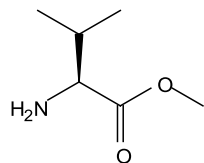


Profiling the Reactivity of Cyclic C-Nucleophiles towards Electrophilic Sulfur in Cysteine Sulfenic Acid

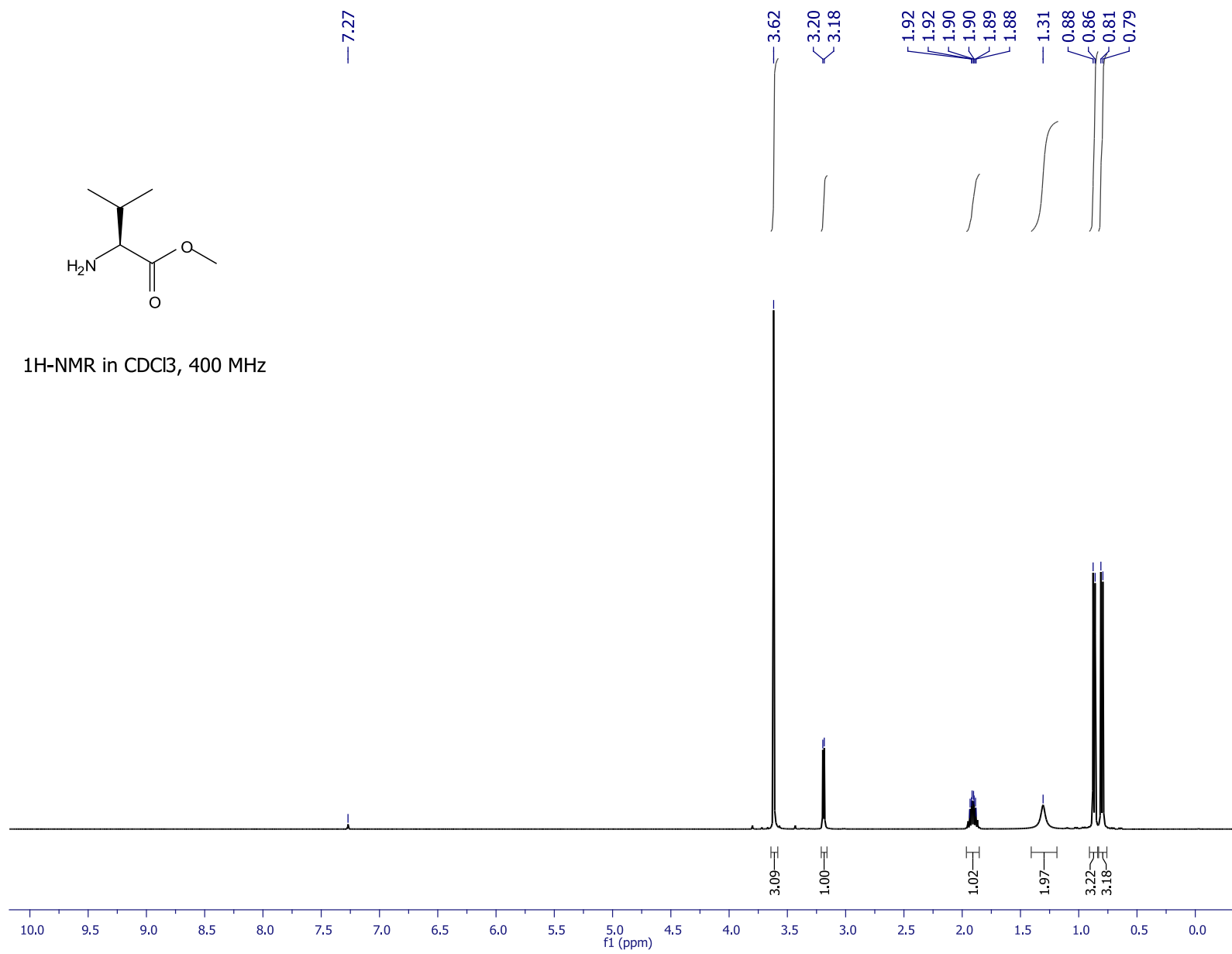
Vinayak Gupta and Kate S. Carroll*

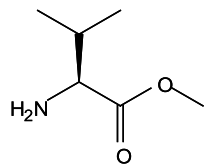
Department of Chemistry, The Scripps Research Institute, Jupiter, Florida, 33458

¹H-NMR and ¹³C-NMR Data

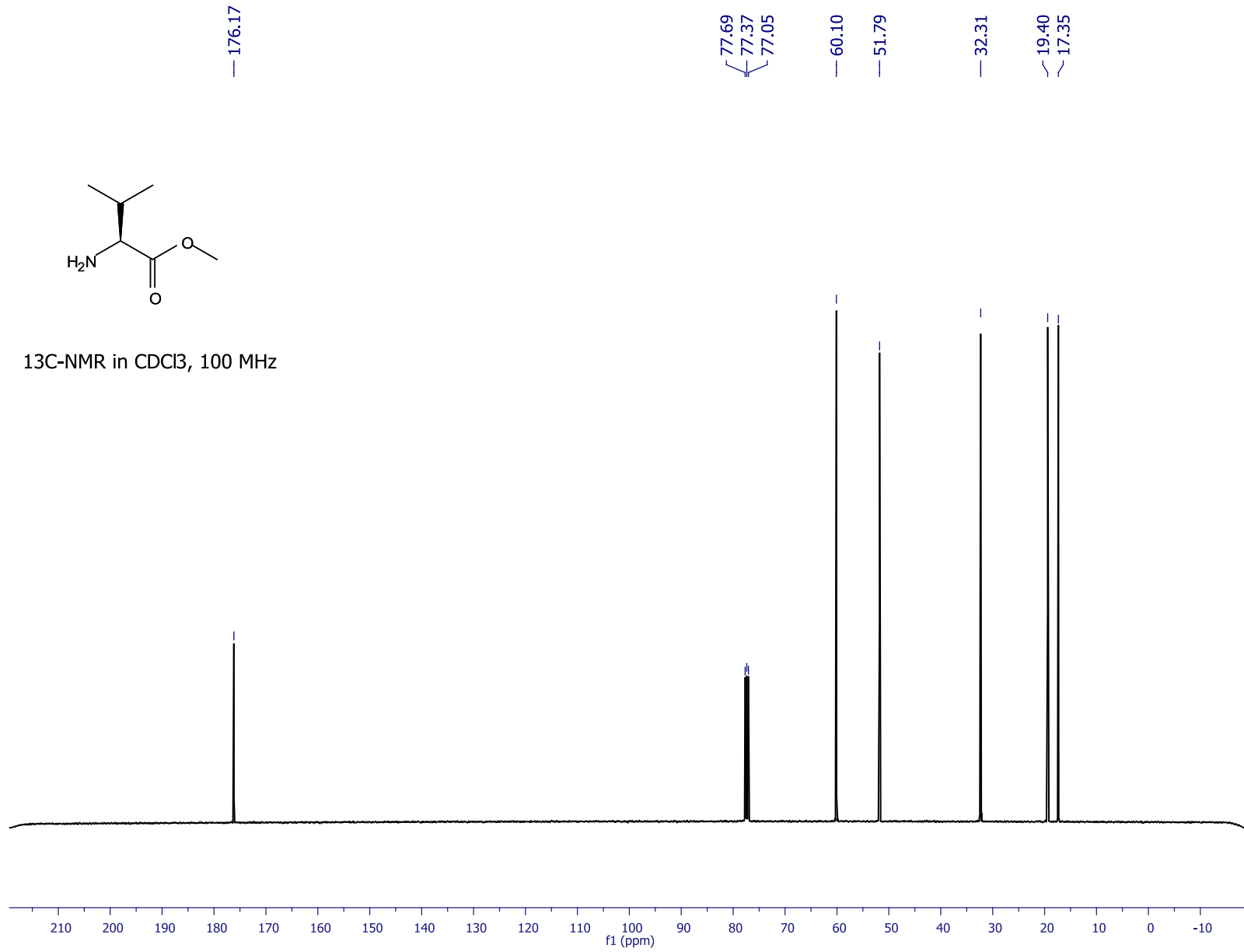


1H-NMR in CDCl3, 400 MHz

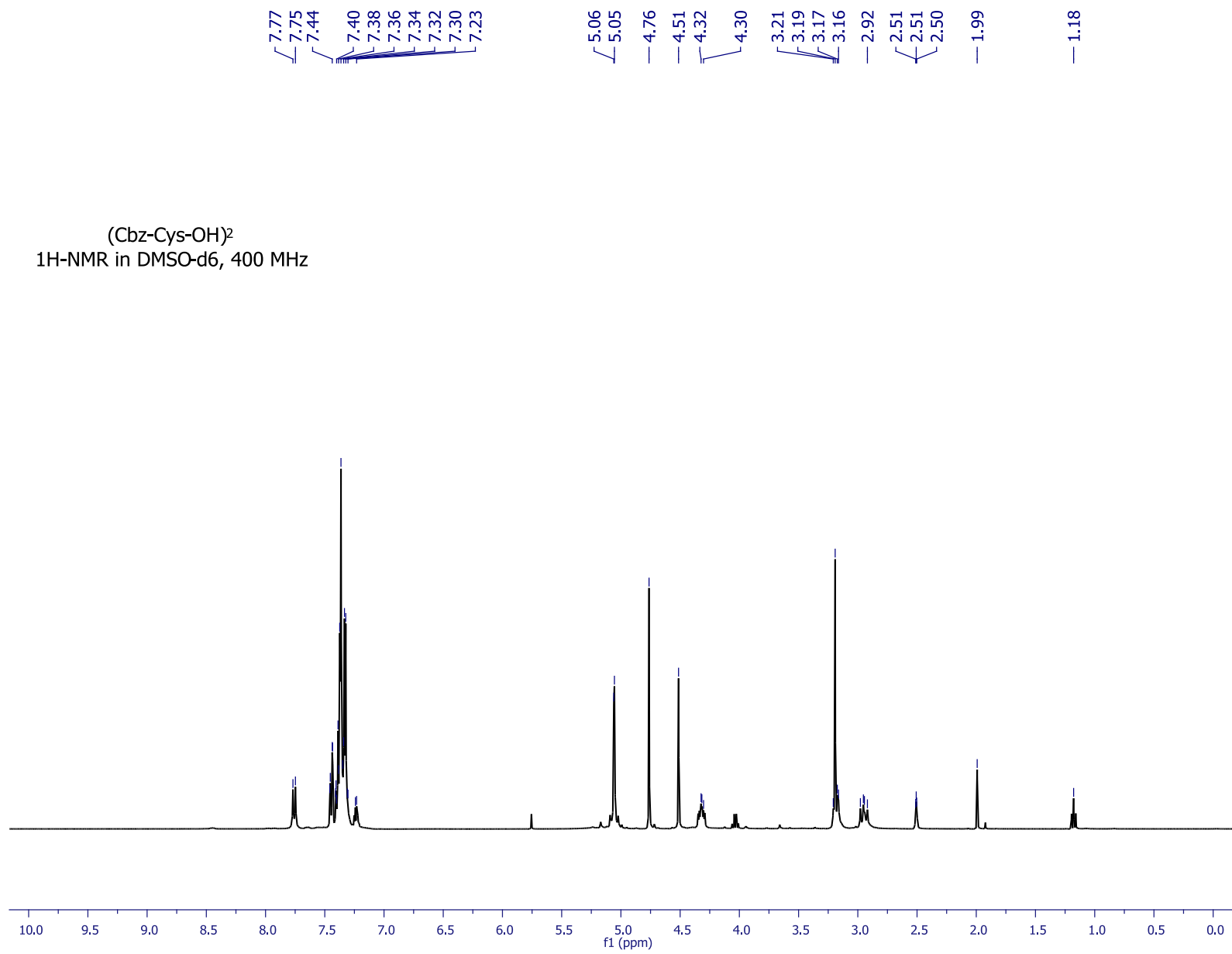




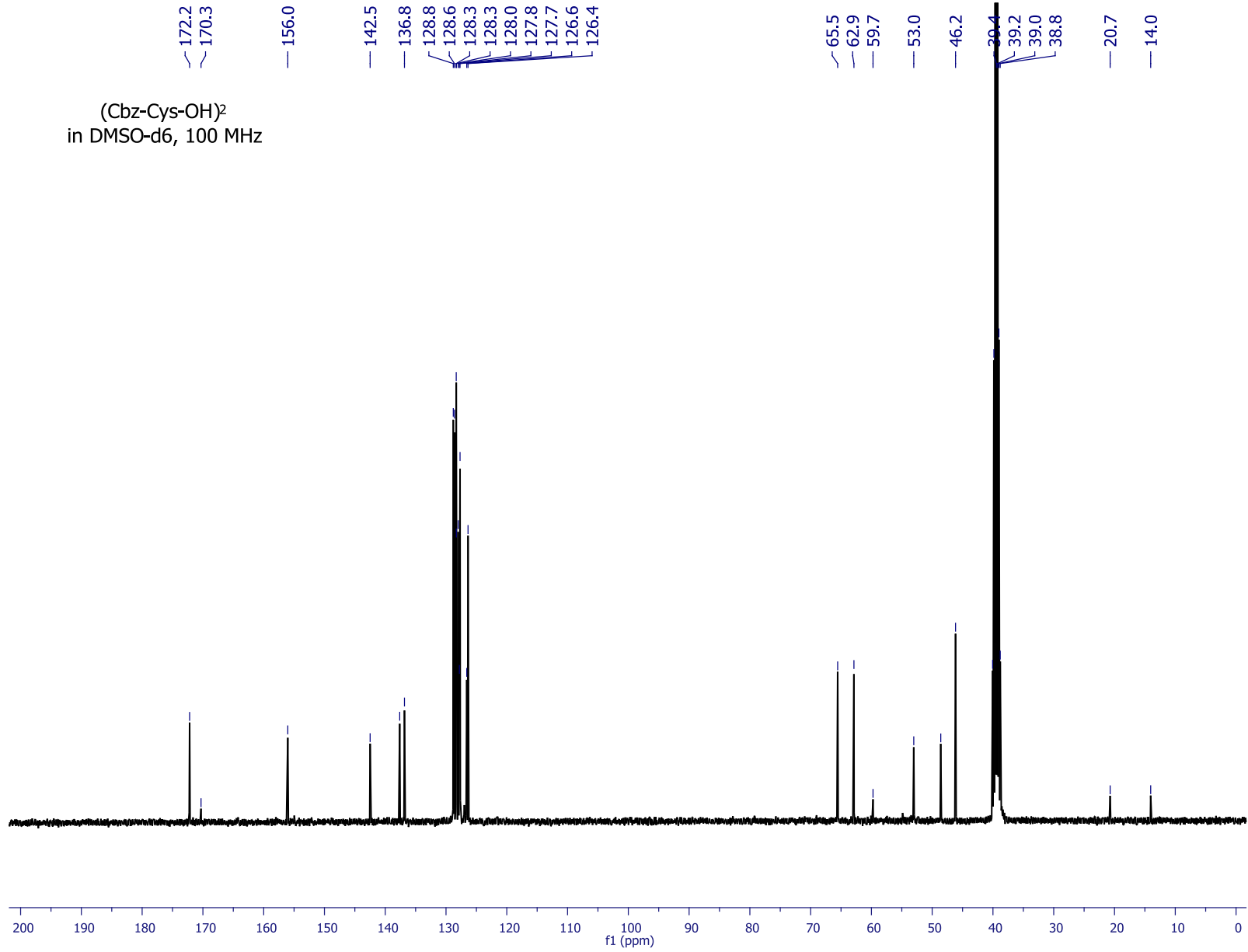
¹³C-NMR in CDCl₃, 100 MHz

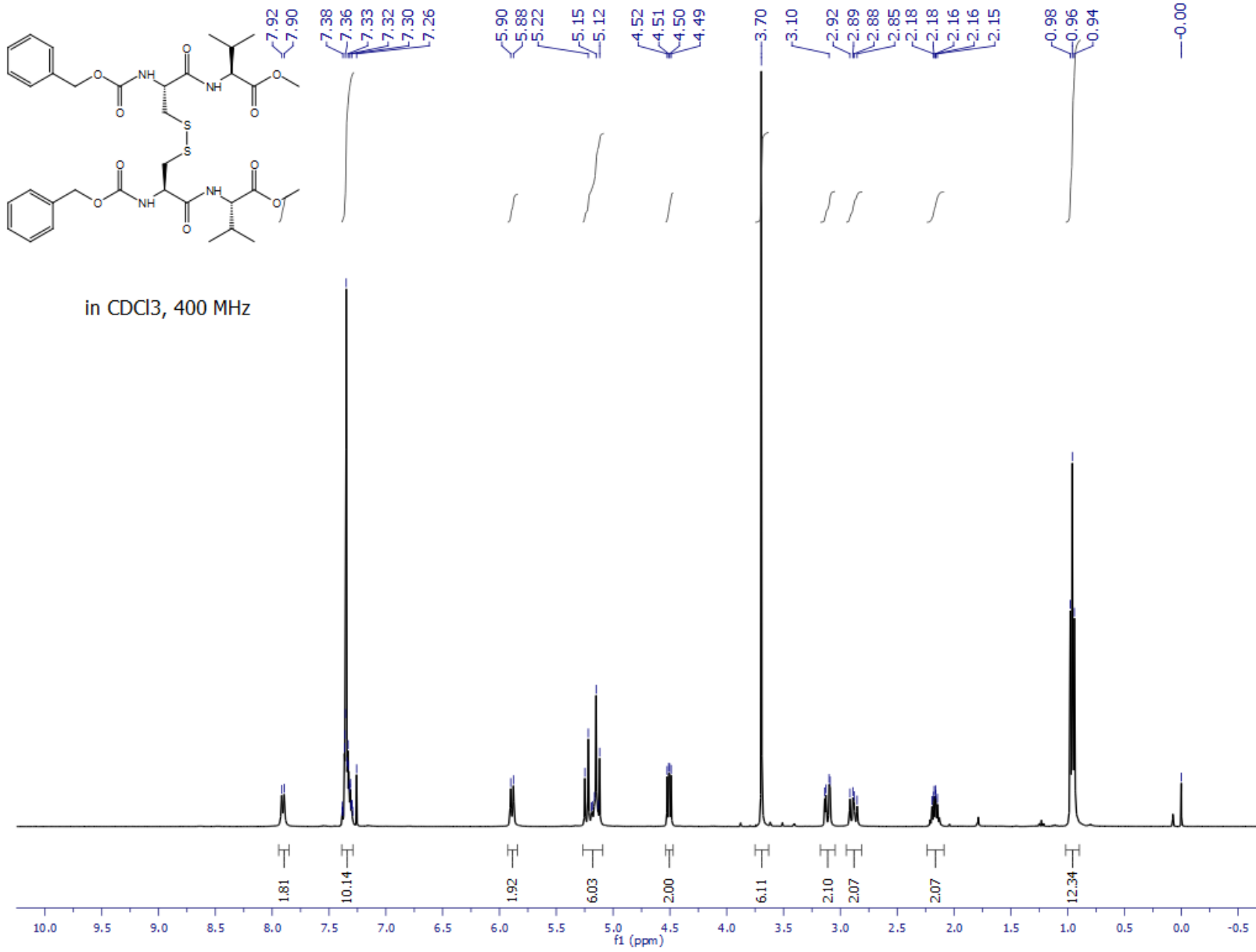


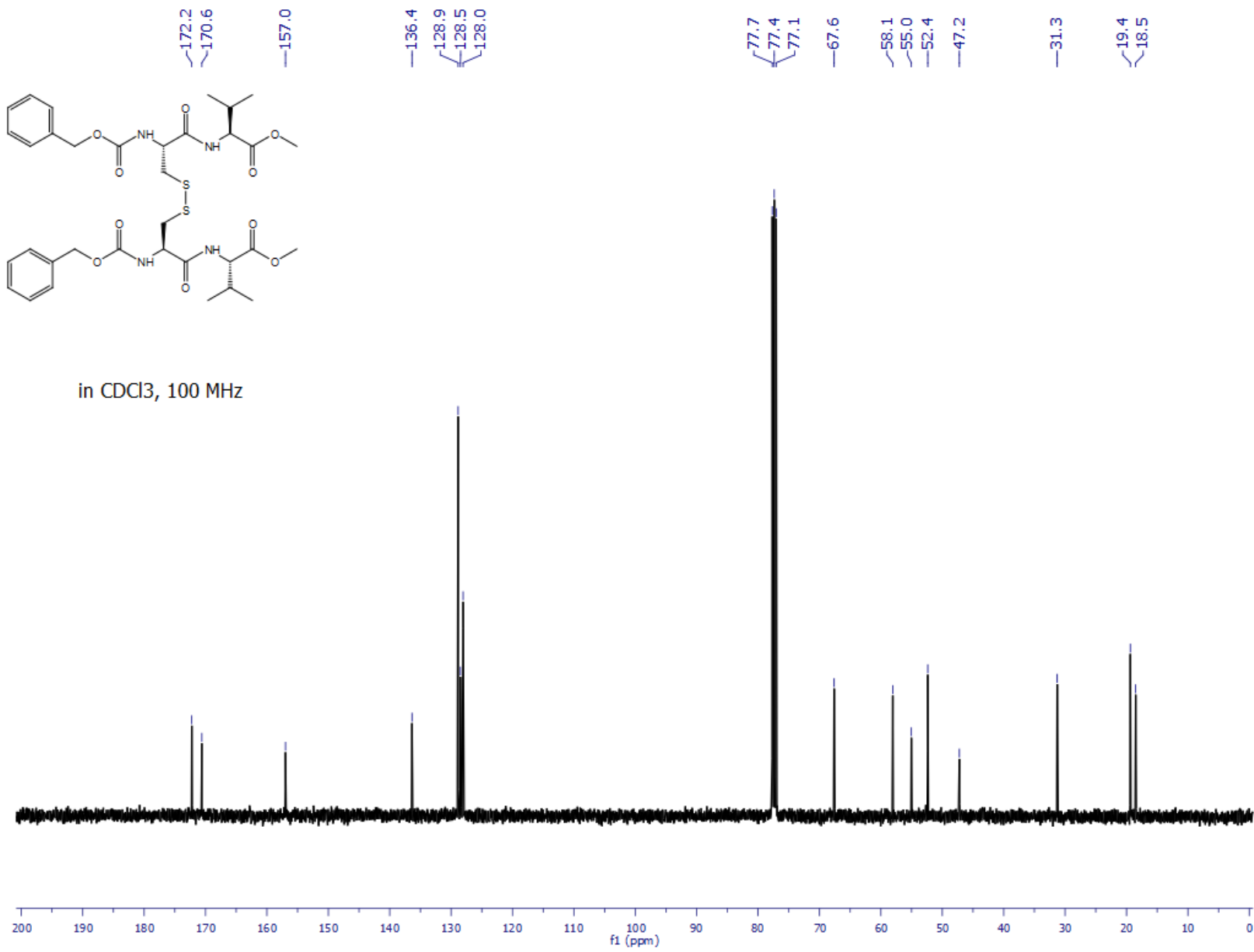
(Cbz-Cys-OH)²
1H-NMR in DMSO-d₆, 400 MHz

