# Synthesis of Dibenzosultams by "Transition-Metal Free" Photoinduced Intramolecular Arylation of *N*-aryl-2-halobenzenesulfonamides

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## Table of Contents

**Experimental Section**

## 1 - Synthesis of 2-halo-*N*-phenylbenzenesulfonamides

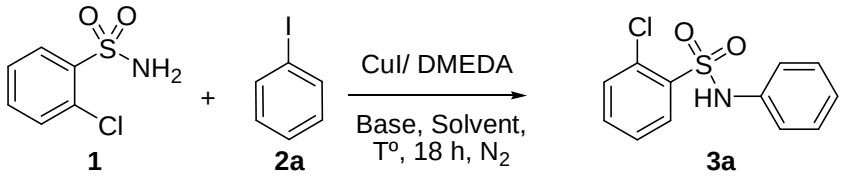
We investigated two methods to obtain *N*-aryl-2-halo-arylsulfonamides: One involves copper-catalyzed *N*-arylation of 2-chlorobenzenesulfonamide with aryl halides (Method A) and the other one involves a known reaction between a substituted benzenesulfonyl chlorides and different anilines (Method B).

### 1.1. *N*-arylation Copper-catalyzed

#### 1.1.1. Screening of Optimal Conditions

The Copper-catalyzed *N*-arylation was initially optimized employing the cross-coupling reaction of 2-chlorobenzenesulfonamide (**1**) with iodobenzene (**2a**).

**Table 1** Optimization of *N*-arylation Copper-catalyzed[a]




**1** **2a** **3a**

| Entry | Conditions | | | | | 3a Yield (%)[b] |
|---|---|---|---|---|---|---|
| | 2a (equiv) | CuI (mol %) | Solvent | Base | Temp (ºC) | |
| 1[c] | 1.2 | 5 | $CH_3CN$ | $K_2CO_3$ | 70 ºC | 15 |
| 2 | 1.2 | 5 | $CH_3CN$ | $K_2CO_3$ | 90 ºC | 25 |
| 3 | 1.2 | 10 | $CH_3CN$ | $K_2CO_3$ | 90 ºC | 40 |
| 4[c] | 1.5 | 10 | $CH_3CN$ | $K_2CO_3$ | 90 ºC | 45 |
| **5** | **2** | **10** | $CH_3CN$ | **$K_2CO_3$** | **90 ºC** | **82** |
| **6**[c] | | | | | | **78** |
| 7 | 2 | 10 | $CH_3CN$ | KOH | 90 ºC | 26 |
| 8 | 2 | 10 | $CH_3CN$ | *t*-BuOK | 90 ºC | <5 |
| 9 | 2 | 10 | Toluene | $K_2CO_3$ | 90 ºC | <5 |
| 10 | 2 | 10 | DMF | $K_2CO_3$ | 90 ºC | 6 |

[a]Reactions carried out under $N_2$ with 0.6 mmol of **1** (2-chlorobenzenesulfonamide), 0.72 – 1.2 mmol of **2a** (iodobenzene**)**, 0.03 – 0.06 mmol of CuI, 0.3 mmol of DMEDA (N,N′-Dimethylethylenediamine), 1.8 mmol of base in 4 mL of solvent. [b]Yields were determined by GC (internal standard method). [c]Isolated yields after column chromatography.

The reaction was also tested with microwave irradiation making no progress even heating at 120 ºC for 30 min obtaining only traces of the corresponding product **3a**.

Microwave-induced reactions were performed in a single mode instrument equipped with a noncontact infrared temperature sensor, direct pressure control system

for measuring the pressure of the reaction vessel contents and a cooling system by compressed air. In the method a temperature controlled reaction at 120ºC, with a maximum power of 150 W.

## 2. Synthesis of Dibenzosultams

### 2.1 Uv-vis spectra for 3a and the corresponding anion

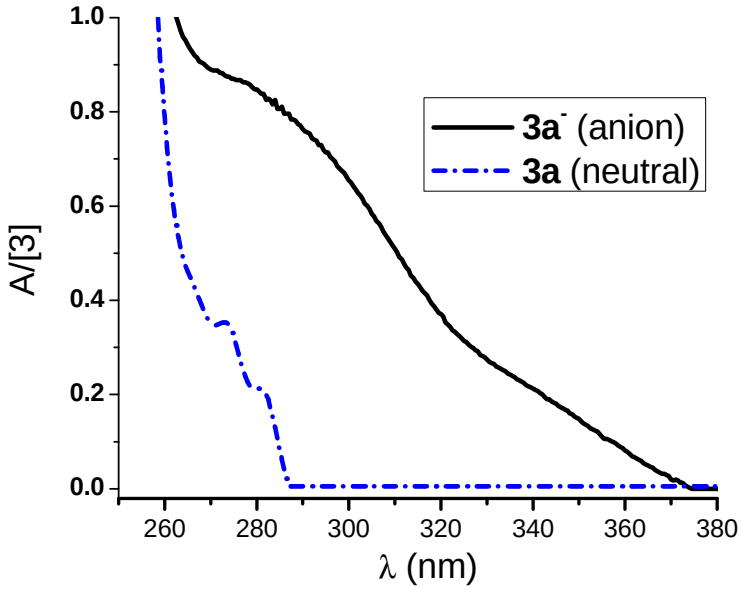
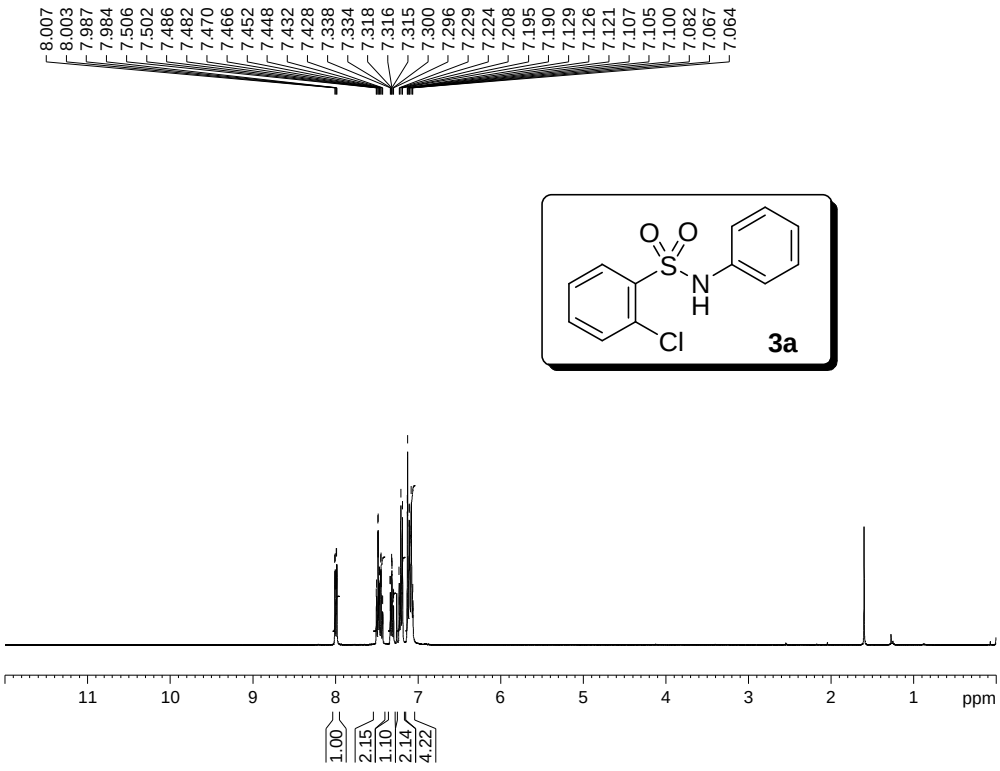
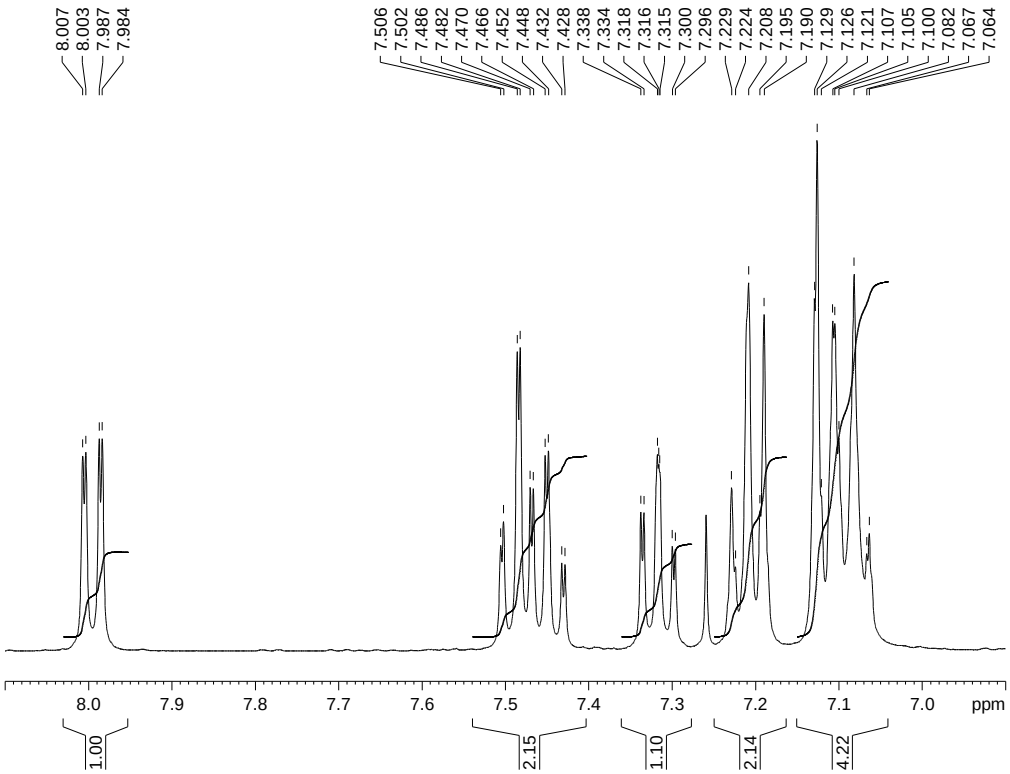



**Figure 1:** Uv-vis spectra for compounds **3a** (7.4 x $10^{-5}$ M) and anion derivative **3a**$^-$. Spectra were performed under $N_2$ in DMSO. To form the anion, a solution of *t*-BuOK 1.35 x $10^{-3}$ M was added and the mixture was incubated for 5 min. Solid line: anion. Dashed line: neutral.

## 3. Copies of $^{1}H$ and $^{13}C$ NMR Spectra of substrates (3a-r)

*2-Chloro-N-phenylbenzenesulfonamide* (**3a**)

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7.428
7.338
7.334
7.318
7.316
7.315
7.300
7.296
7.229
7.224
7.208
7.195
7.190
7.129
7.126
7.121
7.107
7.105
7.100
7.082
7.067
7.064
8.0
7.9
7.8
7.7
7.6
7.5
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7.3
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7.1
7.0
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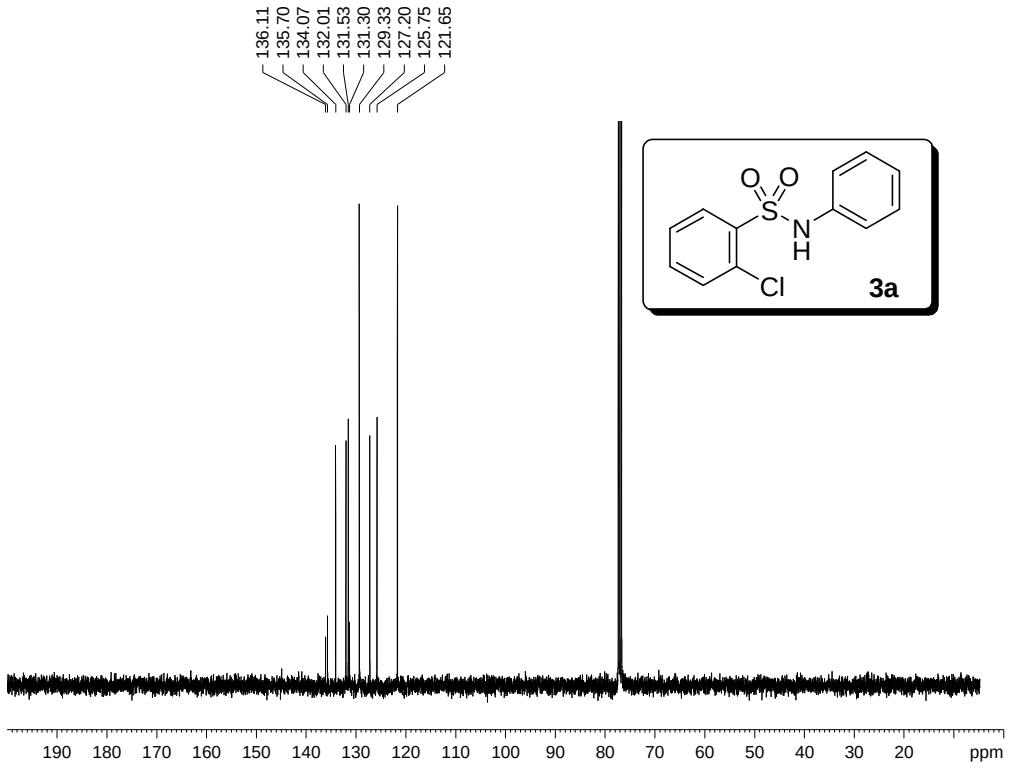
1.10
2.14
4.22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132.01
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131.30
129.33
127.20
125.75
121.65
O
O
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N
H
Cl
3a
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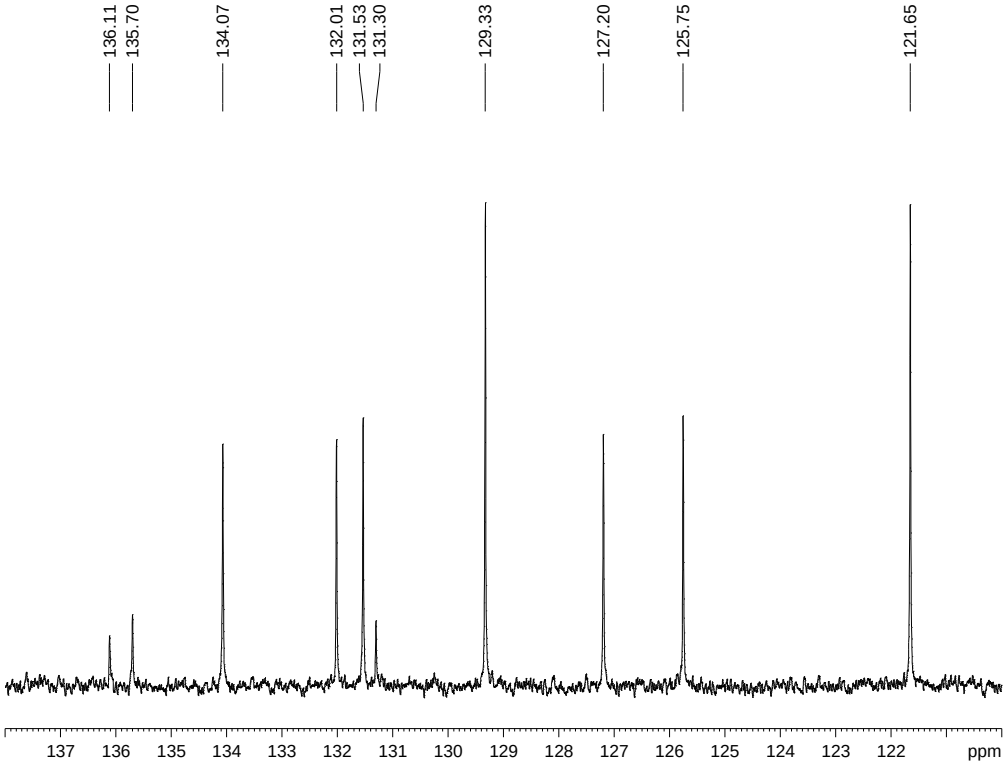
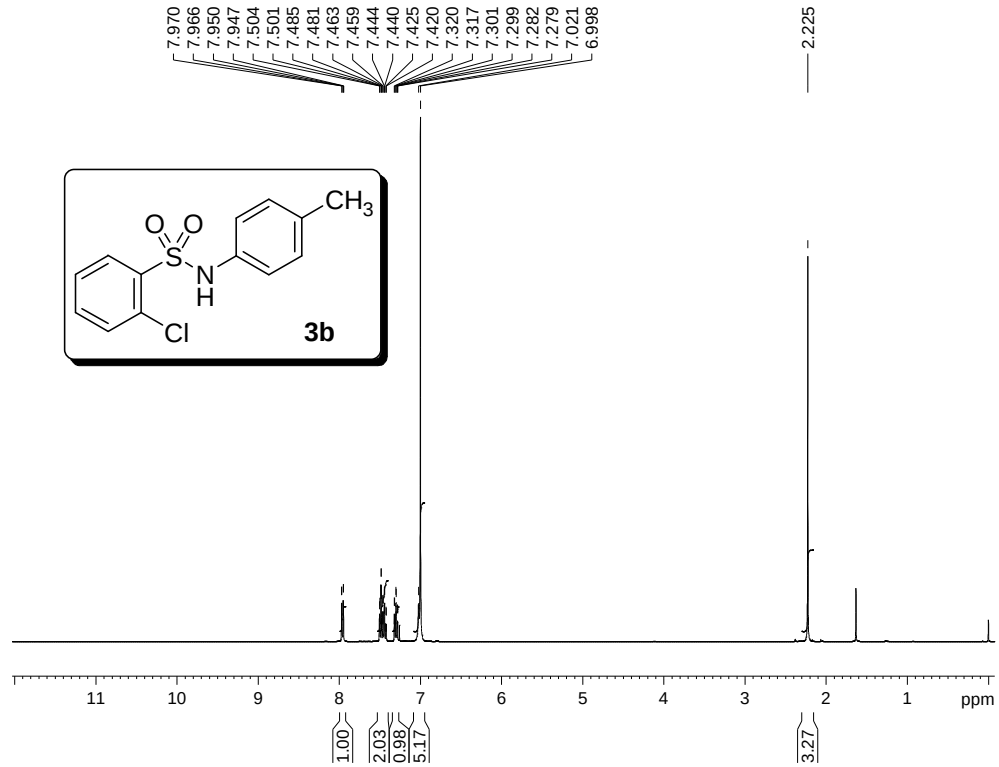
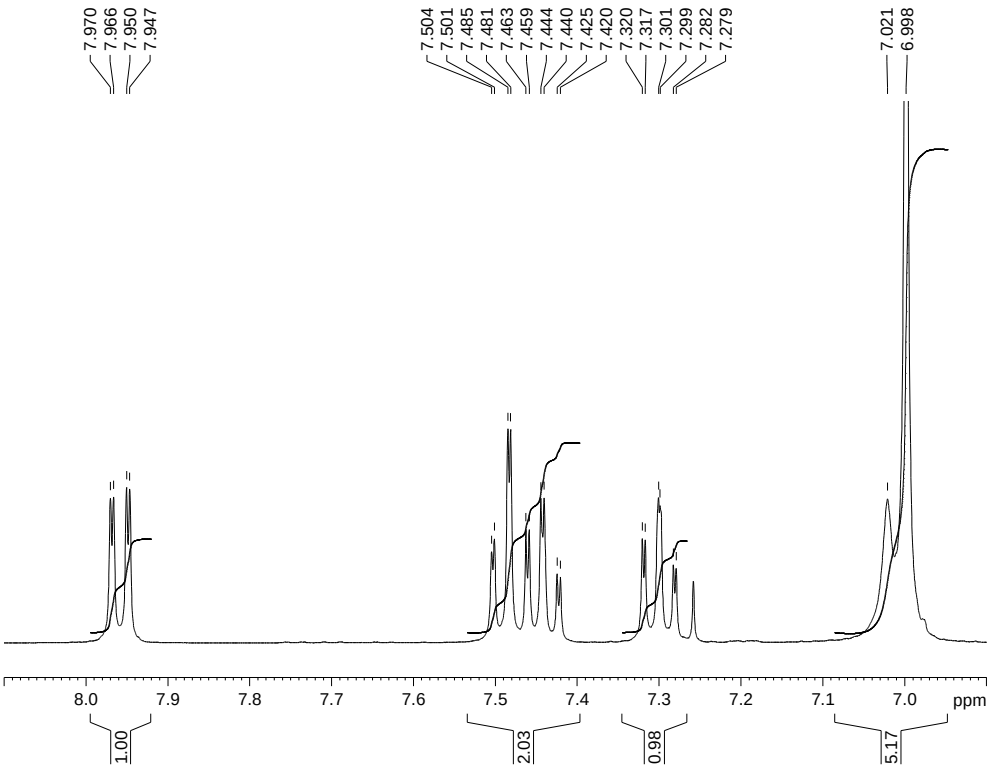
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm




*2-Chloro-N-(p-tolyl)benzenesulfonamide* (**3b**)

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7.501
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7.440
7.425
7.420
7.320
7.317
7.301
7.299
7.282
7.279
7.021
6.998
8.0
7.9
7.8
7.7
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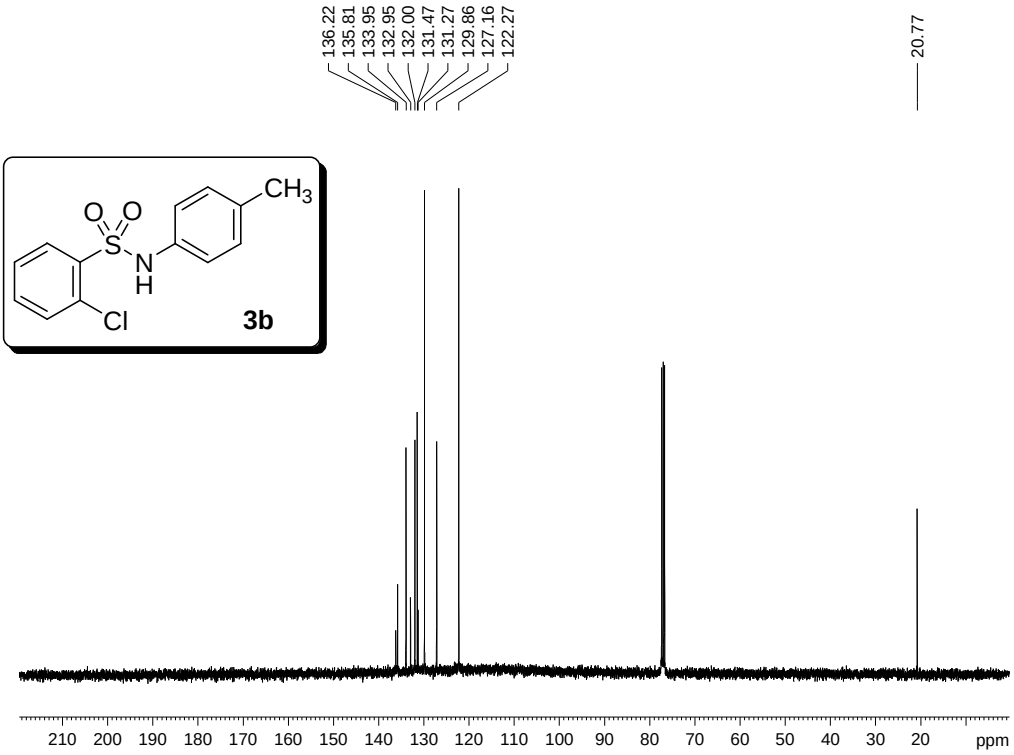
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132.95
132.00
131.47
131.27
129.86
127.16
122.27
20.77
O
O
S
N
H
Cl
CH3
3b
210
200
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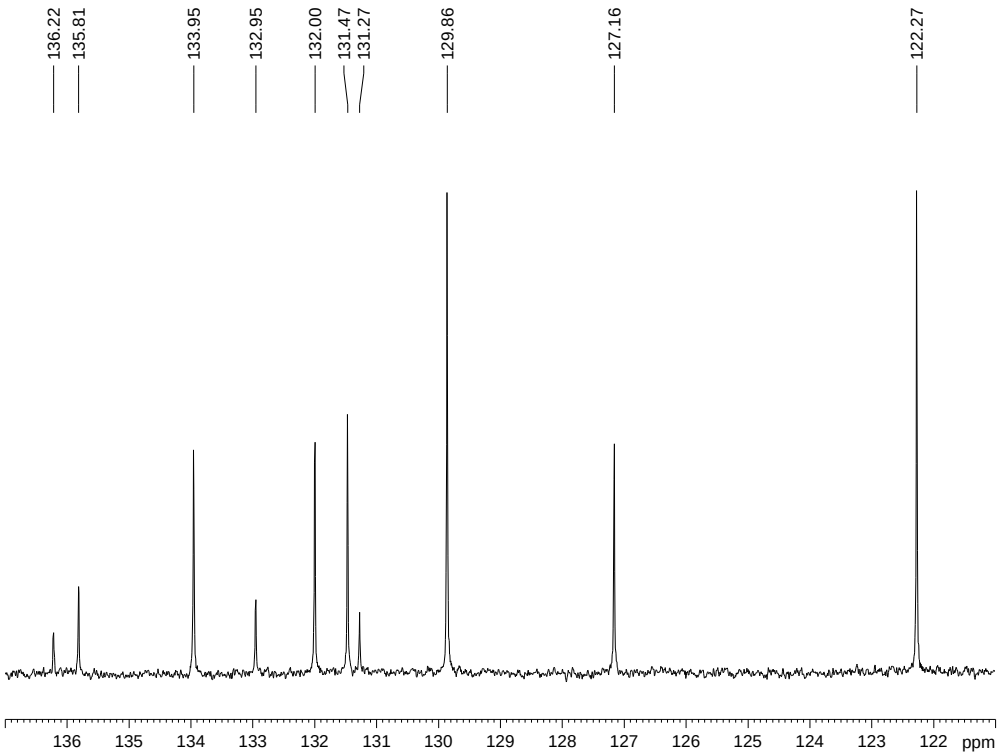
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

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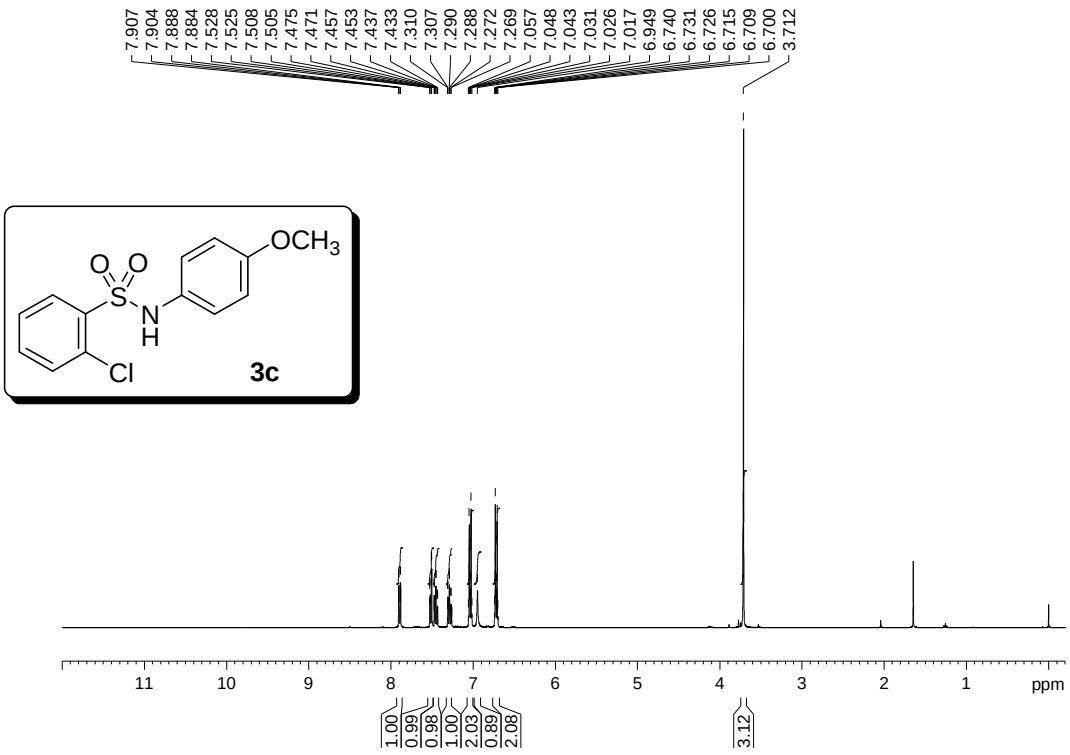

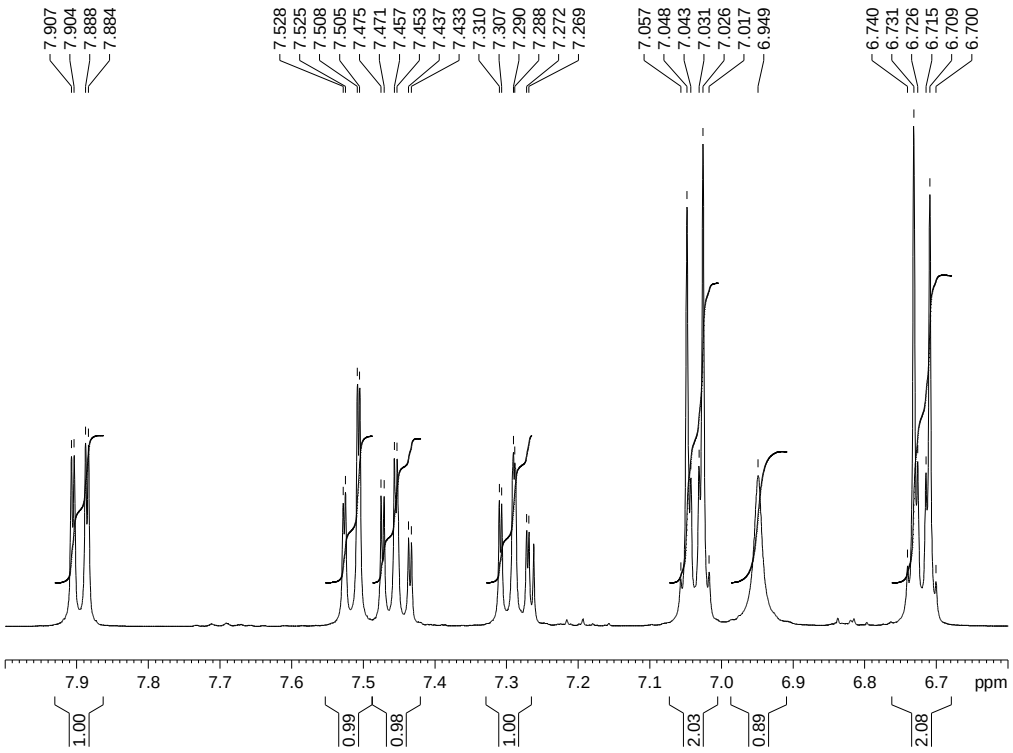
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7.433
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7.307
7.290
7.288
7.272
7.269
7.057
7.048
7.043
7.031
7.026
7.017
6.949
6.740
6.731
6.726
6.715
6.709
6.700
7.9
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7.7
7.6
7.5
7.4
7.3
7.2
7.1
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6.8
6.7
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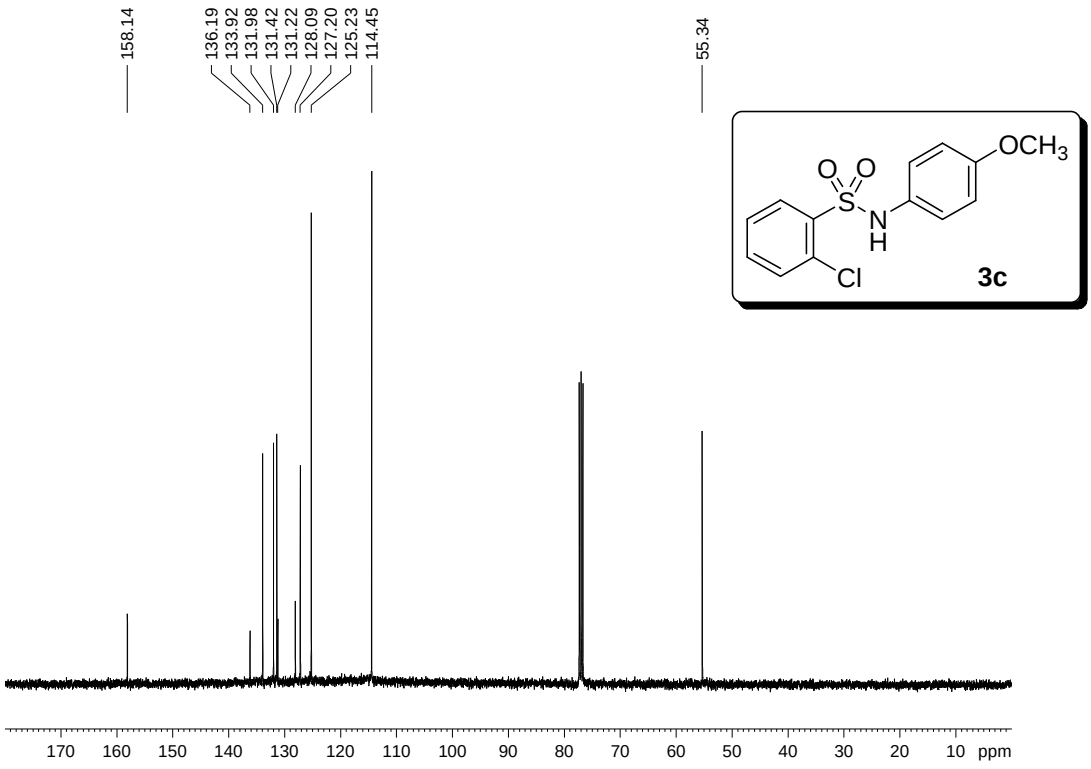
0.89
2.08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125.23
114.45
55.34
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O
O
S
N
H
Cl
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150
140
130
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110
100
90
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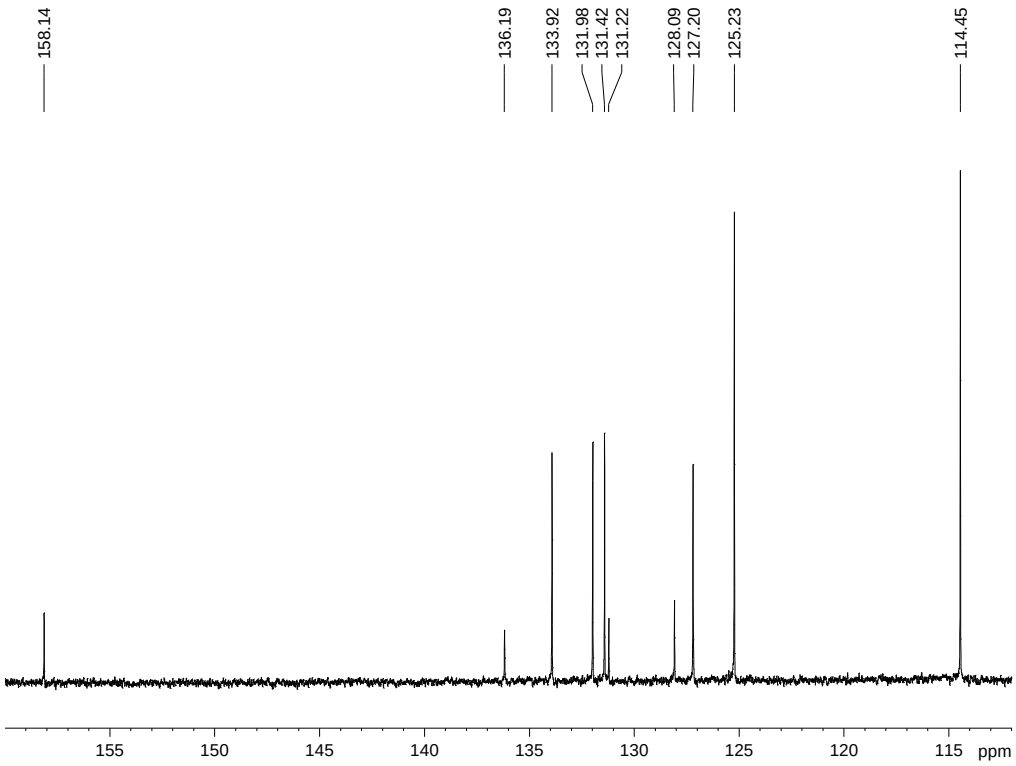
70
60
50
40
30
20
10
ppm

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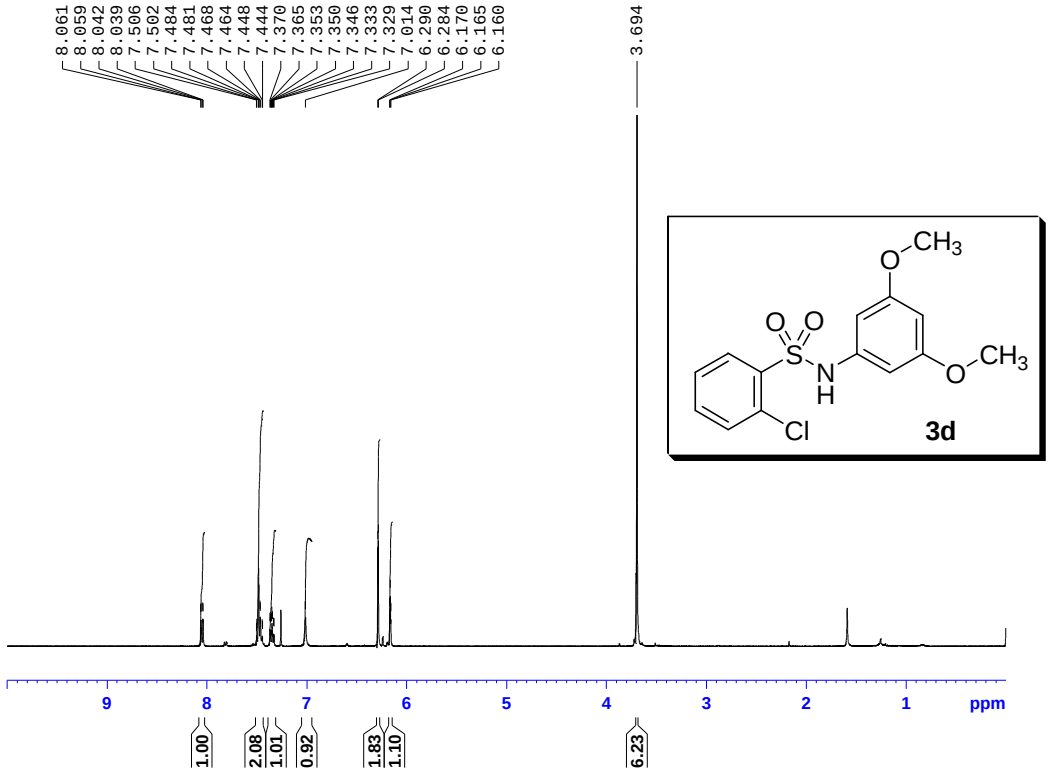
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8.042
8.039
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7.502
7.484
7.481
7.468
7.464
7.448
7.444
7.370
7.365
7.353
7.350
7.346
7.333
7.329
7.014
6.290
6.284
6.170
6.165
6.160
3.694
O
CH3
O
O
S
N
H
O
CH3
Cl
3d
9
8
7
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5
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3
2
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ppm
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1.01
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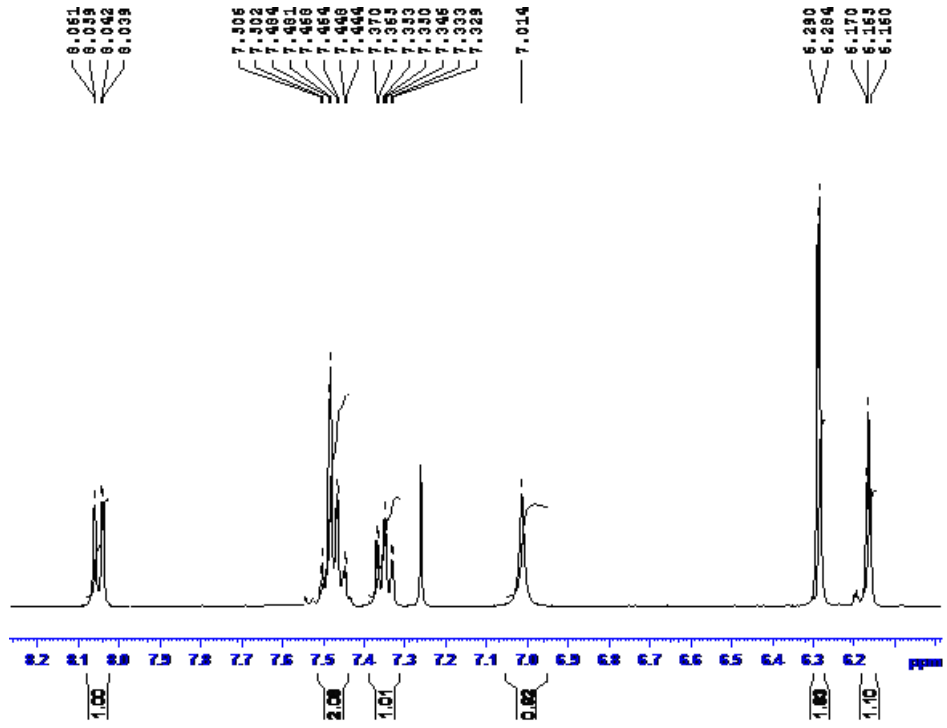
1.83
1.10
6.23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8.042
8.039
7.506
7.502
7.484
7.481
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7.464
7.448
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7.365
7.353
7.350
7.346
7.333
7.329
7.014
6.290
6.284
6.170
6.165
6.160
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
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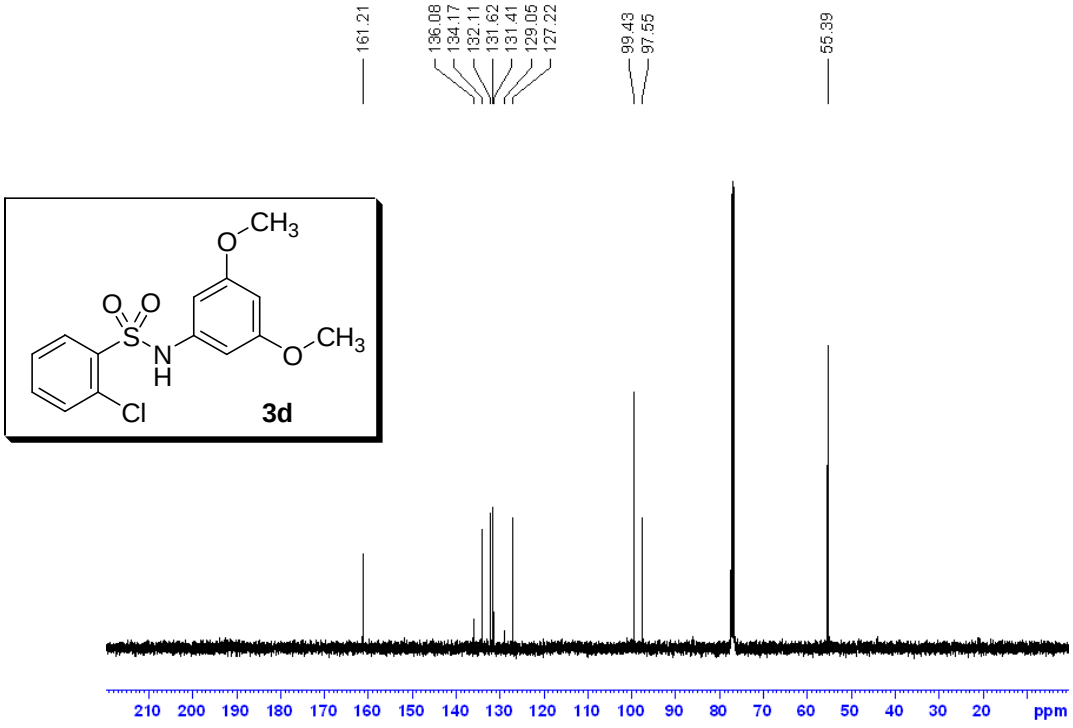
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
6.2
ppm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129.05
127.22
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97.55
55.39
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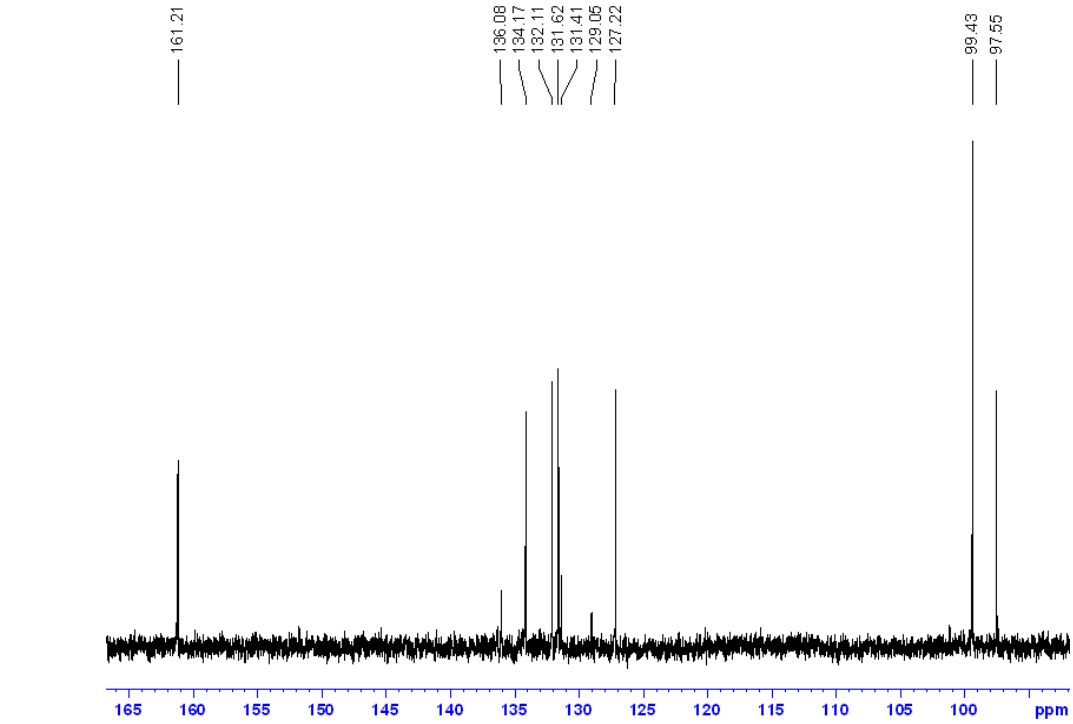
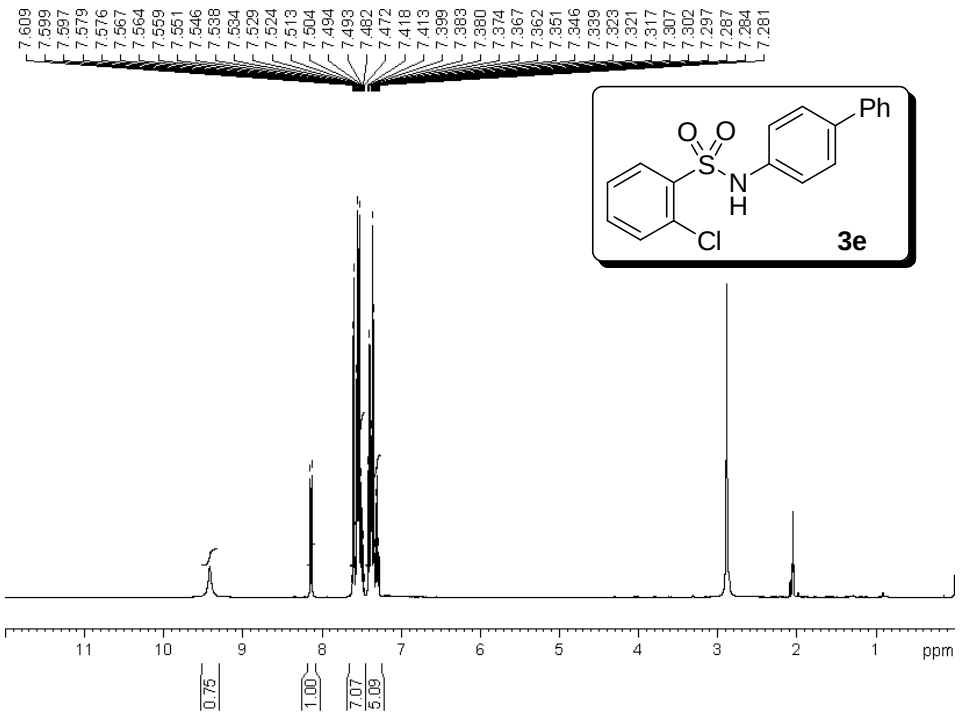
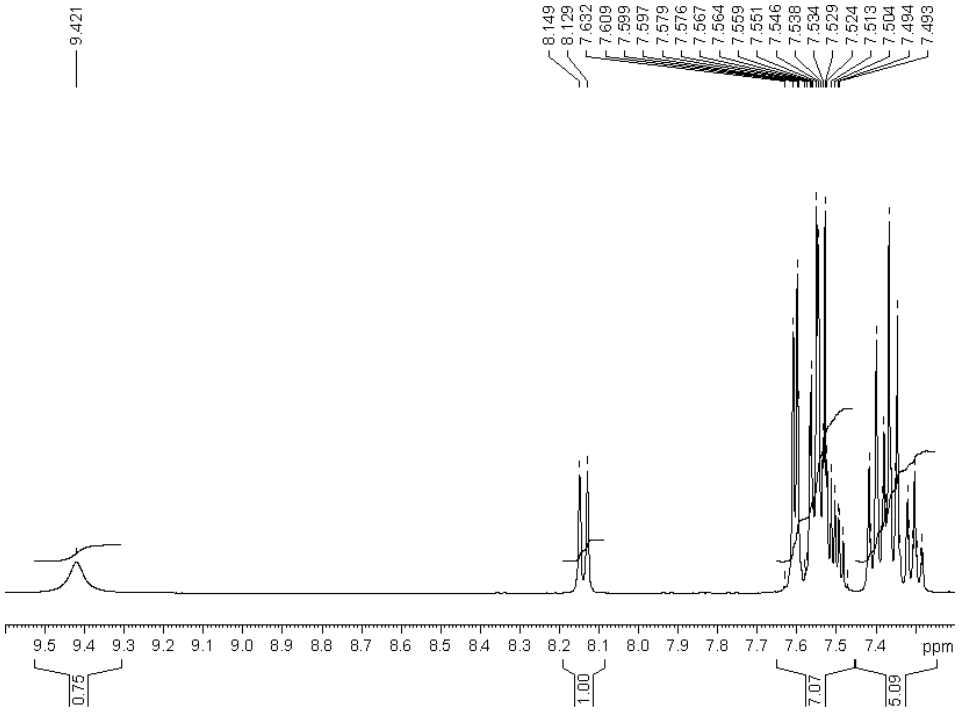
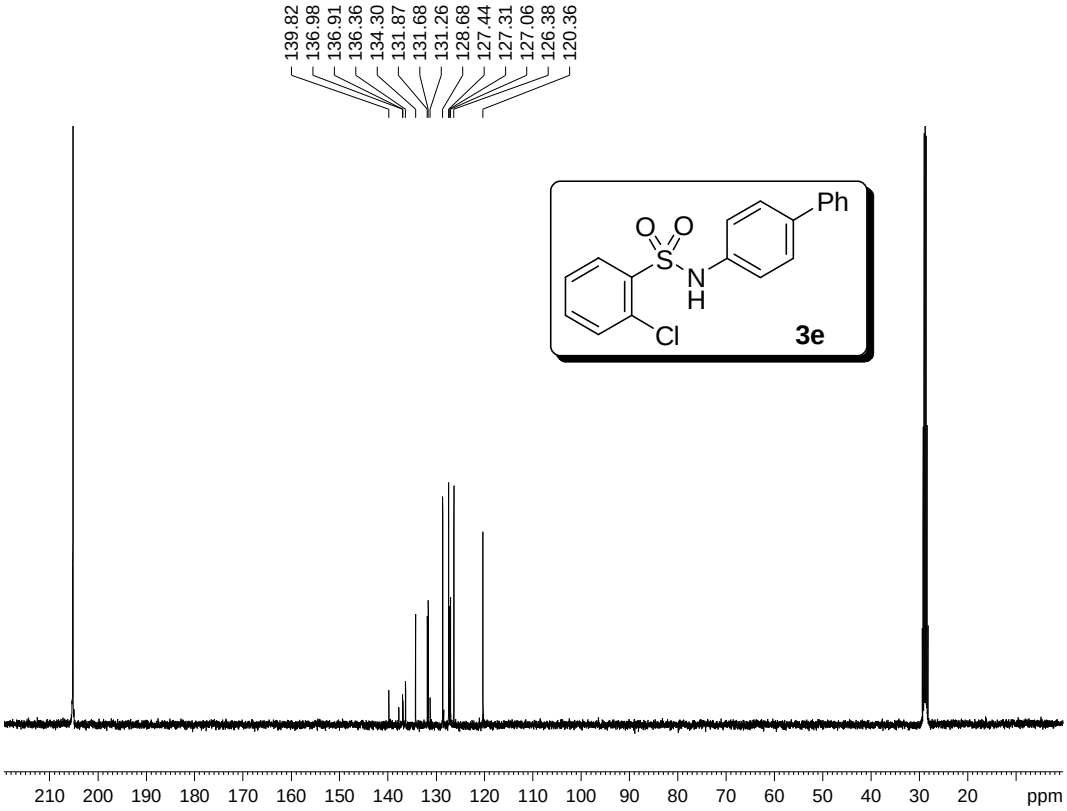
CH3
O
O
S
N
H
O
CH3
Cl
3d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


