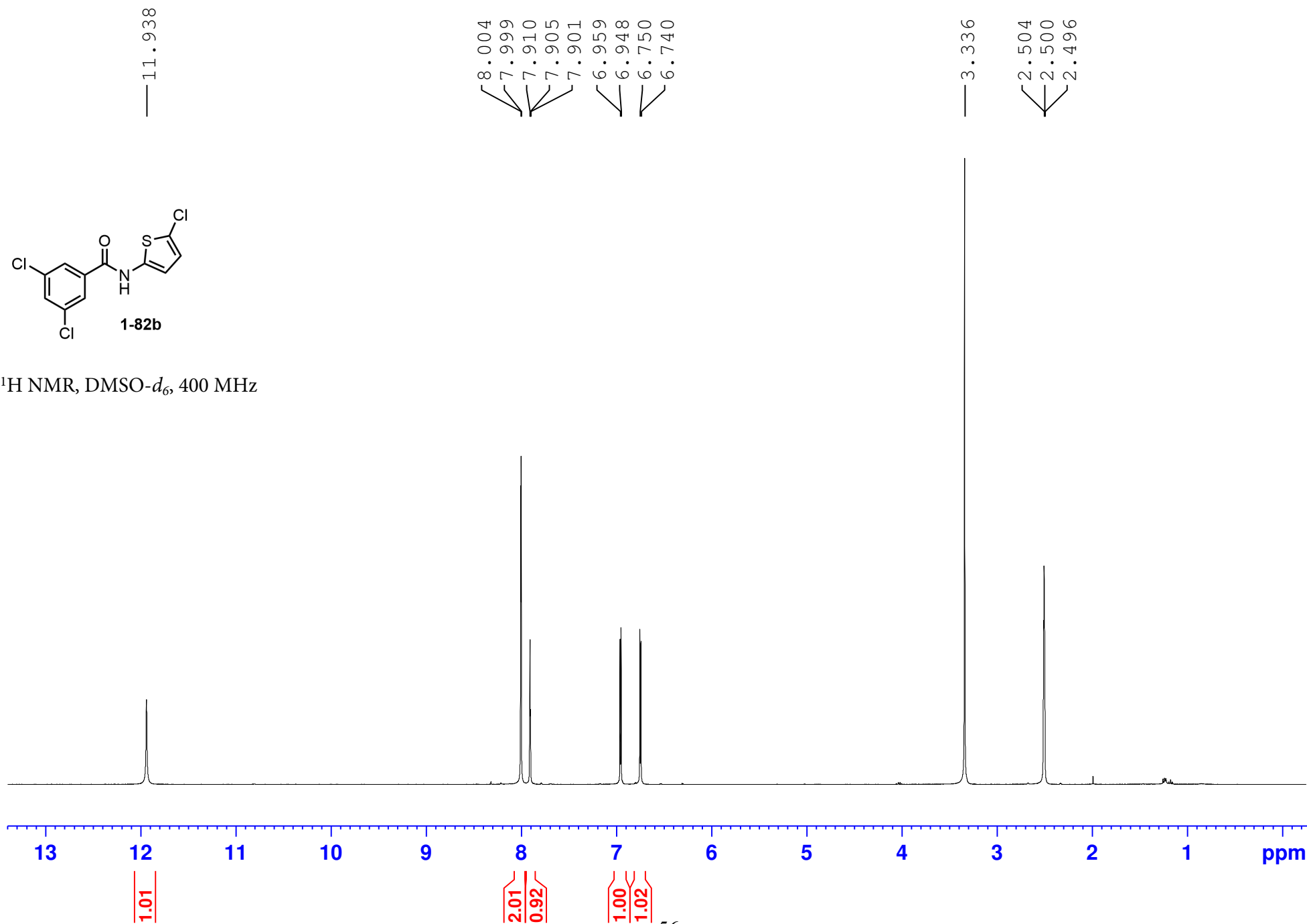


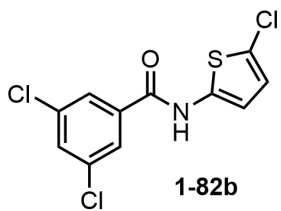
^{13}C NMR, CDCl_3 , 101 MHz



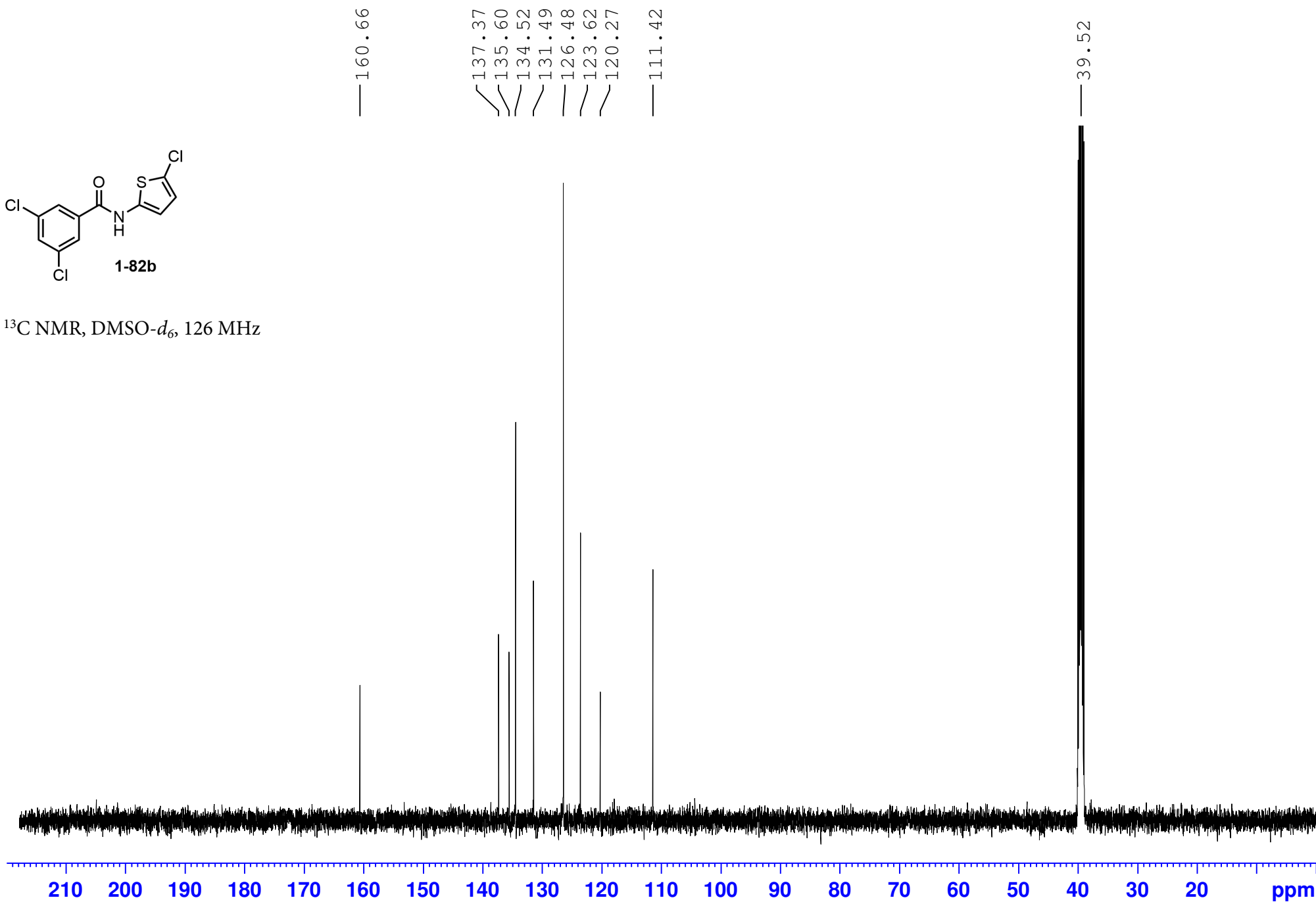


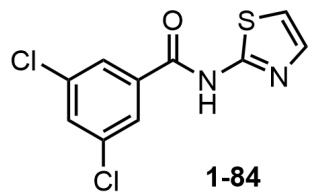
^1H NMR, DMSO- d_6 , 400 MHz



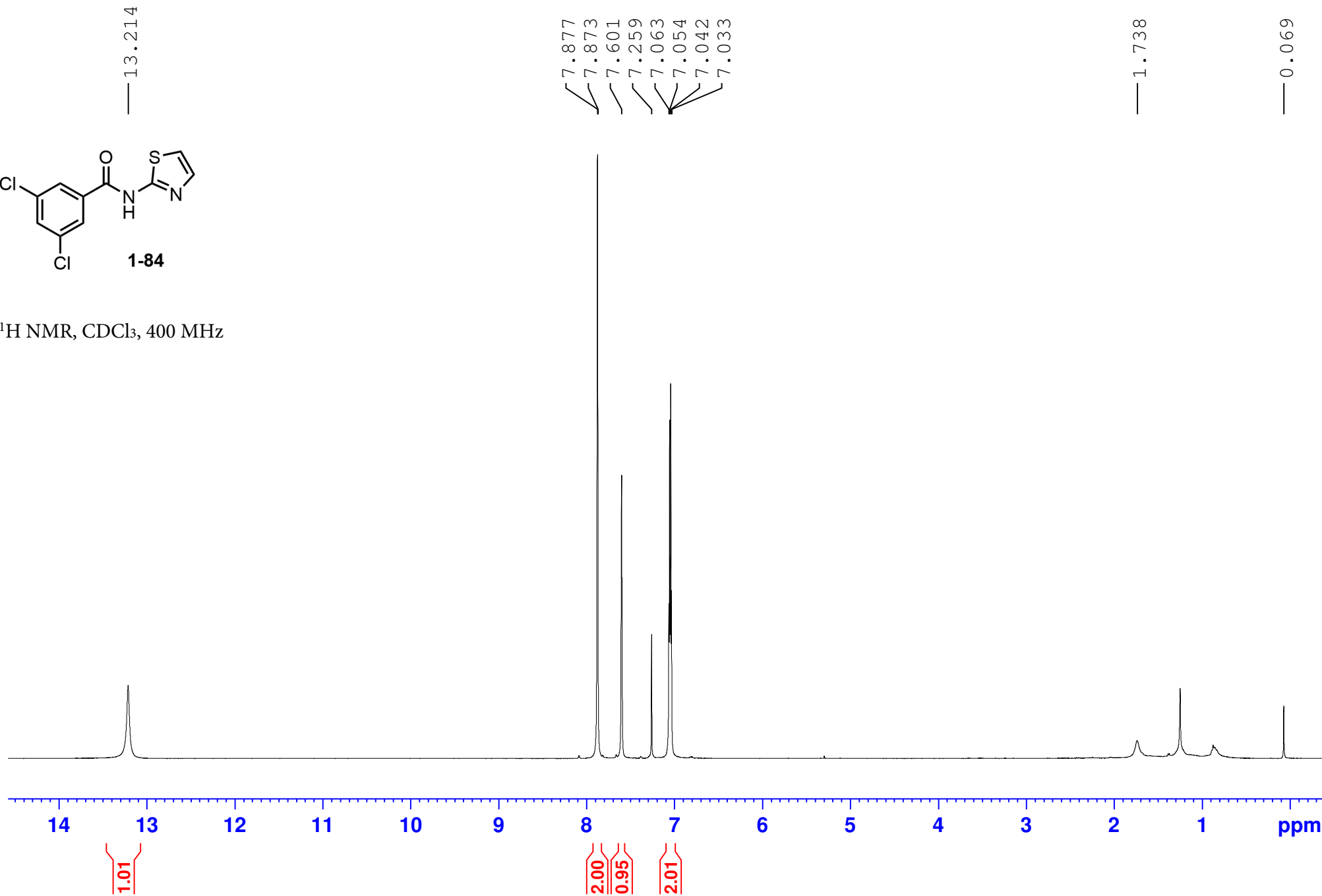


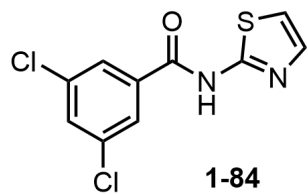
^{13}C NMR, DMSO- d_6 , 126 MHz





¹H NMR, CDCl₃, 400 MHz





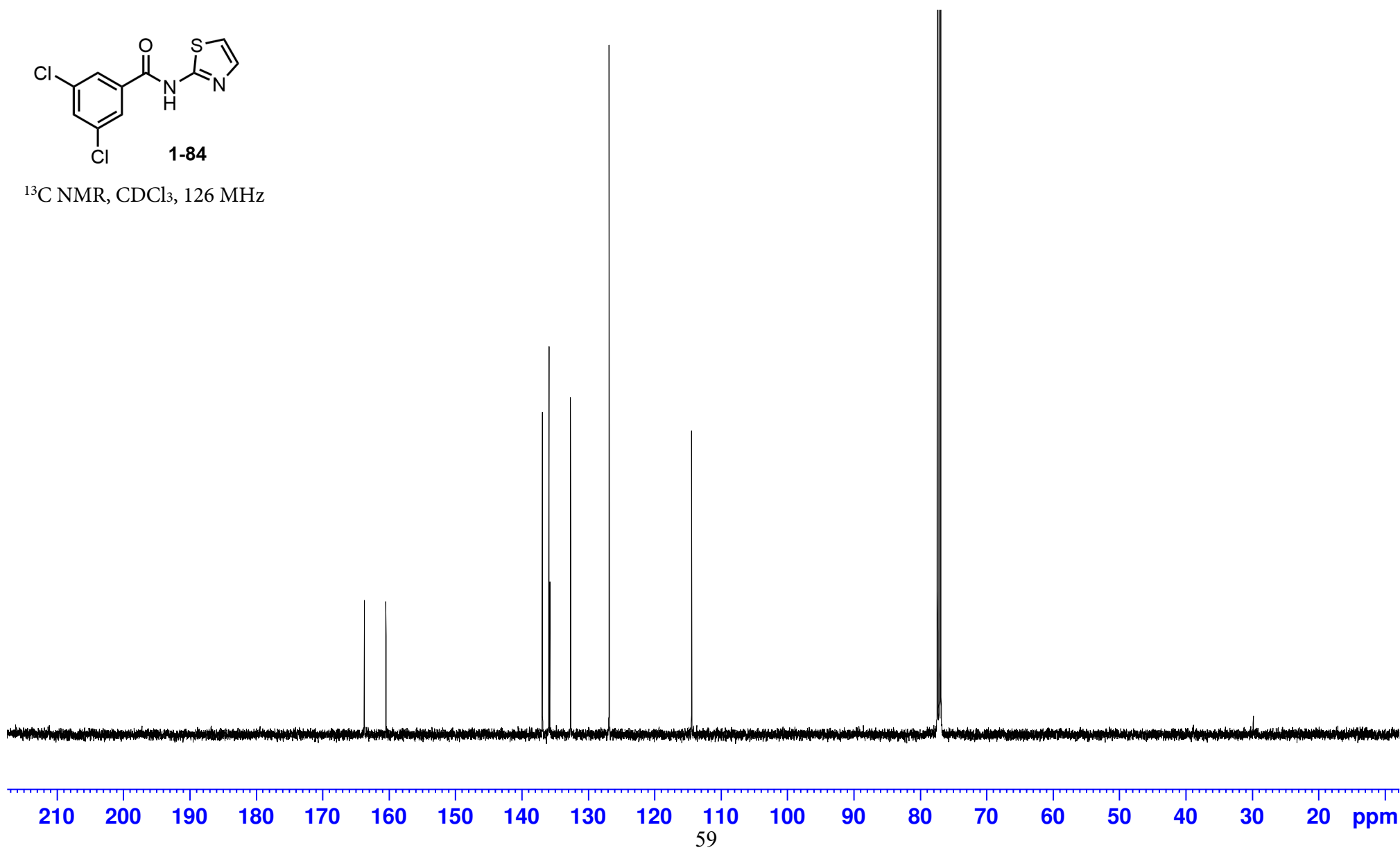
^{13}C NMR, CDCl_3 , 126 MHz

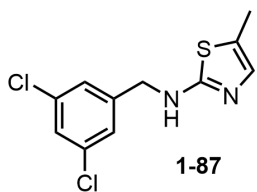
— 163.72
— 160.48

— 136.91
— 135.94
— 132.67
— 126.86

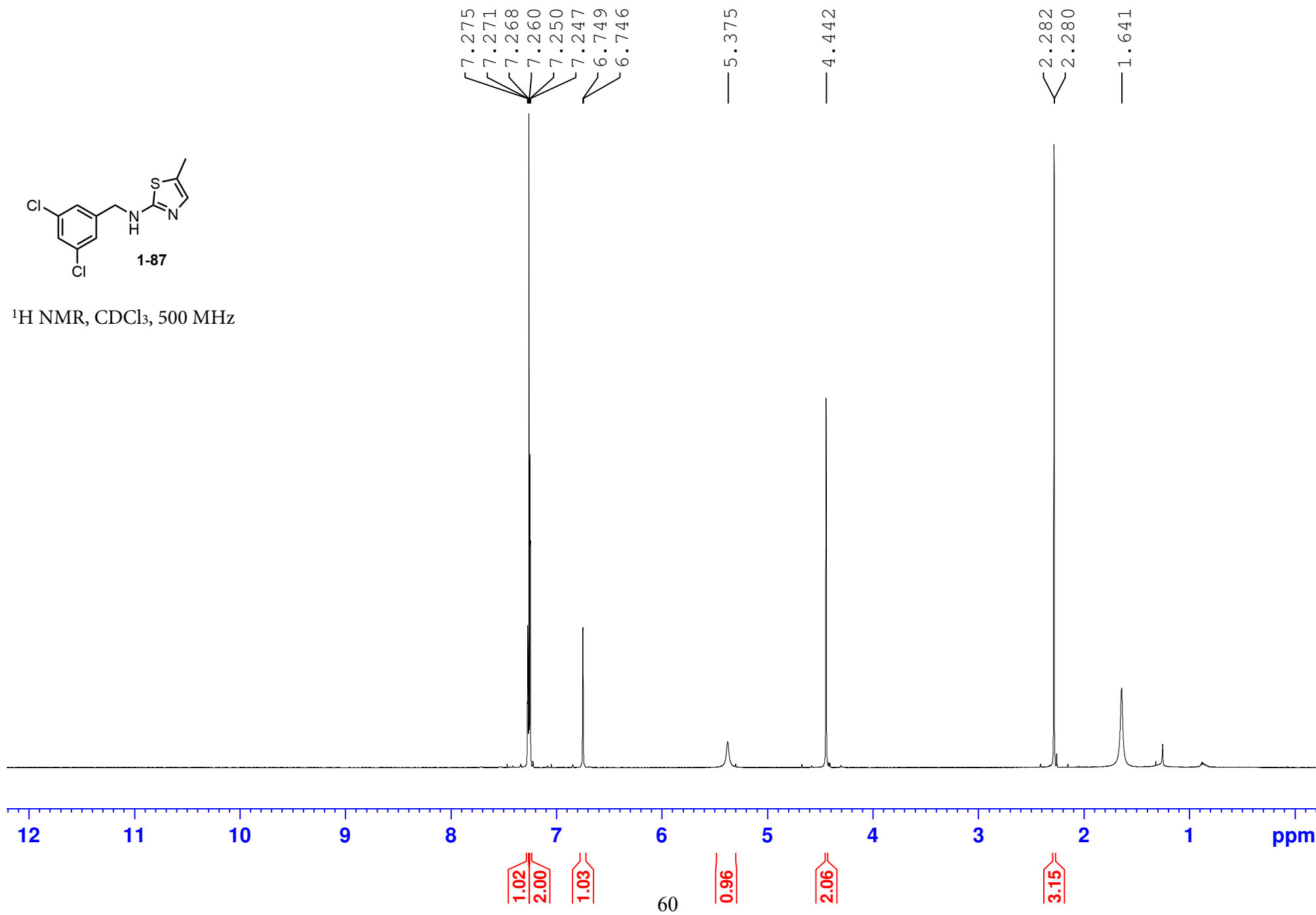
— 114.44

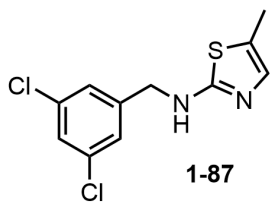
— 77.41
— 77.16
— 76.90



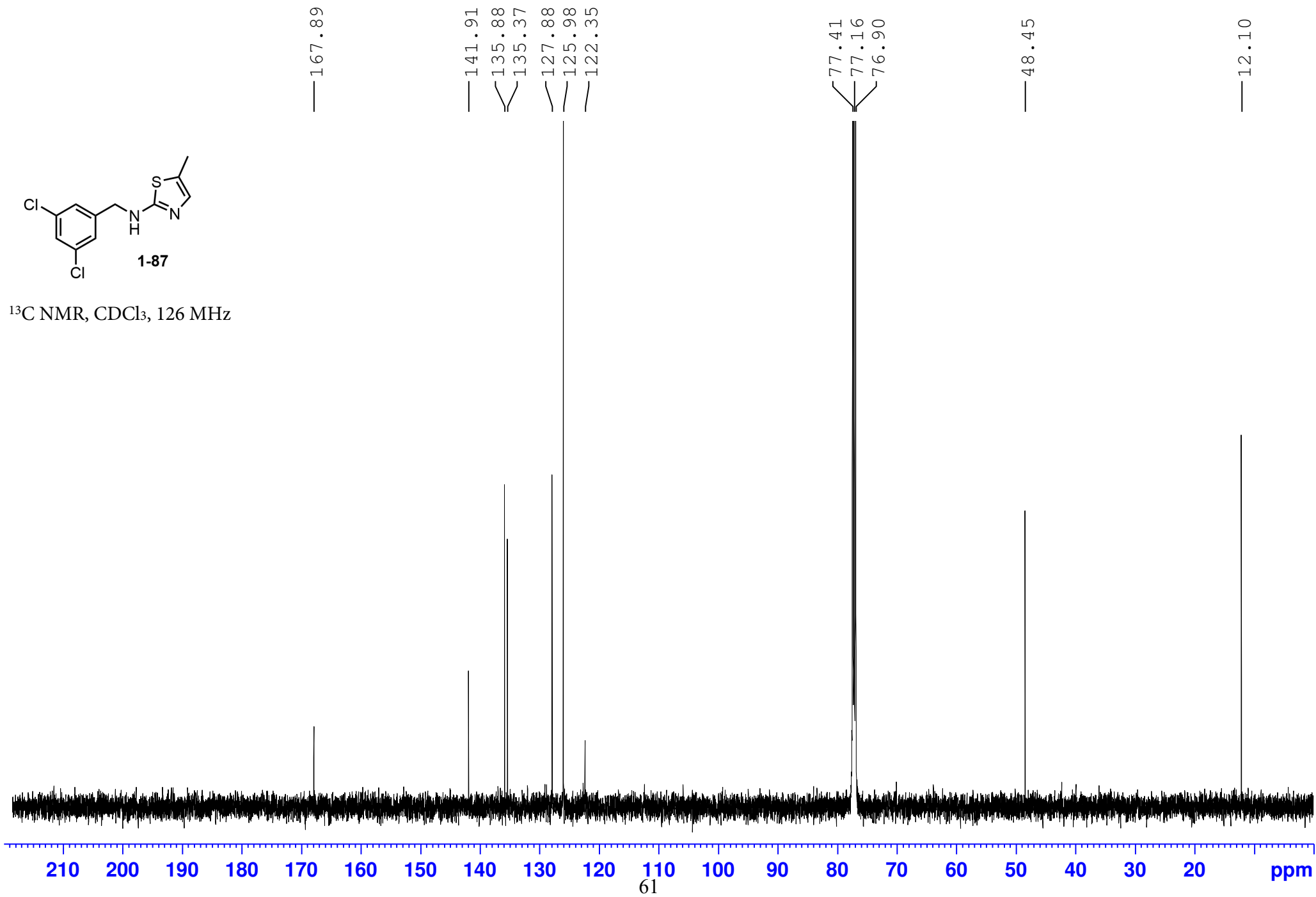


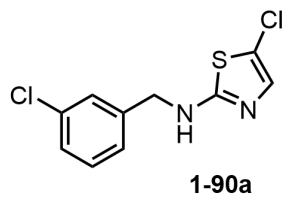
¹H NMR, CDCl₃, 500 MHz



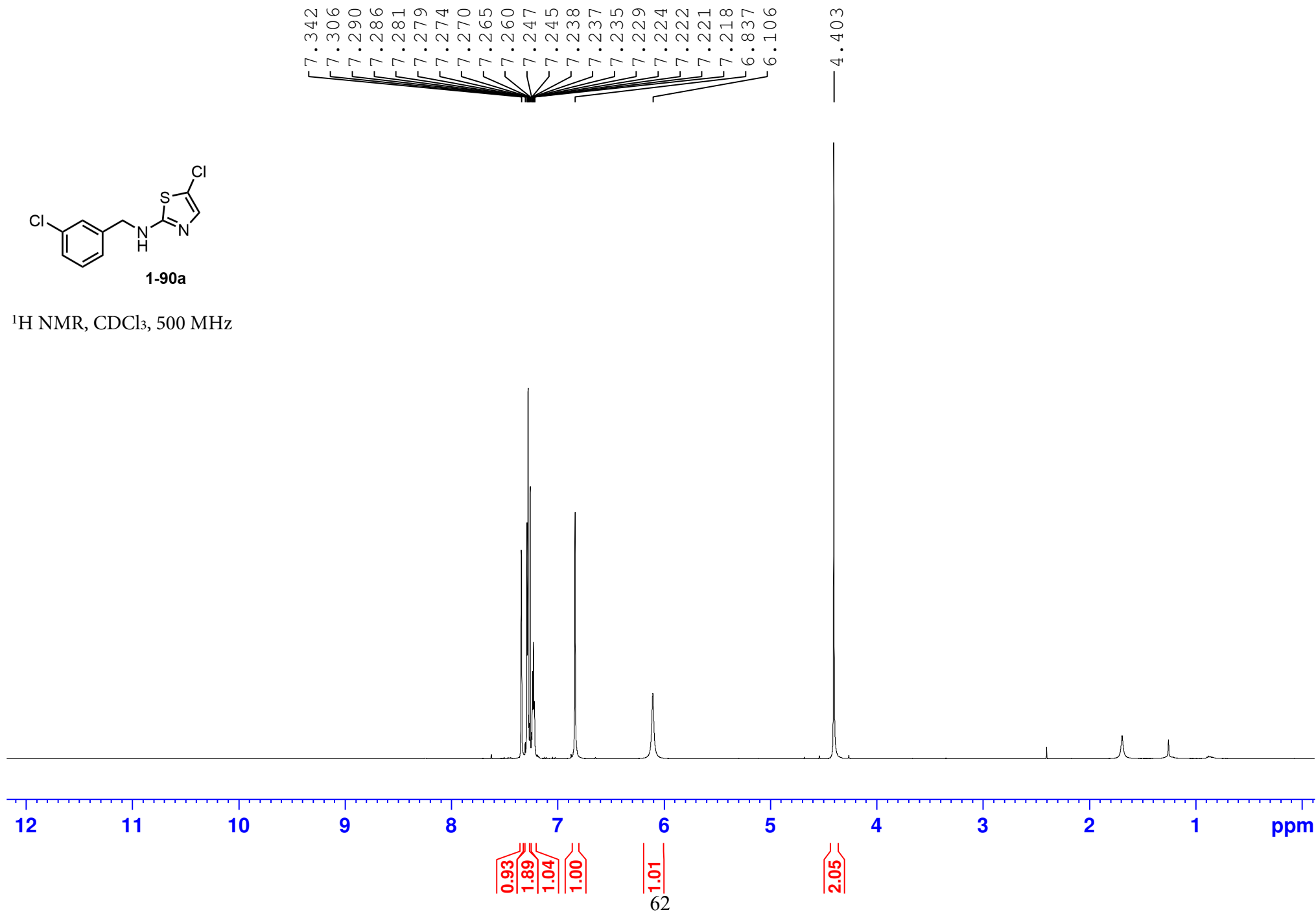


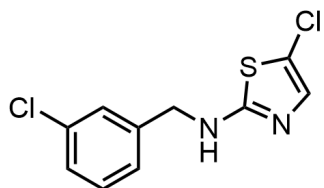
^{13}C NMR, CDCl_3 , 126 MHz





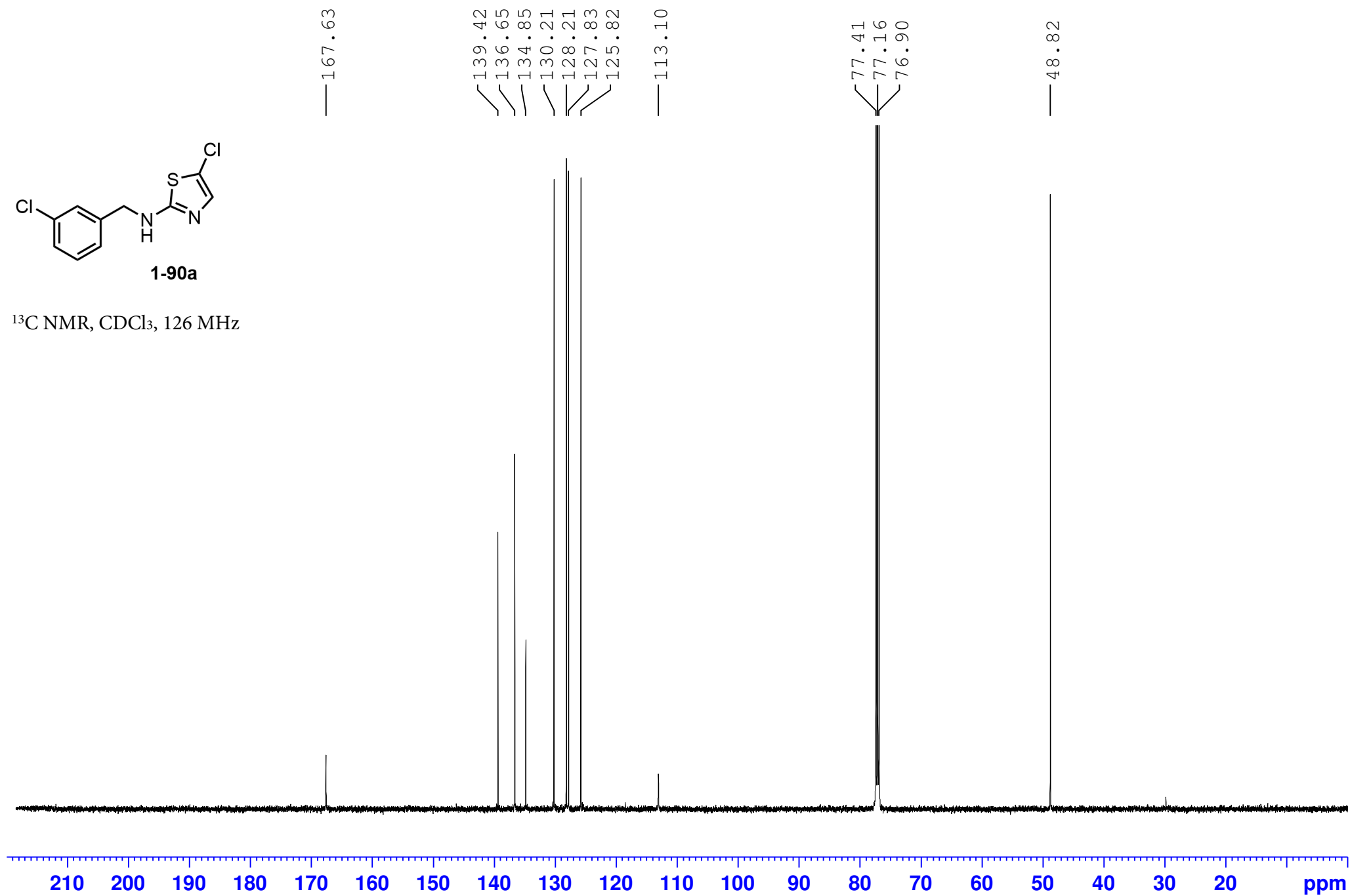
¹H NMR, CDCl₃, 500 MHz

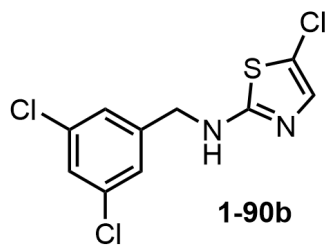




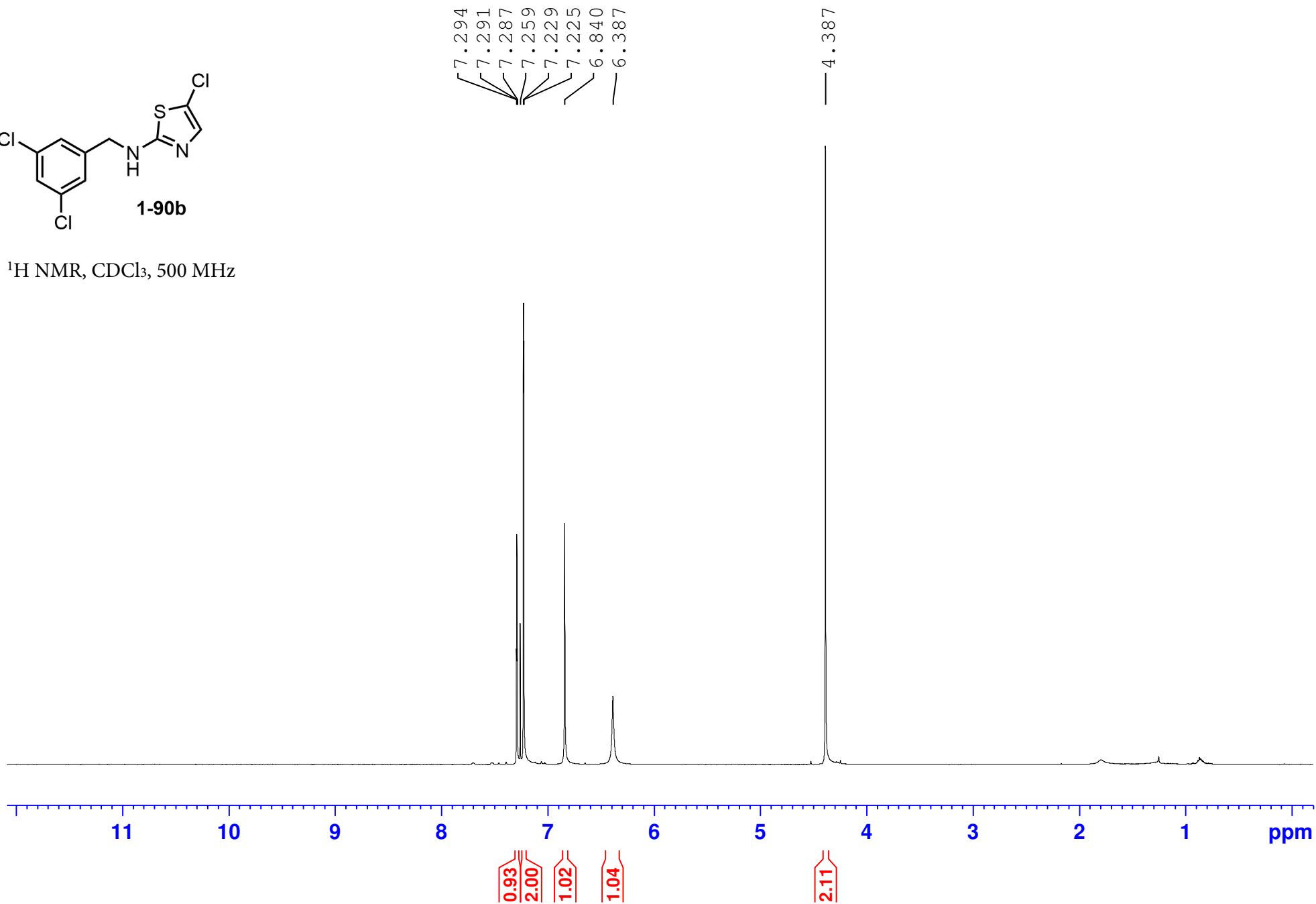
1-90a

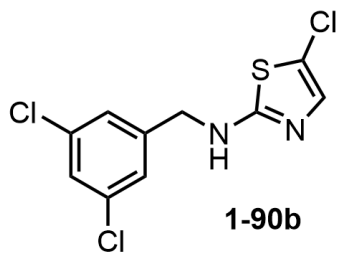
^{13}C NMR, CDCl_3 , 126 MHz



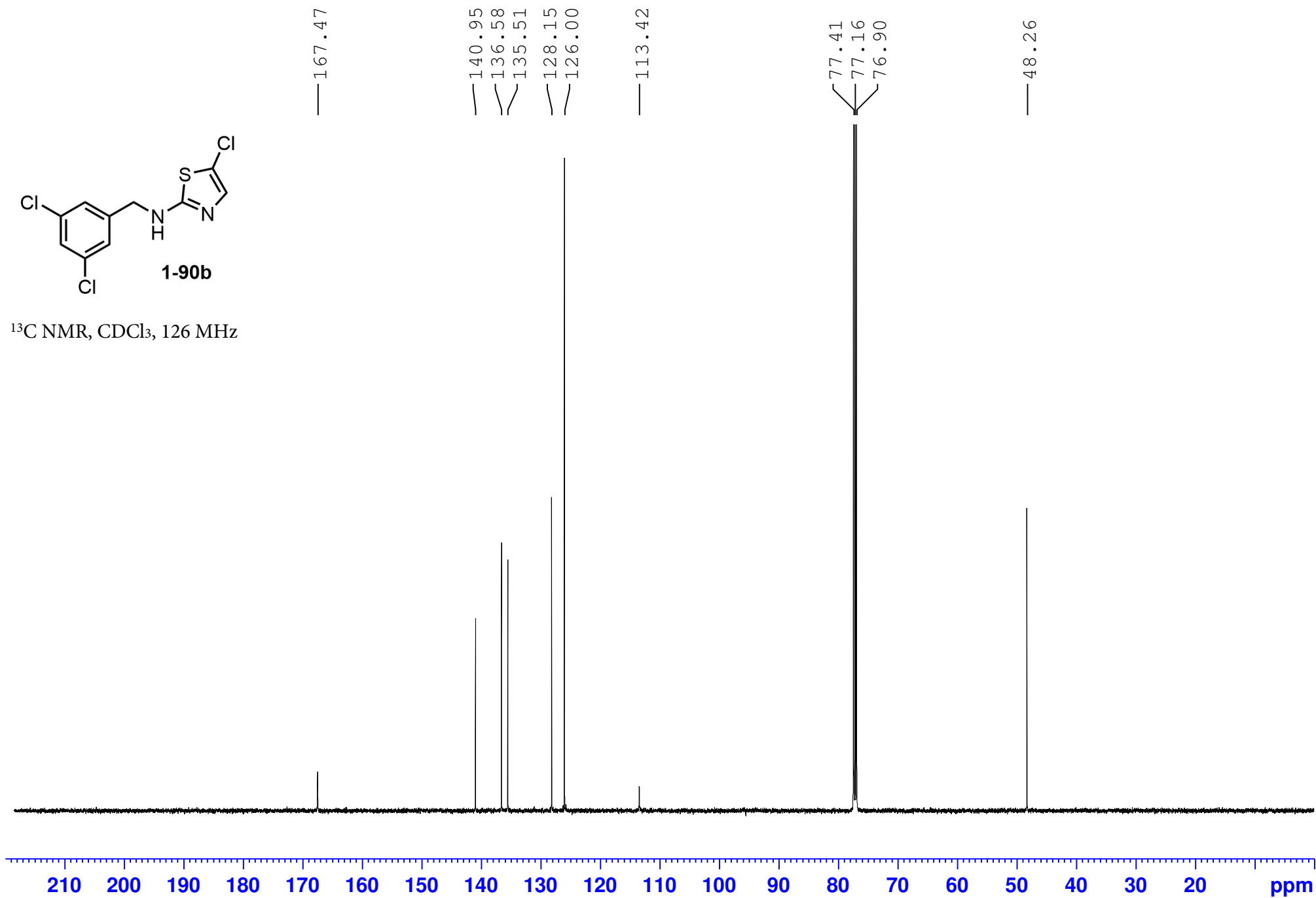


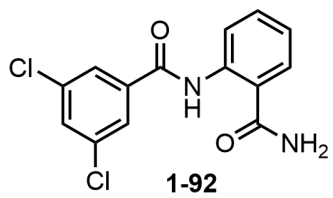
¹H NMR, CDCl₃, 500 MHz



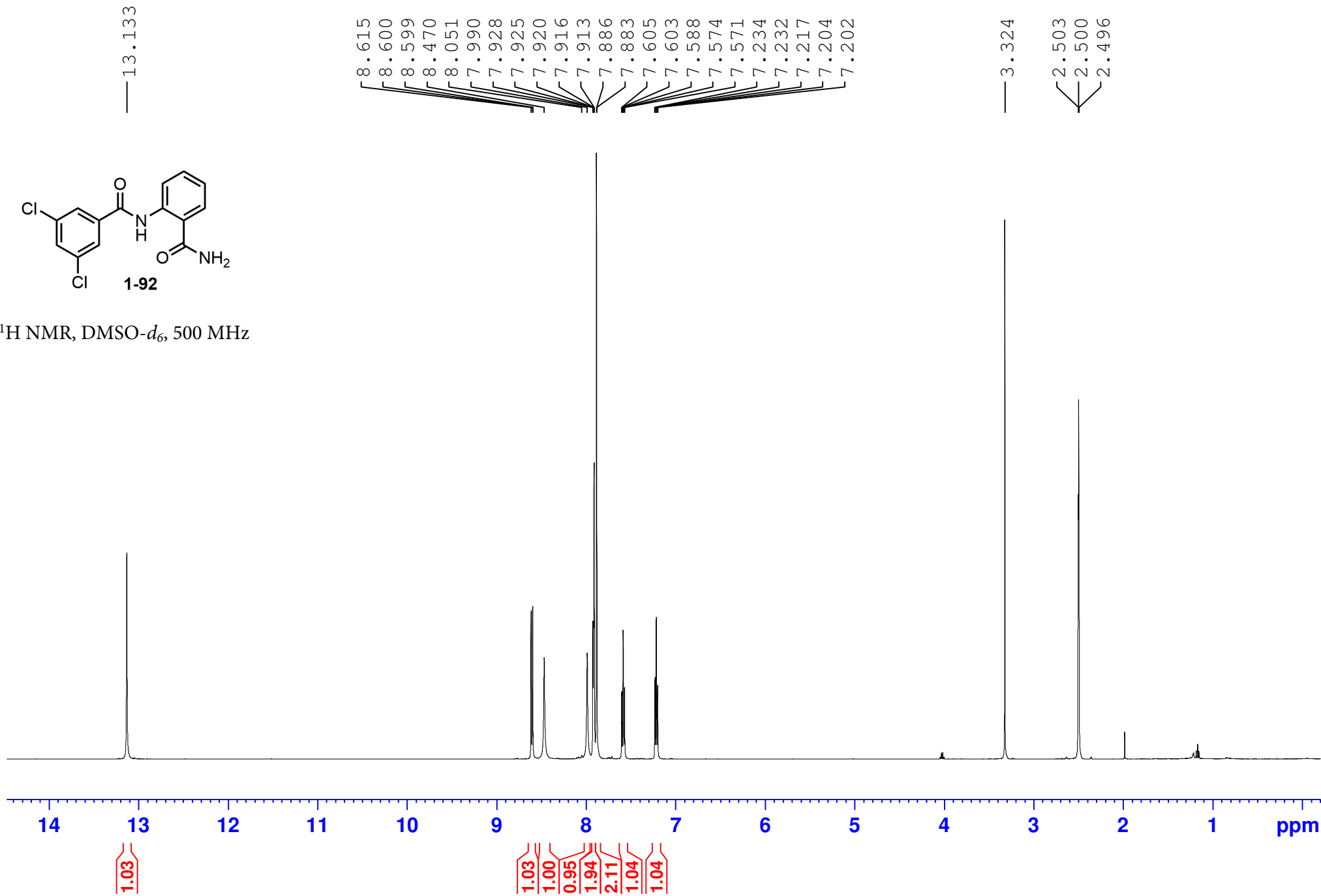


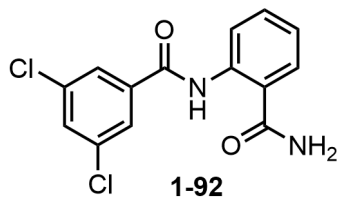
^{13}C NMR, CDCl_3 , 126 MHz



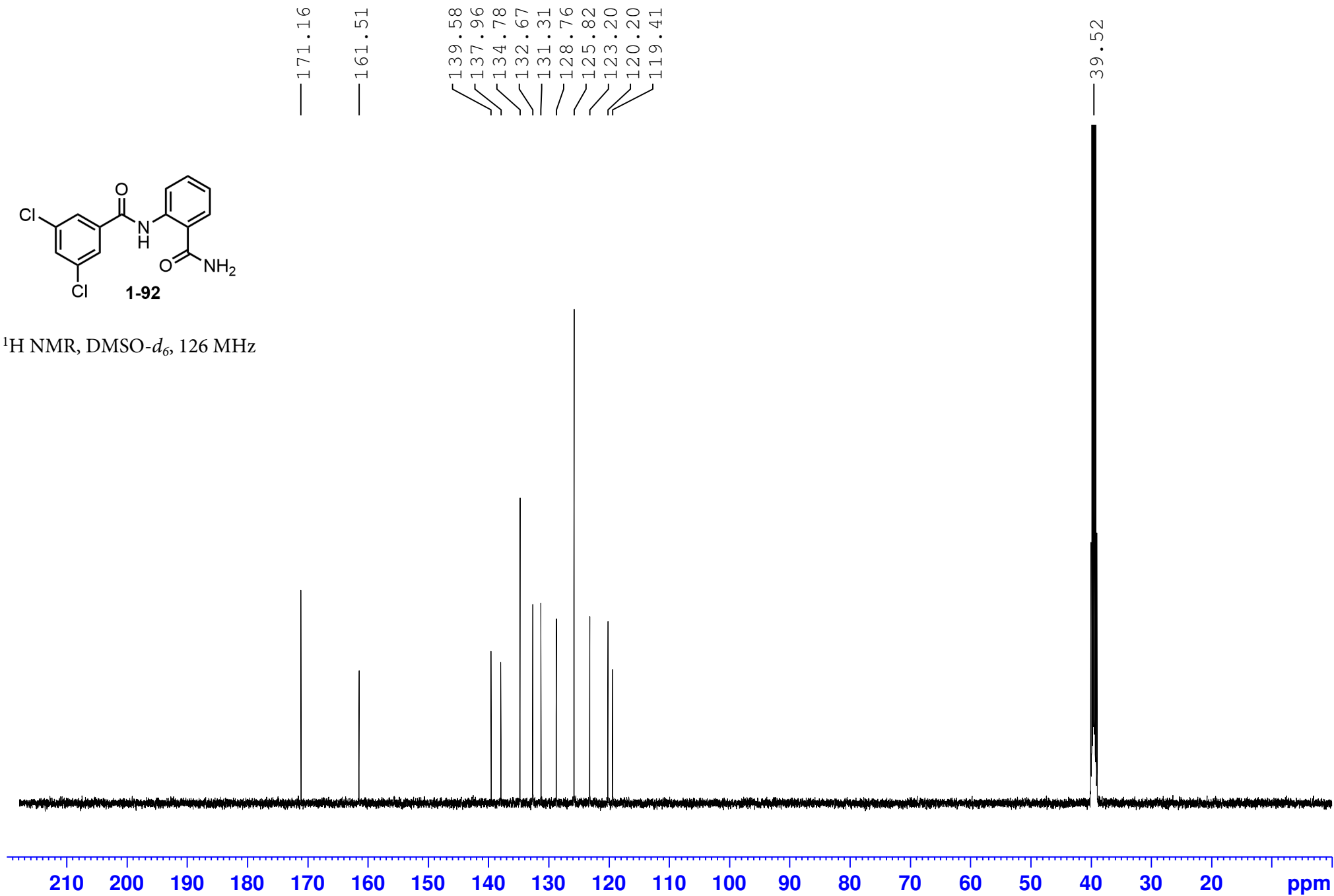


^1H NMR, DMSO- d_6 , 500 MHz

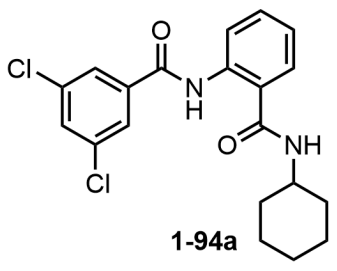




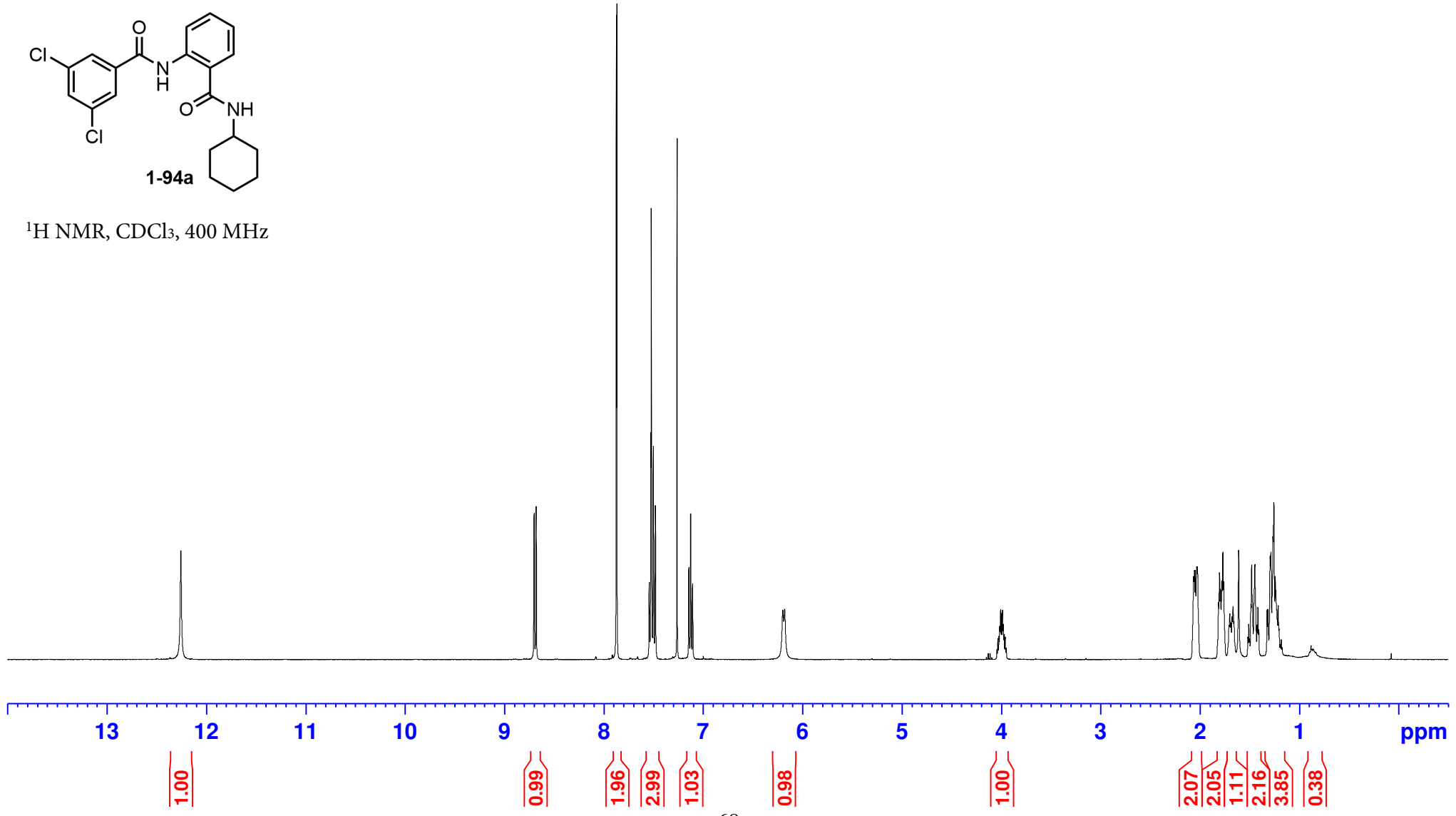
^1H NMR, DMSO- d_6 , 126 MHz

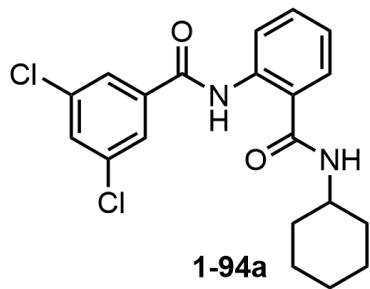


12.254
8.699
8.697
8.678
8.677
7.871
7.866
7.541
7.537
7.524
7.519
7.515
7.498
7.479
7.475
7.259
7.142
7.139
7.122
7.120
7.104
7.101
6.195
6.176
4.002
3.992
3.982
2.059
2.051
2.042
2.028
2.020
1.808
1.799
1.789
1.774
1.765
1.756
1.694
1.685
1.671
1.662
1.653
1.606
1.483
1.475
1.467
1.442
1.412
1.319
1.311
1.288
1.281
1.260
1.251
1.238
1.231
1.223
1.207

