

Supplementary material

Novel methylselenoesters as antiproliferative agents

Nuria Díaz-Argelich^{1,2,3}, Ignacio Encío⁴, Daniel Plano^{1,2}, Aristi P. Fernandes³, Juan Antonio Palop^{1,2}, Carmen Sanmartín^{1,2*}

1) University of Navarra. Faculty of Pharmacy and Nutrition. Department of Organic and Pharmaceutical Chemistry, Irunlarrea 1, 3E-1008 Pamplona, Spain

2) Oncology and Hematology Section, IdiSNA, Navarra Institute for Health Research, Irunlarrea 3, E-31008, Pamplona, Spain

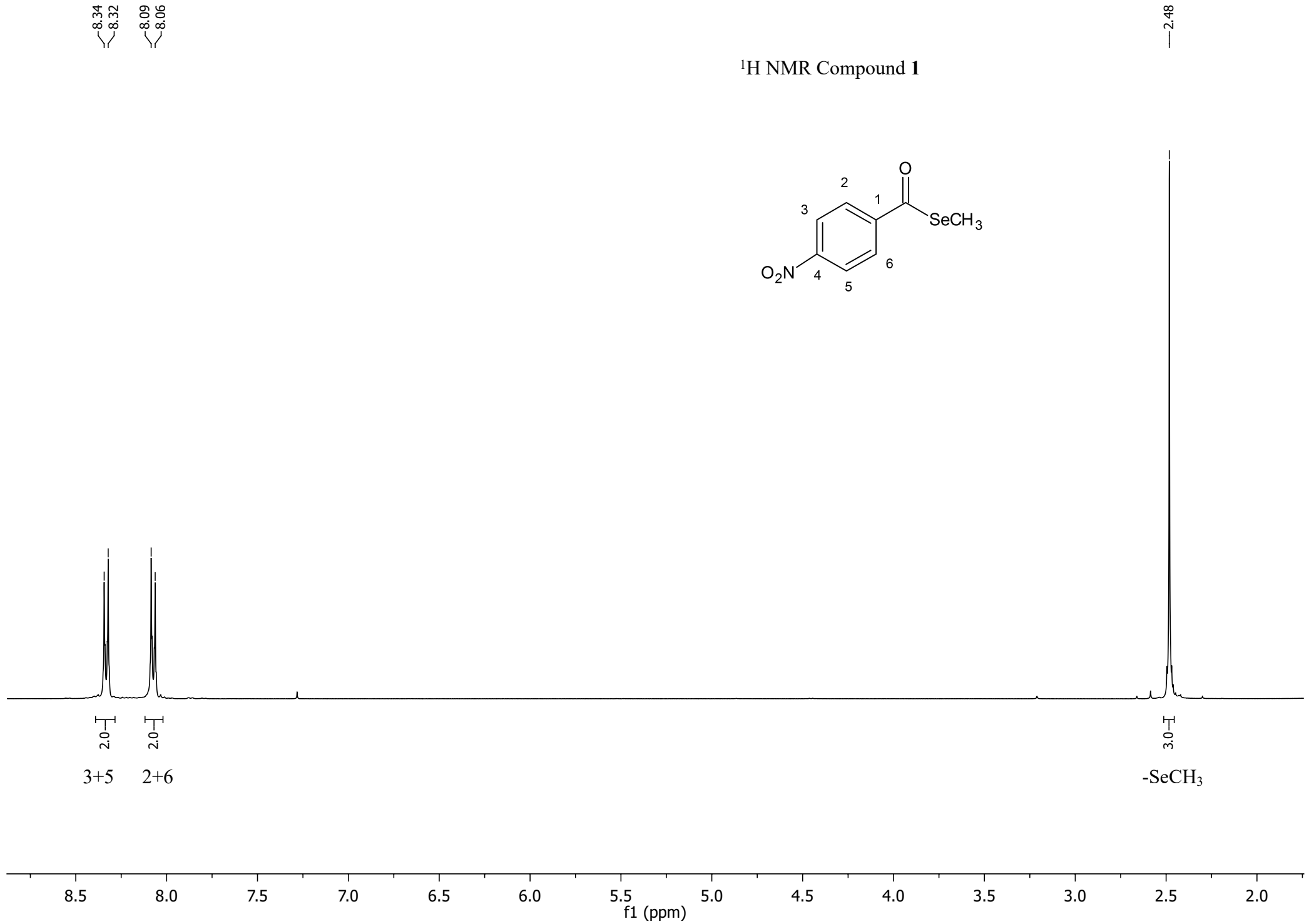
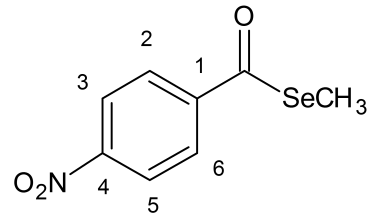
3) Division of Biochemistry, Department of Medical Biochemistry and Biophysics (MBB), Karolinska Institutet, SE-171 77 Stockholm, Sweden

4) Department of Health Sciences, Public University of Navarra, Avda. Barañain s/n, E-31008 Pamplona, Spain

Contents:

Representative spectra (¹H and ¹³C NMR) of the methylselenoesters

¹H NMR Compound 1



—193.72

—150.45

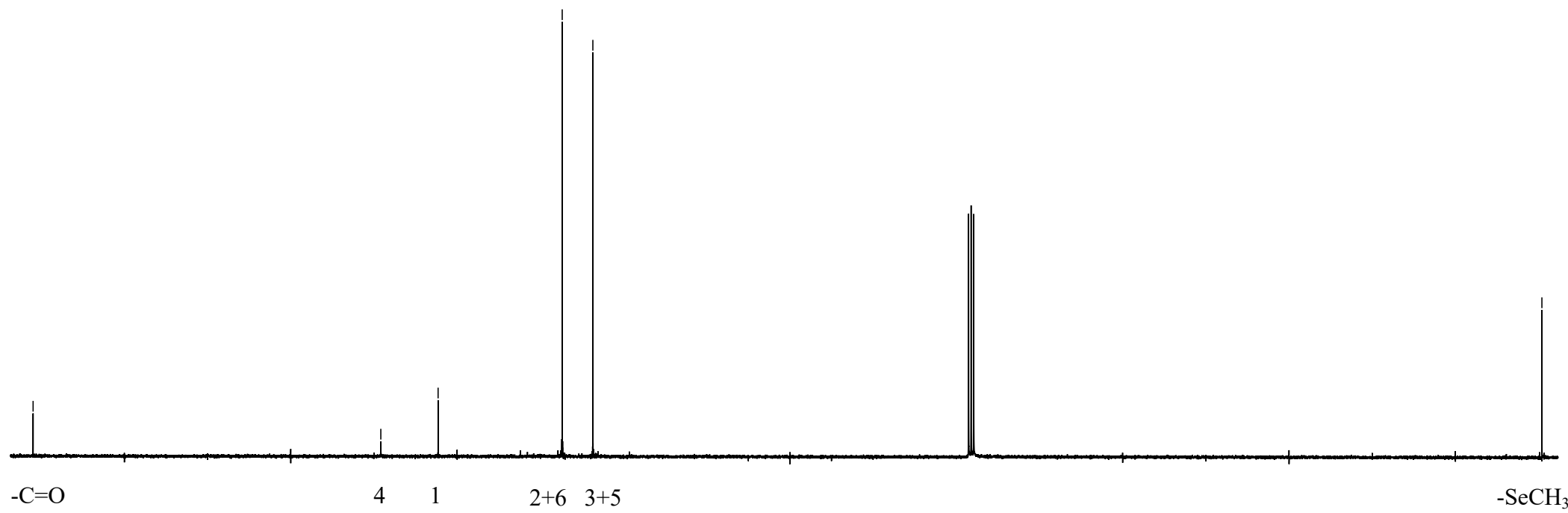
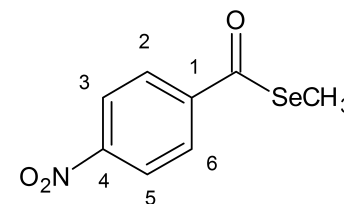
—143.33

—127.88

—124.07

¹³C NMR Compound 1

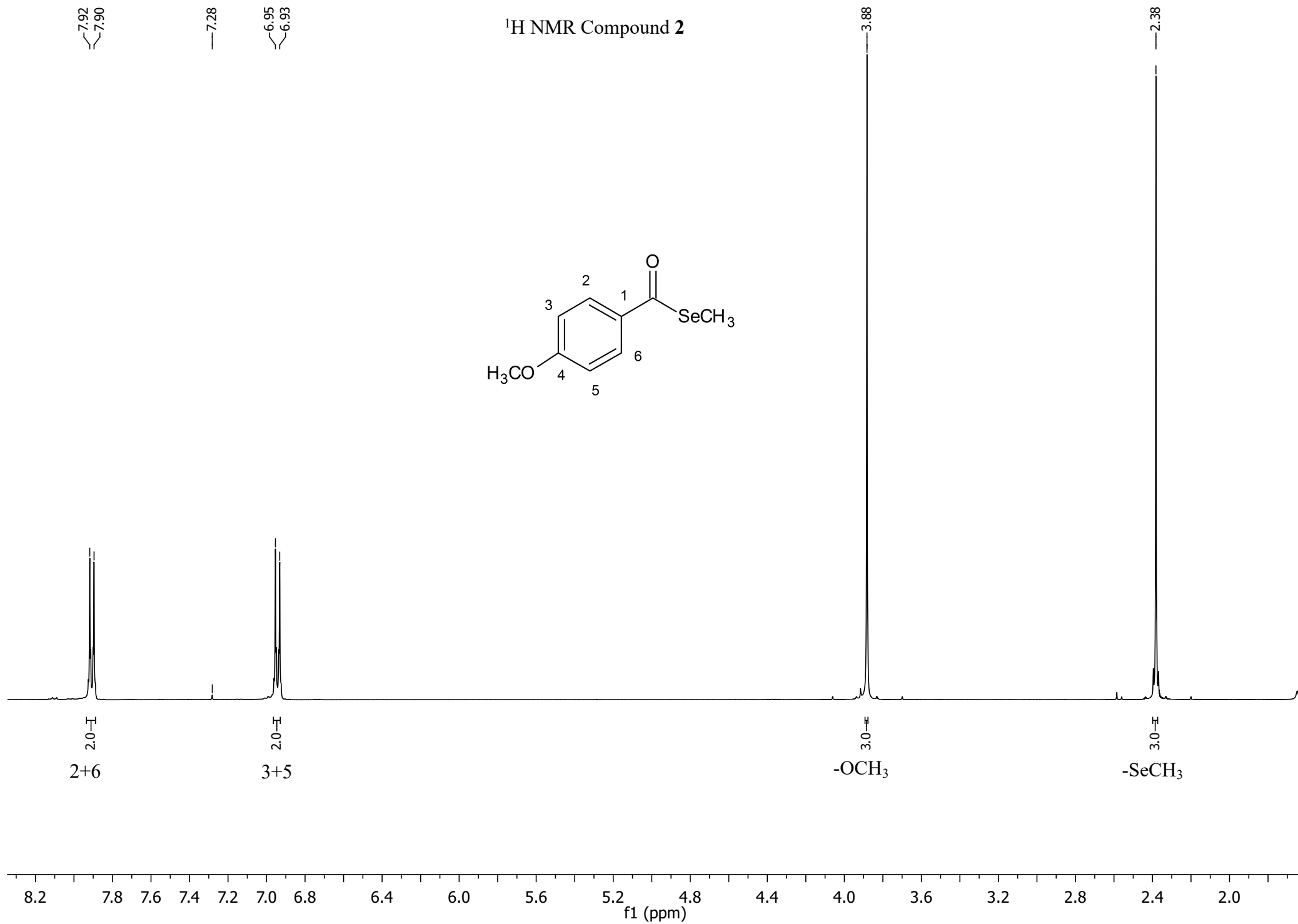
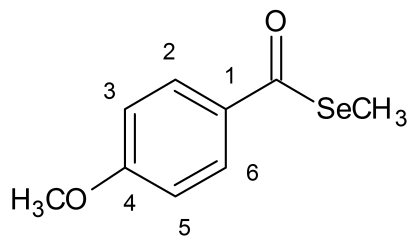
—5.97