161.21
136.08
134.17
132.11
131.62
131.41
129.05
127.22
99.43
97.55
165 160 155 150 145 140 135 130 125 120 115 110 105 100 ppm

*N-([1,1'-Biphenyl]-4-yl)-2-chlorobenzenesulfonamide* (**3e**)

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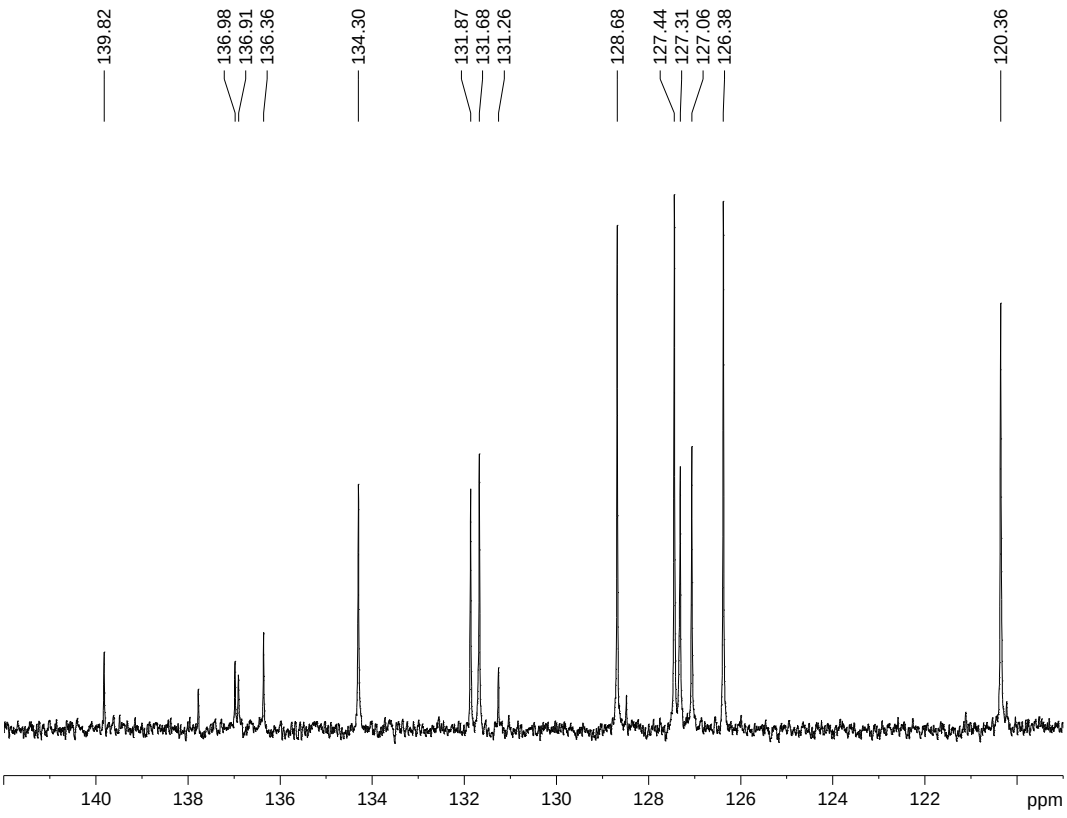
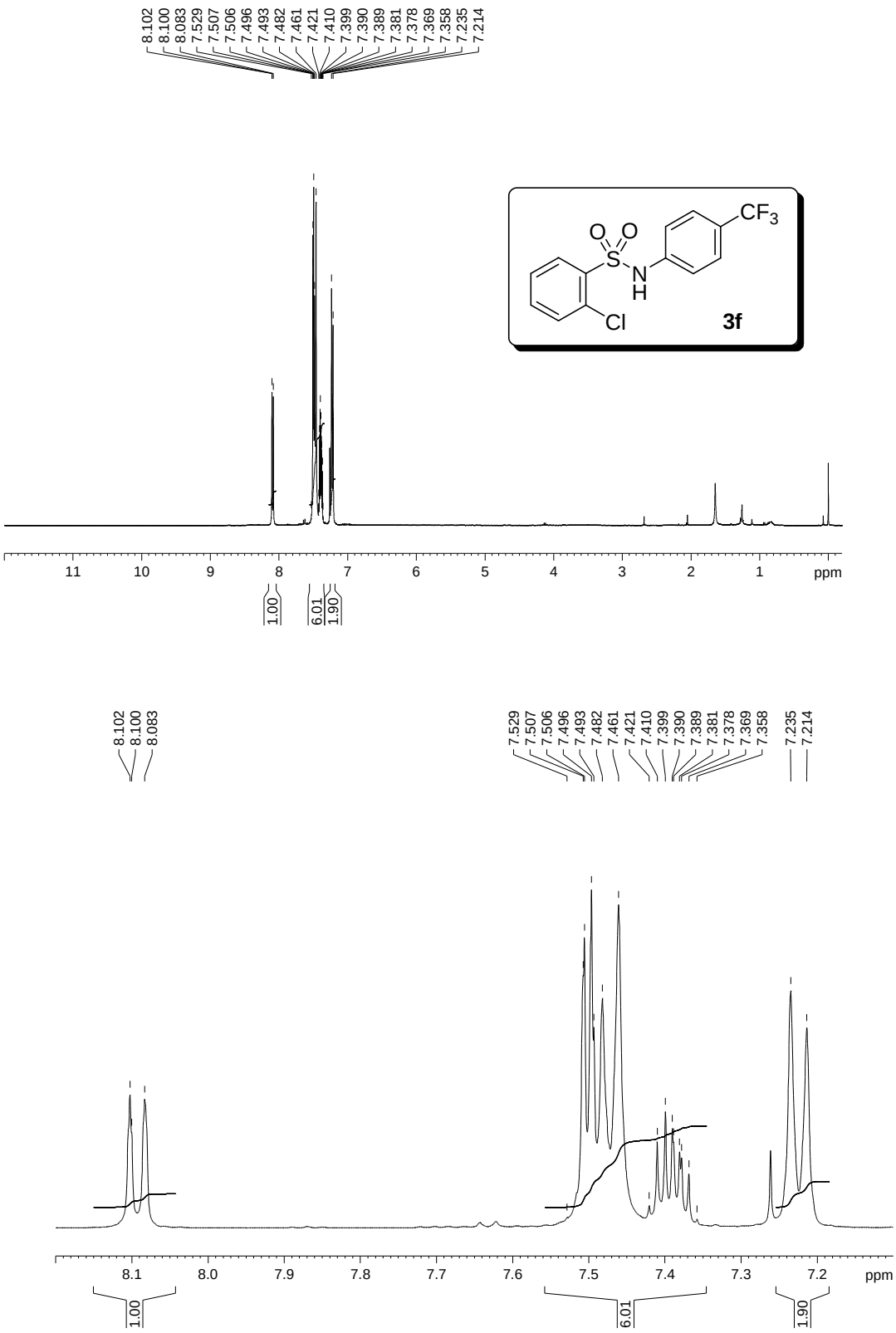
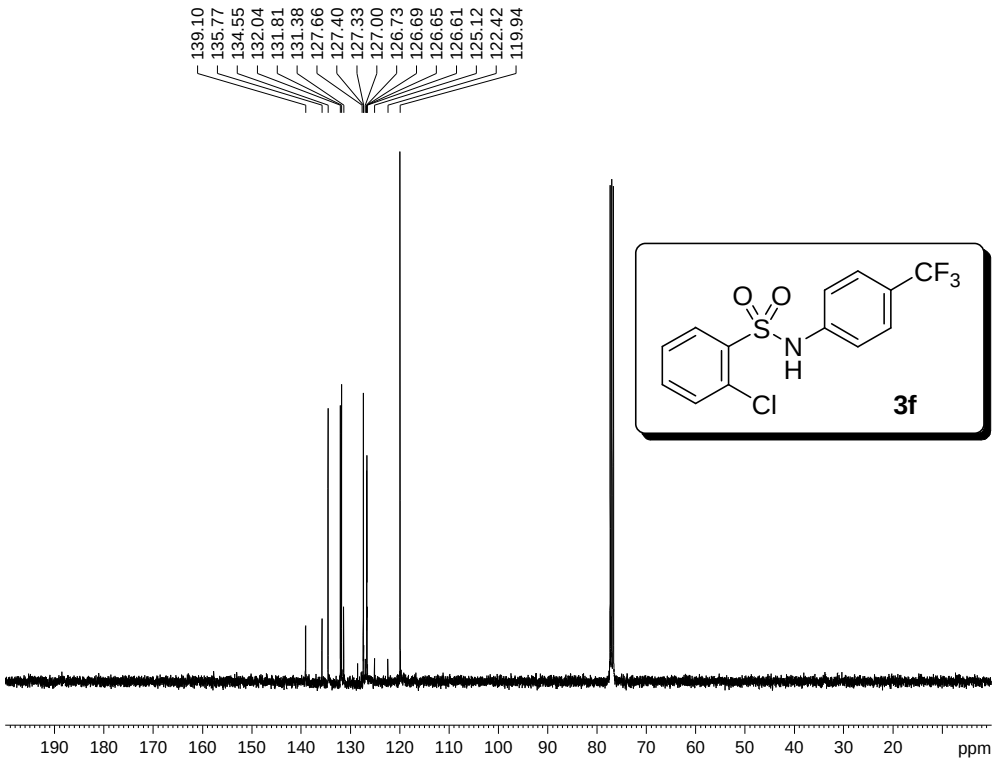
136.98
136.91
136.36
134.30
131.87
131.68
131.26
128.68
127.44
127.31
127.06
126.38
120.36
Ph
O
O
S
N
H
Cl
3e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


139.82
136.98
136.91
136.36
134.30
131.87
131.68
131.26
128.68
127.44
127.31
127.06
126.38
120.36
140 138 136 134 132 130 128 126 124 122 ppm

*2-Chloro-N-(4-(trifluoromethyl)phenyl)benzenesulfonamide* (**3f**)

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135.77
134.55
132.04
131.81
131.38
127.66
127.40
127.33
127.00
126.73
126.69
126.65
126.61
125.12
122.42
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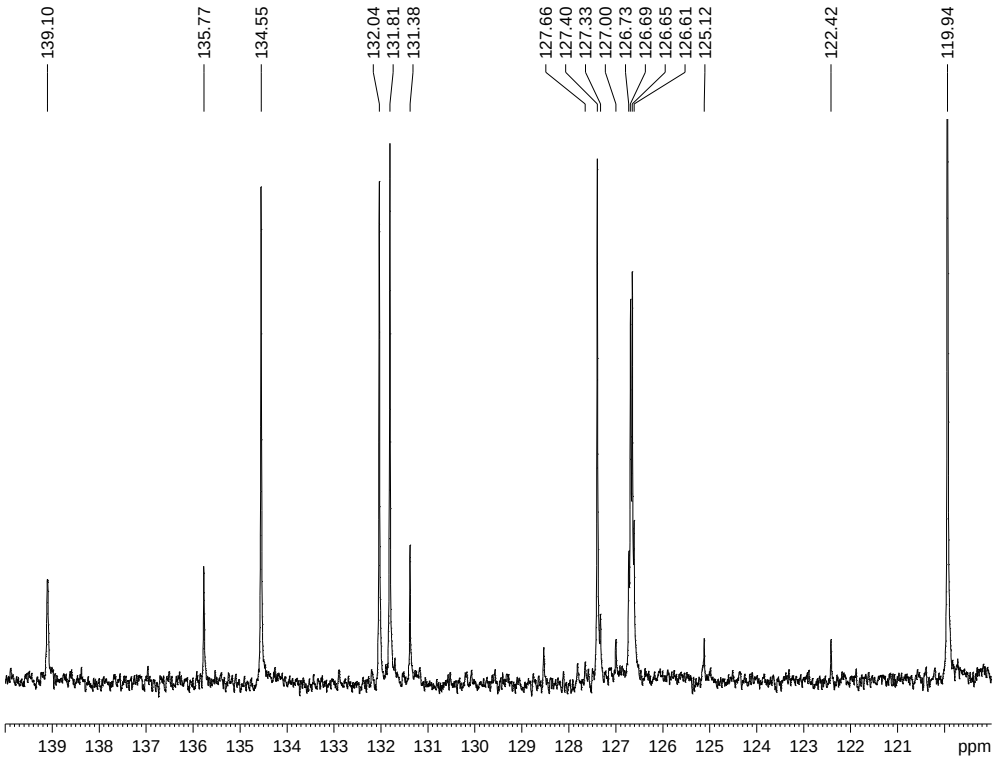
O
O
S
N
H
Cl
CF3
3f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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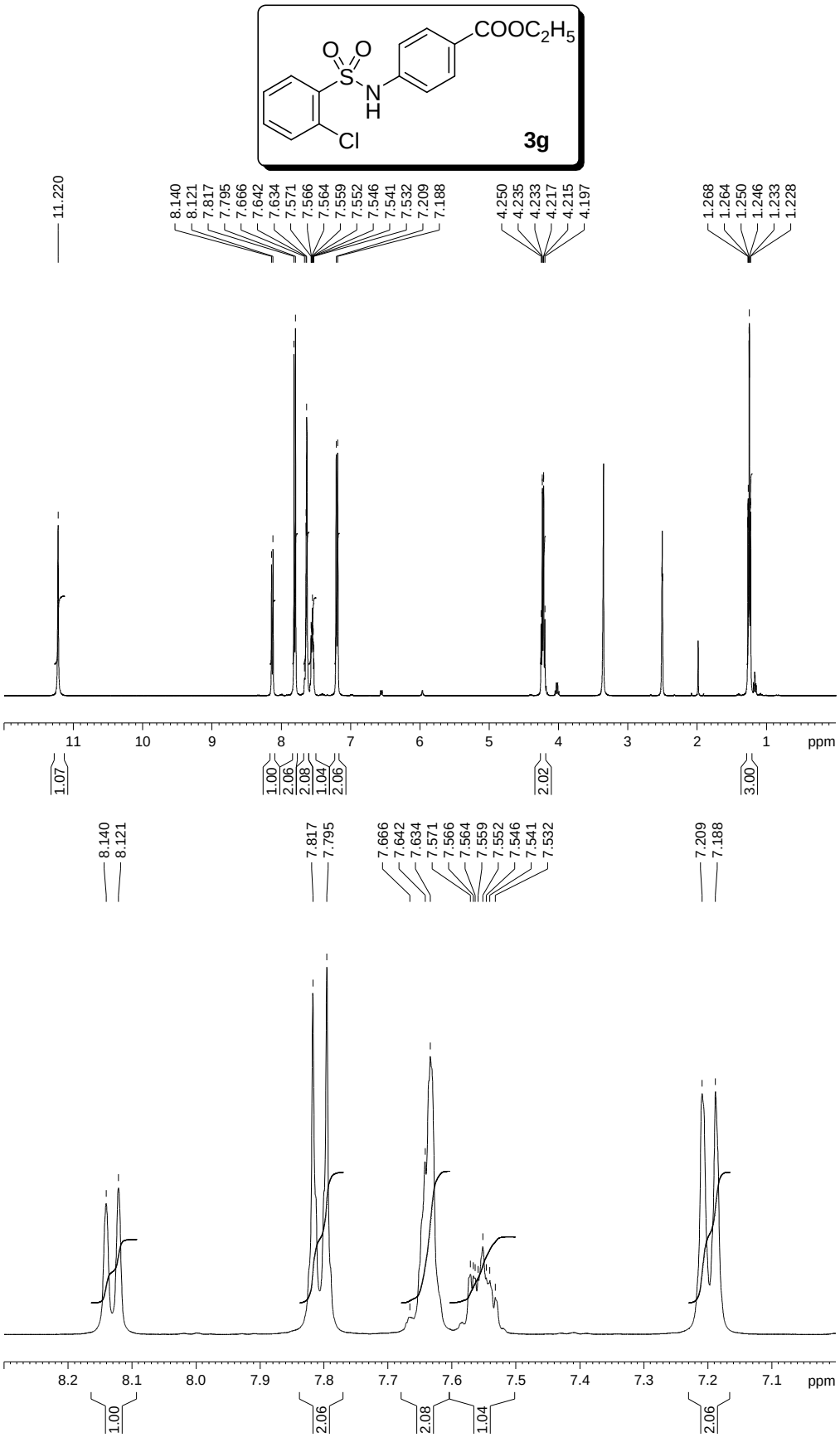
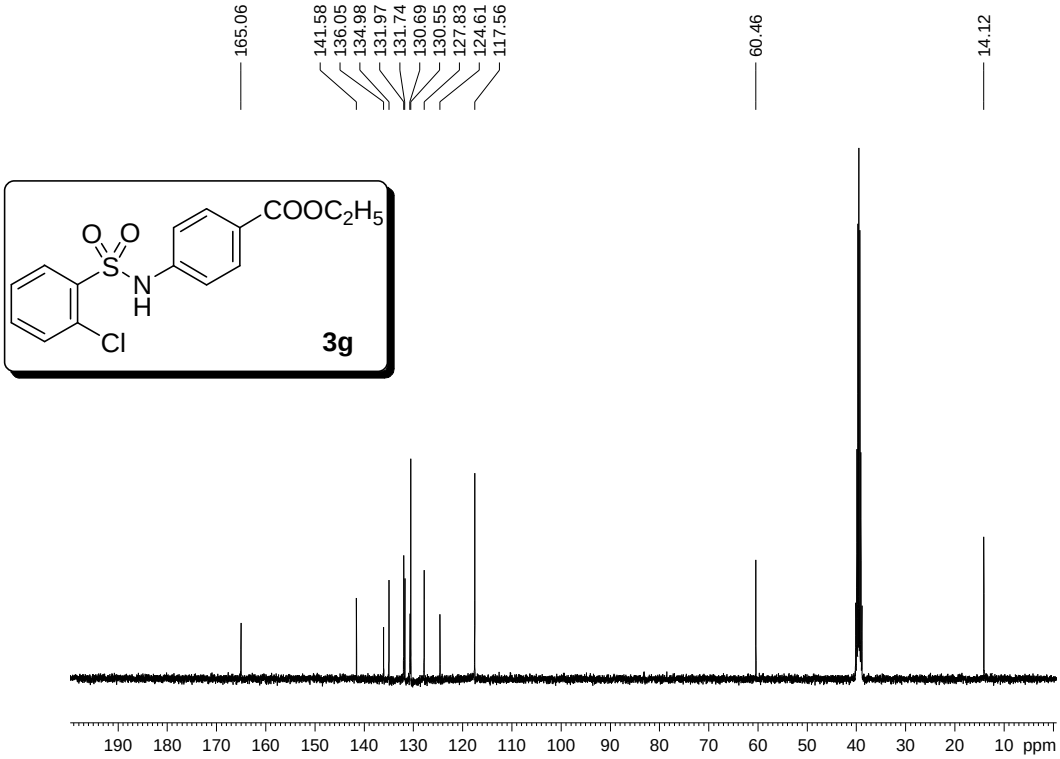
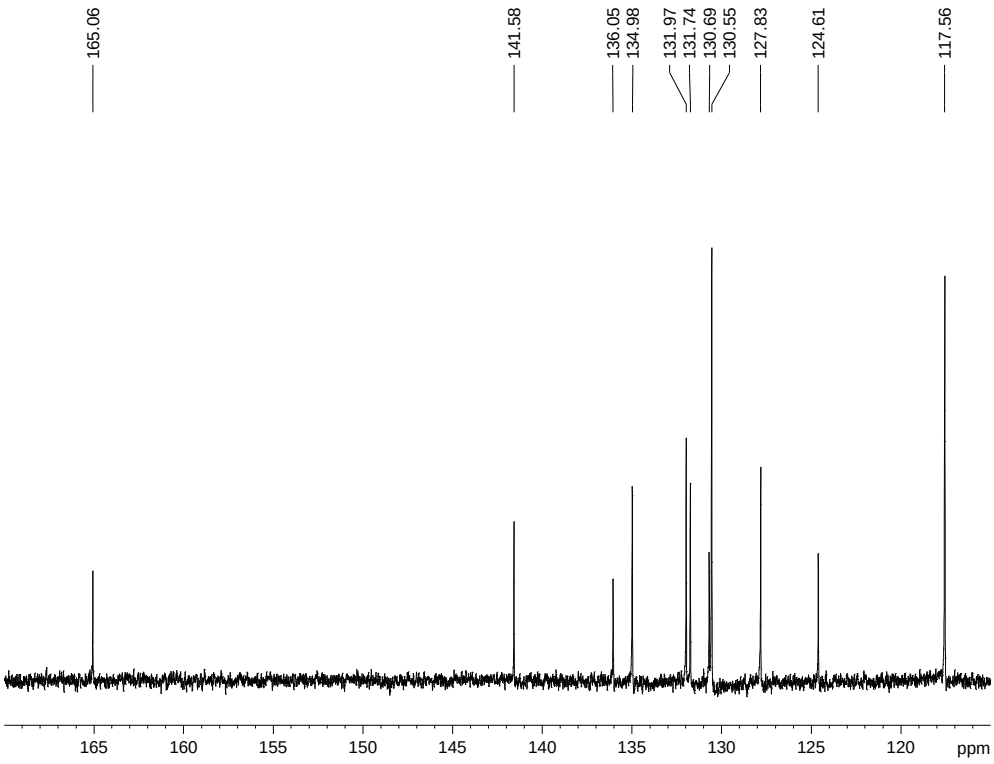
134.55
132.04
131.81
131.38
127.66
127.40
127.33
127.00
126.73
126.69
126.65
126.61
125.12
122.42
119.94
139 138 137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 ppm

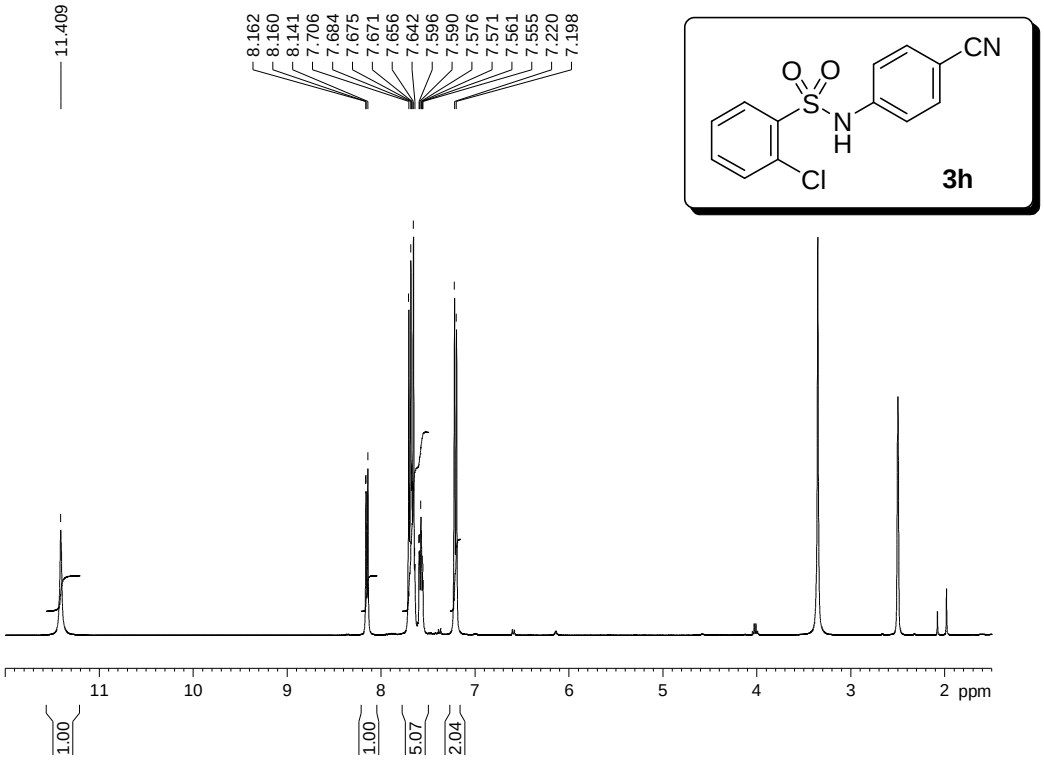
Ethyl 4-(2-chlorophenylsulfonamido)benzoate (**3g**)

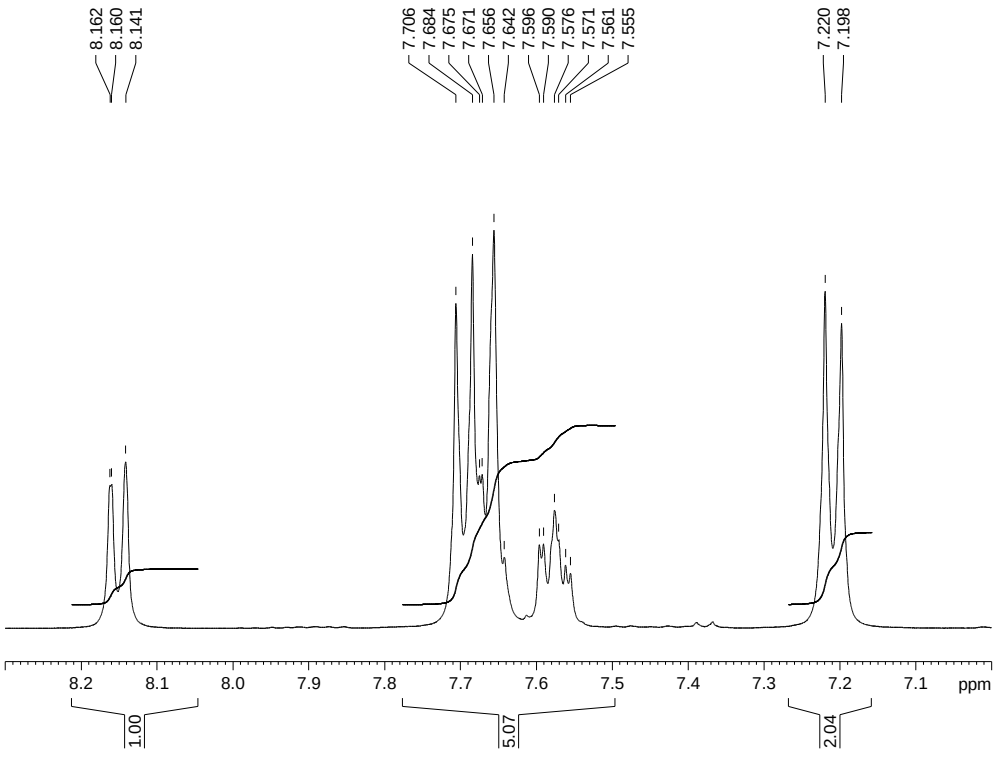


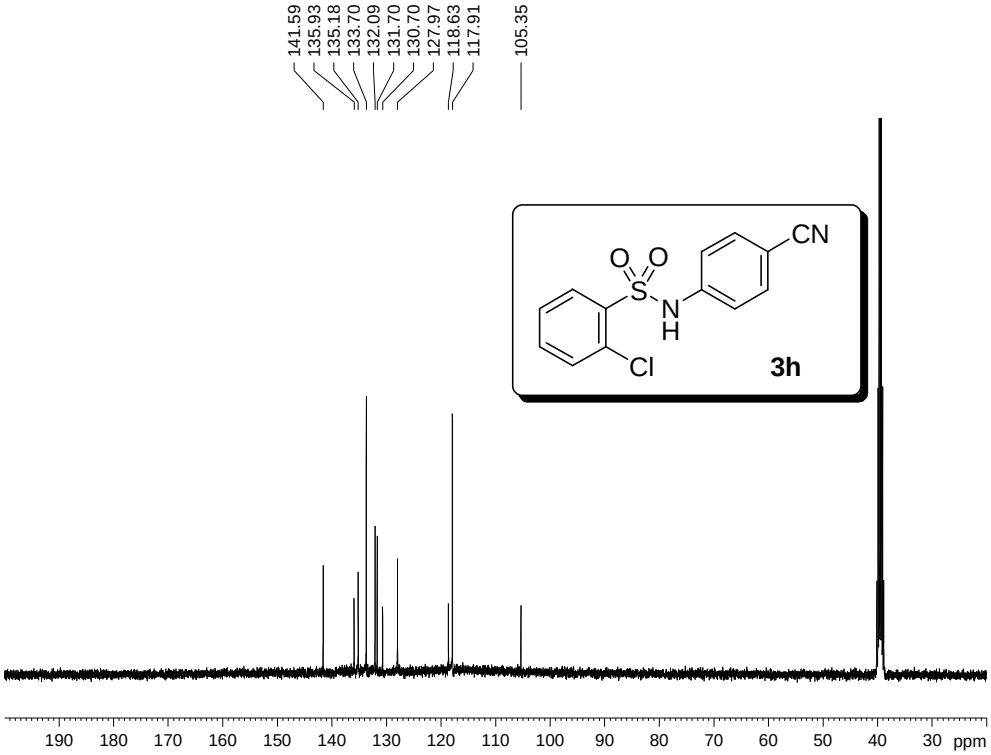

165.06
141.58
136.05
134.98
131.97
131.74
130.69
130.55
127.83
124.61
117.56
60.46
14.12
COOC2H5
O
O
S
N
H
Cl
3g
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

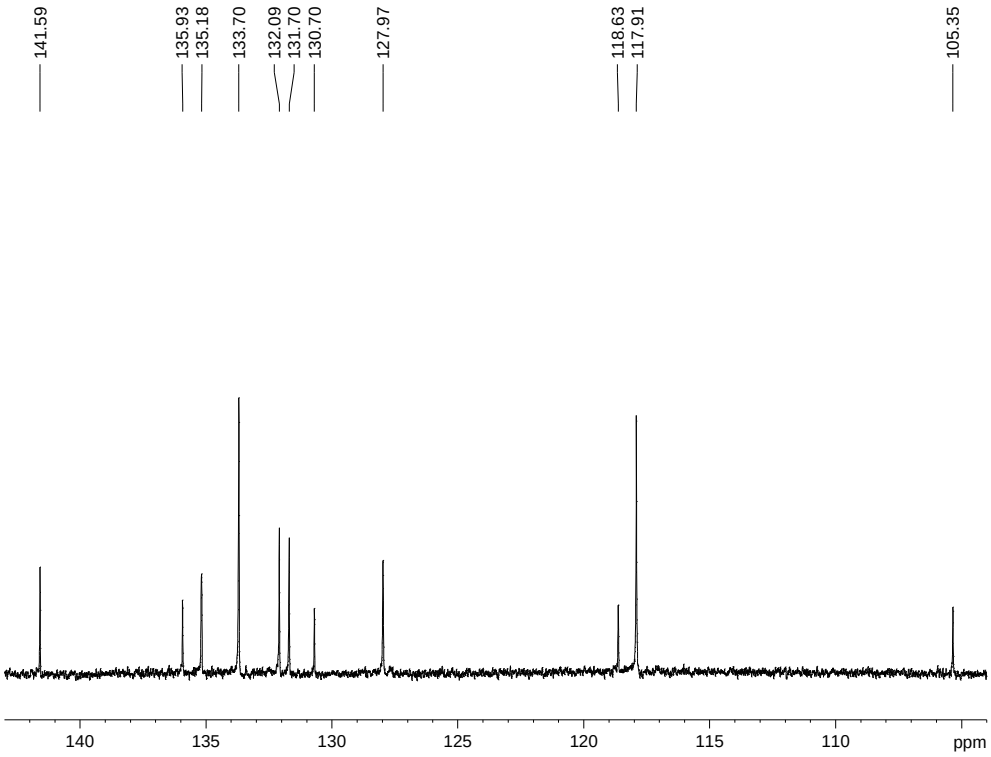

165.06
141.58
136.05
134.98
131.97
131.74
130.69
130.55
127.83
124.61
117.56
165 160 155 150 145 140 135 130 125 120 ppm

*2-Chloro-N-(4-cyanophenyl)benzenesulfonamide* (**3h**)

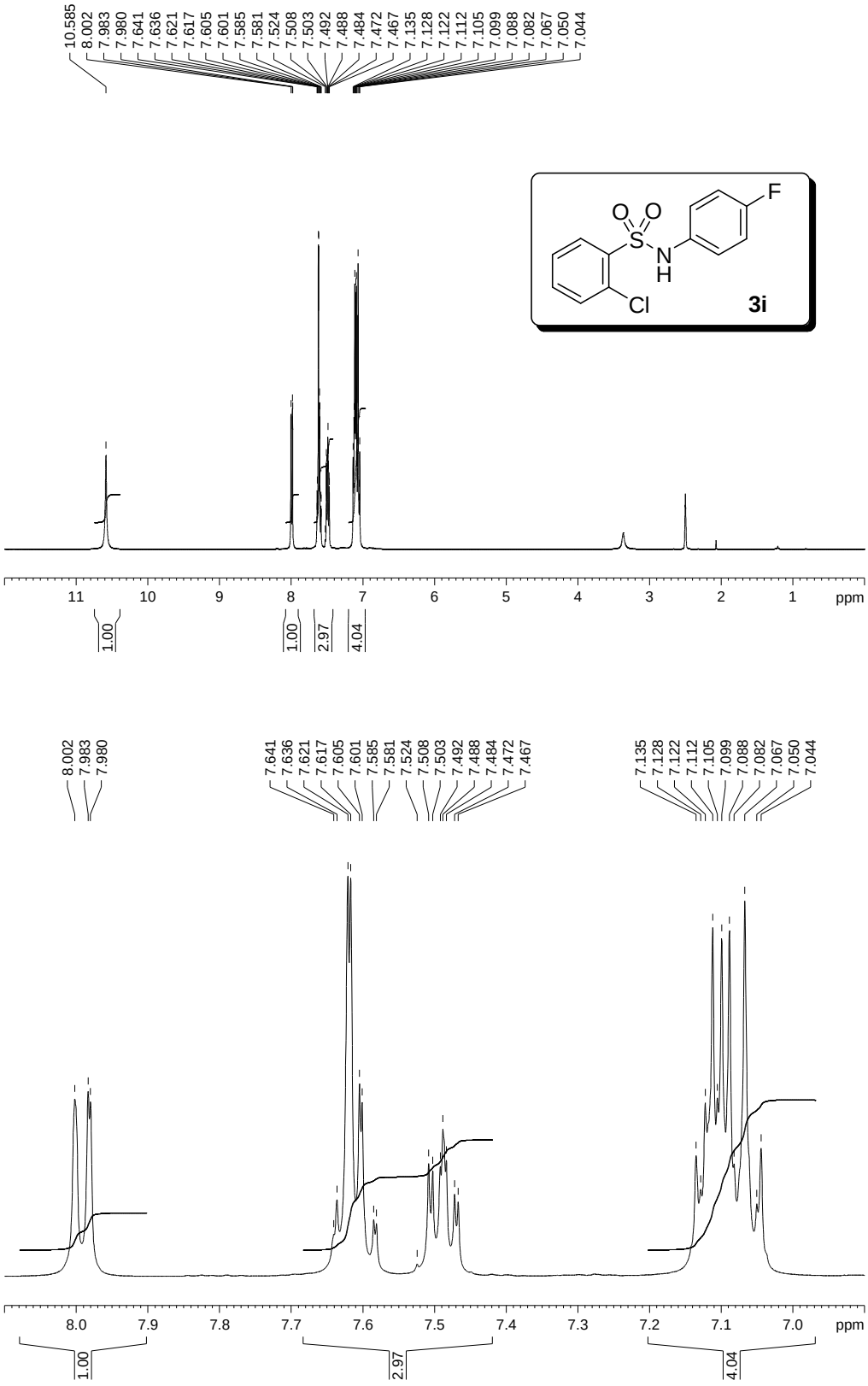


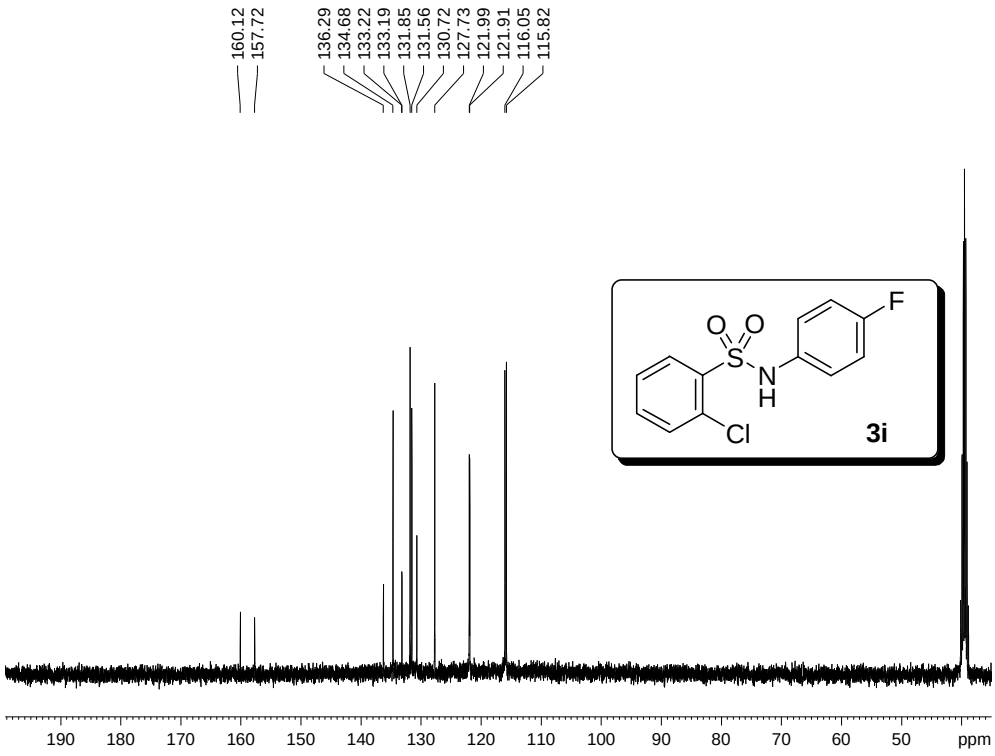



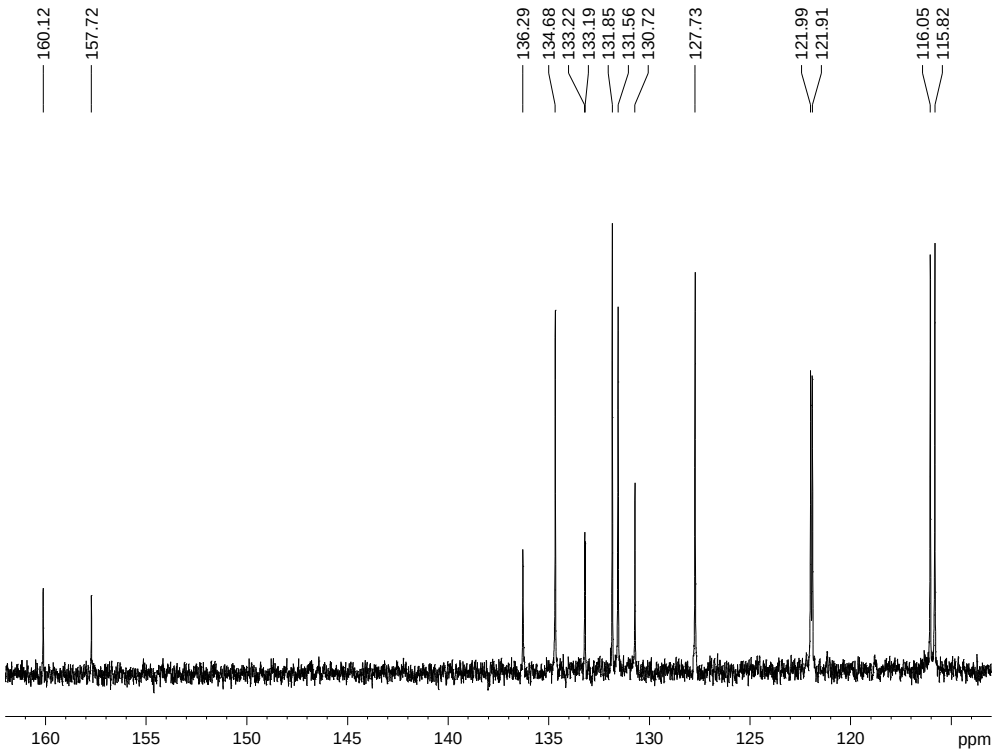

141.59
135.93
135.18
133.70
132.09
131.70
130.70
127.97
118.63
117.91
105.35
CN
O
O
S
N
H
Cl
3h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm


141.59
135.93
135.18
133.70
132.09
131.70
130.70
127.97
118.63
117.91
105.35
140
135
130
125
120
115
110
ppm

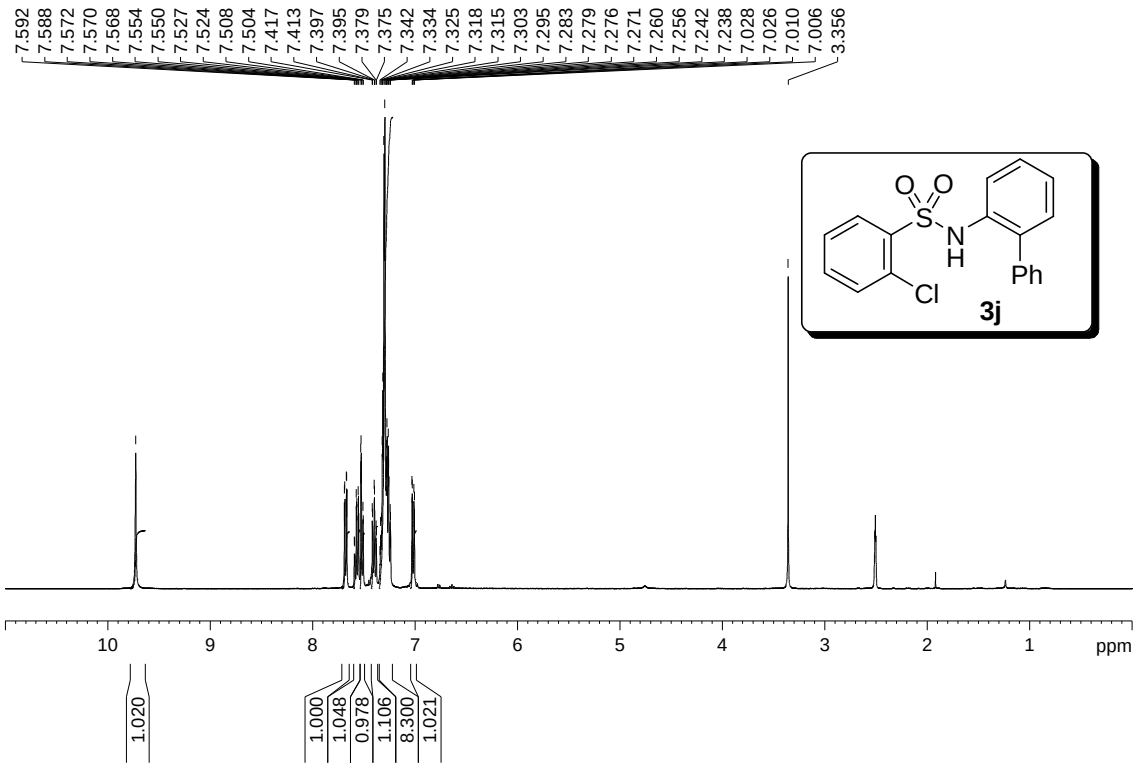
*2-Chloro-N-(4-fluorophenyl)benzenesulfonamide* (**3i**)

