Supporting Information

Photo-sensitized oxy-thiocynation of terminal alkynes / 1,3-aryldienes and their one-pot conversion to 2-hydroxy 4-substitutedaryl thiazoles

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Table of Contents

I. Fluorescence emission spectra of Acr^+ -Mes ClO_4^- - NH_4SCN

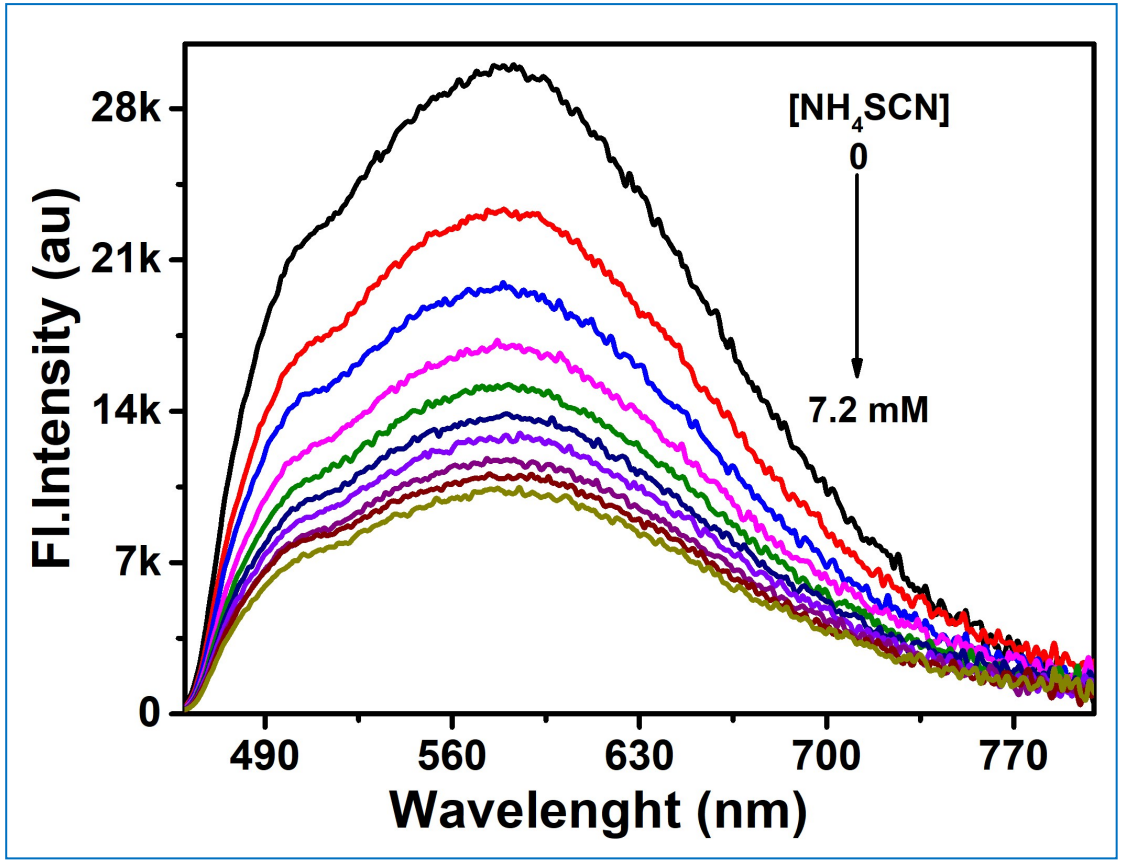


Figure 1: Fluorescence emission quenching of Acr^+-Mes ClO_4^- (10^{-3}M) in acetonitrile solvent with addition of 0.0, 20, 40, 60, 80, 100, 120, 140, 160 µL, 180 µL, of NH_4SCN(10^{-1}M), respectively. The Acr^+-Mes ClO_4^- was excited at 450nm and emission intensity monitored at 580nm.

Stern-Volmer plot

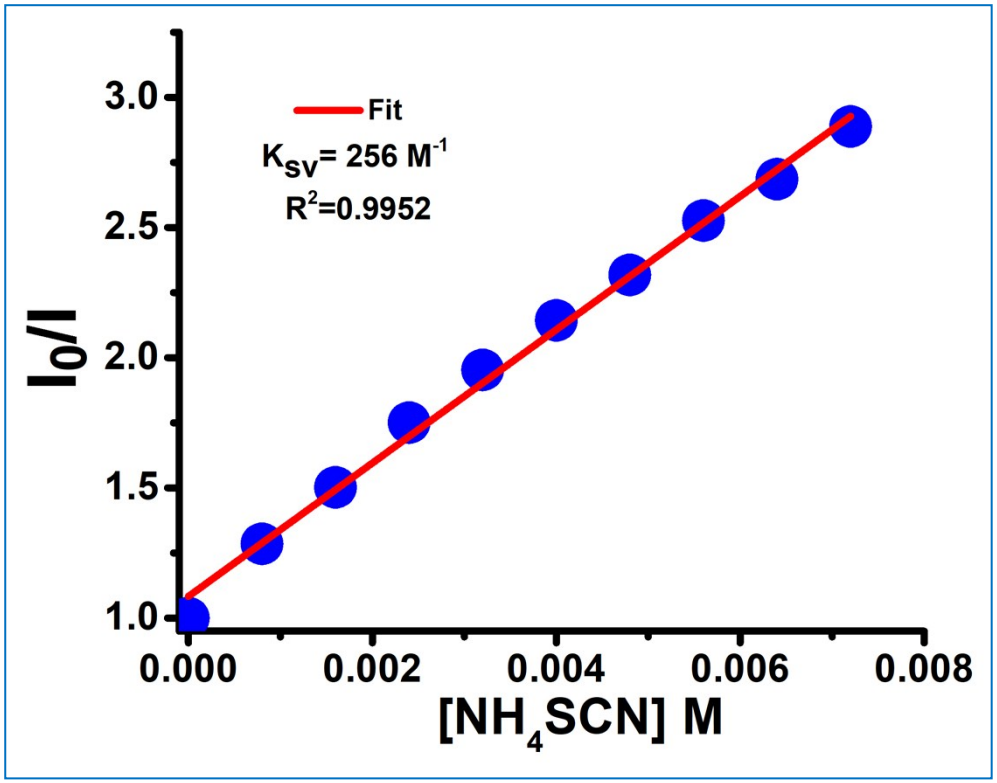


Figure 2: Stern-Volmer plot for Acr^+-Mes ClO_4^- emission quenching by NH_4SCN.

II. Fluorescence emission spectra of Acr^+ -Mes ClO_4^- - 1-Phenyl-1,3-butadiene

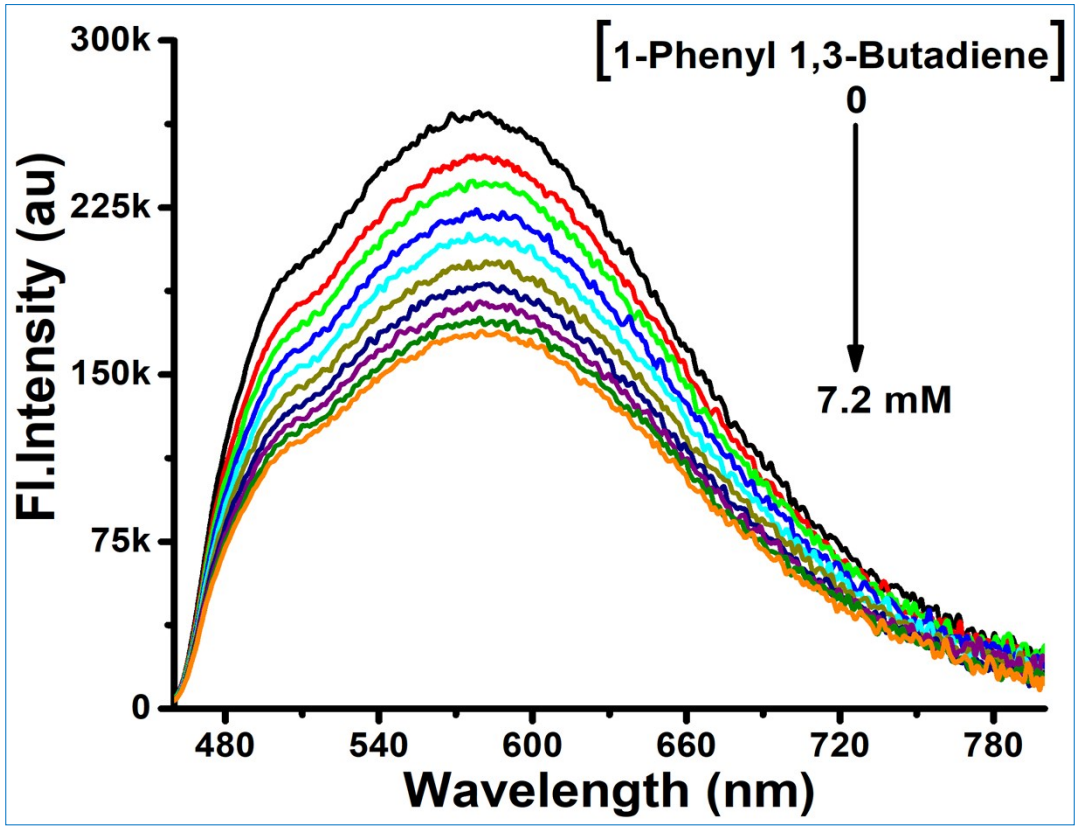


Figure 3: Fluorescence emission quenching of Acr^+-Mes ClO_4^- (10^{-3}M) in acetonitrile solvent with addition of 0.0, 20, 40, 60, 80, 100, 120, 140, 160 µL, 180 µL of 1-Phenyl-1,3-butadiene(10^{-1}M) respectively. The Acr^+-Mes ClO_4^- was excited at 450nm and emission intensity monitored at 580nm.

Stern-Volmer plot of Acr^+ -Mes ClO_4^- - 1-Phenyl-1,3-butadiene

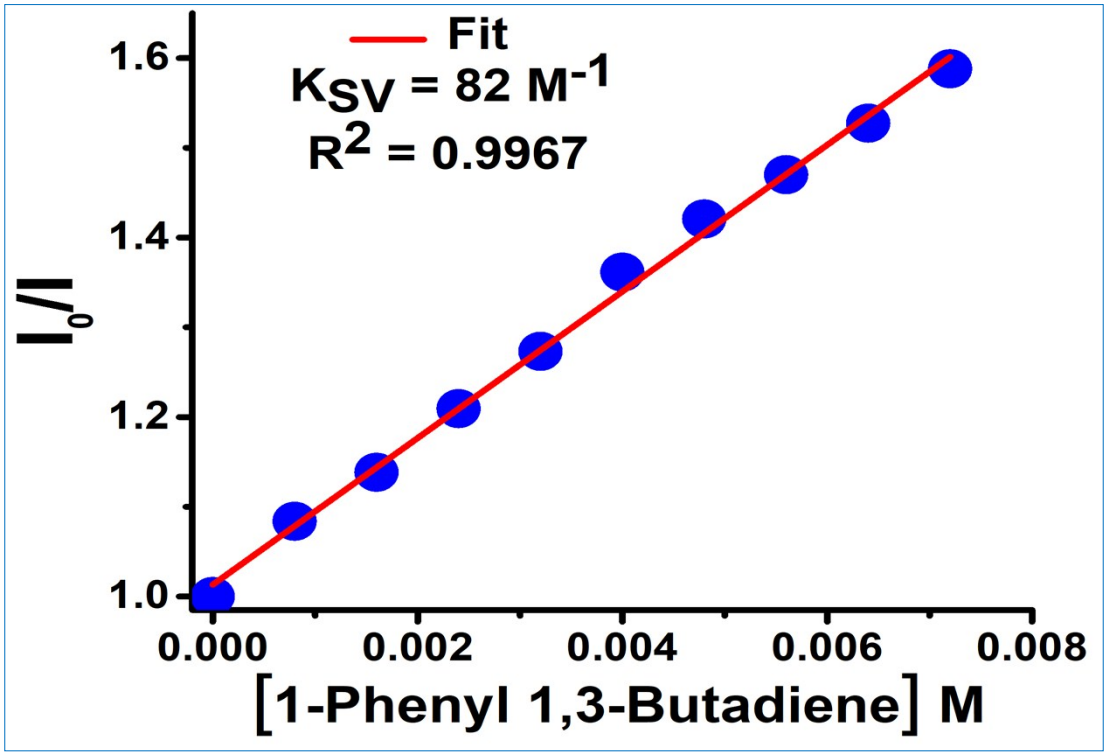


Figure 4: Stern-Volmer plot for Acr^+-Mes ClO_4^- emission quenching by 1-Phenyl-1,3-butadiene. The Stern-Volmer constant (K_{SV}) of 1-Phenyl-1,3-butadiene is three times less than NH_4SCN. Hence NH_4SCN is better quencher than 1-Phenyl -1,3-butadiene.

Cyclic Voltammogram 0f 1-Phenyl-1,3-butadiene.

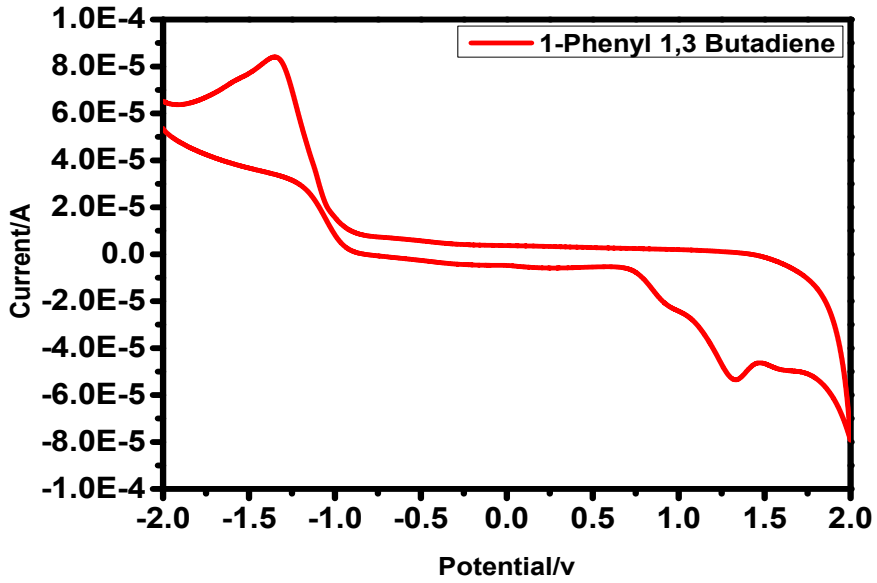


Figure 5. 1-Phenyl-1,3-butadiene oxidation potential (1.32V)in MeCN.

Electrochemical measurements were performed on a PC-controlled CH instruments model CHI 620C electrochemical analyzer. The experiments were performed in a 1 mM 1-Phenyl-1,3-butadiene solution in CAN at scan rate of 100 mV s^{-1} using 0.1 M tetrabutyl ammonium perchlorate (TBAP) as supporting electrolyte, a cyclic voltammogram (CV) had been recorded.The working electrode was glassy carbon, a standard calomel electrode (SCE) was the reference electrode and platinum wire was an auxiliary electrode.

III. Fluorescence emission spectra of Acr^+ -Mes ClO_4^- - Phenyl acetylene

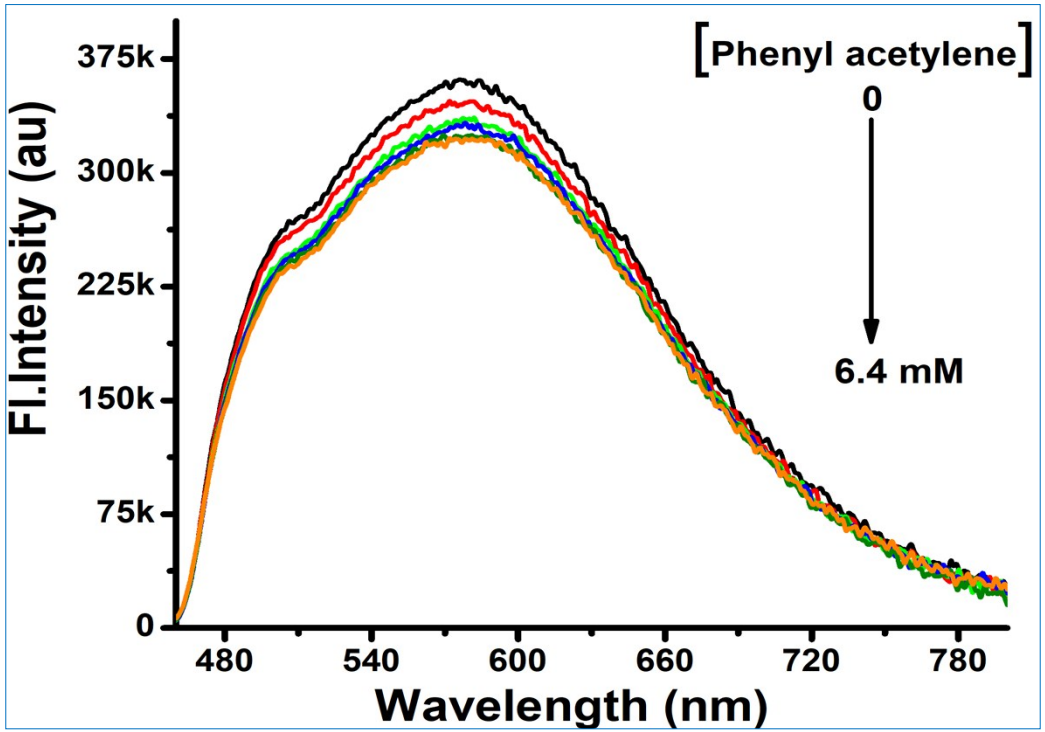


Figure 6: Fluorescence emission quenching of Acr^+-Mes ClO_4^- (10^{-3}M) in acetonitrile solvent with addition of 0.0, 20, 40, 80, 120, 160, of Phenyl acetylene(10^{-1}M), respectively. The Acr^+-Mes ClO_4^- was excited at 450nm and emission intensity monitored at 580nm.