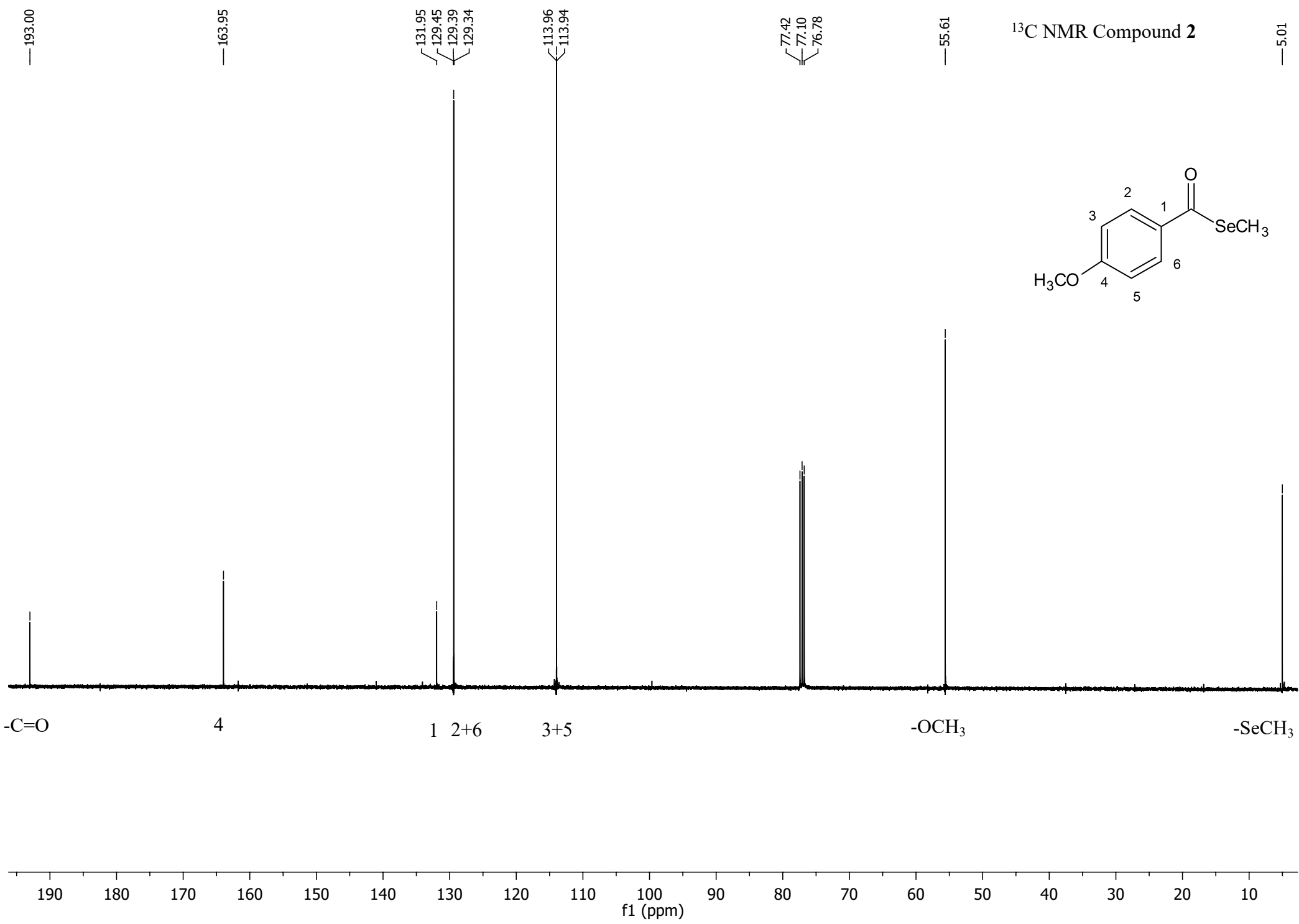
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f1 (ppm)

¹H NMR Compound 2

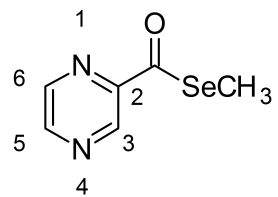


¹³C NMR Compound 2

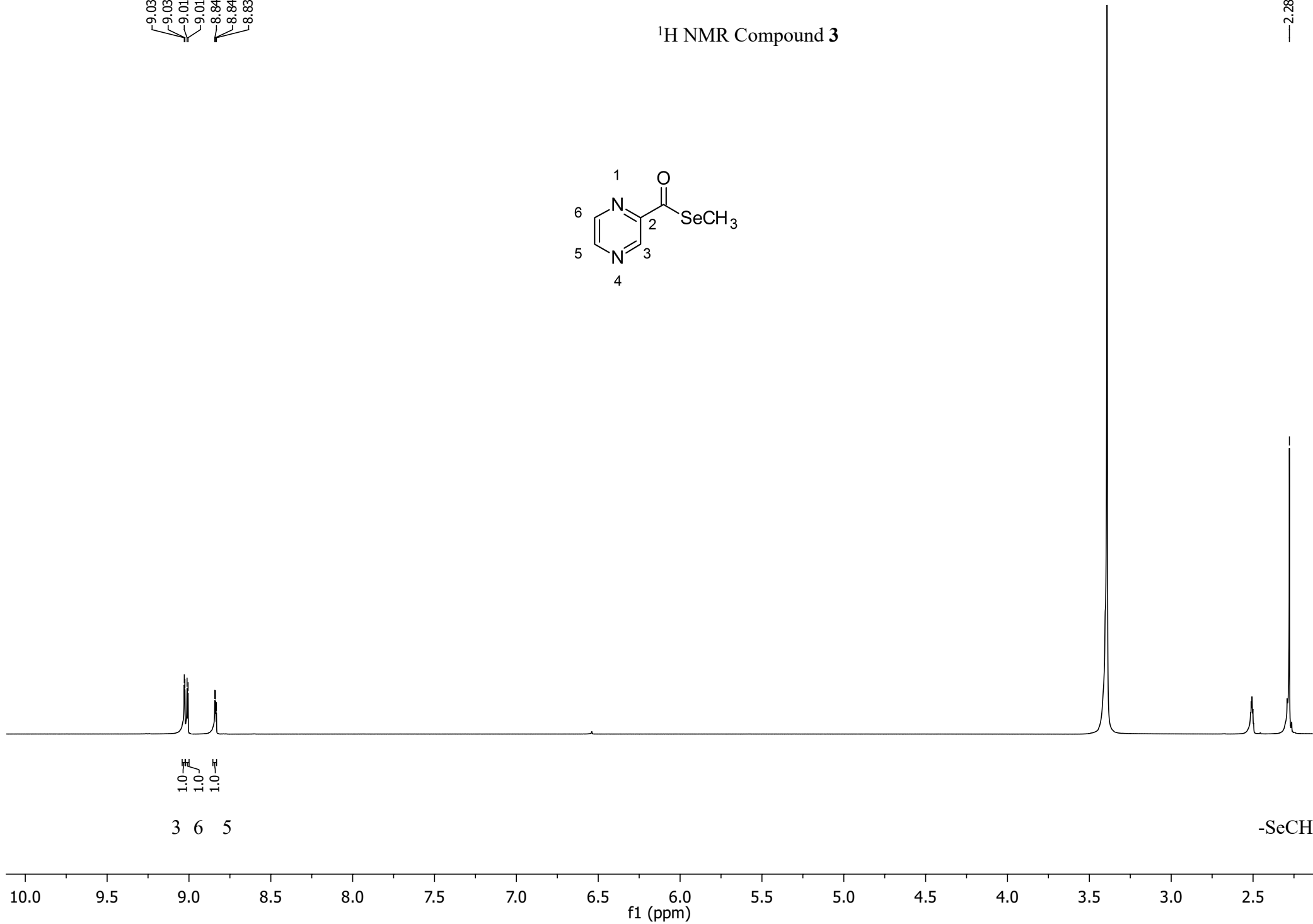


9.03
9.03
9.01
9.01
8.84
8.84
8.83

¹H NMR Compound 3



2.28



1.0
1.0
1.0

3 6 5

-SeCH₃

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5

f1 (ppm)

—198.03

—150.94

—147.15

—145.75

—140.40

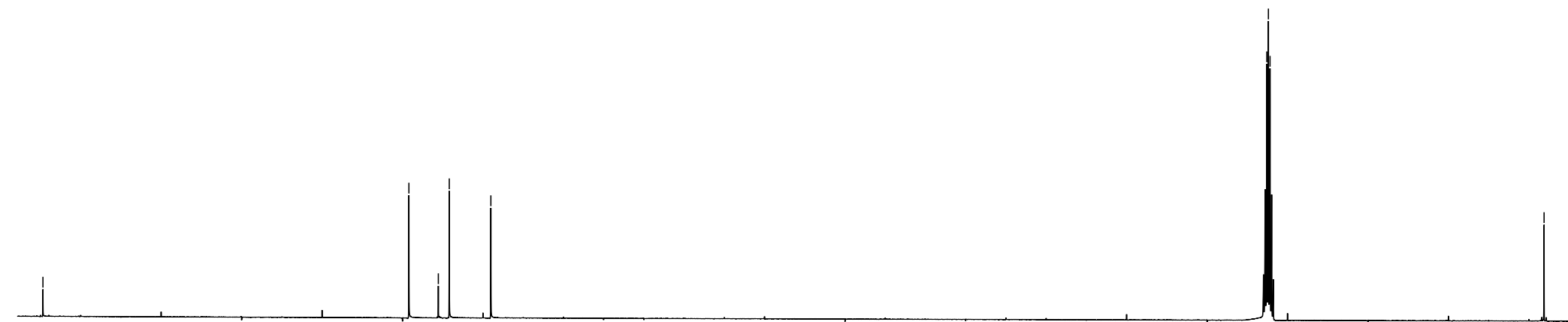
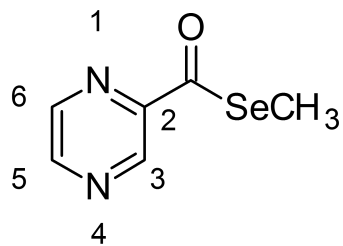
^{13}C NMR Compound 3

—40.56

—40.35

—40.15

—4.88



-C=O

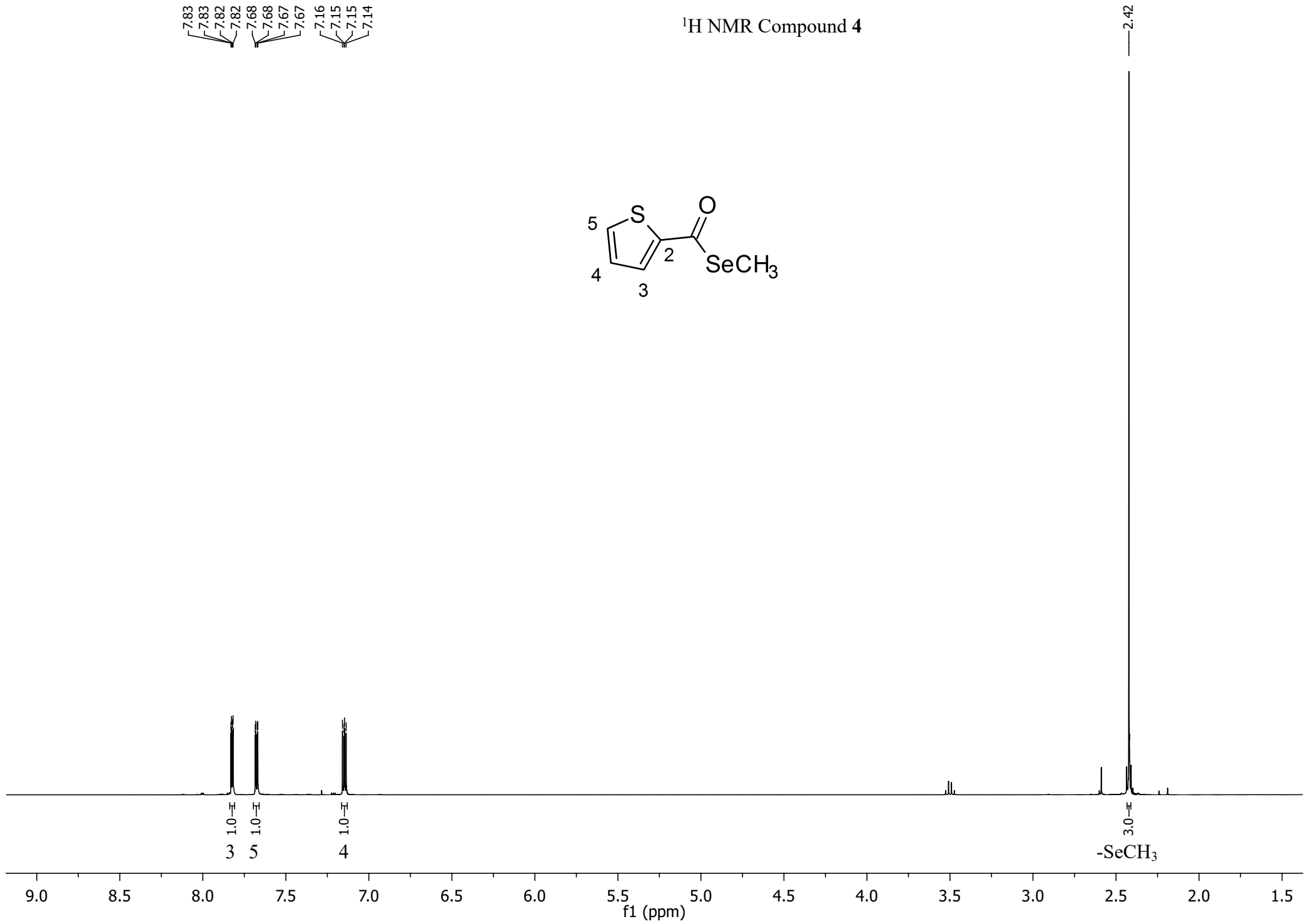
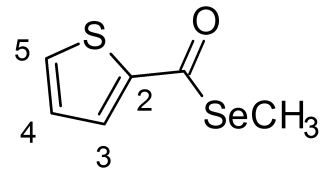
3 5 6 2