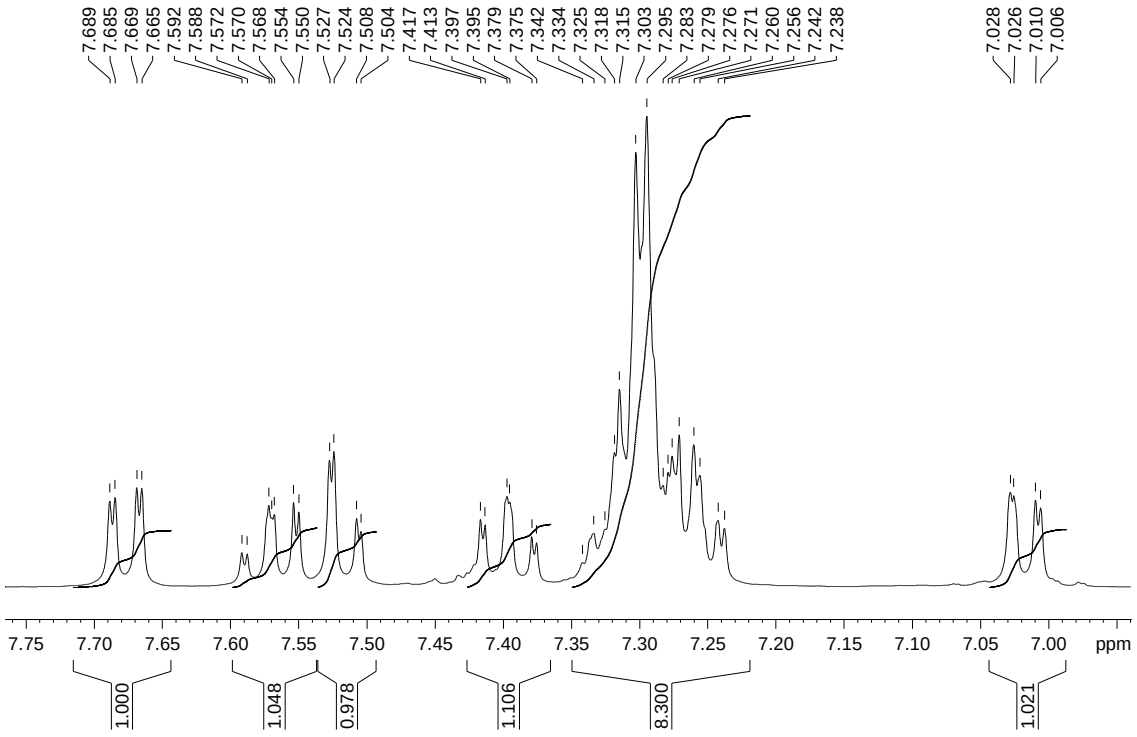


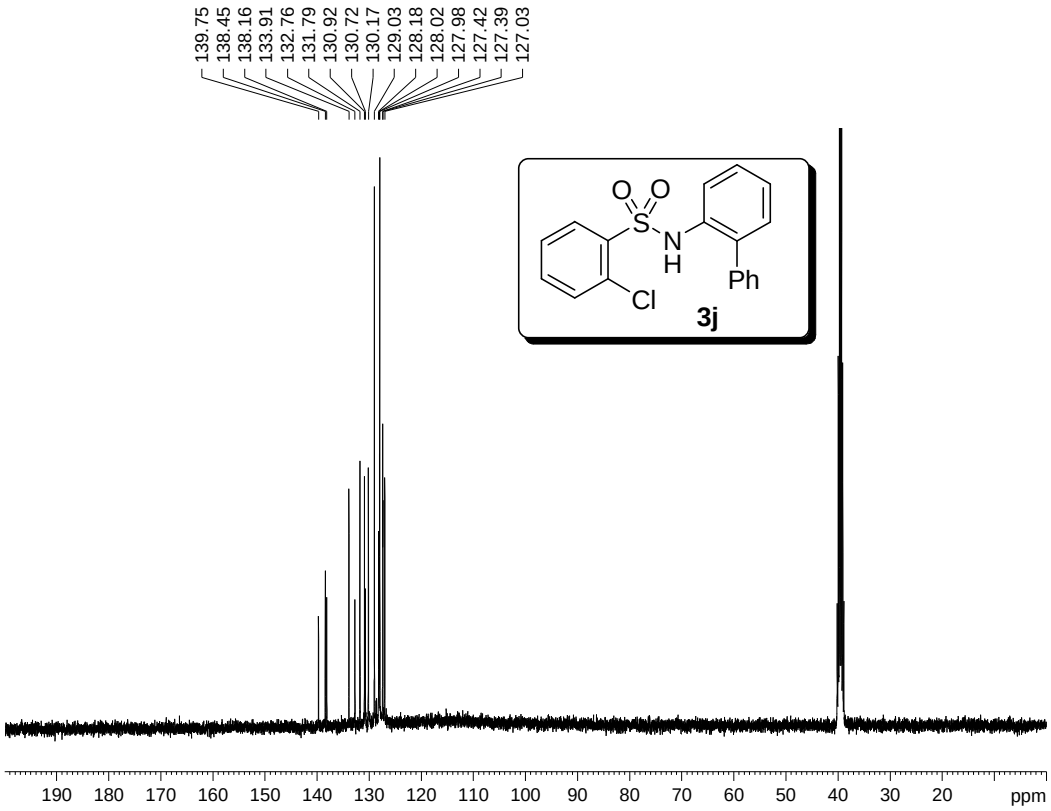

160.12
157.72
136.29
134.68
133.22
133.19
131.85
131.56
130.72
127.73
121.99
121.91
116.05
115.82
O
O
S
N
H
F
Cl
3i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
ppm

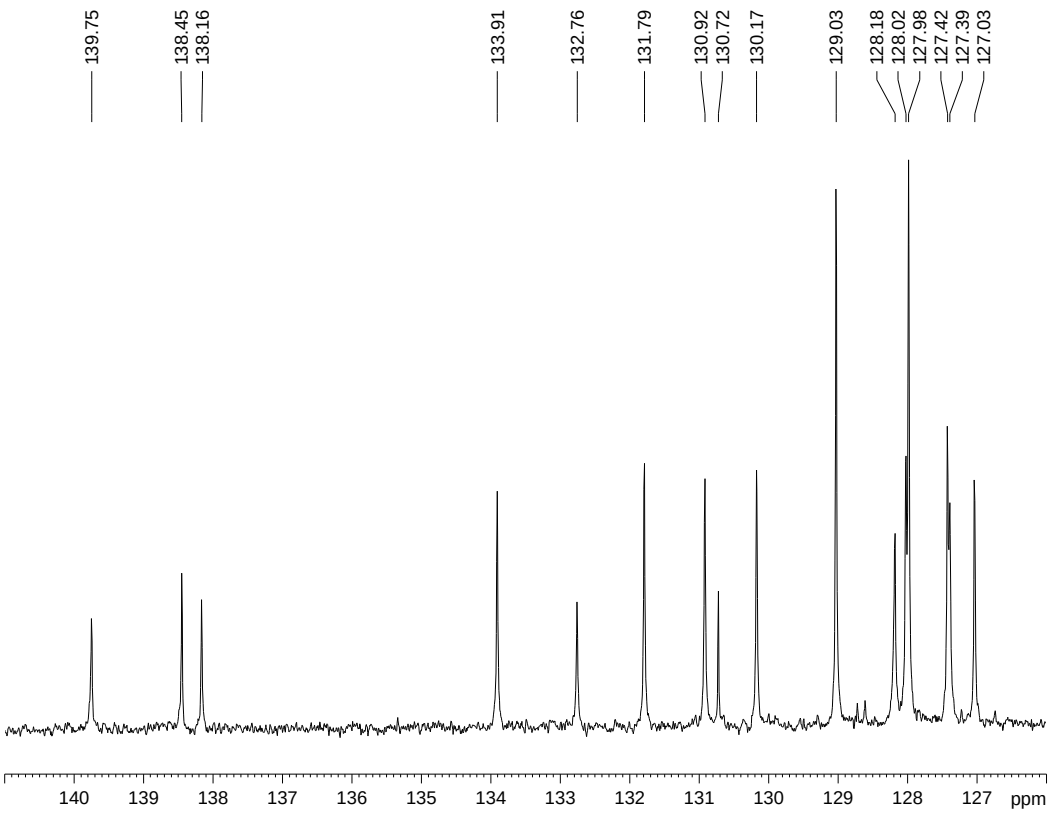

160.12
157.72
136.29
134.68
133.22
133.19
131.85
131.56
130.72
127.73
121.99
121.91
116.05
115.82
160
155
150
145
140
135
130
125
120
ppm

*N-([1,1'-Biphenyl]-2-yl)-2-chlorobenzenesulfonamide* (**3j**)

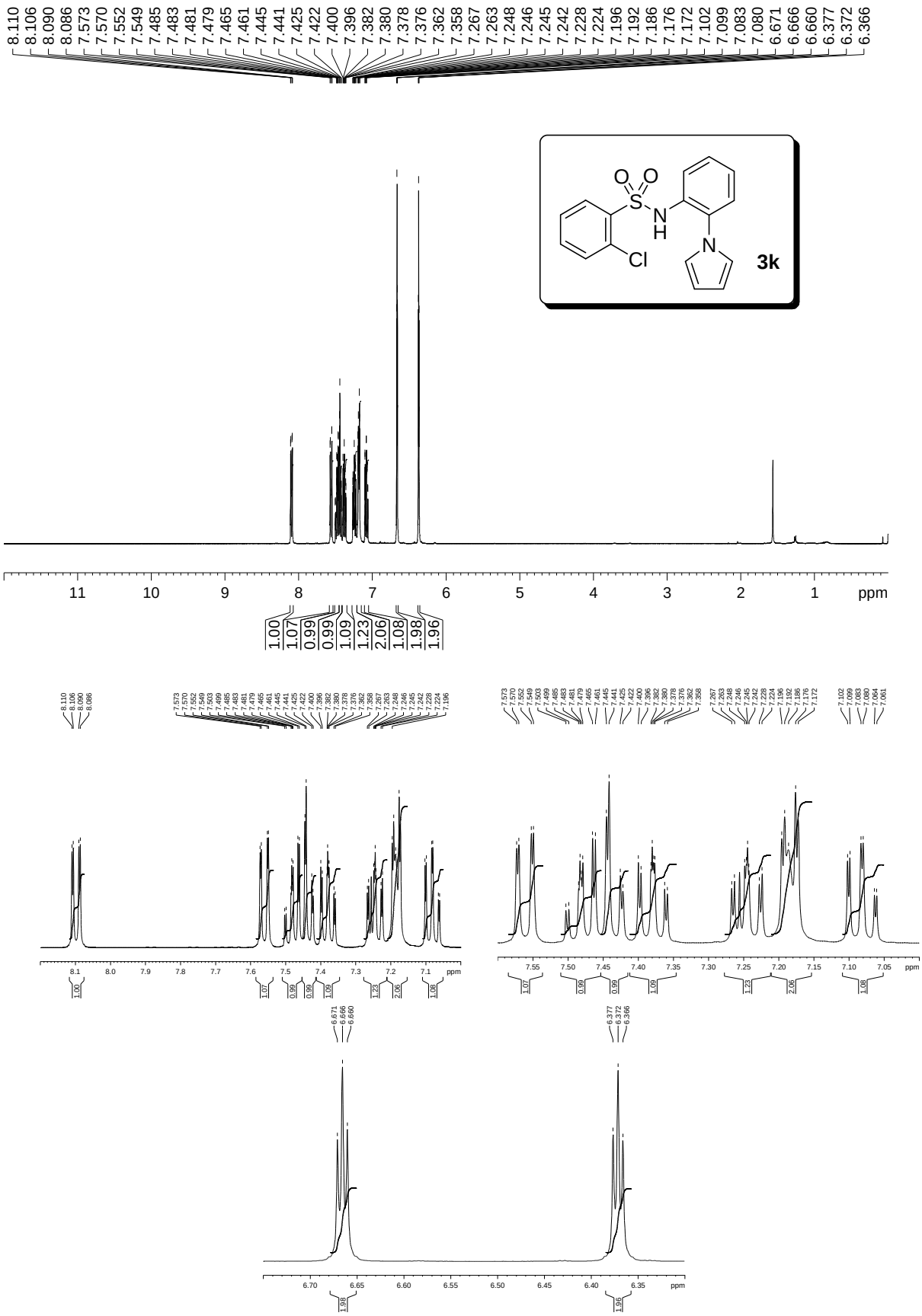


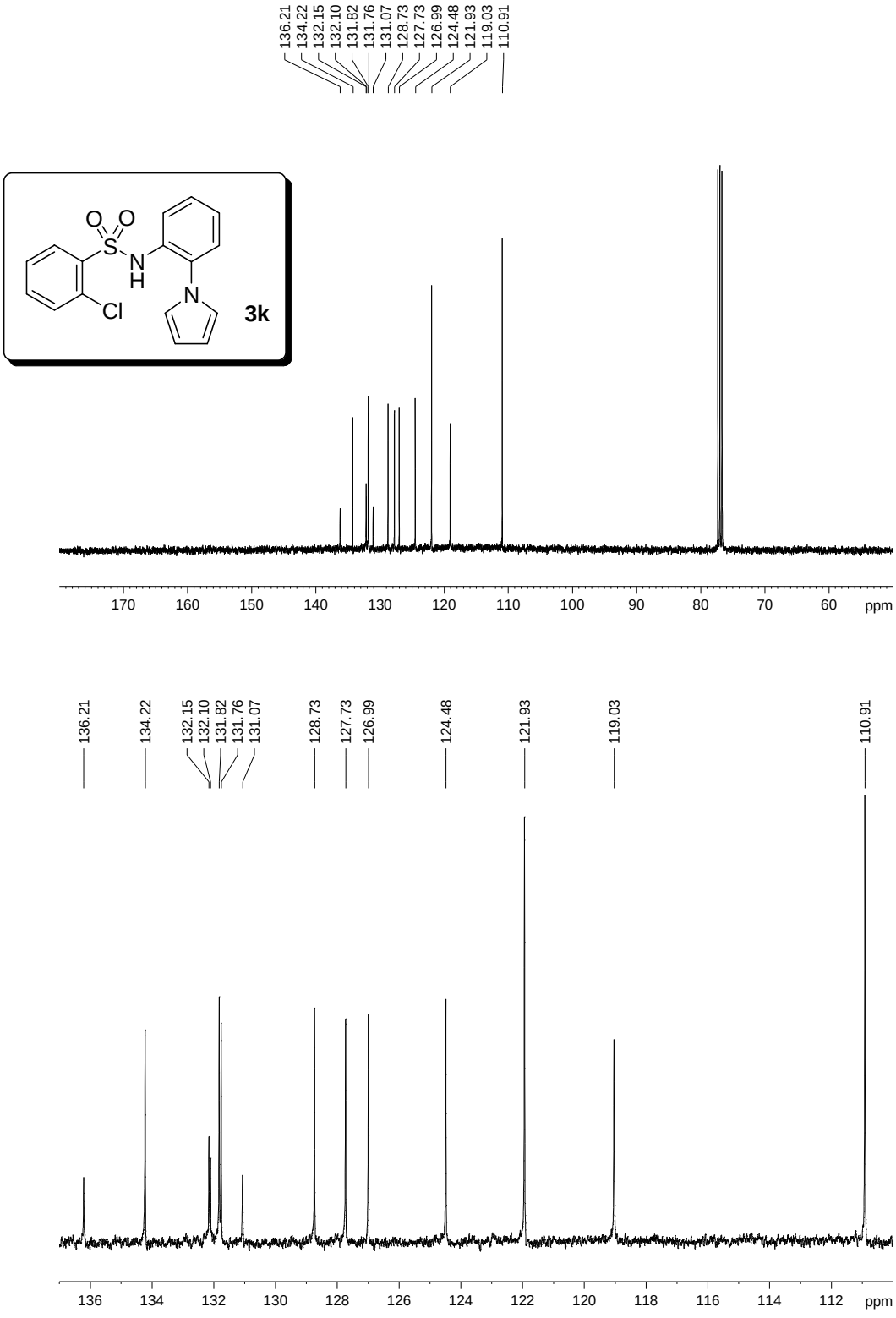




139.75
138.45
138.16
133.91
132.76
131.79
130.92
130.72
130.17
129.03
128.18
128.02
127.98
127.42
127.39
127.03
O
O
S
N
H
Ph
Cl
3j
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

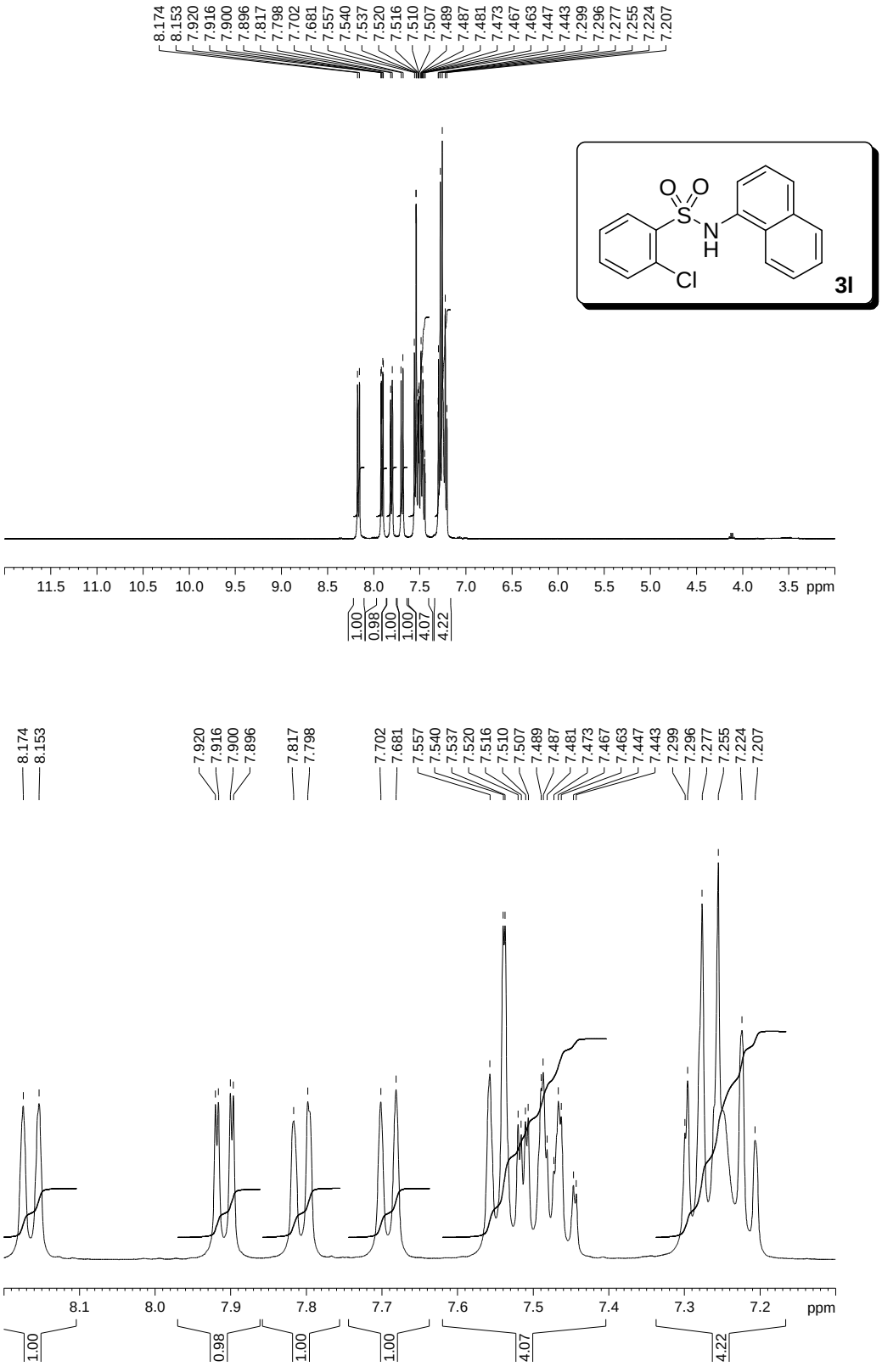

139.75
138.45
138.16
133.91
132.76
131.79
130.92
130.72
130.17
129.03
128.18
128.02
127.98
127.42
127.39
127.03
140 139 138 137 136 135 134 133 132 131 130 129 128 127 ppm

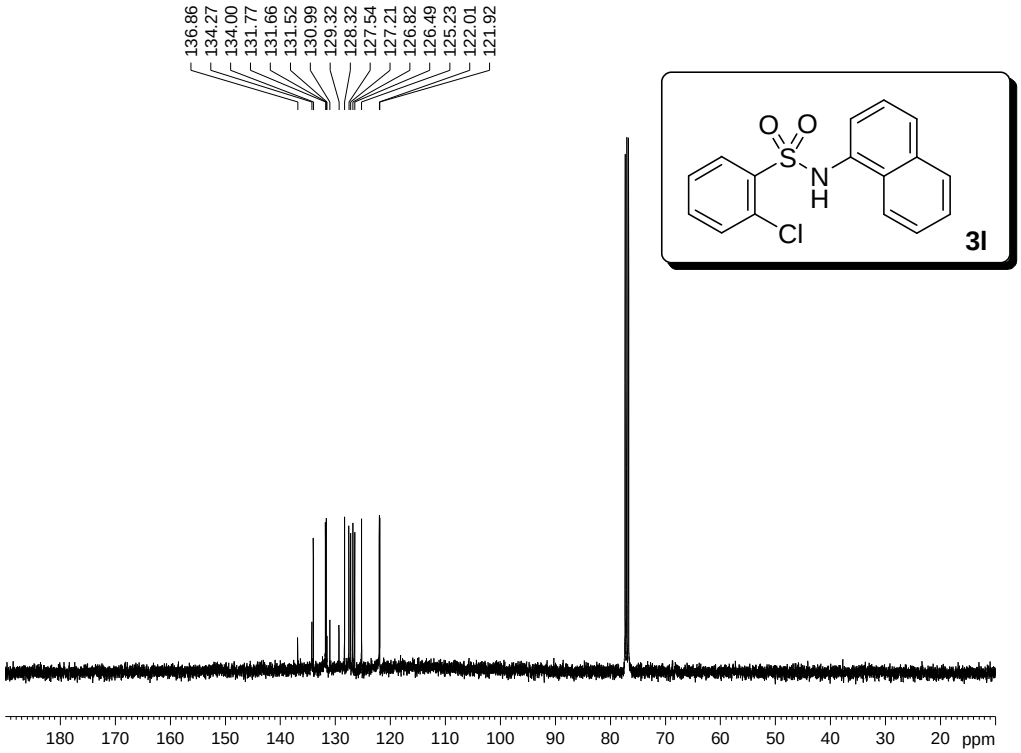
*N-(2-(1H-Pyrrol-1-yl)phenyl)-2-chlorobenzenesulfonamide* (**3k**)

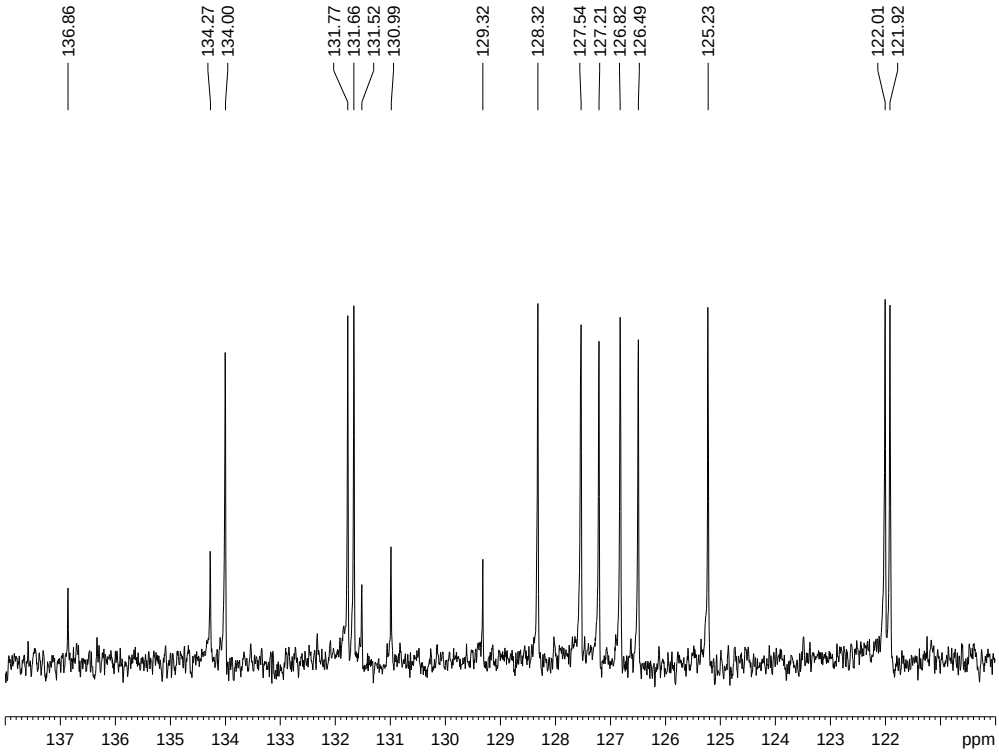



136.21
134.22
132.15
132.10
131.82
131.76
131.07
128.73
127.73
126.99
124.48
121.93
119.03
110.91
O
O
S
N
H
Cl
N
3k
170
160
150
140
130
120
110
100
90
80
70
60
ppm
136
134
132
130
128
126
124
122
120
118
116
114
112
ppm

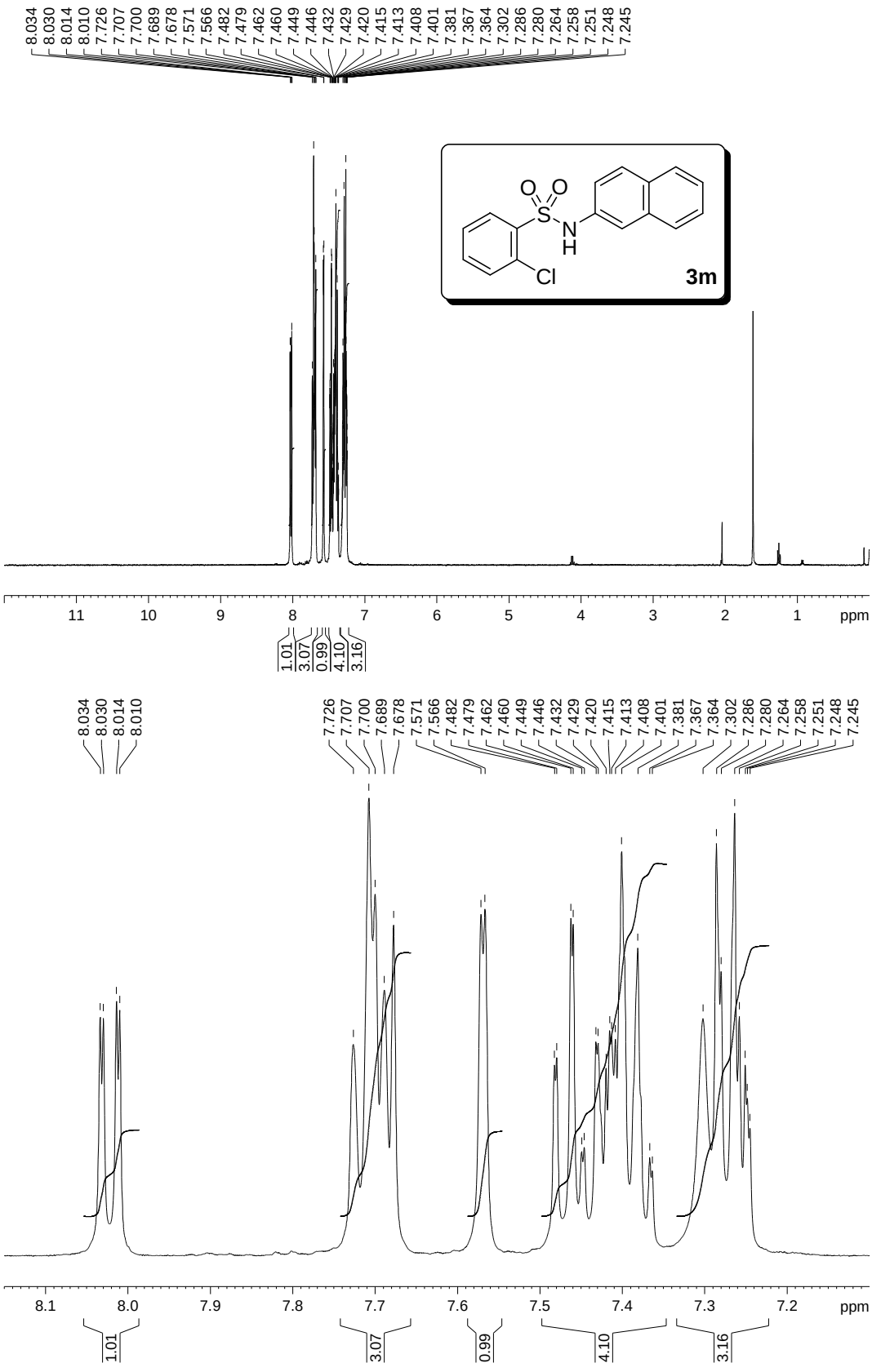
*2-Chloro-N-(naphthalen-1-yl)benzenesulfonamide* (**3l**)

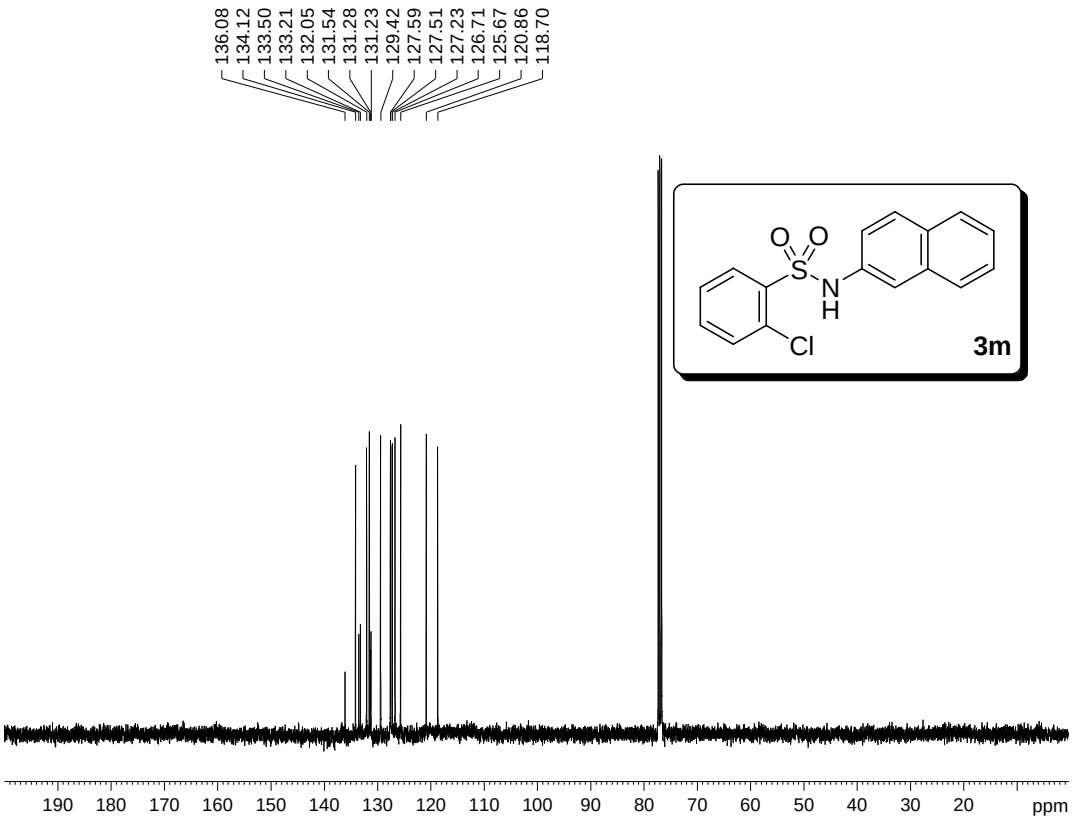


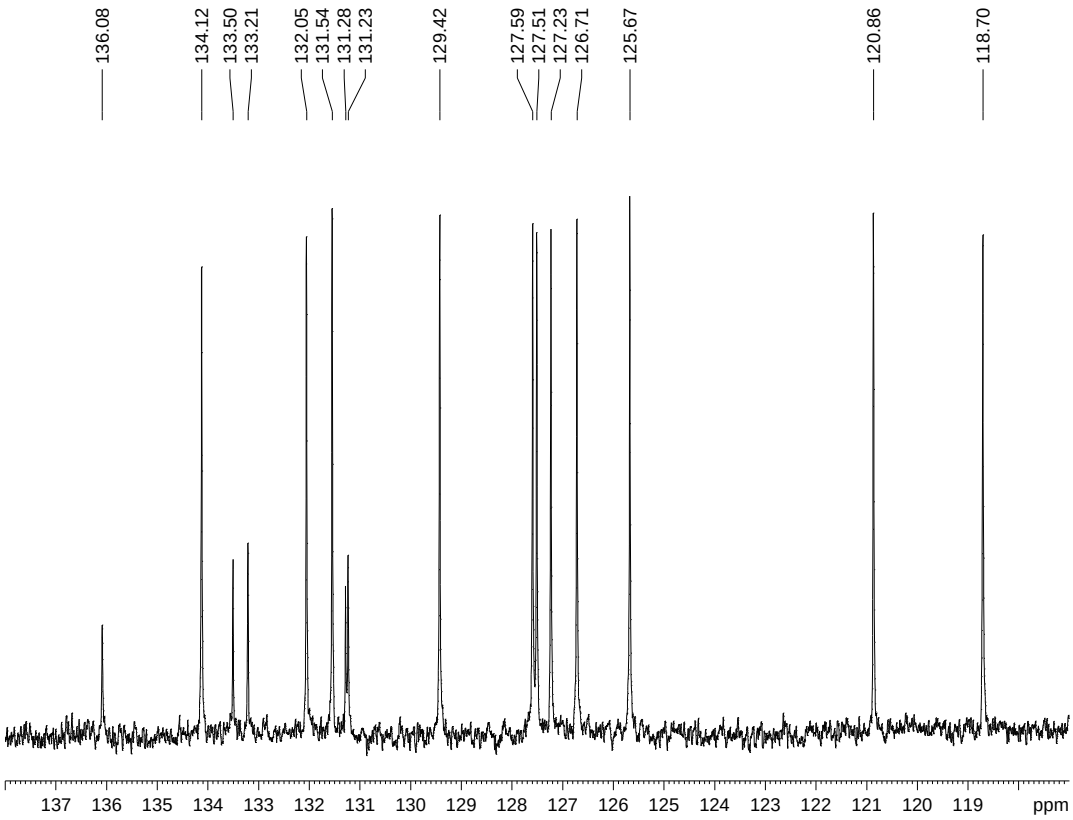

136.86
134.27
134.00
131.77
131.66
131.52
130.99
129.32
128.32
127.54
127.21
126.82
126.49
125.23
122.01
121.92
O
O
S
N
H
Cl
3l
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


136.86
134.27
134.00
131.77
131.66
131.52
130.99
129.32
128.32
127.54
127.21
126.82
126.49
125.23
122.01
121.92
137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 ppm

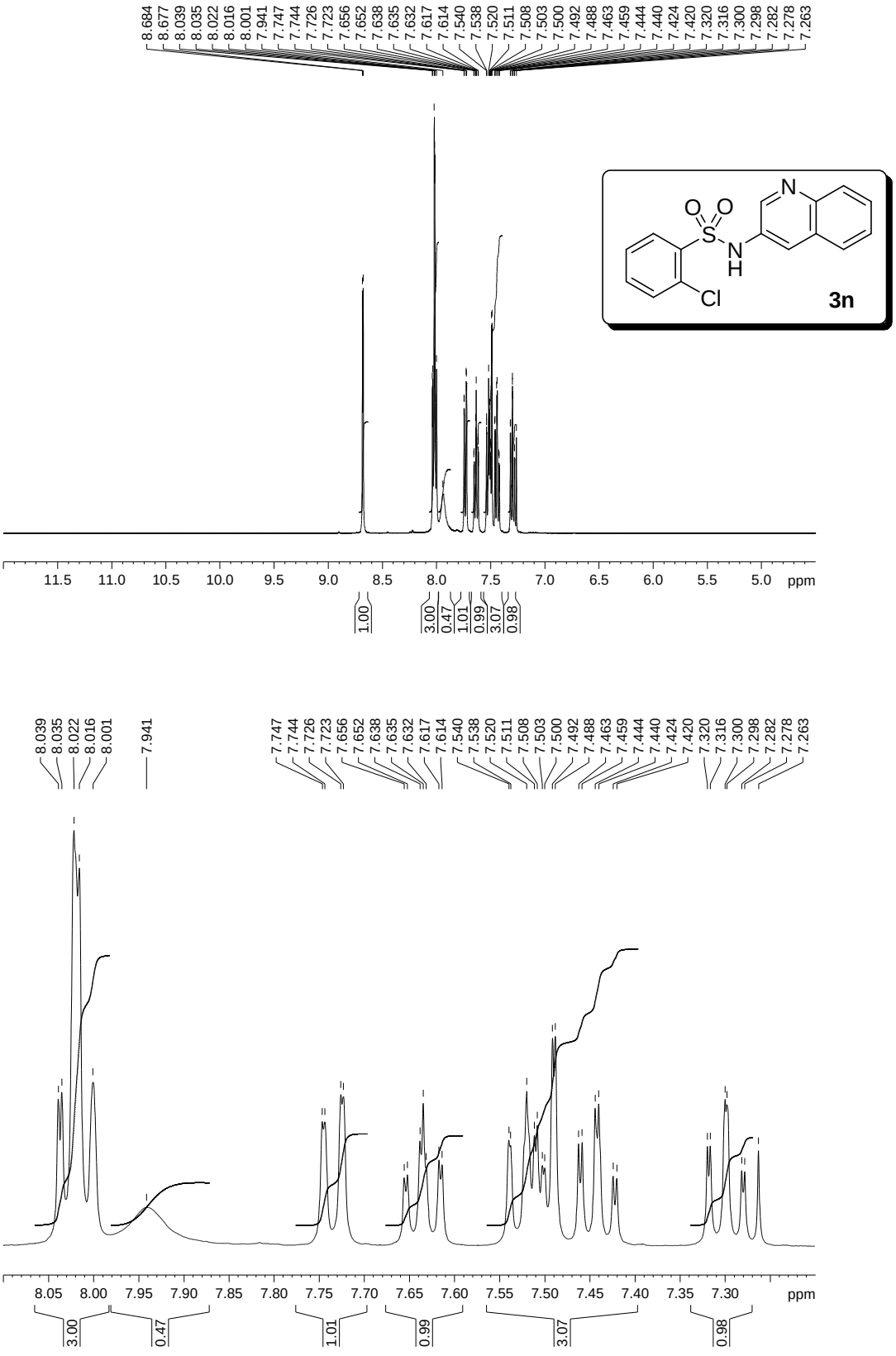
*2-Chloro-N-(naphthalen-2-yl)benzenesulfonamide* (**3m**)

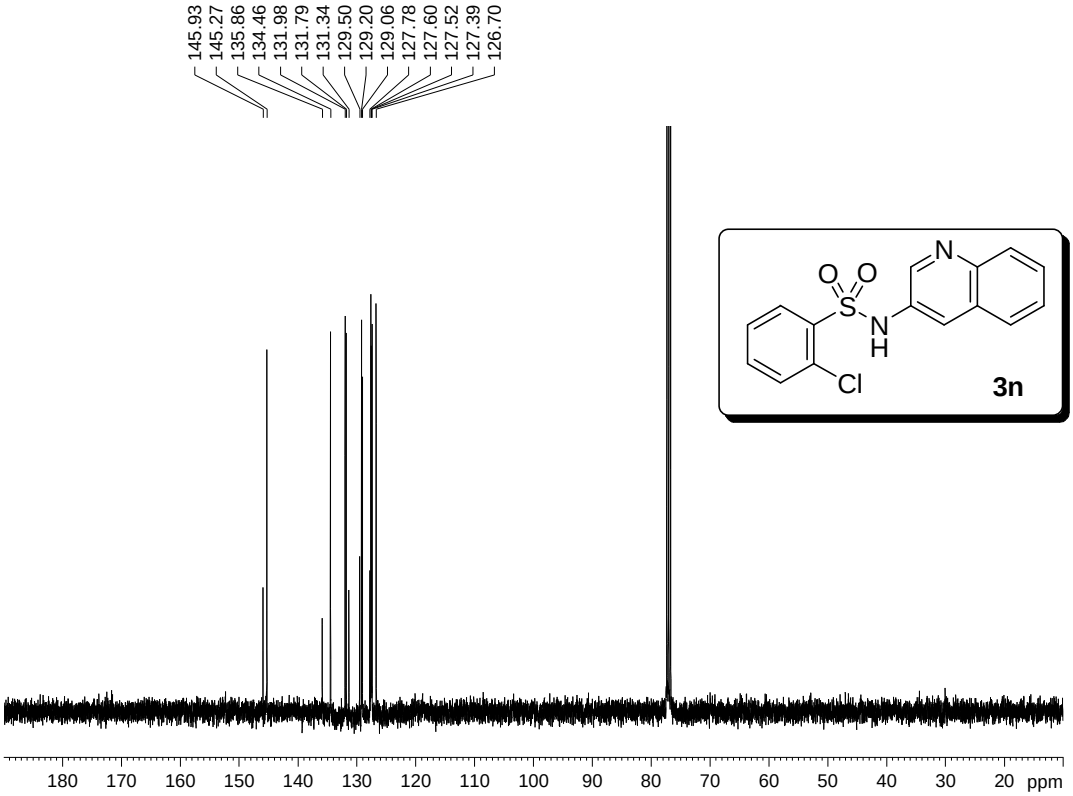


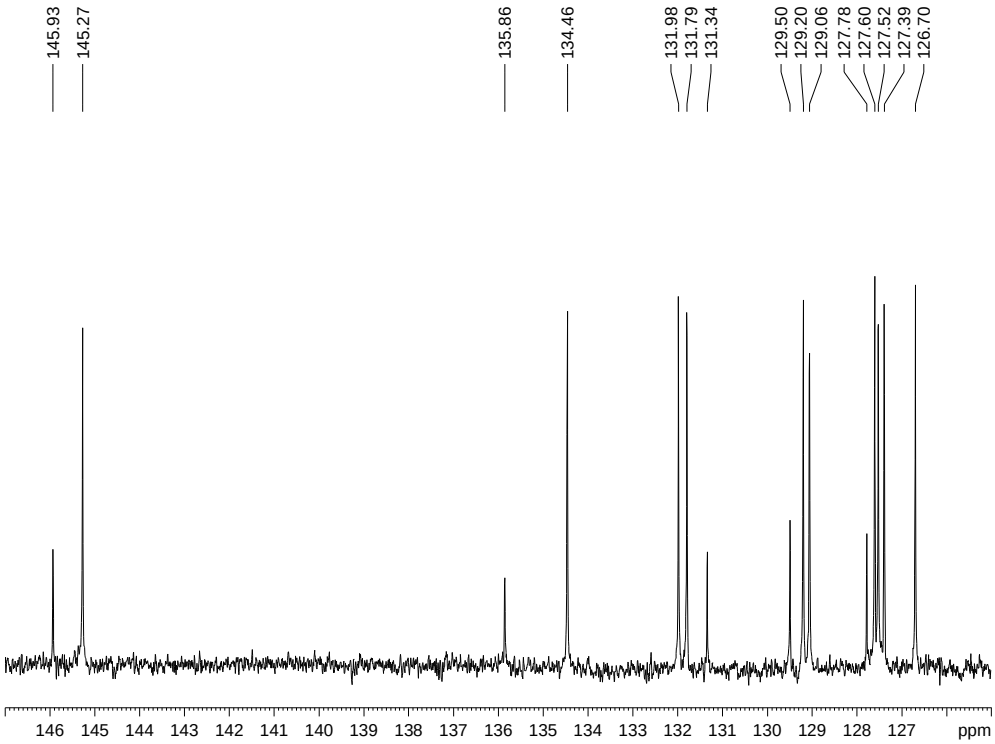

136.08
134.12
133.50
133.21
132.05
131.54
131.28
131.23
129.42
127.59
127.51
127.23
126.71
125.67
120.86
118.70
O
O
S
N
H
Cl
3m
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


136.08
134.12
133.50
133.21
132.05
131.54
131.28
131.23
129.42
127.59
127.51
127.23
126.71
125.67
120.86
118.70
137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 120 119 ppm

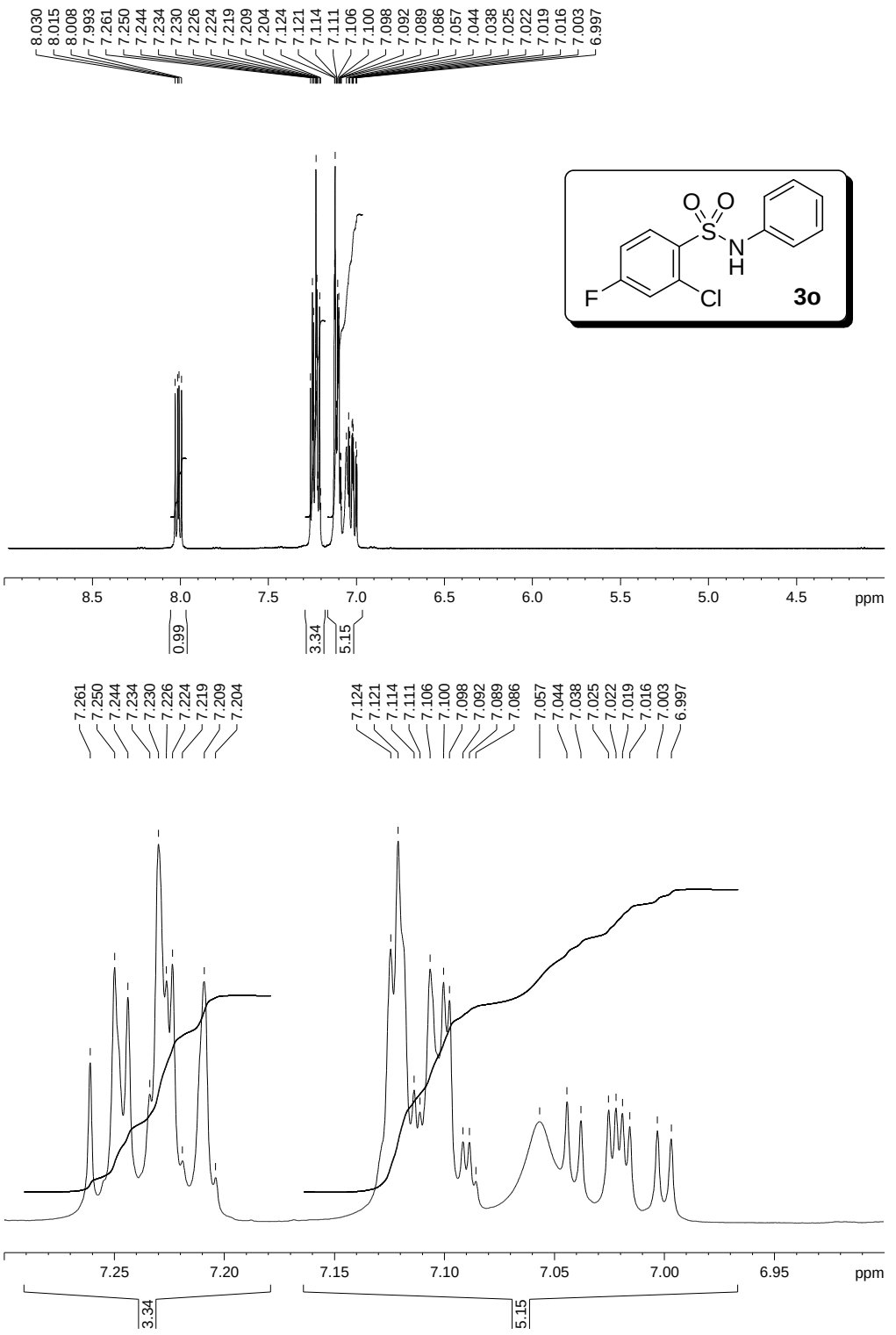
*2-Chloro-N-(quinolin-3-yl)benzenesulfonamide* (**3n**)

