

2-Cl 4-COOMe

9.07
9.05

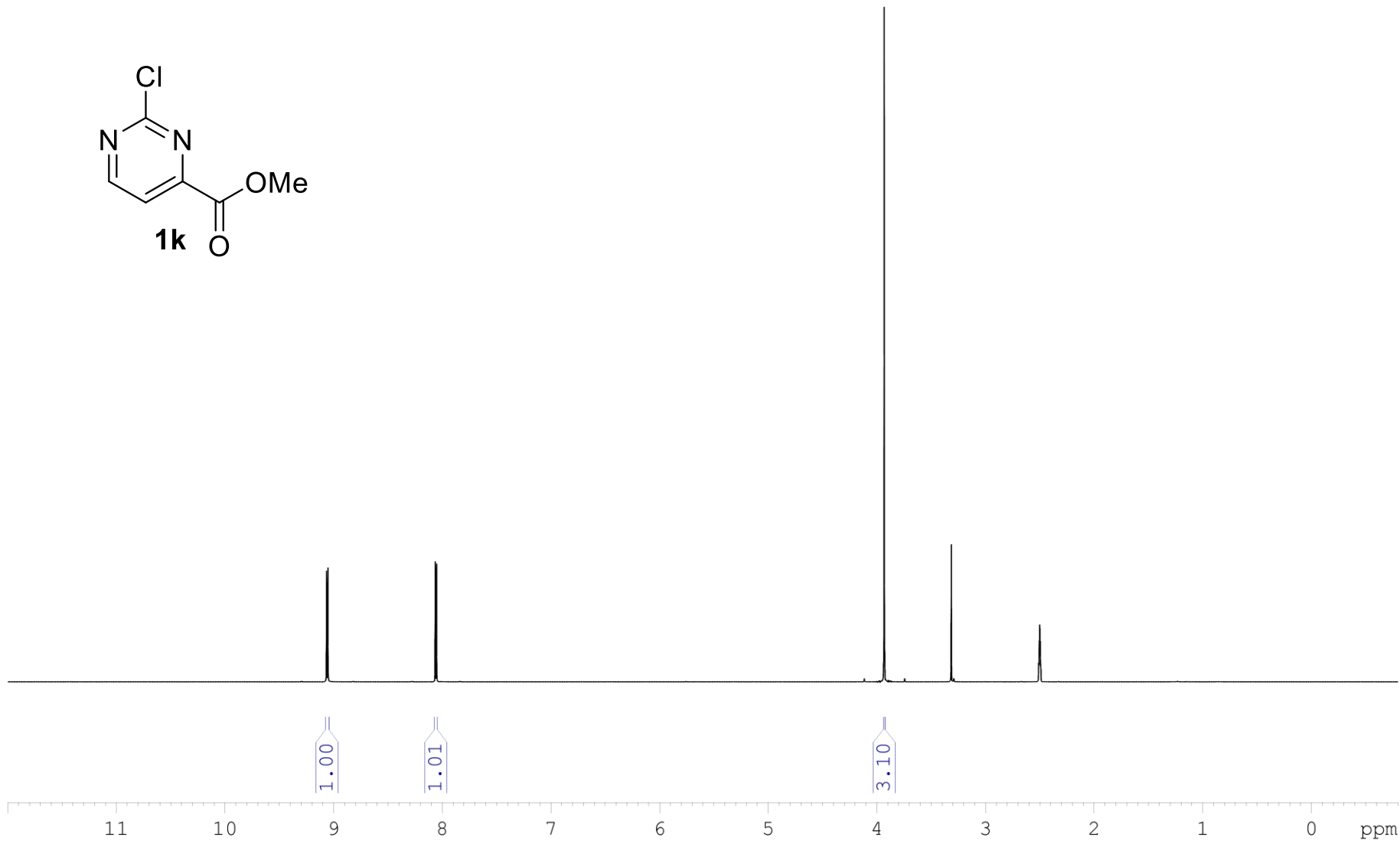
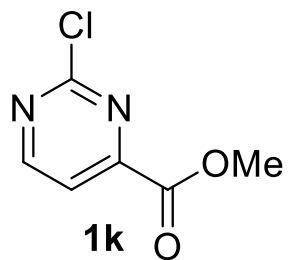
8.07
8.05

1H NMR (400 MHz, DMSO-d6)

3.93

3.31

2.50



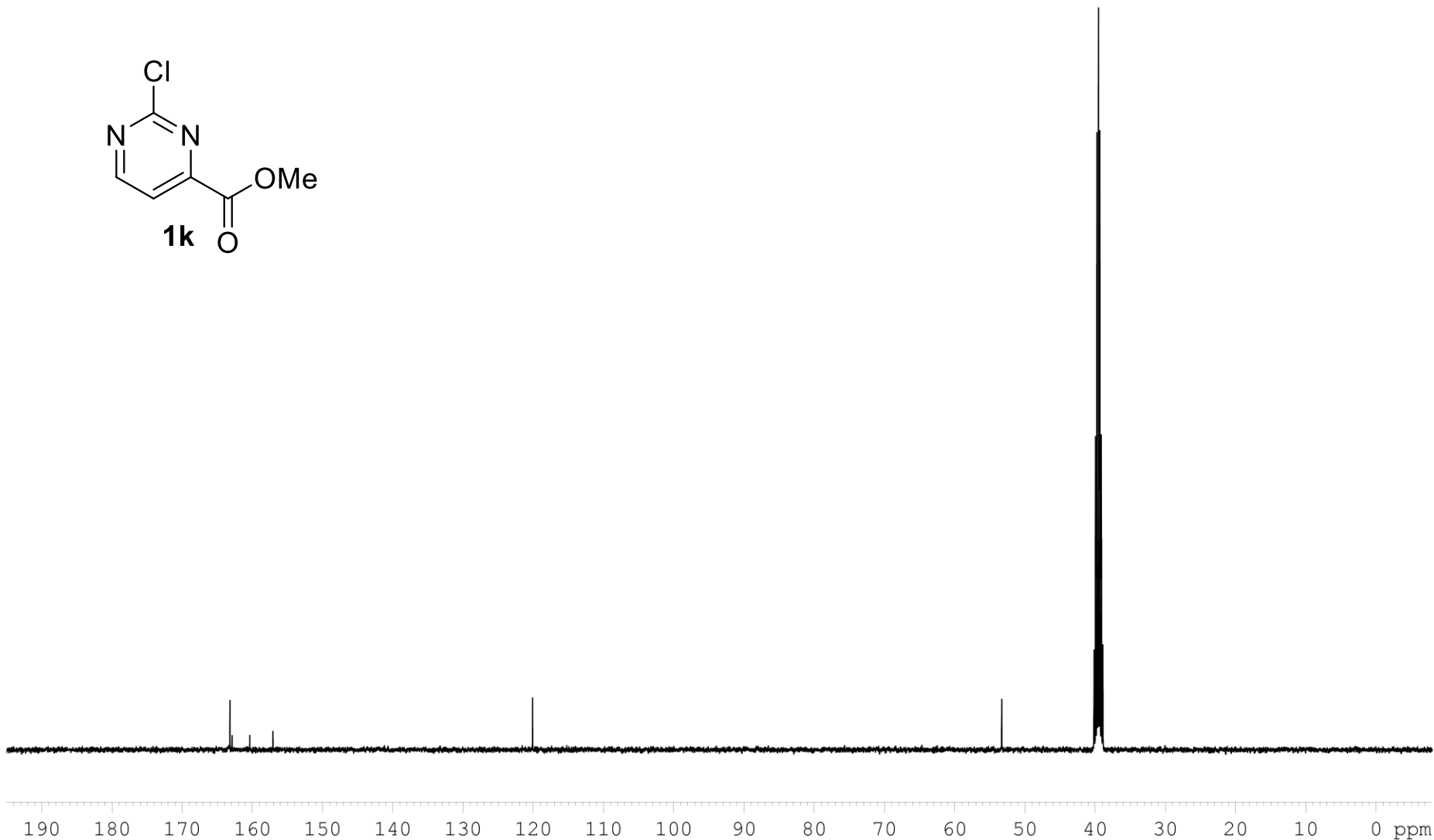
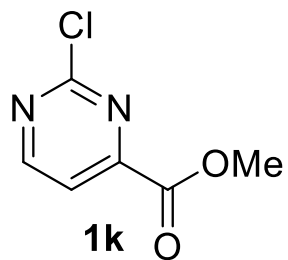
2-Cl 4-COOMe

163.21
162.89
160.37
157.08

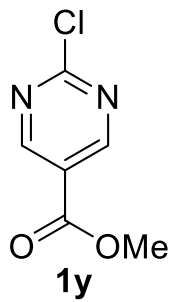
120.09

¹³C NMR (100 MHz, DMSO-d₆)

53.29



2-Cl 5-COOMe
1H NMR (400 MHz, DMSO-d6)

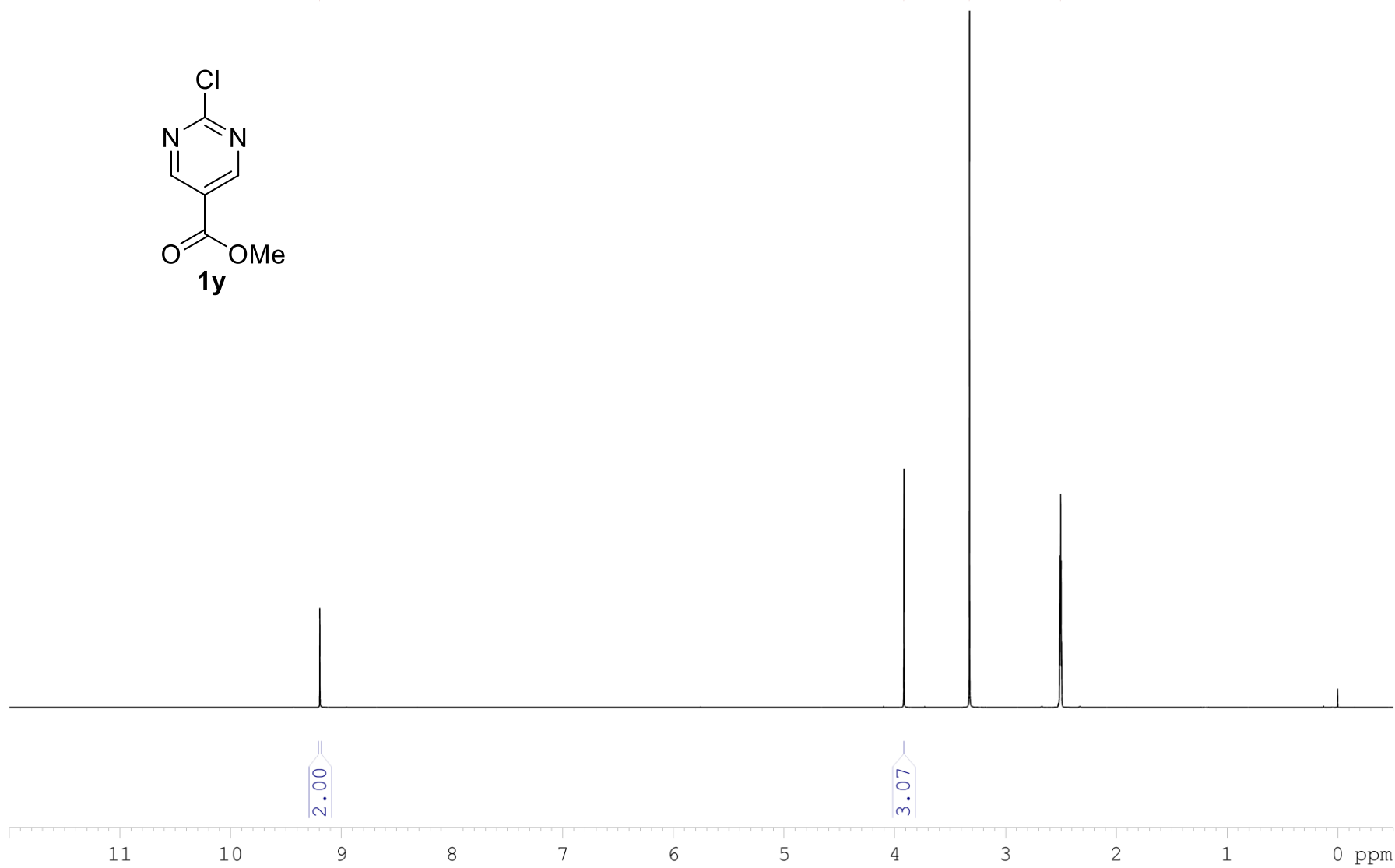


9.19

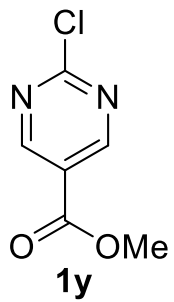
3.92

3.33

2.50



2-Cl 5-COOMe

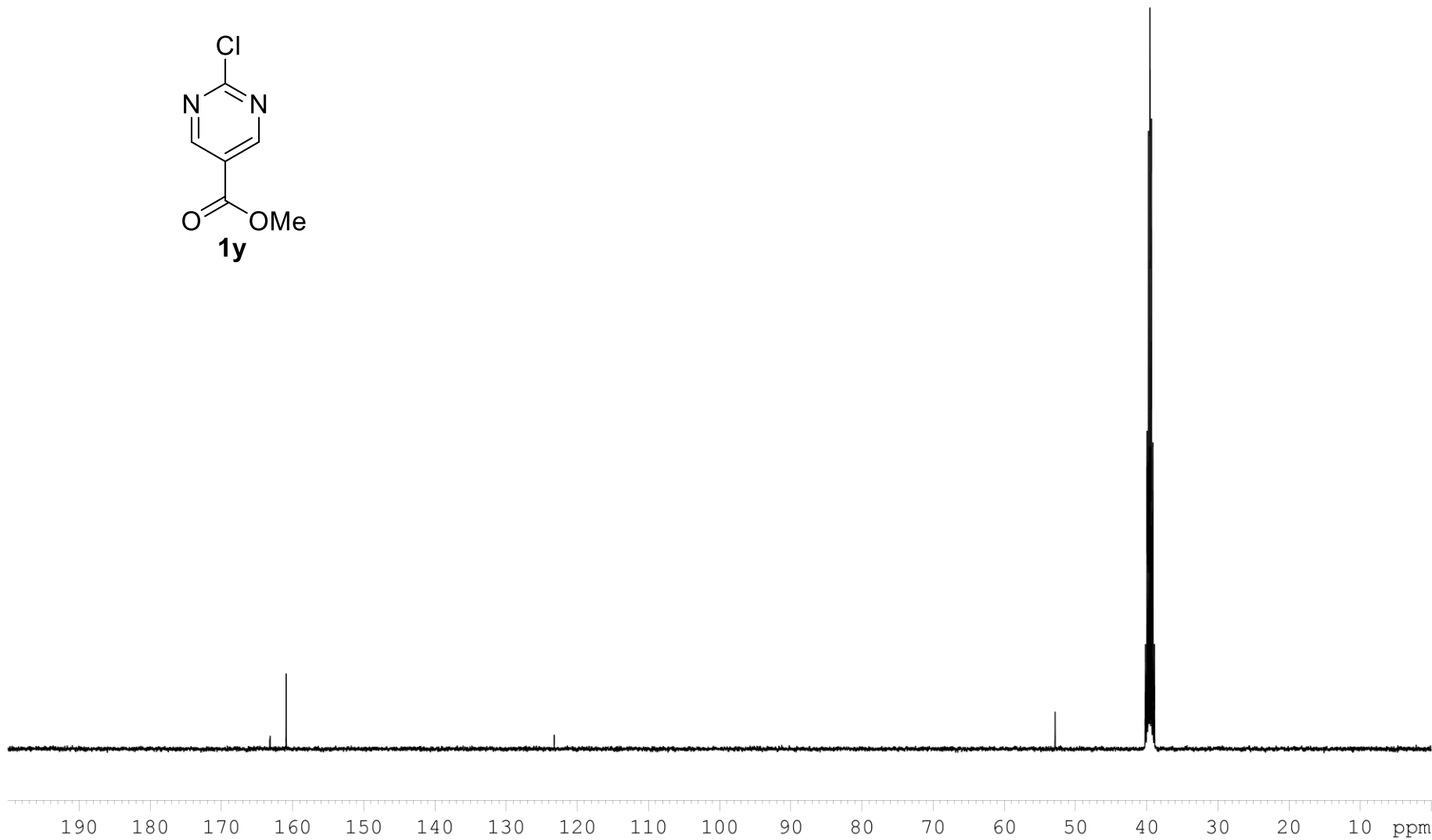


163.20
163.14
160.89

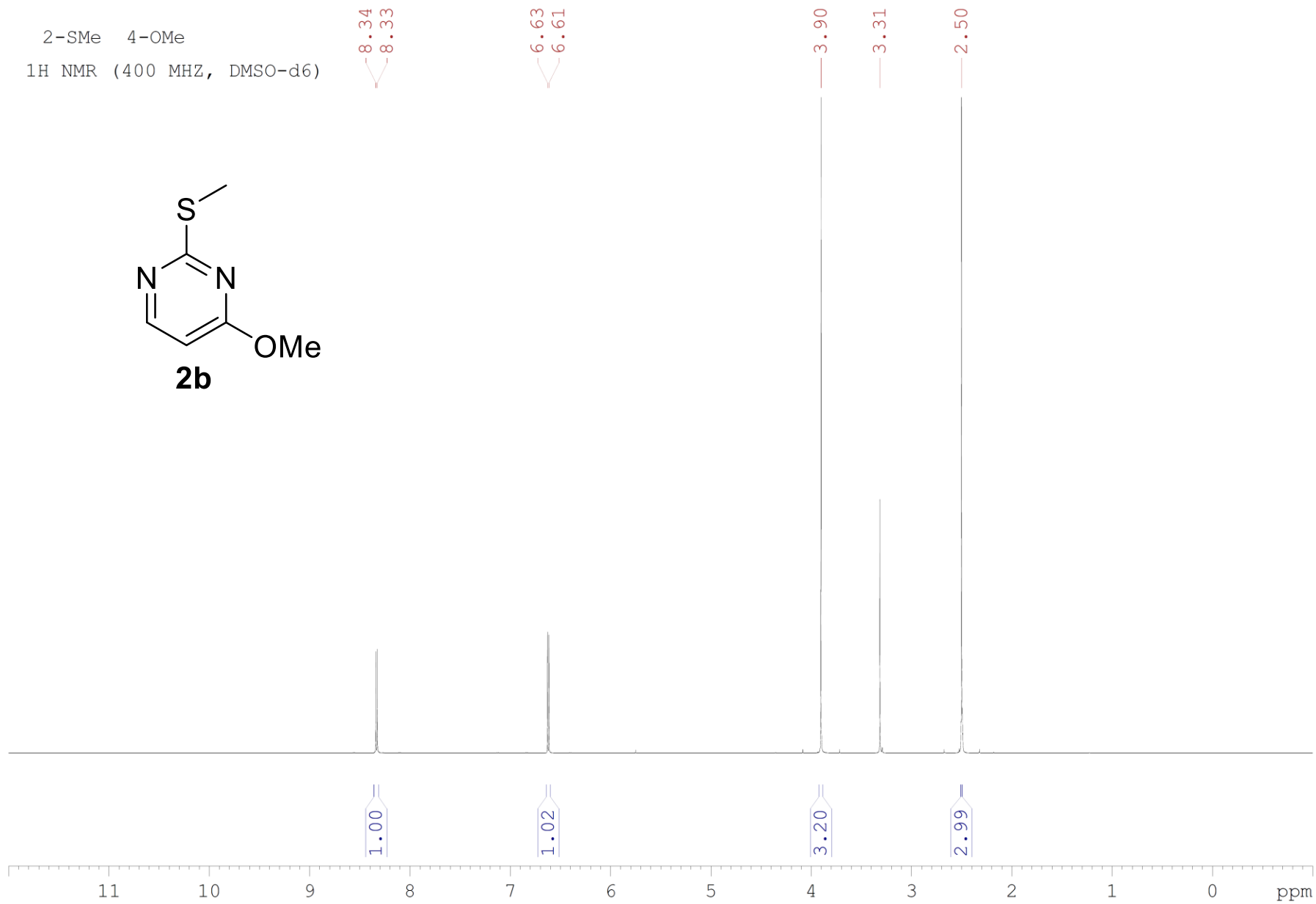
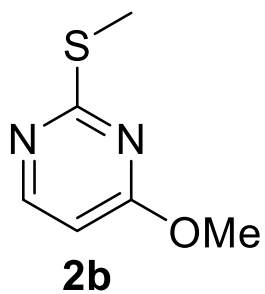
123.24

¹³C NMR (100 MHz, DMSO-d₆)

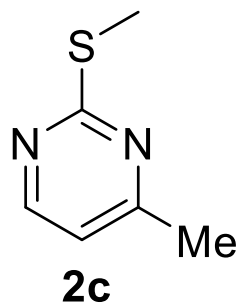
52.85



2-SMe 4-OMe
1H NMR (400 MHz, DMSO-d6)



2-SMe 4-Me
1H NMR (400 MHz, DMSO-d6)



8.48
8.46

7.08
7.07

3.32

2.48
2.40



2-SMe 4-COOH

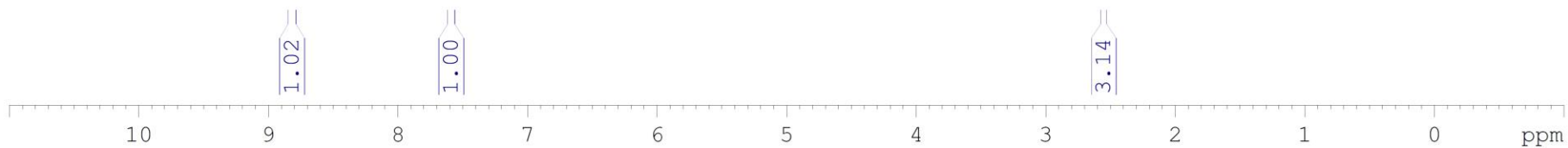
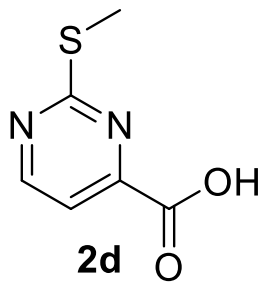
8.82
8.81

7.59
7.58

¹H NMR (400 MHz, DMSO-d₆)

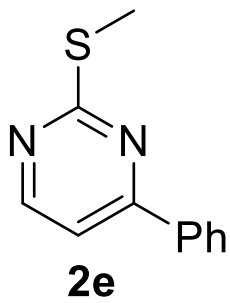
3.39

2.55



2-SMe 4-Ph

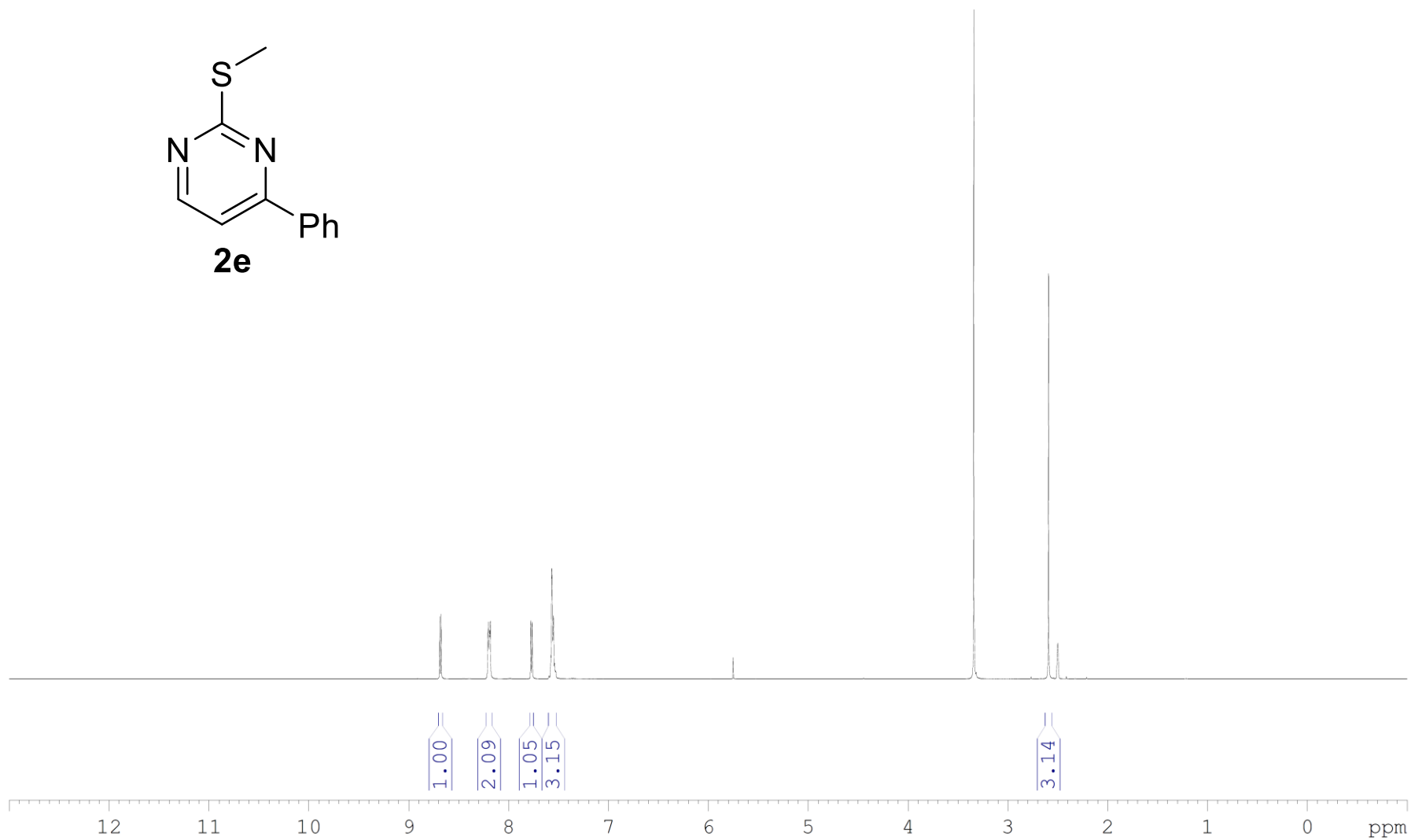
¹H NMR (400 MHz, DMSO-d₆)



8.69
8.67
8.21
8.20
8.19
8.18
7.78
7.76
7.57
7.56
7.55

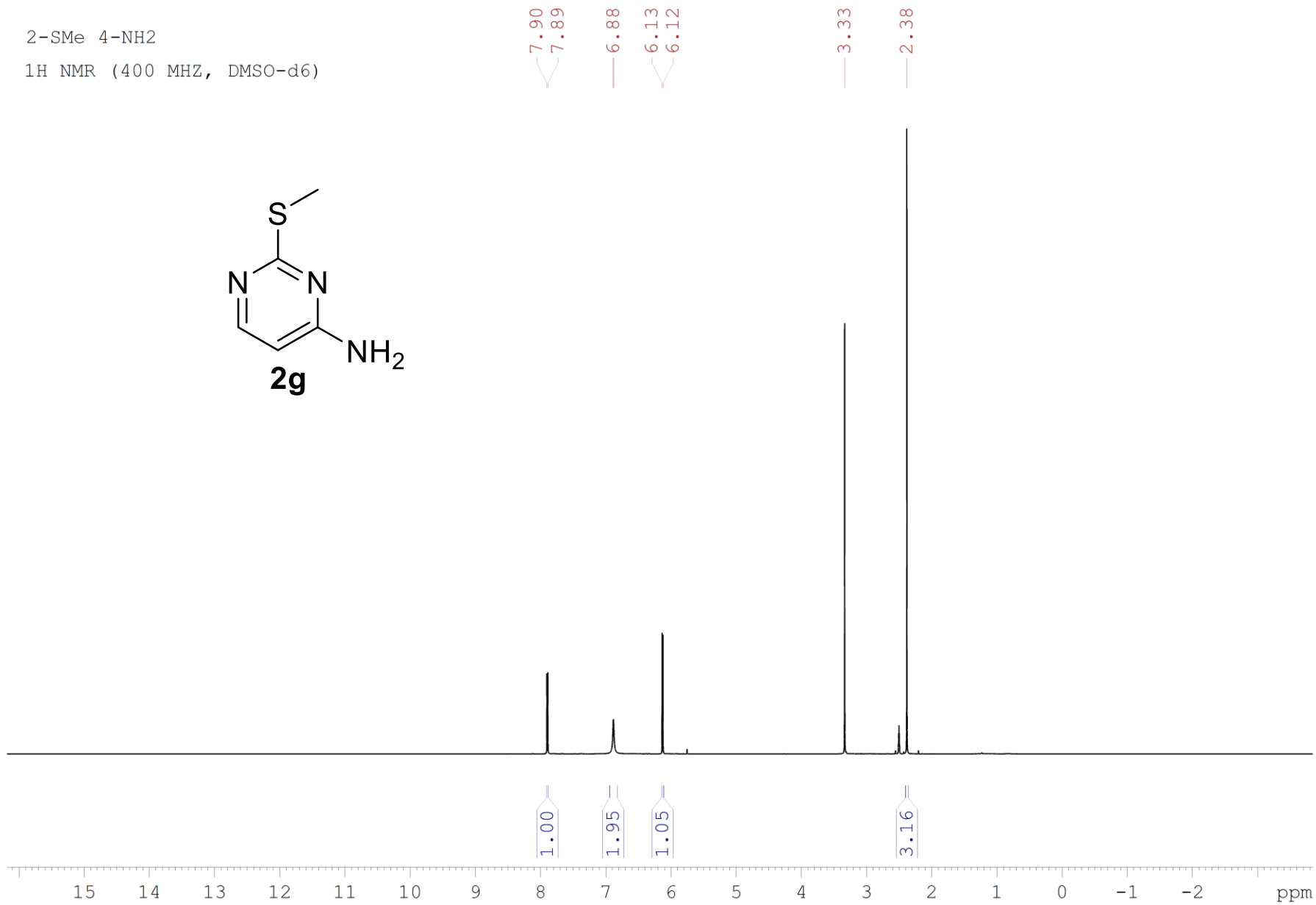
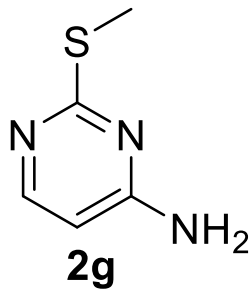
3.34

2.59

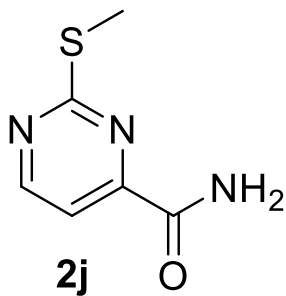


2-SMe 4-NH₂

¹H NMR (400 MHz, DMSO-d₆)



2-SMe 4-C(O)NH₂



¹H NMR (400 MHz, DMSO-d₆)

8.84
8.83

8.20
7.95
7.65
7.64

3.34

2.60

1.00

0.81

0.88

1.04

3.22



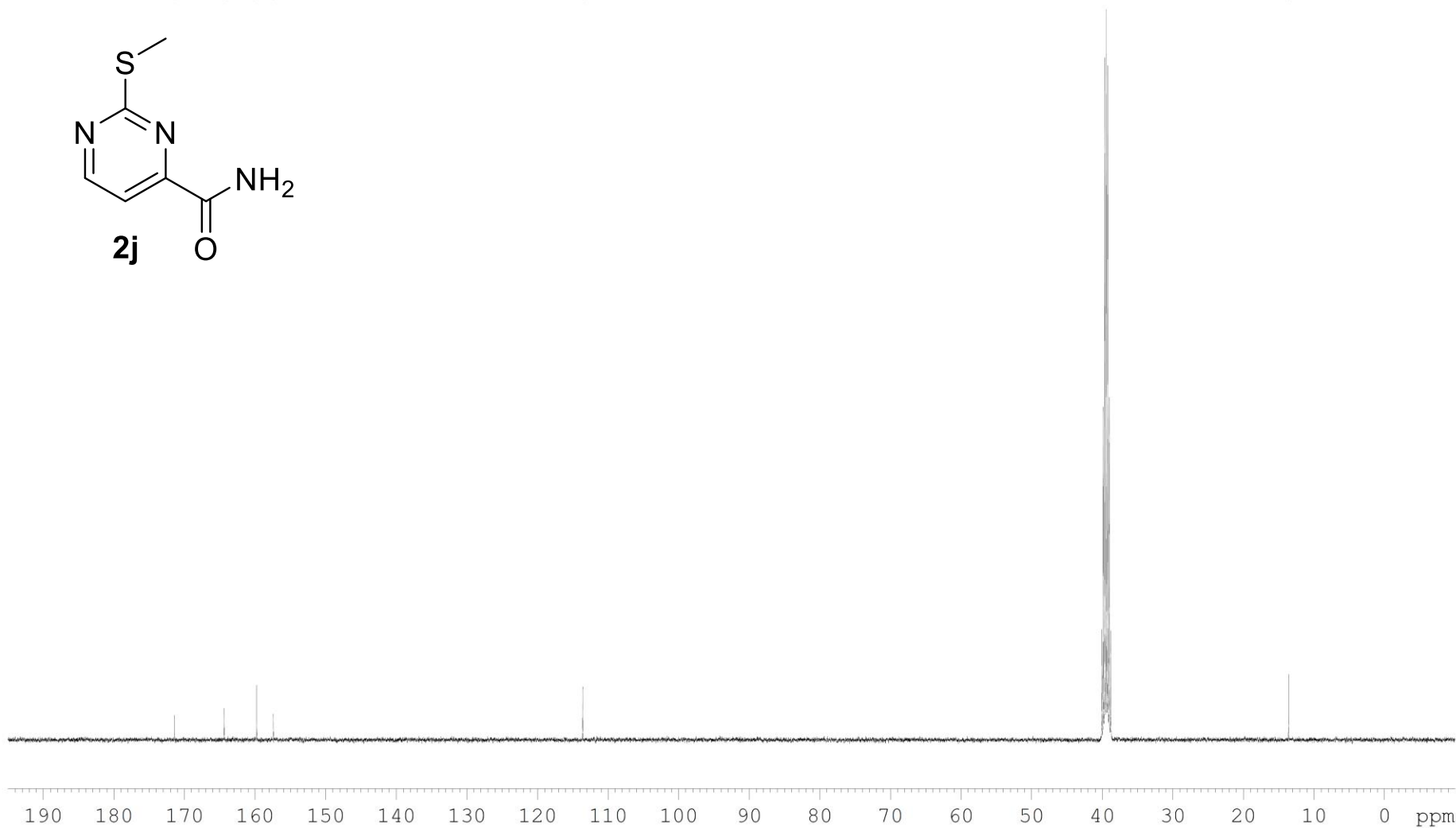
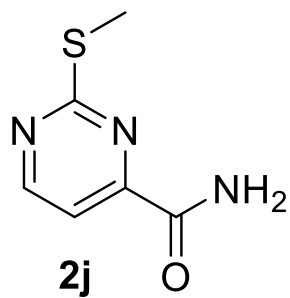
2-SMe 4-C(O)NH₂

¹³C NMR (100 MHz, DMSO-d₆)

— 171.40
— 164.36
— 159.78
— 157.41

— 113.58

— 13.58



2-SMe 4-COOMe

8.91
8.90

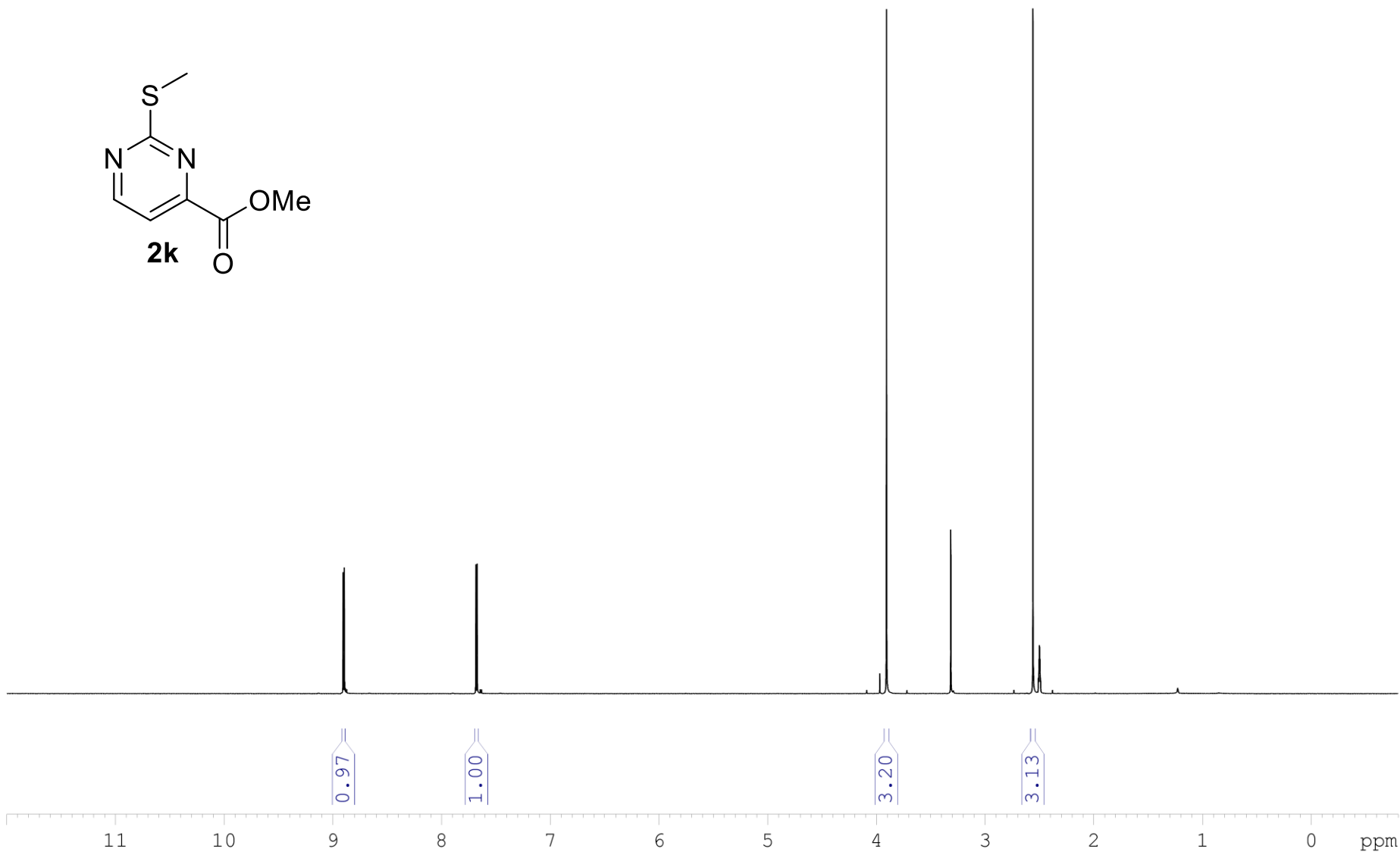
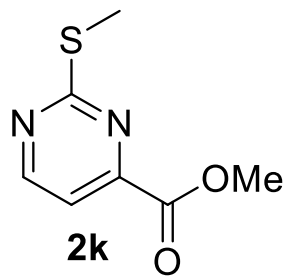
7.69
7.67

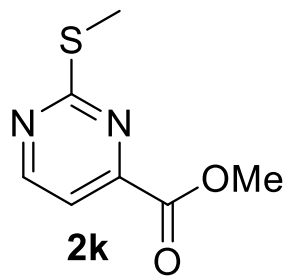
¹H NMR (400 MHz, DMSO-d₆)