Stern-Volmer plot of Acr^+ -Mes ClO_4^- - Phenyl acetylene

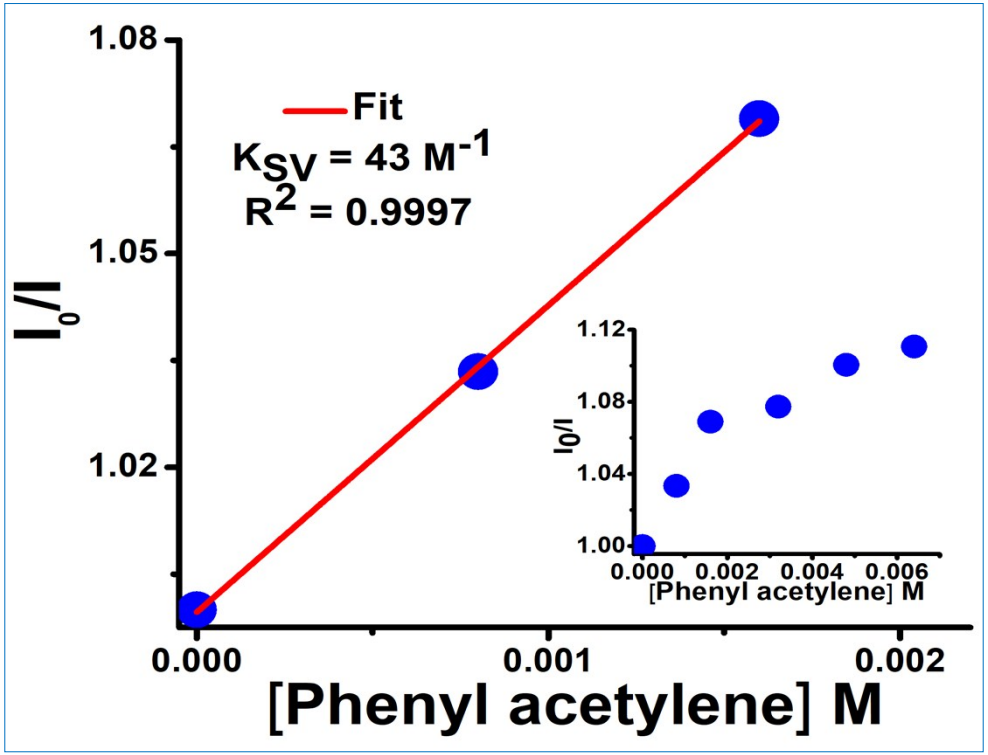
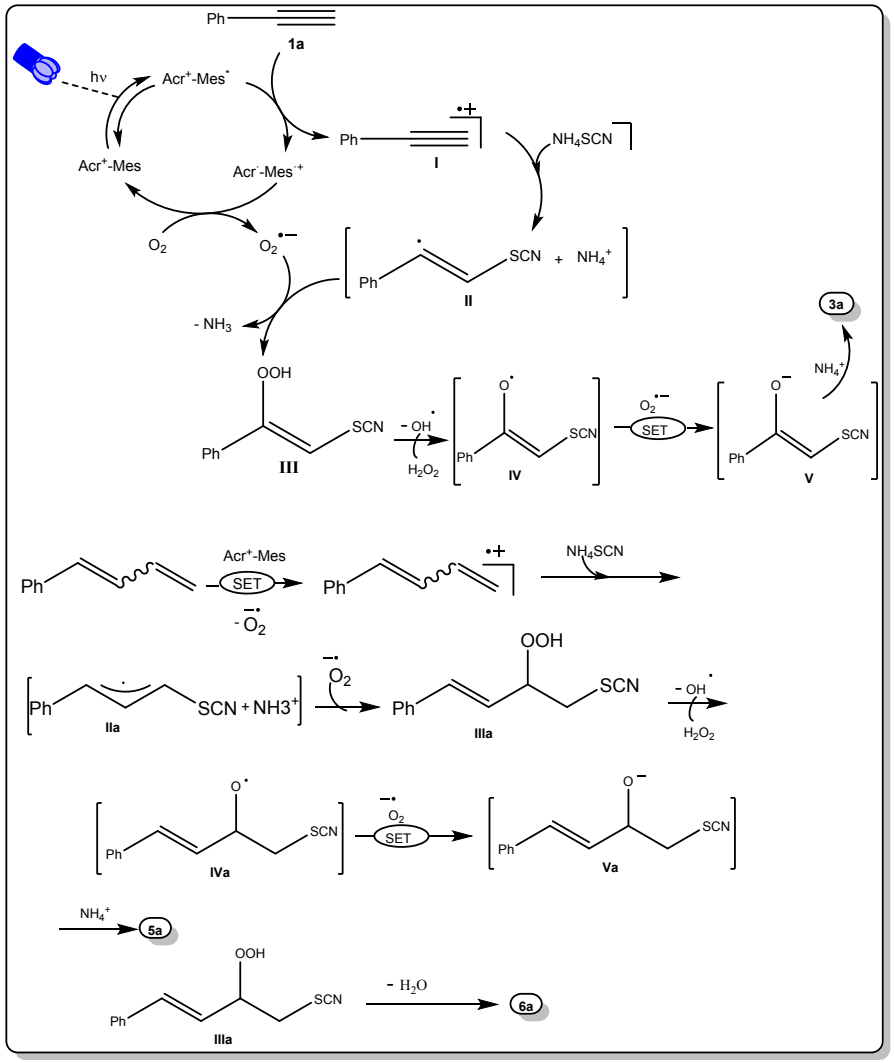


Figure 7: Stern-Volmer plot for Acr^+-Mes ClO_4^- emission quenching by Phenyl acetylene. The efficient quenching of Phenyl acetylene is upto 1.6mM . The Stern-Volmer constant (K_{SV}) of Phenyl acetylene is six times lessthan NH_4SCN. Hence NH_4SCN is better quencher than Phenyl acetylene.

IV. Alternative mechanism



- The excited state of photo-catalyst also quenched by ground state of **1a**. On the basis of this, alternative mechanism cannot be ruled out

V . 5 mmol Scale-up reaction for the synthesis of 4-Phenylthiazol-2-ol(7a)-Image

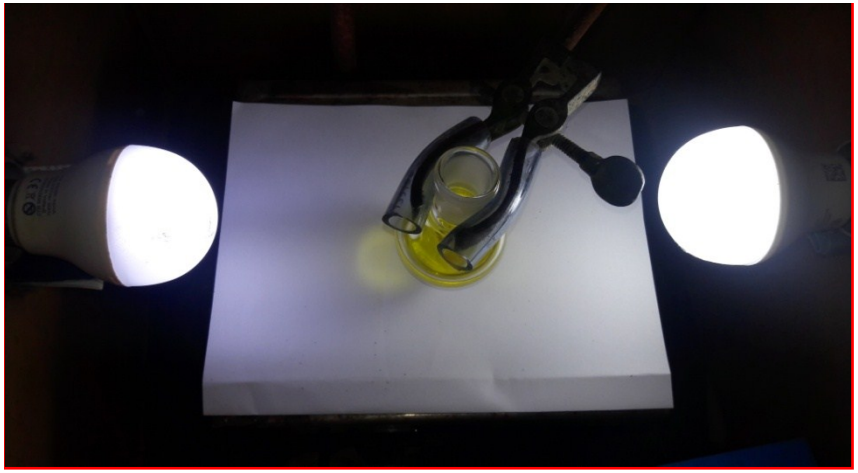
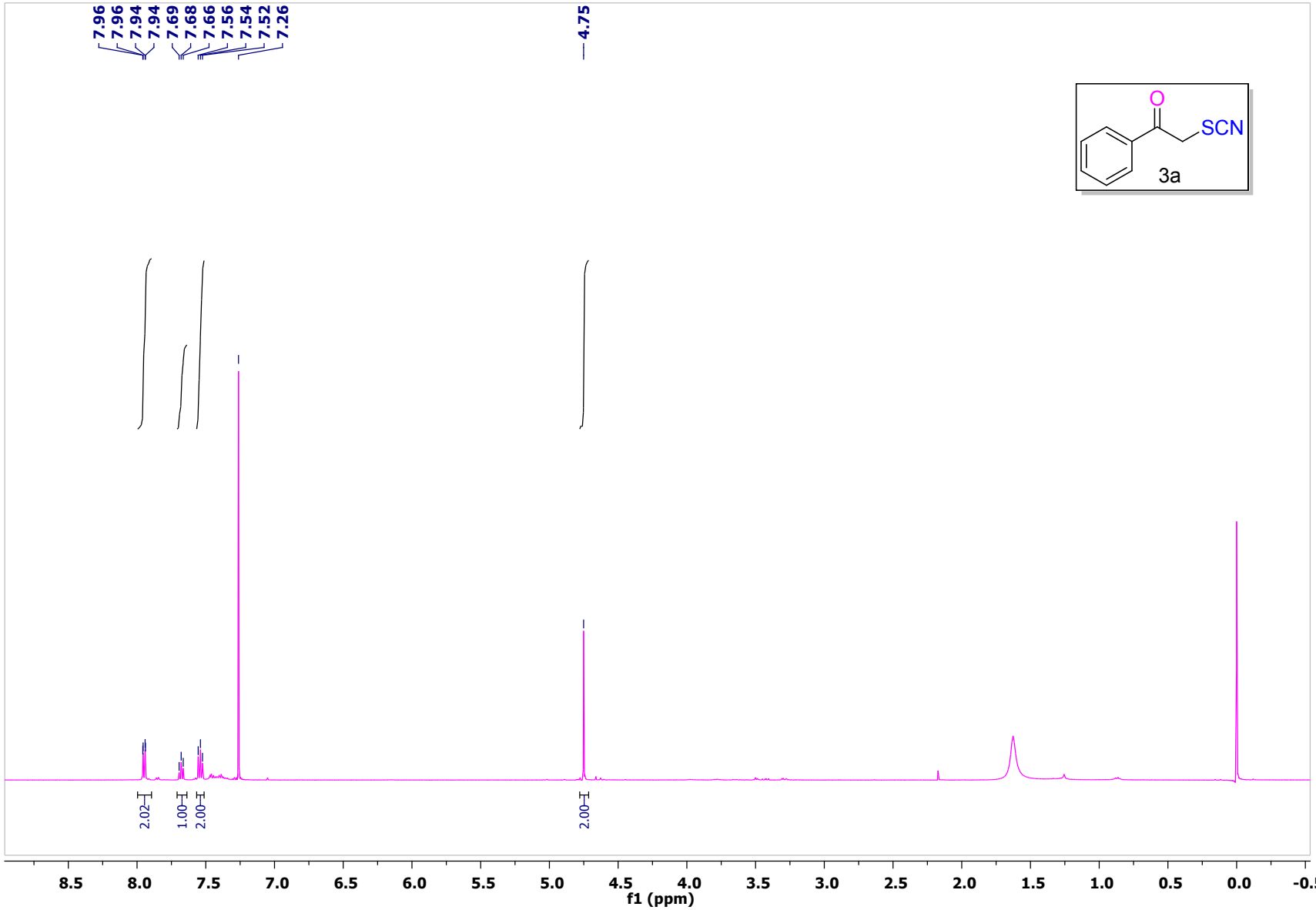