-SeCH₃

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

f1 (ppm)

^1H NMR Compound 4



—185.48

—144.32

—133.33

—131.82

—128.29

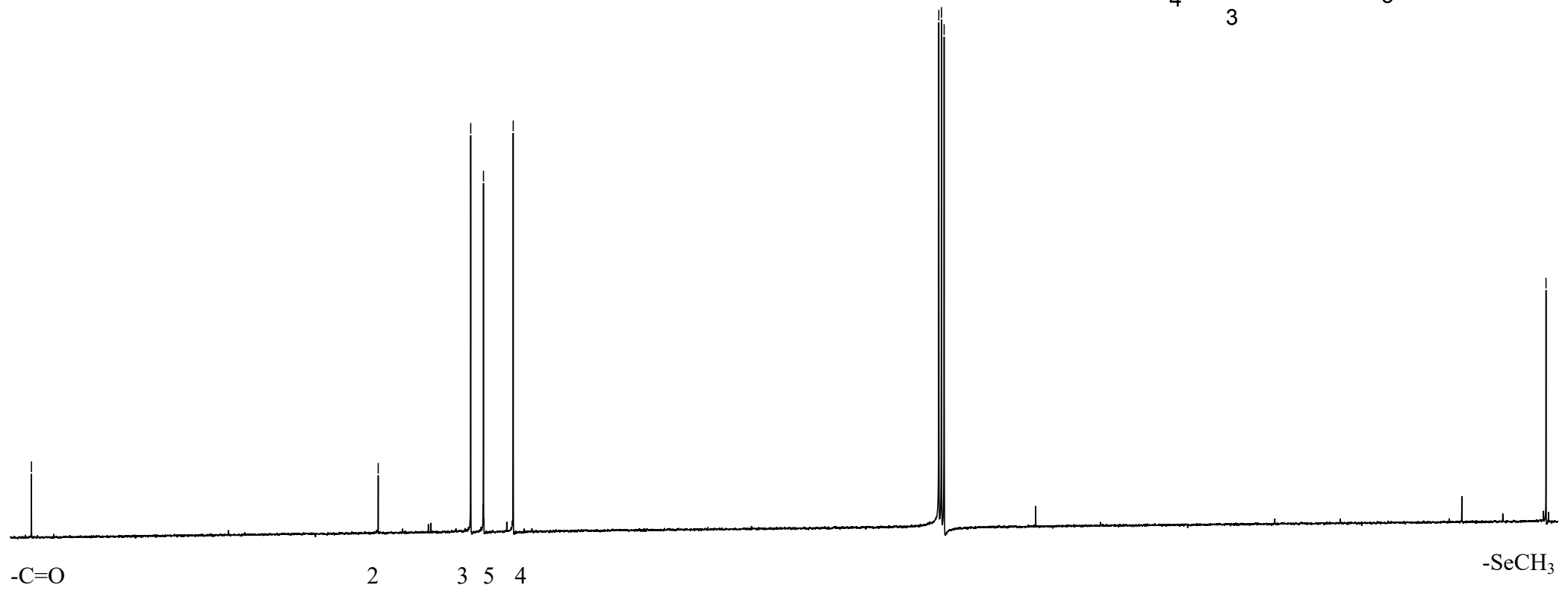
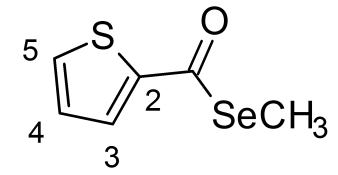
77.78

77.46

77.14

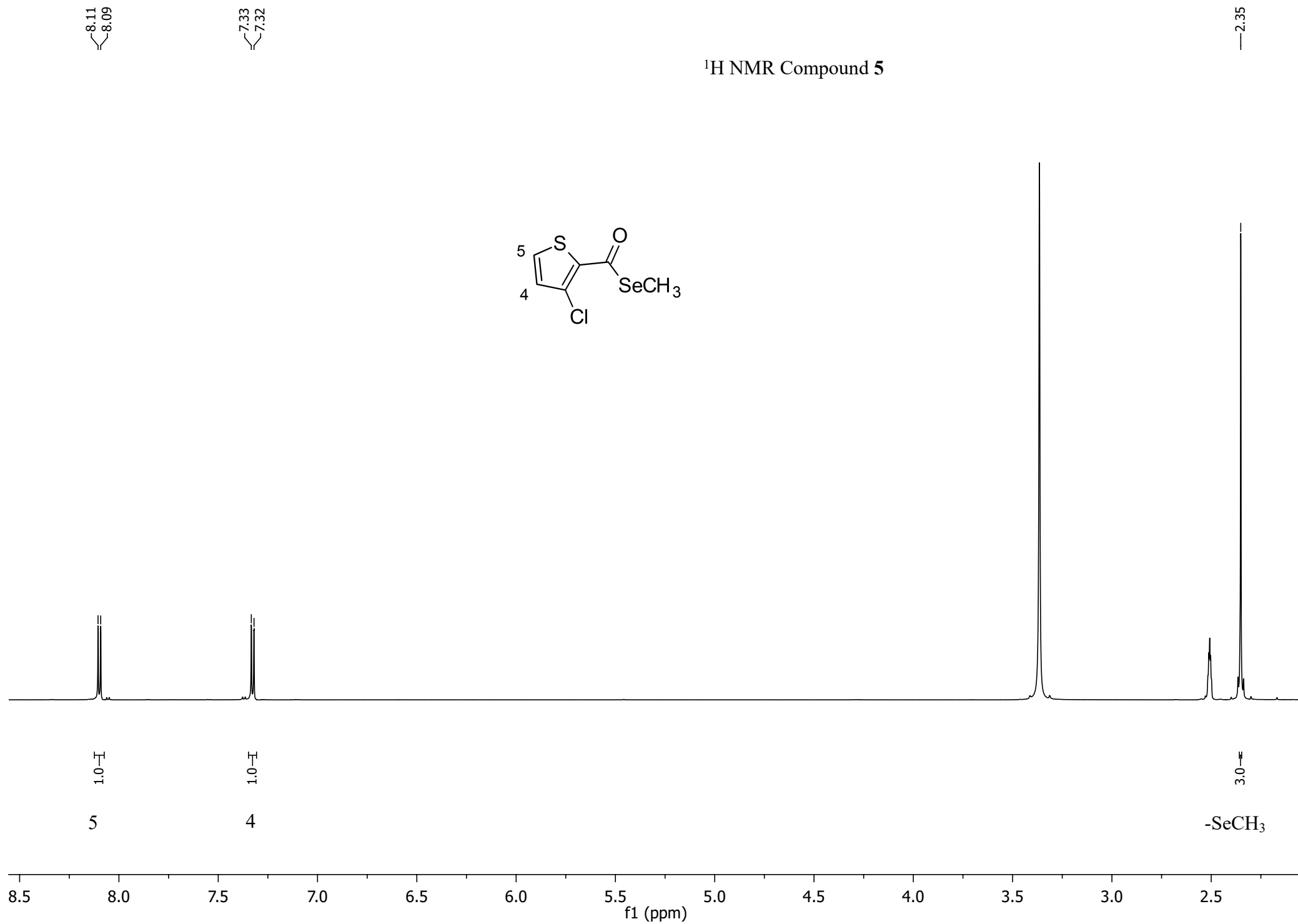
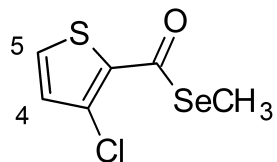
¹³C NMR Compound 4

—5.70



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

¹H NMR Compound 5



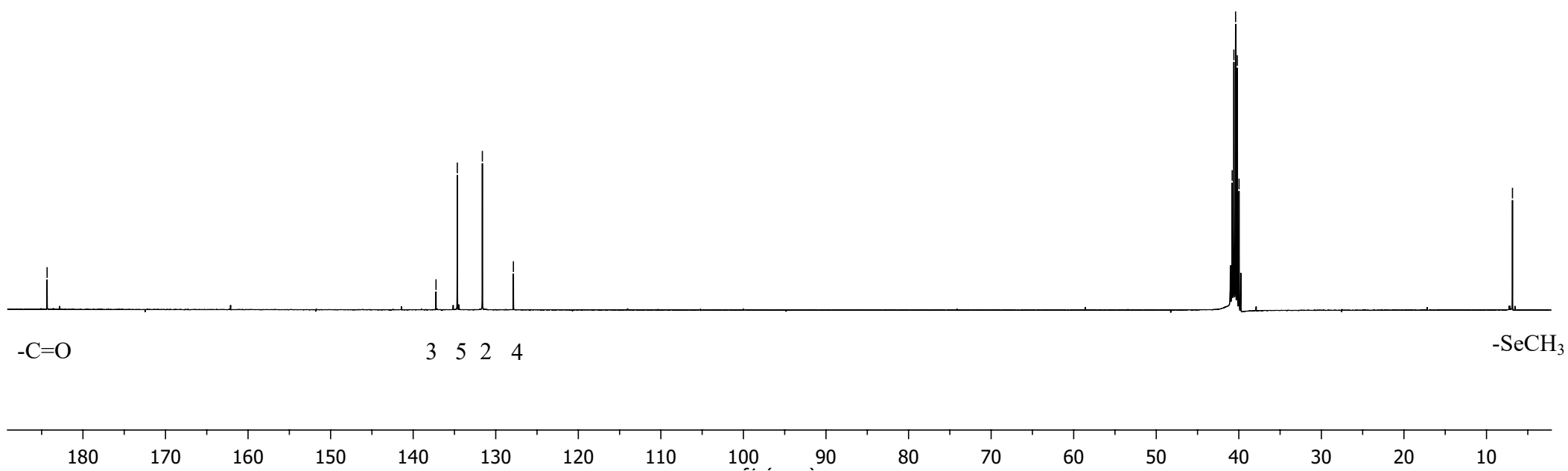
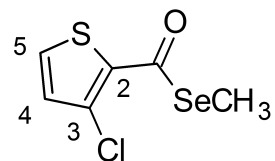
—184.34