3.91

3.32

2.56





2-SMe 4-COOMe
13C NMR (100 MHz, DMSO-d6)

— 172.37

— 163.89

— 160.15

— 154.69

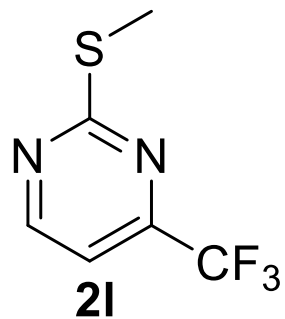
— 116.02

— 53.06

— 13.61

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

2-SMe 4-CF₃
1H NMR (400 MHz, DMSO-d₆)

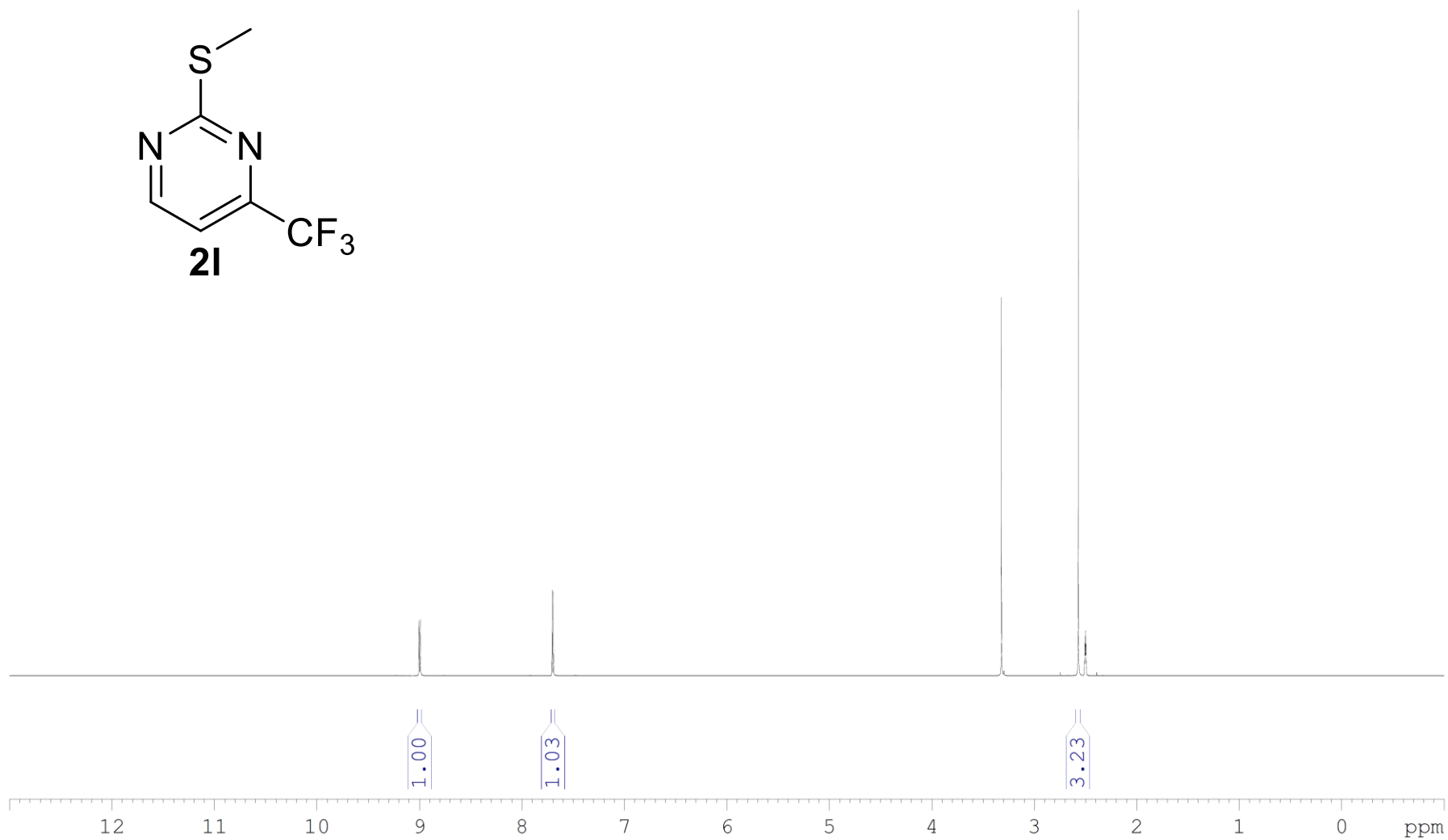


9.00
8.99

7.70
7.69

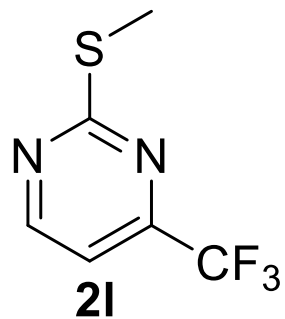
3.32

2.57

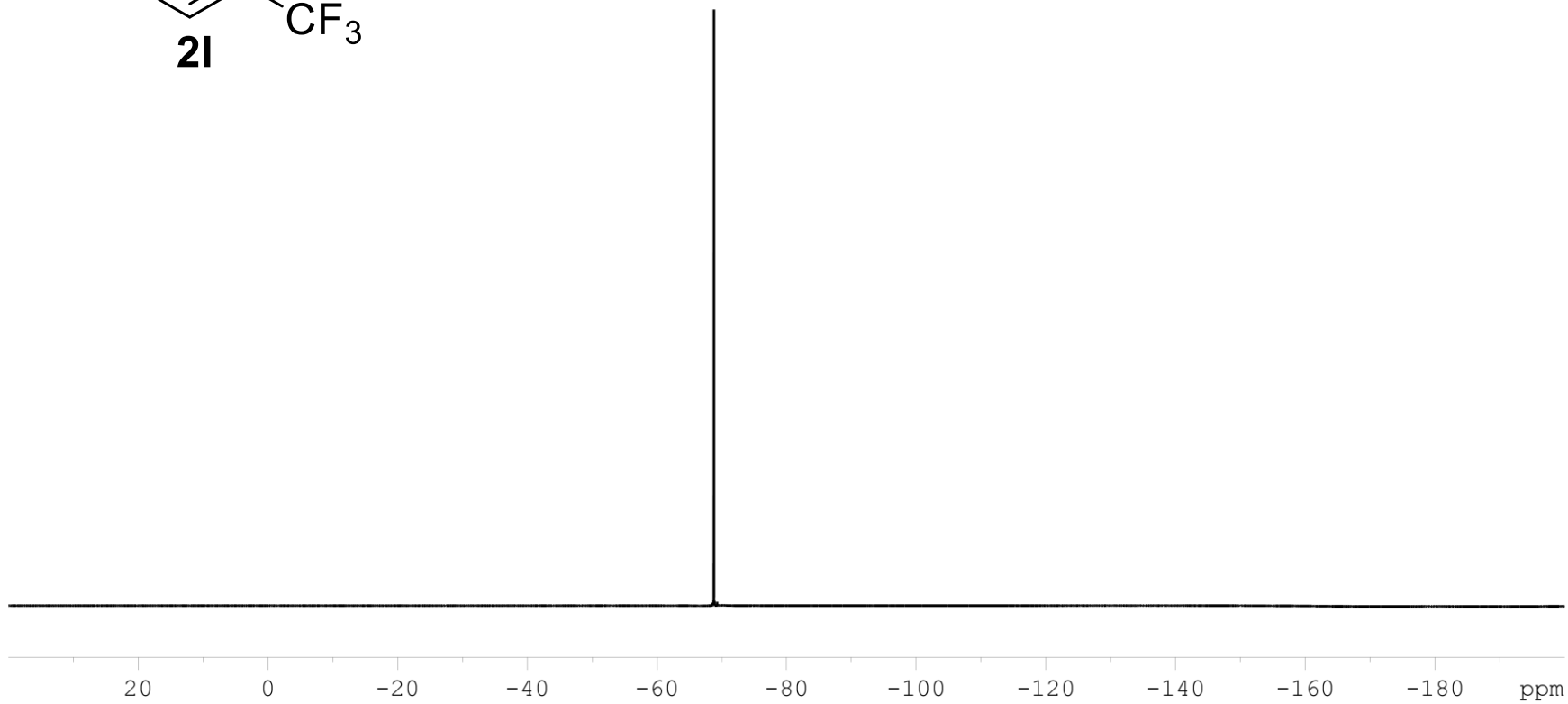


2-SMe 4-CF₃

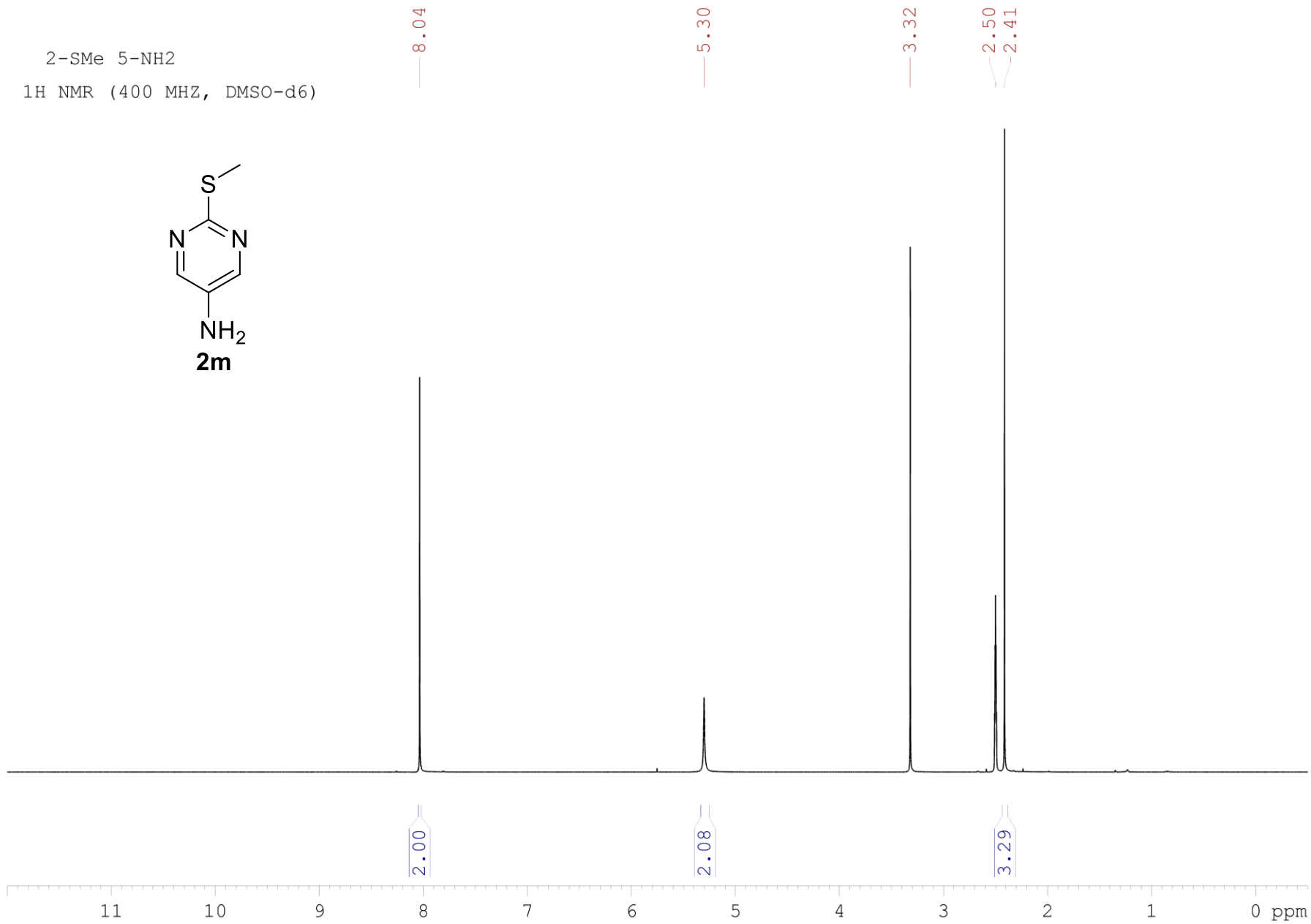
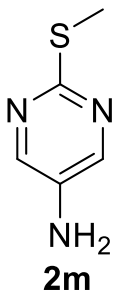
¹⁹F NMR (376 MHz, DMSO-d₆)



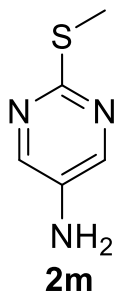
---68.811



2-SMe 5-NH2
1H NMR (400 MHz, DMSO-d6)



2-SMe 5-NH2



¹³C NMR (100 MHz, DMSO-d₆)

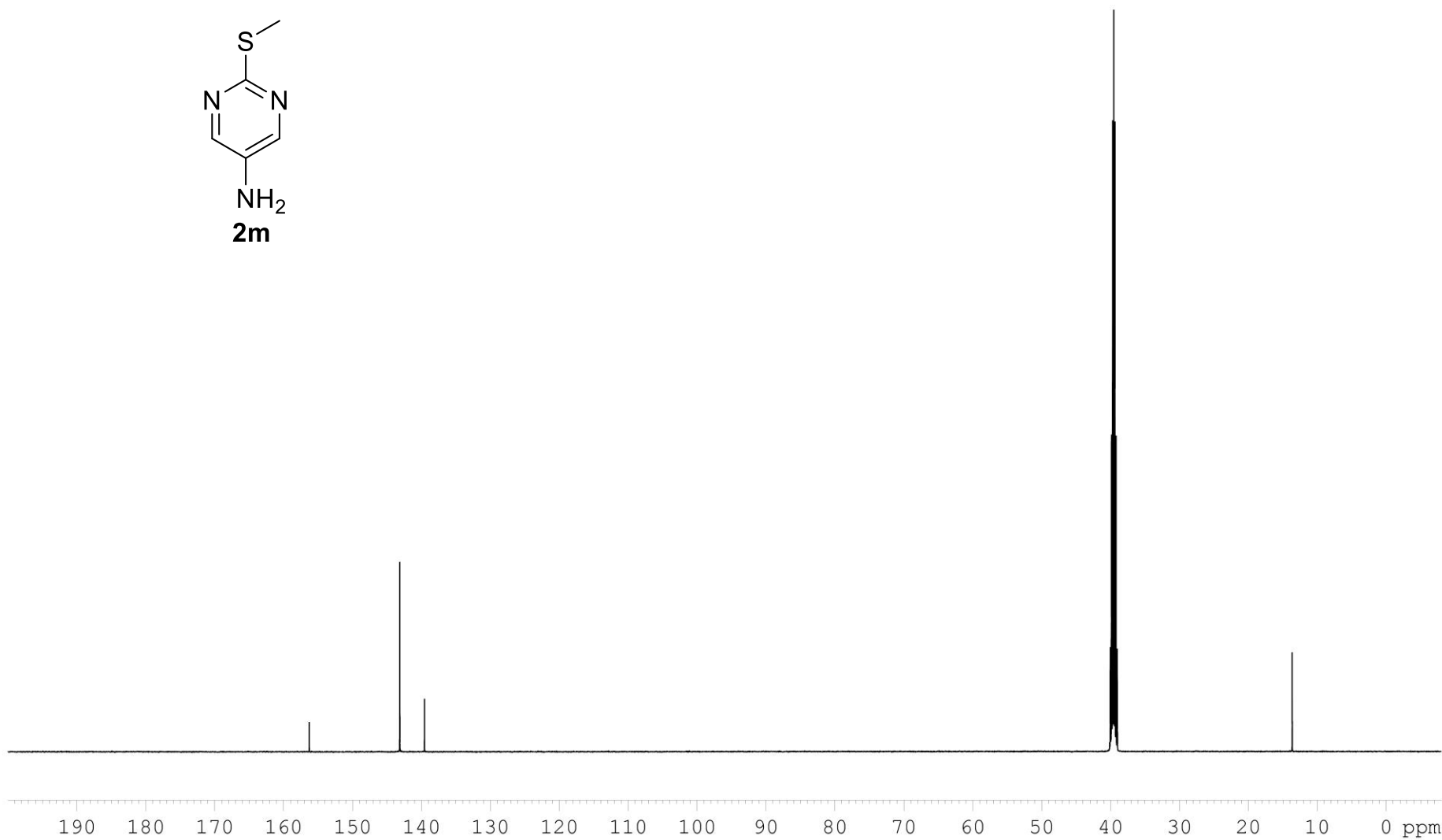
— 156.27

— 143.13

— 139.54

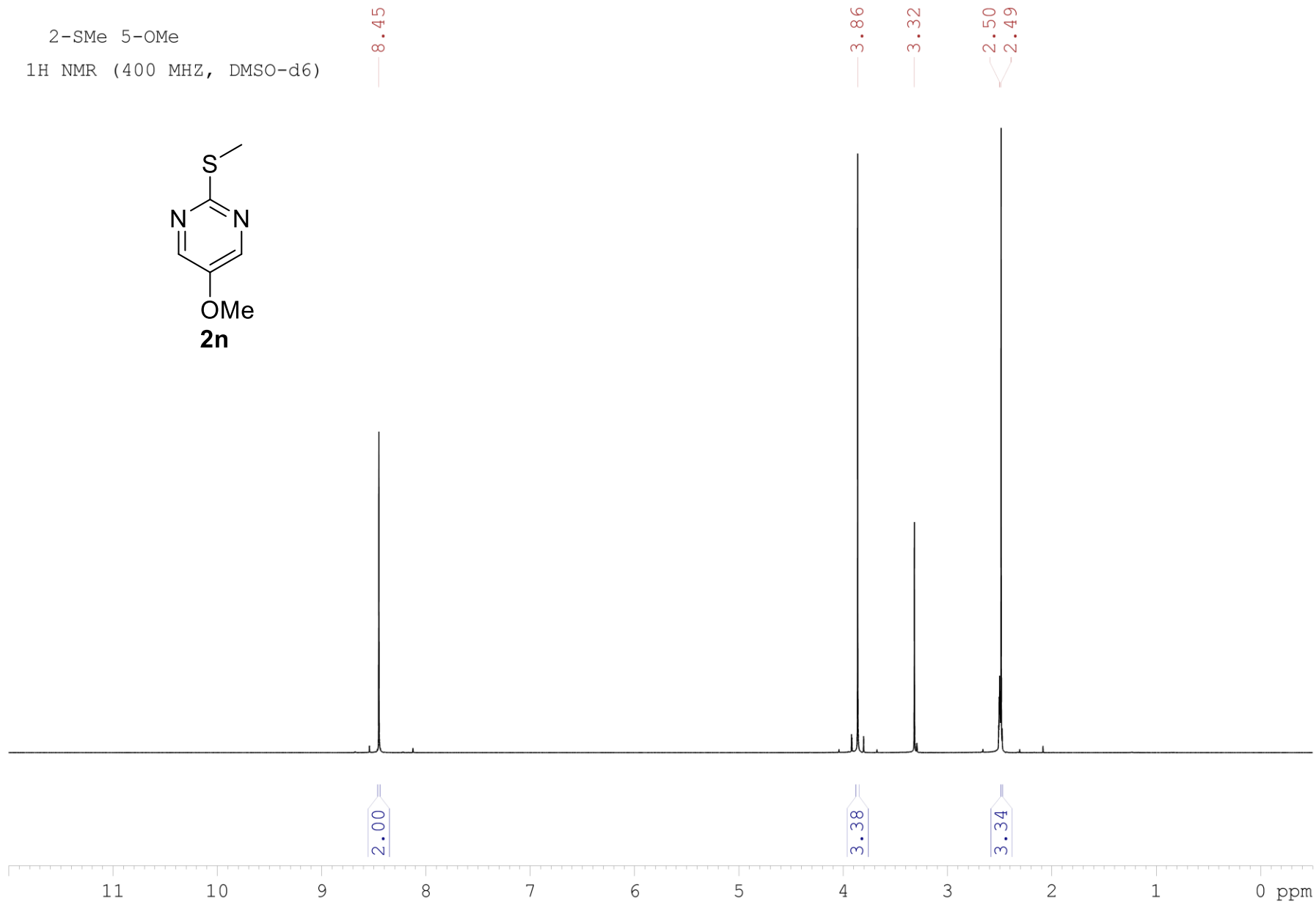
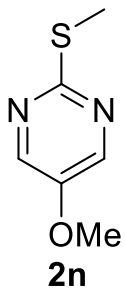
— 39.52

— 13.63



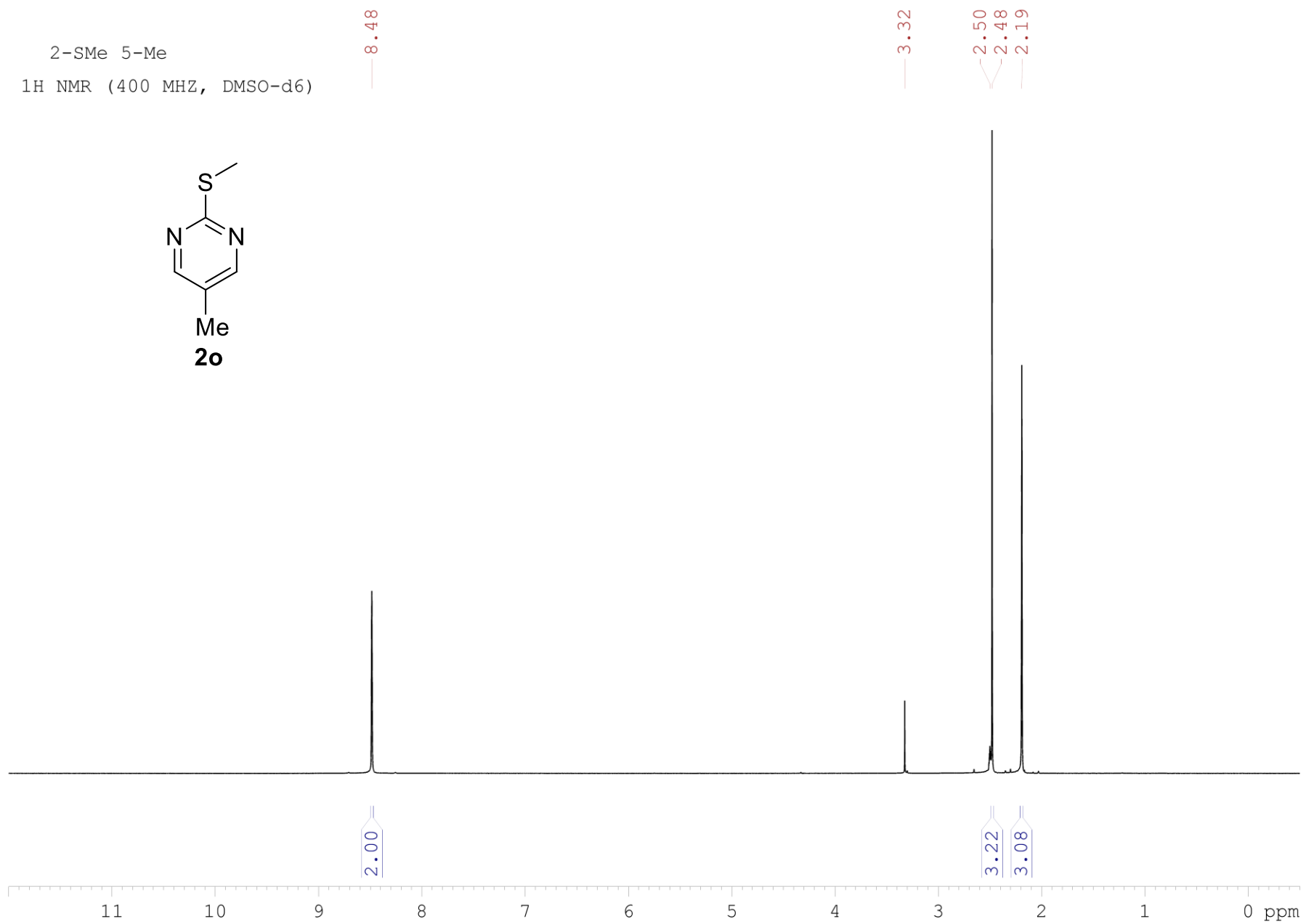
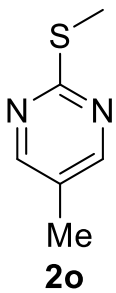
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

2-SMe 5-OMe
1H NMR (400 MHz, DMSO-d6)



2-SMe 5-Me

¹H NMR (400 MHz, DMSO-d₆)



2-SMe 5-Me

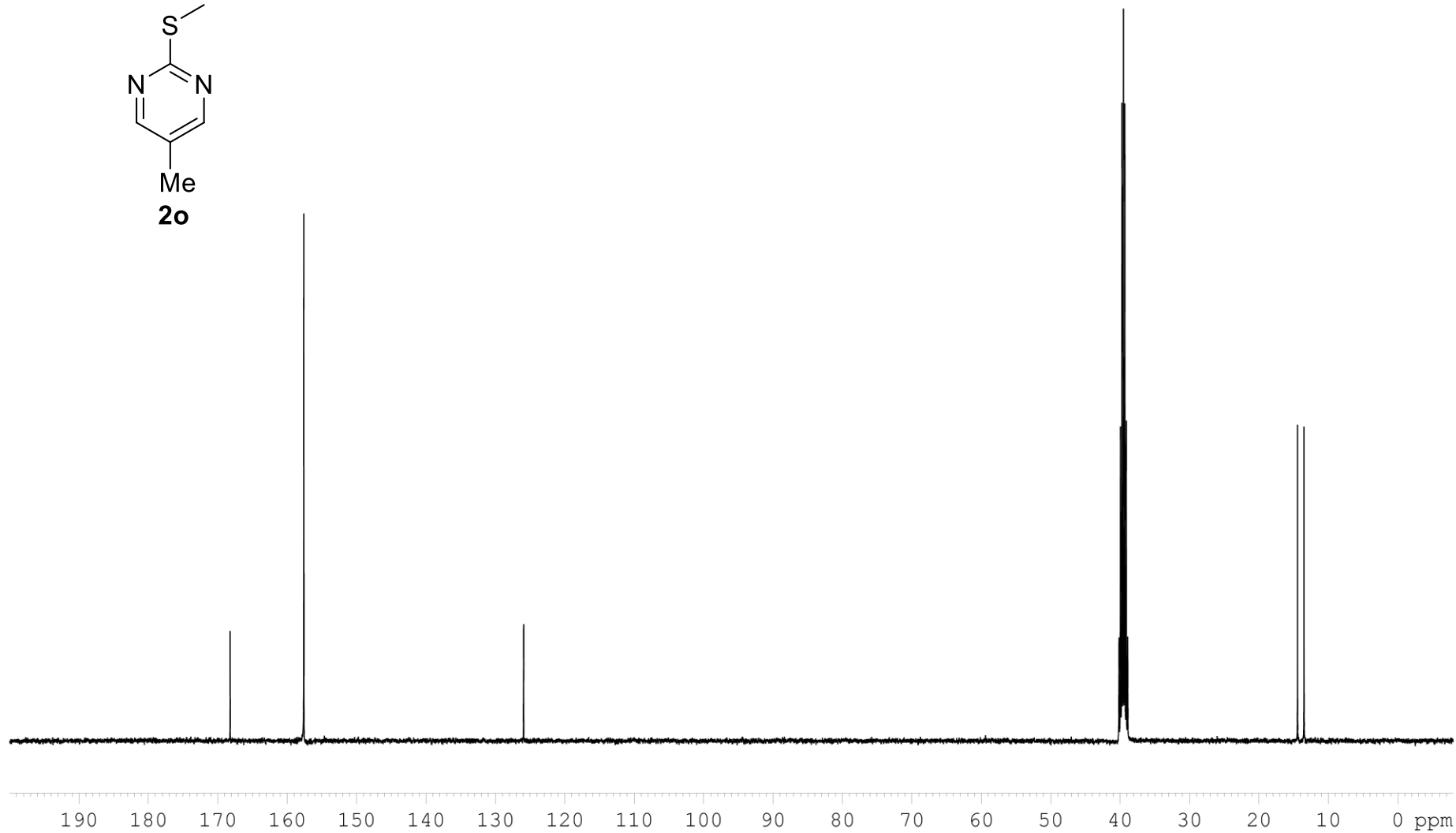
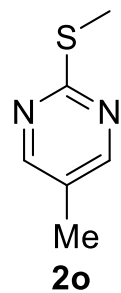
— 168.21

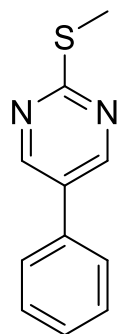
— 157.59

— 125.93

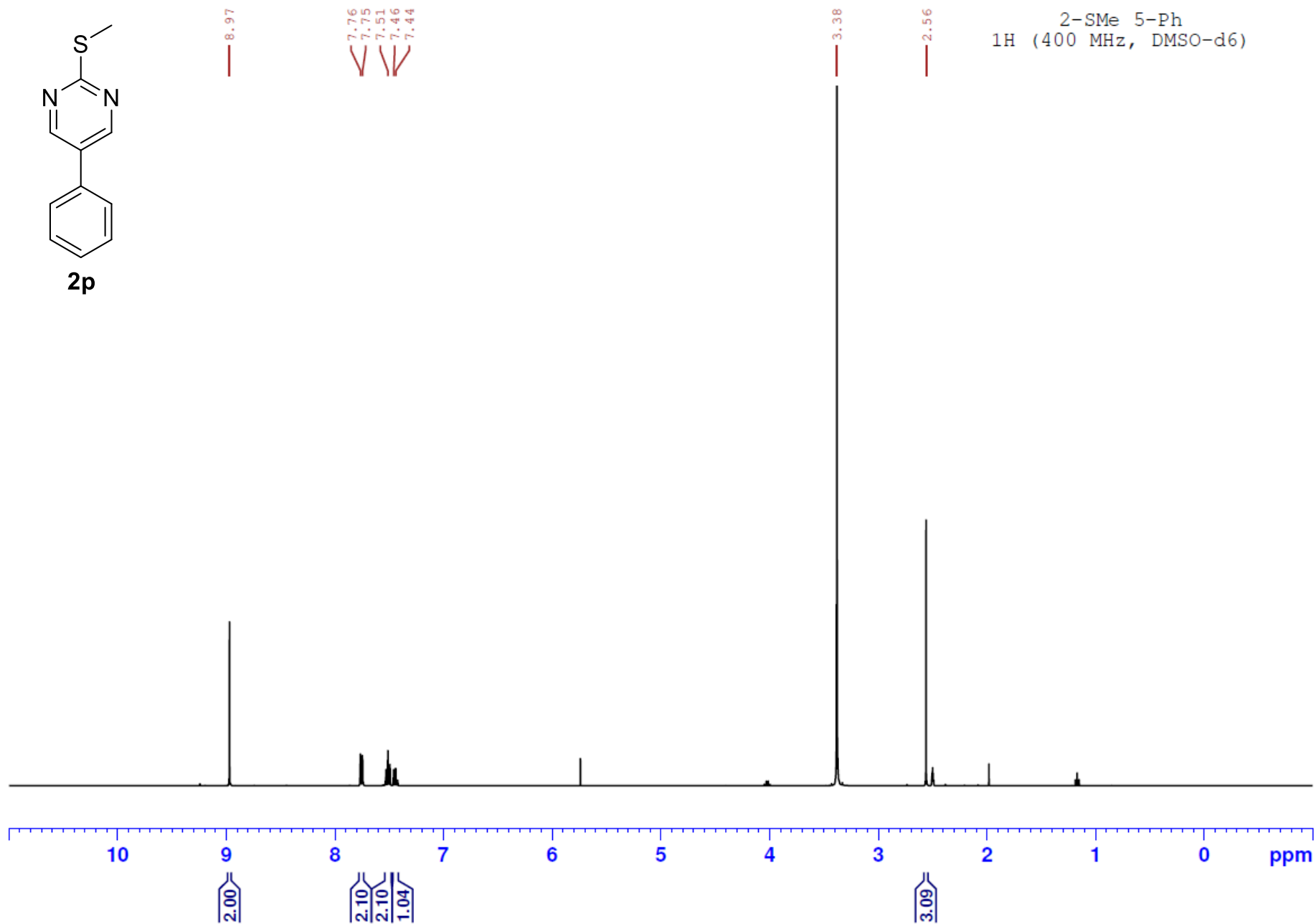
^{13}C NMR (100 MHz, DMSO-d₆)

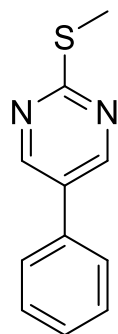
— 14.43
— 13.49





2p





2p

170.24

155.31

133.72

129.29

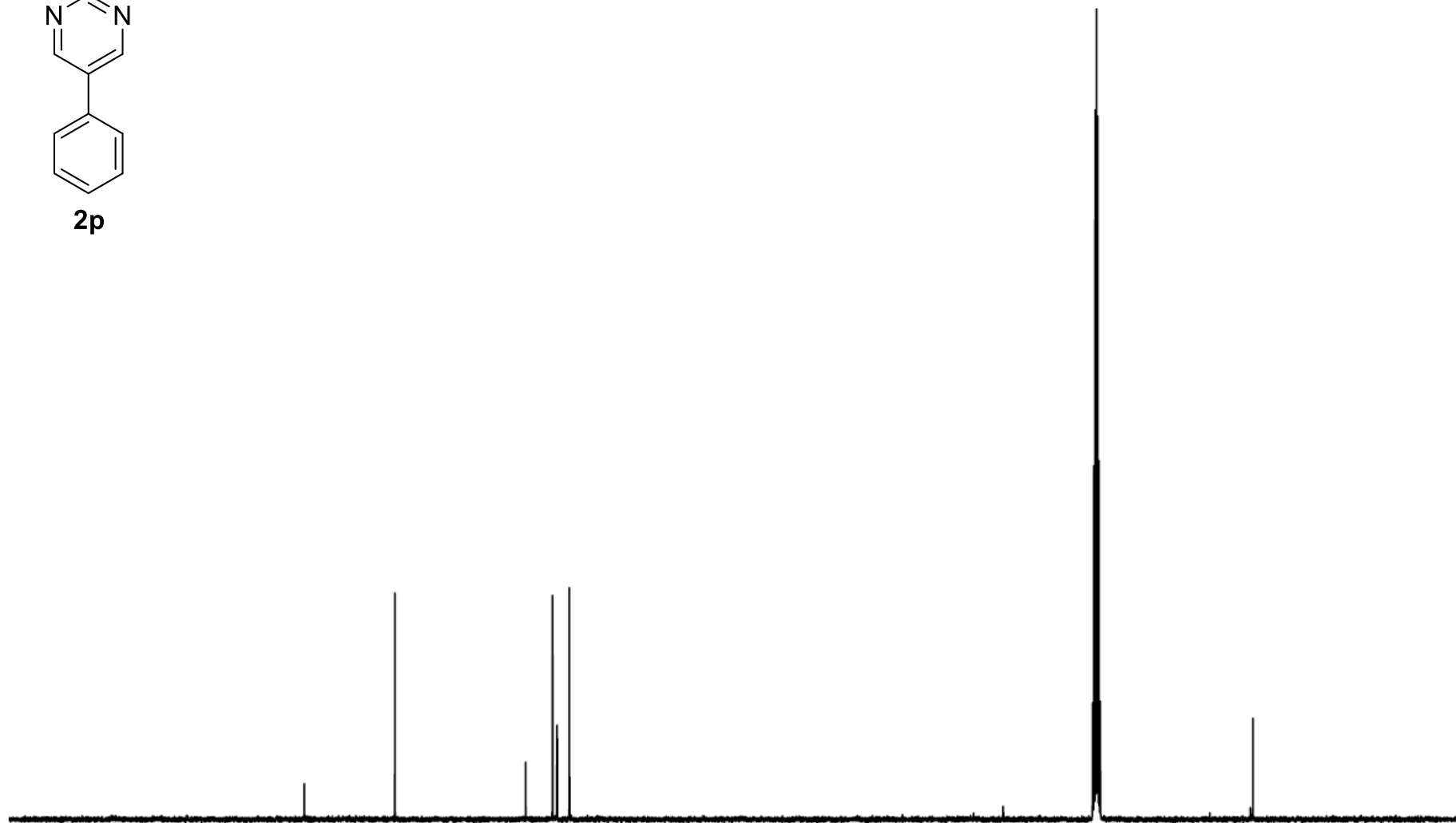
128.62

128.55

126.53

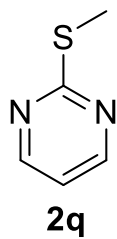
2-SMe 5-Ph
13C (100 MHz, DMSO-d6)

13.69

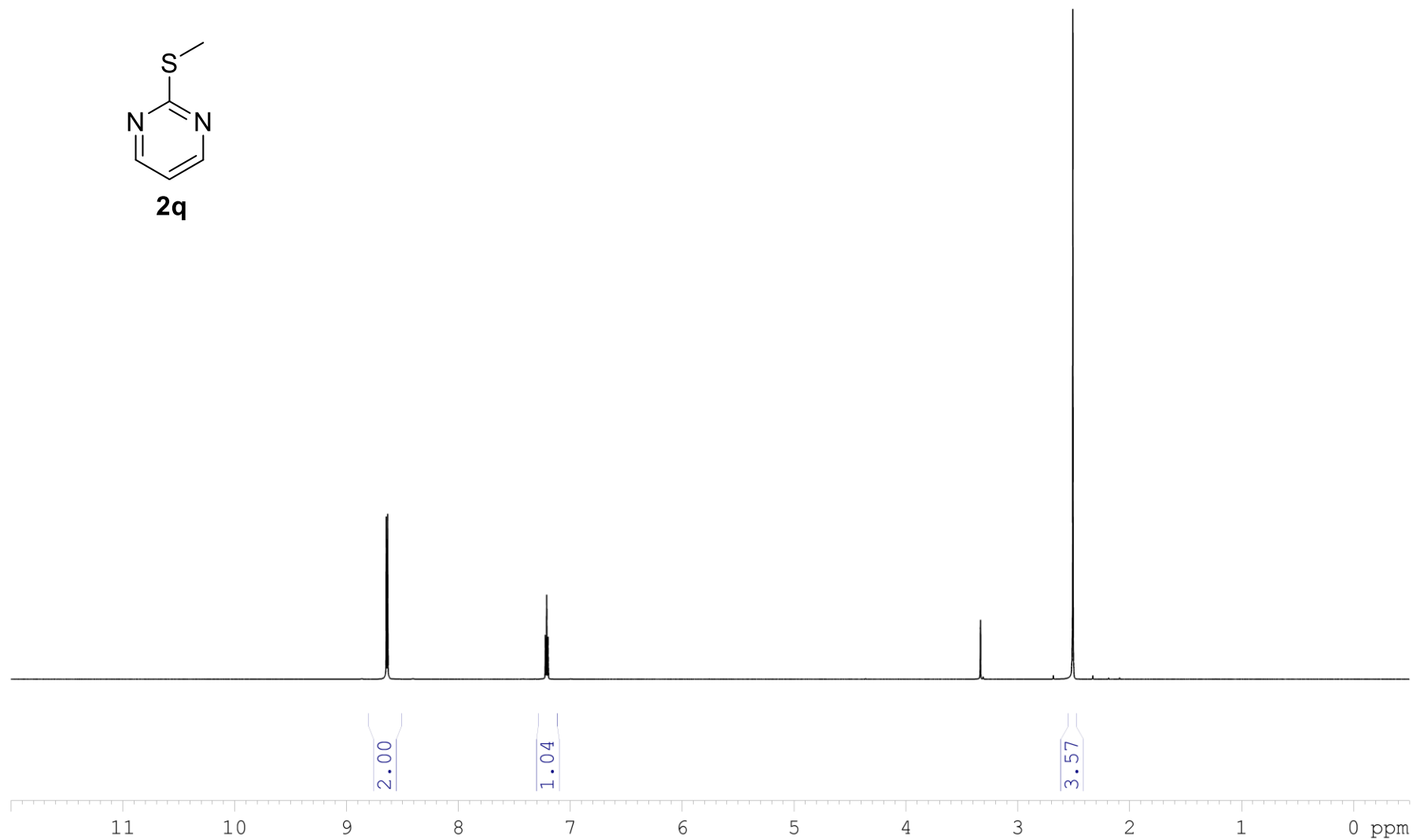


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

2-SMe pyrimidine ref
1H NMR (400 MHz, DMSO-d6)