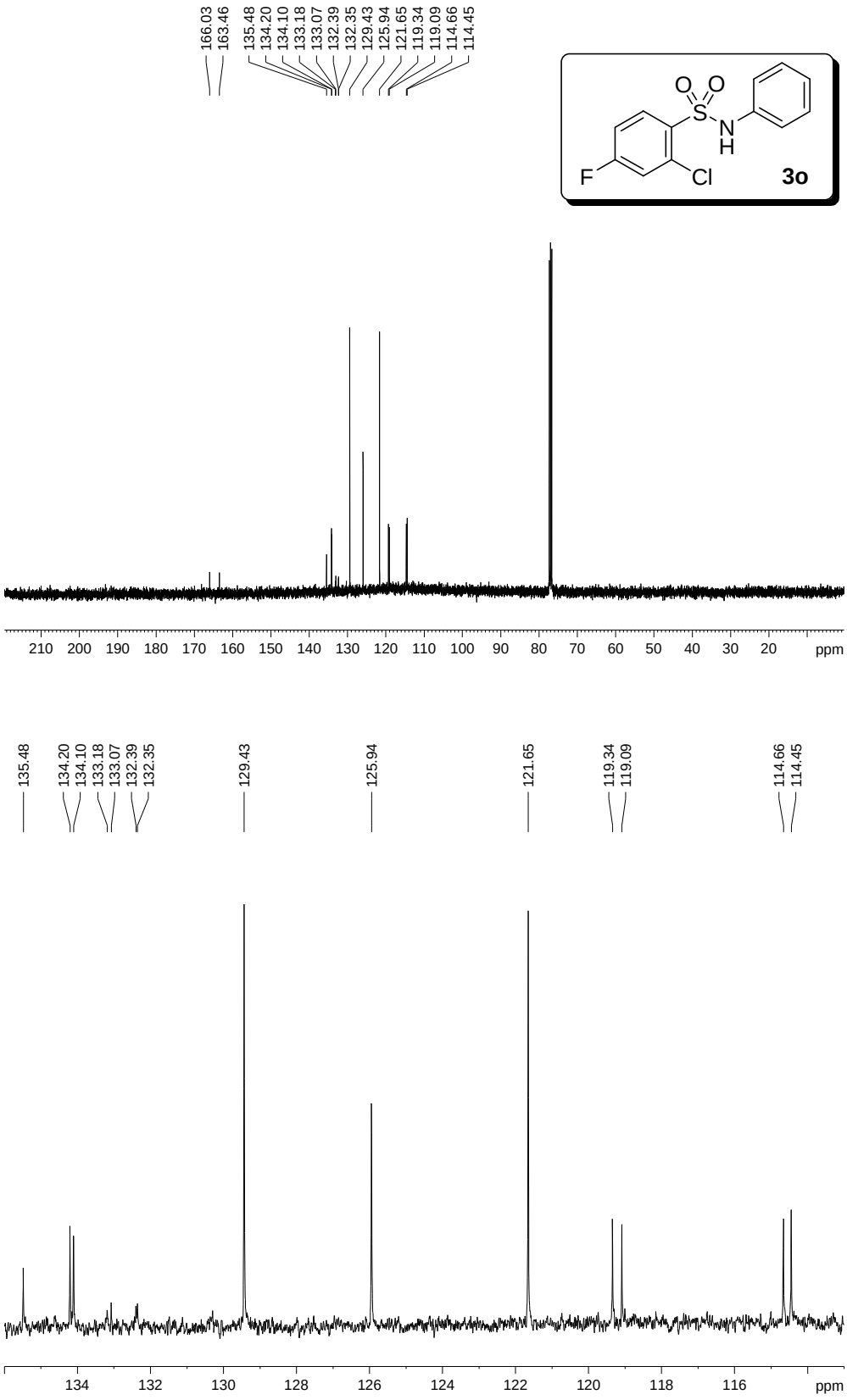



145.93
145.27
135.86
134.46
131.98
131.79
131.34
129.50
129.20
129.06
127.78
127.60
127.52
127.39
126.70
O
O
S
N
H
N
Cl
3n
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

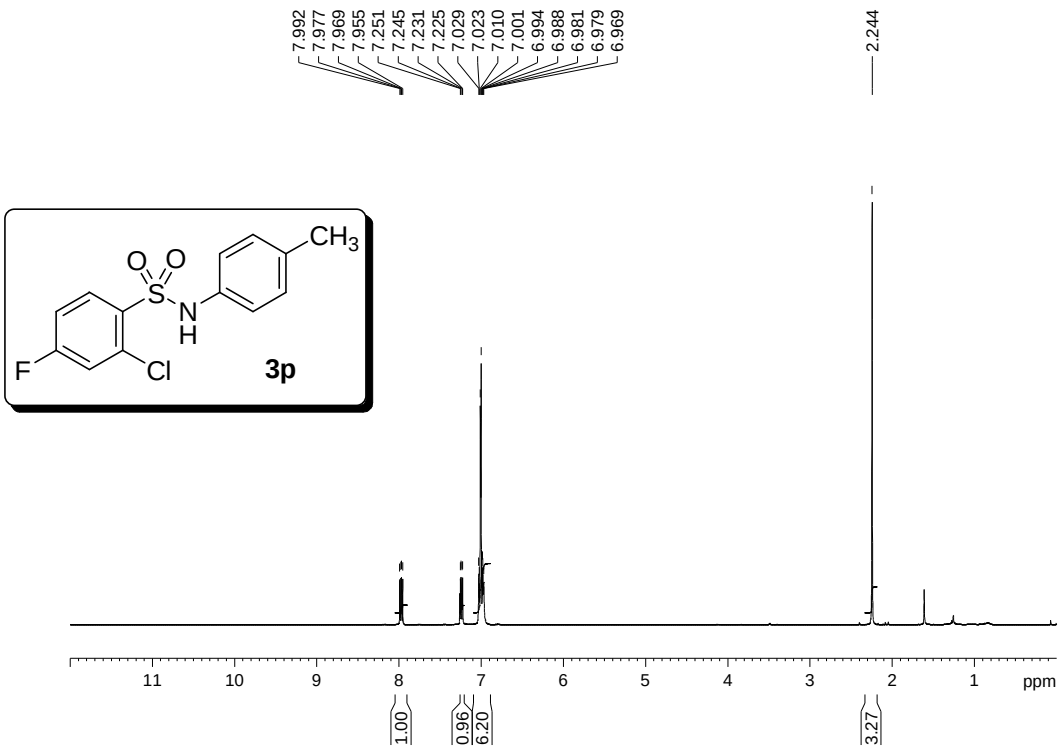

145.93
145.27
135.86
134.46
131.98
131.79
131.34
129.50
129.20
129.06
127.78
127.60
127.52
127.39
126.70
146 145 144 143 142 141 140 139 138 137 136 135 134 133 132 131 130 129 128 127 ppm

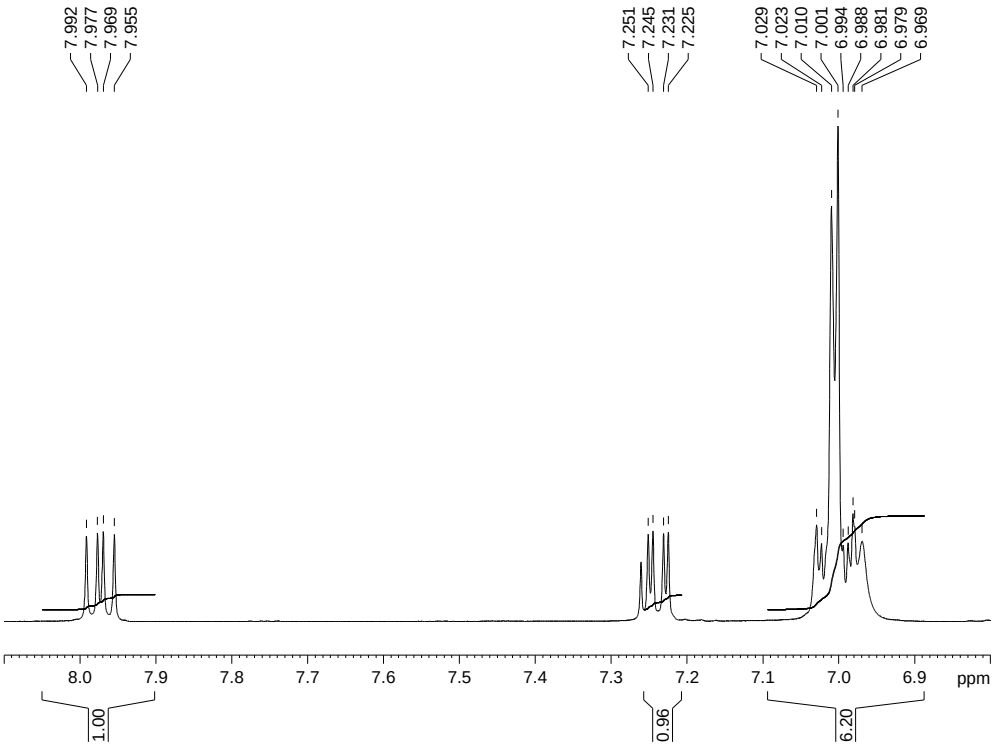
*2-Chloro-4-fluoro-N-phenylbenzenesulfonamide* (**3o**)

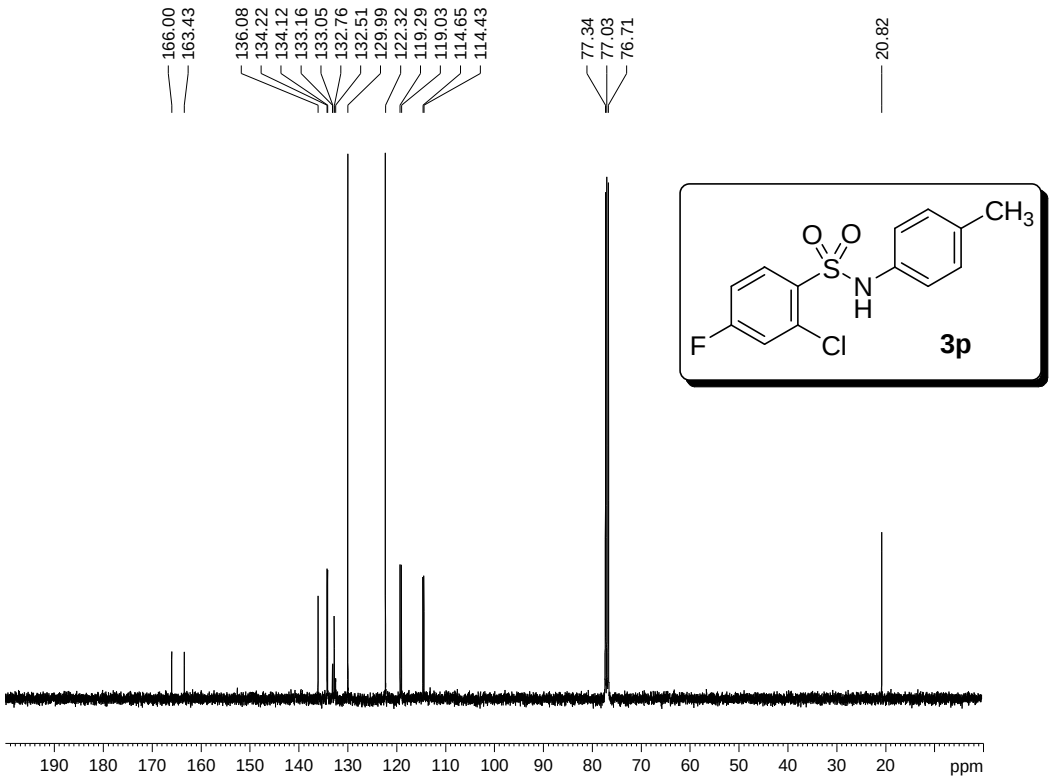


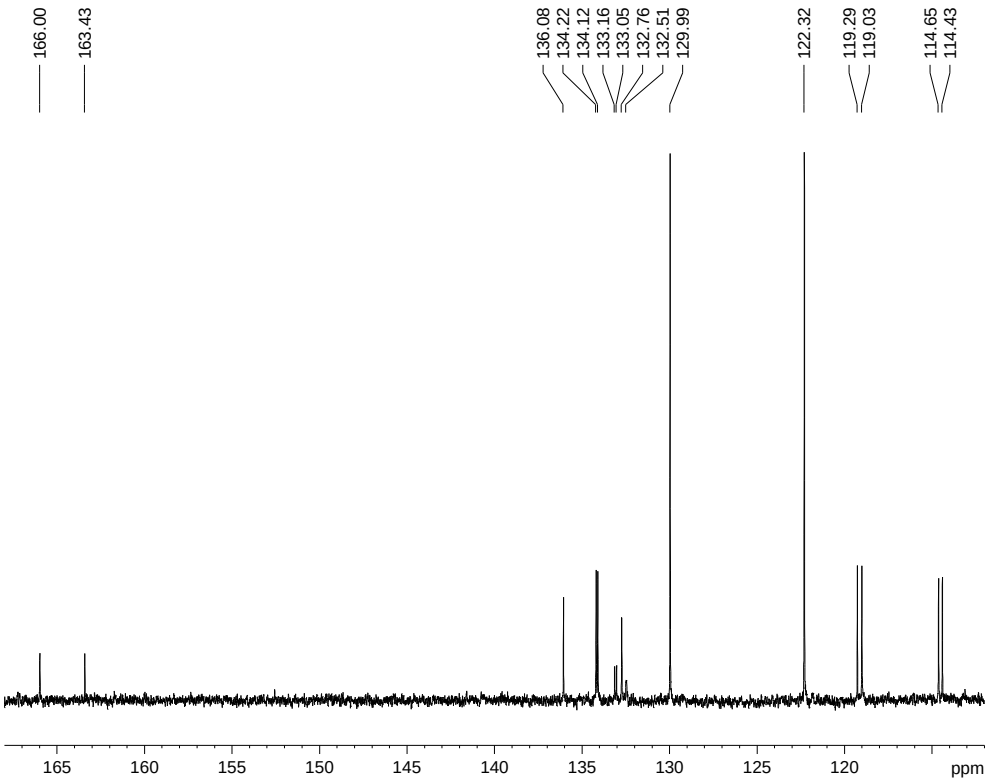

166.03
163.46
135.48
134.20
134.10
133.18
133.07
132.39
132.35
129.43
125.94
121.65
119.34
119.09
114.66
114.45
O
O
S
N
H
F
Cl
3o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
134 132 130 128 126 124 122 120 118 116 ppm

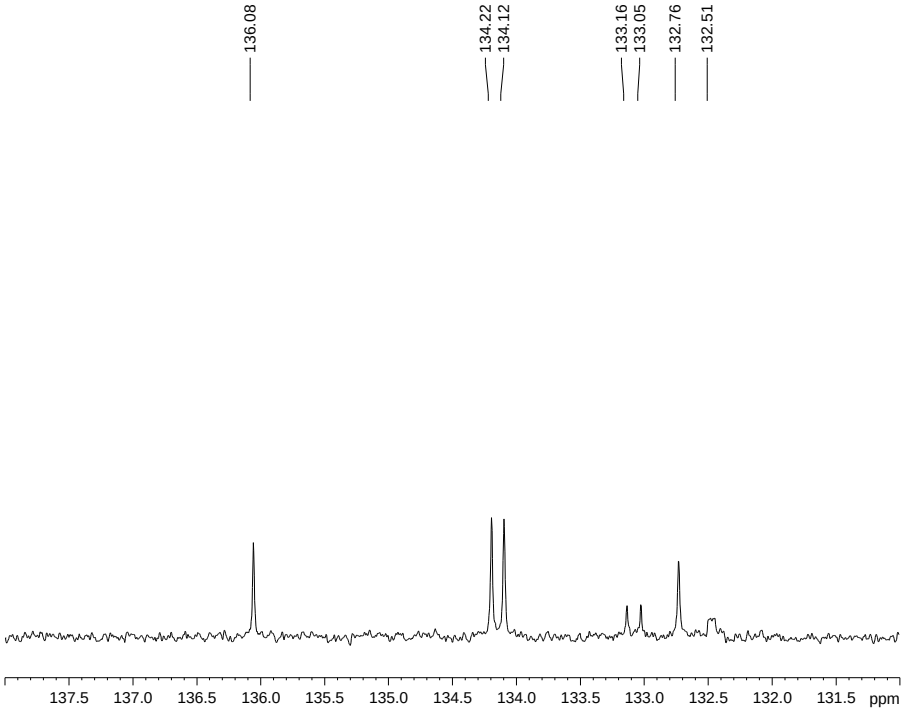
*2-Chloro-4-fluoro-N-(p-tolyl)benzenesulfonamide* (**3p**)



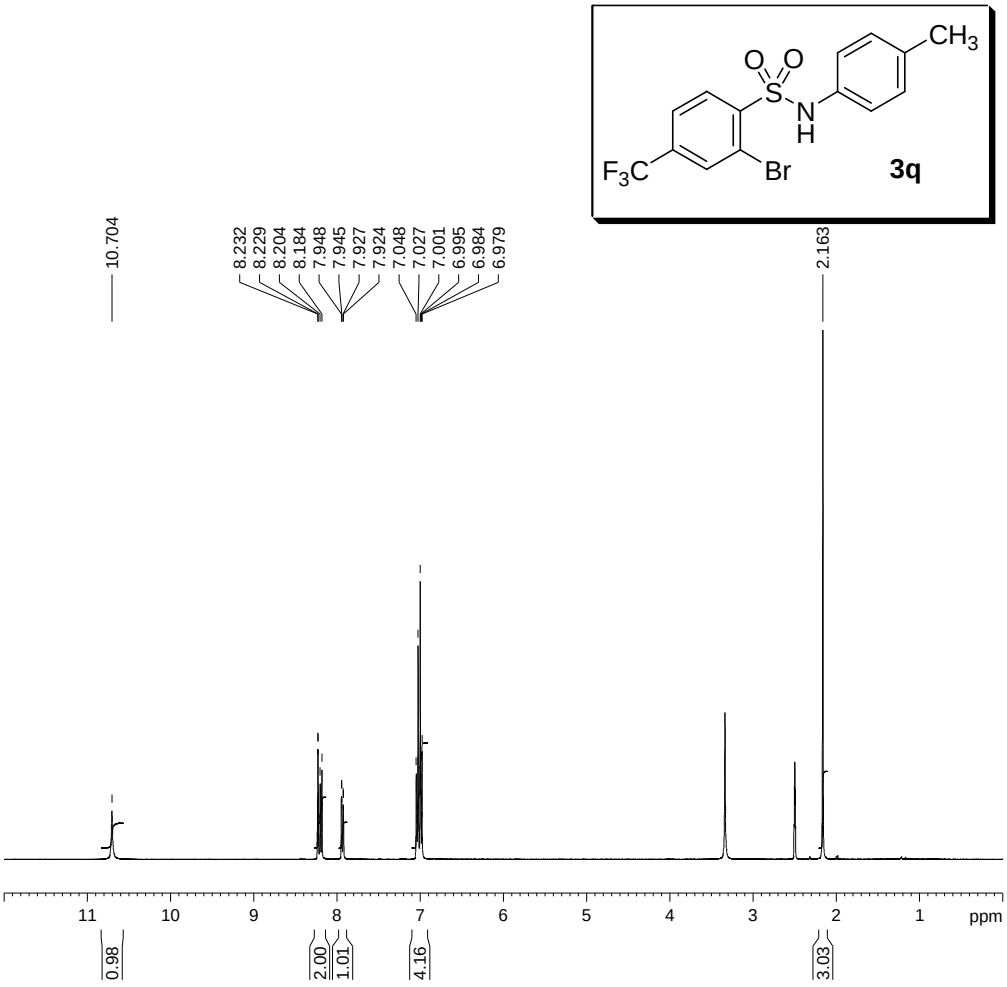



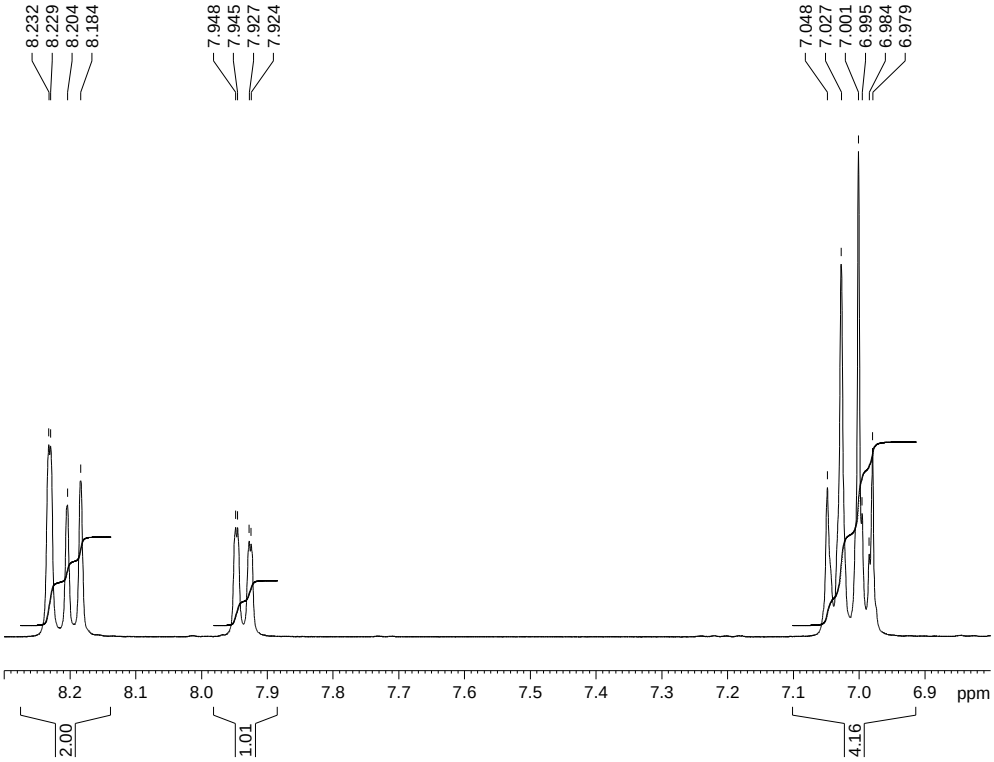

166.00
163.43
136.08
134.22
134.12
133.16
133.05
132.76
132.51
129.99
122.32
119.29
119.03
114.65
114.43
77.34
77.03
76.71
20.82
CH3
O
O
S
N
H
F
Cl
3p
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

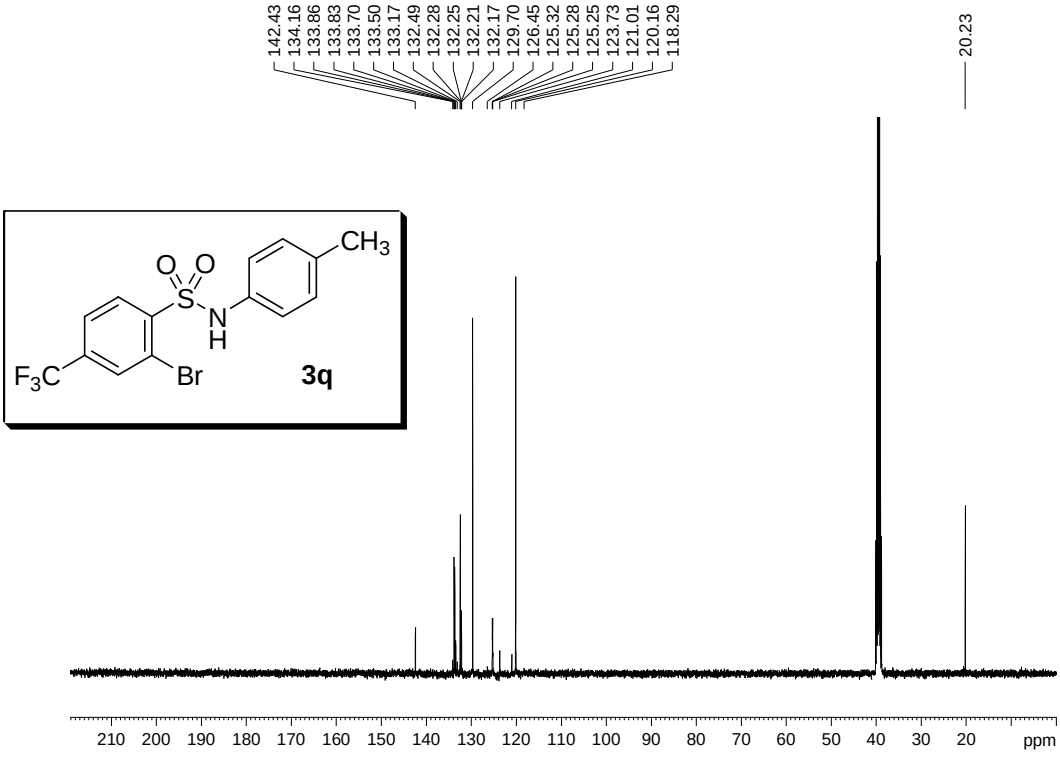

166.00
163.43
136.08
134.22
134.12
133.16
133.05
132.76
132.51
129.99
122.32
119.29
119.03
114.65
114.43
165 160 155 150 145 140 135 130 125 120 ppm

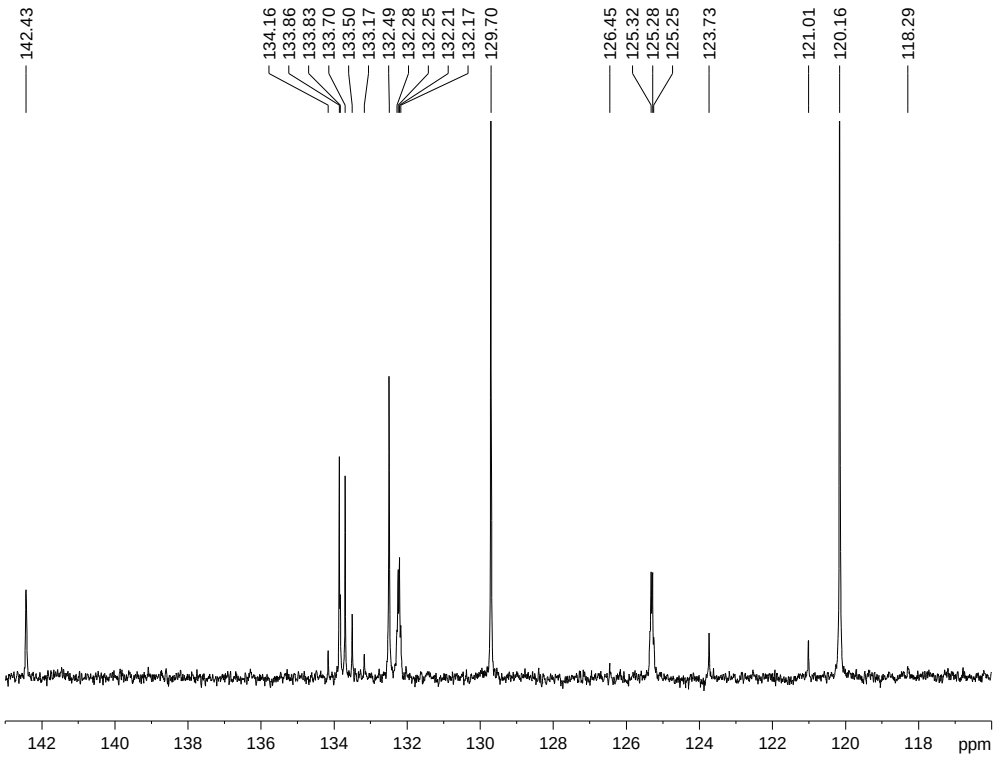


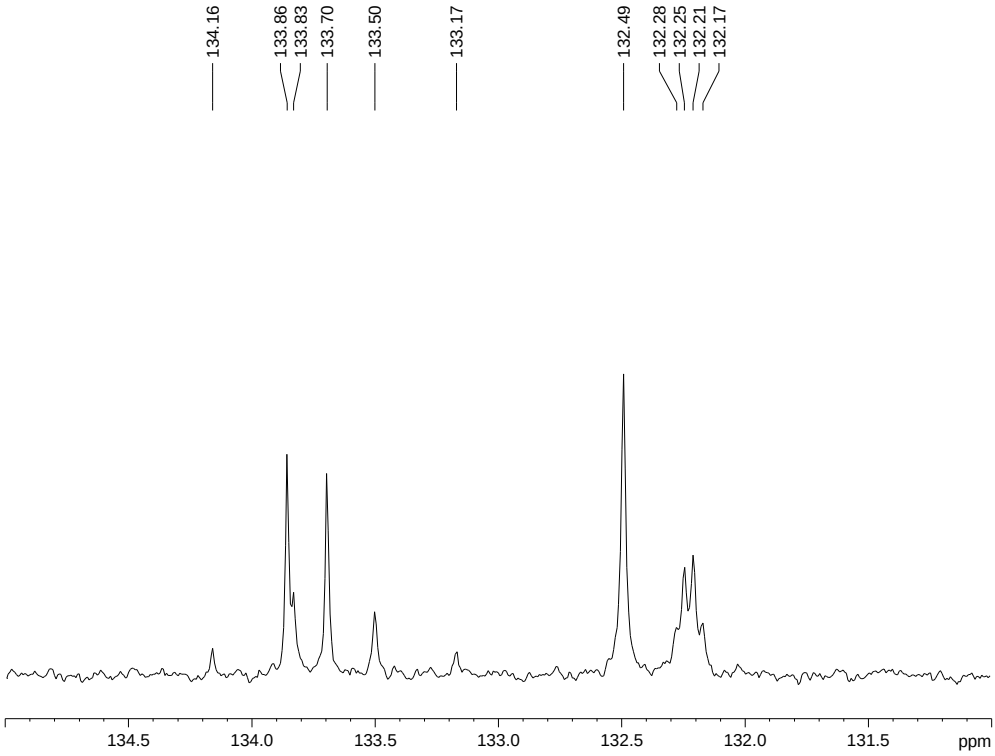

*2-Bromo-N-(p-tolyl)-4-(trifluoromethyl)benzenesulfonamide* (**3q**)

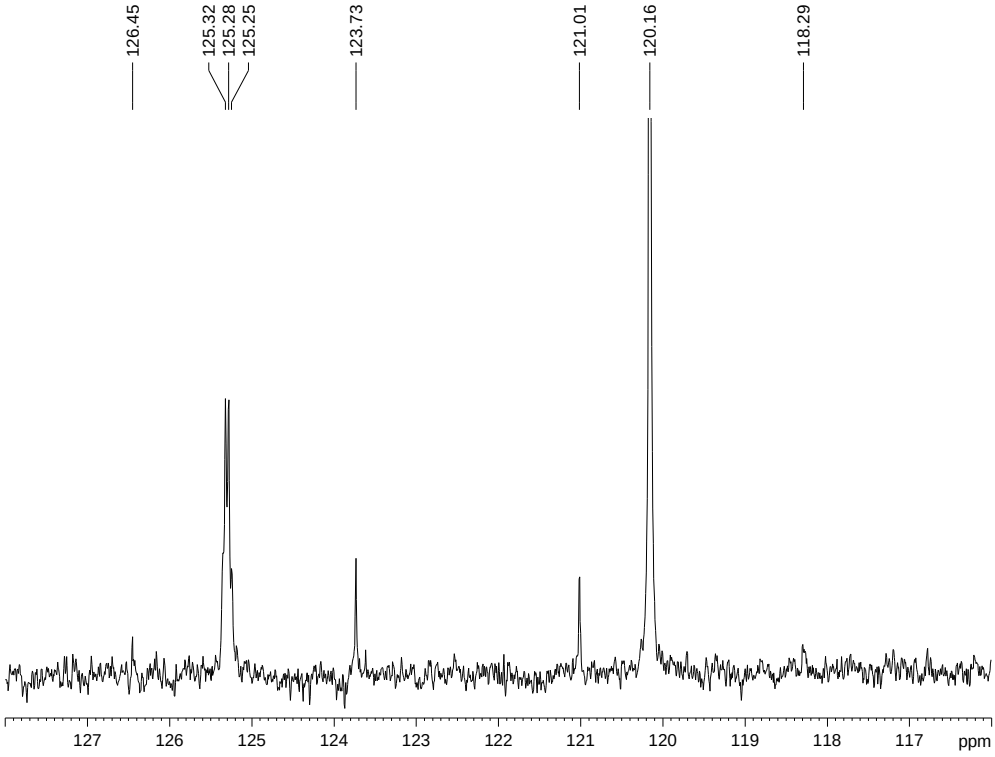



8.232
8.229
8.204
8.184
7.948
7.945
7.927
7.924
7.048
7.027
7.001
6.995
6.984
6.979
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
ppm
2.00
1.01
4.16

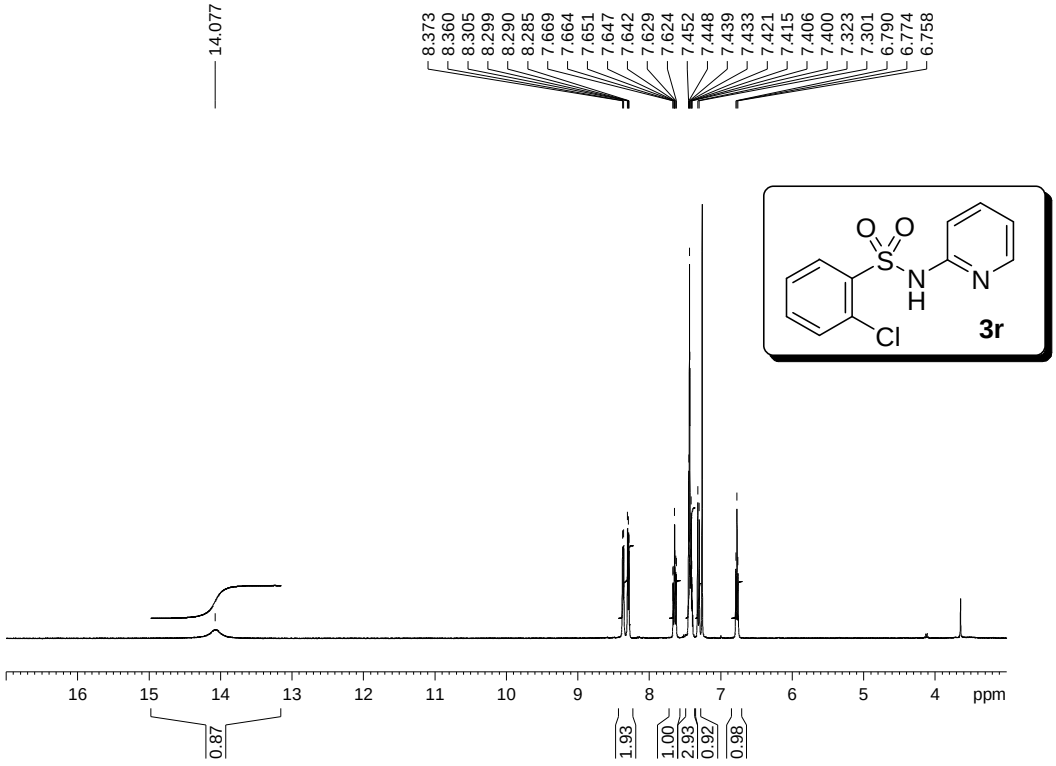

142.43
134.16
133.86
133.83
133.70
133.50
133.17
132.49
132.28
132.25
132.21
132.17
129.70
126.45
125.32
125.28
125.25
123.73
121.01
120.16
118.29
20.23
CH3
O
O
S
N
H
F3C
Br
3q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

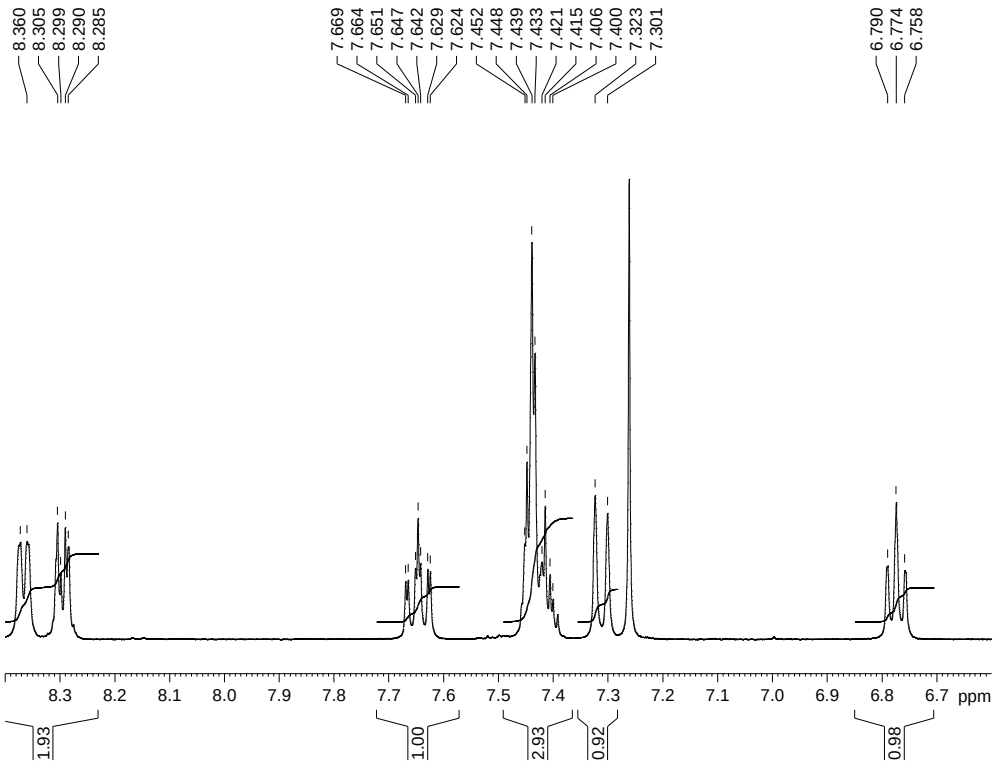

142.43
134.16
133.86
133.83
133.70
133.50
133.17
132.49
132.28
132.25
132.21
132.17
129.70
126.45
125.32
125.28
125.25
123.73
121.01
120.16
118.29
142
140
138
136
134
132
130
128
126
124
122
120
118
ppm

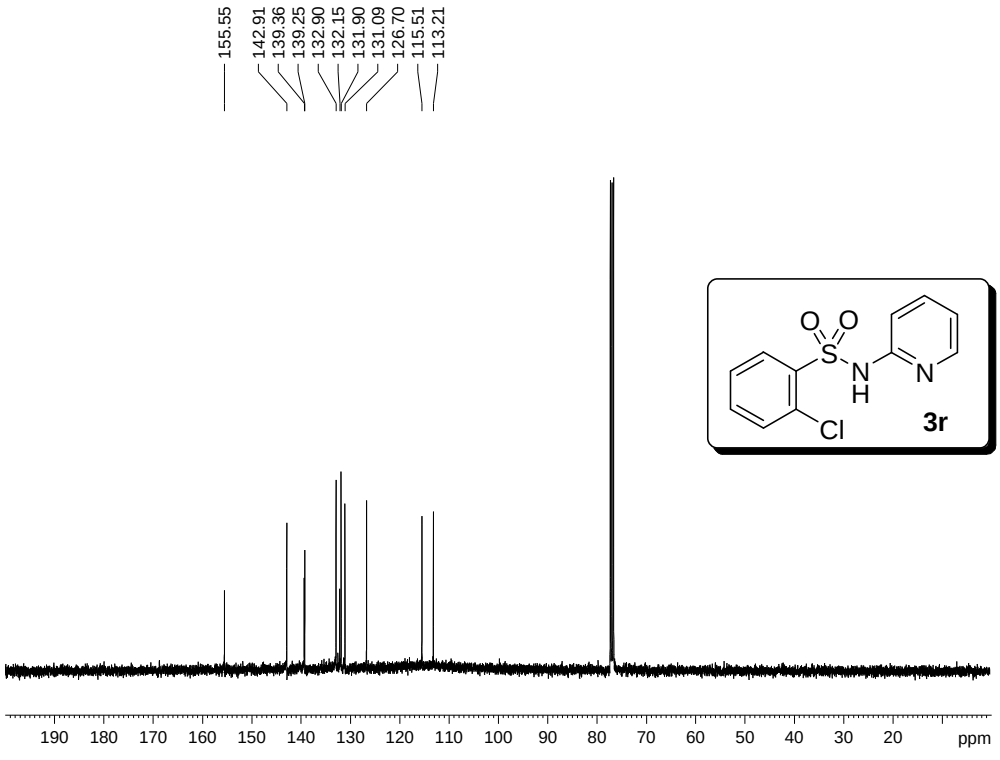

134.16
133.86
133.83
133.70
133.50
133.17
132.49
132.28
132.25
132.21
132.17
134.5
134.0
133.5
133.0
132.5
132.0
131.5
ppm

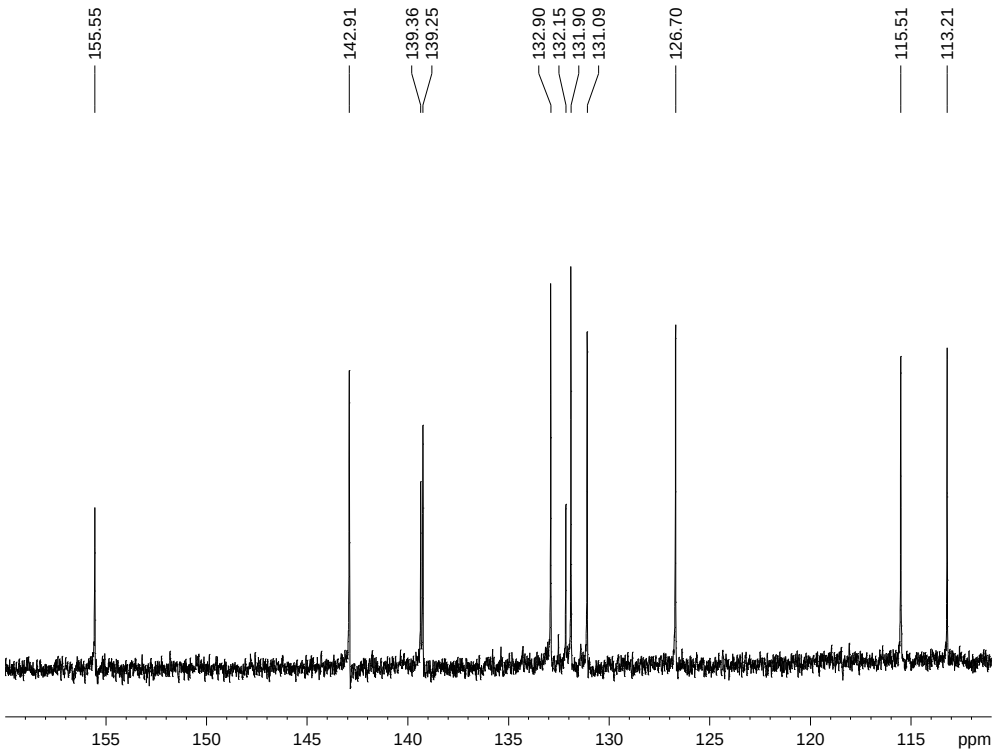



*2-Chloro-N-(pyridin-2-yl)benzenesulfonamide* (**3r**)



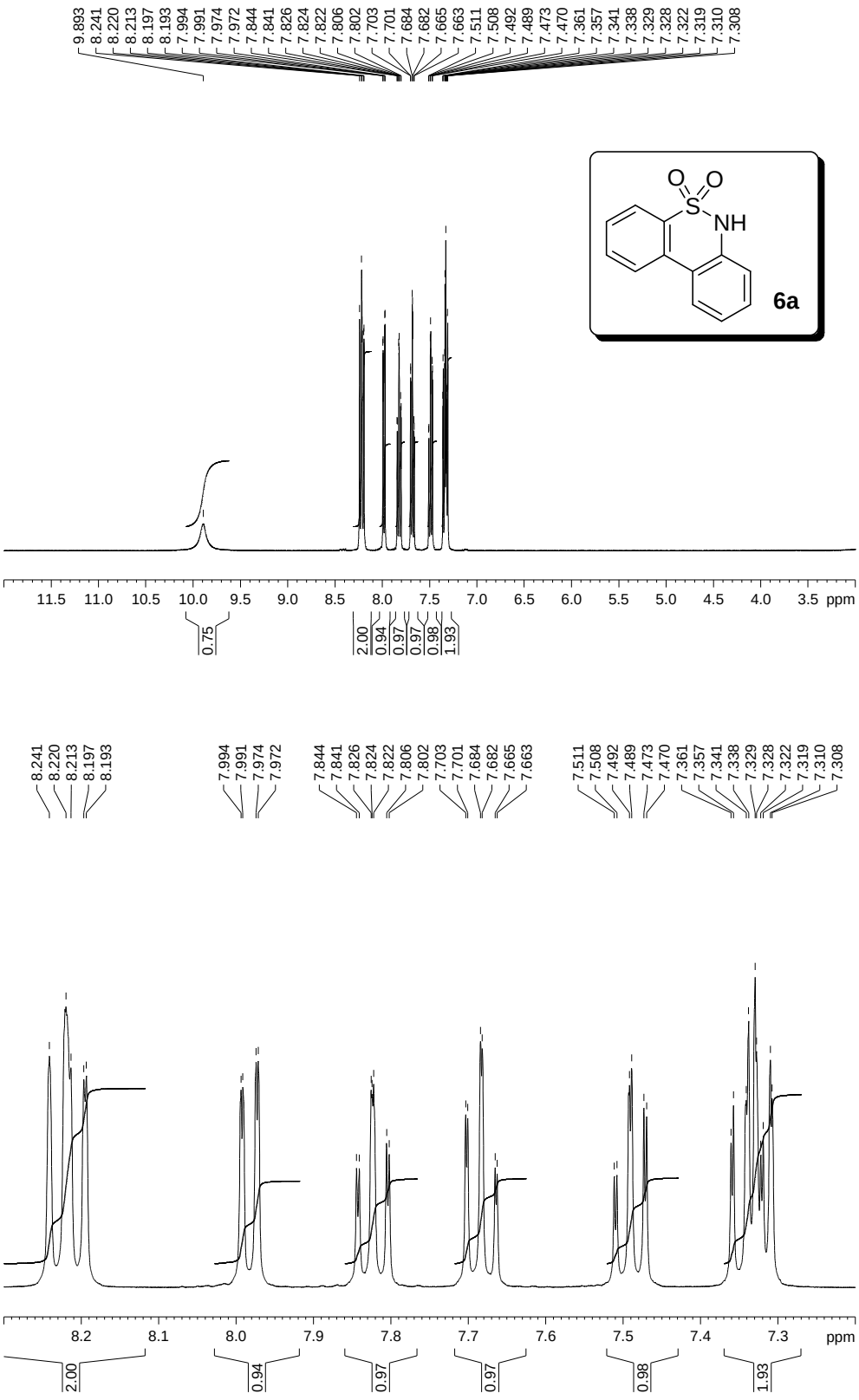

8.360
8.305
8.299
8.290
8.285
7.669
7.664
7.651
7.647
7.642
7.629
7.624
7.452
7.448
7.439
7.433
7.421
7.415
7.406
7.400
7.323
7.301
6.790
6.774
6.758
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 ppm
1.93
1.00
2.93
0.92
0.98

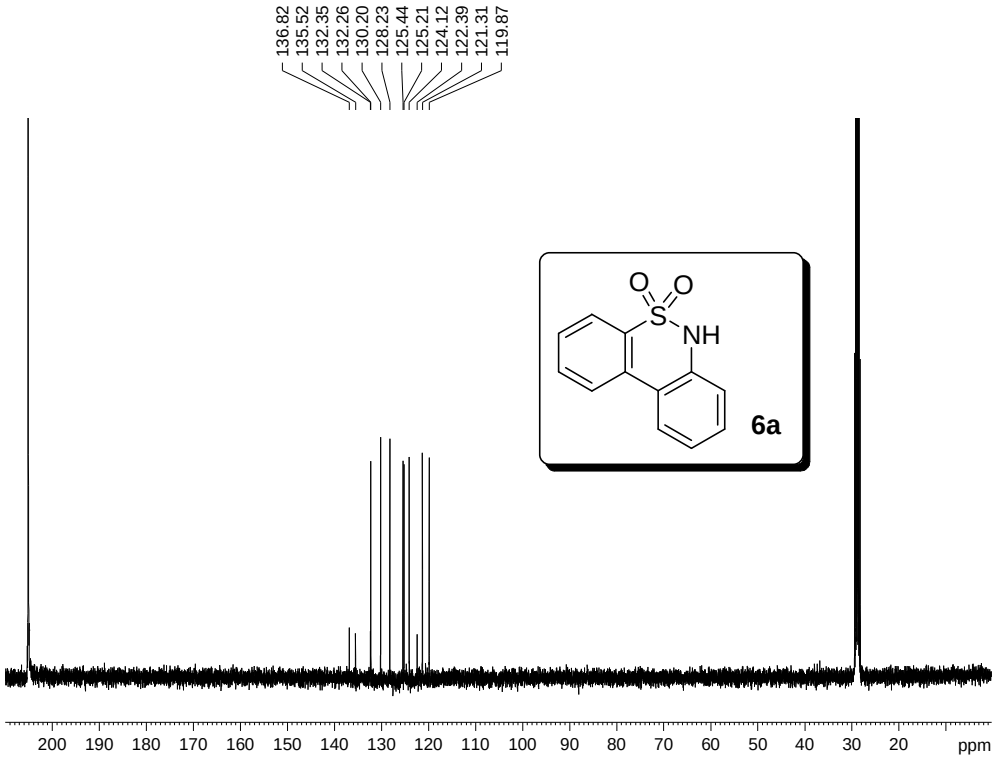

155.55
142.91
139.36
139.25
132.90
132.15
131.90
131.09
126.70
115.51
113.21
O
O
S
N
H
N
Cl
3r
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

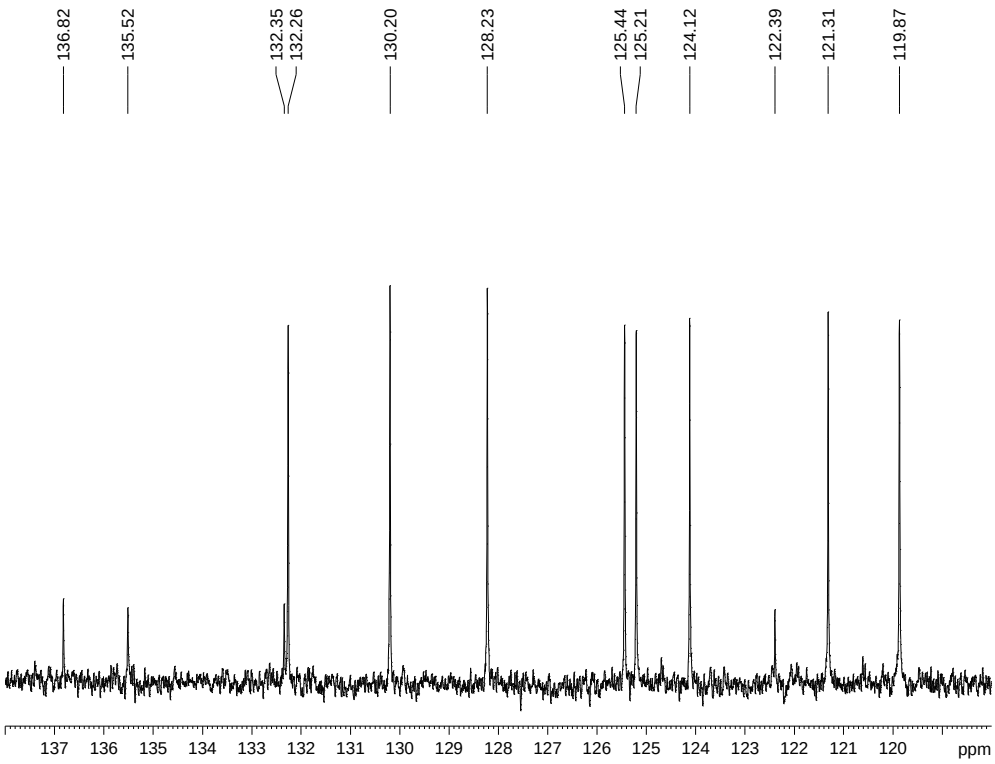

155.55
142.91
139.36
139.25
132.90
132.15
131.90
131.09
126.70
115.51
113.21
155
150
145
140
135
130
125
120
115
ppm