137.24
134.66
131.62
127.86

¹³C NMR Compound 5

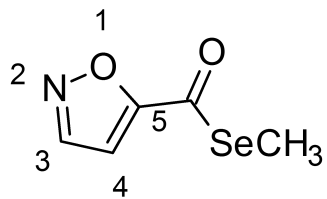
40.81
40.60
40.39
40.18
39.97

—6.85

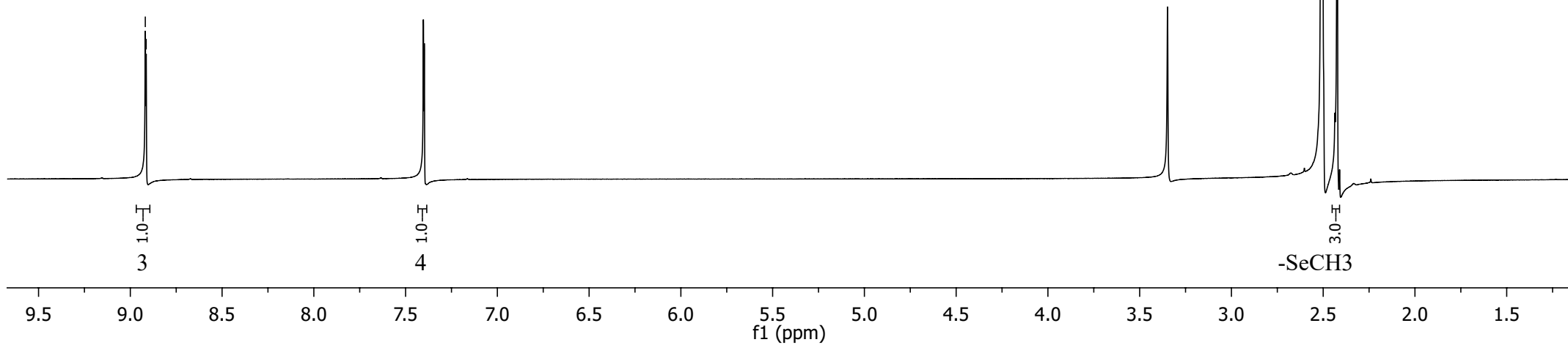


8.92
8.91

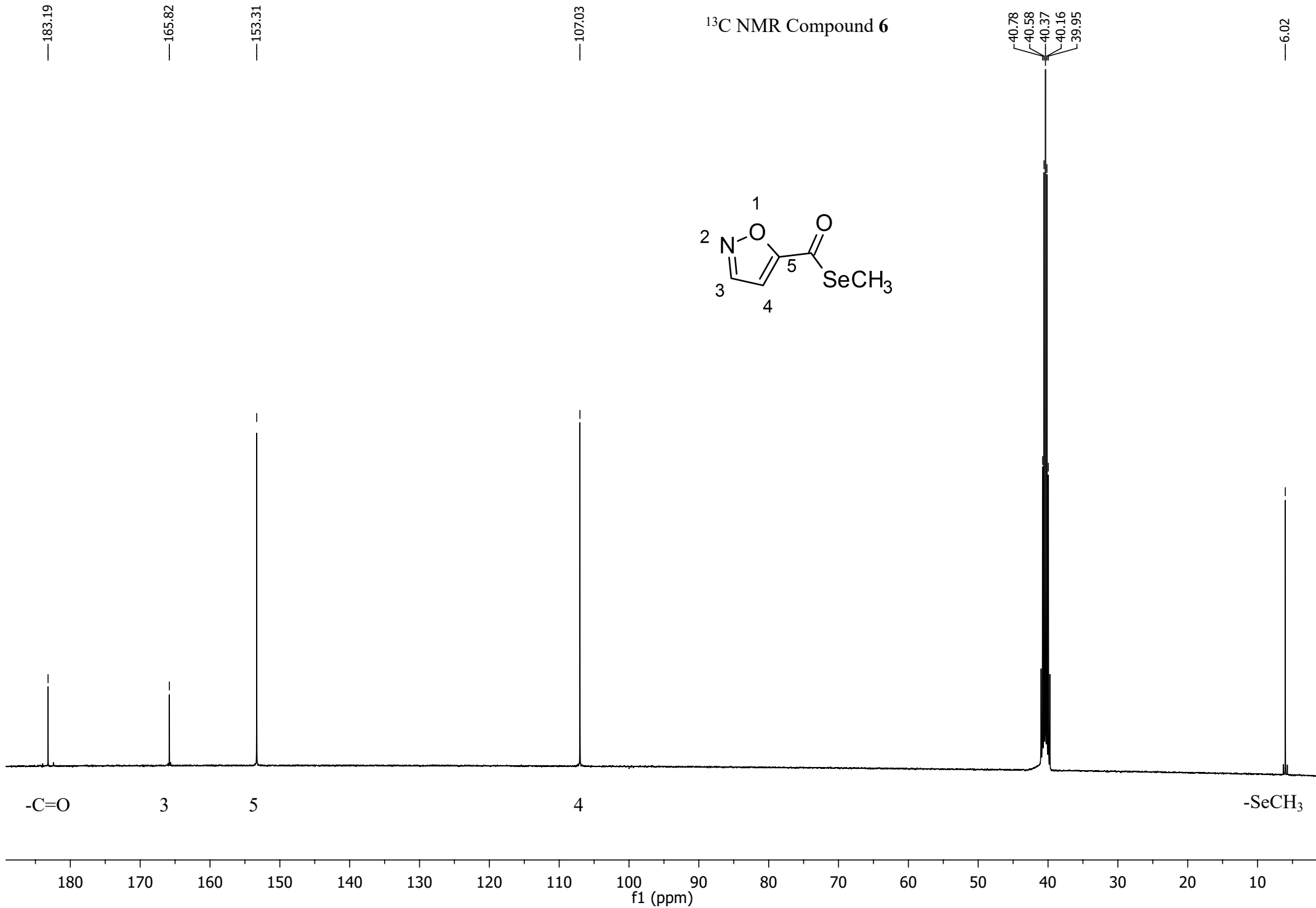
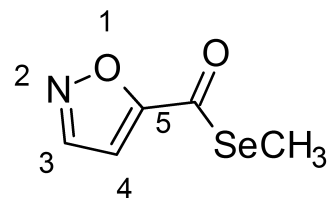
¹H NMR Compound 6



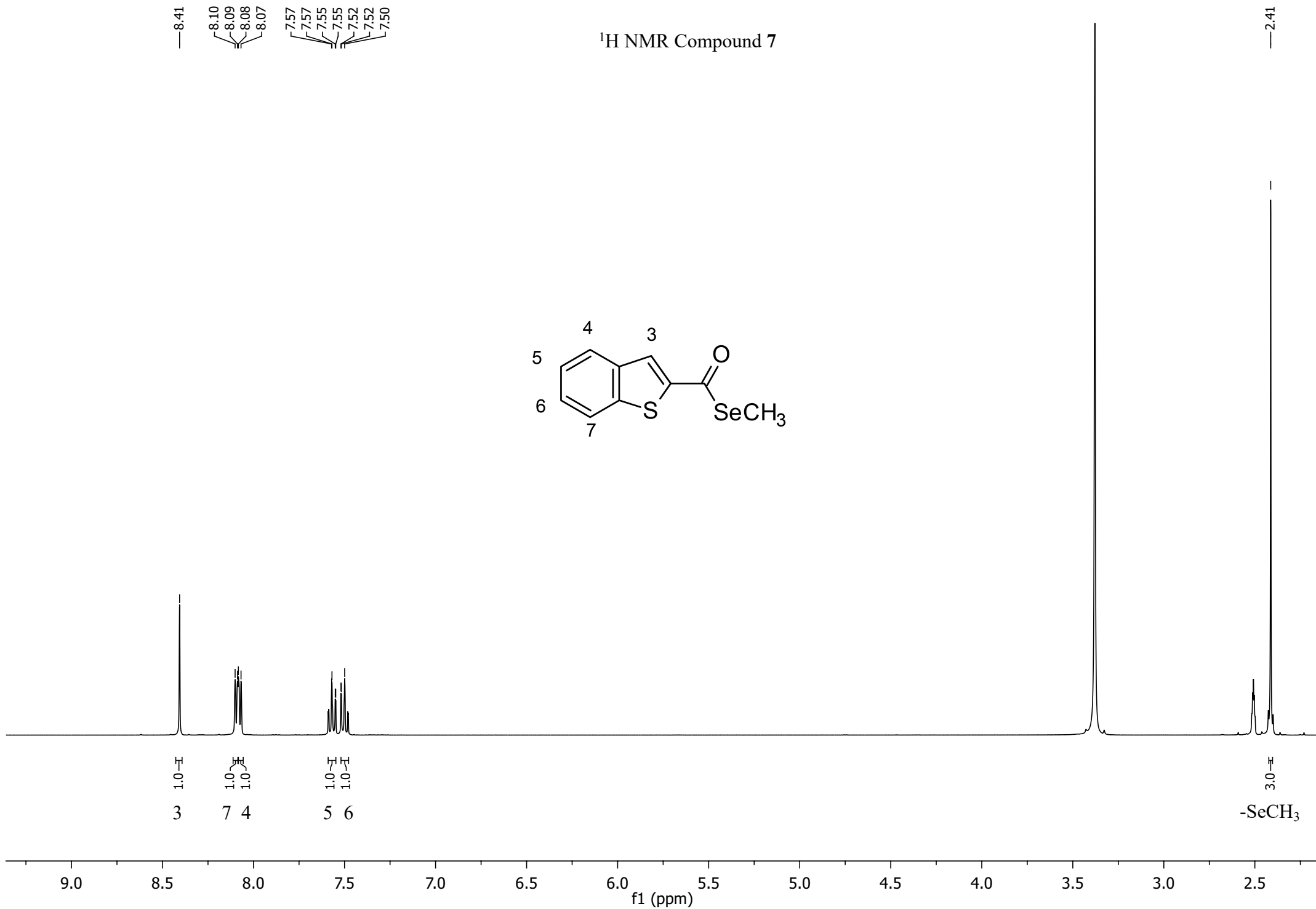
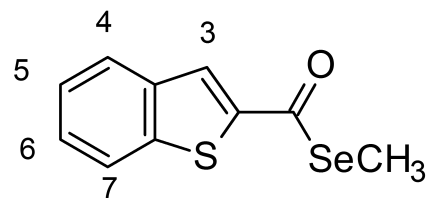
2.42



¹³C NMR Compound 6



¹H NMR Compound 7



—187.57

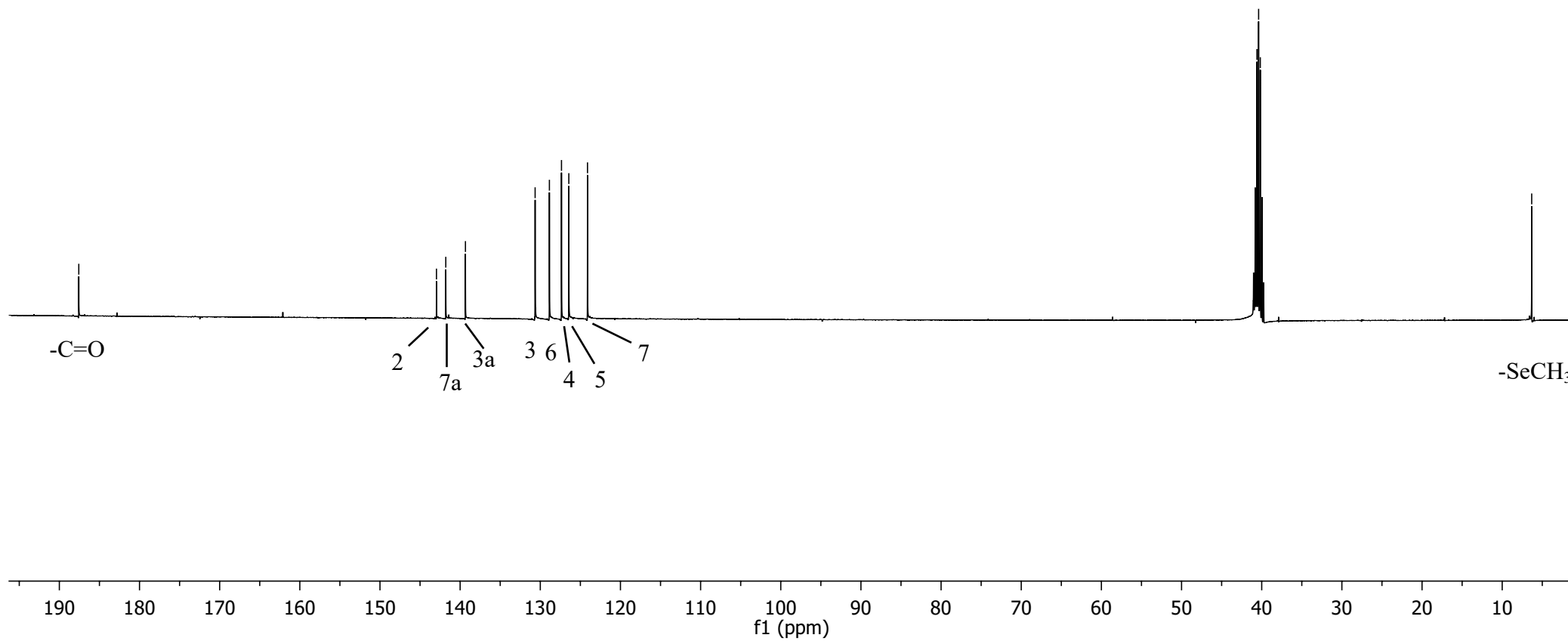
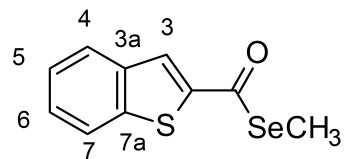
142.95
141.79
139.34