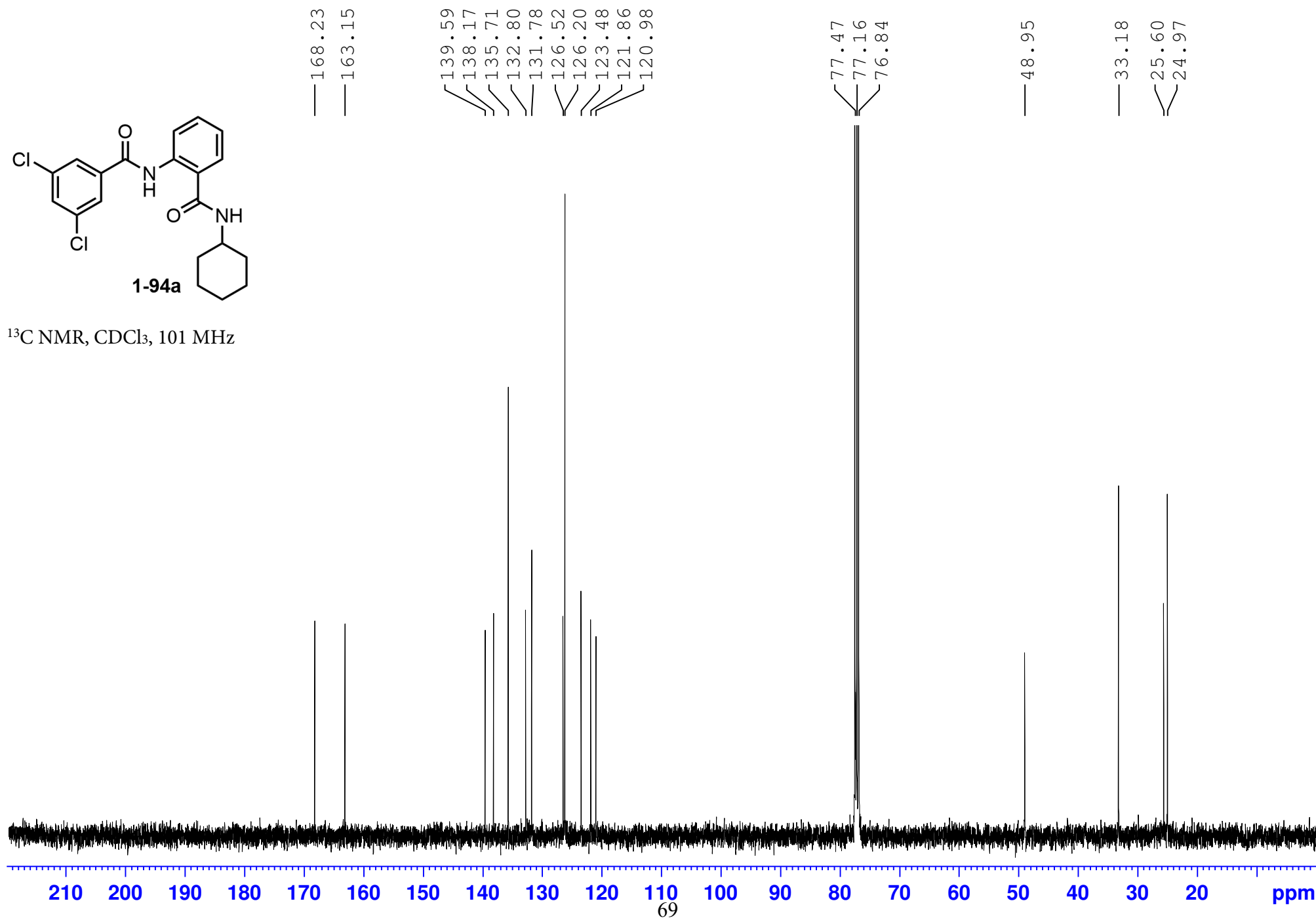


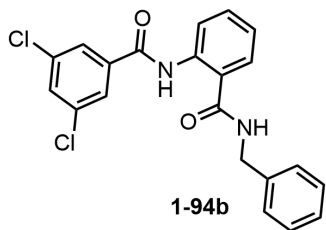
¹H NMR, CDCl₃, 400 MHz



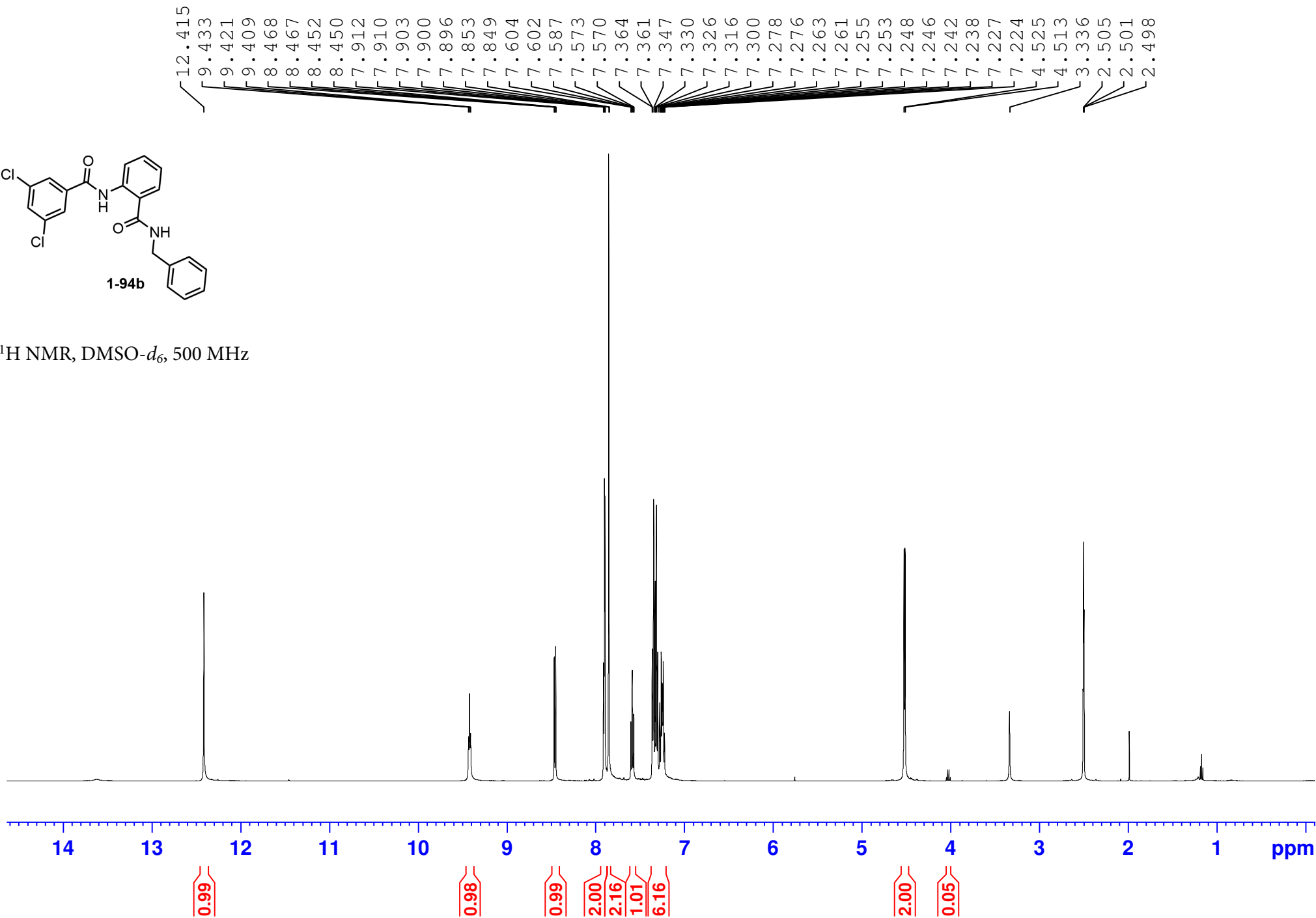


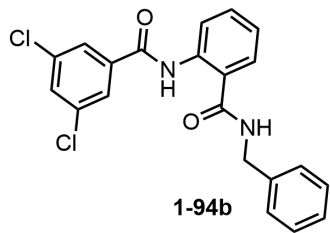
¹³C NMR, CDCl₃, 101 MHz



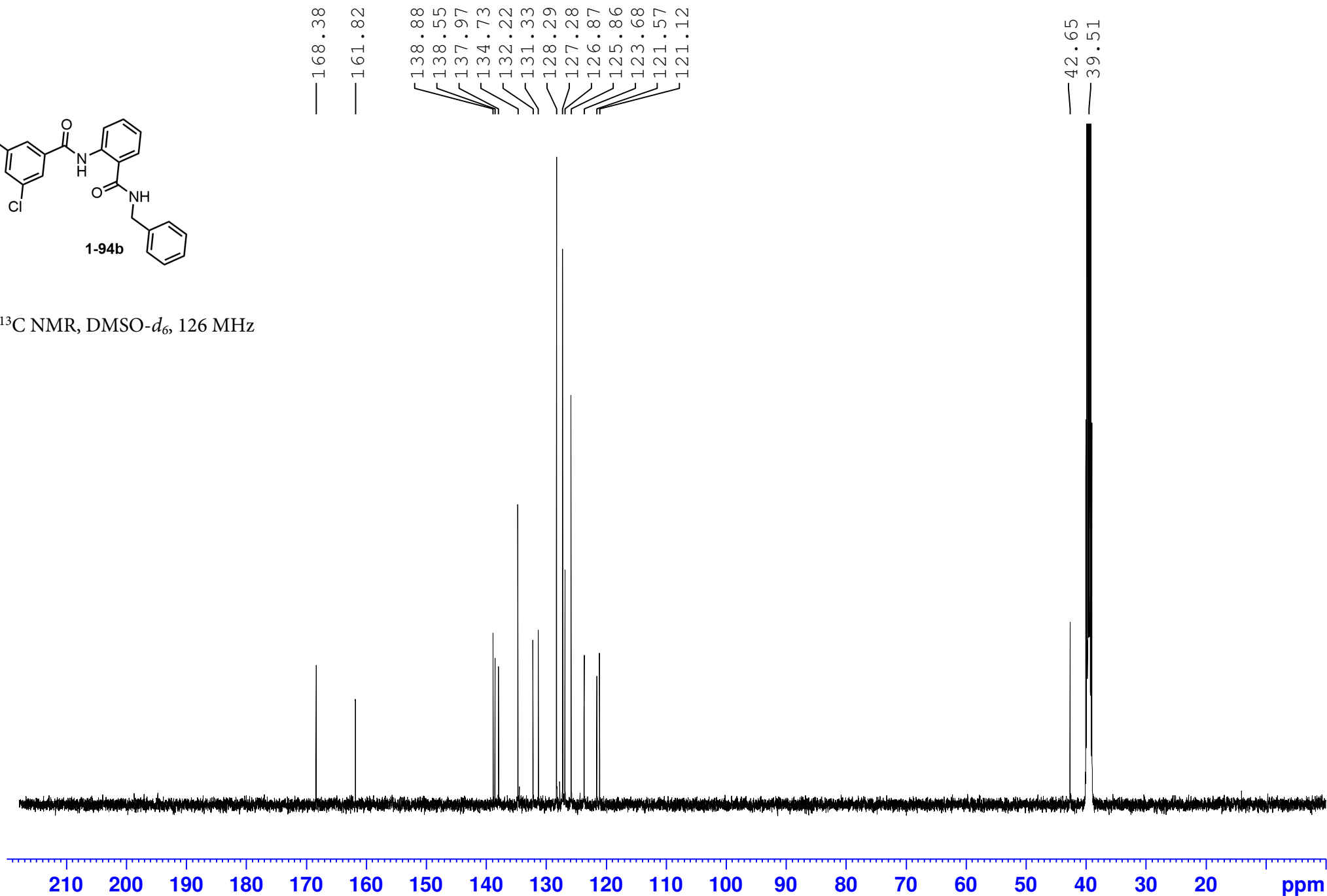


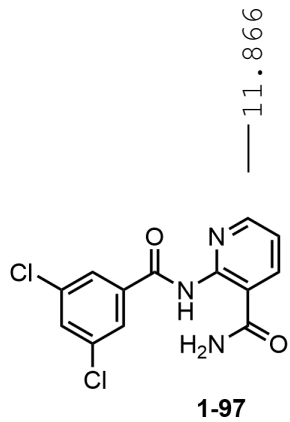
¹H NMR, DMSO-*d*₆, 500 MHz



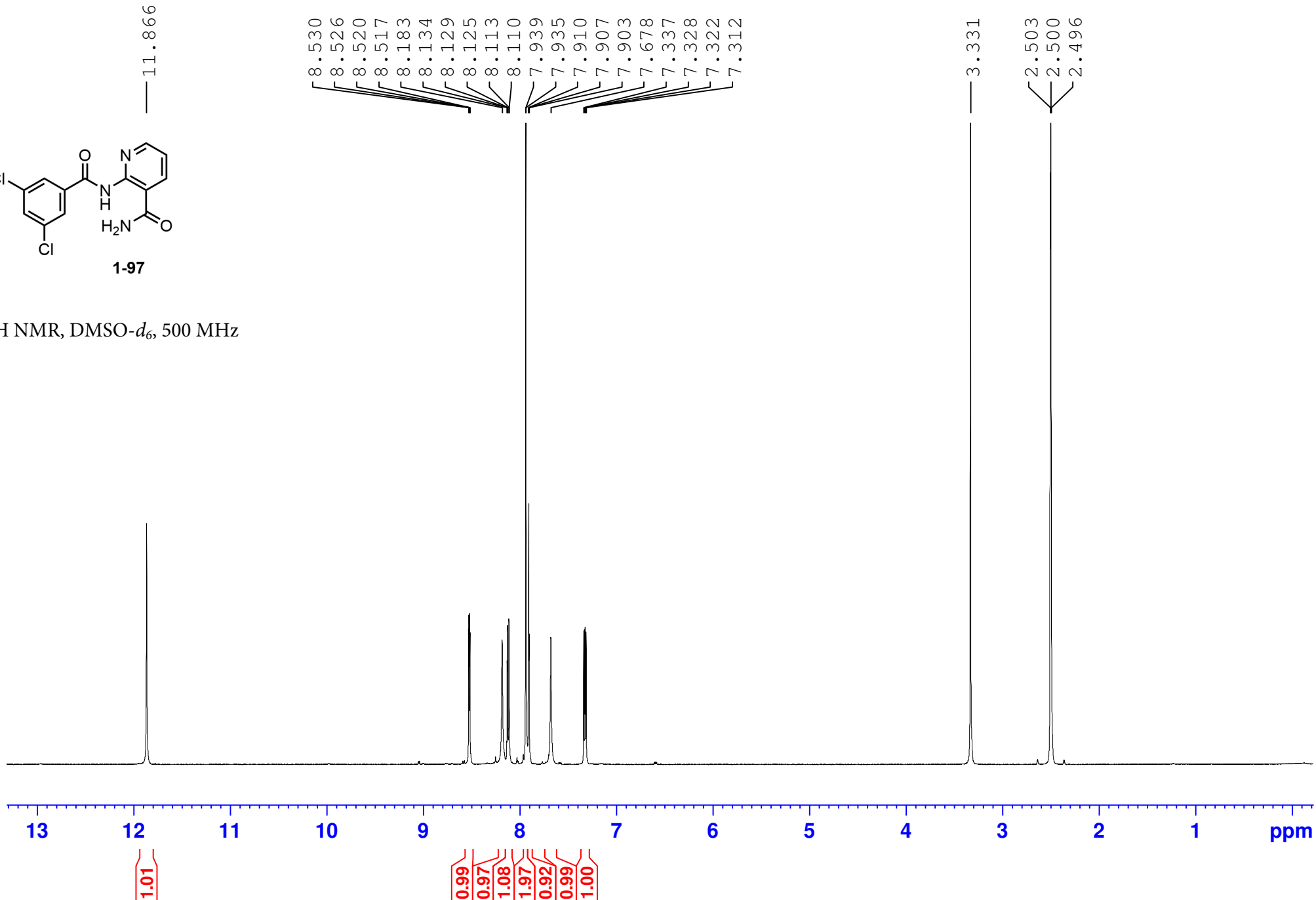


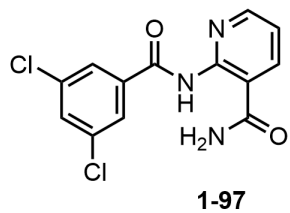
^{13}C NMR, DMSO- d_6 , 126 MHz





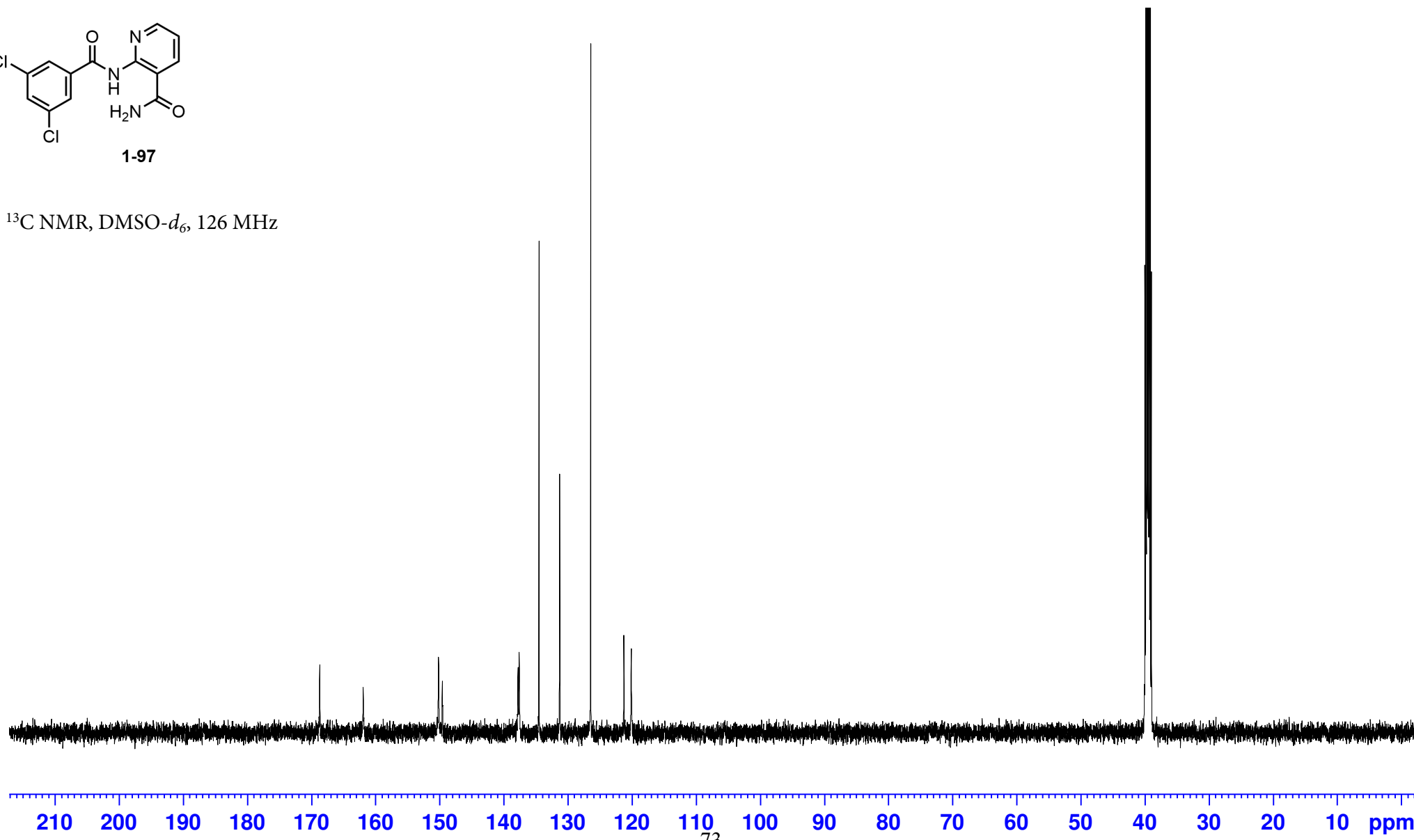
^1H NMR, DMSO- d_6 , 500 MHz

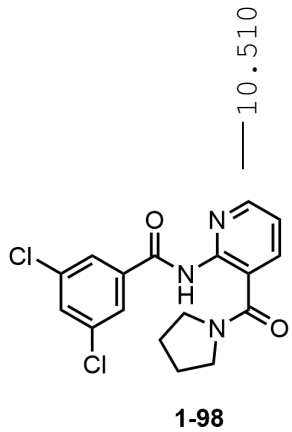




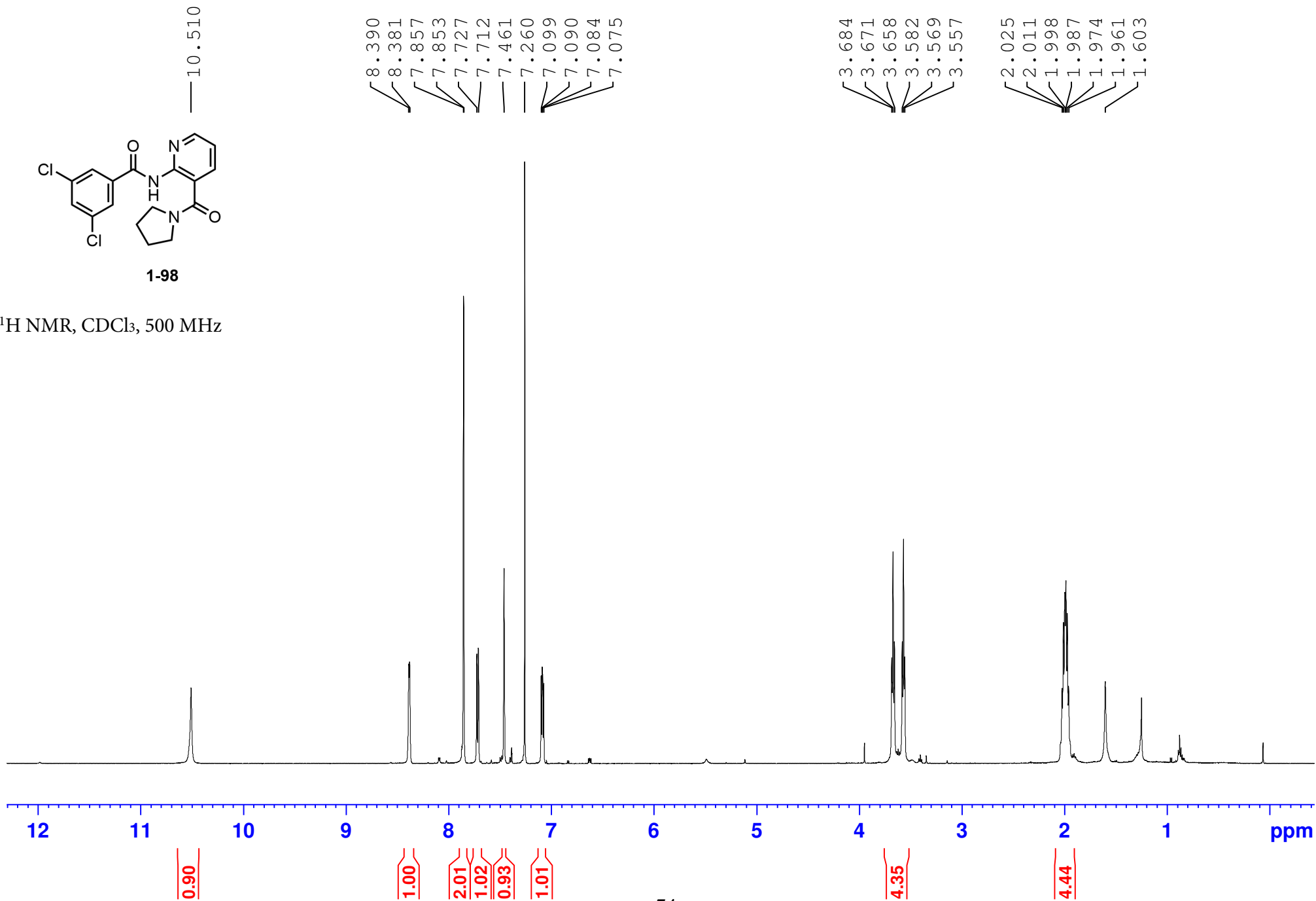
^{13}C NMR, $\text{DMSO-}d_6$, 126 MHz

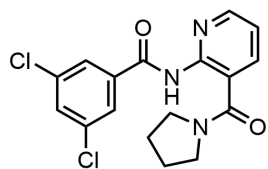
— 168.74
— 161.97
{ 150.20
 149.60
{ 137.82
 137.63
{ 134.53
 131.32
— 126.47
{ 121.29
 120.14





$^1\text{H NMR}$, CDCl_3 , 500 MHz





1-98

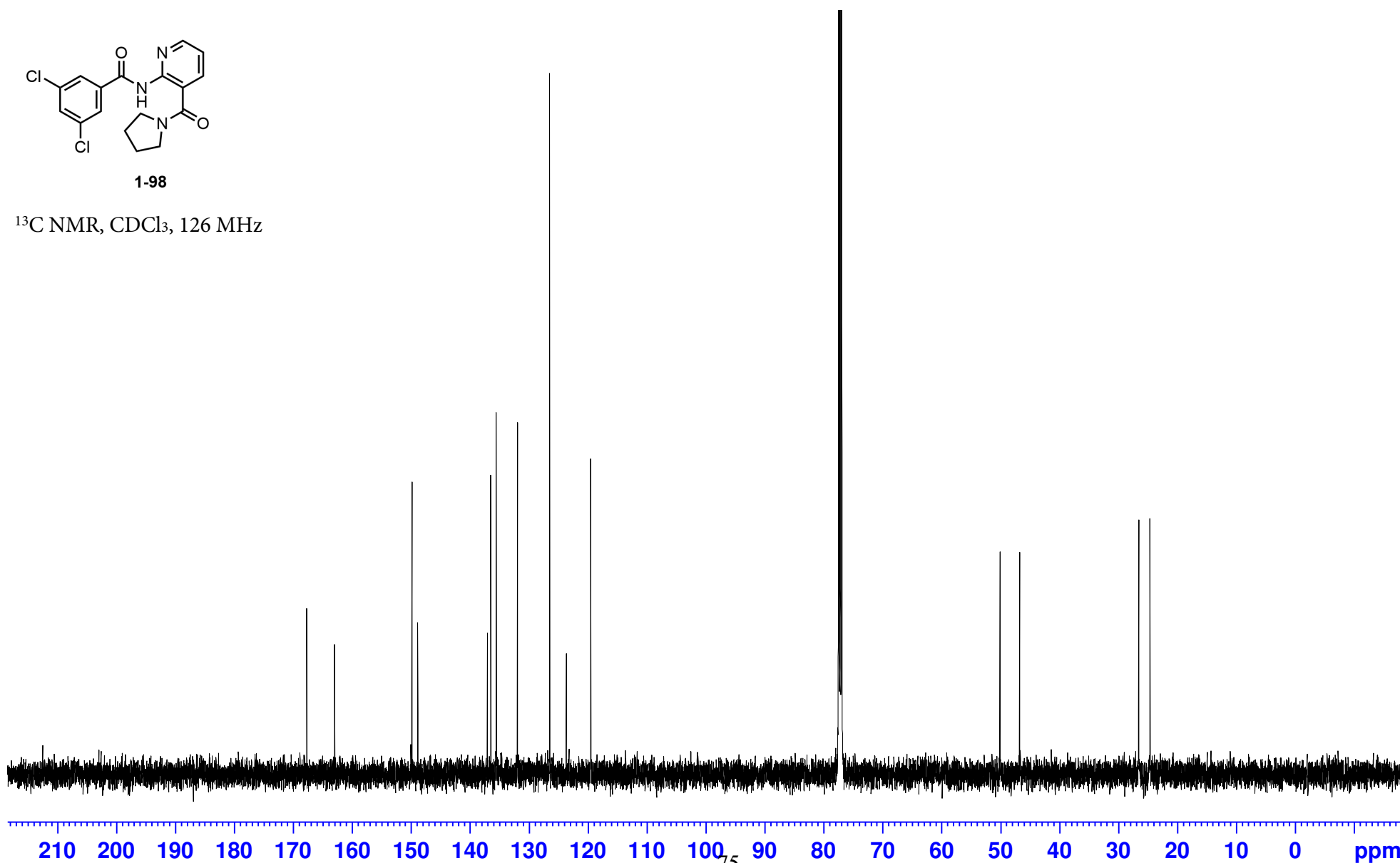
^{13}C NMR, CDCl_3 , 126 MHz

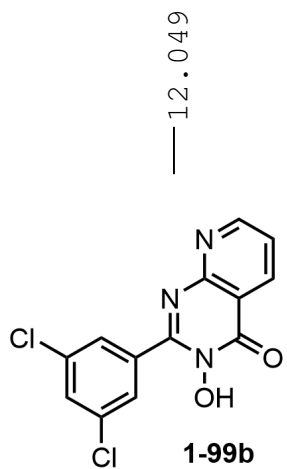
167.68
162.95
149.82
148.83
137.02
136.46
135.52
131.90
126.47
123.61
119.48

77.41
77.16
76.90

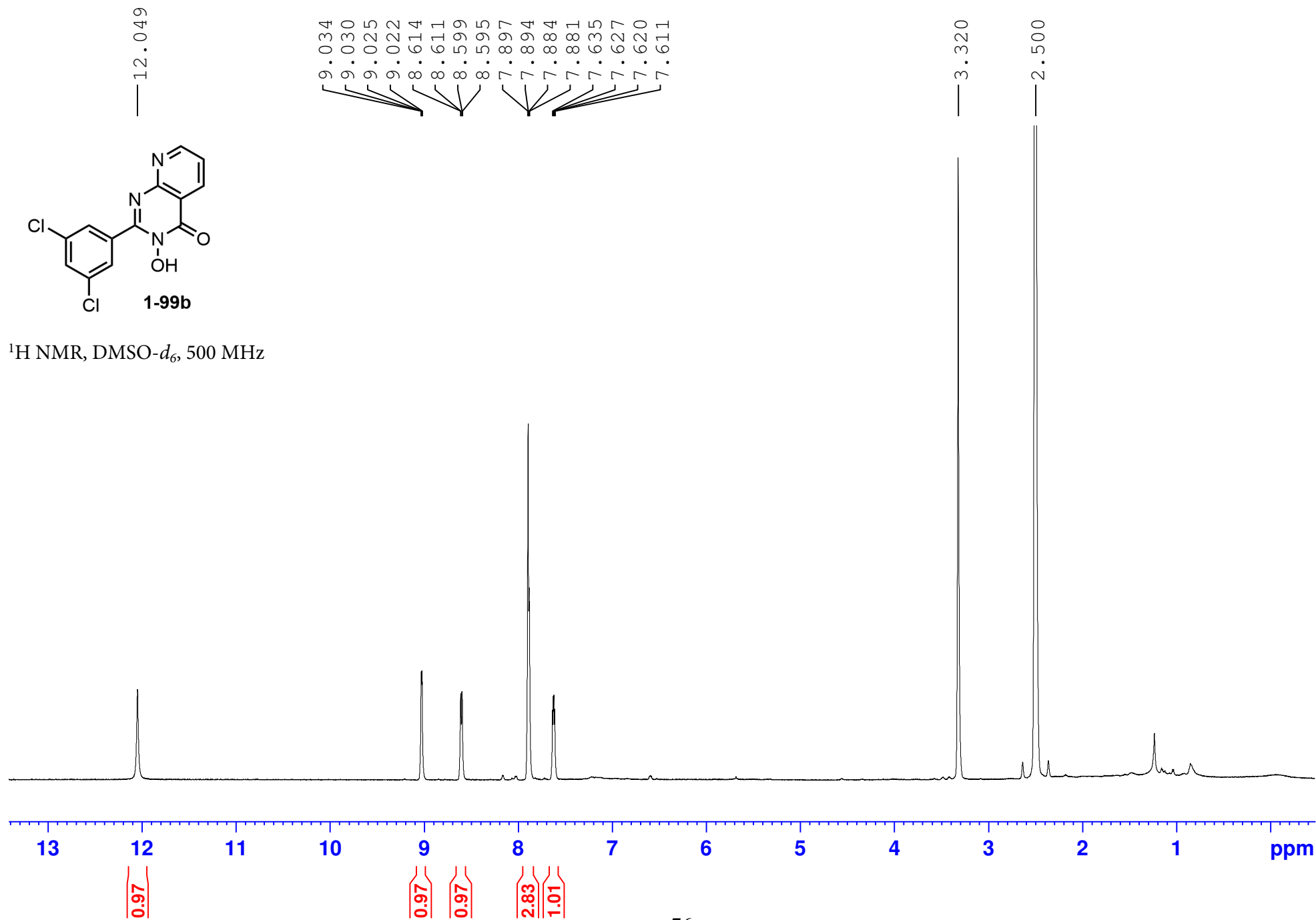
50.04
46.70

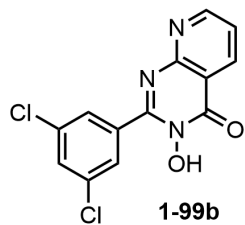
26.50
24.60





$^1\text{H NMR}$, $\text{DMSO-}d_6$, 500 MHz

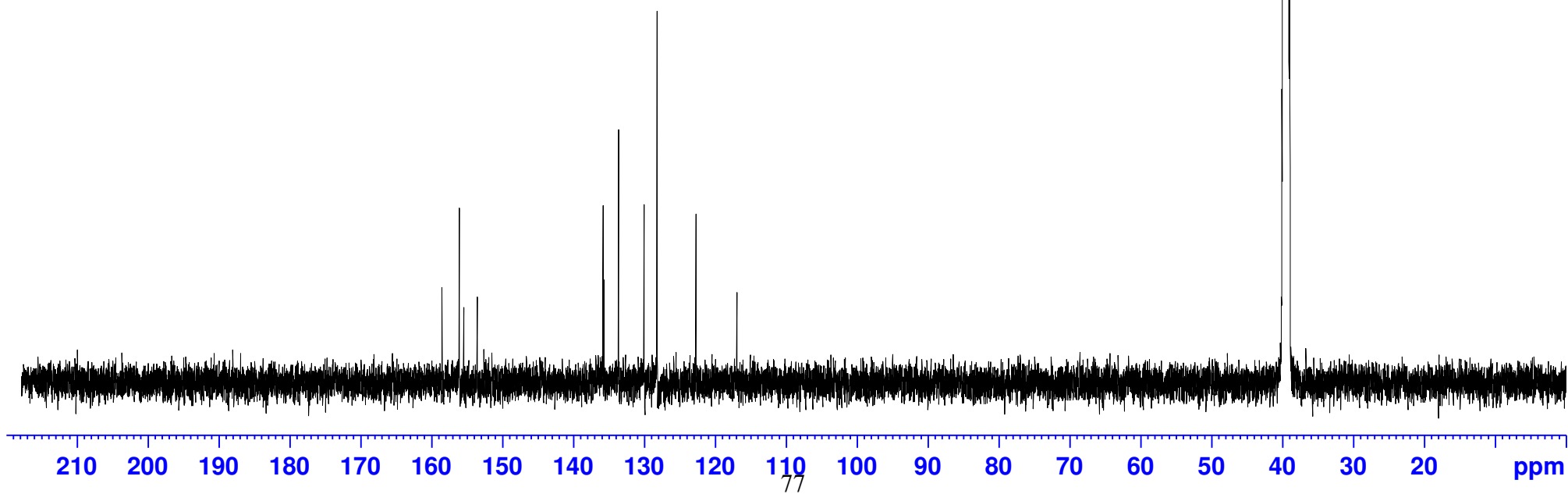


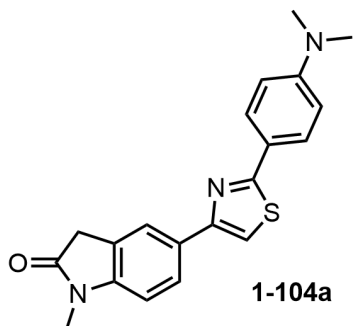


158.54
156.10
155.48
153.55
135.83
135.69
133.64
130.05
128.20
122.71
116.97

39.51

^{13}C NMR, DMSO- d_6 , 126 MHz



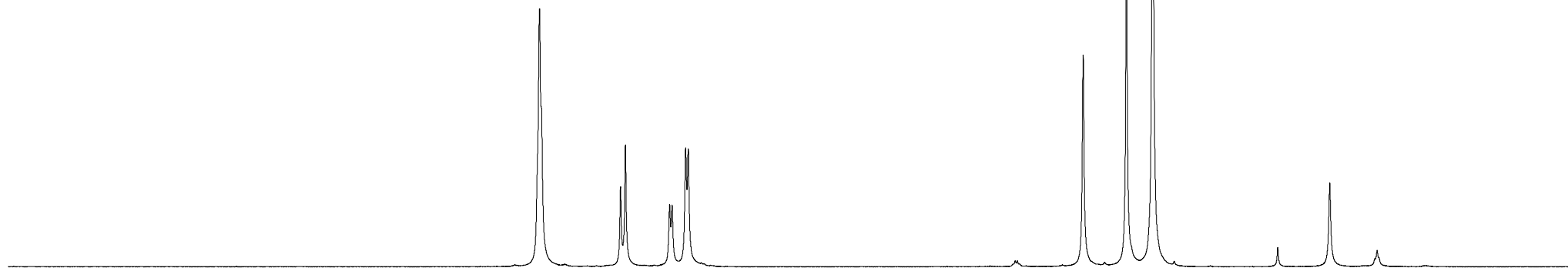


¹H NMR, CDCl₃, 400 MHz

7.904
7.890
7.261
7.222
6.872
6.852
6.744
6.724

3.590
3.247
3.038

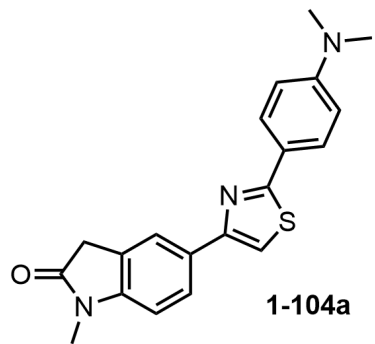
1.633



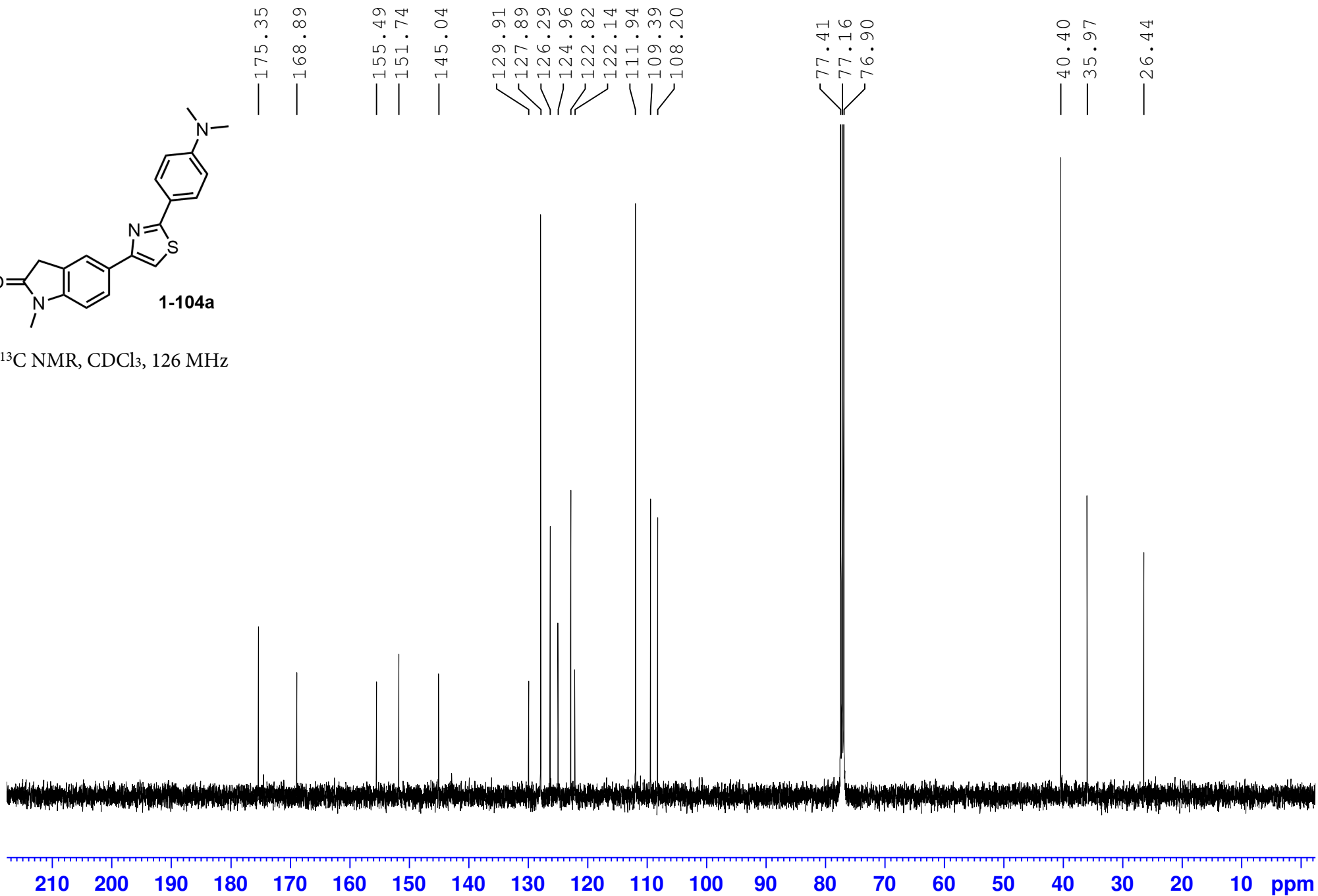
12 11 10 9 8 7 6 5 4 3 2 1 ppm

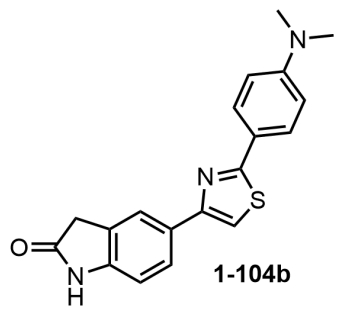
4.01
1.01
1.00
2.08

2.05
3.09
6.25

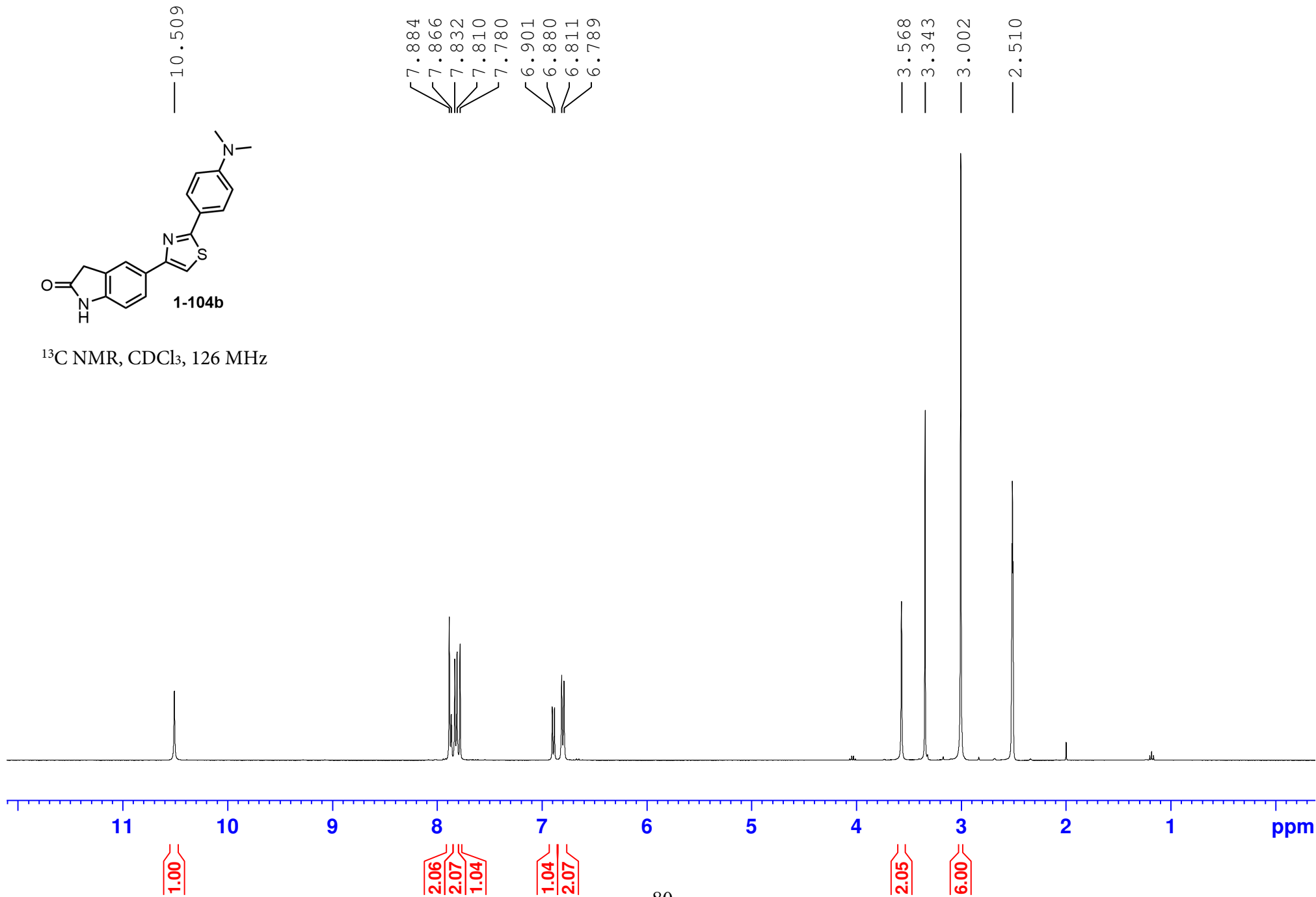


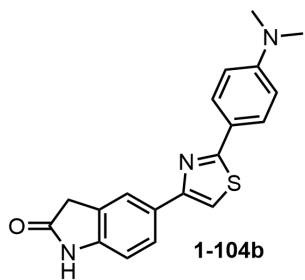
^{13}C NMR, CDCl_3 , 126 MHz



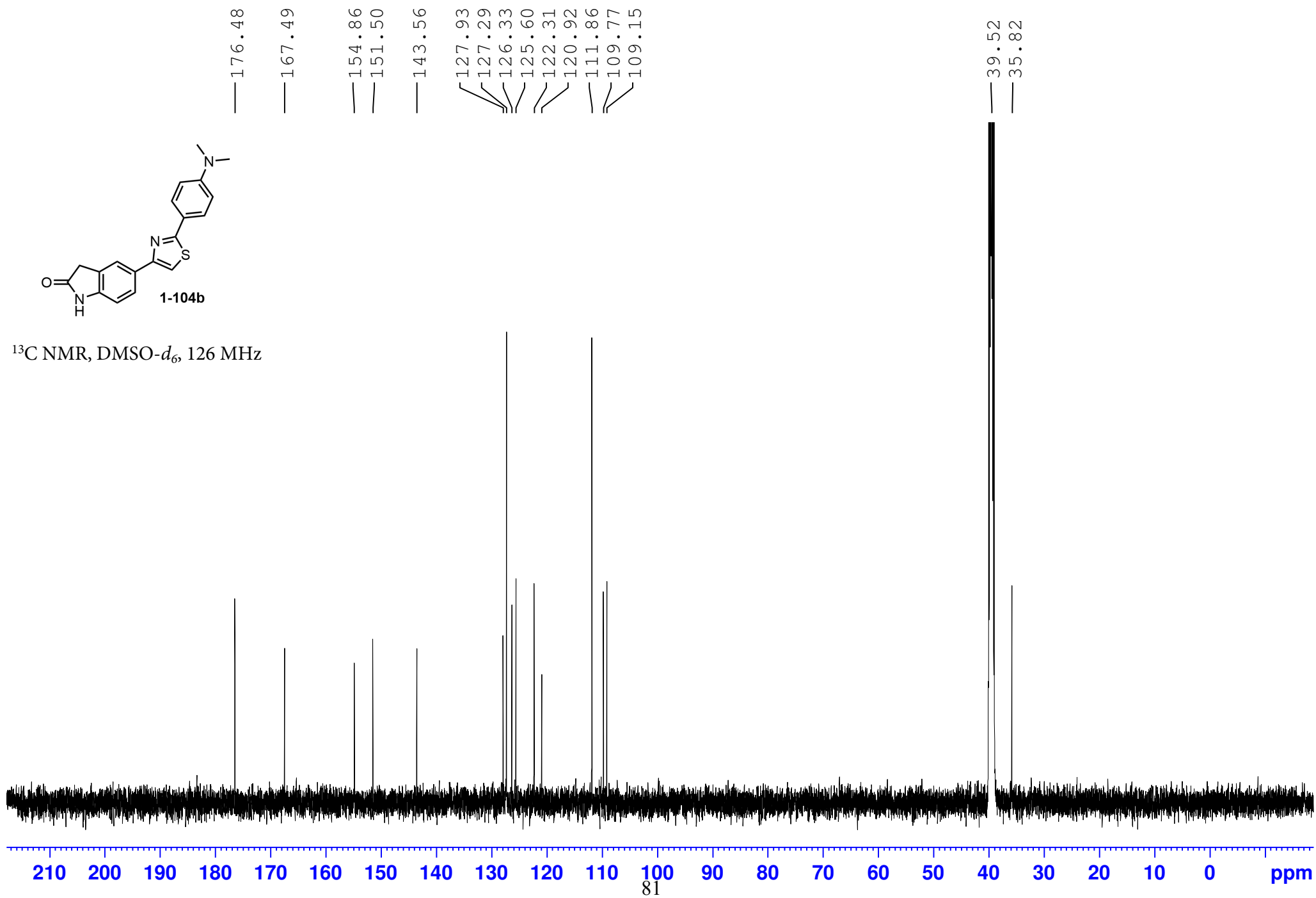


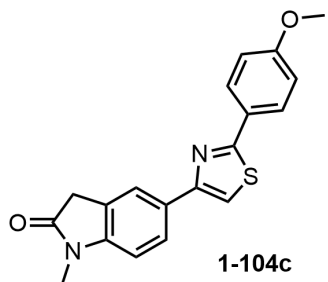
¹³C NMR, CDCl₃, 126 MHz





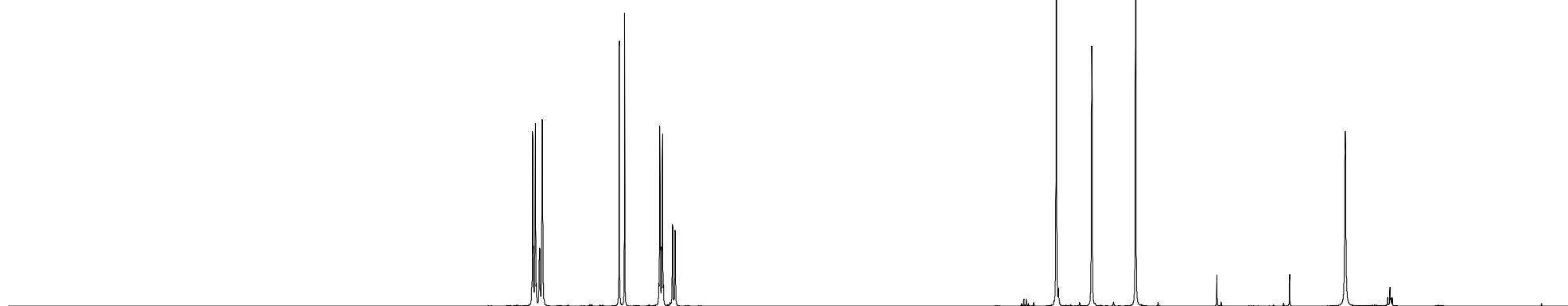
^{13}C NMR, DMSO- d_6 , 126 MHz





¹H NMR, CDCl₃, 400 MHz

7.989
7.982
7.976
7.964
7.959
7.952
7.926
7.906
7.303
7.260
6.992
6.985
6.980
6.968
6.963
6.956
6.884
6.864
3.874
3.596
3.253
1.609