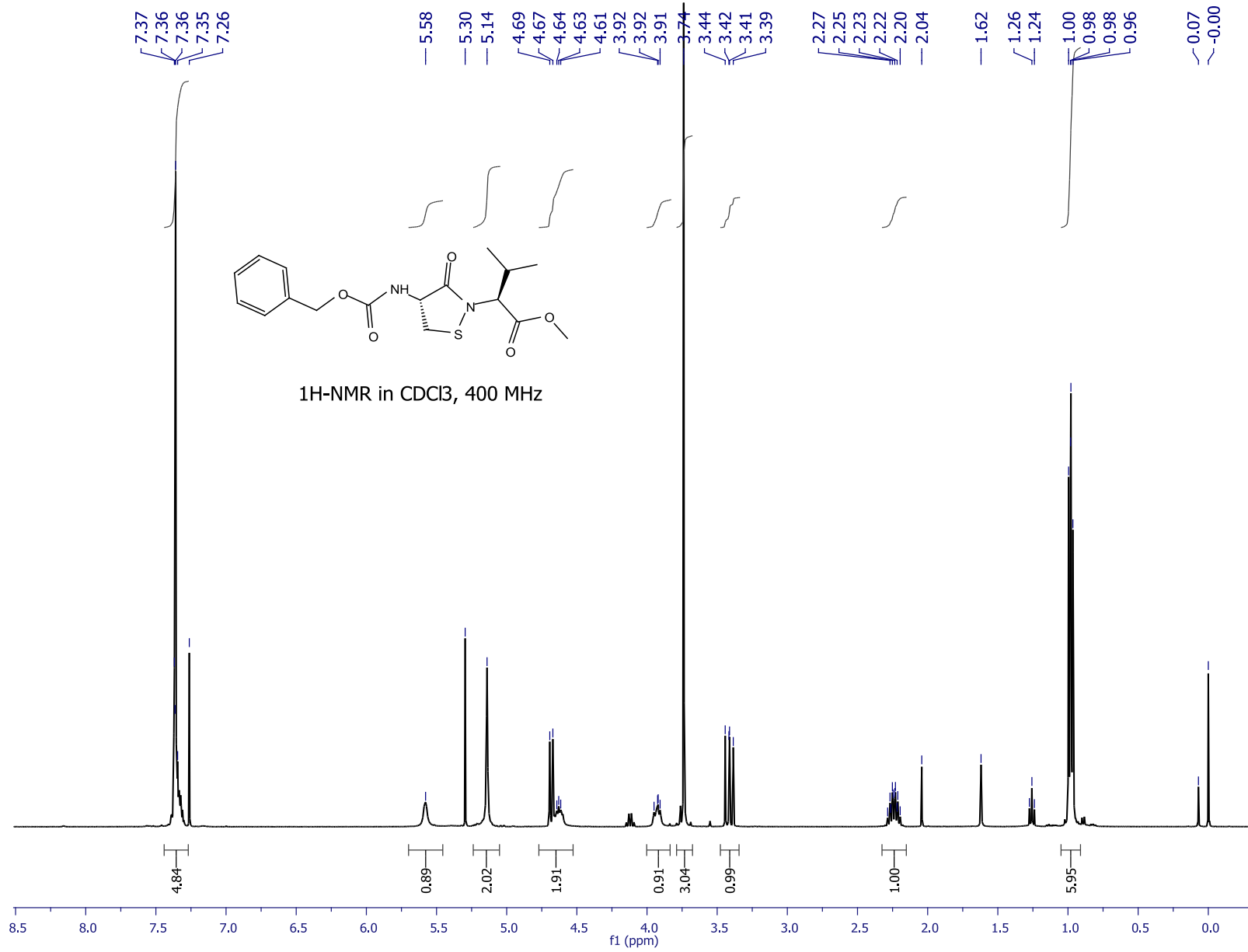


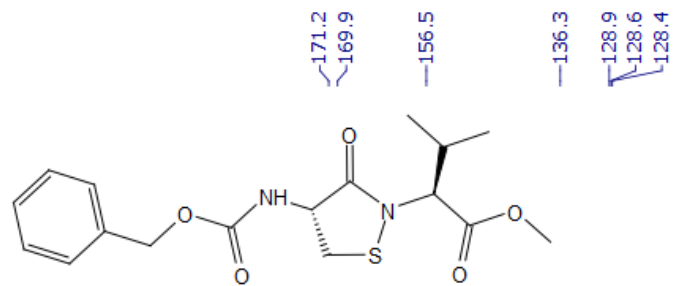
(Cbz-Cys-OH)²
in DMSO-d₆, 100 MHz



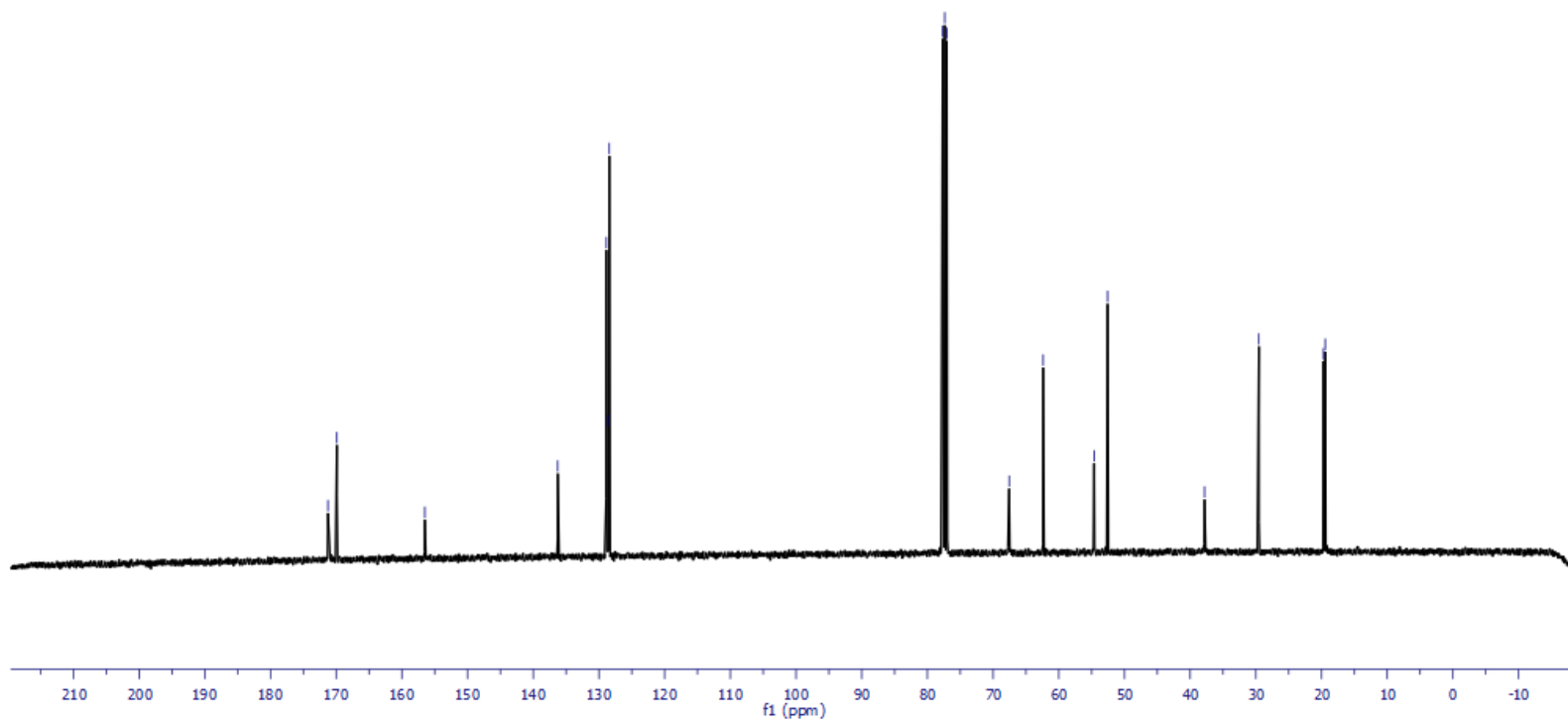


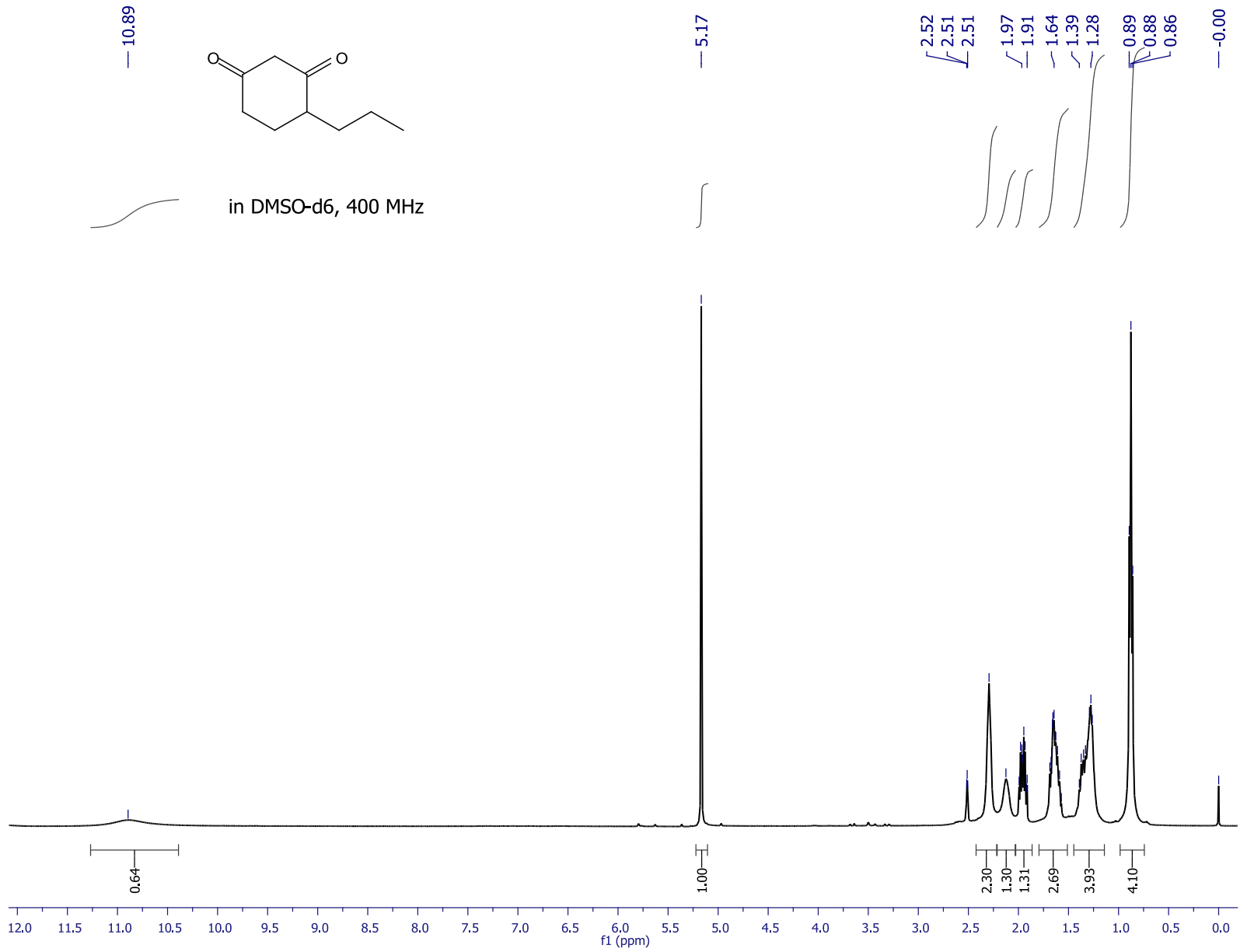


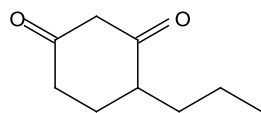




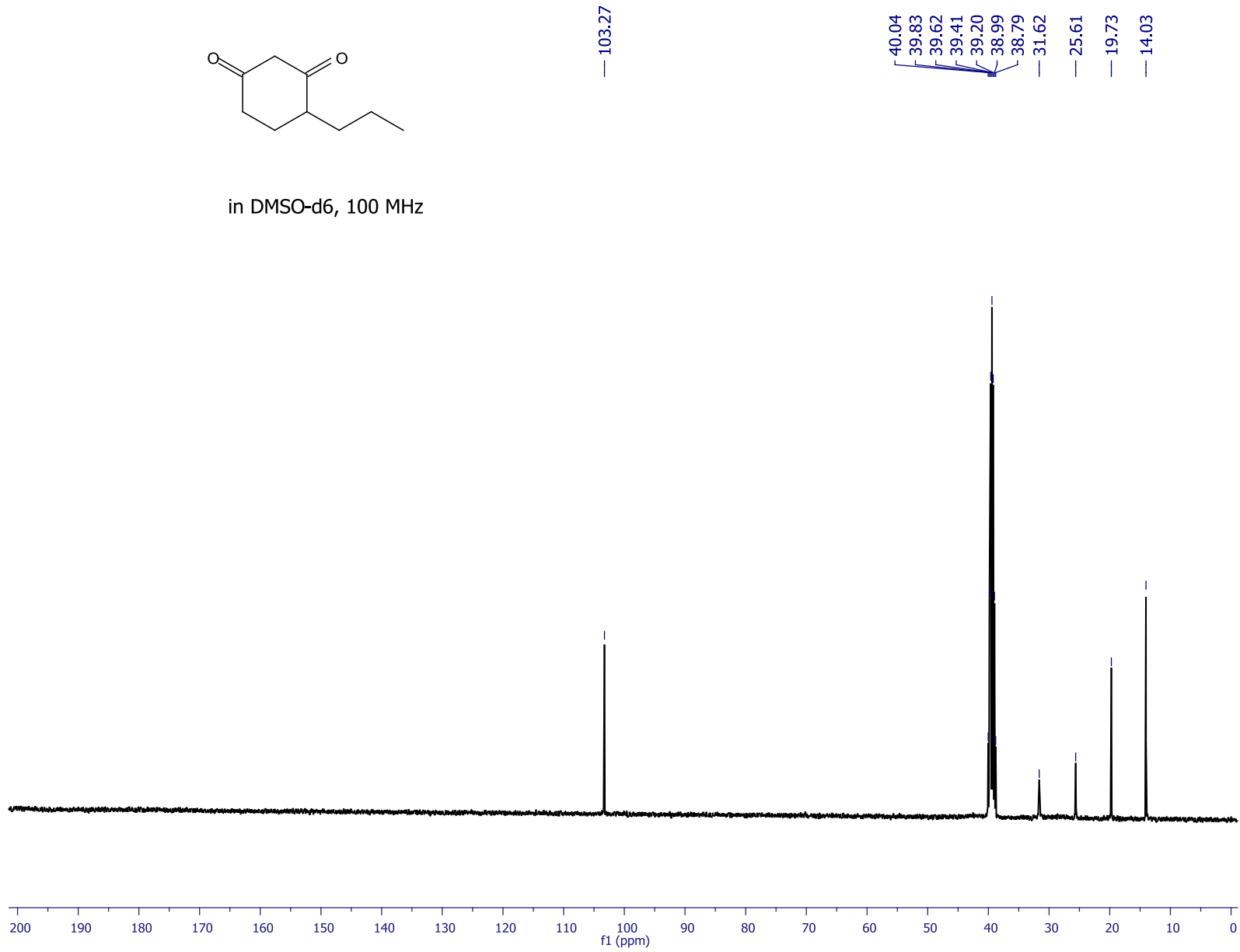
in CDCl₃, 100 MHz

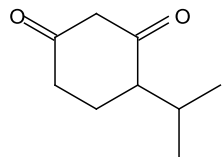




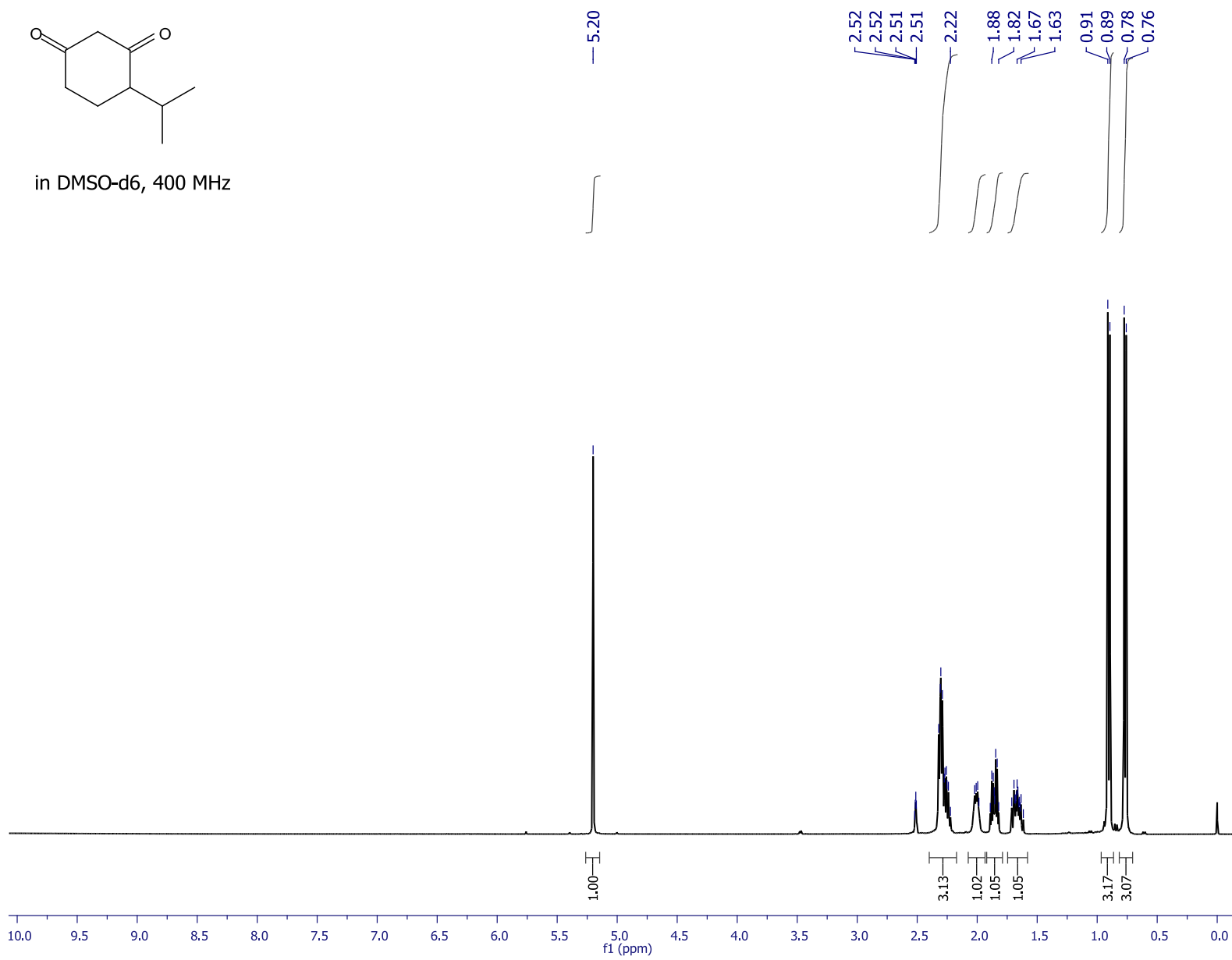


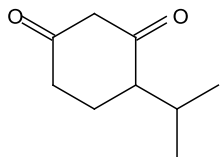
in DMSO-d6, 100 MHz



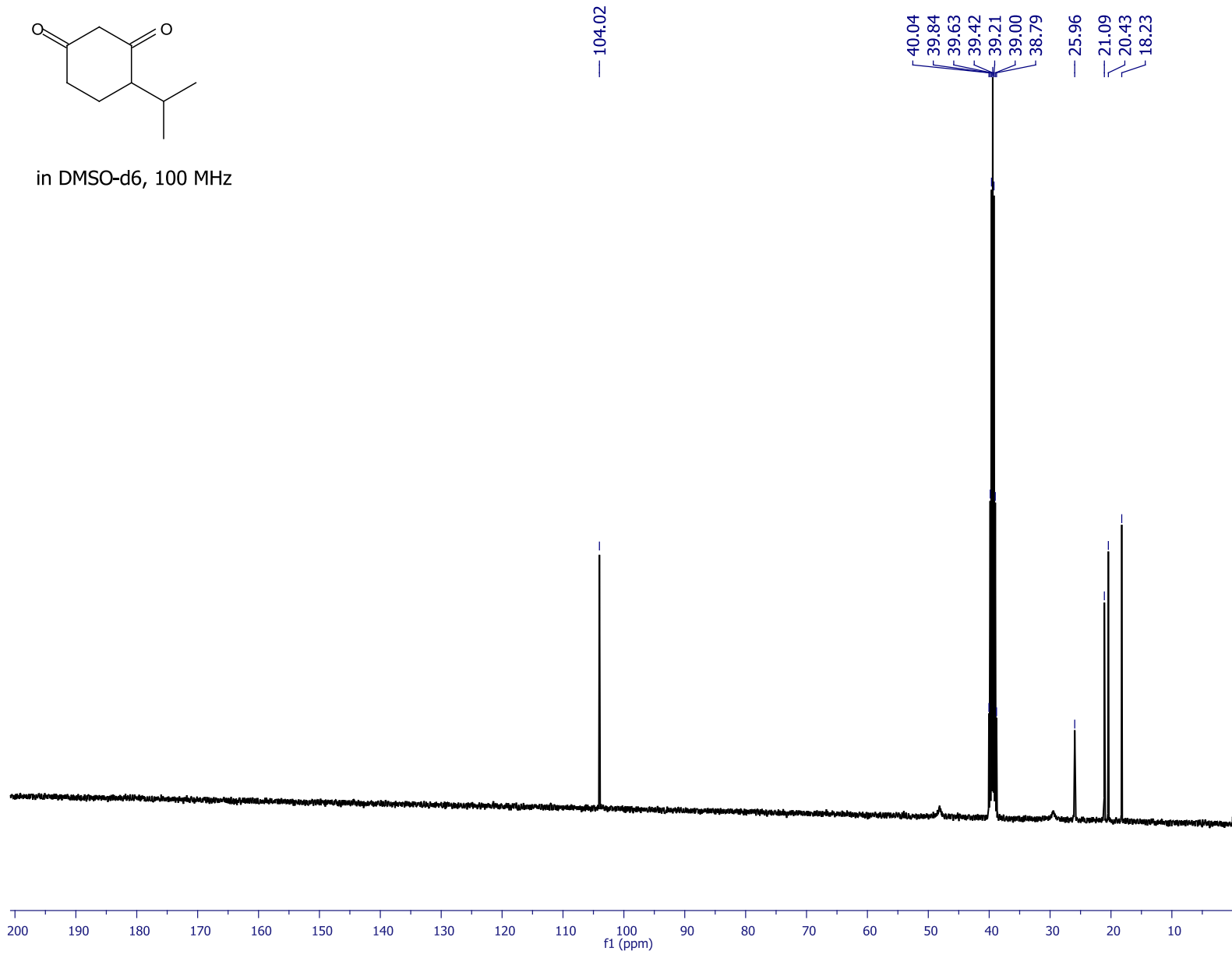


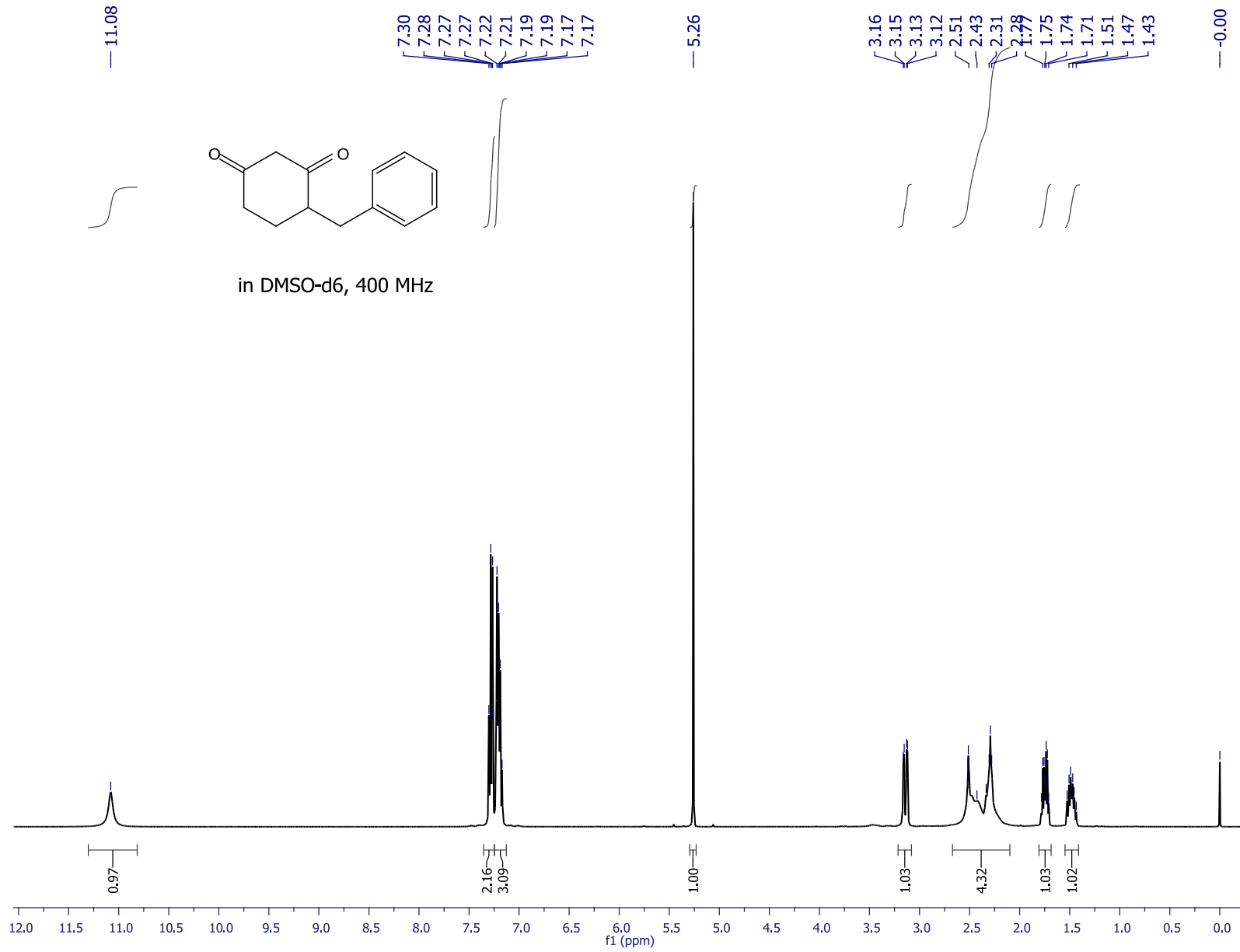
in DMSO-d₆, 400 MHz

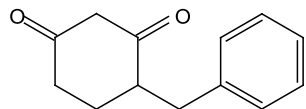




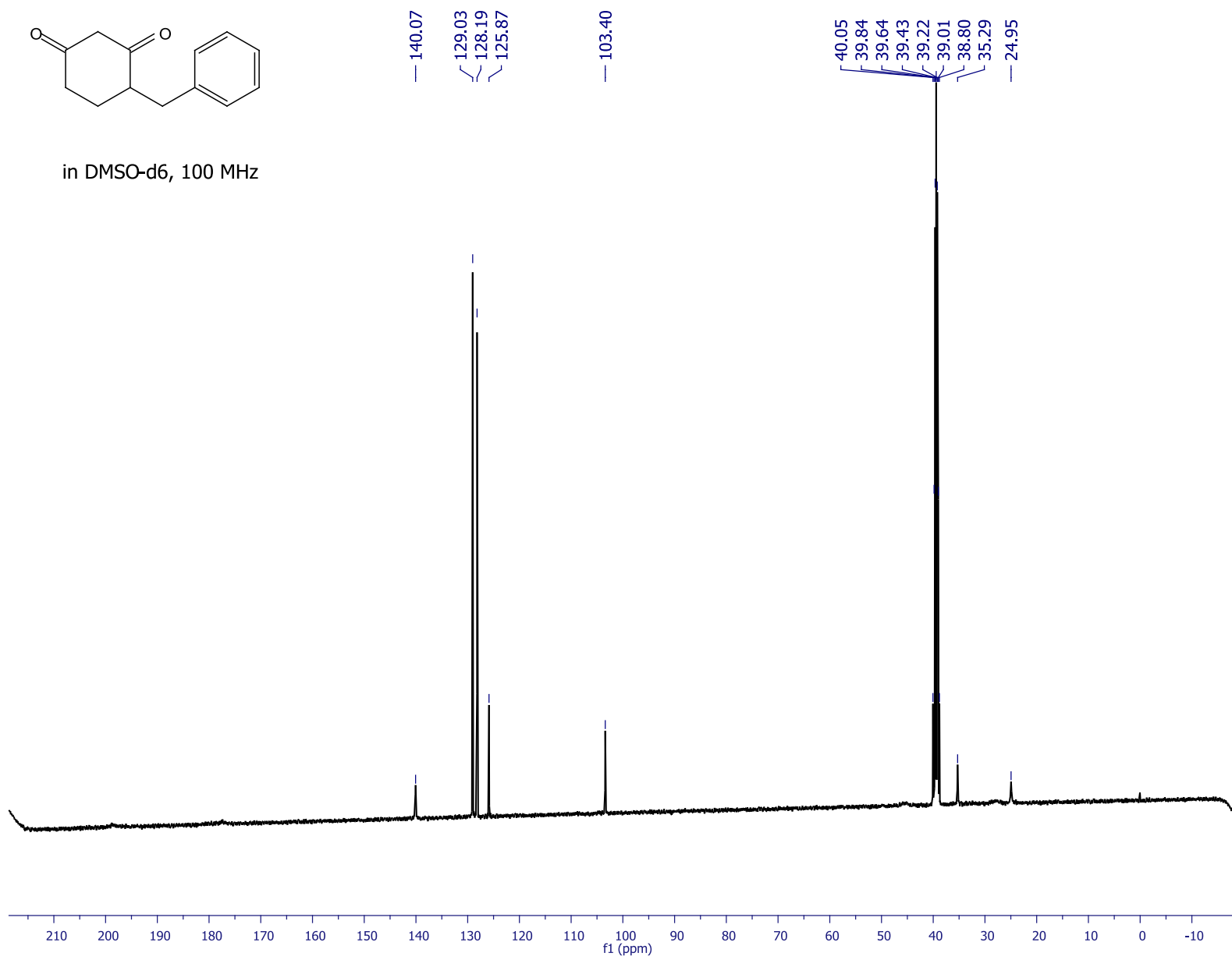
in DMSO-d₆, 100 MHz

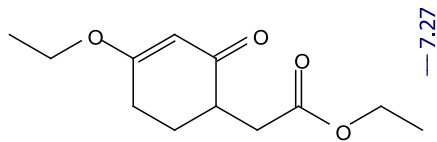




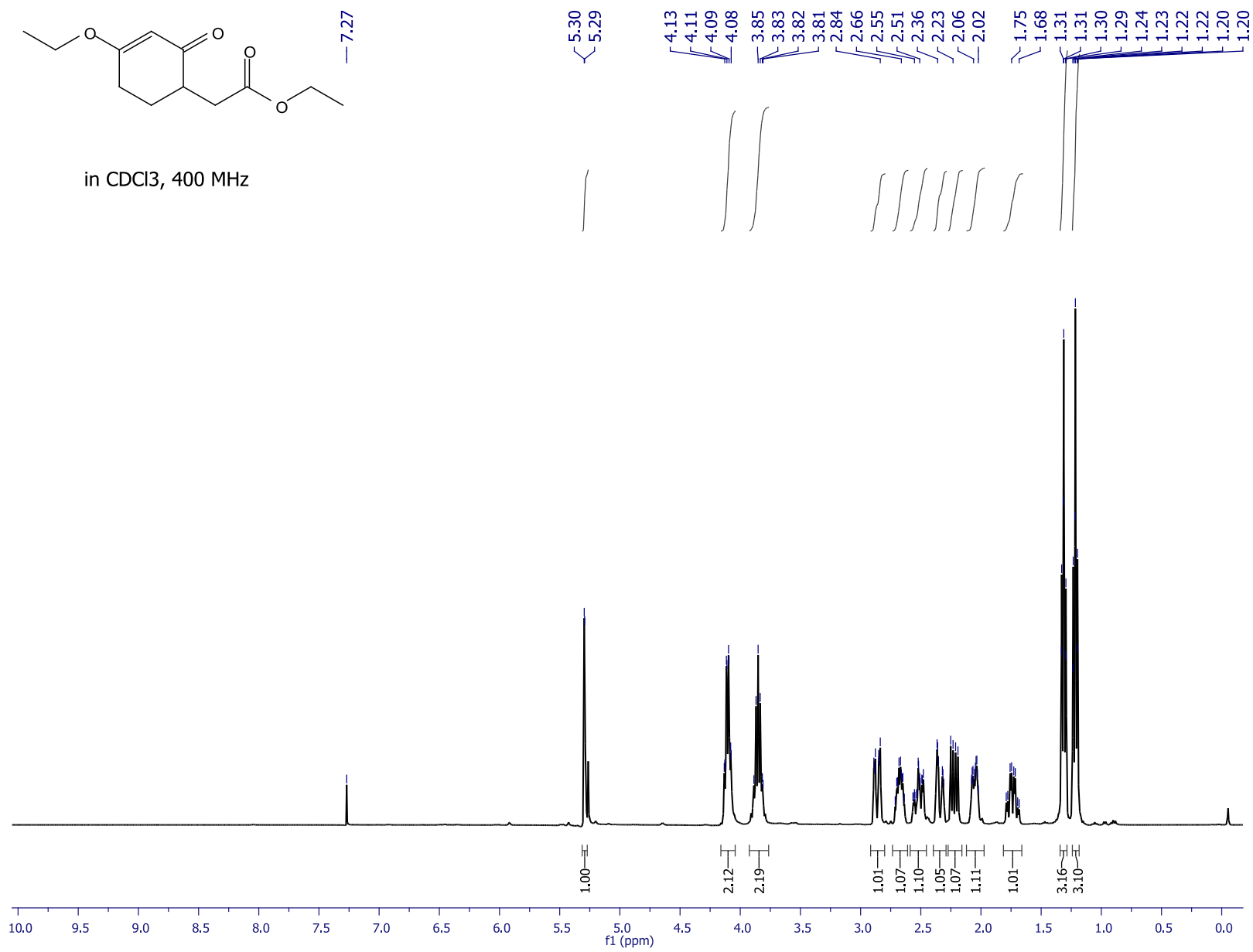


in DMSO-d6, 100 MHz



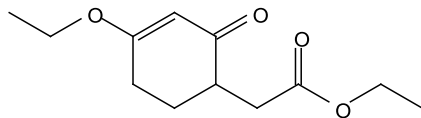


in CDCl₃, 400 MHz



— 199.10

— 177.25
— 172.91



— 102.18

— 77.66
— 77.34
— 77.02

— 64.51
— 60.61

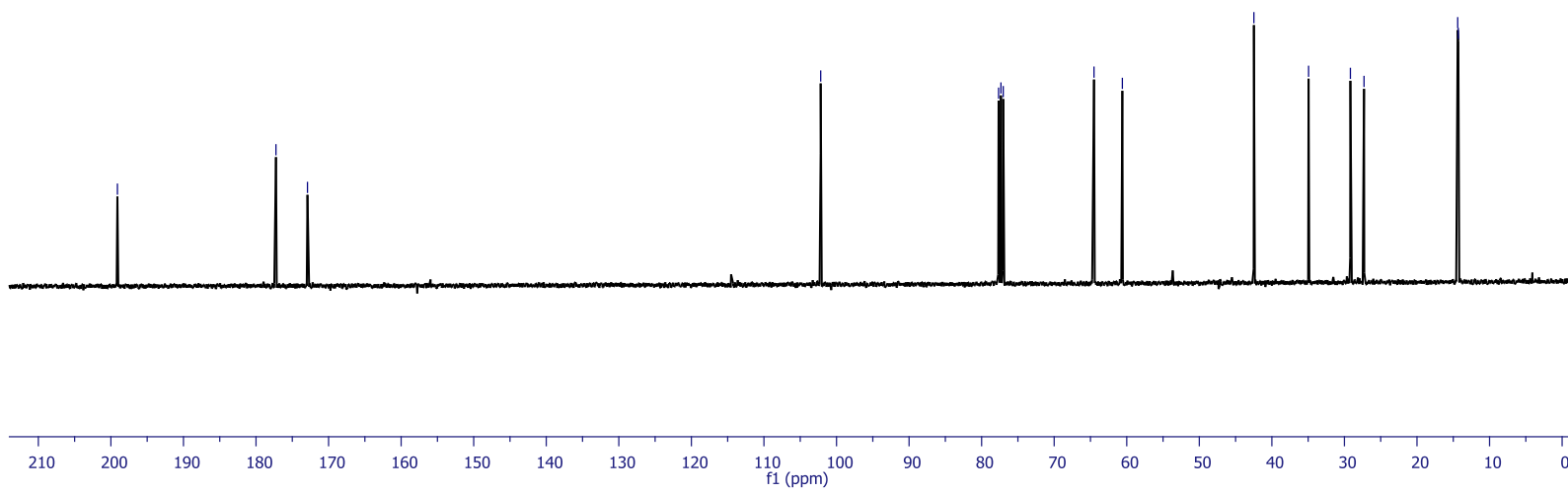
— 42.48

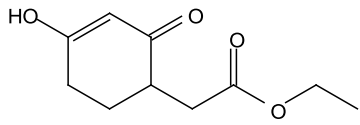
— 34.94

— 29.18
— 27.30

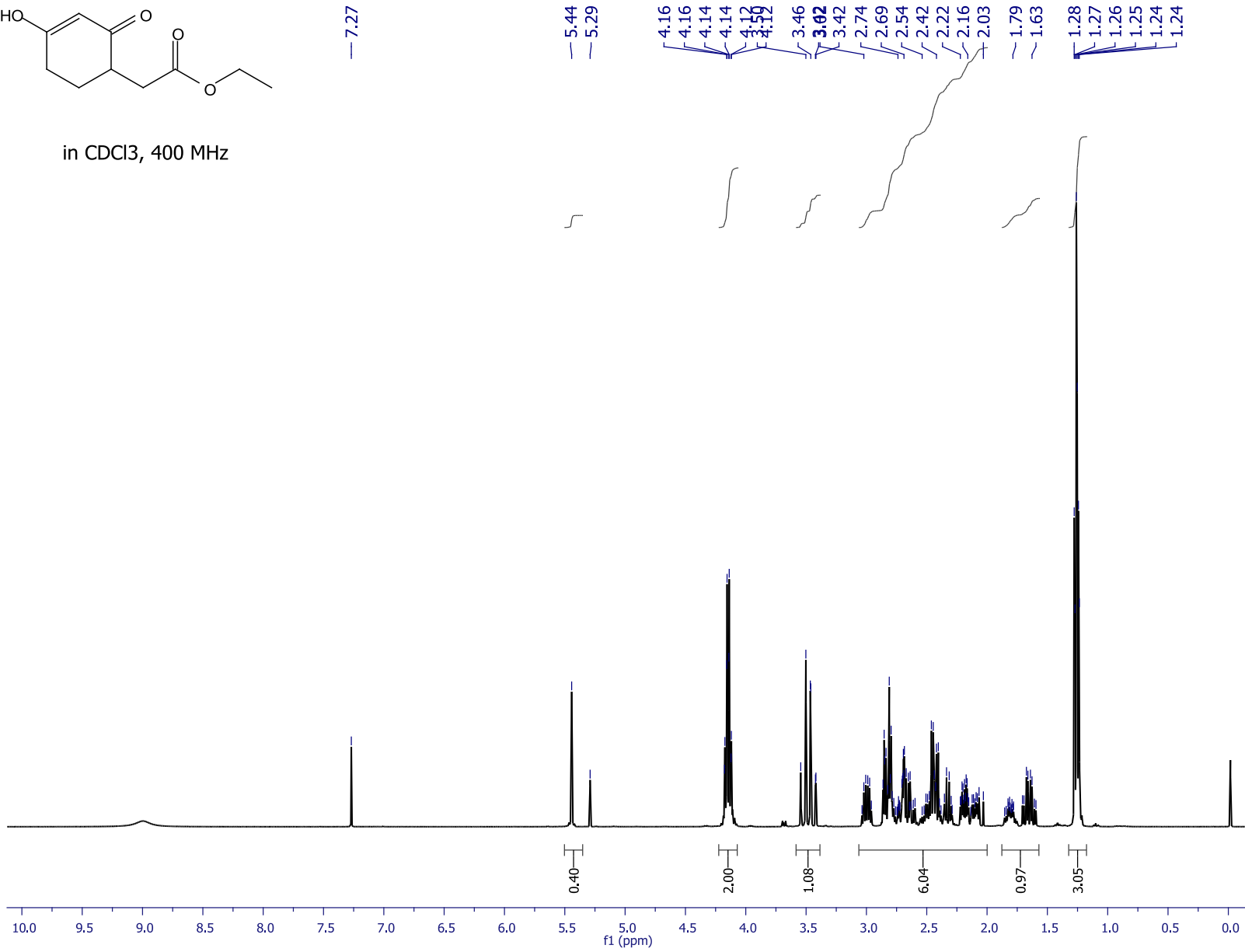
— 14.39
— 14.30

in CDCl₃, 400 MHz

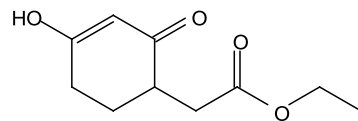




in CDCl₃, 400 MHz



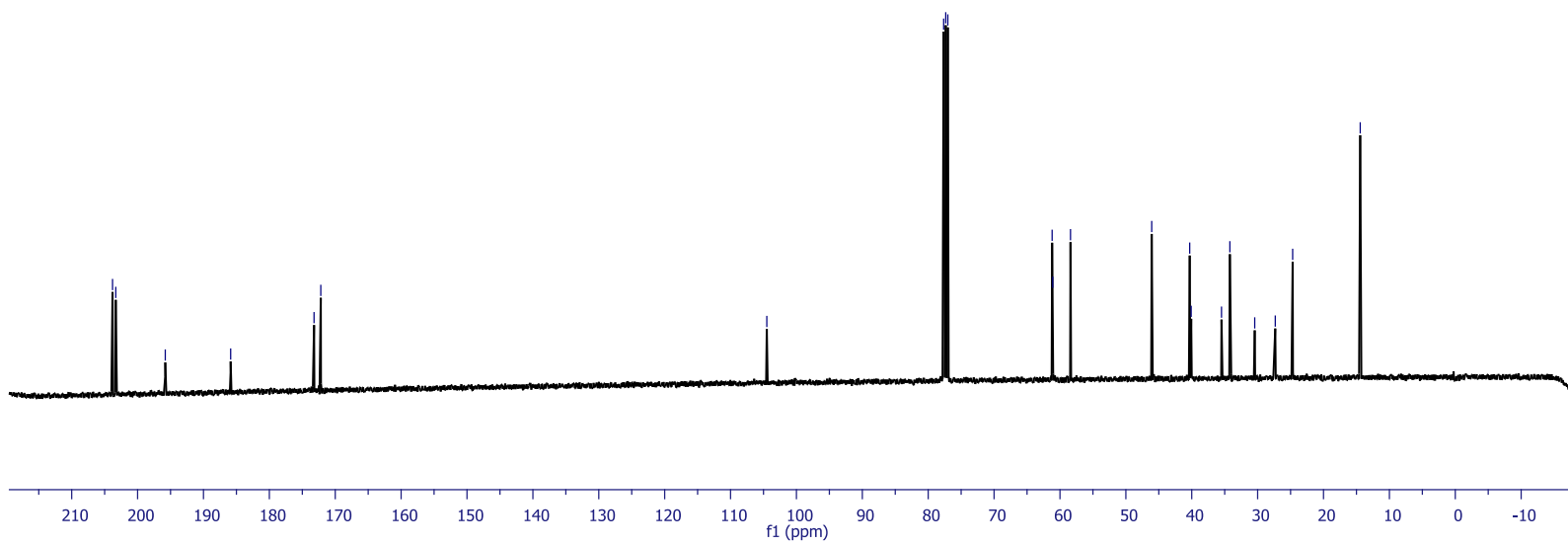
203.80
203.31
195.80
185.87
173.22
172.19

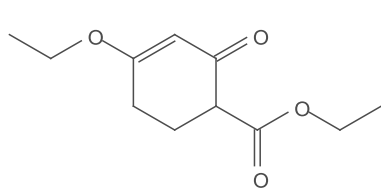


104.50

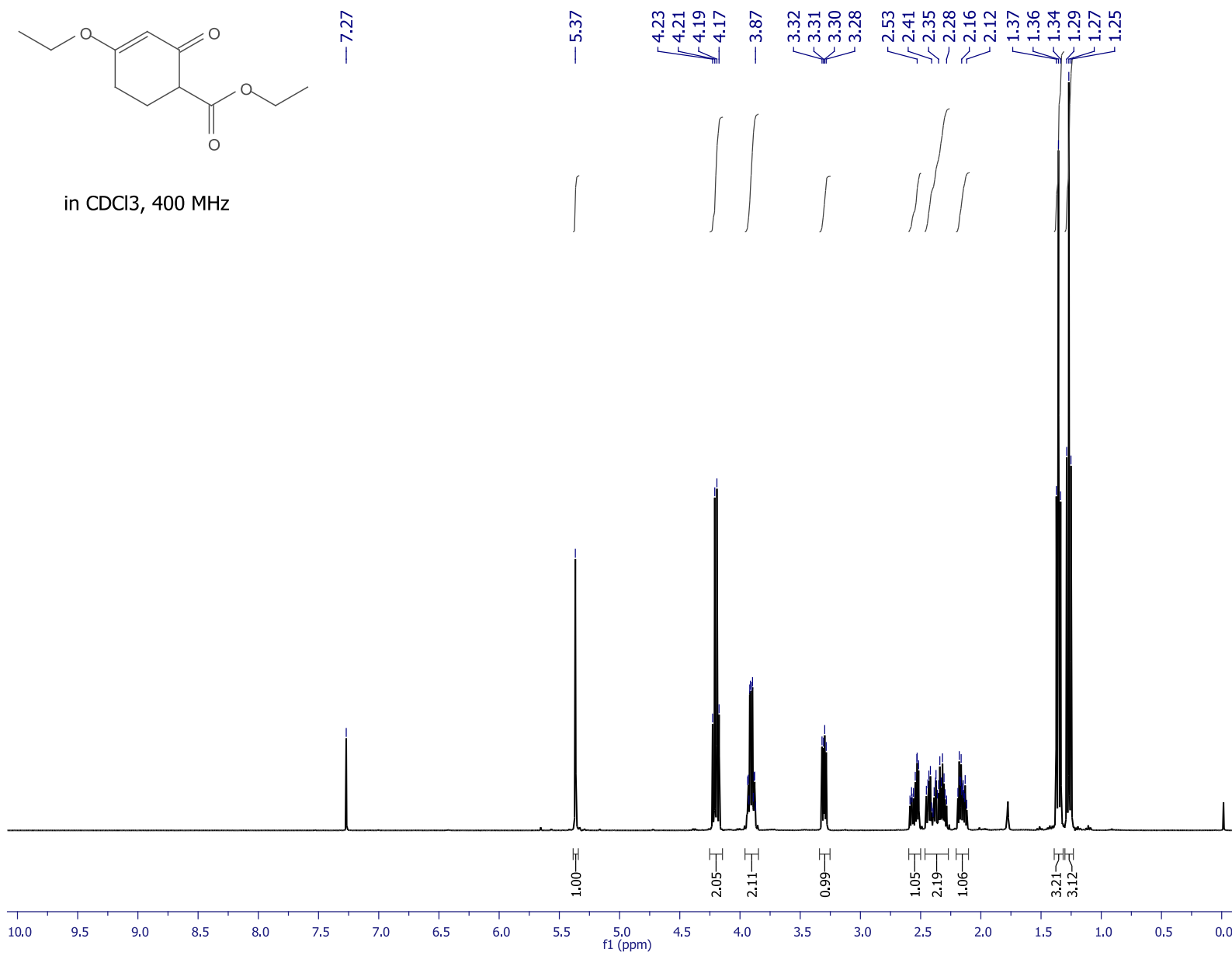
77.66
77.34
77.02
61.19
61.10
58.40
46.07
40.09
35.48
34.21
30.44
27.32
24.68
14.43

