

## Supplementary material

### **Novel methylselenoesters as antiproliferative agents**

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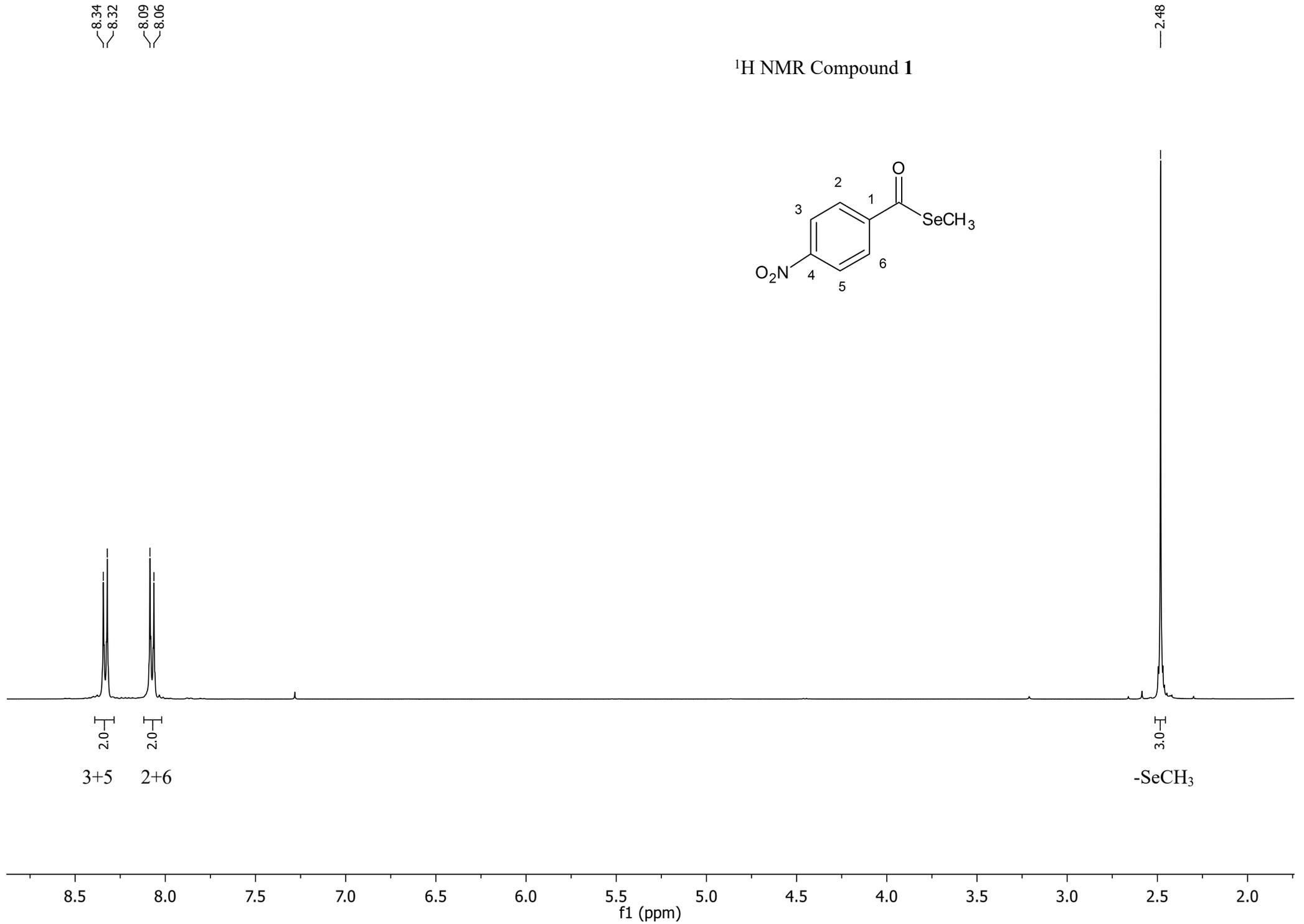
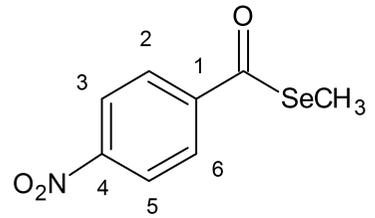
*3) Division of Biochemistry, Department of Medical Biochemistry and Biophysics (MBB), Karolinska Institutet, SE-171 77 Stockholm, Sweden*

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

**Contents:**

**Representative spectra (<sup>1</sup>H and <sup>13</sup>C NMR) of the methylselenoesters**

<sup>1</sup>H NMR Compound 1



—193.72

—150.45

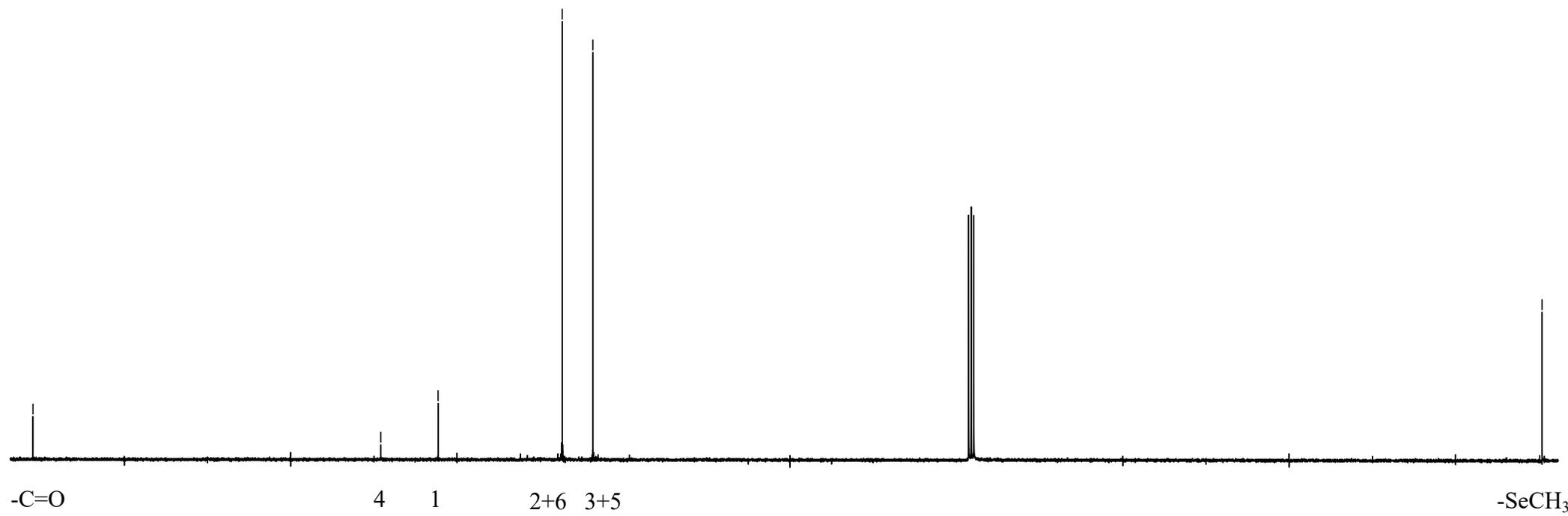
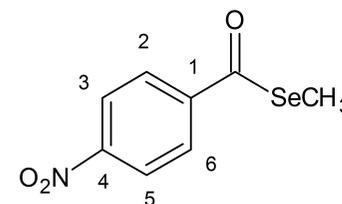
—143.33

—127.88

—124.07

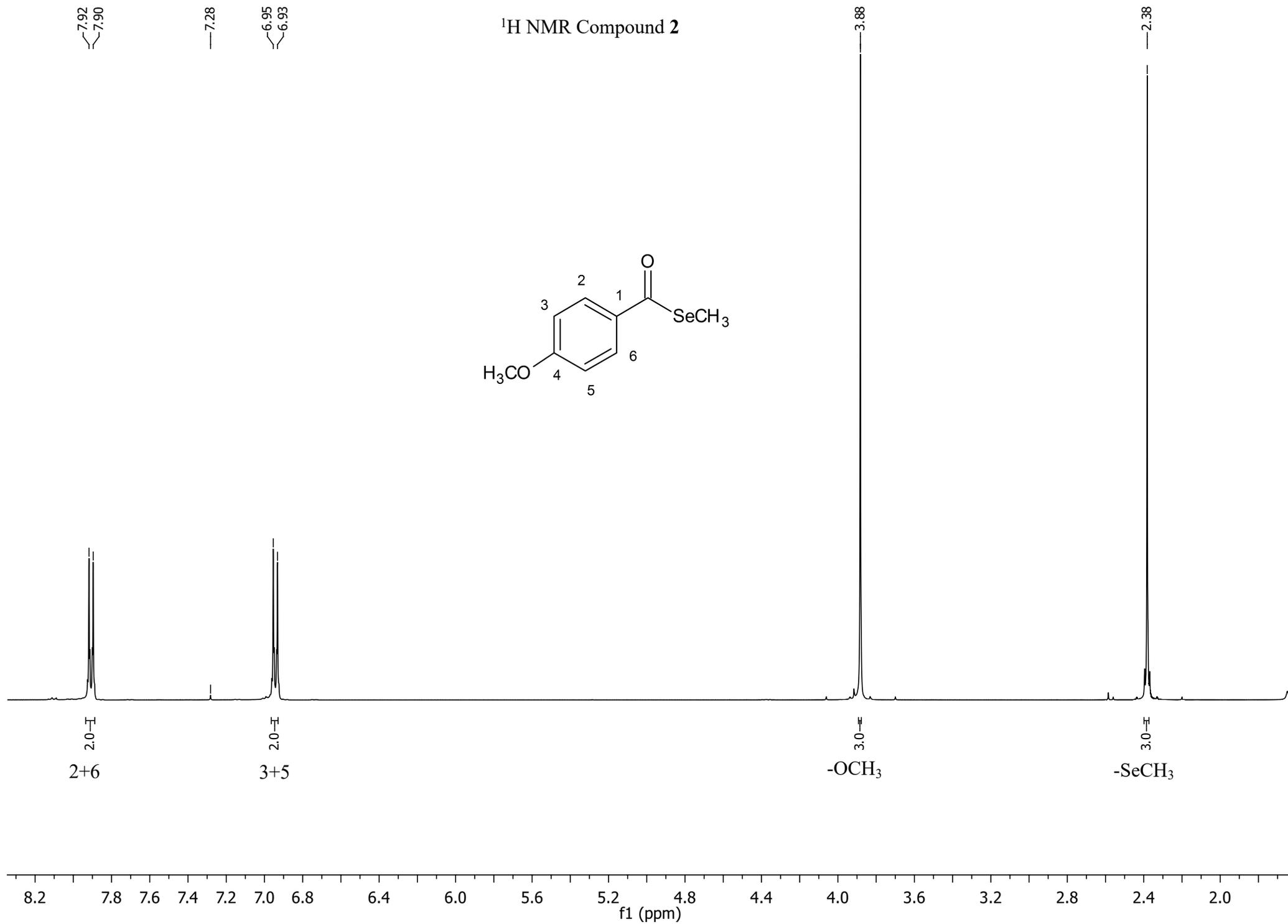
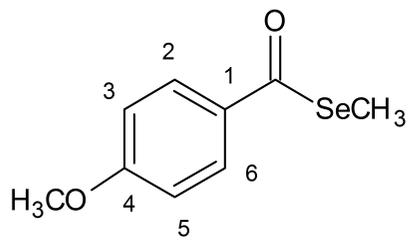
<sup>13</sup>C NMR Compound 1