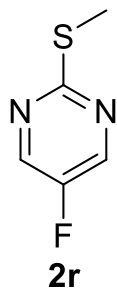


8.64
8.63
7.22
7.21
7.20
2.51



2-SMe 5-F

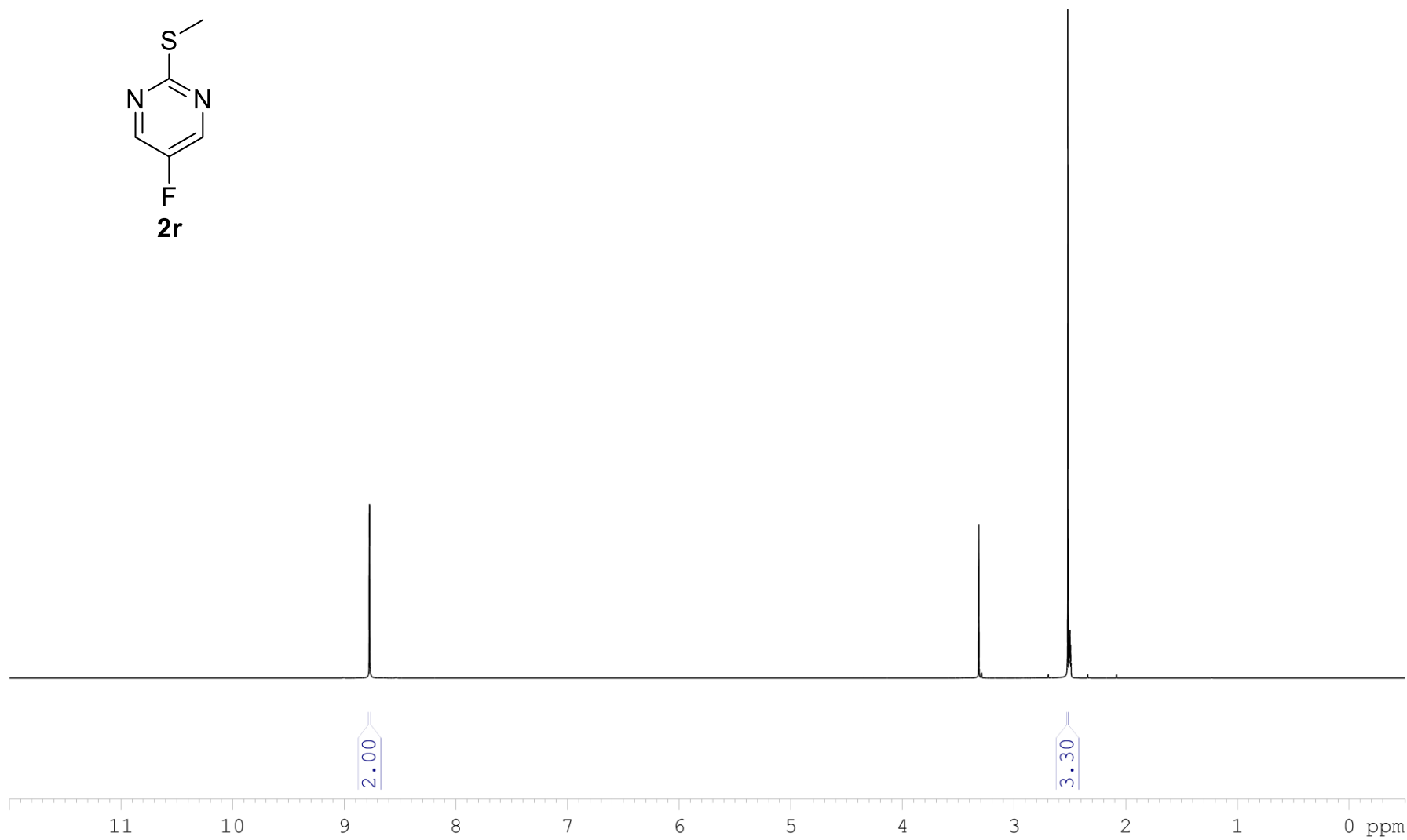
¹H NMR (400 MHz, DMSO-d₆)



8.78
8.77

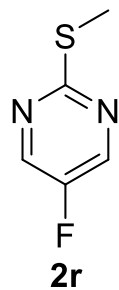
3.32

2.52
2.50



¹³C NMR (100 MHz, DMSO-d₆)

2-SMe 5-F

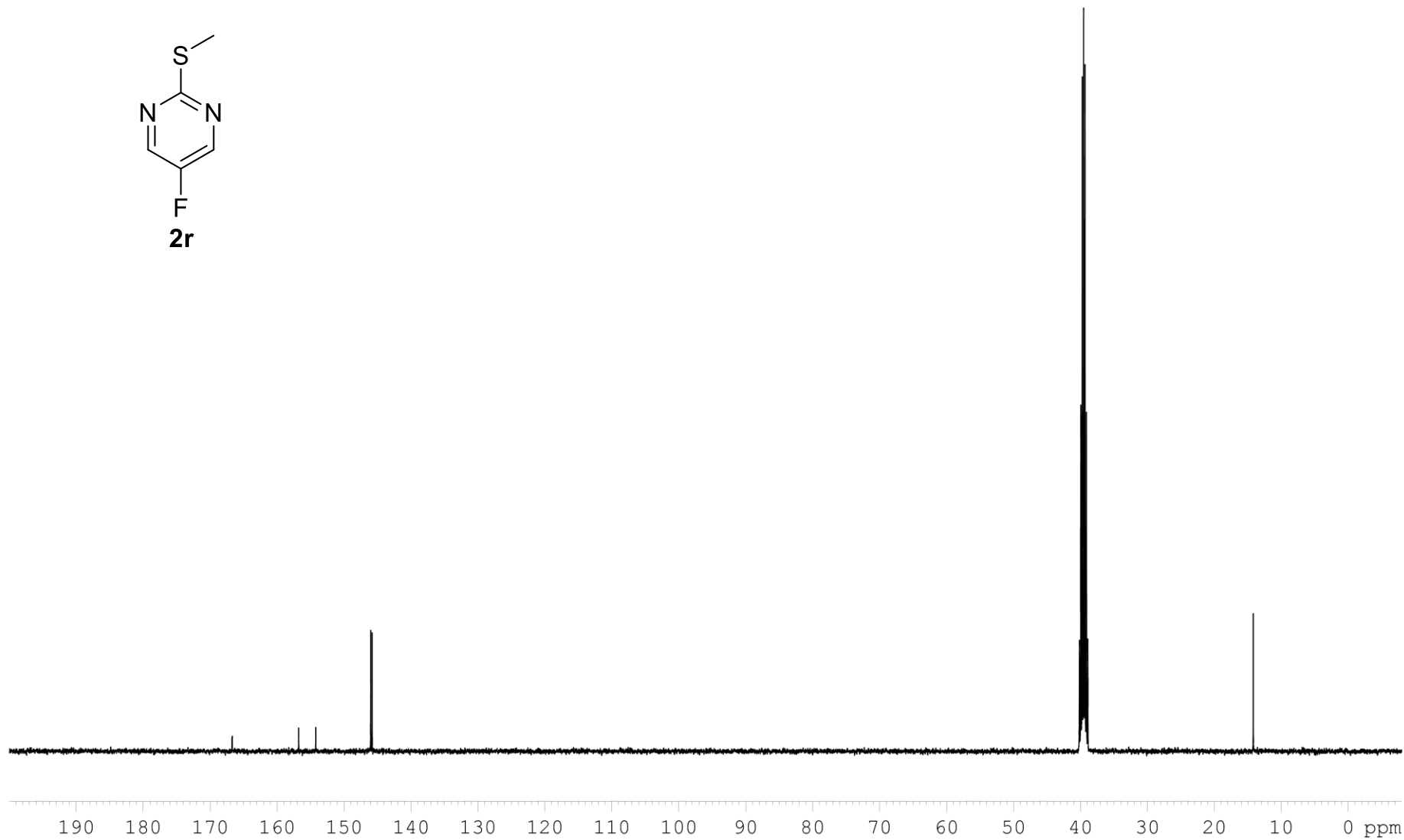


166.73
166.69

156.78
154.22

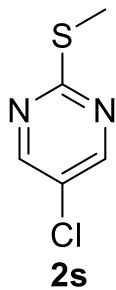
146.01
145.80

14.18



2-SMe 5-Cl

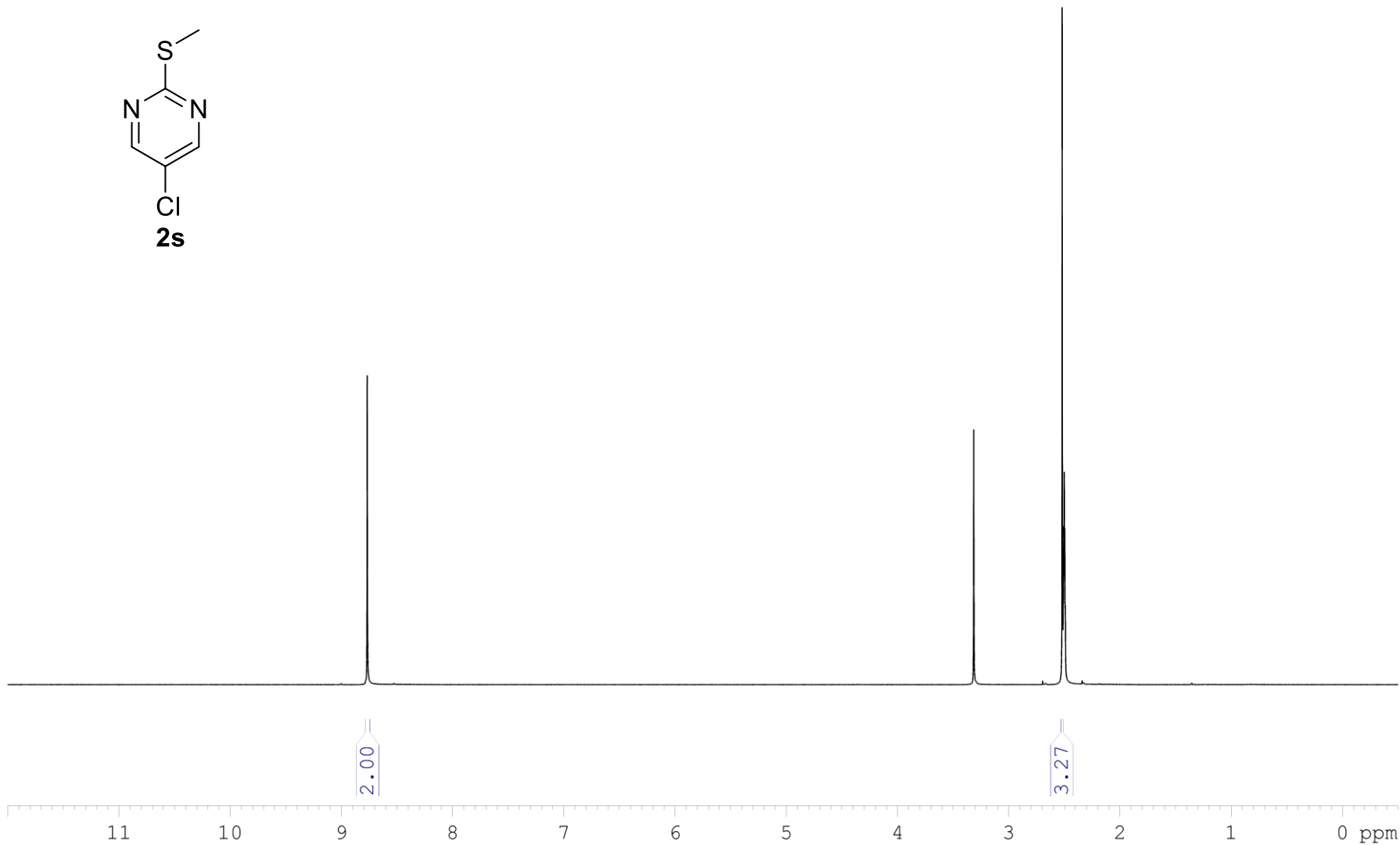
¹H NMR (400 MHz, DMSO-d₆)



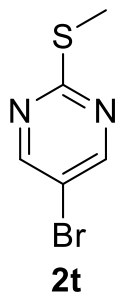
8.77

3.31

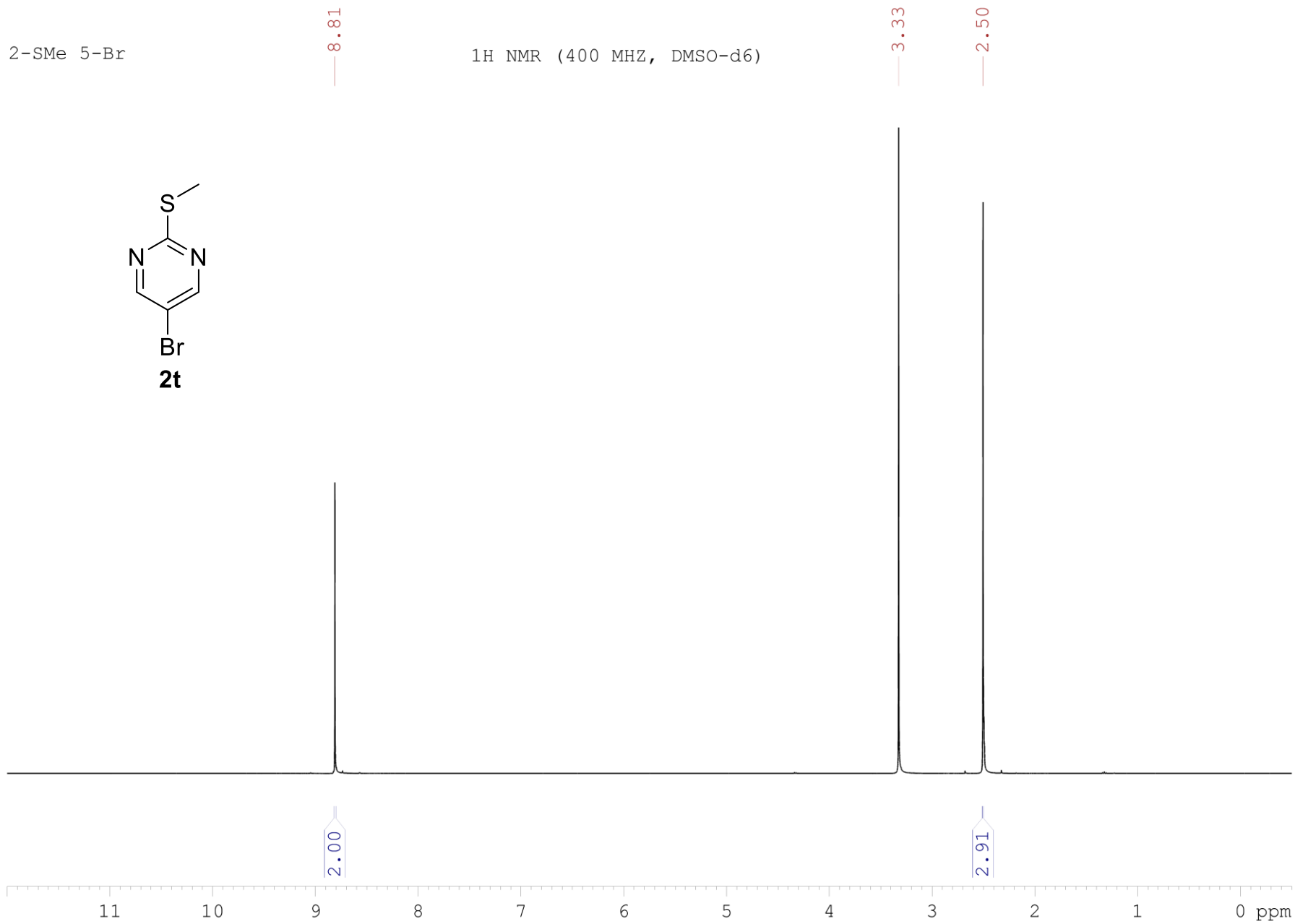
2.52
2.50

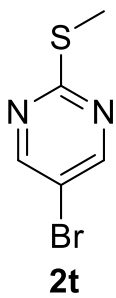


2-SMe 5-Br



1H NMR (400 MHz, DMSO-d6)





2-SMe 5-Br

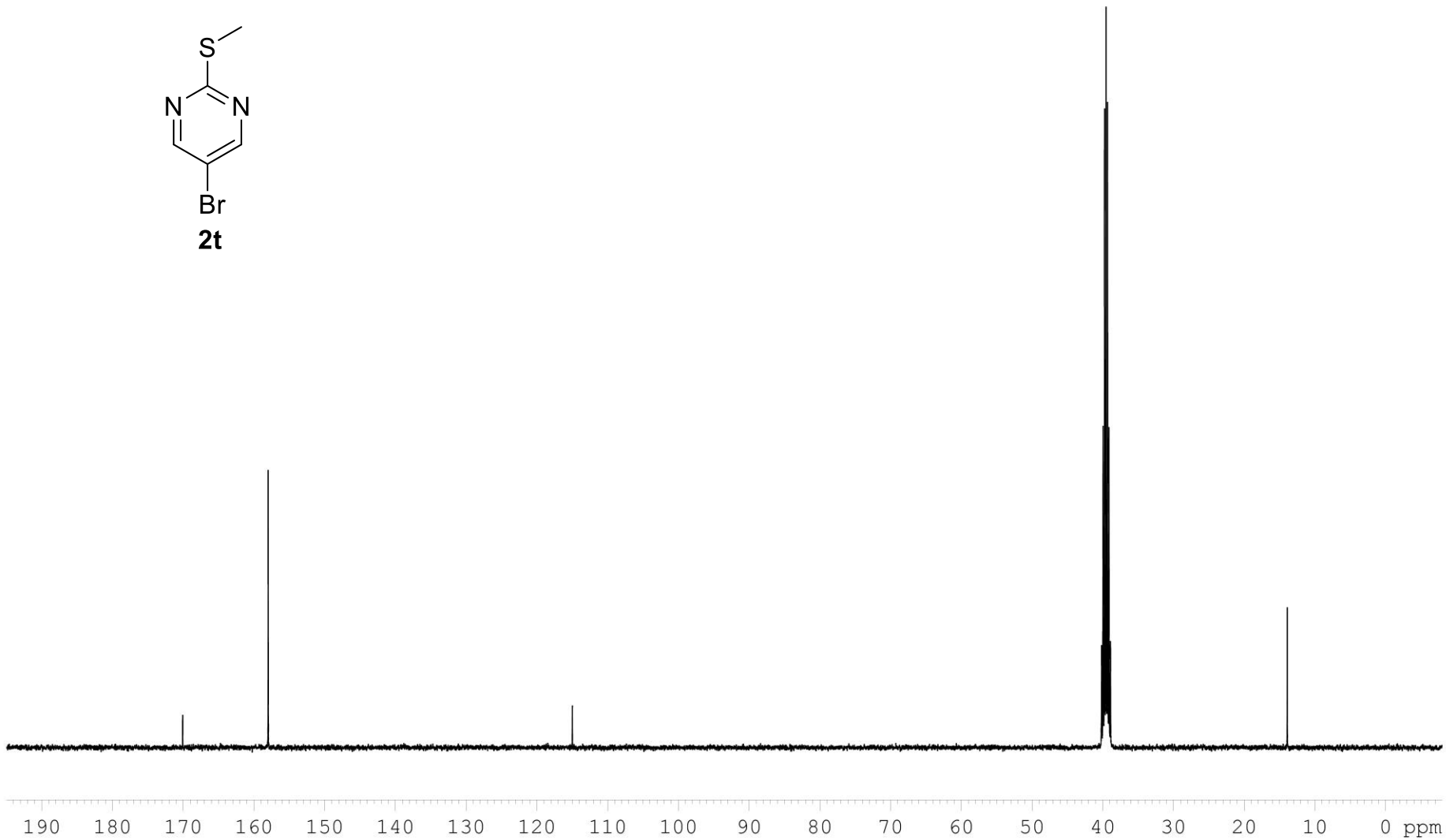
¹³C NMR (100 MHz, DMSO-d₆)

— 170.06

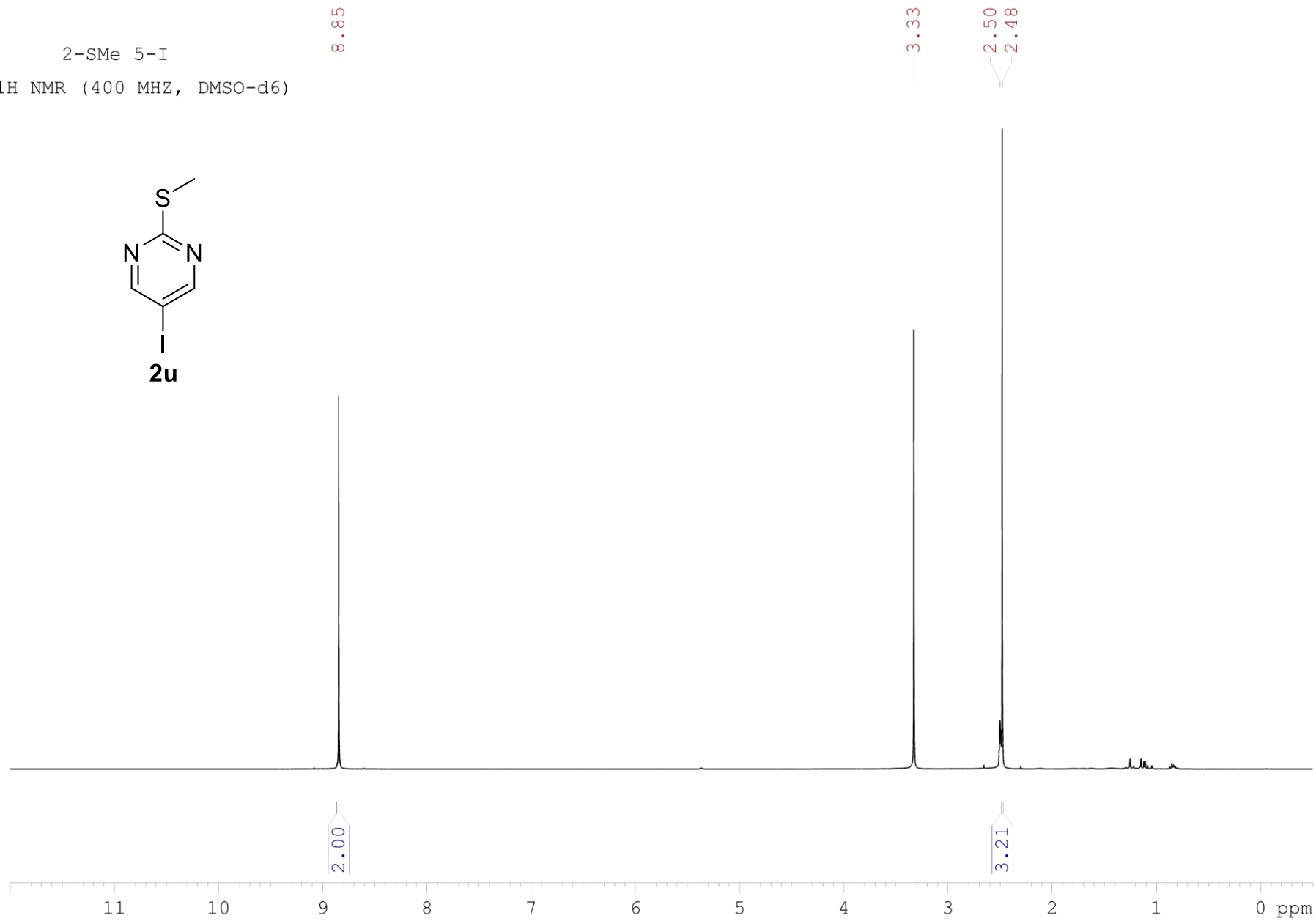
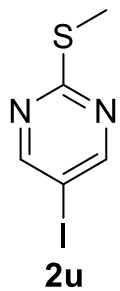
— 157.98

— 114.97

— 13.90



2-SMe 5-I
1H NMR (400 MHz, DMSO-d6)



2-SMe 5-I

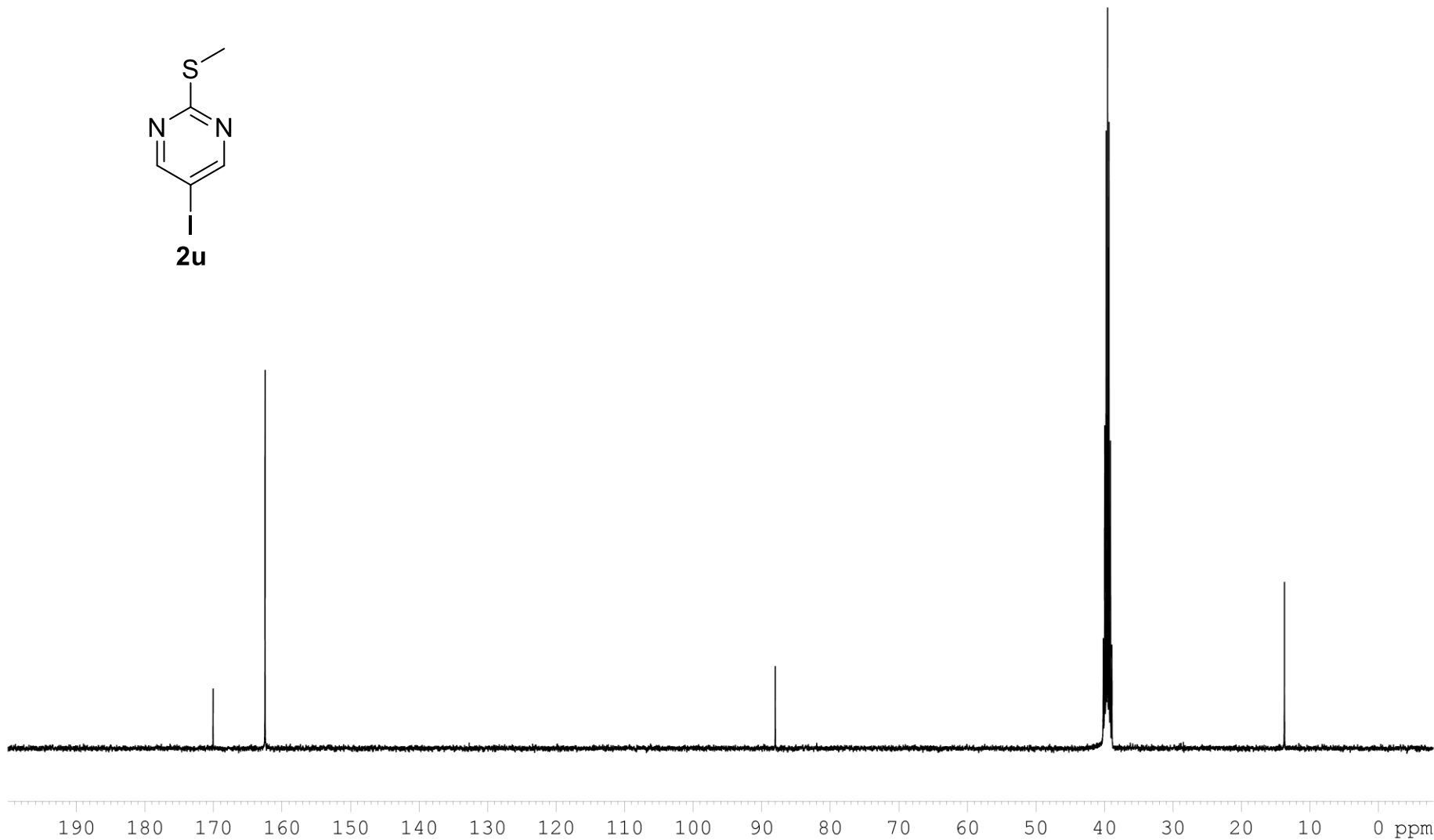
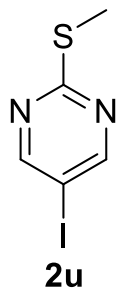
—170.05

—162.47

¹³C NMR (100 MHz, DMSO-d₆)

—88.02

—13.71



13.60

2-SMe 5-COOH

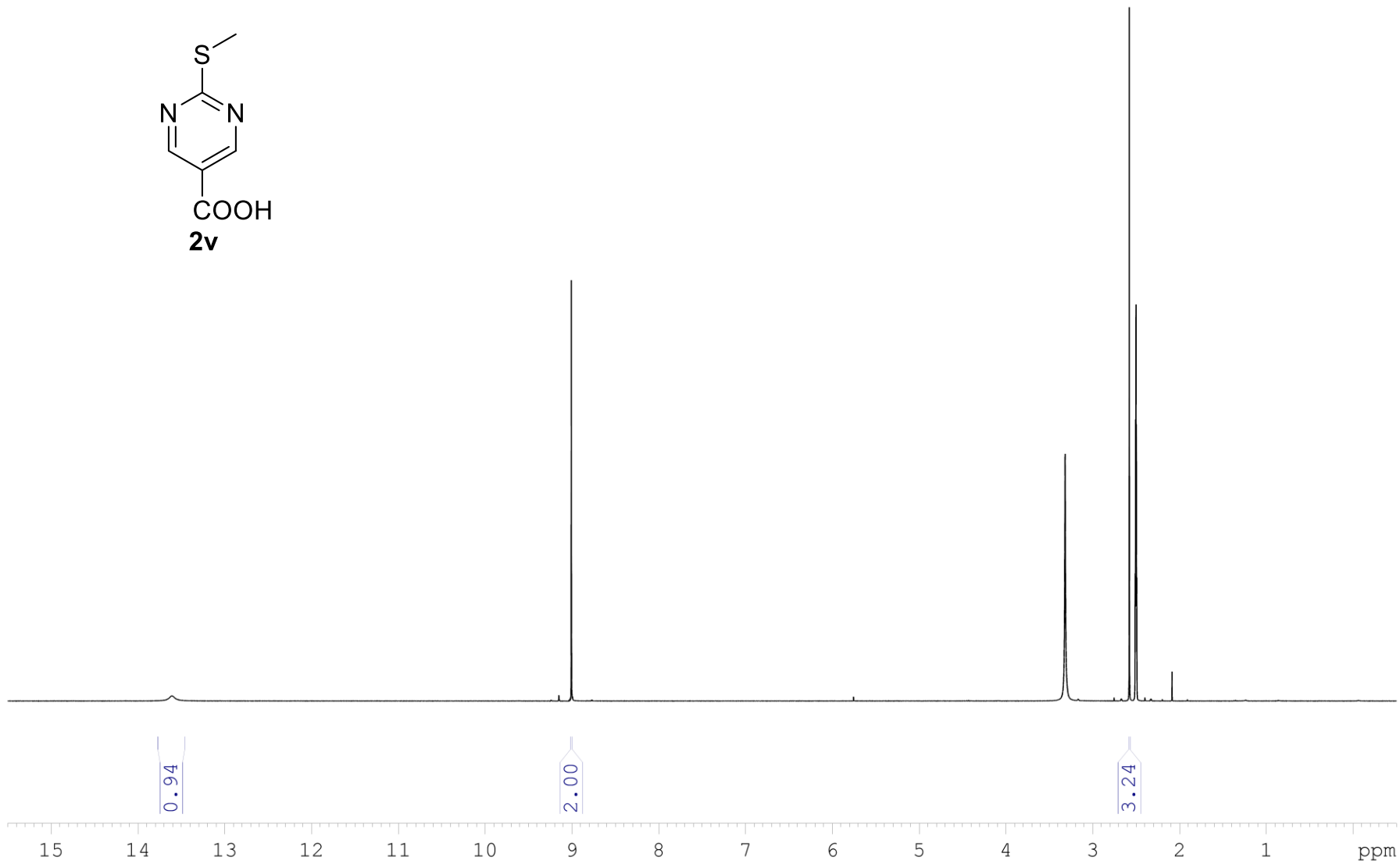
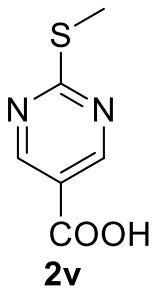
9.01

1H NMR (400 MHz, DMSO-d6)

3.32

2.58

2.50



—175.80
—164.94
—158.11

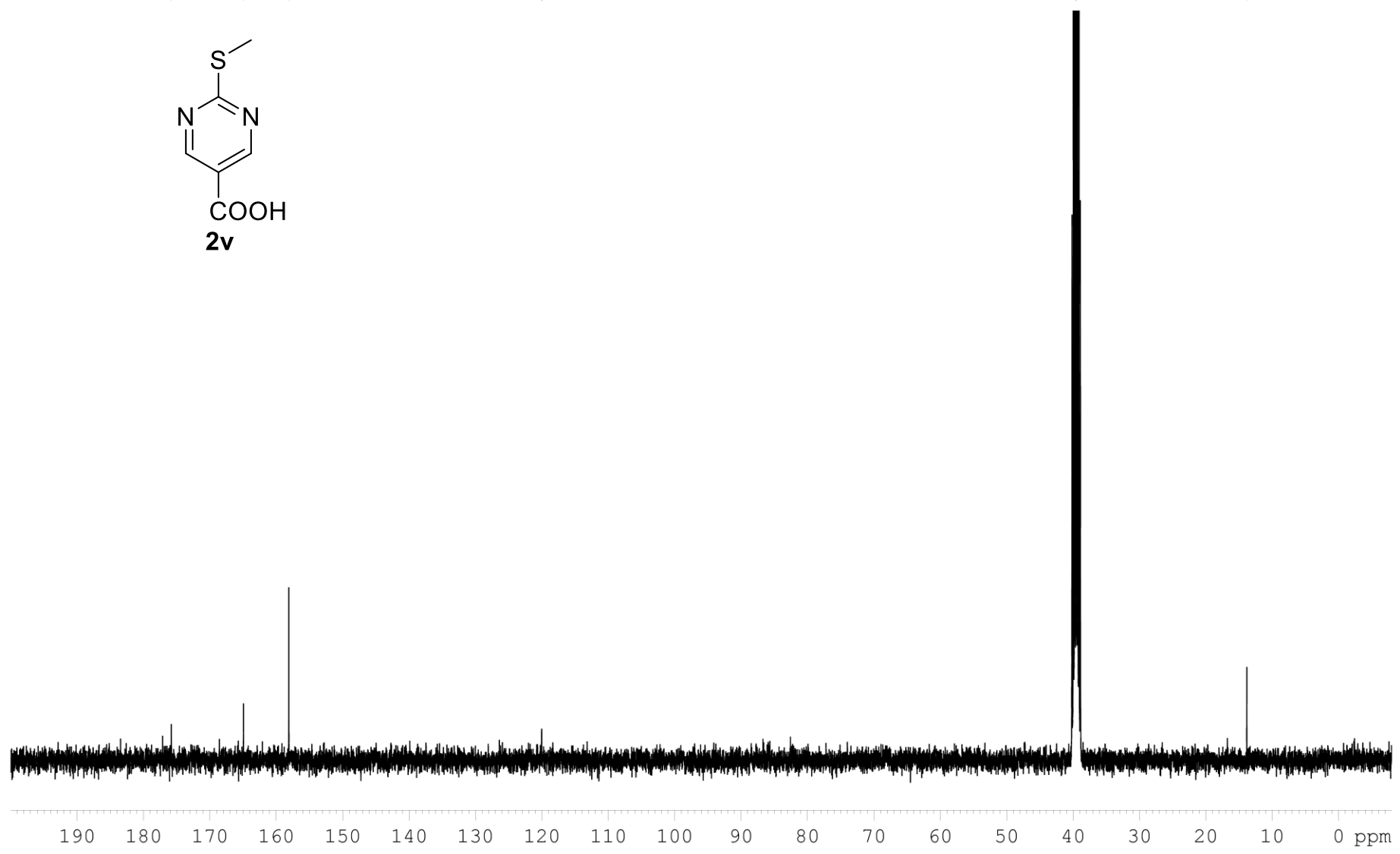
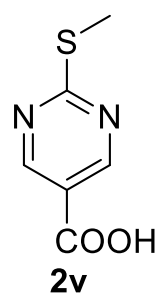
2-SMe 5-COOH

¹³C NMR (100 MHz, DMSO-d₆)

—120.03

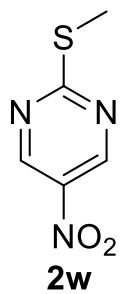
—39.52

—13.82

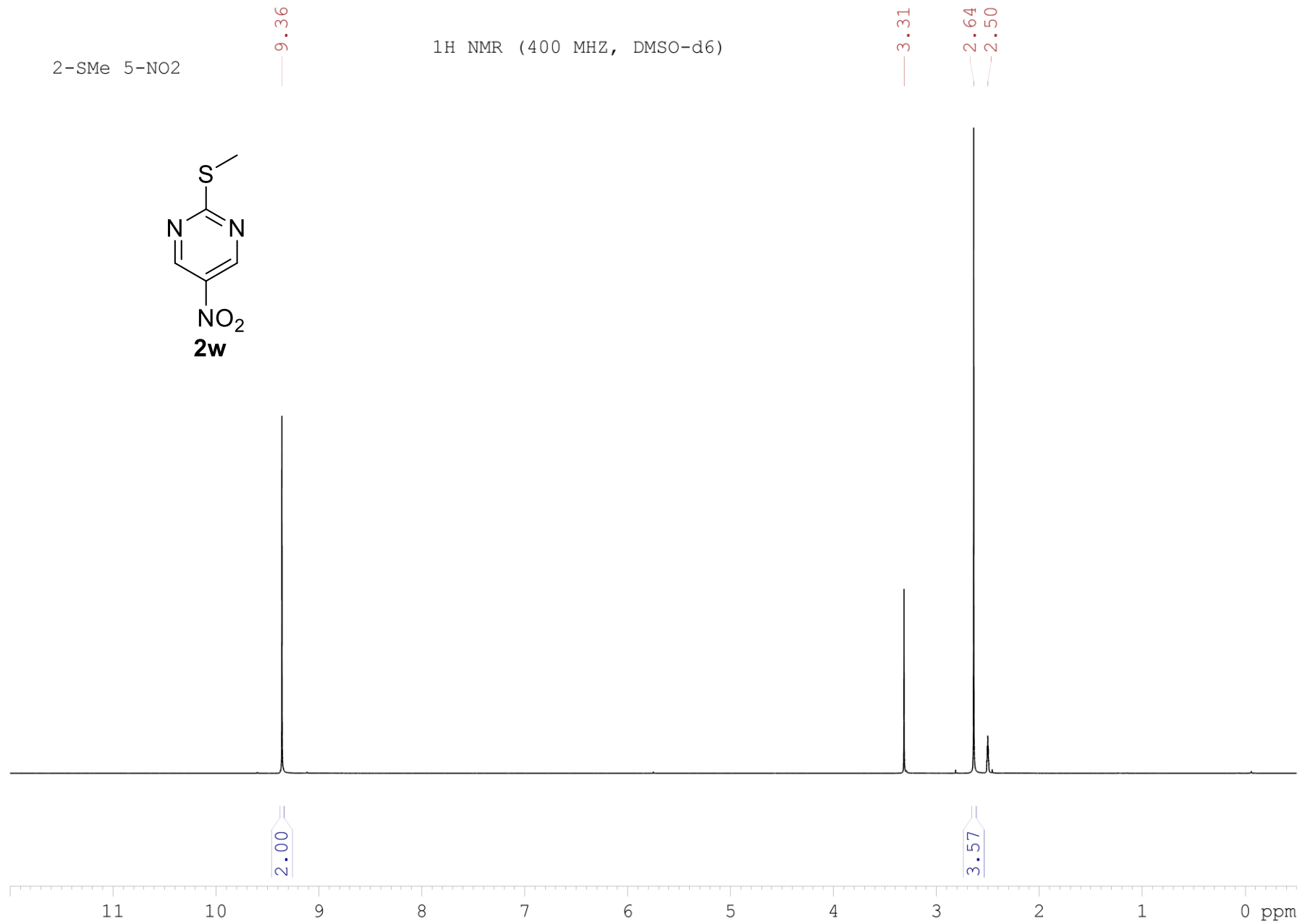


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

2-SMe 5-NO2



1H NMR (400 MHz, DMSO-d6)