Figure 8: 5 mmol Scale-up reaction for the synthesis of 4-Phenylthiazol-2-ol, (**7a**) with two 7W day light white LED lamps (PHILIPS 6500K, 42mA 220-240V, Made in India).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3a
2.02
1.00
2.00
2.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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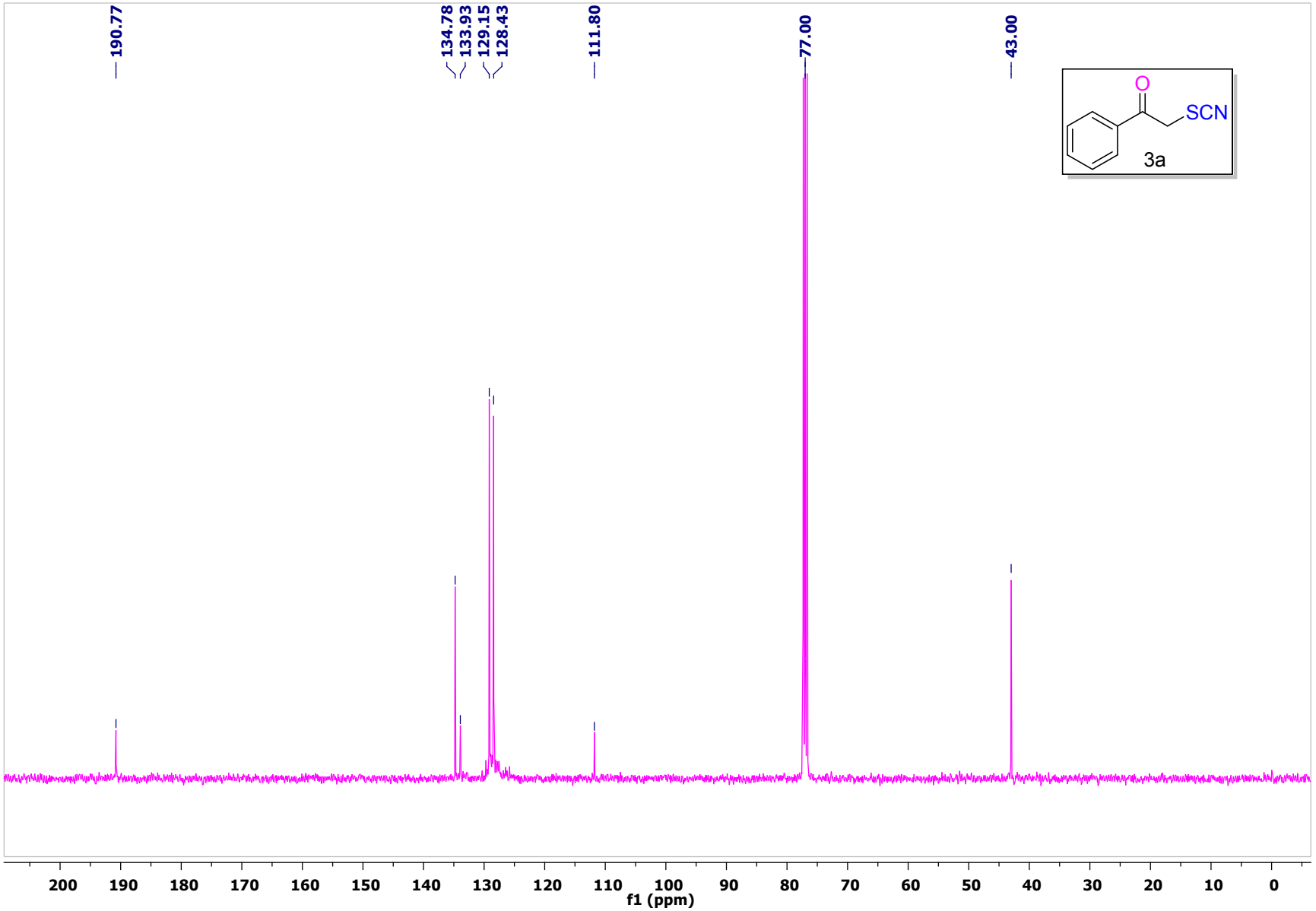
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SCN
3a
200
190
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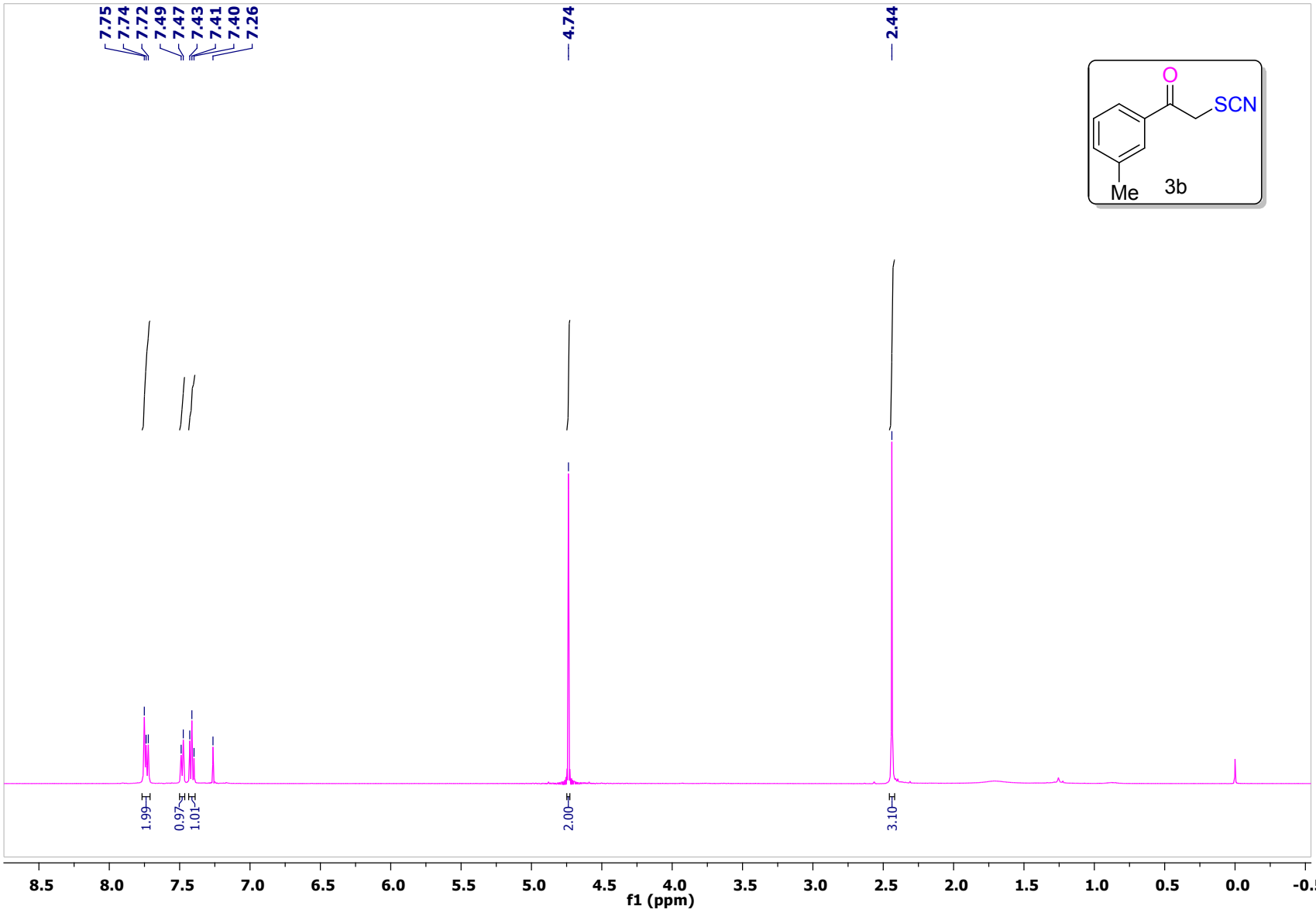
10
0
f1 (ppm)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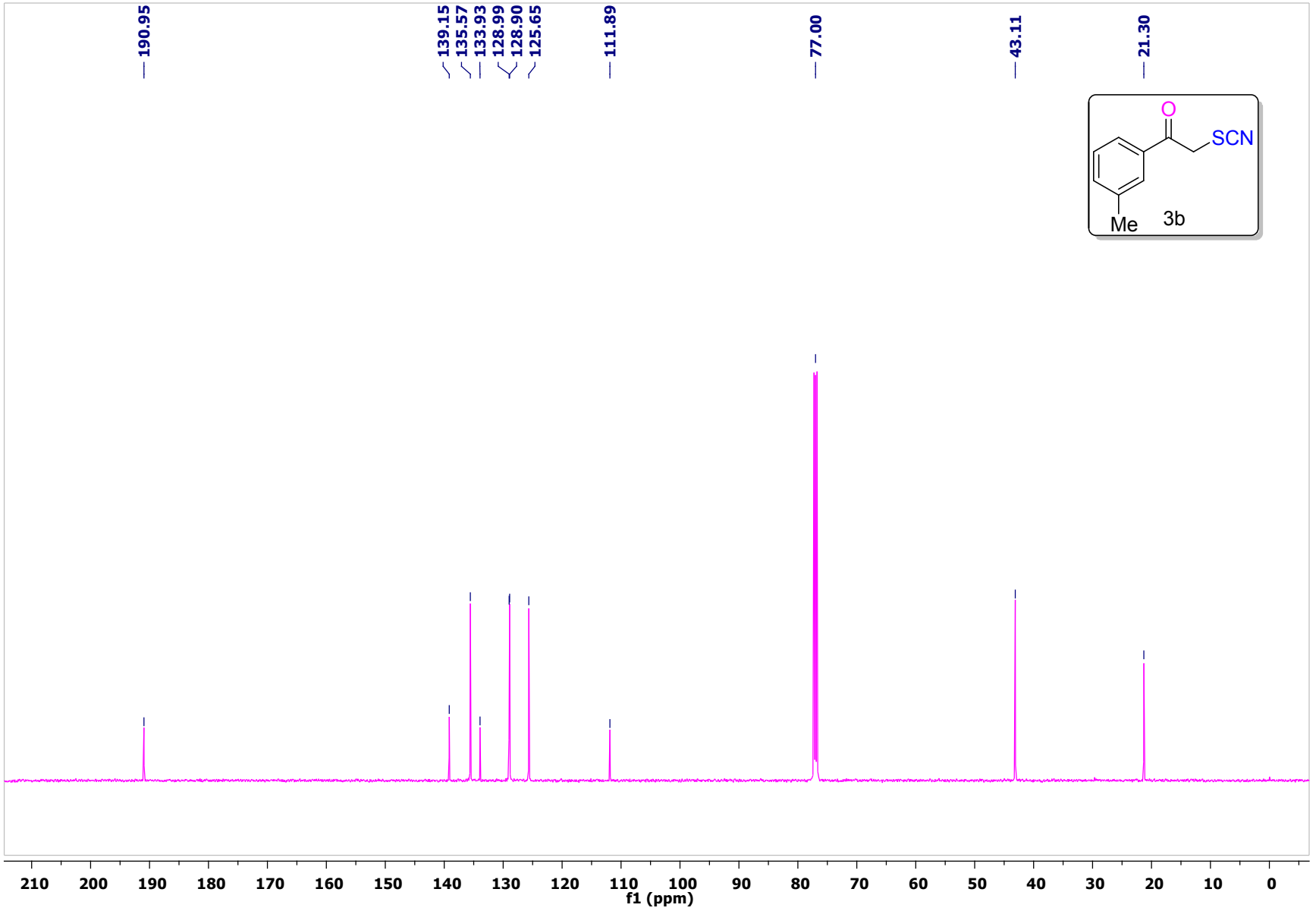
f1 (ppm)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21.30
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SCN
Me
3b
210
200
190
180
170
160
150
140
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120
110
100
90
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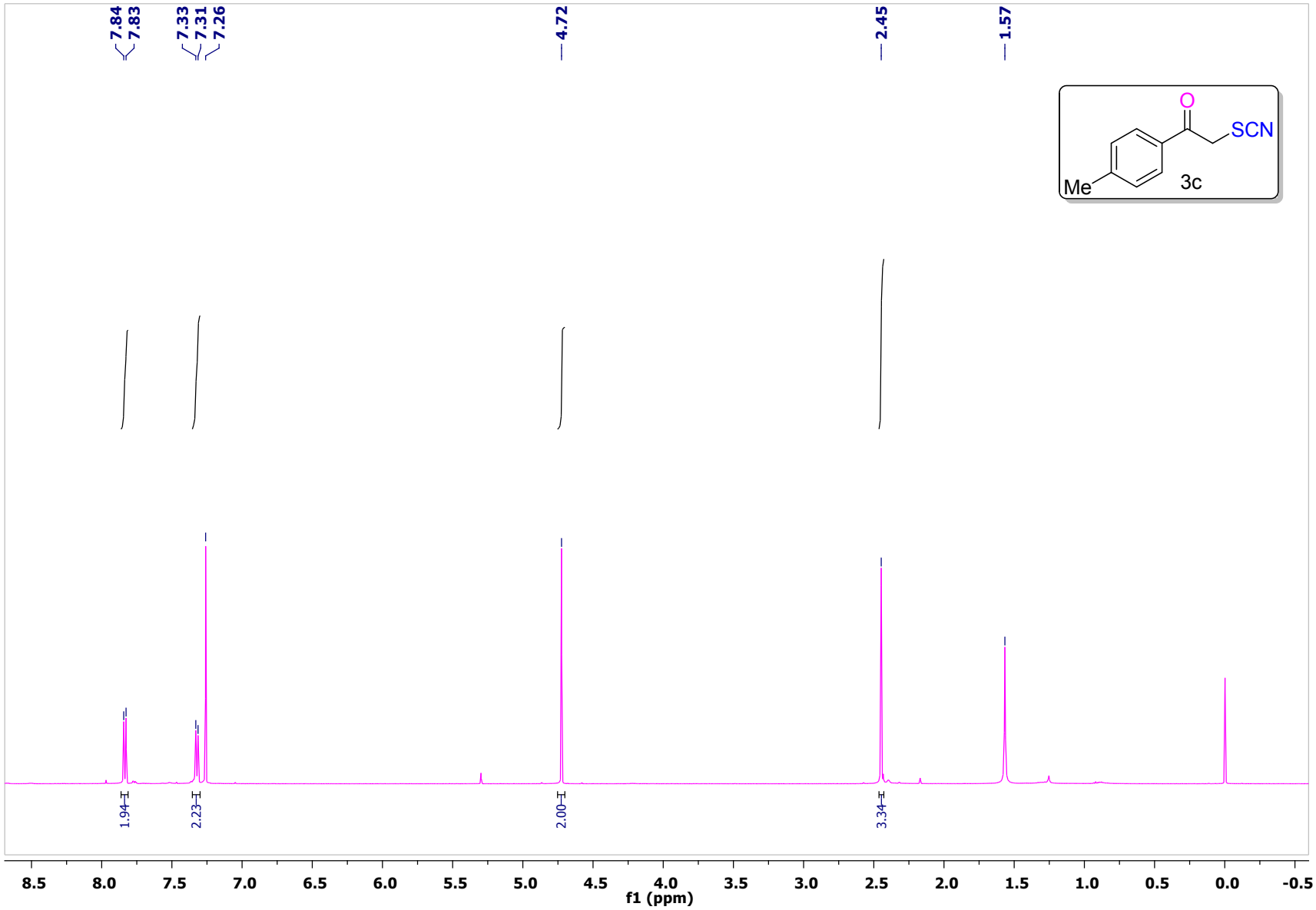
60
50
40
30
20
10
0