11

10

9

2.04
2.04

1.00
2.07
1.04

6

5

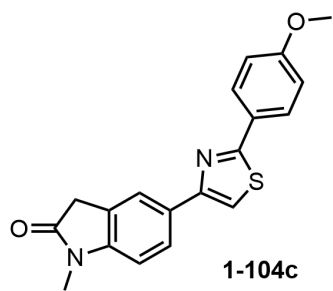
3.06
2.08
3.06

4

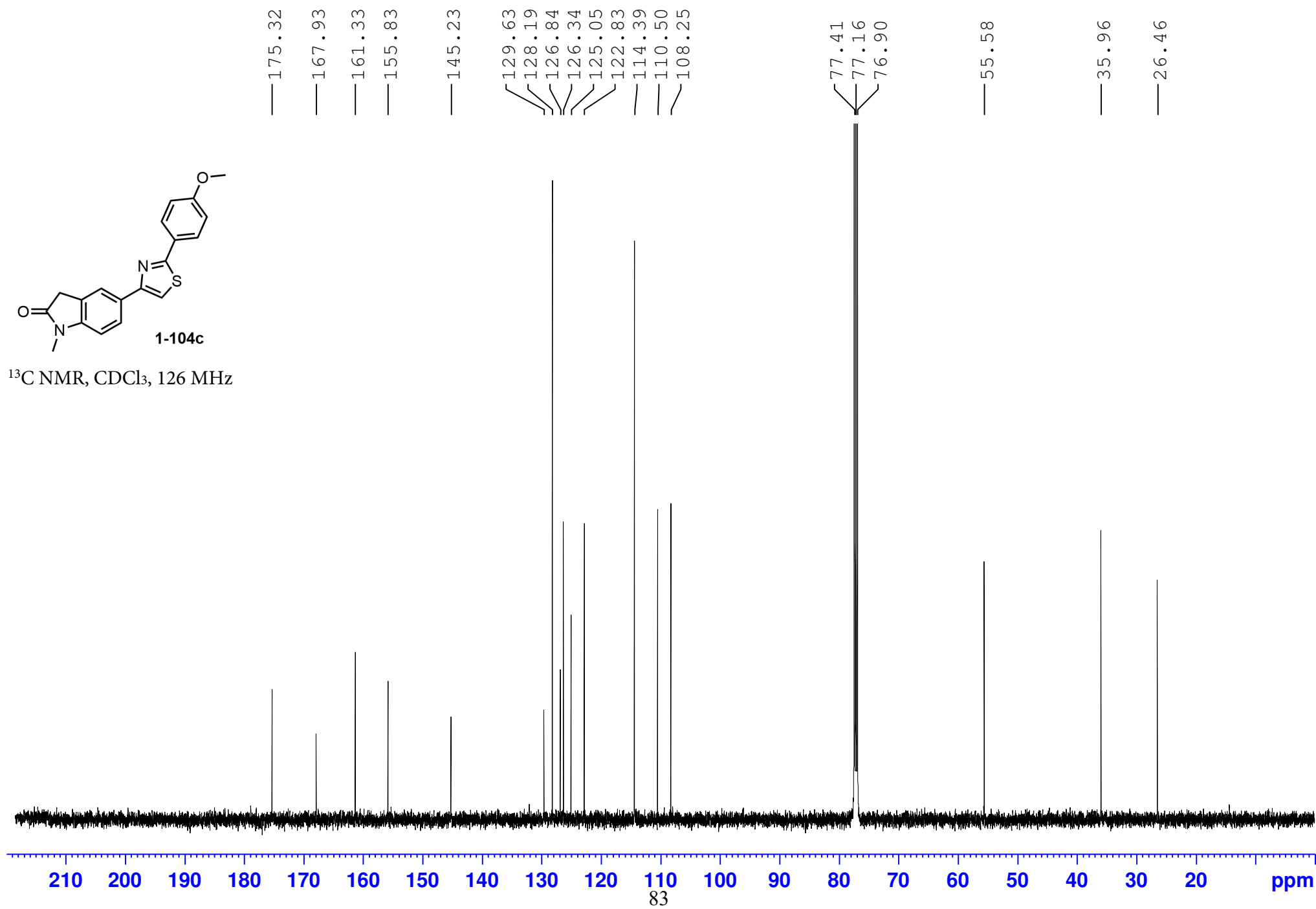
3

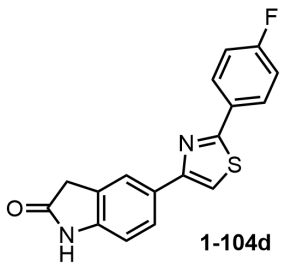
2

1 ppm

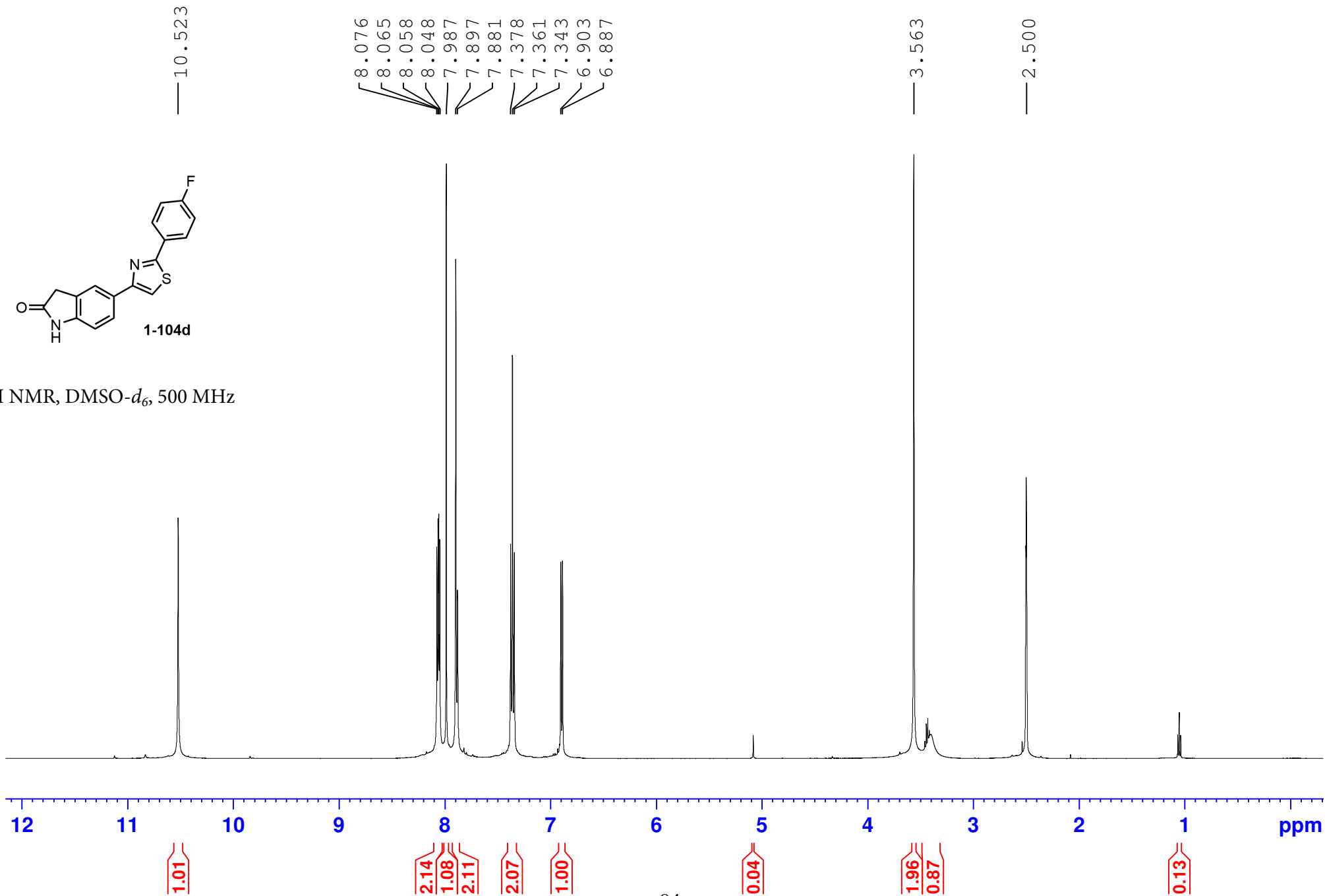


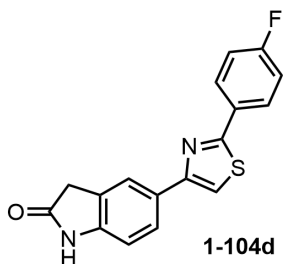
¹³C NMR, CDCl₃, 126 MHz





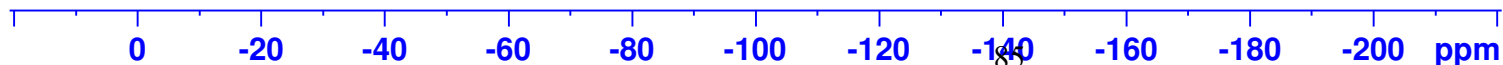
^1H NMR, DMSO- d_6 , 500 MHz





^{16}F NMR, DMSO- d_6 , 471 MHz

-110.64



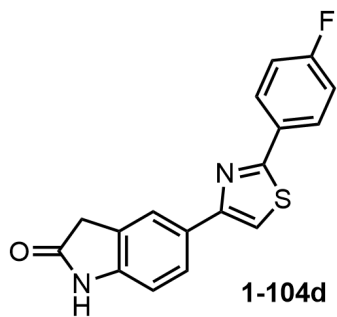
Current Data Parameters
 NAME LT-667-93-Fluorine
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160824
 Time 12.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgfhigqn.2
 TD 131072
 SOLVENT DMSO
 NS 16
 DS 4
 SWH 113636.367 Hz
 FIDRES 0.866977 Hz
 AQ 0.5767168 sec
 RG 203
 DW 4.400 usec
 DE 6.50 usec
 TE 295.5 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 470.5735434 MHz
 NUC1 19F
 P1 5.00 usec
 PLW1 10.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1620006 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.00000000 W
 PLW12 0.37195000 W

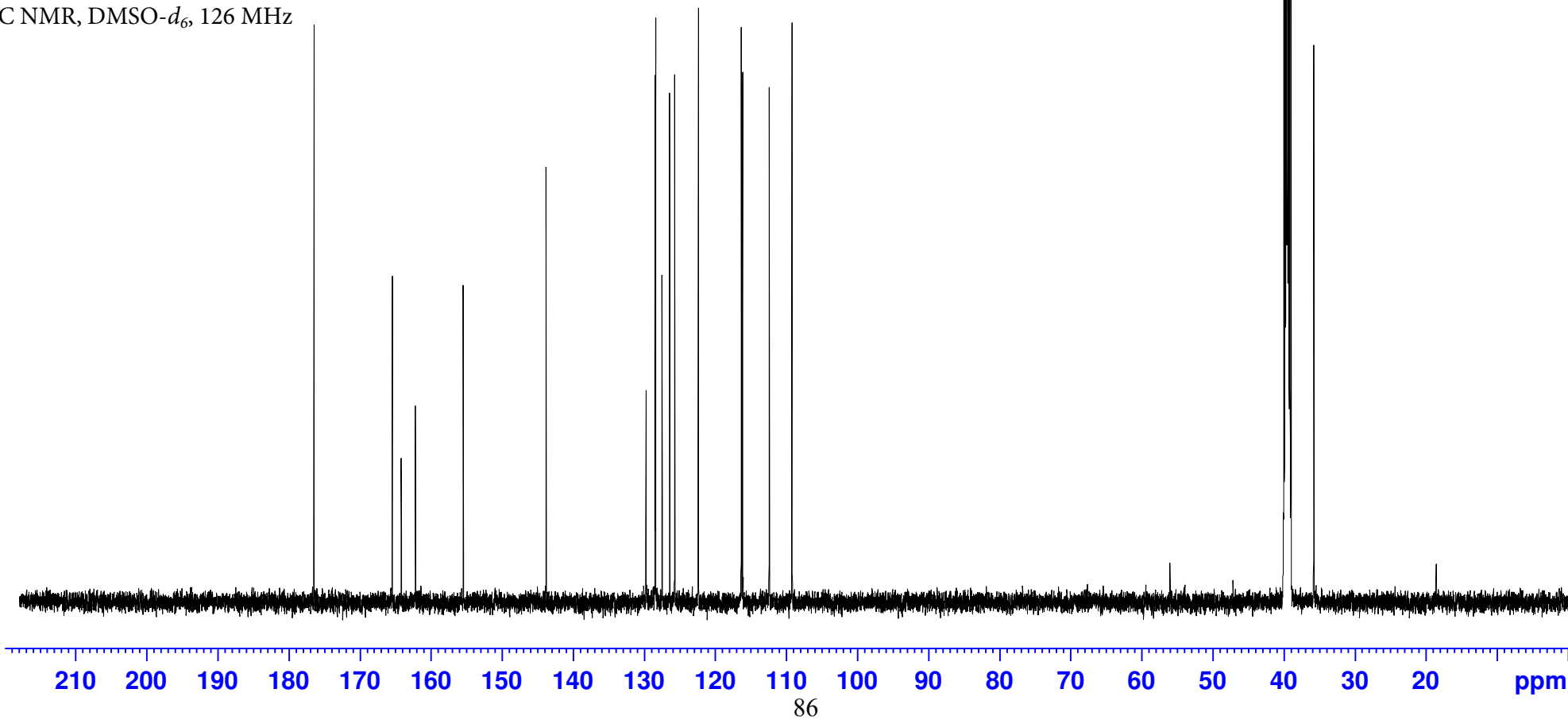
F2 - Processing parameters
 SI 65536
 SF 470.6206054 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

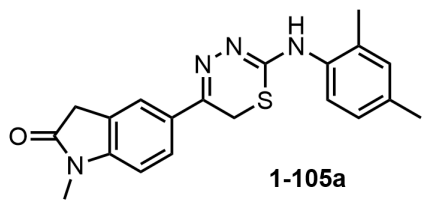


¹³C NMR, DMSO-*d*₆, 126 MHz

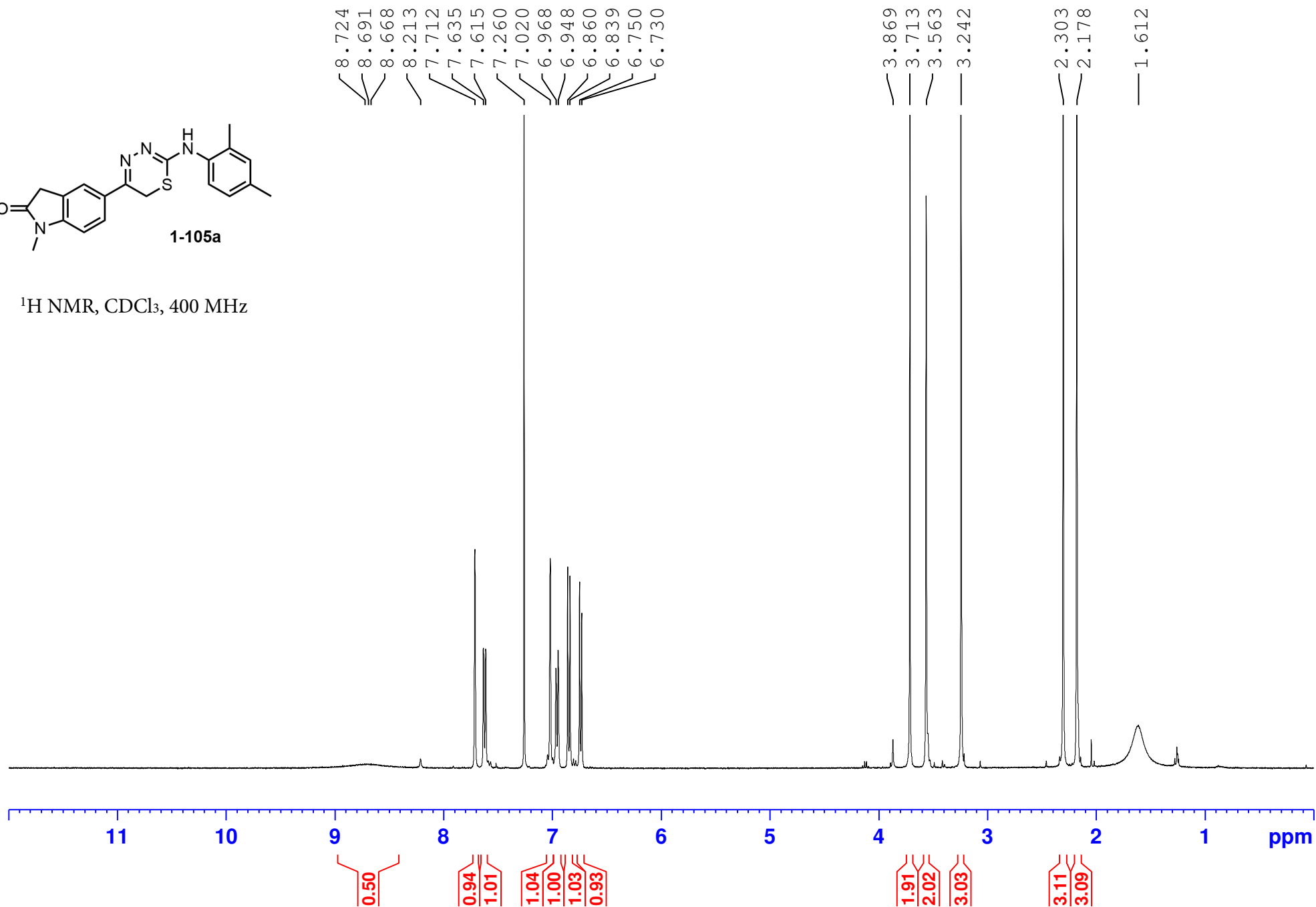
- 176.47
- 165.45
- 164.20
- 162.23
- 155.48
- 143.83
- 129.77
- 129.75
- 128.48
- 128.41
- 127.50
- 126.43
- 125.73
- 122.40
- 116.36
- 116.18
- 112.42
- 109.22

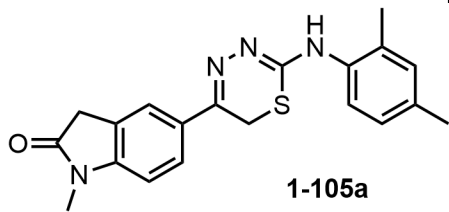
- 39.52
- 35.80



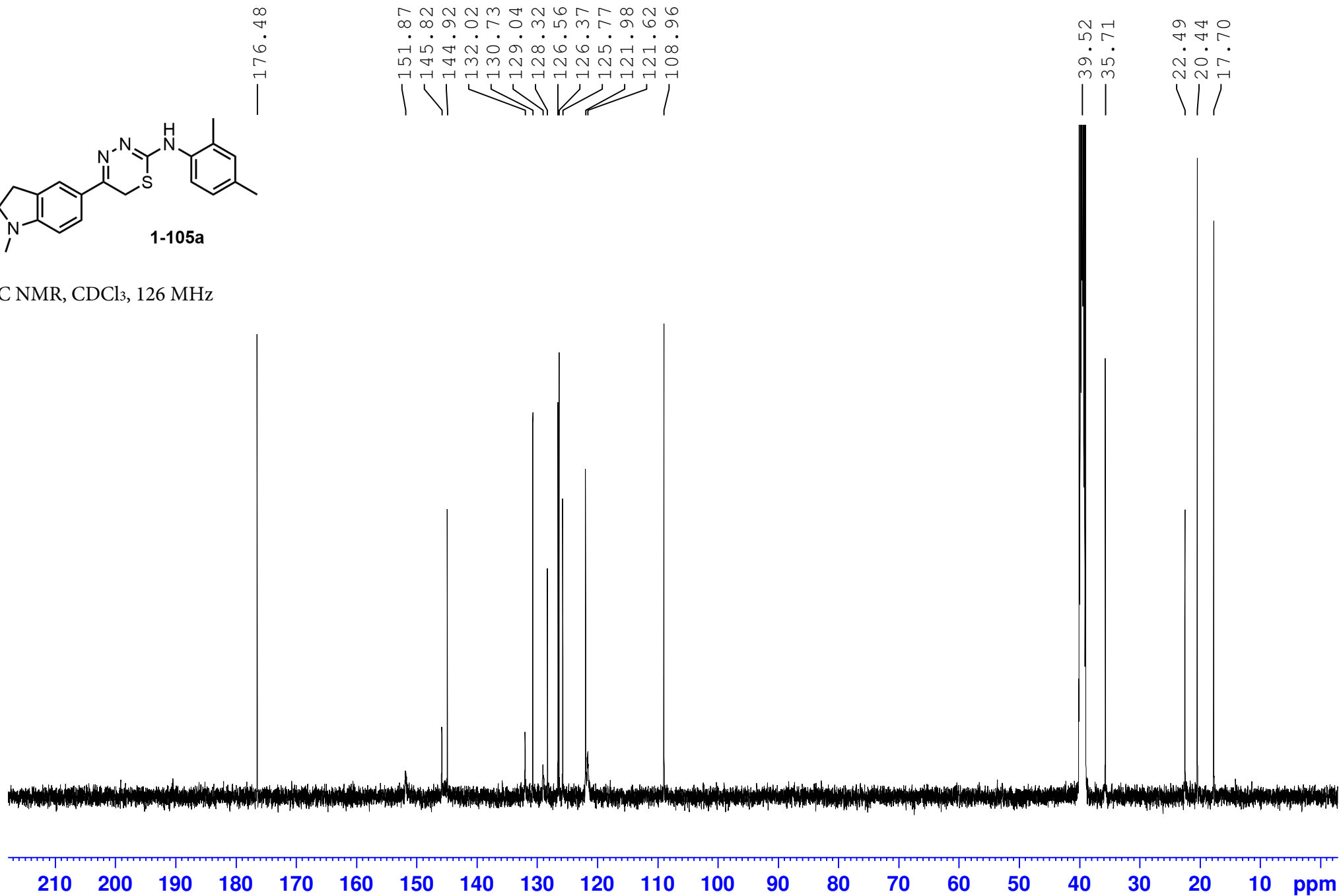


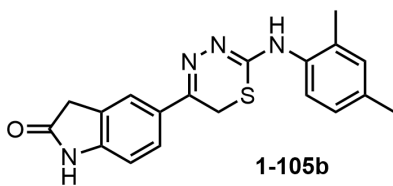
¹H NMR, CDCl₃, 400 MHz



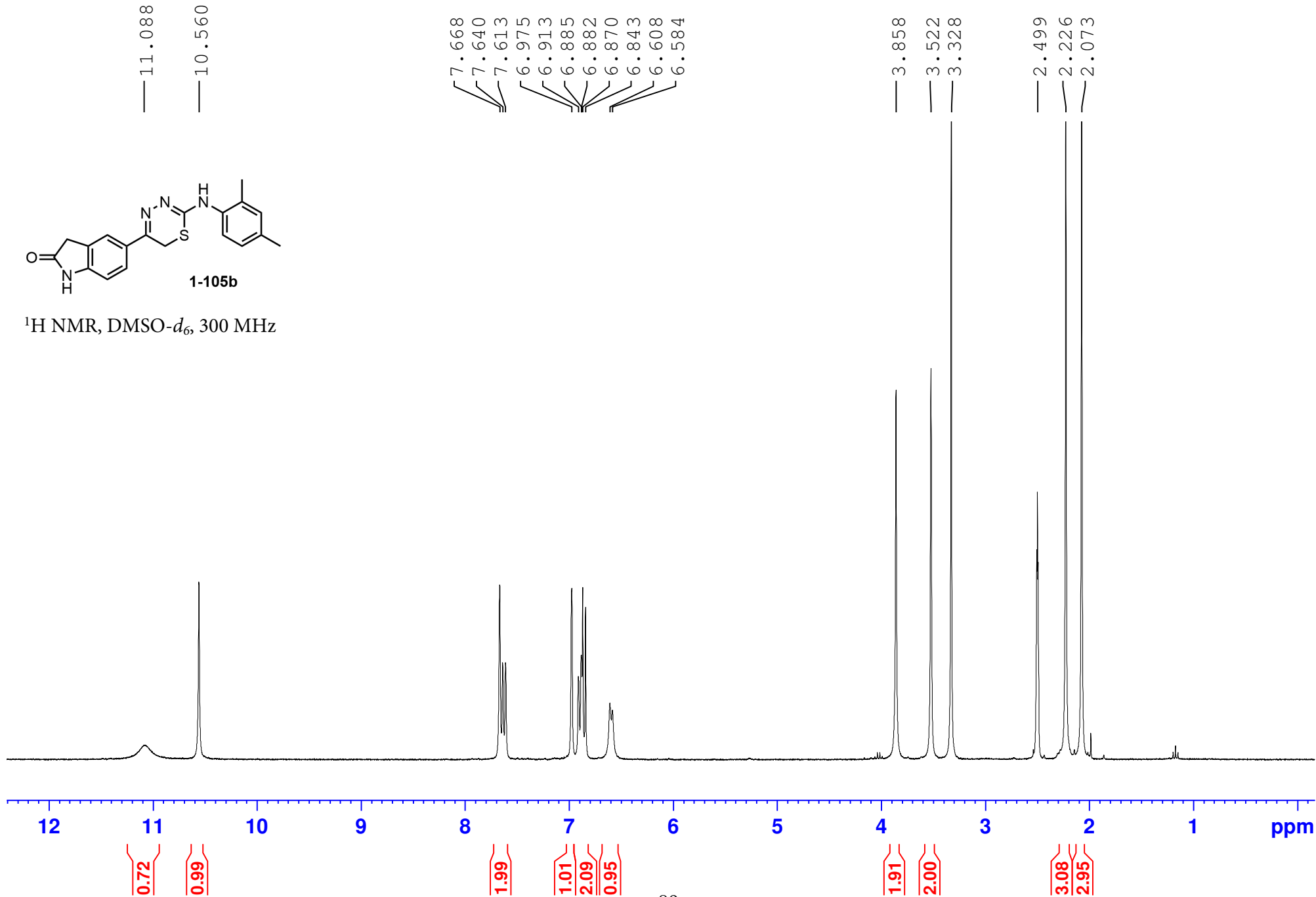


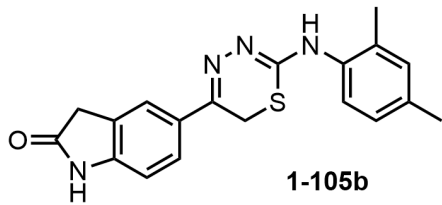
^{13}C NMR, CDCl_3 , 126 MHz



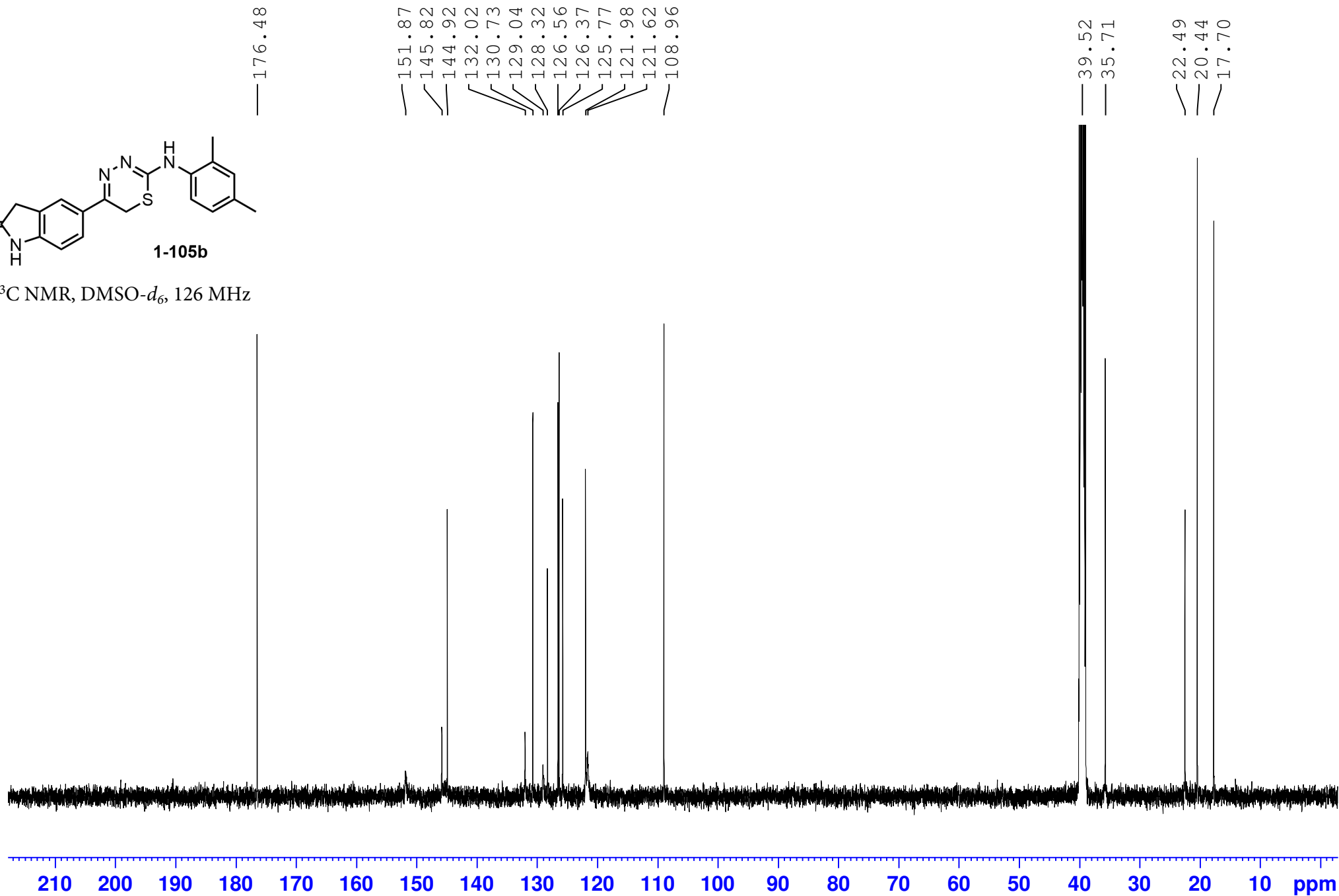


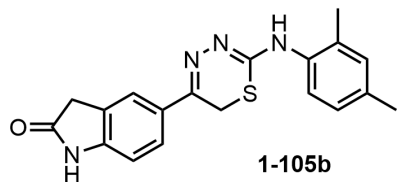
^1H NMR, DMSO- d_6 , 300 MHz



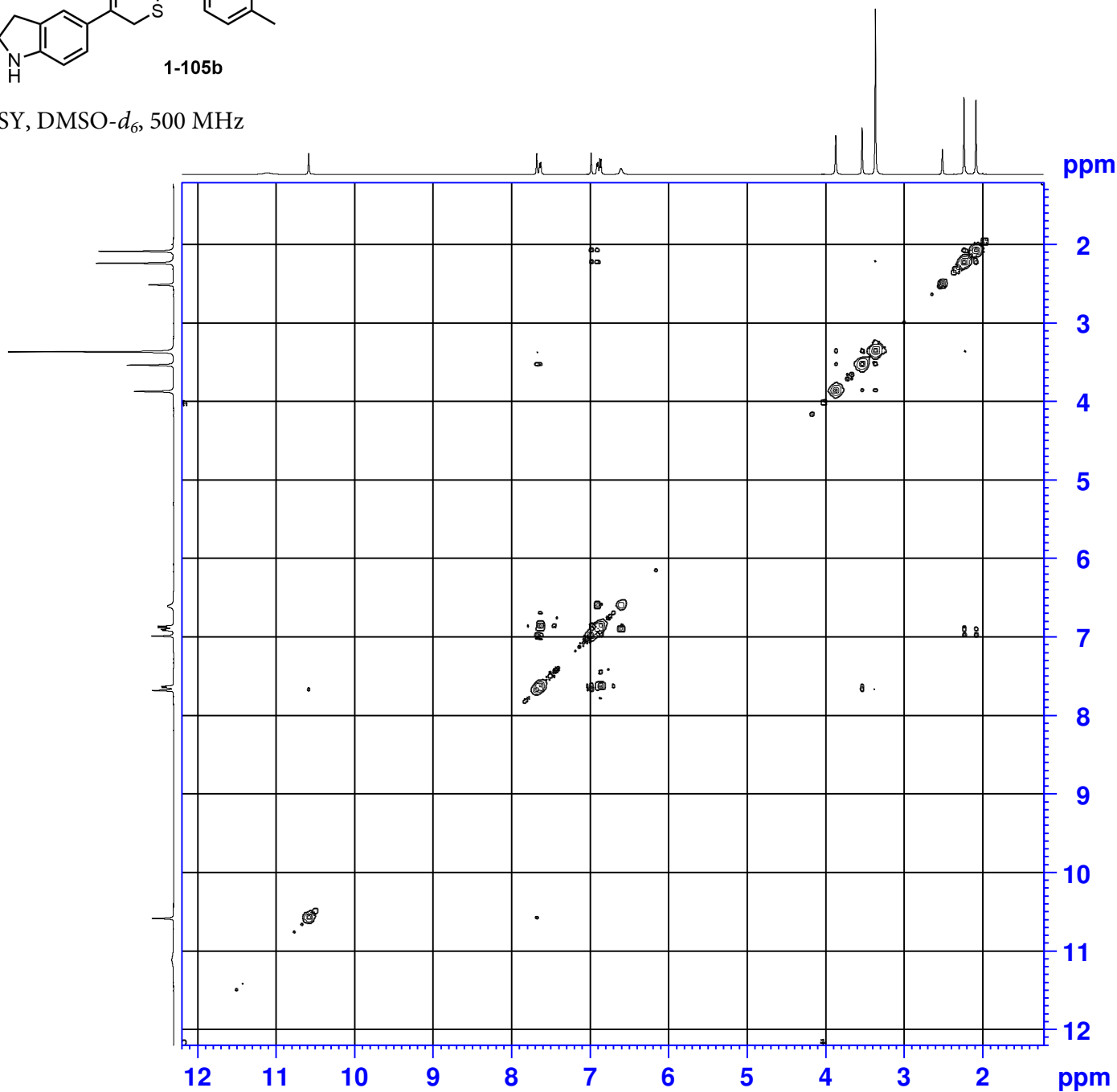


^{13}C NMR, DMSO- d_6 , 126 MHz





COSY, DMSO-*d*₆, 500 MHz



```

Current Data Parameters
NAME      LT-667-94_COSY
EXPNO     11
PROCNO    1

F2 - Acquisition Parameters
Date_     20160830
Time      13.48
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   cosygpppqf
TD         2048
SOLVENT   DMSO
NS         2
DS         8
SWH       5494.505 Hz
FIDRES    2.682864 Hz
AQ         0.1863680 sec
RG         64
DW         91.000 usec
DE         6.50 usec
TE         294.9 K
D0         0.0000300 sec
D1         1.96682203 sec
D11        0.03000000 sec
D12        0.00002000 sec
D13        0.00000400 sec
D16        0.00020000 sec
INO        0.00018200 sec

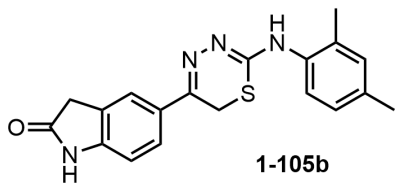
===== CHANNEL f1 =====
SF01      500.1633555 MHz
NUC1       1H
P0         11.50 usec
P1         11.50 usec
P17        2500.00 usec
PLW1       18.00000000 W
PLW10      3.52139997 W

===== GRADIENT CHANNEL =====
GPNAM[1]  SMSQ10.100
GPZ1      10.00 %
P16       1000.00 usec

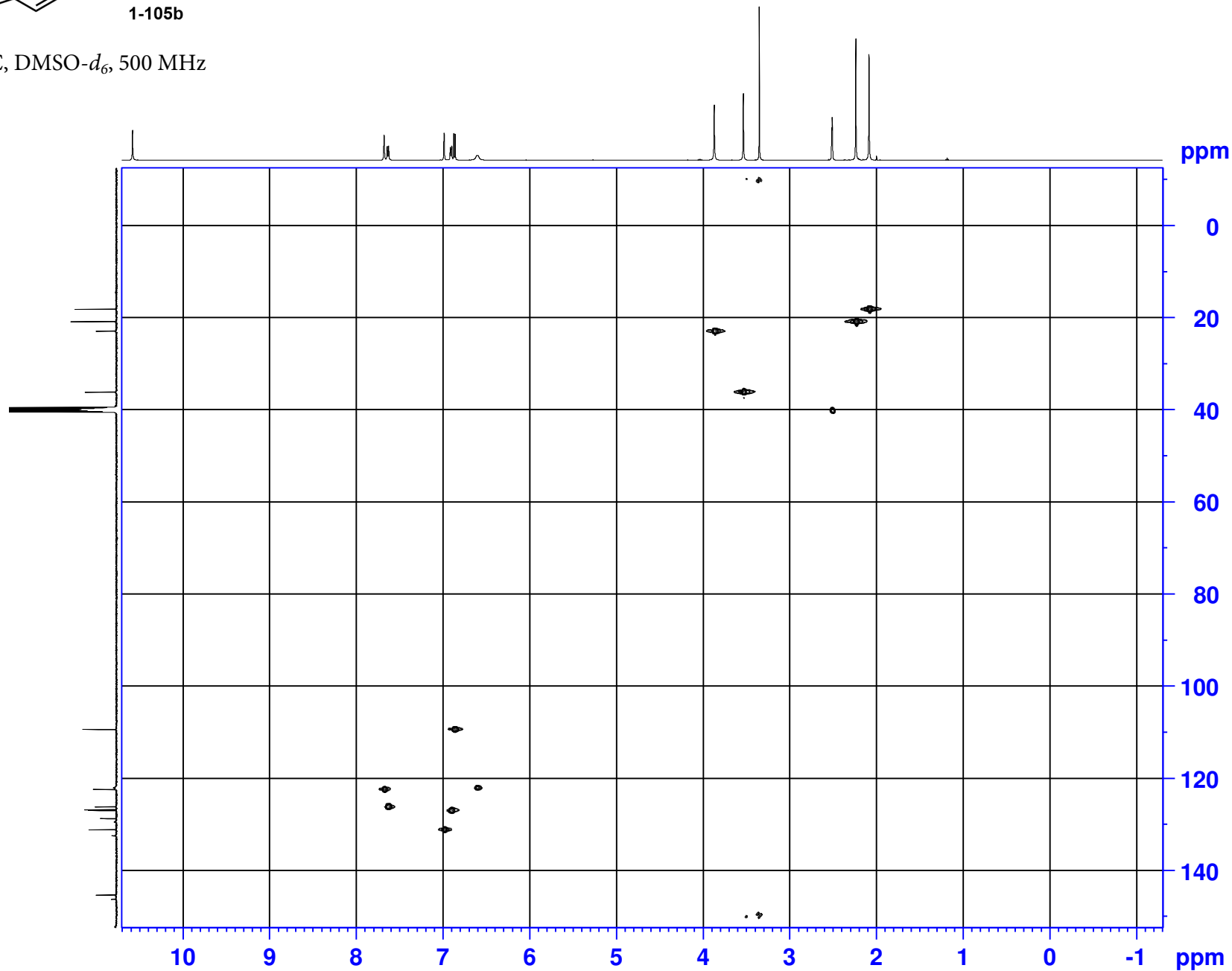
F1 - Acquisition parameters
TD         128
SF01      500.1634 MHz
FIDRES    85.851646 Hz
SW         10.985 ppm
FnMODE     QF

F2 - Processing parameters
SI         1024
SF         500.1600000 MHz
WDW        QSINE
SSB        0
LB         0 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        QF
SF         500.1600000 MHz
WDW        QSINE
SSB        0
LB         0 Hz
GB         0
  
```



HSQC, DMSO-*d*₆, 500 MHz



```

Current Data Parameters
NAME      LT-667-94_HSQC
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20160829
Time      13.03
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   hsqcetgpcisp2.2
TD         1024
SOLVENT   DMSO
NS         13
DS         16
SWH        6009.615 Hz
FIDRES     5.868765 Hz
AQ         0.0851968 sec
RG         128
DW         83.200 usec
DE         6.50 usec
TE         295.1 K
CNST2     145.000000
CNST17    -0.500000
DO         0.00000300 sec
D1         2.00000000 sec
D4         0.00172414 sec
D11        0.03000000 sec
D16        0.00200000 sec
D24        0.00089000 sec
RG         0.00022410 sec

===== CHANNEL f1 =====
SFO1      500.1623508 MHz
NUC1       1H
P1         11.50 usec
P2         23.00 usec
P28        1000.00 usec
PLW1       18.00000000 W

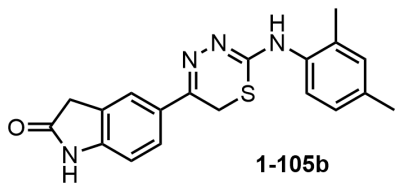
===== CHANNEL f2 =====
SFO2      125.7741356 MHz
NUC2       13C
CPDPRG2   bi_p5m4sp_4sp.2
P3         10.50 usec
P14        500.00 usec
P24        2000.00 usec
P63        1500.00 usec
PLW0       0 W
PLW2       110.00000000 W
PLW12      2.47499990 W
SPNAM[3]   Crp60,0.5,20.1
SFOAL3     0 Hz
SPOFFS3    0 Hz
SPW3       18.52899933 W
SFOAL7     0 Hz
SPOFFS7    0 Hz
SPW7       18.52899933 W
SPNAM[14]  Crp32,1.5,20.2
SFOAL14    0 Hz
SPOFFS14   0 Hz
SPW14      7.90590000 W
SPNAM[31]  Crp32,1.5,20.2
SFOAL31    0 Hz
SPOFFS31   0 Hz
SPW31      1.97650003 W

===== GRADIENT CHANNEL =====
GPNAM[1]   SMSQ10.100
GPNAM[2]   SMSQ10.100
GPNAM[3]   SMSQ10.100
GPNAM[4]   SMSQ10.100
GP21       80.00 %
GP22       20.10 %
GP23       11.00 %
GP24       -5.00 %
P16        1000.00 usec
P19        600.00 usec

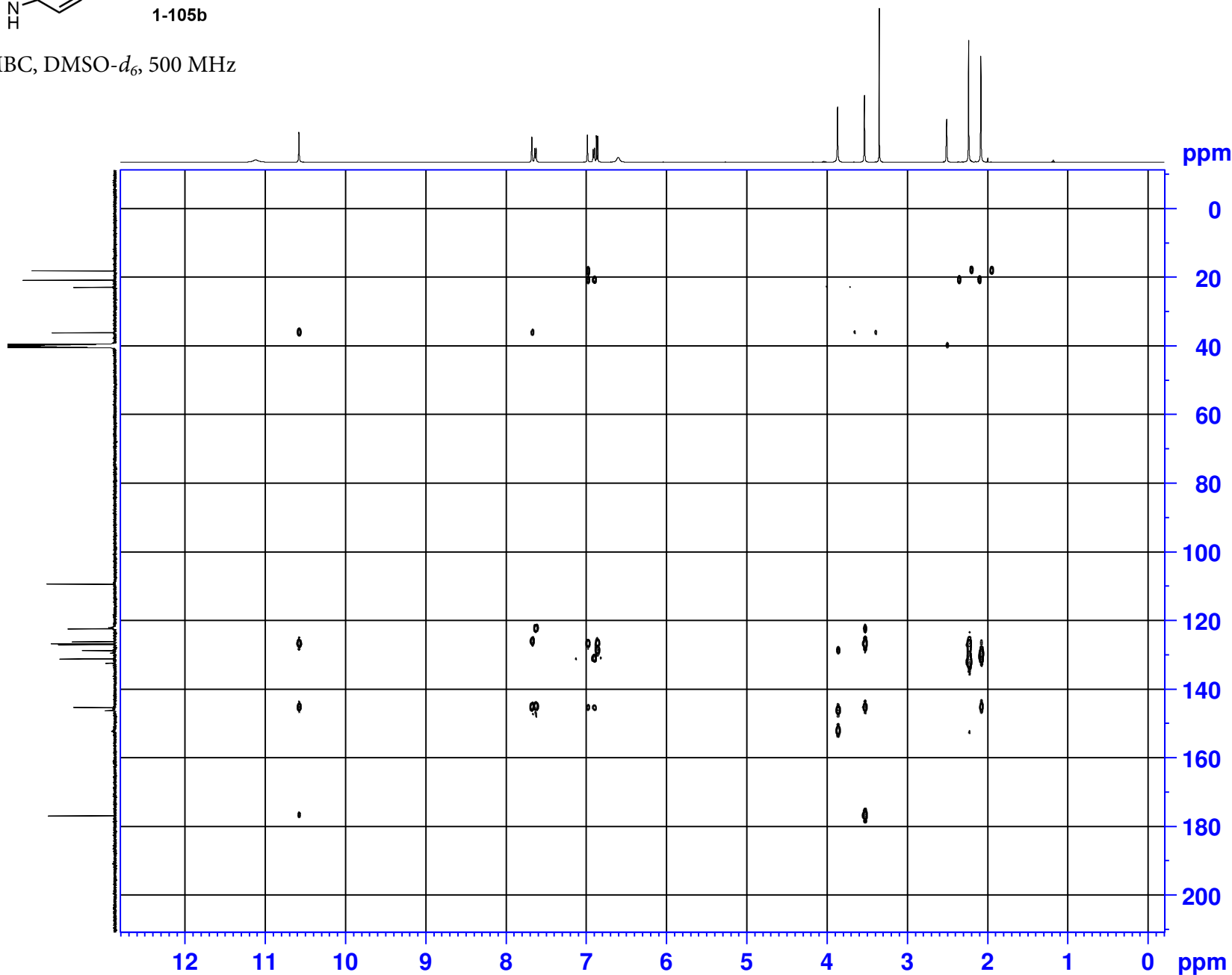
F1 - Acquisition parameters
TD         64
SFO1      125.7741 MHz
FIDRES     648.340271 Hz
SW         164.954 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI         1024
SF         500.1600000 MHz
WDW        QSINE
SSB        2
LB         0 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        echo-antiecho
SF         125.7653320 MHz
WDW        QSINE
SSB        2
LB         0 Hz
GB         0
  