## 4. Copies of $^{1}H$ and $^{13}C$ NMR Spectra of products

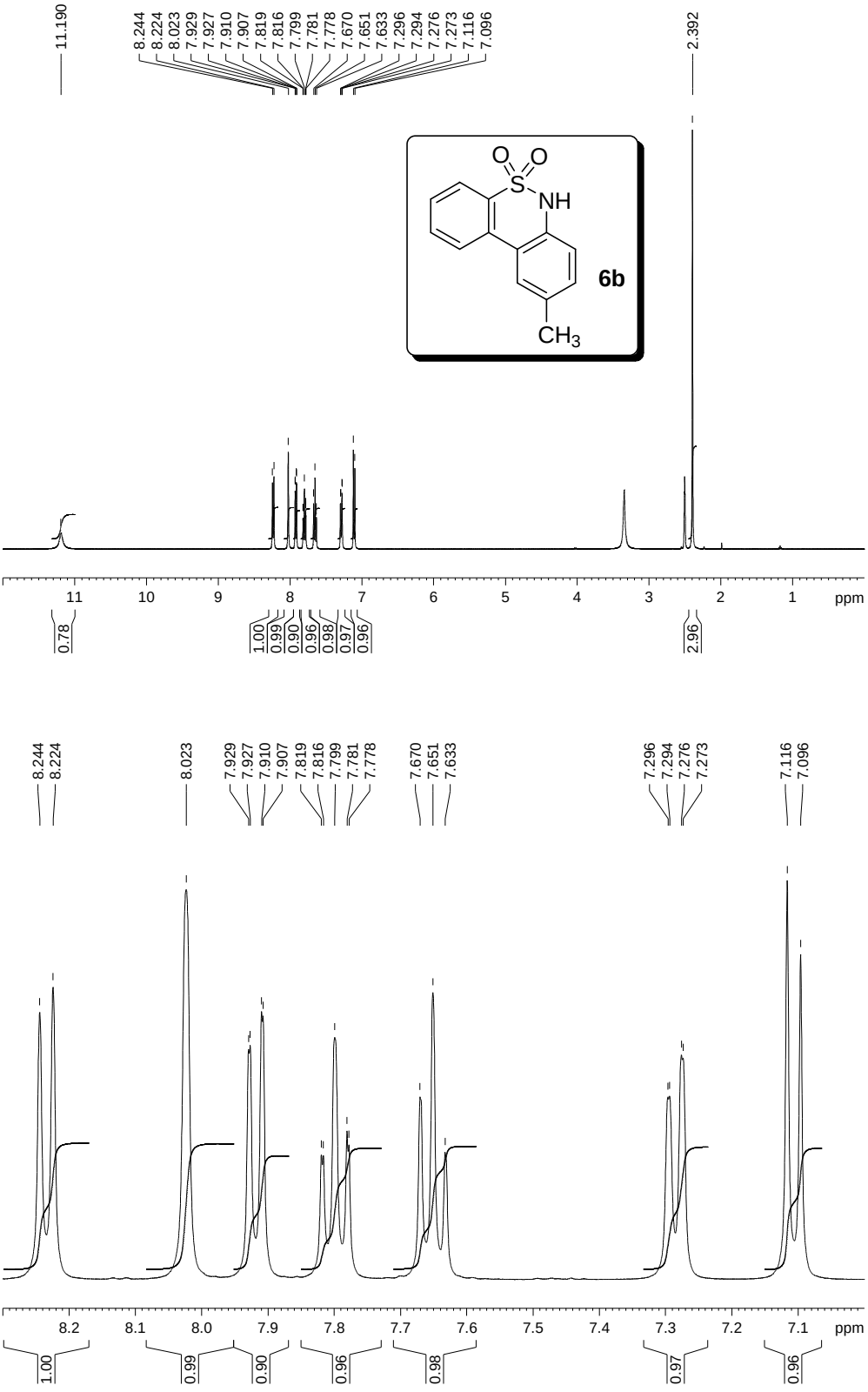
*6H-Dibenzo[c,e][1,2]thiazine 5,5-dioxide* (**6a**)

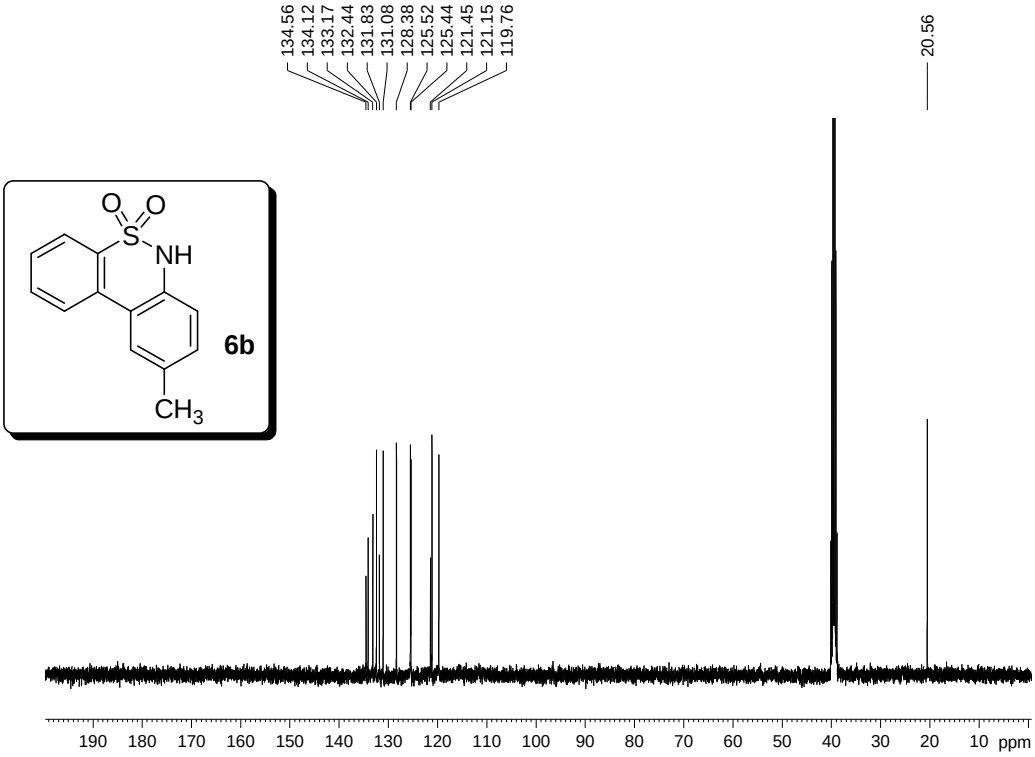


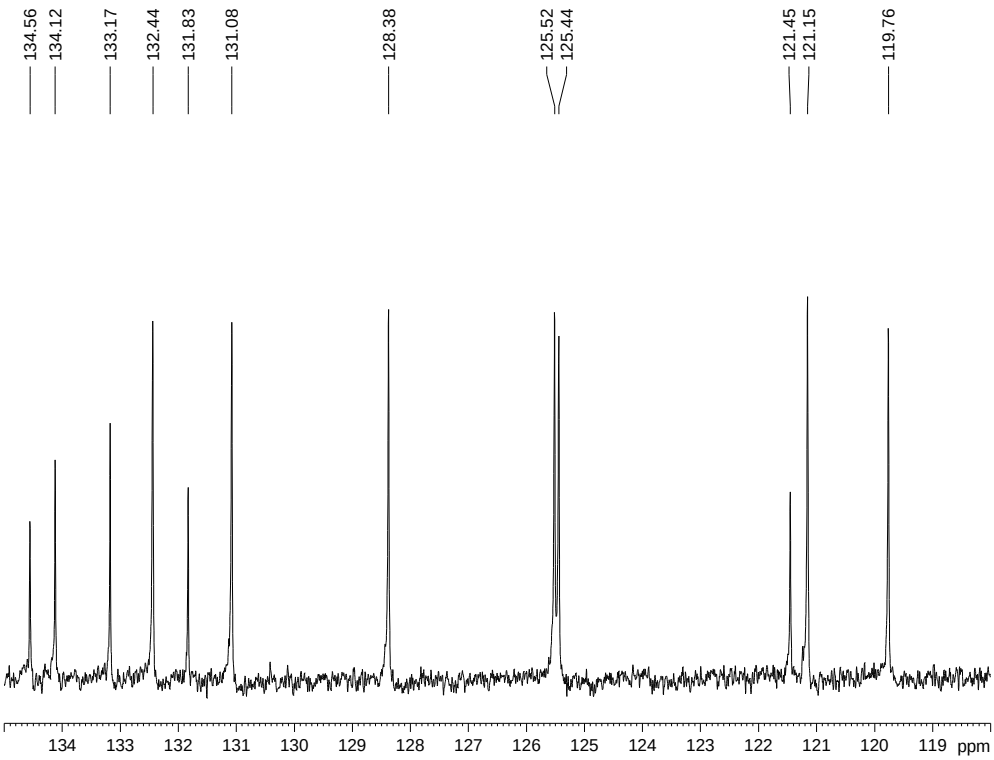

136.82
135.52
132.35
132.26
130.20
128.23
125.44
125.21
124.12
122.39
121.31
119.87
O
O
S
NH
6a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


136.82
135.52
132.35
132.26
130.20
128.23
125.44
125.21
124.12
122.39
121.31
119.87
137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 120 ppm

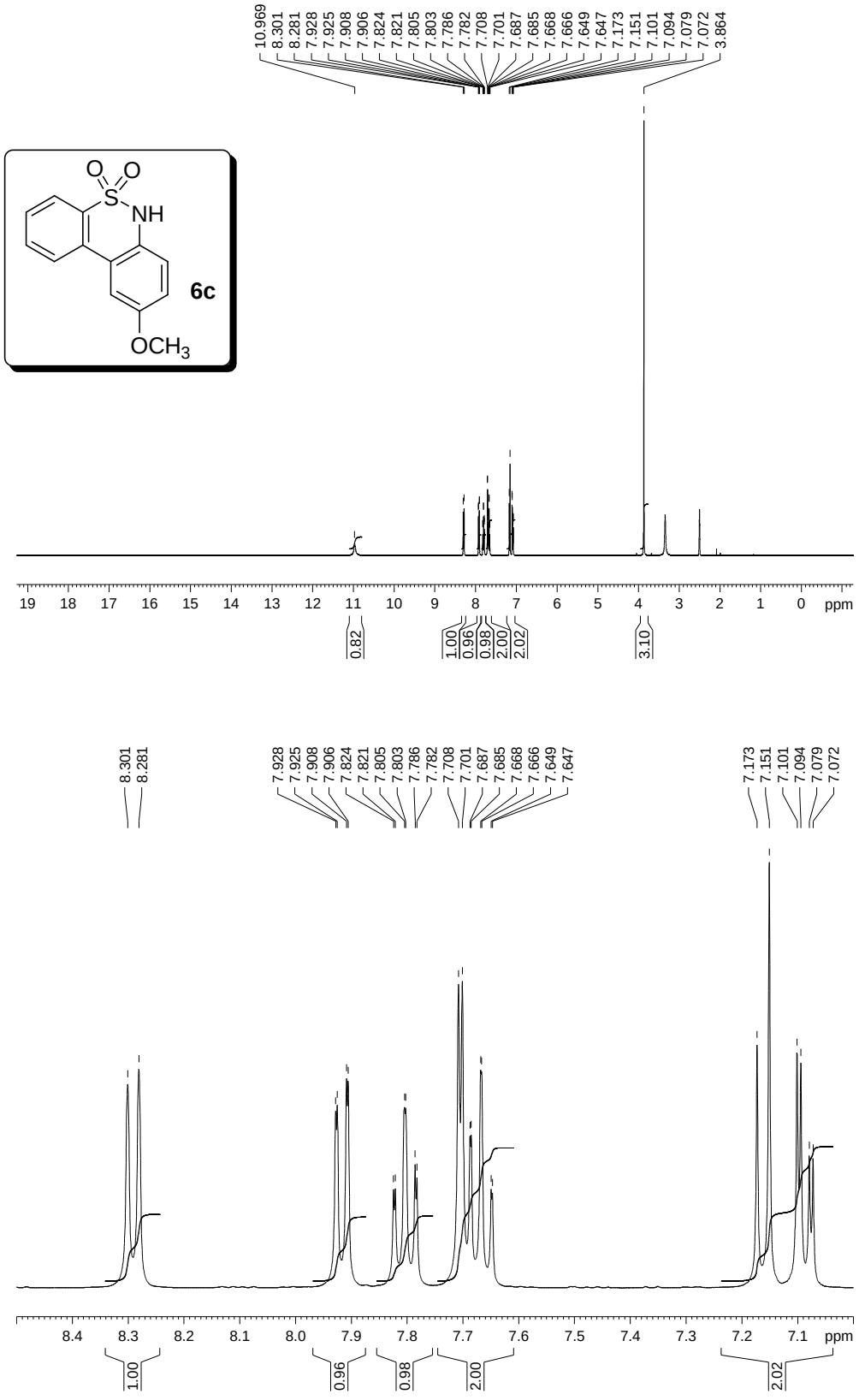
*9-Methyl-6H-dibenzo[c,e][1,2]thiazine 5,5-dioxide* (**6b**)

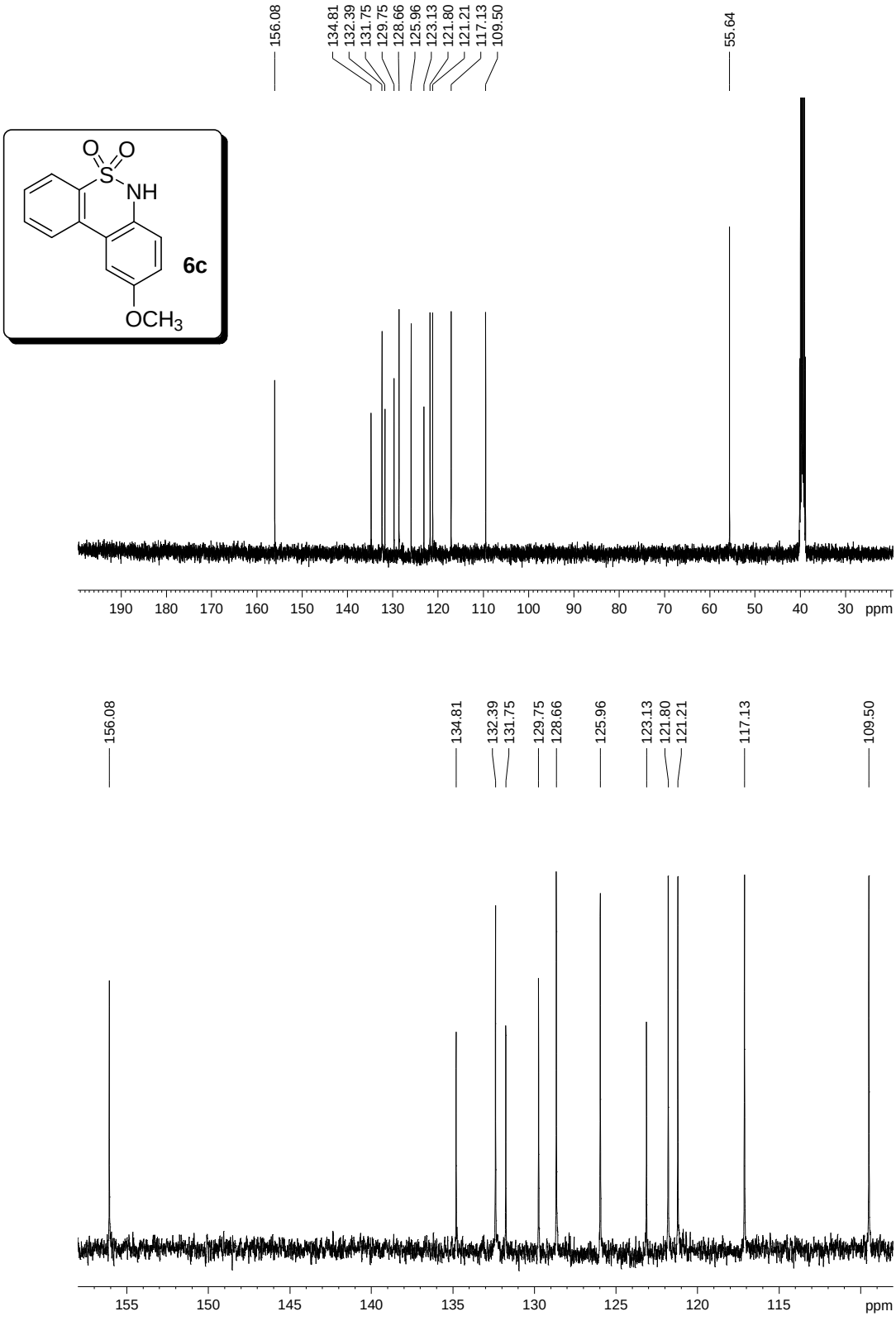



134.56
134.12
133.17
132.44
131.83
131.08
128.38
125.52
125.44
121.45
121.15
119.76
20.56
O
O
S
NH
6b
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

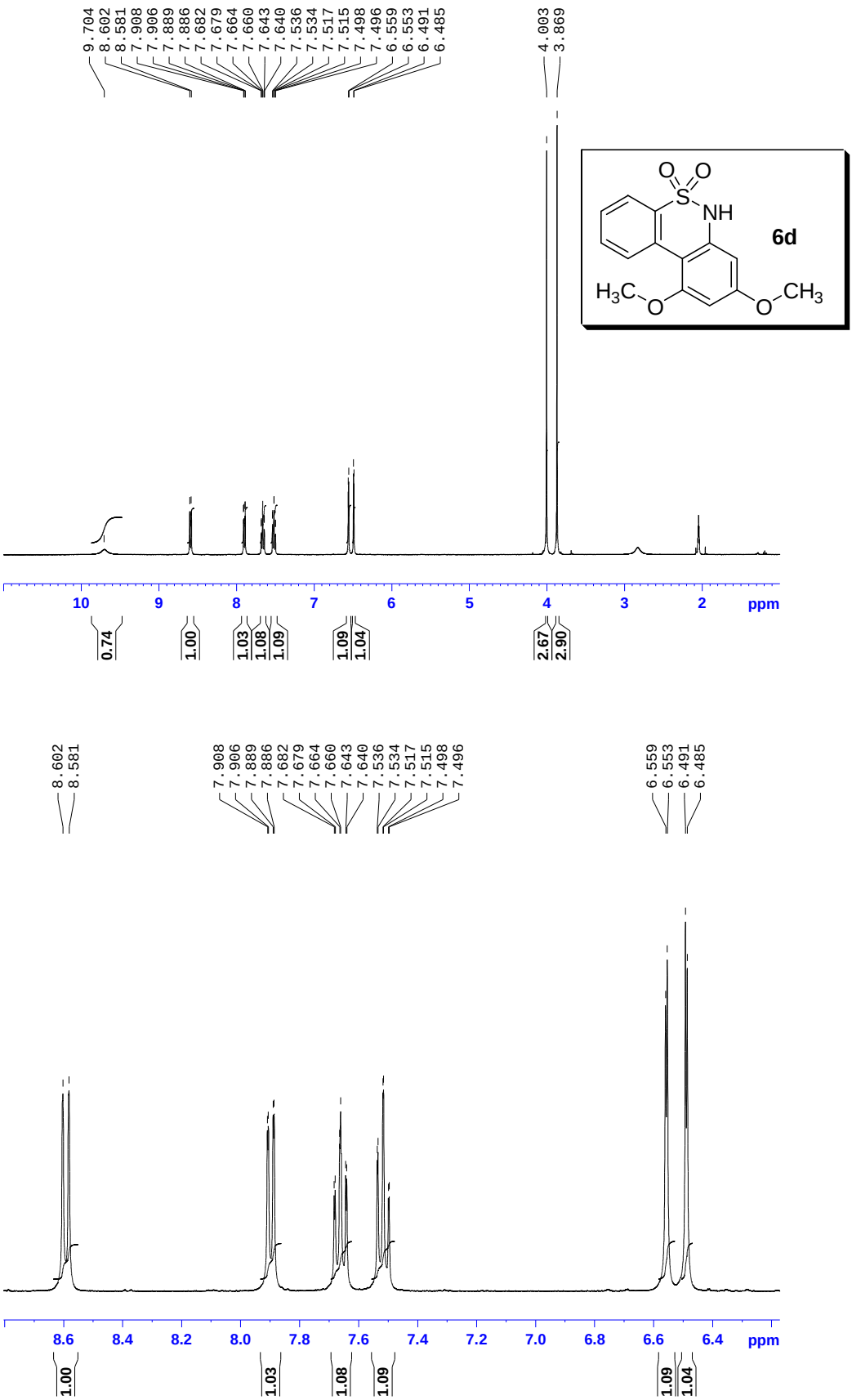

134.56
134.12
133.17
132.44
131.83
131.08
128.38
125.52
125.44
121.45
121.15
119.76
134 133 132 131 130 129 128 127 126 125 124 123 122 121 120 119 ppm

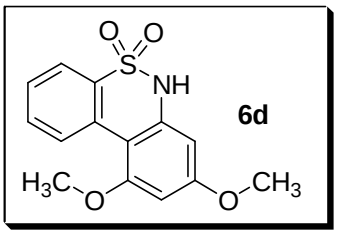
*9-Methoxy-6H-dibenzo[c,e][1,2]thiazine 5,5-dioxide* (**6c**)

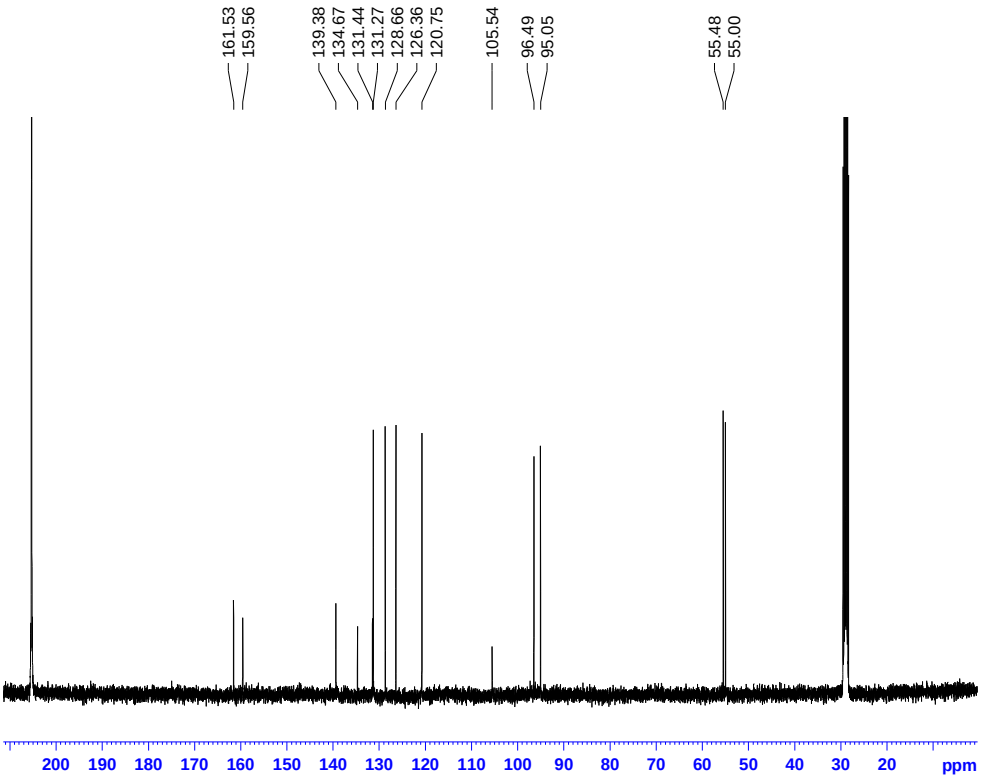


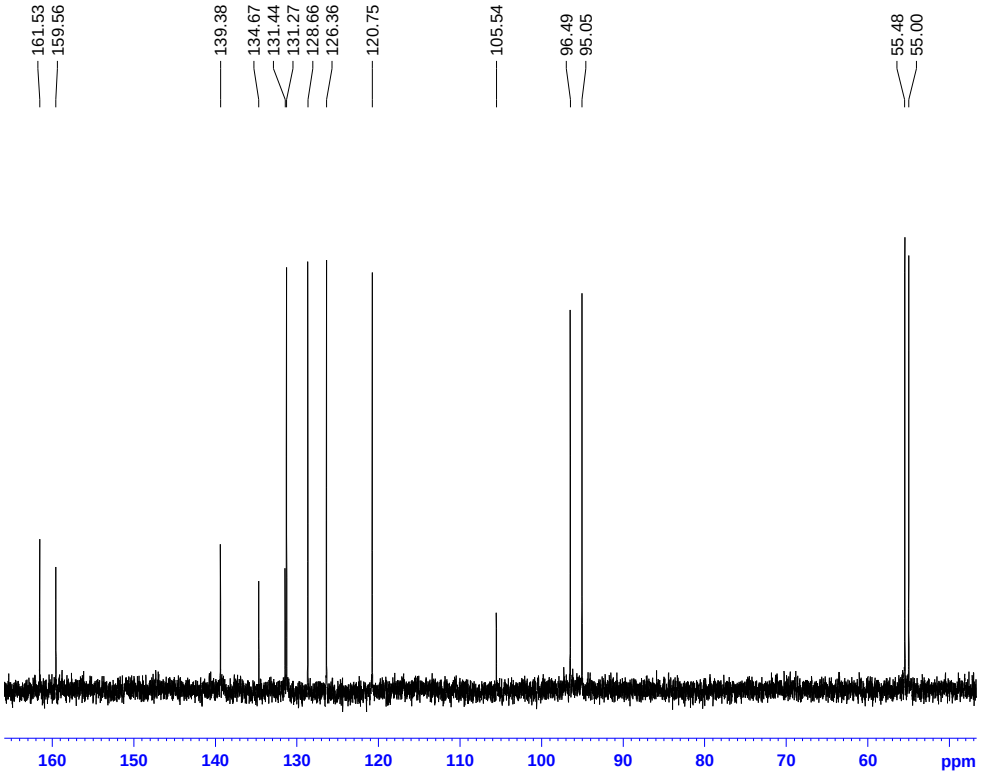

156.08
134.81
132.39
131.75
129.75
128.66
125.96
123.13
121.80
121.21
117.13
109.50
55.64
O
O
S
NH
6c
OCH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm
156.08
134.81
132.39
131.75
129.75
128.66
125.96
123.13
121.80
121.21
117.13
109.50
155 150 145 140 135 130 125 120 115 ppm

*8,10-Di-methoxy-6H-dibenzo[c,e][1,2]thiazine 5,5-dioxide* (**6d**)

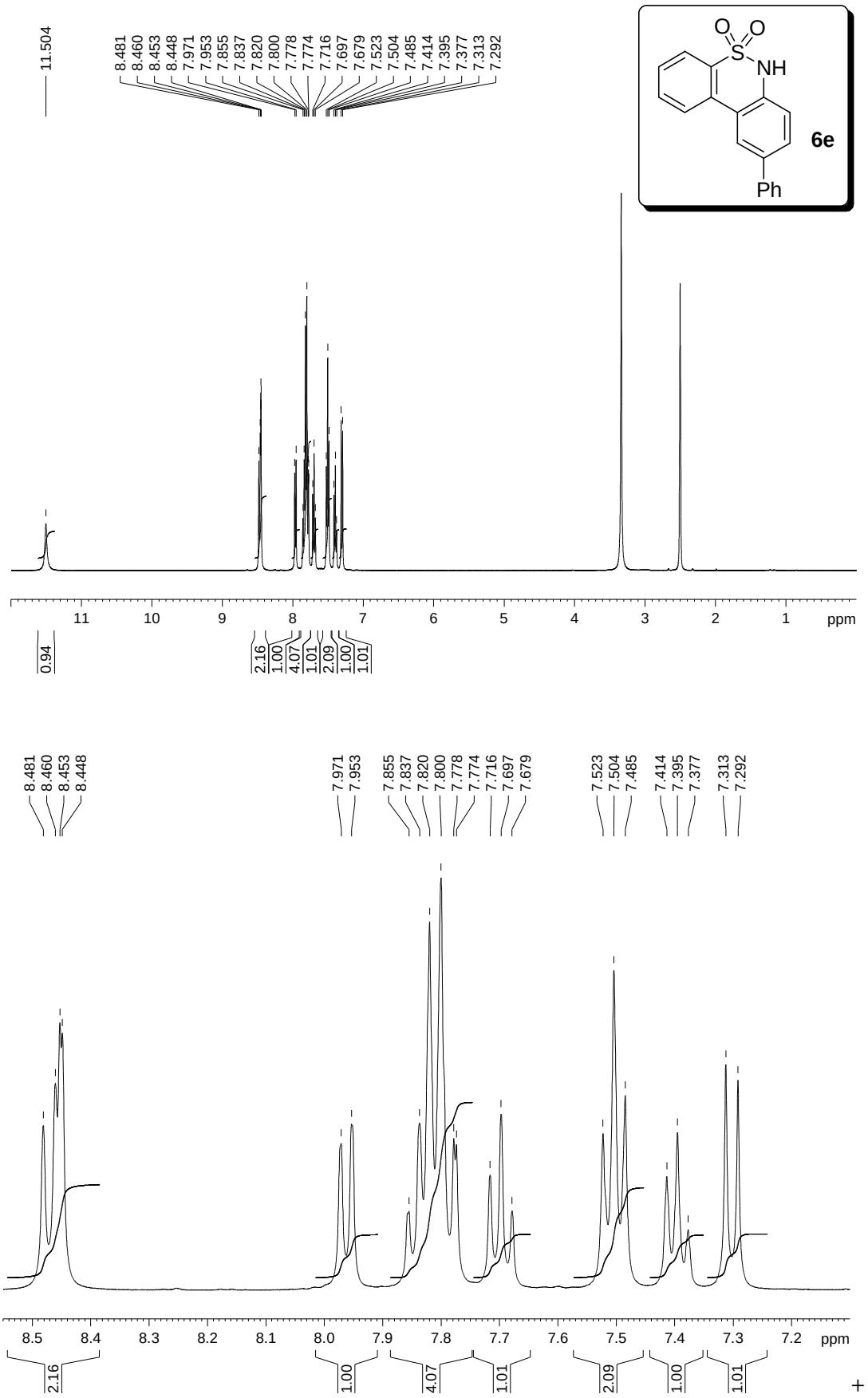


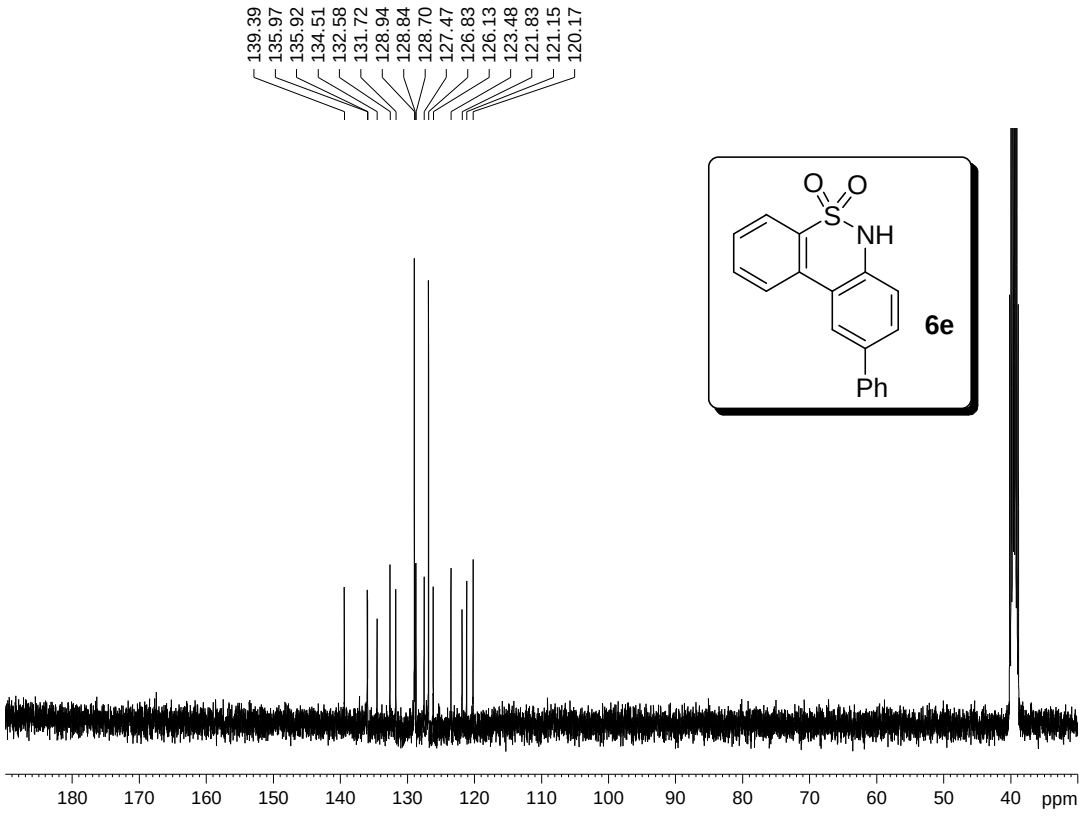

O
O
S
NH
6d
H3C
O
O
CH3

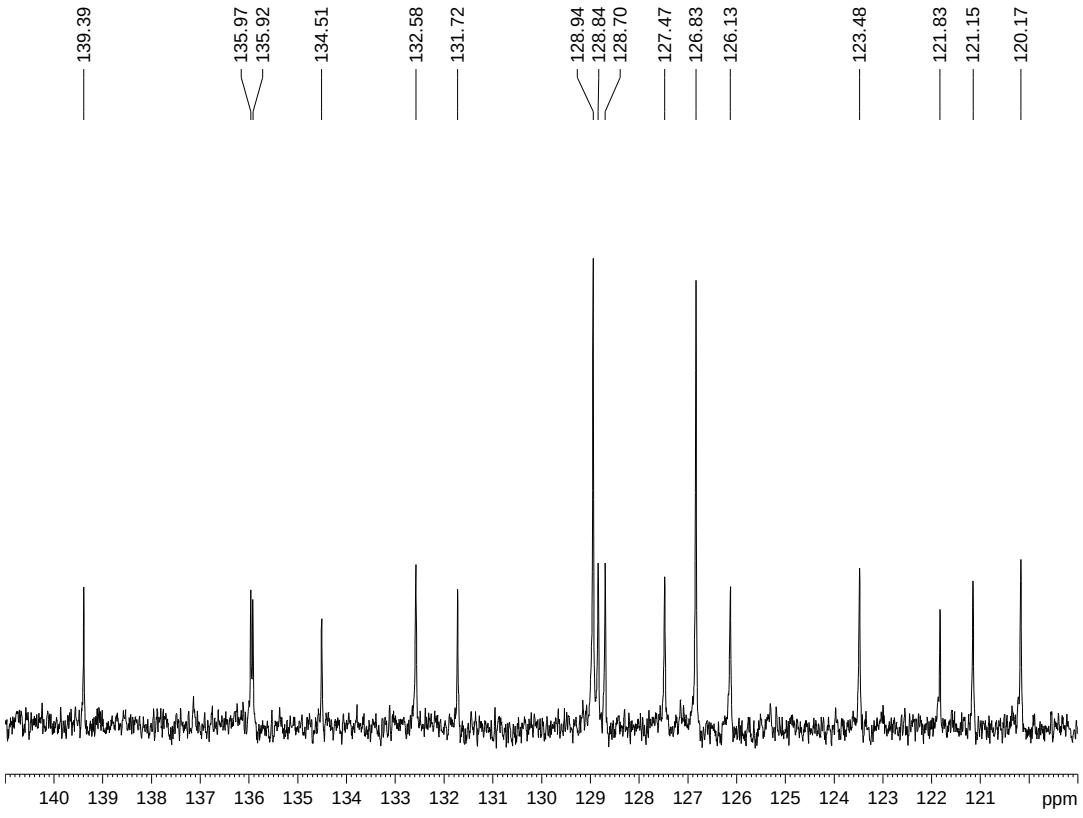

161.53
159.56
139.38
134.67
131.44
131.27
128.66
126.36
120.75
105.54
96.49
95.05
55.48
55.00
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


161.53
159.56
139.38
134.67
131.44
131.27
128.66
126.36
120.75
105.54
96.49
95.05
55.48
55.00
160 150 140 130 120 110 100 90 80 70 60 ppm

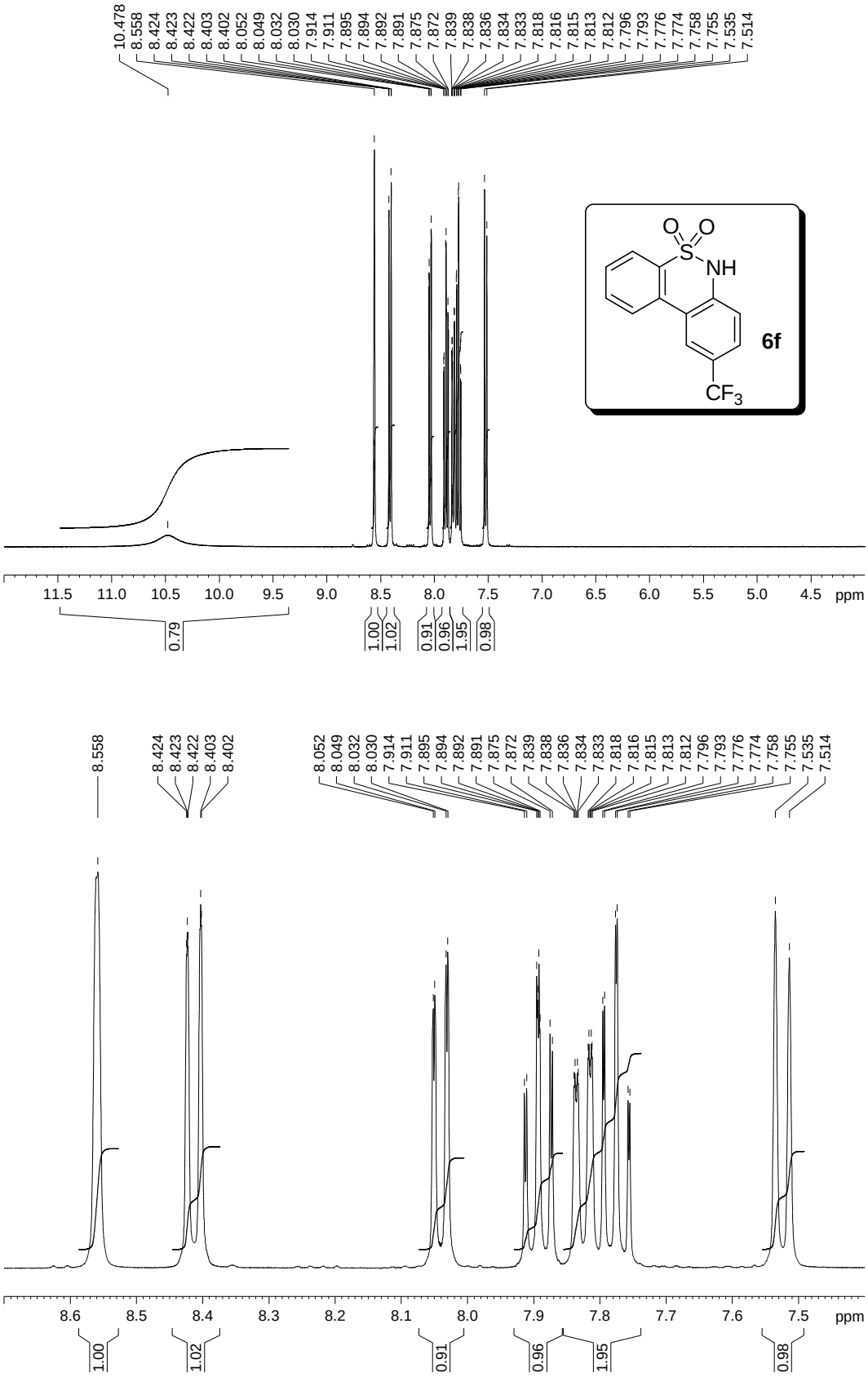
*9-Phenyl-6H-dibenzo[c,e][1,2]thiazine 5,5-dioxide* (**6e**)

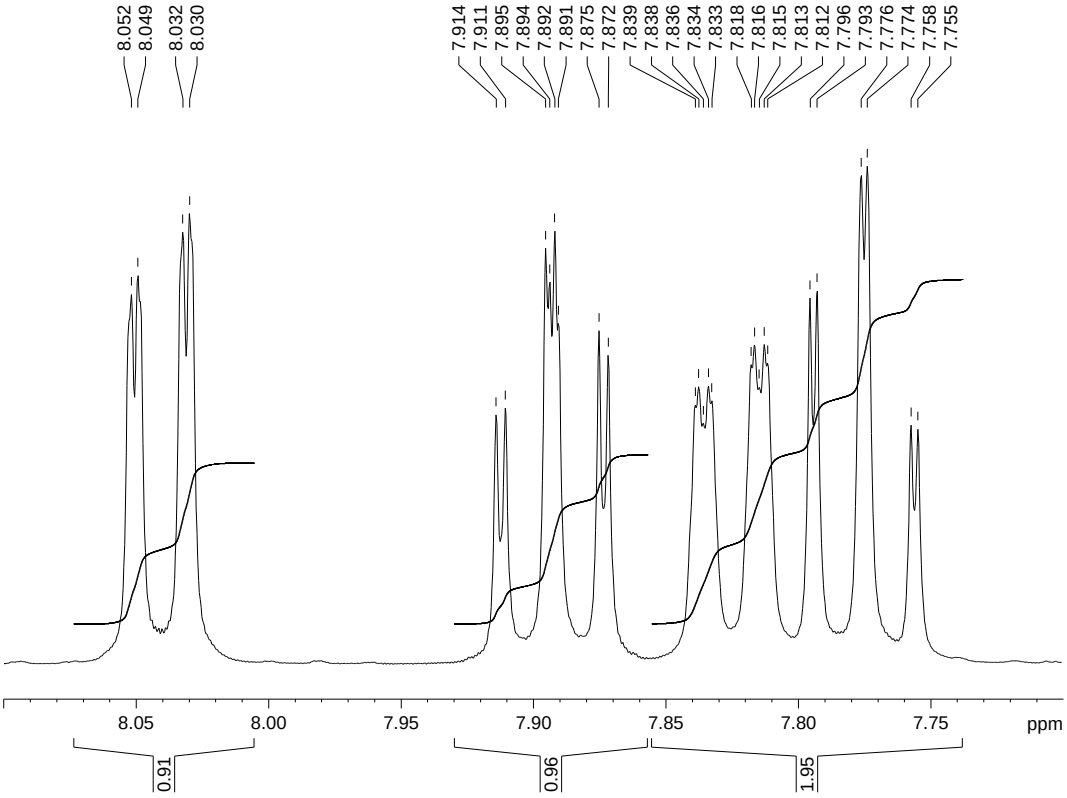


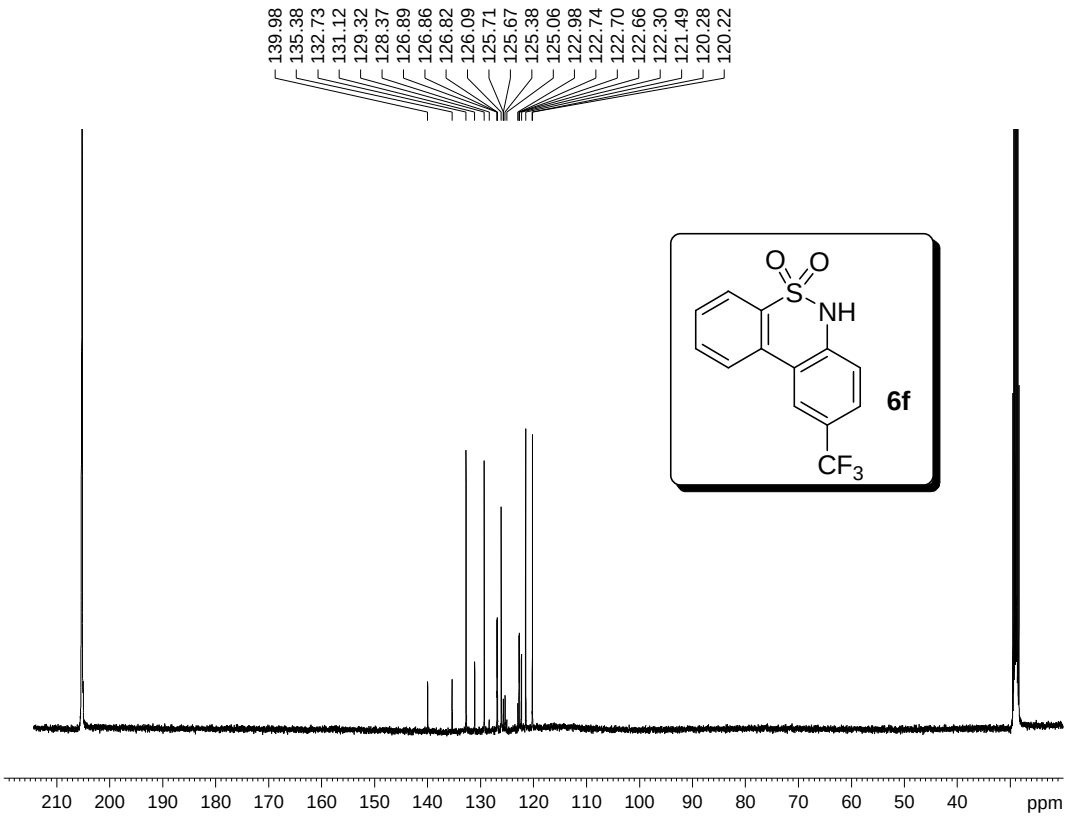

139.39
135.97
135.92
134.51
132.58
131.72
128.94
128.84
128.70
127.47
126.83
126.13
123.48
121.83
121.15
120.17
O
O
S
NH
Ph
6e
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

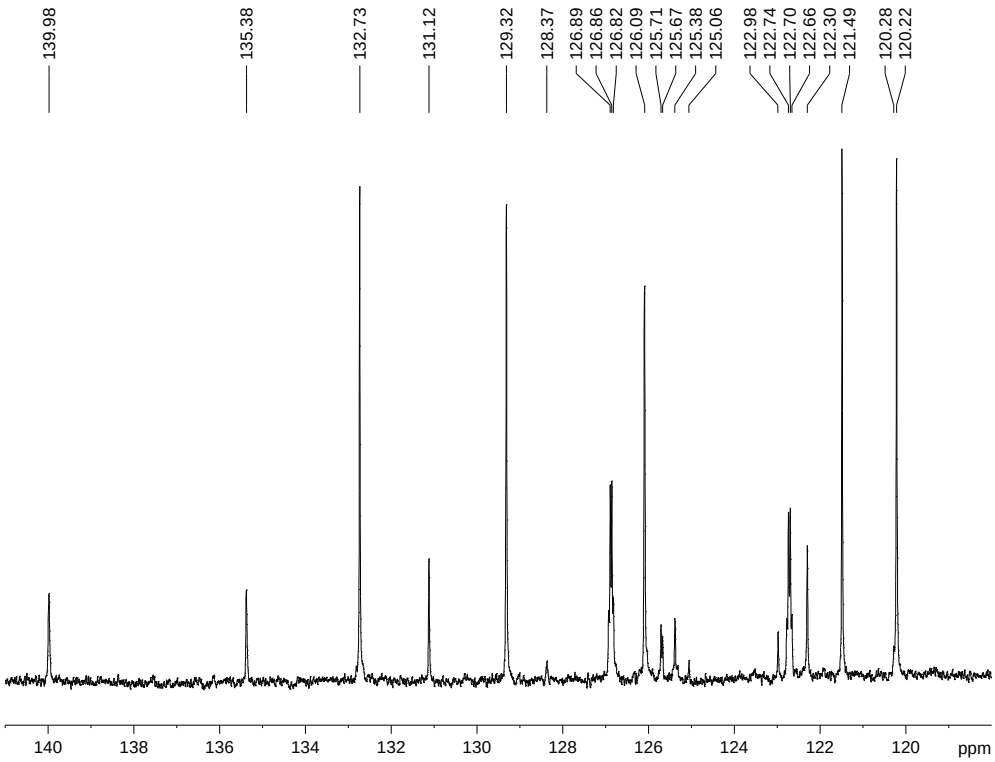

139.39
135.97
135.92
134.51
132.58
131.72
128.94
128.84
128.70
127.47
126.83
126.13
123.48
121.83
121.15
120.17
140
139
138
137
136
135
134
133
132
131
130
129
128
127
126
125
124
123
122
121
ppm