— 177.73

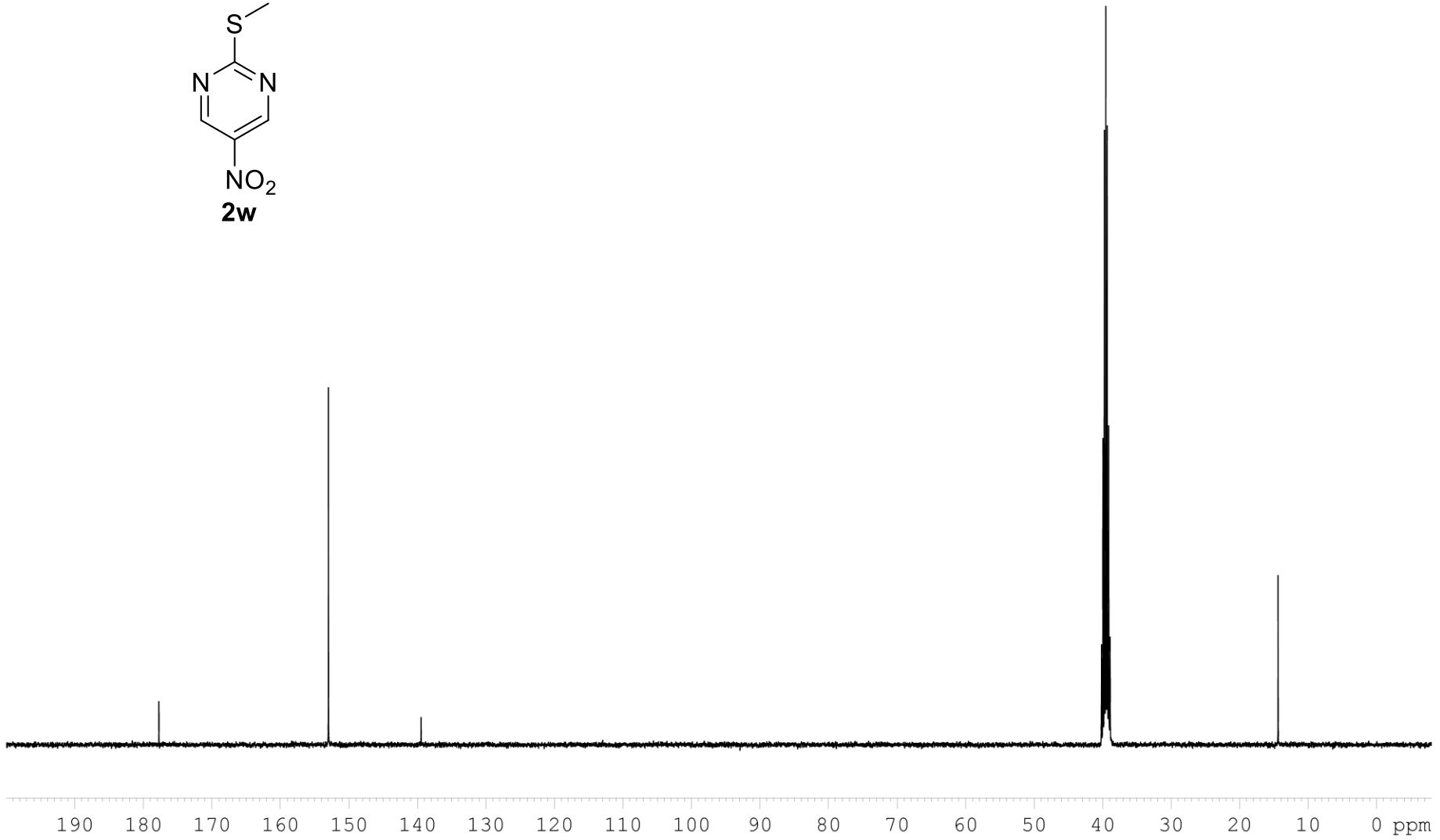
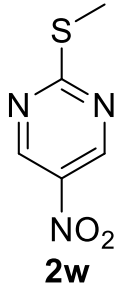
— 152.98

— 139.45

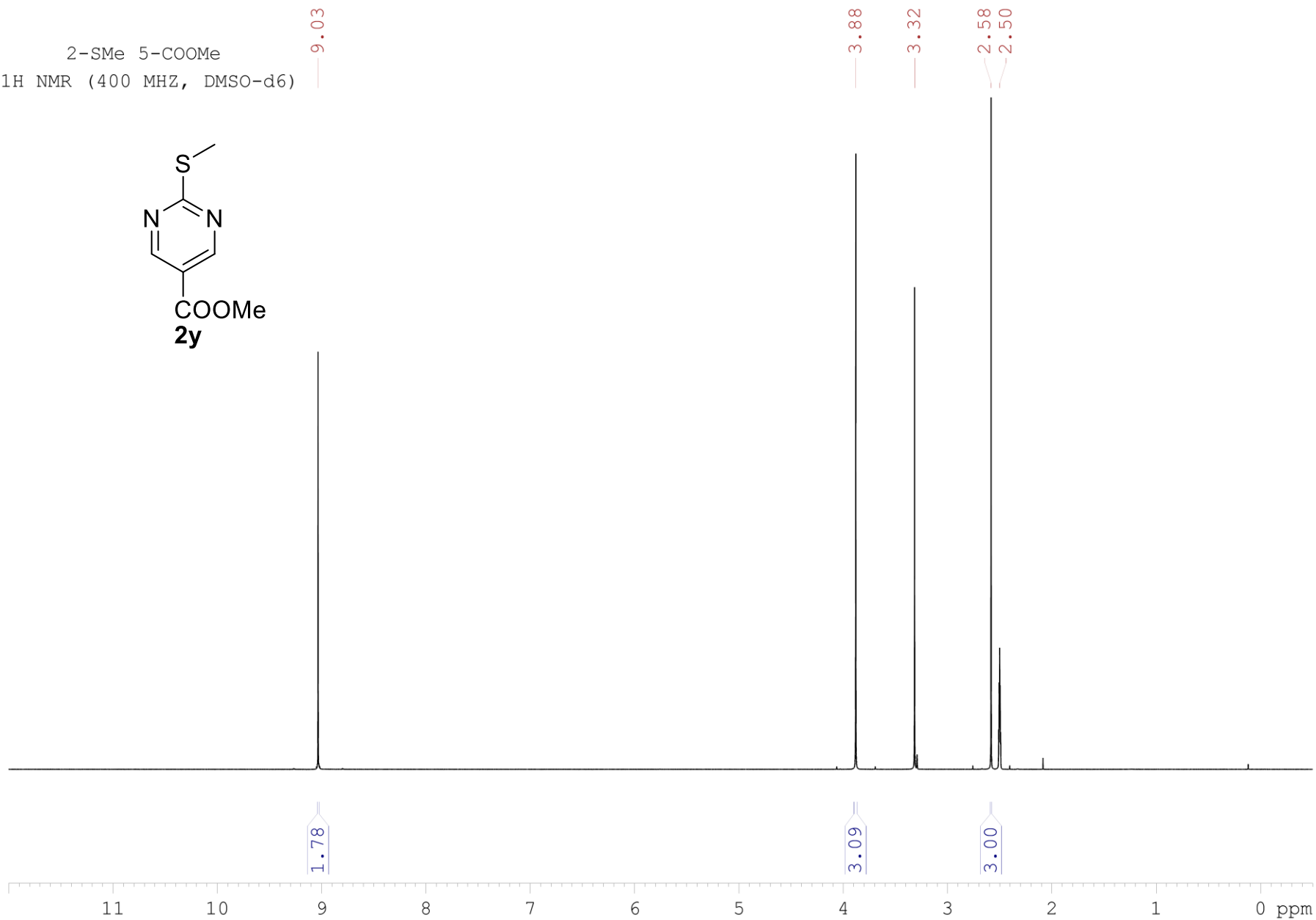
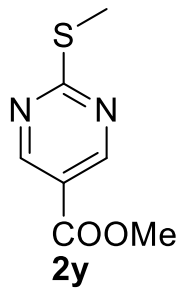
13C NMR (100 MHz, DMSO-d6)

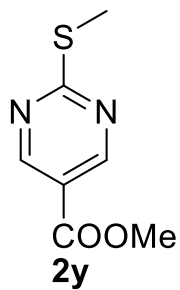
2-SMe 5-NO2

— 14.37



2-SMe 5-COOMe
1H NMR (400 MHz, DMSO-d6)





2-SMe 5-COOMe

¹³C NMR (100 MHz, DMSO-d₆)

— 176.23

— 163.96

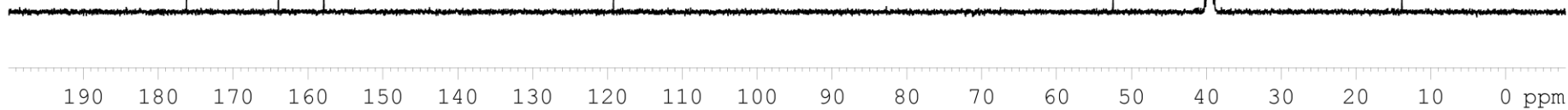
— 157.87

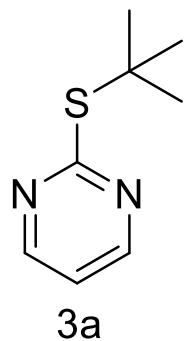
— 119.18

— 52.44

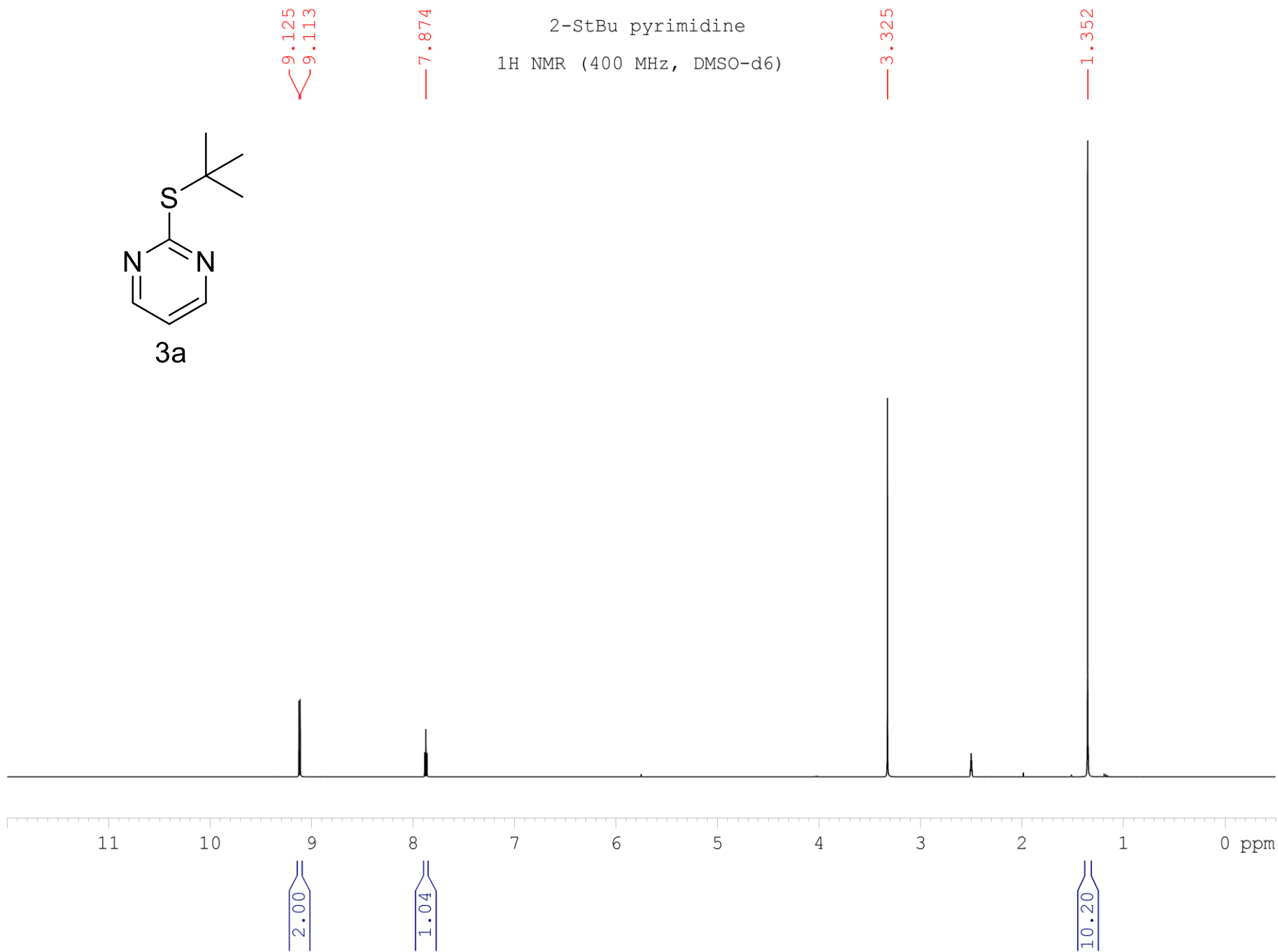
— 39.52

— 13.84



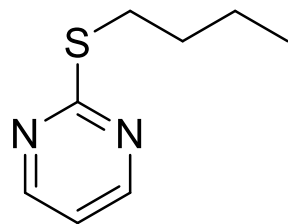


2-StBu pyrimidine
1H NMR (400 MHz, DMSO-d6)



2-SnBu pyrimidine

¹H NMR (400 MHz, DMSO-d₆)

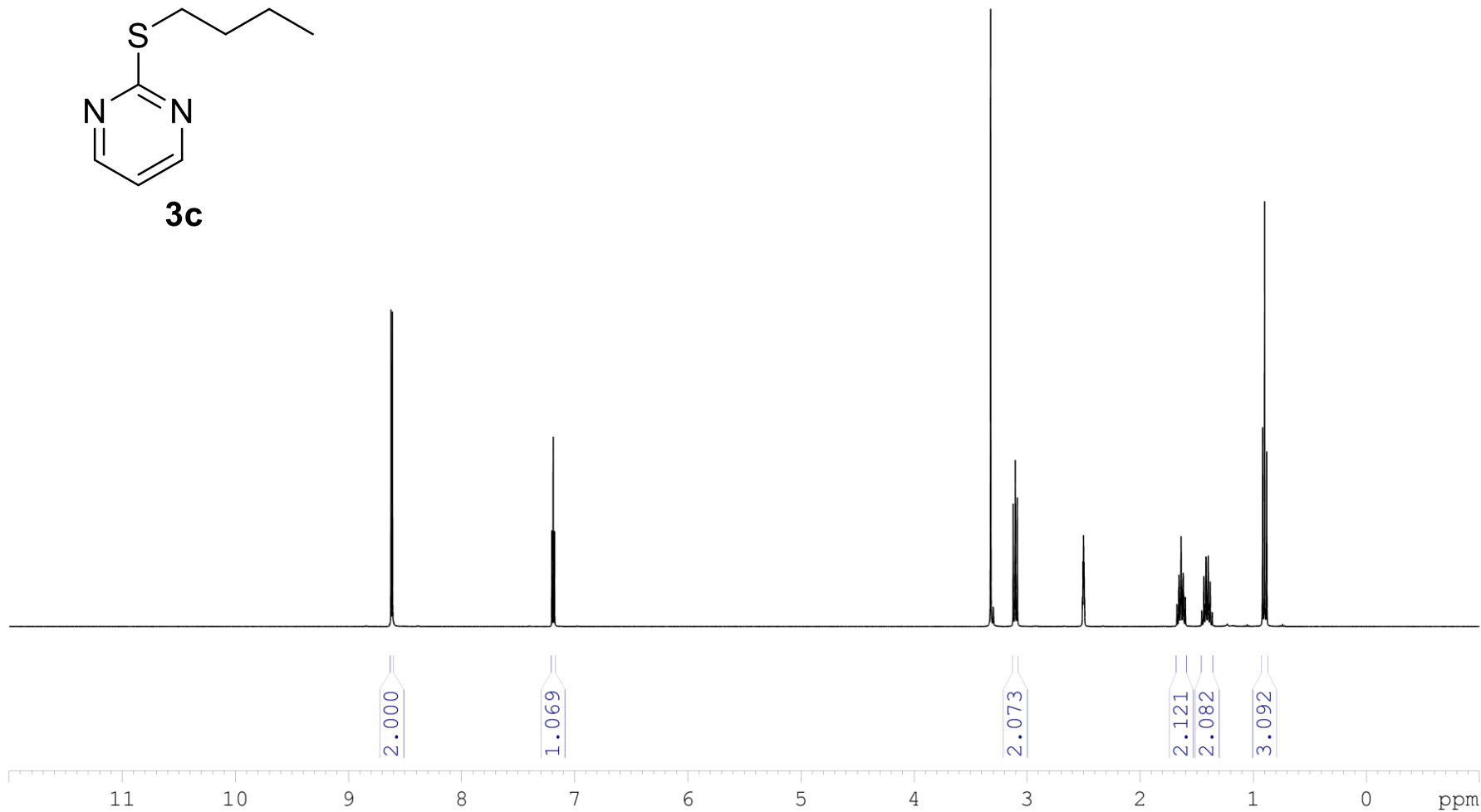


3c

8.62
8.61

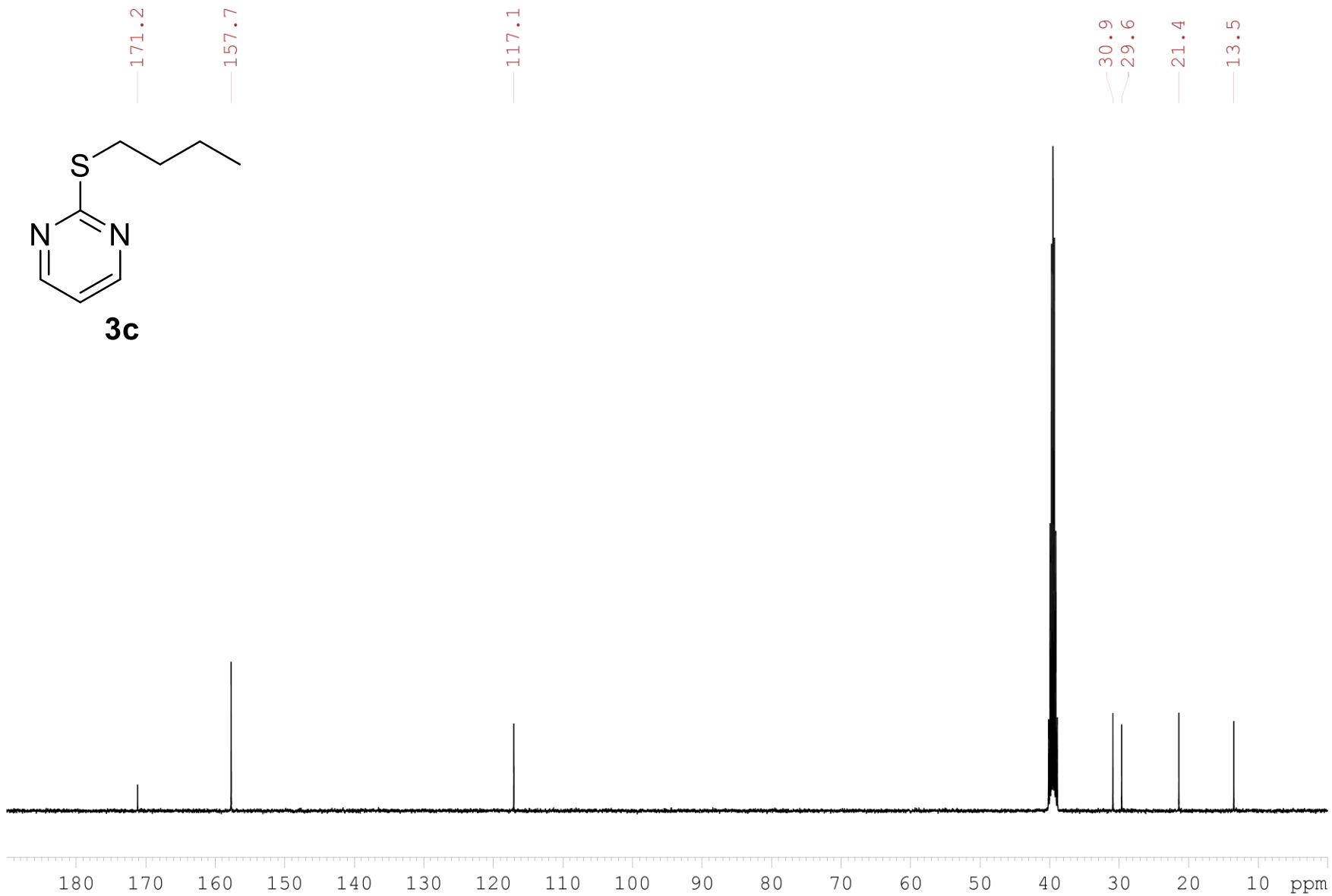
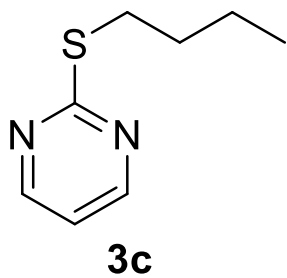
7.20
7.19
7.18

3.32
3.12
3.10
3.09
1.67
1.66
1.62
1.60
1.45
1.44
1.42
1.40
1.38
1.36
0.92
0.90
0.88



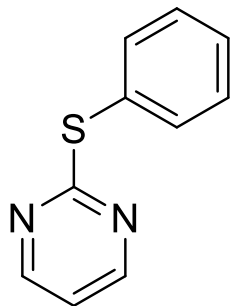
2-SnBu pyrimidine

^{13}C NMR (100 MHz, DMSO- d_6)



2-SPh pyrimidine

¹H NMR (400 MHz, DMSO-d₆)

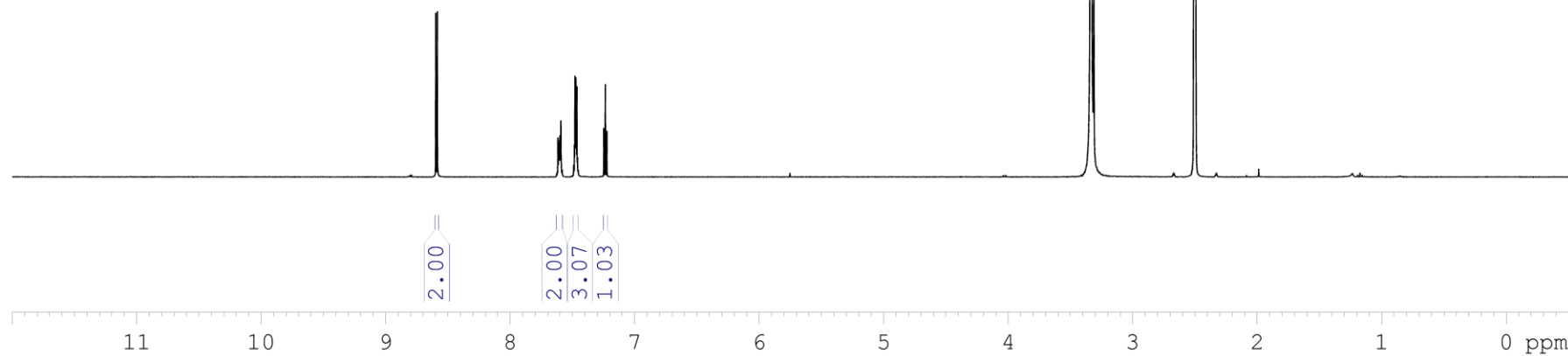


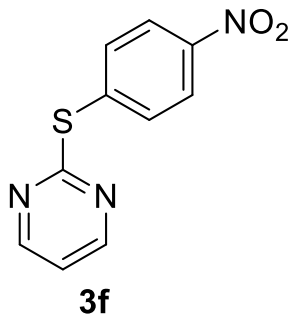
3d

8.60
8.58
7.62
7.60
7.59
7.48
7.47
7.46
7.25
7.23
7.22

3.33

2.50



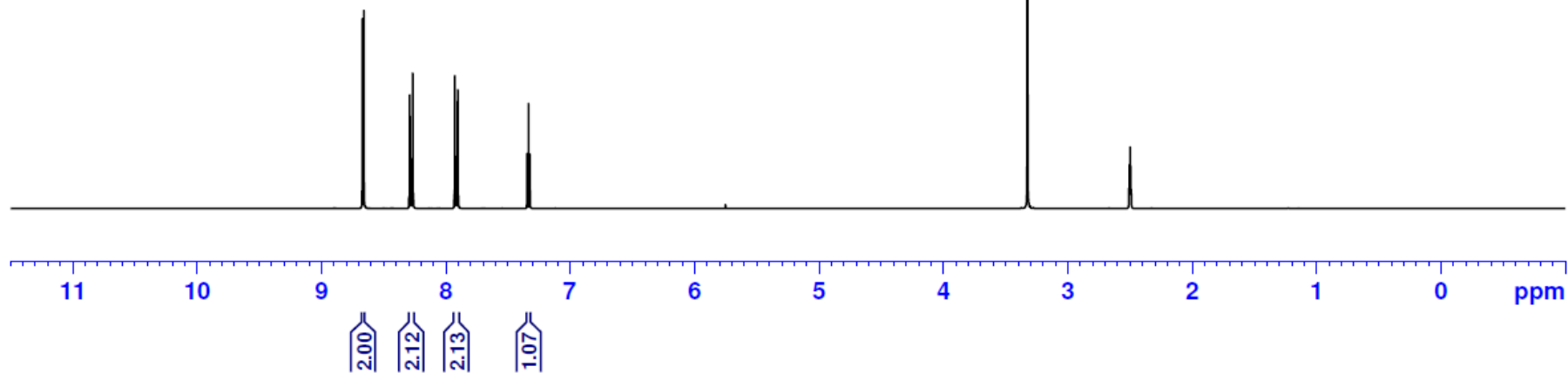


8.67
8.66
8.29
8.27
7.93
7.90
7.35
7.33
7.32

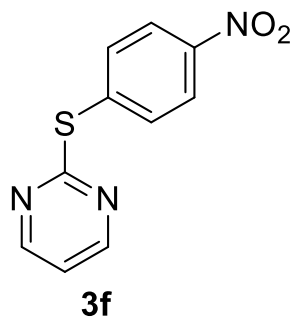
2-S (p-NO₂Ph)
1H (400 MHz, DMSO-d₆)

3.33

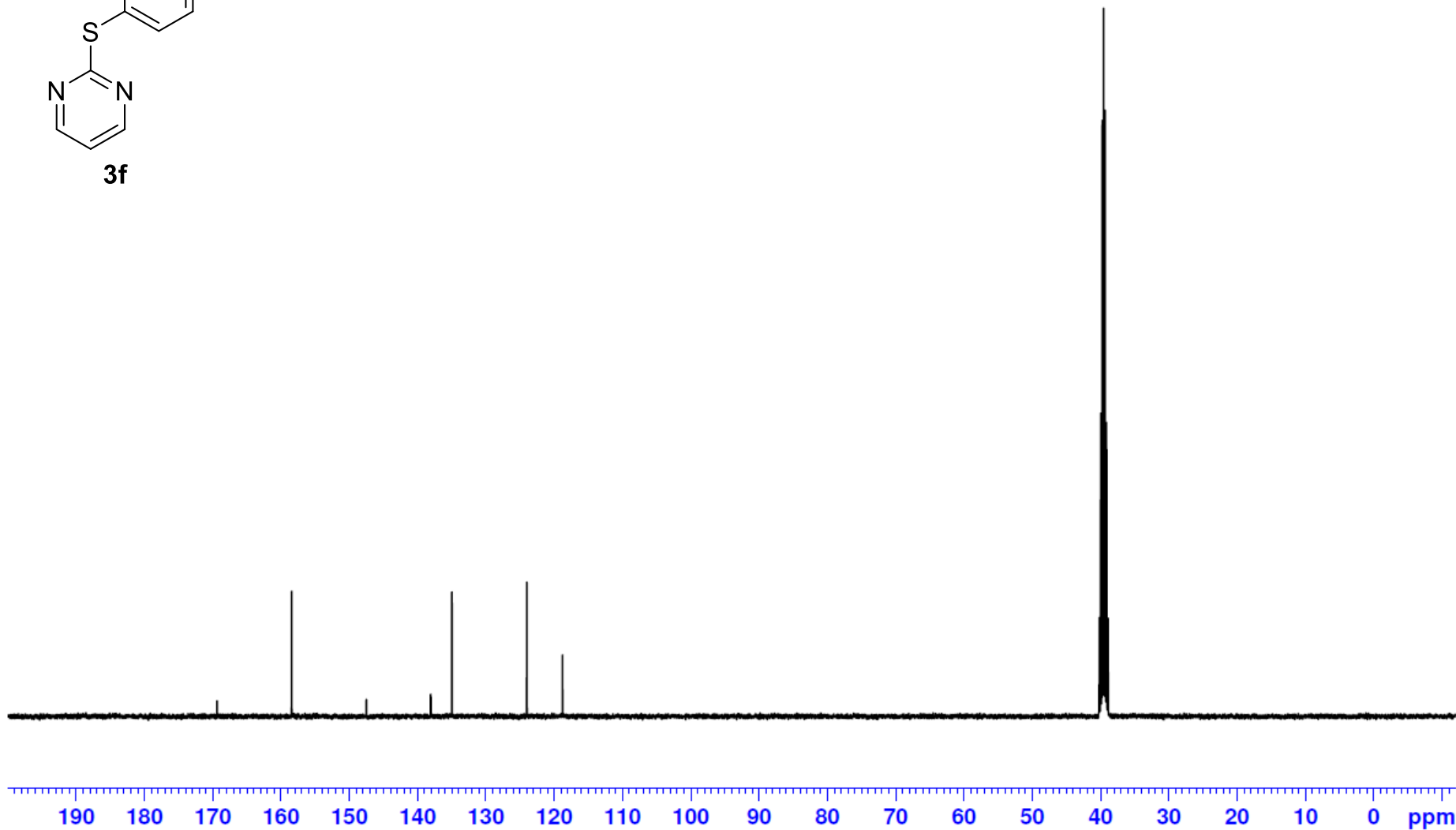
2.50

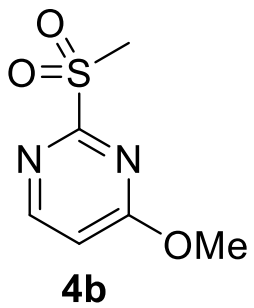


2-S (p-NO₂Ph)
13C (100 MHz, DMSO-d₆)



169.33
158.42
147.49
138.06
134.96
123.99
118.77





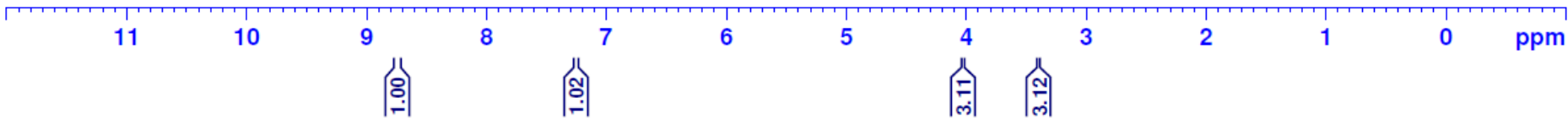
2-SO₂Me 4-OMe
1H NMR (400 MHz, DMSO-d₆)

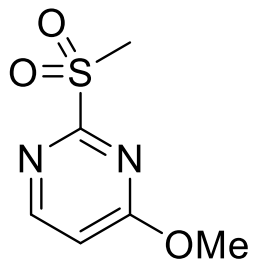
8.75
8.74

7.26
7.25

4.03

3.40
3.32





4b

170.11
165.01
158.60

111.23

2-SO₂Me 4-OMe
13C (100MHz, DMSO-d₆)

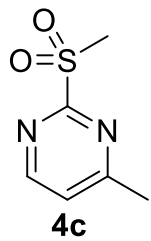
54.89

38.89



190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

2-SO₂Me 4-Me pyrimidine



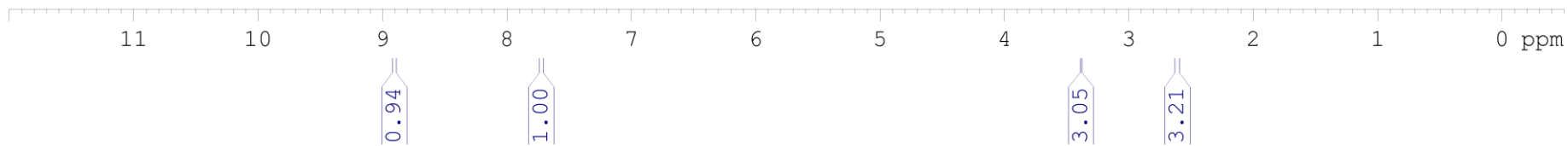
¹H NMR (400 MHz, DMSO-d₆)

8.911
8.898

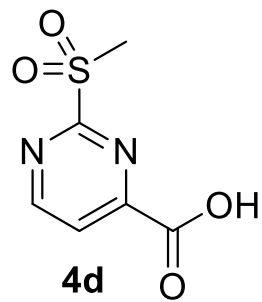
7.730
7.729
7.718
7.716

3.385
3.323

2.611
2.610
2.500



2-SO₂Me 4-COOH



¹H NMR (400 MHz, DMSO-d₆)

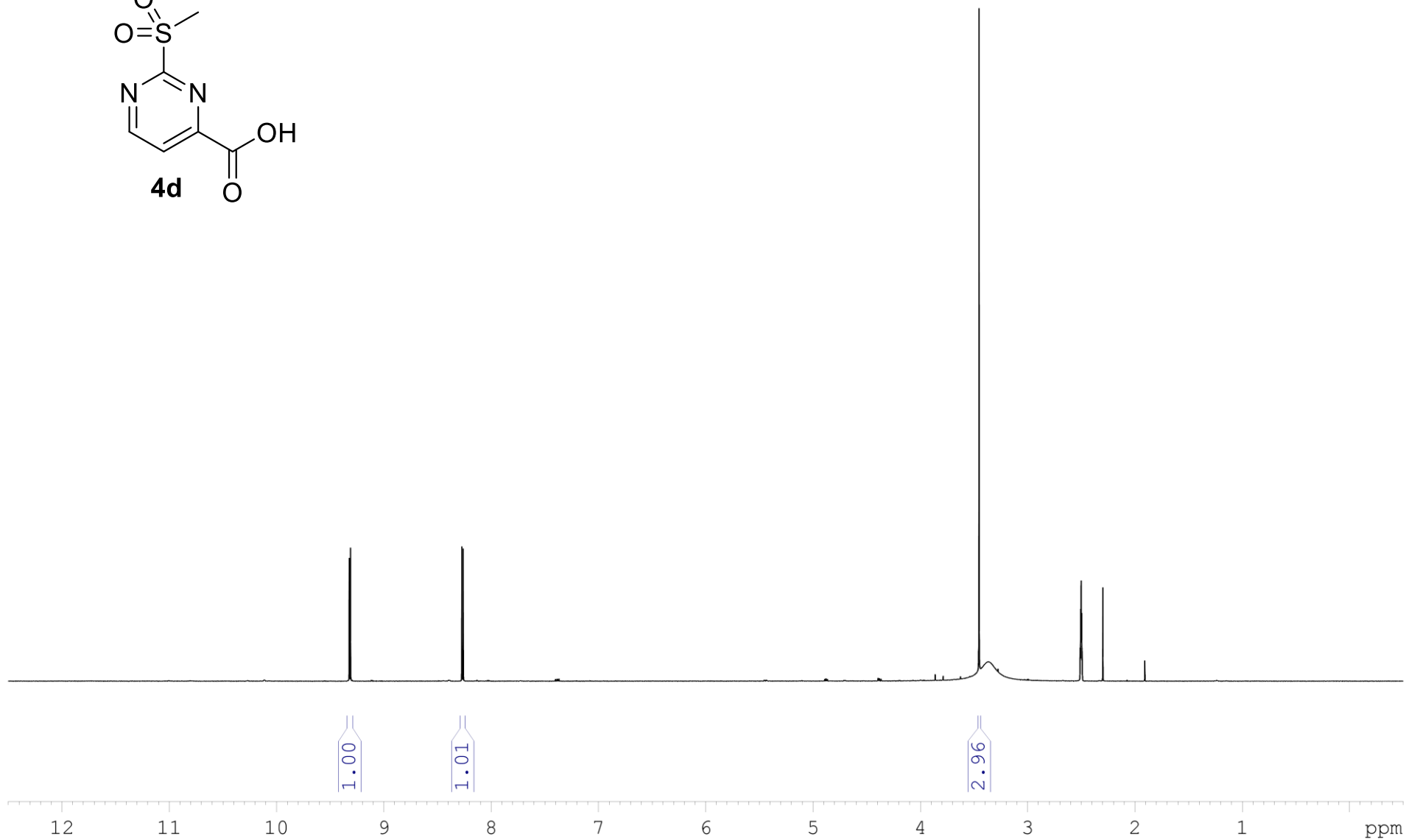
9.32
9.31

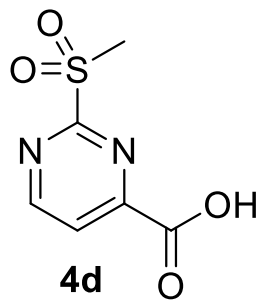
8.27
8.26

3.45
3.37

2.50
2.30

1.91



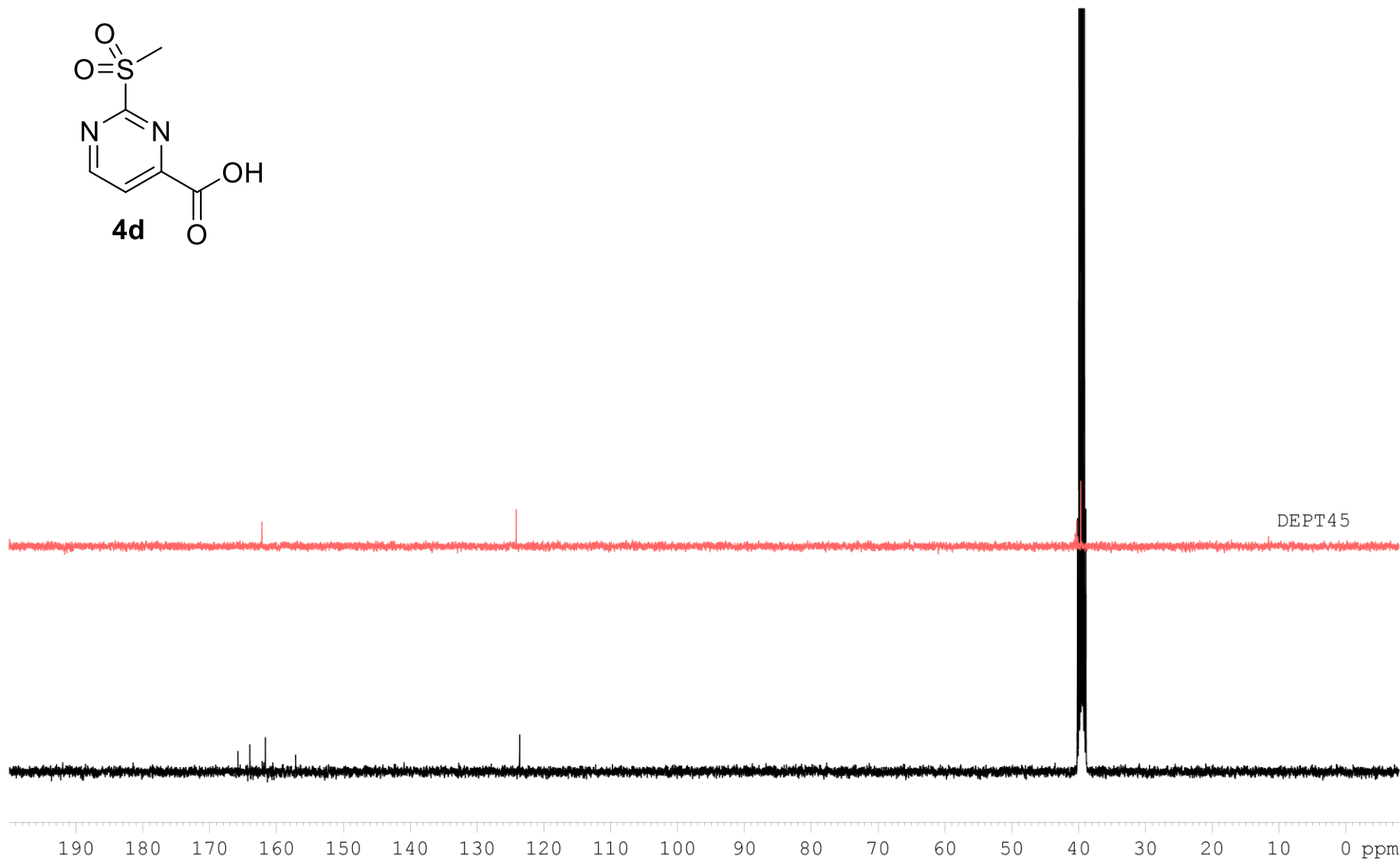


165.76
163.99
161.67
157.13

123.61

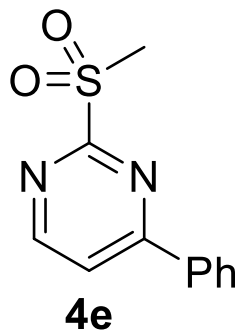
¹³C NMR (100 MHz, DMSO-d₆)