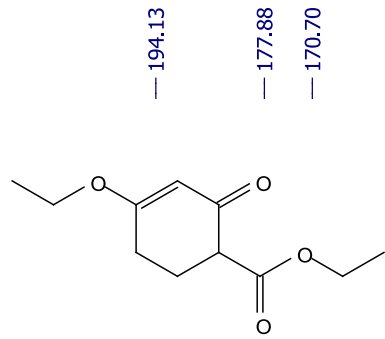
in CDCl₃, 100 MHz



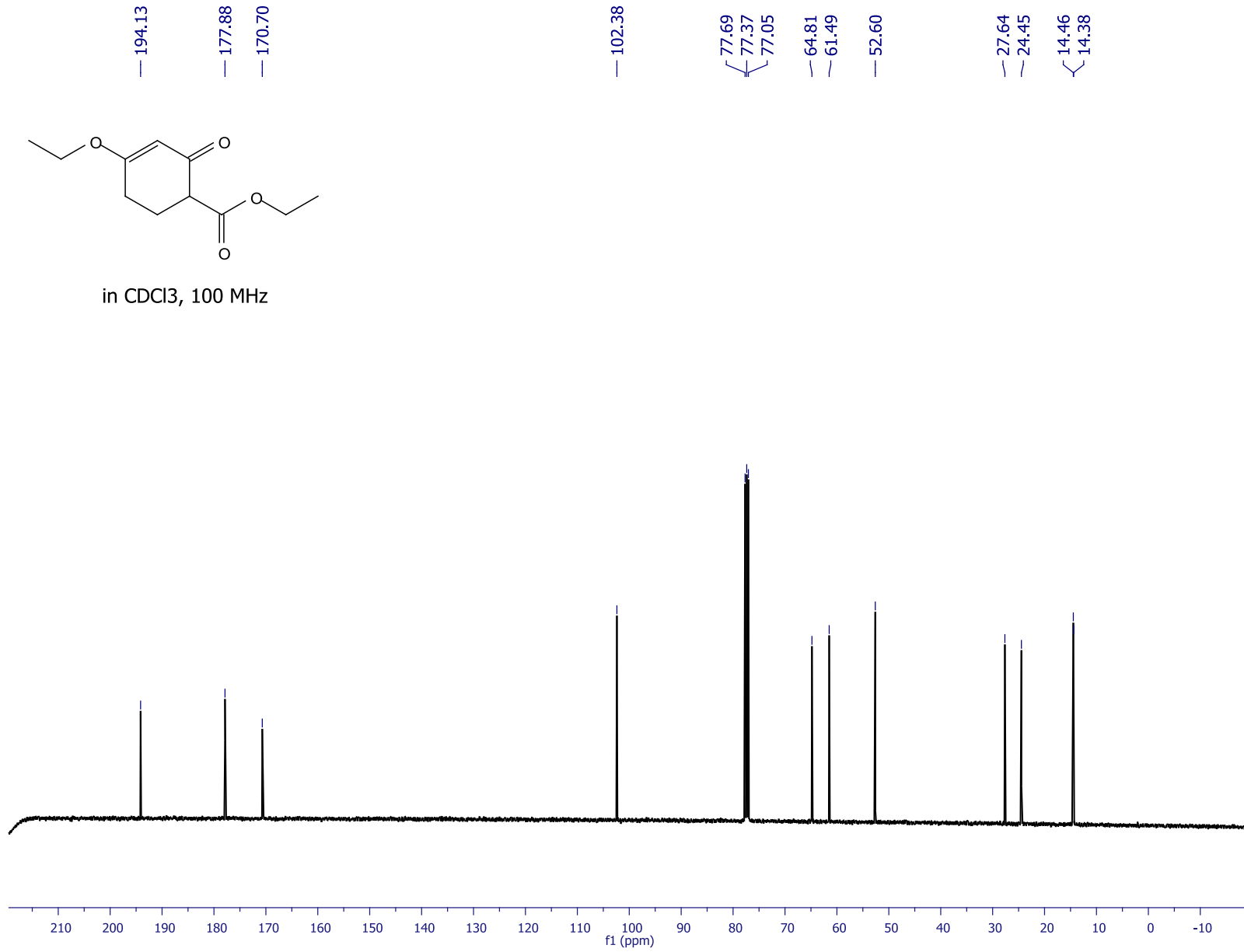


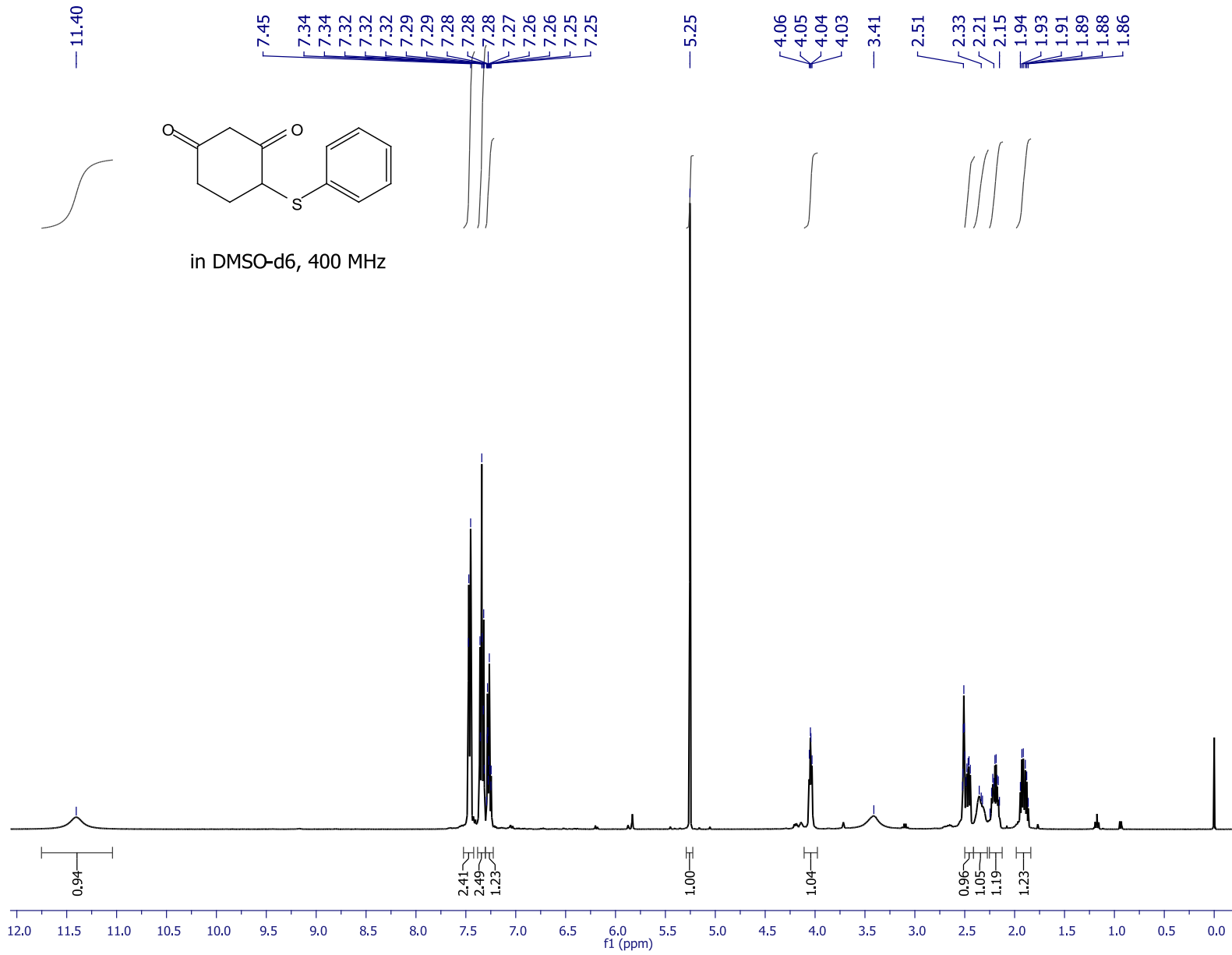
in CDCl₃, 400 MHz

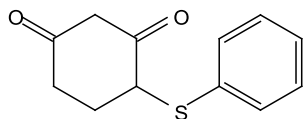




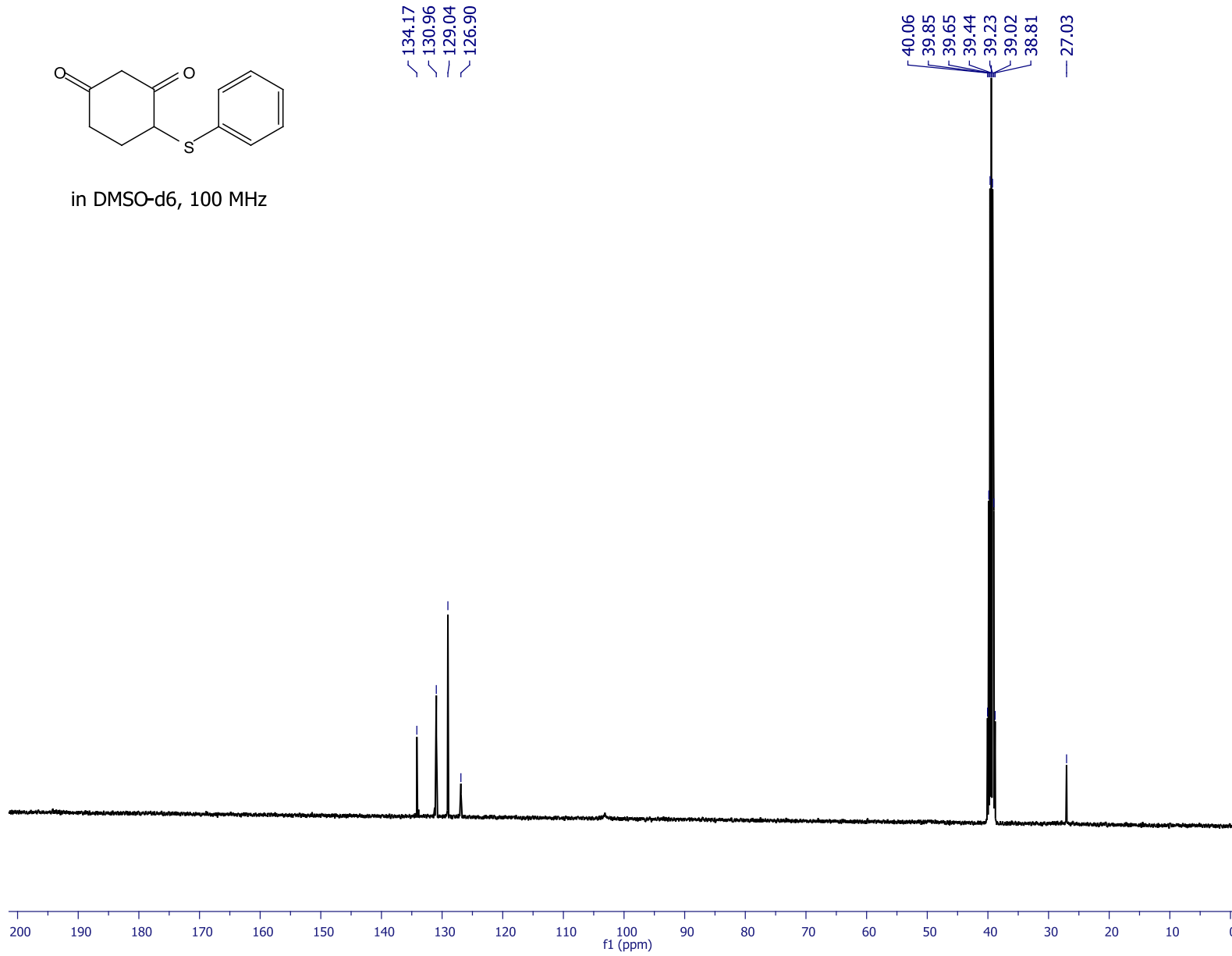
in CDCl₃, 100 MHz

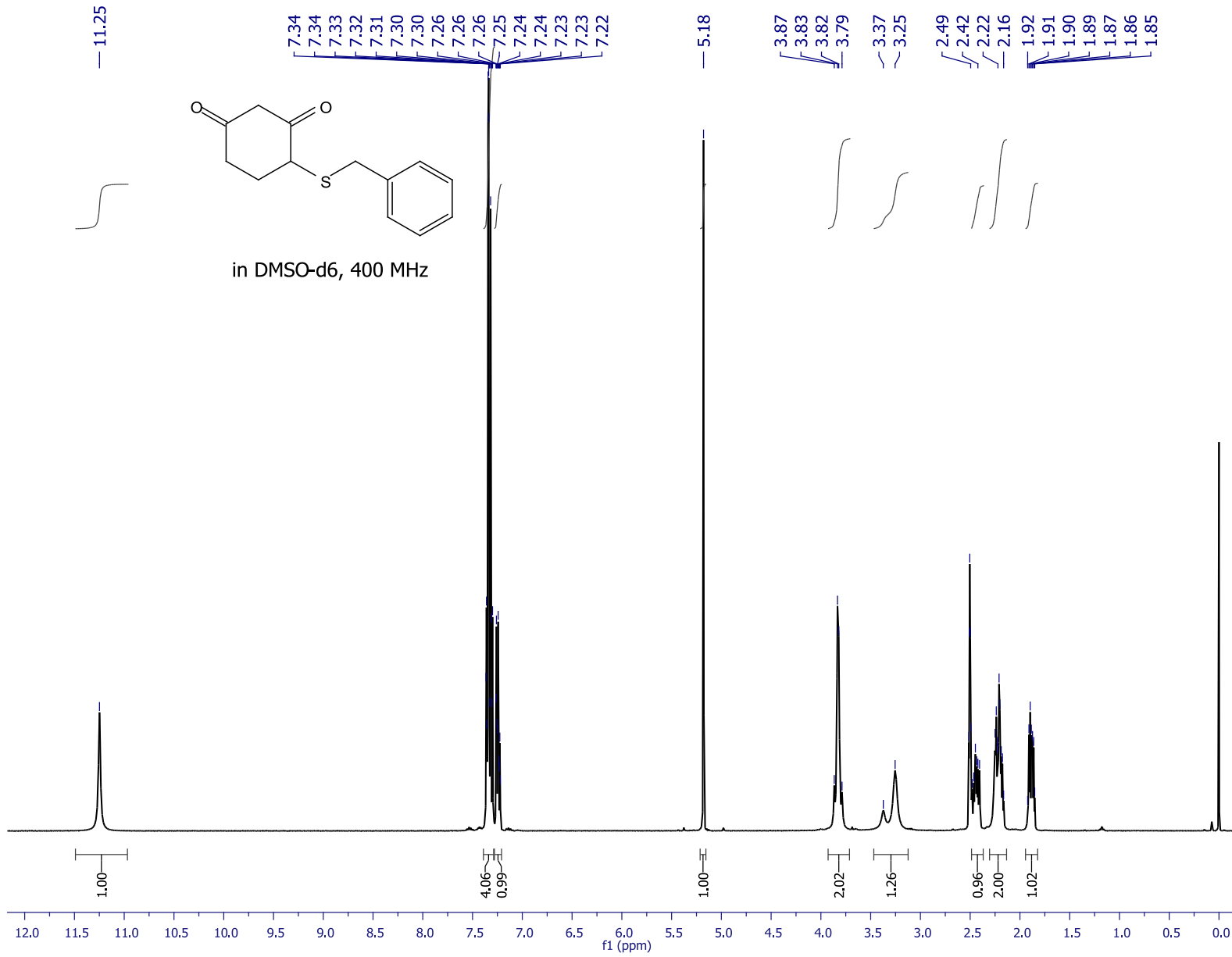


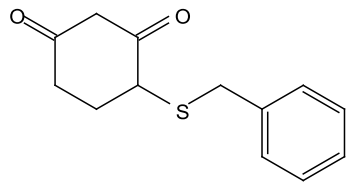




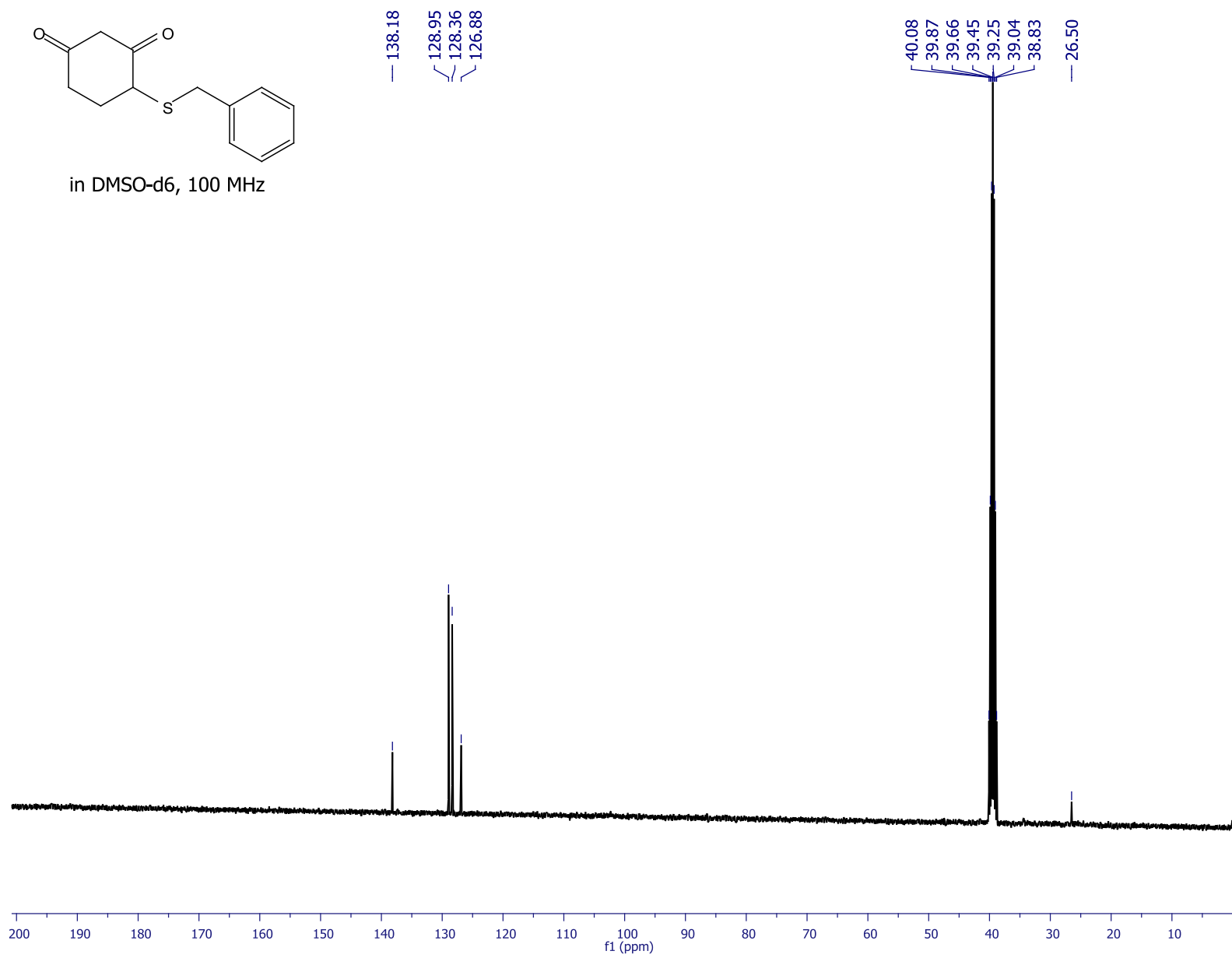
in DMSO-d6, 100 MHz

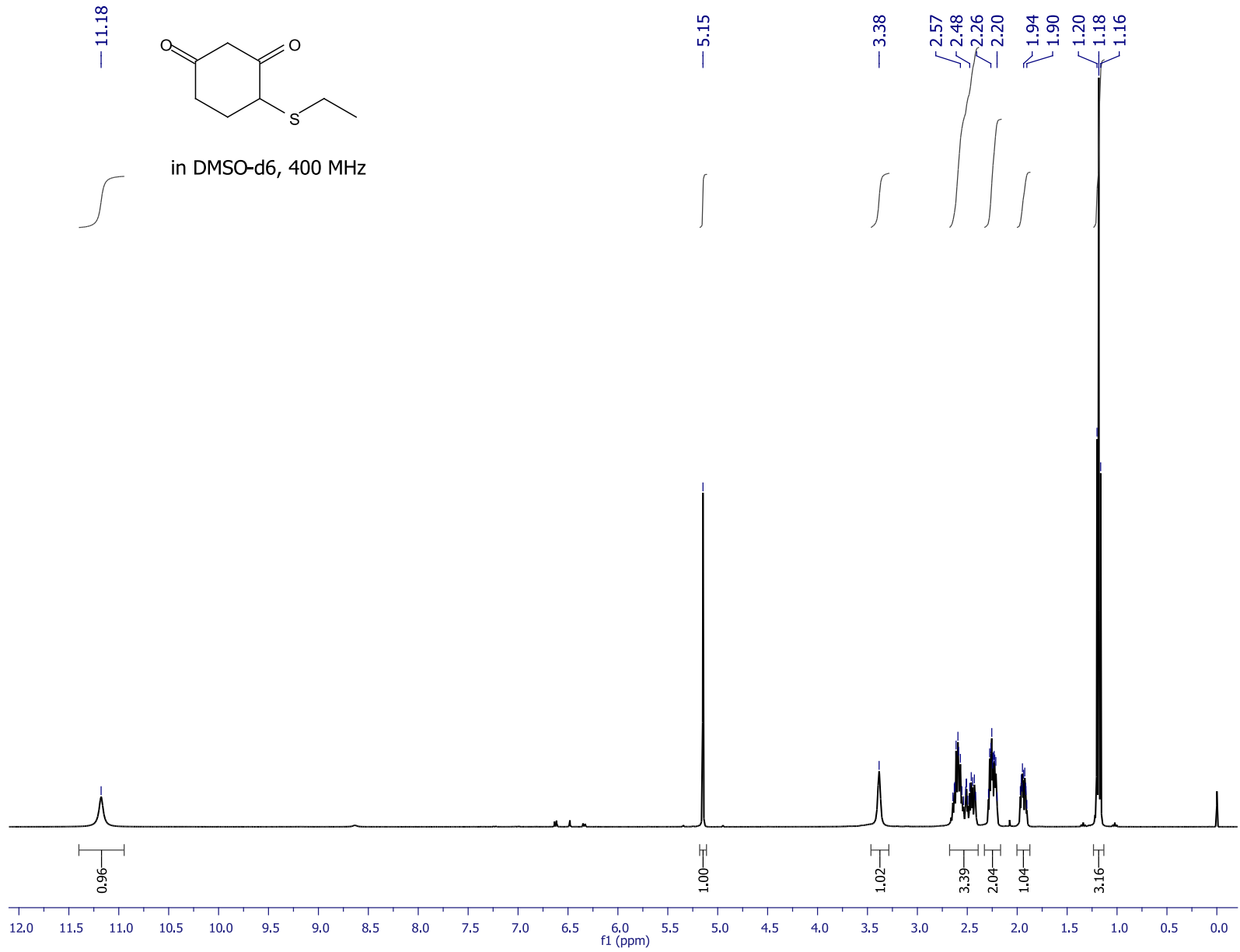


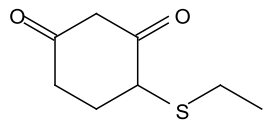




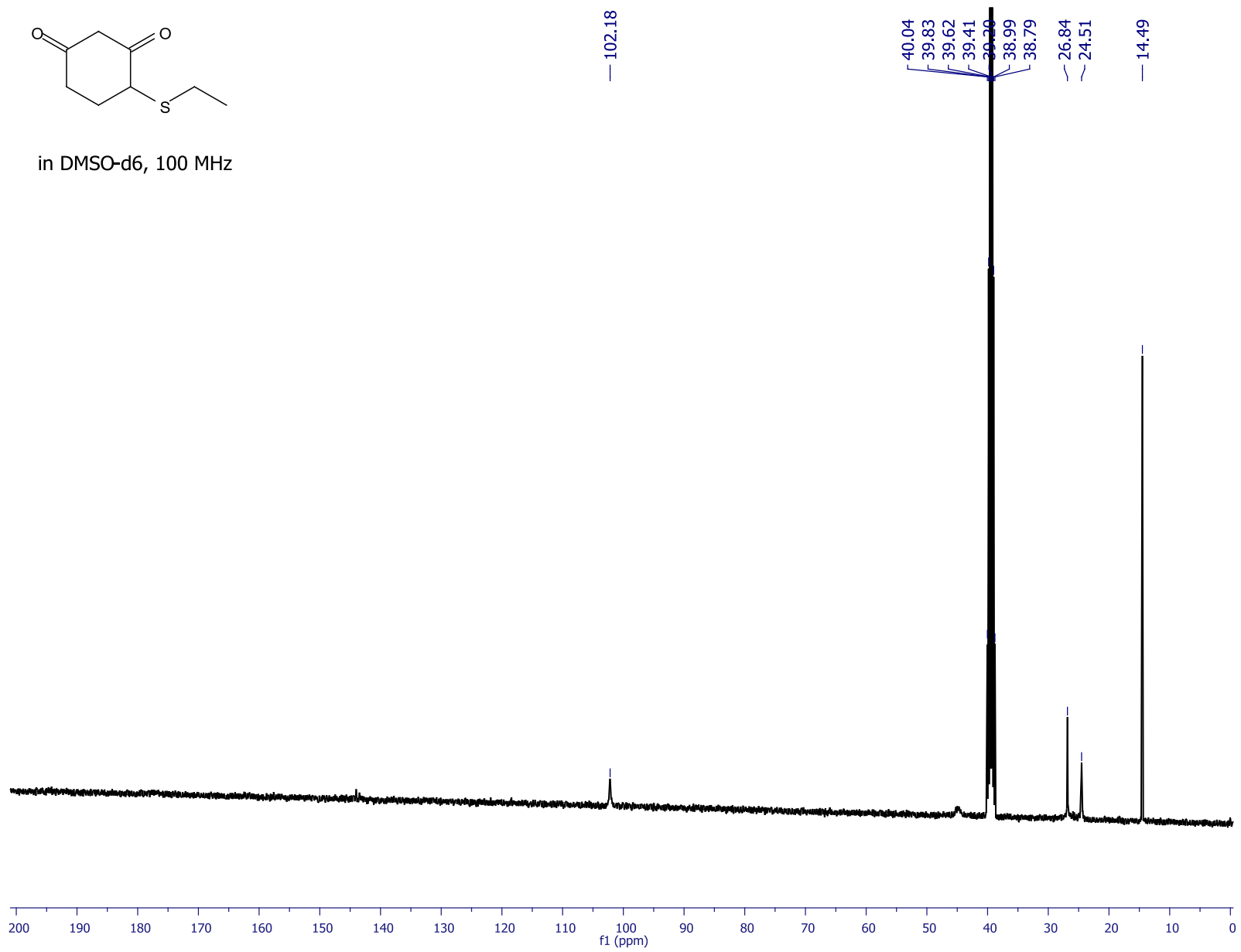
in DMSO-d6, 100 MHz

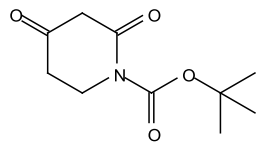




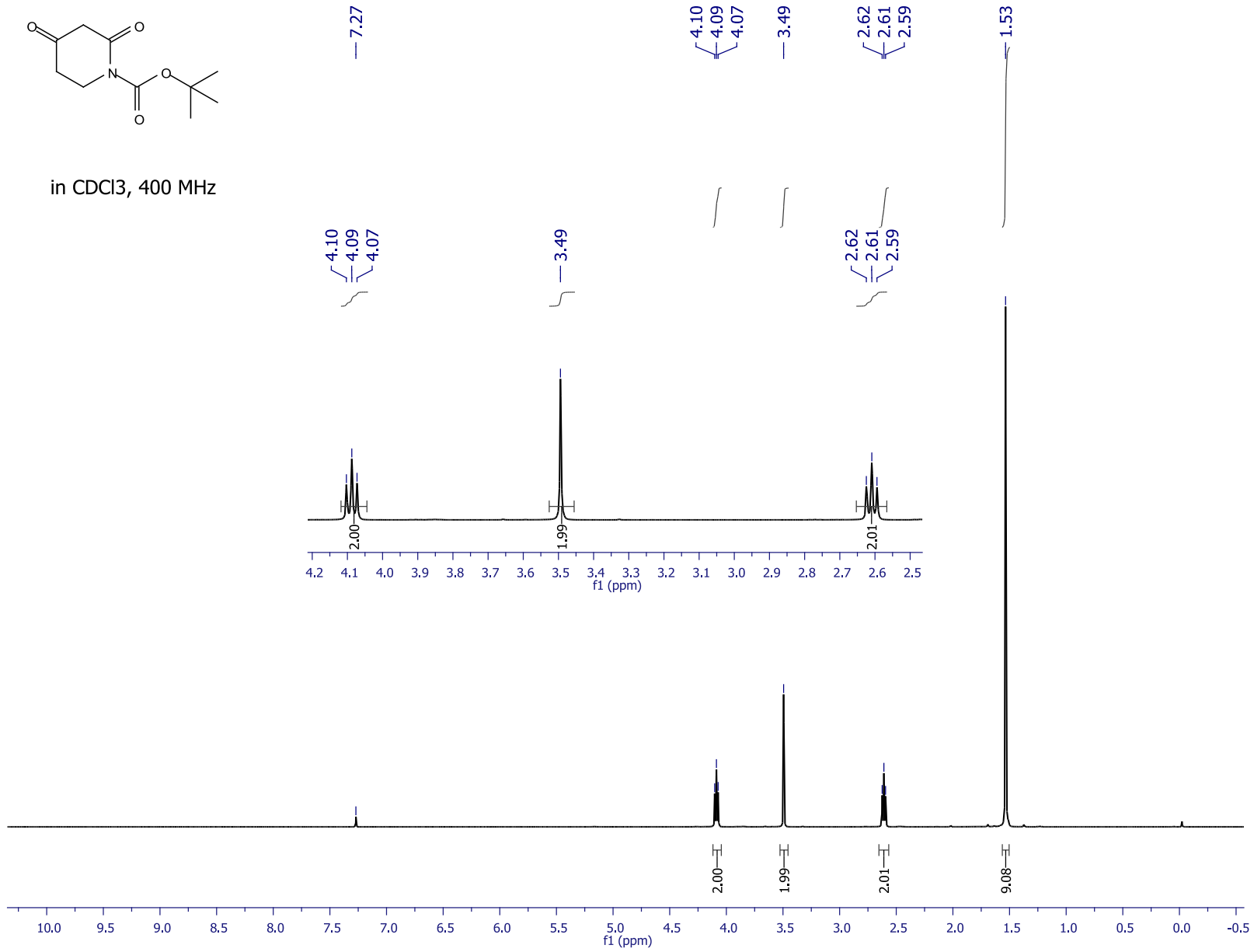


in DMSO-d6, 100 MHz





in CDCl₃, 400 MHz



— 202.42

— 165.60

— 151.54

— 84.51

77.66

77.34

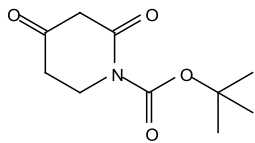
77.02

— 52.47

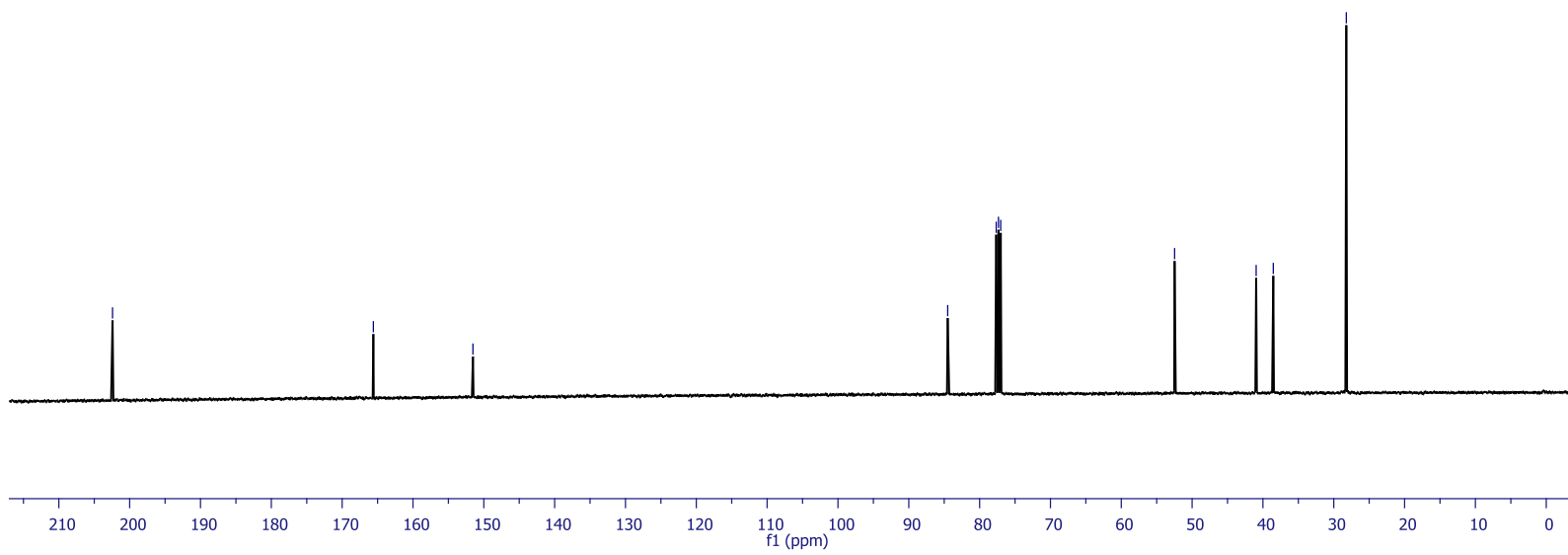
— 40.96

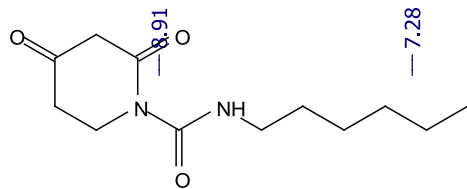
— 38.54

— 28.23

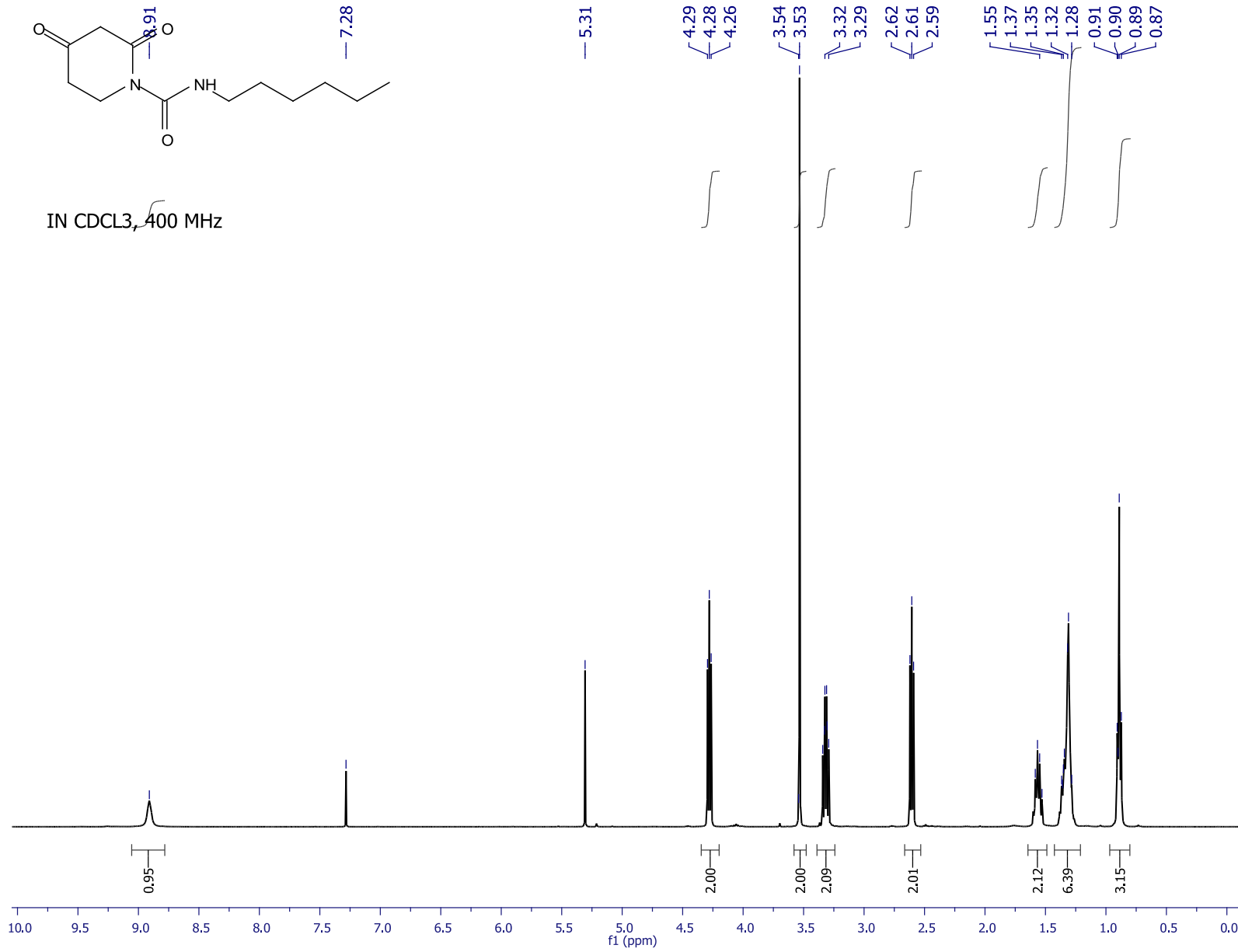


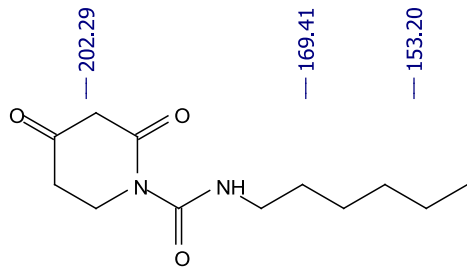
in CDCl₃, 100 MHz





IN CDCl₃, 400 MHz





77.37
77.05
76.74

51.59

40.71

38.37

38.08

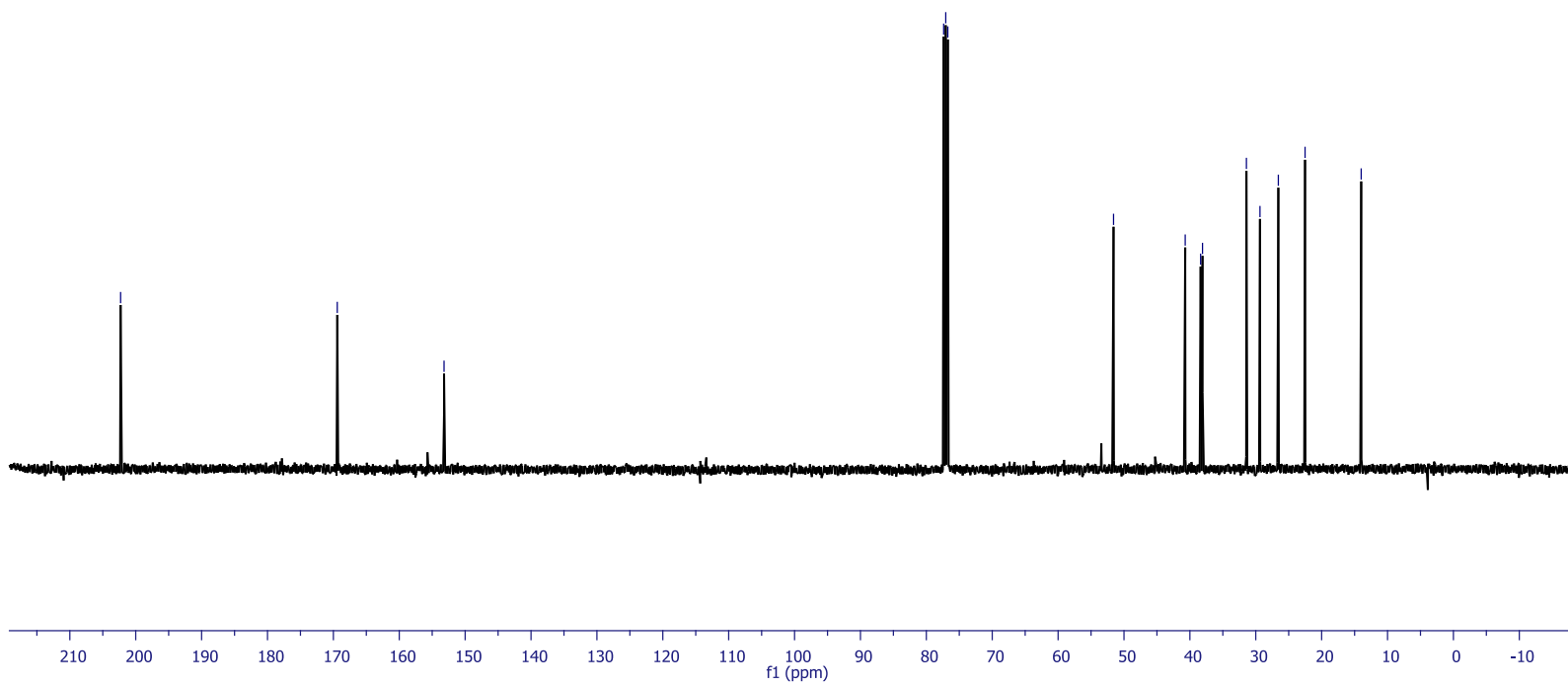
31.42

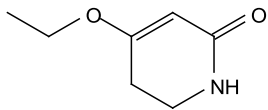
26.57

22.52

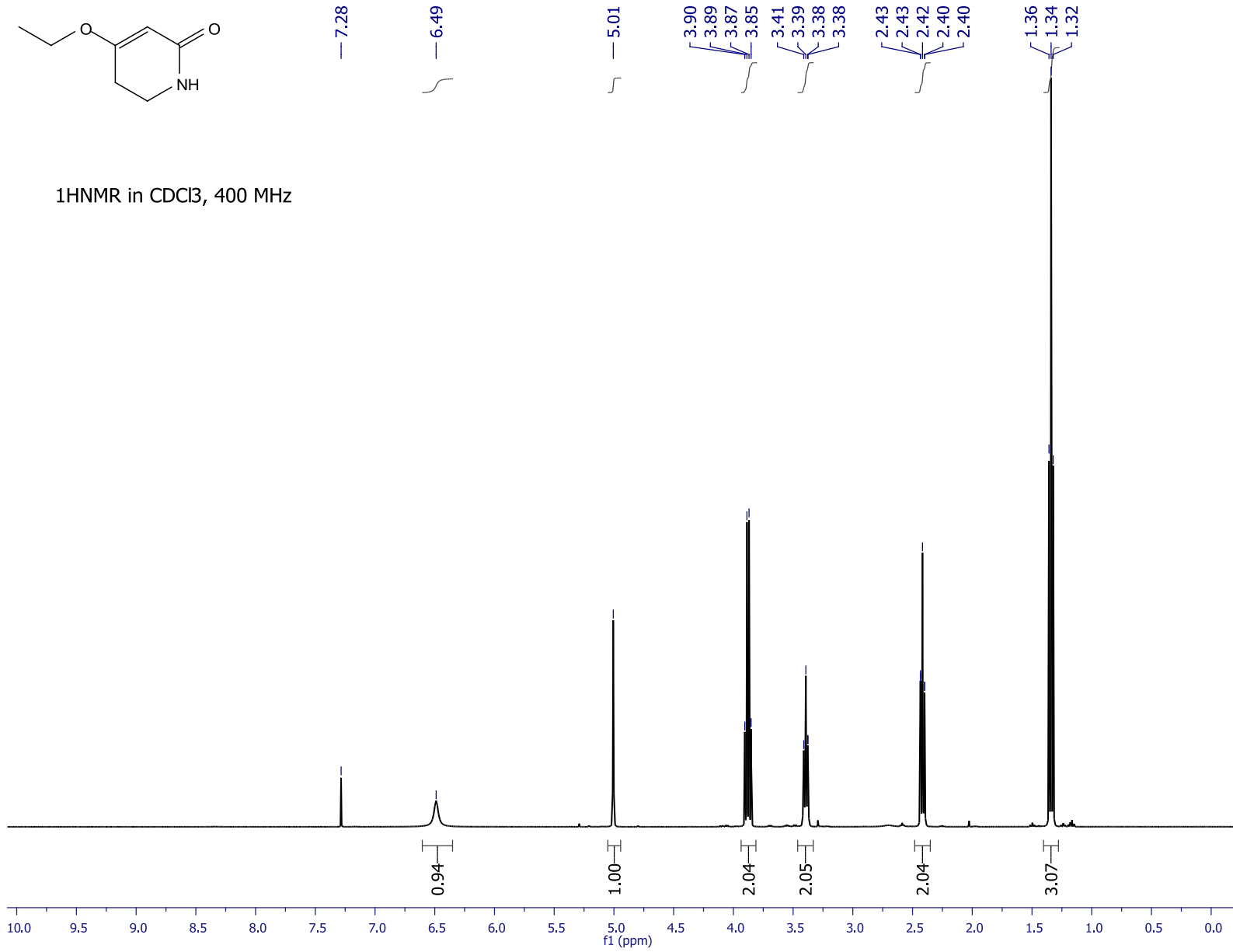
14.00

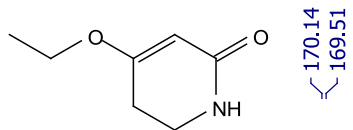
IN CDCl₃, 100 MHz





¹HNMR in CDCl₃, 400 MHz





93.85

77.41

77.09

76.77

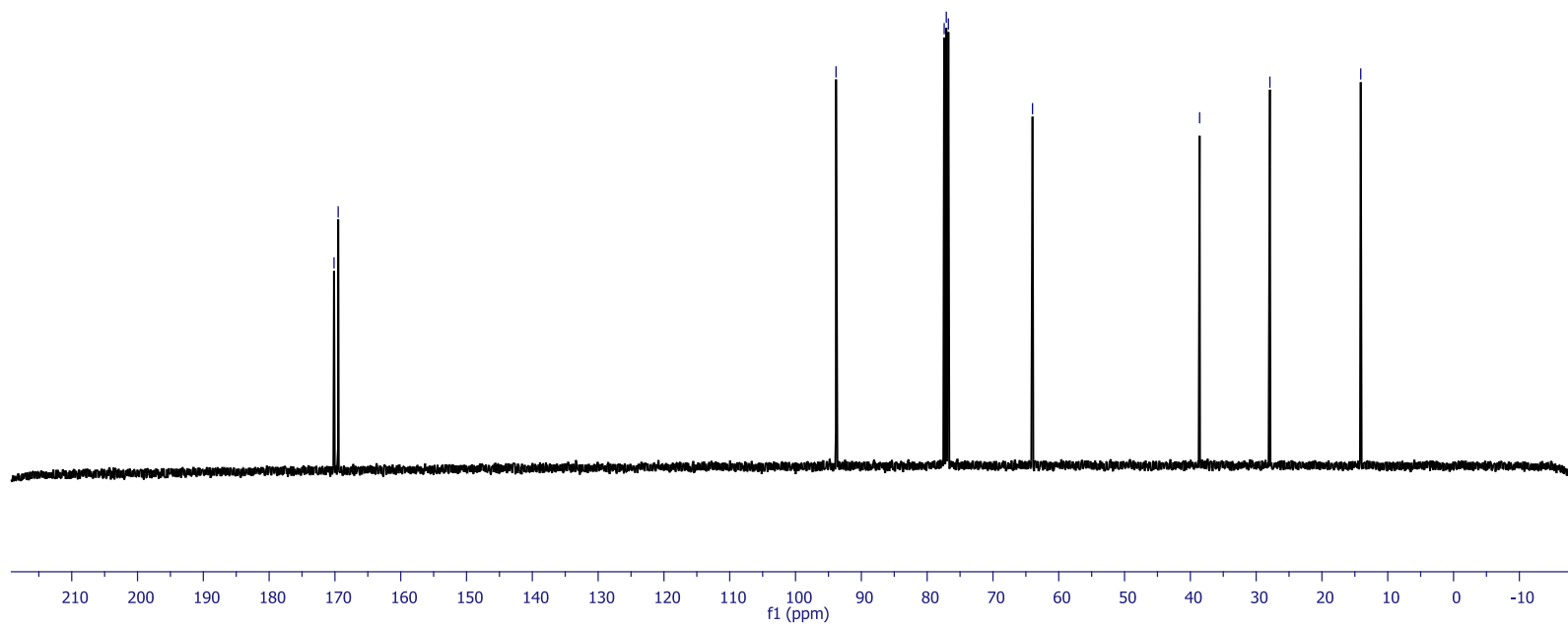
63.98

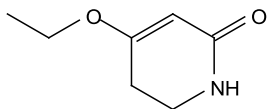
38.59