—5.97

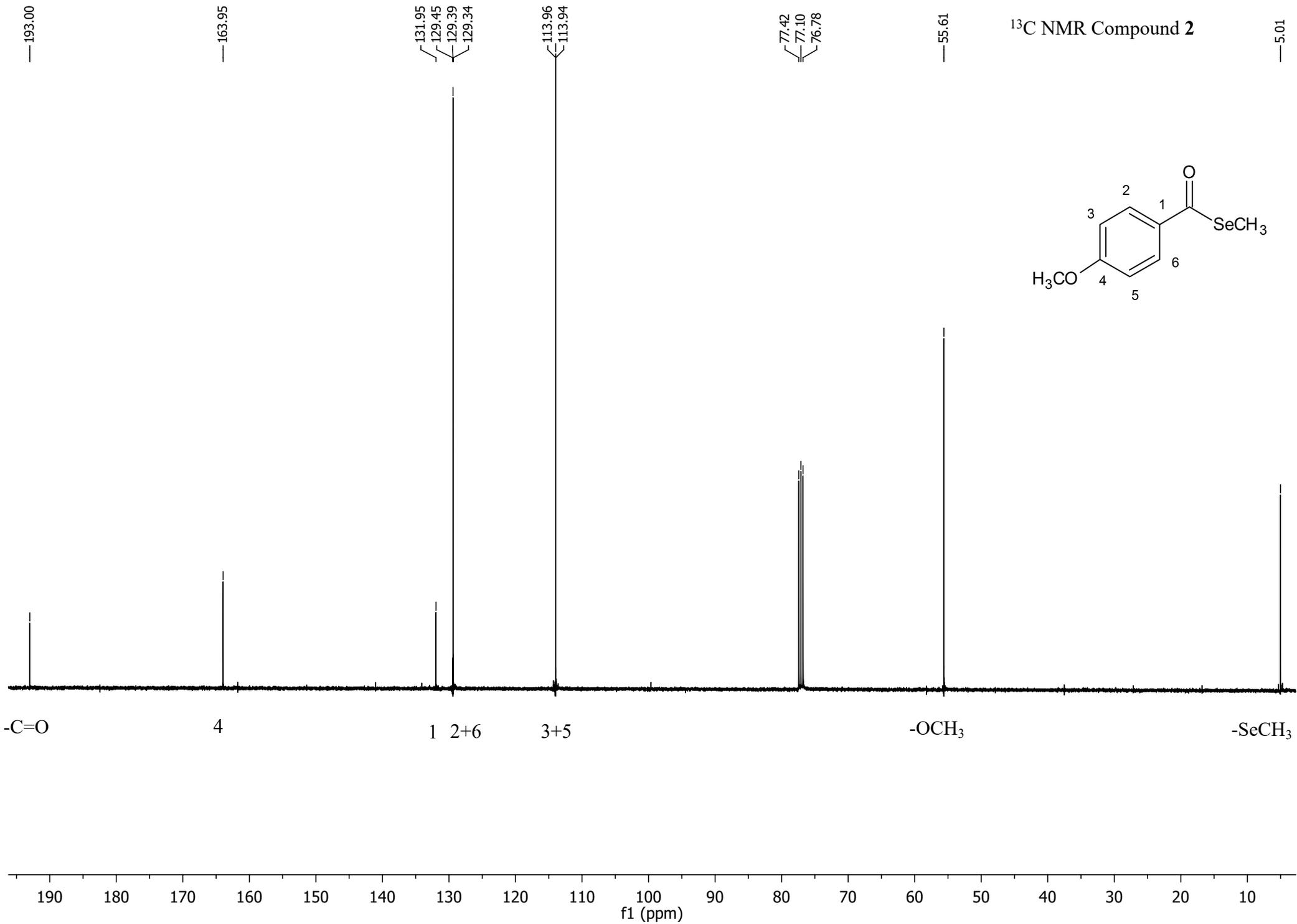


f1 (ppm)

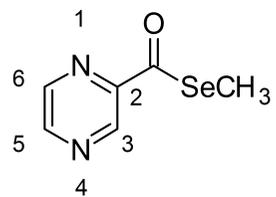
<sup>1</sup>H NMR Compound 2



<sup>13</sup>C NMR Compound 2

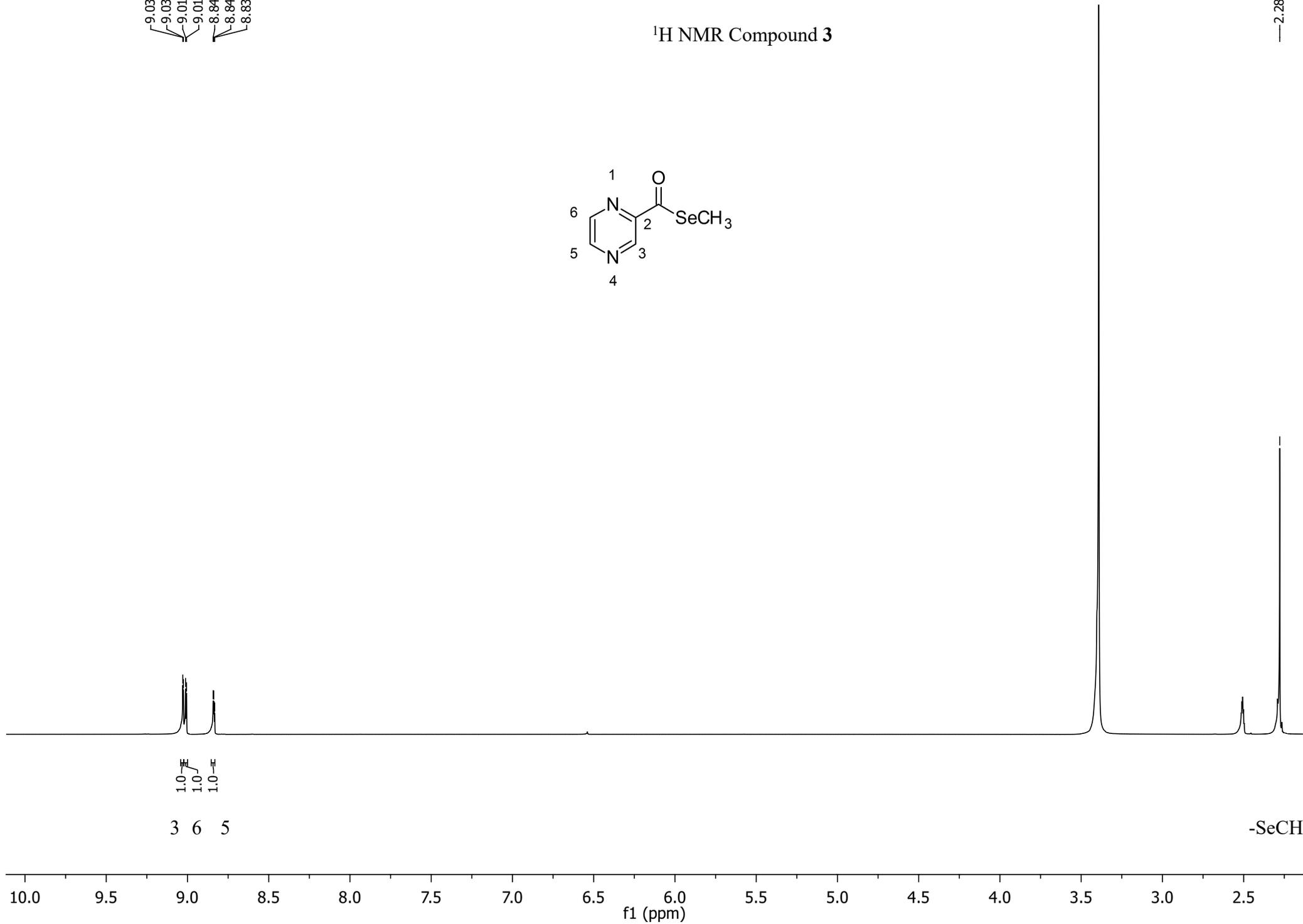


<sup>1</sup>H NMR Compound 3



9.03  
9.03  
9.01  
9.01  
8.84  
8.84  
8.83

2.28



—198.03

—150.94

—147.15

—145.75

—140.40

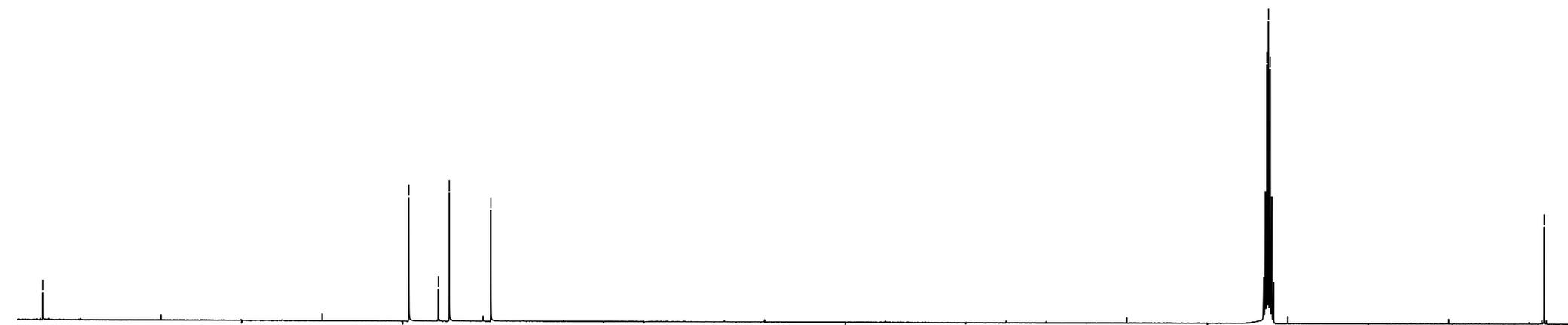
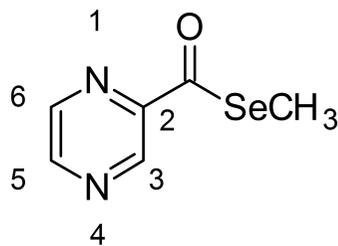
### $^{13}\text{C}$ NMR Compound 3

—40.56

—40.35

—40.15

—4.88



-C=O

3

5

6

2

-SeCH<sub>3</sub>

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

f1 (ppm)



—185.48

—144.32

—133.33

—131.82

—128.29

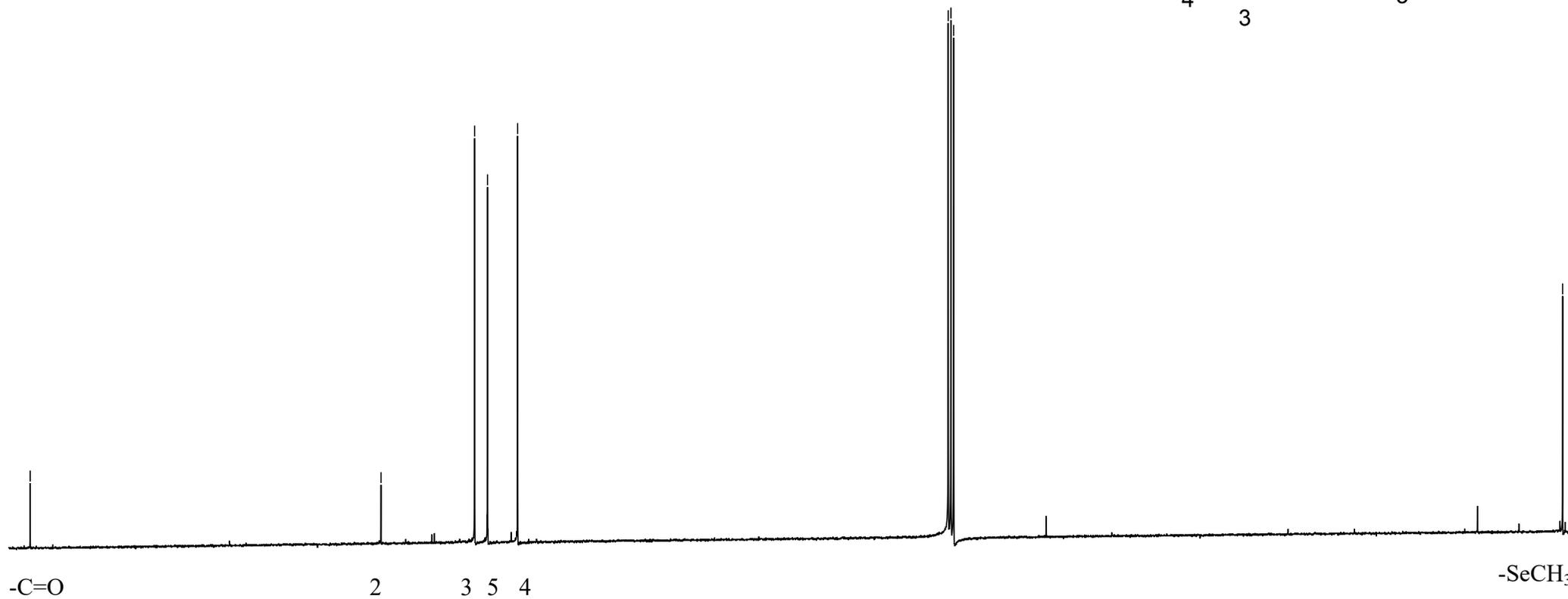
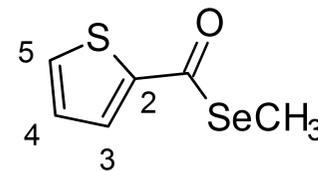
—77.78