f1 (ppm)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Me
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2.23
2.00
3.34
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8.0
7.5
7.0
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5.0
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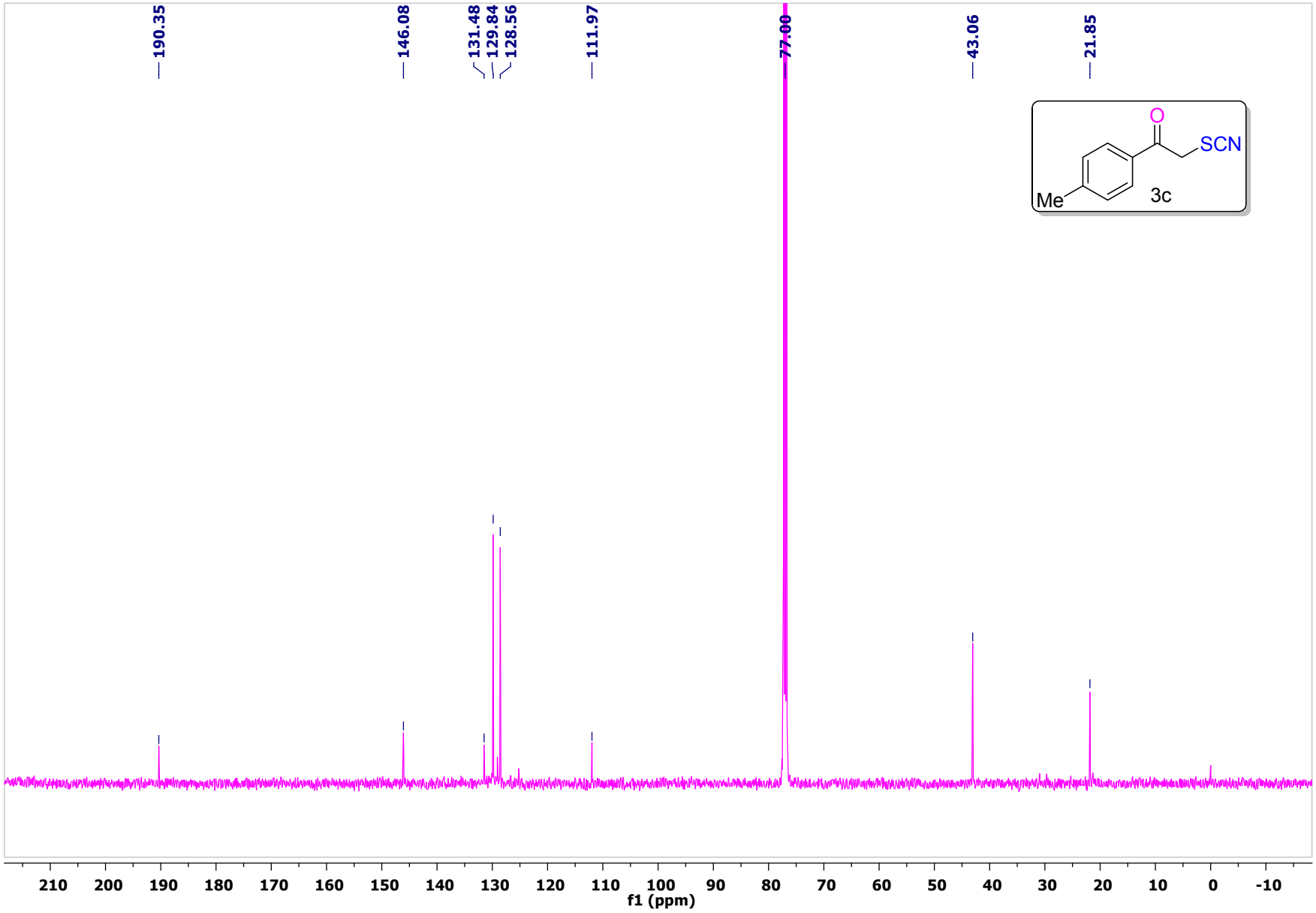
f1 (ppm)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200
190
180
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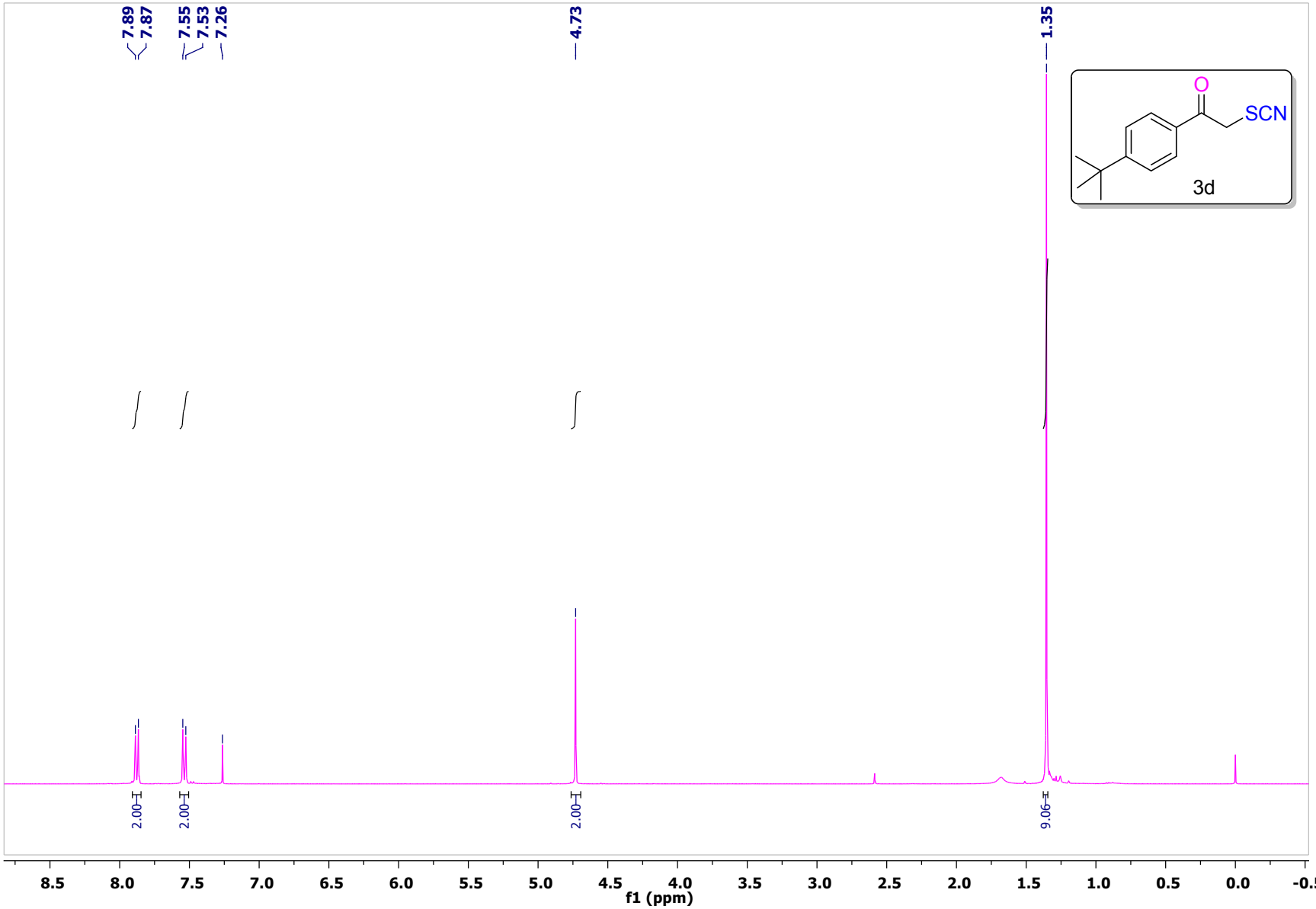
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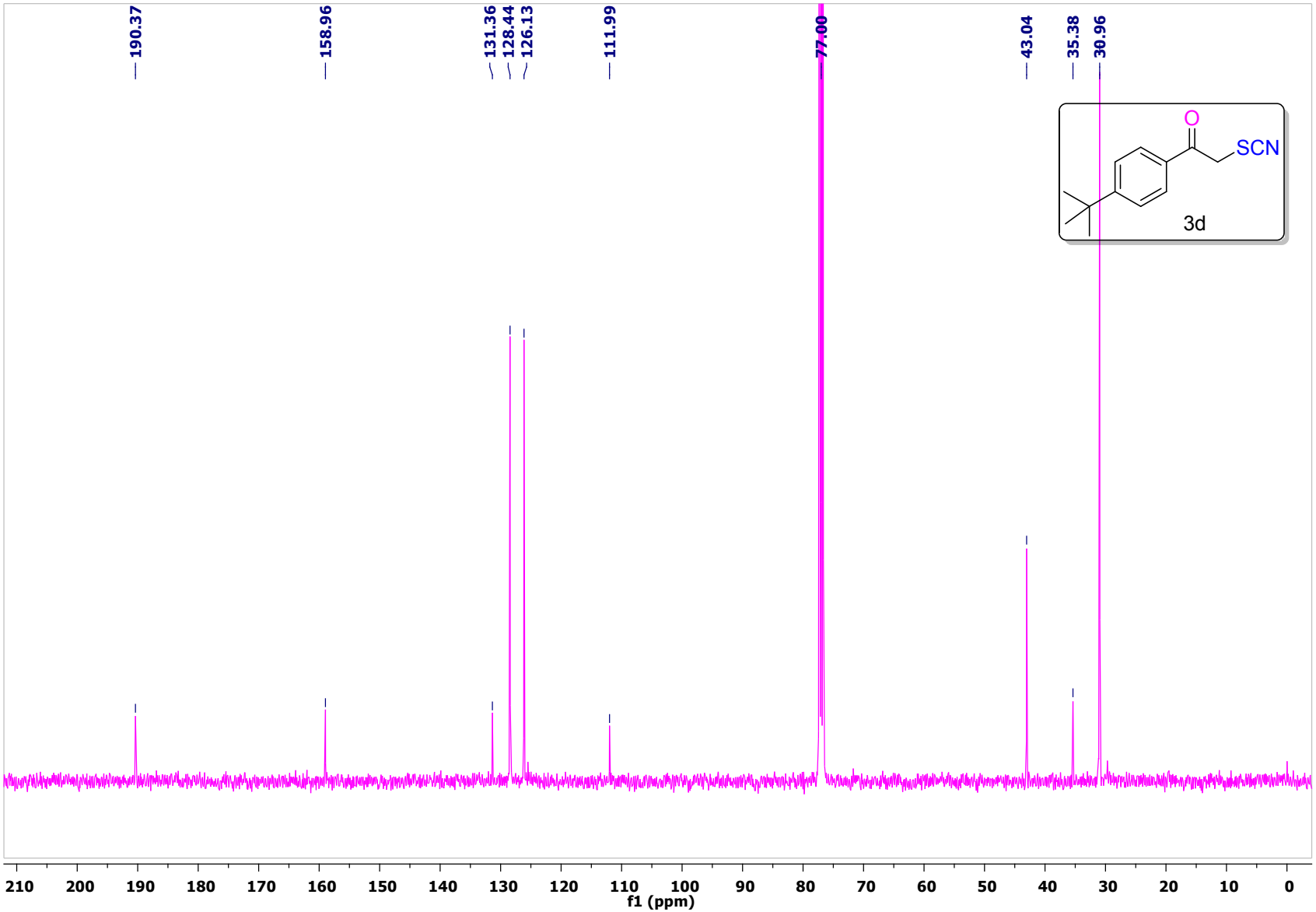
f1 (ppm)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200
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180
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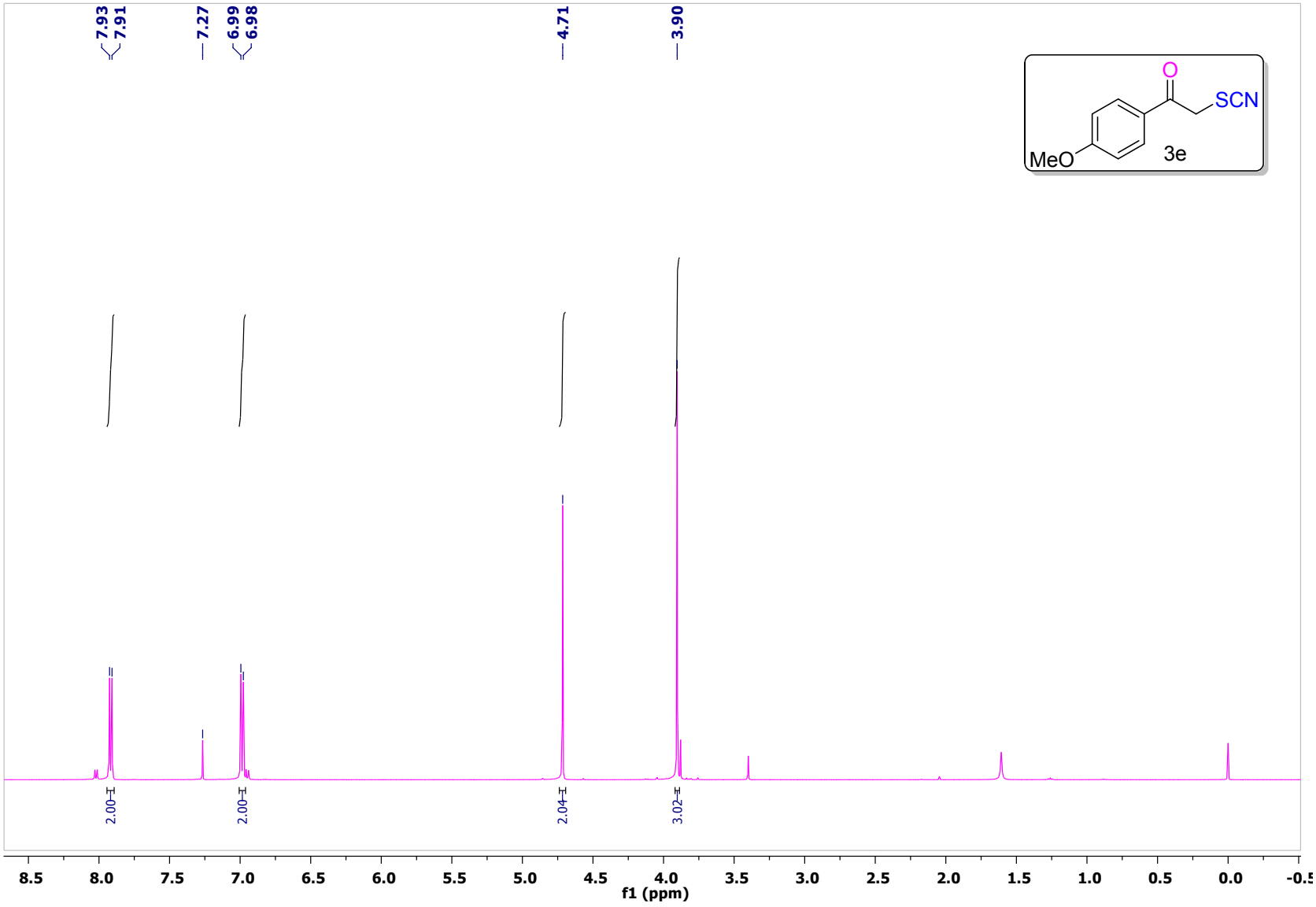
f1 (ppm)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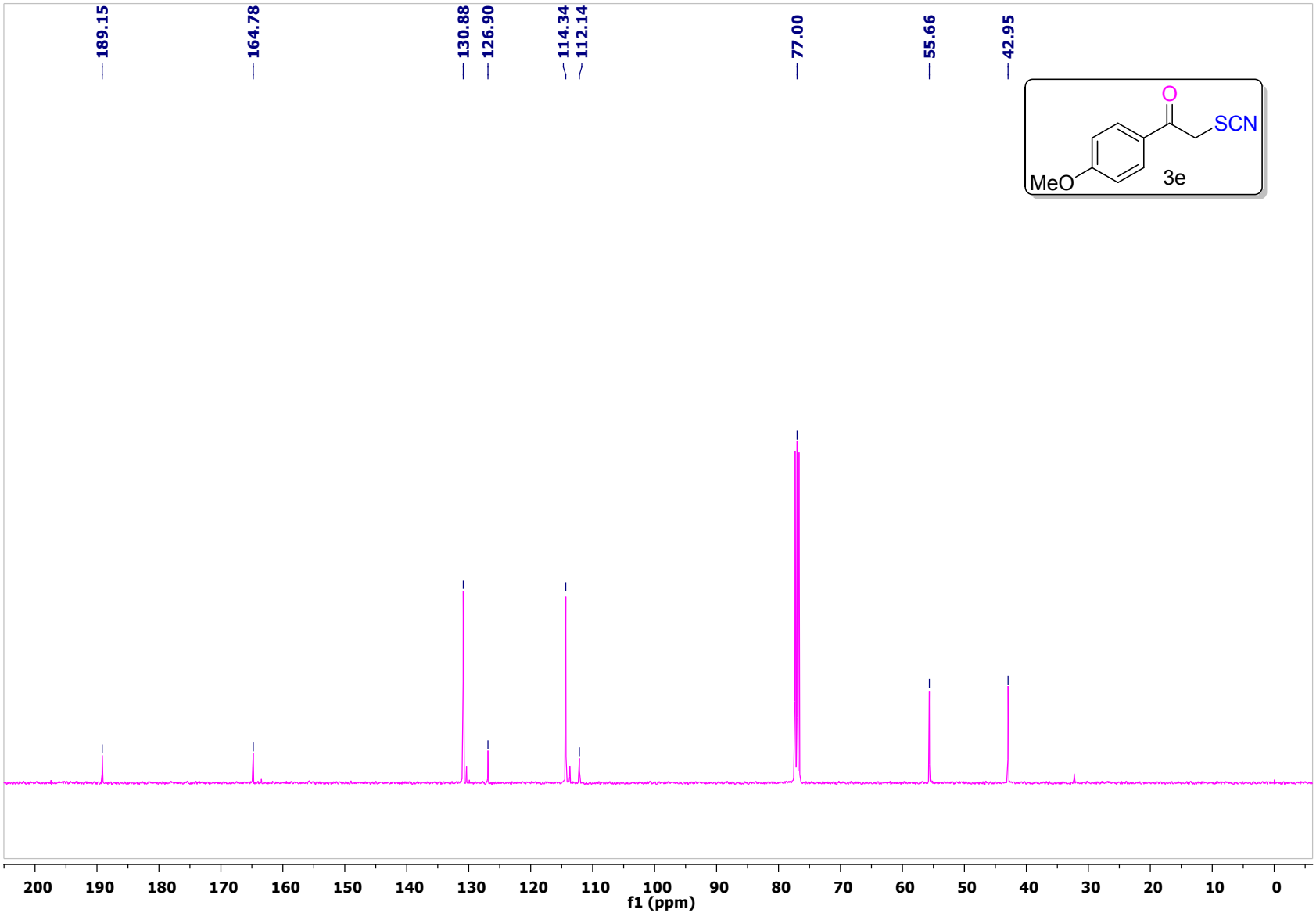
f1 (ppm)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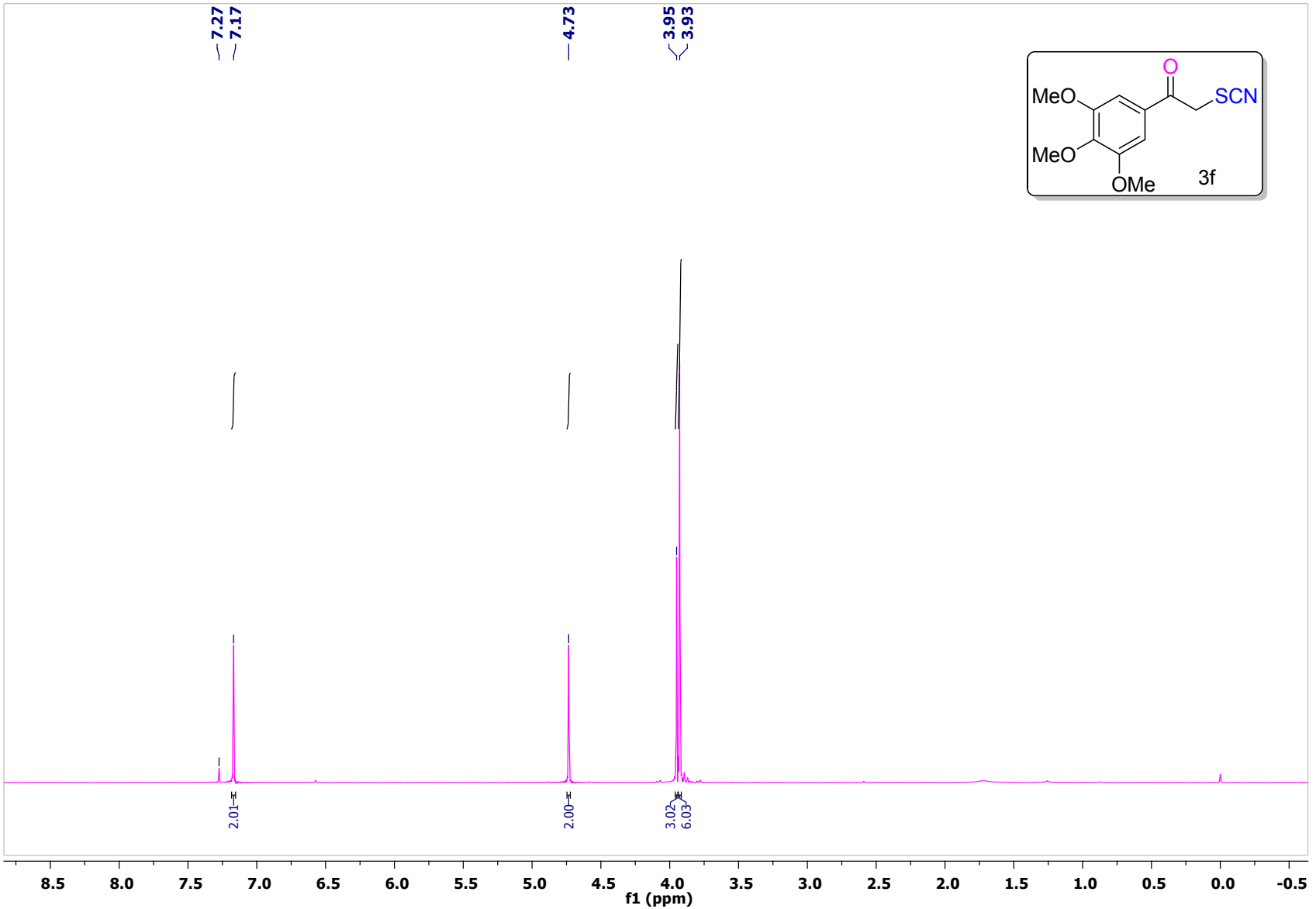