27.91

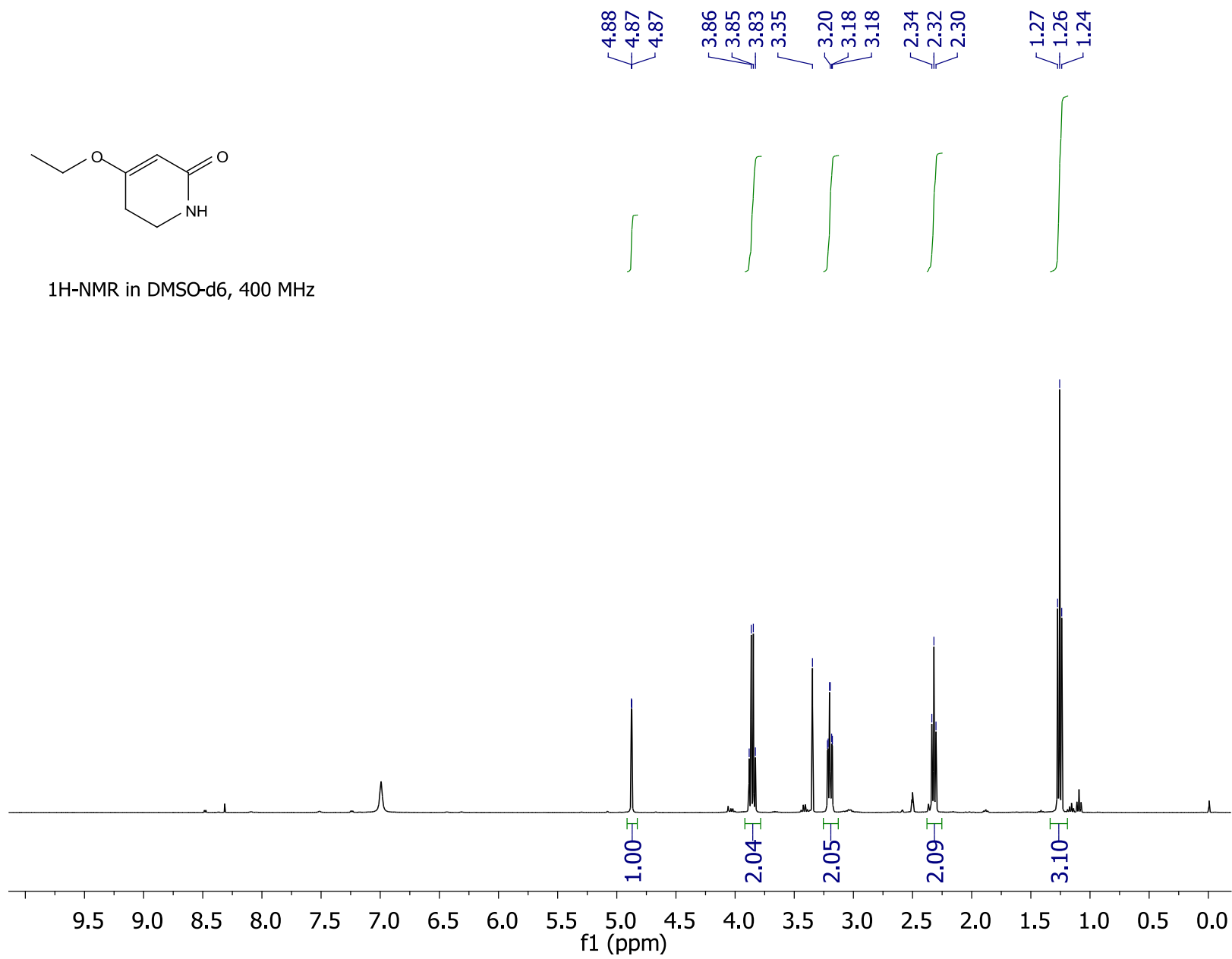
14.10

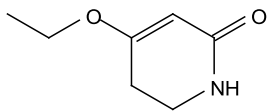
13-CNMR in CDCl₃, 100 MHz





¹H-NMR in DMSO-d₆, 400 MHz





168.48
167.90

94.07

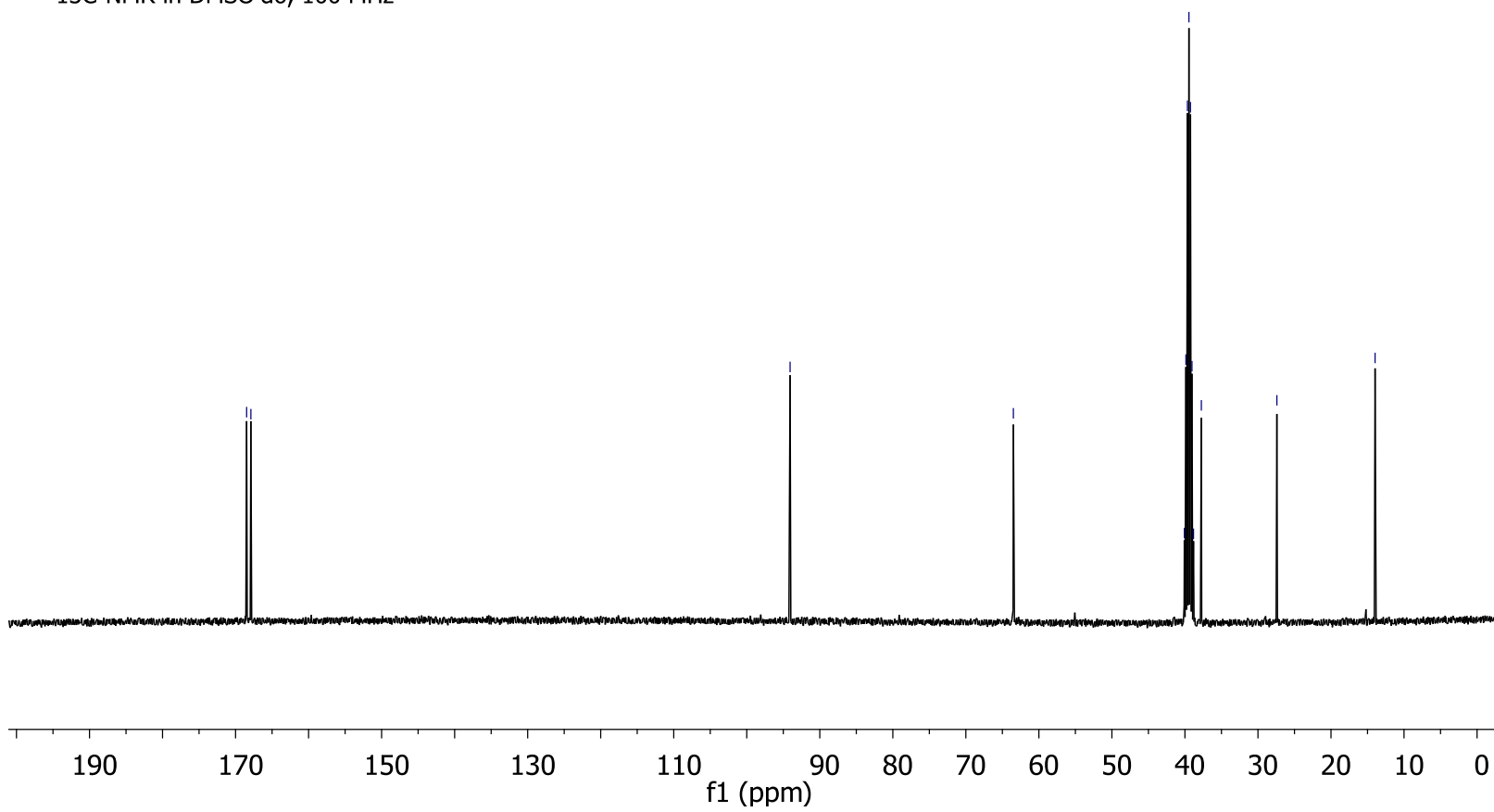
63.49

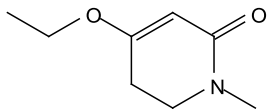
39.45
39.24
39.04
38.83
37.75

27.41

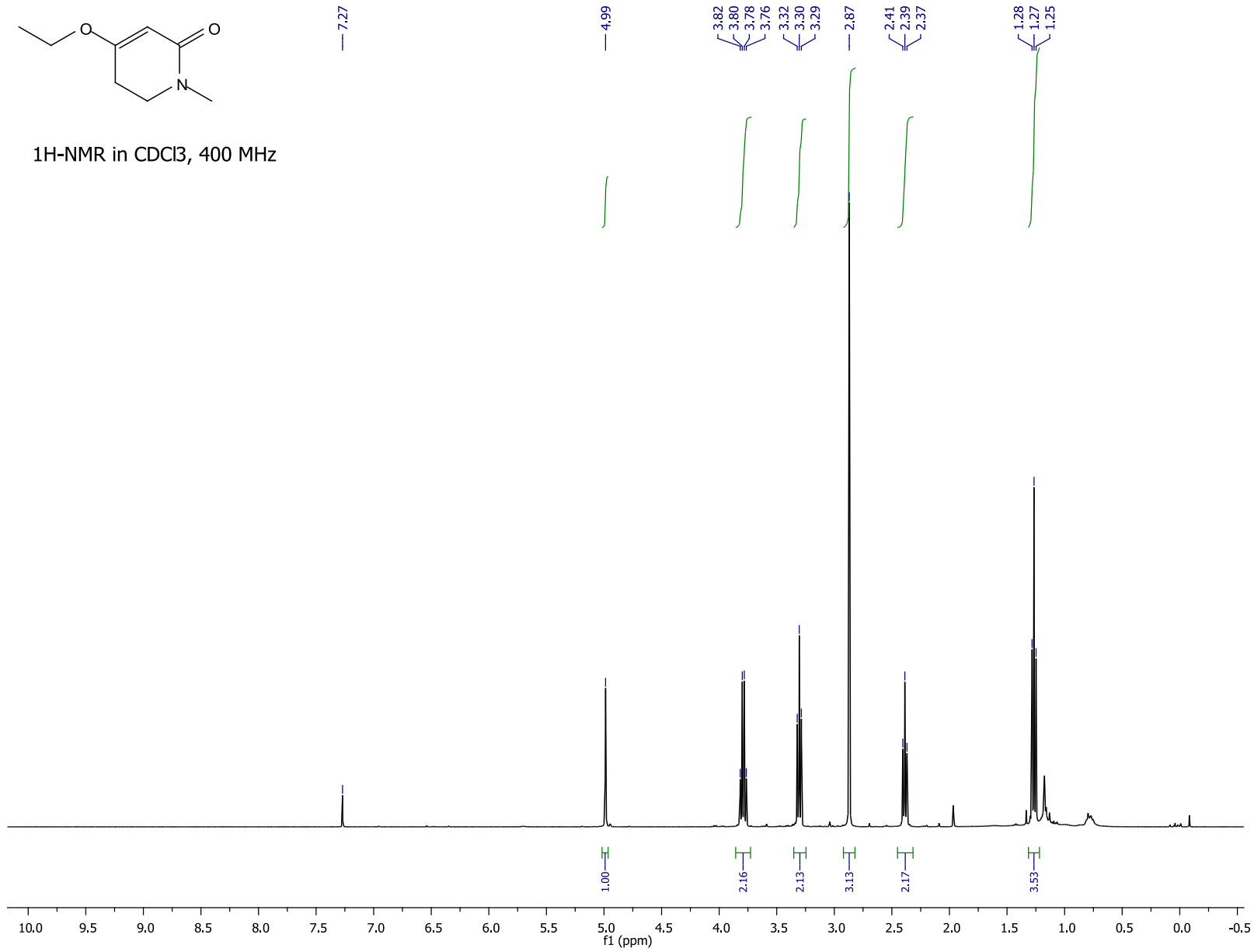
13.96

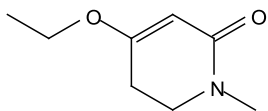
¹³C-NMR in DMSO-d₆, 100 MHz





¹H-NMR in CDCl₃, 400 MHz





13-CNMR in CDCl₃, 100 MHz

167.7
167.5

94.5

77.5
77.2
76.8

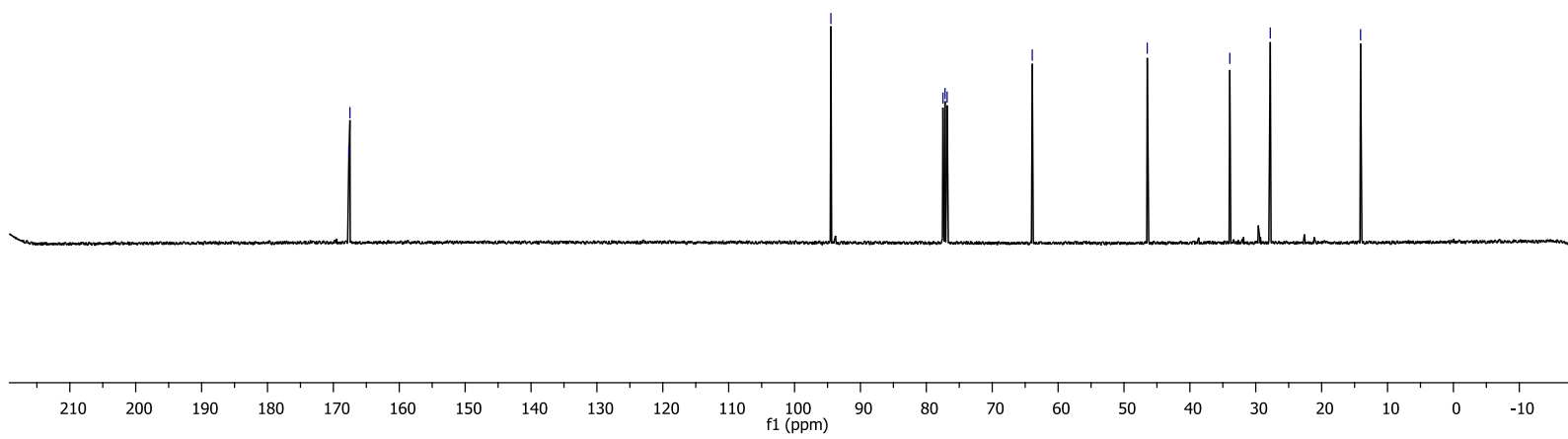
63.9

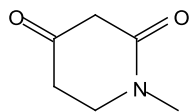
46.5

33.9

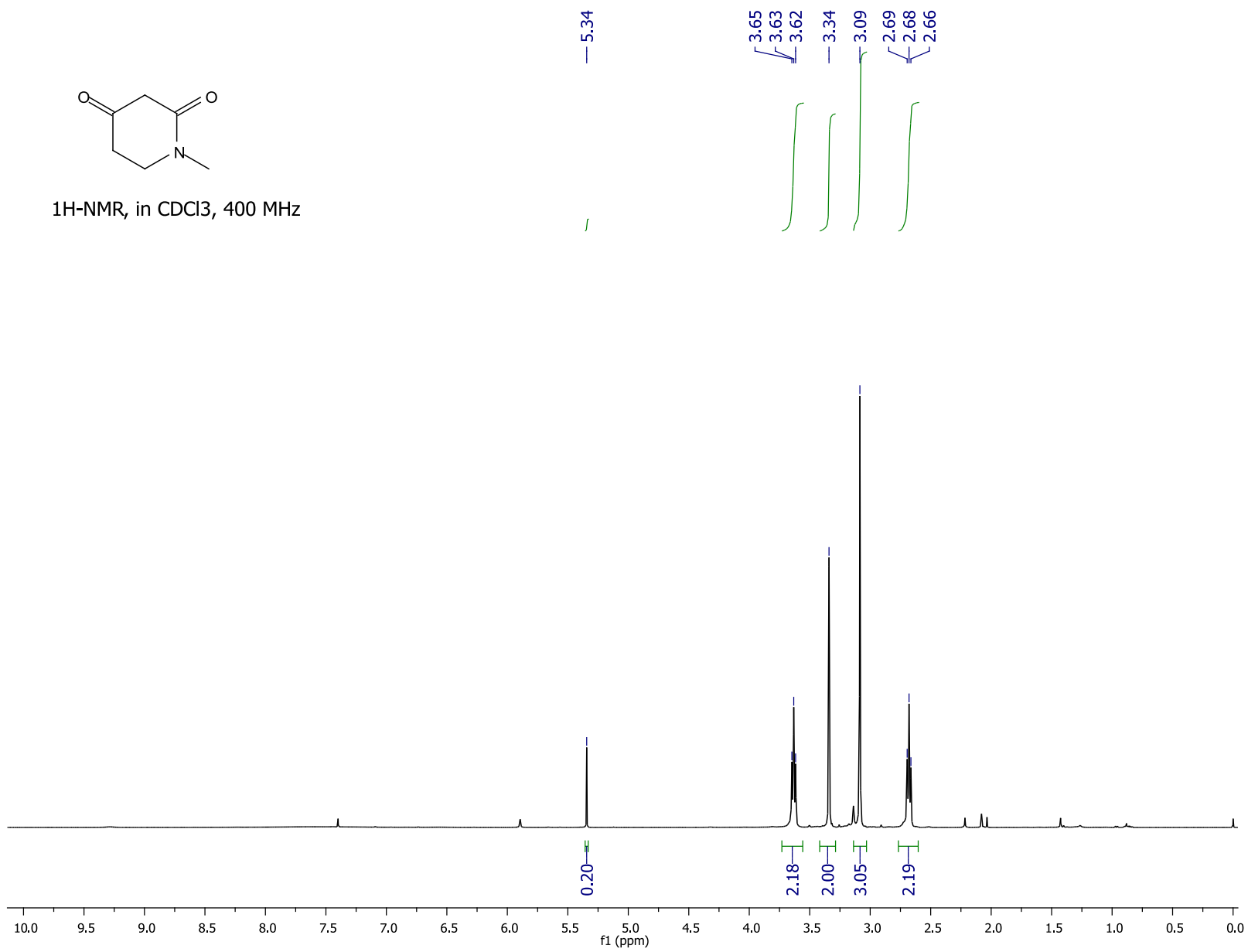
27.8

14.1

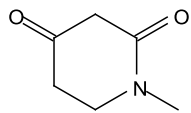




¹H-NMR, in CDCl₃, 400 MHz



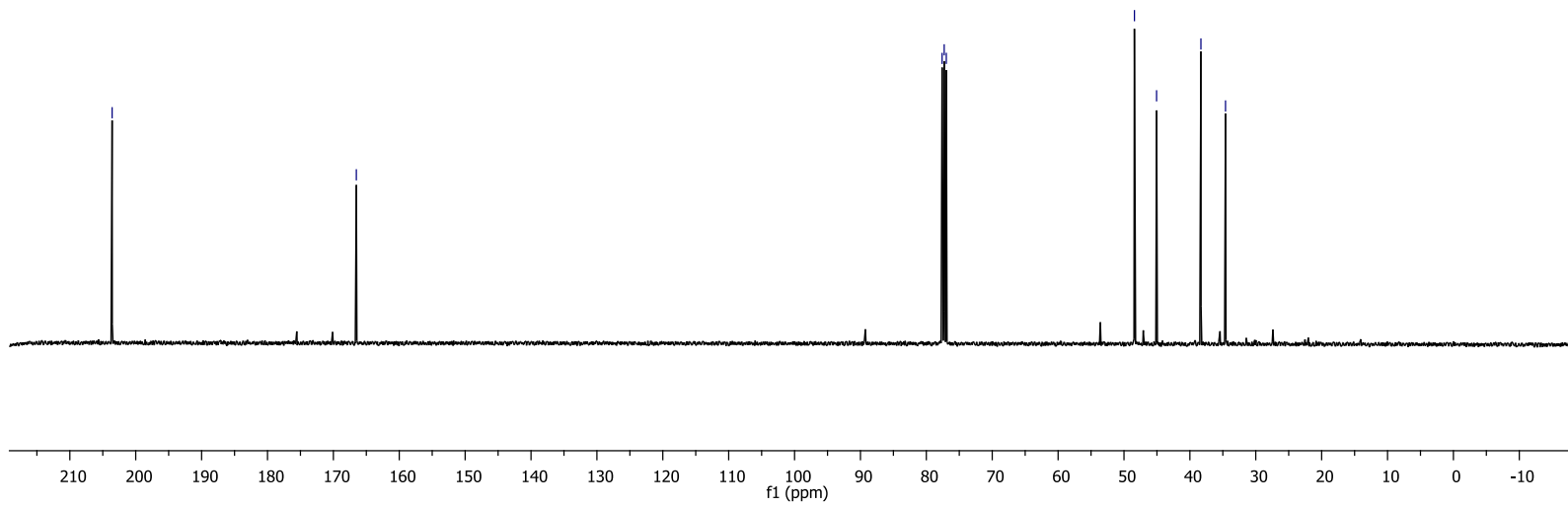
— 203.6
— 166.5

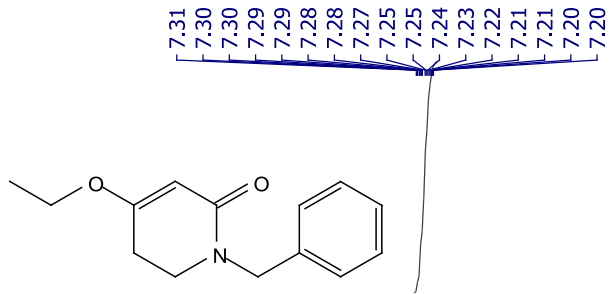


¹³C-NMR, in CDCl₃, 100 MHz

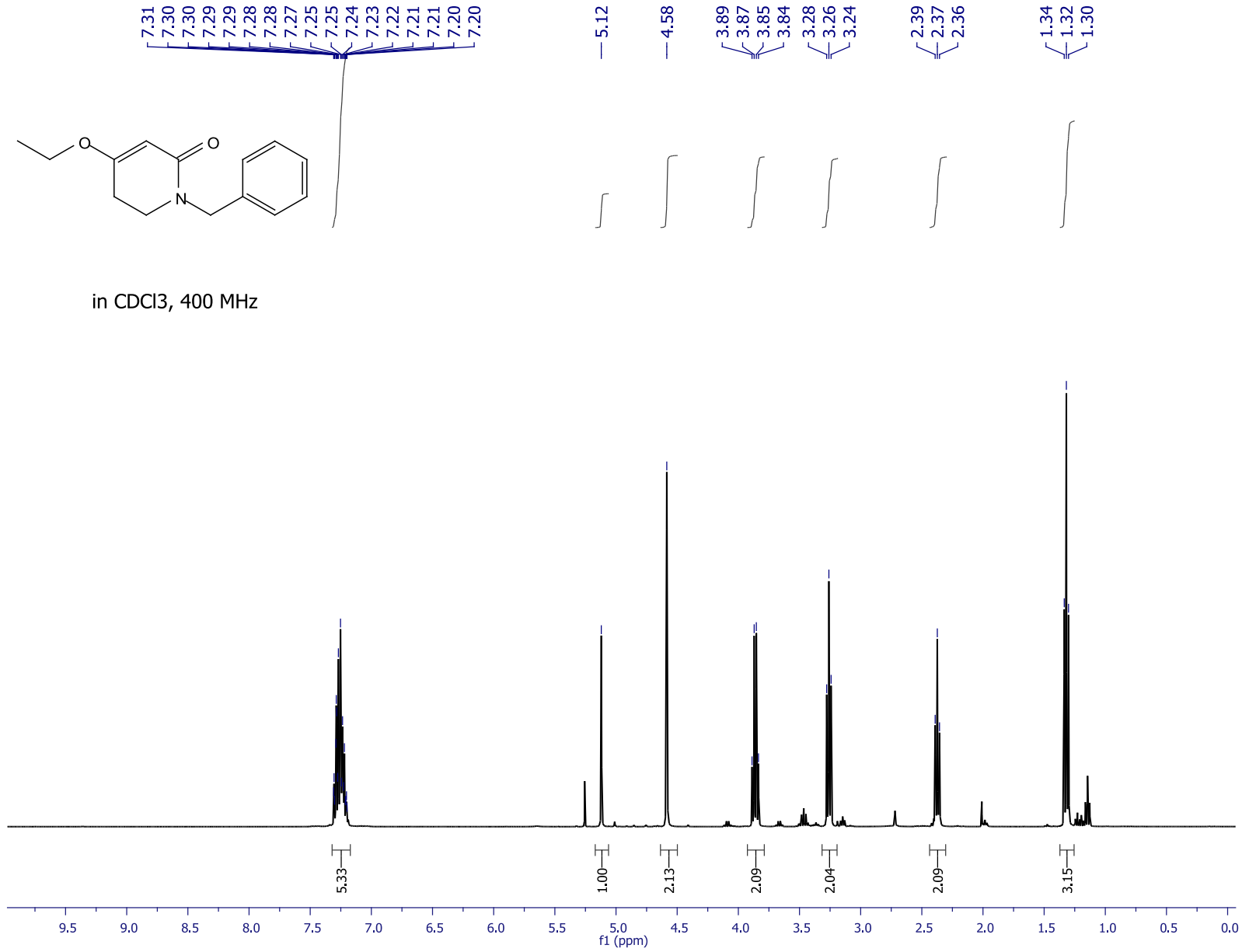
77.6
77.3
77.0

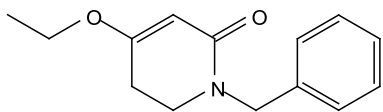
48.4
45.1
38.3
34.6



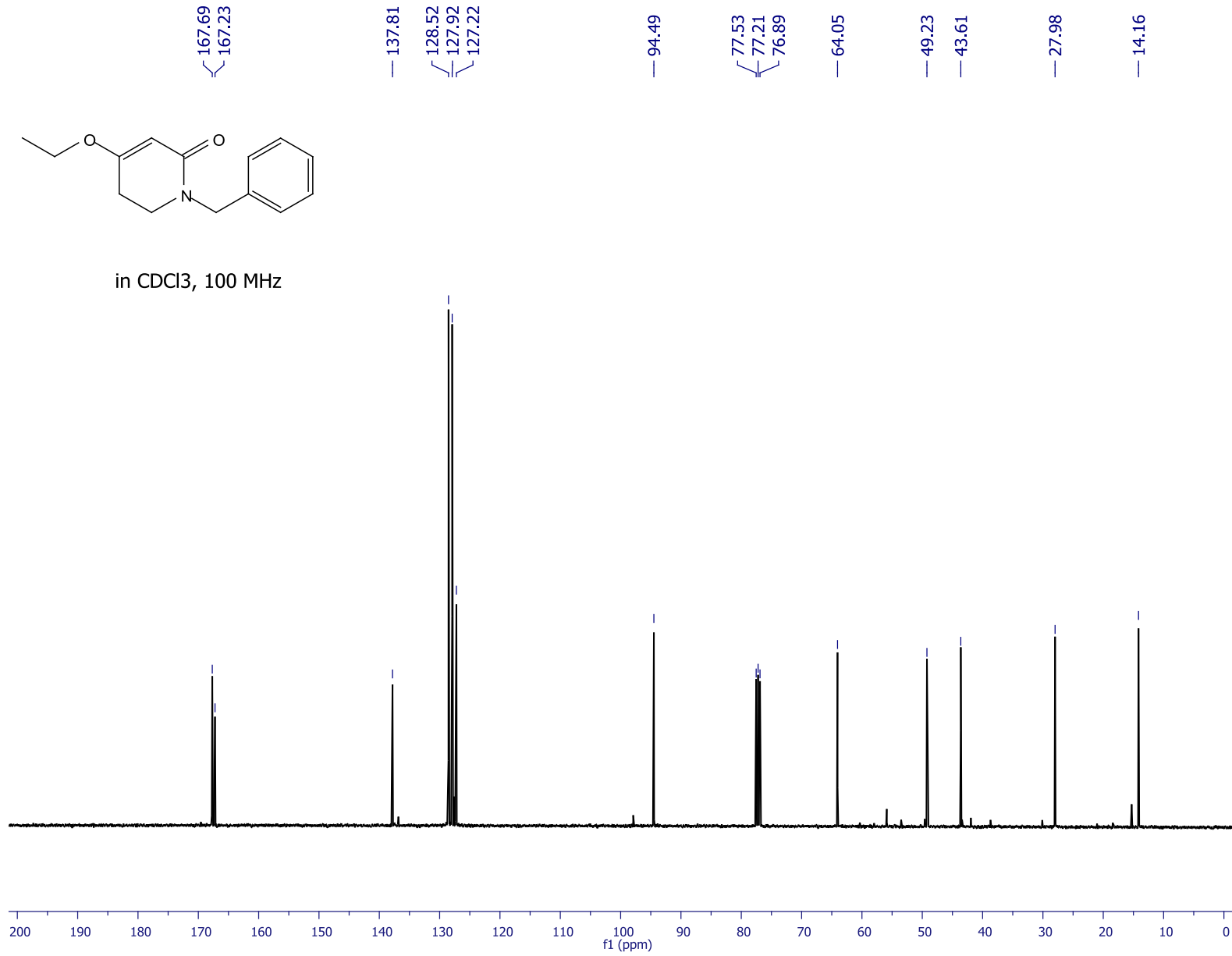


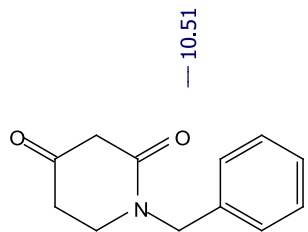
in CDCl₃, 400 MHz



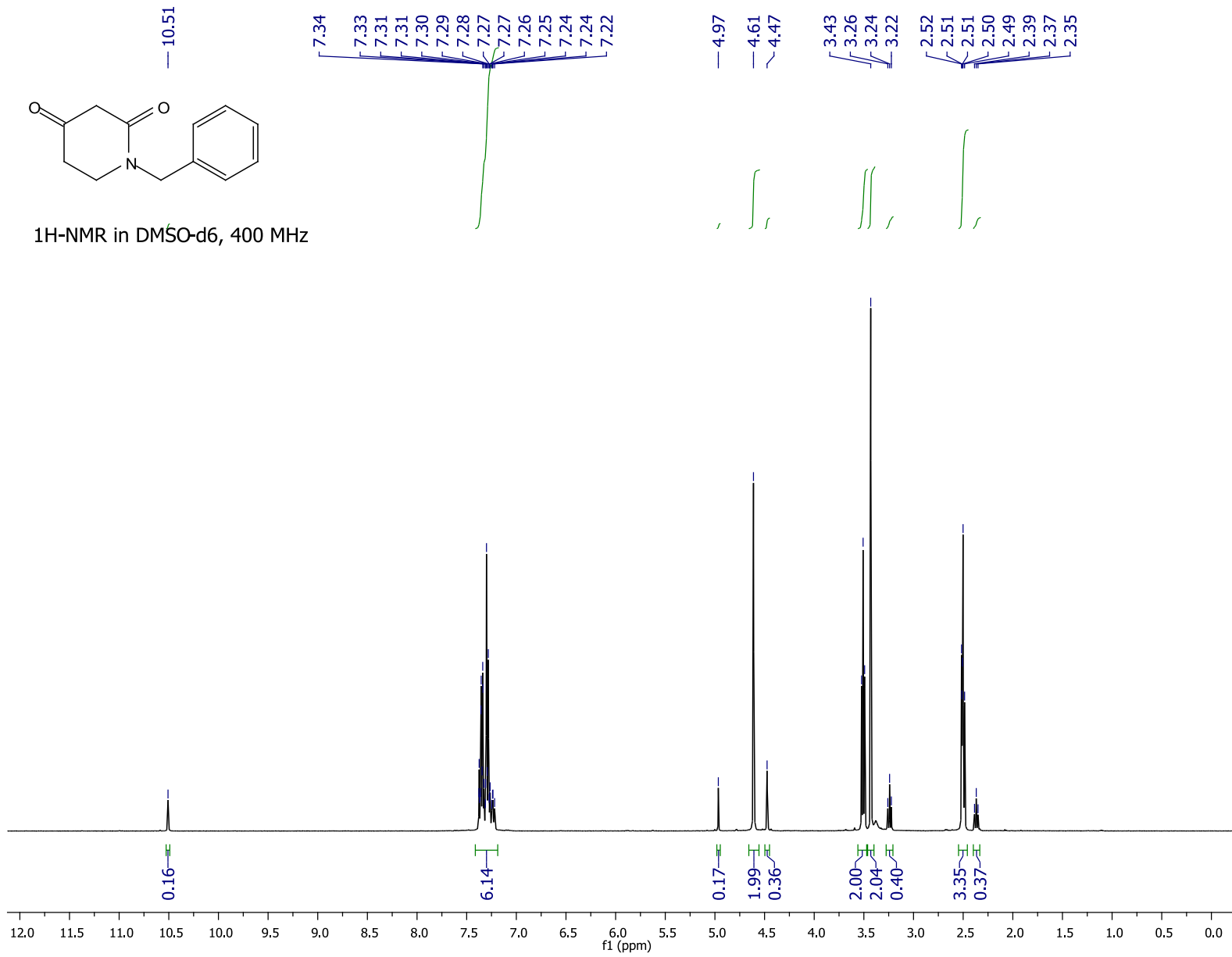


in CDCl₃, 100 MHz

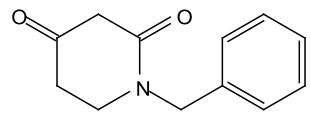




¹H-NMR in DMSO-d₆, 400 MHz



— 204.8
167.6
166.7
166.2

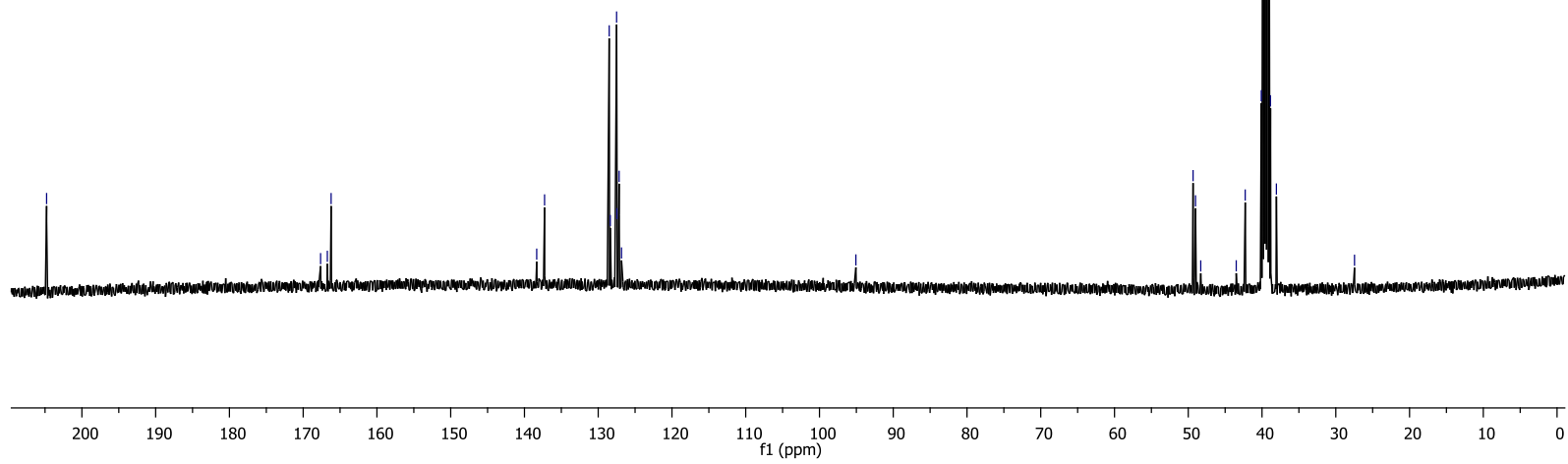


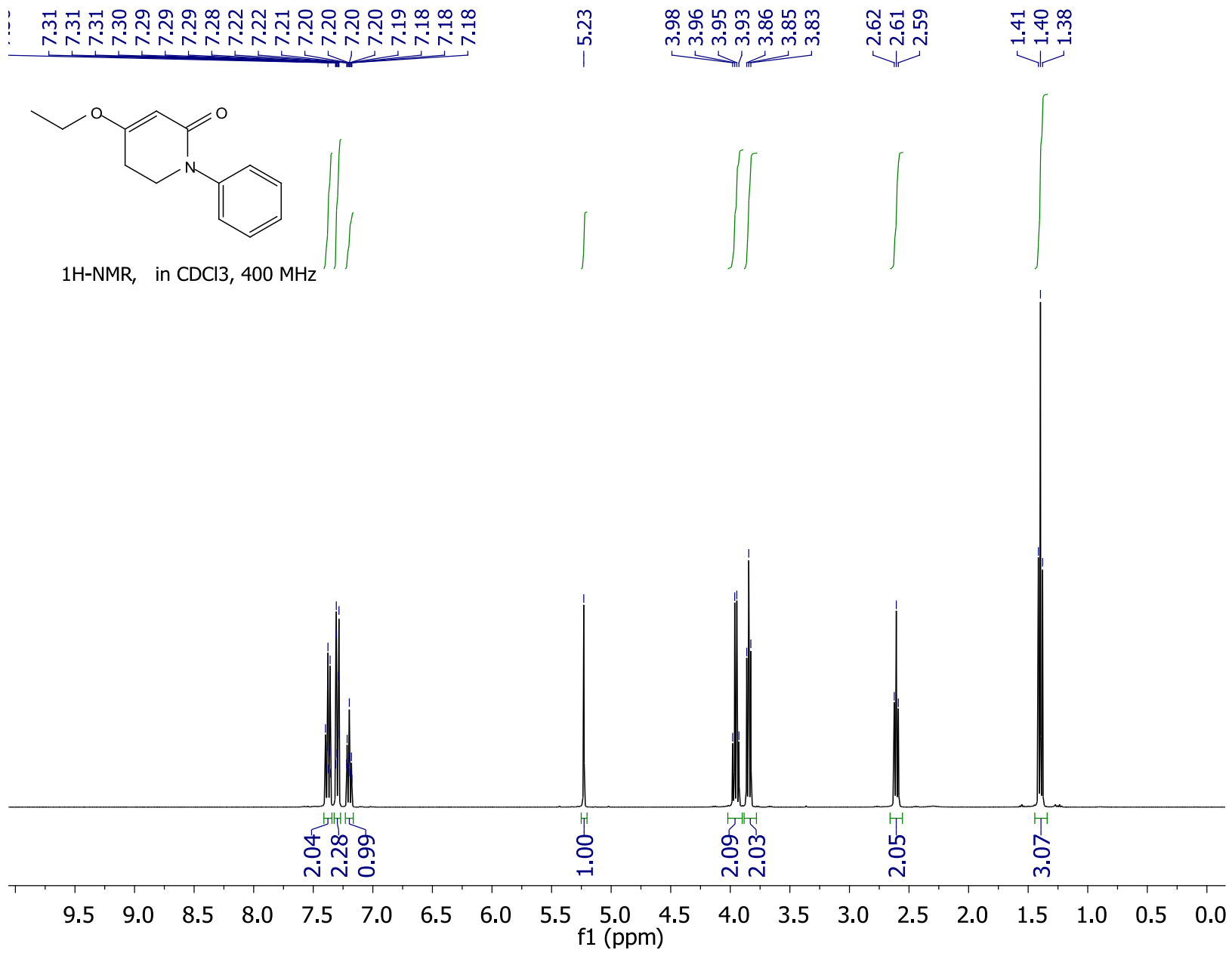
13C-NMR in DMSO-d6,100 MHz

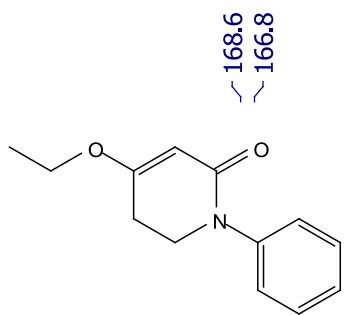
138.3
137.3
128.5
128.4
127.5
127.5
127.2
126.8