130.64
128.86
127.36
126.44
124.11

^{13}C NMR Compound 7

40.59
40.39
40.18

—6.32



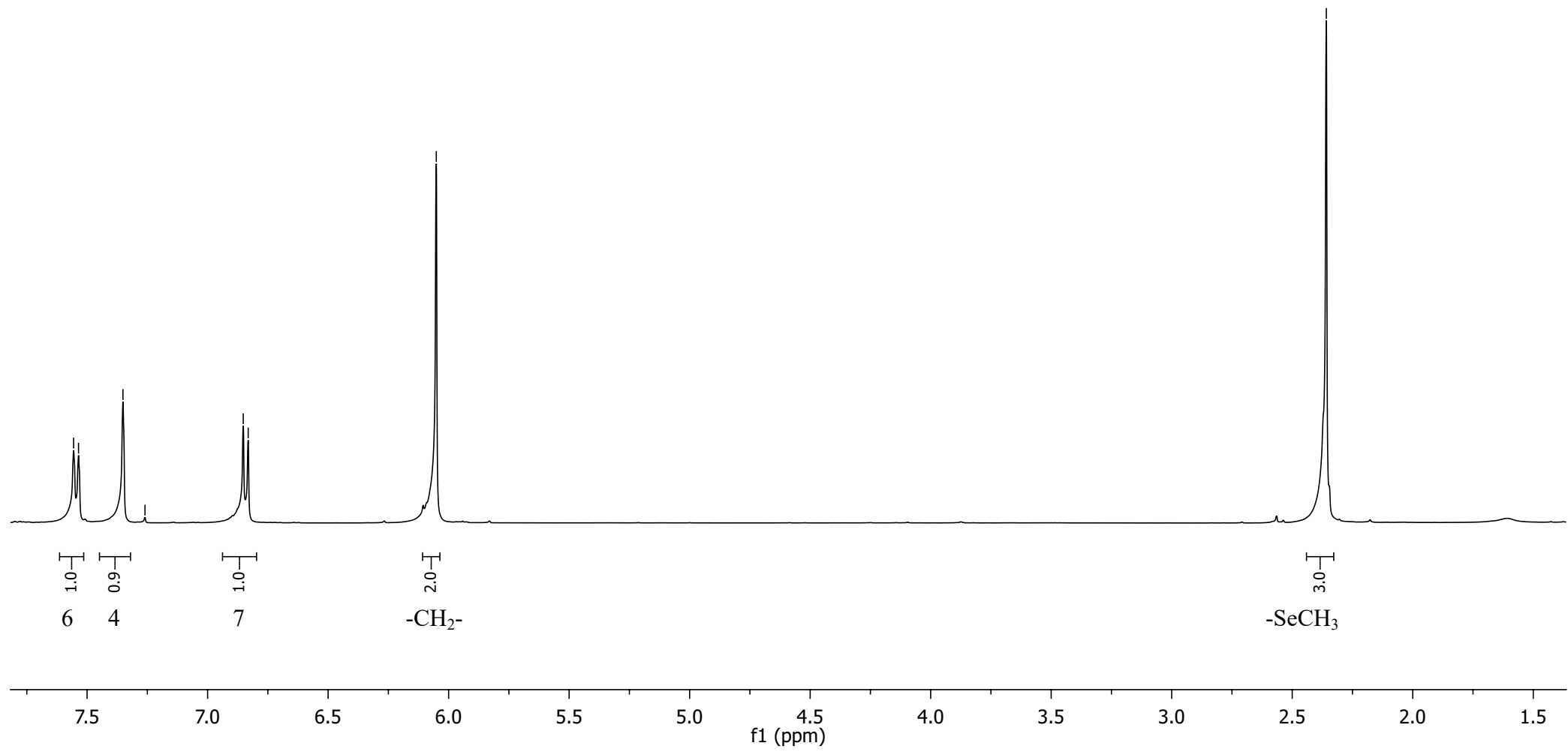
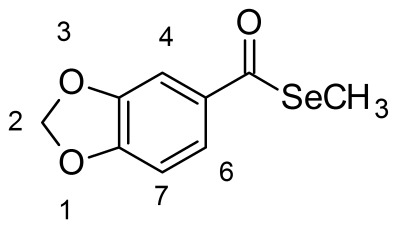
7.56
7.54
7.35
7.26

6.85
6.83

6.05

¹H NMR Compound 8

2.36



—192.32

—151.79

—147.83

—133.21

—123.19

—107.77

—106.48

—101.68

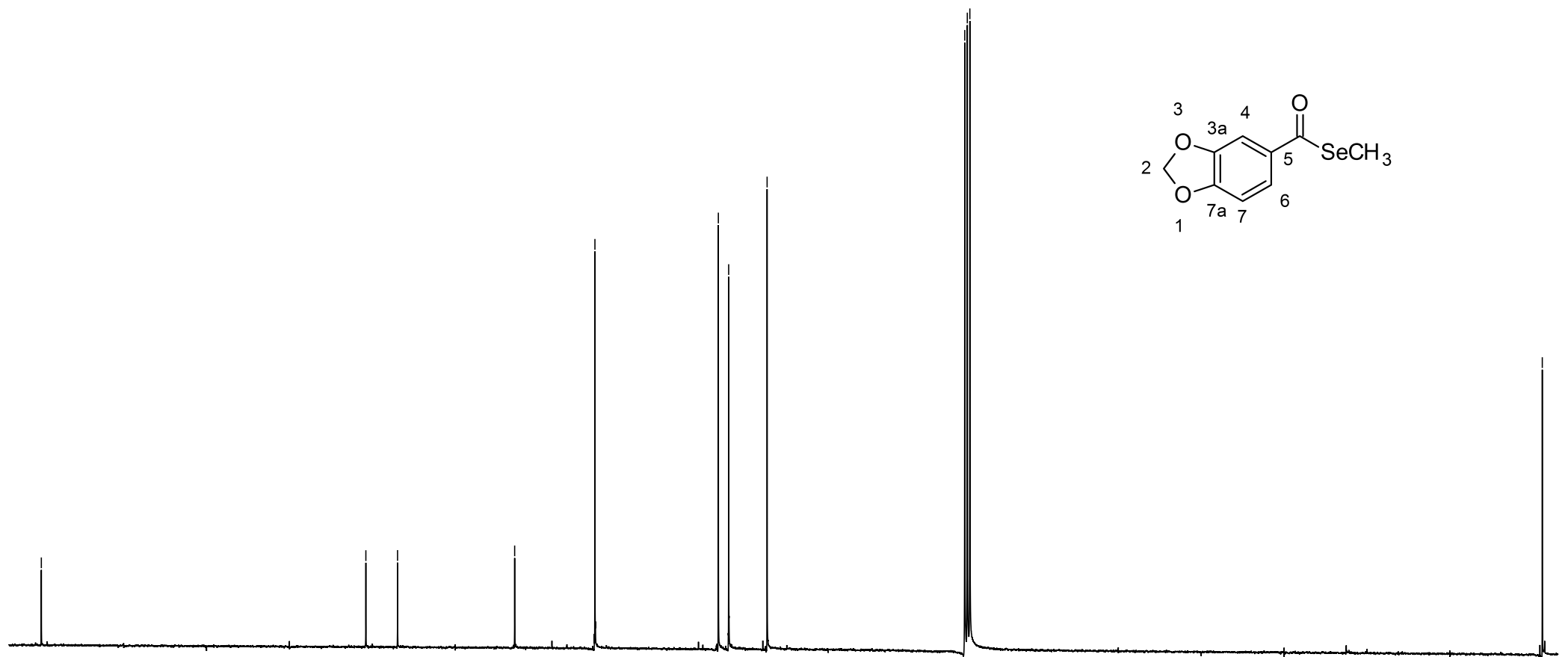
—77.00

—76.68

—76.36

¹³C NMR Compound **8**

—4.87



-C=O

7a 3a

5

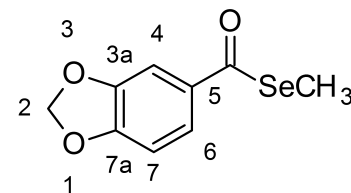
6

4

7

2

-SeCH₃



f1 (ppm)

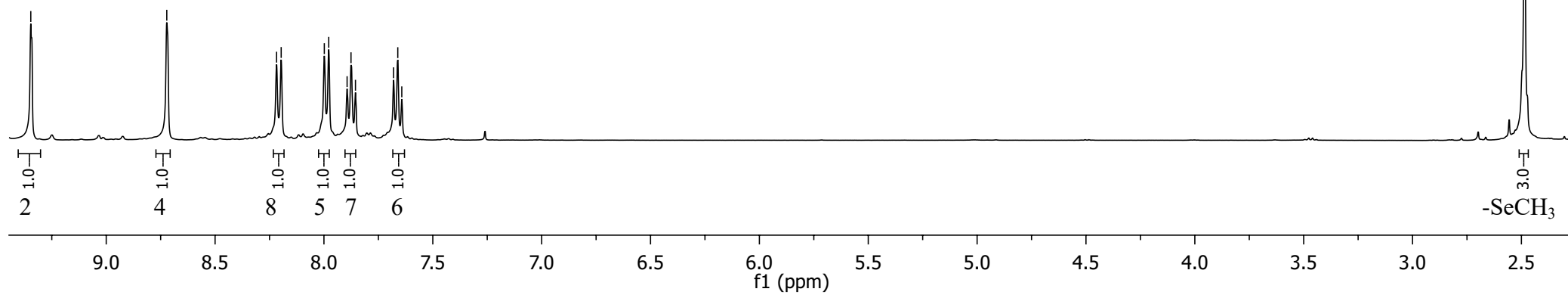
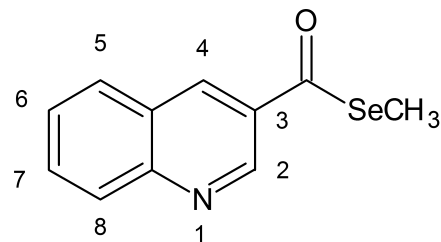
—9.35

—8.72

8.22
8.20
8.00
7.98
7.89
7.88
7.86
7.68
7.66
7.64

—2.48

¹H NMR Compound 9



—193.47

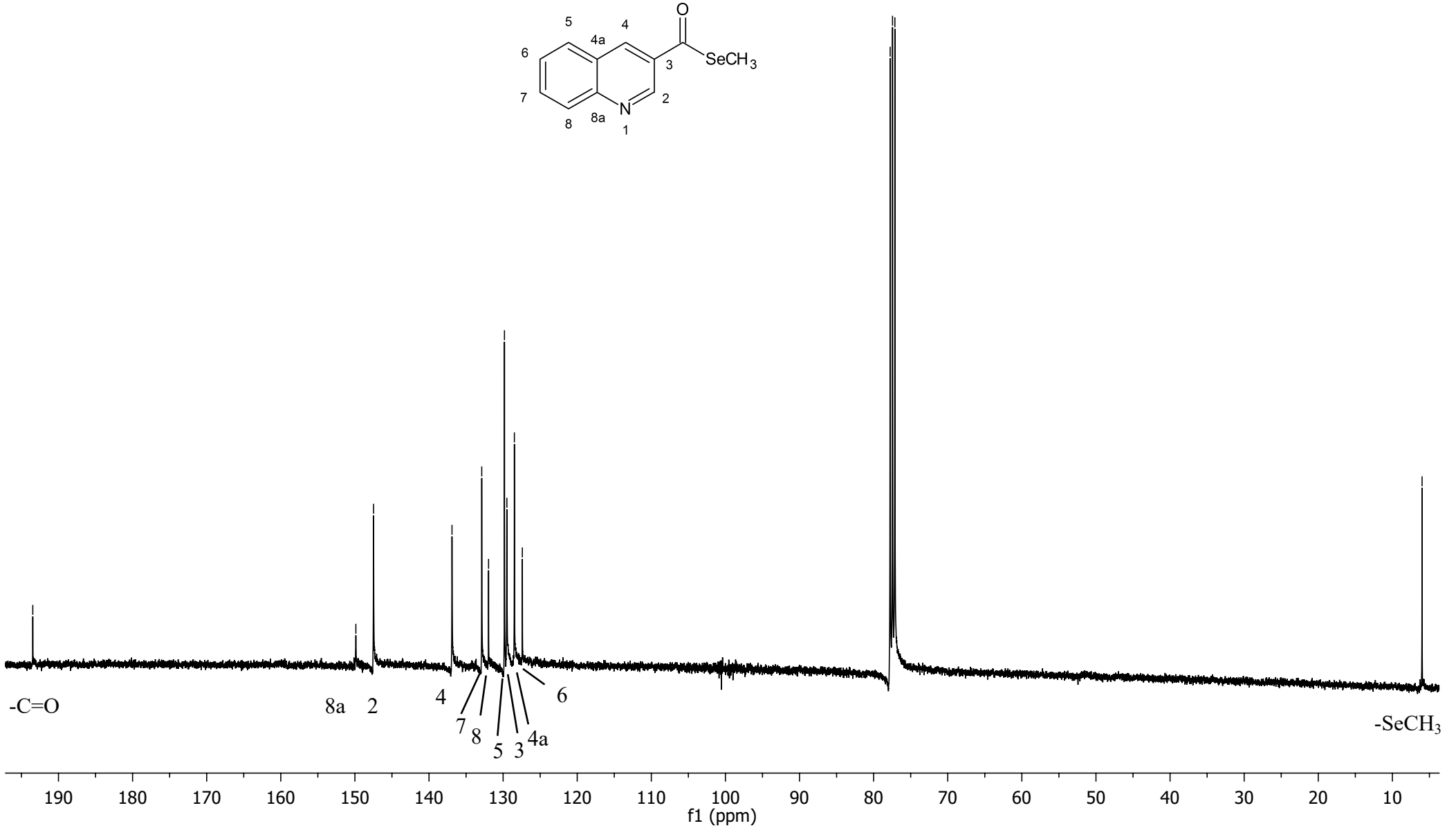
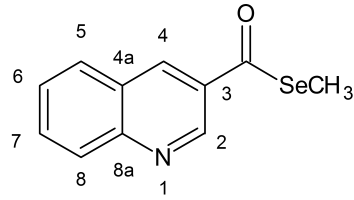
—149.87
—147.48