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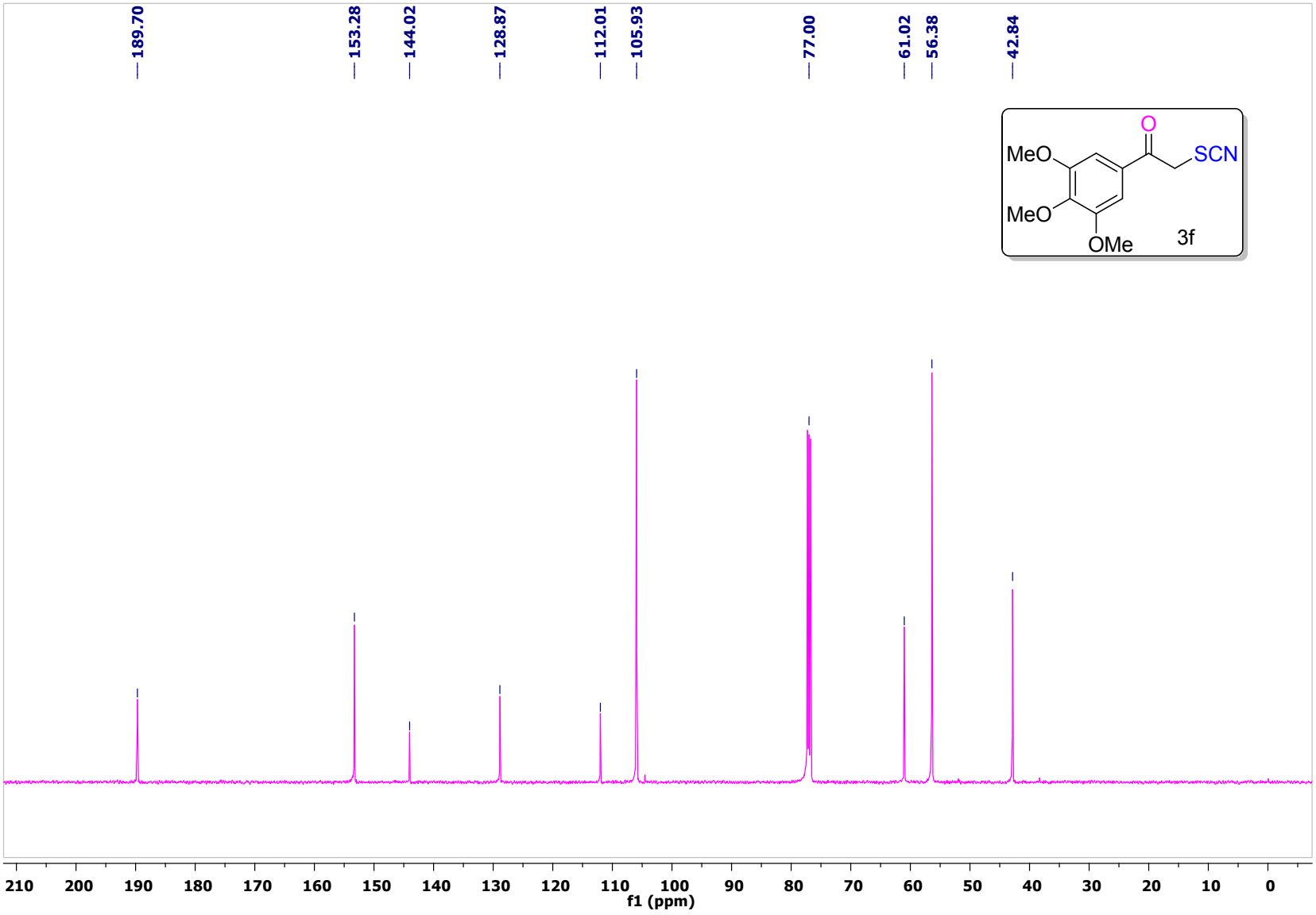
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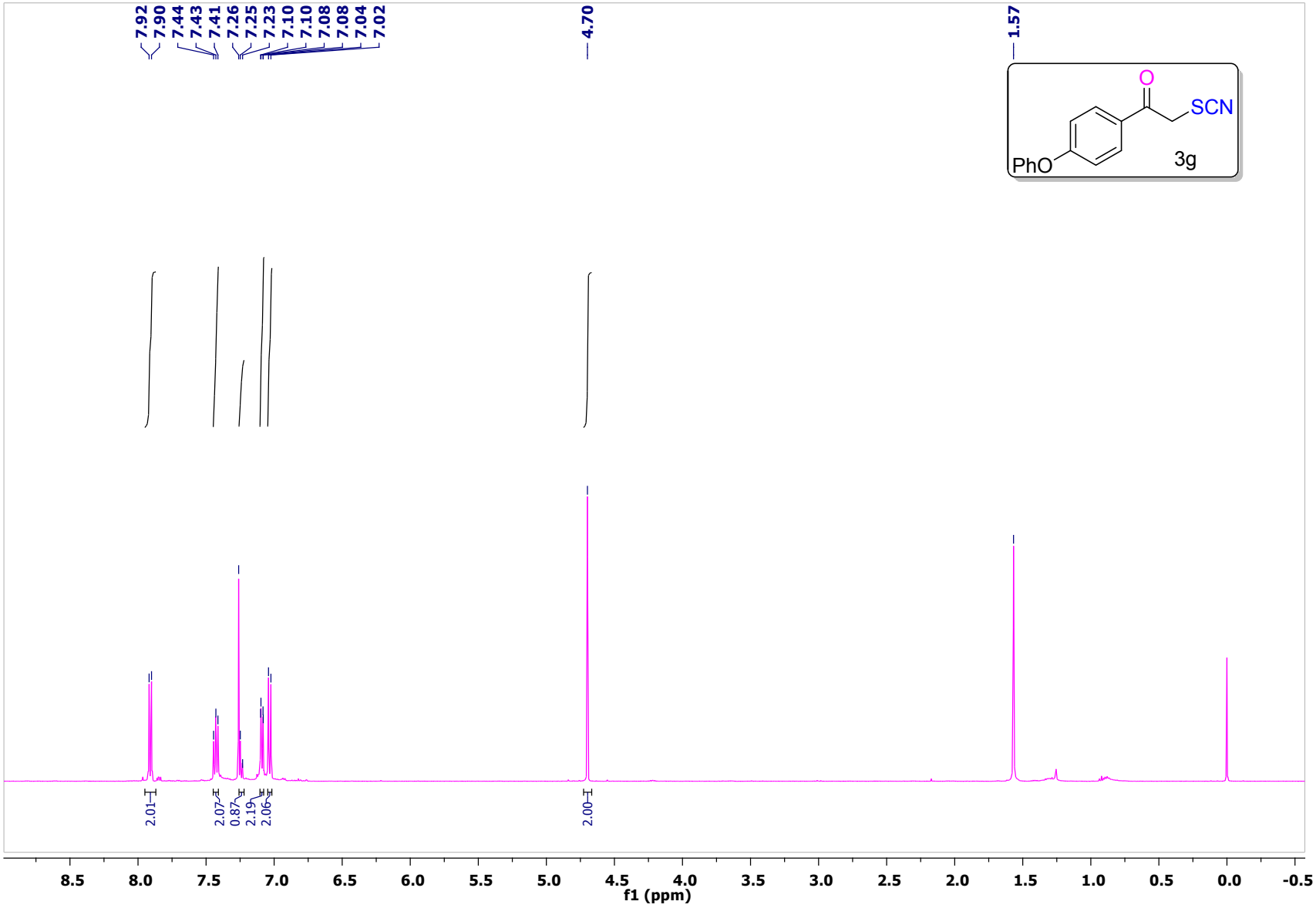
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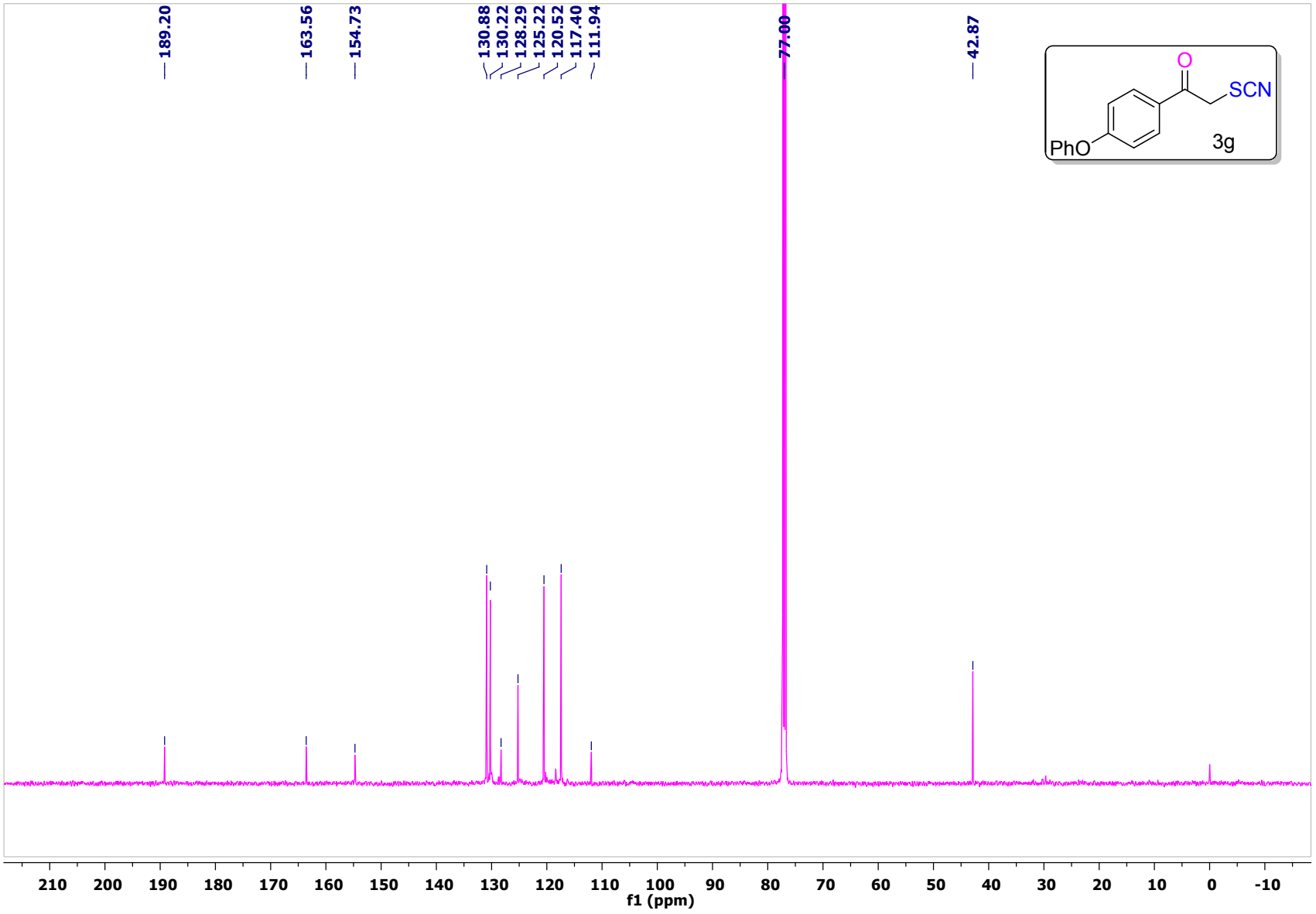
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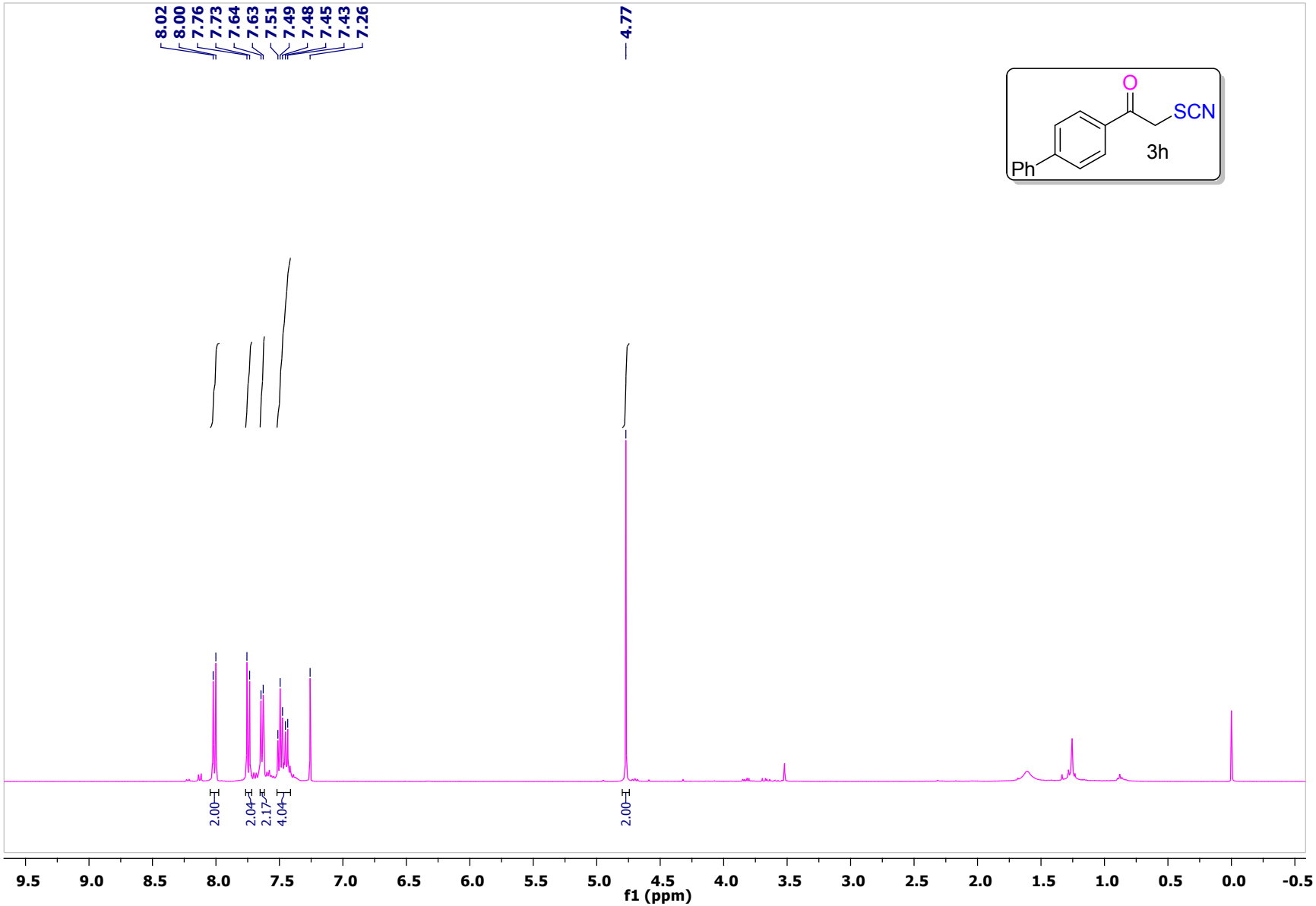
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2.17
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7.0
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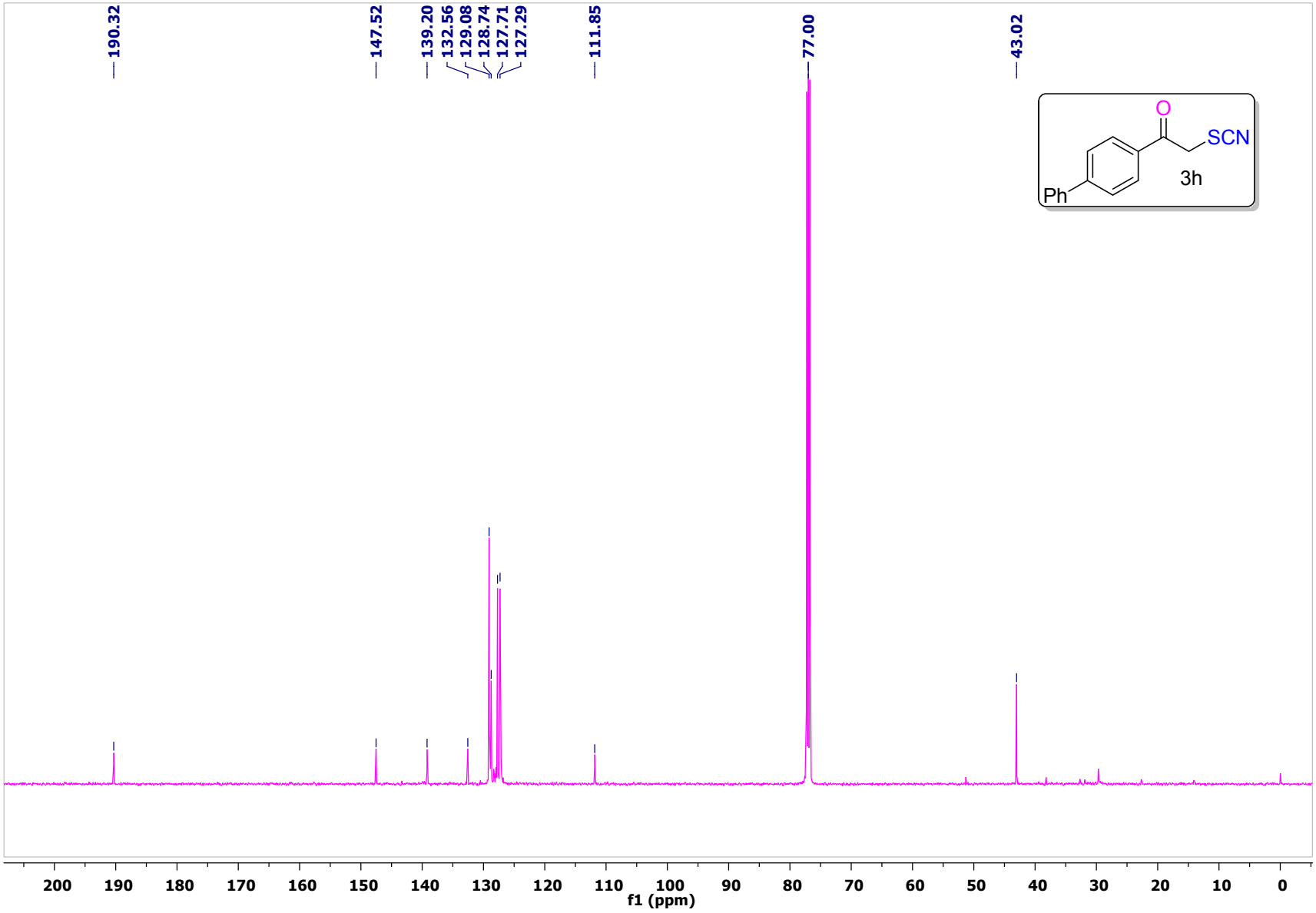
f1 (ppm)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3h
200
190
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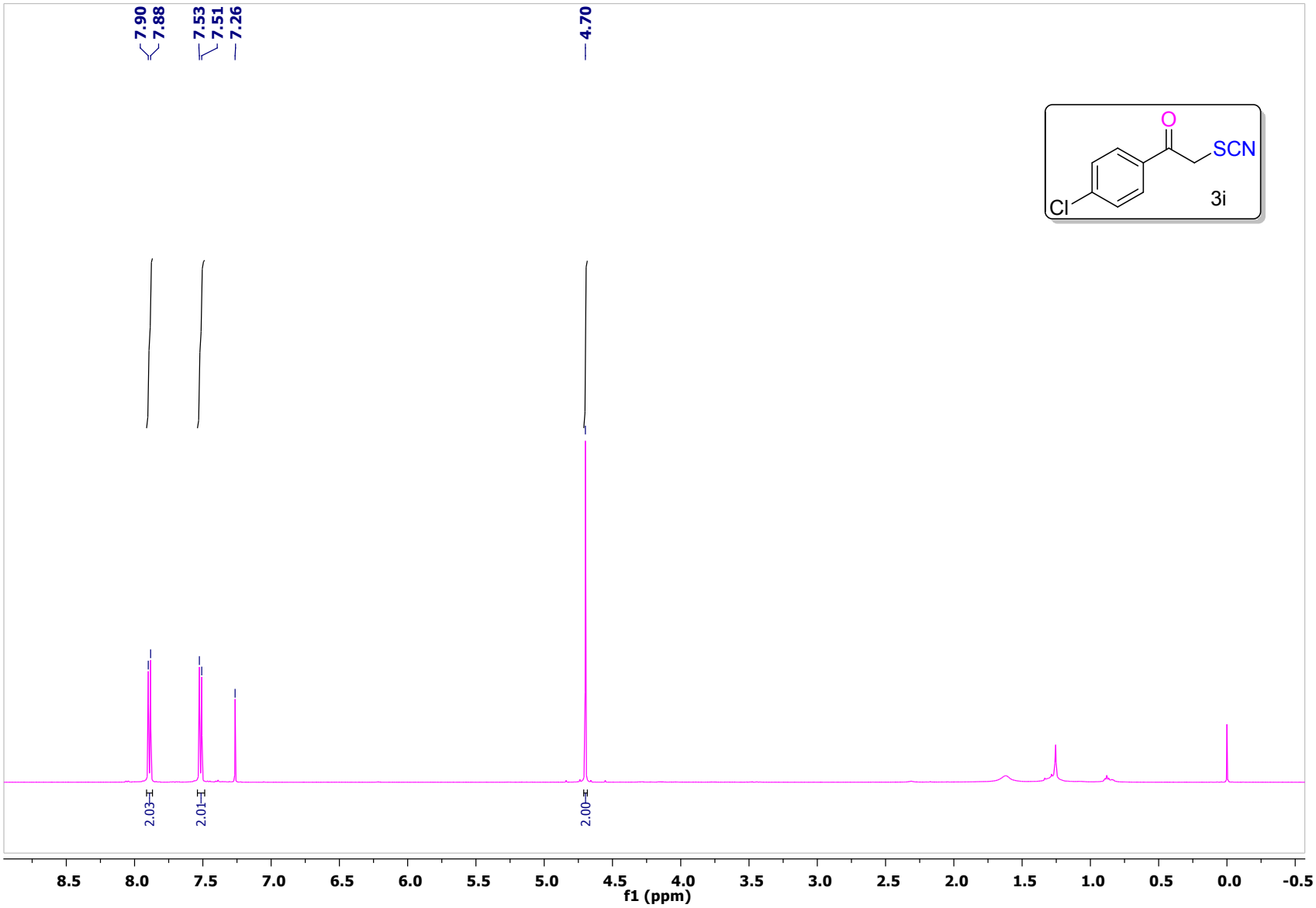
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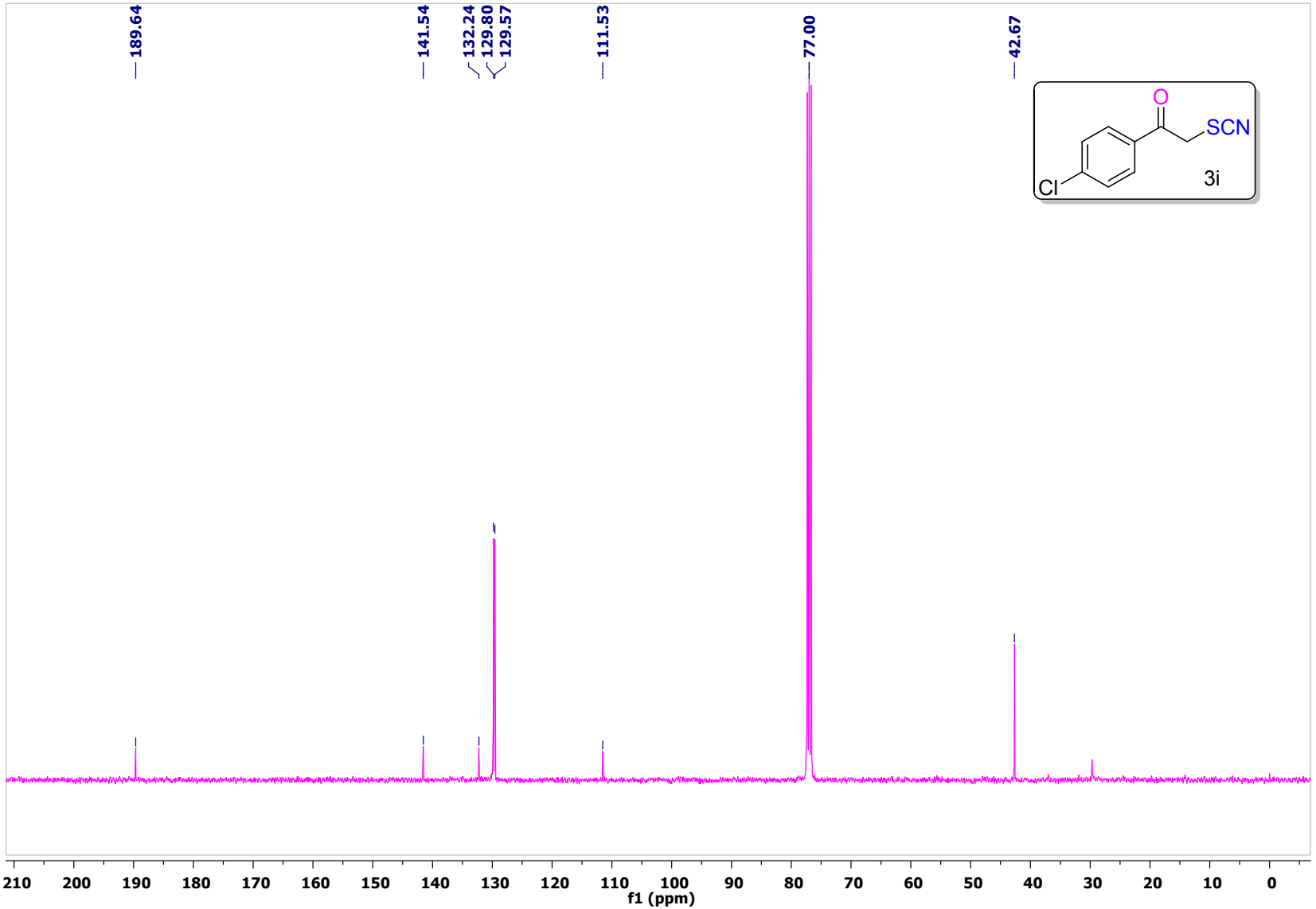
f1 (ppm)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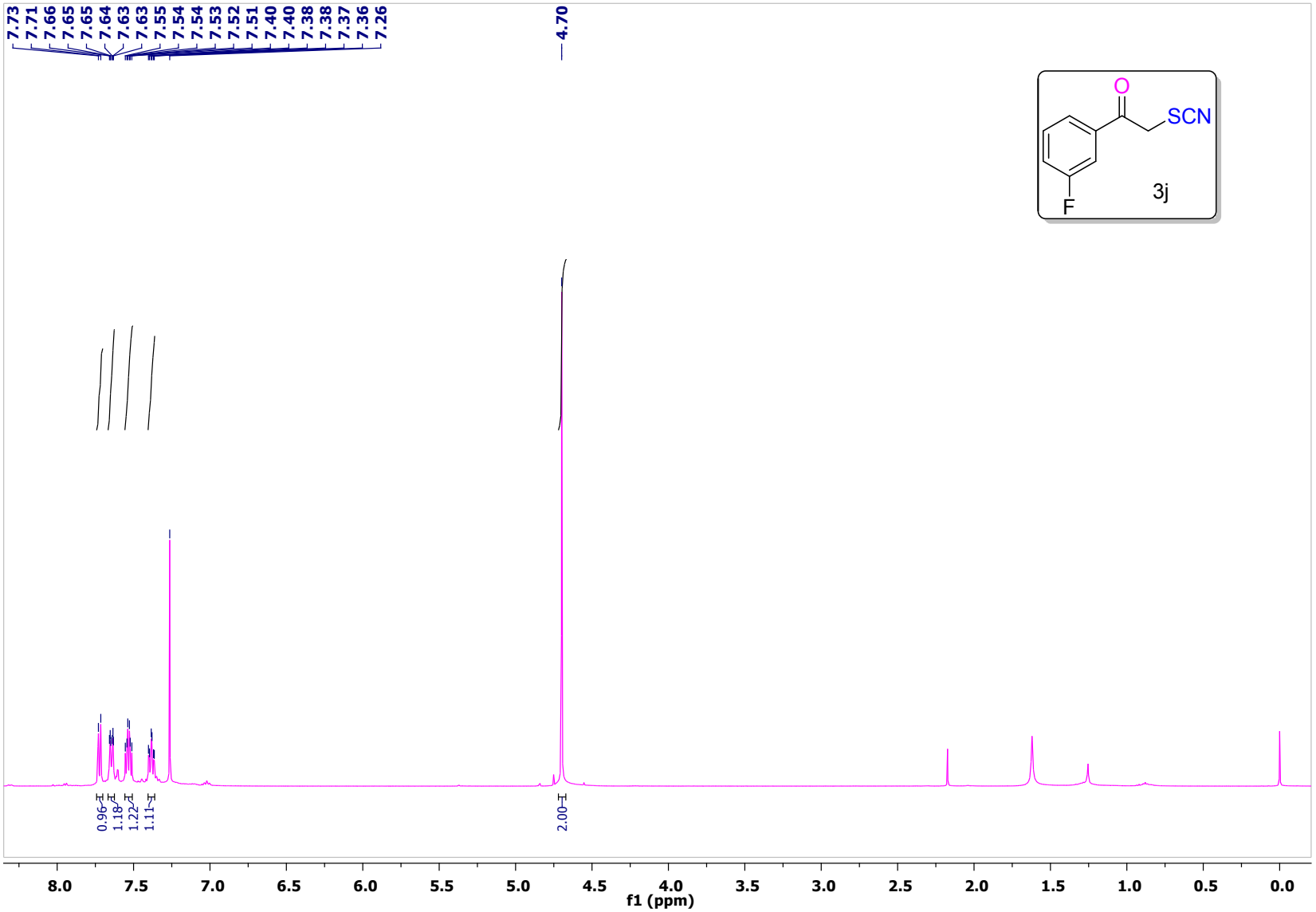
f1 (ppm)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7.40