— 95.1

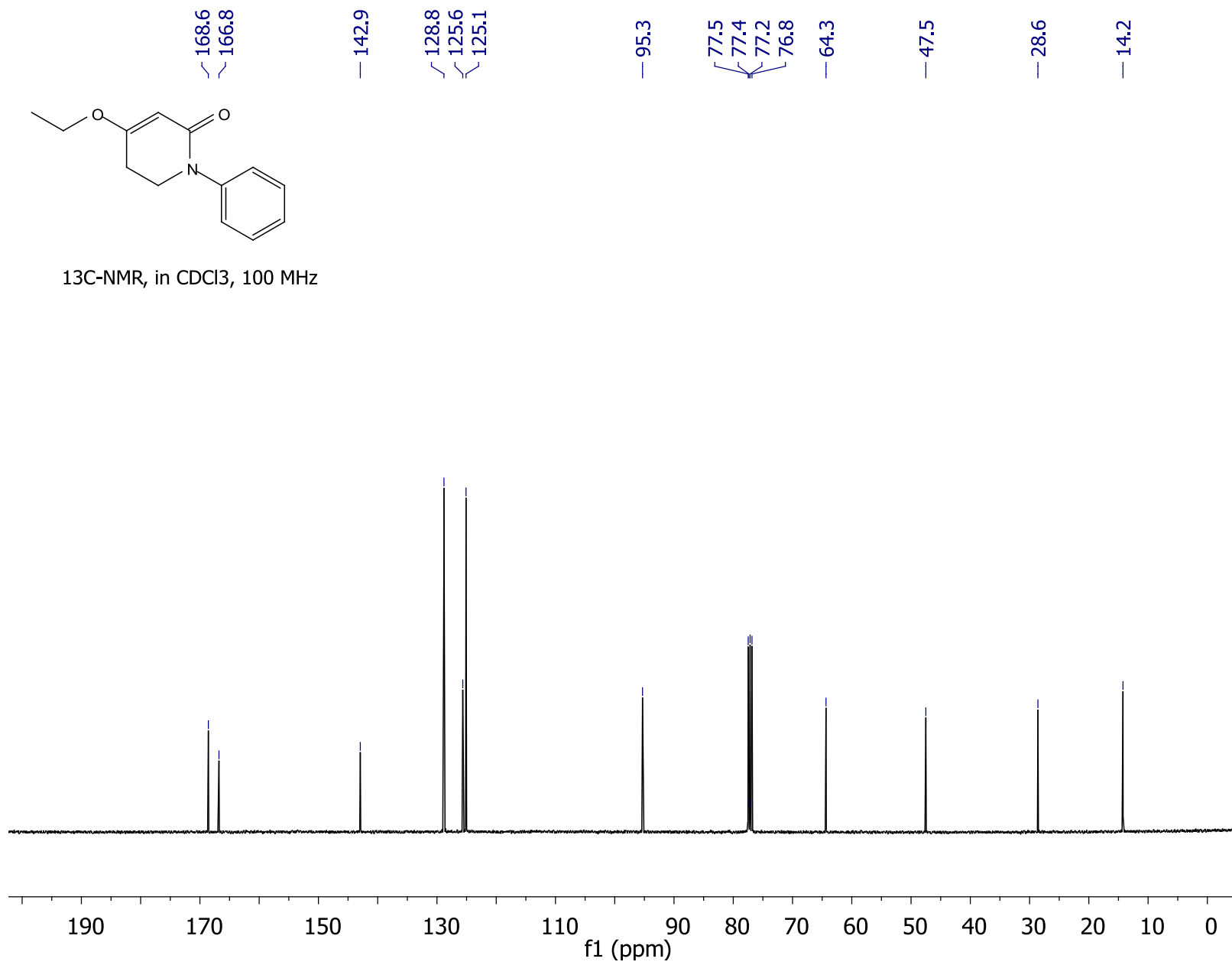
49.3
49.0
48.3
39.9
39.5
39.1
38.1
— 27.5

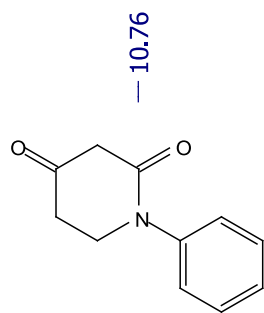




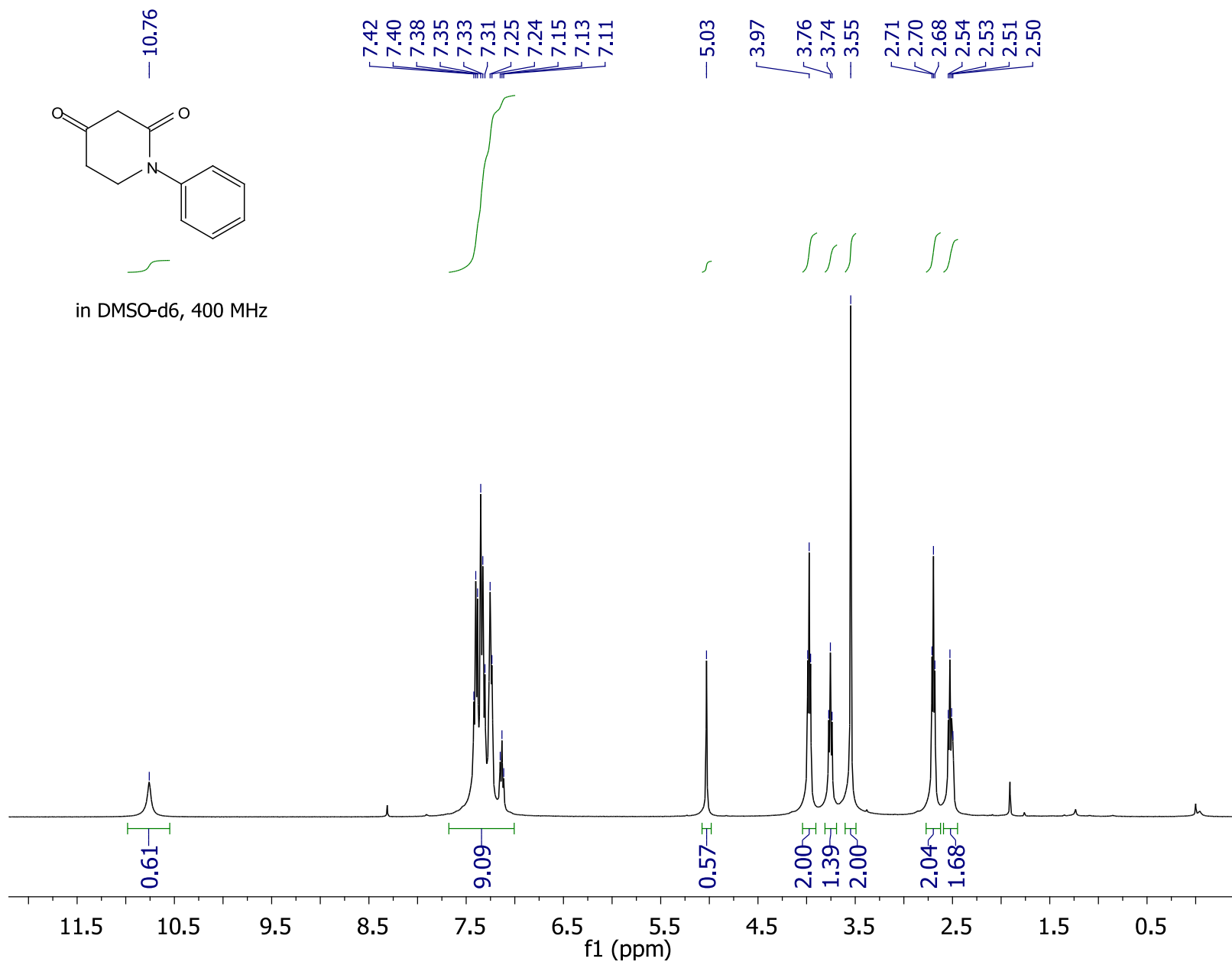


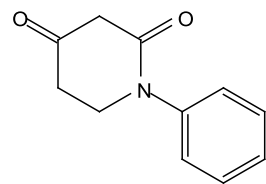
¹³C-NMR, in CDCl₃, 100 MHz



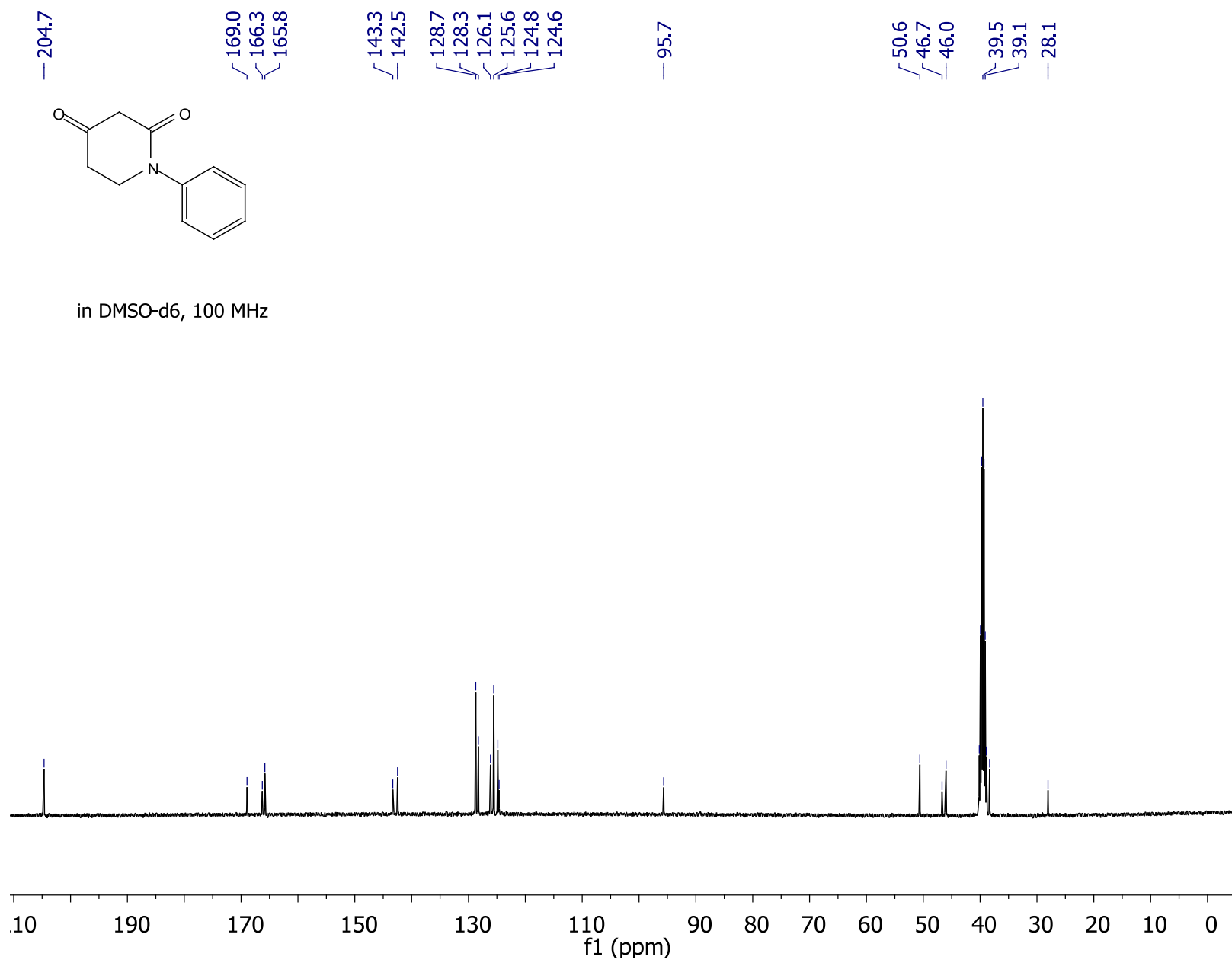


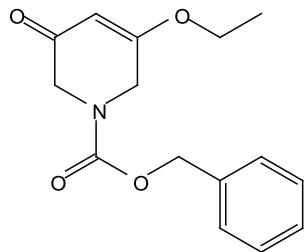
in DMSO-d6, 400 MHz



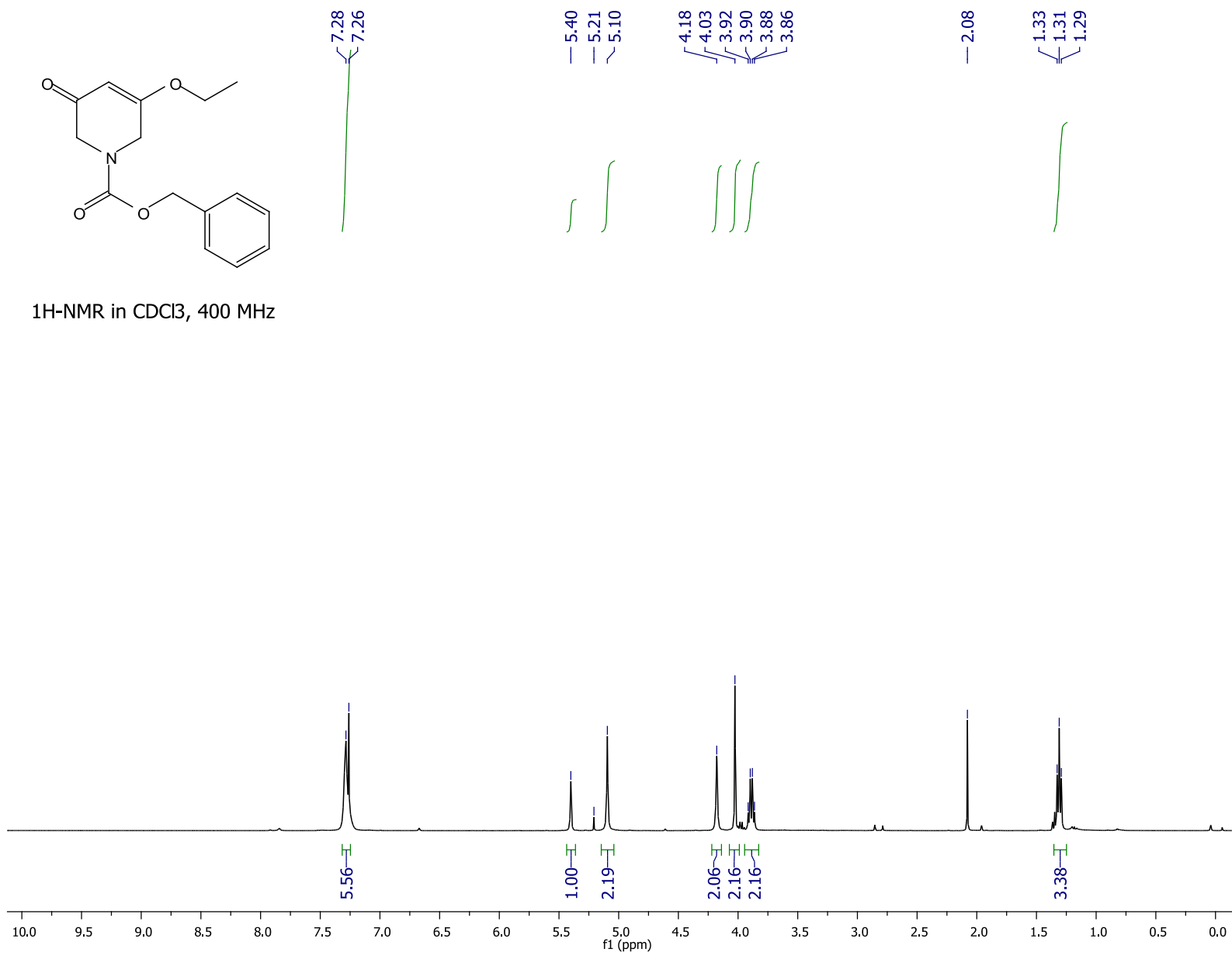


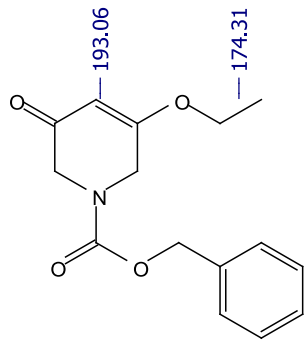
in DMSO-d6, 100 MHz



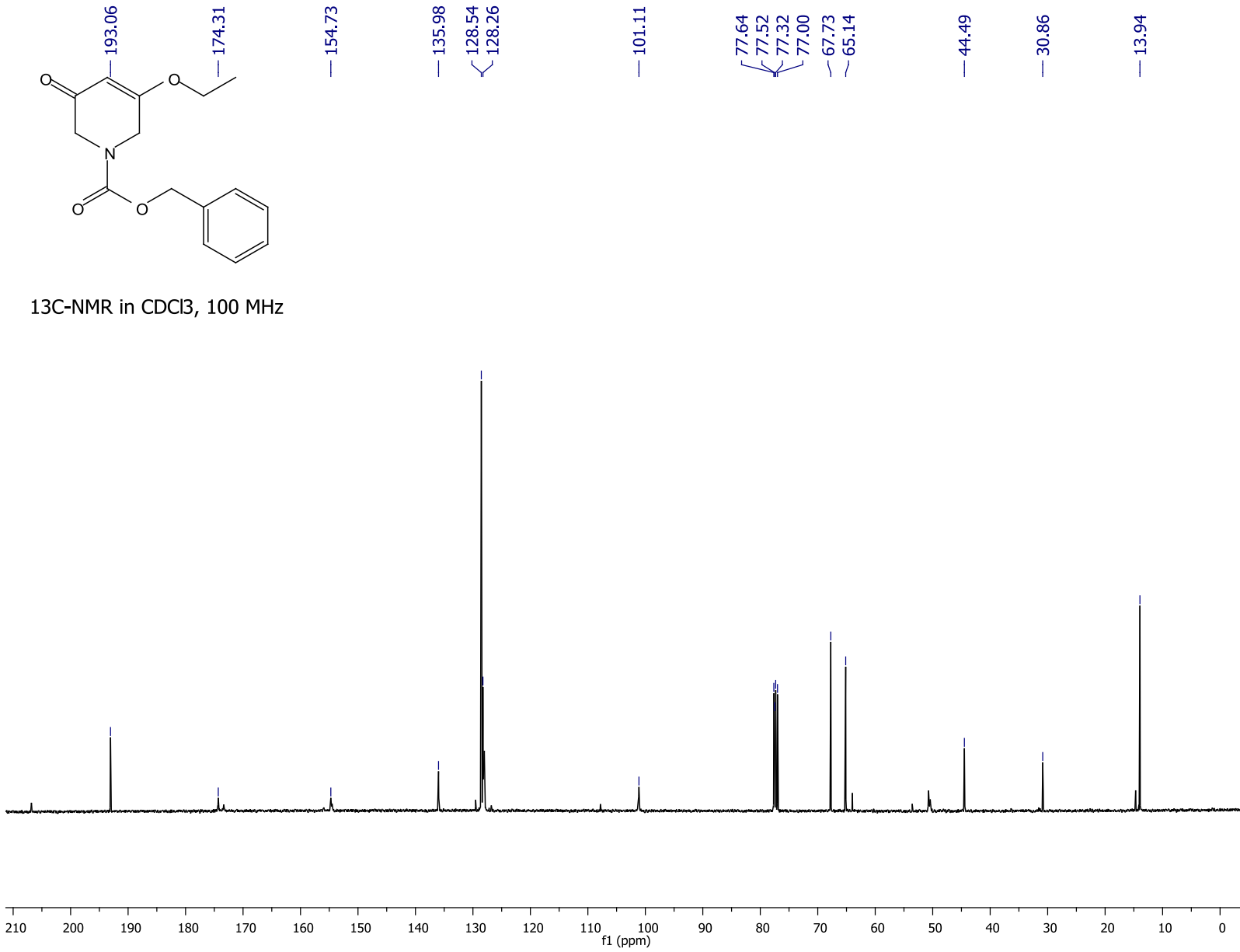


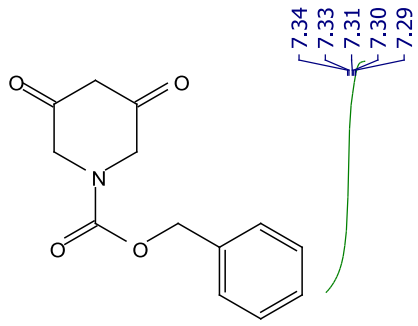
¹H-NMR in CDCl₃, 400 MHz



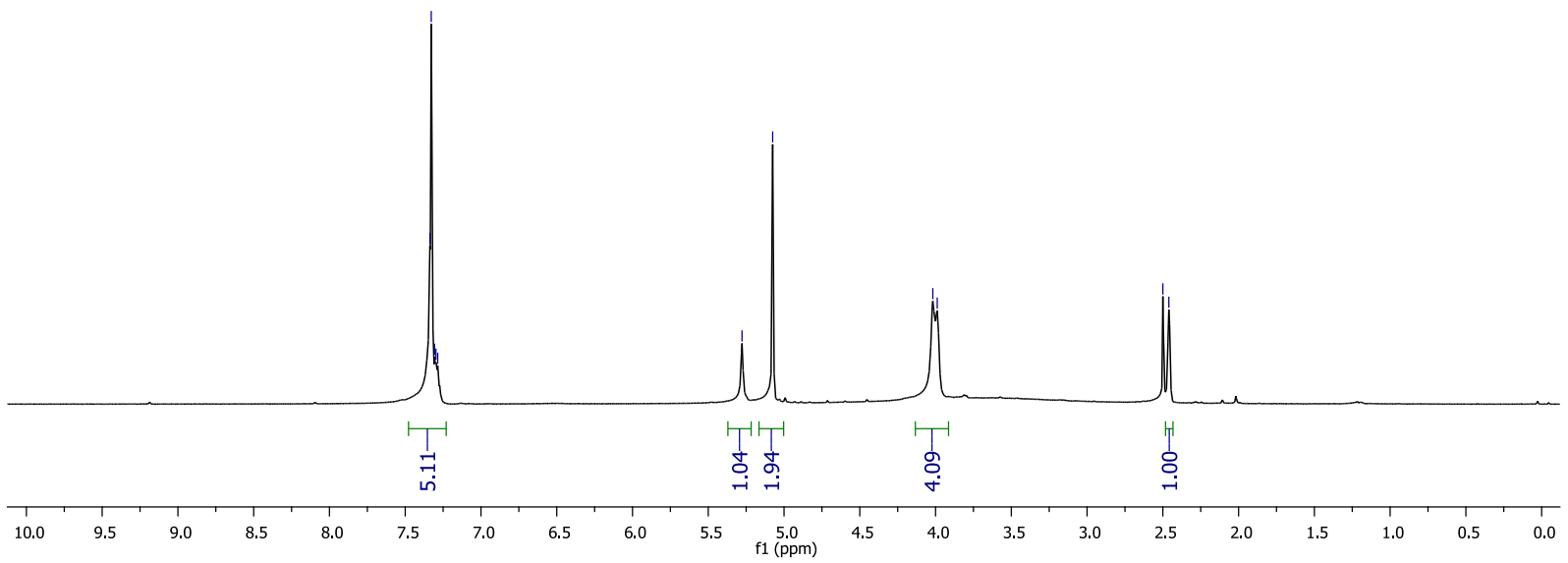
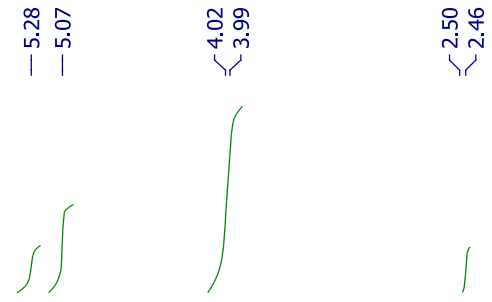


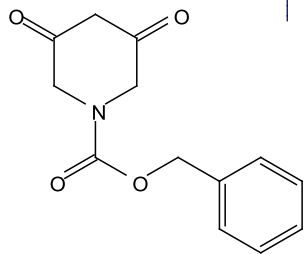
¹³C-NMR in CDCl₃, 100 MHz



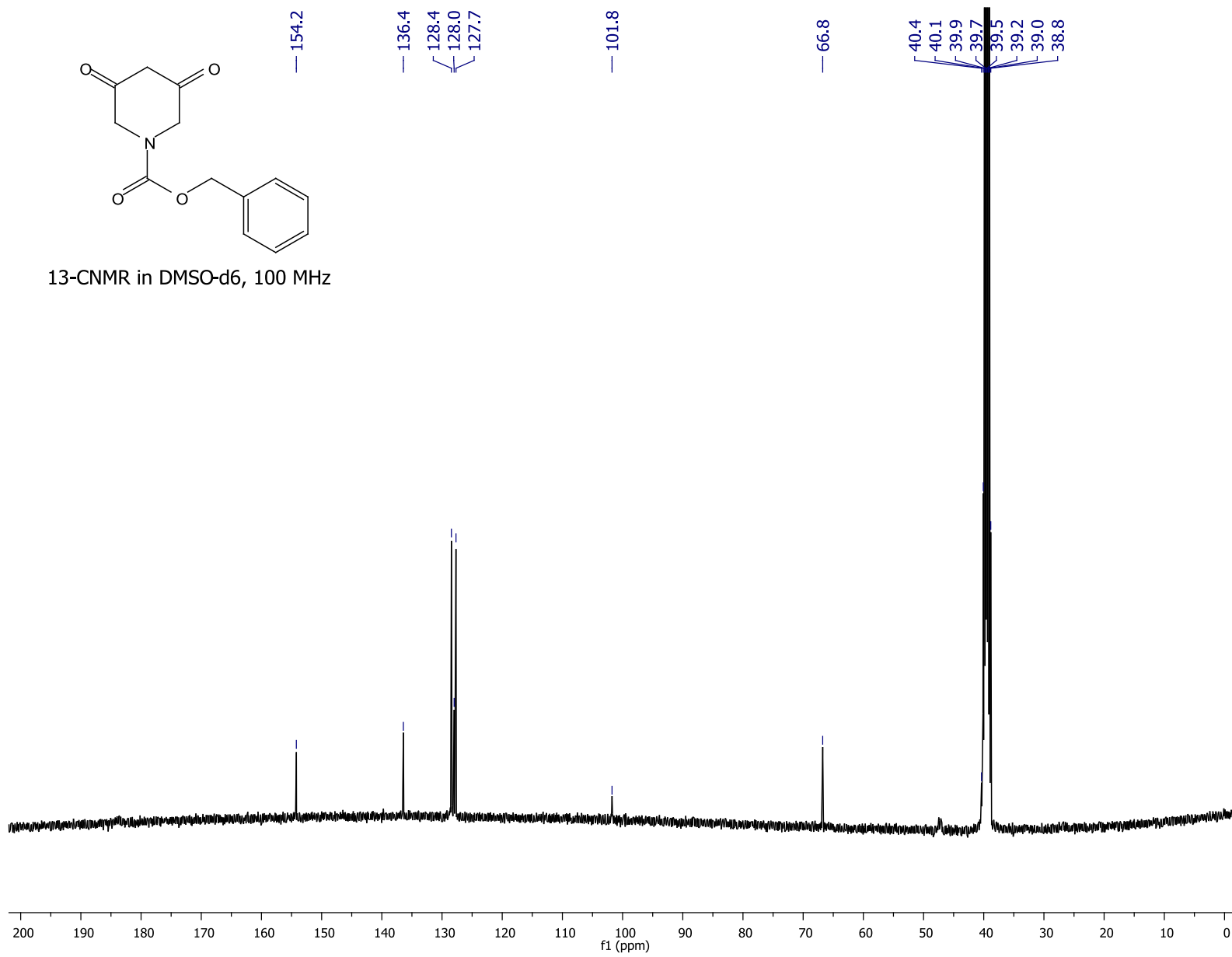


1-HNMR in DMSO-d6, 400 MHz

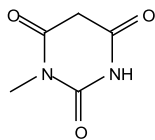




13-CNMR in DMSO-d6, 100 MHz



11.33



3.58

3.05

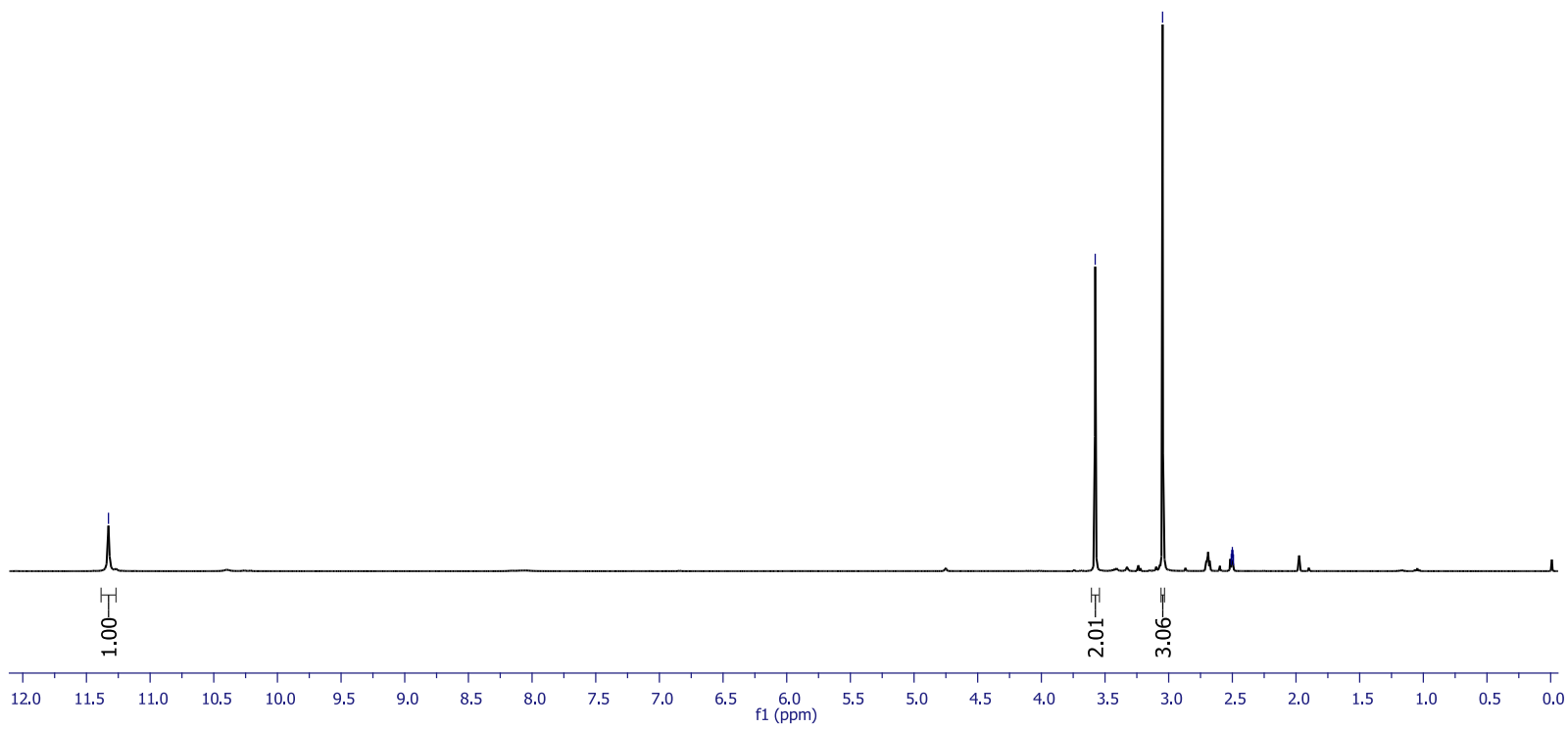
2.51

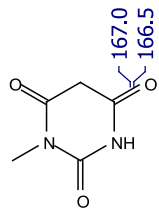
2.50

2.50

2.49

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

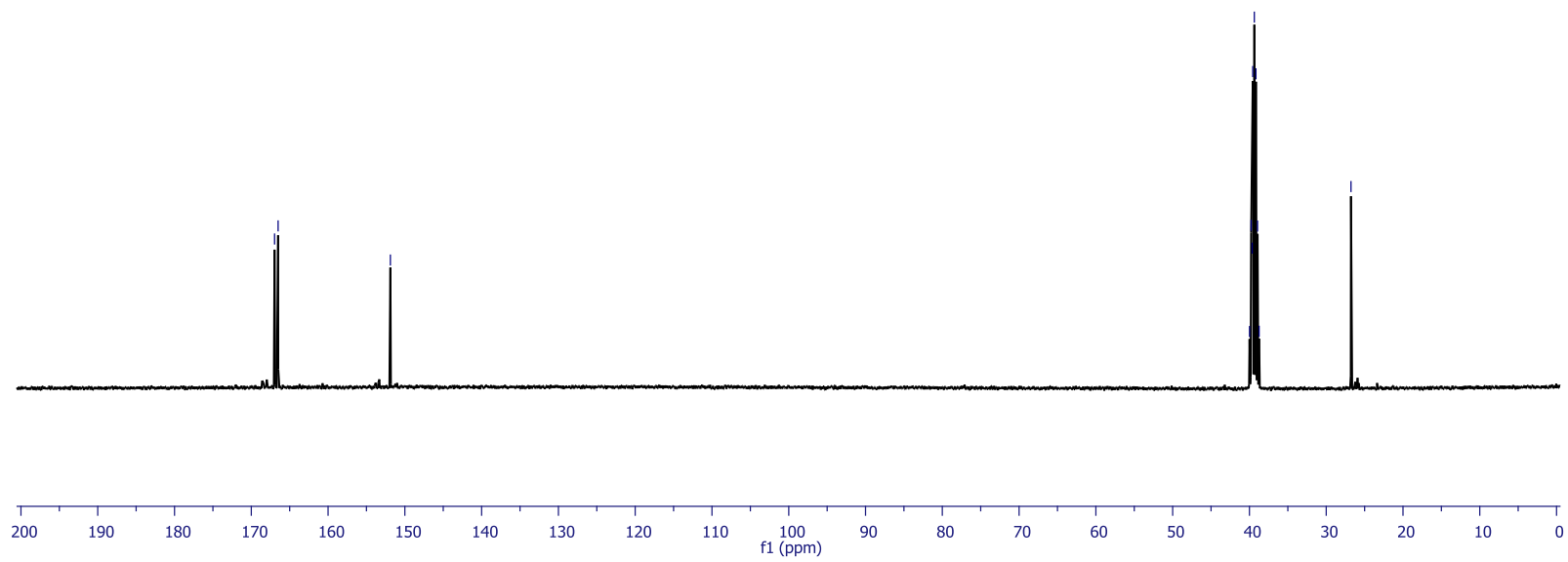


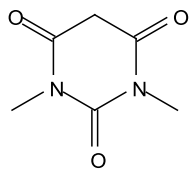


— 151.9

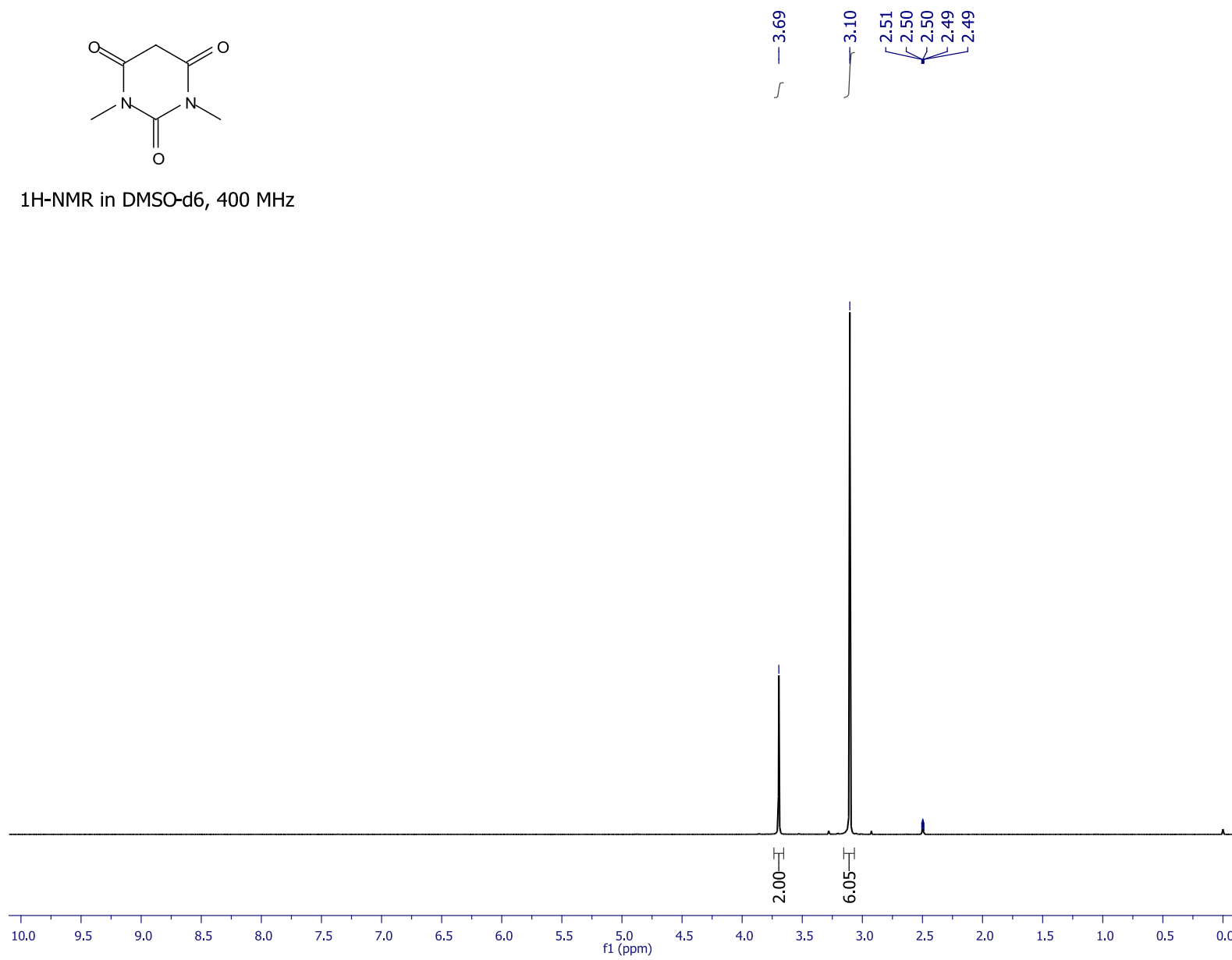
40.0
39.8
39.6
39.6
39.4
39.2
38.9
38.7
— 26.8