2-SO₂Me 4-COOH



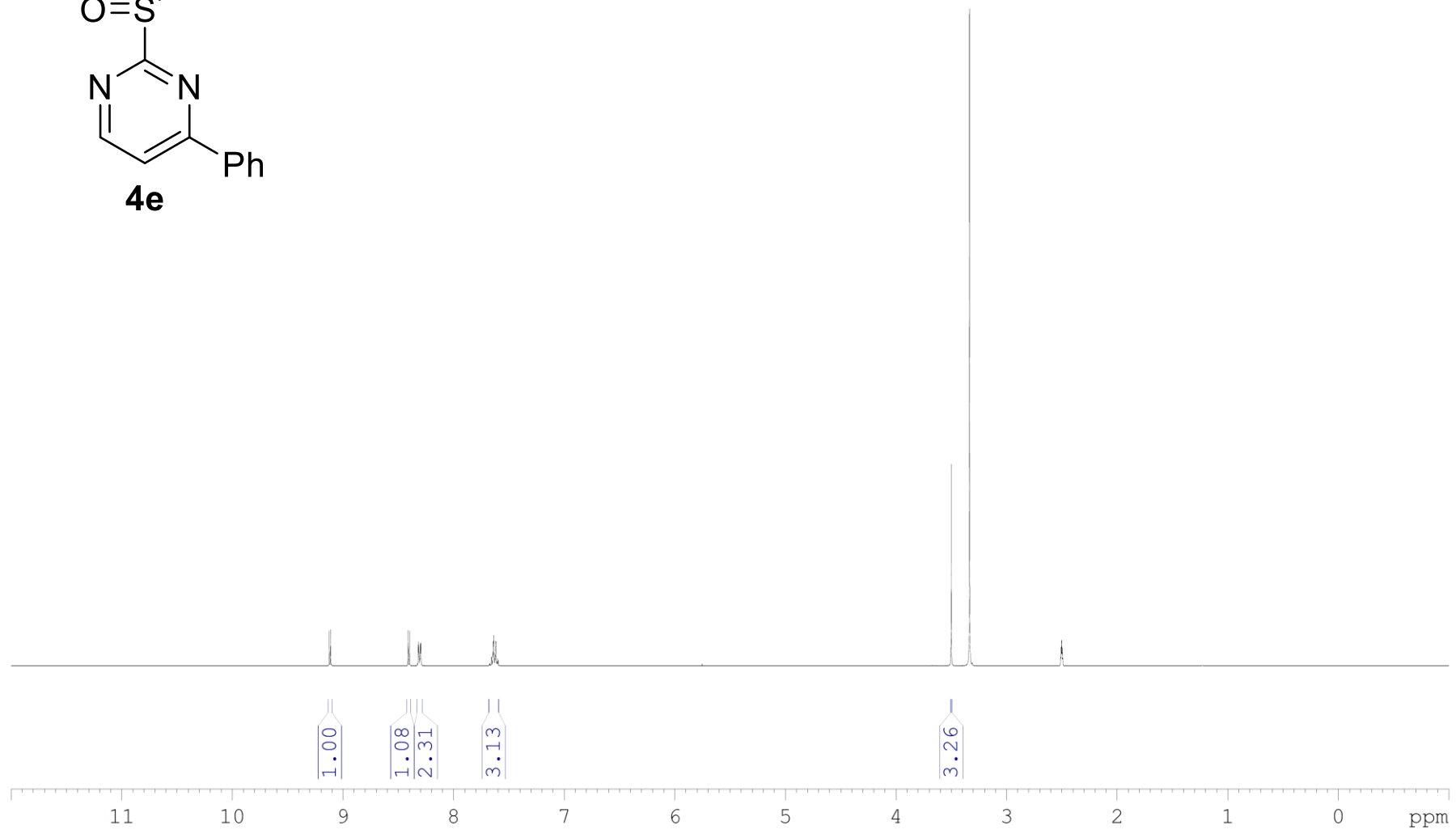
¹H NMR (400 MHz, DMSO-d₆)

2-SO₂Me 4-Ph

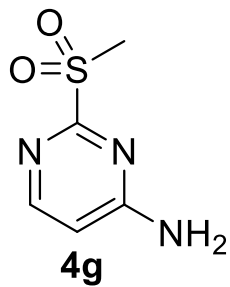


9.12
9.11
8.41
8.40
8.32
8.32
8.30
8.29
7.66
7.64
7.64
7.62
7.60

3.50
3.33



2-SO₂Me 4-NH₂
1H NMR (400 MHz, DMSO-d₆)



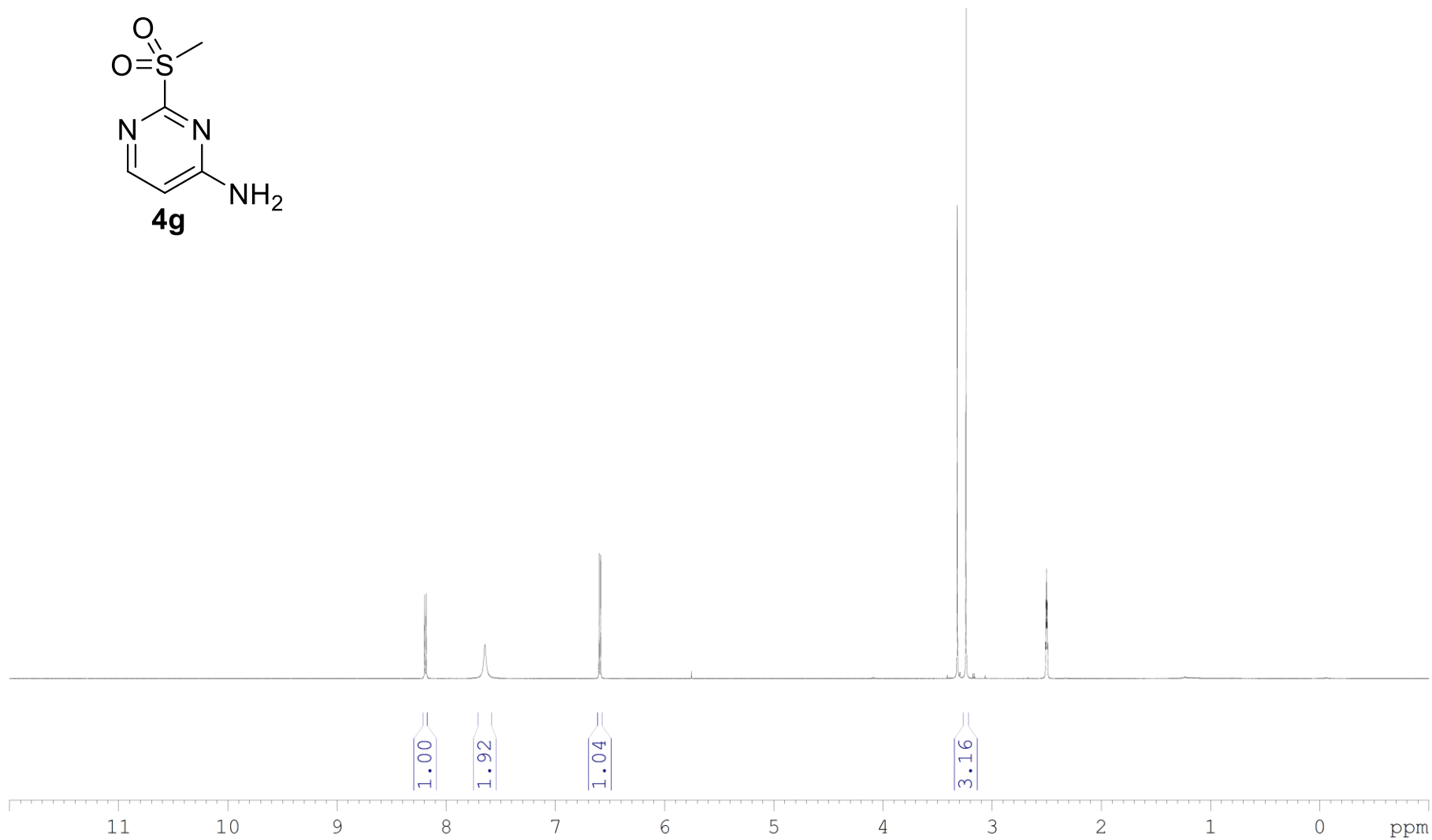
8.20
8.18

7.64

6.60
6.59

3.32
3.24

2.50



2-SO₂Me 4-NH₂

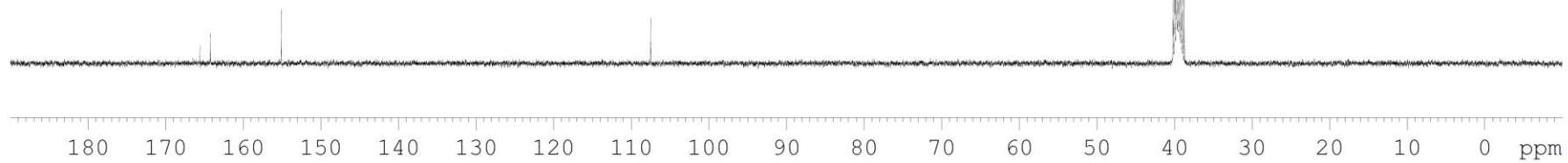
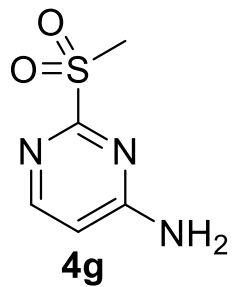
¹³C NMR (100 MHz, DMSO-d₆)

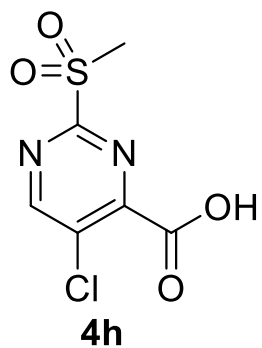
165.56
164.22

155.06

107.47

38.69





2-SO₂Me 4-COOH 5-Cl
1H NMR (400 MHz, DMSO-d₆)

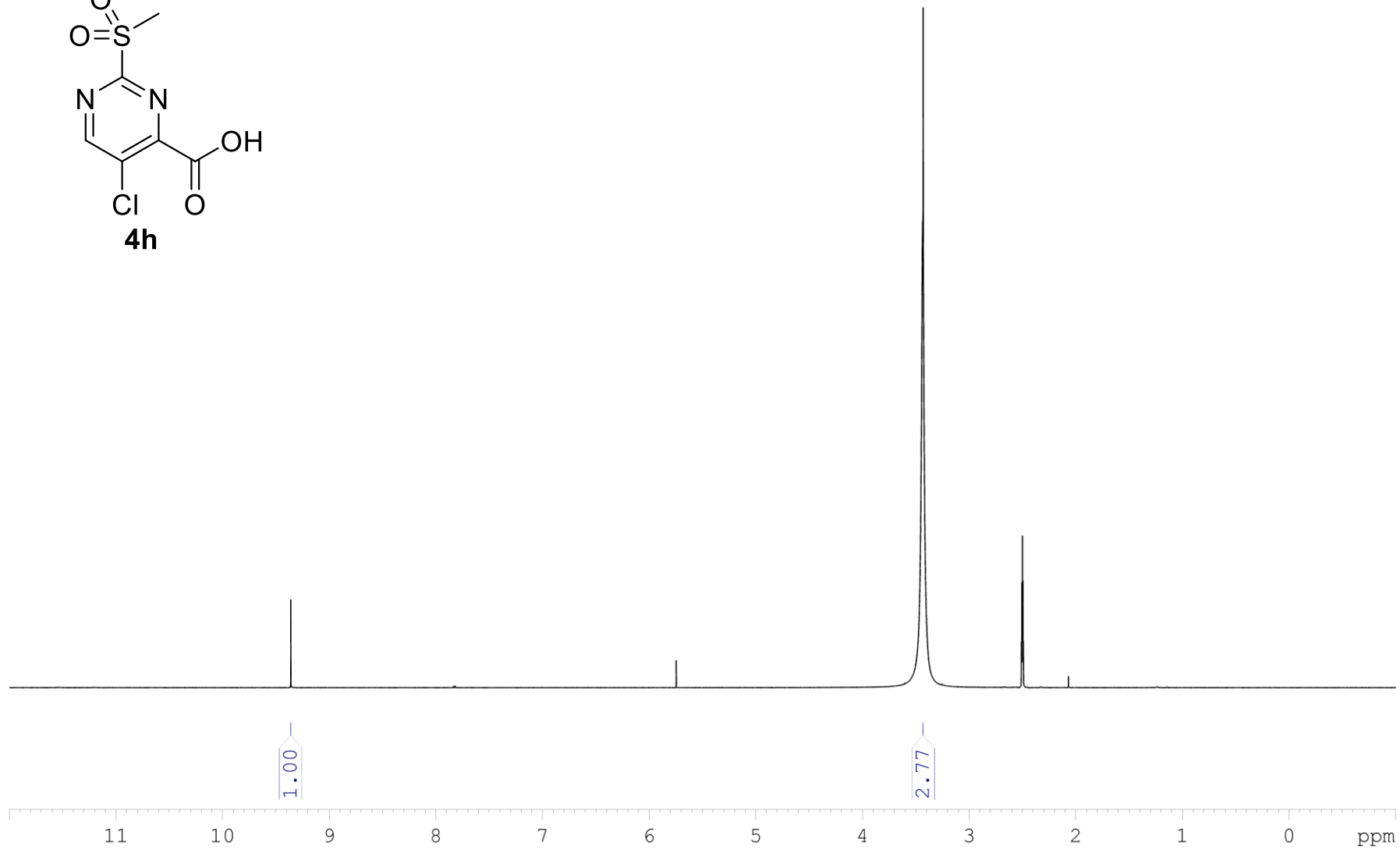
9.36

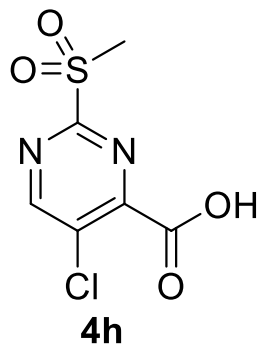
5.75

3.43

2.50

2.07



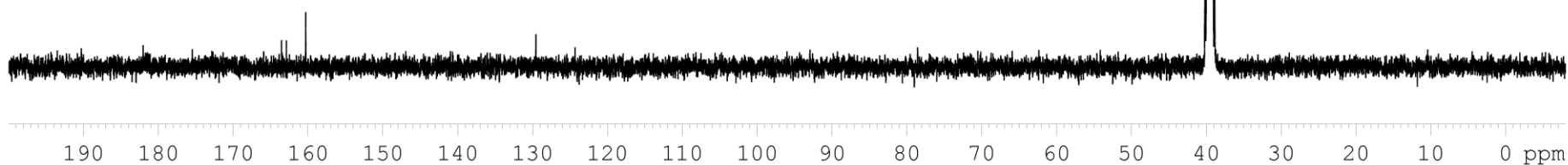


163.55
162.90
160.32

129.56

2-SO₂Me 4-COOH 5-Cl
13C NMR (100 MHz, DMSO-d₆)

39.44



1H NMR (400 MHz, DMSO-d6)

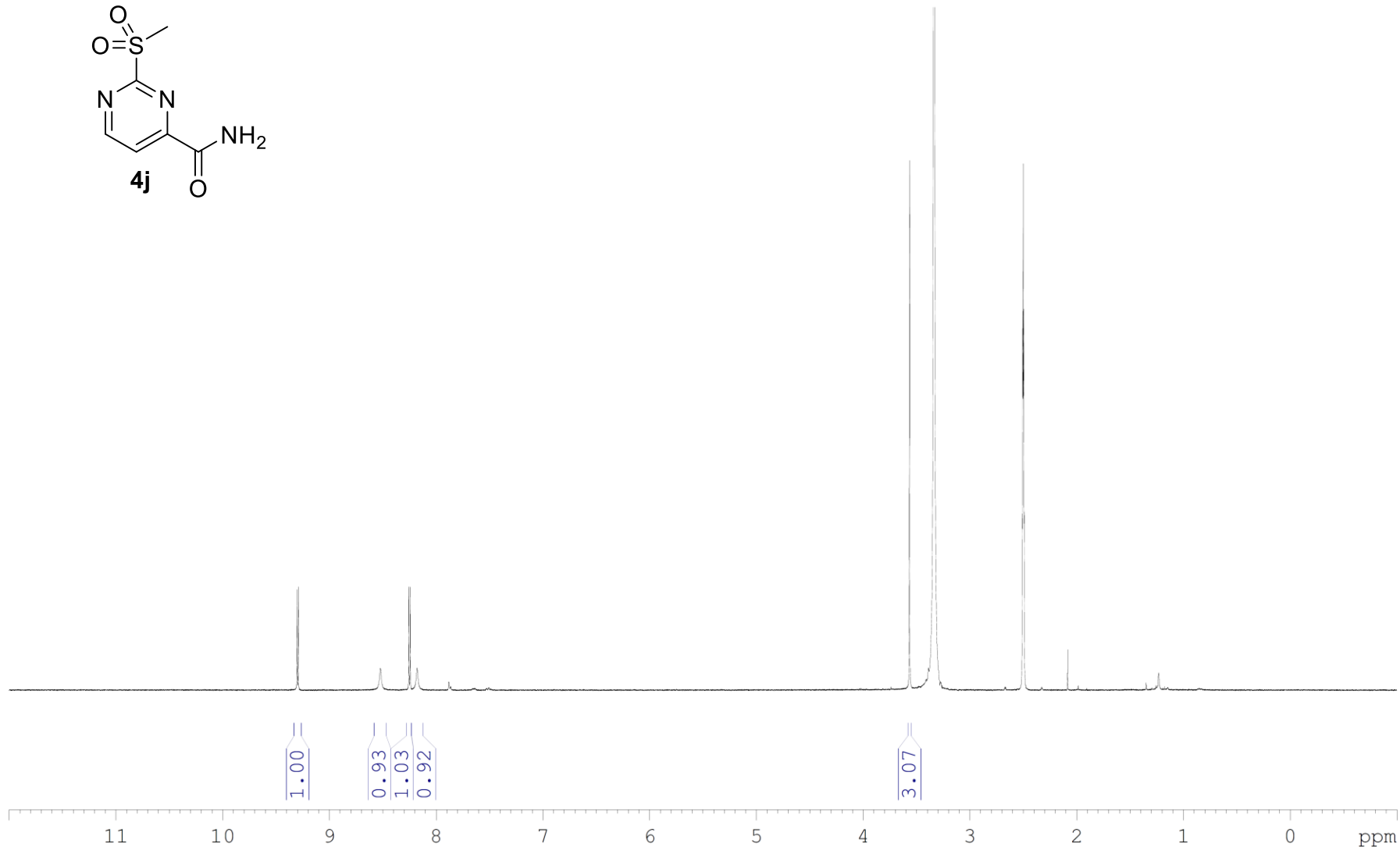
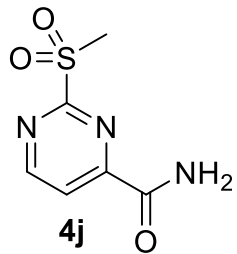
2-SO2Me 4-C(O)NH2

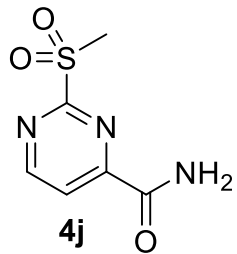
9.30
9.29

8.52
8.25
8.24
8.18

3.57
3.34

2.50



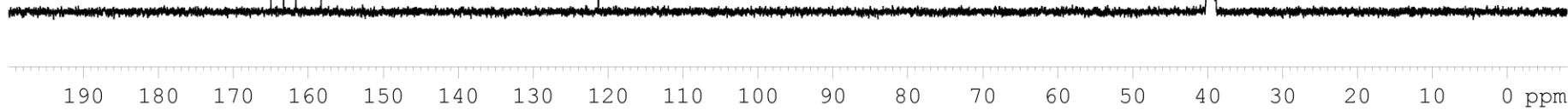


165.00
163.30
161.68
158.29

121.29

13C NMR (100 MHz, DMSO-d6)
2-SO2Me 4-C(O)NH2

38.93



2-SO₂Me 4-COOMe

9.36
9.35

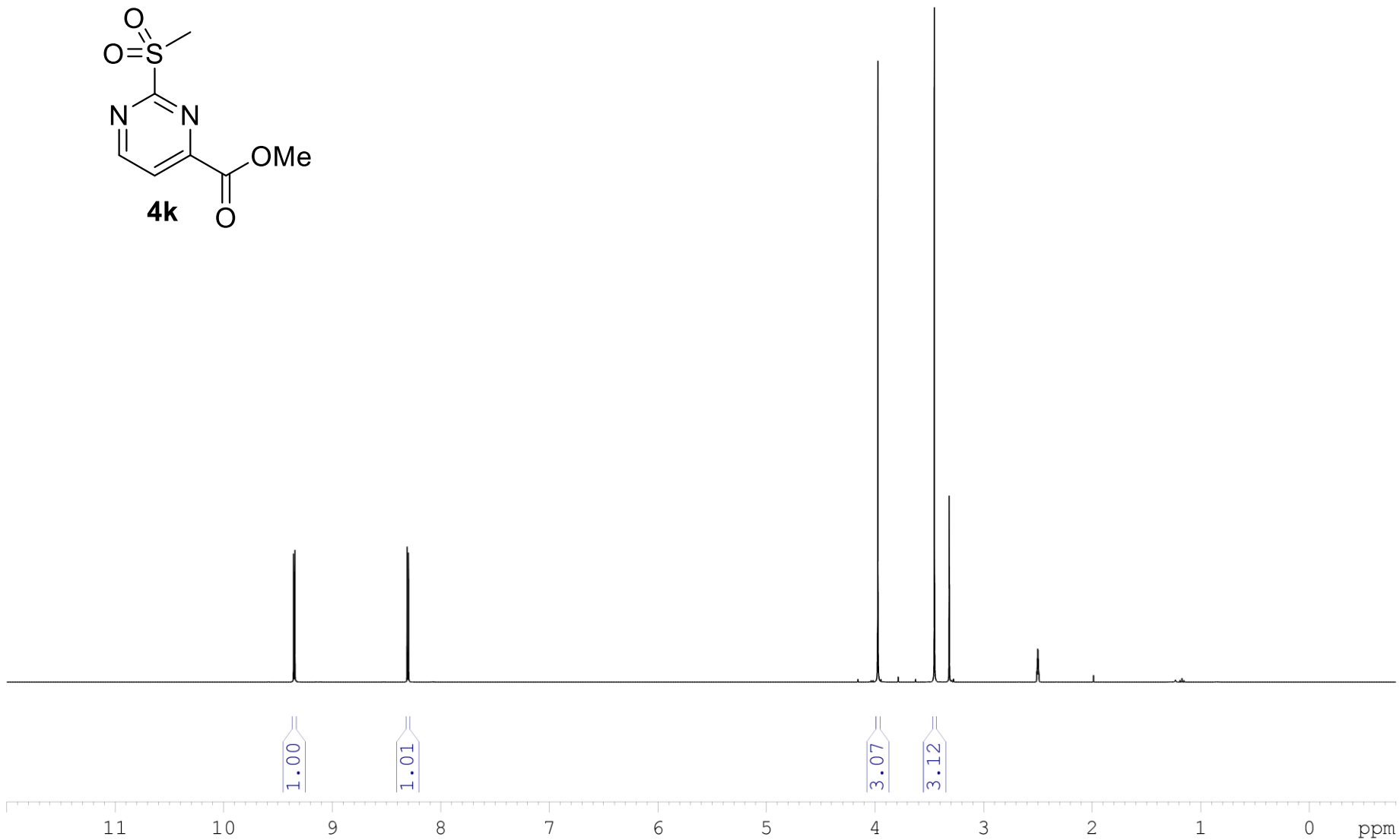
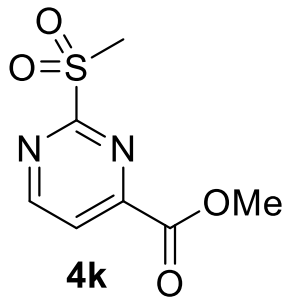
8.31
8.30

¹H NMR (400 MHz, DMSO-d₆)

3.97

3.32

2.50



2-SO₂Me 4-CO₂Me

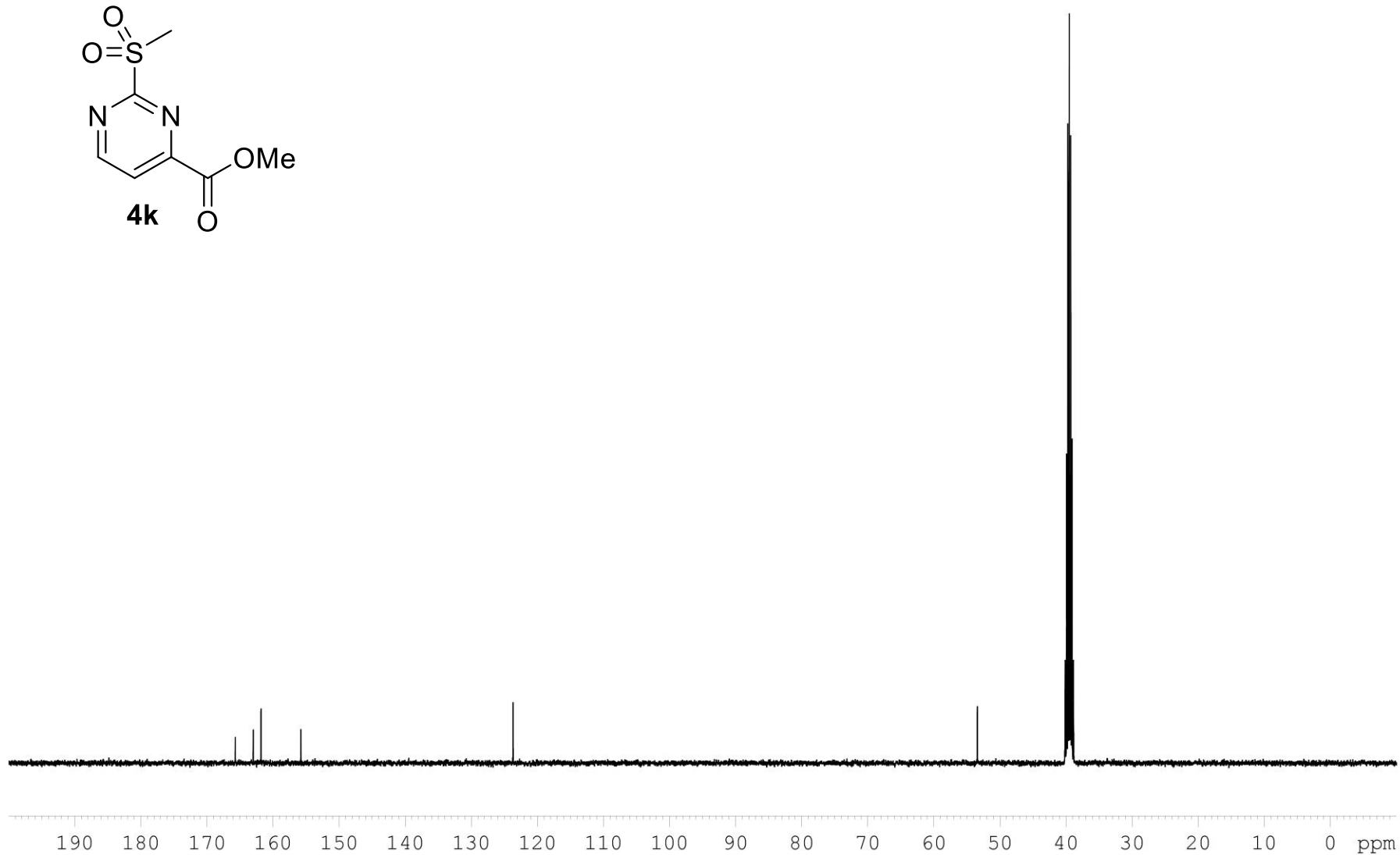
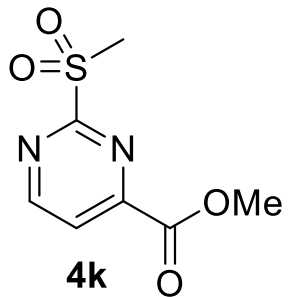
165.73
163.01
161.83
155.80

123.70

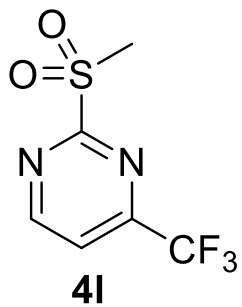
¹³C NMR (100 MHz, DMSO-d₆)

53.44

39.17



2-SO₂Me 4-CF₃



¹H NMR (400 MHz, DMSO-d₆)

9.48
9.47

8.40
8.39

3.48
3.35

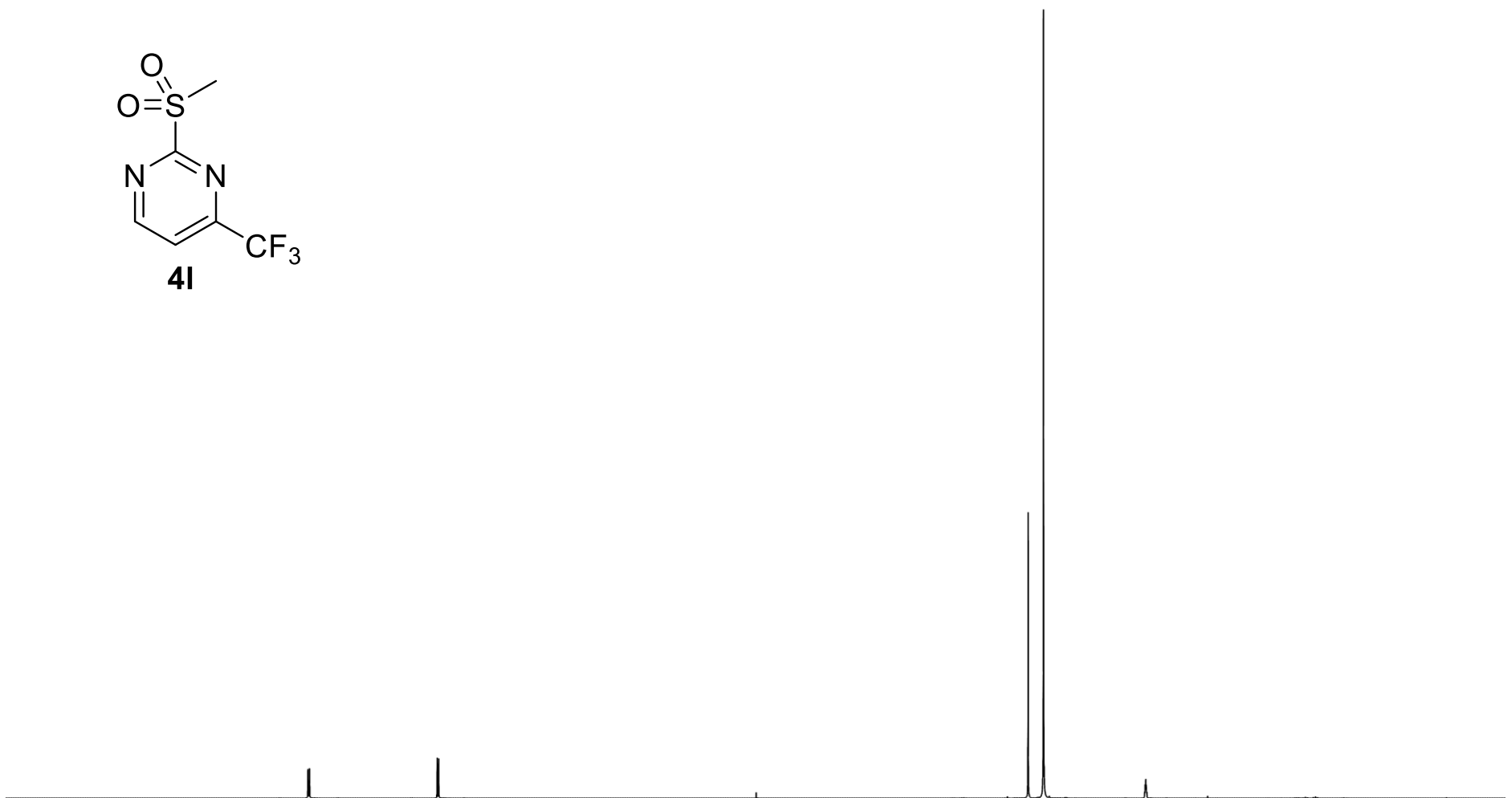
2.50

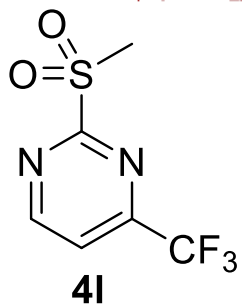
1.00

1.02

3.16

11 10 9 8 7 6 5 4 3 2 1 0 ppm



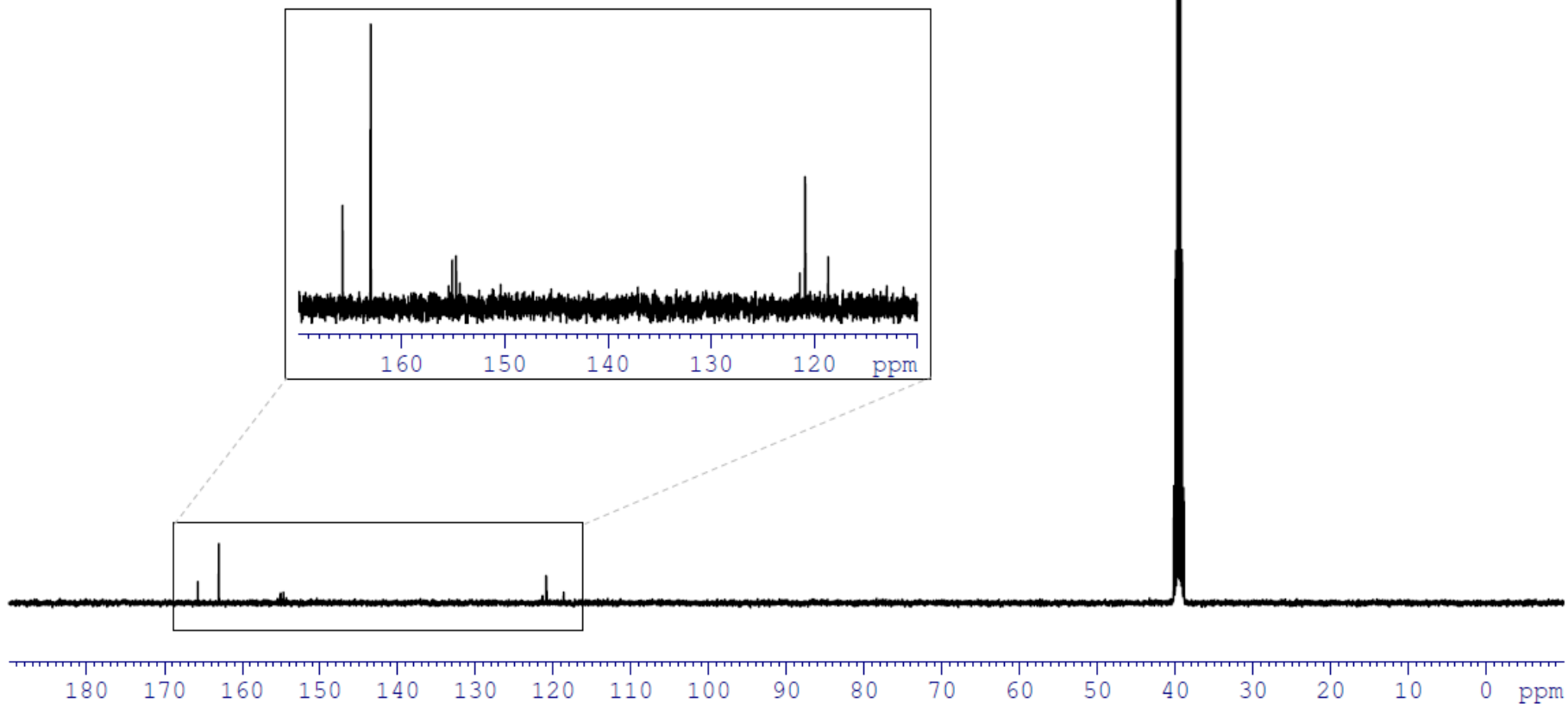


165.723
162.997
155.449
155.077
154.711
154.348

121.379
120.919
120.887
120.862
120.839
118.642

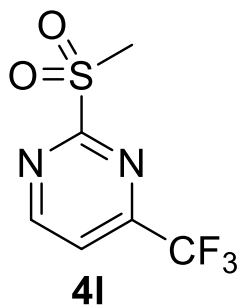
2-SO₂Me 4-CF₃
13C (100MHz, DMSO-D₆)