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O
SCN
F
3j
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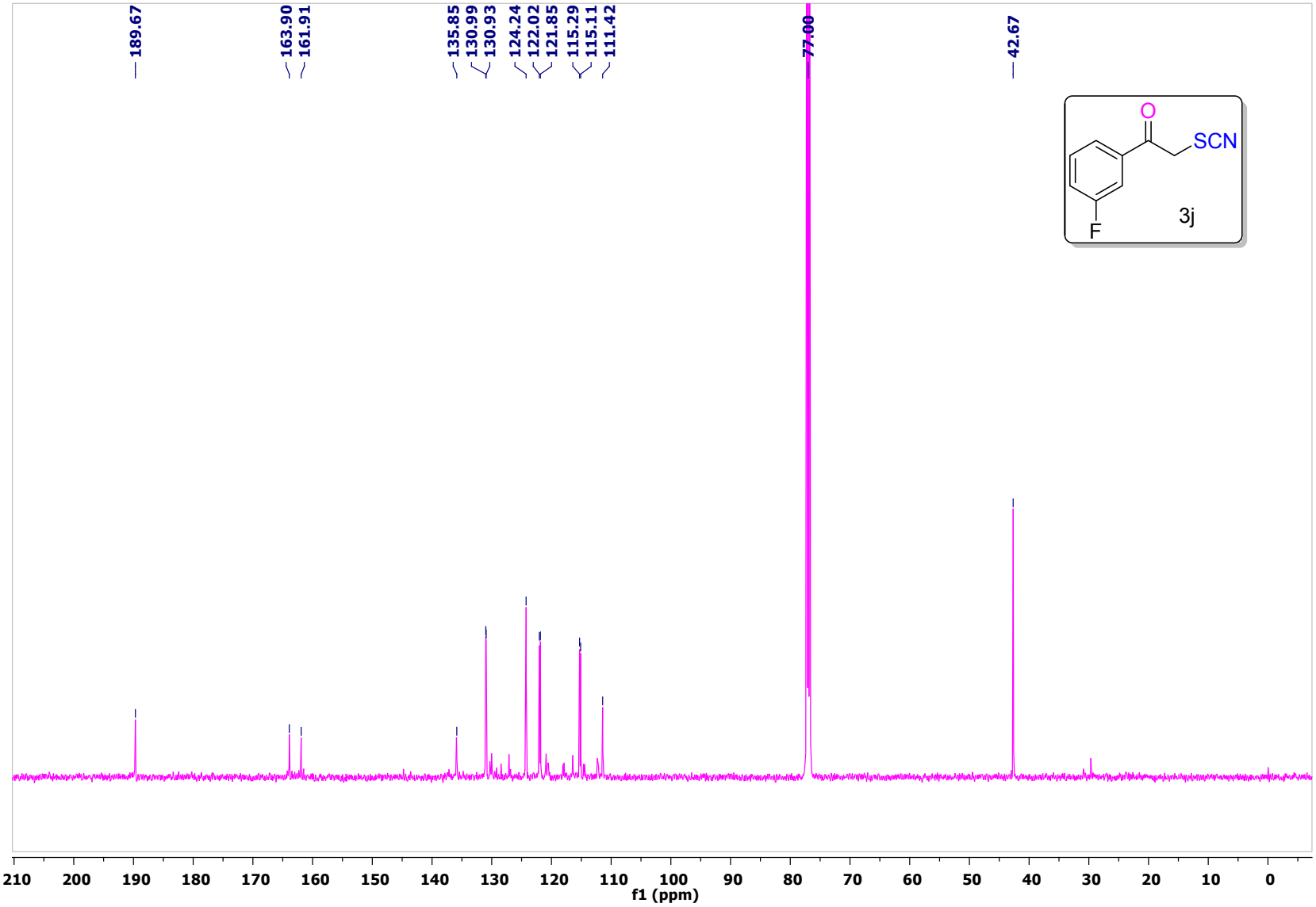
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O
SCN
F
3j
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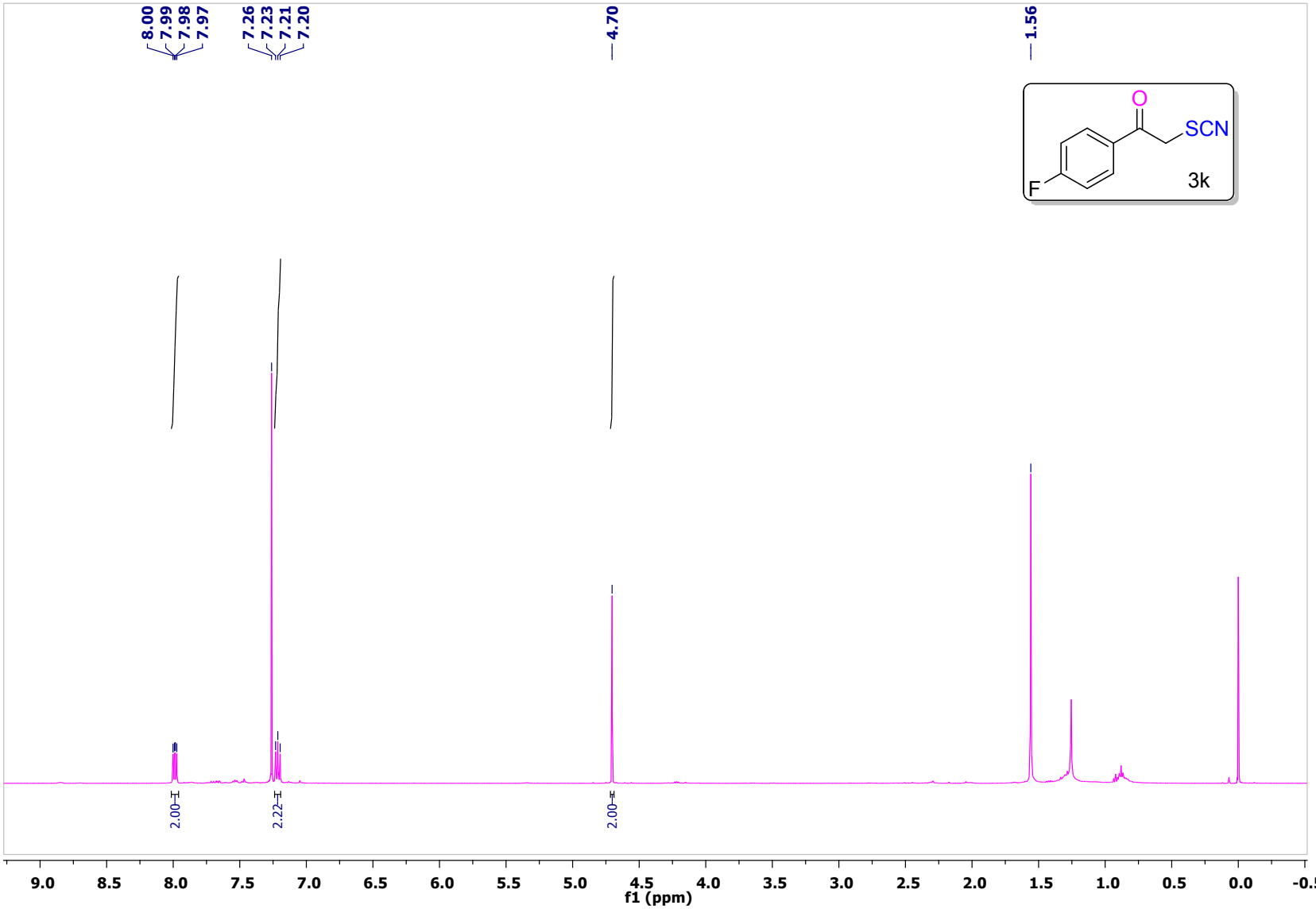
f1 (ppm)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7.97
7.26
7.23
7.21
7.20
4.70
1.56
O
SCN
F
3k
2.00
2.22
2.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.0
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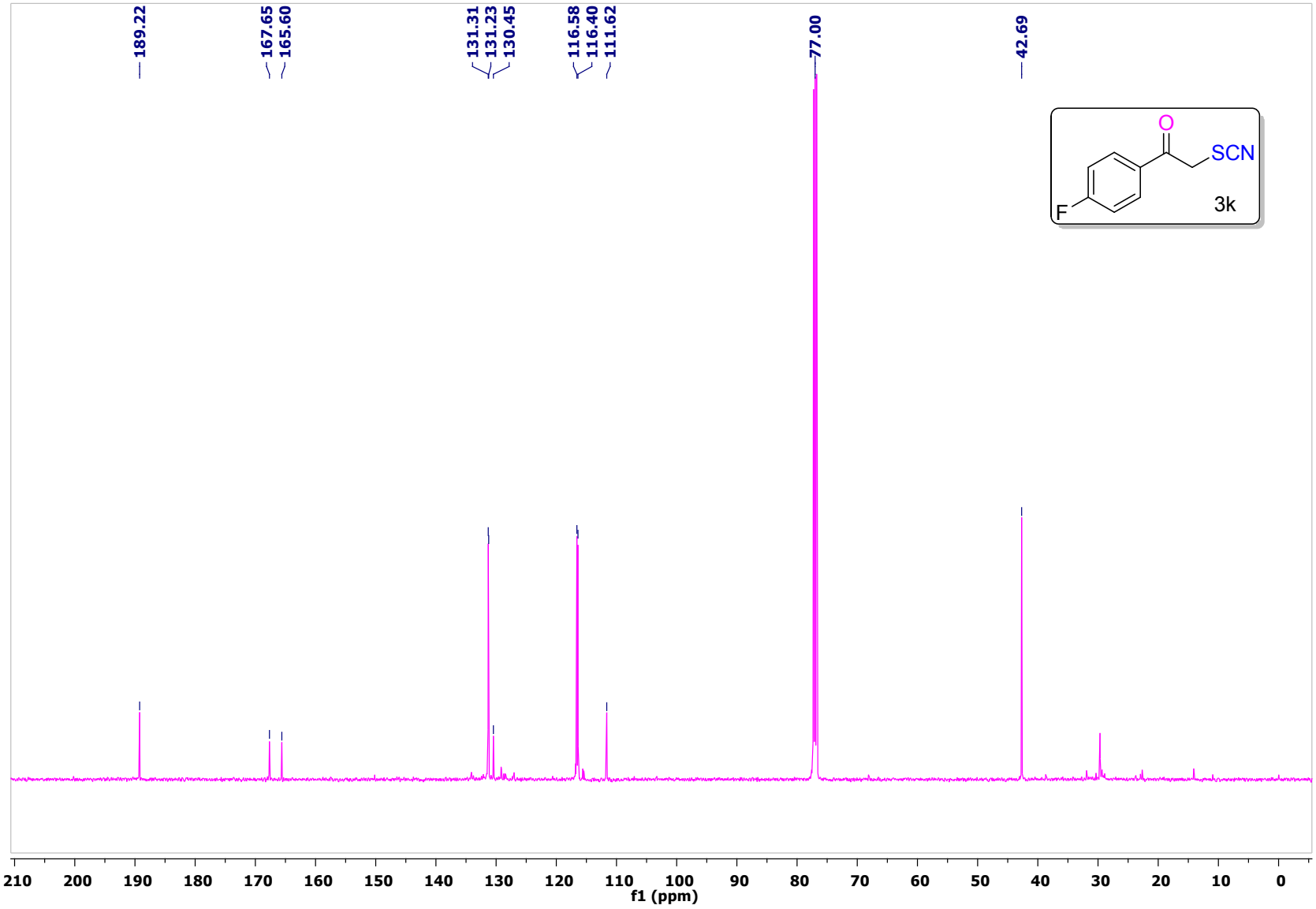
f1 (ppm)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165.60
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131.23
130.45
116.58
116.40
111.62
77.00
42.69
O
SCN
F
3k
210
200
190
180
170
160
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130
120
110
100
90
80
70
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50
40
30
20
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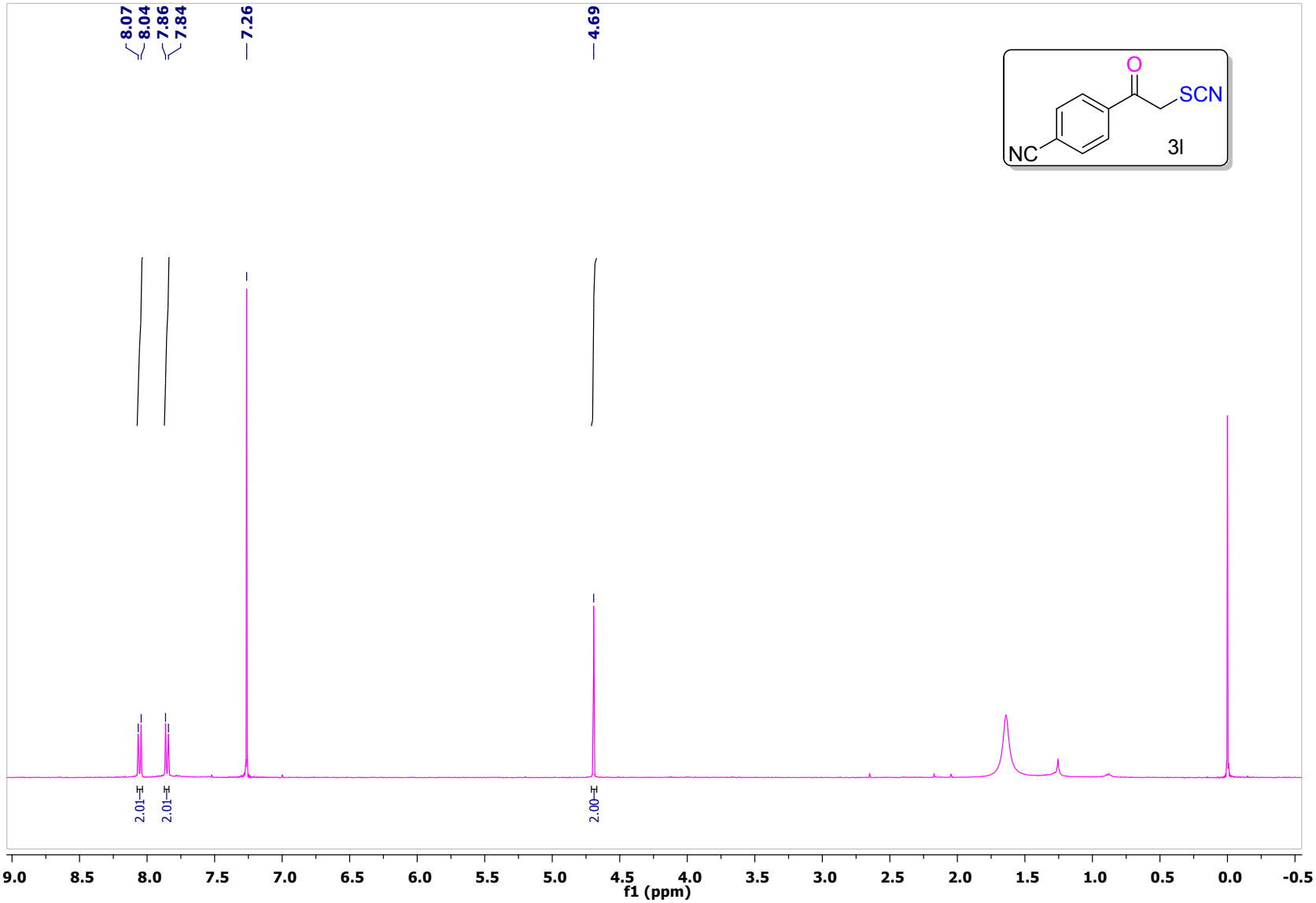