*9-(Trifluoromethyl)-6H-dibenzo[c,e][1,2]thiazine 5,5-dioxide* (**6f**)

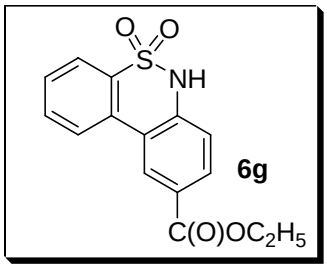


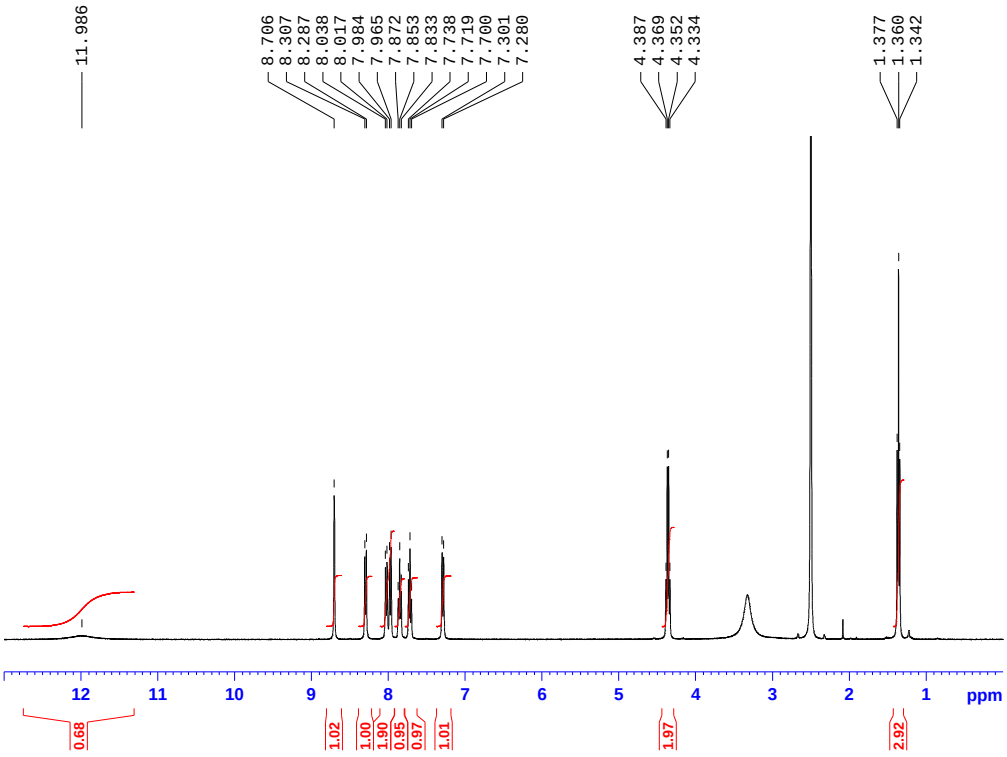

8.052
8.049
8.032
8.030
7.914
7.911
7.895
7.894
7.892
7.891
7.875
7.872
7.839
7.838
7.836
7.834
7.833
7.818
7.816
7.815
7.813
7.812
7.796
7.793
7.776
7.774
7.758
7.755
8.05
8.00
7.95
7.90
7.85
7.80
7.75
ppm
0.91
0.96
1.95

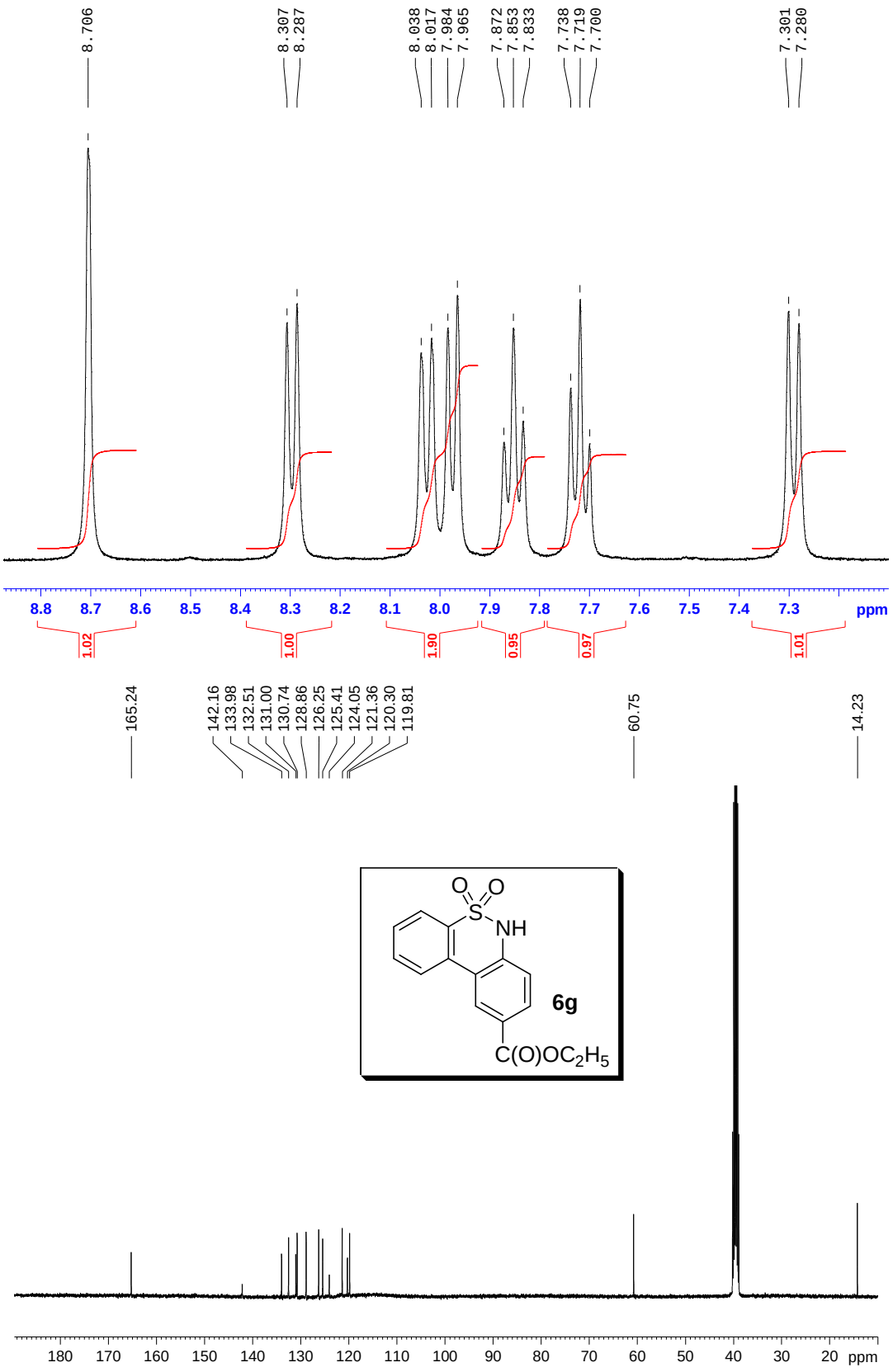

139.98
135.38
132.73
131.12
129.32
128.37
126.89
126.86
126.82
126.09
125.71
125.67
125.38
125.06
122.98
122.74
122.70
122.66
122.30
121.49
120.28
120.22
O
O
S
NH
6f
CF3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

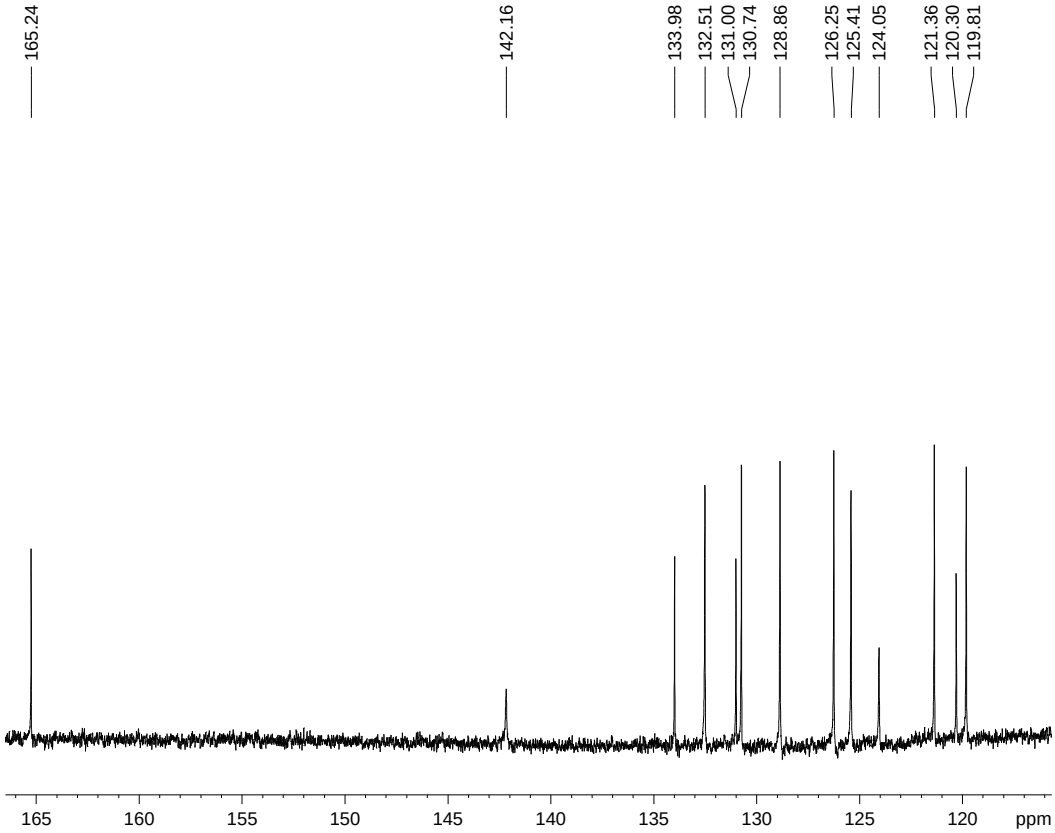



*Ethyl 6H-dibenzo[c,e][1,2]thiazine-9-carboxylate 5,5-dioxide* (**6g**)

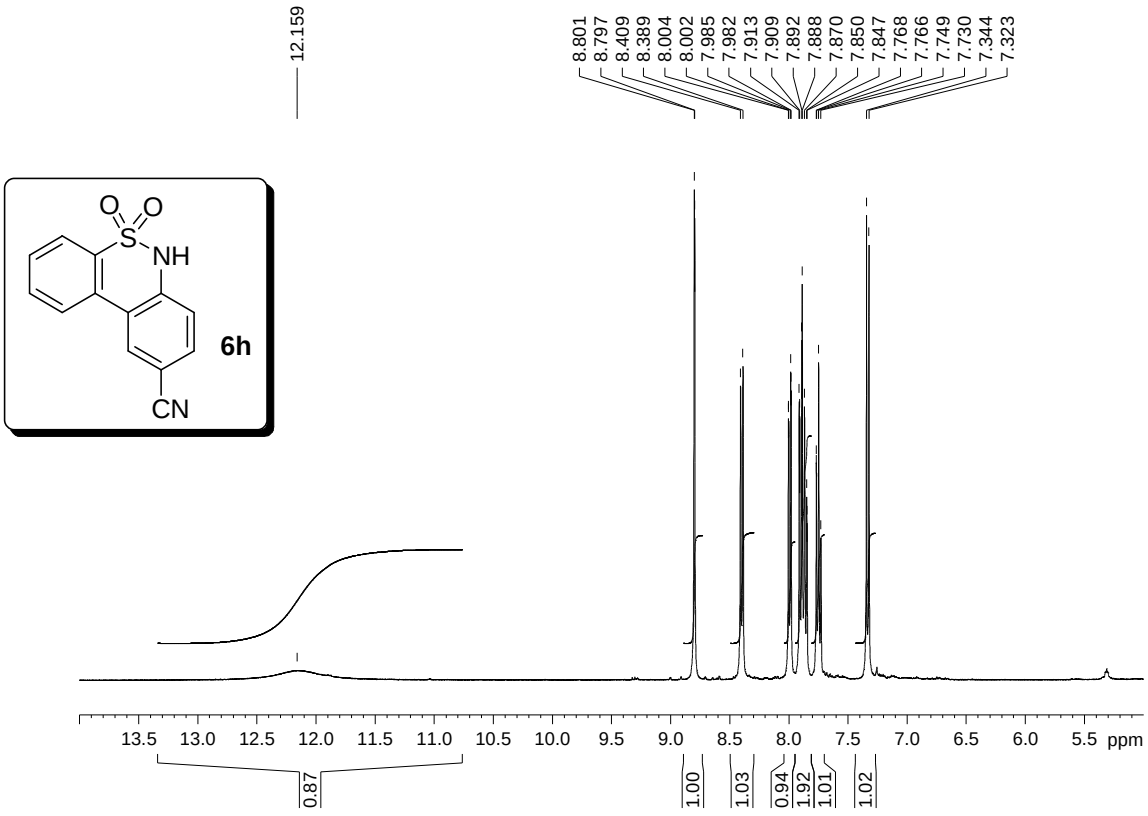


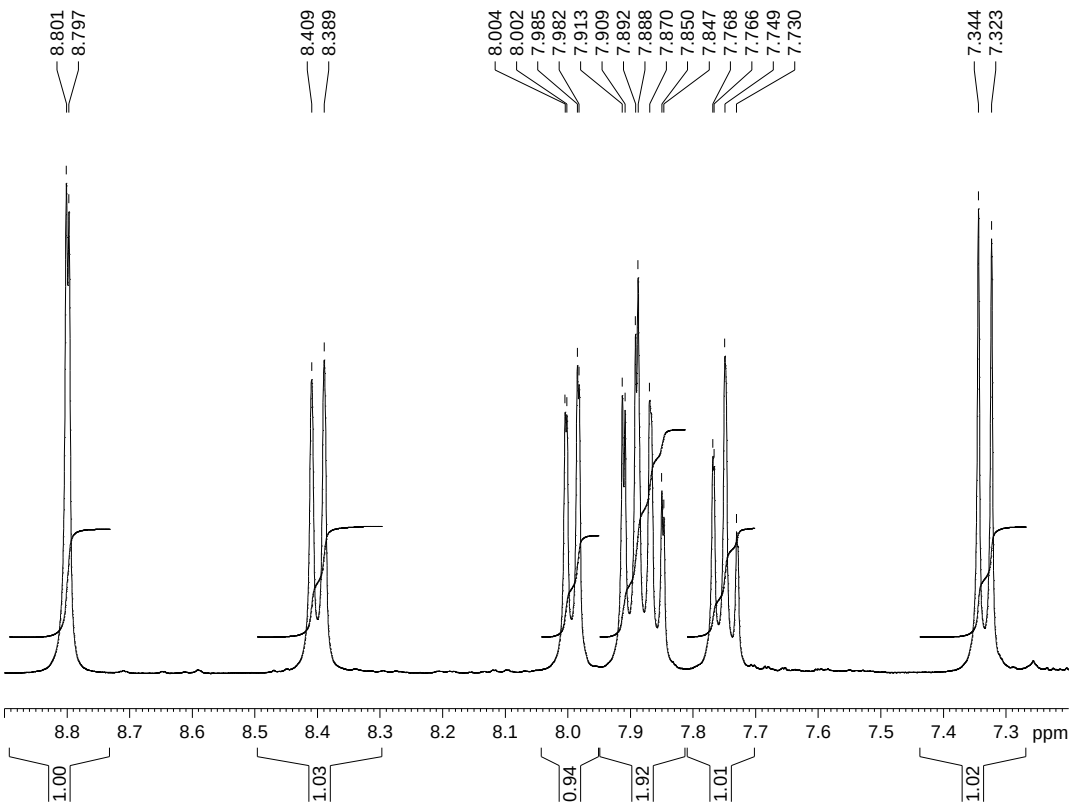



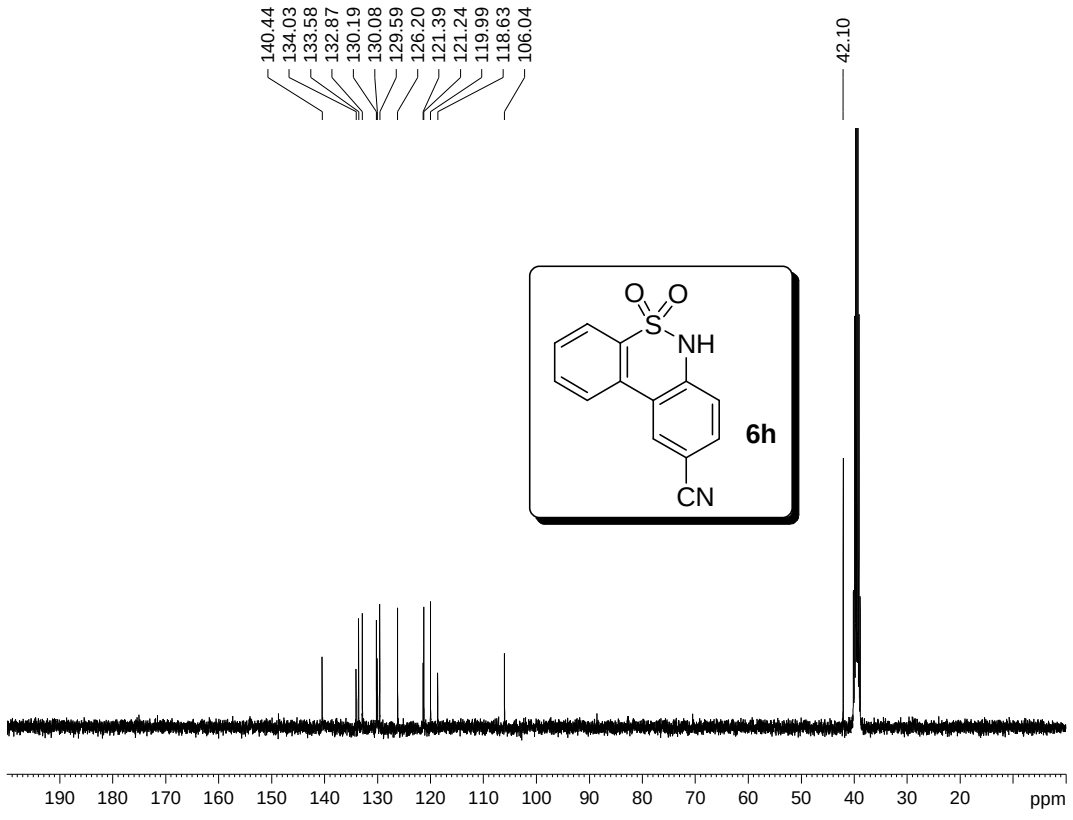

8.706
8.307
8.287
8.038
8.017
7.984
7.965
7.872
7.853
7.833
7.738
7.719
7.700
7.301
7.280
8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 ppm
1.02
1.00
1.90
0.95
0.97
1.01
165.24
142.16
133.98
132.51
131.00
130.74
128.86
126.25
125.41
124.05
121.36
120.30
119.81
60.75
14.23
O
O
S
NH
6g
C(O)OC2H5
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

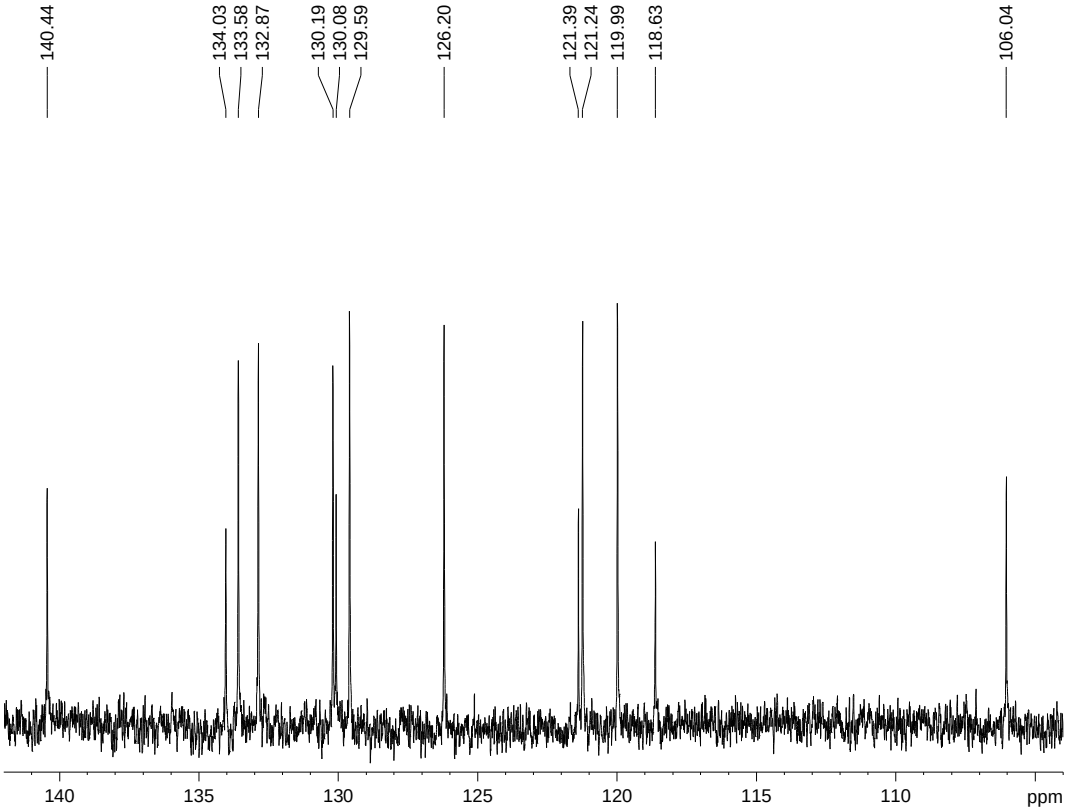



*6H-Dibenzo[c,e][1,2]thiazine-9-carbonitrile 5,5-dioxide* (**6h**)

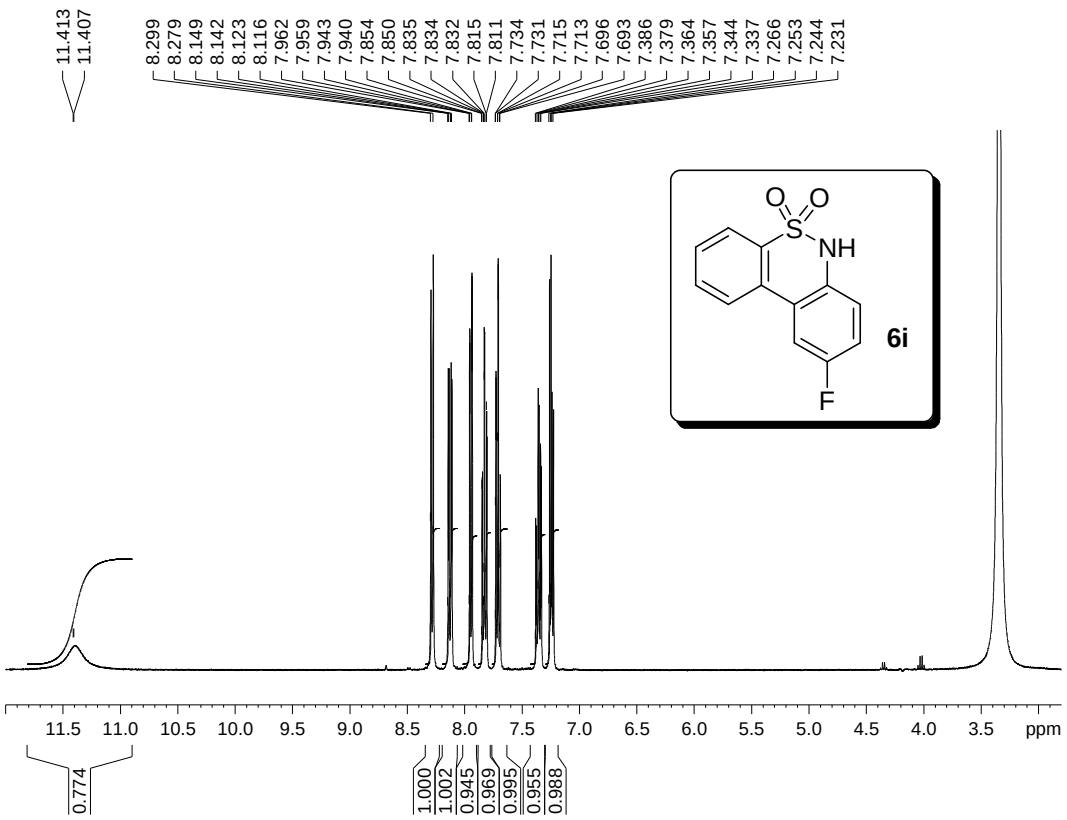


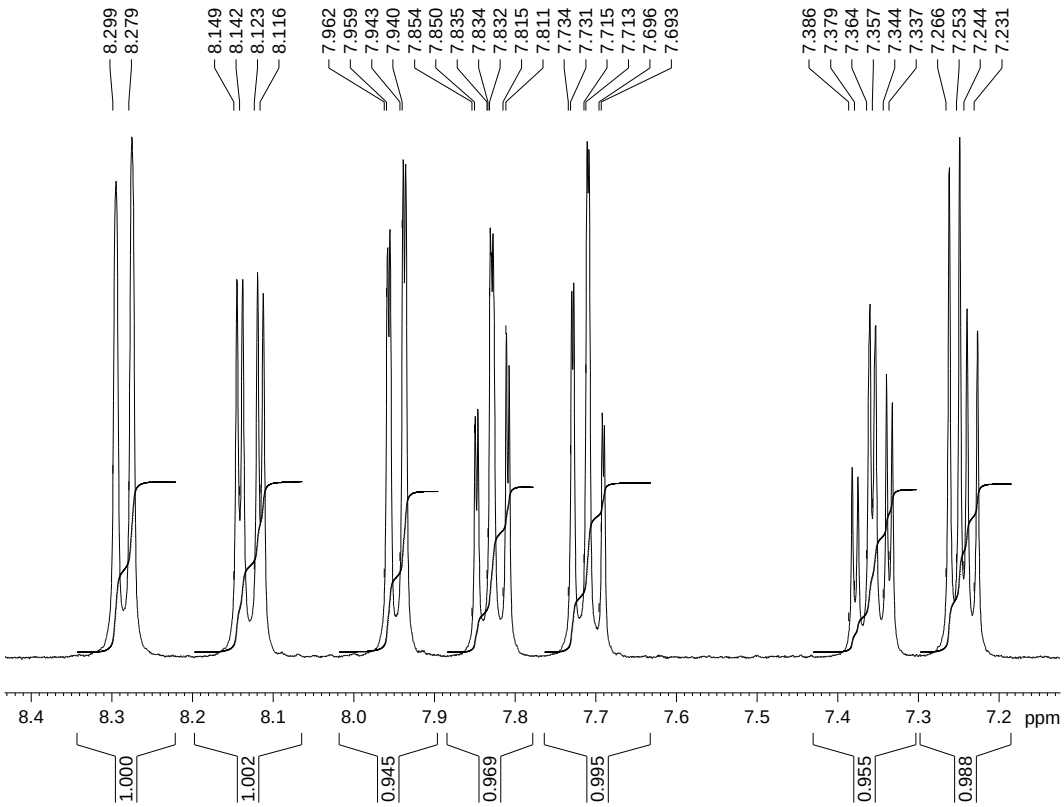

8.801
8.797
8.409
8.389
8.004
8.002
7.985
7.982
7.913
7.909
7.892
7.888
7.870
7.850
7.847
7.768
7.766
7.749
7.730
7.344
7.323
8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 ppm
1.00
1.03
0.94
1.92
1.01
1.02

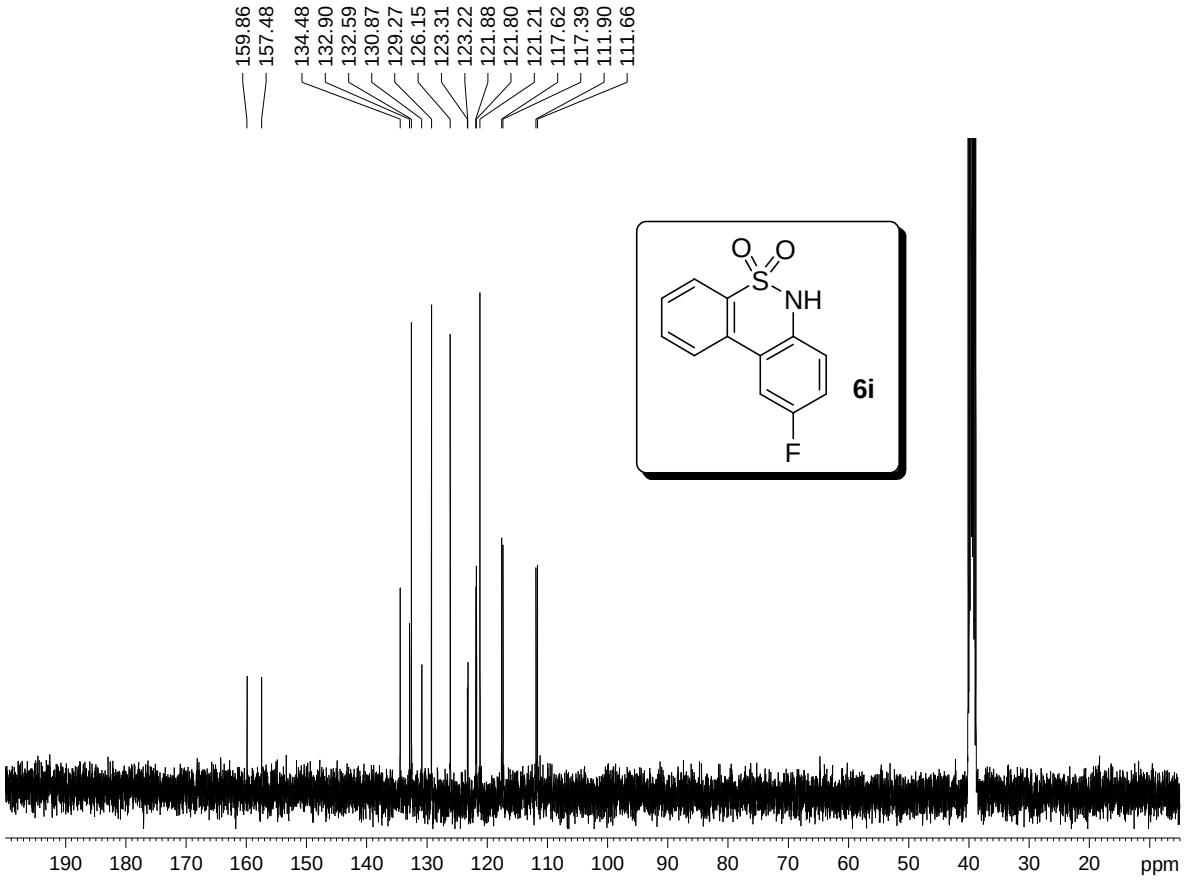

140.44
134.03
133.58
132.87
130.19
130.08
129.59
126.20
121.39
121.24
119.99
118.63
106.04
42.10
O
O
S
NH
CN
6h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

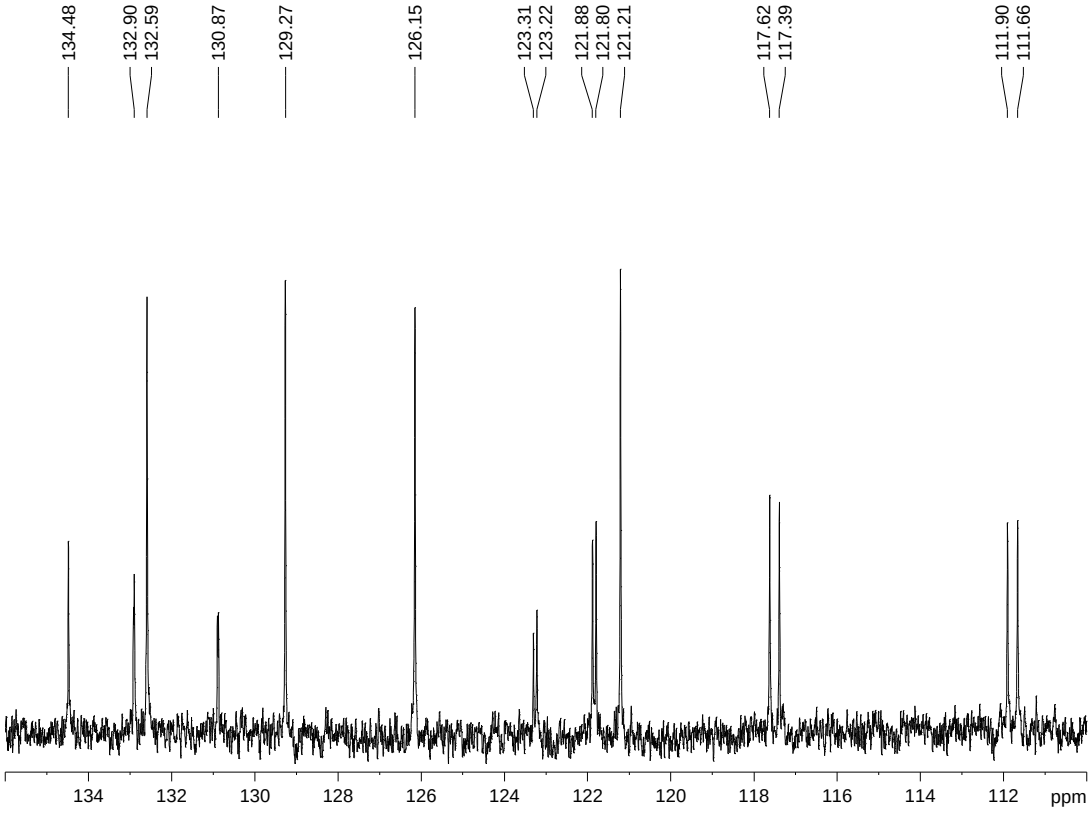



*9-Fluoro-6H-dibenzo[c,e][1,2]thiazine 5,5-dioxide* (**6i**)

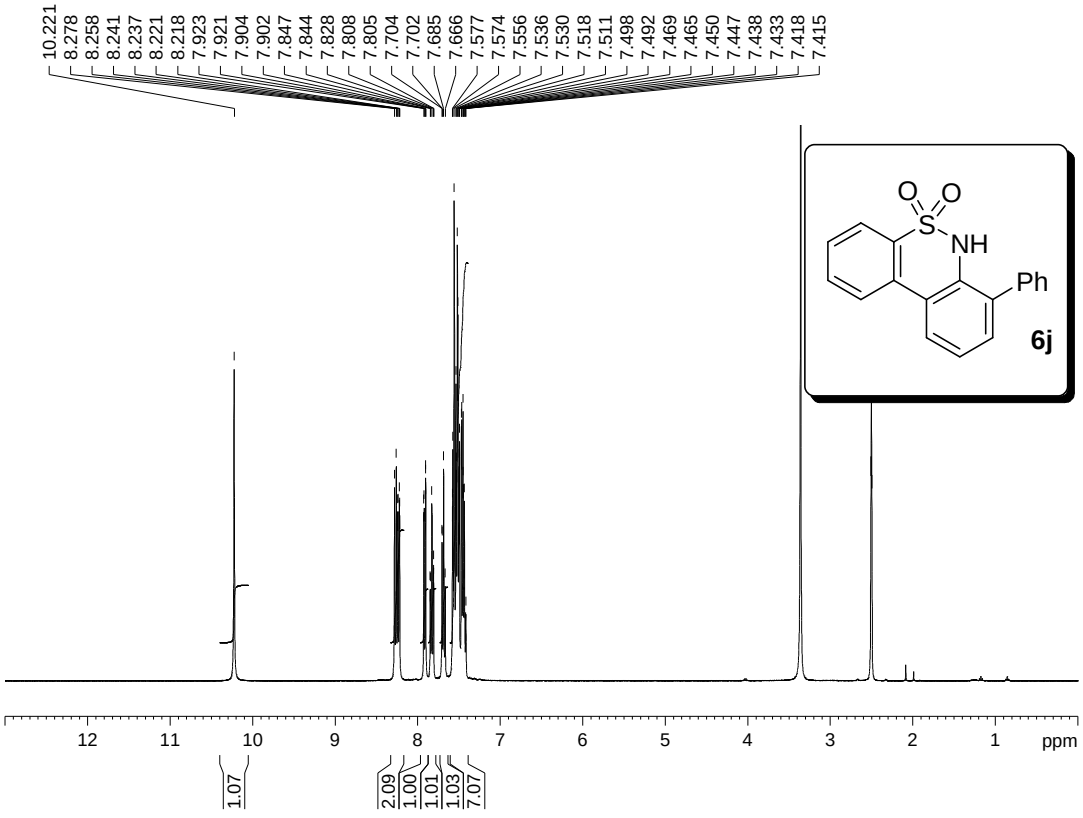


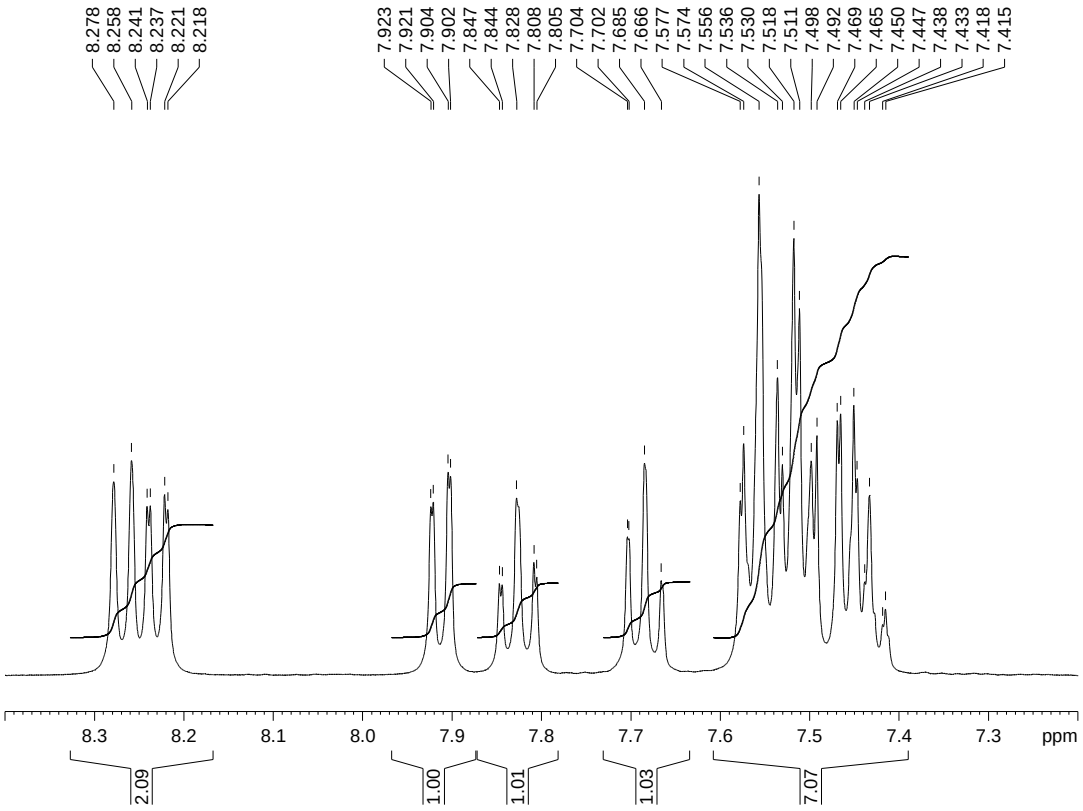

8.299
8.279
8.149
8.142
8.123
8.116
7.962
7.959
7.943
7.940
7.854
7.850
7.835
7.834
7.832
7.815
7.811
7.734
7.731
7.715
7.713
7.696
7.693
7.386
7.379
7.364
7.357
7.344
7.337
7.266
7.253
7.244
7.231
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
1.000
1.002
0.945
0.969
0.995
0.955
0.988

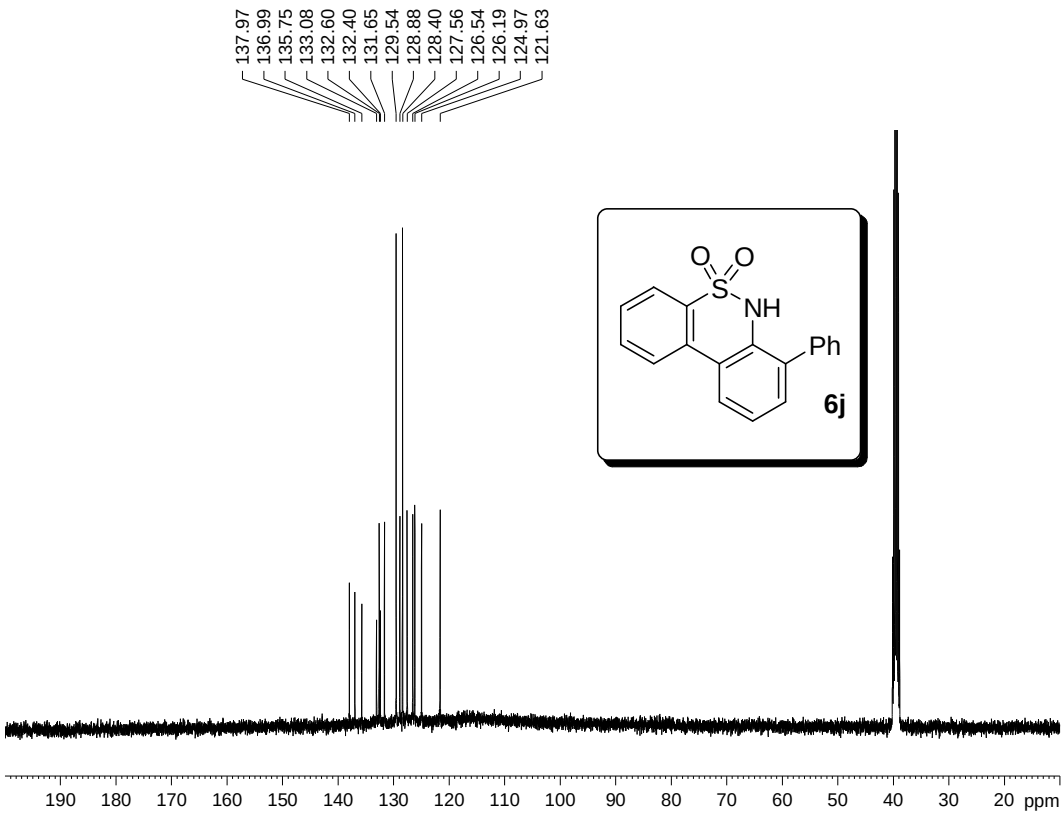

159.86
157.48
134.48
132.90
132.59
130.87
129.27
126.15
123.31
123.22
121.88
121.80
121.21
117.62
117.39
111.90
111.66
O
O
S
NH
F
6i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

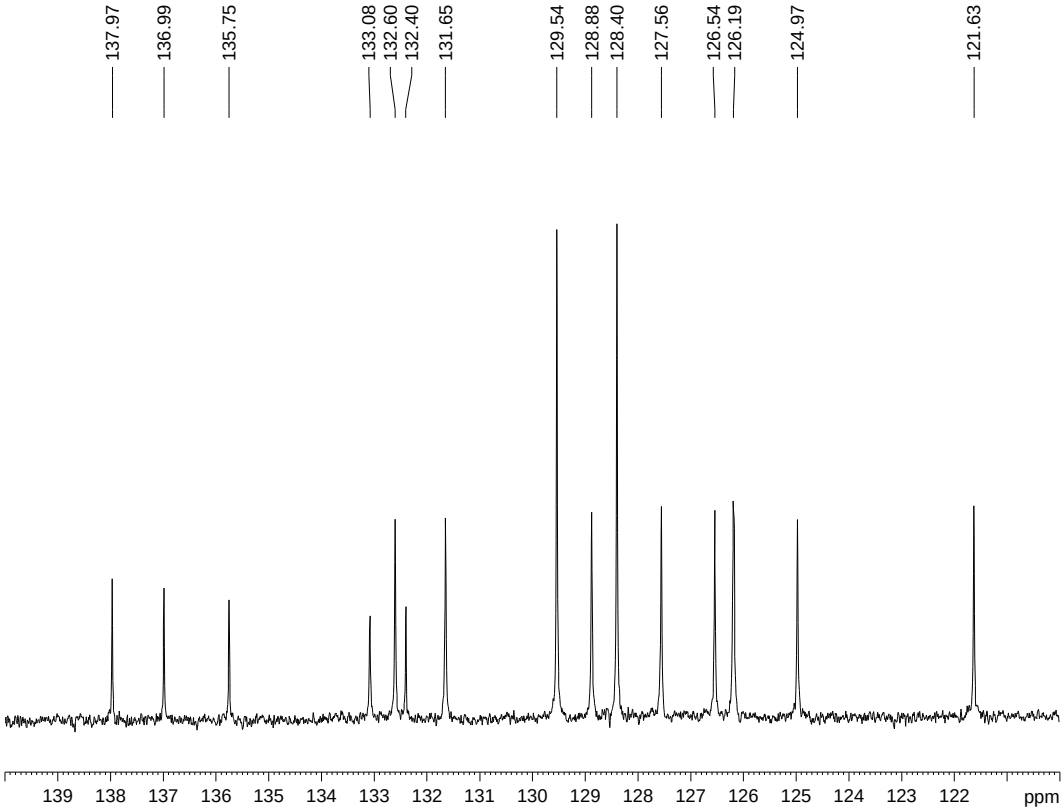



*7-Phenyl-6H-dibenzo[c,e][1,2]thiazine 5,5-dioxide* (**6j**)