39.135

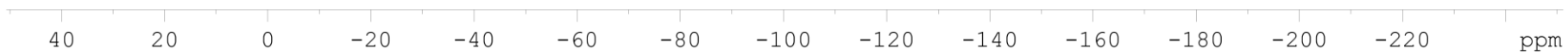


2-SO₂Me 4-CF₃

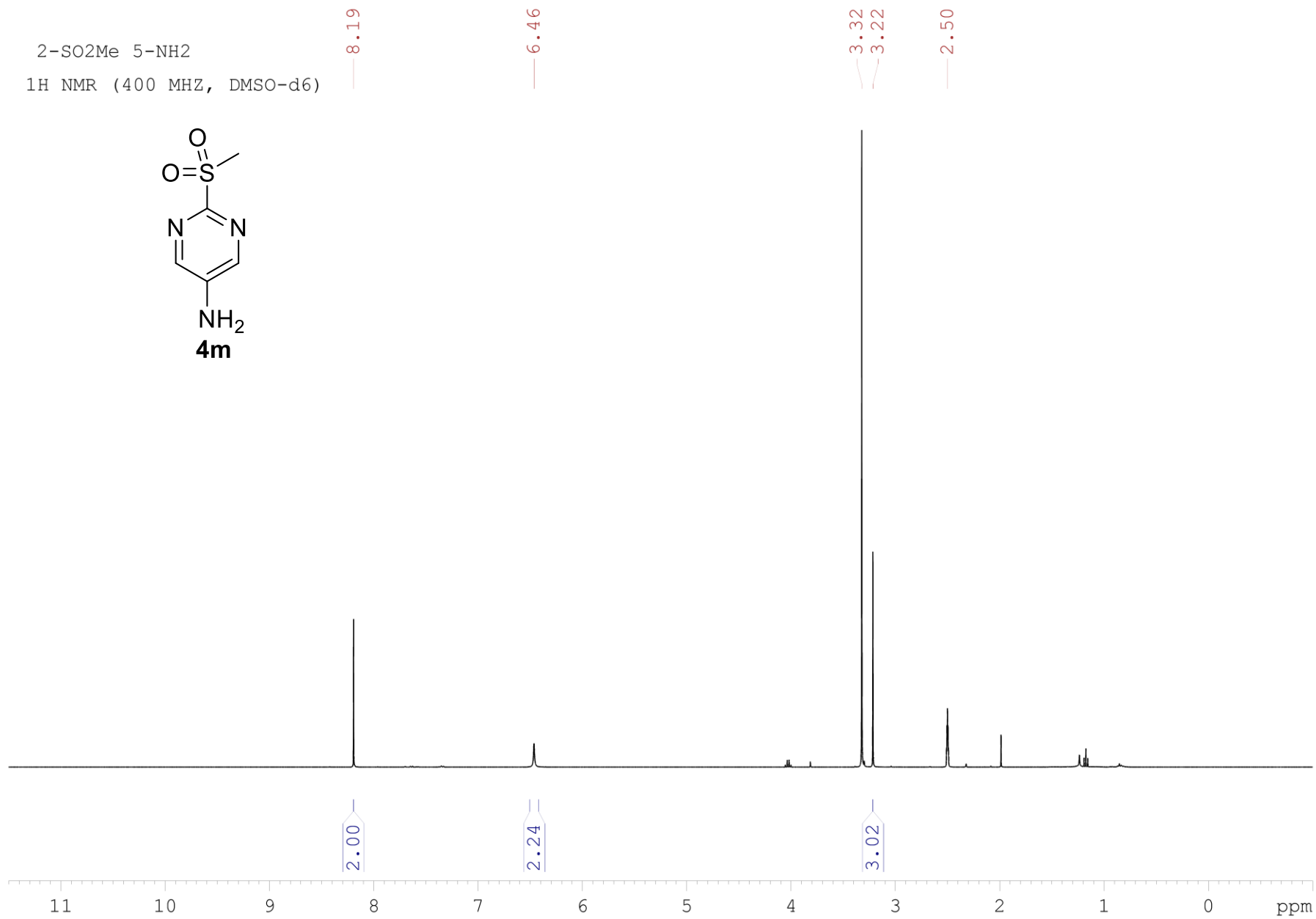
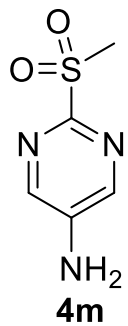
¹⁹F NMR (376 MHz, DMSO-d₆)



— -68.59



2-SO₂Me 5-NH₂
1H NMR (400 MHz, DMSO-d₆)

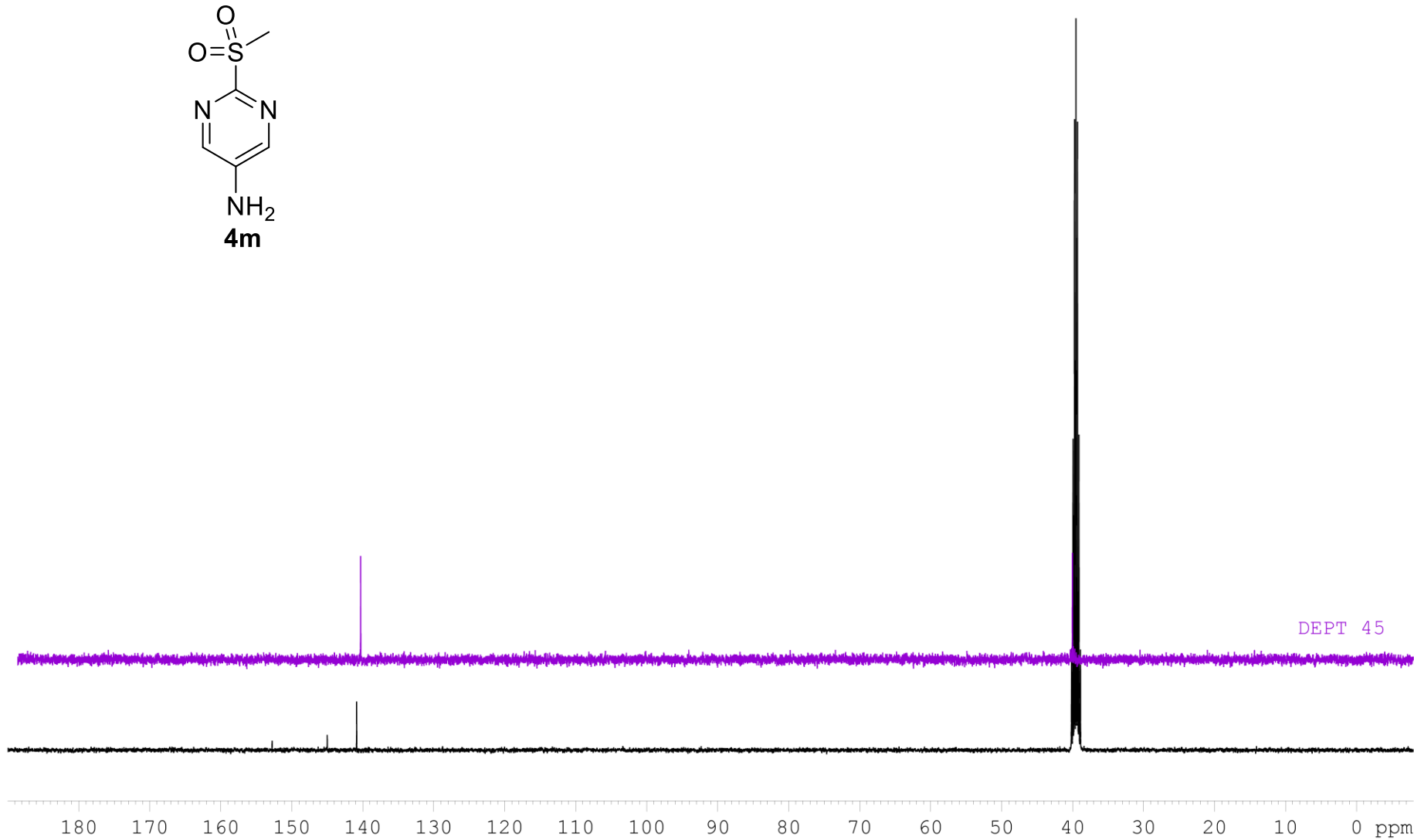
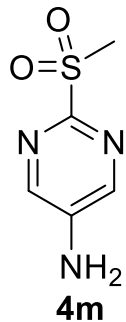


2-SO₂Me 5-NH₂

— 152.76
— 144.99
— 140.85

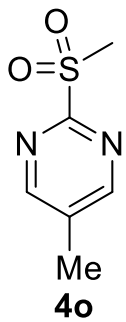
¹³C NMR (100 MHz, DMSO-d₆)

— 39.9

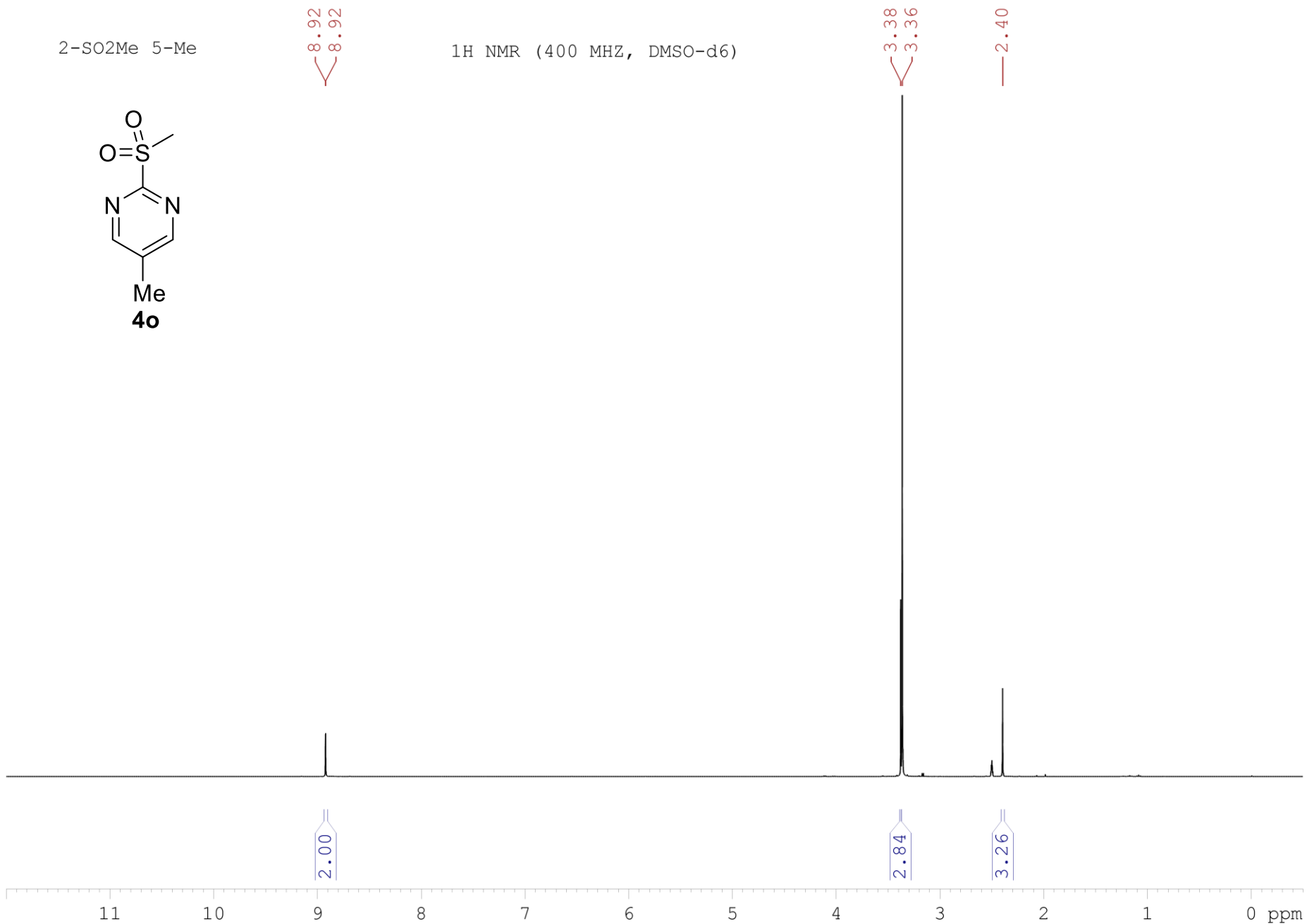


DEPT 45

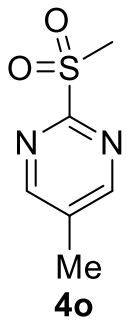
2-SO₂Me 5-Me



¹H NMR (400 MHz, DMSO-d₆)



2-SO₂Me 5-Me



¹³C NMR (100 MHz, DMSO-d₆)

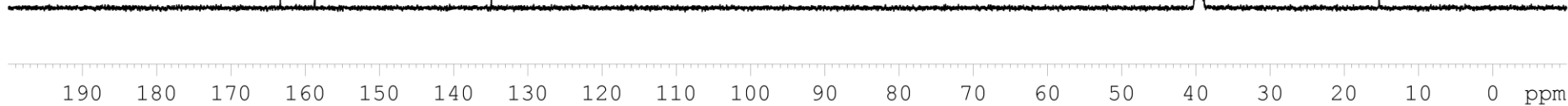
— 163.33

— 158.66

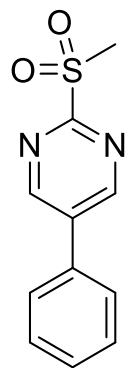
— 134.88

— 39.23

— 15.26



2-SO₂Me 5-Ph



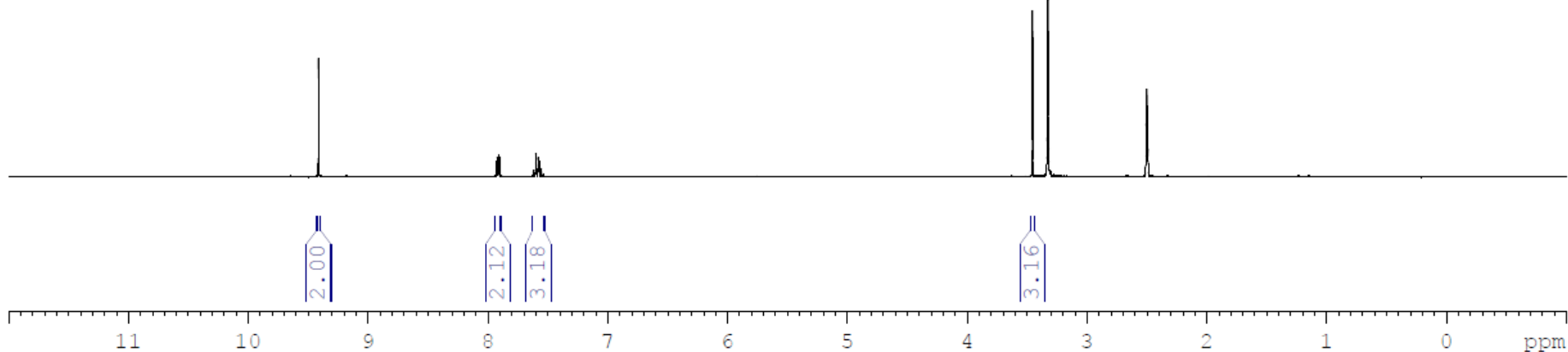
4p

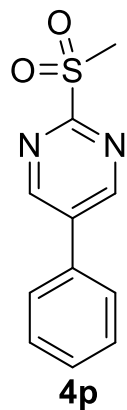
9.42

7.92
7.91
7.90
7.60
7.58
7.57

1H NMR (400 MHz, DMSO-d₆)

3.45
3.33





— 164.17

— 156.43

— 135.53

— 132.46

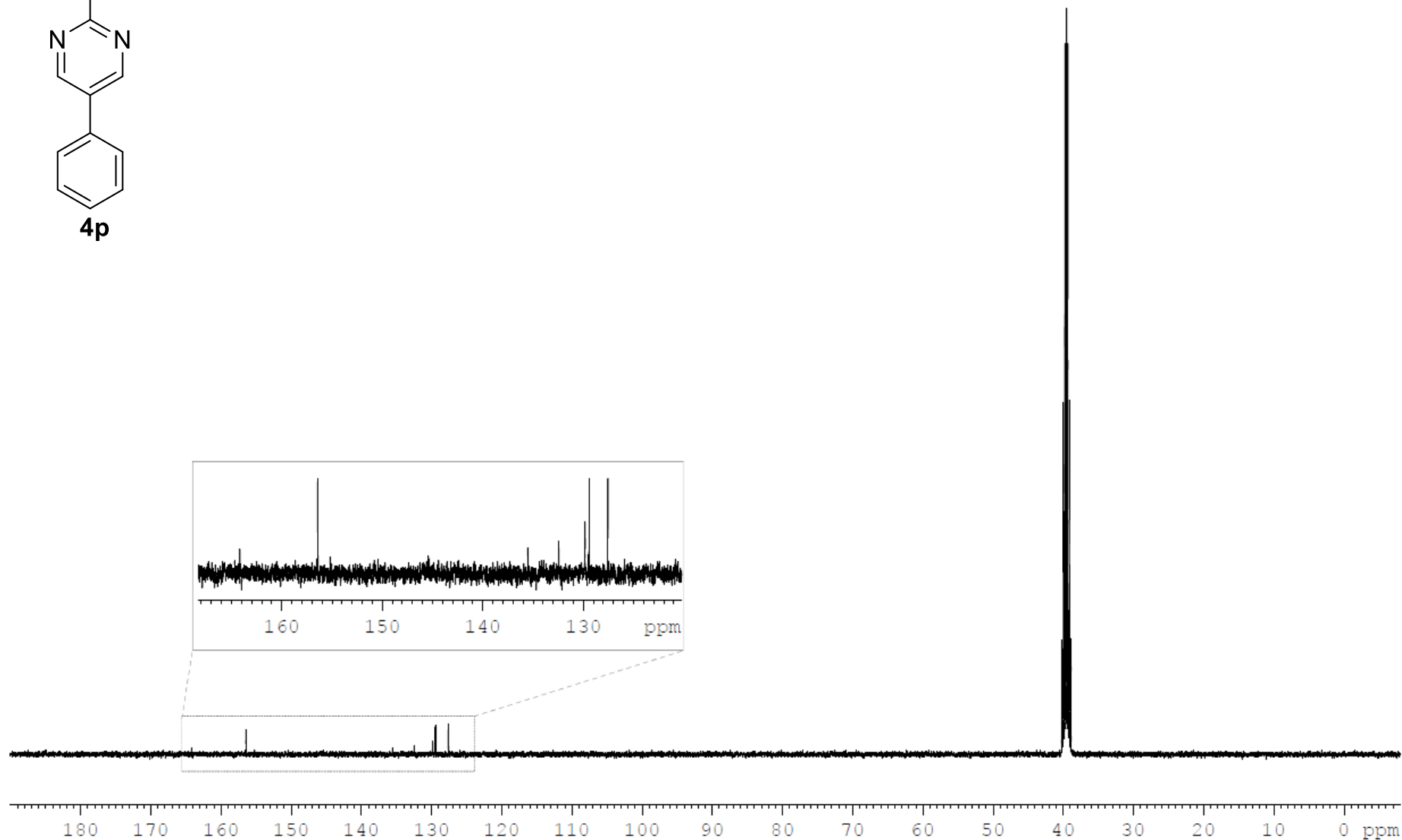
— 129.84

— 129.44

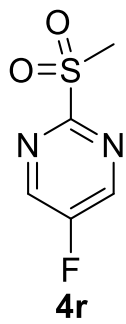
— 127.58

2-SO₂Me 5-Ph

¹³C NMR (100 MHz, DMSO-d₆)



2-SO₂Me 5-F



¹H NMR (400 MHz, DMSO-d₆)

9.19
9.19

3.43
3.31

2.50

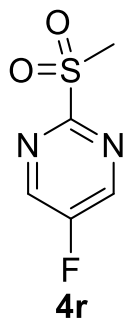


2.00

3.07

11 10 9 8 7 6 5 4 3 2 1 0 ppm

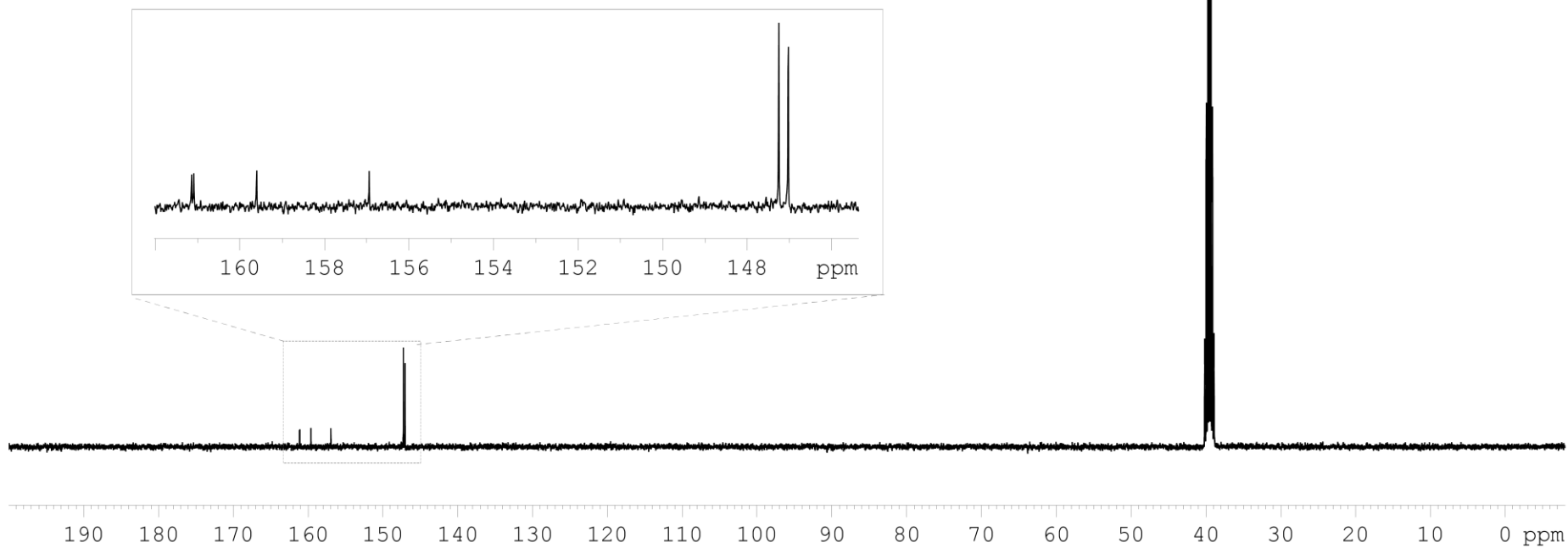
2-SO₂Me 5-F



161.14
161.09
159.61
156.94
147.25
147.03

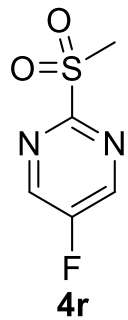
¹³C NMR (100 MHz, DMSO-d₆)

39.7

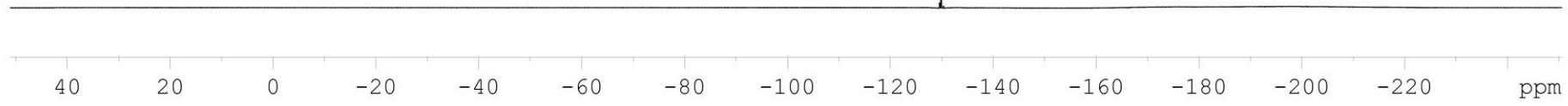


2-SO₂Me 5-F

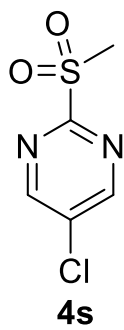
¹⁹F NMR (376 MHz, DMSO-d₆)



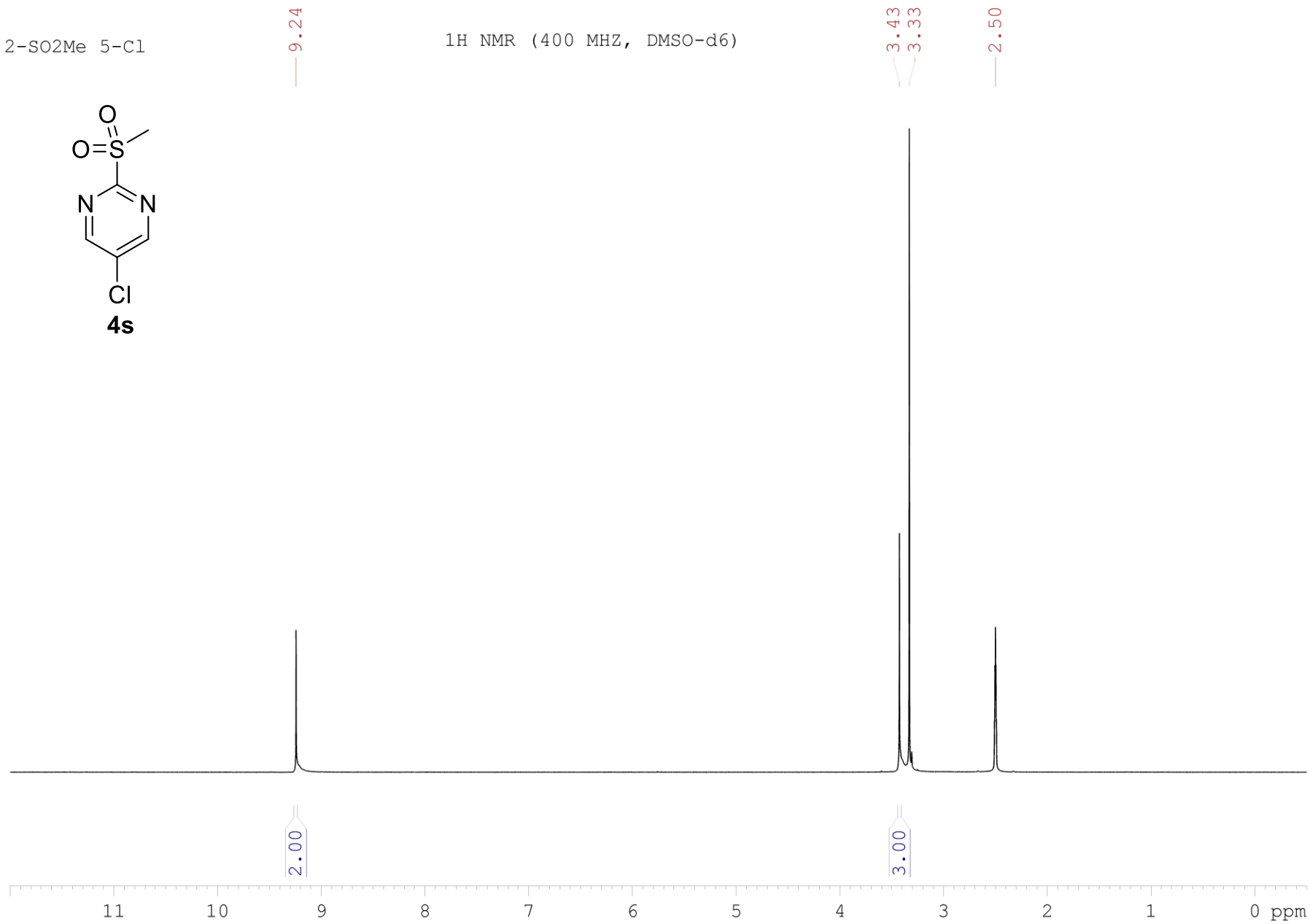
-129.88



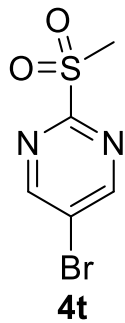
2-SO₂Me 5-Cl



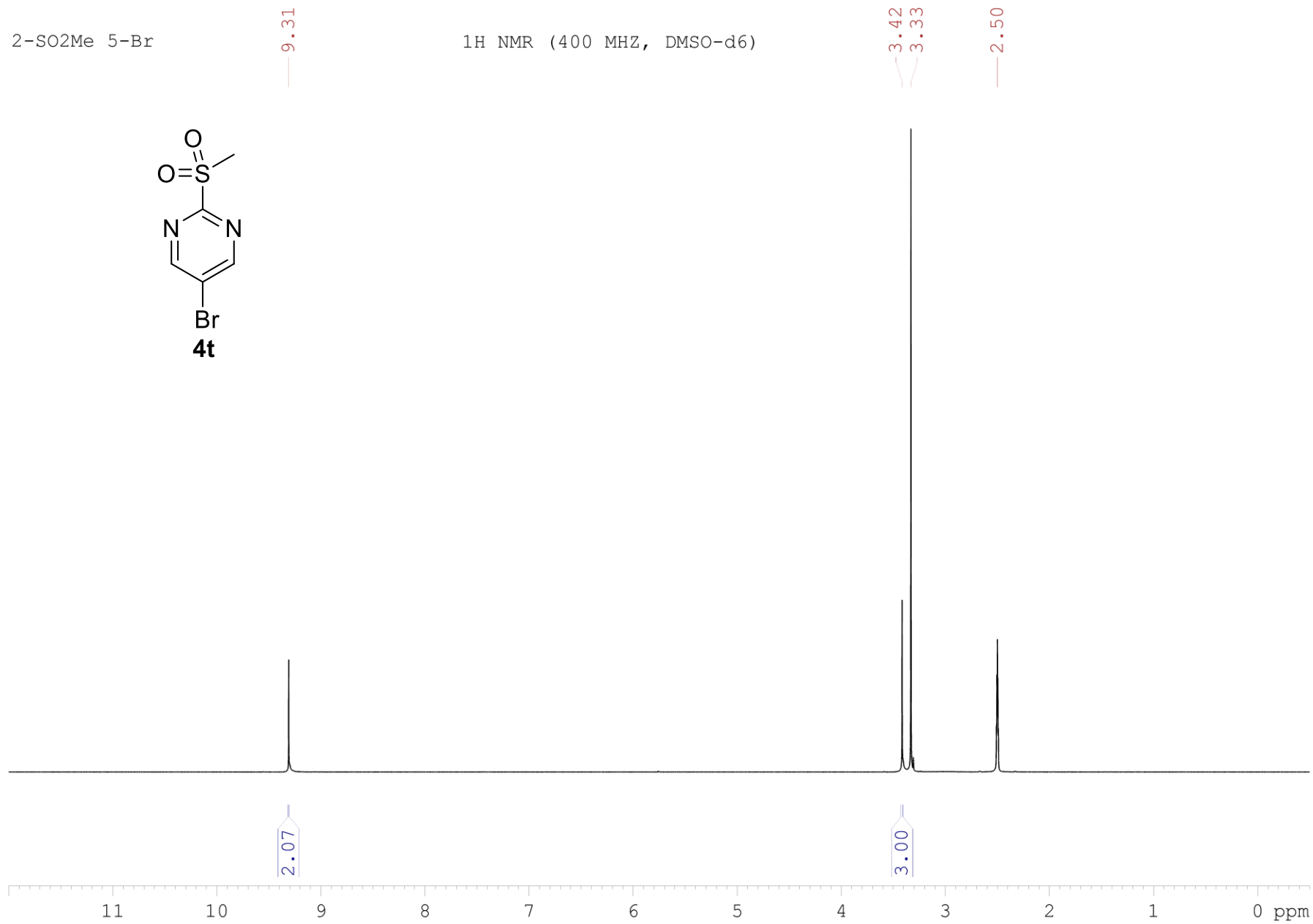
¹H NMR (400 MHz, DMSO-d₆)



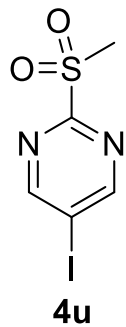
2-SO₂Me 5-Br



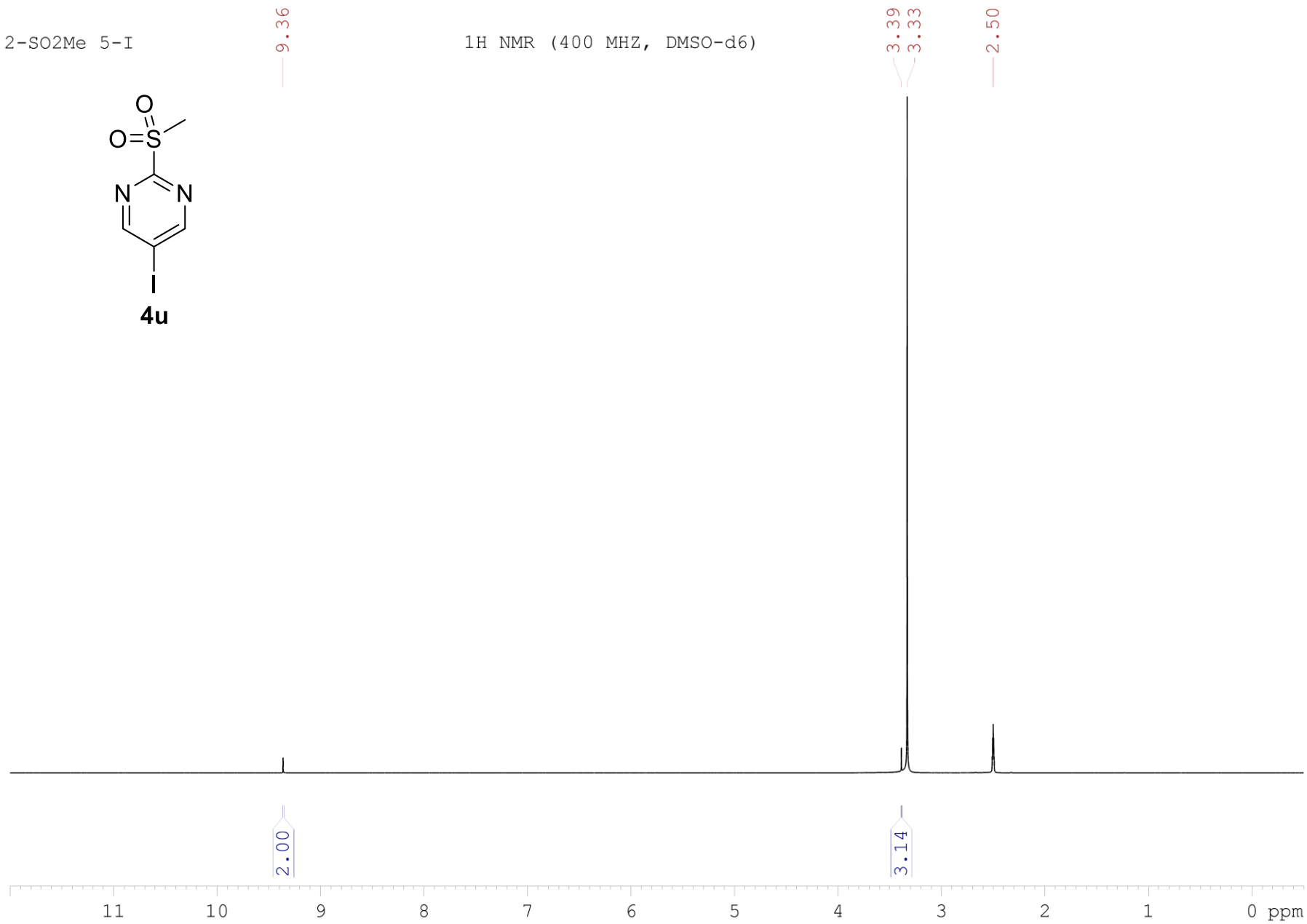
¹H NMR (400 MHz, DMSO-d₆)

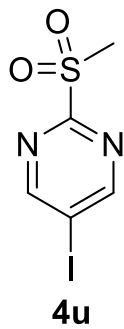


2-SO₂Me 5-I



¹H NMR (400 MHz, DMSO-d₆)





164.19
163.96

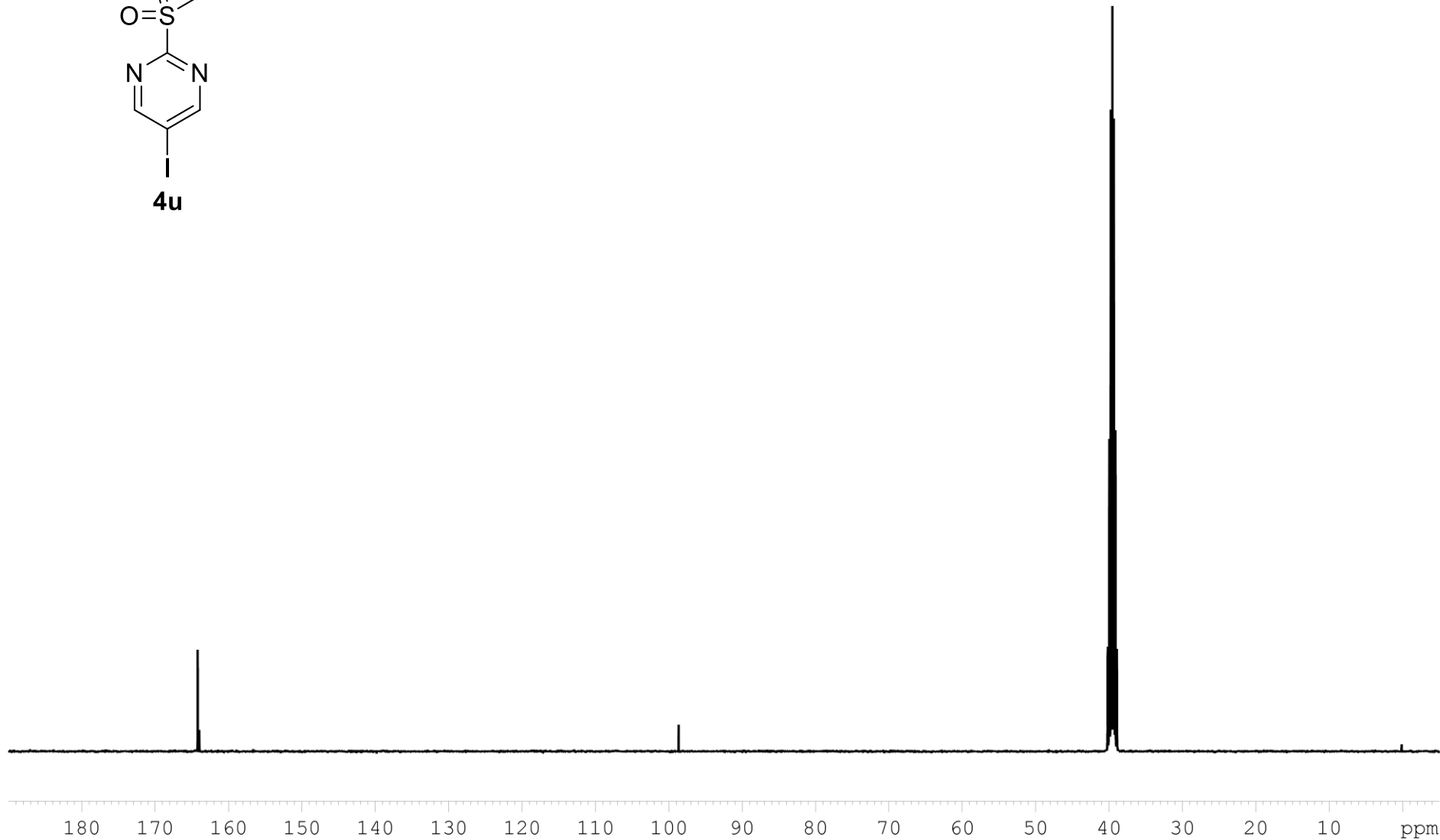
¹³C NMR (100 MHz, DMSO-d₆)