```



HMBC, DMSO-*d*₆, 500 MHz



Current Data Parameters
 NAME LT-667-94_HMBC
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160829
 Time 15.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG hmbcgp1pndqf
 TD 2048
 SOLVENT DMSO
 NS 32
 DS 8
 SWH 6510.417 Hz
 FIDRES 3.178914 Hz
 AQ 0.1572864 sec
 RG 203
 DW 76.800 usec
 DE 6.50 usec
 TE 294.9 K
 CNST2 145.0000000
 CNST13 10.0000000
 D0 0.0000300 sec
 D1 1.5000000 sec
 D2 0.00344828 sec
 D6 0.05000000 sec
 D16 0.00020000 sec
 IN0 0.00001790 sec

==== CHANNEL f1 =====
 SFO1 500.1631510 MHz
 NUC1 1H
 P1 11.50 usec
 P2 23.00 usec
 PLW1 18.00000000 W

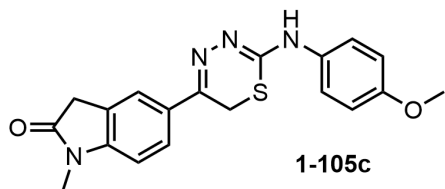
==== CHANNEL f2 =====
 SFO2 125.7778879 MHz
 NUC2 13C
 P3 10.50 usec
 PLW2 110.00000000 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P16 1000.00 usec

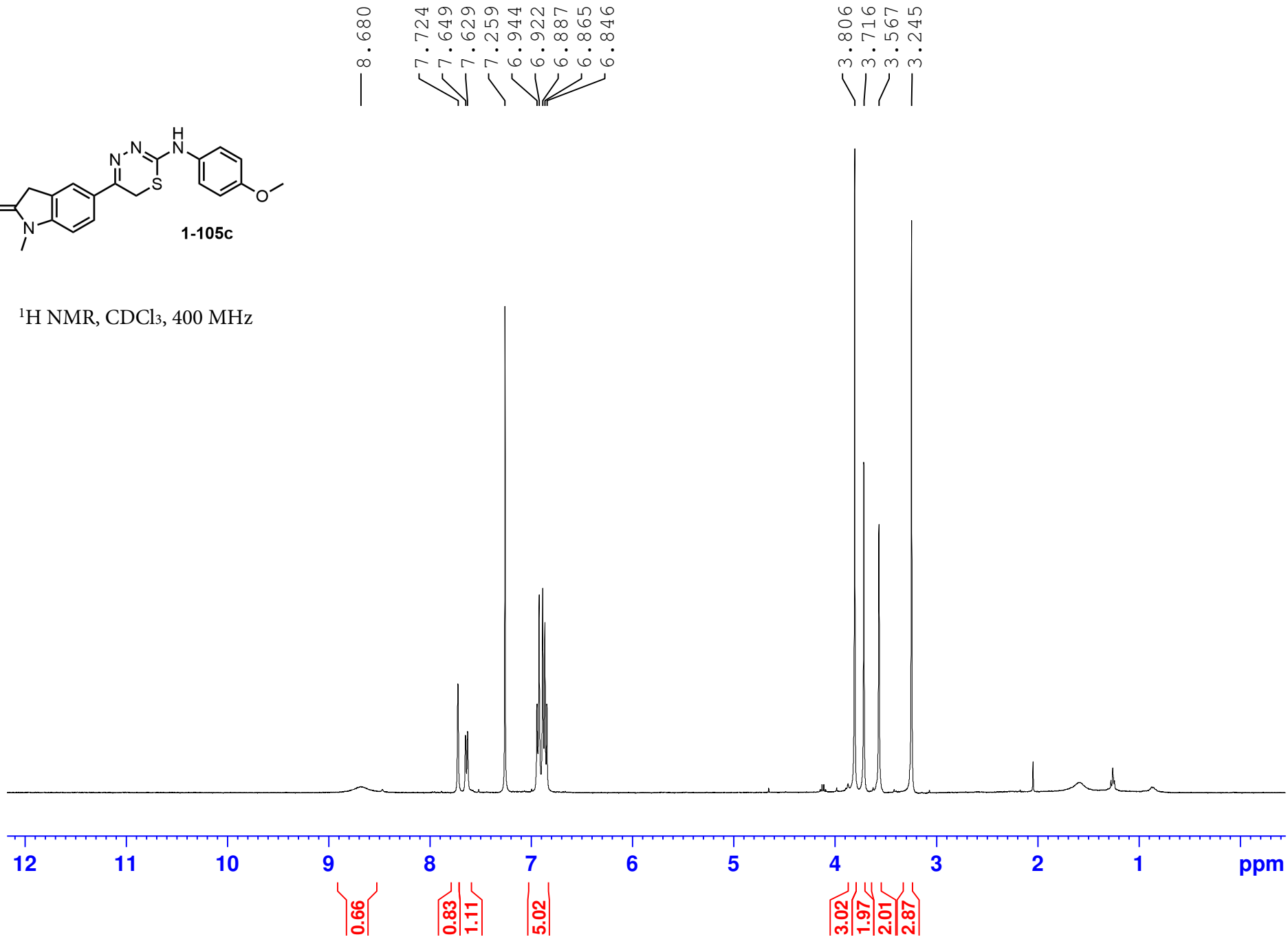
F1 - Acquisition parameters
 TD 32
 SFO1 125.7779 MHz
 FIDRES 1745.810059 Hz
 SW 222.082 ppm
 FhMODE QF

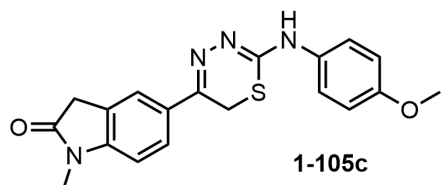
F2 - Processing parameters
 SI 2048
 SF 500.1600000 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 125.7653320 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0

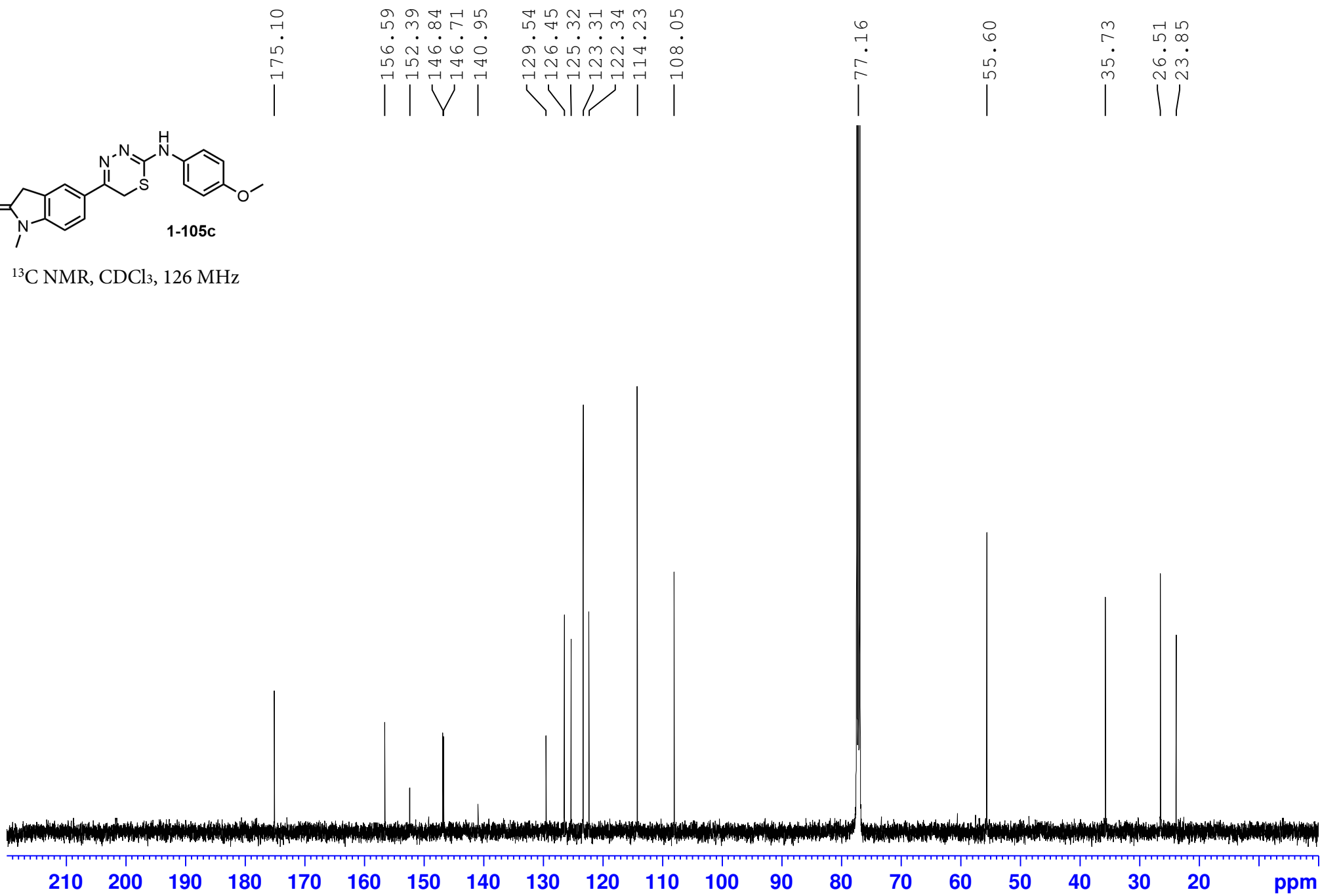


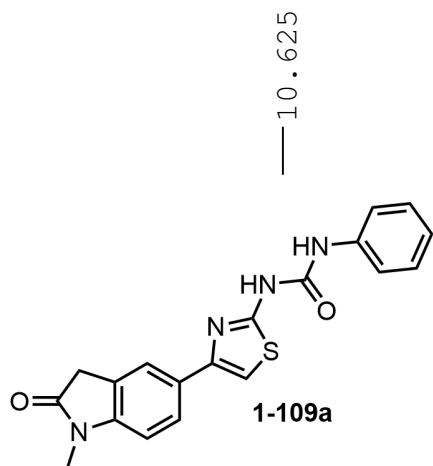
¹H NMR, CDCl₃, 400 MHz



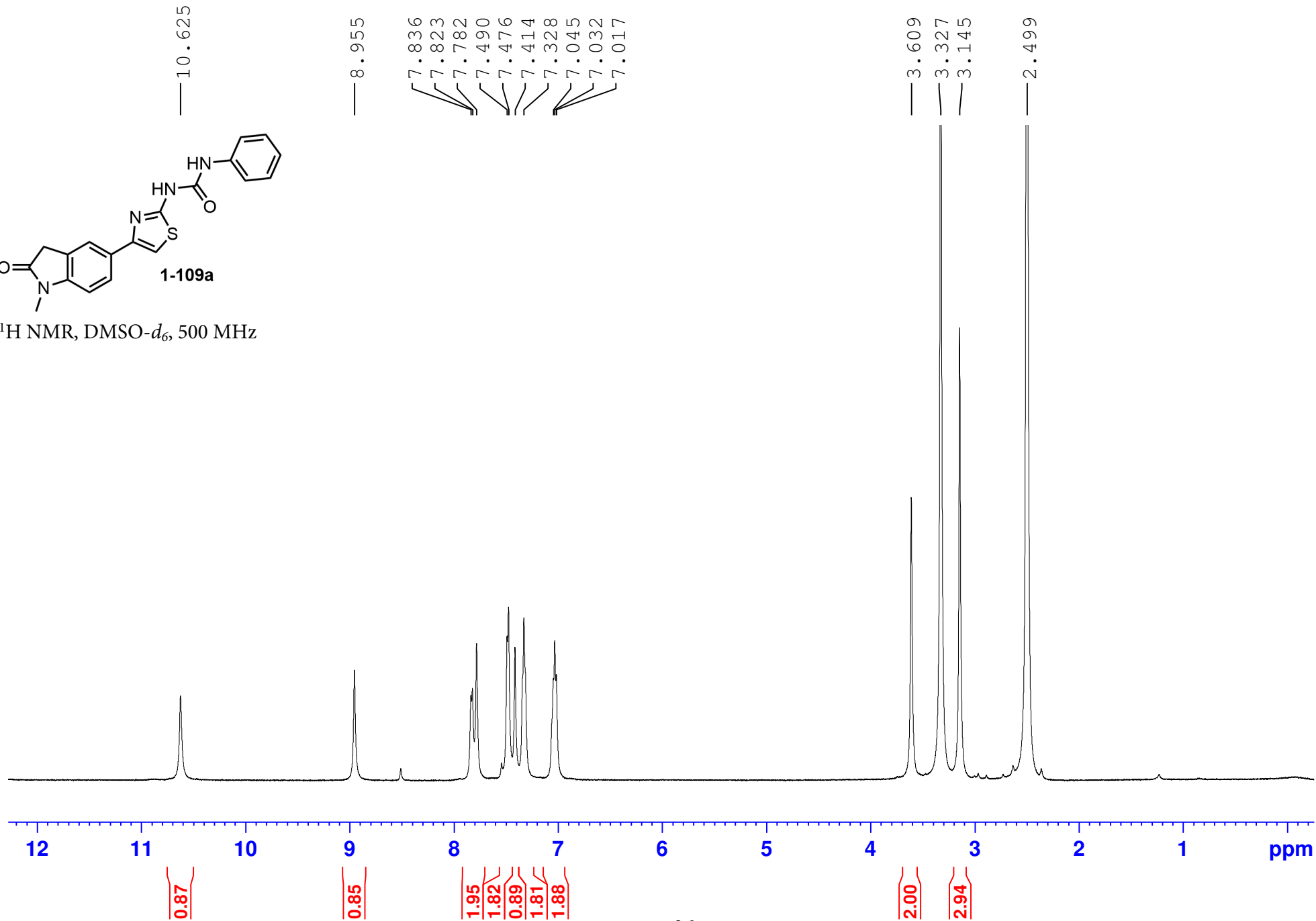


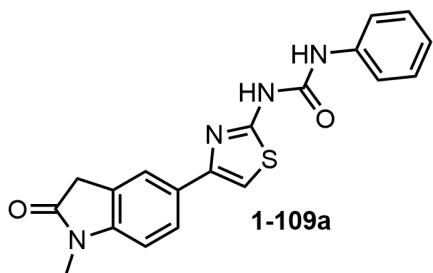
^{13}C NMR, CDCl_3 , 126 MHz



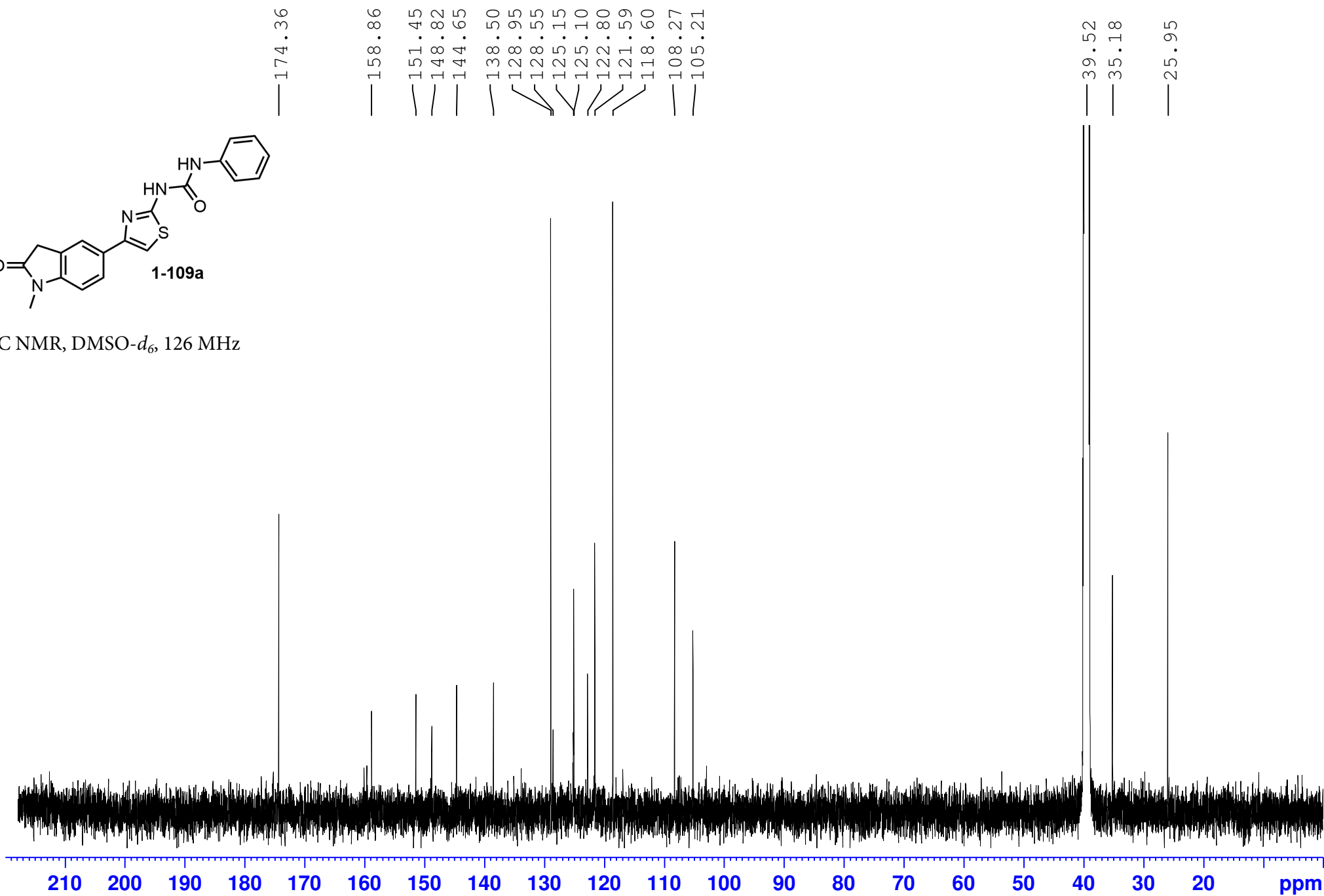


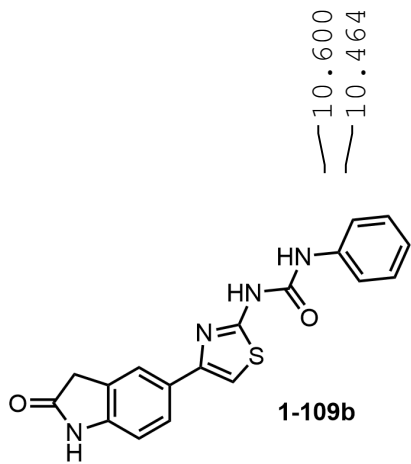
¹H NMR, DMSO-*d*₆, 500 MHz



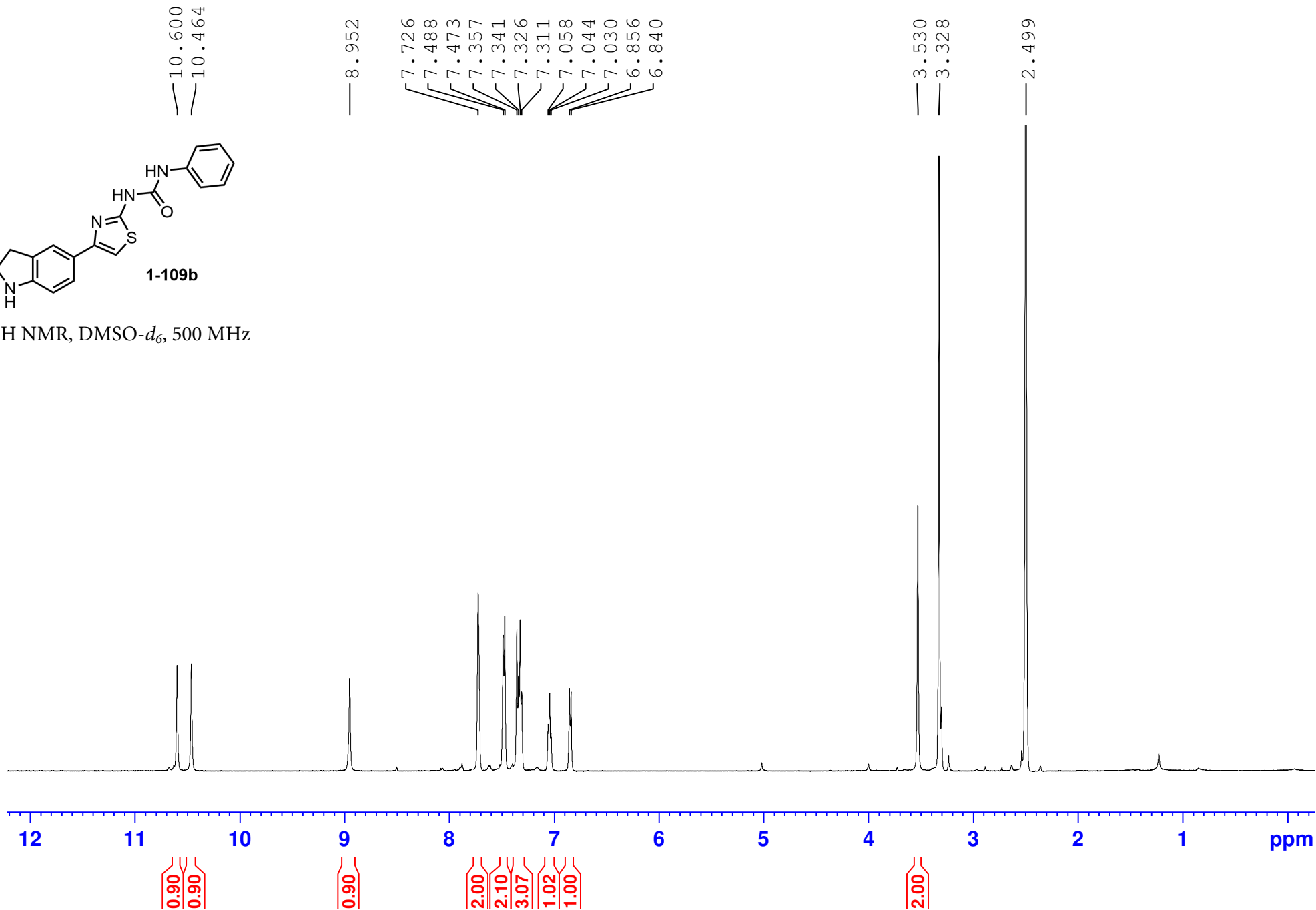


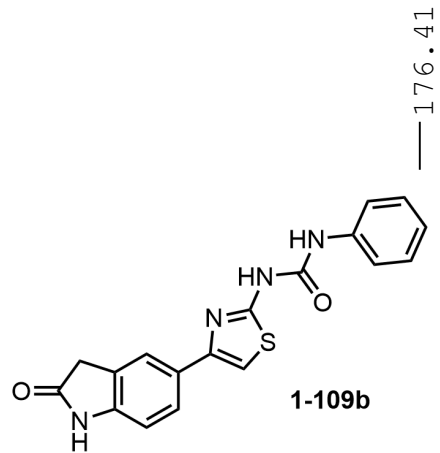
^{13}C NMR, DMSO- d_6 , 126 MHz



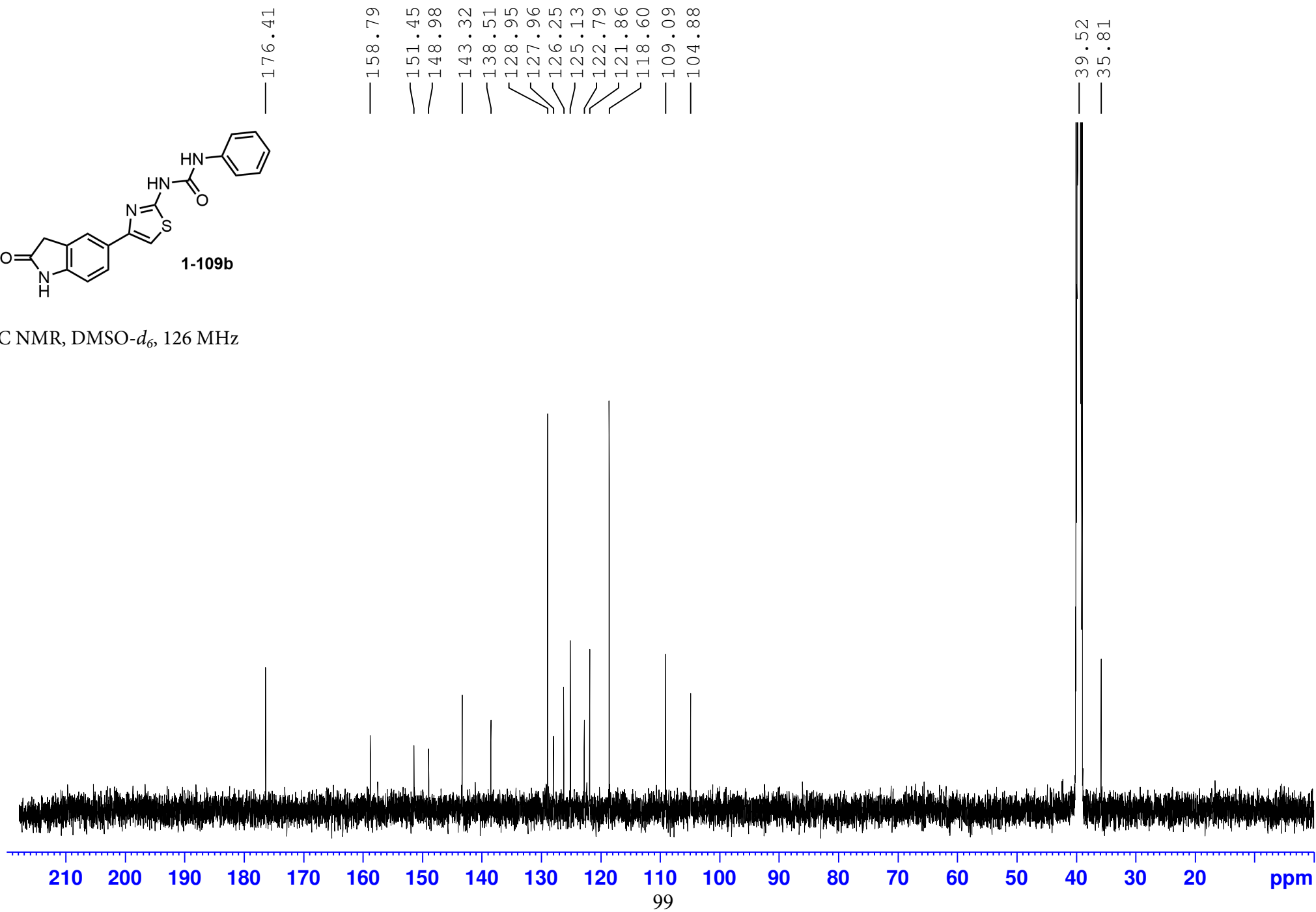


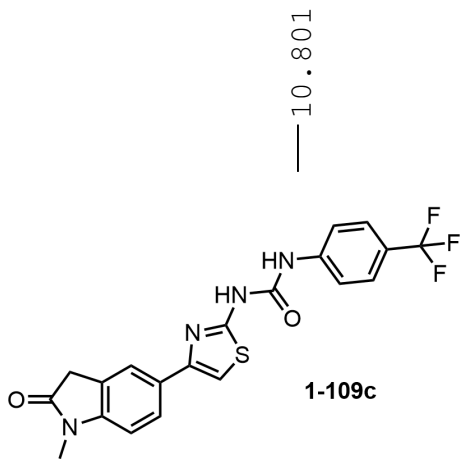
¹H NMR, DMSO-*d*₆, 500 MHz



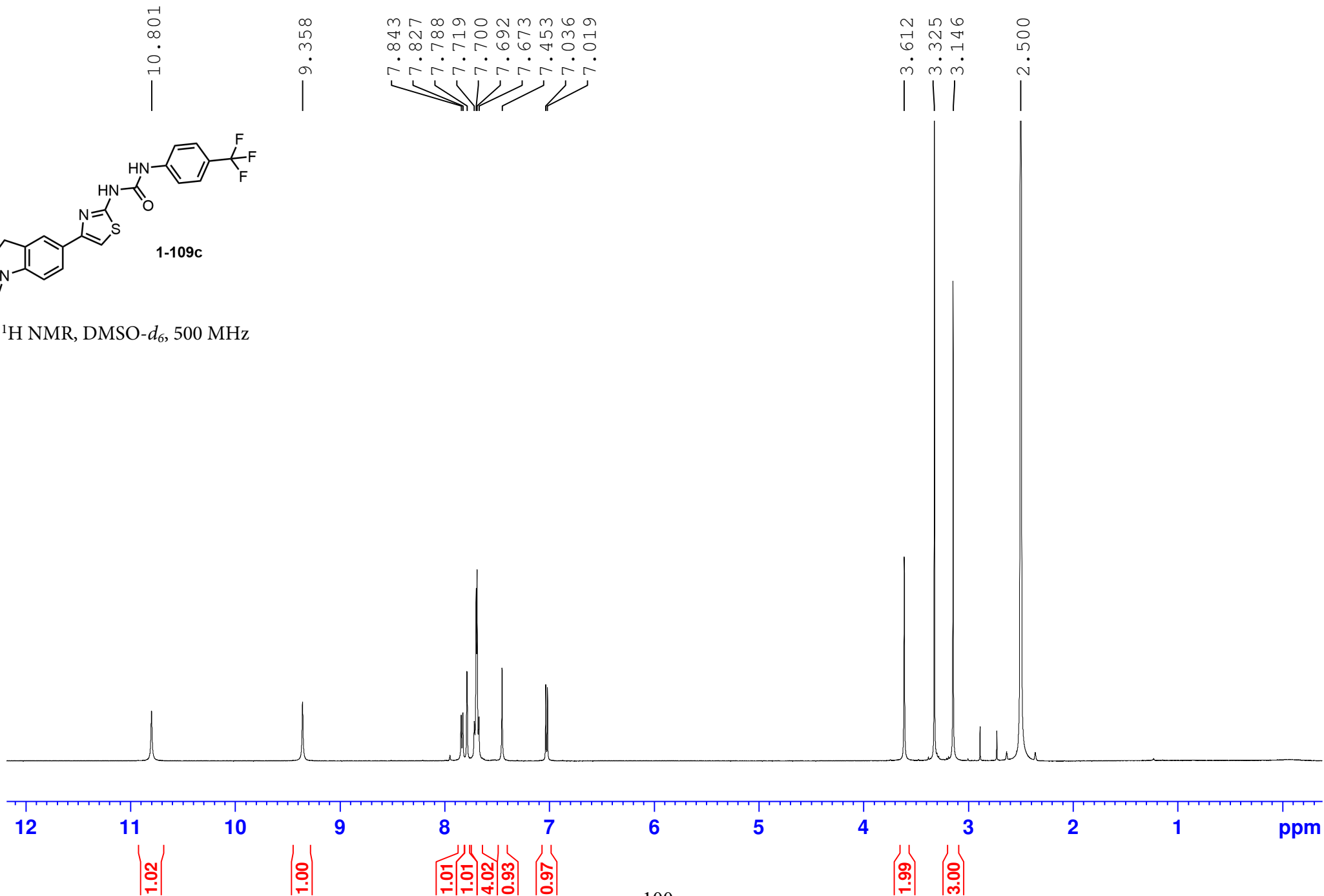


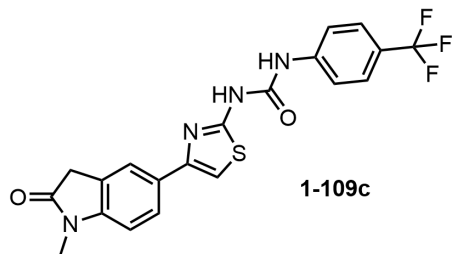
¹³C NMR, DMSO-*d*₆, 126 MHz



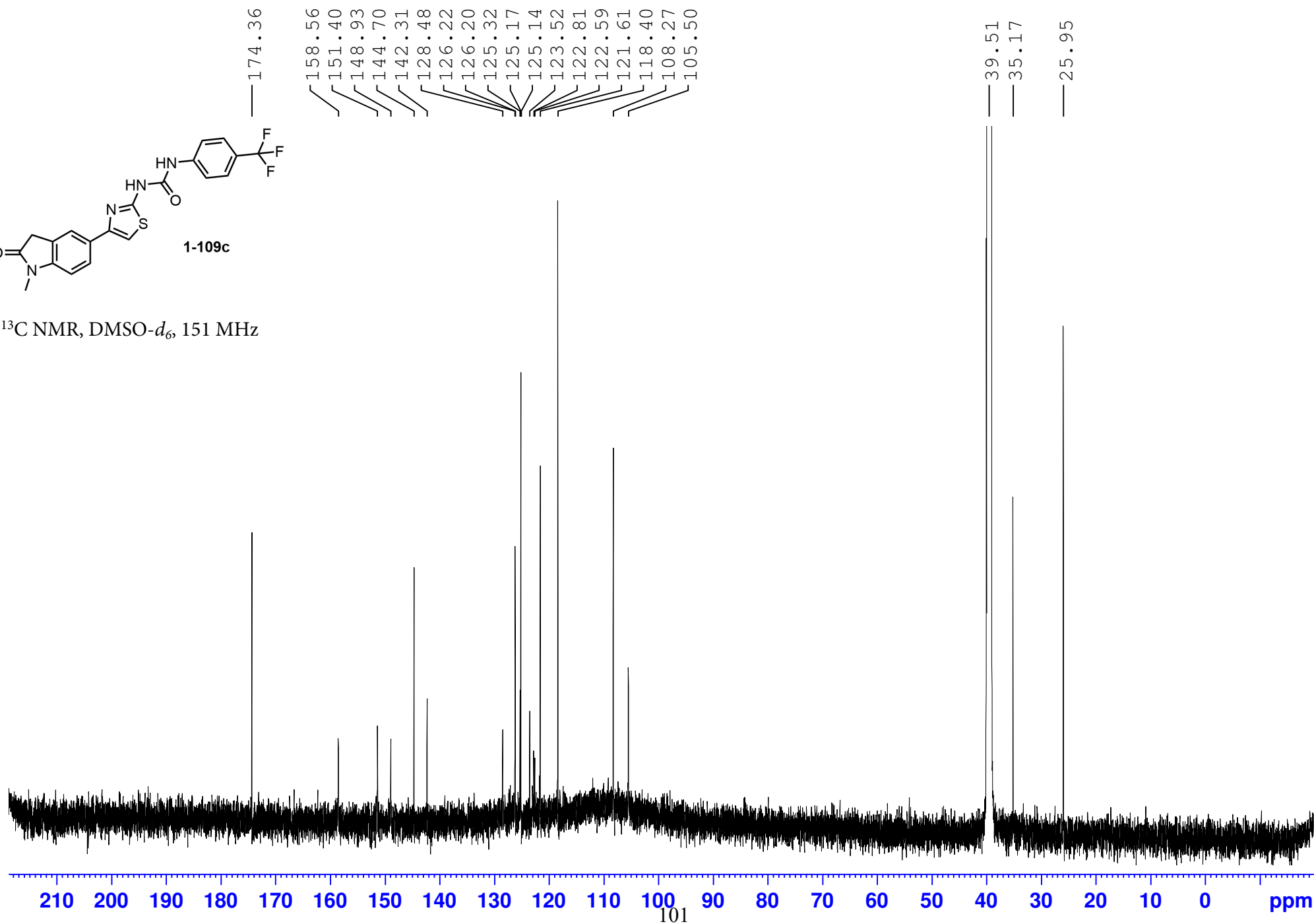


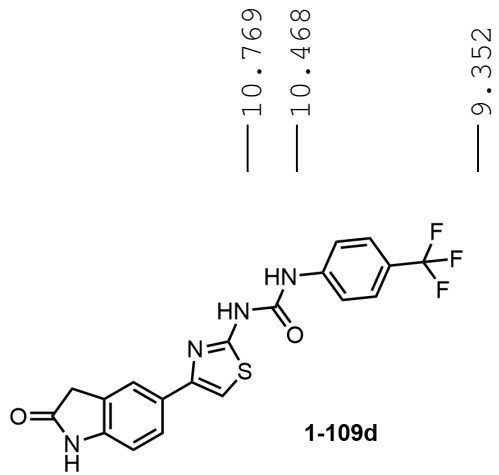
^1H NMR, DMSO- d_6 , 500 MHz



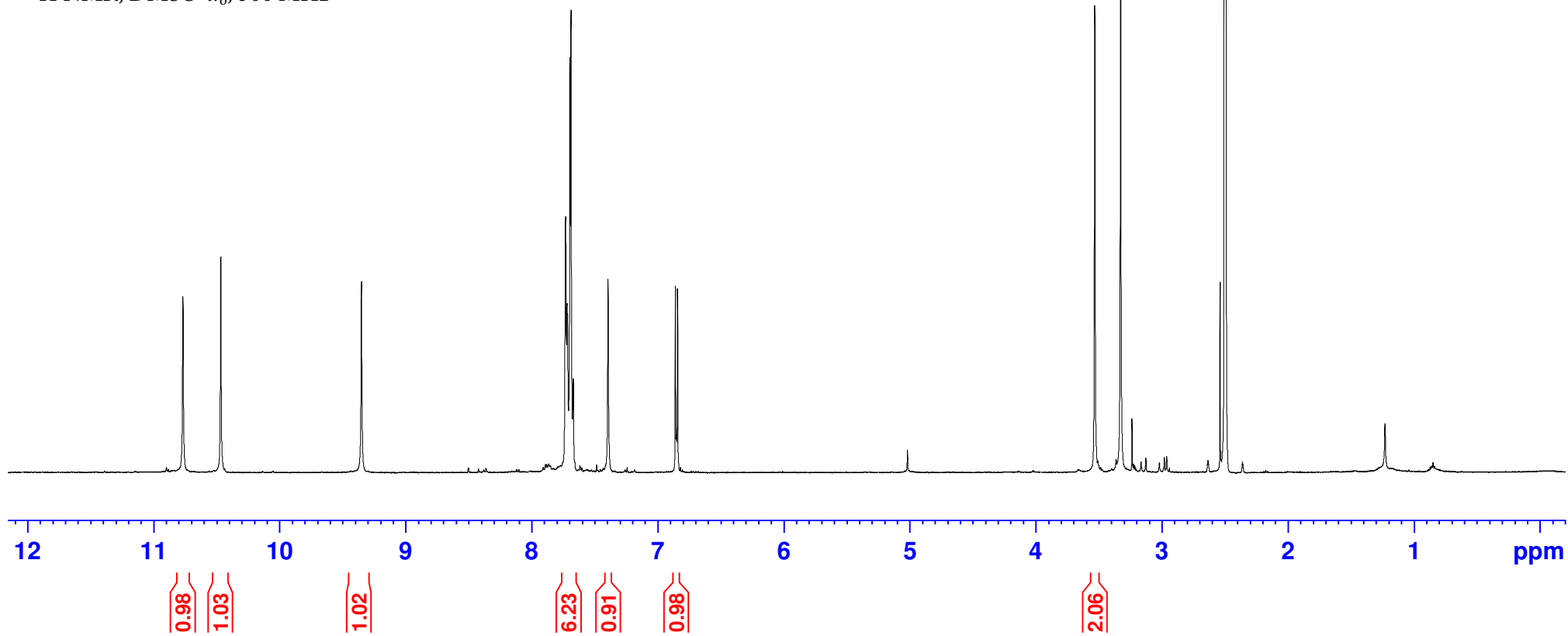


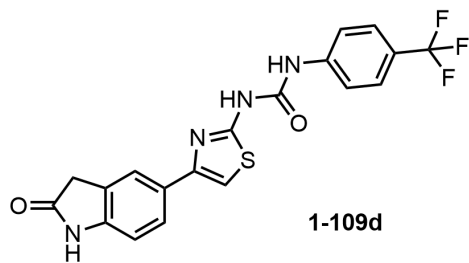
^{13}C NMR, DMSO- d_6 , 151 MHz



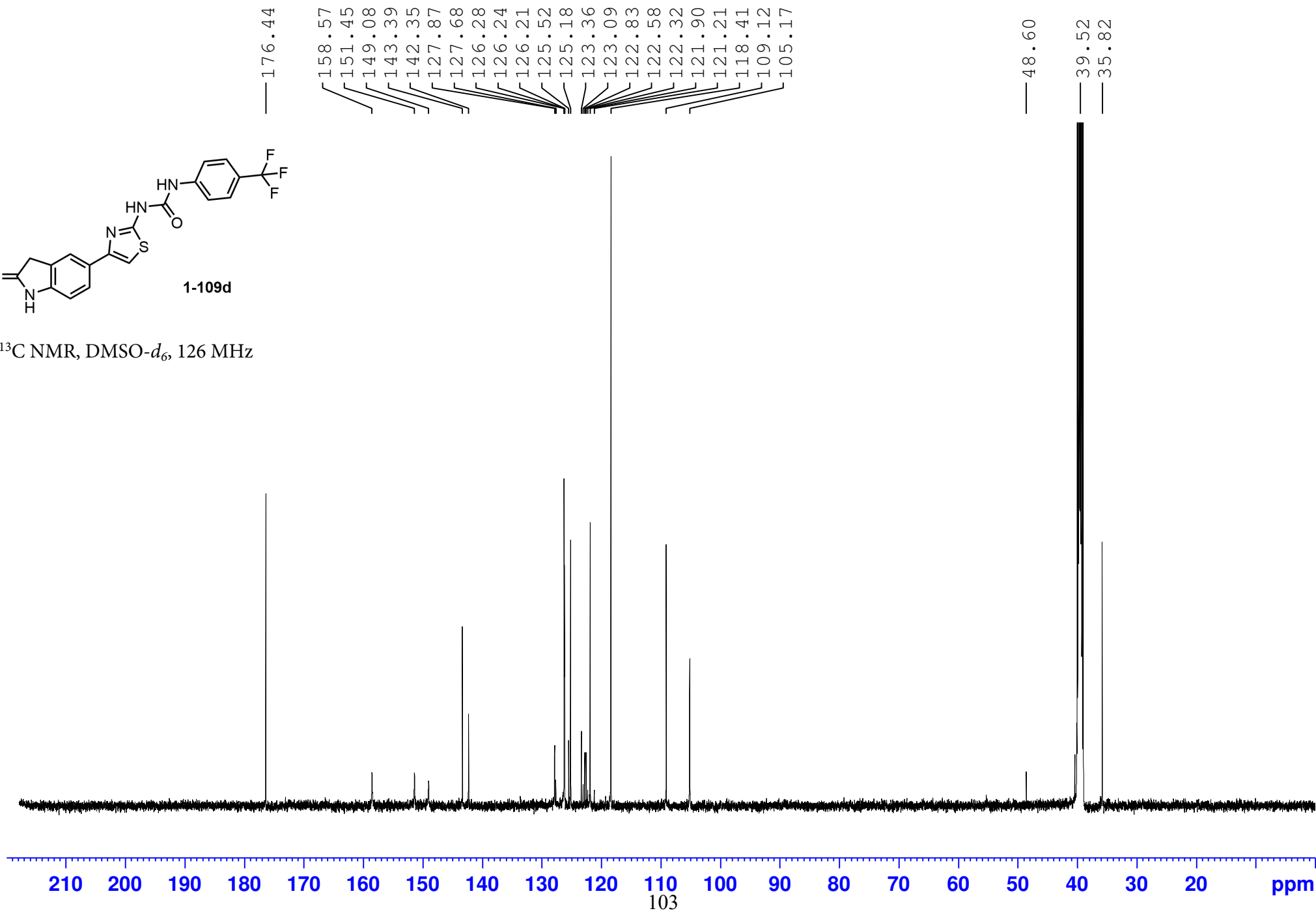


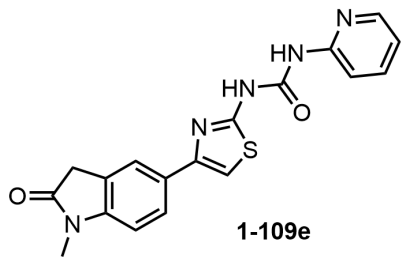
^1H NMR, DMSO- d_6 , 500 MHz



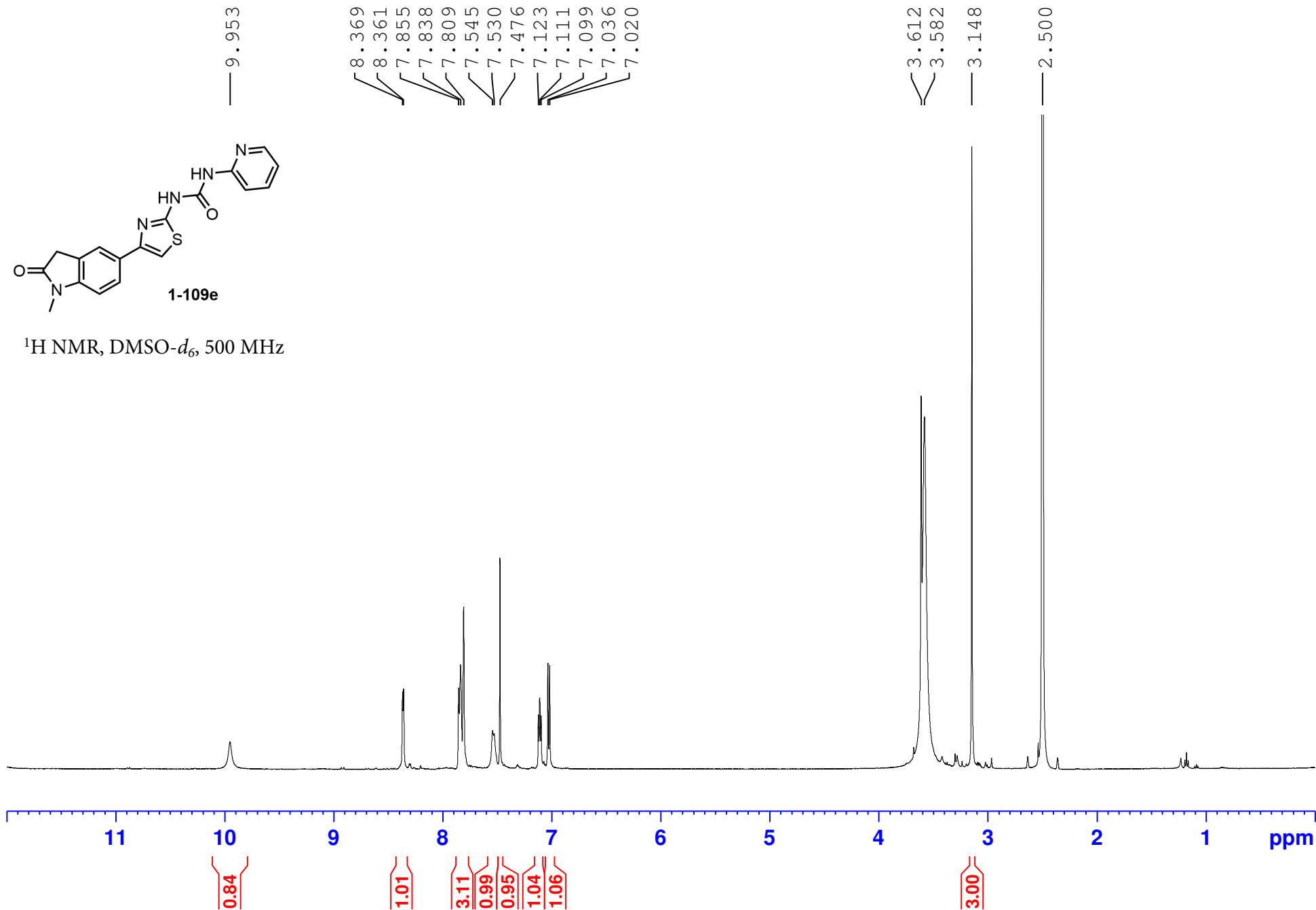


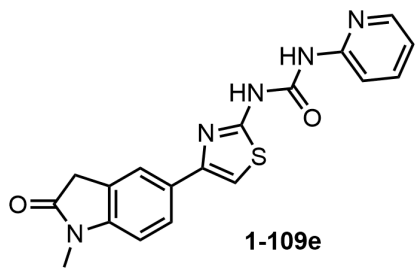
^{13}C NMR, DMSO- d_6 , 126 MHz



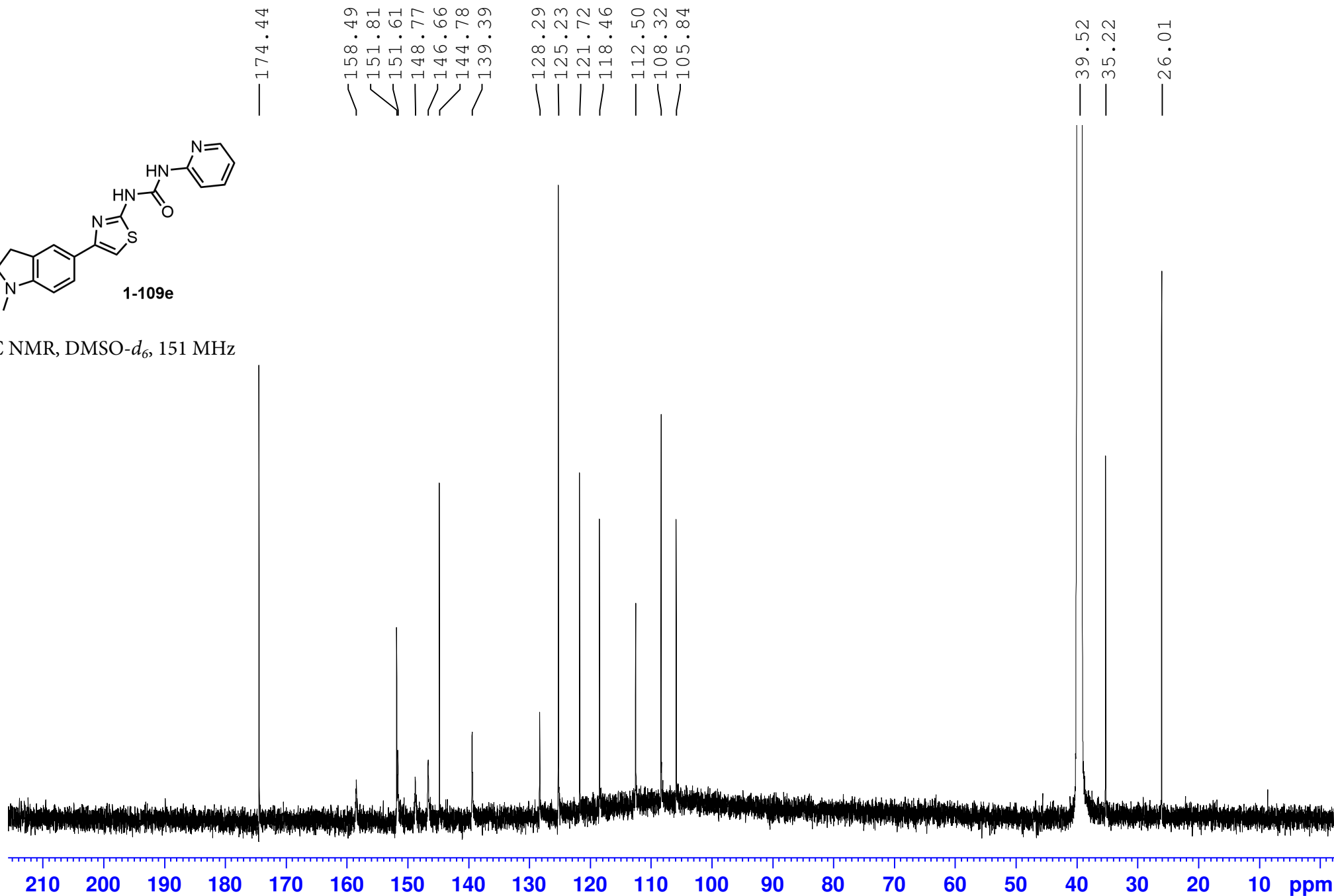


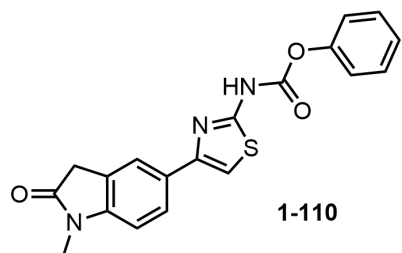
$^1\text{H NMR}$, $\text{DMSO-}d_6$, 500 MHz