136.90
132.88
131.96
129.82
129.49
128.48
127.40

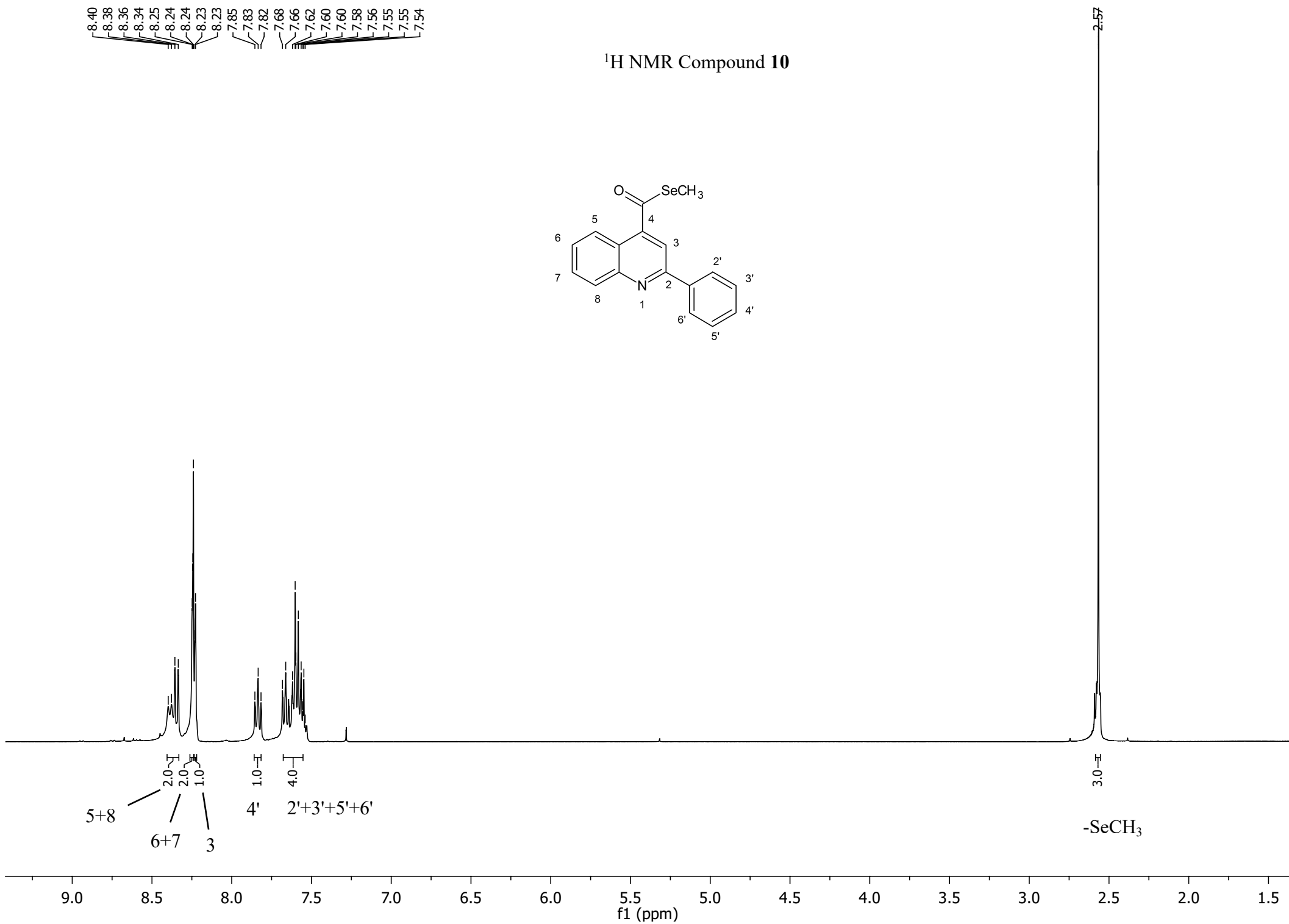
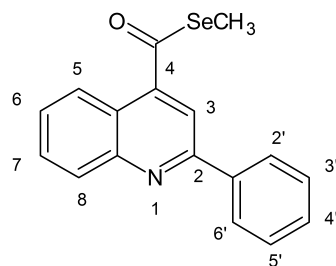
¹³C NMR Compound 9

77.77
77.45
77.13

—5.99



¹H NMR Compound 10



—197.10

—157.26

—148.70

—146.28

—138.17

—131.29

—130.72

—129.82

—129.53

—128.77

—128.22

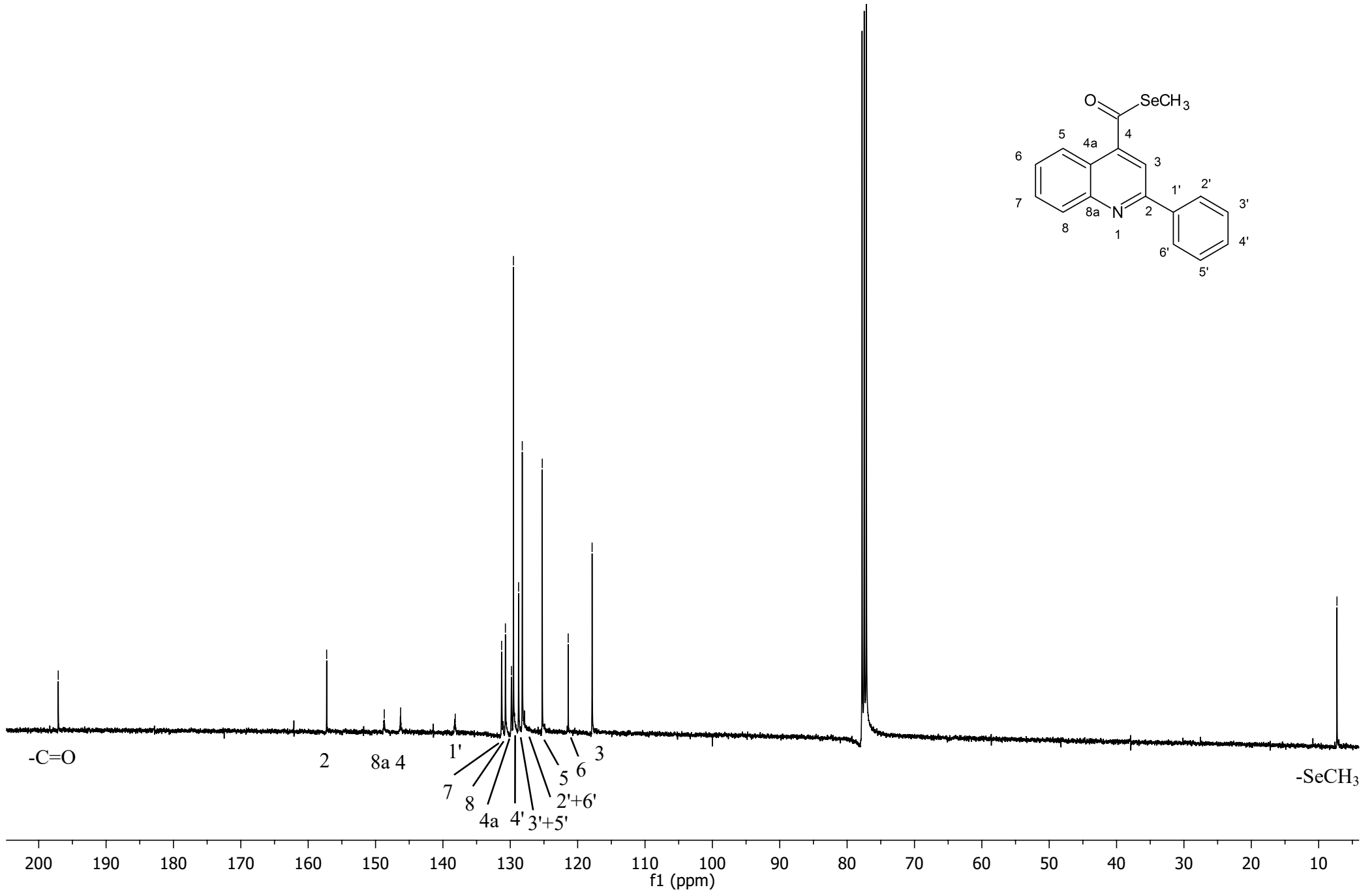
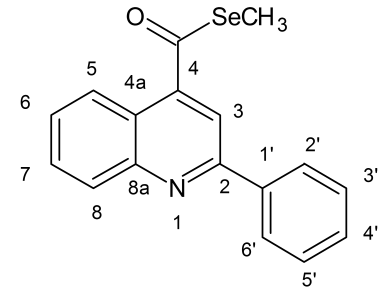
—125.25

—121.40

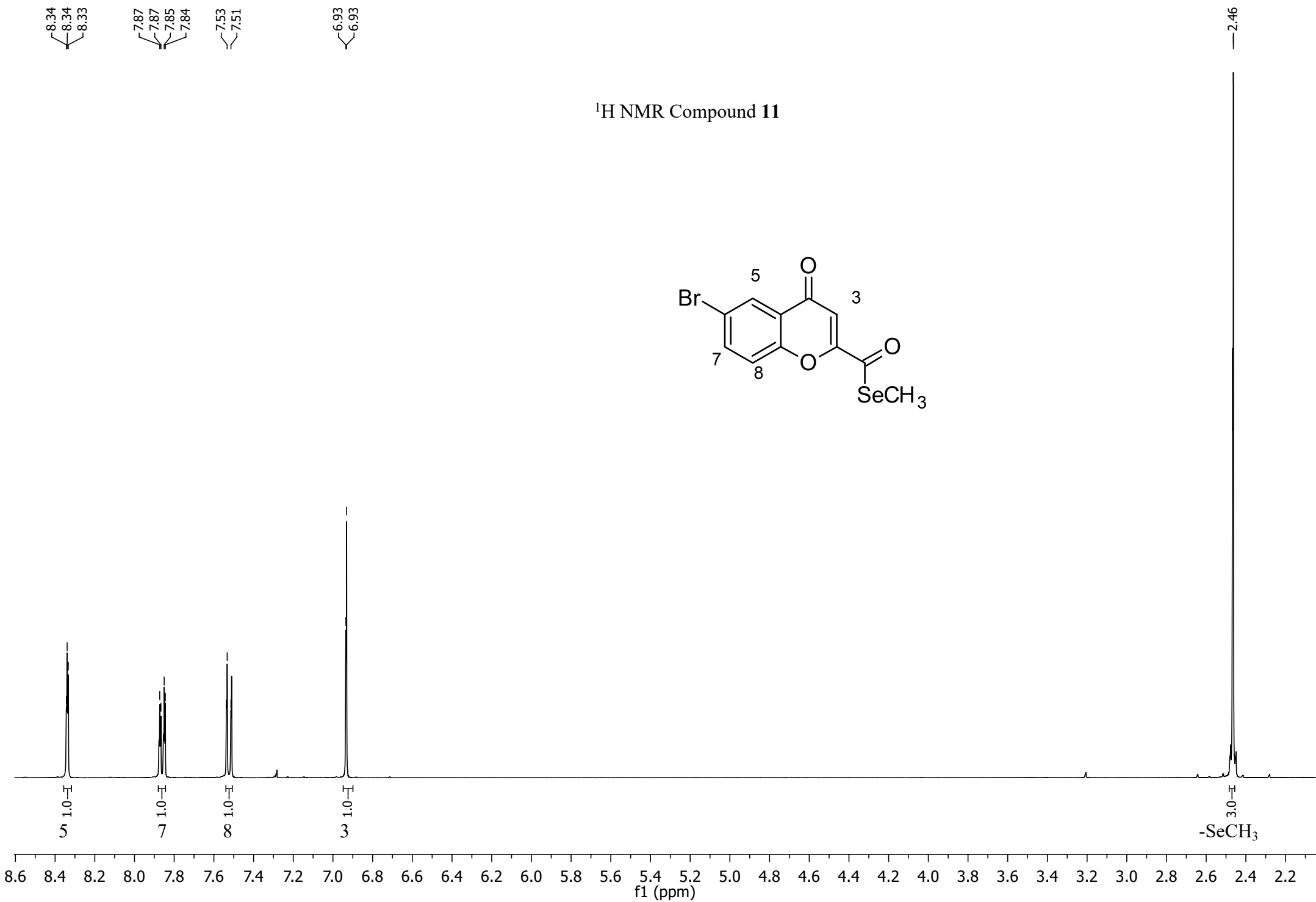
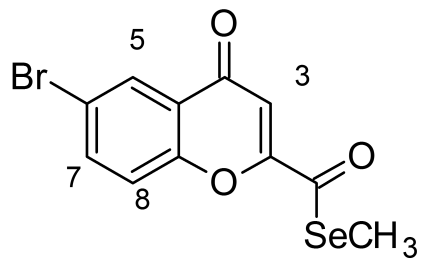
—117.85