f1 (ppm)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8.04
7.86
7.84
7.26
4.69
O
SCN
NC
3l
2.01
2.01
2.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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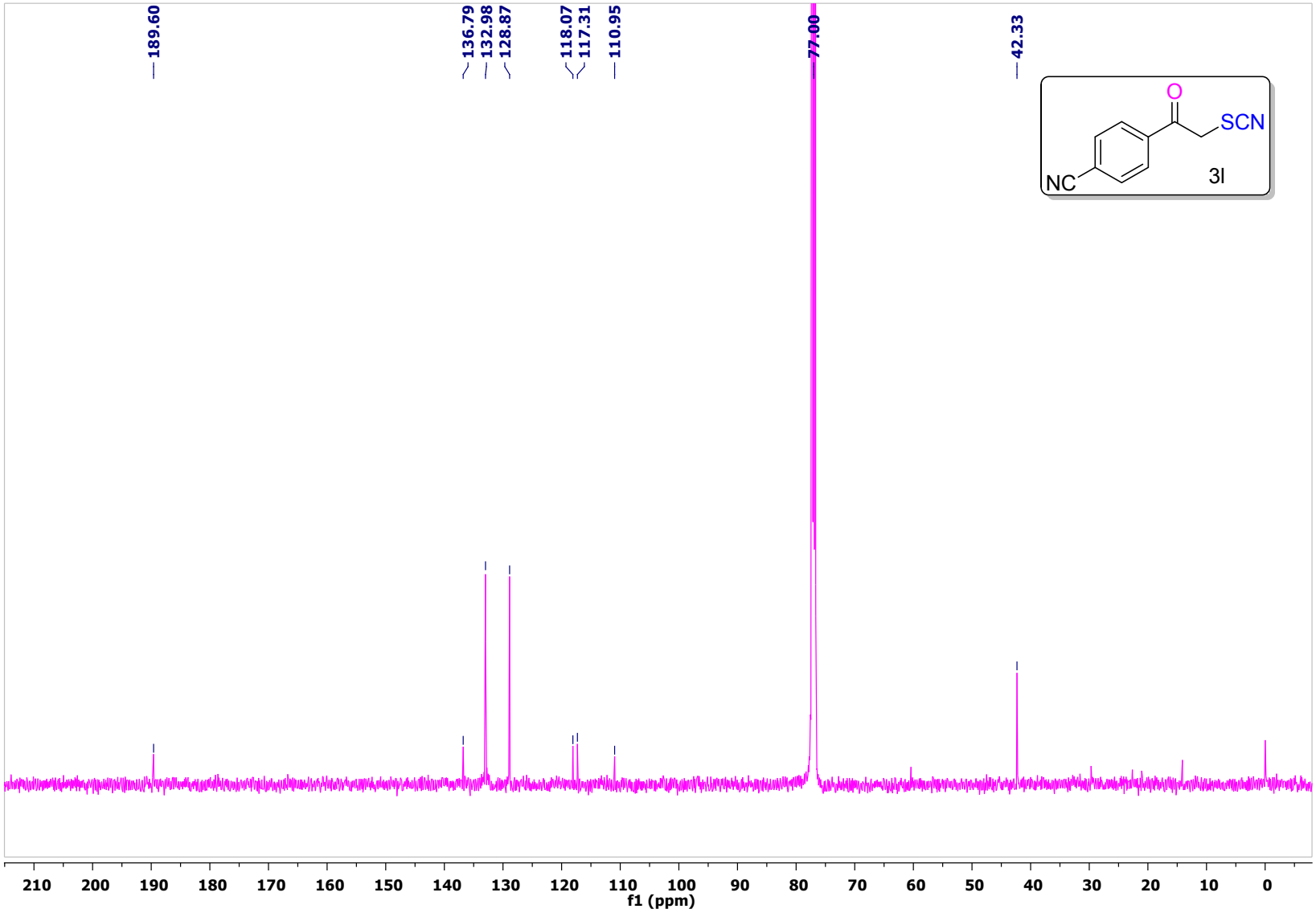
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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118.07
117.31
110.95
77.00
42.33
O
SCN
NC
3l
210
200
190
180
170
160
150
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130
120
110
100
90
80
70
60
50
40
30
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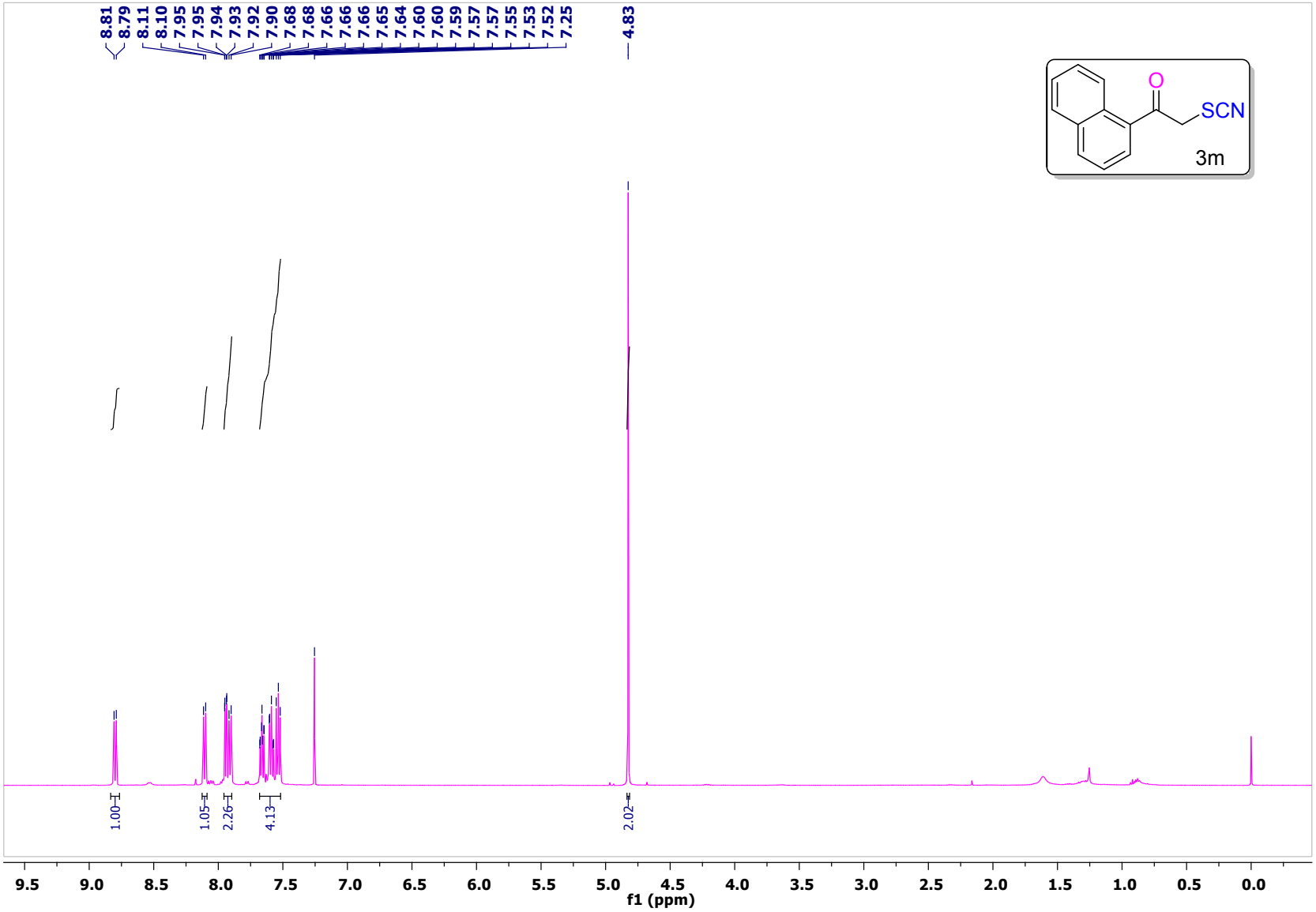
10
0
f1 (ppm)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7.93
7.92
7.90
7.68
7.68
7.66
7.66
7.65
7.64
7.60
7.60
7.59
7.57
7.57
7.55
7.53
7.52
7.25
4.83
O
SCN
3m
1.00
1.05
2.26
4.13
2.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
3.0
2.5
2.0
1.5
1.0
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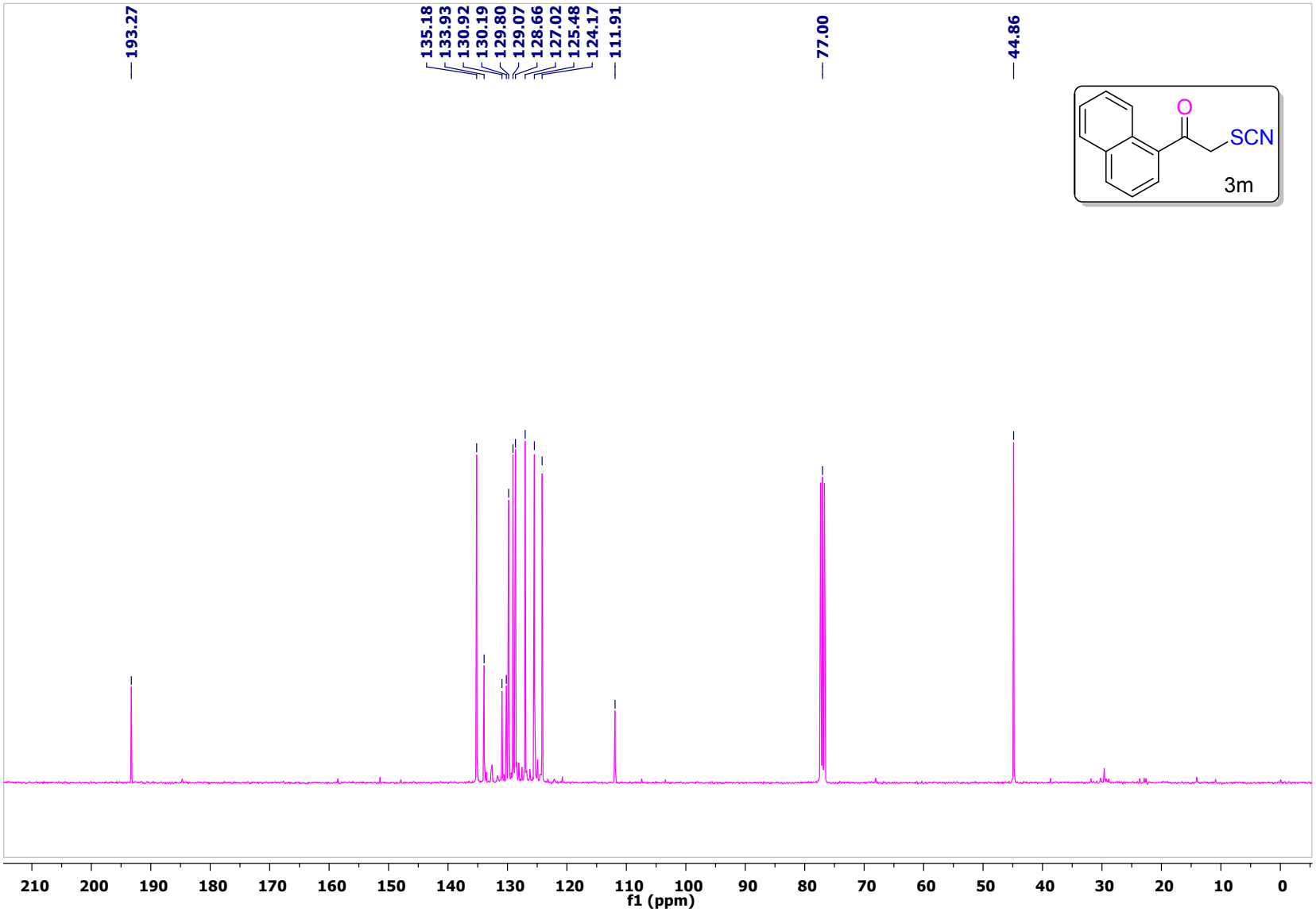
0.0