—77.46

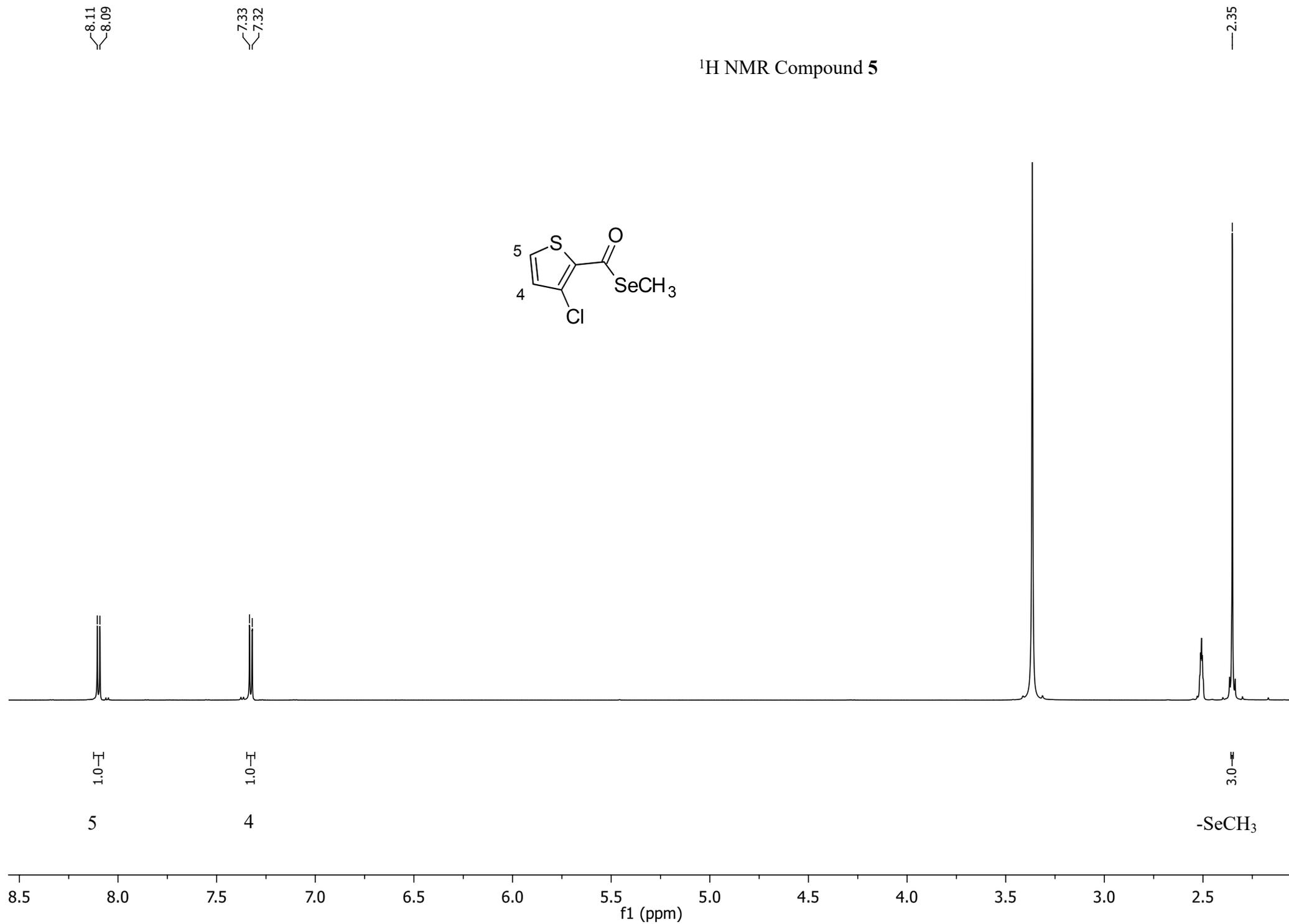
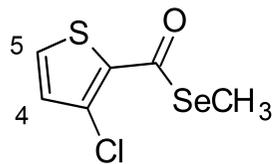
—77.14

<sup>13</sup>C NMR Compound 4

—5.70



<sup>1</sup>H NMR Compound 5



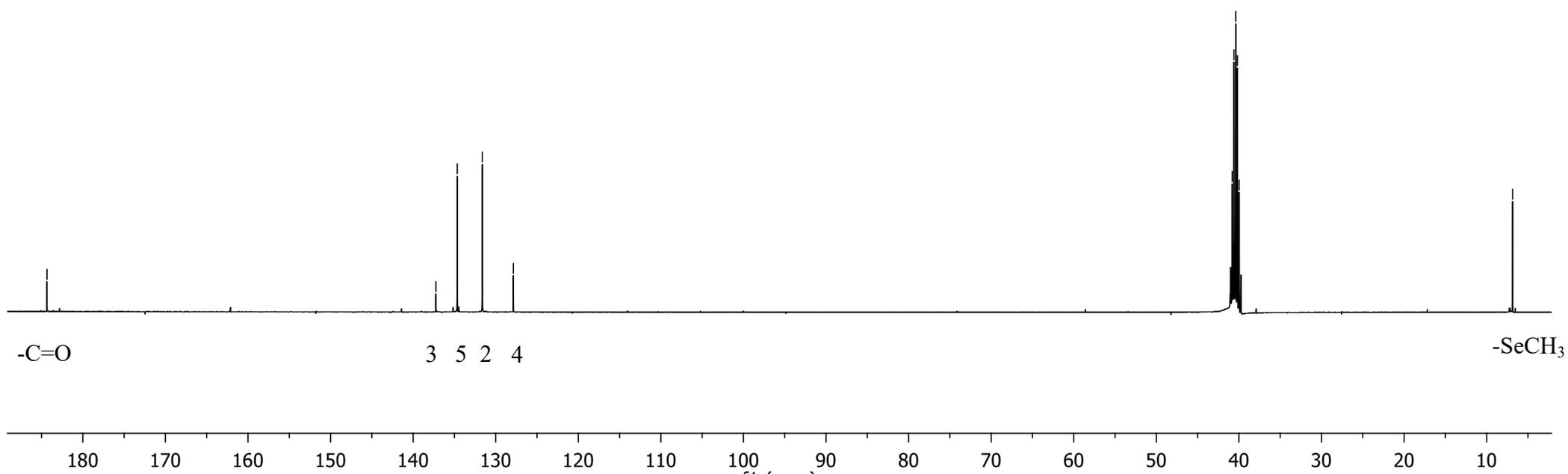
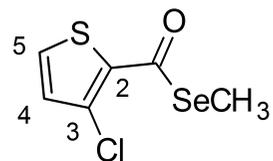
—184.34

137.24  
134.66  
131.62  
127.86

<sup>13</sup>C NMR Compound 5

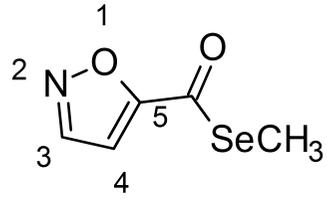
40.81  
40.60  
40.39  
40.18  
39.97

—6.85

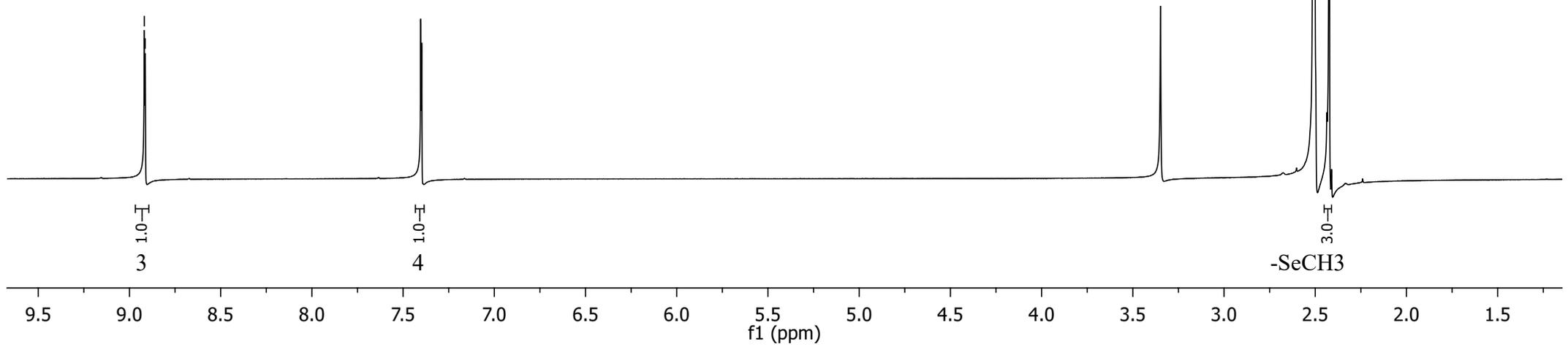


8.92  
8.91

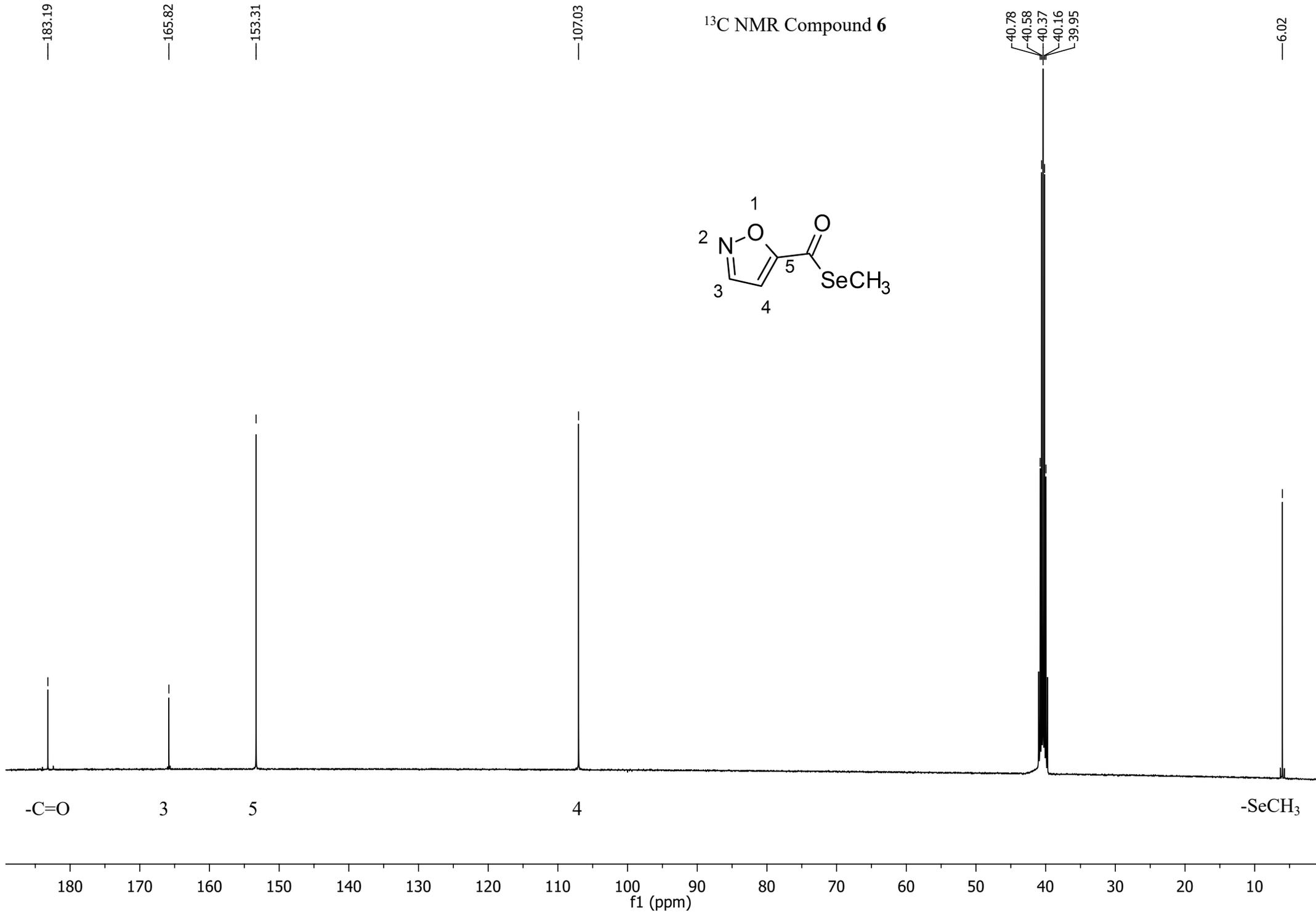
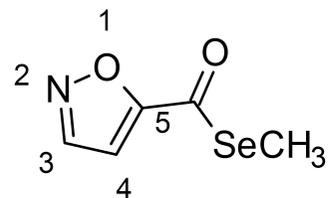
<sup>1</sup>H NMR Compound 6