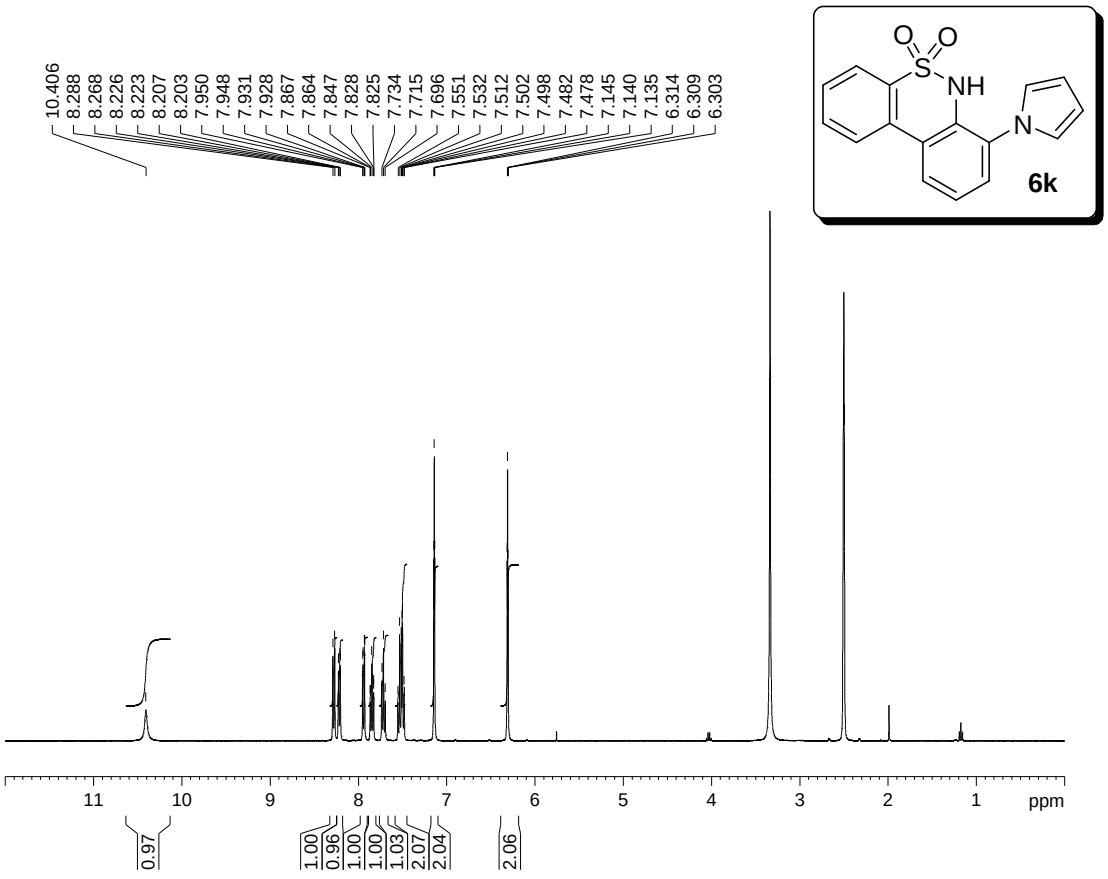


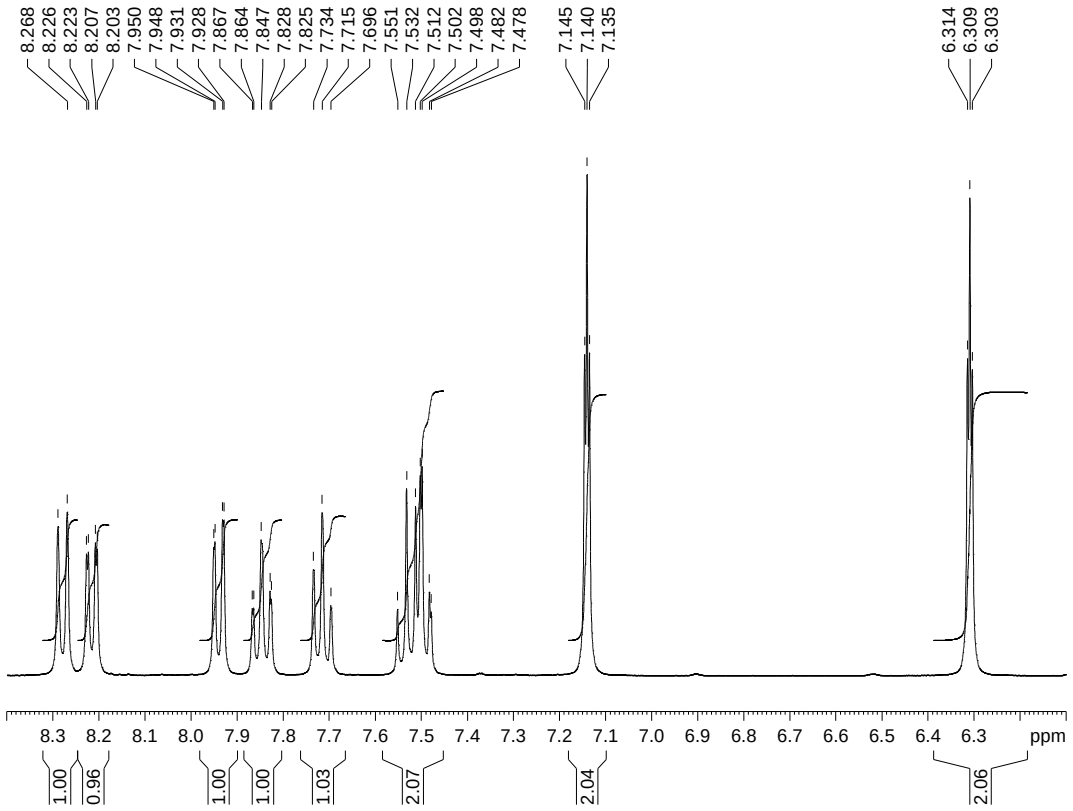

8.278
8.258
8.241
8.237
8.221
8.218
7.923
7.921
7.904
7.902
7.847
7.844
7.828
7.808
7.805
7.704
7.702
7.685
7.666
7.577
7.574
7.556
7.536
7.530
7.518
7.511
7.498
7.492
7.469
7.465
7.450
7.447
7.438
7.433
7.418
7.415
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm
2.09
1.00
1.01
1.03
7.07

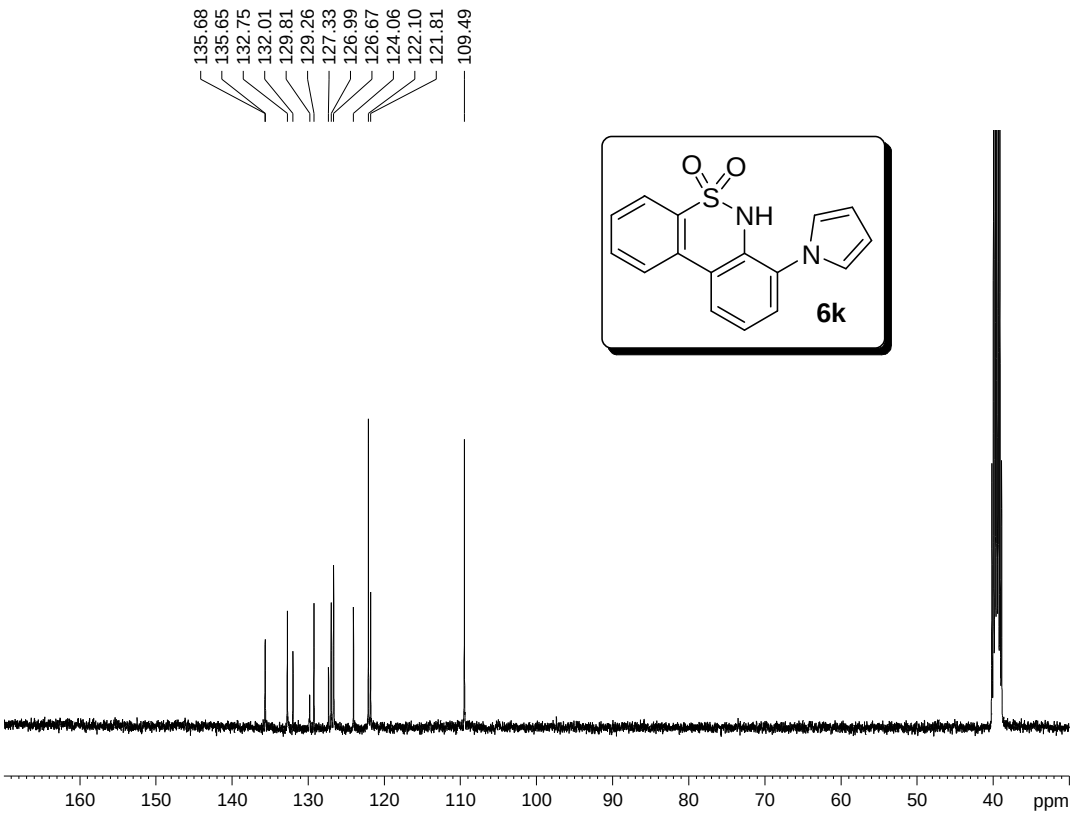

137.97
136.99
135.75
133.08
132.60
132.40
131.65
129.54
128.88
128.40
127.56
126.54
126.19
124.97
121.63
O
O
S
NH
Ph
6j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

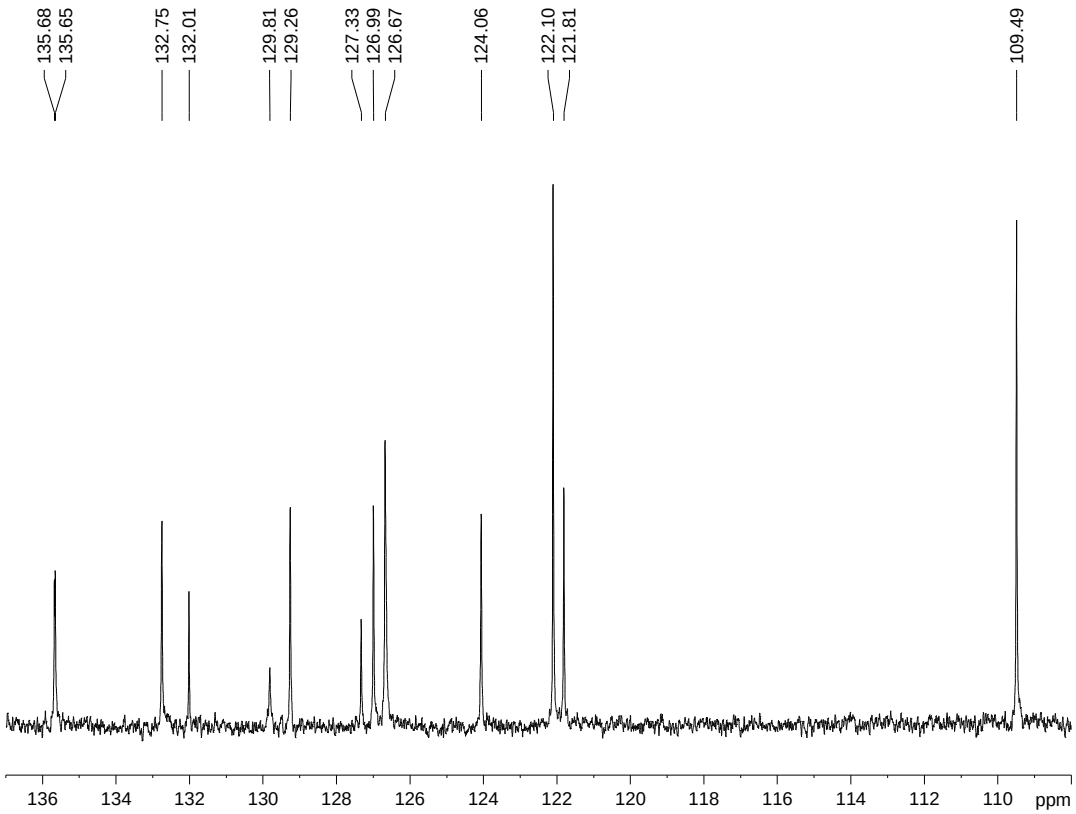



*7-(1H-Pyrrol-1-yl)-6H-dibenzo[c,e][1,2]thiazine 5,5-dioxide* (**6k**)

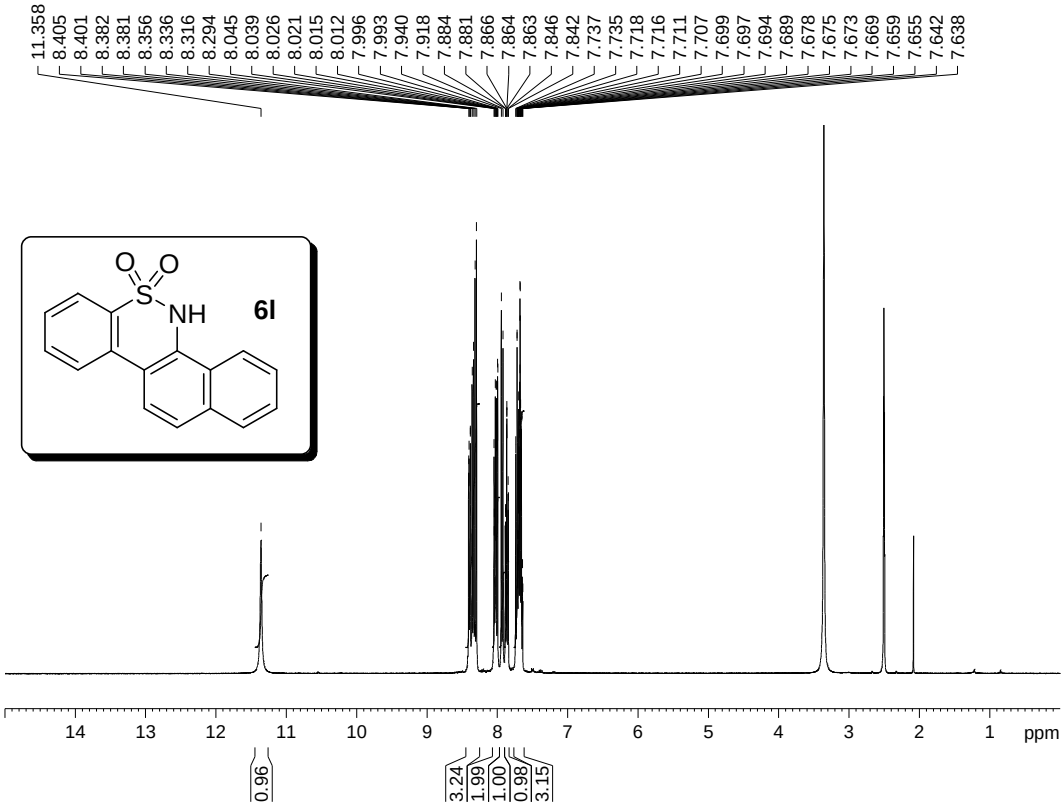


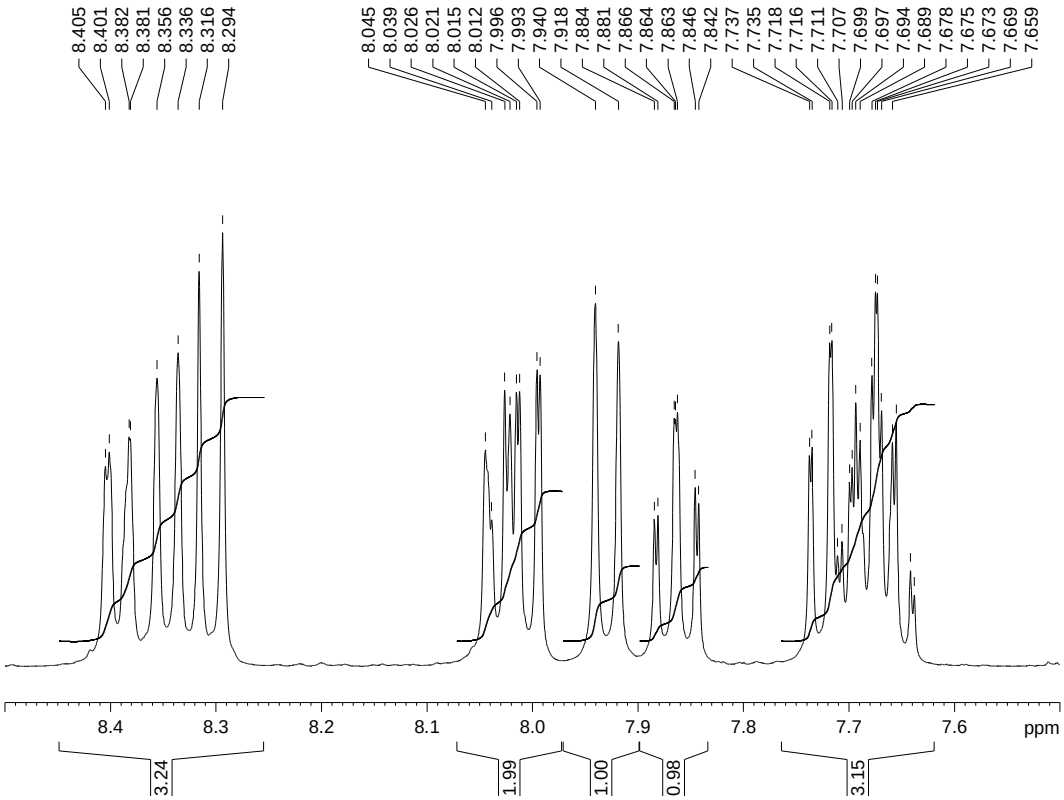

8.268
8.226
8.223
8.207
8.203
7.950
7.948
7.931
7.928
7.867
7.864
7.847
7.828
7.825
7.734
7.715
7.696
7.551
7.532
7.512
7.502
7.498
7.482
7.478
7.145
7.140
7.135
6.314
6.309
6.303
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 ppm
1.00
0.96
1.00
1.00
1.03
2.07
2.04
2.06

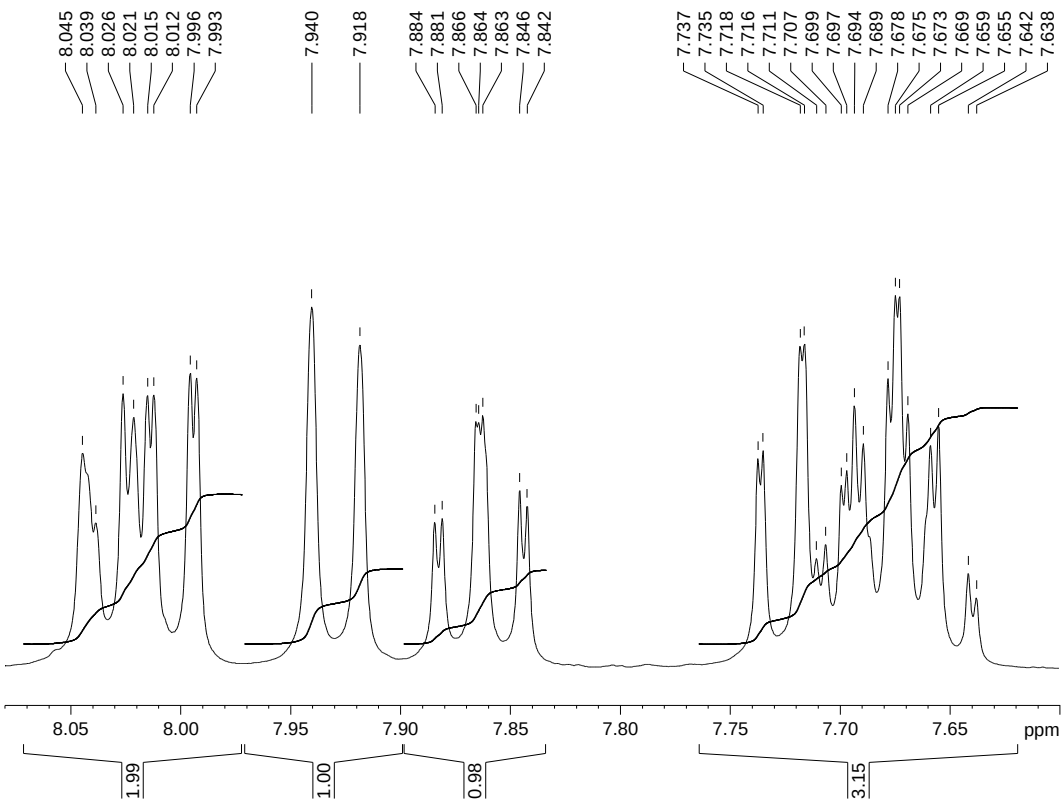

135.68
135.65
132.75
132.01
129.81
129.26
127.33
126.99
126.67
124.06
122.10
121.81
109.49
O
O
S
NH
N
6k
160 150 140 130 120 110 100 90 80 70 60 50 40 ppm

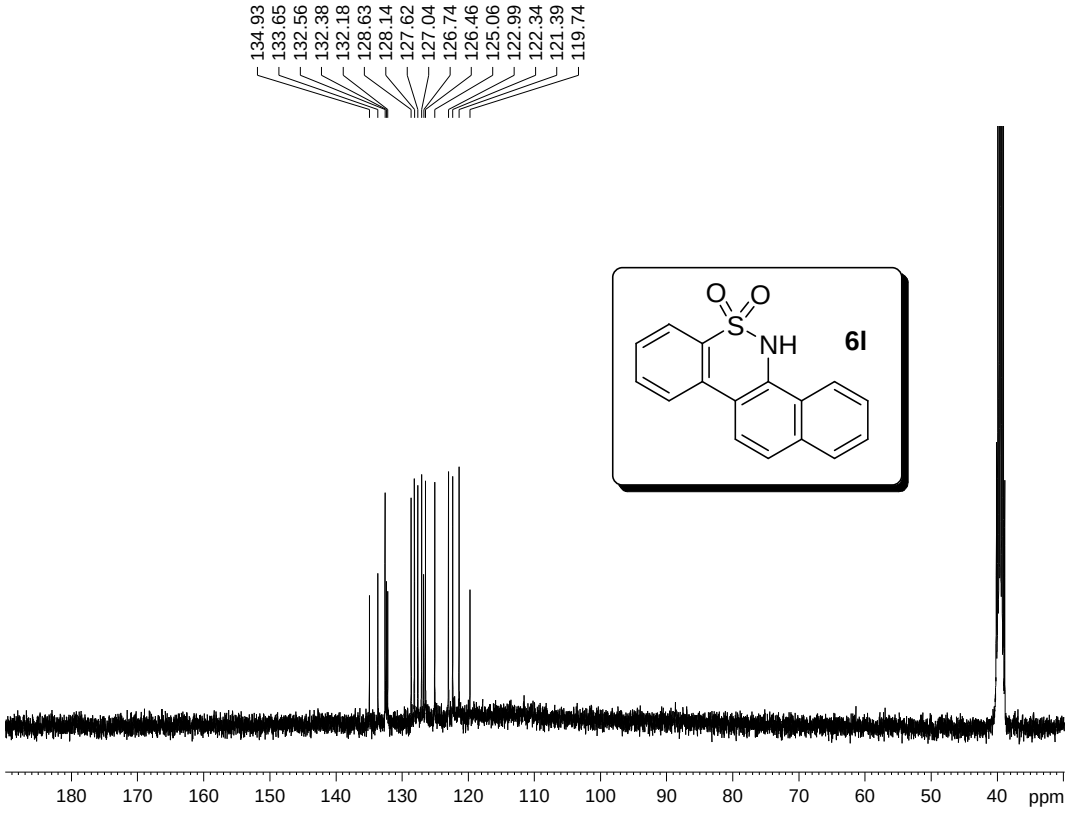


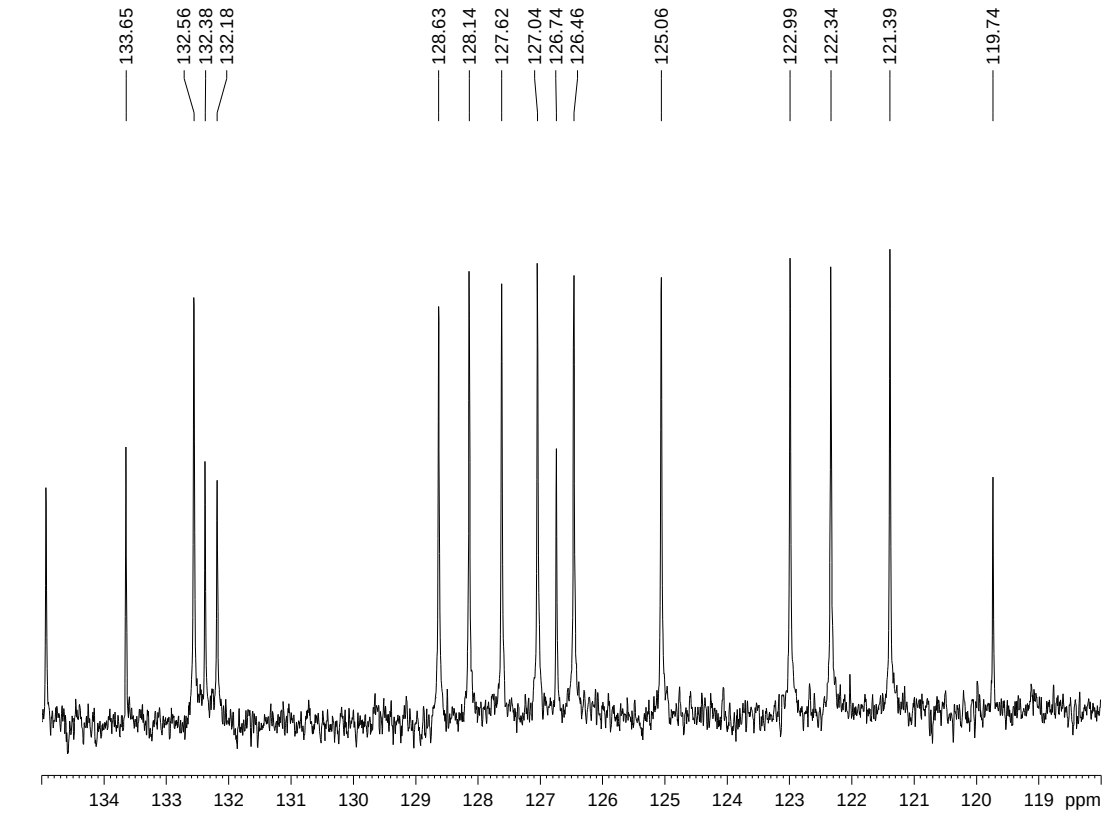

*5H-Benzo[e]naphtho[1,2-c][1,2]thiazine 6,6-dioxide* (**6l**)



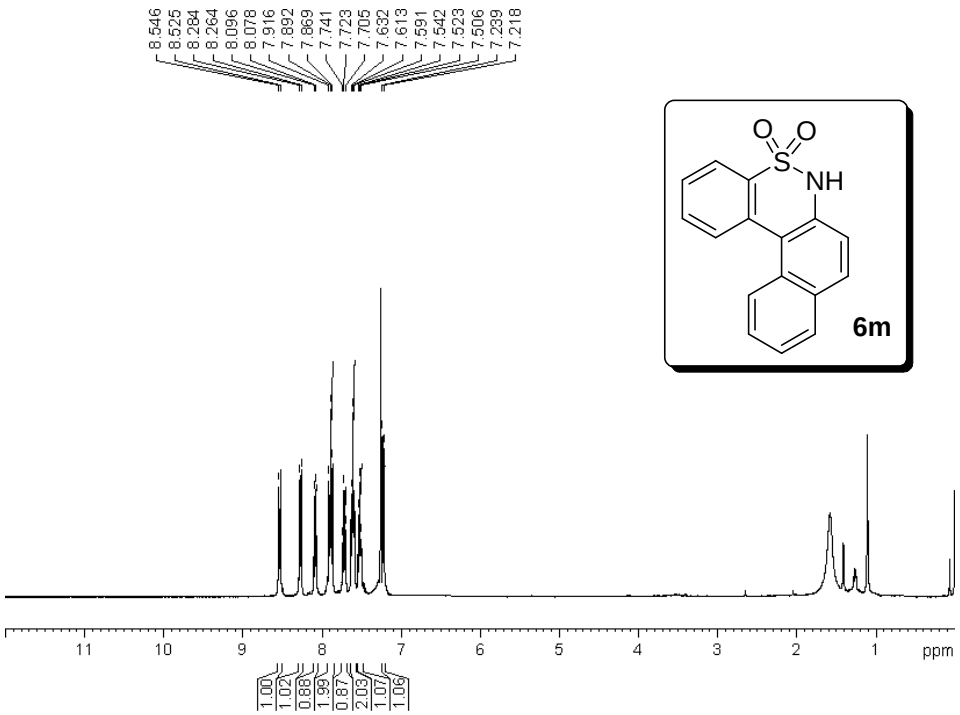

8.405
8.401
8.382
8.381
8.356
8.336
8.316
8.294
8.045
8.039
8.026
8.021
8.015
8.012
7.996
7.993
7.940
7.918
7.884
7.881
7.866
7.864
7.863
7.846
7.842
7.737
7.735
7.718
7.716
7.711
7.707
7.699
7.697
7.694
7.689
7.678
7.675
7.673
7.669
7.659
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
ppm
3.24
1.99
1.00
0.98
3.15

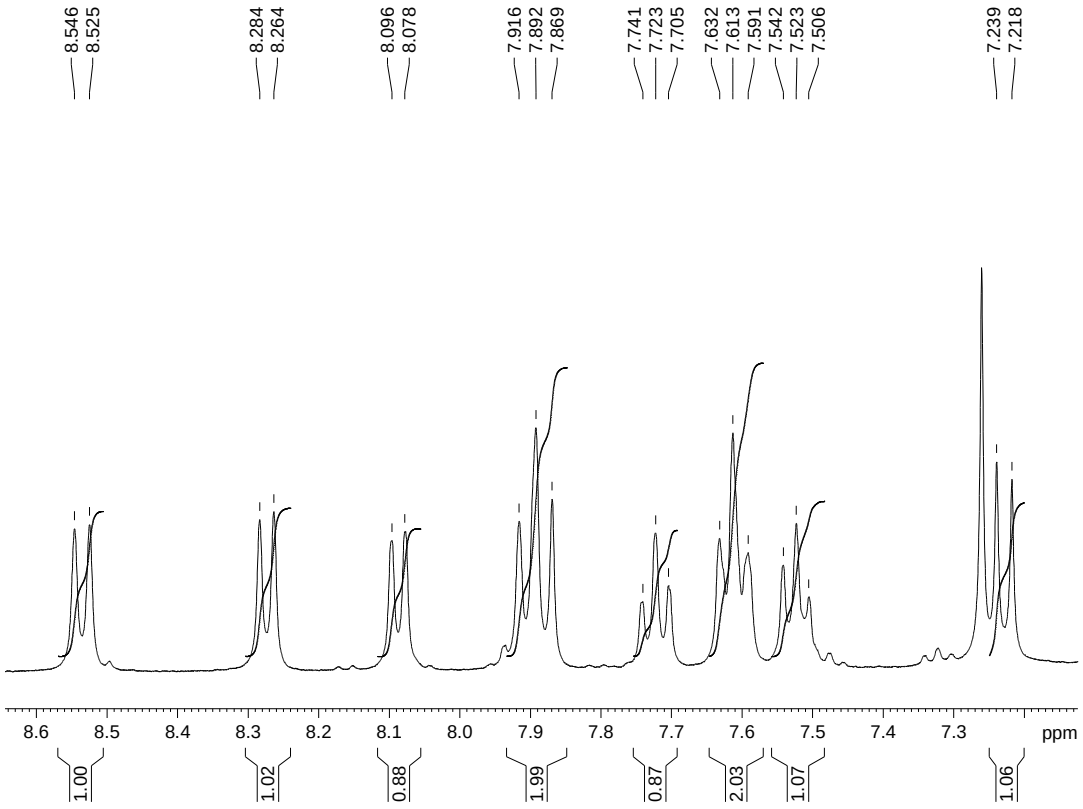

8.045
8.039
8.026
8.021
8.015
8.012
7.996
7.993
7.940
7.918
7.884
7.881
7.866
7.864
7.863
7.846
7.842
7.737
7.735
7.718
7.716
7.711
7.707
7.699
7.697
7.694
7.689
7.678
7.675
7.673
7.669
7.659
7.655
7.642
7.638
8.05
8.00
7.95
7.90
7.85
7.80
7.75
7.70
7.65
ppm
1.99
1.00
0.98
3.15


134.93
133.65
132.56
132.38
132.18
128.63
128.14
127.62
127.04
126.74
126.46
125.06
122.99
122.34
121.39
119.74
O
O
S
NH
6l
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

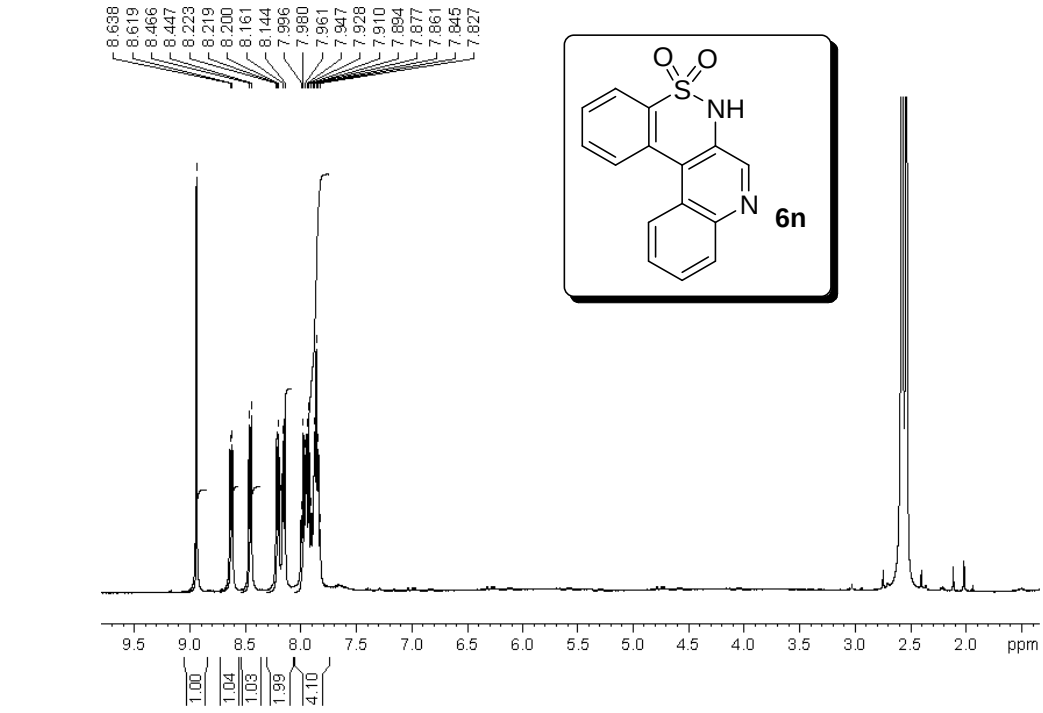

133.65
132.56
132.38
132.18
128.63
128.14
127.62
127.04
126.74
126.46
125.06
122.99
122.34
121.39
119.74
134
133
132
131
130
129
128
127
126
125
124
123
122
121
120
119
ppm

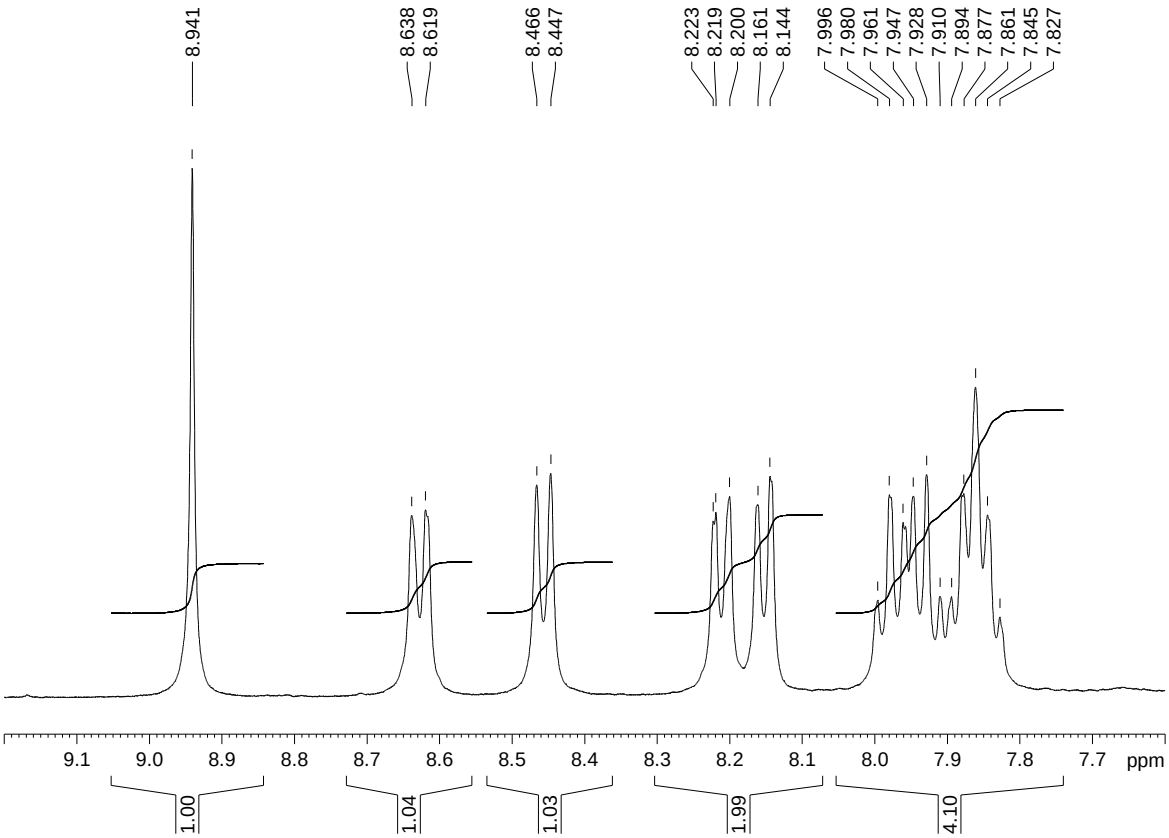
*6H-Benzo[e]naphtho[2,1-c][1,2]thiazine 5,5-dioxide* (**6m**)

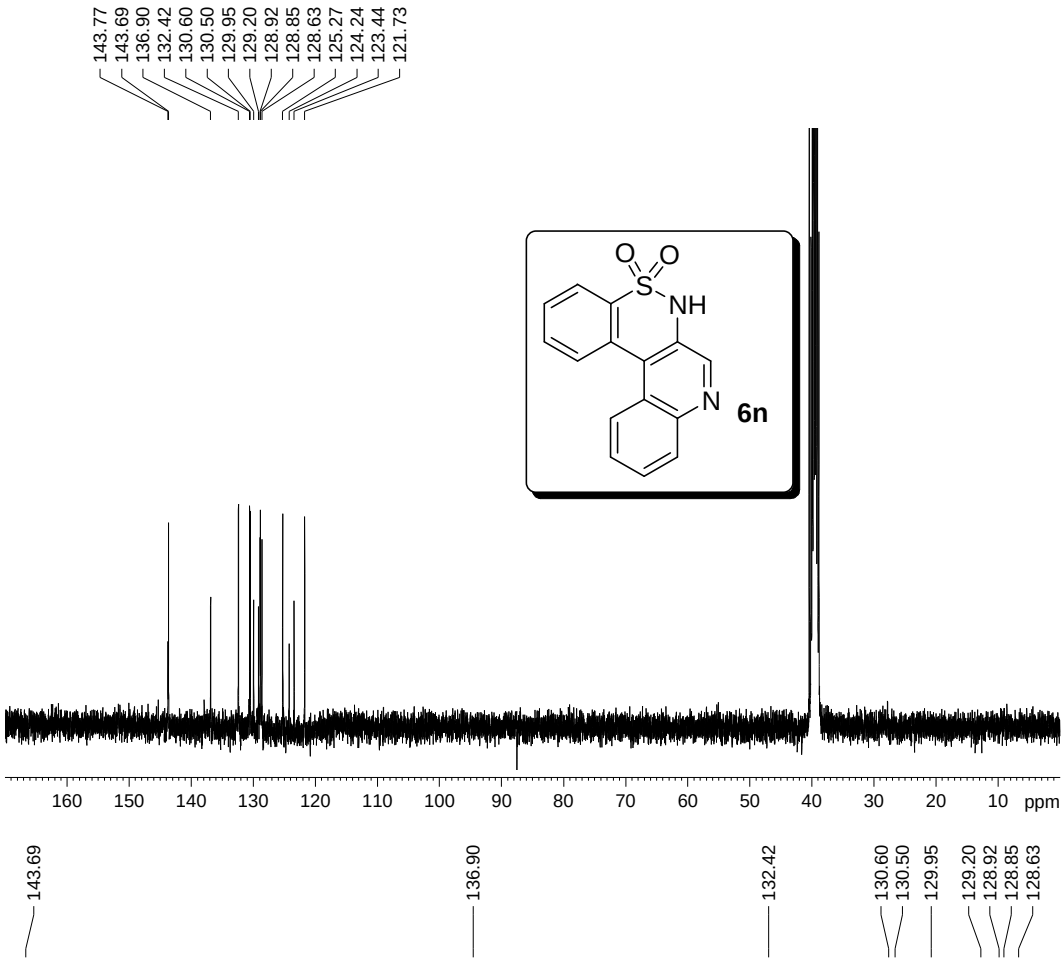


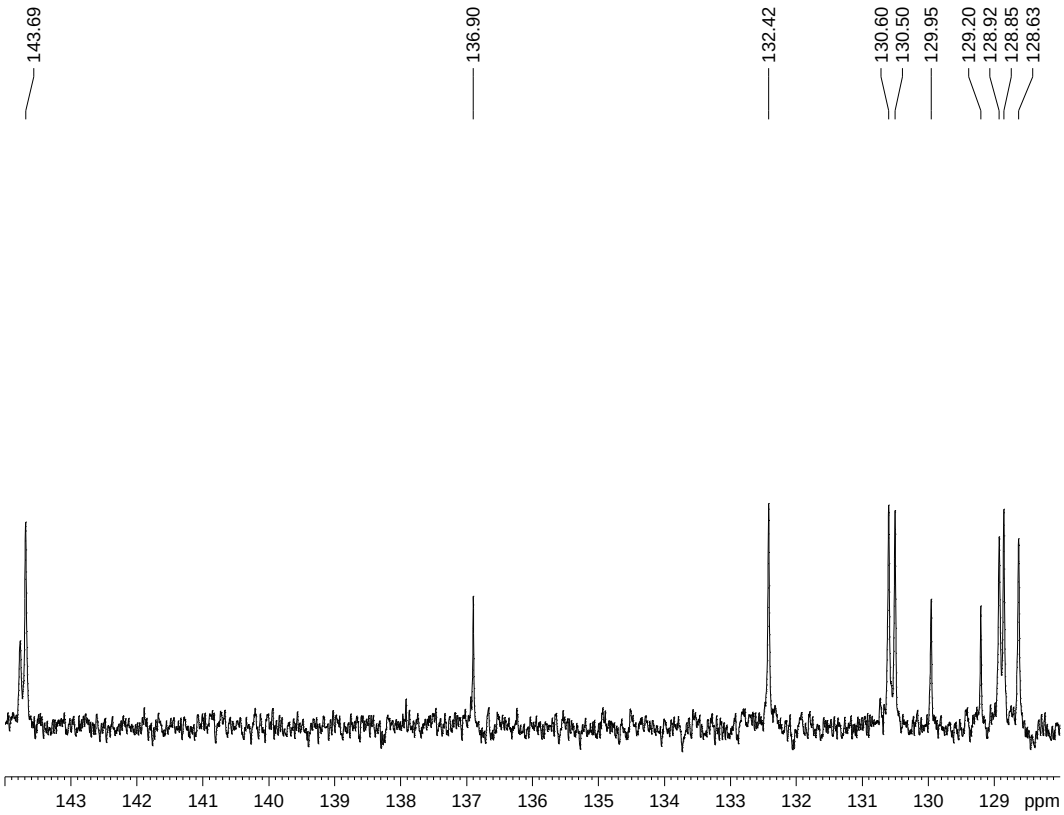



*6H-Benzo[5,6][1,2]thiazino[3,4-c]quinoline 5,5-dioxide* (**6n**)

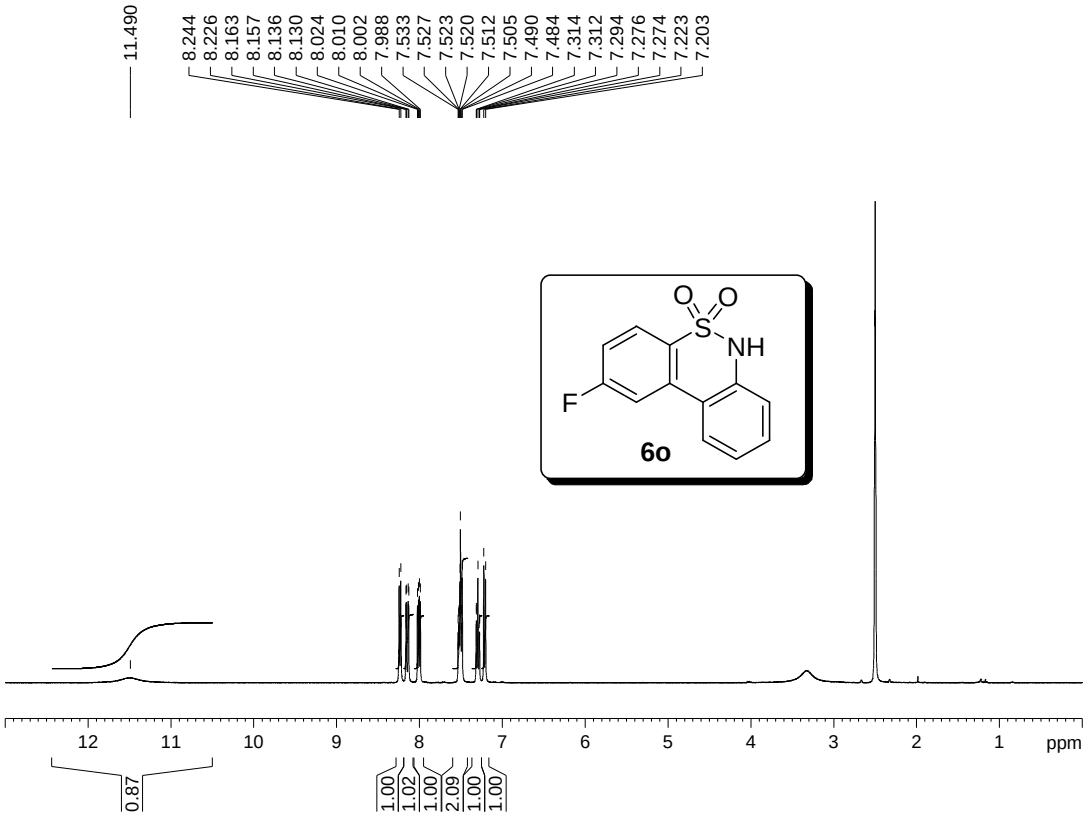


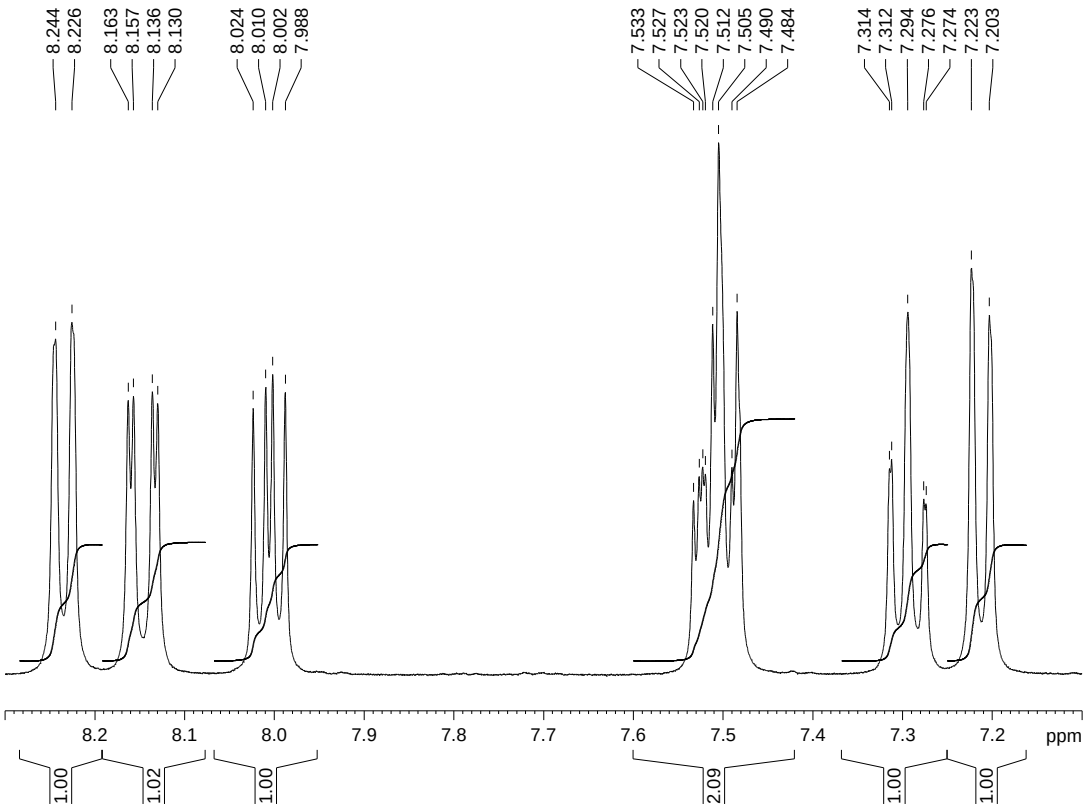



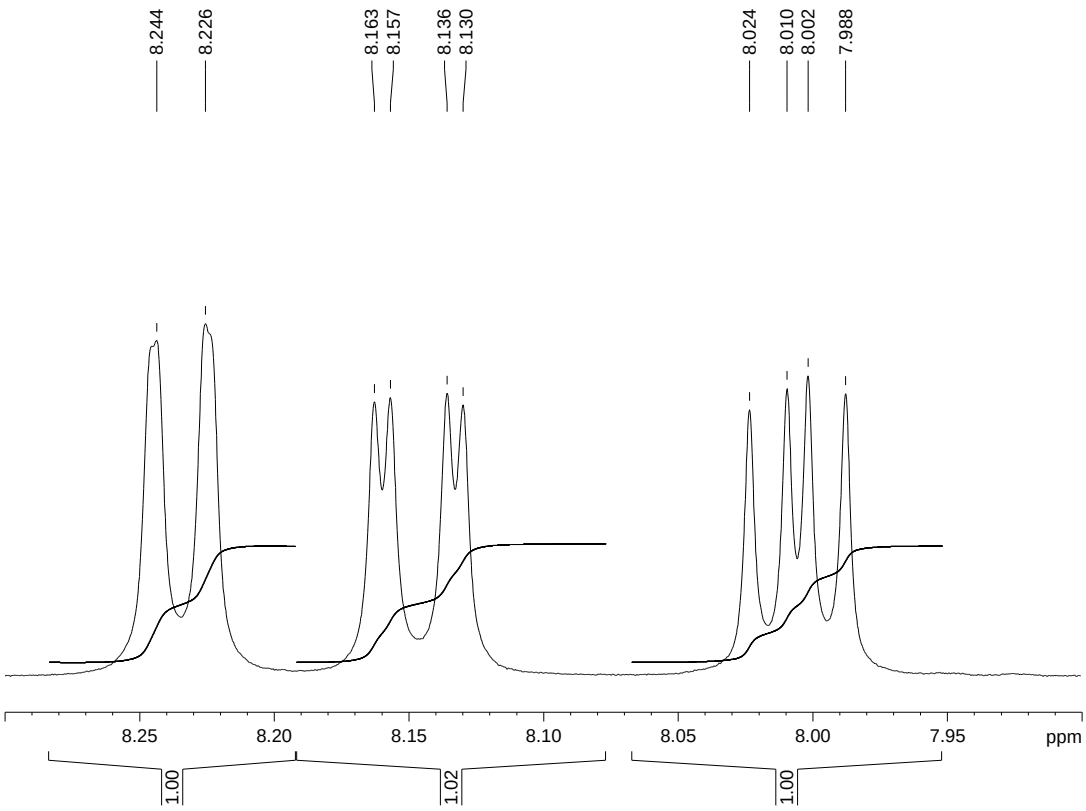

143.77
143.69
136.90
132.42
130.60
130.50
129.95
129.20
128.92
128.85
128.63
125.27
124.24
123.44
121.73
O
O
S
NH
N
6n
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