¹³C NMR Compound 10

—7.28



¹H NMR Compound 11



—190.55

—177.15

—157.09
—154.58

—138.23

—129.04
—126.25

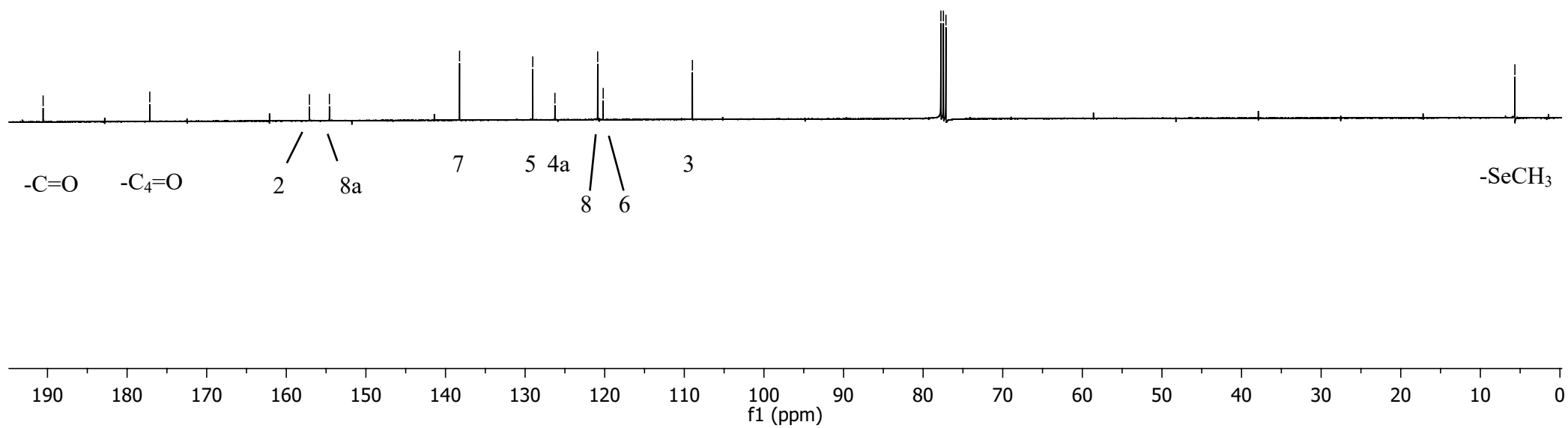
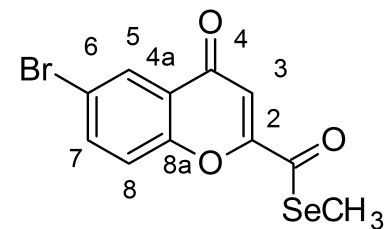
—120.88
—120.19

—108.98

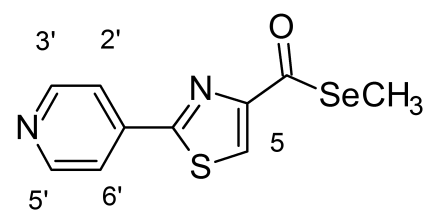
—77.77
—77.45
—77.13

¹³C NMR Compound 11

—5.66



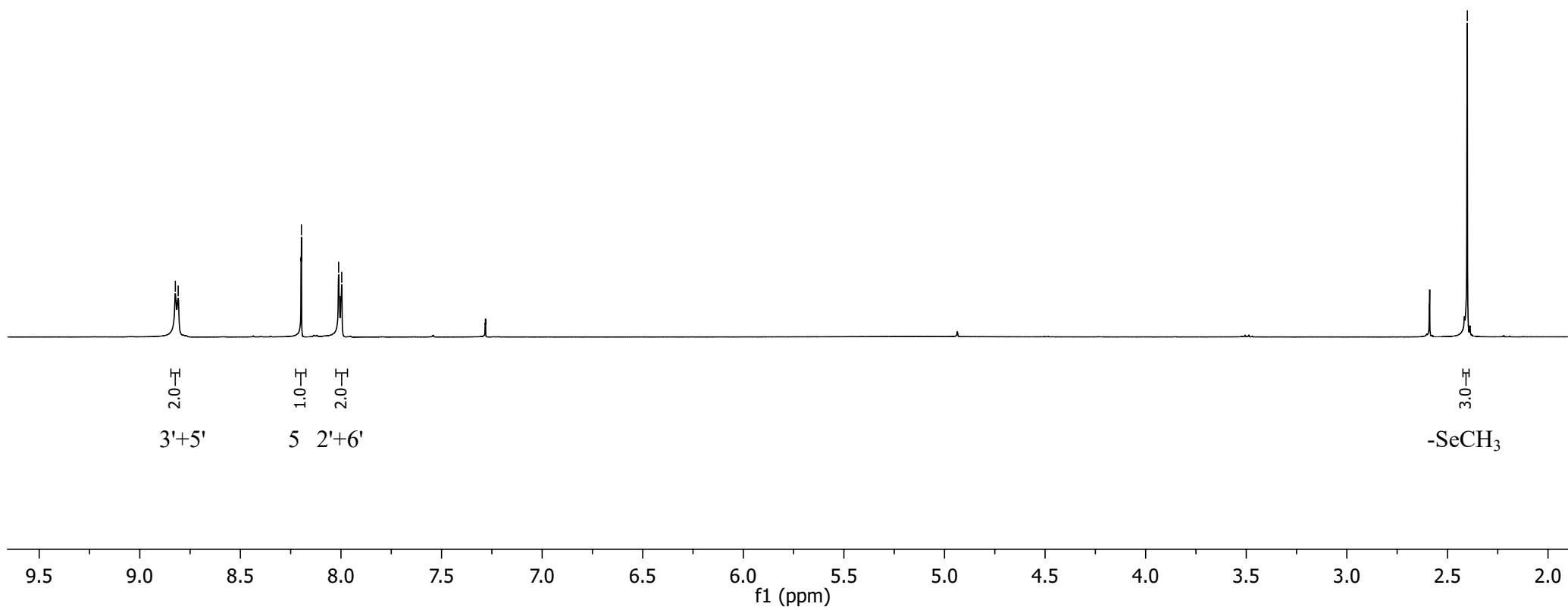
¹H NMR Compound 12



8.82
8.81

8.20
8.01
8.00

2.40



—189.66

—164.89

—156.45

—149.61

—141.11

—122.68

—121.39

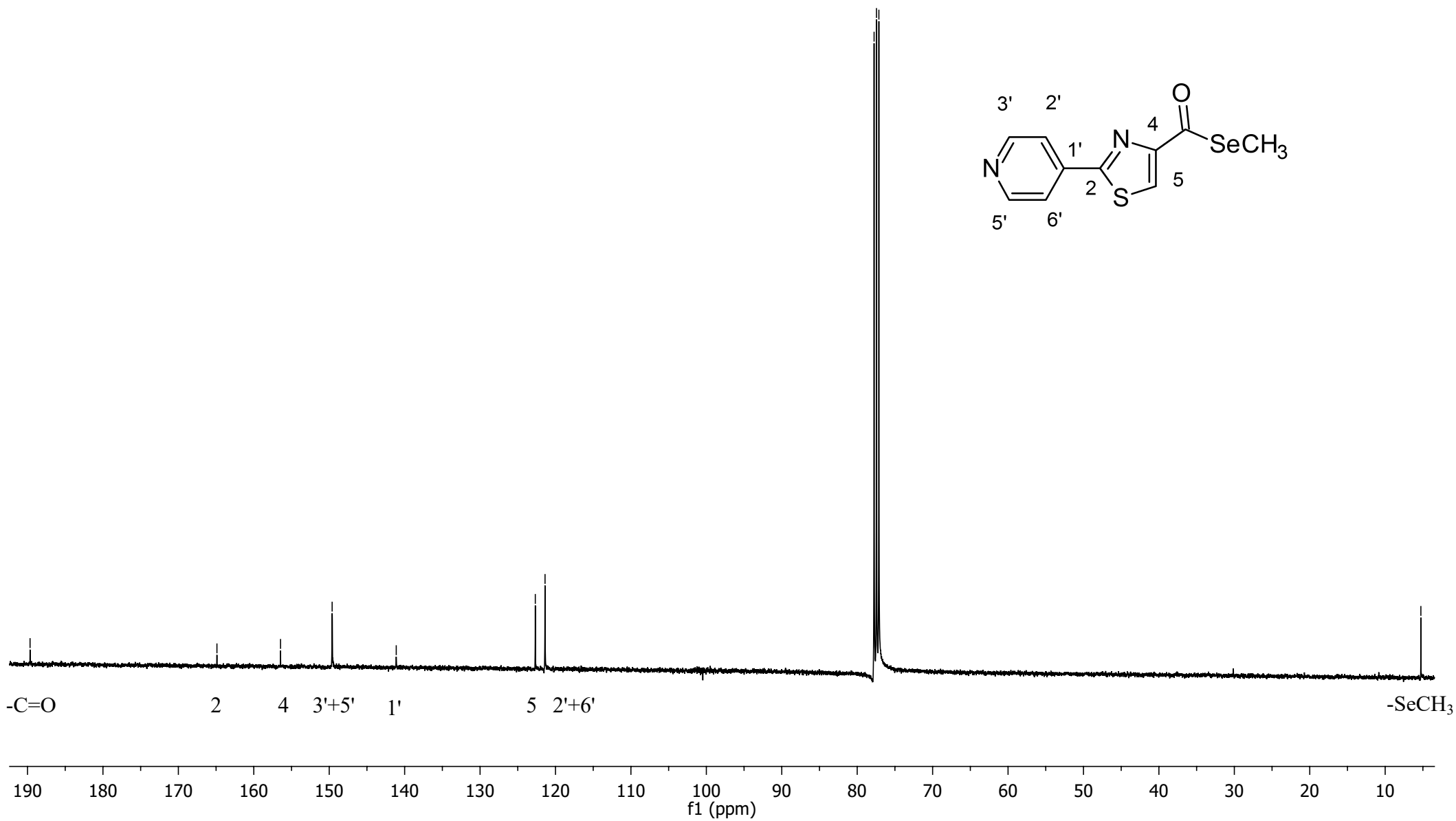
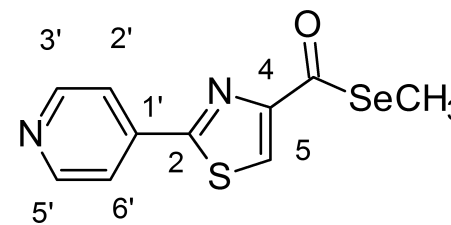
77.76