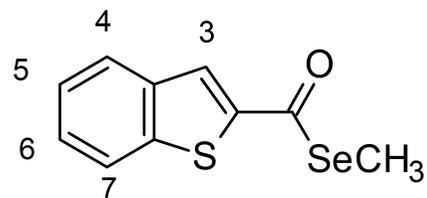
2.42



<sup>13</sup>C NMR Compound 6

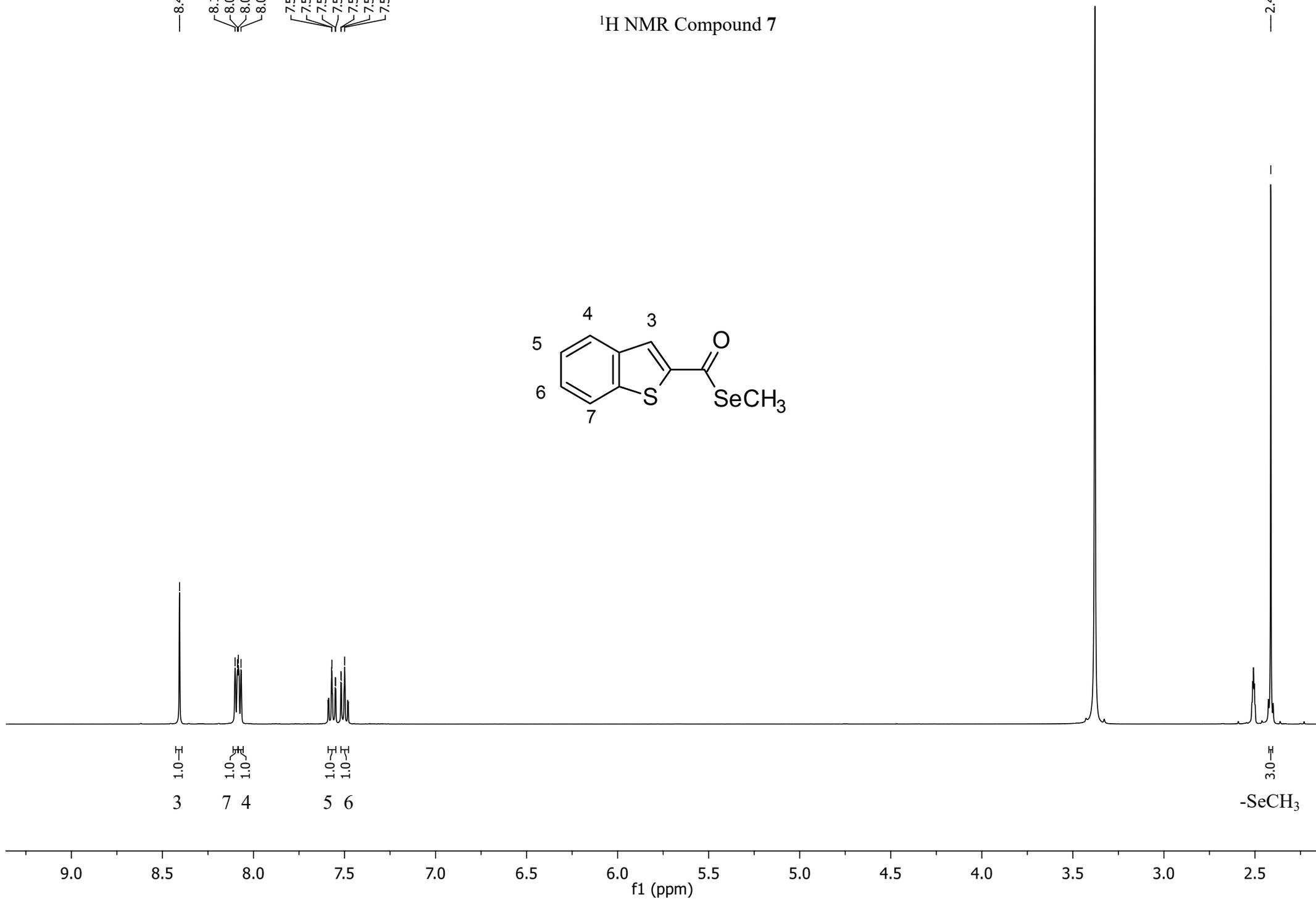


<sup>1</sup>H NMR Compound 7



8.41  
8.10  
8.09  
8.08  
8.07  
7.57  
7.57  
7.55  
7.55  
7.52  
7.52  
7.50

2.41



—187.57

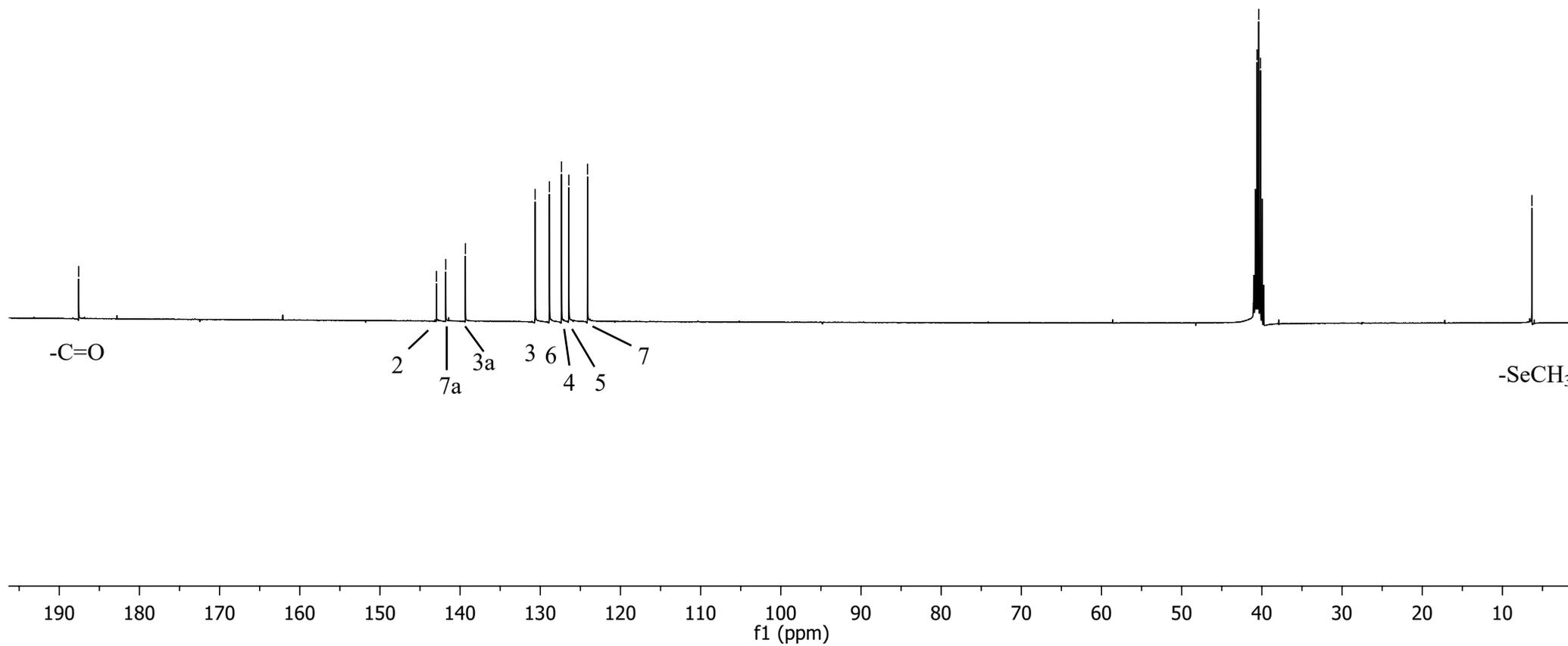
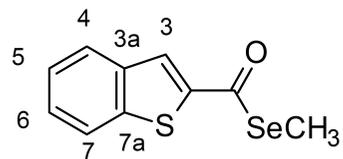
142.95  
141.79  
139.34

130.64  
128.86  
127.36  
126.44  
124.11

### <sup>13</sup>C NMR Compound 7

40.59  
40.39  
40.18

—6.32



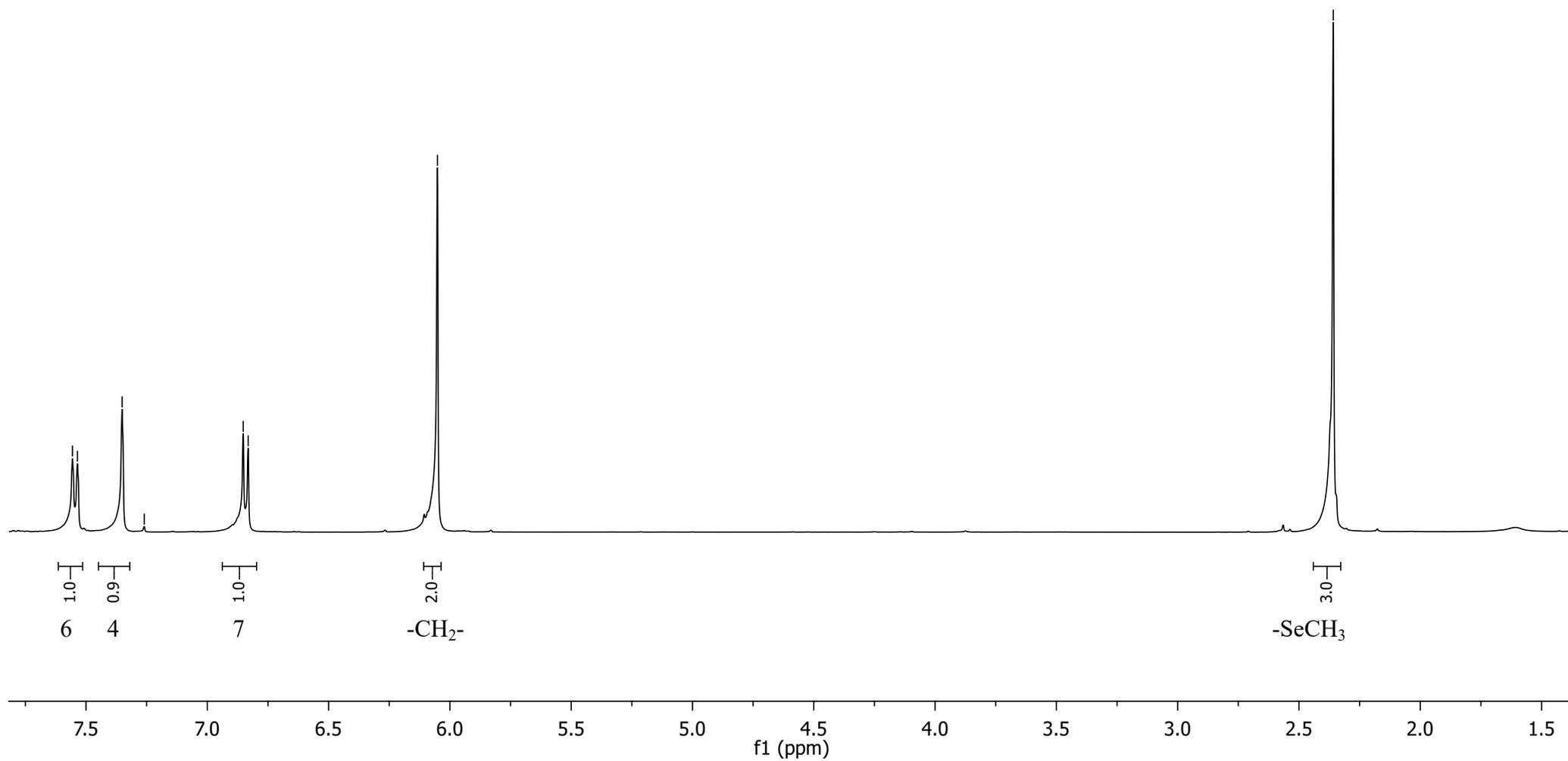
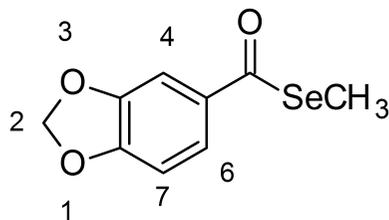
7.56  
7.54  
7.35  
7.26