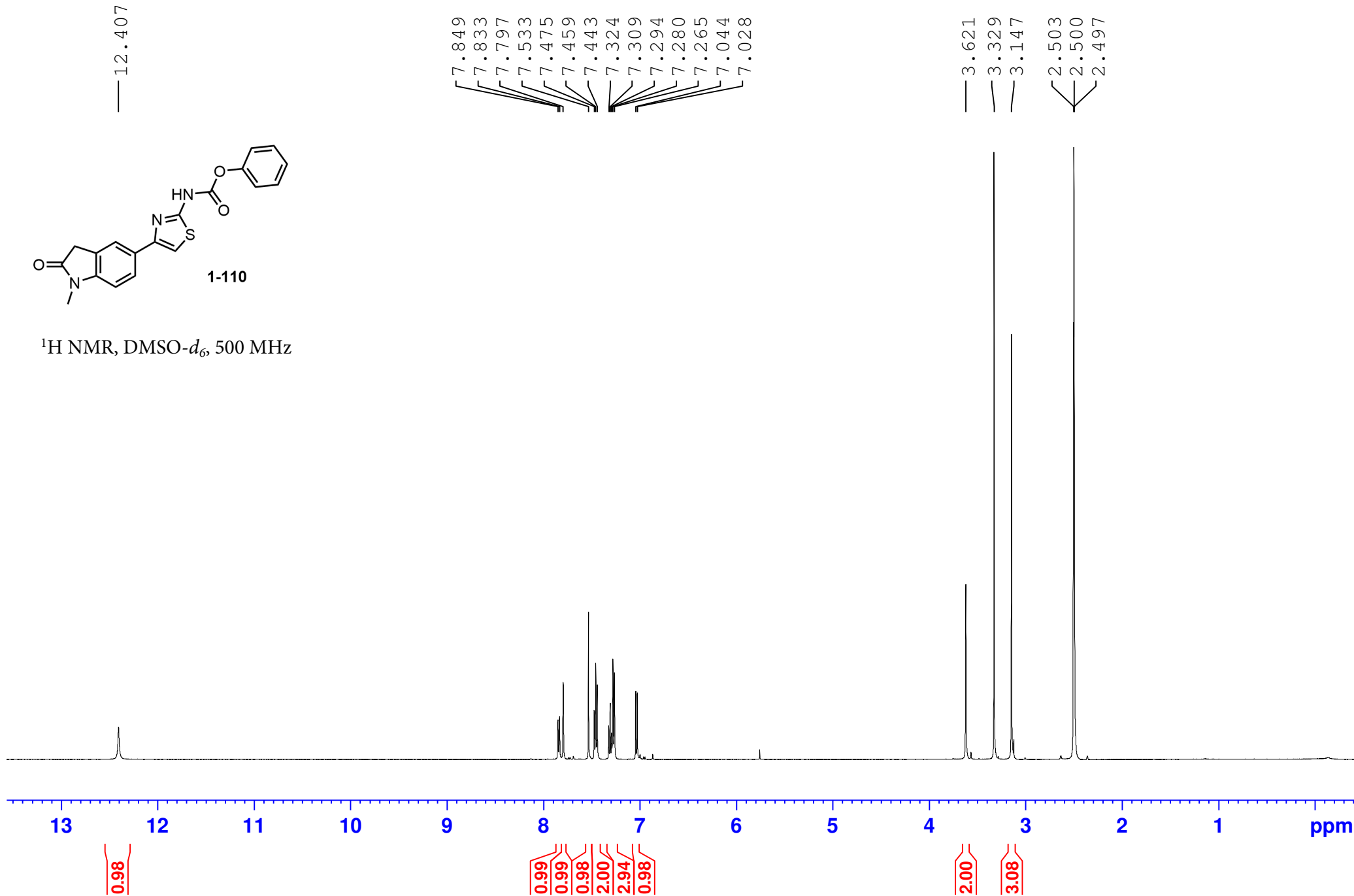


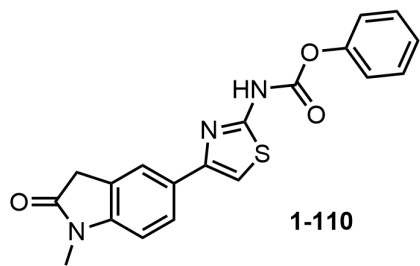
¹³C NMR, DMSO-*d*₆, 151 MHz



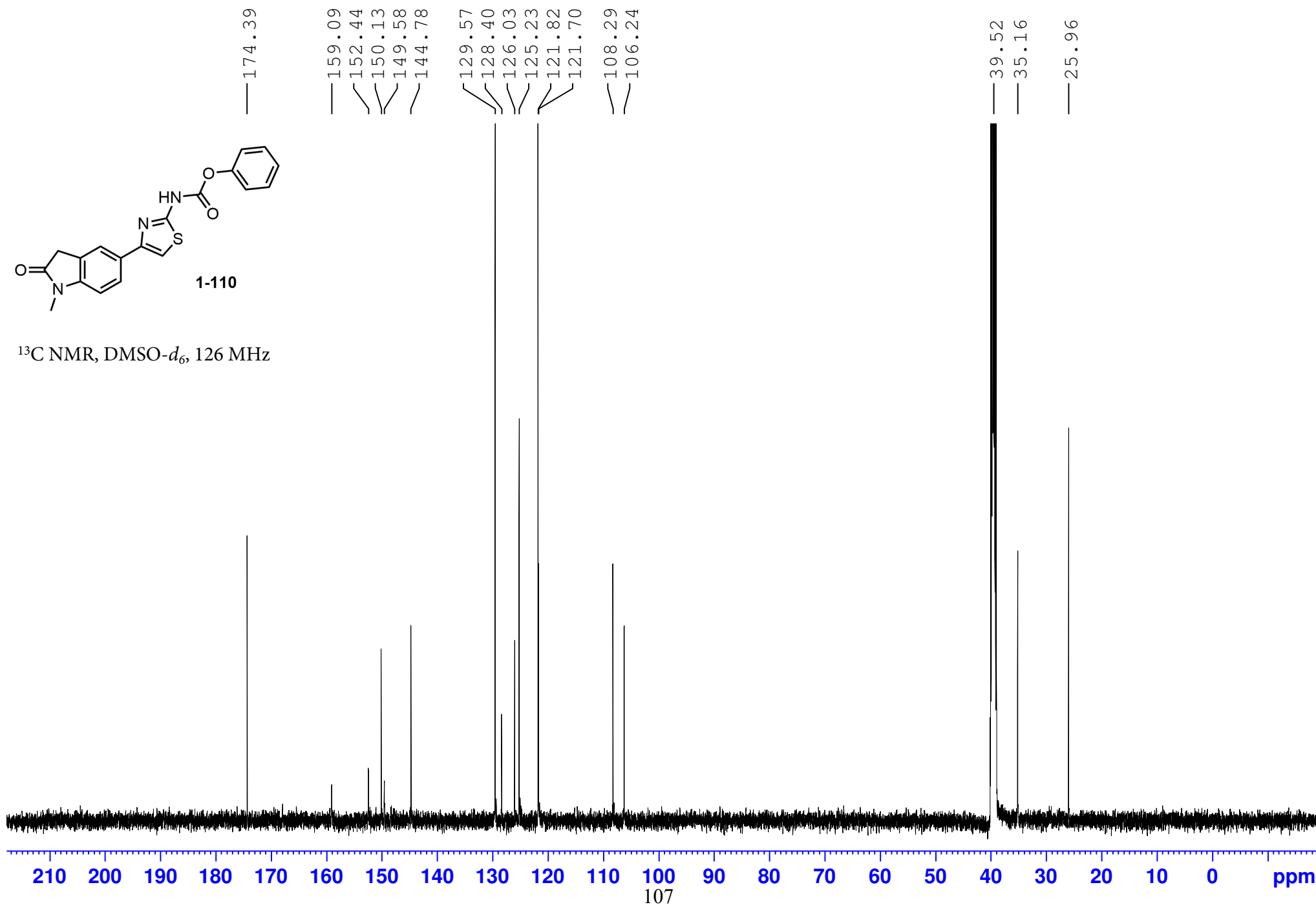


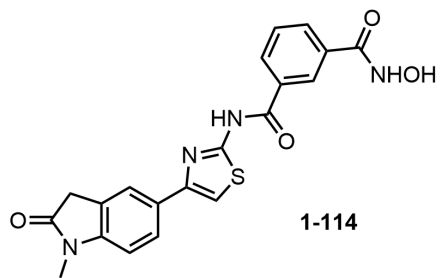
¹H NMR, DMSO-d₆, 500 MHz



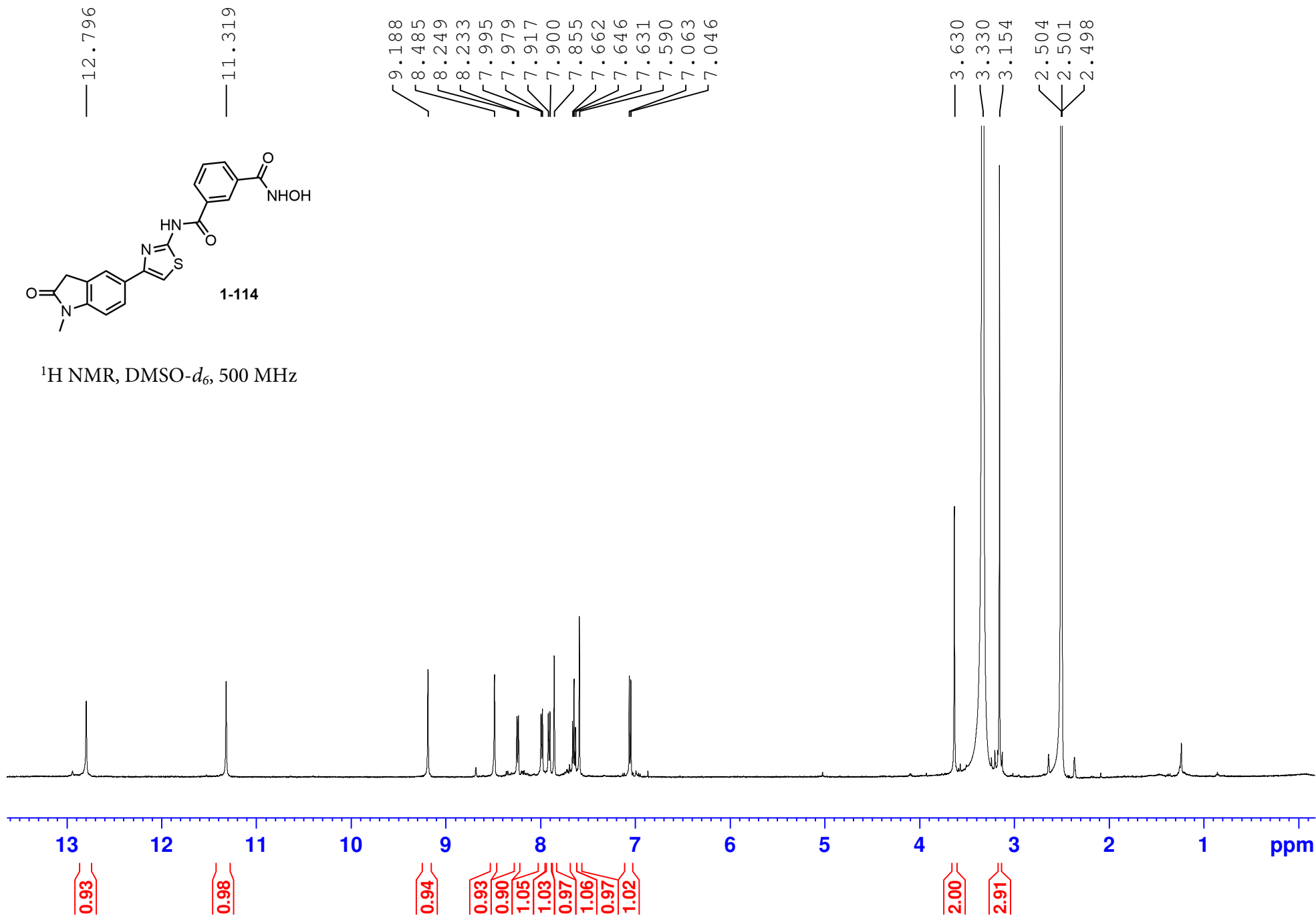


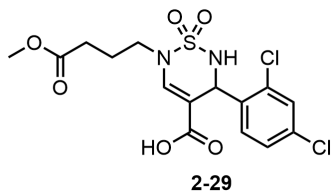
^{13}C NMR, DMSO- d_6 , 126 MHz



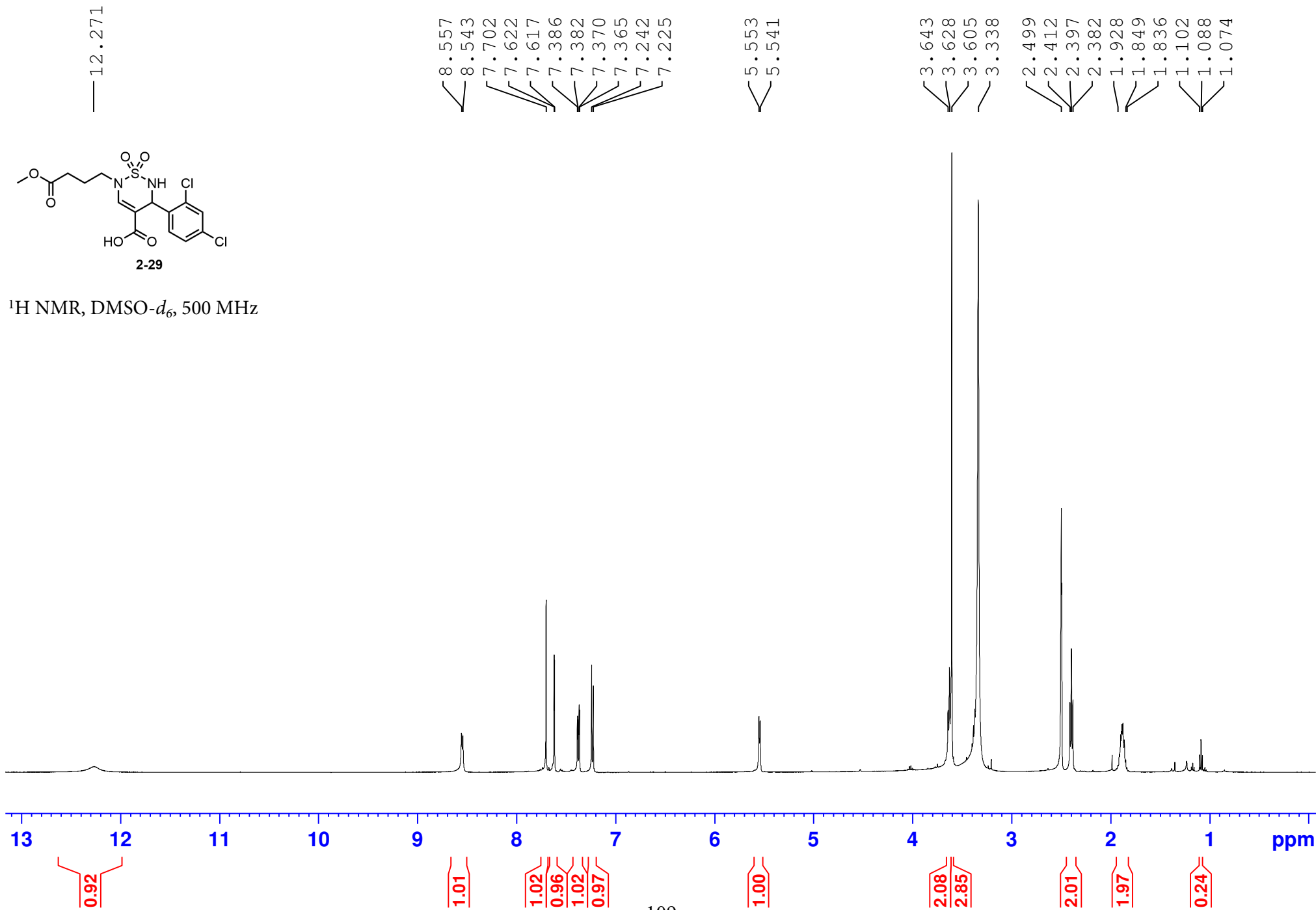


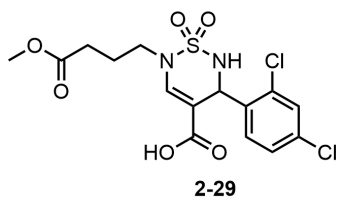
^1H NMR, DMSO- d_6 , 500 MHz





¹H NMR, DMSO-*d*₆, 500 MHz





— 172.73

— 166.09

— 142.98

— 134.93

— 133.88

— 133.08

— 131.41

— 128.72

— 126.64

— 102.67

— 53.84

— 51.38

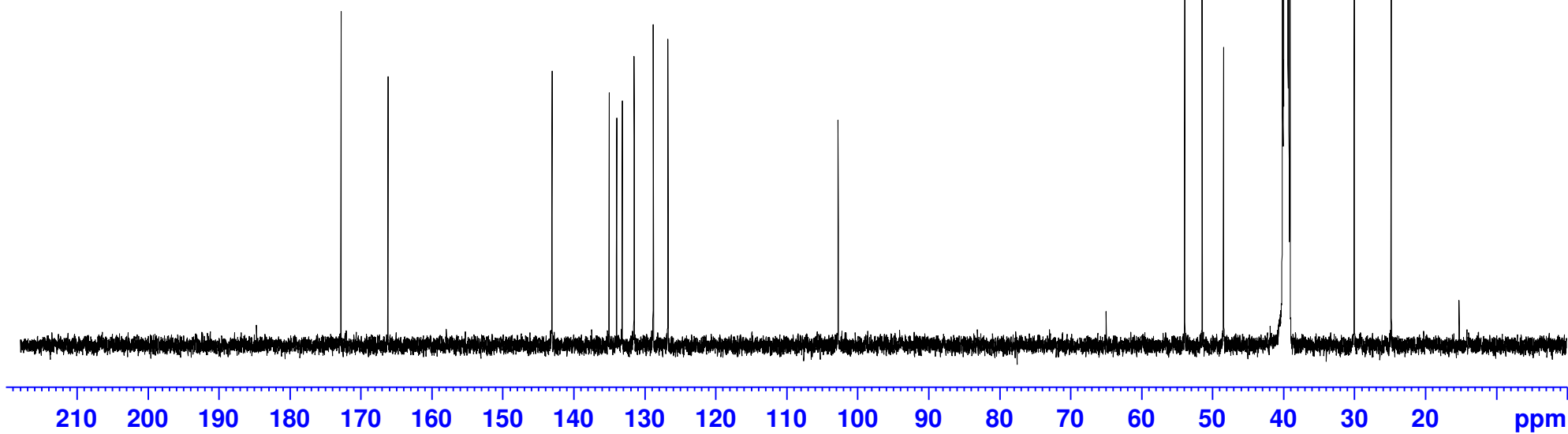
— 48.36

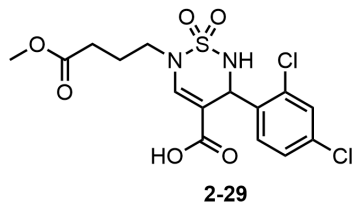
— 39.52

— 29.94

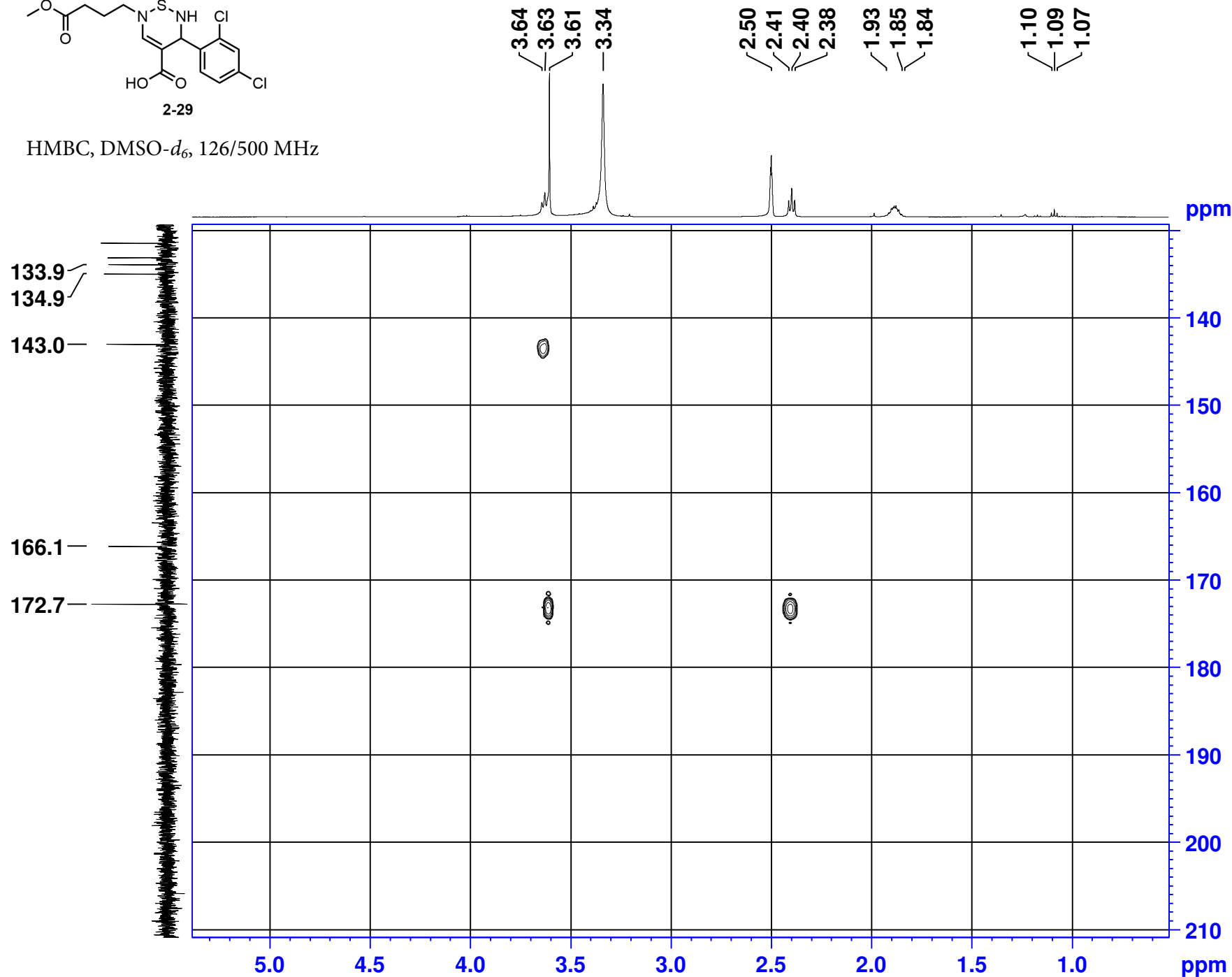
— 24.73

¹³C NMR, DMSO-*d*₆, 126 MHz





HMBC, DMSO-*d*₆, 126/500 MHz



Current Data Parameters
 NAME LT-930-24
 EXPNO 31
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190702
 Time 5.17
 INSTRUM spect
 PROBD 5 mm PABBO BB/
 PULPROG hmbcgp1pndqf
 TD 2048
 SOLVENT DMSO
 NS 8
 DS 16
 SWH 6756.757 Hz
 FIDRES 3.299198 Hz
 AQ 0.1515520 sec
 RG 203
 DW 74.000 usec
 DE 6.50 usec
 TE 296.3 K
 CNST2 145.0000000
 CNST13 10.0000000
 D0 0.00000300 sec
 D1 1.50573397 sec
 D2 0.00344828 sec
 D6 0.05000000 sec
 D16 0.00020000 sec
 IN0 0.00001790 sec

==== CHANNEL f1 =====
 SFO1 500.1633957 MHz
 NUC1 1H
 P1 11.50 usec
 P2 23.00 usec
 PLW1 18.00000000 W

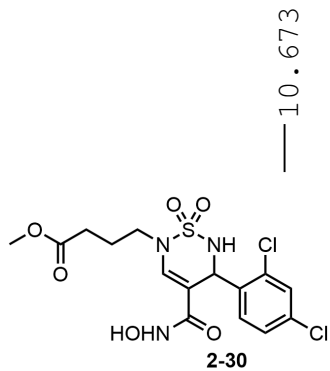
==== CHANNEL f2 =====
 SFO2 125.7778879 MHz
 NUC2 13C
 P3 10.50 usec
 PLW2 110.00000000 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P16 1000.00 usec

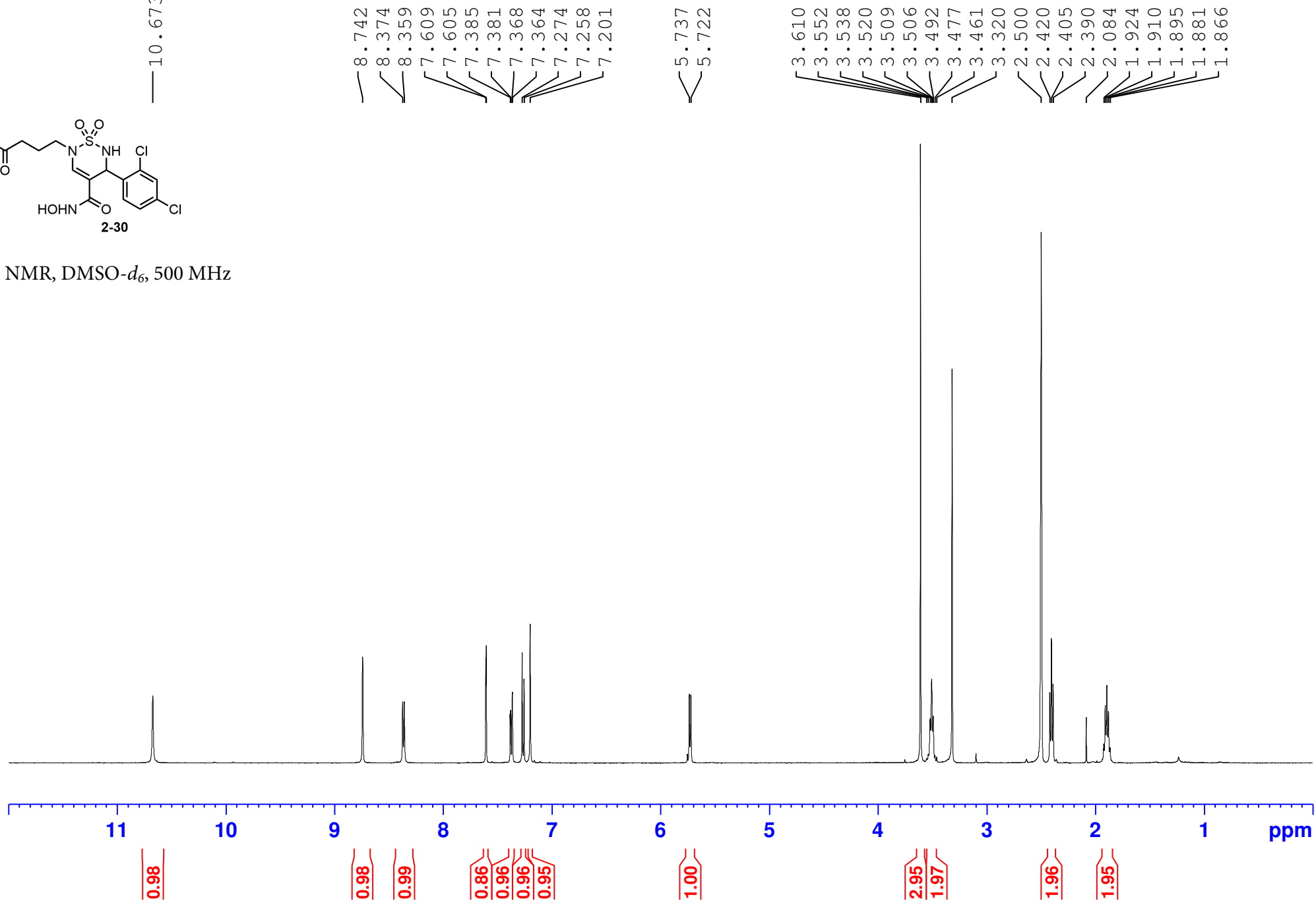
F1 - Acquisition parameters
 TD 128
 SFO1 125.7779 MHz
 FIDRES 436.452515 Hz
 SW 222.082 ppm
 FnmODE QF

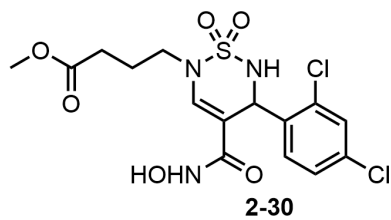
F2 - Processing parameters
 SI 2048
 SF 500.1600000 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 125.7653320 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0