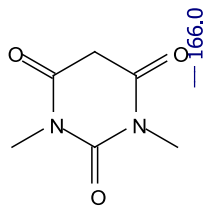
¹³C-NMR in DMSO-d₆, 100 MHz





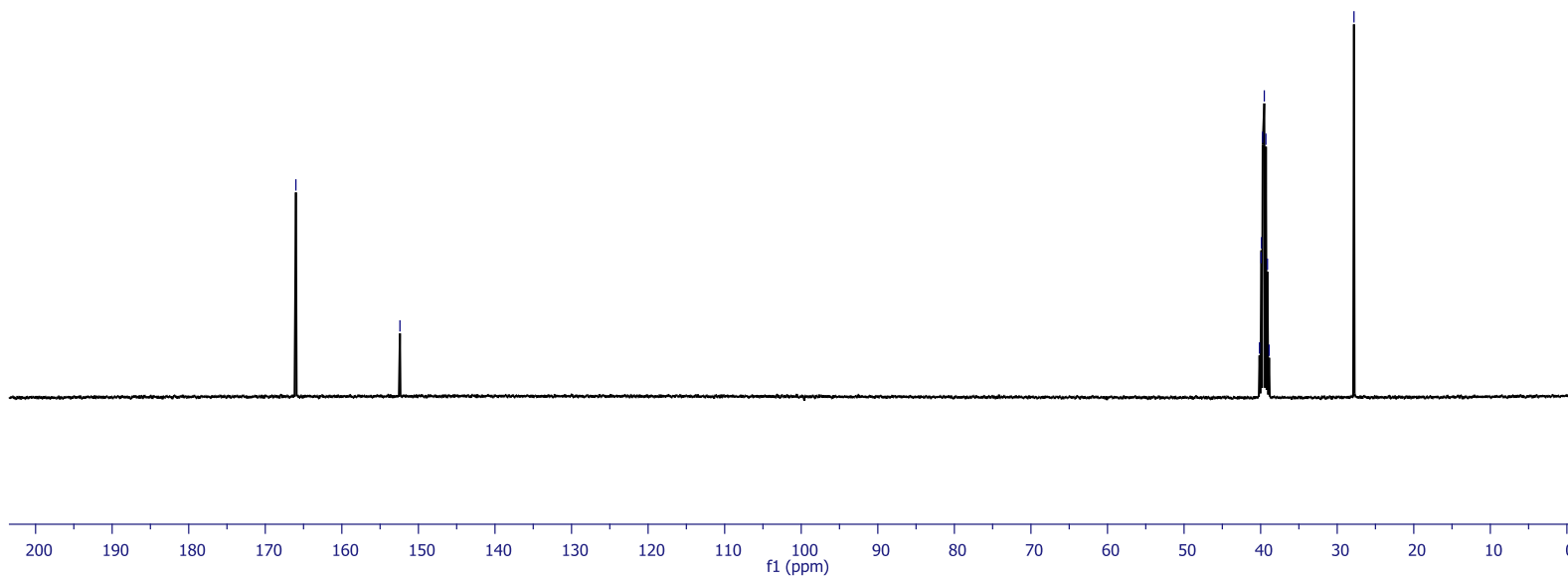
1H-NMR in DMSO-d6, 400 MHz

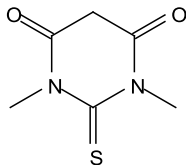




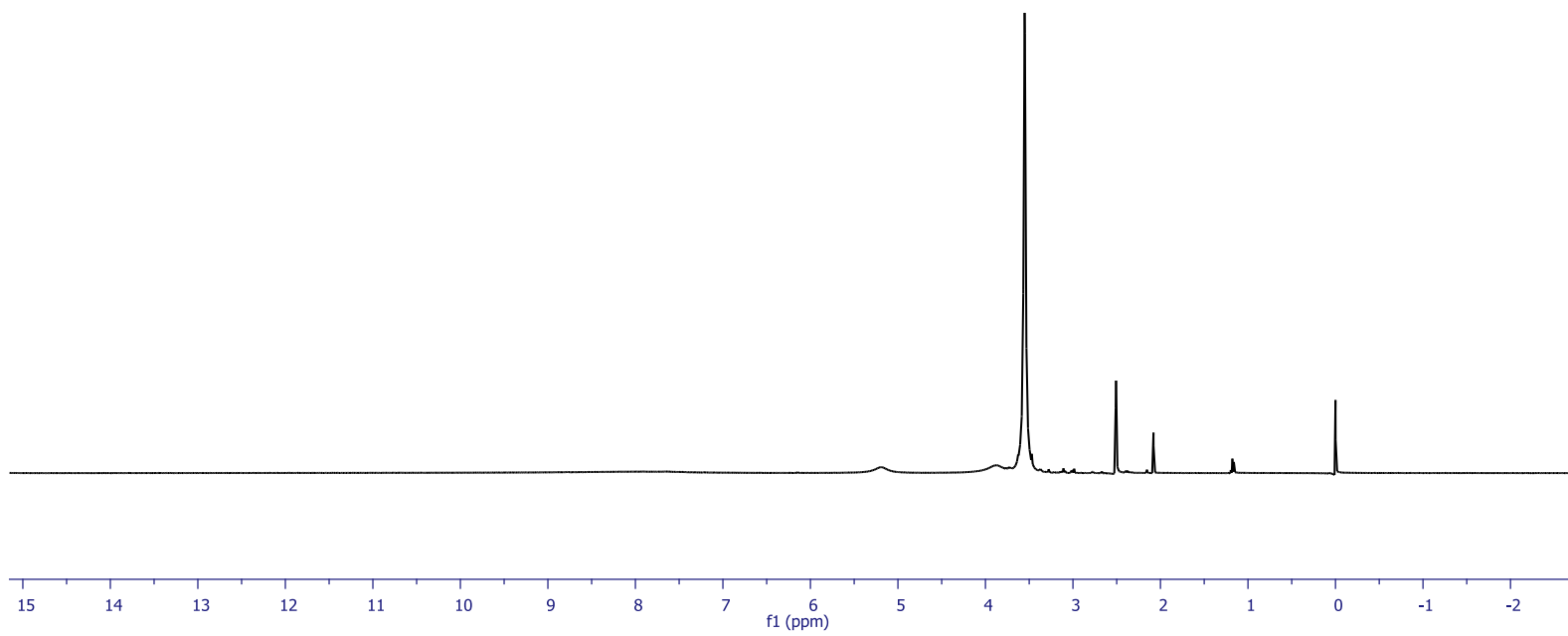
¹³C-NMR in DMSO-d₆, 100 MHz

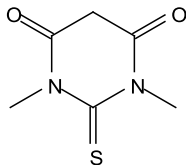
40.1
39.9
39.9
39.7
39.5
39.3
39.1
38.9
27.8





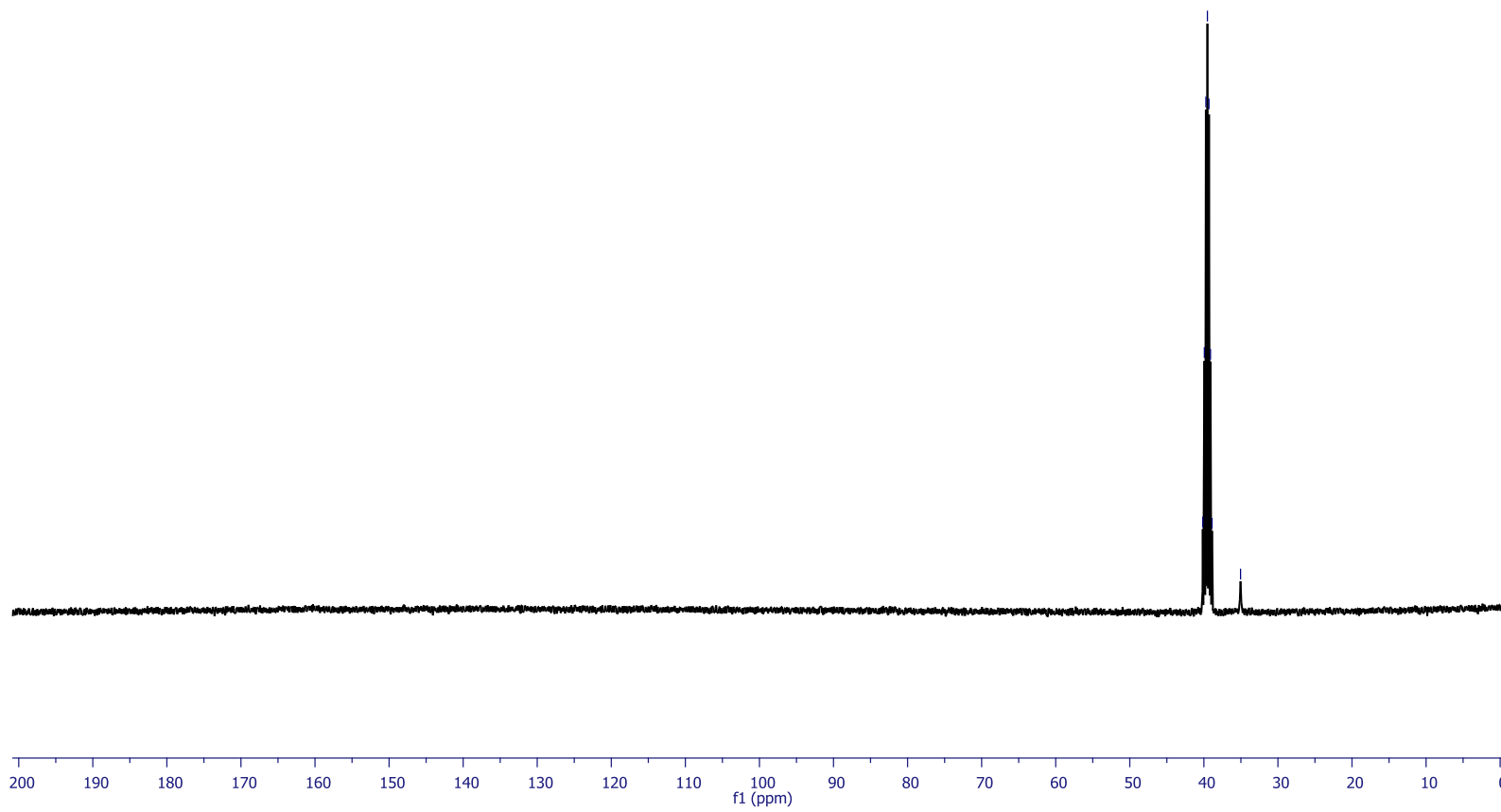
¹H-NMR, in DMSO-d₆, 400 MHz

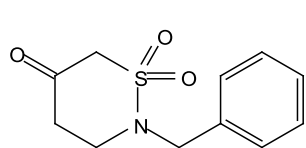




^{13}C -NMR, in DMSO- d_6 , 100 MHz

40.1
39.9
39.7
39.5
39.3
39.1
38.9
35.0





¹H-NMR, in CDCl₃, 400 MHz

7.32
7.28
7.27
7.24

4.40

3.92

3.33

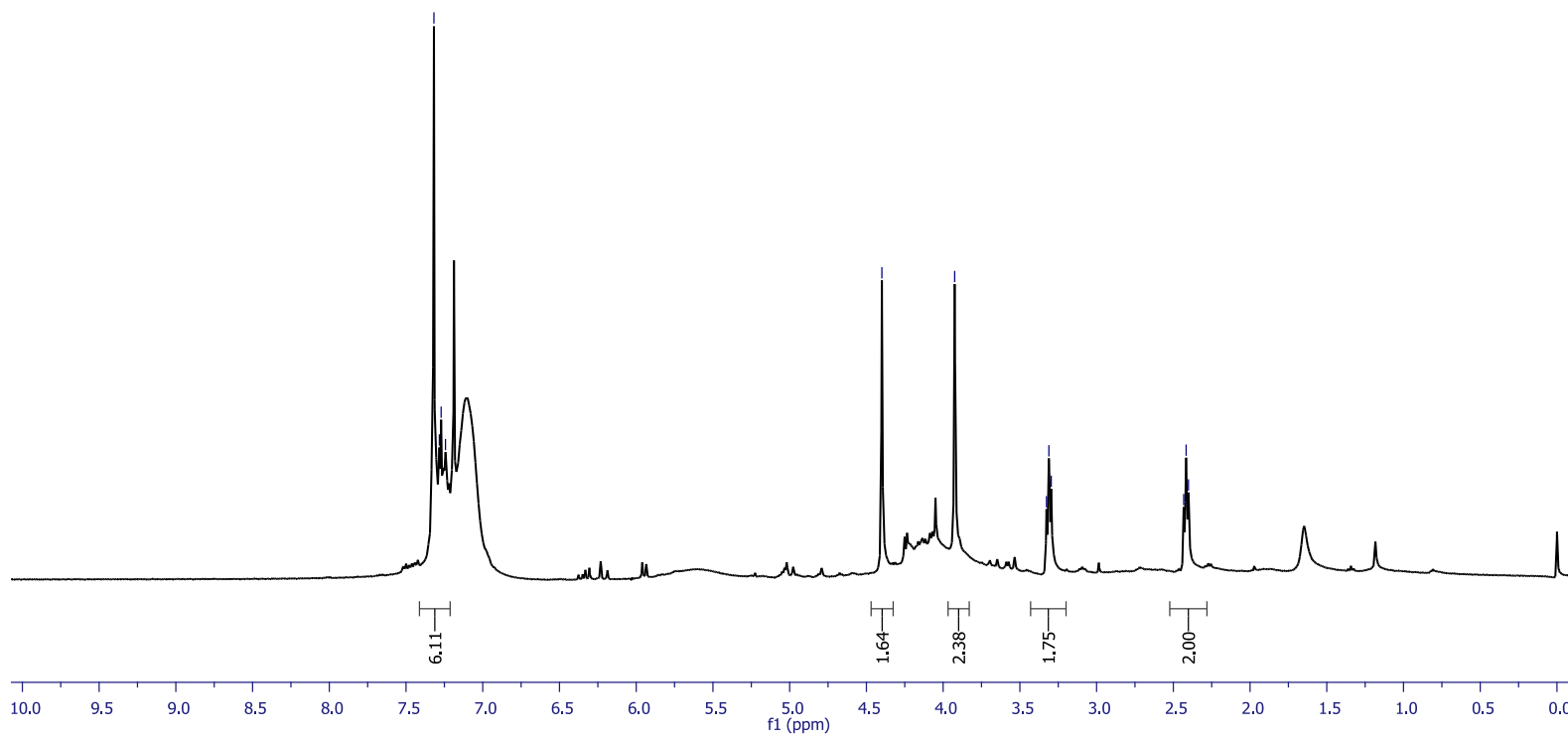
3.31

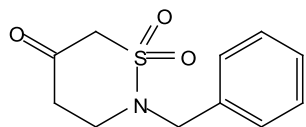
3.30

2.43

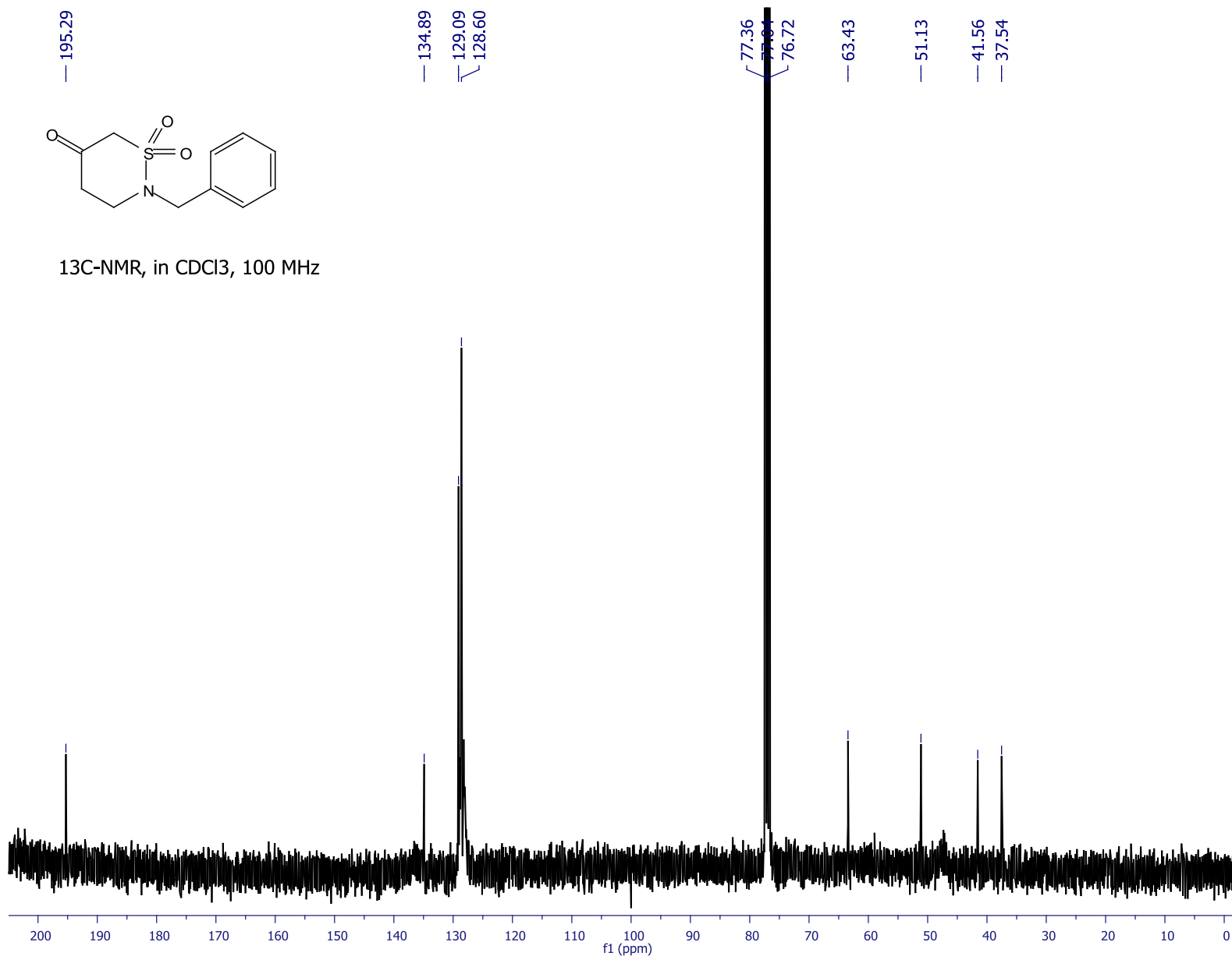
2.42

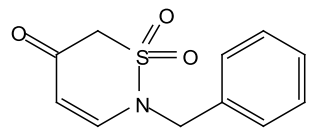
2.40



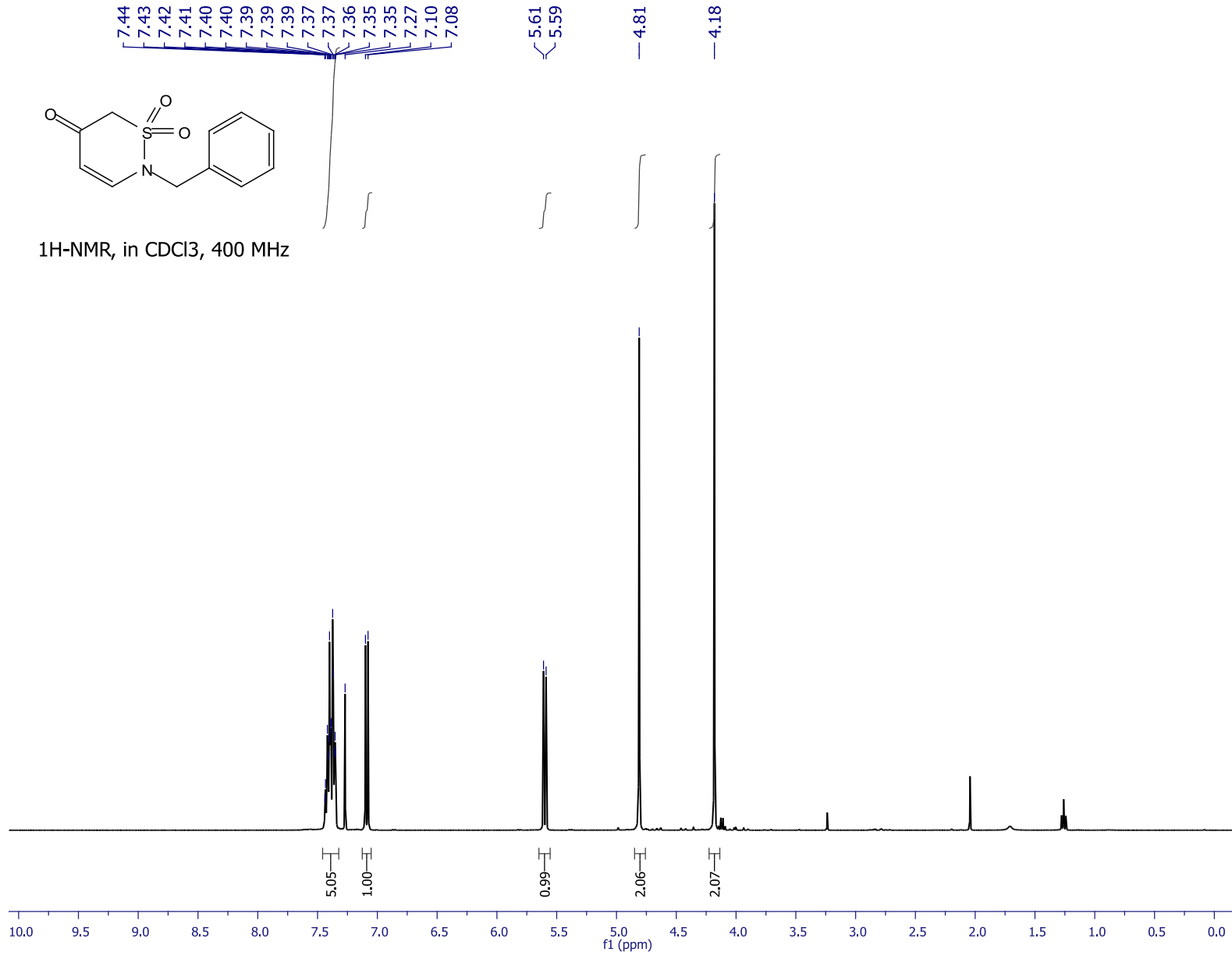


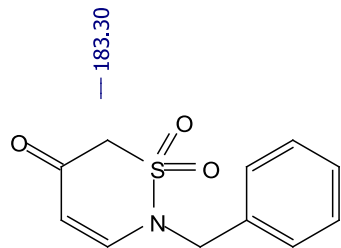
¹³C-NMR, in CDCl₃, 100 MHz



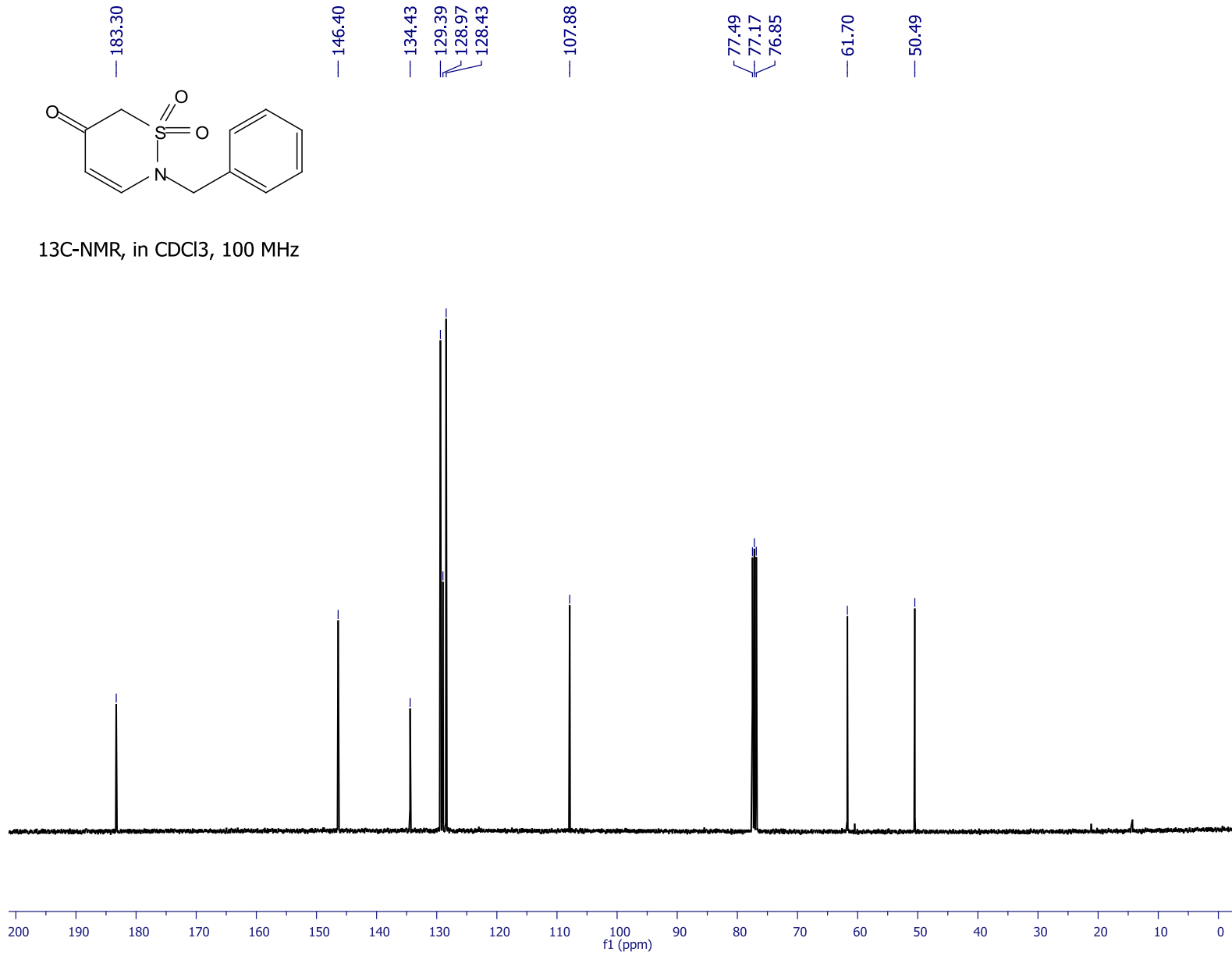


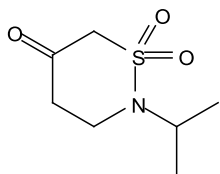
¹H-NMR, in CDCl₃, 400 MHz



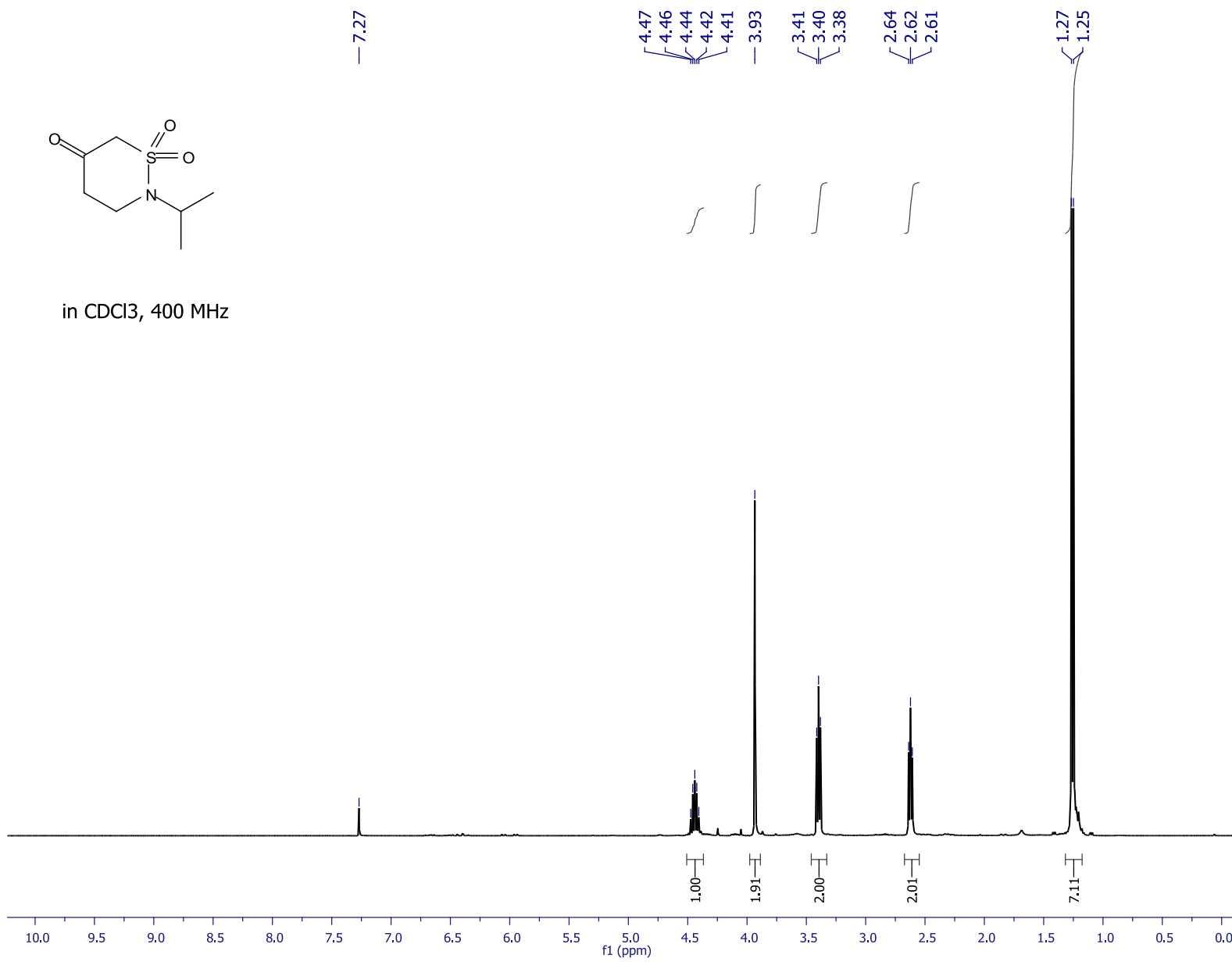


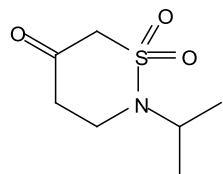
$^{13}\text{C-NMR}$, in CDCl_3 , 100 MHz