6.85  
6.83

6.05

<sup>1</sup>H NMR Compound 8

2.36



—192.32

—151.79

—147.83

—133.21

—123.19

—107.77

—106.48

—101.68

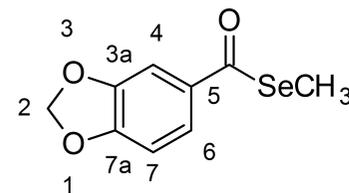
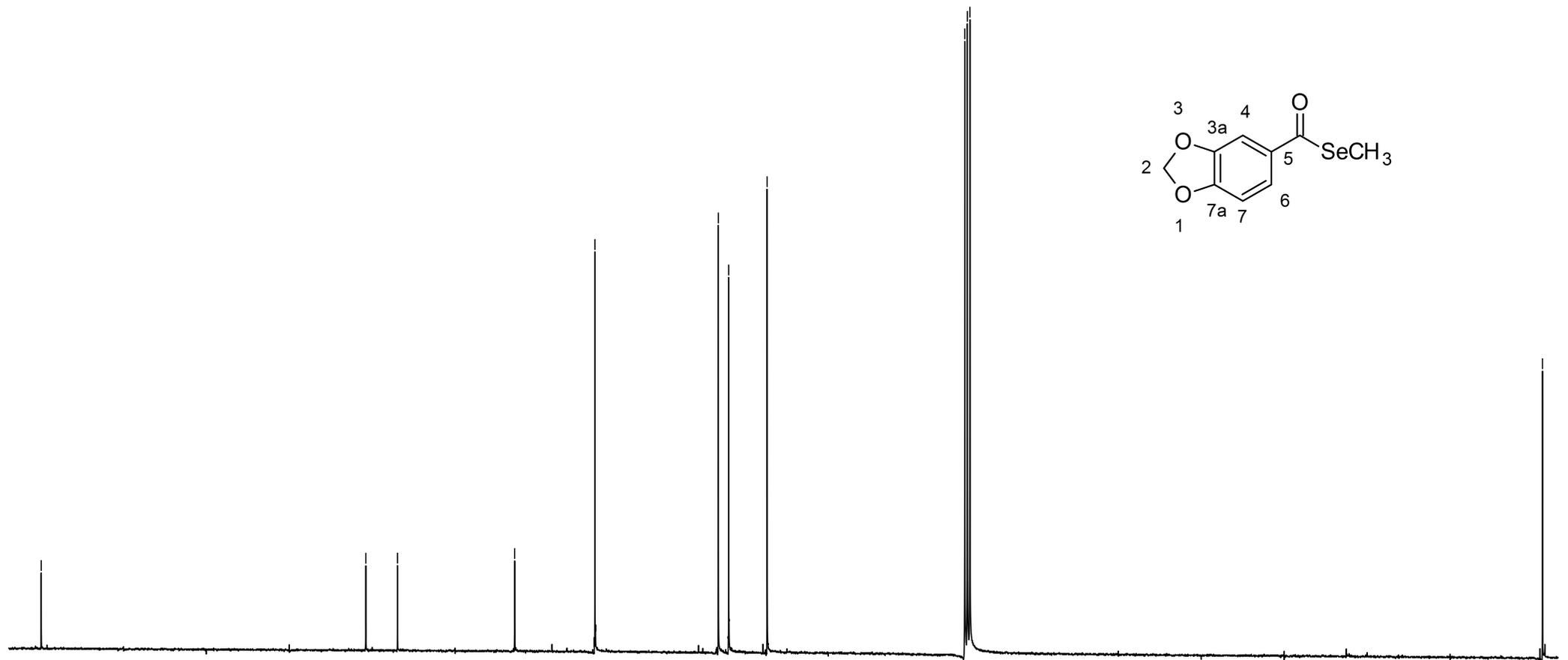
—77.00

—76.68

—76.36

<sup>13</sup>C NMR Compound **8**

—4.87



-C=O

7a 3a

5

6

4

7

2

-SeCH<sub>3</sub>

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

f1 (ppm)

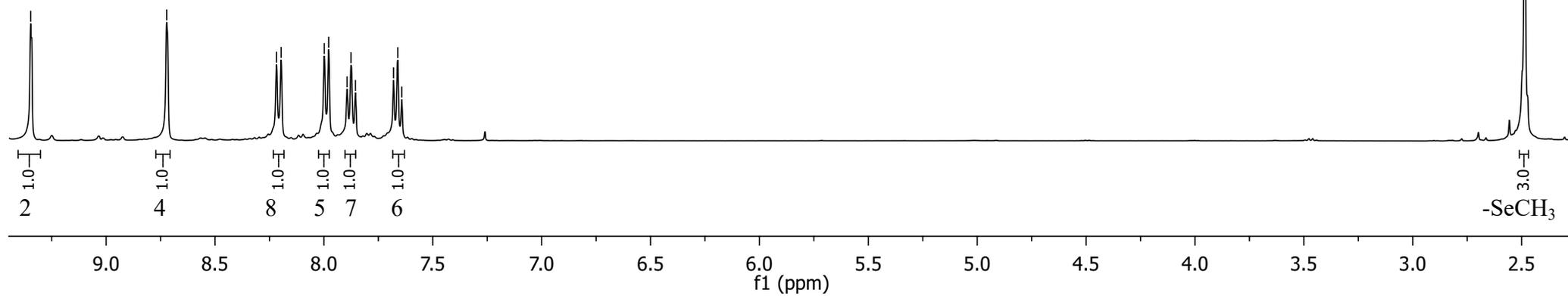
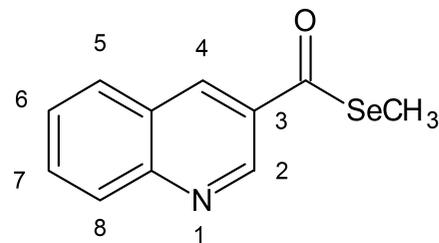
—9.35

—8.72

8.22  
8.20  
8.00  
7.98  
7.89  
7.88  
7.86  
7.68  
7.66  
7.64

—2.48

### <sup>1</sup>H NMR Compound 9



—193.47

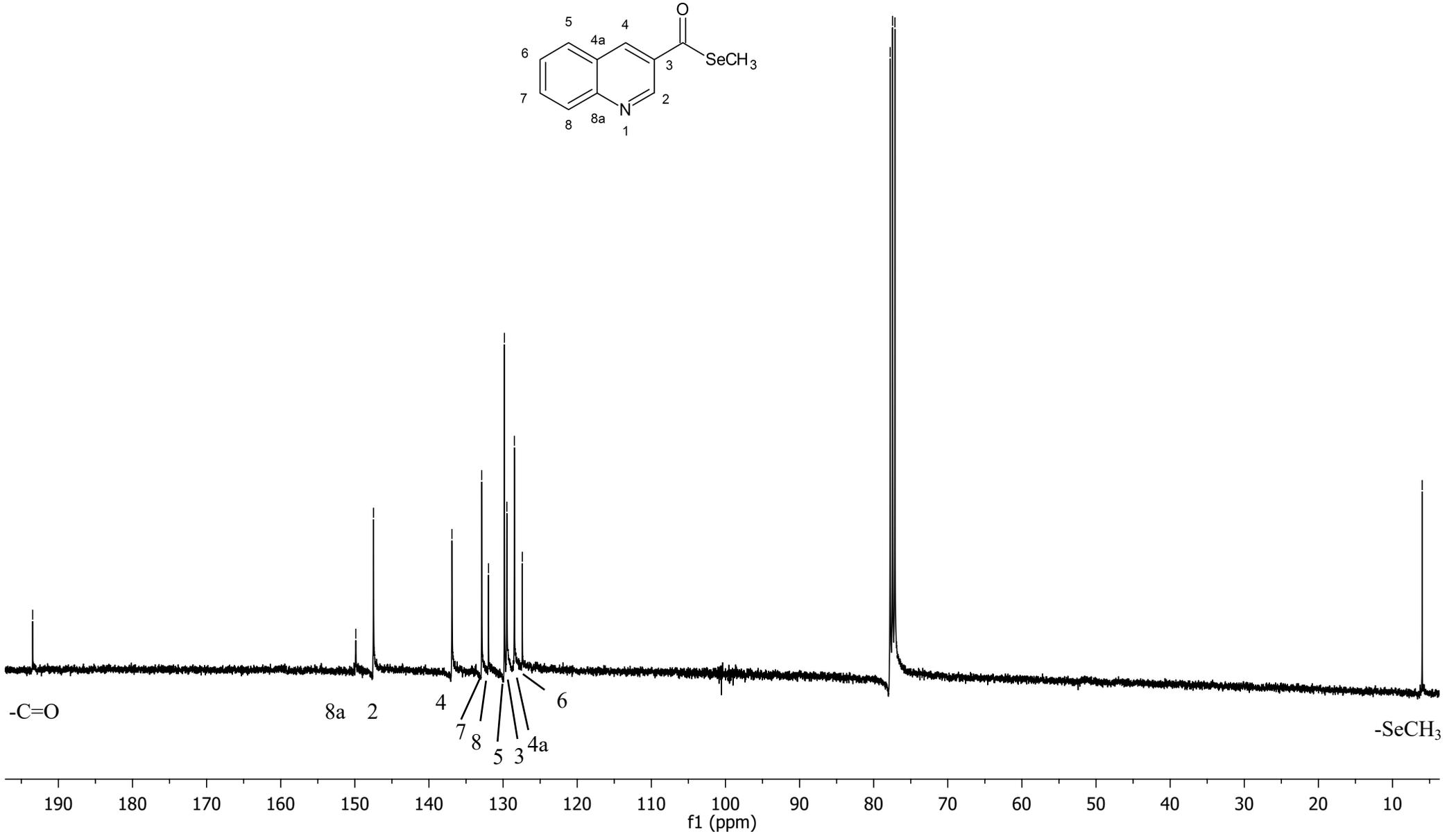
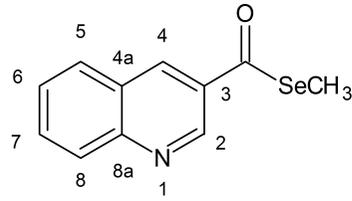
—149.87  
—147.48

136.90  
132.88  
131.96  
129.82  
129.49  
128.48  
127.40

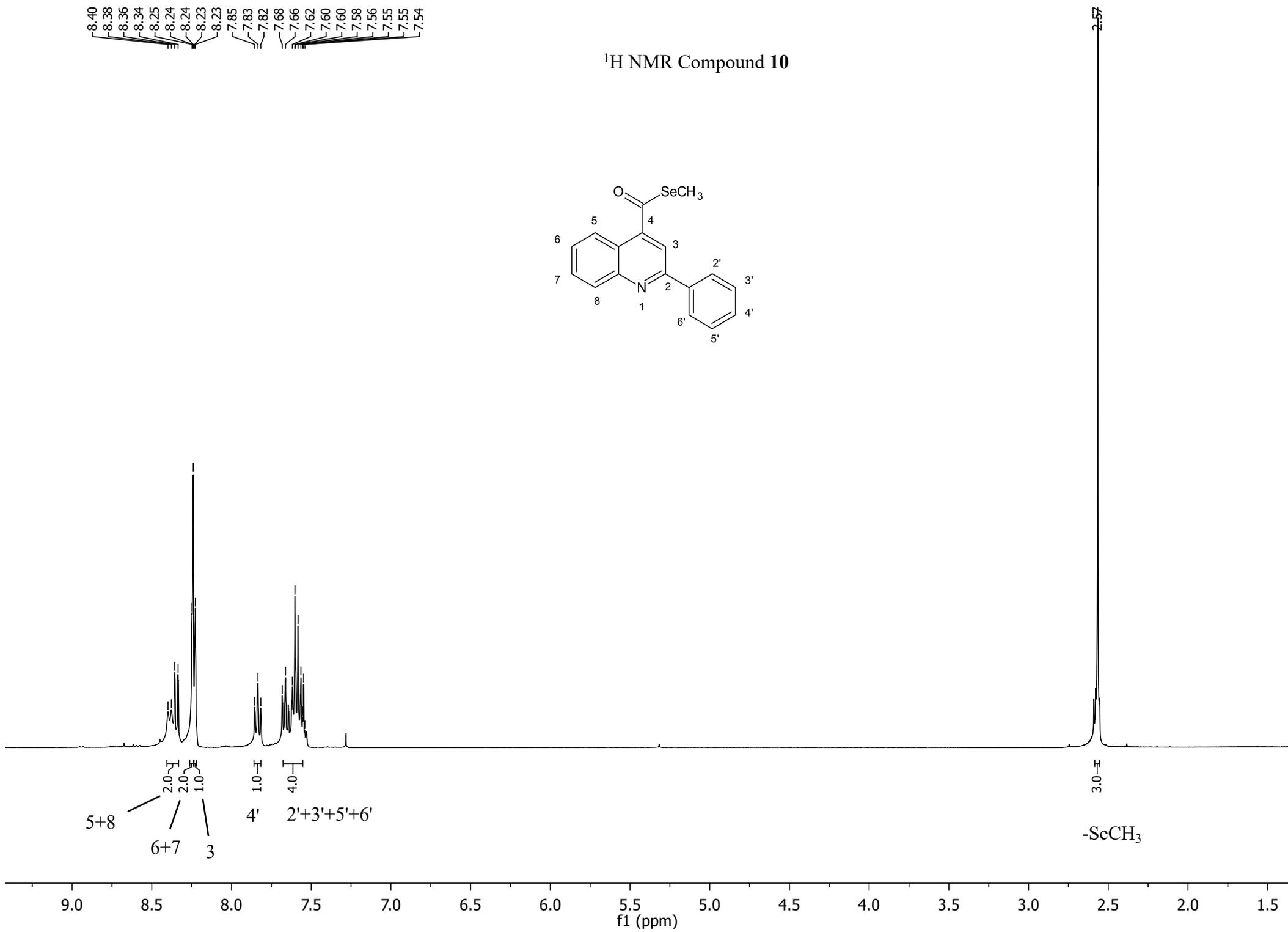
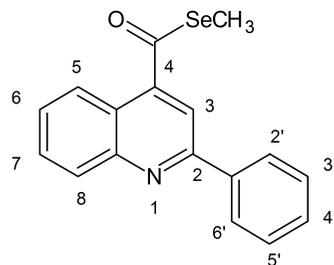
<sup>13</sup>C NMR Compound 9