$^1\text{H NMR}$, $\text{DMSO-}d_6$, 500 MHz





^{13}C NMR, DMSO- d_6 , 126 MHz

— 172.86

— 164.01

136.39
134.71
134.21
133.22
131.62
128.74
126.53

— 106.34

— 53.87

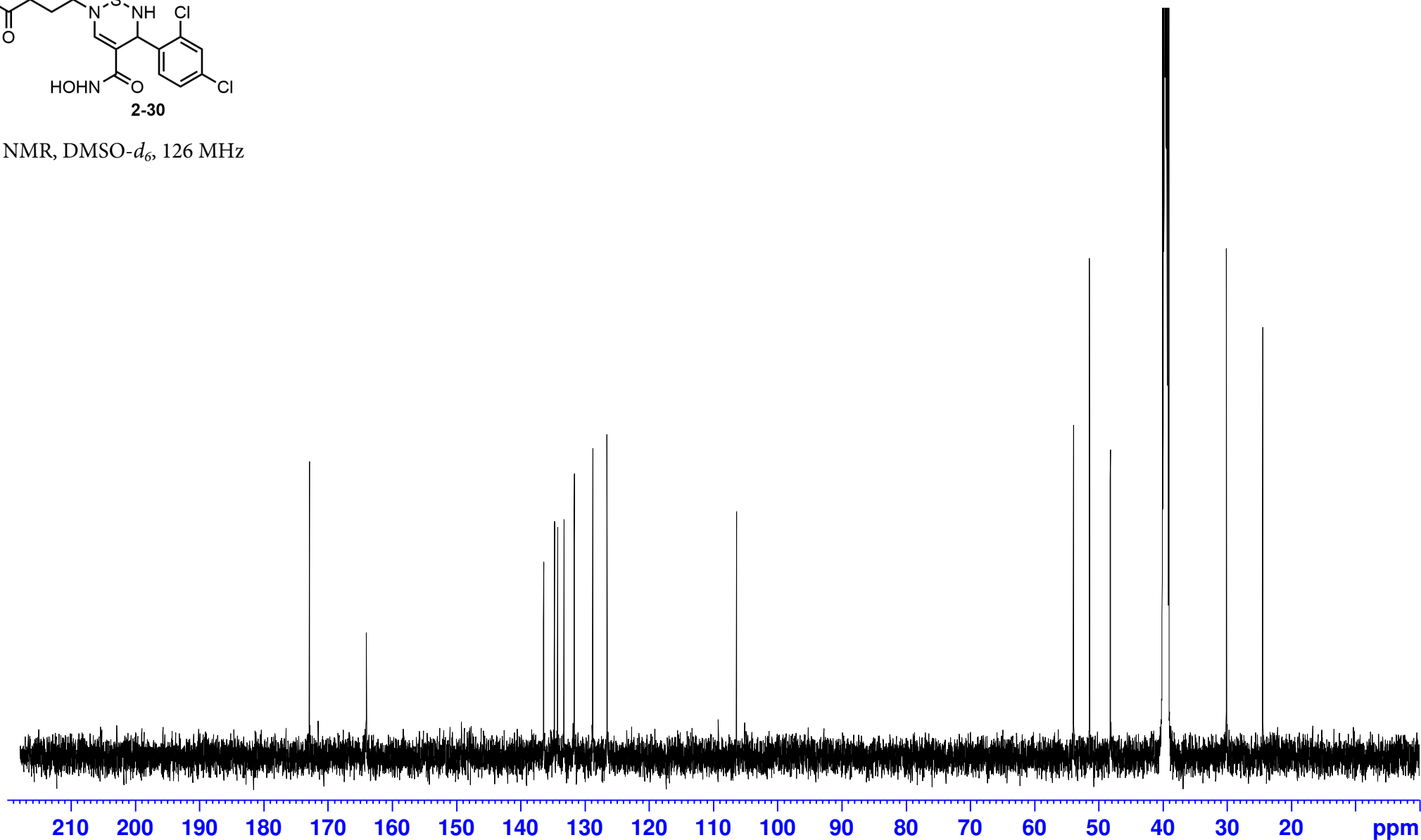
— 51.39

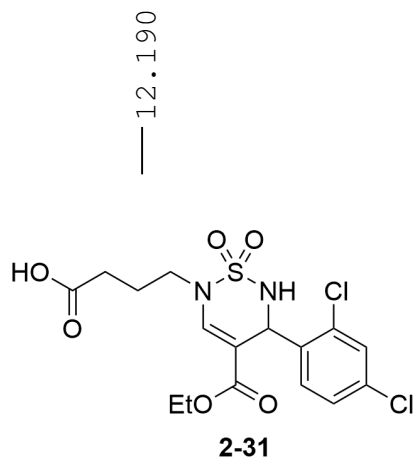
— 48.13

— 39.52

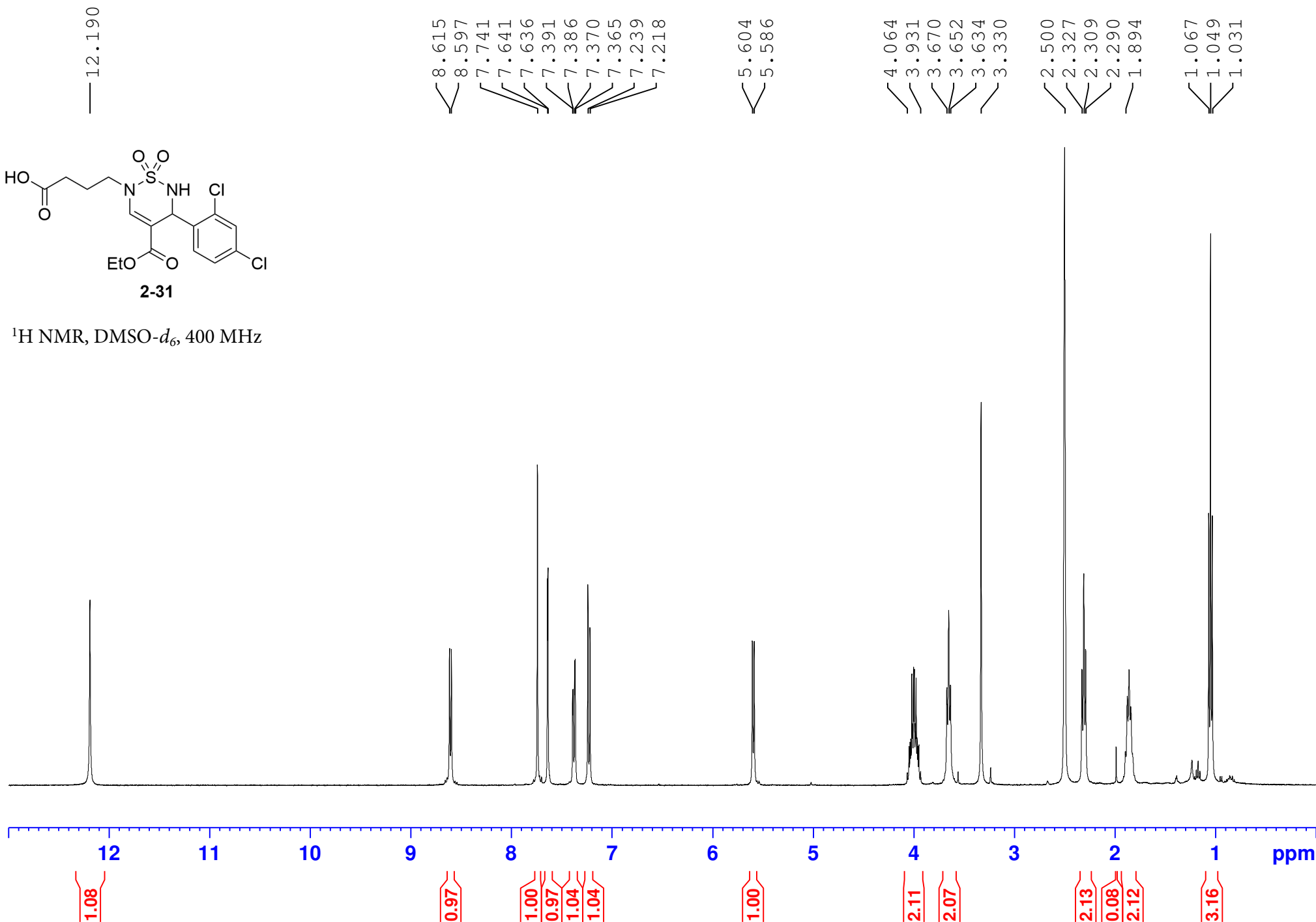
— 30.06

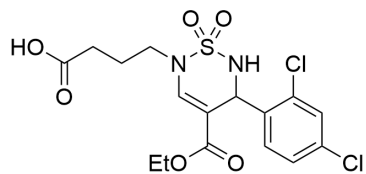
— 24.39





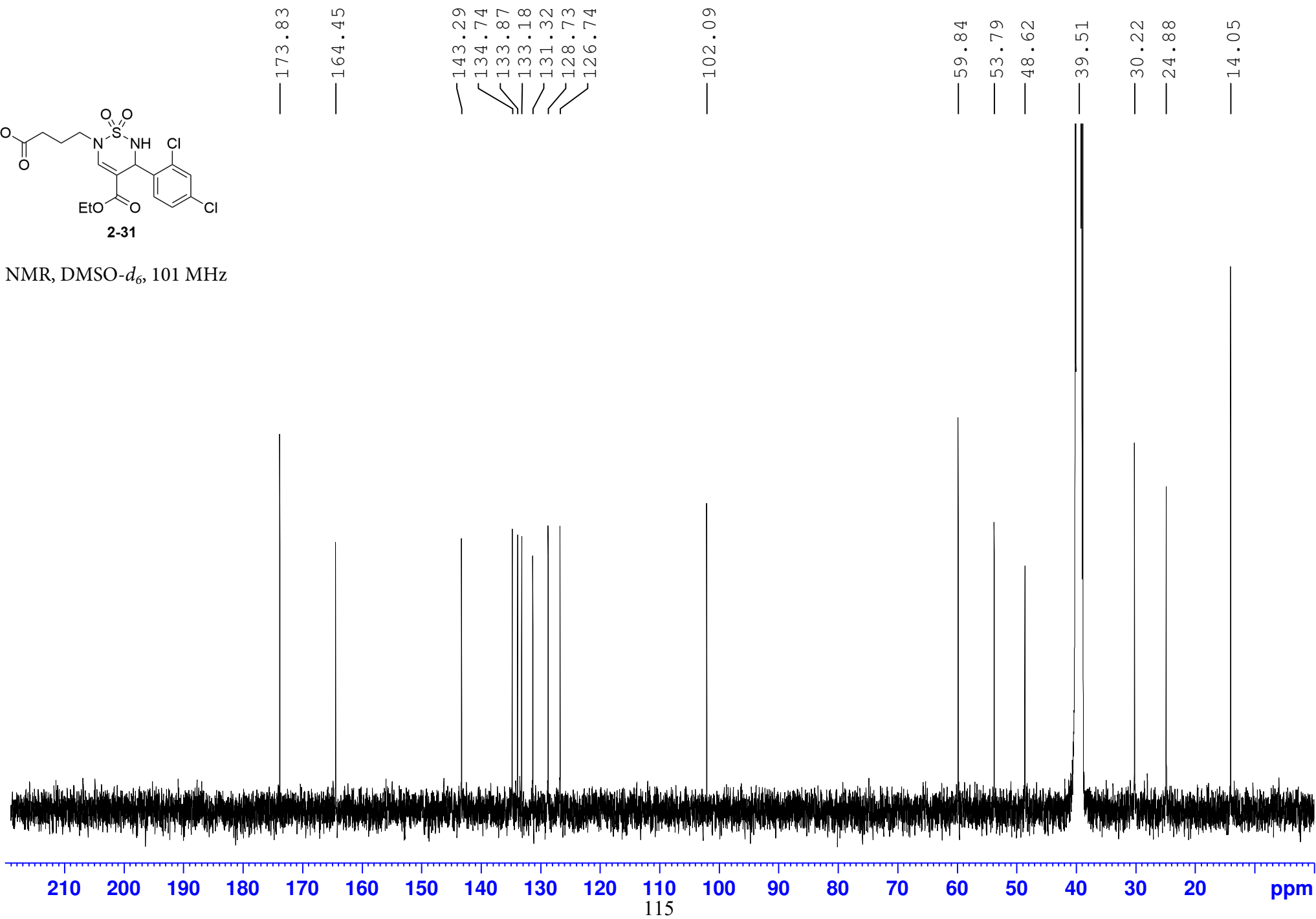
¹H NMR, DMSO-*d*₆, 400 MHz

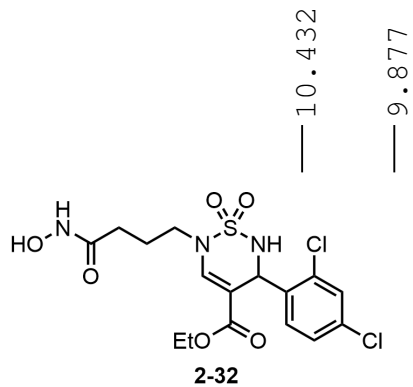




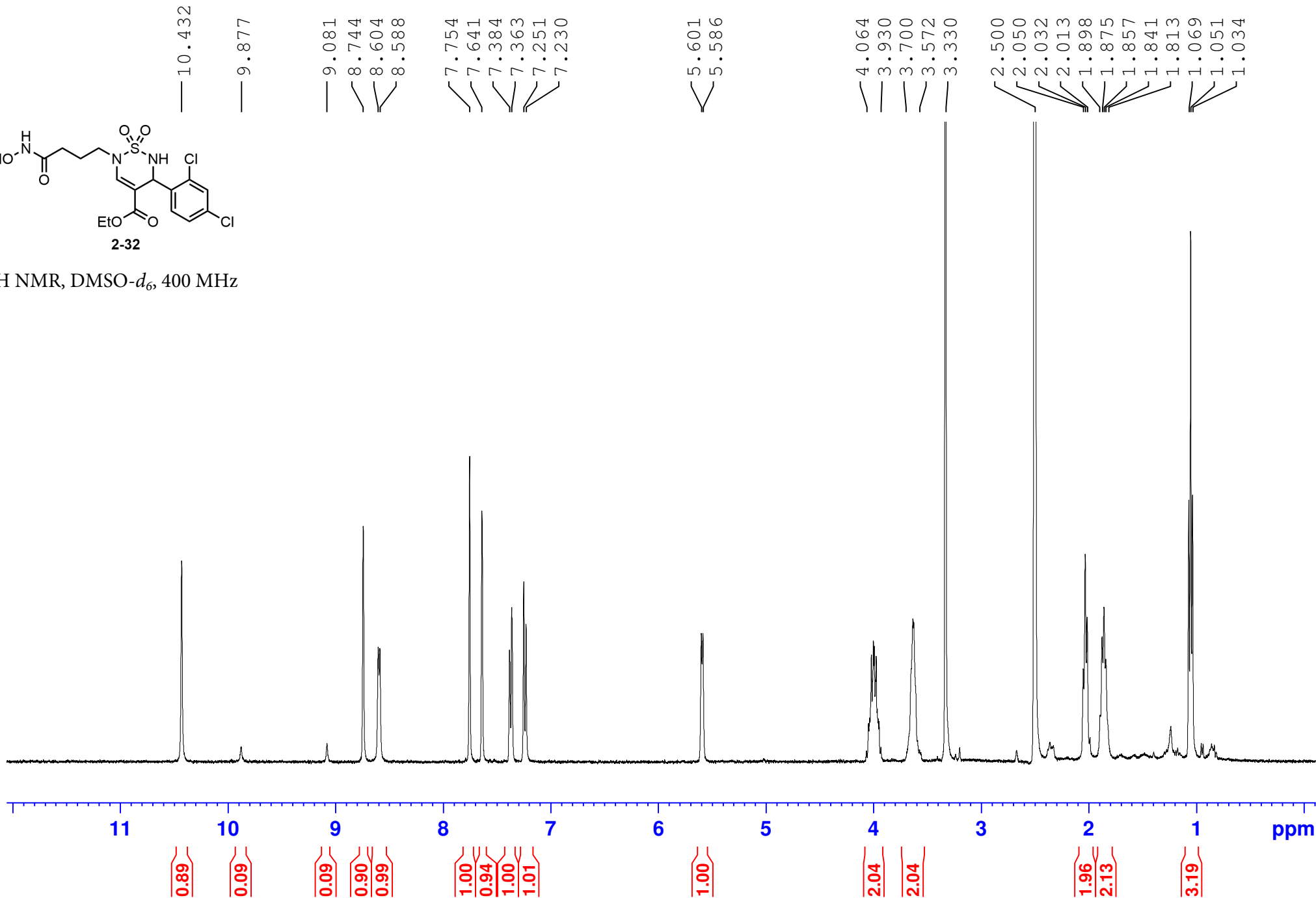
2-31

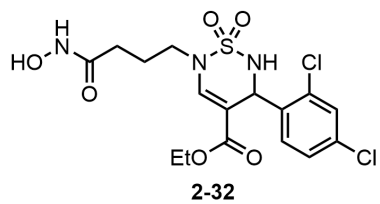
^1H NMR, DMSO- d_6 , 101 MHz





^1H NMR, DMSO- d_6 , 400 MHz





— 168.32
— 164.49

— 143.37
— 134.76
— 133.89
— 133.20
— 131.38
— 128.74
— 126.75

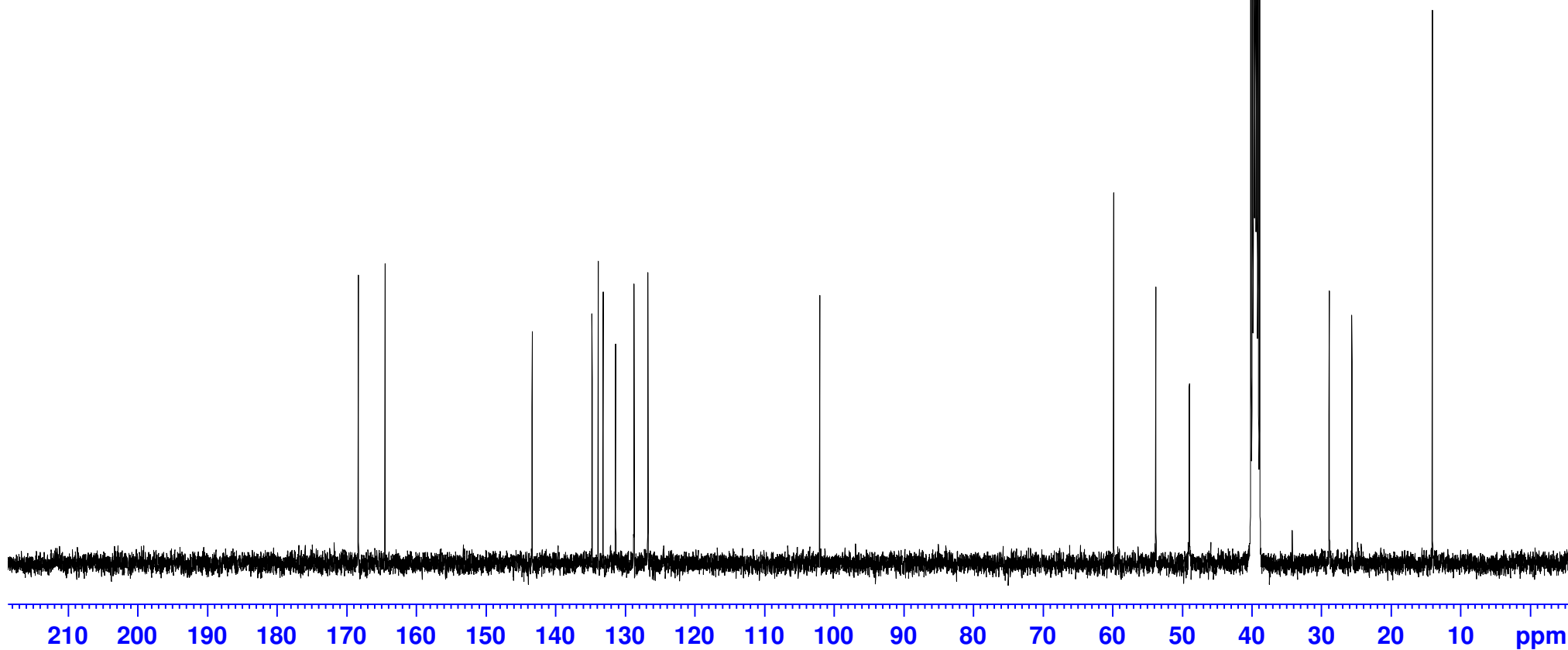
— 102.06

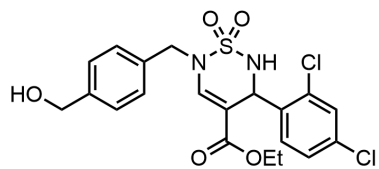
— 59.86
— 53.79
— 48.99
— 39.52

— 28.91
— 25.64

— 14.08

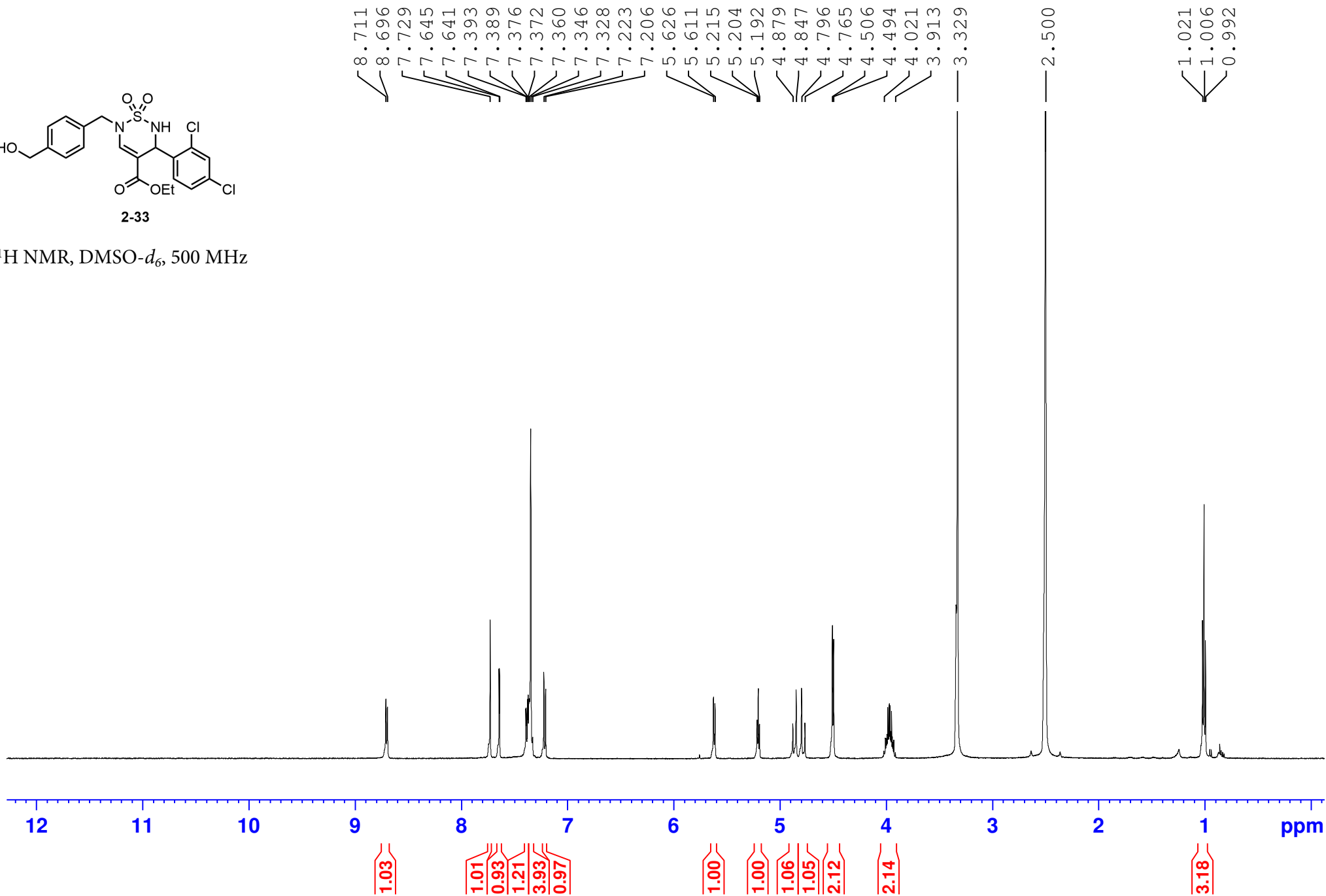
^1H NMR, DMSO- d_6 , 101 MHz

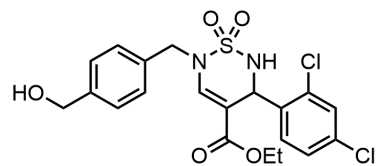




2-33

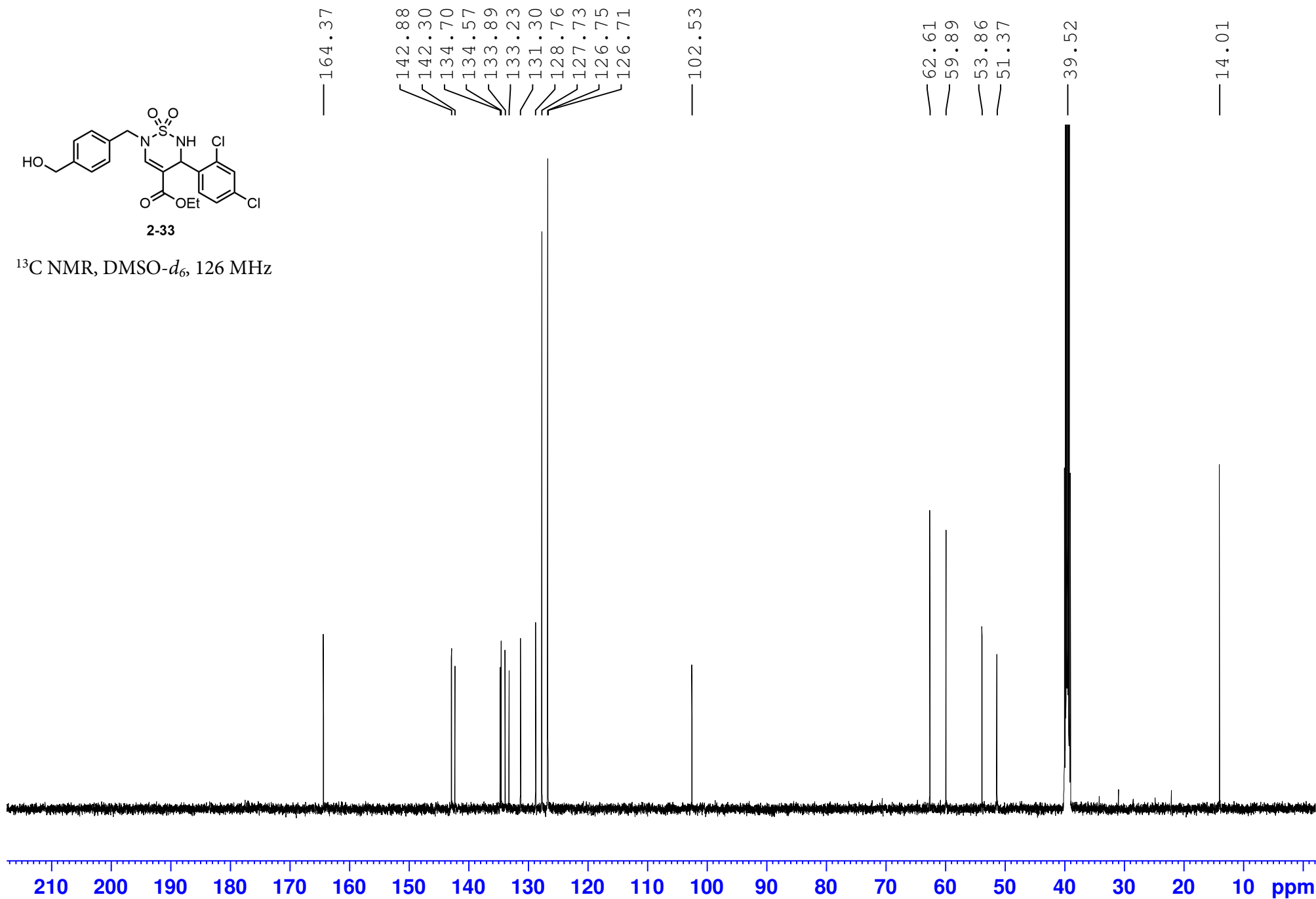
¹H NMR, DMSO-*d*₆, 500 MHz

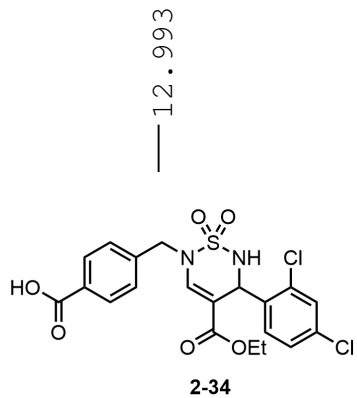




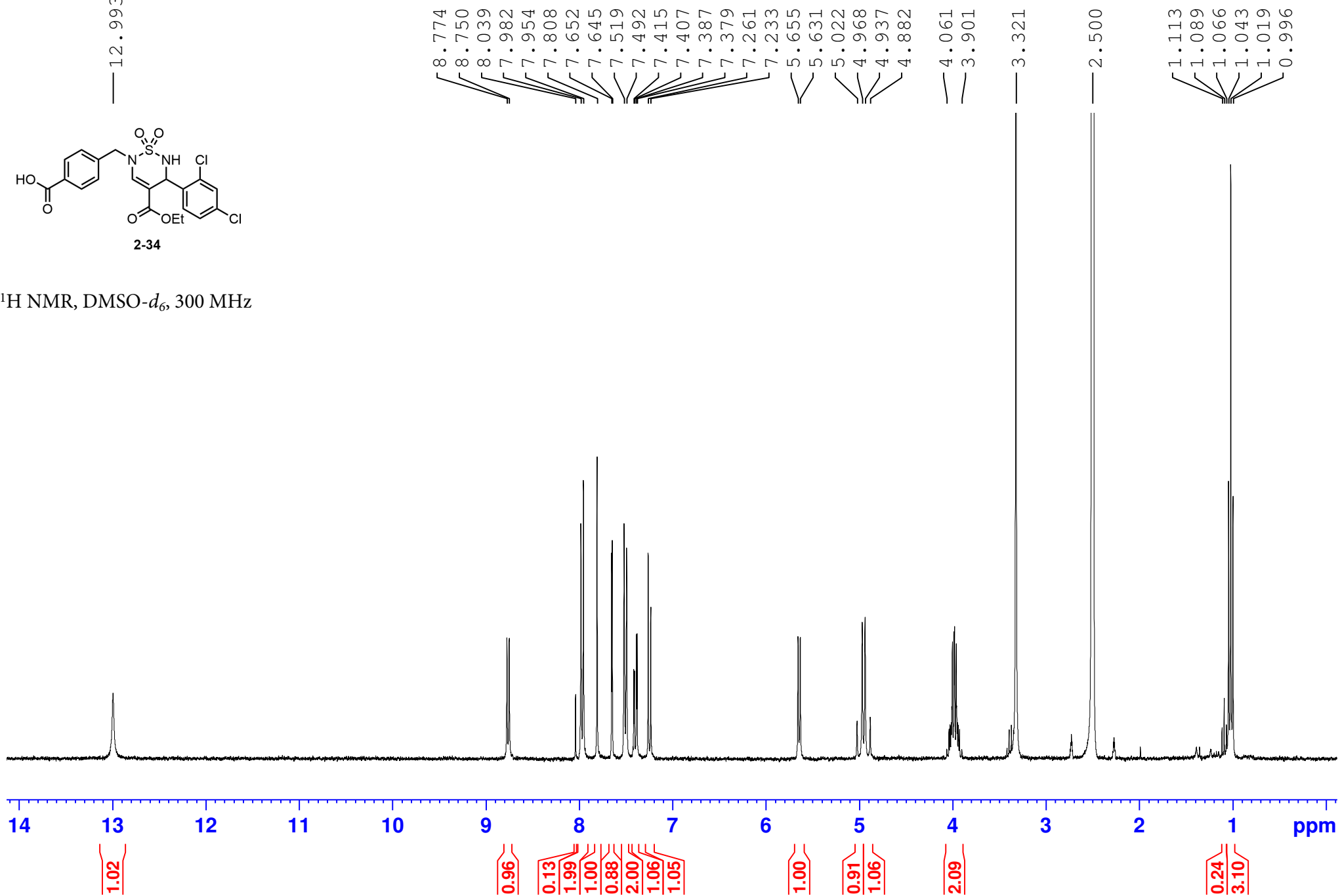
2-33

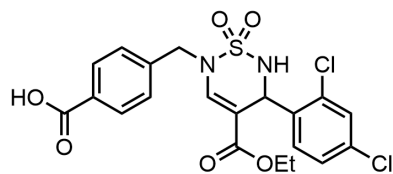
^{13}C NMR, DMSO- d_6 , 126 MHz





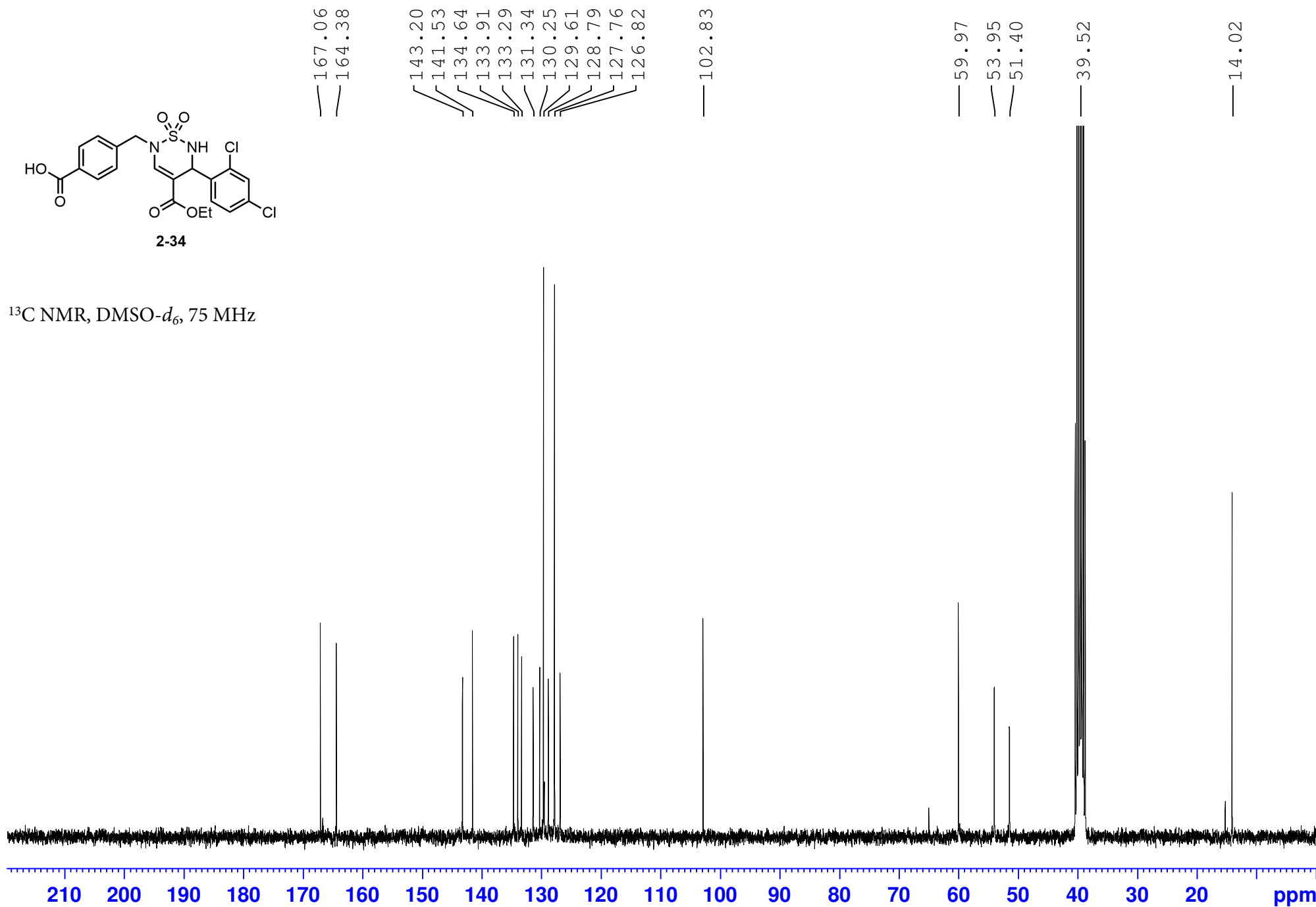
¹H NMR, DMSO-*d*₆, 300 MHz

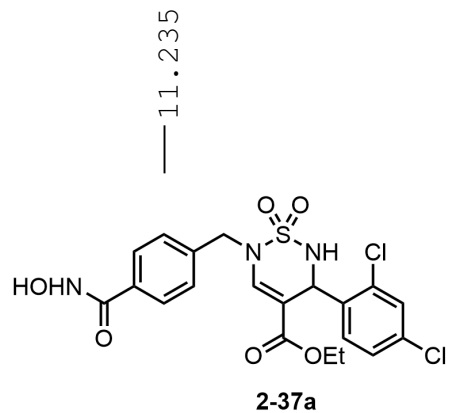




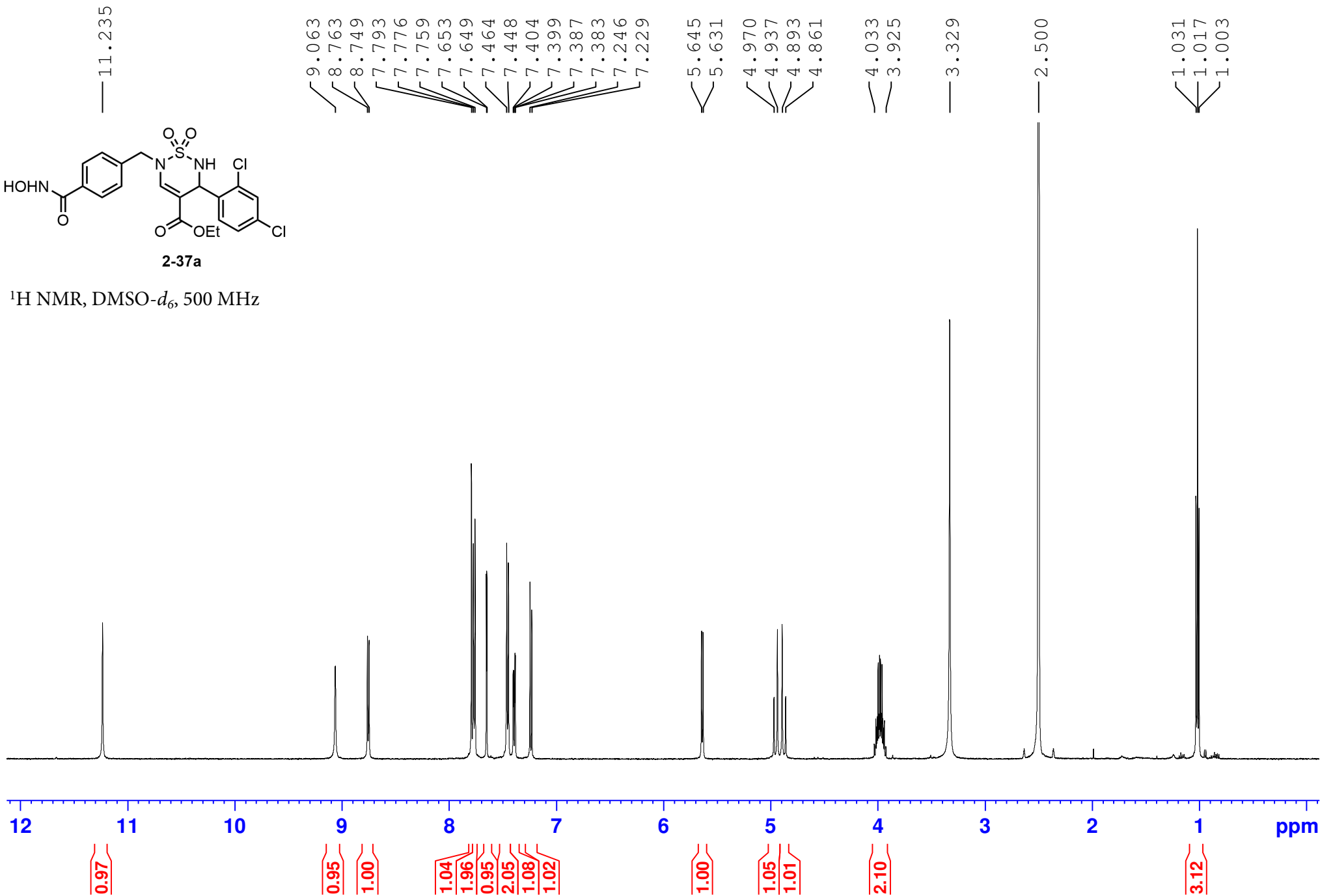
2-34

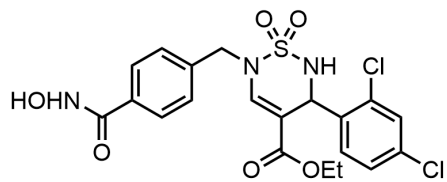
^{13}C NMR, DMSO- d_6 , 75 MHz





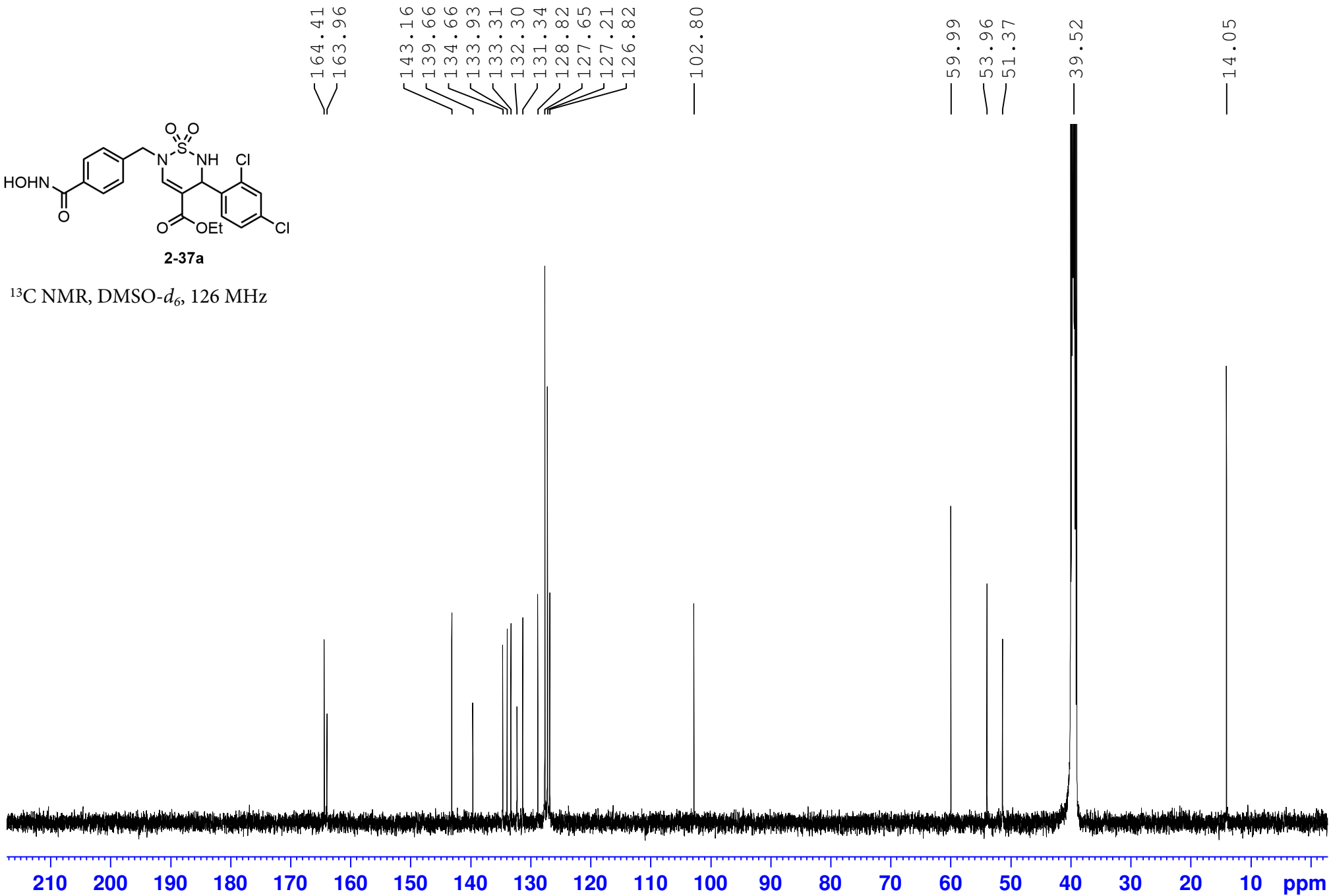
¹H NMR, DMSO-*d*₆, 500 MHz

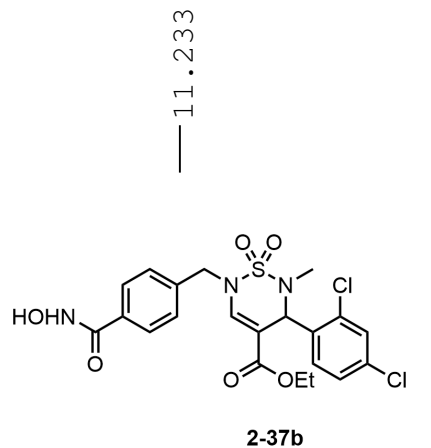




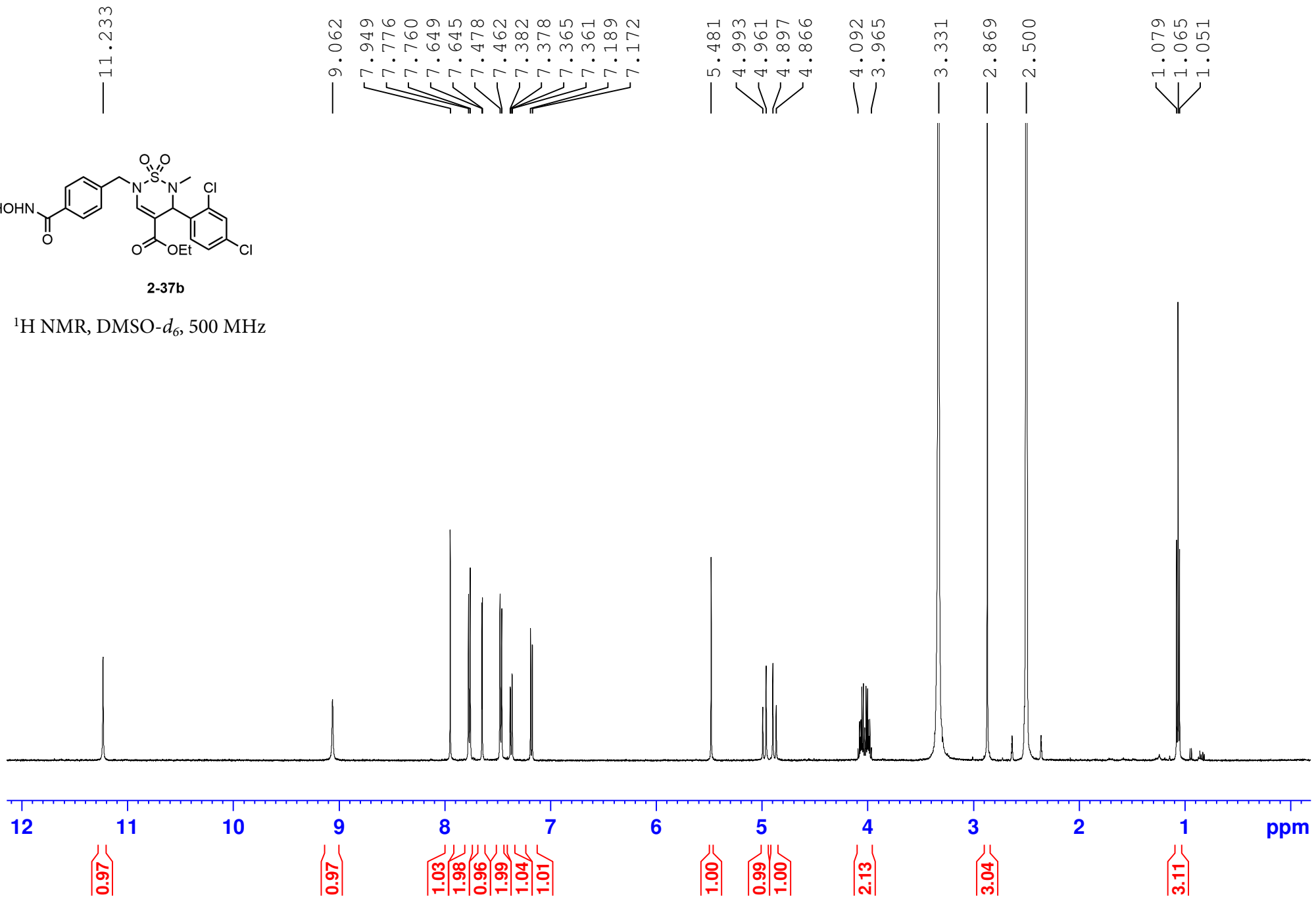
2-37a

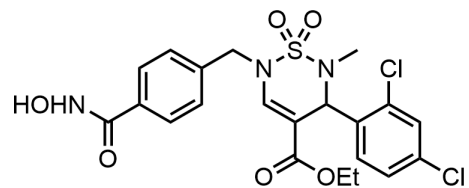
^{13}C NMR, DMSO- d_6 , 126 MHz





¹H NMR, DMSO-*d*₆, 500 MHz





2-37b

^{13}C NMR, DMSO- d_6 , 126 MHz

164.60
163.86

142.34
139.44
134.61
134.13
133.22
132.48
131.52
128.67
127.83
127.28
126.63

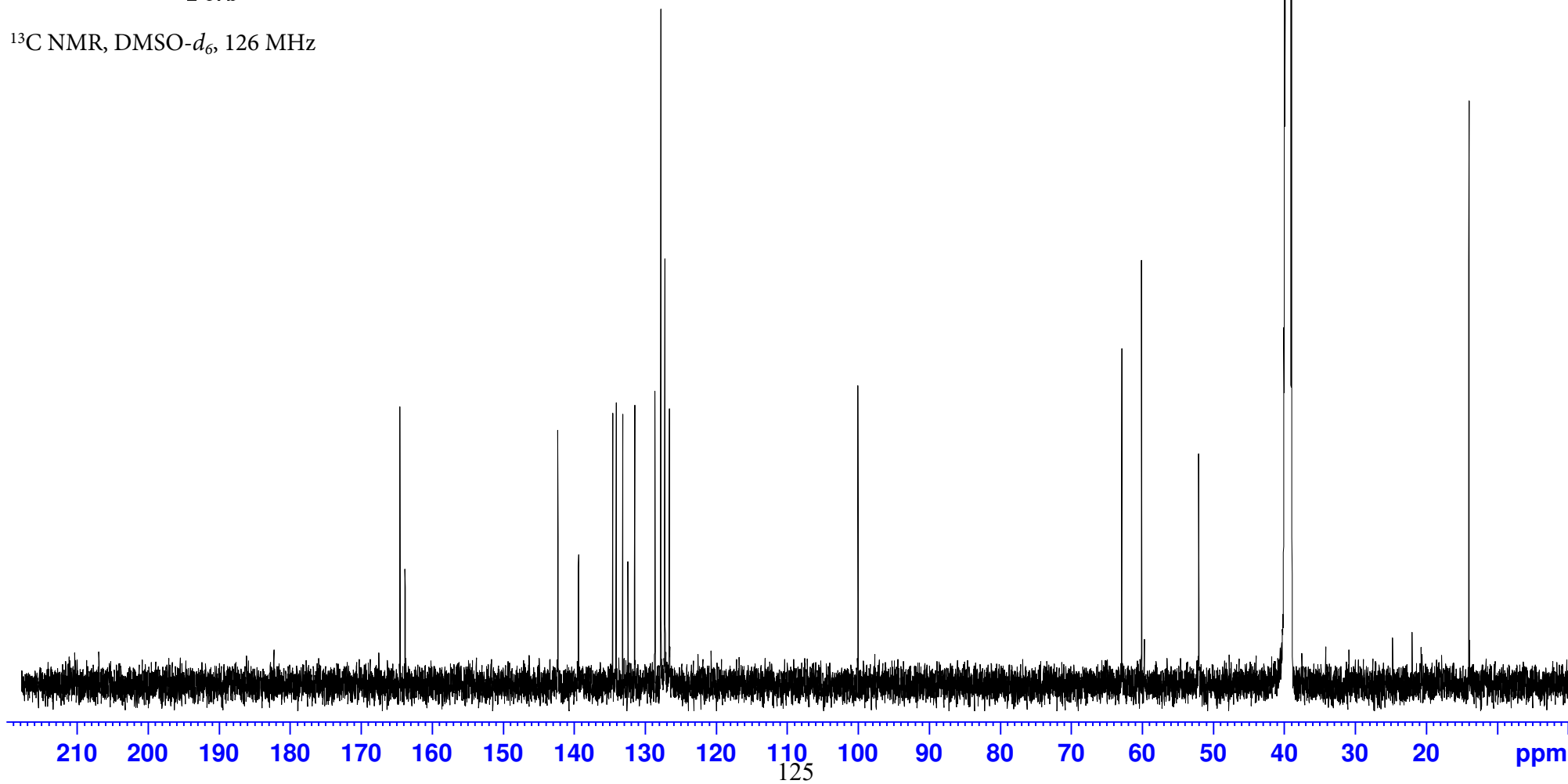
100.07

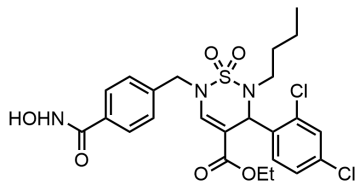
62.92
60.15

52.09

39.52

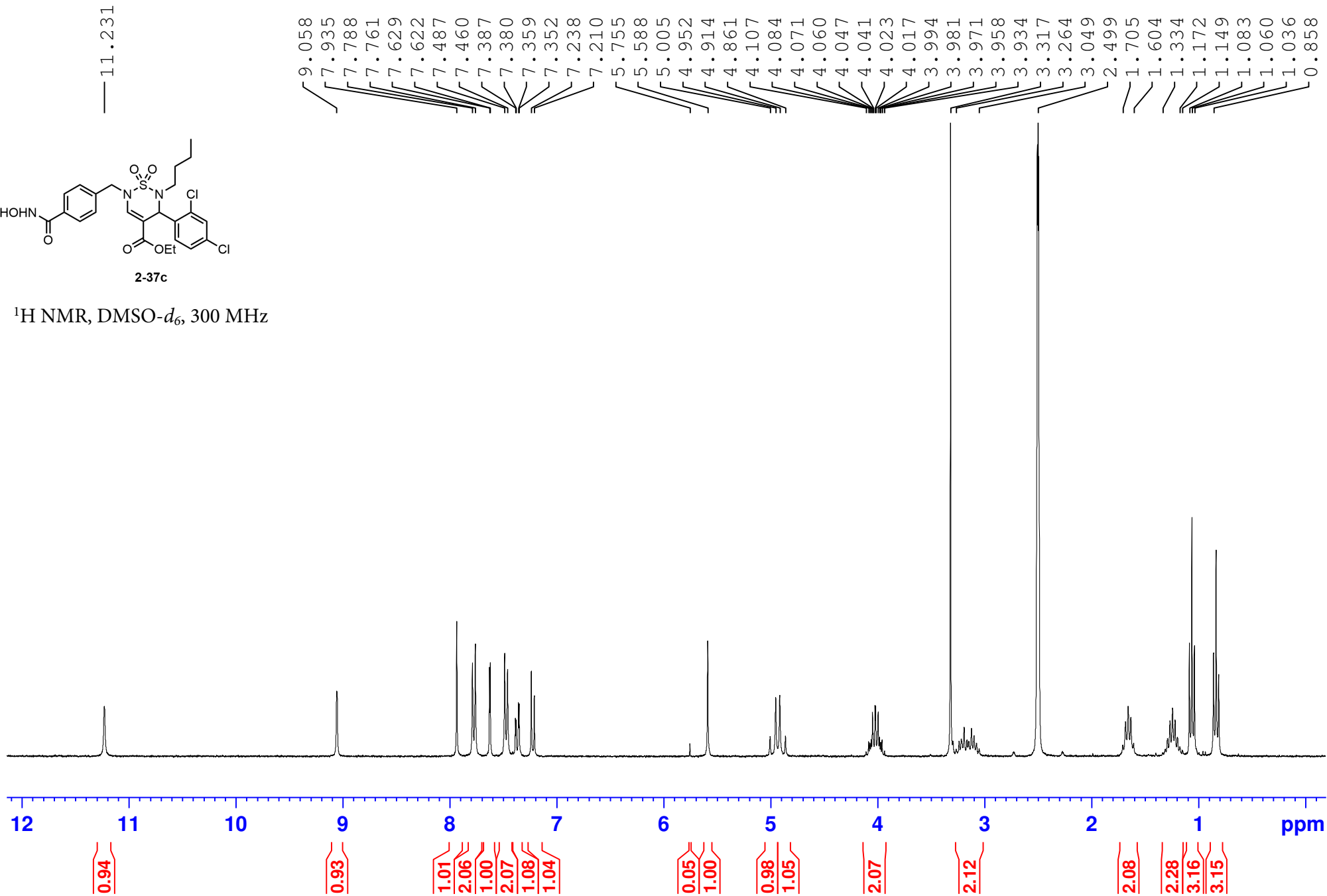
14.04

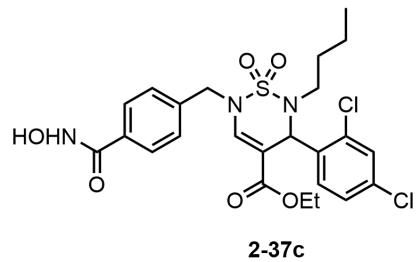




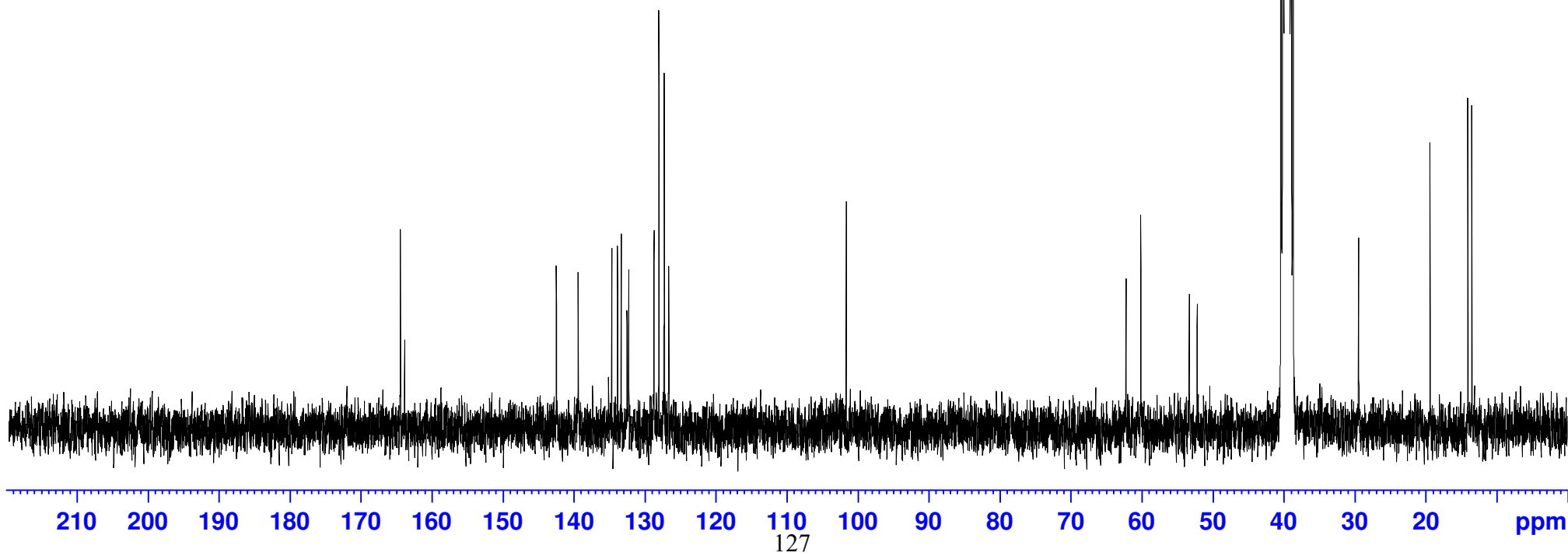
2-37c