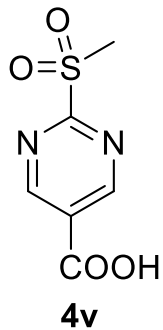
98.64

2-SO₂Me 5-I

39.22

0.10



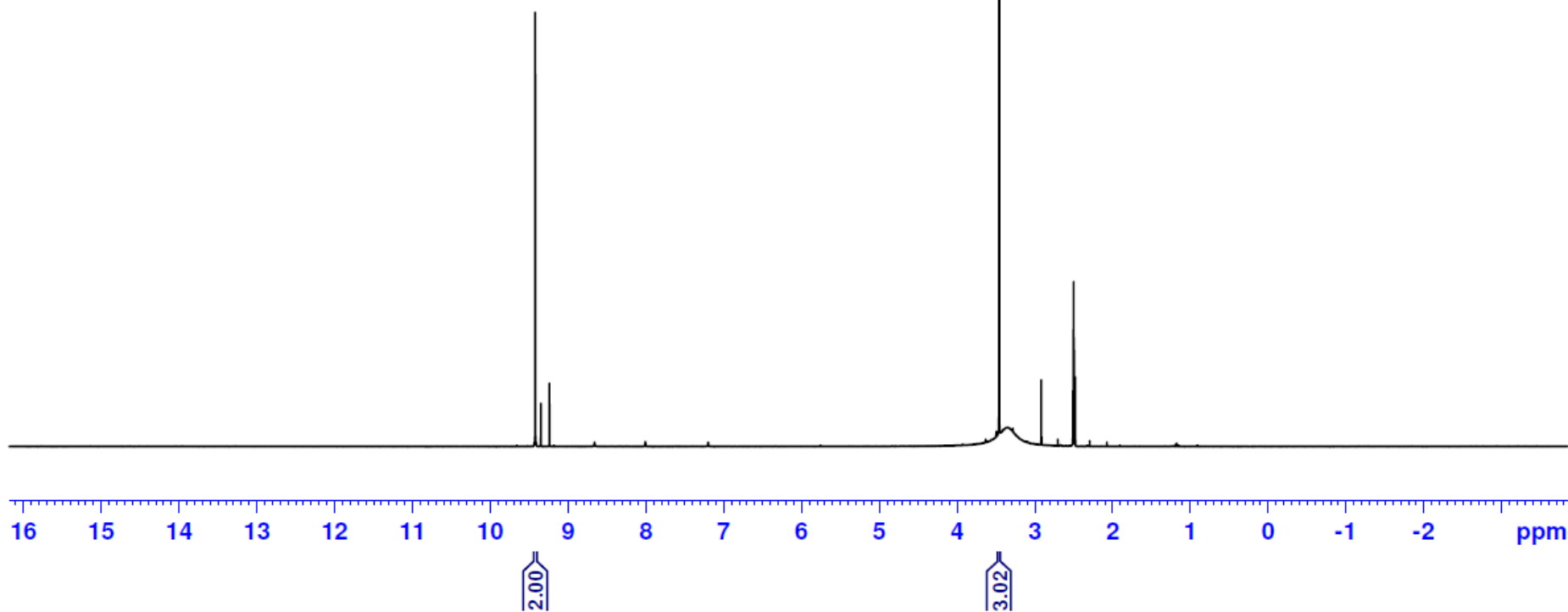


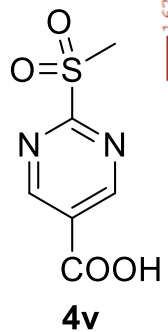
9.42

2-SO₂Me 5-COOH
1H (400 MHz, DMSO-d₆)

3.46

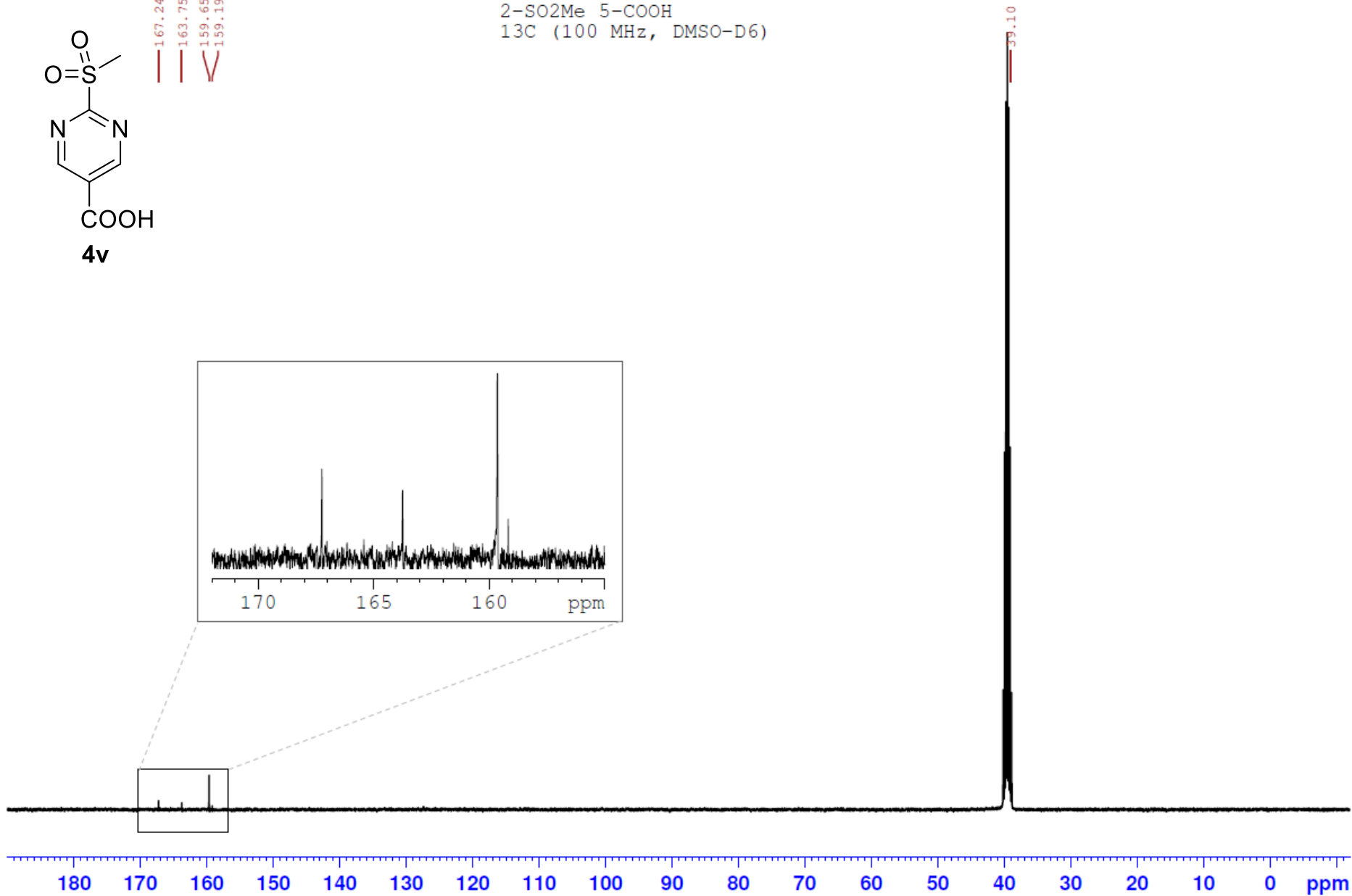
2.50



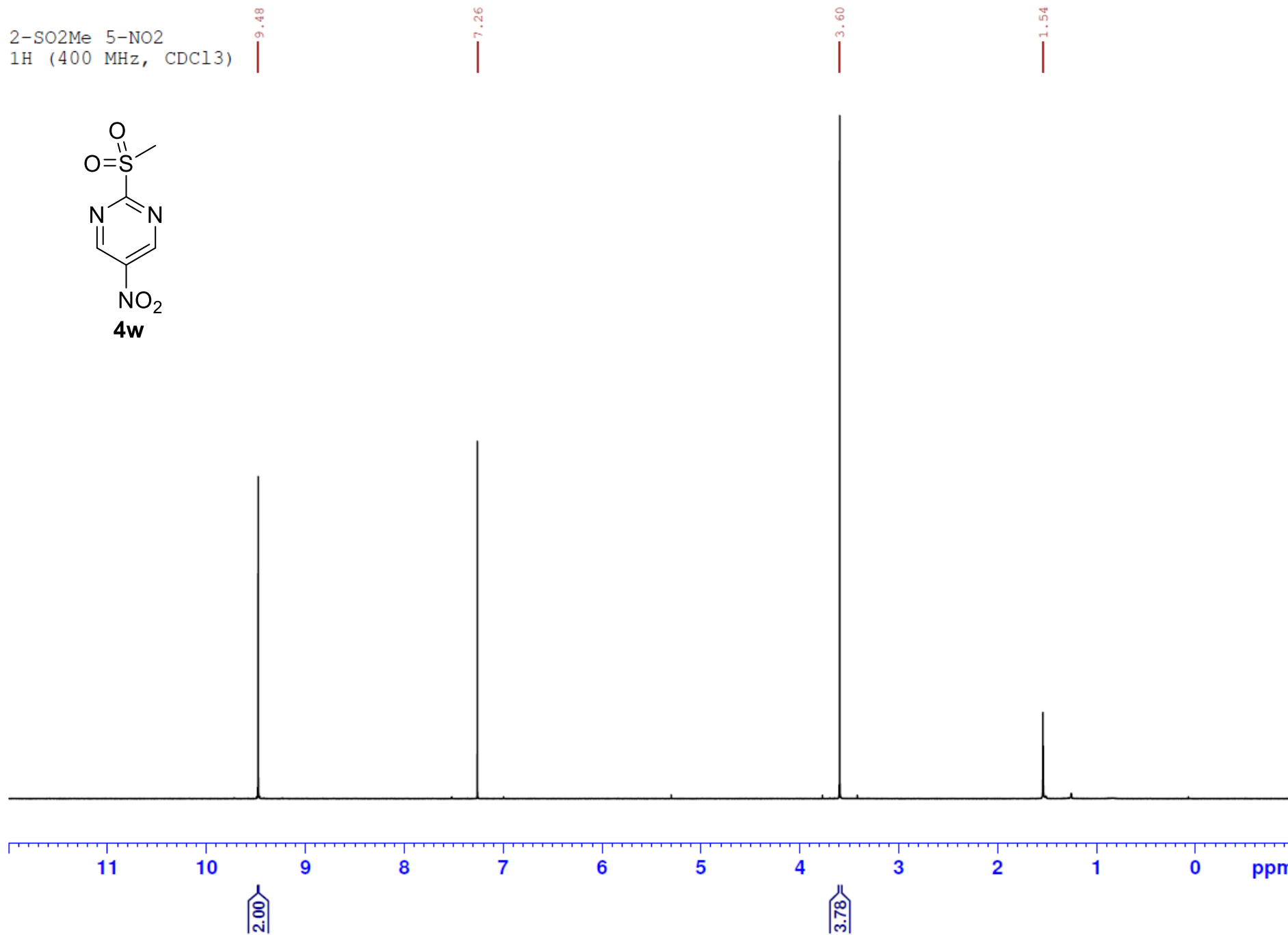
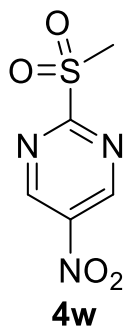


167.24
163.75
159.65
159.19

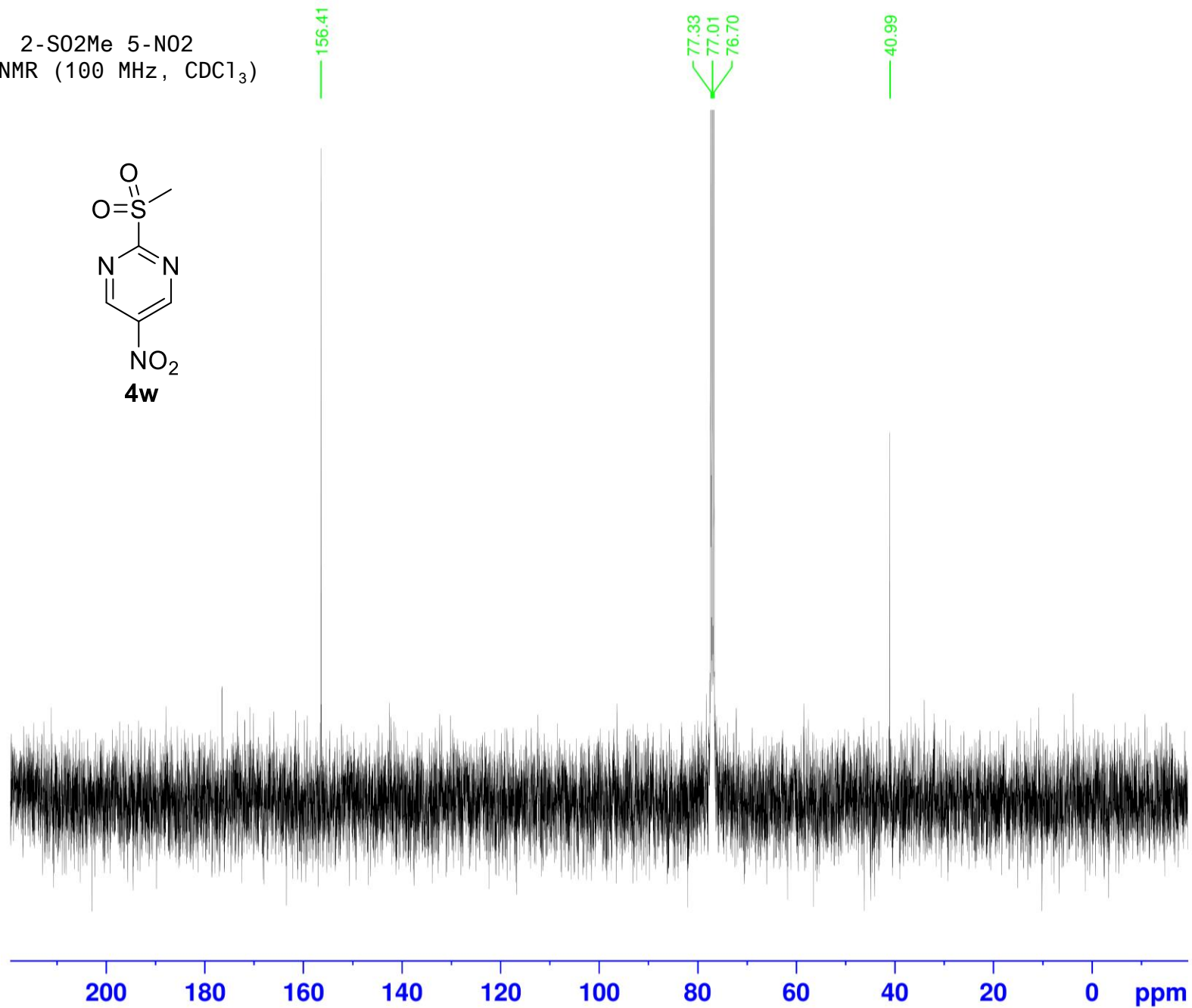
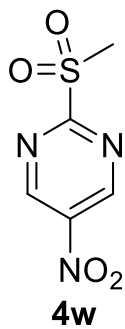
2-SO₂Me 5-COOH
13C (100 MHz, DMSO-D₆)



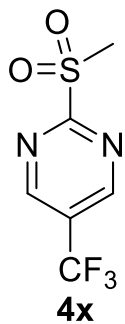
2-SO₂Me 5-NO₂
1H (400 MHz, CDCl₃)



2-SO₂Me 5-NO₂
¹³C NMR (100 MHz, CDCl₃)



2-SO₂Me 5-CF₃



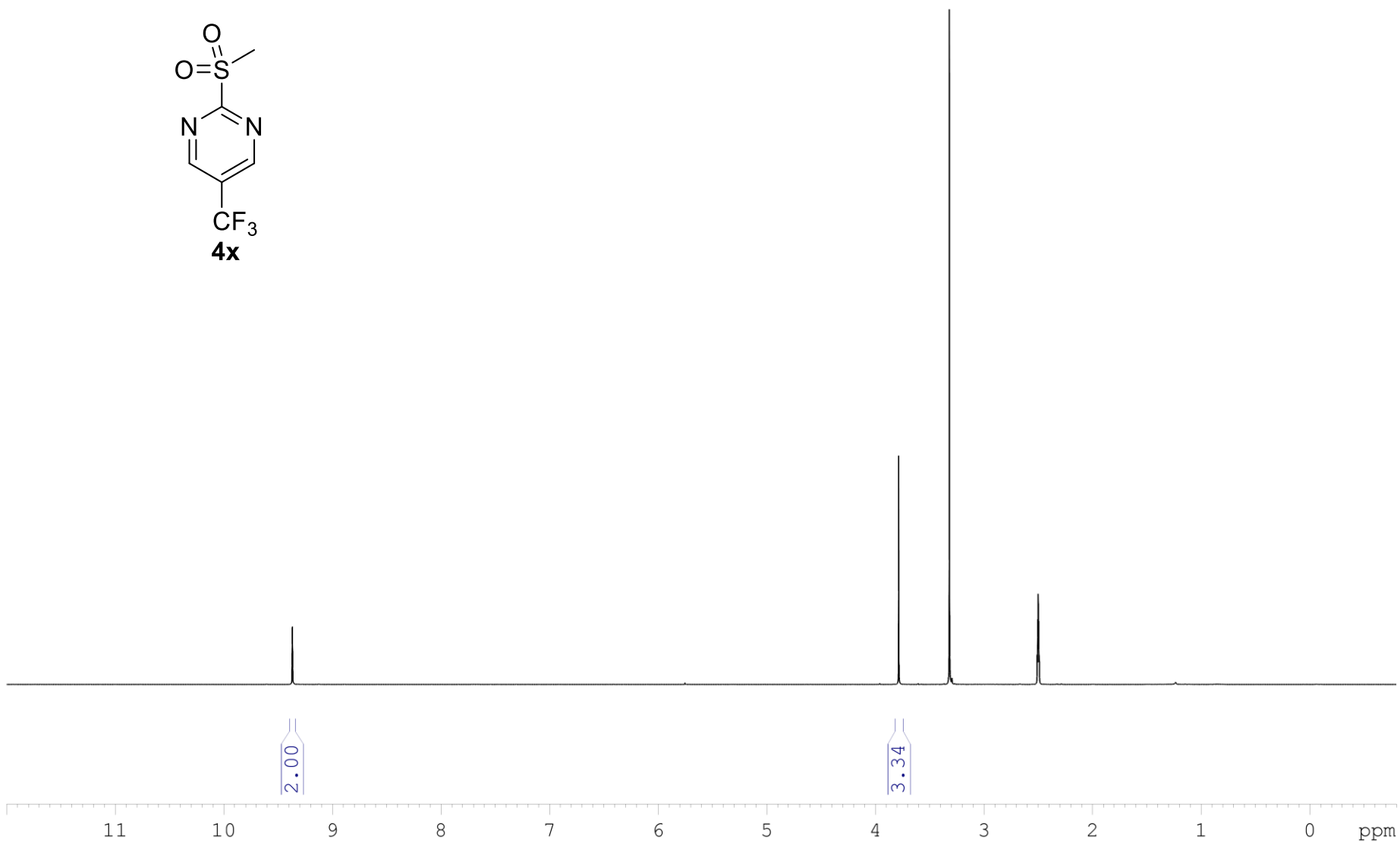
¹H NMR (400 MHz, DMSO-d₆)

9.37
9.37

3.78

3.32

2.50

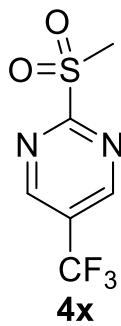


2.00

3.34

11 10 9 8 7 6 5 4 3 2 1 0 ppm

2-SO2Me 5-CF3

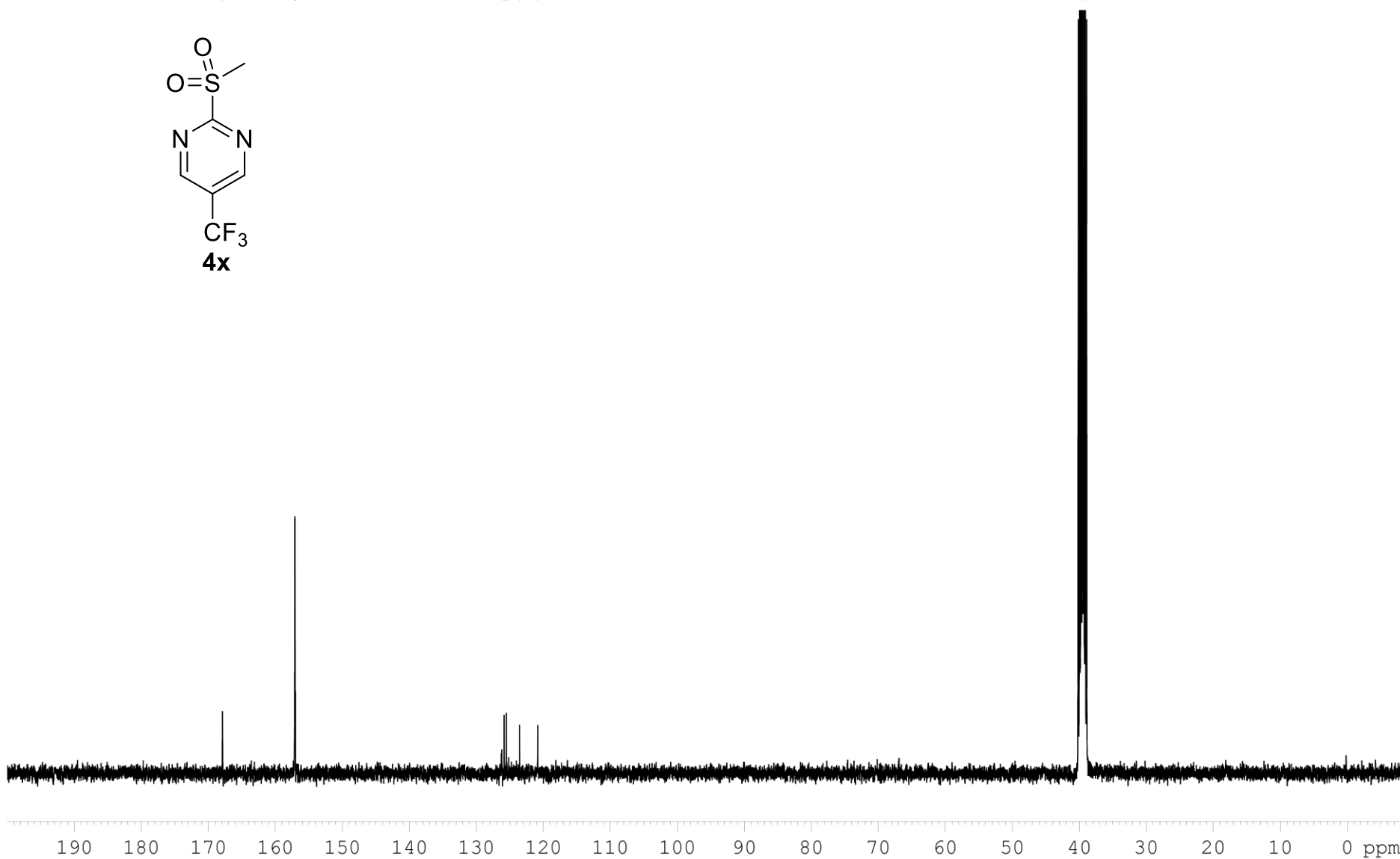


167.89
157.12
157.08
157.05
157.01

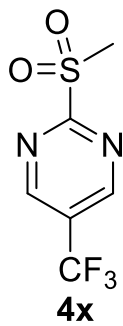
126.19
125.85
125.51
125.18
123.54
120.82

¹³C NMR (100 MHz, DMSO-d₆)

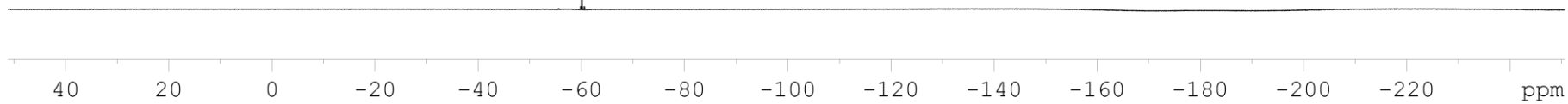
39.07



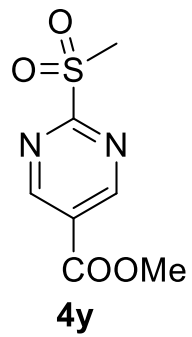
2-SO₂Me 5-CF₃
19F NMR (376 MHz, DMSO-d₆)



-60.08



2-SO₂Me 5-COOMe

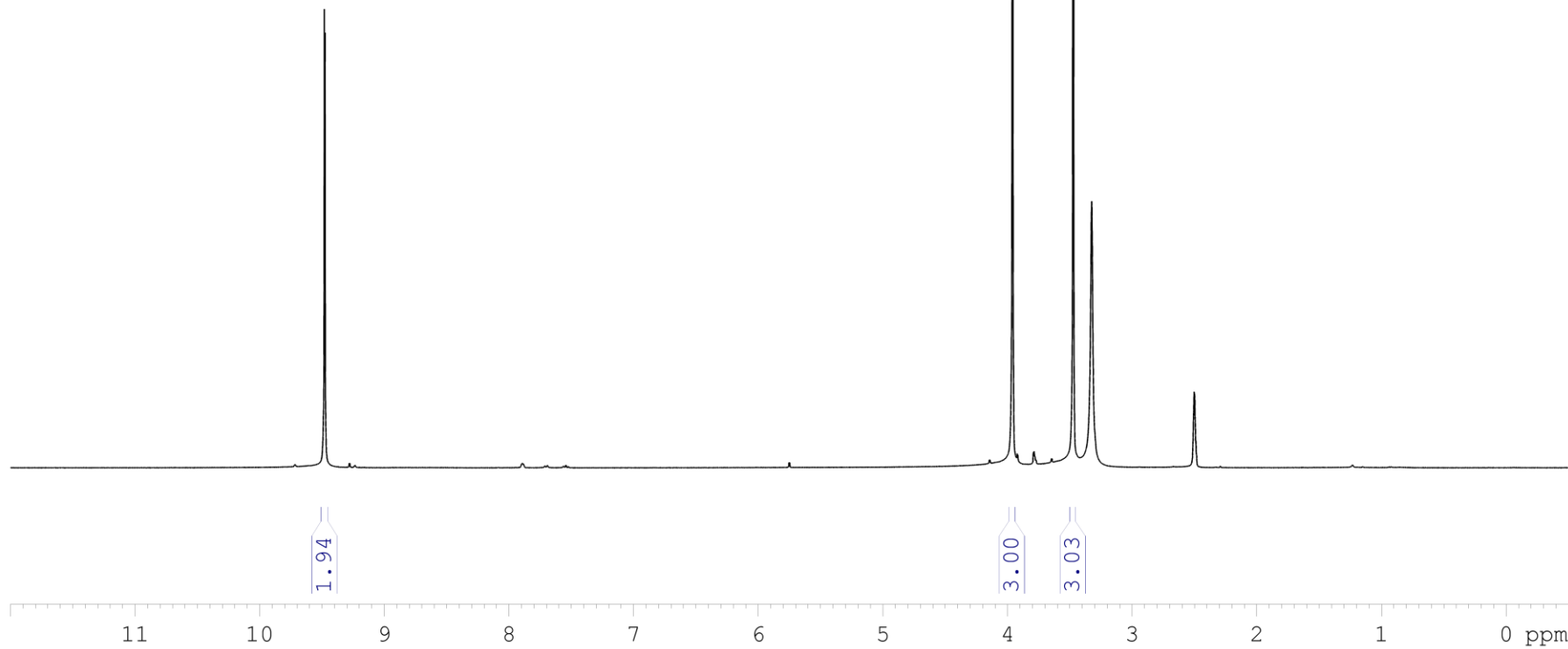


¹H NMR (400 MHz, DMSO-d₆)

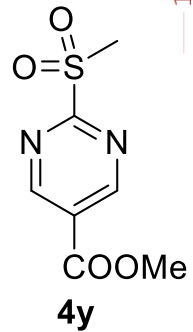
9.48
9.47

3.96
3.96
3.47
3.47
3.32

2.50



2-SO₂Me 5-COOMe



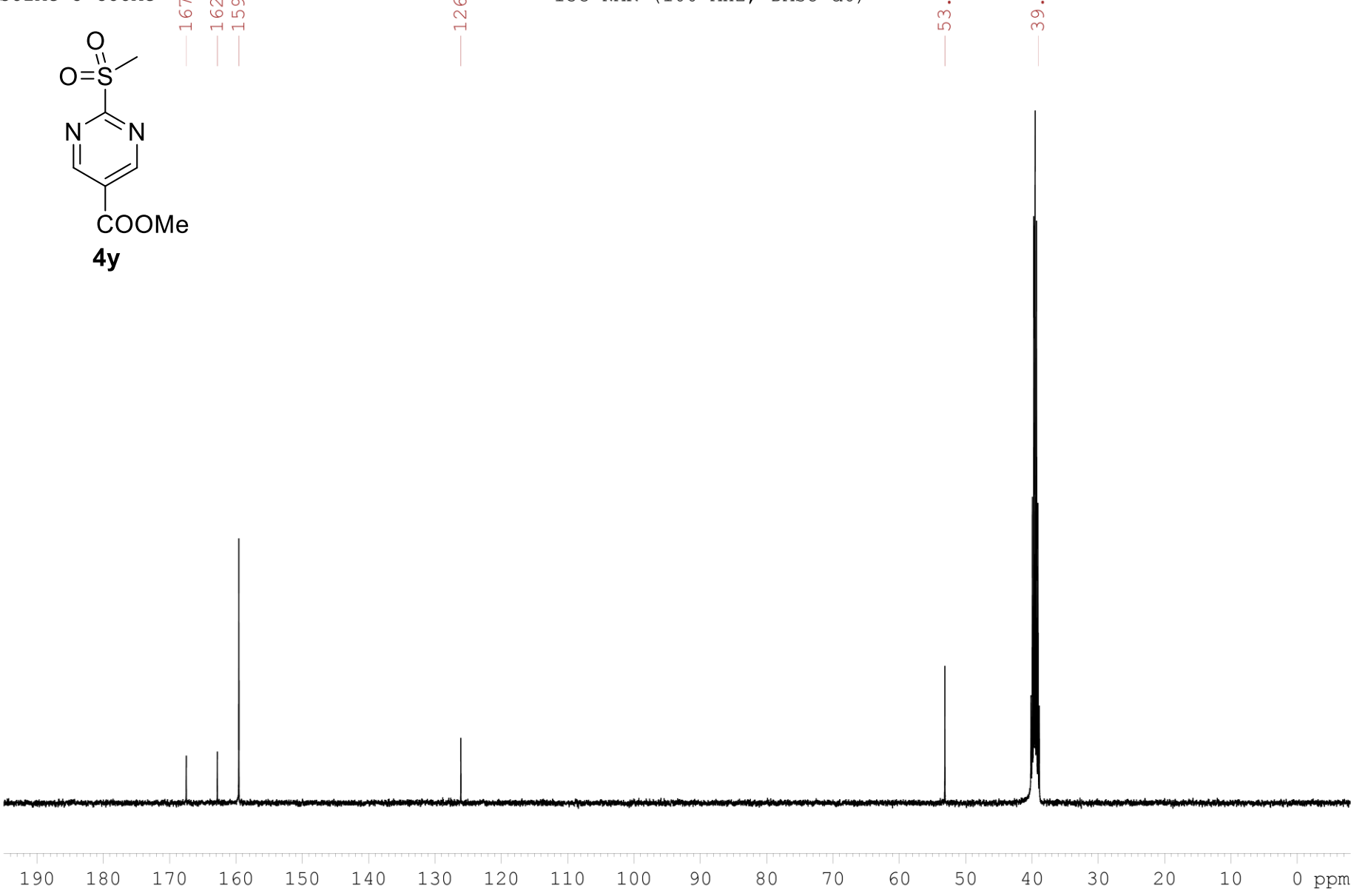
— 167.49
— 162.80
— 159.56

— 126.09

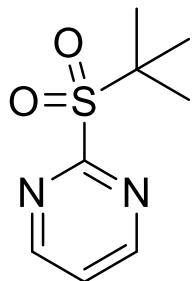
¹³C NMR (100 MHz, DMSO-d₆)

— 53.12

— 39.05



2-SO₂tBu pyrimidine



5a

¹H NMR (400 MHz, DMSO-d₆)

9.12
9.11

7.87

3.33

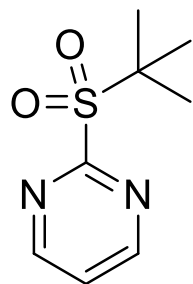
1.35

2.00

1.04

10.20

11 10 9 8 7 6 5 4 3 2 1 0 ppm



5a

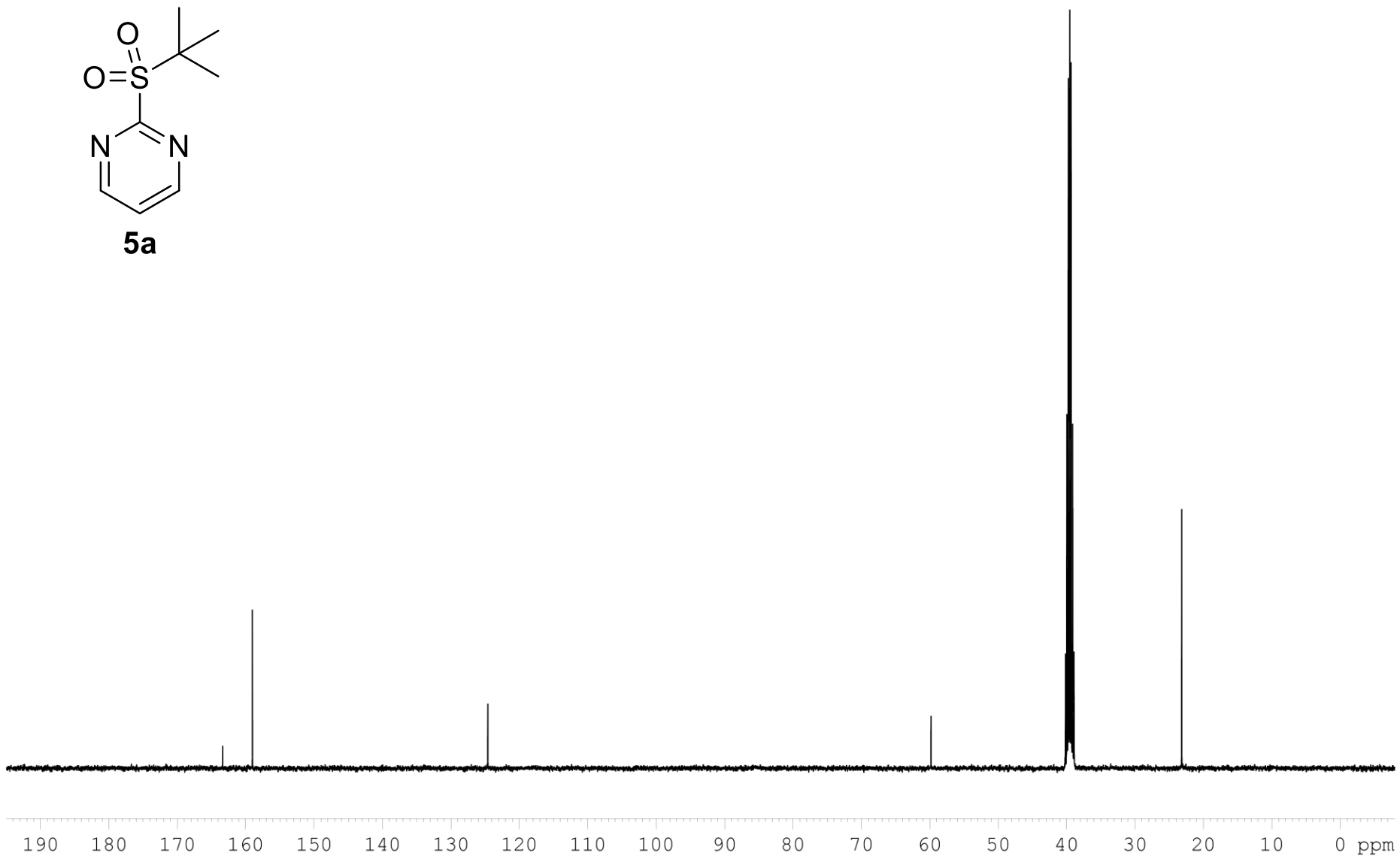
2-SO₂tBu pyrimidine
13C NMR (100 MHz, DMSO-d₆)