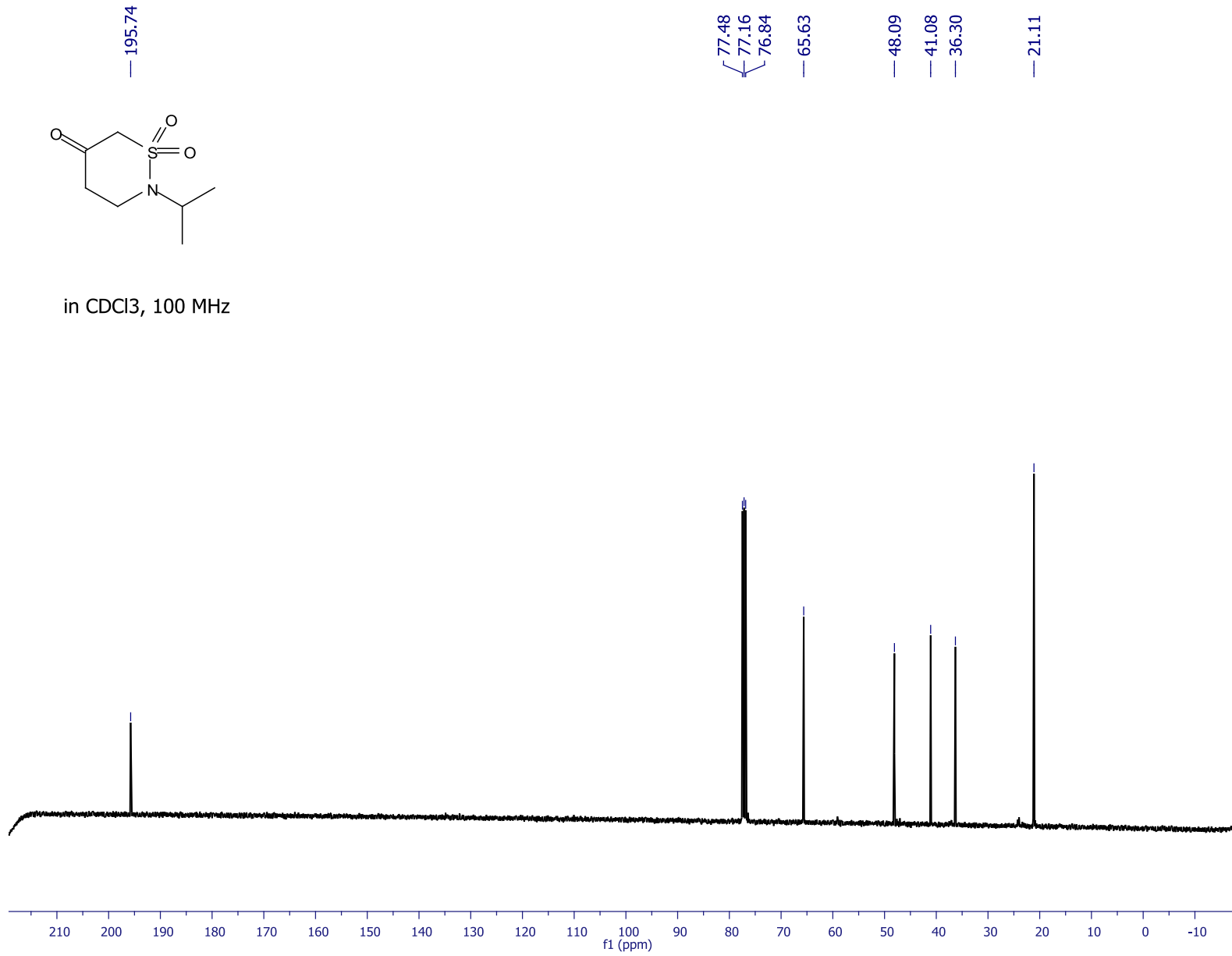


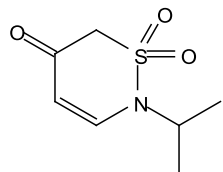
in CDCl₃, 400 MHz



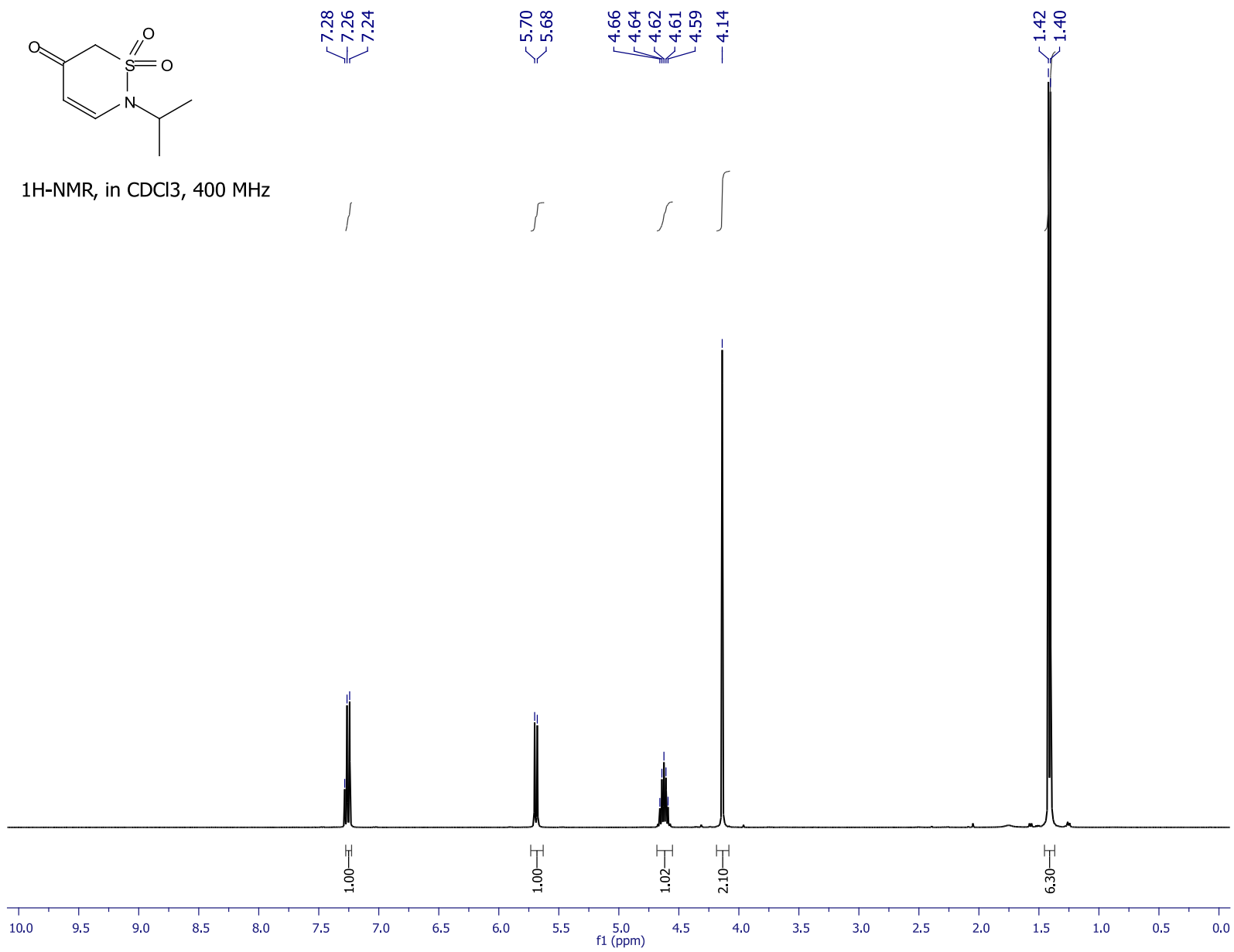


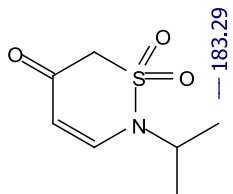
in CDCl₃, 100 MHz



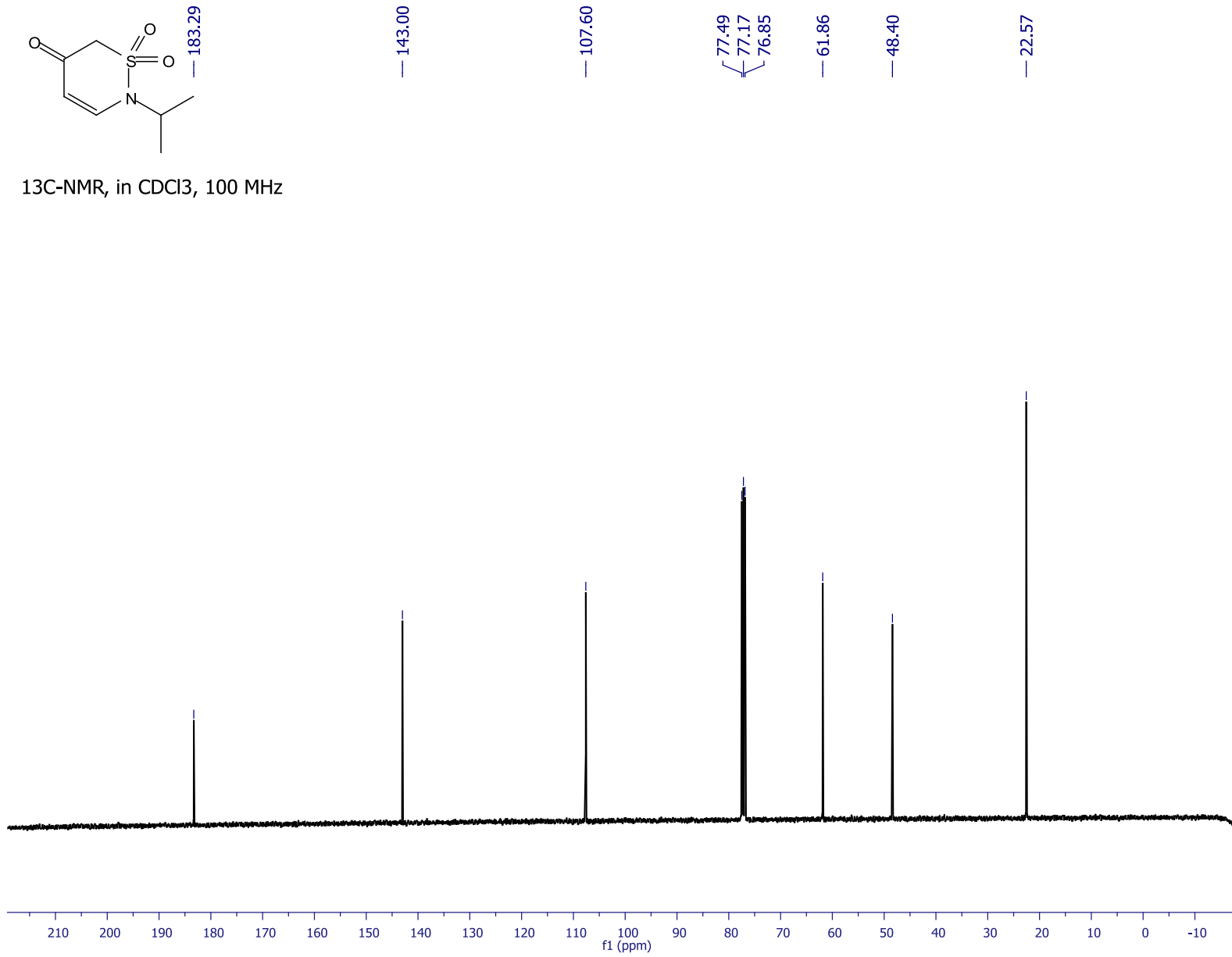


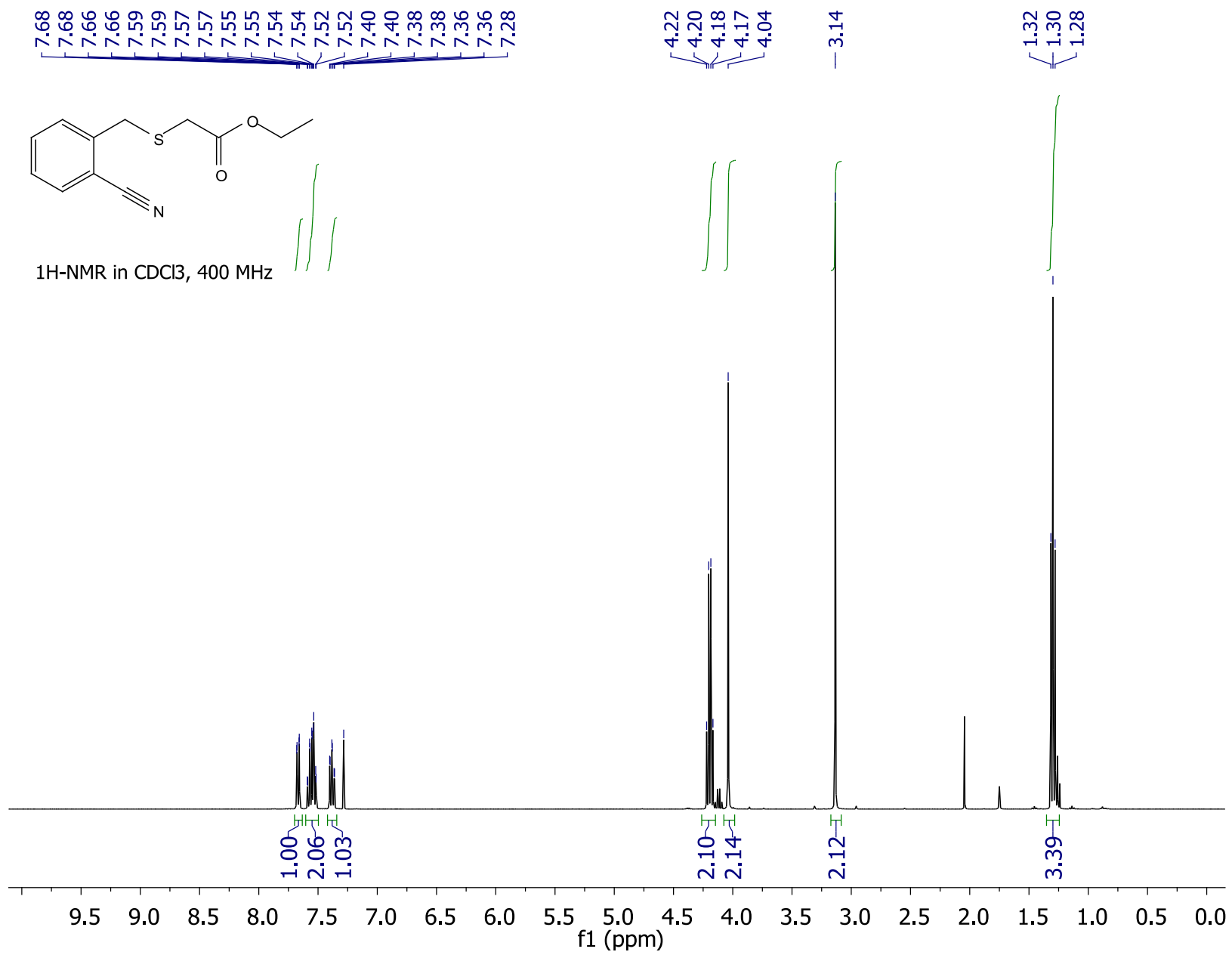
¹H-NMR, in CDCl₃, 400 MHz

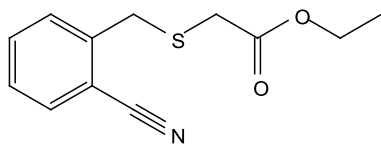




$^{13}\text{C-NMR}$, in CDCl_3 , 100 MHz







— 169.94

— 141.34

— 133.30

— 132.76

— 130.31

— 127.87

— 117.38

— 112.79

— 77.42

— 77.10

— 76.78

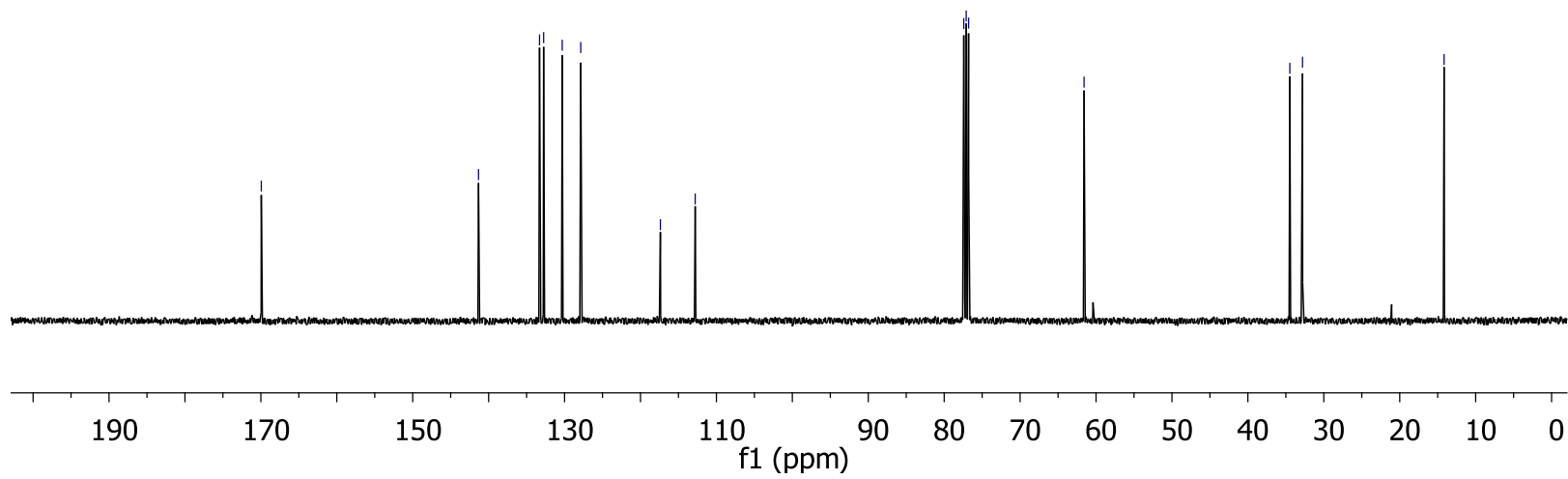
— 61.58

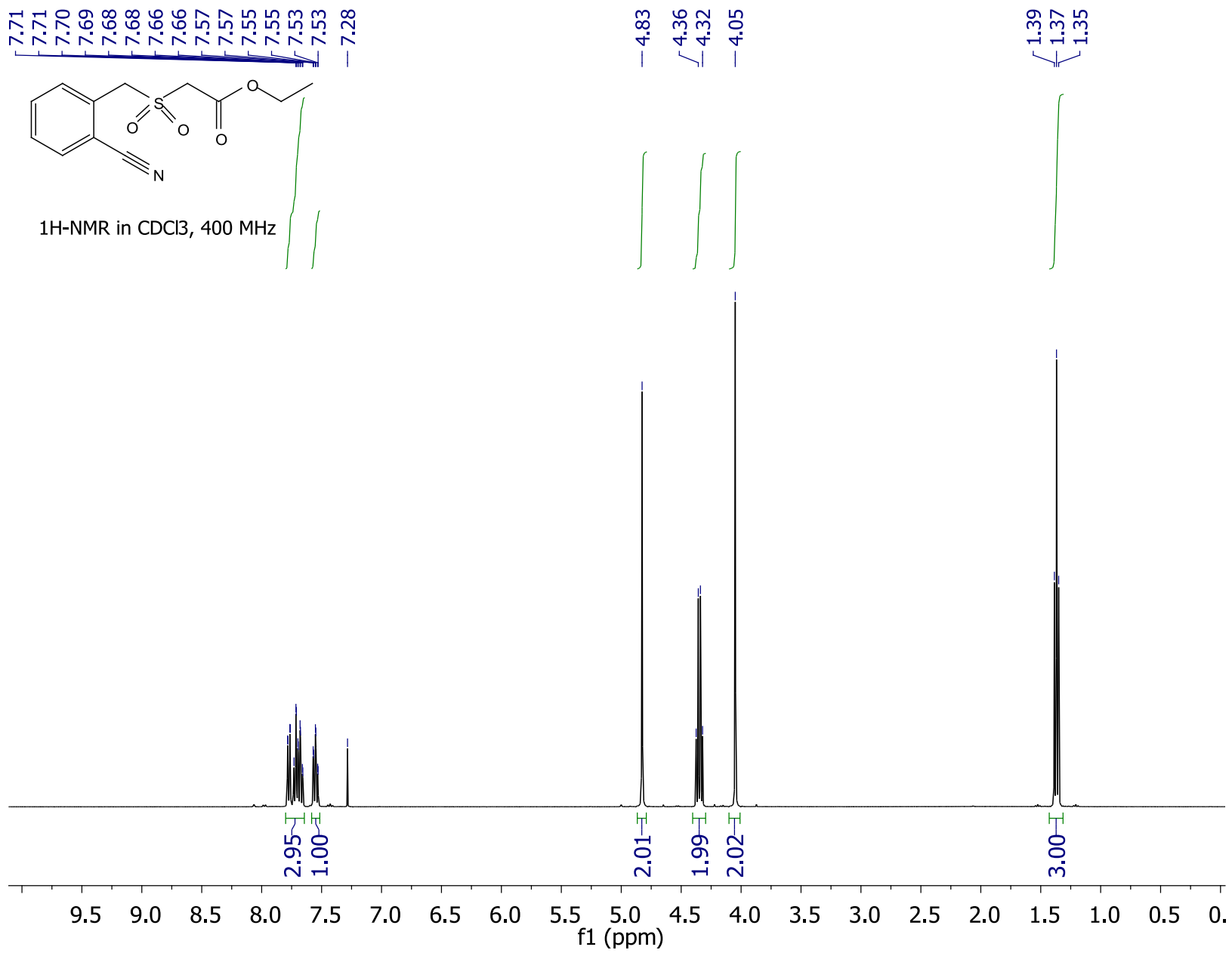
— 34.48

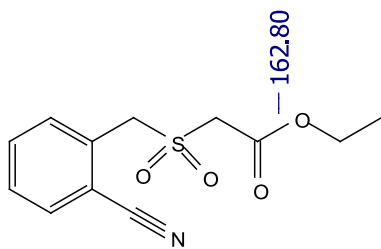
— 32.81

— 14.16

¹³C-NMR in CDCl₃, 100 MHz







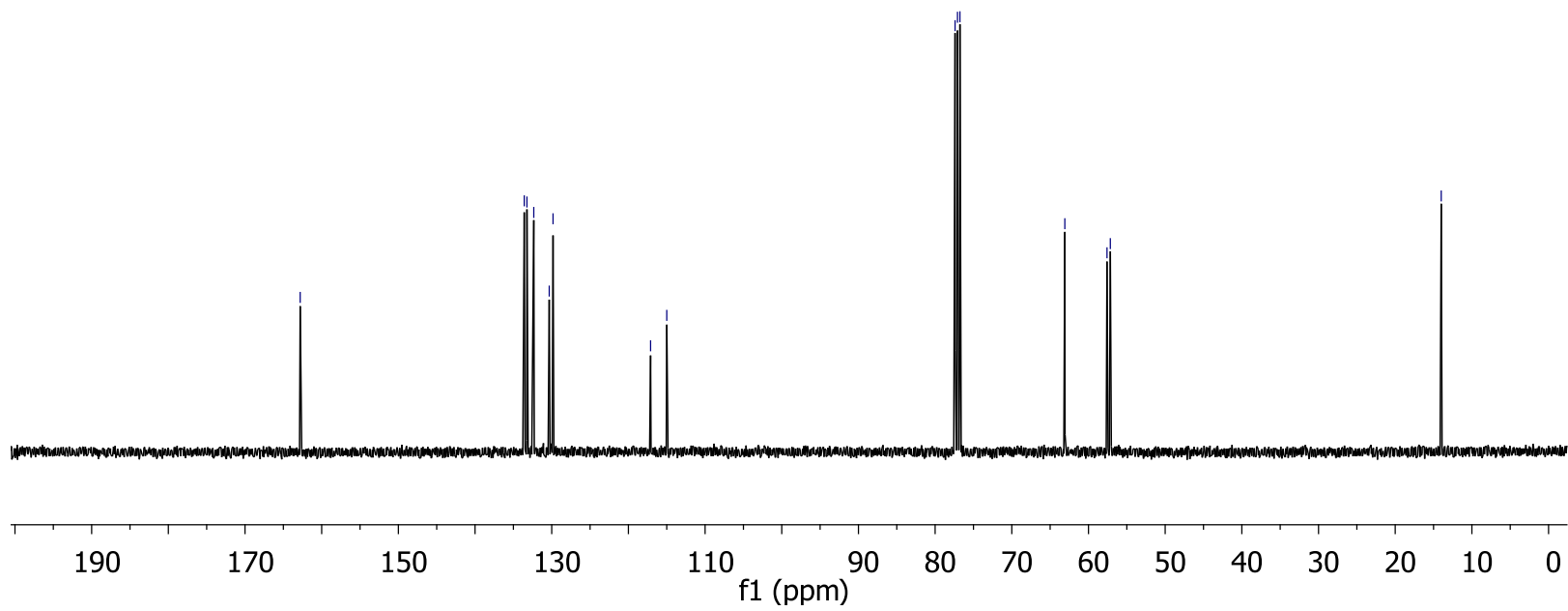
¹³C-NMR in CDCl₃, 100 MHz

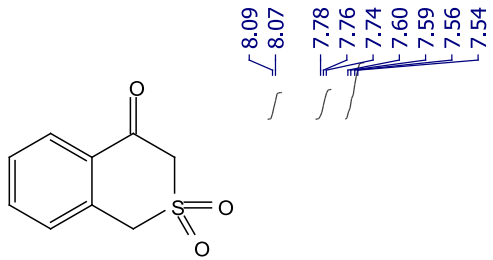
133.58
133.23
132.34
130.32
129.83
117.11
115.00

77.40
77.08
76.76

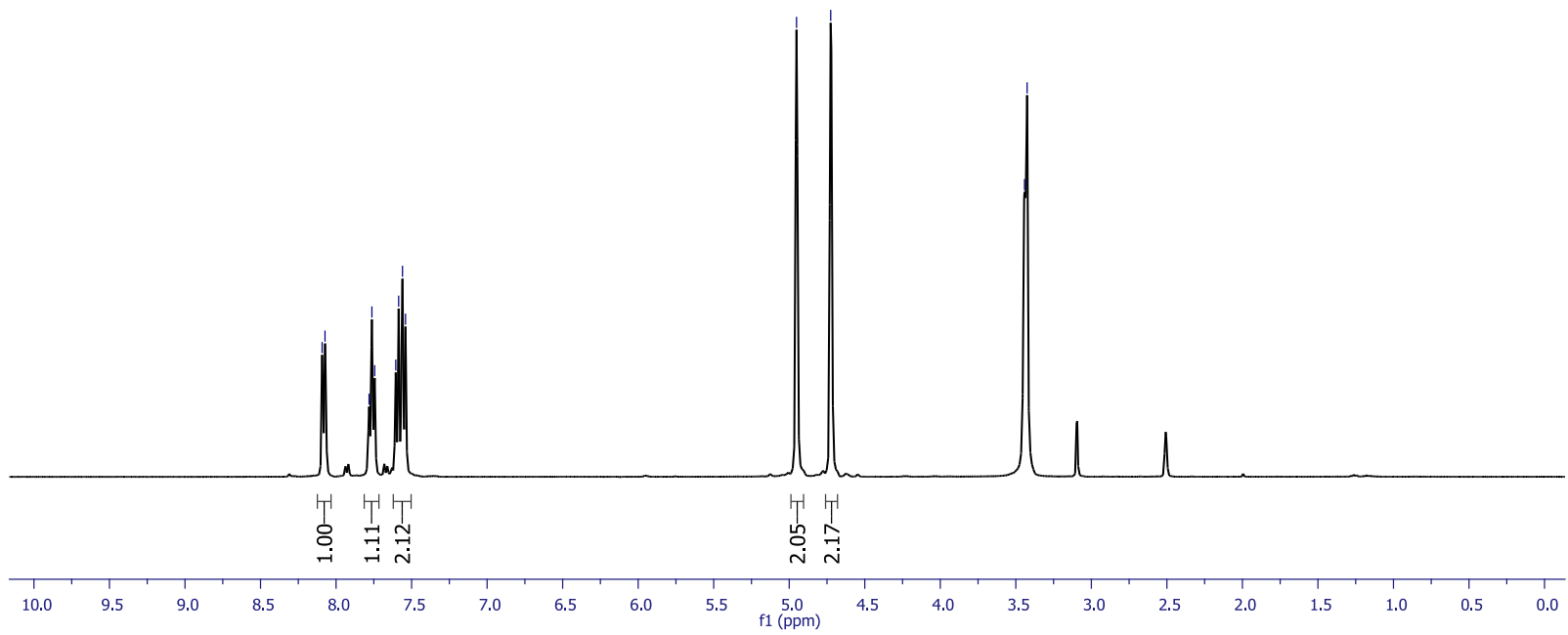
63.09
57.59
57.15

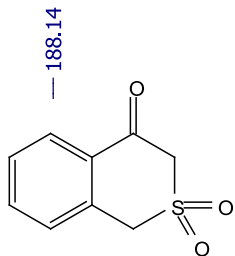
14.00





¹H-NMR in DMSO-d₆, 400 MHz

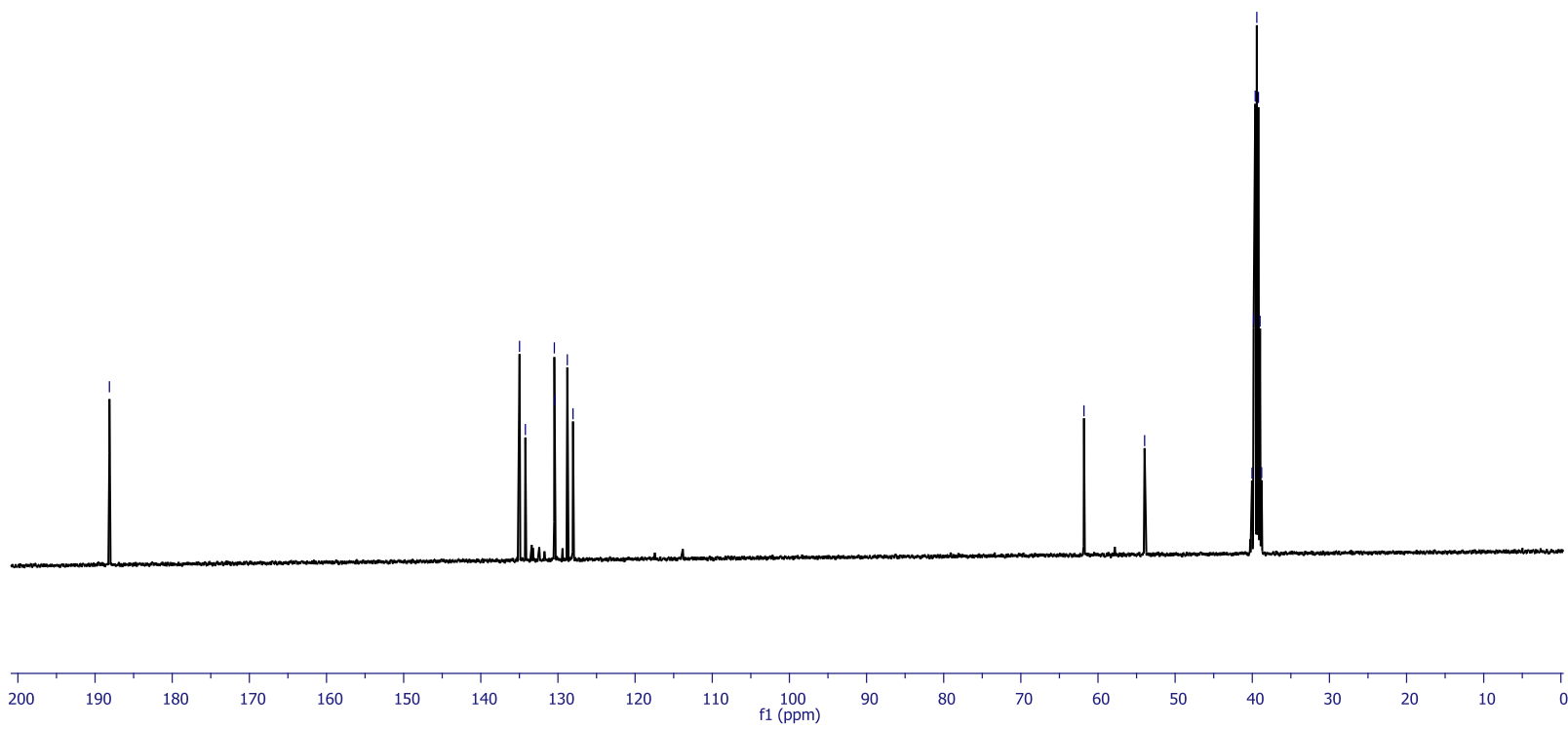


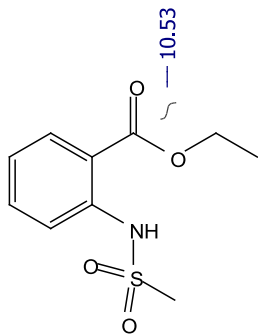


¹³C-NMR in DMSO-d₆, 100 MHz

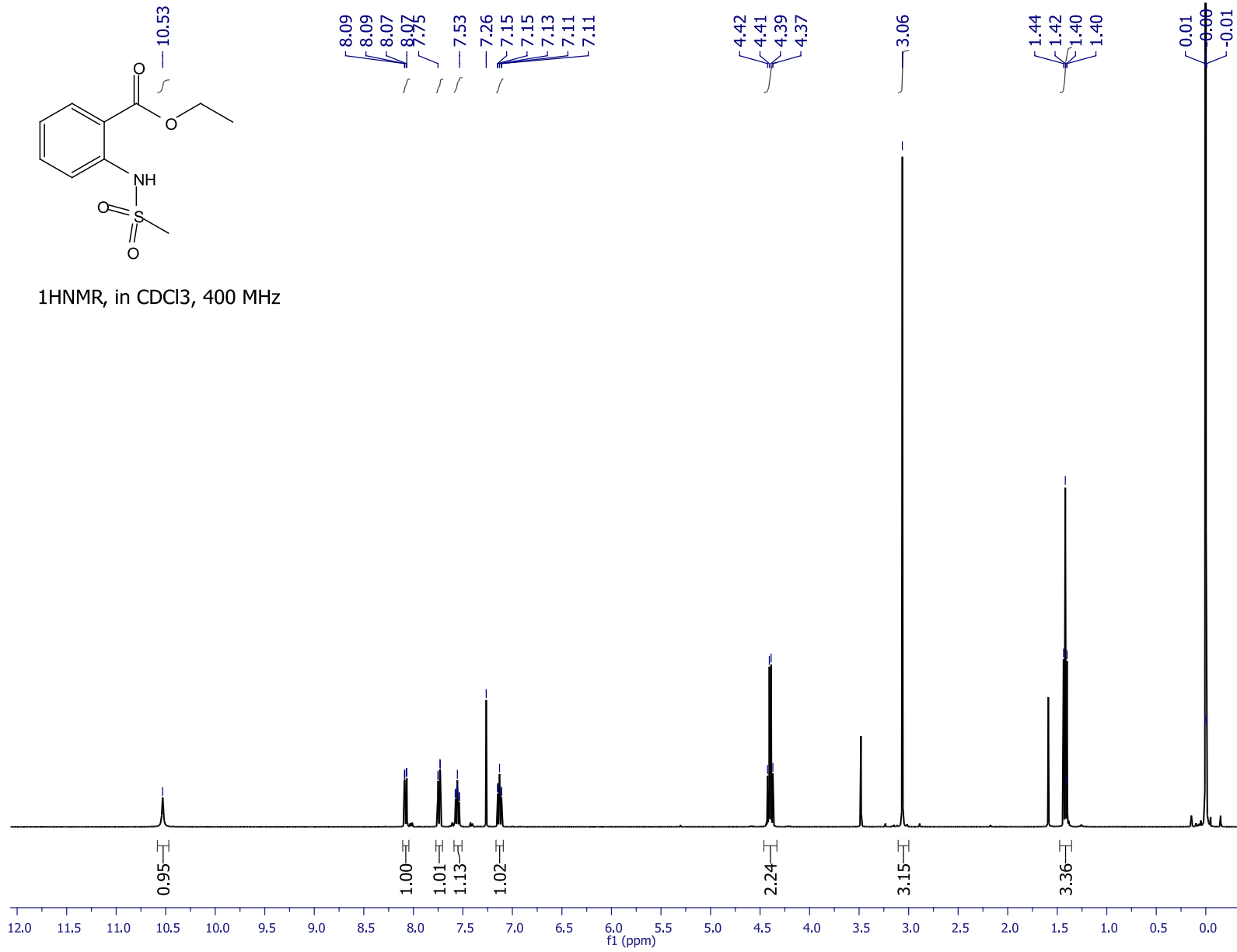
134.98
134.22
130.47
130.43
128.79
128.05

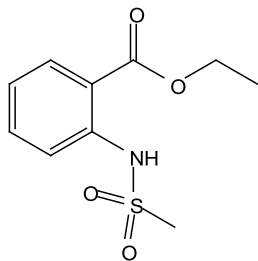
61.81
53.96
40.04
39.83
39.62
39.41
39.20
38.99
38.78