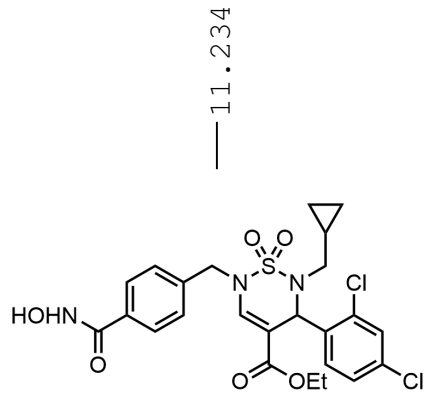
¹H NMR, DMSO-*d*₆, 300 MHz





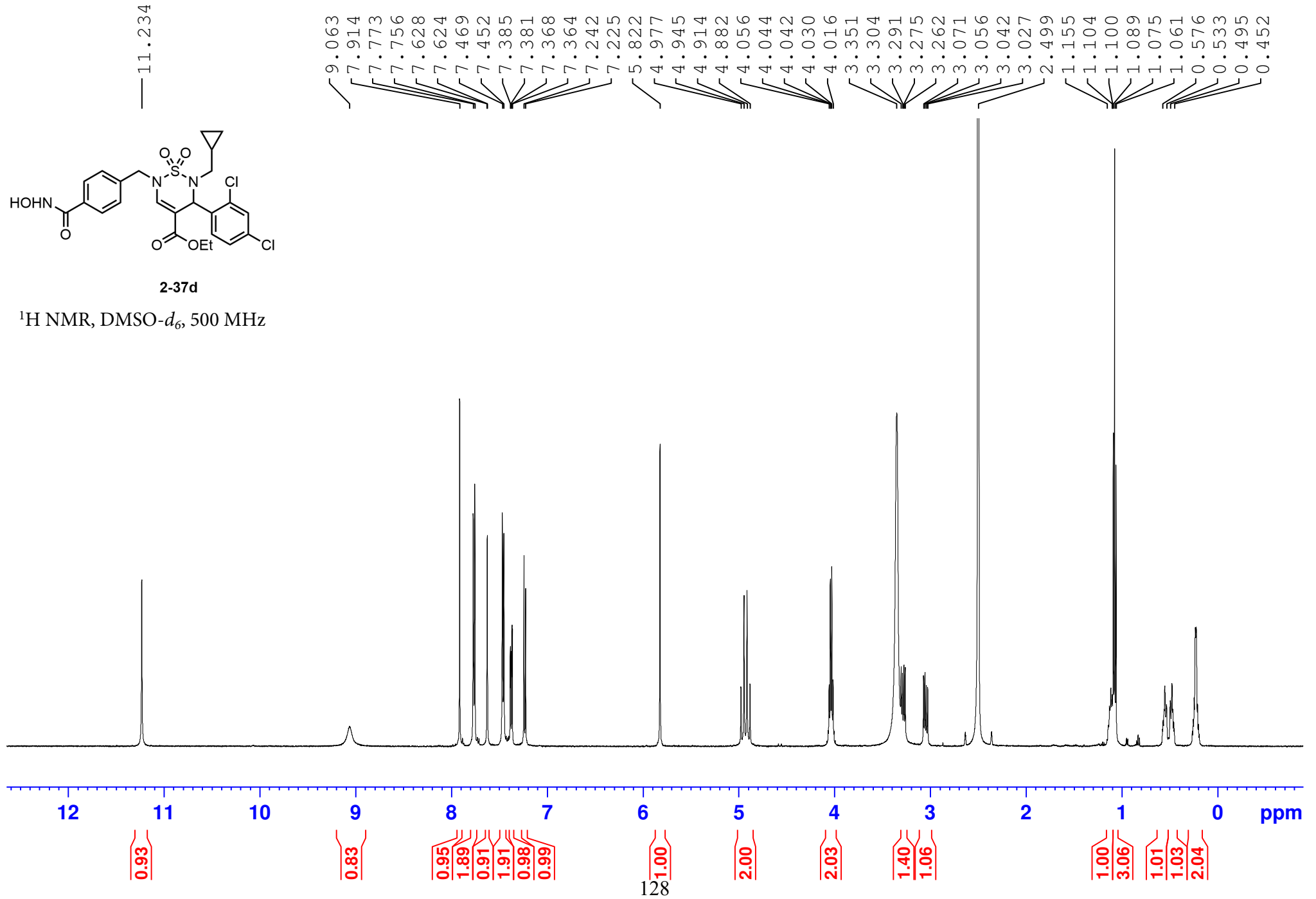
^{13}C NMR, DMSO- d_6 , 75 MHz

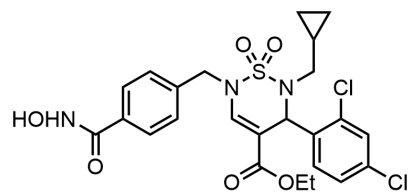




2-37d

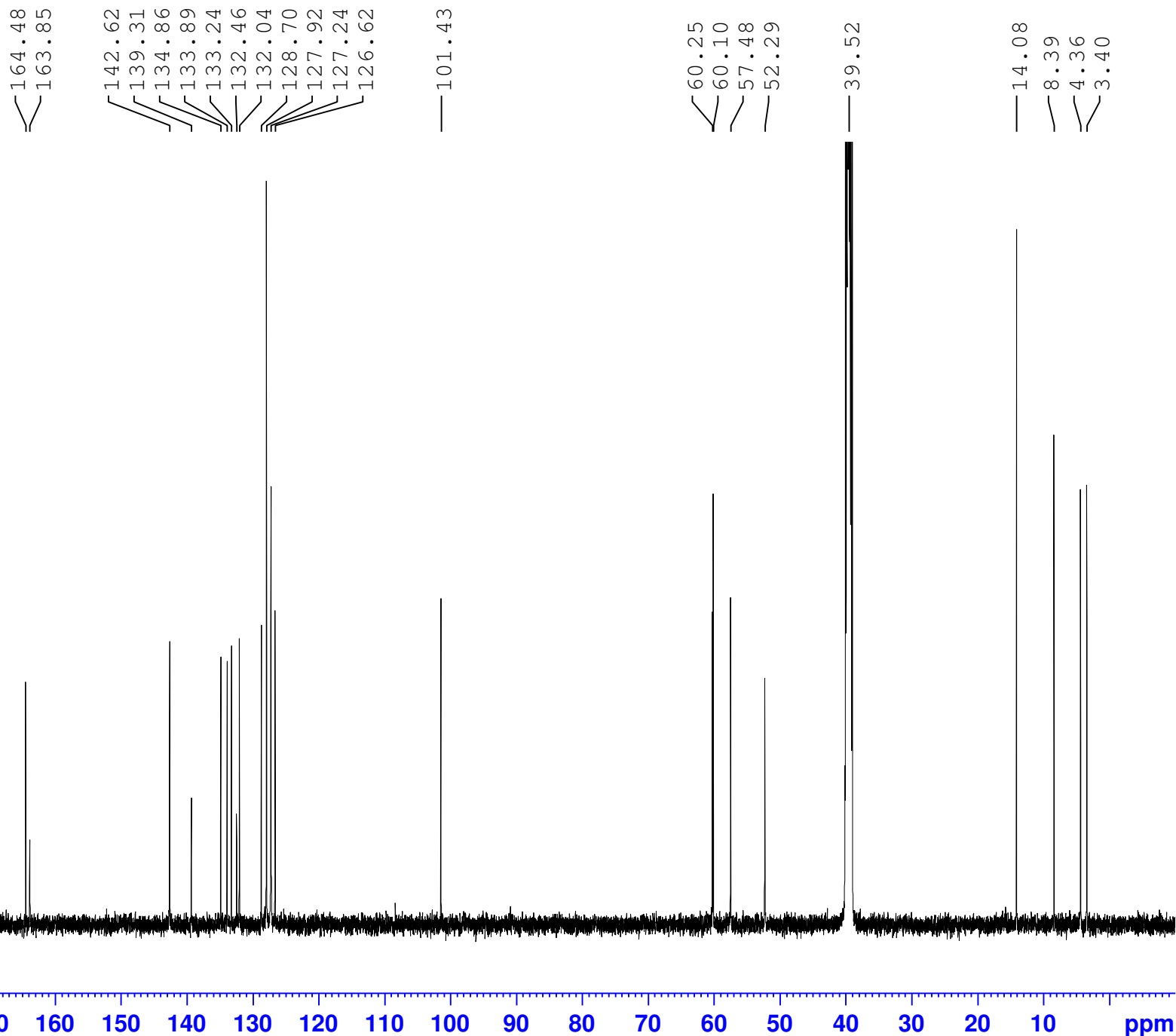
¹H NMR, DMSO-*d*₆, 500 MHz

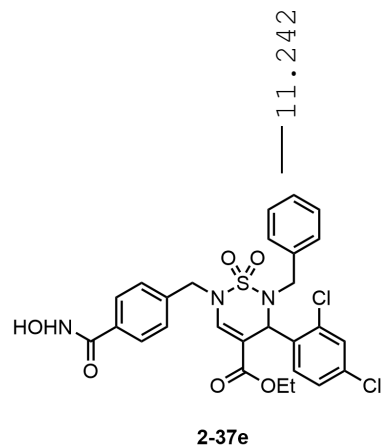




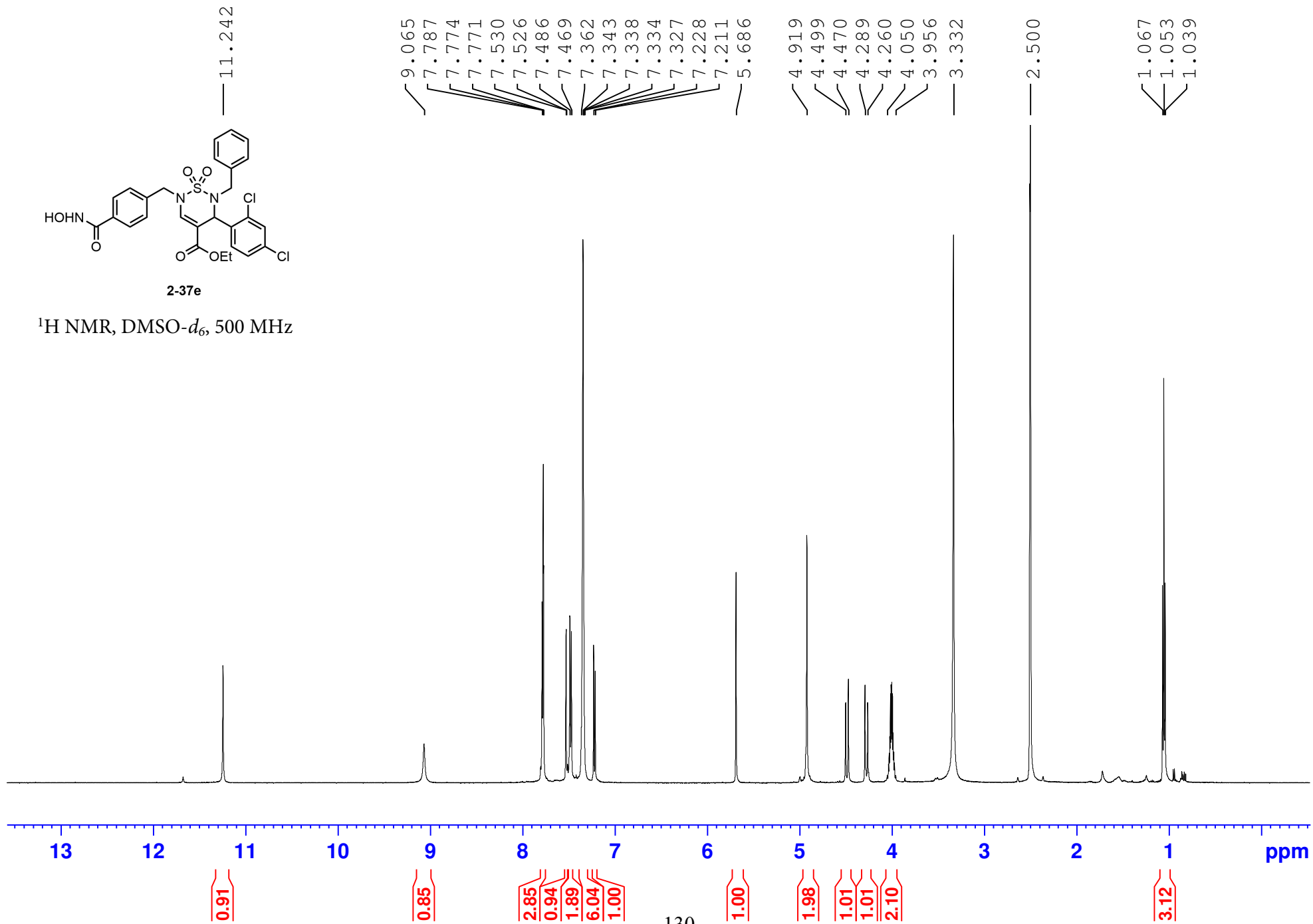
2-37d

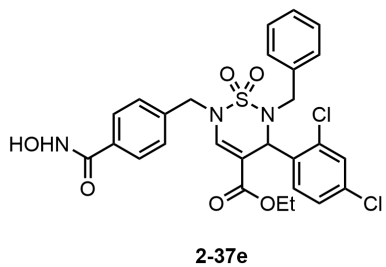
^{13}C NMR, DMSO- d_6 , 126 MHz



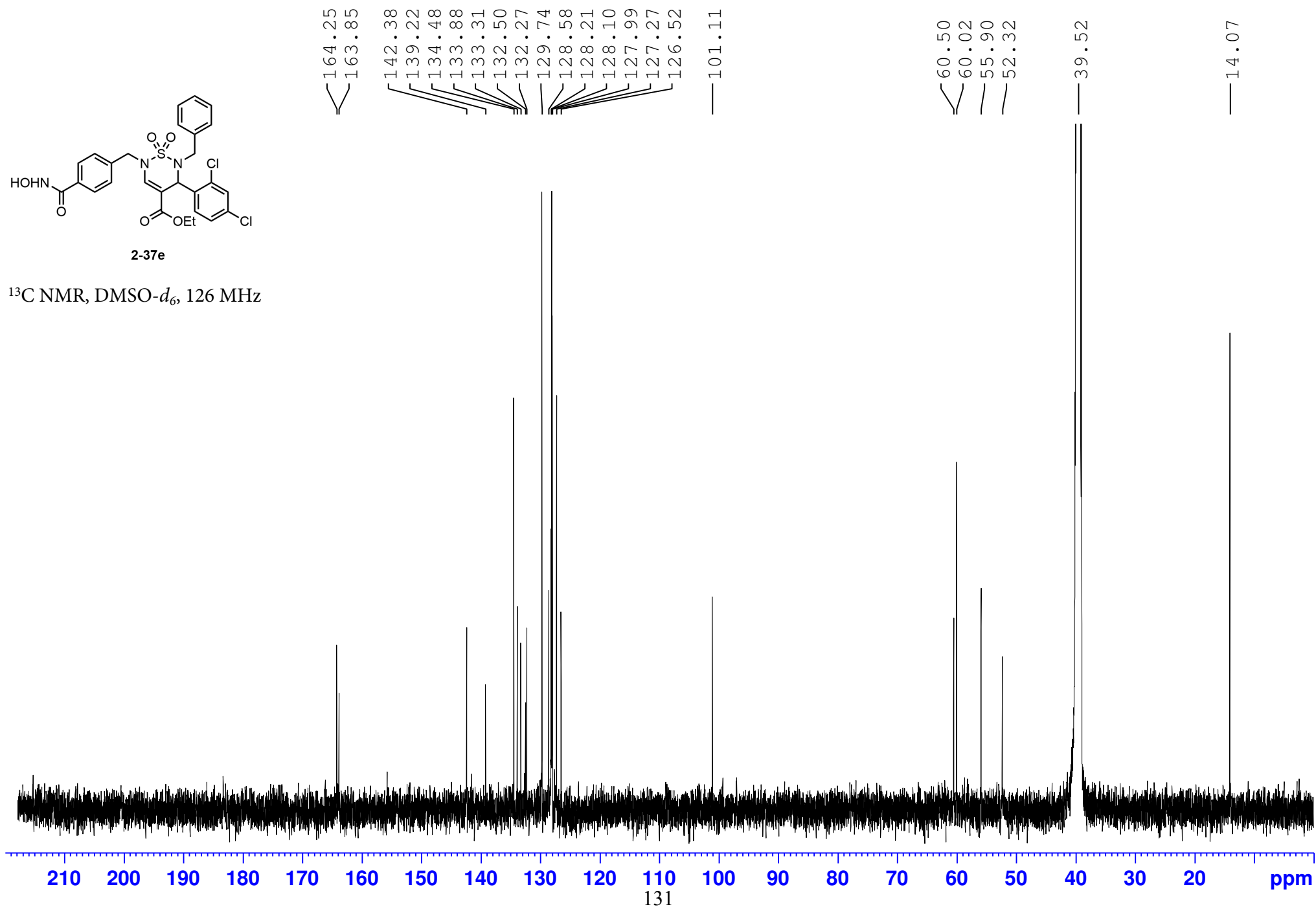


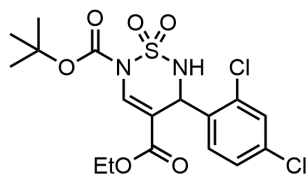
¹H NMR, DMSO-*d*₆, 500 MHz





¹³C NMR, DMSO-*d*₆, 126 MHz

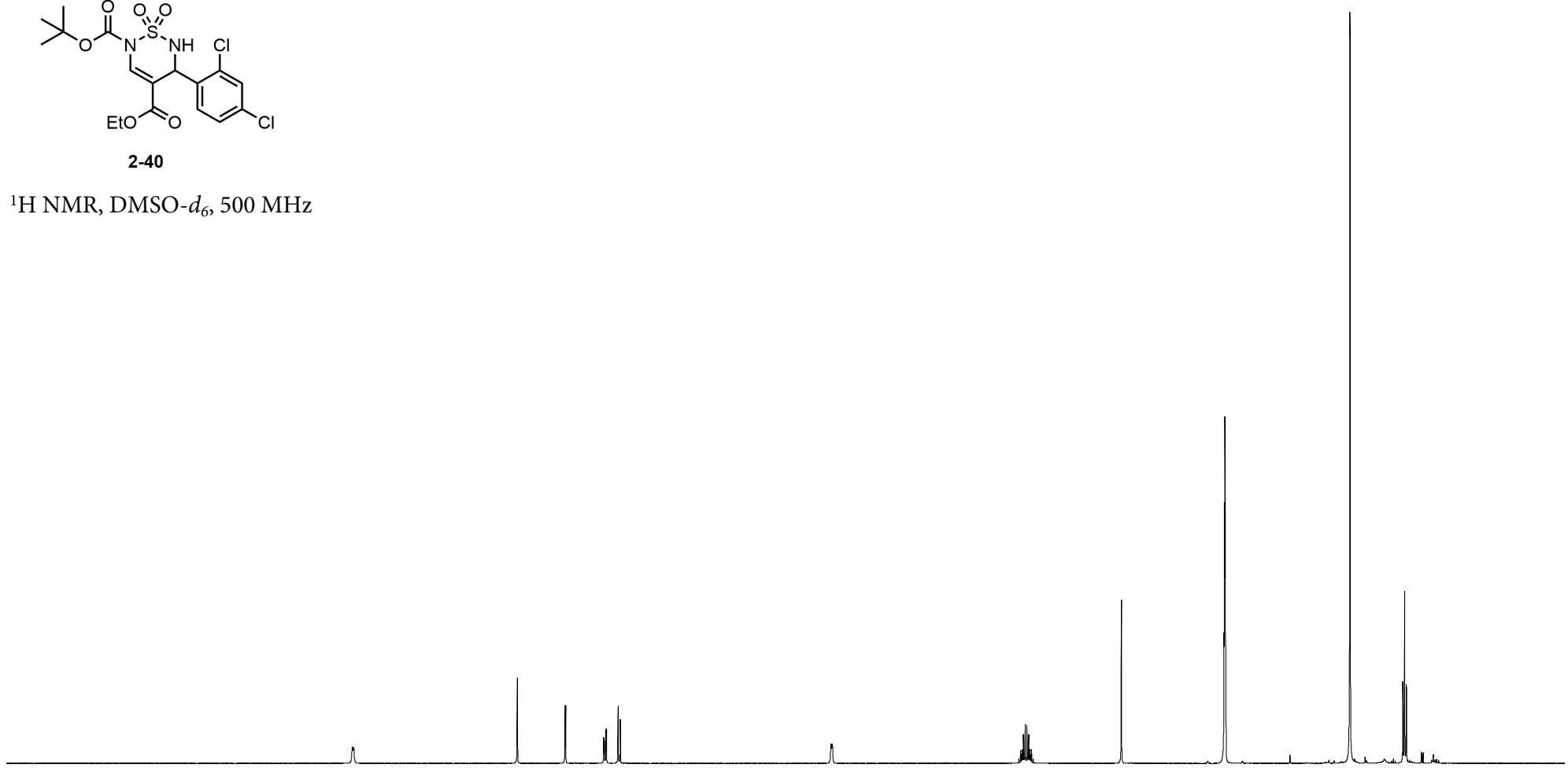




2-40

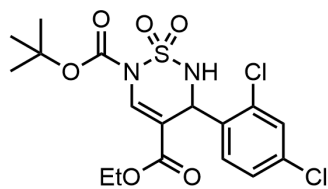
¹H NMR, DMSO-*d*₆, 500 MHz

9.367
9.356
8.068
8.068
7.692
7.688
7.388
7.384
7.371
7.367
7.275
7.258
5.600
5.589
4.122
4.008
3.314
2.500
1.515
1.099
1.085
1.071



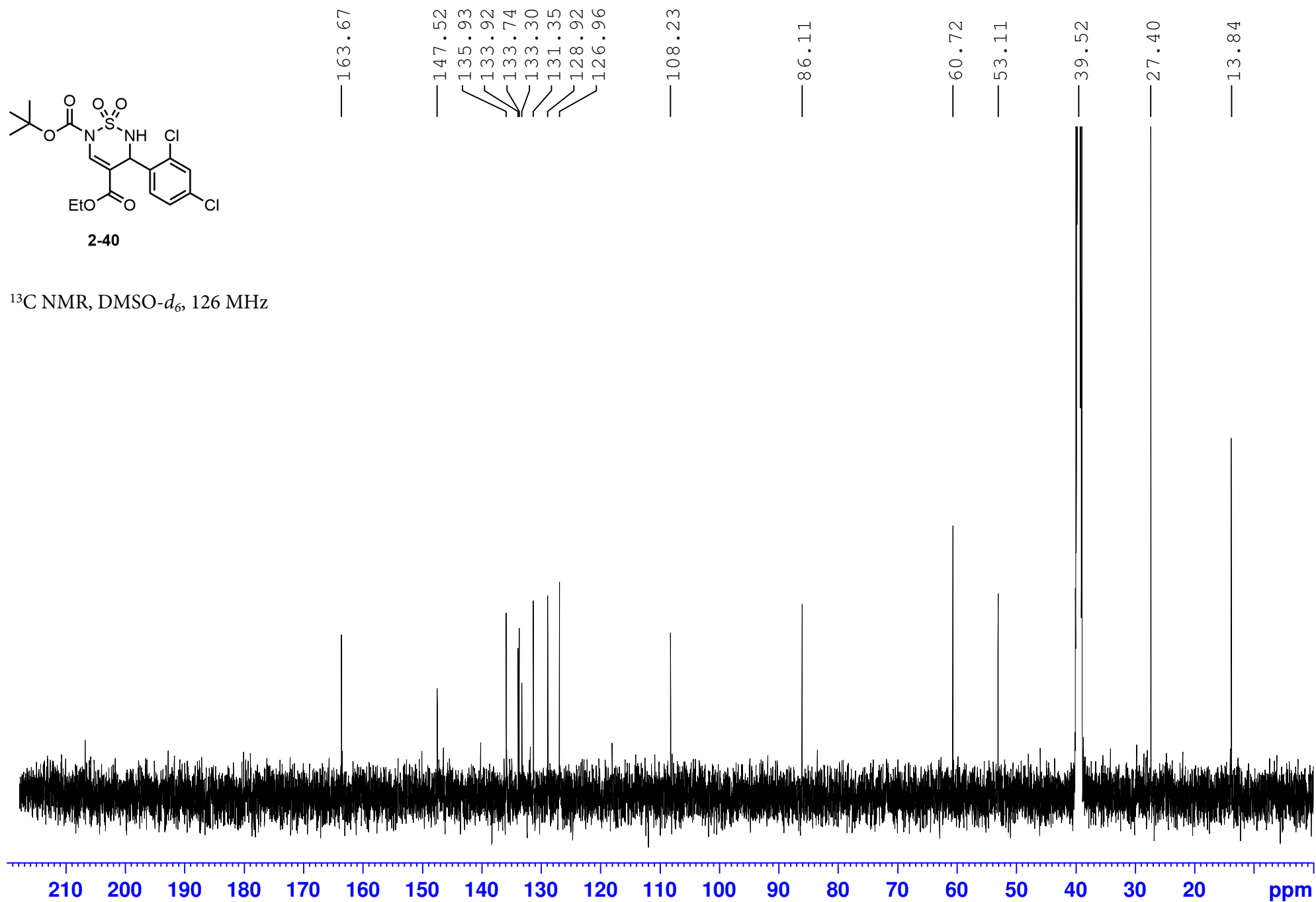
11 10 9 8 7 6 5 4 3 2 1 ppm

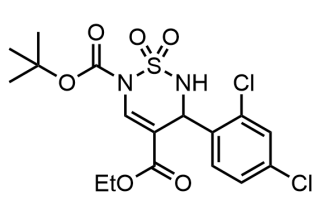
0.99
0.94
0.90
0.98
0.98
1.00
2.07
9.17
3.03



2-40

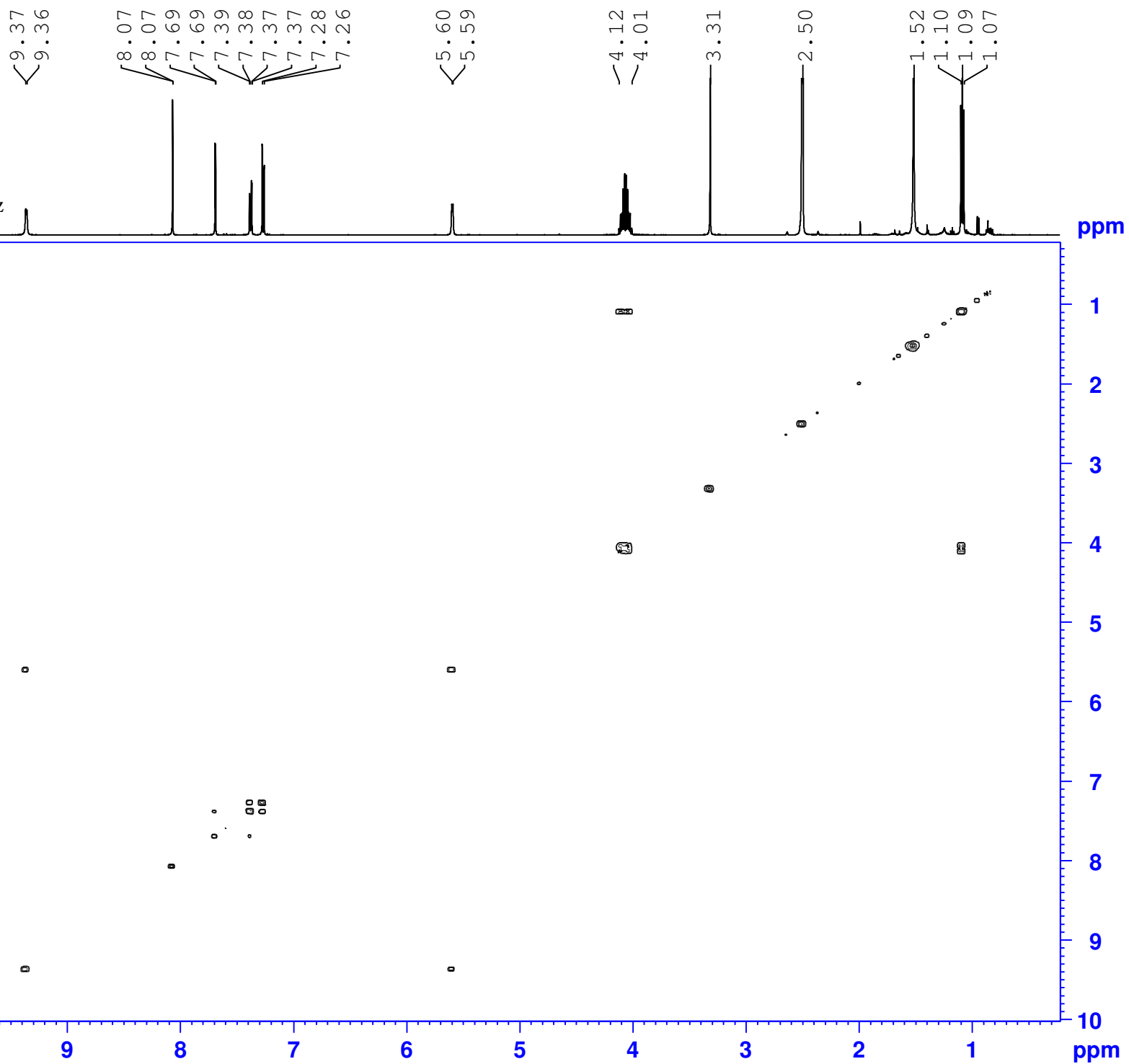
^{13}C NMR, DMSO- d_6 , 126 MHz

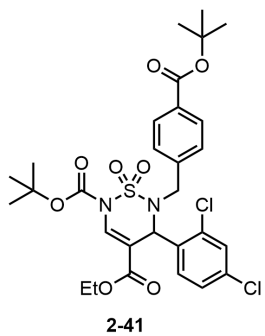




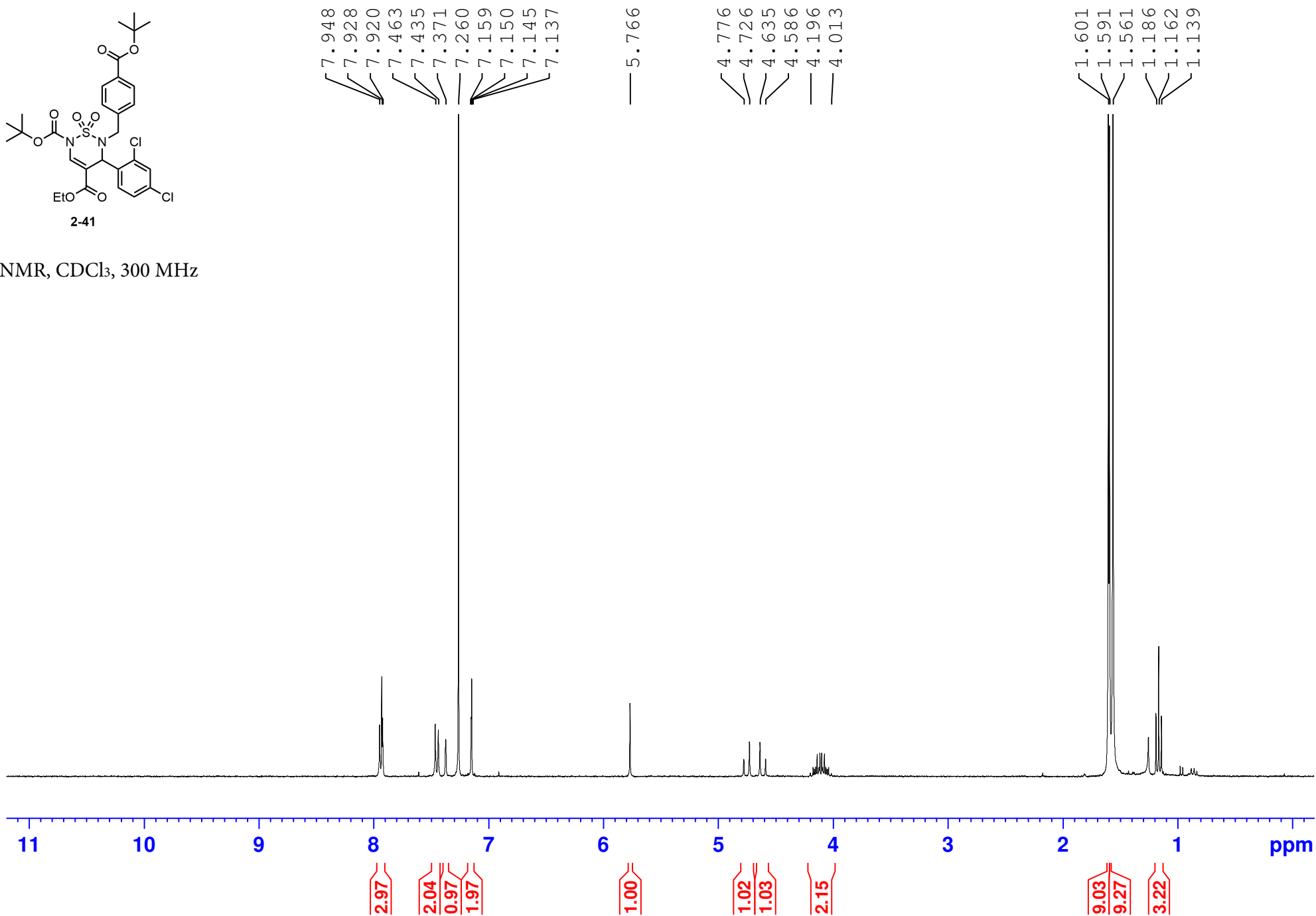
2-40

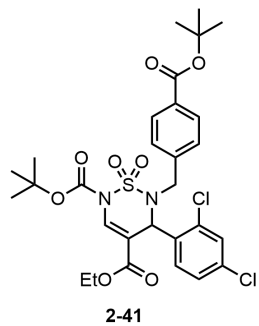
COSY NMR, DMSO-*d*₆, 500 MHz





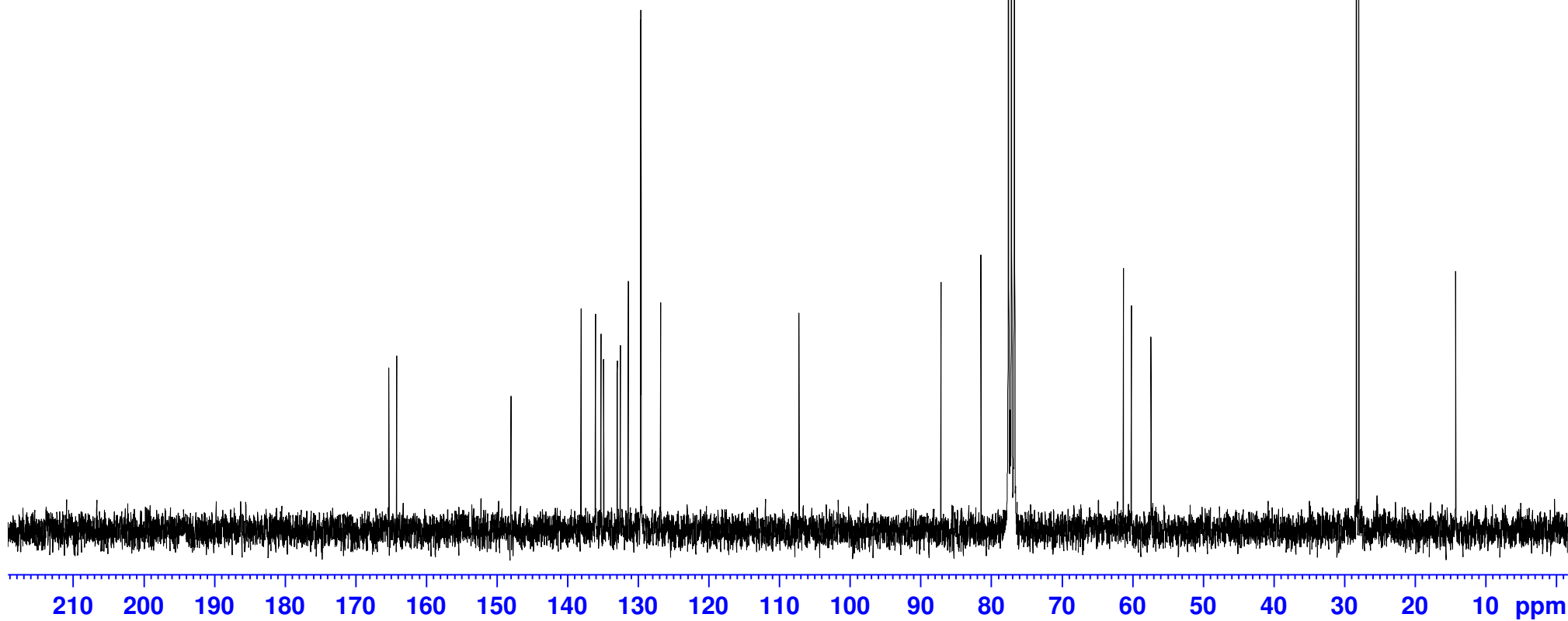
$^1\text{H NMR}$, CDCl_3 , 300 MHz

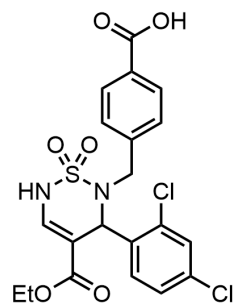




- 165.32
- 164.21
- 148.03
- 138.08
- 136.07
- 135.29
- 134.90
- 132.98
- 132.53
- 131.42
- 129.70
- 129.65
- 129.61
- 126.83
- 107.25
- 87.14
- 81.47
- 77.16
- 61.31
- 60.19
- 57.40
- 28.32
- 27.98
- 14.27

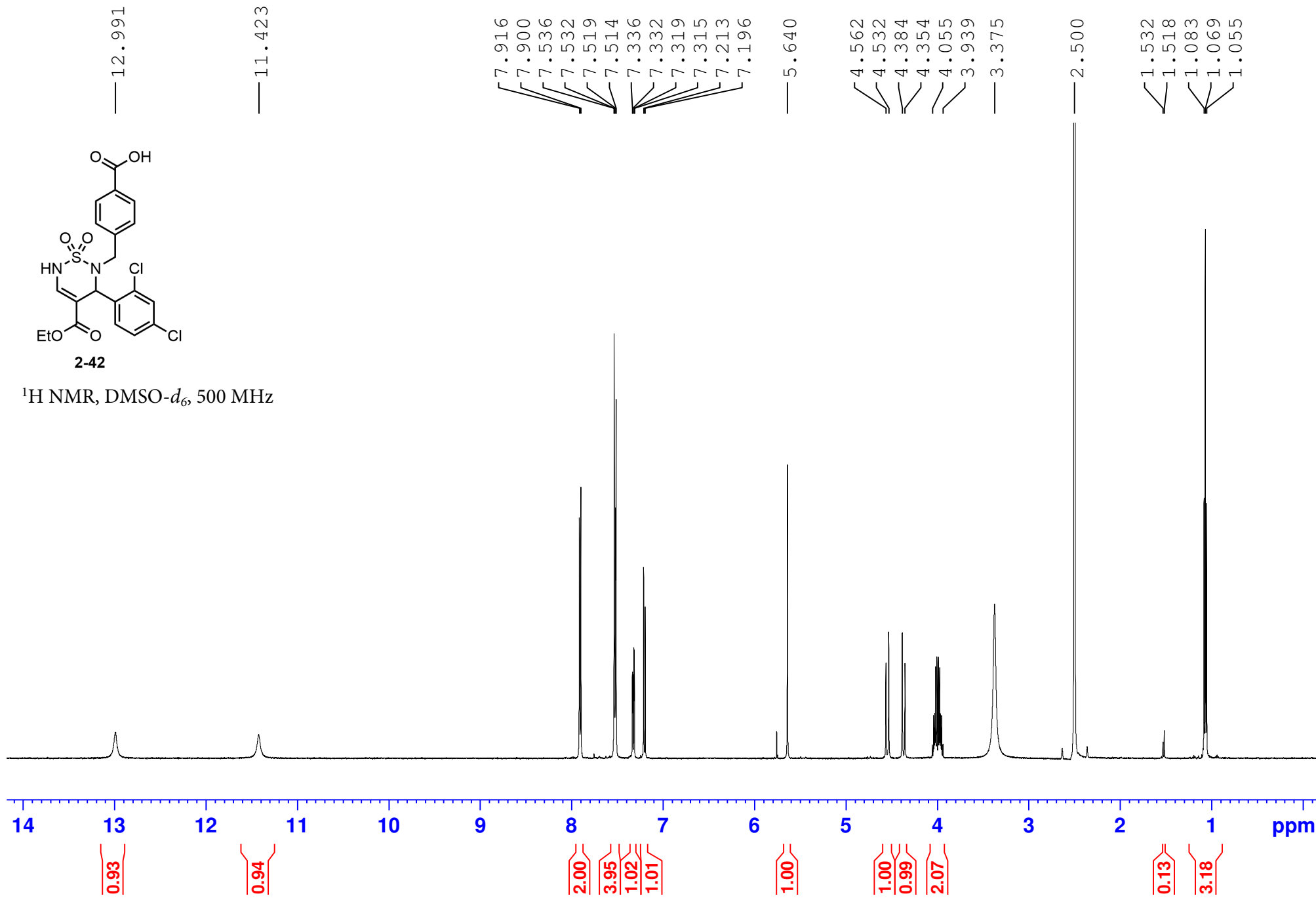
^{13}C NMR, CDCl_3 , 75 MHz

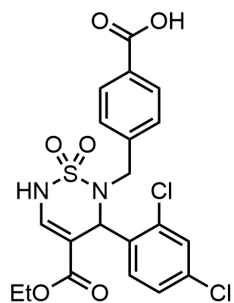




2-42

¹H NMR, DMSO-*d*₆, 500 MHz





2-42

^{13}C NMR, DMSO- d_6 , 126 MHz

167.09
164.48

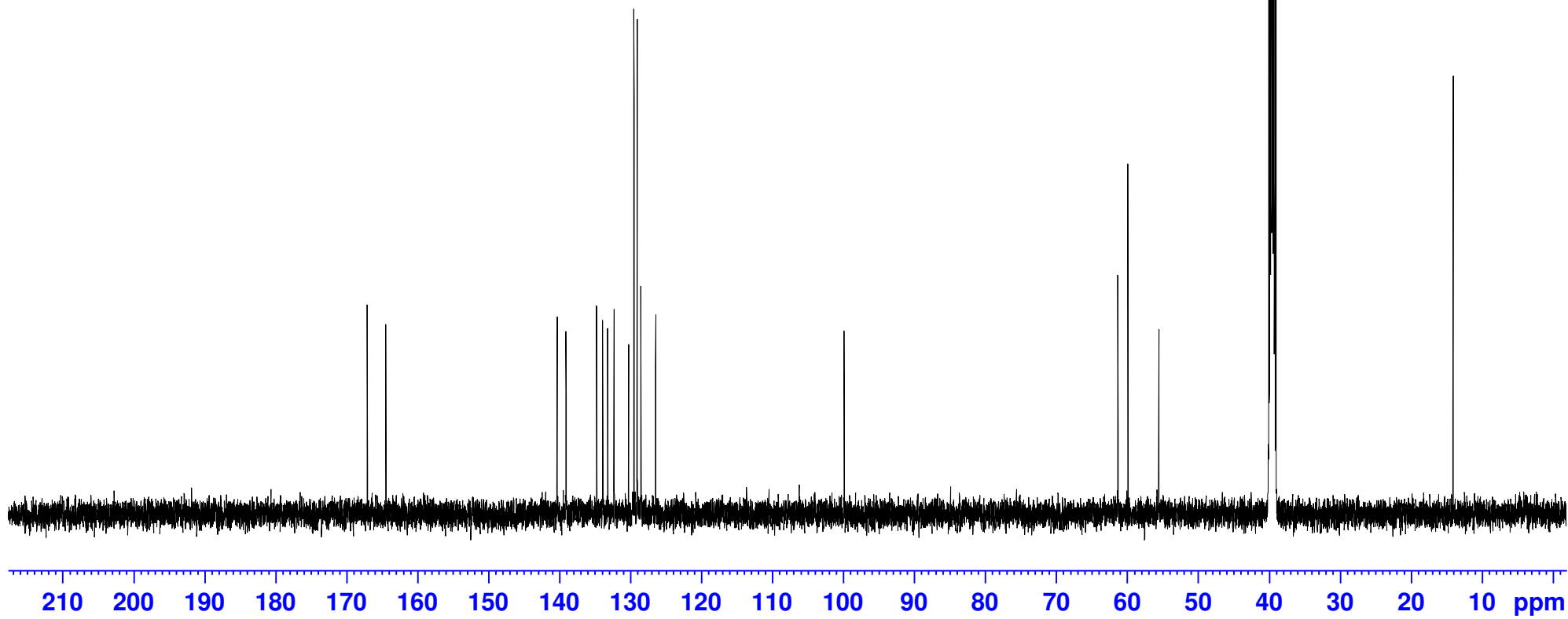
140.33
139.08
134.77
133.91
133.21
132.30
130.25
129.50
129.04
128.53
126.45

99.88

61.29
59.89
55.52

39.52

14.04



11.410
11.242
11.100

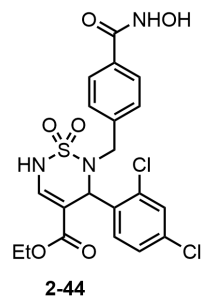
9.027
7.740
7.724
7.536
7.519
7.478
7.462
7.331
7.328
7.315
7.311
7.217
7.200
6.961
6.945

5.630

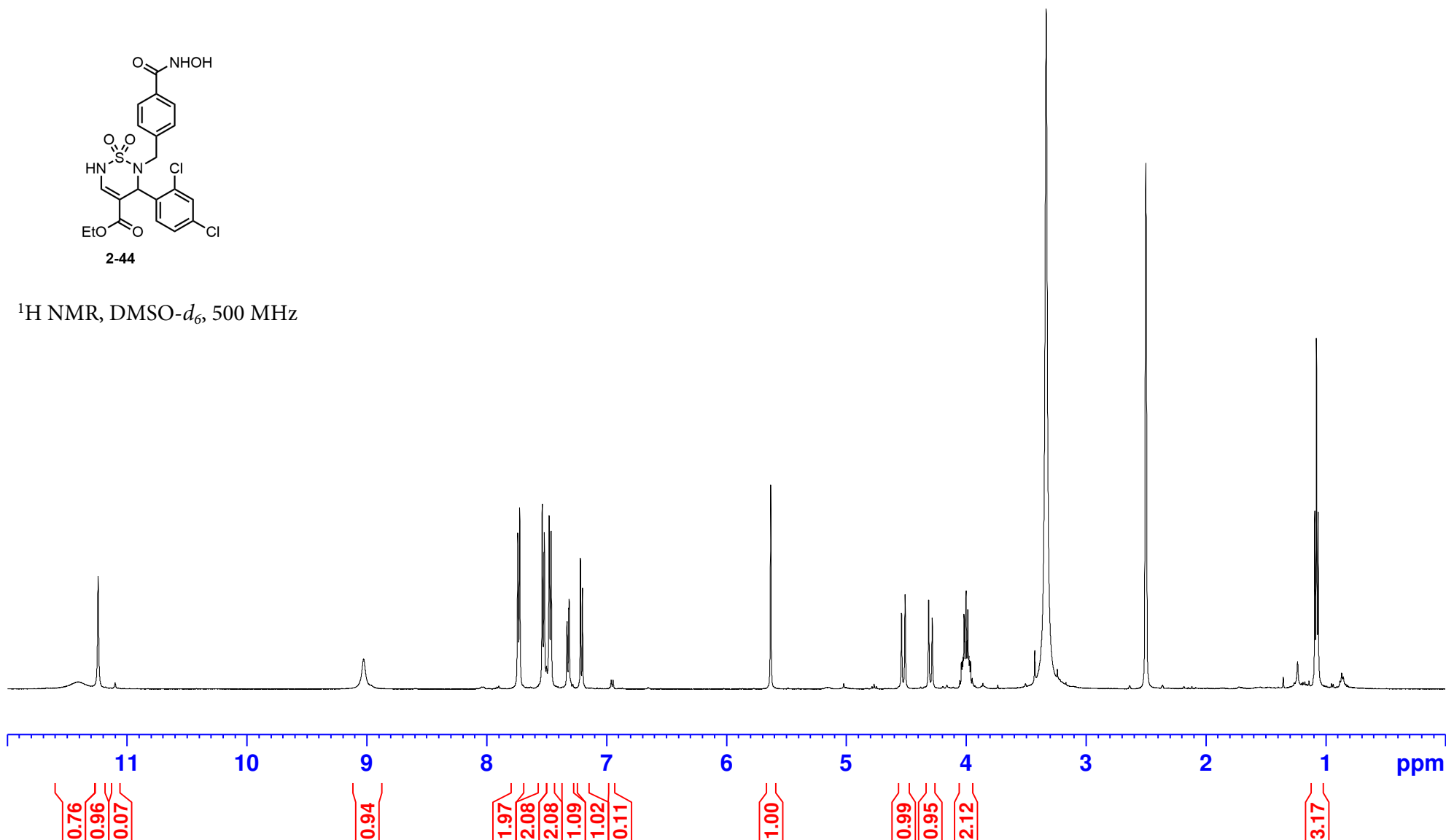
4.538
4.508
4.312
4.282
4.052
3.948
3.426
3.331