77.77  
77.45  
77.13

—5.99



<sup>1</sup>H 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

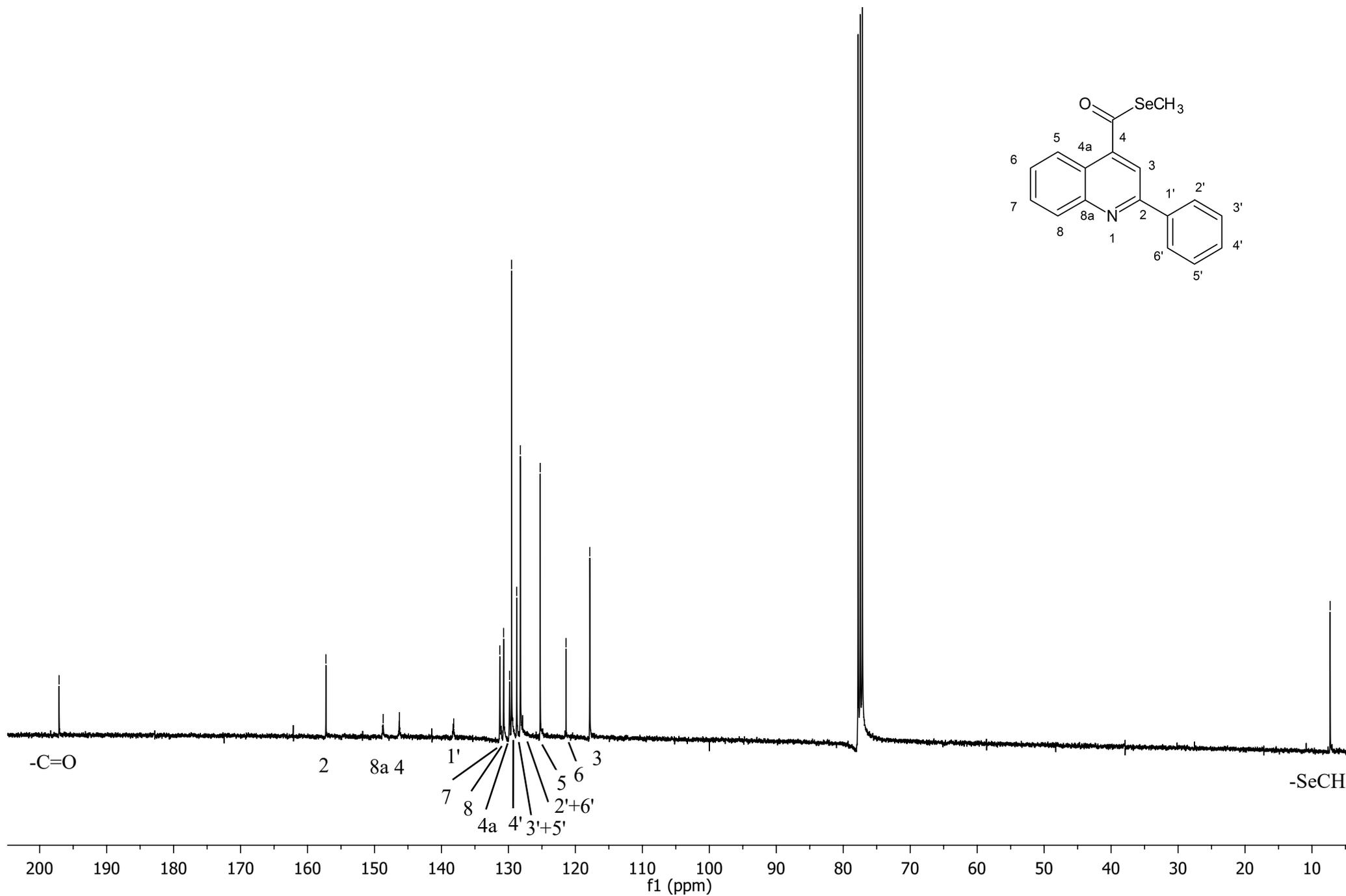
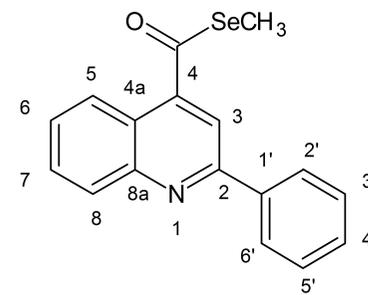
—125.25

—121.40

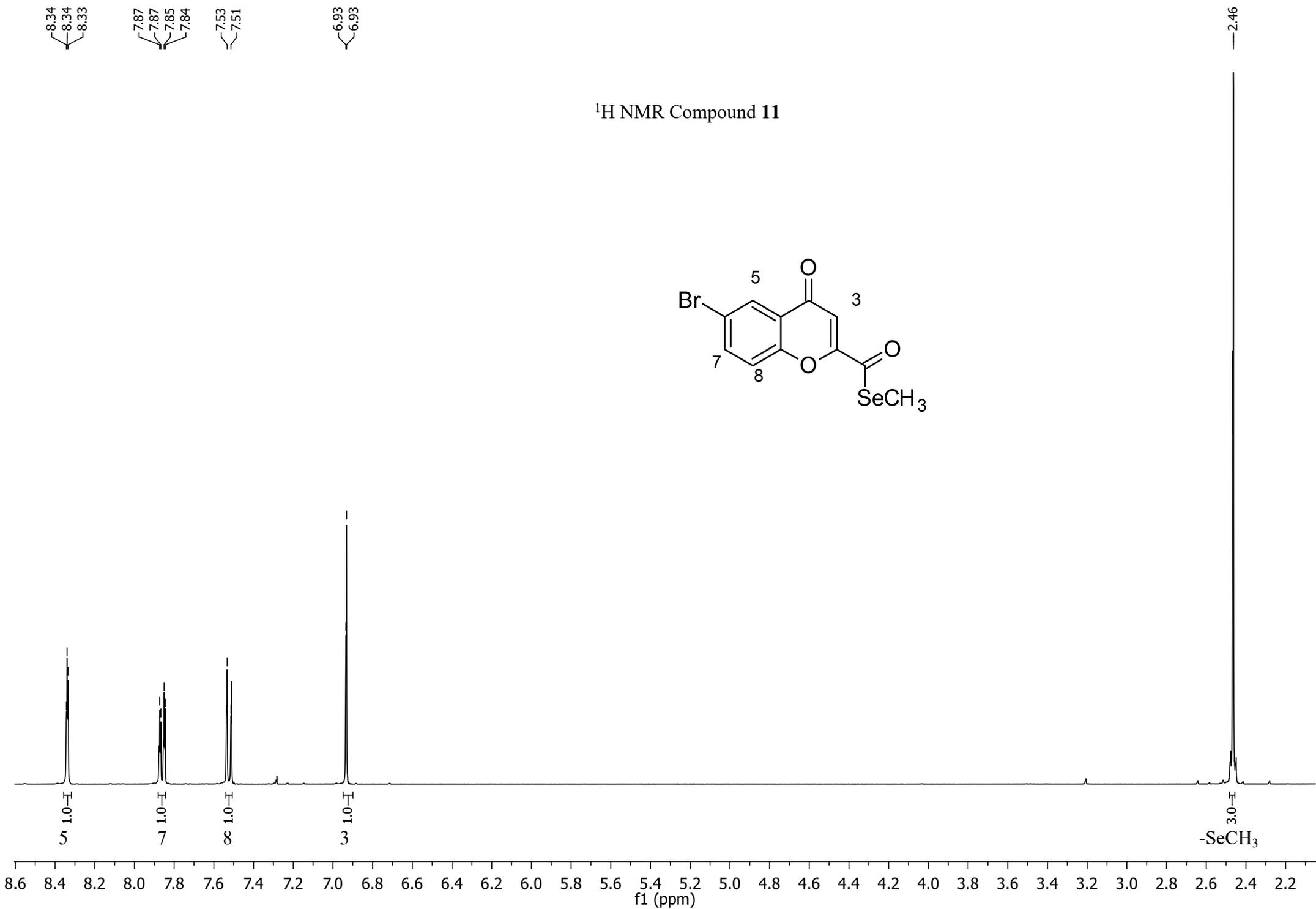
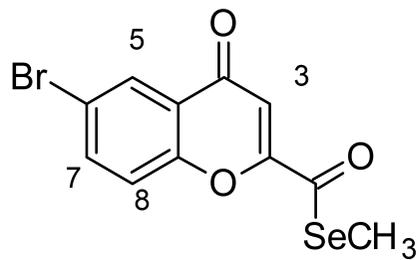
—117.85

<sup>13</sup>C NMR Compound 10

—7.28



<sup>1</sup>H NMR Compound 11



—190.55

—177.15

—157.09

—154.58

—138.23

—129.04

—126.25

—120.88

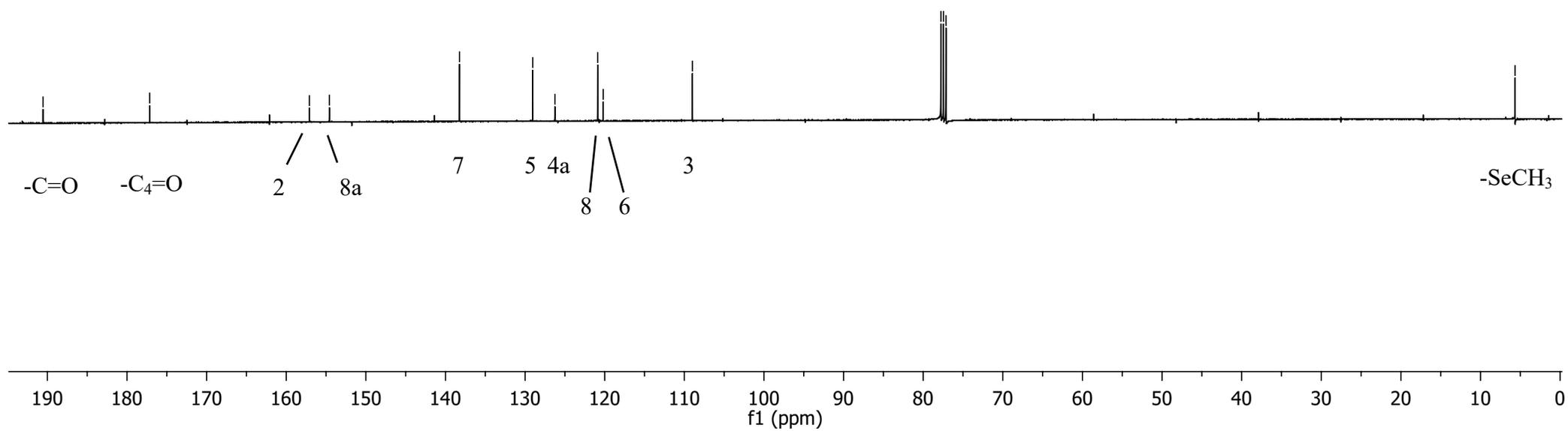
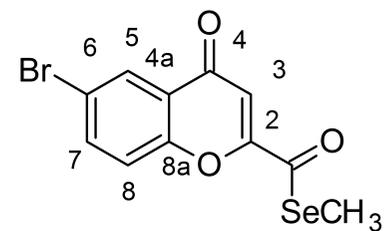
—120.19