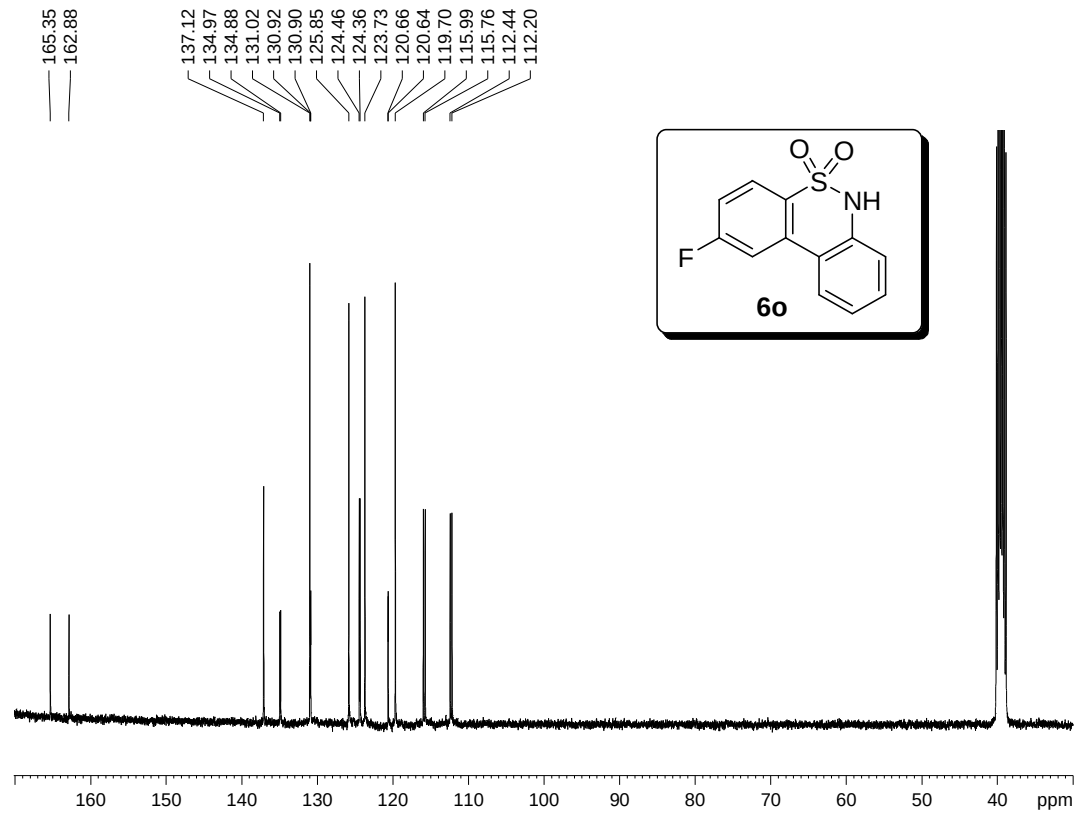

143.69
136.90
132.42
130.60
130.50
129.95
129.20
128.92
128.85
128.63
143
142
141
140
139
138
137
136
135
134
133
132
131
130
129
ppm

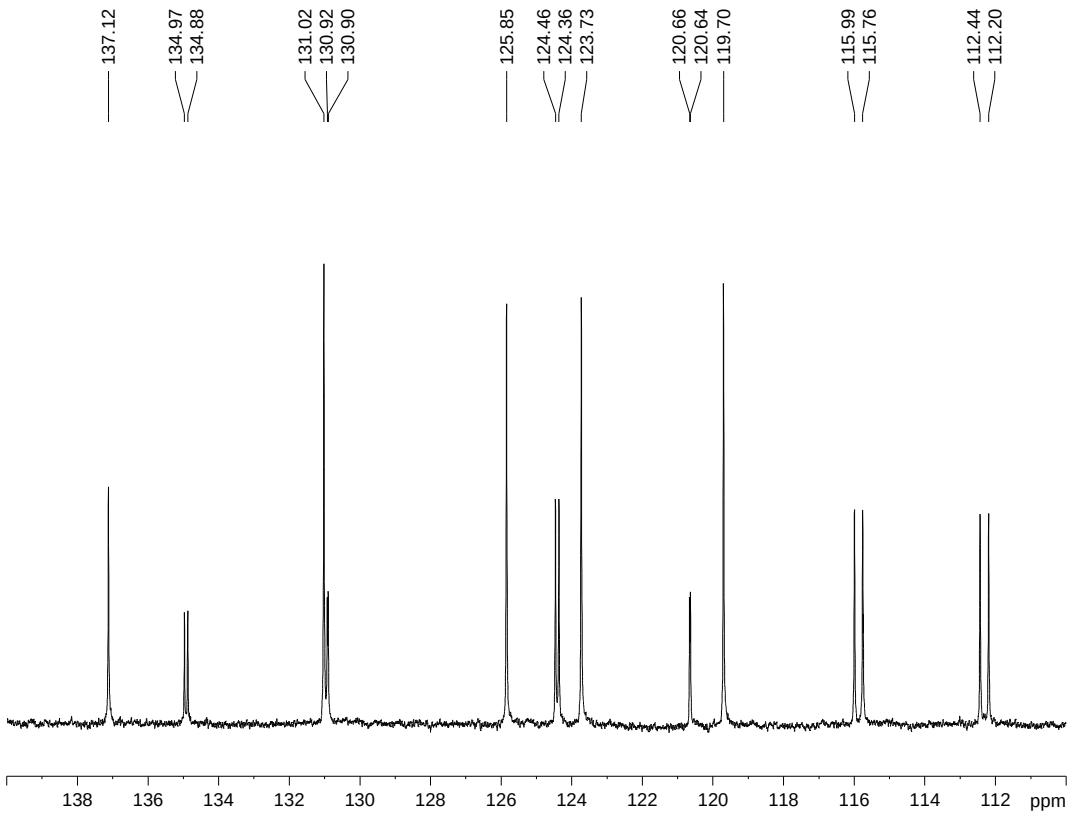
*2-Fluoro-6H-dibenzo[c,e][1,2]thiazine 5,5-dioxide* (**6o**)



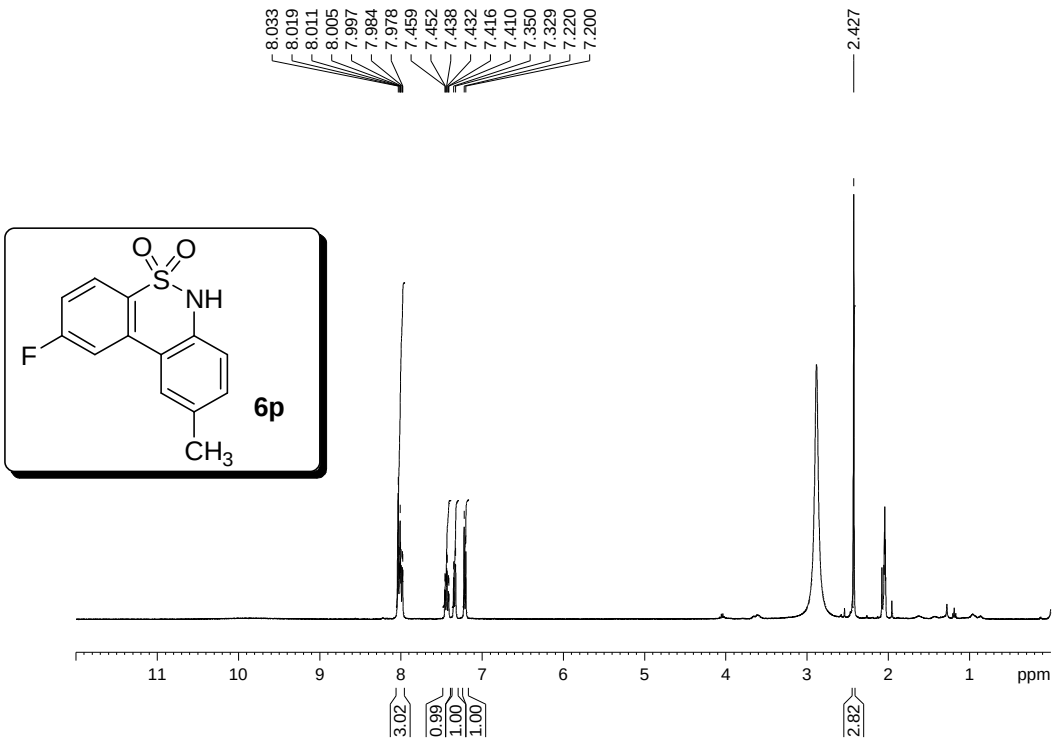



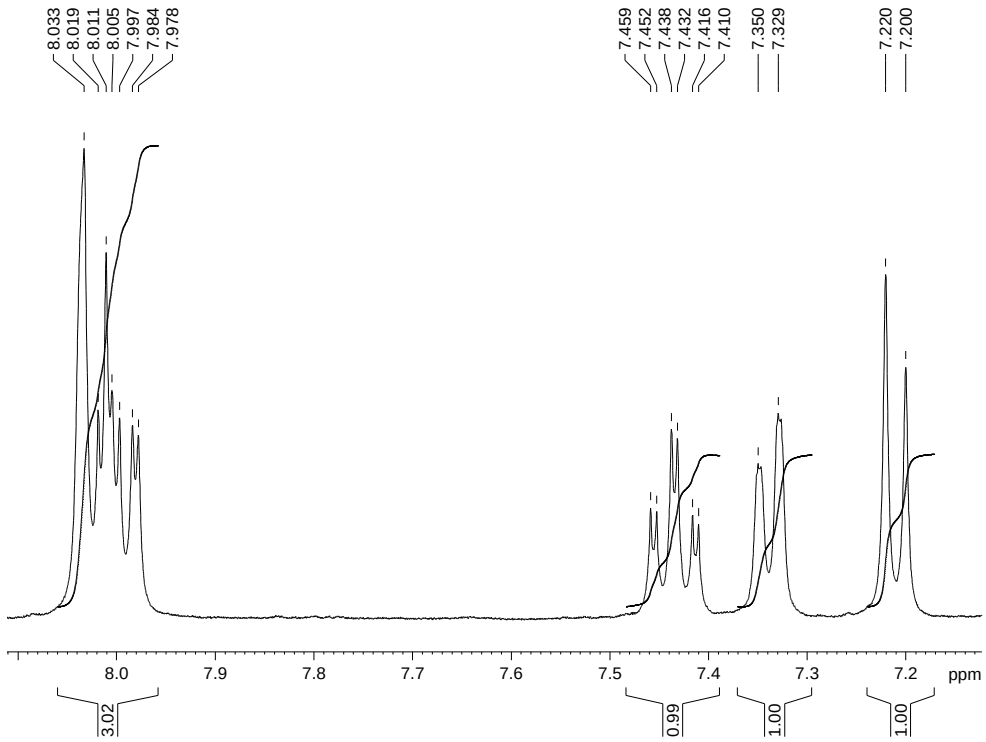

8.244
8.226
8.163
8.157
8.136
8.130
8.024
8.010
8.002
7.988
8.25
8.20
8.15
8.10
8.05
8.00
7.95
ppm
1.00
1.02
1.00

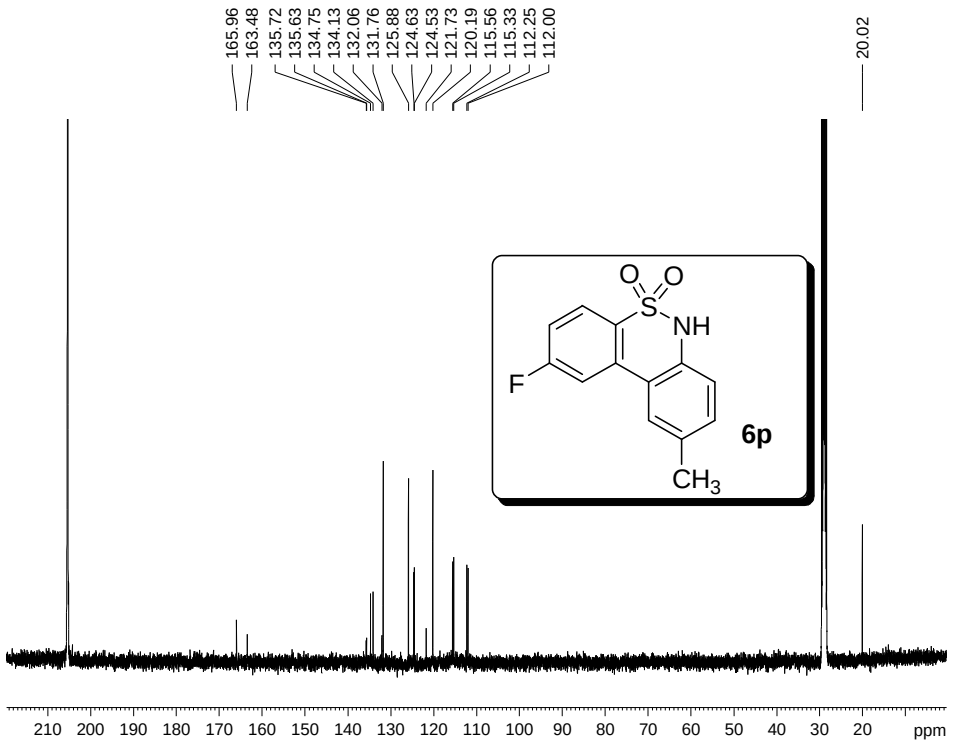

165.35
162.88
137.12
134.97
134.88
131.02
130.92
130.90
125.85
124.46
124.36
123.73
120.66
120.64
119.70
115.99
115.76
112.44
112.20
O
O
S
NH
F
6o
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

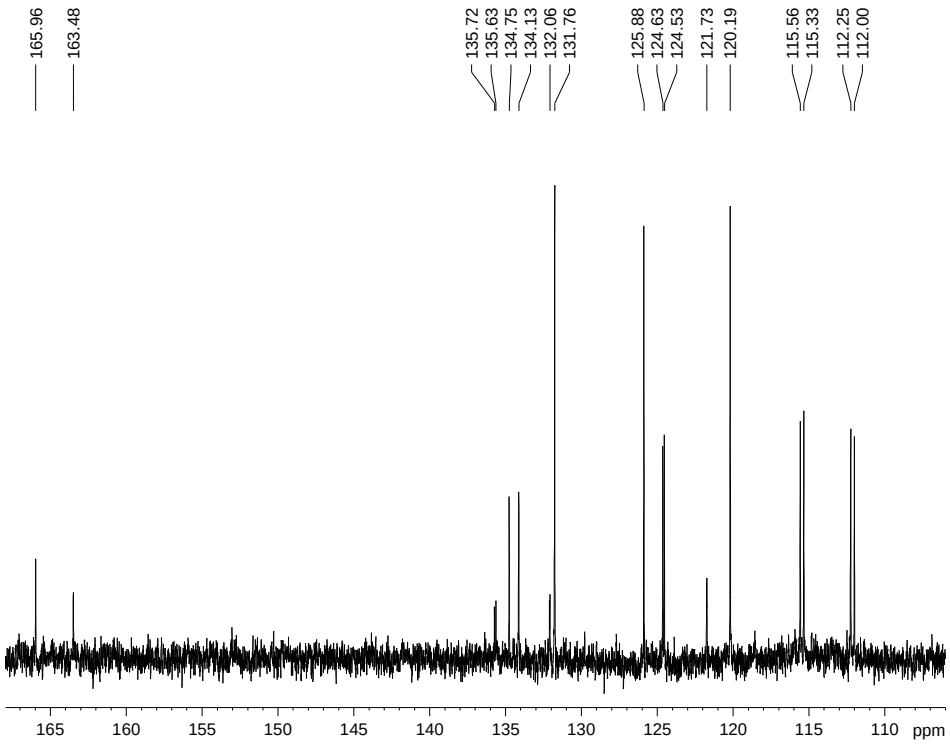



*2-Fluoro-9-methyl-6H-dibenzo[c,e][1,2]thiazine 5,5-dioxide* (**6p**)

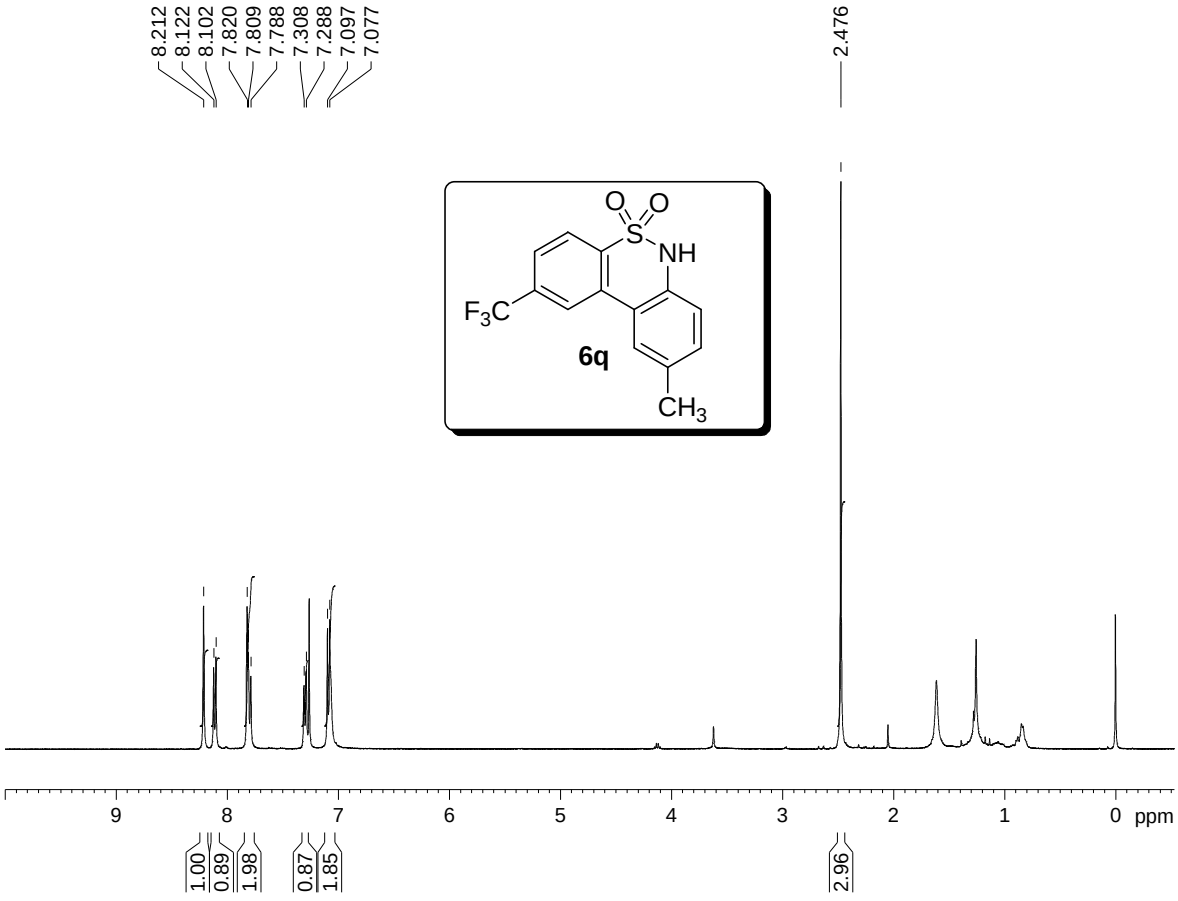


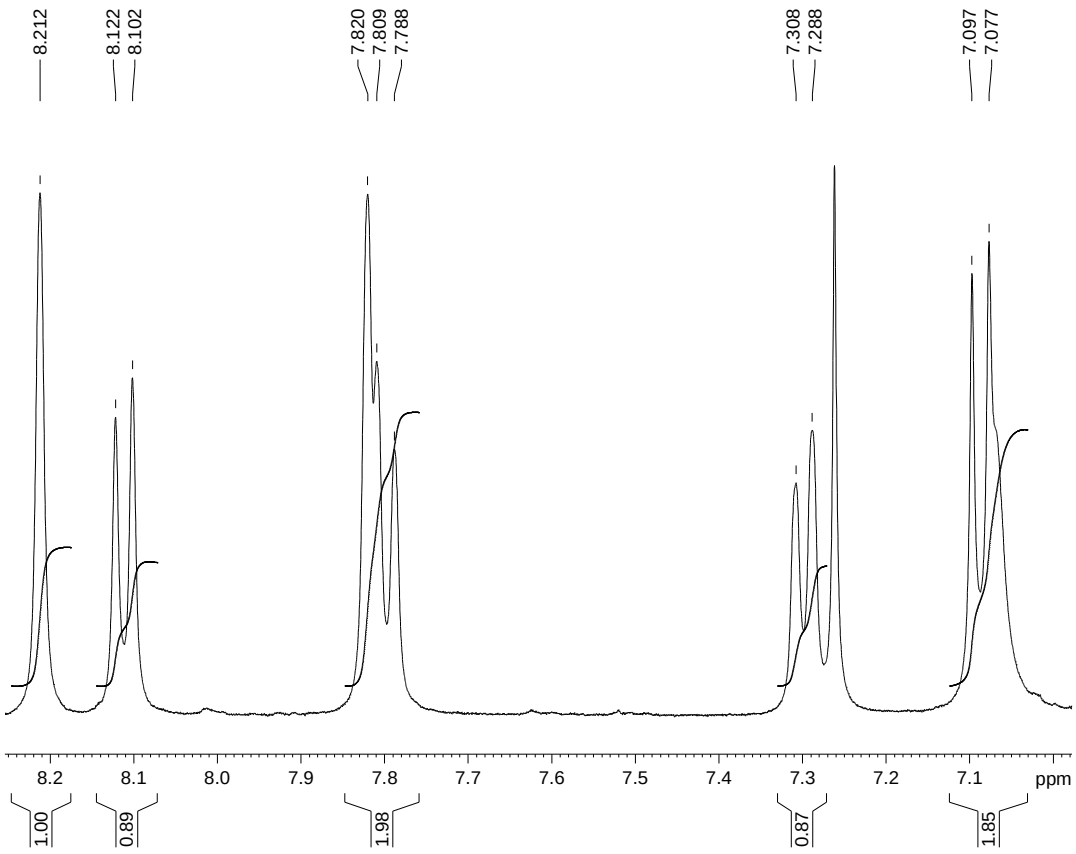

8.033
8.019
8.011
8.005
7.997
7.984
7.978
7.459
7.452
7.438
7.432
7.416
7.410
7.350
7.329
7.220
7.200
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
3.02
0.99
1.00
1.00

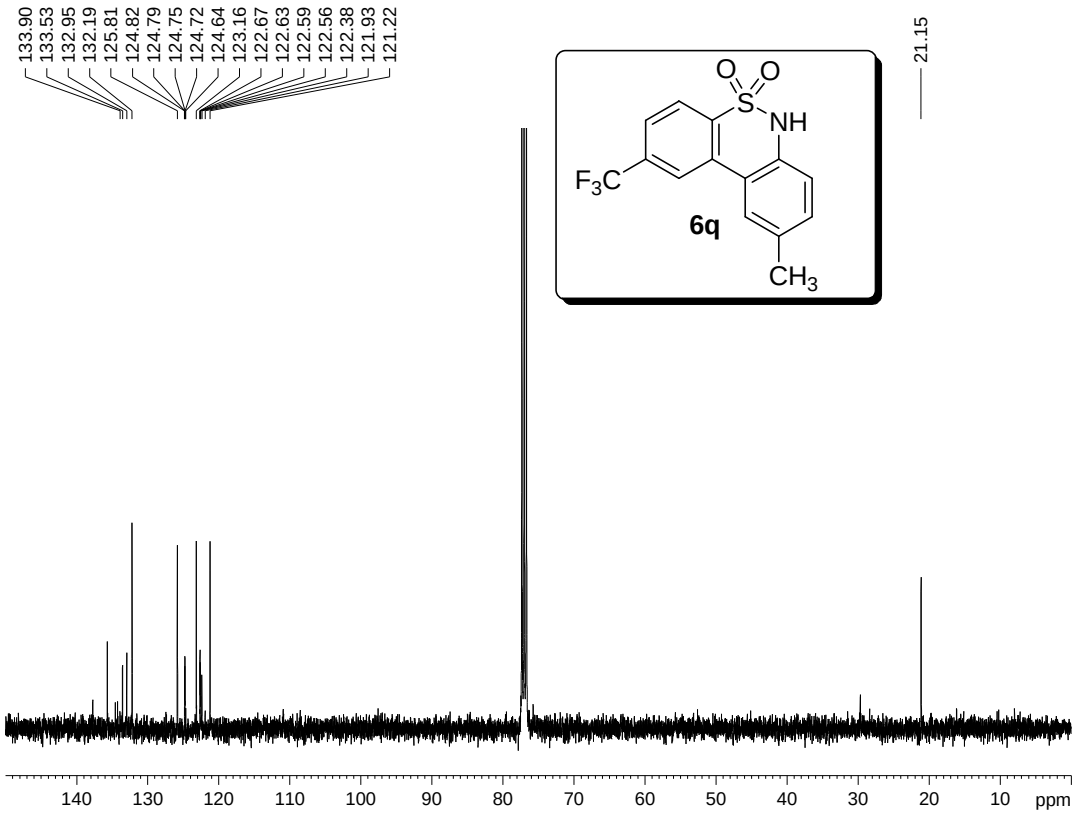

165.96
163.48
135.72
135.63
134.75
134.13
132.06
131.76
125.88
124.63
124.53
121.73
120.19
115.56
115.33
112.25
112.00
20.02
O
O
S
NH
F
CH3
6p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

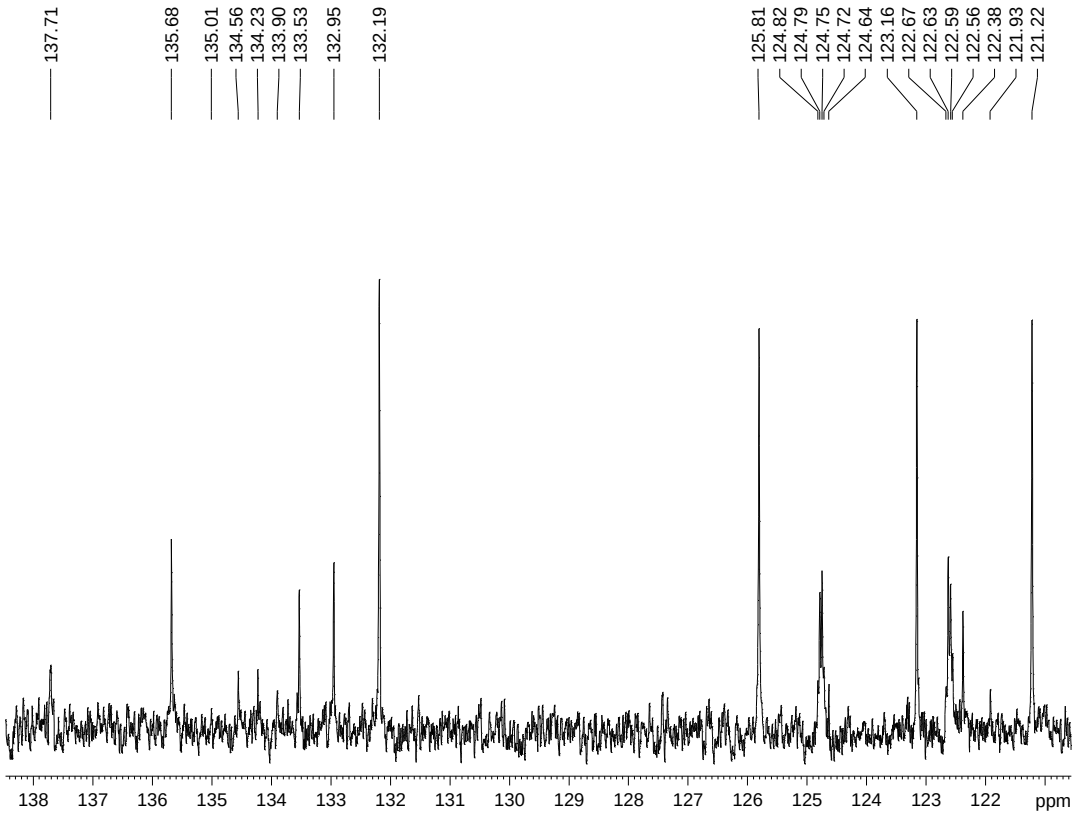



*9-Methyl-2-(trifluoromethyl)-6H-dibenzo[c,e][1,2]thiazine 5,5-dioxide* (**6q**)




8.212
8.122
8.102
7.820
7.809
7.788
7.308
7.288
7.097
7.077
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
ppm
1.00
0.89
1.98
0.87
1.85

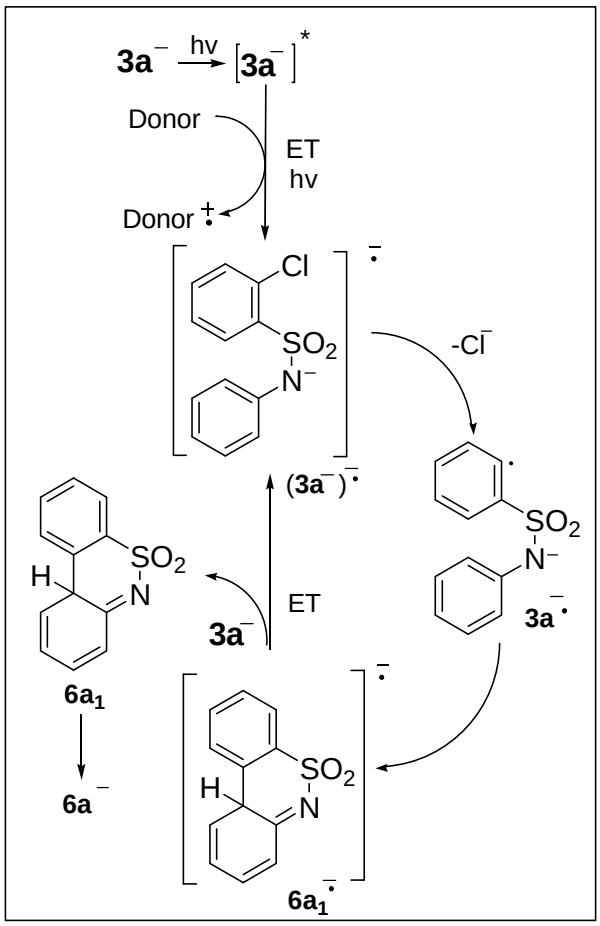

133.90
133.53
132.95
132.19
125.81
124.82
124.79
124.75
124.72
124.64
123.16
122.67
122.63
122.59
122.56
122.38
121.93
121.22
21.15
O
O
S
NH
F3C
6q
CH3
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm




## 5. Theoretical Section

**Full *Gaussian09* Reference**

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.




**3a**$^{-}$ (anion 3a)
m06-2x/6-311+g(d) scrf=(solvent=dmso,pcm)
Sum of electronic and zero-point Energies= -1526.065603 a.u.
Charge = -1 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 0.13270 | 0.53200 | 0.66039 |
| C | 1.16273 | 0.59909 | 1.59665 |
| C | 2.43800 | 0.15018 | 1.26237 |
| C | 2.68103 | -0.36793 | -0.00705 |
| C | 1.64620 | -0.43174 | -0.93677 |
| C | 0.36006 | 0.01443 | -0.62025 |
| H | 0.96114 | 1.00080 | 2.58253 |
| H | 3.23360 | 0.20717 | 1.99717 |
| H | 3.67006 | -0.72178 | -0.27639 |
| H | 1.82002 | -0.83536 | -1.92585 |
| Cl | -1.44611 | 1.11611 | 1.18056 |
| S | -0.93377 | -0.11655 | -1.92400 |
| O | -0.21921 | -0.75646 | -3.06597 |
| O | -2.00845 | -0.95622 | -1.34035 |
| N | -1.53620 | 1.31682 | -2.21281 |
| C | -0.80156 | 2.36423 | -2.76767 |
| C | 0.52104 | 2.31646 | -3.26510 |
| C | -1.46734 | 3.61089 | -2.83682 |
| C | 1.13393 | 3.45781 | -3.78376 |
| H | 1.06700 | 1.38208 | -3.26289 |

| | | | |
|---|---|---|---|
| C | -0.85115 | 4.73933 | -3.36347 |
| H | -2.48449 | 3.66718 | -2.46170 |
| C | 0.46207 | 4.67817 | -3.84111 |
| H | 2.15276 | 3.38346 | -4.15417 |
| H | -1.39925 | 5.67671 | -3.39812 |
| H | 0.94580 | 5.55958 | -4.24906 |

(**3a**$^{-}$)*(anion 3a $S_1$)
TD DFT m06-2x/6-311+g(d) scrf=(solvent=dmso,pcm)
The total energy including the PCM contribution is -1526.090199236 a.u.
Charge = -1 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 0.13270 | 0.53200 | 0.66039 |
| C | 1.16273 | 0.59909 | 1.59665 |
| C | 2.43800 | 0.15018 | 1.26237 |
| C | 2.68103 | -0.36793 | -0.00705 |
| C | 1.64620 | -0.43174 | -0.93677 |
| C | 0.36006 | 0.01443 | -0.62025 |
| H | 0.96114 | 1.00080 | 2.58253 |
| H | 3.23360 | 0.20717 | 1.99717 |
| H | 3.67006 | -0.72178 | -0.27639 |
| H | 1.82002 | -0.83536 | -1.92585 |
| Cl | -1.44611 | 1.11611 | 1.18056 |
| S | -0.93377 | -0.11655 | -1.92400 |
| O | -0.21921 | -0.75646 | -3.06597 |
| O | -2.00845 | -0.95622 | -1.34035 |
| N | -1.53620 | 1.31682 | -2.21281 |
| C | -0.80156 | 2.36423 | -2.76767 |
| C | 0.52104 | 2.31646 | -3.26510 |
| C | -1.46734 | 3.61089 | -2.83682 |
| C | 1.13393 | 3.45781 | -3.78376 |
| H | 1.06700 | 1.38208 | -3.26289 |
| C | -0.85115 | 4.73933 | -3.36347 |
| H | -2.48449 | 3.66718 | -2.46170 |
| C | 0.46207 | 4.67817 | -3.84111 |
| H | 2.15276 | 3.38346 | -4.15417 |
| H | -1.39925 | 5.67671 | -3.39812 |
| H | 0.94580 | 5.55958 | -4.24906 |

(**3a**$^{-}$)$^{\bullet-}$ (dianion radical 3a)
m06-2x/6-311+g(d) scrf=(solvent=dmso,pcm)
Sum of electronic and zero-point Energies= -1526.131042 a.u.
Charge = -2 Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.05330 | 0.47402 | 0.58983 |
| C | 1.11829 | 0.81895 | 1.38929 |
| C | 2.45188 | 0.55895 | 0.98635 |
| C | 2.64764 | -0.12197 | -0.25365 |
| C | 1.58577 | -0.47408 | -1.05194 |
| C | 0.21985 | -0.19083 | -0.68301 |
| H | 0.91097 | 1.27615 | 2.36032 |
| H | 3.29056 | 0.85532 | 1.61589 |

| | | | |
|---|---|---|---|
| H | 3.66071 | -0.38055 | -0.57501 |
| H | 1.74988 | -0.99296 | -1.99801 |
| Cl | -1.57448 | 0.72568 | 1.23416 |
| S | -1.02839 | -0.19458 | -1.91238 |
| O | -0.38919 | -0.77315 | -3.12791 |
| O | -2.18122 | -0.98426 | -1.42809 |
| N | -1.62172 | 1.28491 | -2.16854 |
| C | -0.82723 | 2.28405 | -2.64792 |
| C | 0.54241 | 2.18871 | -3.03261 |
| C | -1.41627 | 3.57477 | -2.78502 |
| C | 1.24470 | 3.30084 | -3.49382 |
| H | 1.04495 | 1.22460 | -2.97732 |
| C | -0.70581 | 4.67158 | -3.25234 |
| H | -2.46668 | 3.67400 | -2.50186 |
| C | 0.64290 | 4.55505 | -3.61233 |
| H | 2.29476 | 3.17758 | -3.77360 |
| H | -1.21103 | 5.63743 | -3.33654 |
| H | 1.20404 | 5.41627 | -3.97759 |

**TS C-Cl** (Transition State for C-Cl fragmentation)
m06-2x/6-311+g(d) scrf=(solvent=dmso,pcm)
Sum of electronic and zero-point Energies= -1526.131649 a.u.
Charge = -2 Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.01172 | 0.79536 | 0.31345 |
| C | 1.12292 | 1.21356 | 1.05771 |
| C | 2.39947 | 0.78722 | 0.74248 |
| C | 2.57969 | -0.18349 | -0.29219 |
| C | 1.49143 | -0.62757 | -1.00805 |
| C | 0.18059 | -0.16102 | -0.74630 |
| H | 0.96735 | 1.89297 | 1.89229 |
| H | 3.25423 | 1.19002 | 1.27528 |
| H | 3.56800 | -0.57479 | -0.50837 |
| H | 1.63114 | -1.34156 | -1.81348 |
| Cl | -1.58170 | 0.85044 | 1.23399 |
| S | -1.03529 | -0.30755 | -2.02544 |
| O | -0.34690 | -0.95090 | -3.18343 |
| O | -2.17647 | -1.13043 | -1.54859 |
| N | -1.64765 | 1.13493 | -2.34617 |
| C | -0.80868 | 2.18611 | -2.66530 |
| C | 0.56242 | 2.10899 | -3.00901 |
| C | -1.38697 | 3.47736 | -2.67118 |
| C | 1.29451 | 3.25536 | -3.30621 |
| H | 1.05362 | 1.14508 | -3.04889 |
| C | -0.65076 | 4.61121 | -2.97988 |
| H | -2.43869 | 3.56137 | -2.41563 |
| C | 0.70631 | 4.51740 | -3.29688 |
| H | 2.34571 | 3.15288 | -3.55980 |
| H | -1.13977 | 5.58068 | -2.96809 |
| H | 1.28435 | 5.40286 | -3.53598 |

**3a**$^{\bullet-}$ (radical anion 3a)
m06-2x/6-311+g(d) scrf=(solvent=dmso,pcm)
Sum of electronic and zero-point Energies= -1065.787758 a.u.
Charge = -1 Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 2.07937 | 0.74349 | -1.36146 |
| C | 2.82856 | 1.03541 | -0.24673 |
| C | 2.50976 | 0.34090 | 0.92503 |
| C | 1.47580 | -0.59553 | 0.93015 |
| C | 0.74544 | -0.85549 | -0.22629 |
| C | 1.05823 | -0.16934 | -1.40302 |
| H | 3.62938 | 1.76602 | -0.26410 |
| H | 3.07156 | 0.53447 | 1.83215 |
| H | 1.23975 | -1.13104 | 1.84227 |
| H | -0.05401 | -1.58801 | -0.23337 |
| S | 0.08103 | -0.42870 | -2.89884 |
| O | 1.05652 | -0.40875 | -4.00876 |
| O | -0.59615 | -1.72001 | -2.70097 |
| N | -1.02085 | 0.69599 | -2.93692 |
| C | -0.69249 | 2.04060 | -3.08705 |
| C | 0.55704 | 2.57578 | -3.46532 |
| C | -1.73581 | 2.95882 | -2.84064 |
| C | 0.74174 | 3.95376 | -3.56621 |
| H | 1.37974 | 1.91459 | -3.70487 |
| C | -1.54335 | 4.32675 | -2.95308 |
| H | -2.70353 | 2.56172 | -2.55281 |
| C | -0.29671 | 4.84290 | -3.31323 |
| H | 1.71718 | 4.33043 | -3.85751 |
| H | -2.37225 | 4.99834 | -2.75391 |
| H | -0.14372 | 5.91253 | -3.39841 |

**TS C-C** (Transition State for C-C coupling)
m06-2x/6-311+g(d) scrf=(solvent=dmso,pcm)
Sum of electronic and zero-point Energies= -1065.773184 a.u.
Charge = -1 Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.46176 | 1.32920 | -0.97103 |
| C | 1.03560 | 1.79248 | 0.19743 |
| C | 1.73252 | 0.88435 | 0.99749 |
| C | 1.83532 | -0.45458 | 0.61619 |
| C | 1.25399 | -0.89646 | -0.56825 |
| C | 0.56289 | 0.01629 | -1.36938 |
| H | 0.94586 | 2.83471 | 0.49116 |
| H | 2.19312 | 1.22023 | 1.92087 |
| H | 2.37200 | -1.15583 | 1.24492 |
| H | 1.33412 | -1.93582 | -0.87196 |
| S | -0.13486 | -0.52346 | -2.95022 |
| O | 1.04467 | -0.69260 | -3.83040 |
| O | -0.86226 | -1.78279 | -2.70743 |
| N | -1.14990 | 0.59906 | -3.37267 |
| C | -0.59926 | 1.89212 | -3.33871 |

| | | | |
|---|---|---|---|
| C | 0.23746 | 2.40986 | -4.32647 |
| C | -0.83864 | 2.67311 | -2.17159 |
| C | 0.79744 | 3.68150 | -4.19047 |
| H | 0.45731 | 1.79964 | -5.19557 |
| C | -0.33185 | 3.98527 | -2.08227 |
| H | -1.63653 | 2.35679 | -1.50872 |
| C | 0.51173 | 4.46893 | -3.07112 |
| H | 1.44850 | 4.06610 | -4.96807 |
| H | -0.58797 | 4.60082 | -1.22668 |
| H | 0.92918 | 5.46670 | -2.99095 |

**$6a_1^{\bullet-}$** (radical anion $6a_1$)
m06-2x/6-311+g(d) scrf=(solvent=dmso,pcm)
Sum of electronic and zero-point Energies= -1065.825920 a.u.
Charge = -1 Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.46526 | 1.32619 | -1.10793 |
| C | 1.13041 | 1.84937 | -0.00271 |
| C | 1.79720 | 1.00468 | 0.88463 |
| C | 1.83032 | -0.37025 | 0.67082 |
| C | 1.19178 | -0.91075 | -0.44228 |
| C | 0.51173 | -0.05746 | -1.29848 |
| H | 1.14045 | 2.91988 | 0.16556 |
| H | 2.30332 | 1.42911 | 1.74454 |
| H | 2.35930 | -1.01791 | 1.36021 |
| H | 1.22204 | -1.97433 | -0.64994 |
| S | -0.28605 | -0.65203 | -2.77583 |
| O | 0.26960 | -1.97010 | -3.11011 |
| O | -1.74166 | -0.65768 | -2.51386 |
| N | 0.15872 | 0.40298 | -3.88726 |
| C | 0.12733 | 1.73065 | -3.54832 |
| C | 0.49510 | 2.68509 | -4.48350 |
| C | -0.29318 | 2.15913 | -2.14137 |
| C | 0.51659 | 4.05630 | -4.19539 |
| H | 0.77438 | 2.33109 | -5.47130 |
| C | -0.21441 | 3.64279 | -1.92011 |
| H | -1.34709 | 1.84287 | -2.02720 |
| C | 0.15222 | 4.51039 | -2.89890 |
| H | 0.81174 | 4.76667 | -4.95816 |
| H | -0.52477 | 4.01337 | -0.94853 |
| H | 0.16187 | 5.57561 | -2.68848 |

**$6a_1$** ($6a_1$ neutral)
m06-2x/6-311+g(d) scrf=(solvent=dmso,pcm)
Sum of electronic and zero-point Energies= -1065.698372 a.u.
Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 0.48002 | 1.32431 | -1.09786 |
| C | 1.12577 | 1.84518 | 0.01850 |
| C | 1.77834 | 0.99315 | 0.90799 |
| C | 1.81352 | -0.38074 | 0.69108 |

| | | | |
|---|---|---|---|
| C | 1.19509 | -0.91786 | -0.43278 |
| C | 0.53155 | -0.05523 | -1.29205 |
| H | 1.14148 | 2.91307 | 0.19682 |
| H | 2.27650 | 1.41477 | 1.77312 |
| H | 2.33081 | -1.03092 | 1.38588 |
| H | 1.22512 | -1.98044 | -0.64309 |
| S | -0.27360 | -0.66672 | -2.74479 |
| O | 0.31212 | -1.93938 | -3.12783 |
| O | -1.72231 | -0.61073 | -2.55565 |
| N | 0.15169 | 0.45886 | -3.89978 |
| C | 0.12825 | 1.70433 | -3.54205 |
| C | 0.46655 | 2.70208 | -4.53411 |
| C | -0.24766 | 2.16489 | -2.13948 |
| C | 0.48190 | 4.01174 | -4.21756 |
| H | 0.72106 | 2.34721 | -5.52524 |
| C | -0.17671 | 3.64174 | -1.91380 |
| H | -1.31592 | 1.89576 | -2.05017 |
| C | 0.14595 | 4.49742 | -2.88761 |
| H | 0.74774 | 4.73856 | -4.97740 |
| H | -0.45852 | 3.99965 | -0.93004 |
| H | 0.15344 | 5.56494 | -2.70600 |

**6a**$^{-}$ (anion 6a)
m06-2x/6-311+g(d) scrf=(solvent=dmso,pcm)
Sum of electronic and zero-point Energies= -1065.299912 a.u.
Charge = -1 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 3.83017 | -0.13449 | -0.04985 |
| C | 2.82625 | -1.05561 | -0.27749 |
| C | 1.46348 | -0.70734 | -0.16826 |
| C | 1.14051 | 0.64892 | 0.11594 |
| C | 2.18135 | 1.55668 | 0.37123 |
| C | 3.51153 | 1.18330 | 0.29910 |
| C | -0.26213 | 1.09390 | 0.05351 |
| C | -1.30743 | 0.15957 | 0.06670 |
| C | -2.64470 | 0.52142 | -0.06653 |
| H | -3.40870 | -0.24817 | -0.06105 |
| C | -2.97483 | 1.86086 | -0.20360 |
| C | -1.95687 | 2.81743 | -0.22079 |
| C | -0.62740 | 2.44220 | -0.10663 |
| H | 4.86792 | -0.44224 | -0.12428 |
| H | 3.06209 | -2.08509 | -0.52504 |
| H | 1.94059 | 2.57925 | 0.64044 |
| H | 4.29339 | 1.90403 | 0.50774 |
| H | -4.01118 | 2.16093 | -0.30434 |
| H | -2.20366 | 3.86598 | -0.34402 |
| H | 0.13800 | 3.20594 | -0.17272 |
| S | -0.86255 | -1.53760 | 0.31947 |
| O | -1.87031 | -2.39268 | -0.32775 |
| O | -0.77991 | -1.72592 | 1.78450 |
| N | 0.53109 | -1.70274 | -0.41007 |

**6a** (6a neutral)
m06-2x/6-311+g(d) scrf=(solvent=dmso,pcm)
Sum of electronic and zero-point Energies= -1065.743453 a.u.
Charge = 0 Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 3.83143 | -0.15555 | 0.01495 |
| C | 2.82845 | -1.06679 | -0.28025 |
| C | 1.49580 | -0.66131 | -0.26170 |
| C | 1.14777 | 0.66688 | 0.04173 |
| C | 2.17858 | 1.55593 | 0.36808 |
| C | 3.50613 | 1.15705 | 0.35284 |
| C | -0.26451 | 1.09754 | -0.00794 |
| C | -1.31199 | 0.16906 | 0.06567 |
| C | -2.65366 | 0.51966 | -0.01094 |
| H | -3.41959 | -0.24569 | 0.04222 |
| C | -2.98403 | 1.85905 | -0.16091 |
| C | -1.96907 | 2.81077 | -0.24410 |
| C | -0.63344 | 2.43756 | -0.17892 |
| H | 4.86632 | -0.47687 | 0.00079 |
| H | 3.07122 | -2.09611 | -0.52069 |
| H | 1.93607 | 2.57373 | 0.64946 |
| H | 4.28542 | 1.86439 | 0.60901 |
| H | -4.02337 | 2.15705 | -0.22368 |
| H | -2.22042 | 3.85639 | -0.37766 |
| H | 0.13150 | 3.19646 | -0.28812 |
| S | -0.90699 | -1.52738 | 0.33655 |
| O | -1.87884 | -2.41247 | -0.28181 |
| O | -0.60805 | -1.73119 | 1.74681 |
| N | 0.47197 | -1.57962 | -0.59518 |
| H | 0.76452 | -2.52967 | -0.80756 |