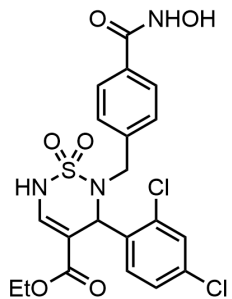
2.500

1.090
1.076
1.062



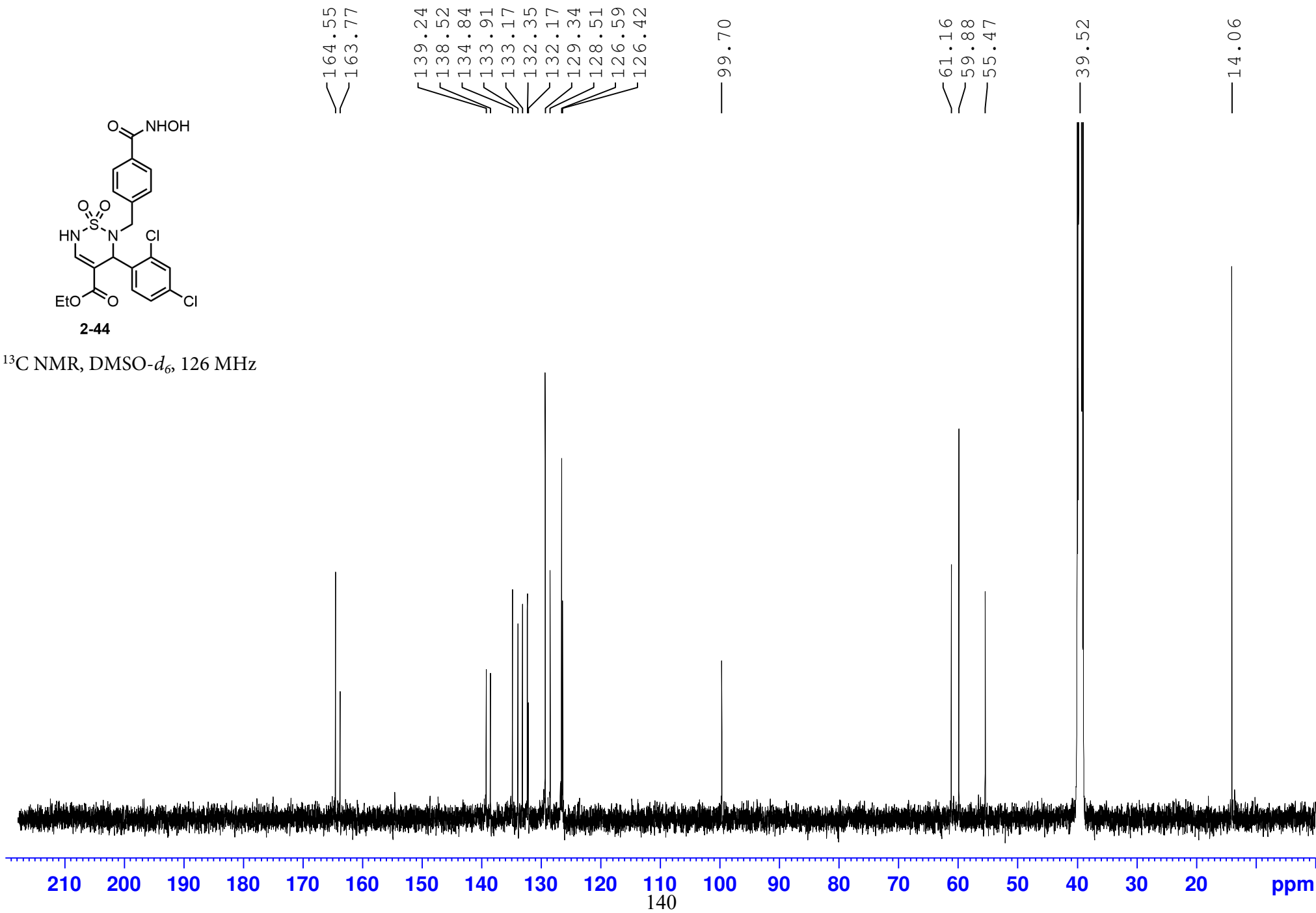
¹H NMR, DMSO-d₆, 500 MHz

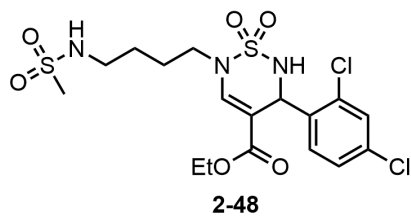




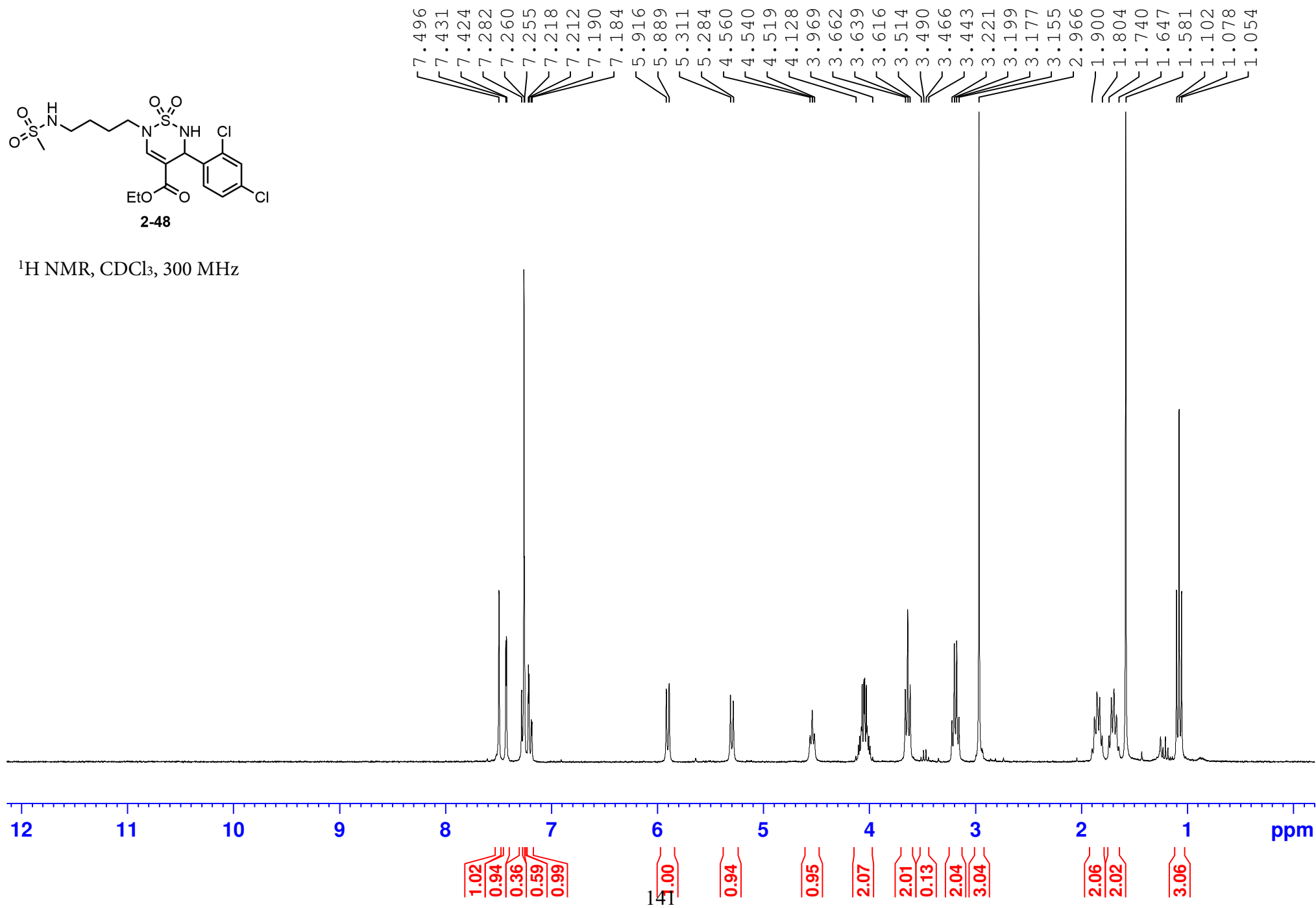
2-44

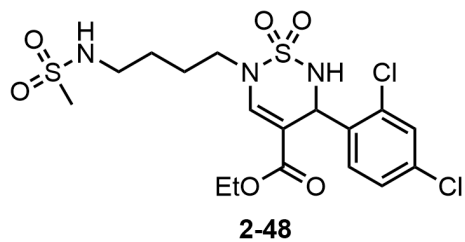
^{13}C NMR, $\text{DMSO-}d_6$, 126 MHz



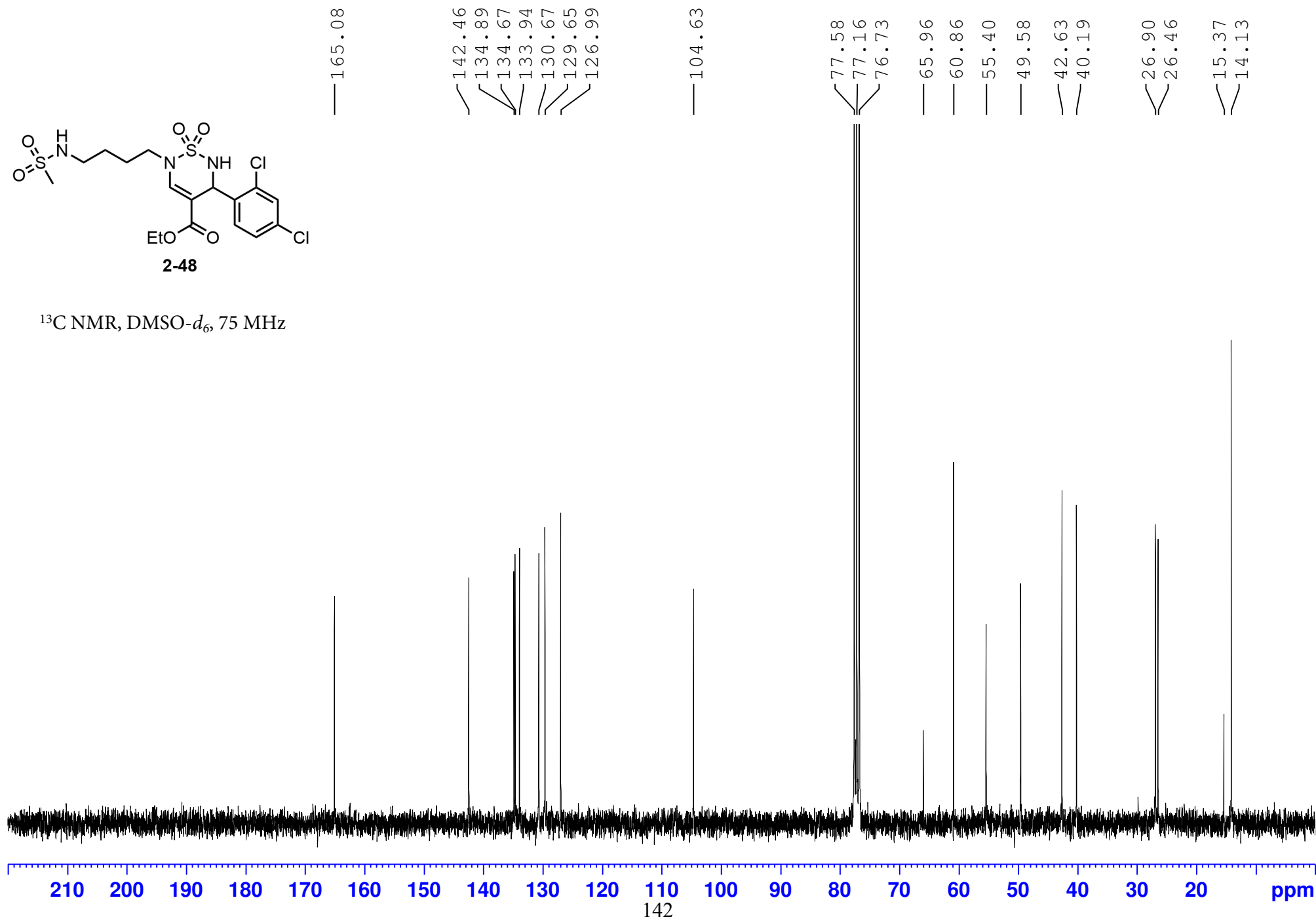


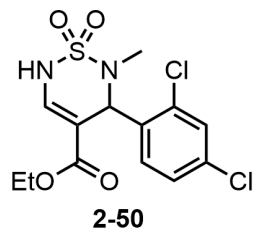
¹H NMR, CDCl₃, 300 MHz



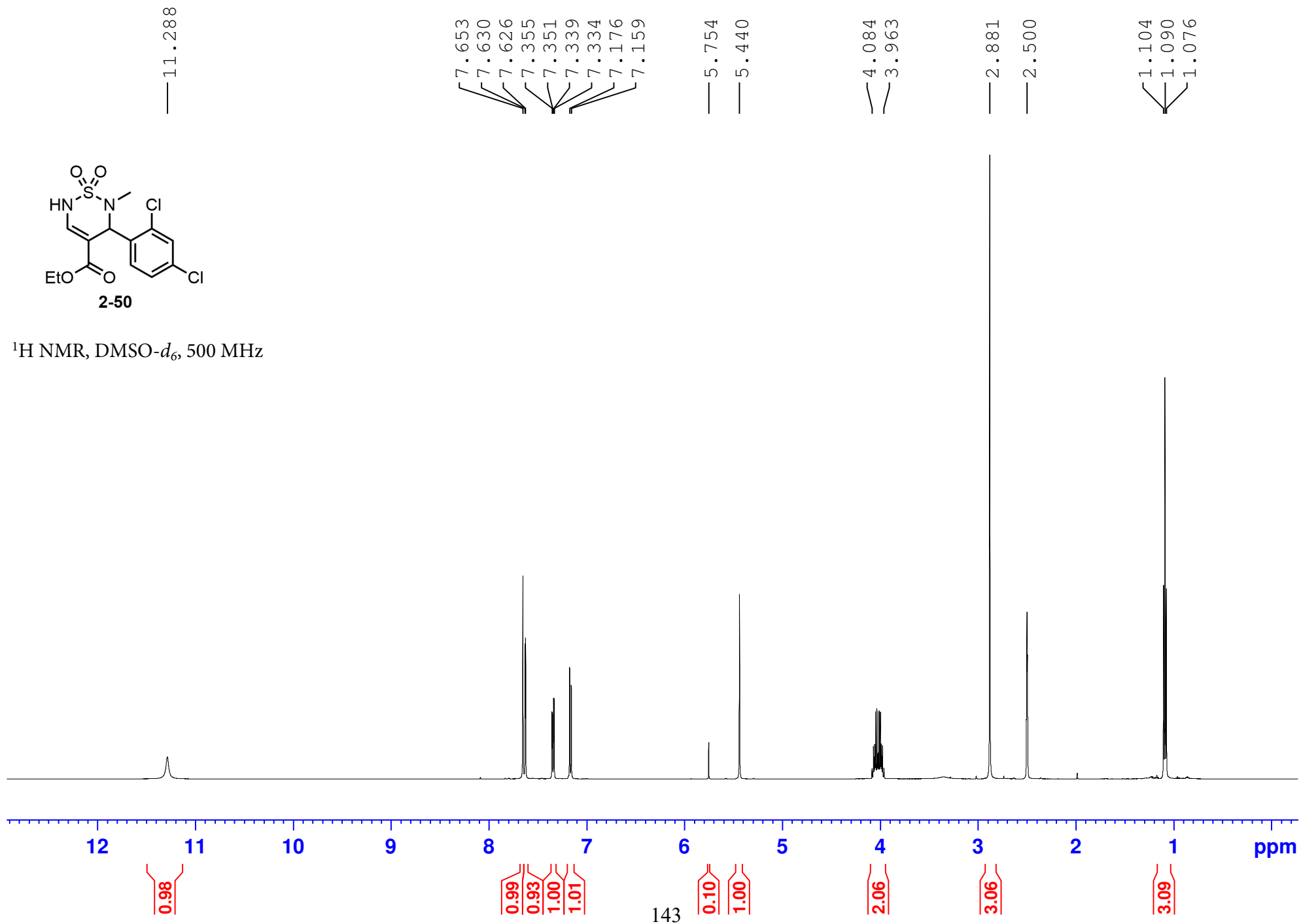


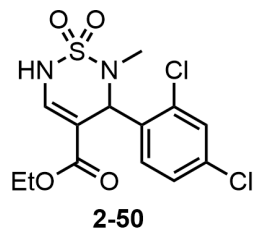
^{13}C NMR, DMSO- d_6 , 75 MHz



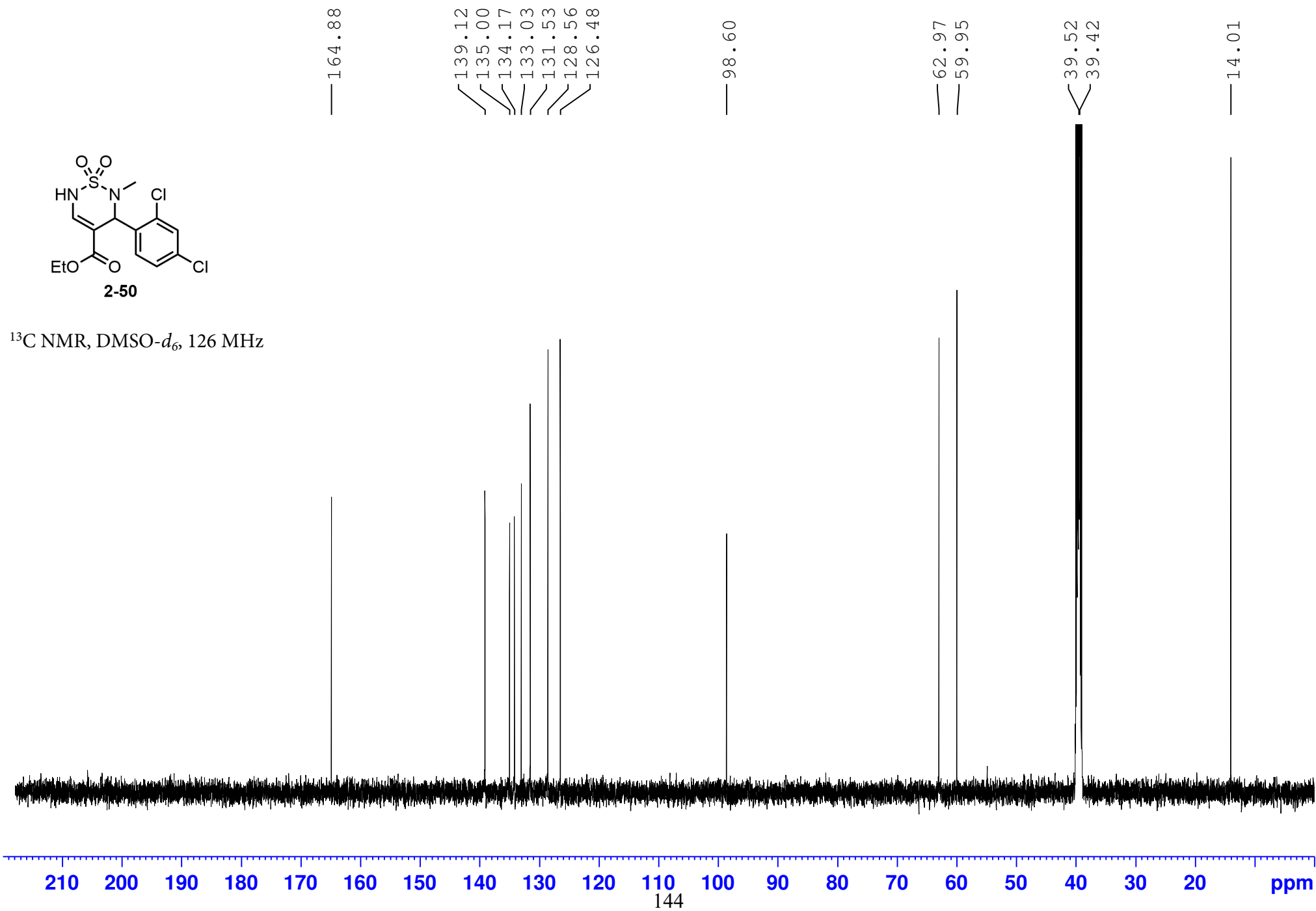


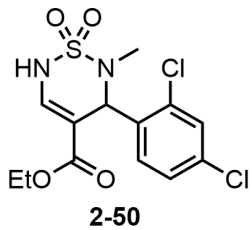
$^1\text{H NMR}$, $\text{DMSO-}d_6$, 500 MHz



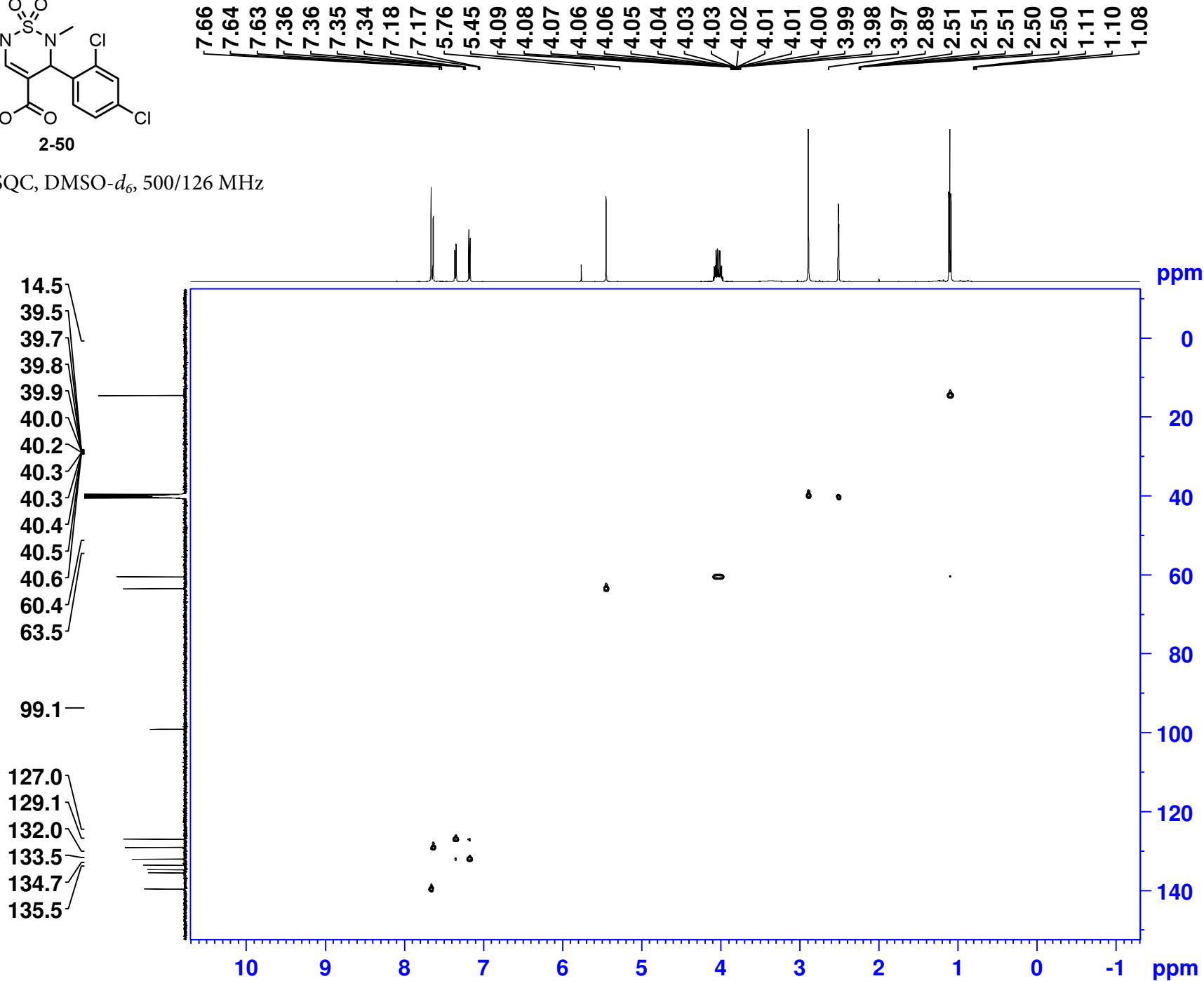


^{13}C NMR, DMSO- d_6 , 126 MHz





HSQC, DMSO-*d*₆, 500/126 MHz



```

Current Data Parameters
NAME          LT-951-42
EXPNO         20
PROCNO        1

F2 - Acquisition Parameters
Date_         20191204
Time          13.26
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       hsqcetgpsisp2.2
TD            1024
SOLVENT       DMSO
NS            4
DS            16
SWH           6009.615 Hz
FIDRES        5.868765 Hz
AQ            0.0851968 sec
RG            203
DW            83.200 usec
DE            6.50 usec
TE            297.5 K
CNST2         145.000000
CNST17        -0.500000
D0            0.00000300 sec
D1            2.00000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00089000 sec
INO           0.00002410 sec

===== CHANNEL f1 =====
SFO1          500.1623508 MHz
NUC1           1H
P1            11.50 usec
P2            23.00 usec
P28           1000.00 usec
PLW1          18.00000000 W

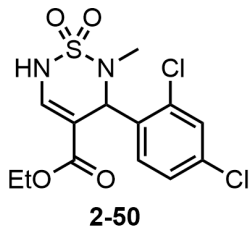
===== CHANNEL f2 =====
SFO2          125.7741356 MHz
NUC2           13C
CPDPRG2       bi_p5m4sp_4sp.2
P3            10.50 usec
P14           500.00 usec
P24           2000.00 usec
P63           1500.00 usec
PLMG          0 W
PLW2          110.00000000 W
PLW12         2.47499990 W
SPNAM[3]      Crp60,0.5,20.1
SFOAL3        0 Hz
SPOFFS3       0 Hz
SPW3          18.52899933 W
SPNAM[7]      Crp60comp,4
SFOAL7        0 Hz
SPOFFS7       0 Hz
SPW7          18.52899933 W
SPNAM[14]     Crp32,1.5,20.2
SFOAL14       0 Hz
SPOFFS14      0 Hz
SPW14         7.90590000 W
SPNAM[31]     Crp32,1.5,20.2
SFOAL31       0 Hz
SPOFFS31      0 Hz
SPW31         1.97650003 W

===== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1          80.00 %
GPZ2          20.10 %
GPZ3          11.00 %
GPZ4          -5.00 %
P16           1000.00 usec
P19           500.00 usec

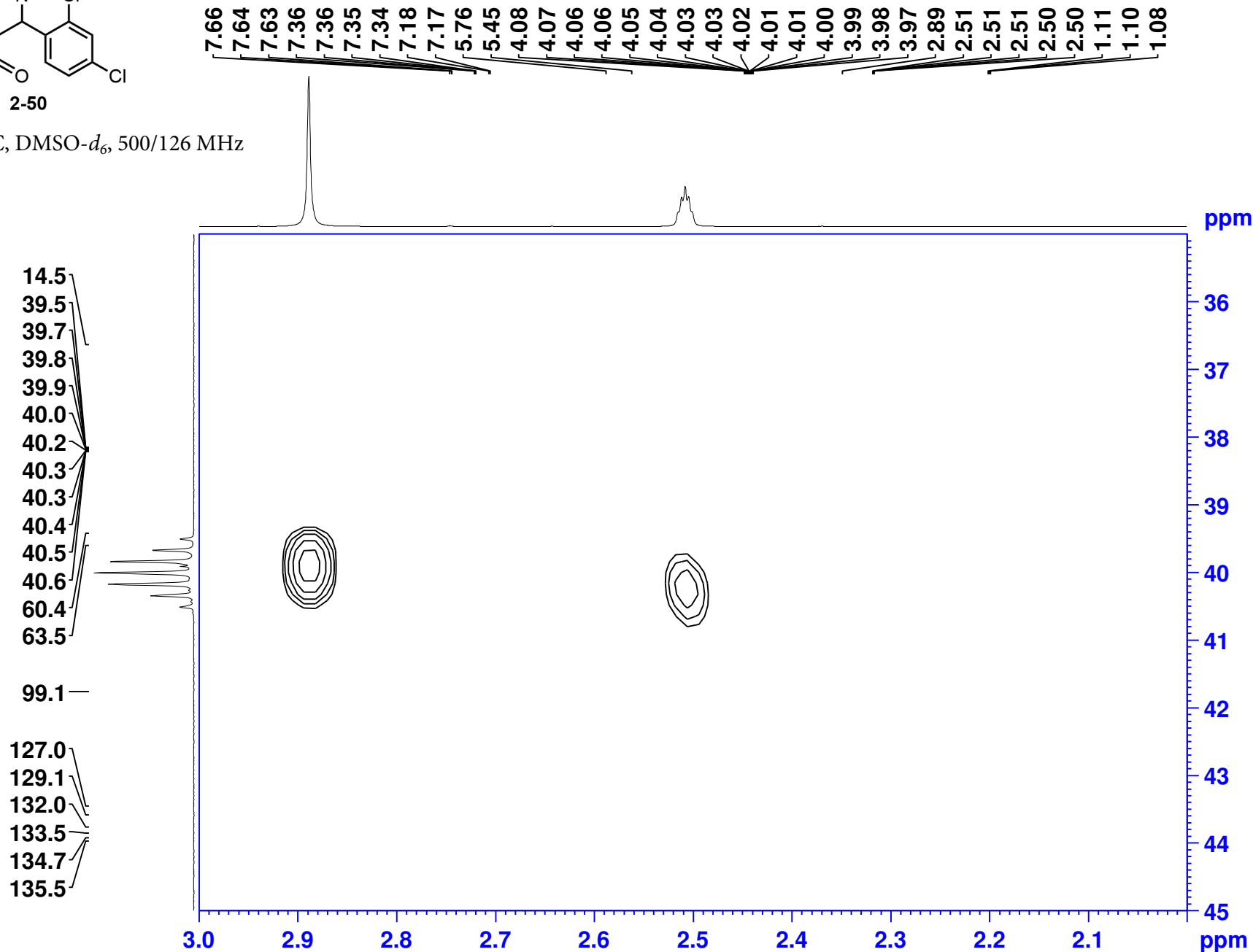
F1 - Acquisition parameters
TD            64
SFO1          125.7741 MHz
FIDRES        648.340271 Hz
SW            164.954 ppm
FnMODE        Echo-Antiecho

F2 - Processing parameters
SI            1024
SF            500.1600000 MHz
WDW           QSINE
SSB           2
LB            0 Hz
GB            0
PC            1.40

F1 - Processing parameters
SI            1024
MC2           echo-antiecho
SF            125.7653320 MHz
WDW           QSINE
SSB           2
LB            0 Hz
GB            0
  
```



HSQC, DMSO-*d*₆, 500/126 MHz



```

Current Data Parameters
NAME          LI-951-42
EXPNO         20
PROCNO        1

F2 - Acquisition Parameters
Date_         20191204
Time          13.26
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       hsqcetgpsisp2.2
TD            1024
SOLVENT       DMSO
NS            4
DS            16
SWH           6009.615 Hz
FIDRES        5.868765 Hz
AQ            0.0851968 sec
RG            203
DW            83.200 usec
DE            6.50 usec
TE            297.5 K
CNST2         145.0000000
CNST17        -0.5000000
DO            0.00000300 sec
D1            2.00000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00089000 sec
INO           0.00002410 sec

===== CHANNEL f1 =====
SFO1          500.1623508 MHz
NUC1          1H
P1            11.50 usec
P2            23.00 usec
P28           1000.00 usec
PLW1          18.00000000 W

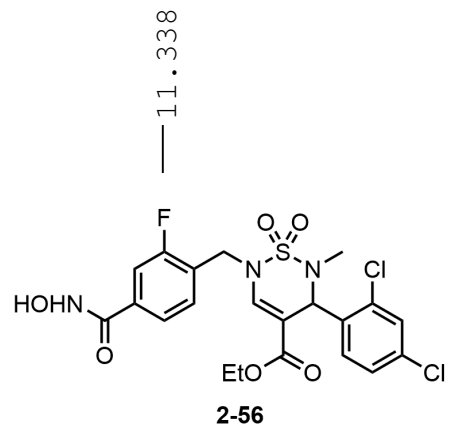
===== CHANNEL f2 =====
SFO2          125.7741356 MHz
NUC2          13C
CPDPRG2       bi_p5m4sp_4sp.2
P3            10.50 usec
P14           500.00 usec
P24           2000.00 usec
P63           1500.00 usec
PLM0          0 W
PLW2          110.00000000 W
PLW12         2.47499990 W
SPNAM[3]      Crp60,0.5,20.1
SFOAL3        0.500
SPOFFS3       0 Hz
SPW3          18.52899933 W
SPNAM[7]      Crp60comp,4
SFOAL7        0.500
SPOFFS7       0 Hz
SPW7          18.52899933 W
SPNAM[14]     Crp32,1.5,20.2
SFOAL14       0.500
SPOFFS14      0 Hz
SPW14         7.90590000 W
SPNAM[31]     Crp32,1.5,20.2
SFOAL31       0.500
SPOFFS31      0 Hz
SPW31         1.97650003 W

===== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GP21          80.00 %
GP22          20.10 %
GP23          11.00 %
GP24          -5.00 %
P16           1000.00 usec
P19           500.00 usec

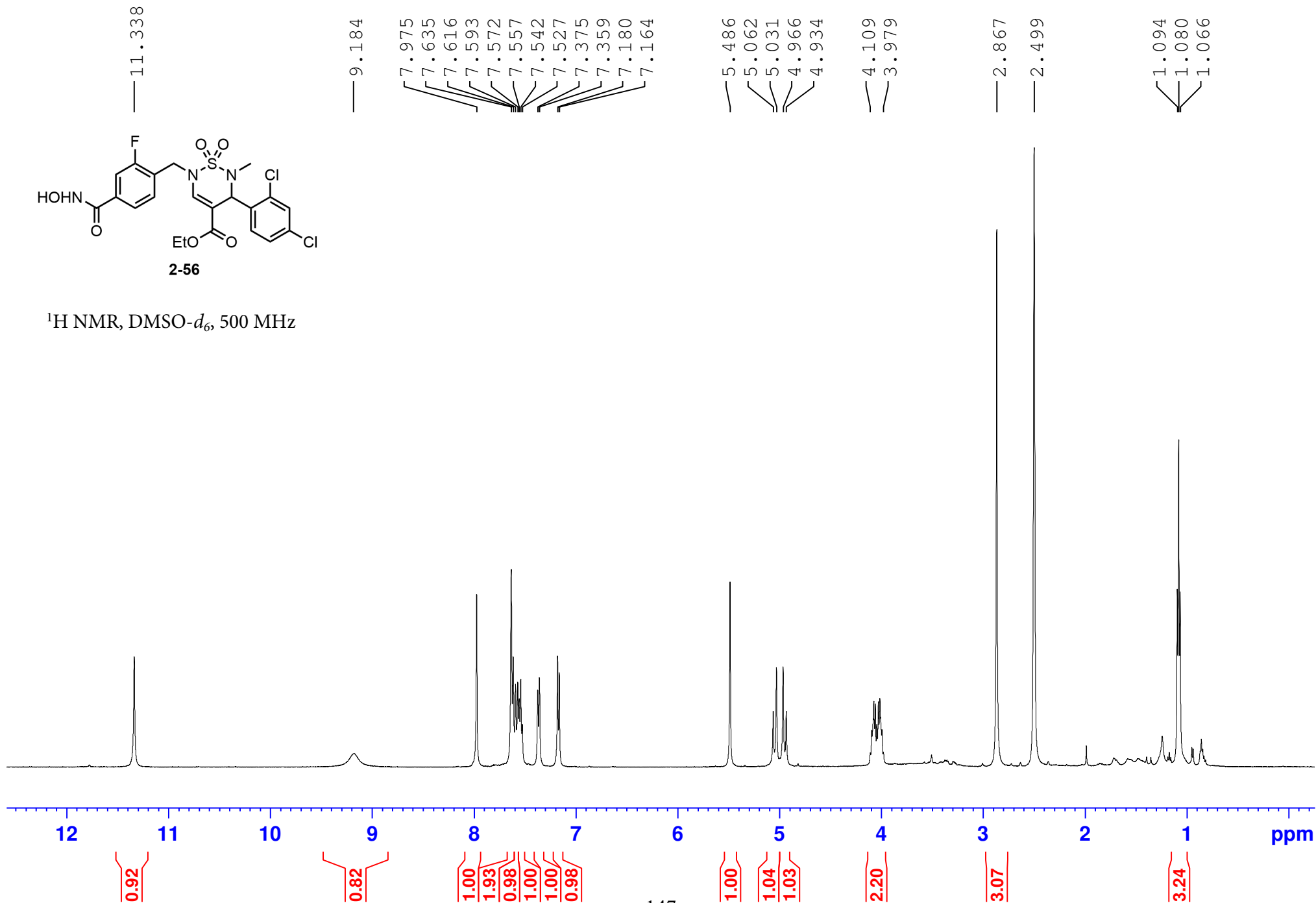
F1 - Acquisition parameters
TD            64
SFO1          125.7741 MHz
FIDRES        648.340271 Hz
SW            164.954 ppm
FnMODE        Echo-Antiecho

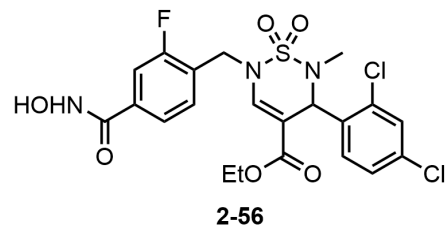
F2 - Processing parameters
SI            1024
SF            500.1600000 MHz
WDW           QSINE
SSB           2
LB            0 Hz
GB            0
PC            1.40

F1 - Processing parameters
SI            1024
MC2           echo-antiecho
SF            125.7653320 MHz
WDW           QSINE
SSB           2
LB            0 Hz
GB            0
  
```

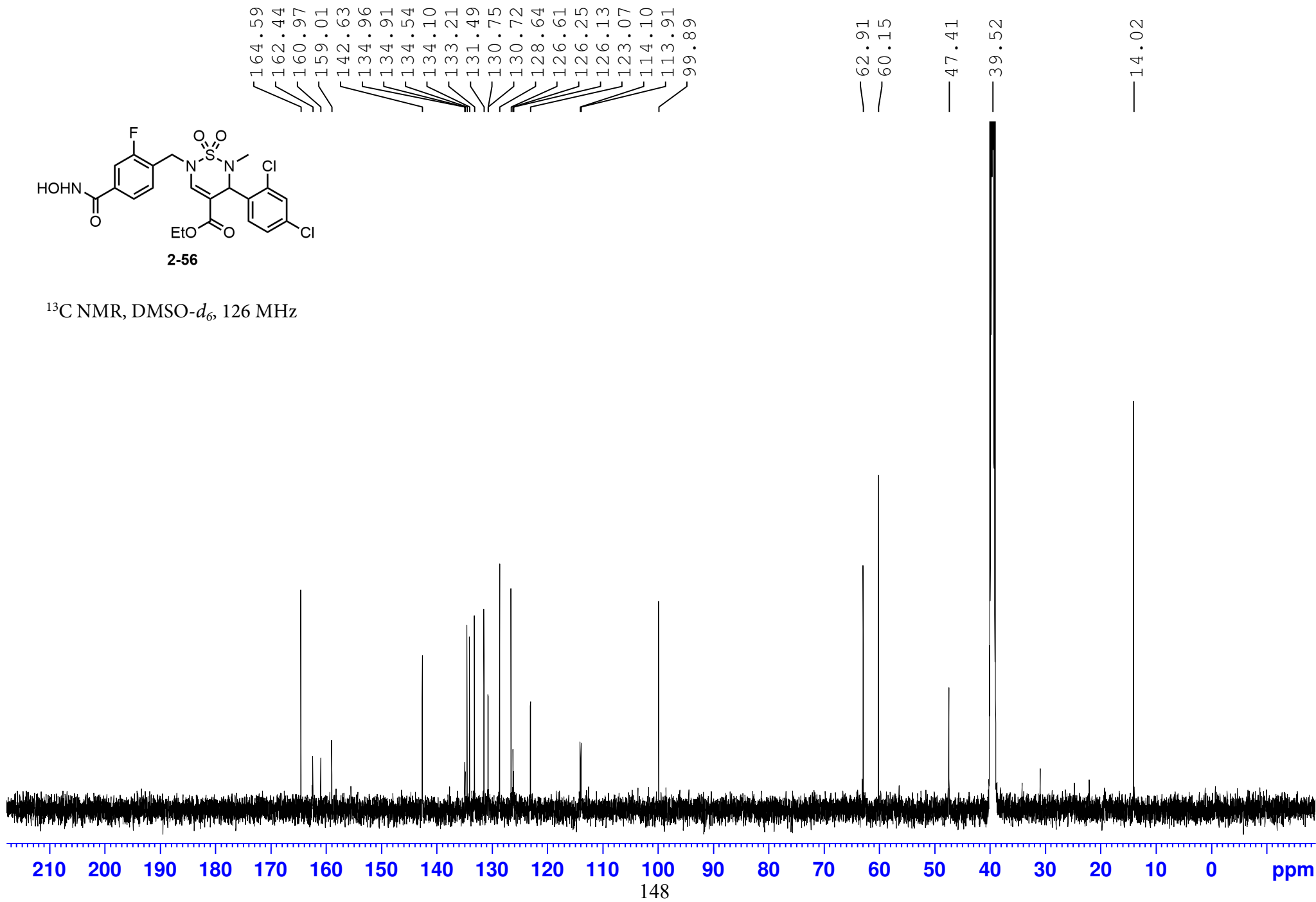


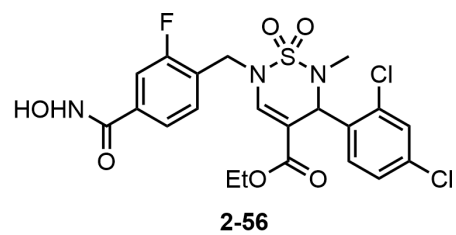
¹H NMR, DMSO-*d*₆, 500 MHz



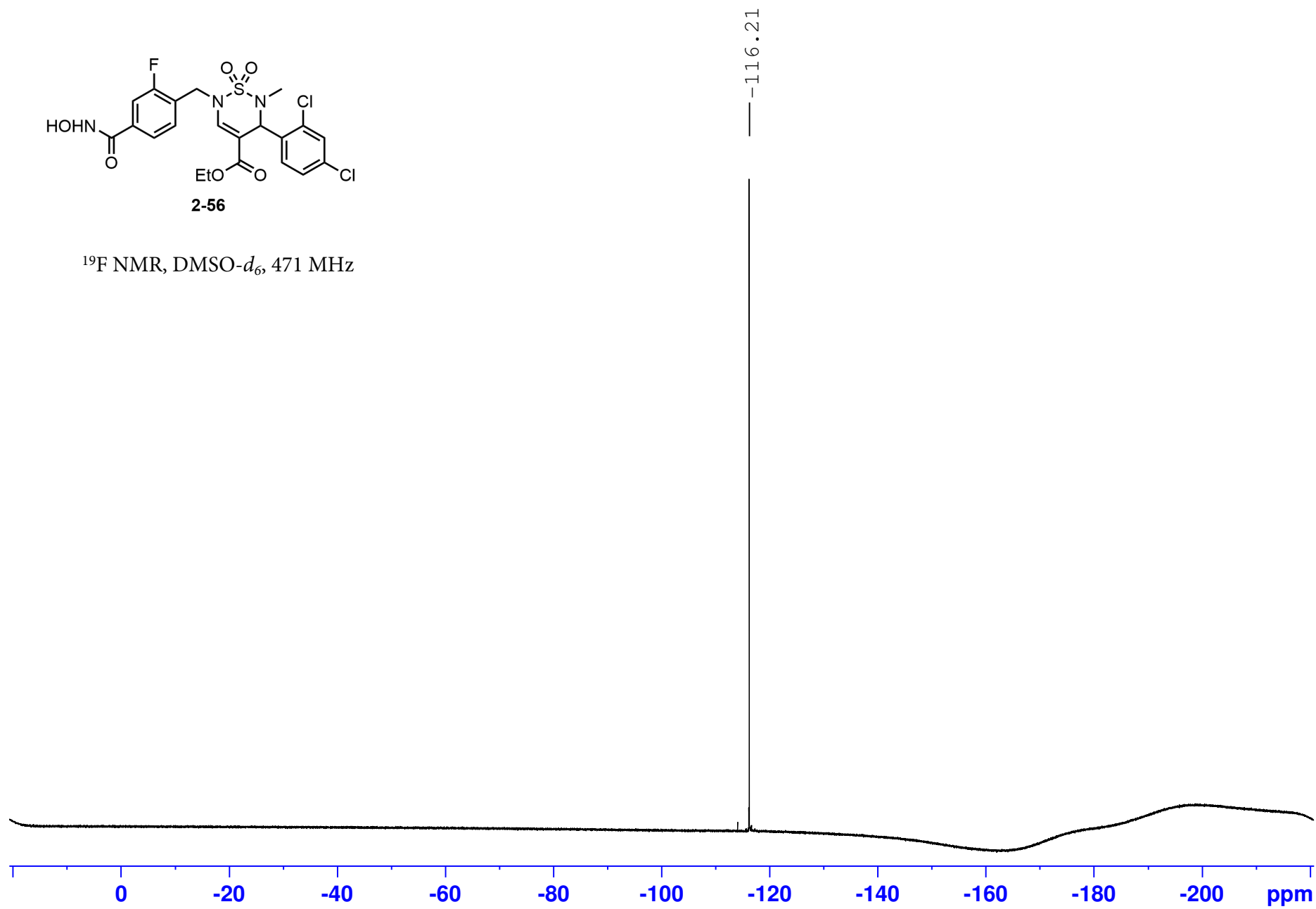


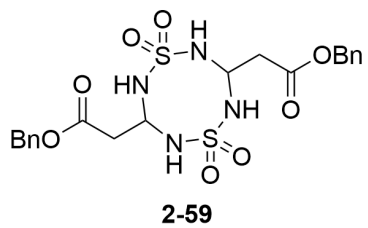
^{13}C NMR, DMSO- d_6 , 126 MHz



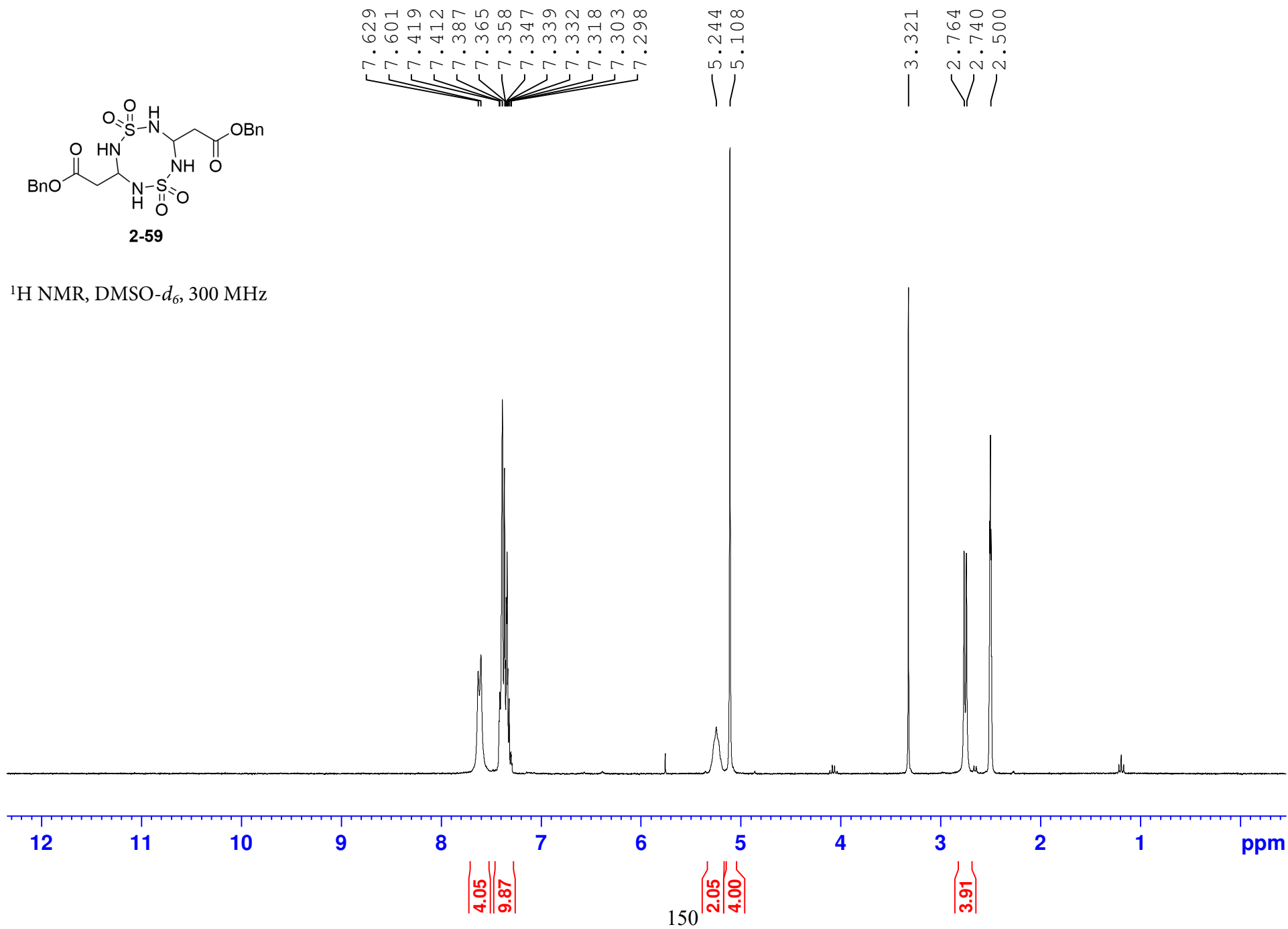


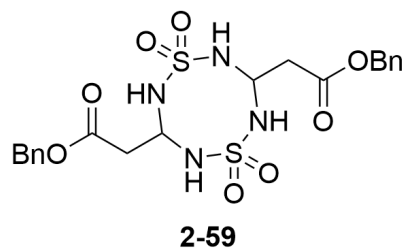
^{19}F NMR, DMSO- d_6 , 471 MHz



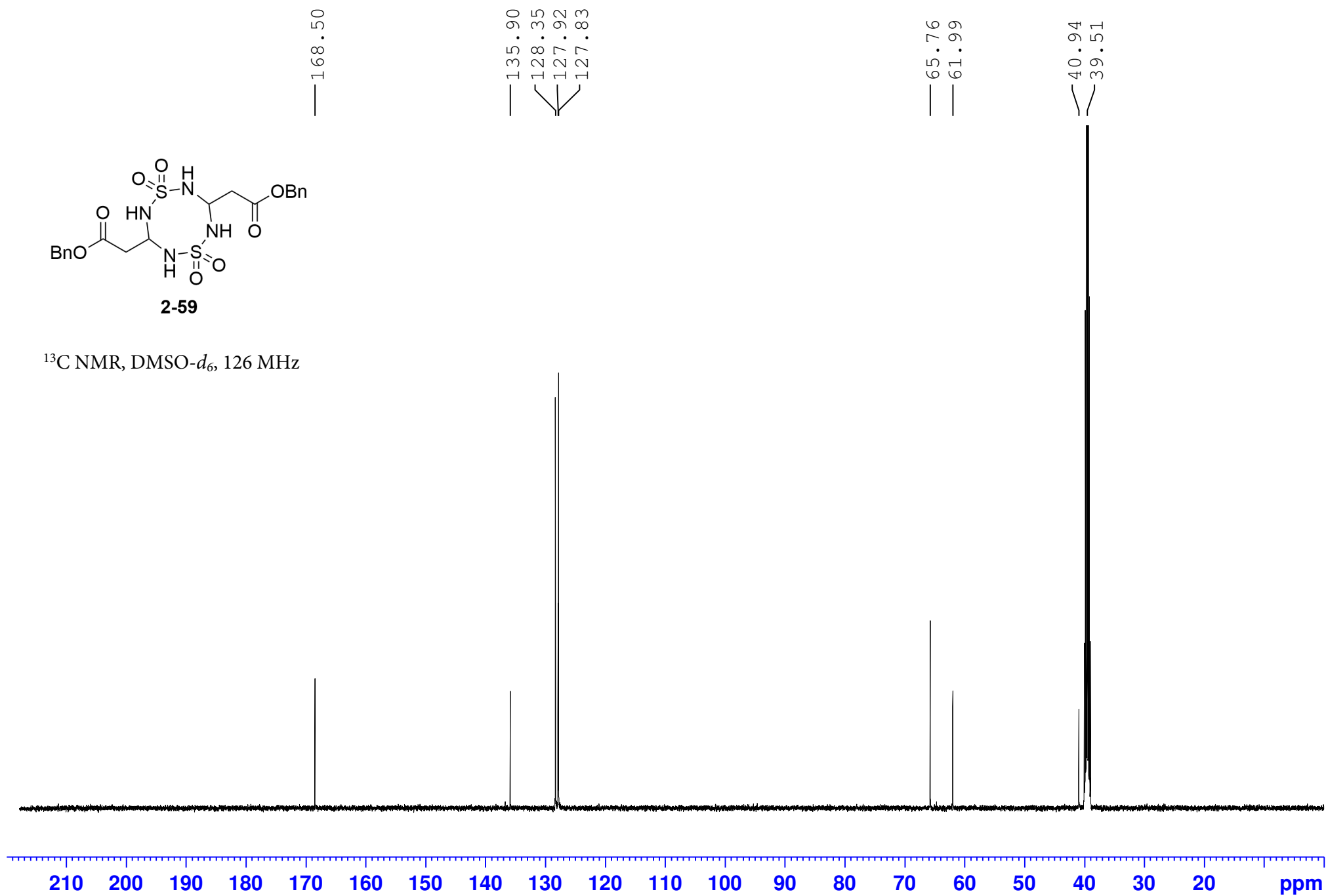


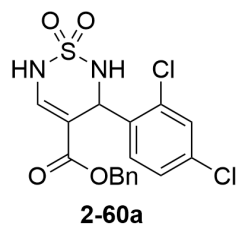
¹H NMR, DMSO-*d*₆, 300 MHz



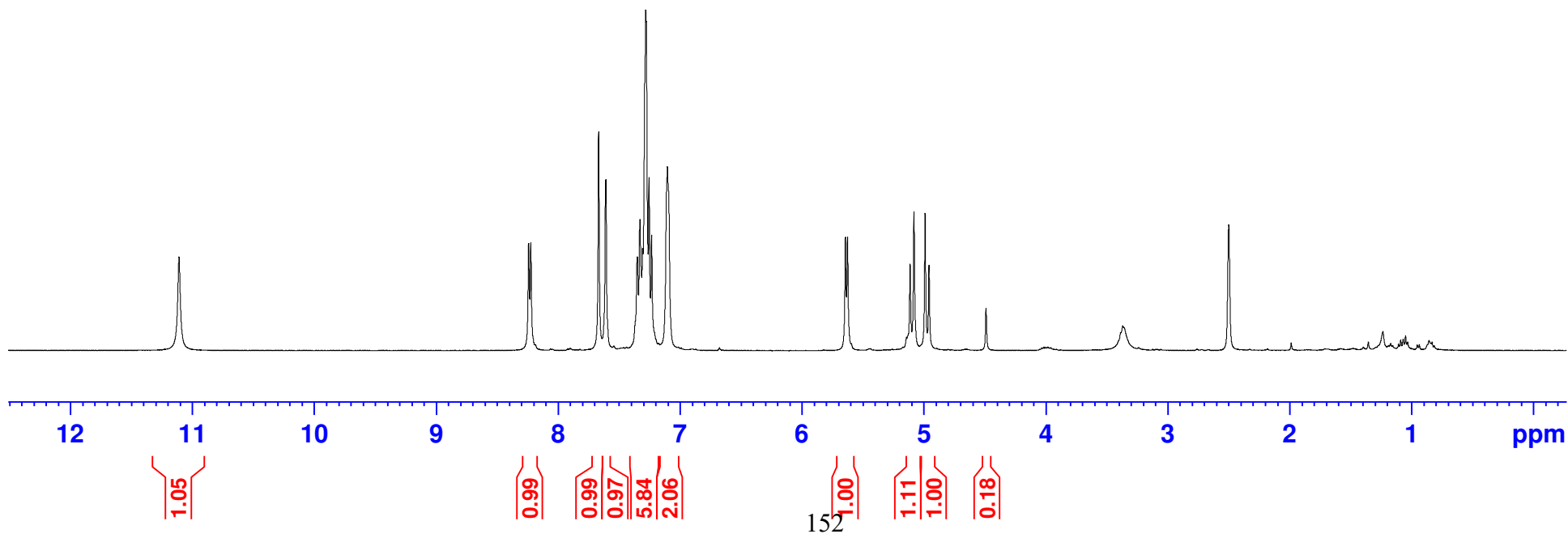


^{13}C NMR, DMSO- d_6 , 126 MHz





$^1\text{H NMR}$, $\text{DMSO-}d_6$, 400 MHz



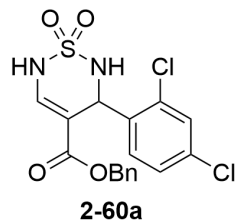
— 11.110

8.242
8.224
7.668
7.609
7.352
7.328
7.307
7.282
7.277
7.254
7.233
7.104

5.644
5.626
5.113
5.081
4.990
4.958
4.490

— 3.370

— 2.499



^{13}C NMR, DMSO- d_6 , 126 MHz