—108.98

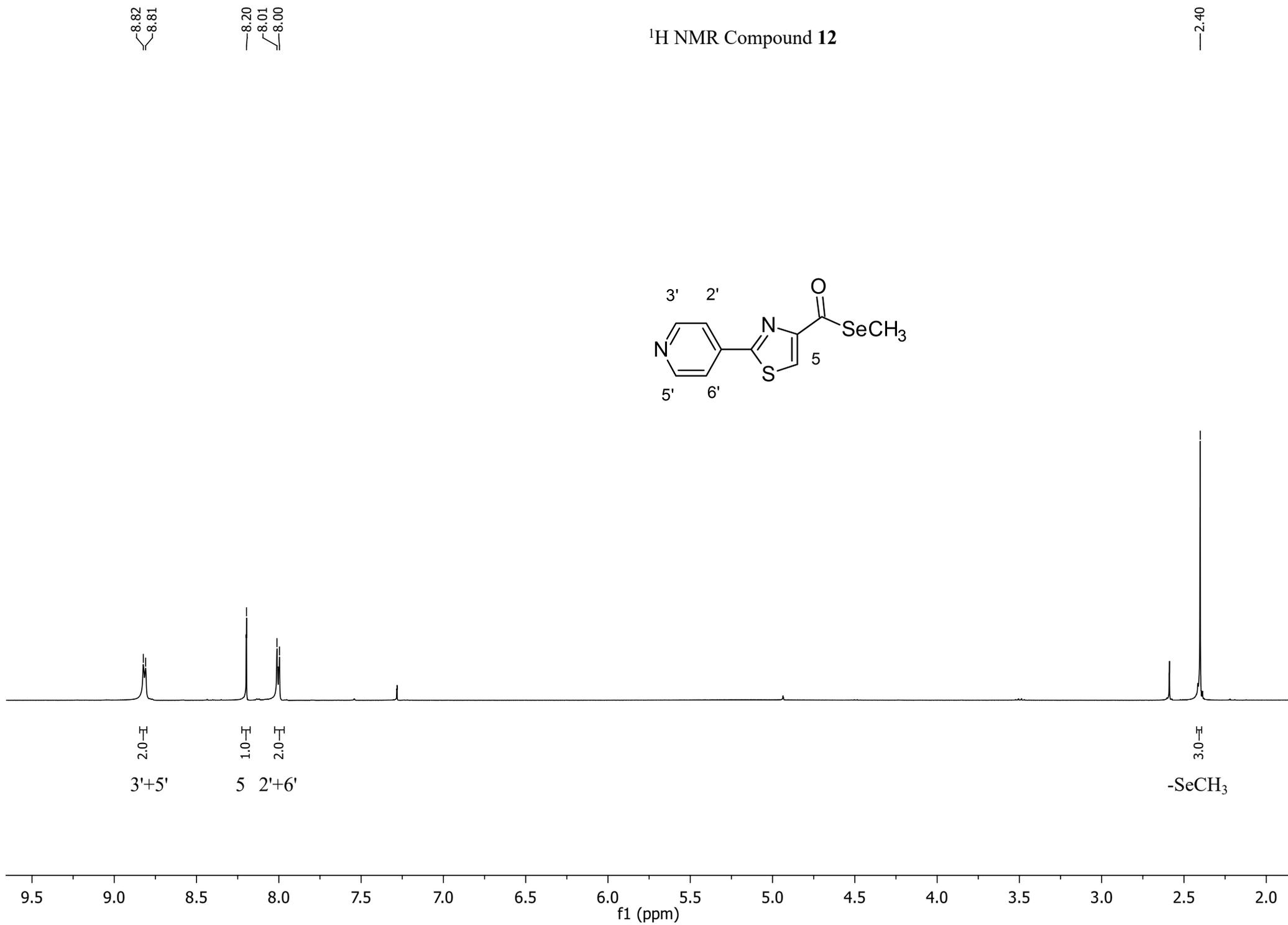
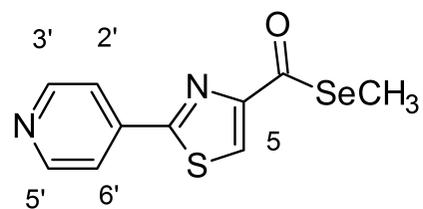
—77.77  
—77.45  
—77.13

<sup>13</sup>C NMR Compound **11**

—5.66



<sup>1</sup>H NMR Compound 12



—189.66

—164.89

—156.45

—149.61

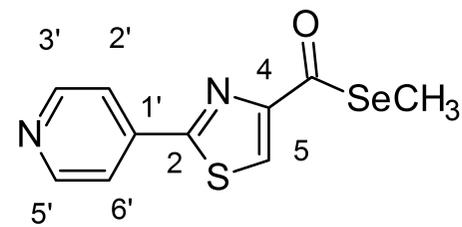
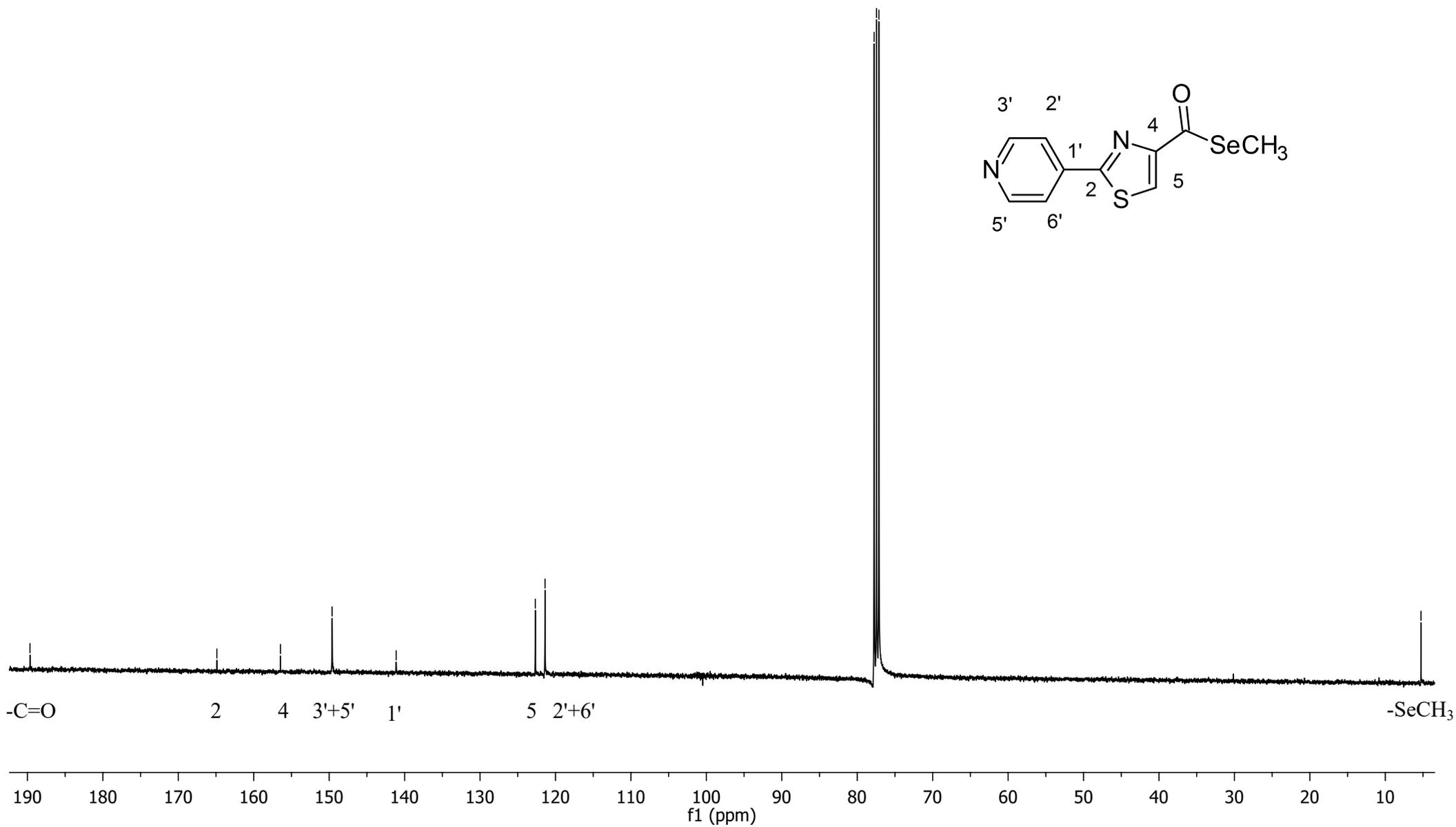
—141.11

—122.68  
—121.39

77.76  
77.44  
77.13

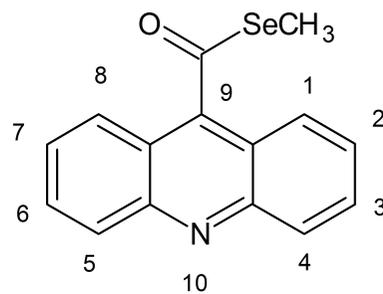
<sup>13</sup>C NMR Compound **12**

—5.27

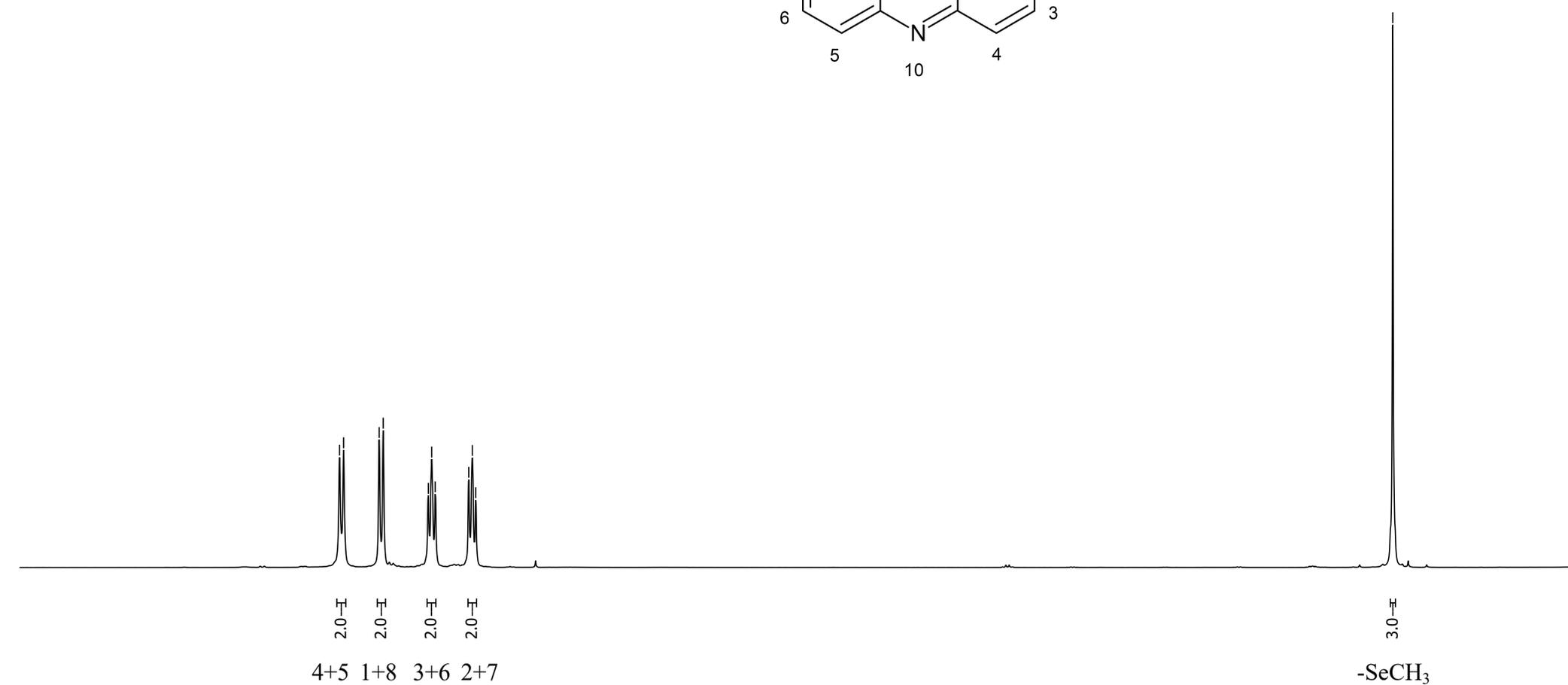


<sup>1</sup>H NMR Compound 13

—2.64



8.32  
8.30  
8.10  
8.08  
7.84  
7.82  
7.80  
7.62  
7.60  
7.58



10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0

f1 (ppm)