77.44

77.13

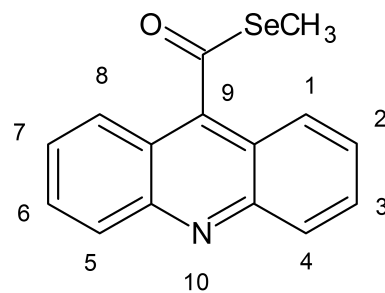
¹³C NMR Compound **12**

—5.27

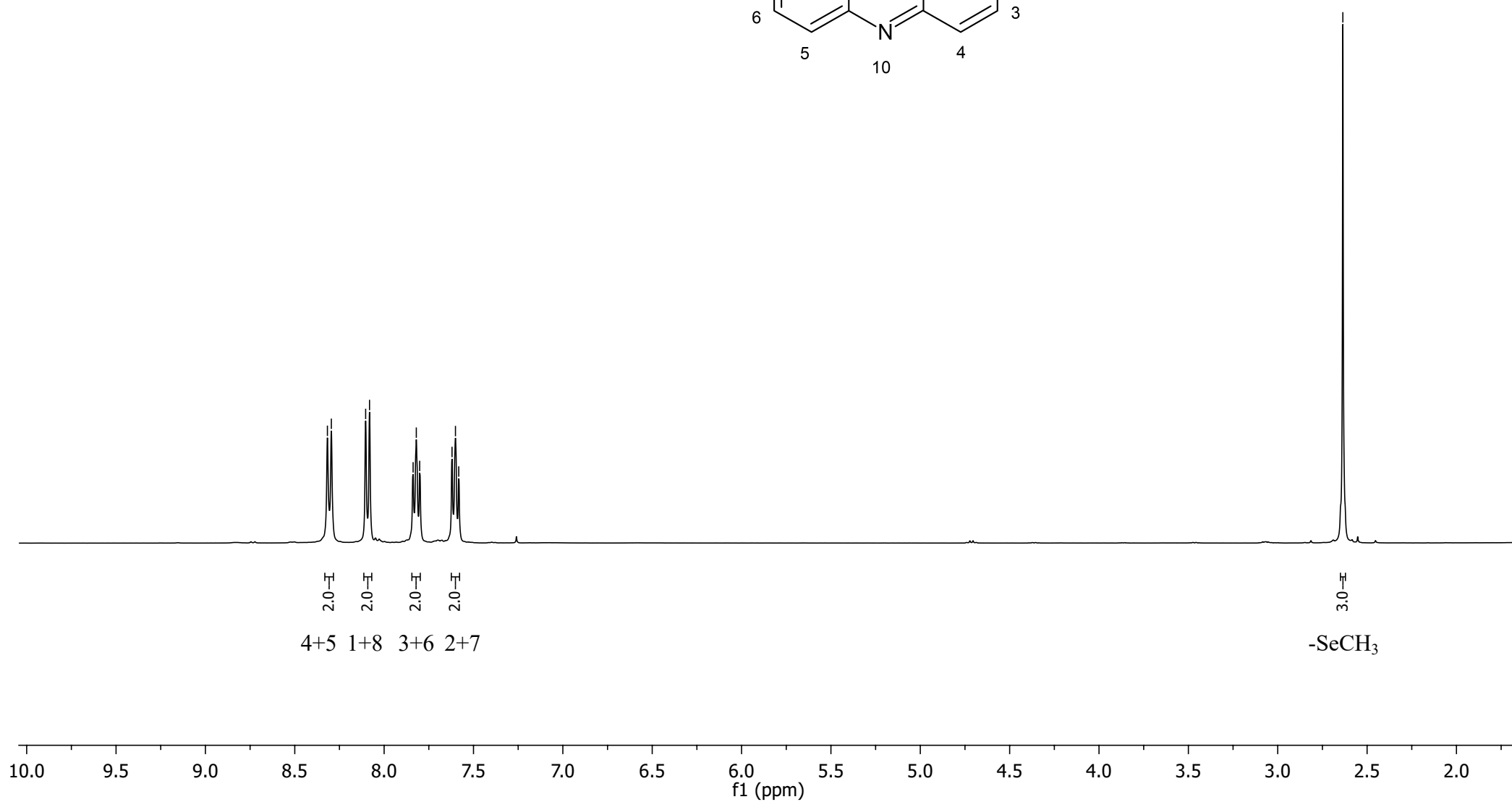


¹H NMR Compound 13

—2.64



8.32
8.30
8.10
8.08
7.84
7.82
7.80
7.62
7.60
7.58



—198.40

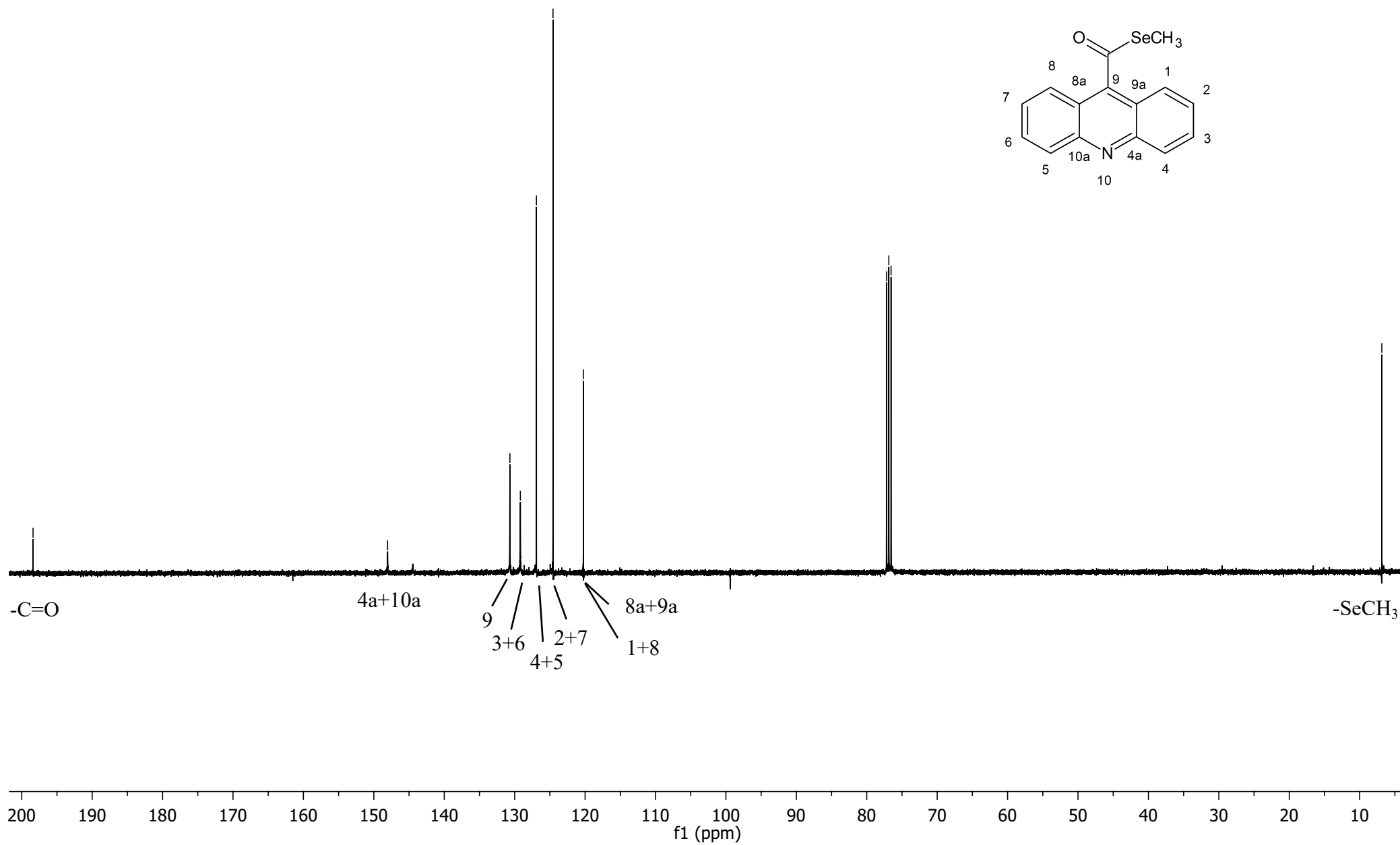
—148.05

130.68
129.19
126.91
124.56
120.24
120.23

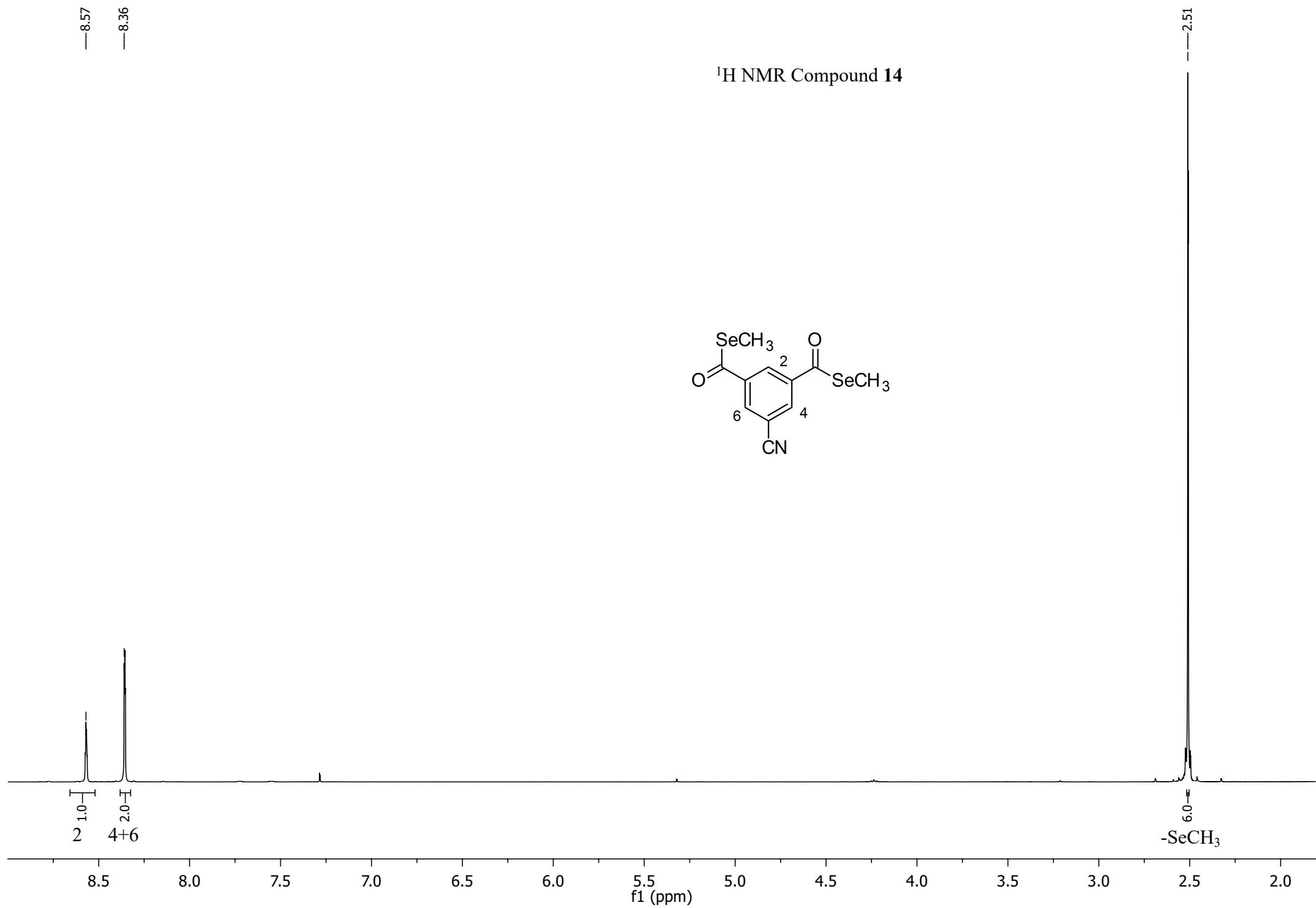
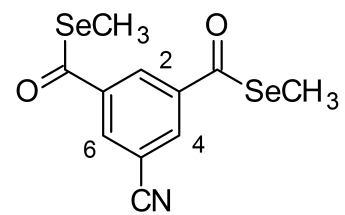
77.18
76.87
76.55

¹³C NMR Compound 13

—6.86



¹H NMR Compound 14



—192.85

—141.02

—134.47

—129.11

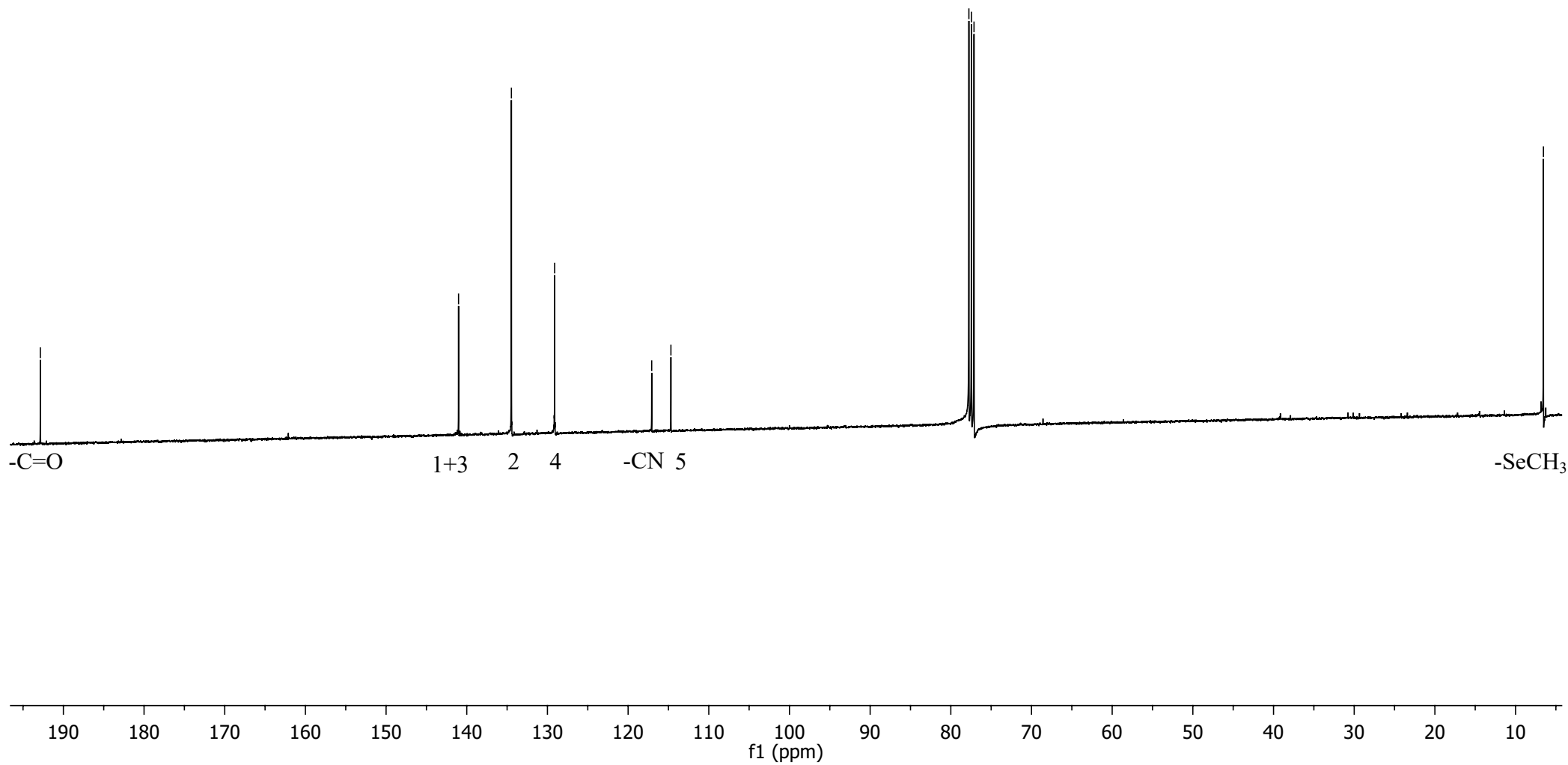
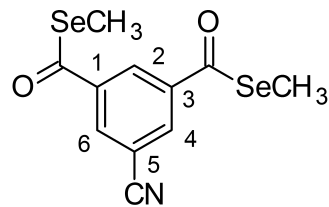
—117.08

—114.69

{ 77.76
77.44
77.12 }

¹³C NMR Compound **14**

—6.55



—7.21

^1H NMR Compound **15**

—2.43