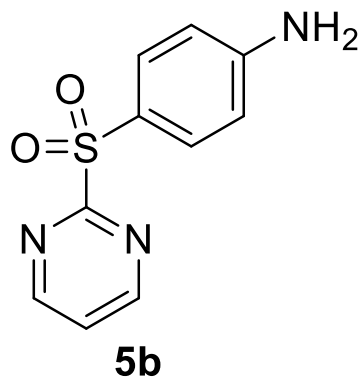
163.35
159.01

124.60

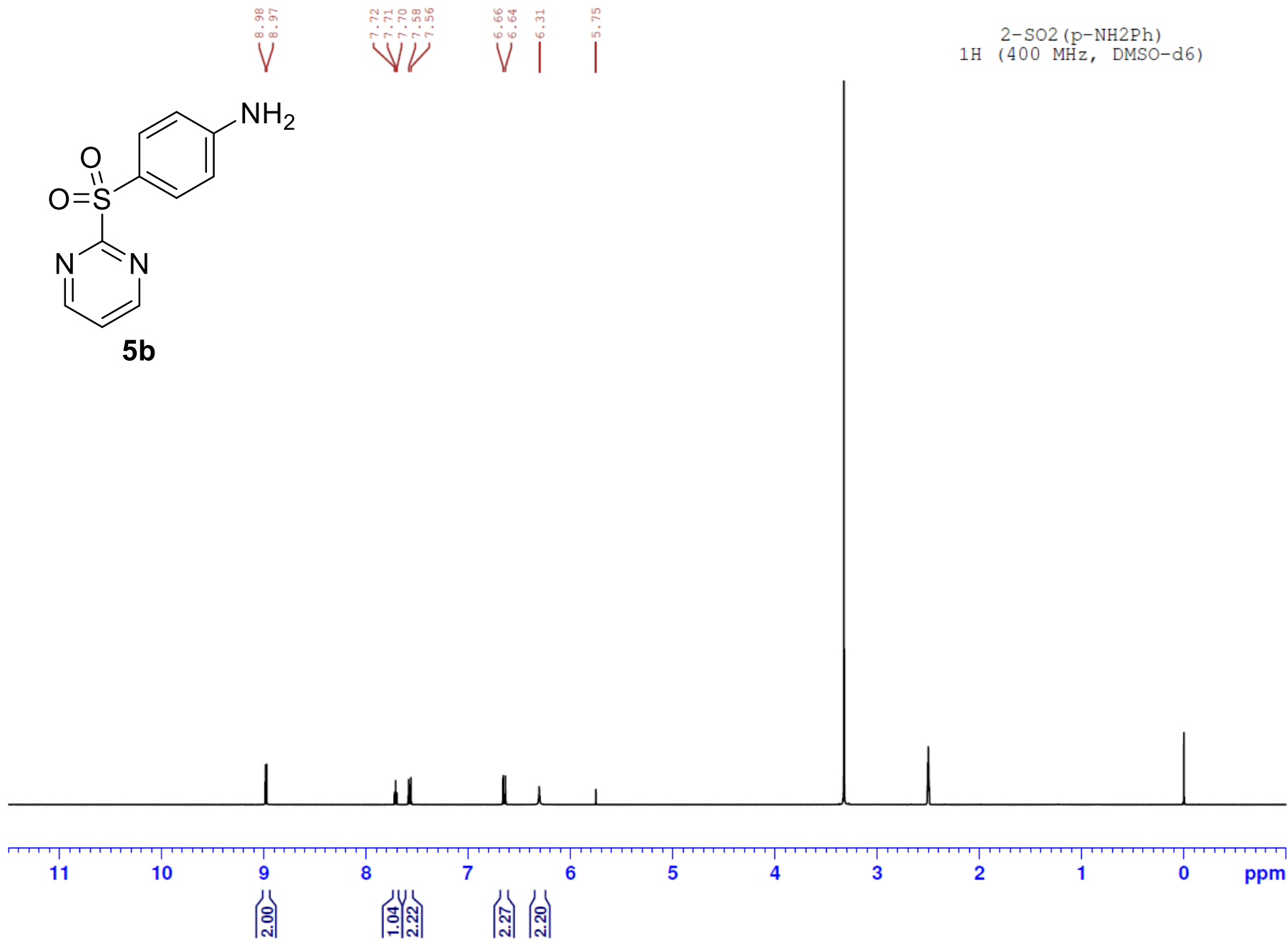
59.79

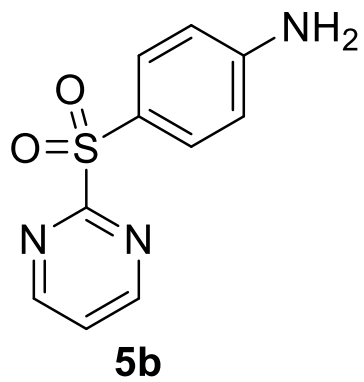
23.15



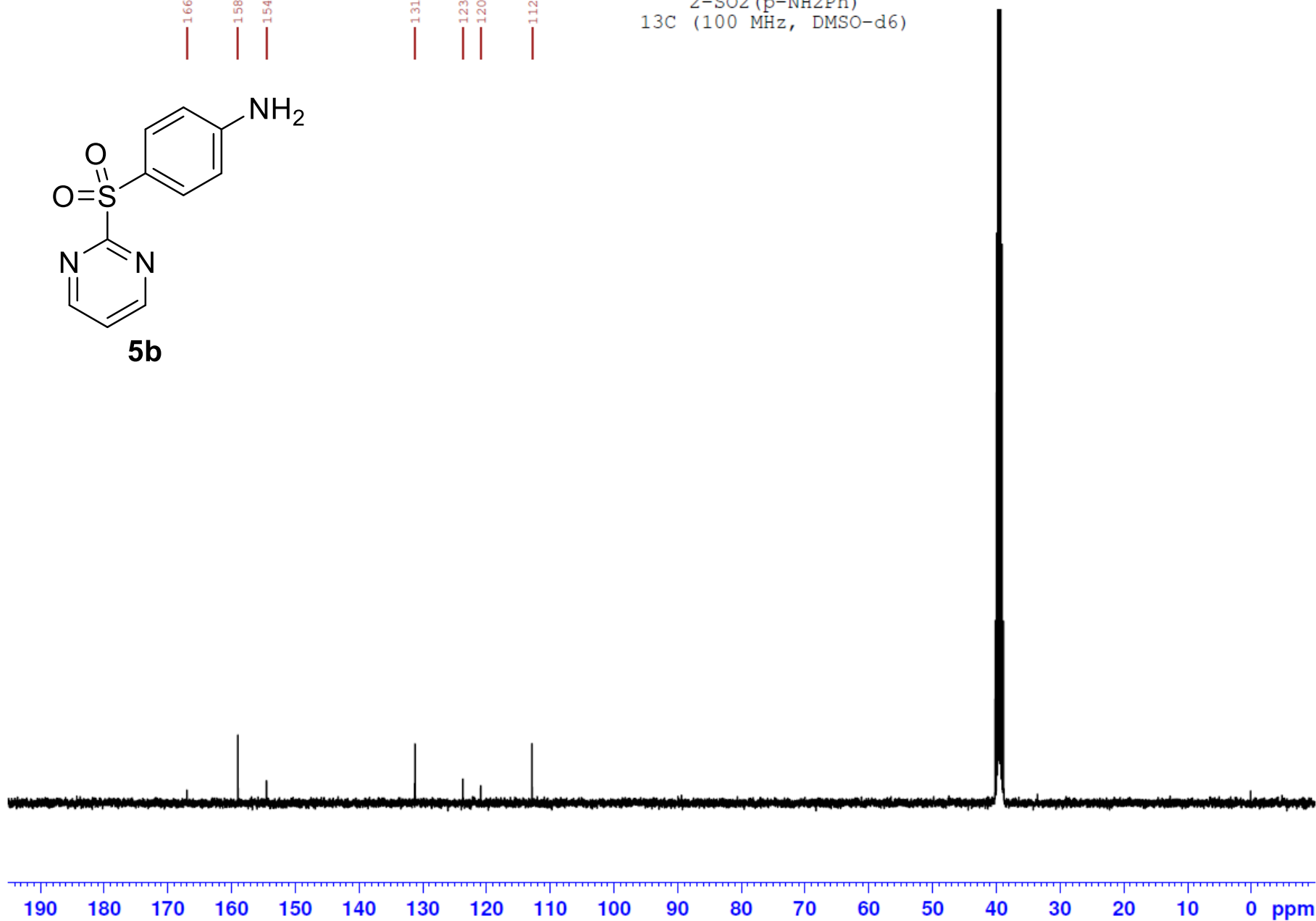


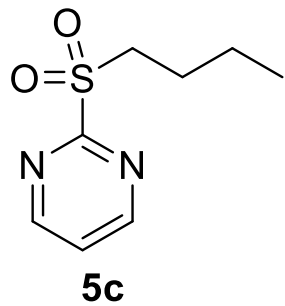
2-SO₂(p-NH₂Ph)
1H (400 MHz, DMSO-d₆)



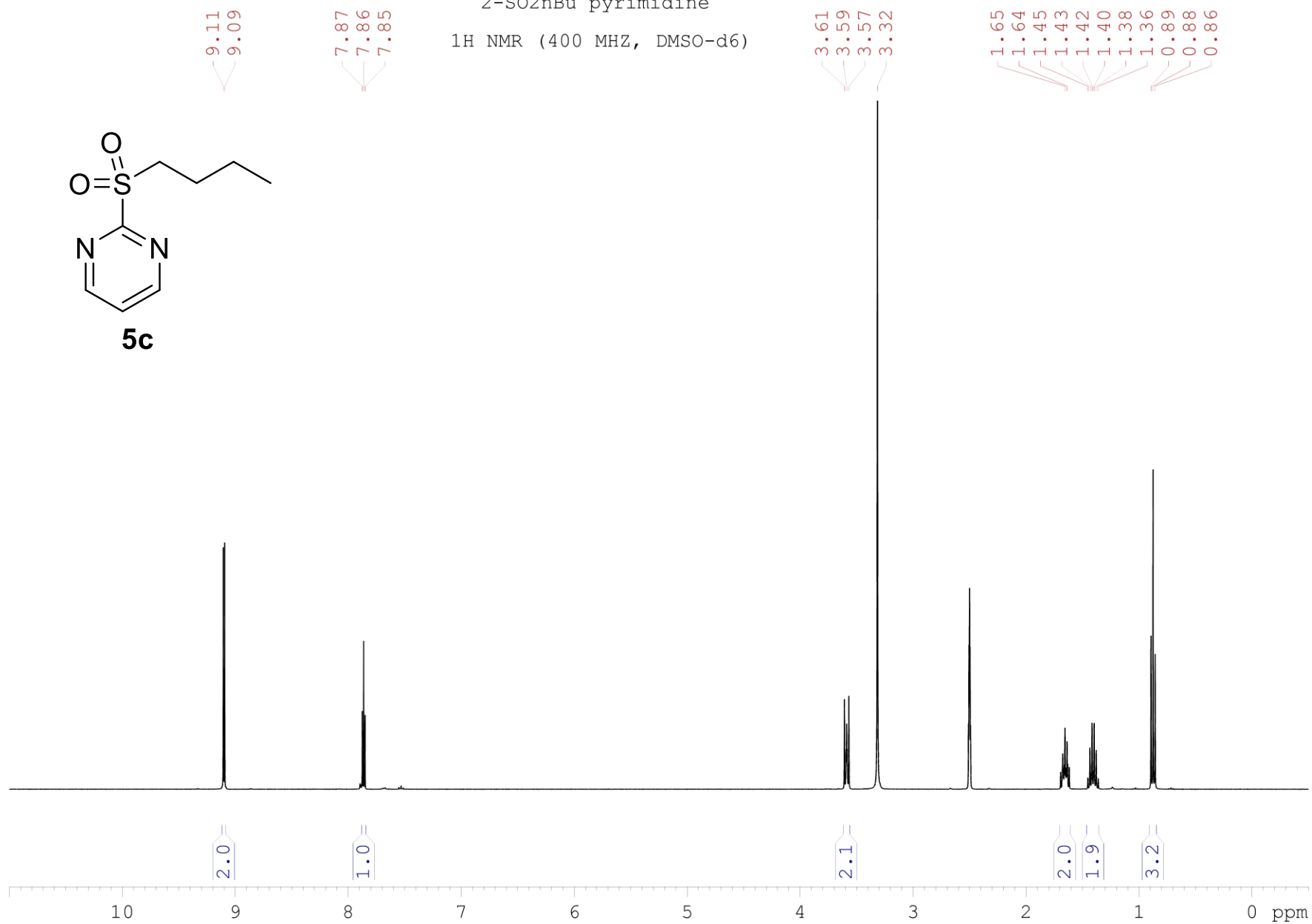


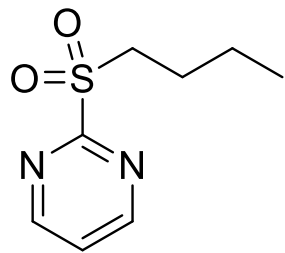
2-SO₂ (p-NH₂Ph)
13C (100 MHz, DMSO-d₆)





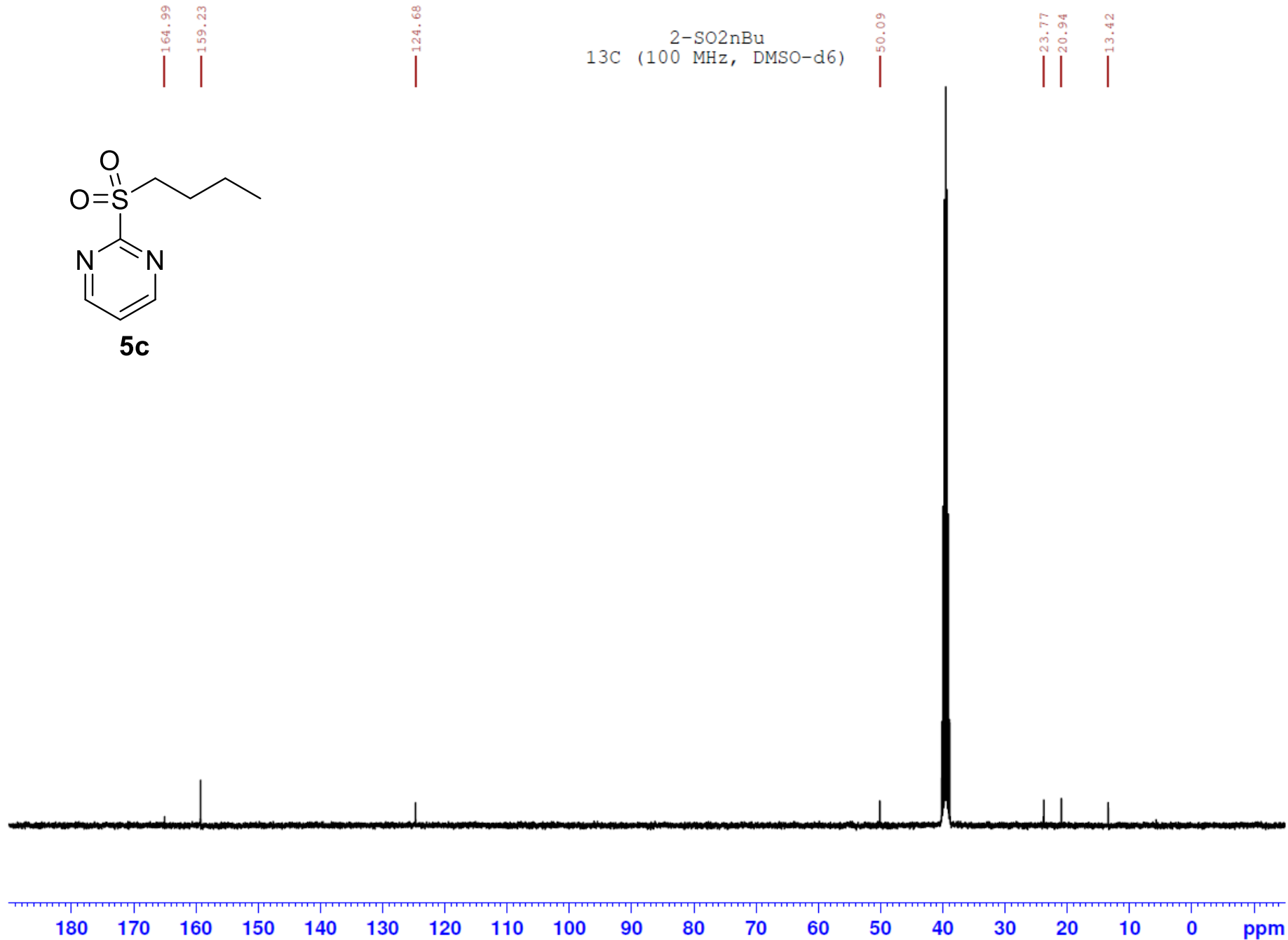
2-SO₂nBu pyrimidine
1H NMR (400 MHz, DMSO-d₆)

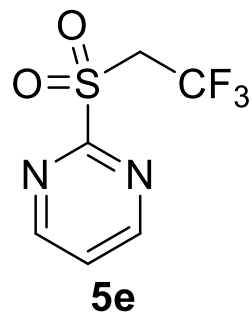




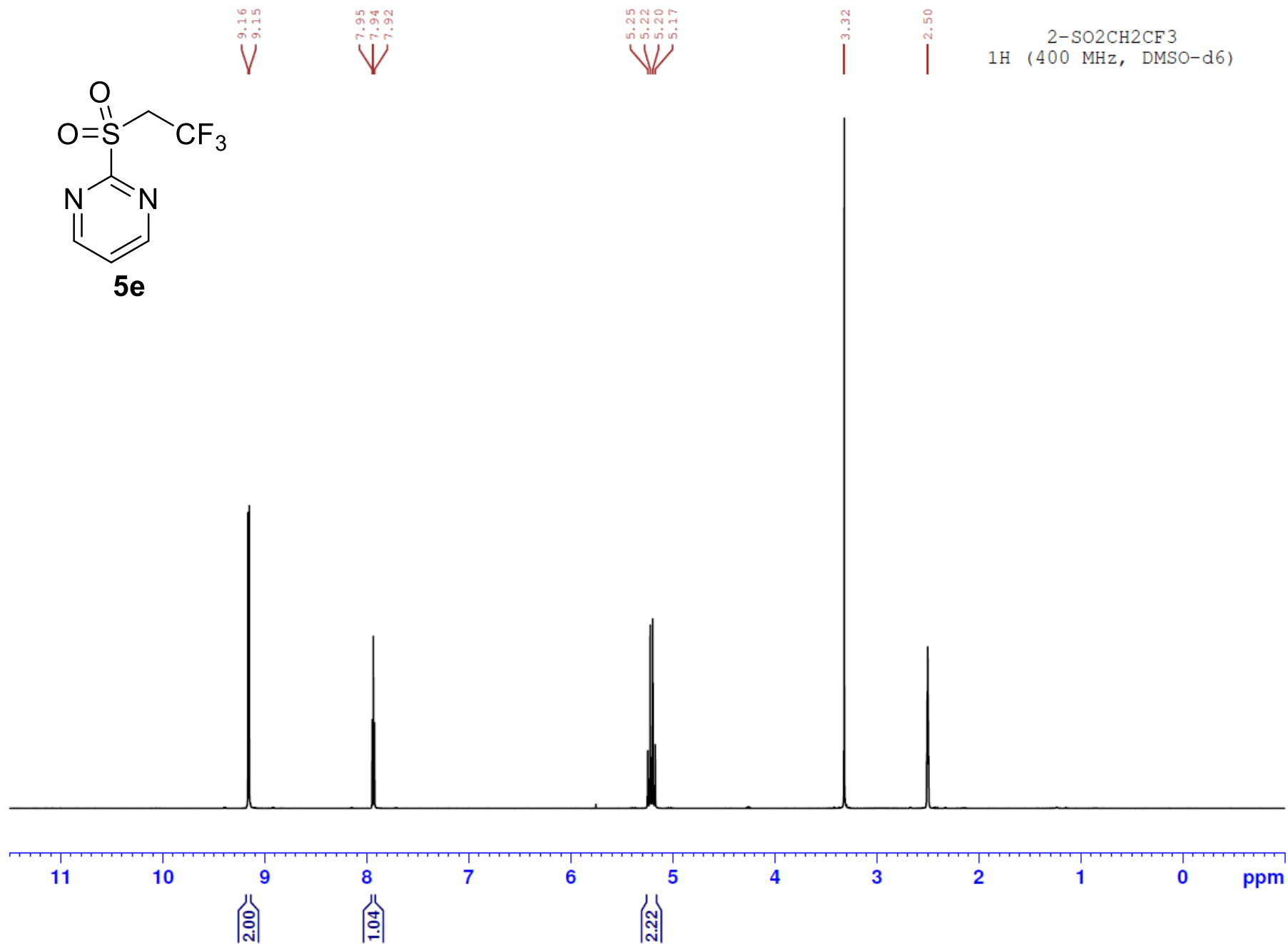
5c

2-SO₂nBu
13C (100 MHz, DMSO-d₆)

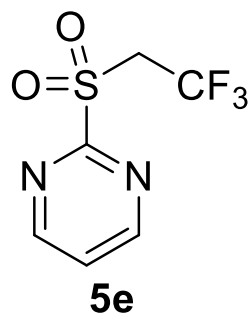




2-SO₂CH₂CF₃
1H (400 MHz, DMSO-d₆)



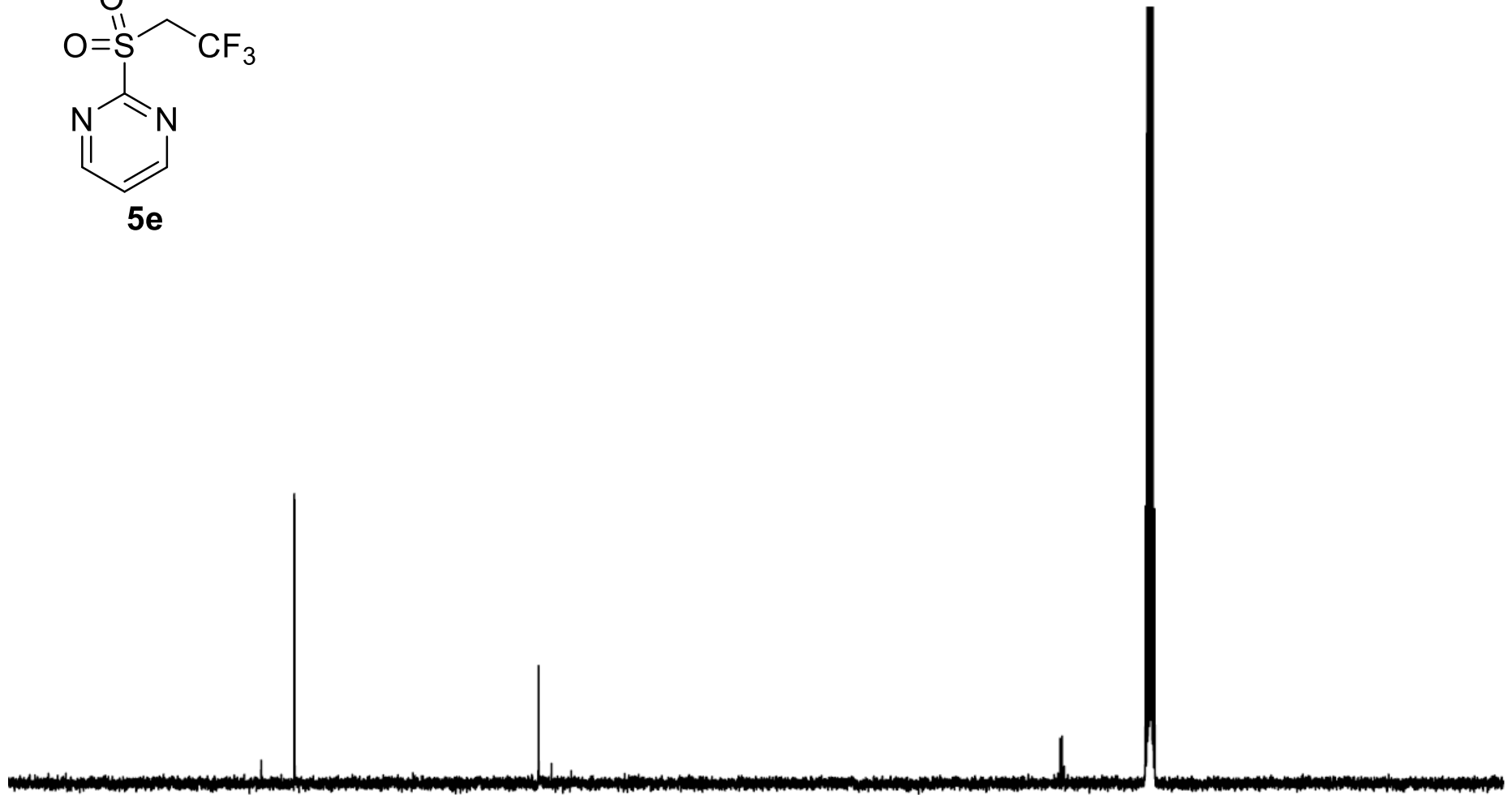
2-SO₂CH₂CF₃
13C (100 MHz, DMSO-d₆)



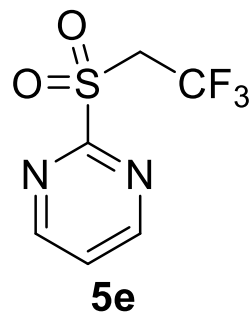
164.18
159.51

125.28
123.46

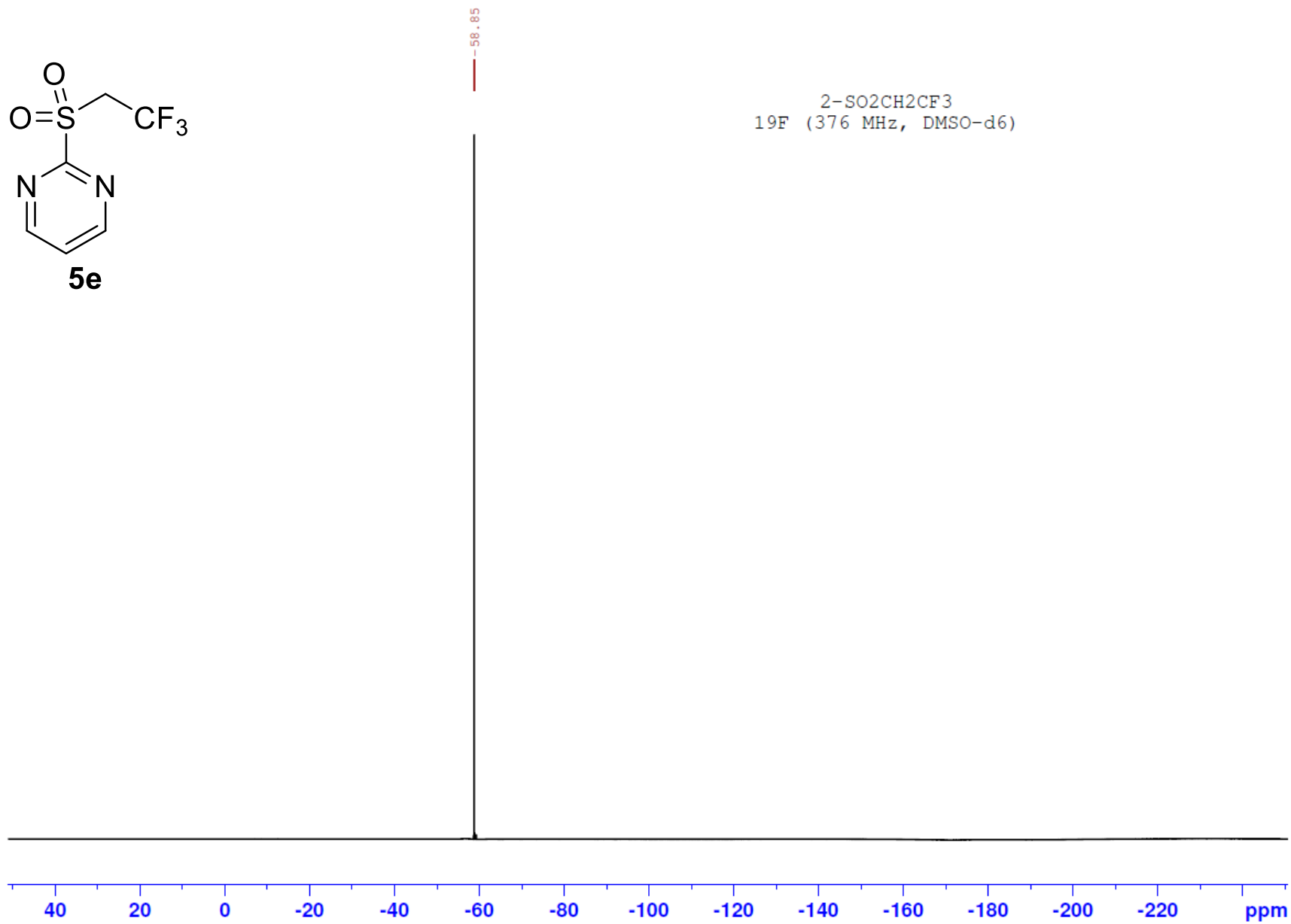
52.45
52.14
51.84
51.55



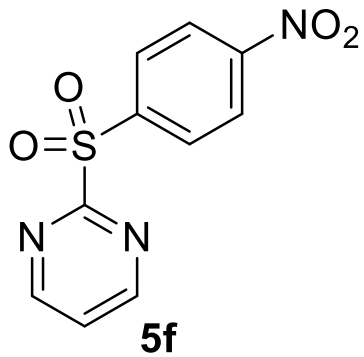
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



2-SO₂CH₂CF₃
19F (376 MHz, DMSO-d₆)



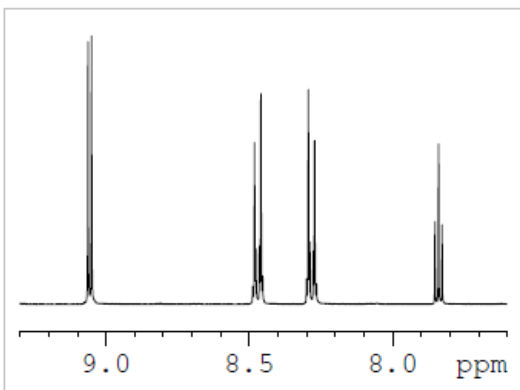
2-SO₂ (p-NO₂Ph)
1H (400 MHz, DMSO-d₆)



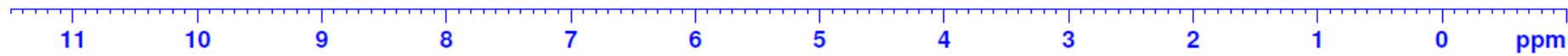
9.06
9.05
8.48
8.46
8.29
8.27
7.85
7.84
7.83

3.34

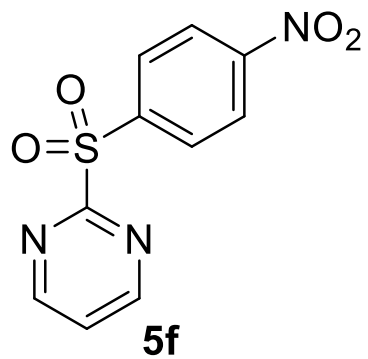
2.50



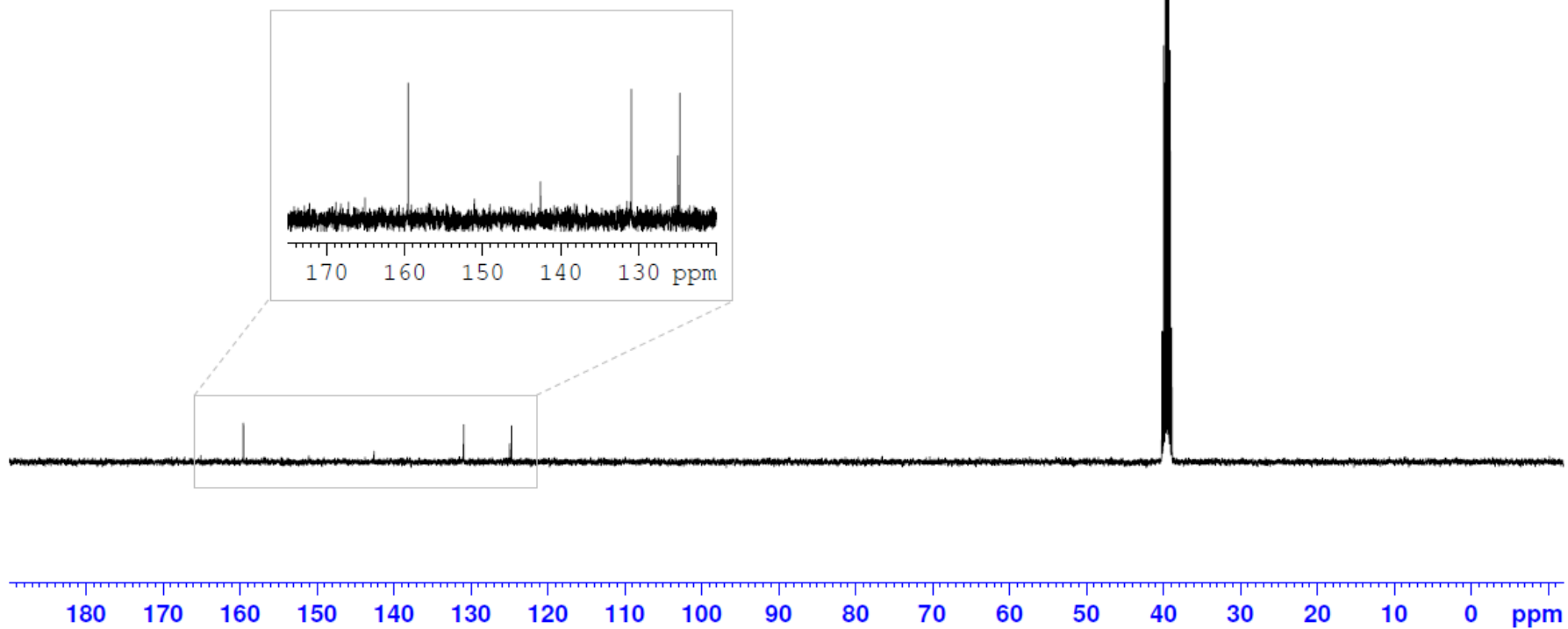
1.90
2.07
2.11
1.00

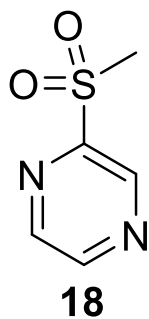


2-SO₂ (p-NO₂Ph)
13C (100 MHz, DMSO-d₆)



165.07
159.53
151.04
142.57
130.91
124.94
124.70



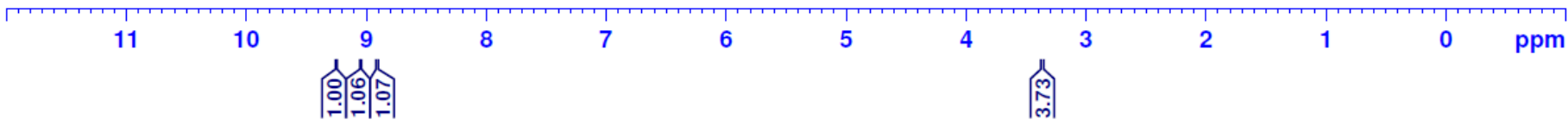


9.25
9.25
9.05
9.04
8.91
8.91
8.90

2-SO₂Me pyrazine
1H (400 MHz, DMSO-d₆)

3.36
3.32

2.50

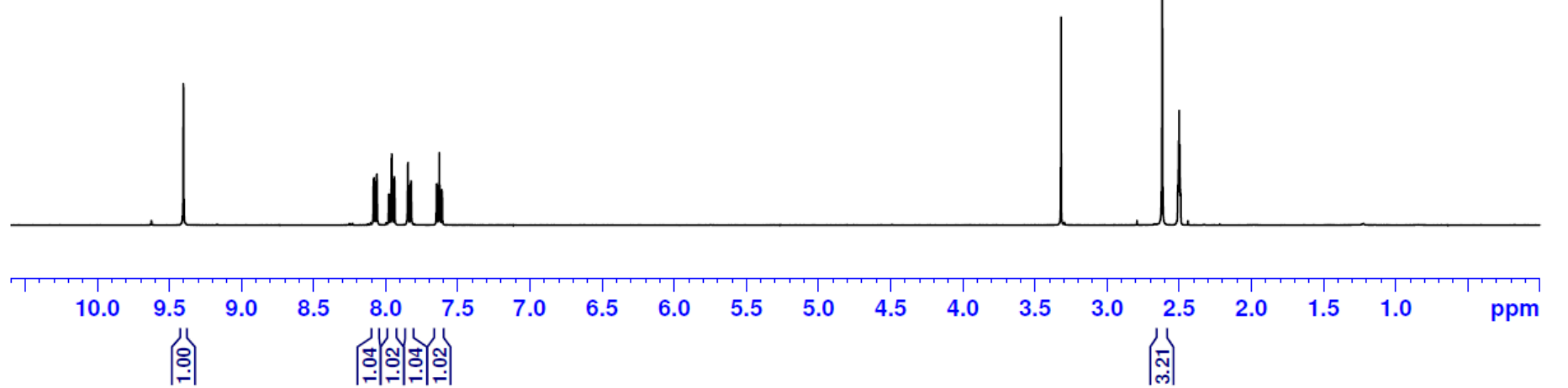
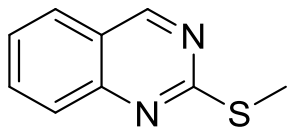


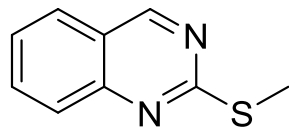
2-SMe Quinazoline
1H NMR (400 MHz, DMSO-d6)

9.40
9.40
8.08
8.08
8.07
8.06
8.06
8.06
7.98
7.96
7.96
7.94
7.94
7.94
7.85
7.85
7.83
7.82
7.65
7.65
7.63
7.63
7.63
7.61
7.61

3.32

2.62
2.50





2-SMe quinazoline
13C NMR (100 MHz, DMSO-d6)

167.87

160.89

149.97

135.07

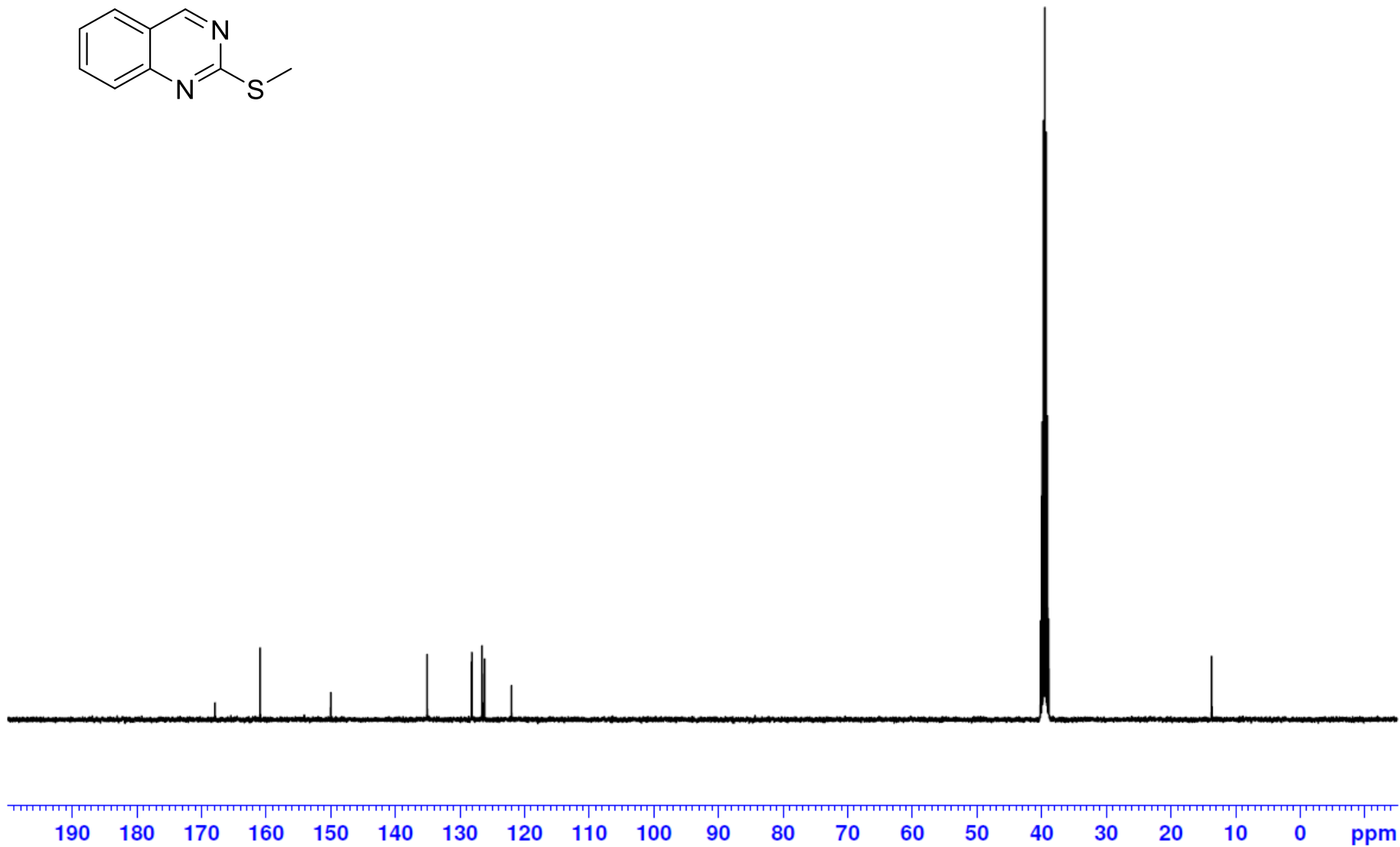
128.16

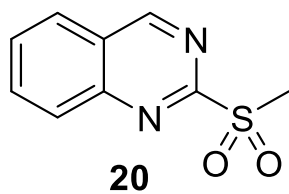
126.56

126.17

122.02

13.67





2-(methylsulfonyl)quinazoline
1H (400 MHz, CDCl3)