—198.40

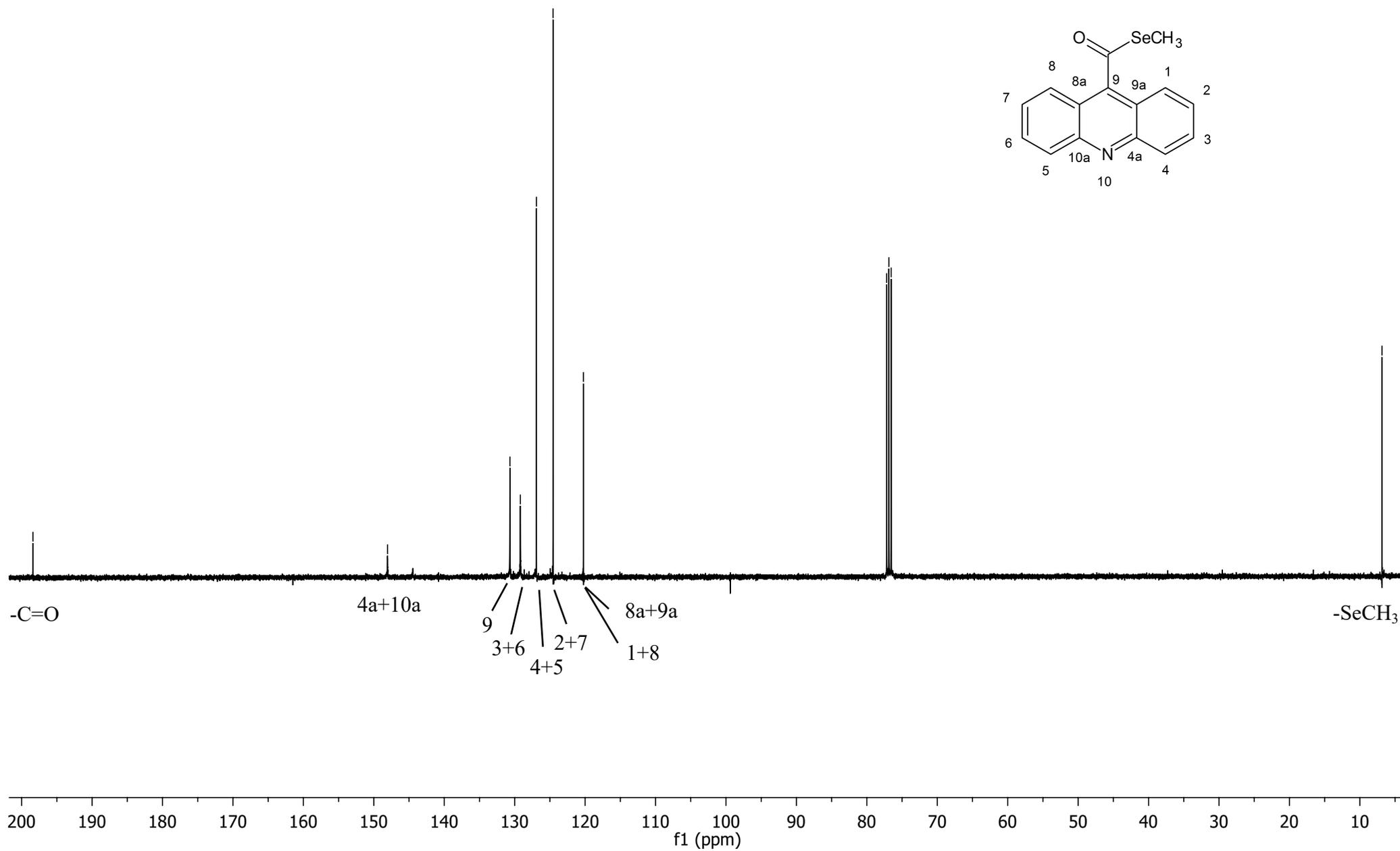
—148.05

130.68  
129.19  
126.91  
124.56  
120.24  
120.23

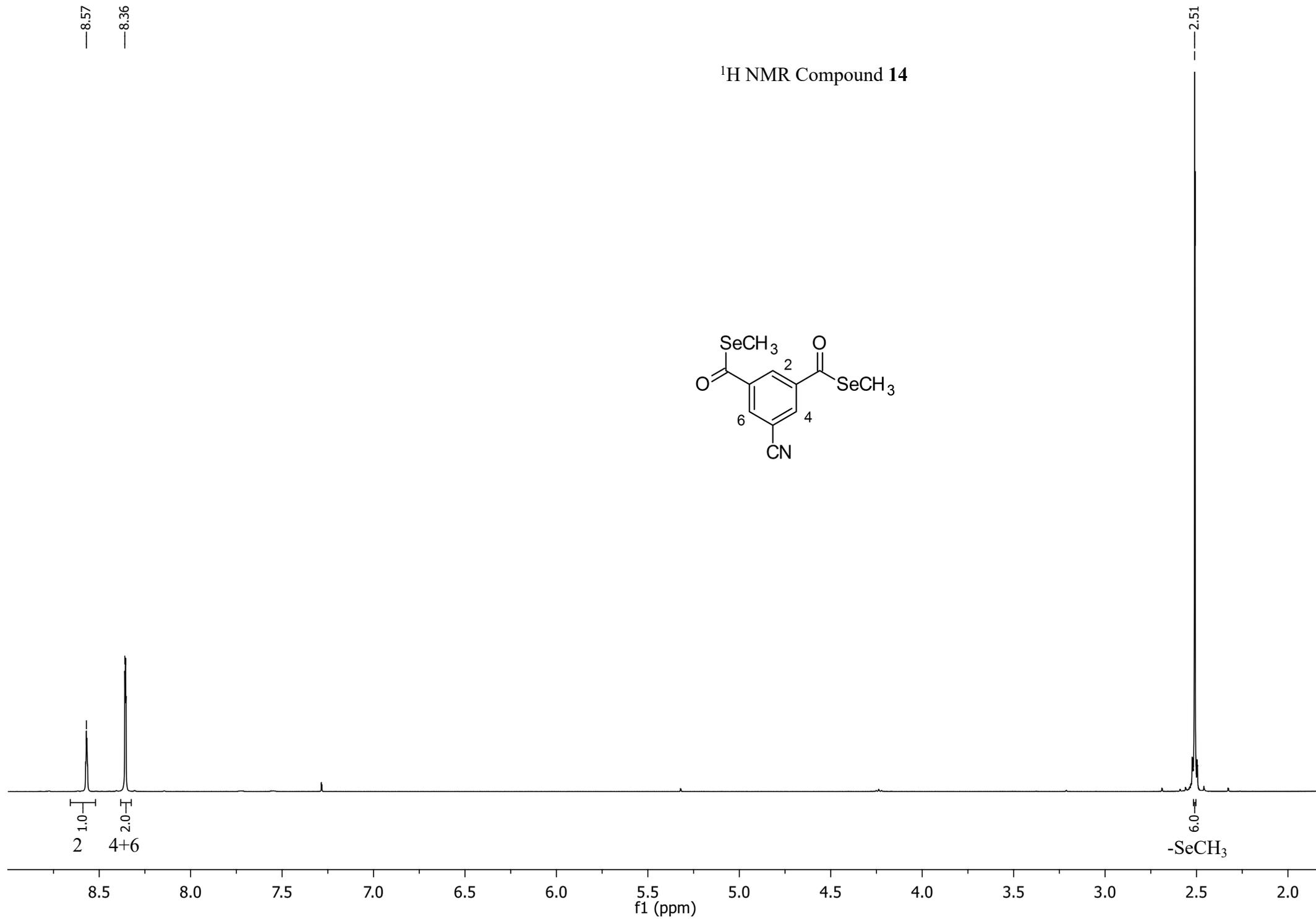
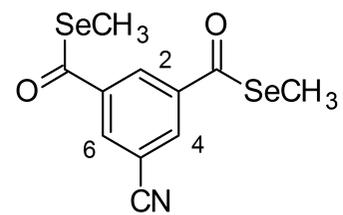
77.18  
76.87  
76.55

### <sup>13</sup>C NMR Compound 13

—6.86



<sup>1</sup>H NMR Compound 14



—192.85

—141.02

—134.47

—129.11

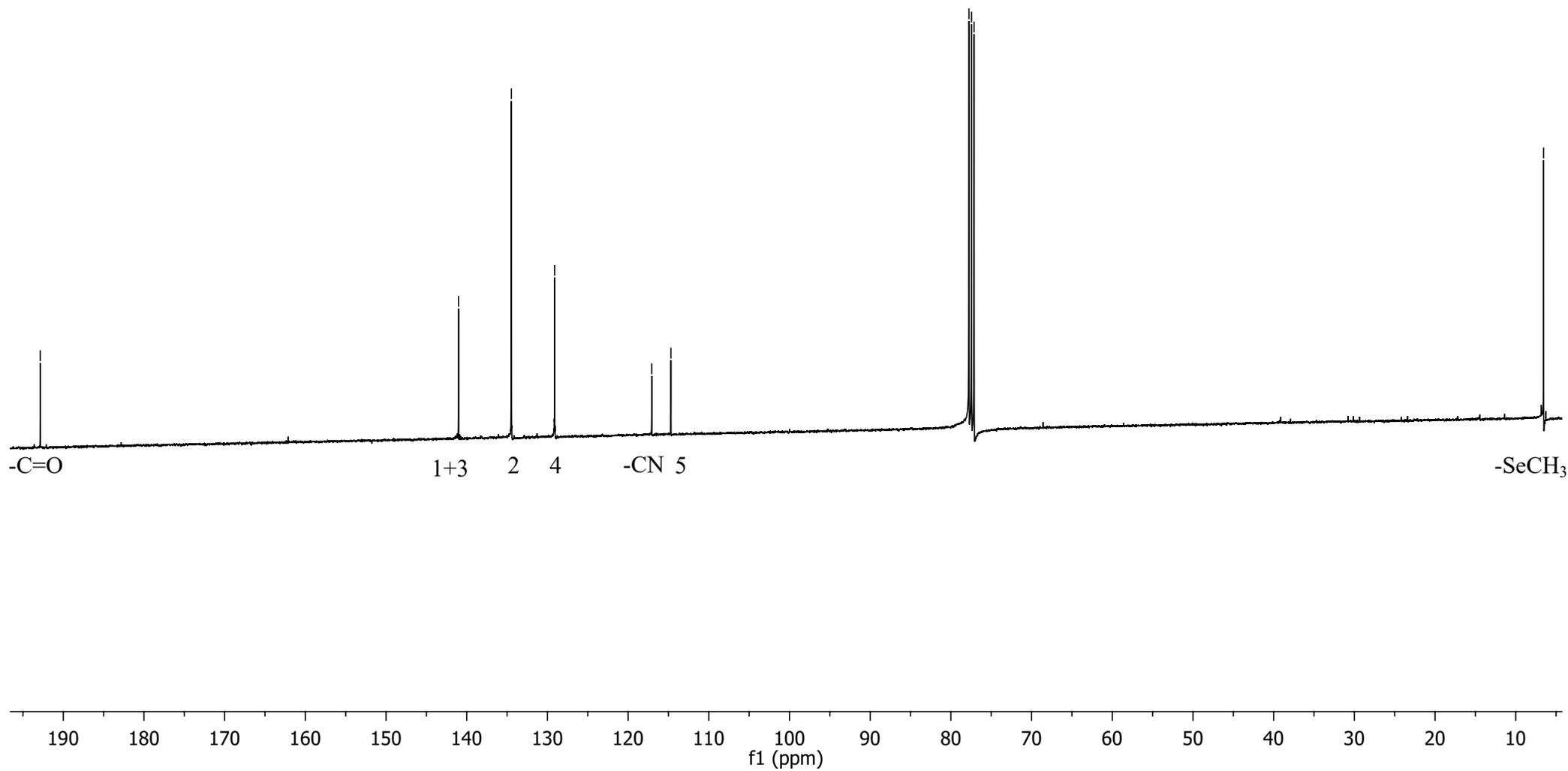
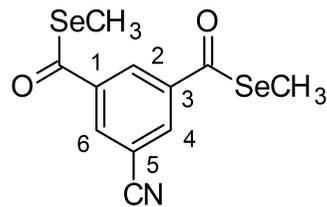
—117.08

—114.69

{ 77.76  
77.44  
77.12 }

<sup>13</sup>C NMR Compound **14**

—6.55



—7.21

$^1\text{H}$  NMR Compound **15**

—2.43