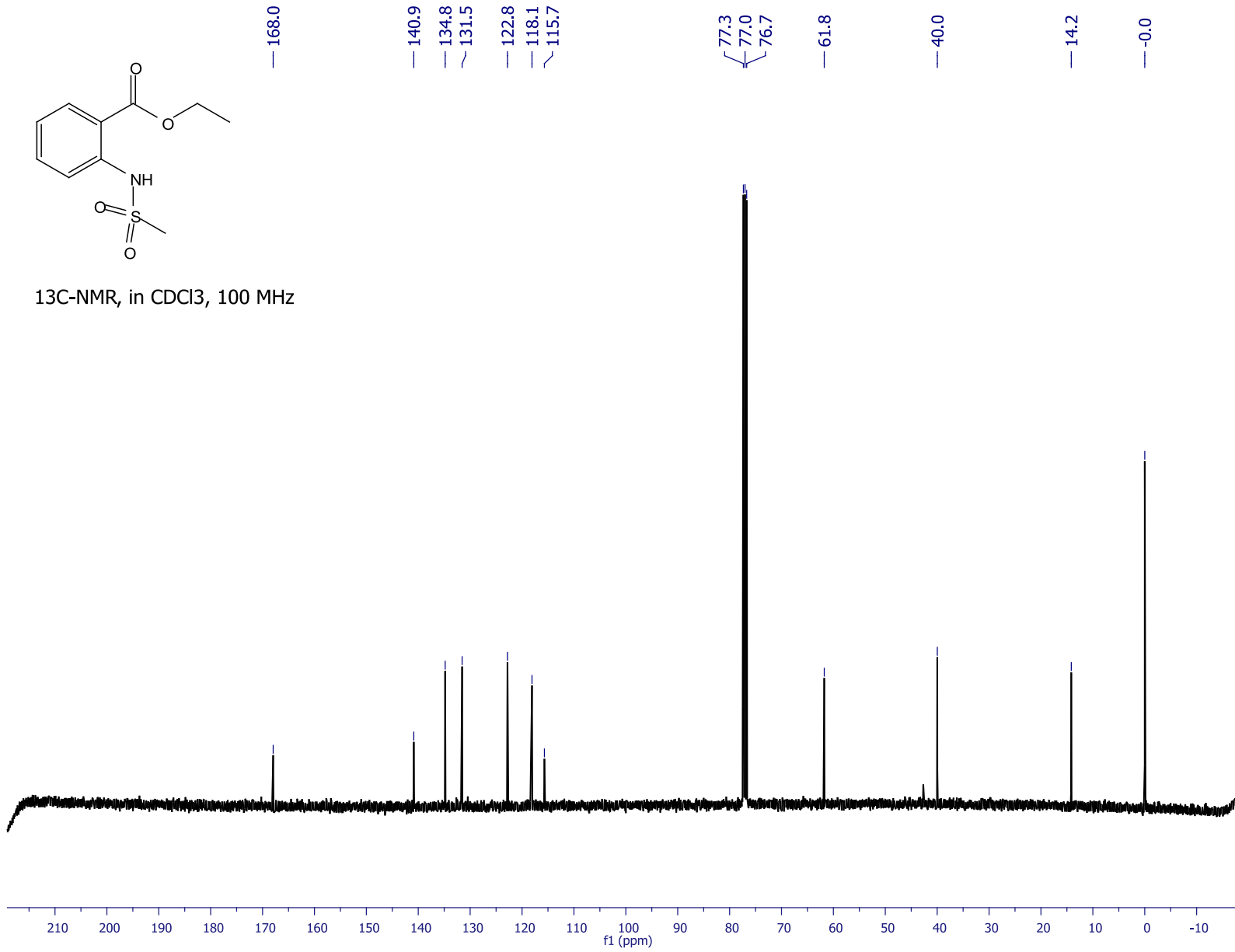


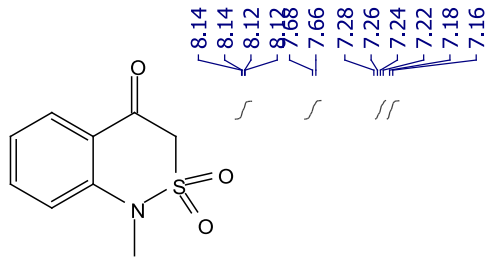
¹HNMR, in CDCl₃, 400 MHz



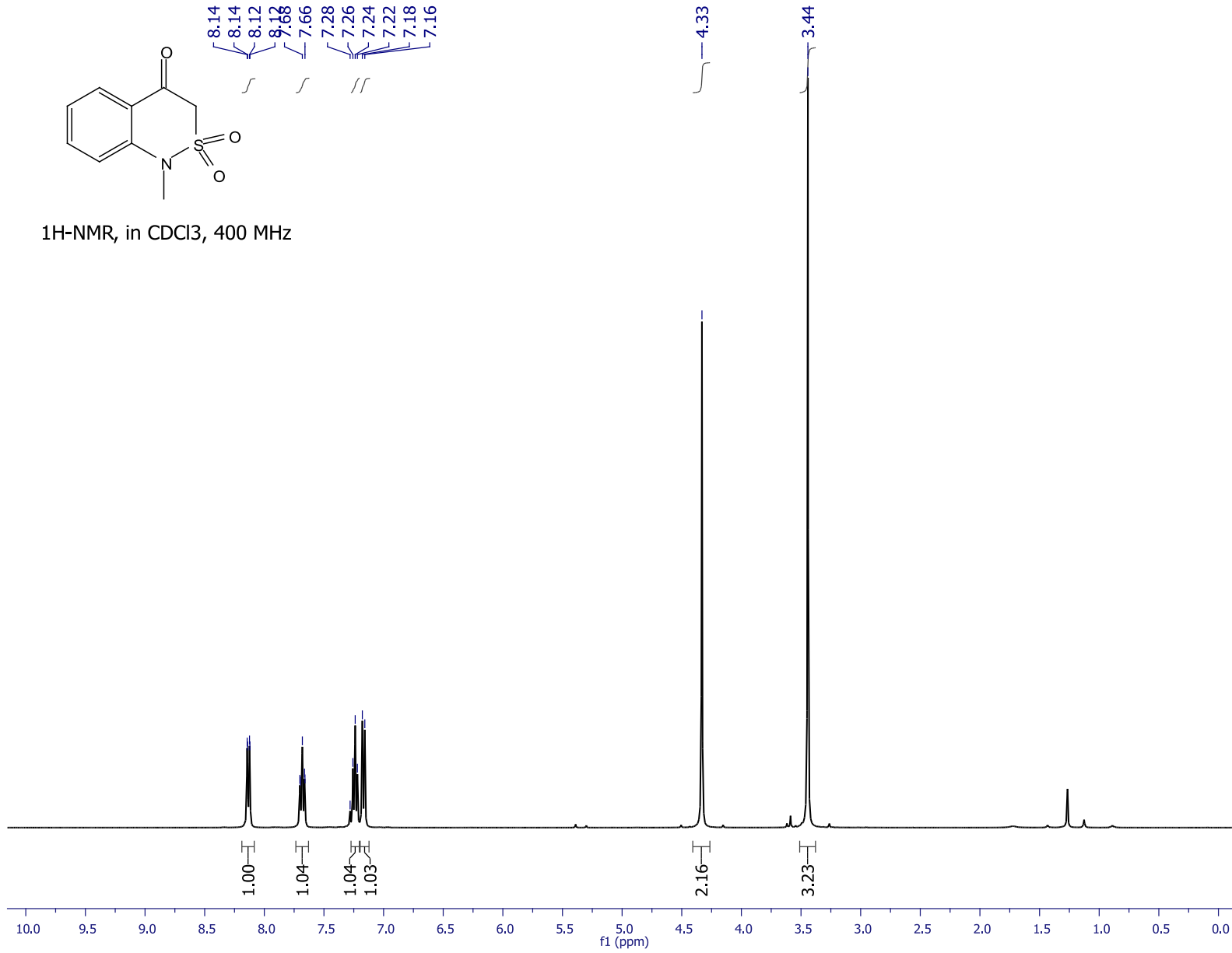


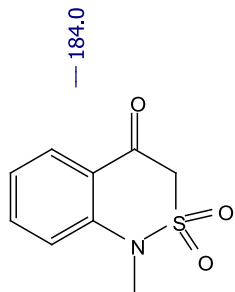
¹³C-NMR, in CDCl₃, 100 MHz



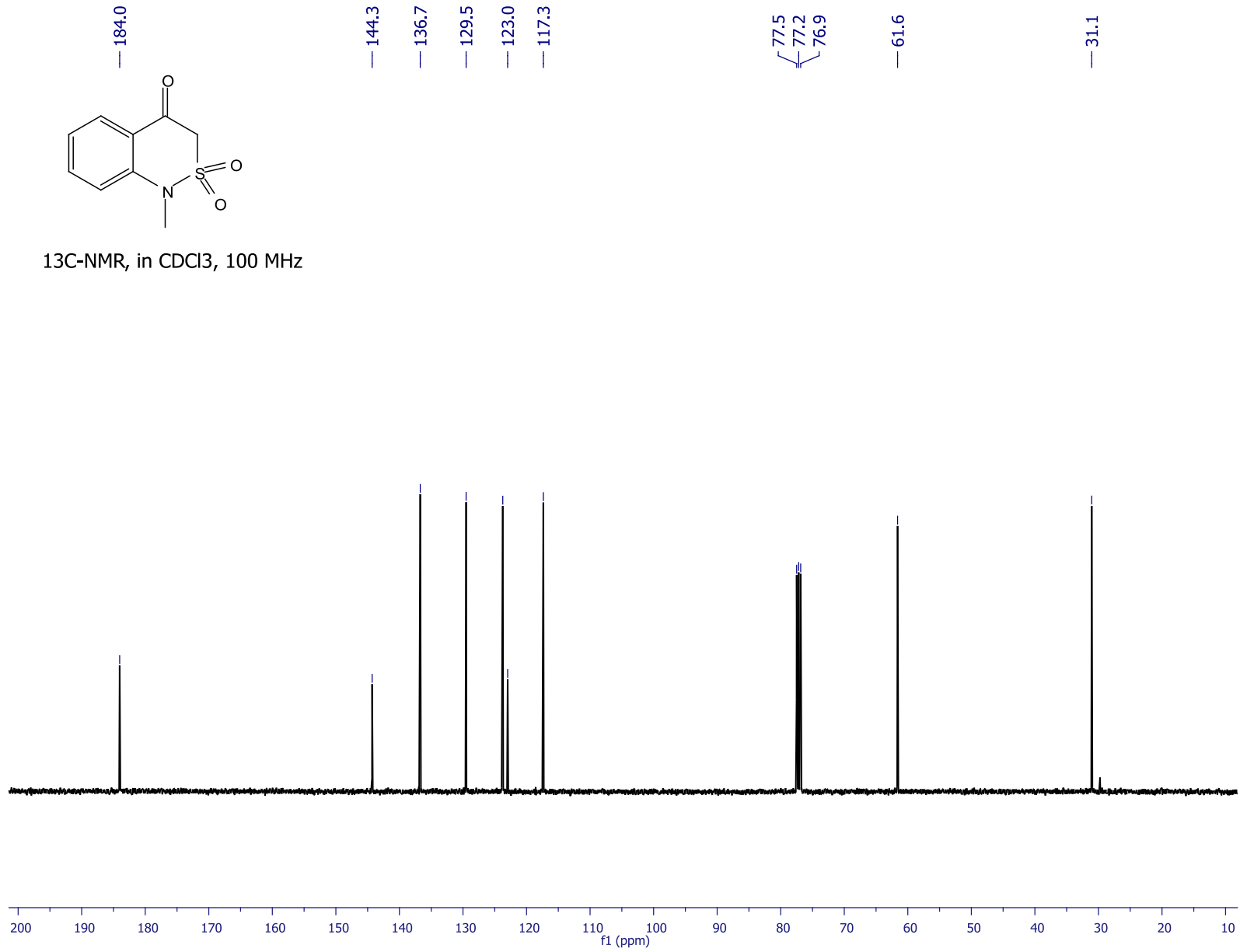


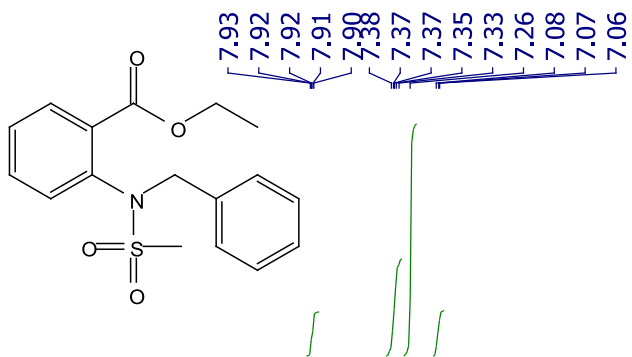
¹H-NMR, in CDCl₃, 400 MHz



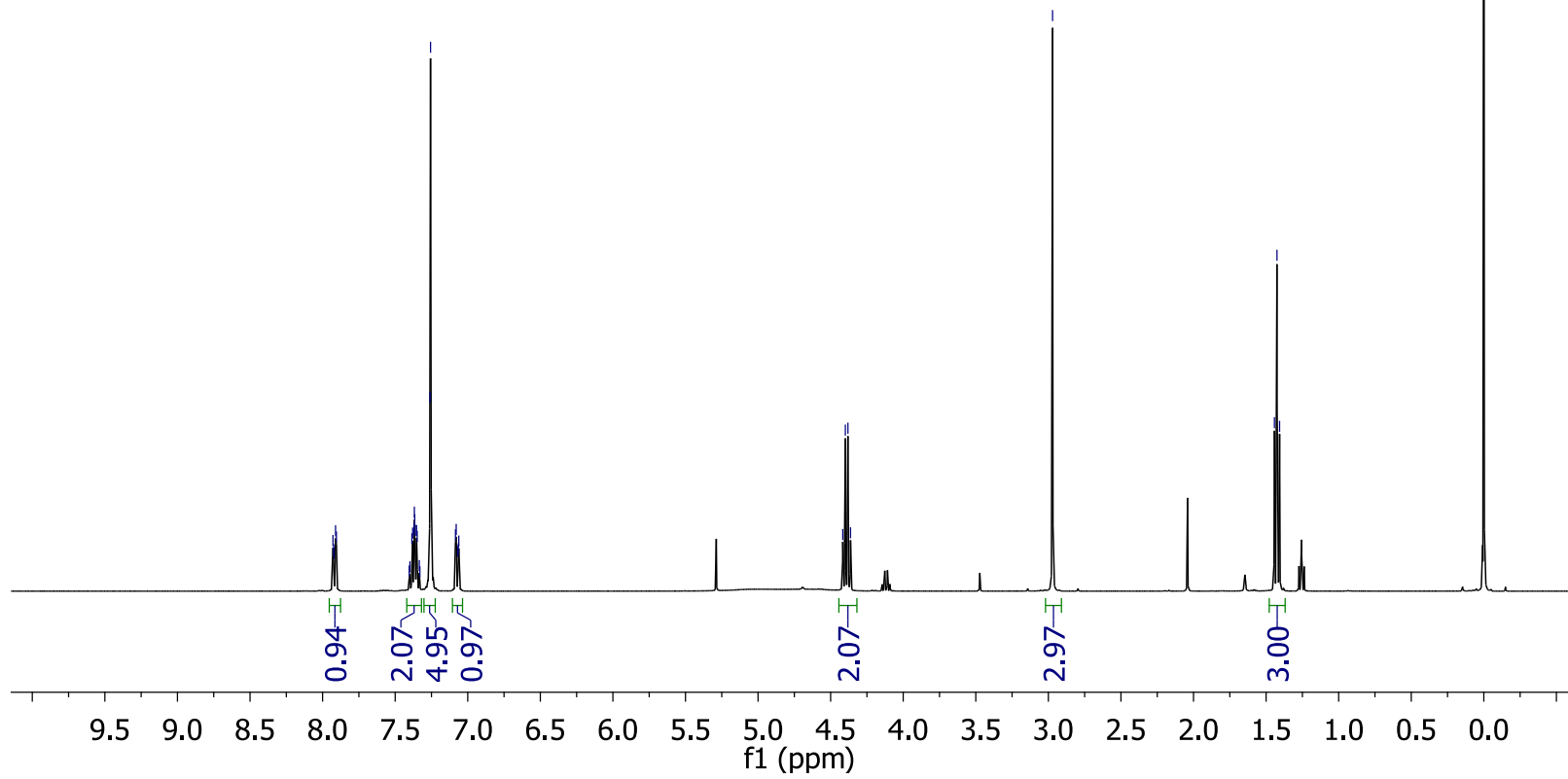


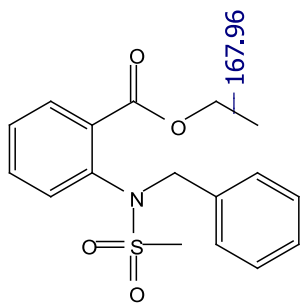
^{13}C -NMR, in CDCl_3 , 100 MHz





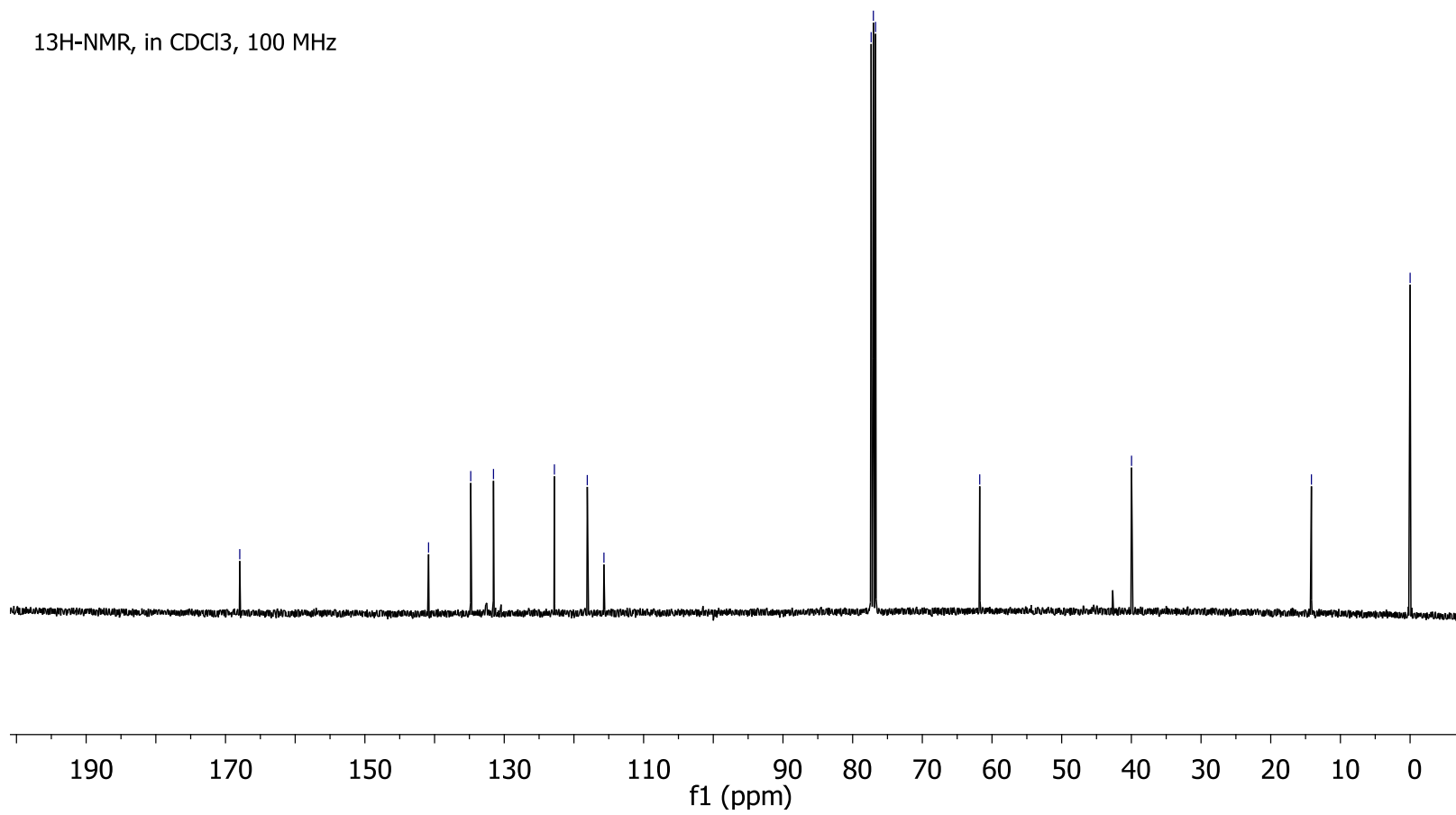
¹H-NMR, in CDCl₃, 400 MHz

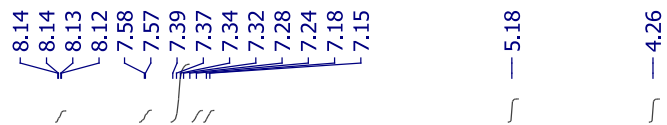
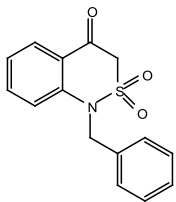




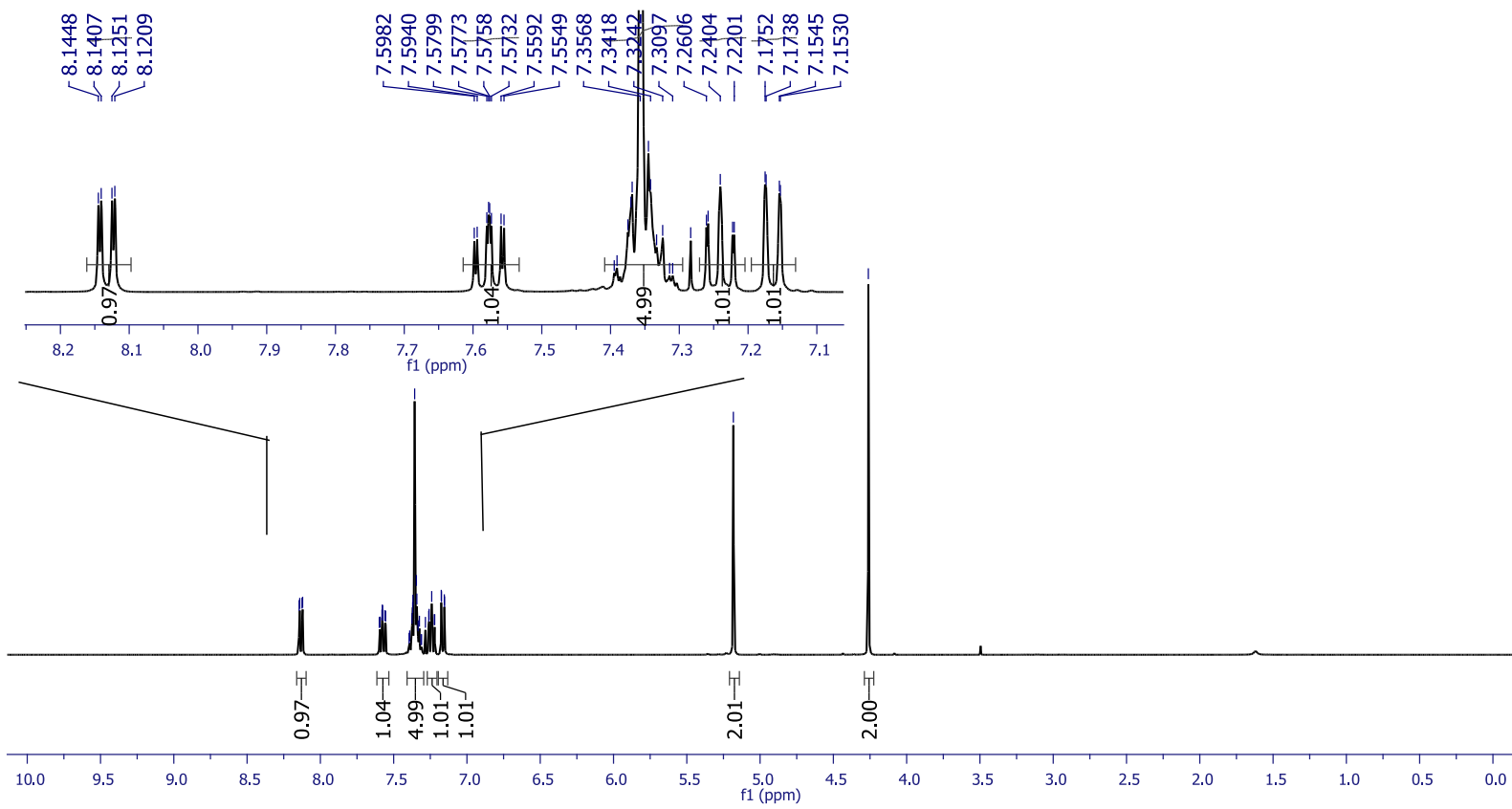
- 140.86
- 134.81
- 131.54
- 122.80
- 118.08
- 115.69
- 77.34
- 77.03
- 76.71
- 61.76
- 39.97
- 14.16
- 0.00

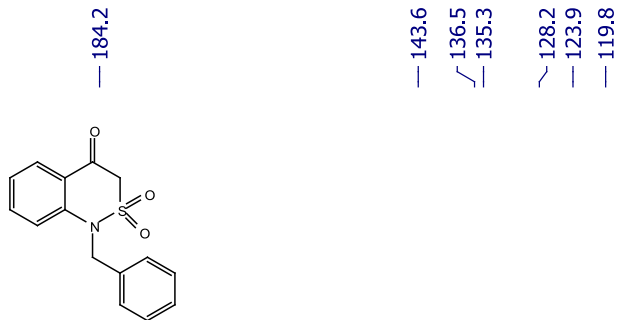
¹³H-NMR, in CDCl₃, 100 MHz



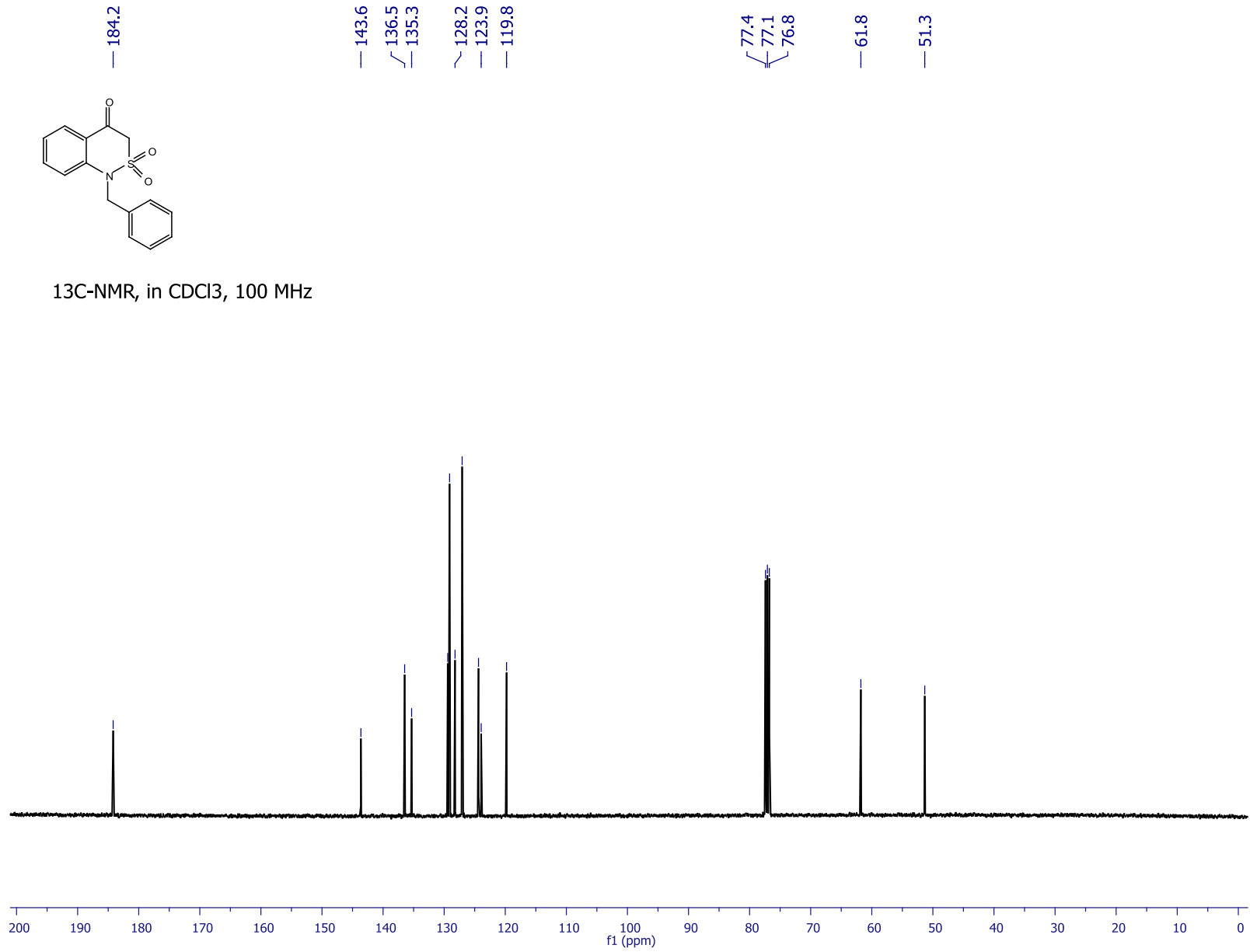


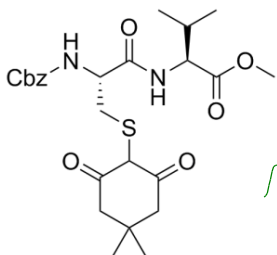
1H-NMR, in CDCl₃, 400 MHz





¹³C-NMR, in CDCl₃, 100 MHz





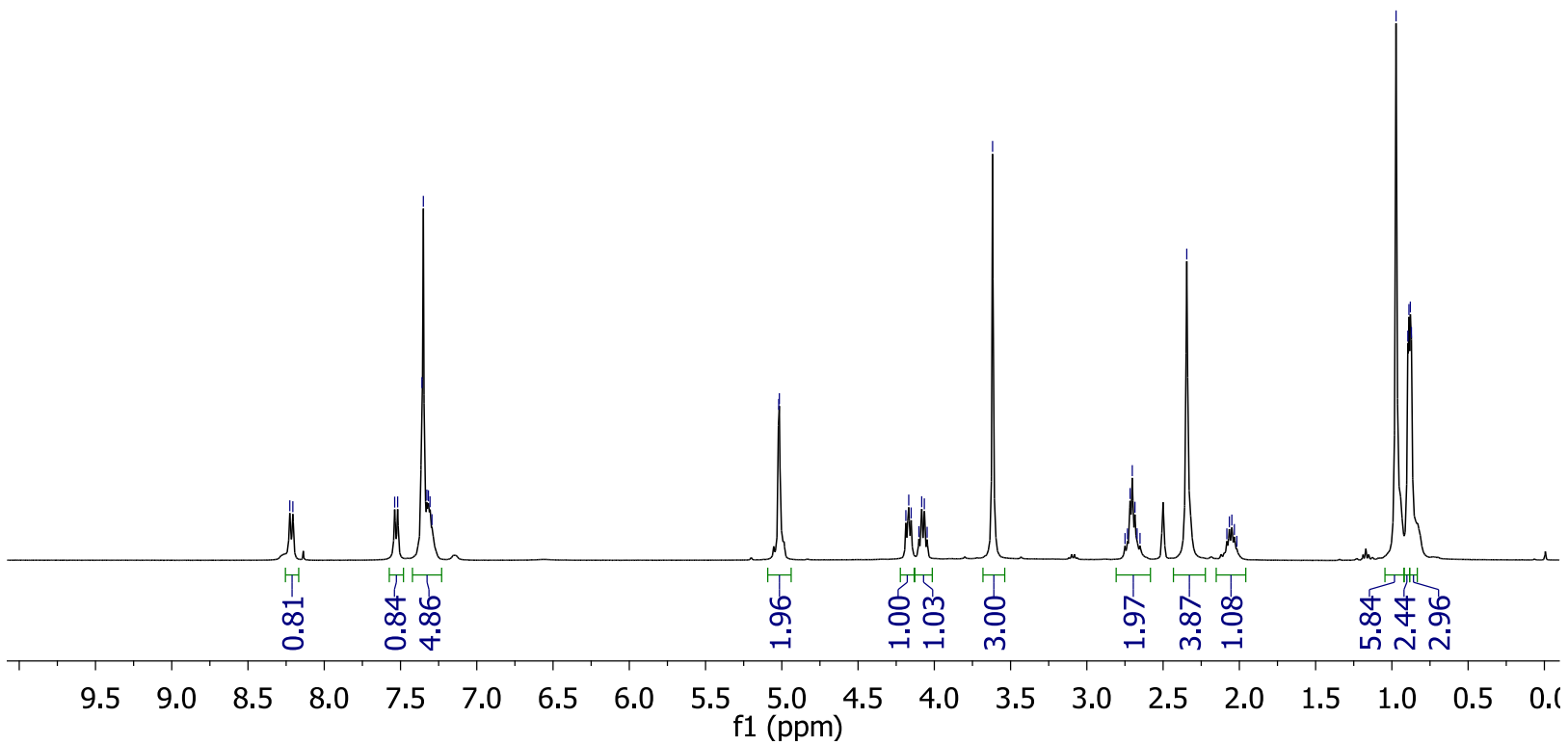
8.23
8.21
7.54
7.52
7.36
7.35
7.33
7.32
7.31
7.29

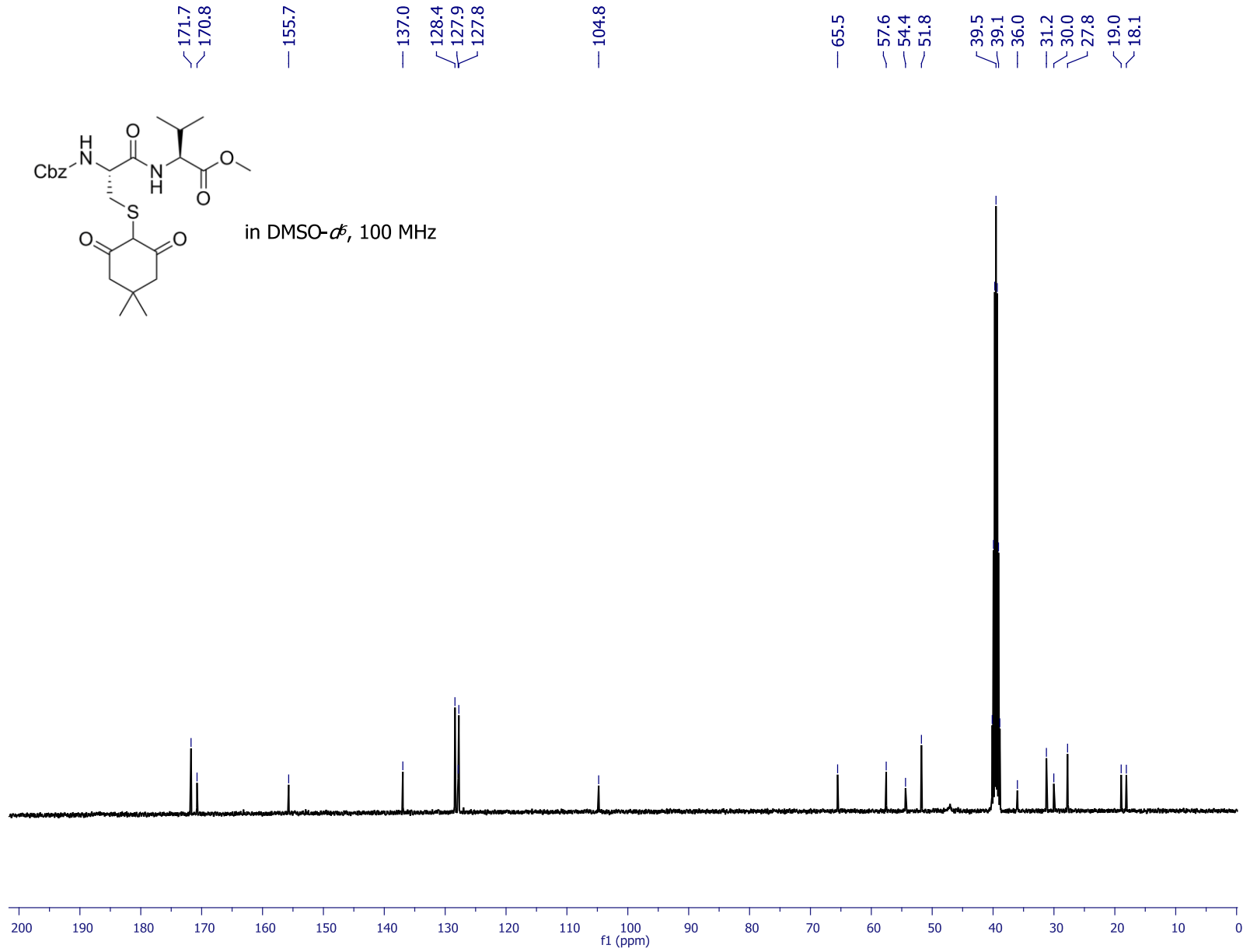
5.02
5.02
4.17
4.08
4.07
4.05
3.62

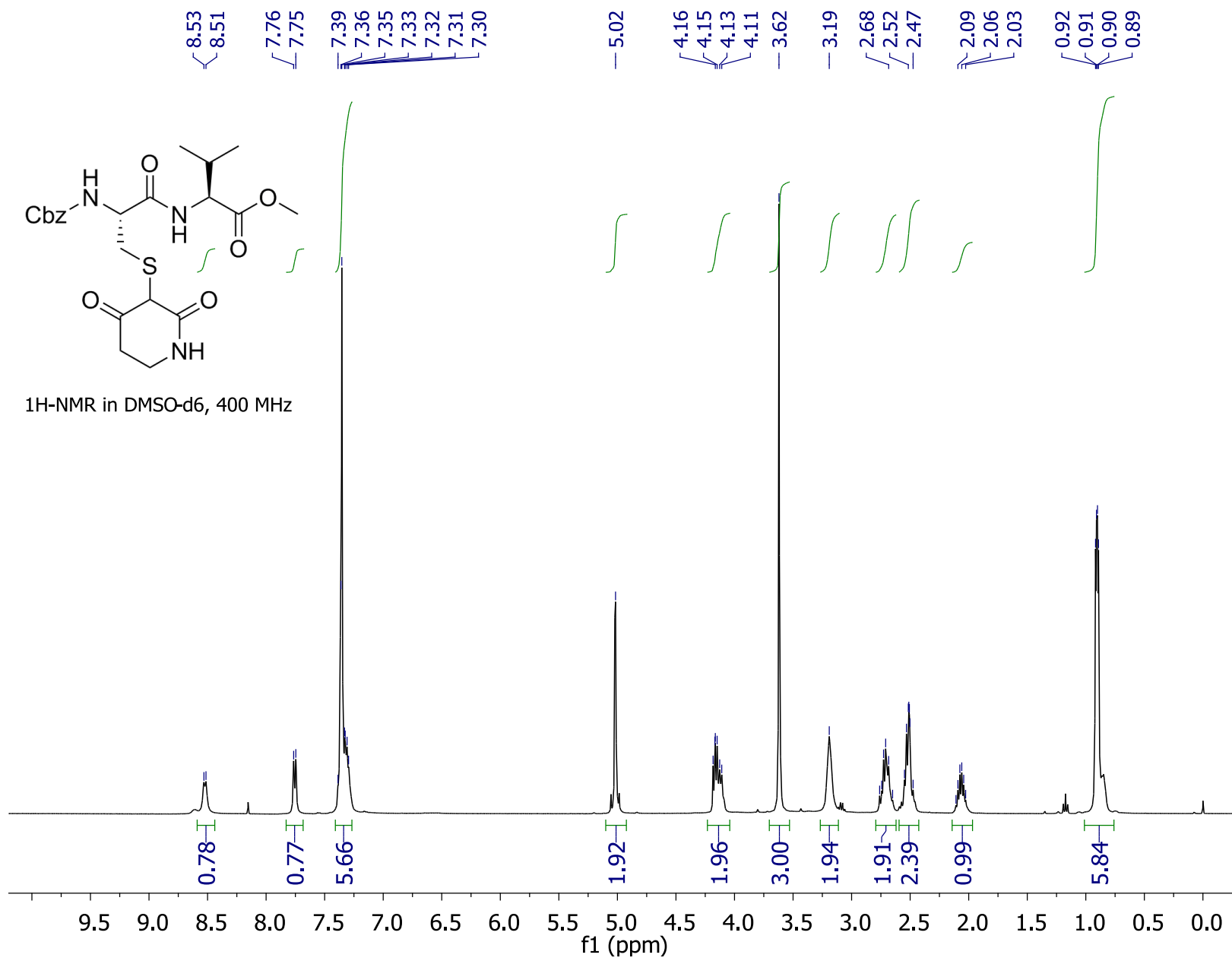
2.72
2.68
2.65
2.34
2.05
2.03
2.02

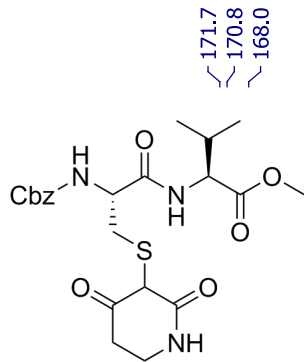
0.97
0.90
0.89
0.88
0.87

¹H-NMR in DMSO-d₆, 400 MHz

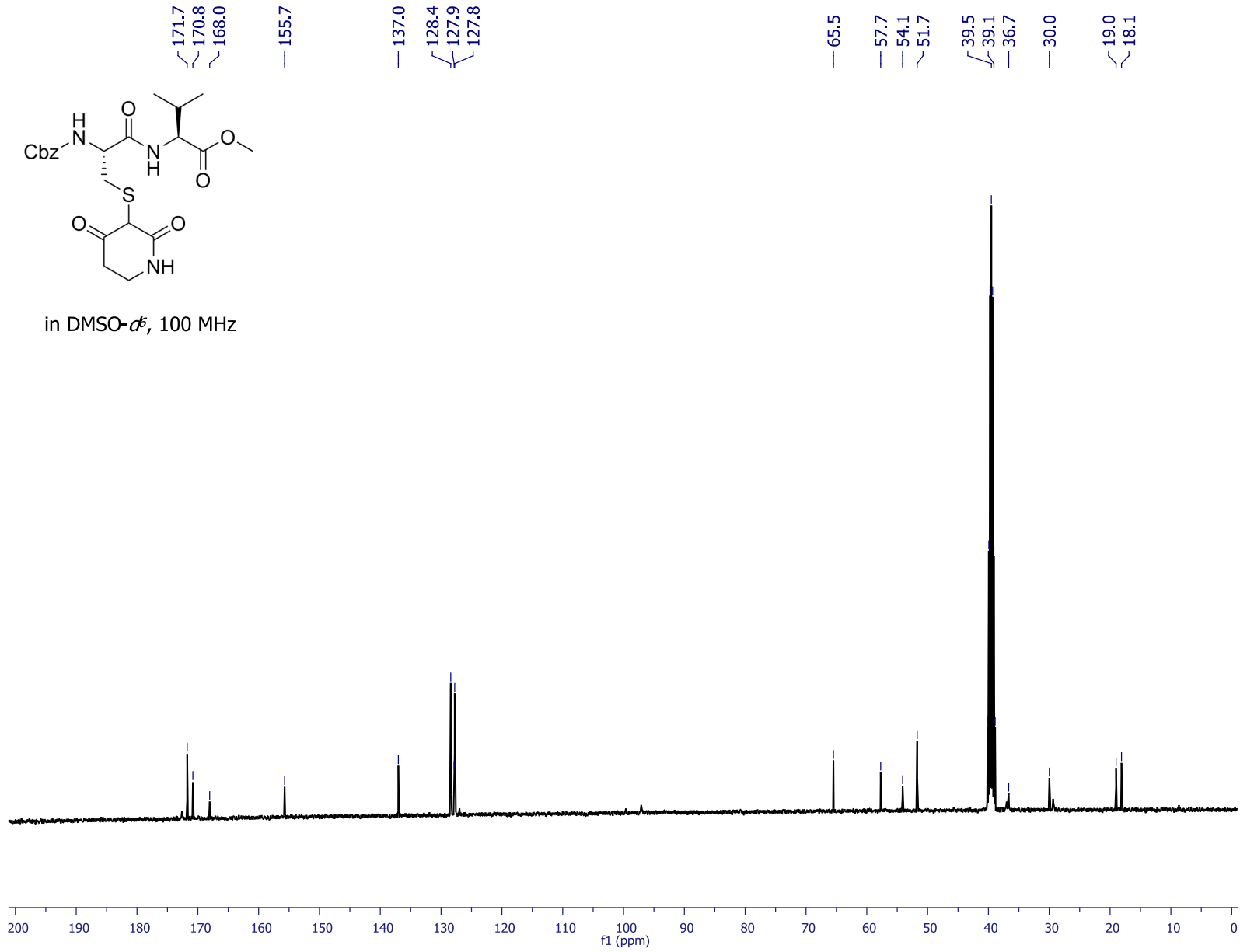


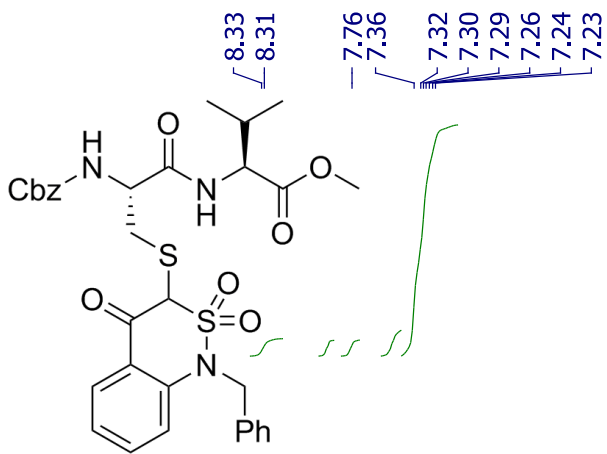






in DMSO- d_6 , 100 MHz





1H-NMR in DMSO-d₆, 400 MHz