f1 (ppm)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129.80
129.07
128.66
127.02
125.48
124.17
111.91
77.00
44.86
O
SCN
3m
210
200
190
180
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130
120
110
100
90
80
70
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50
40
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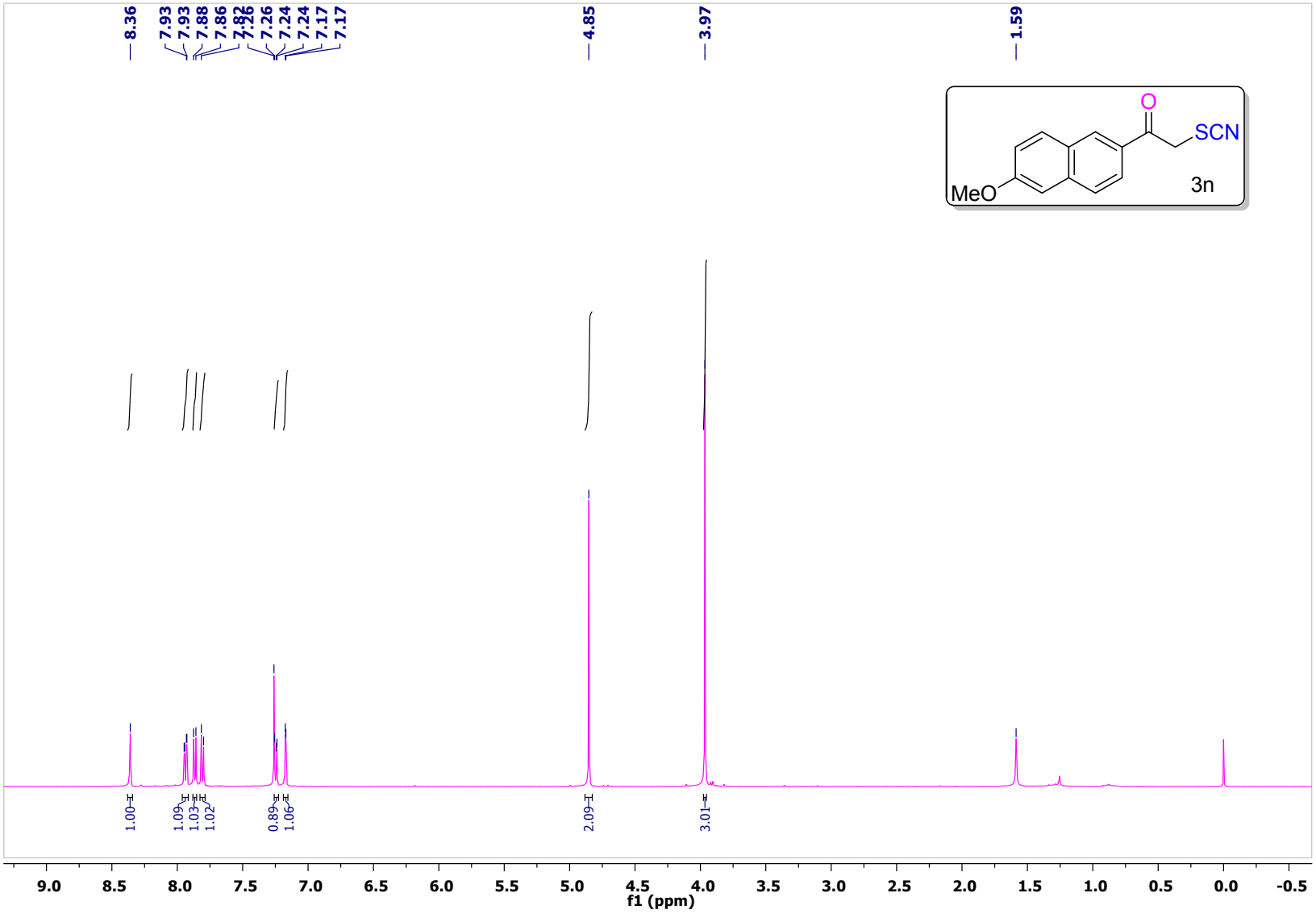
10
0
f1 (ppm)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7.93
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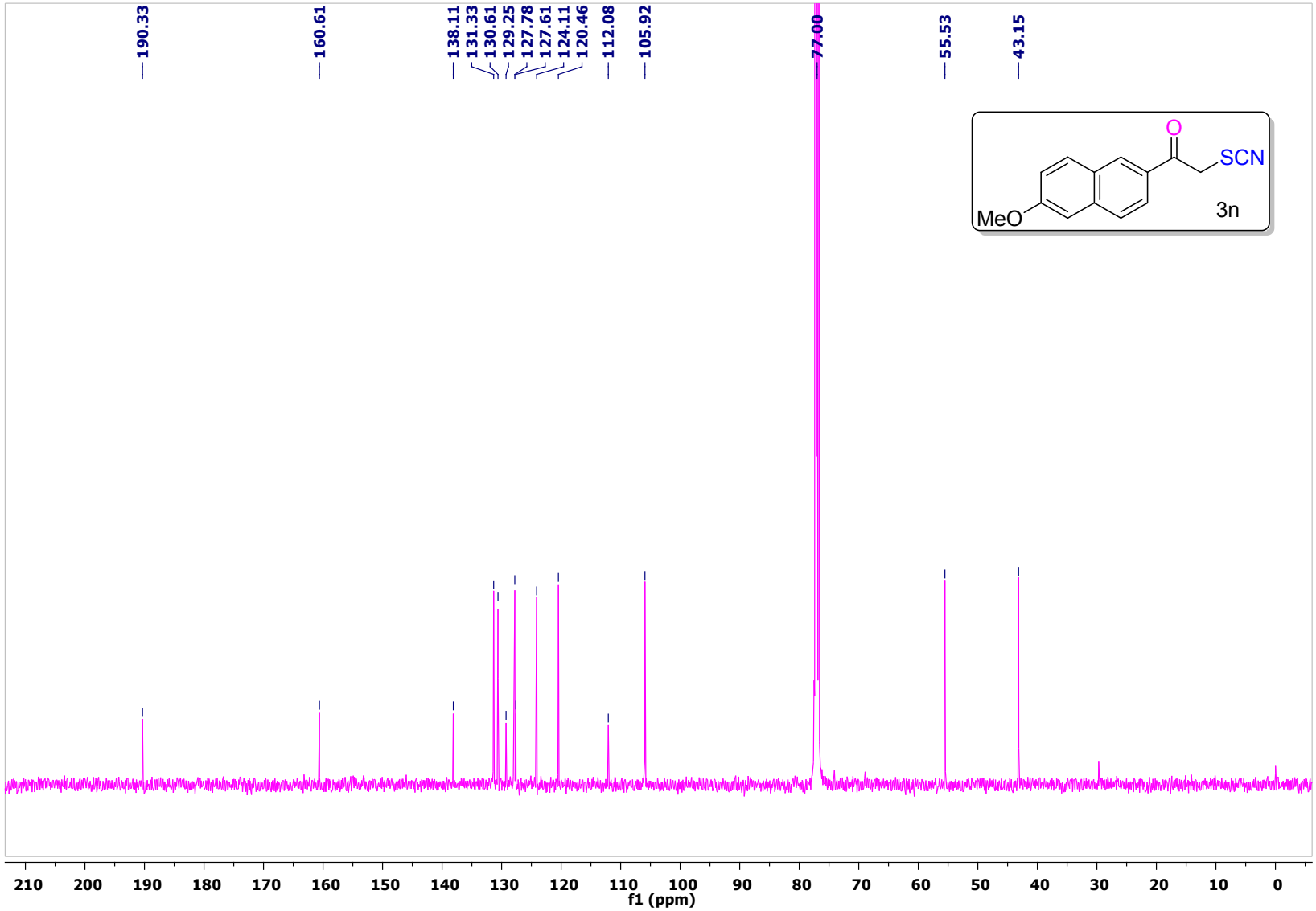
7.26
7.24
7.24
7.17
7.17
4.85
3.97
1.59
O
SCN
MeO
3n
1.00
1.09
1.03
1.02
0.89
1.06
2.09
3.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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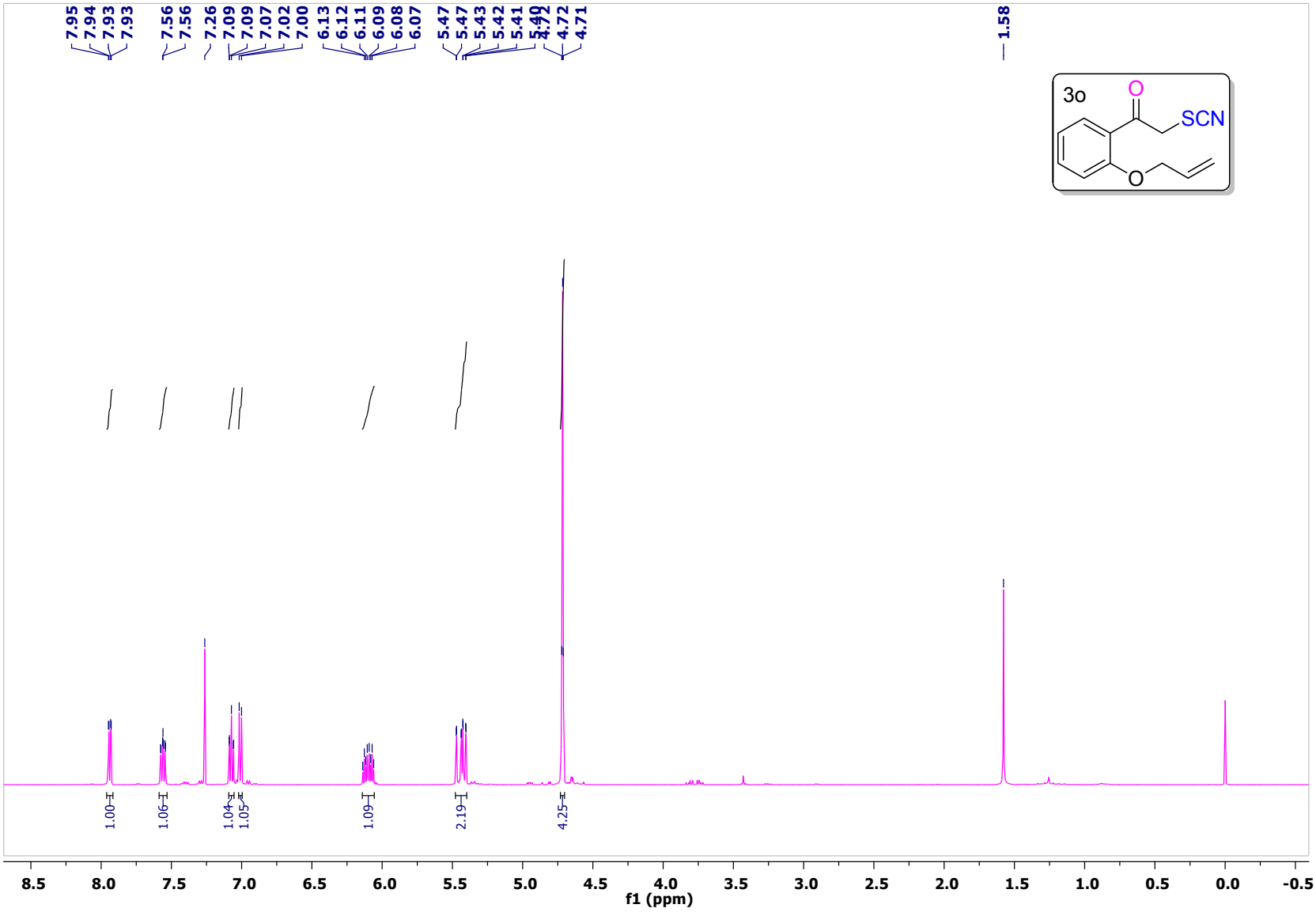
131.33
130.61
129.25
127.78
127.61
124.11
120.46
112.08
105.92
77.00
55.53
43.15
O
SCN
MeO
3n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.94
7.93
7.93
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7.56
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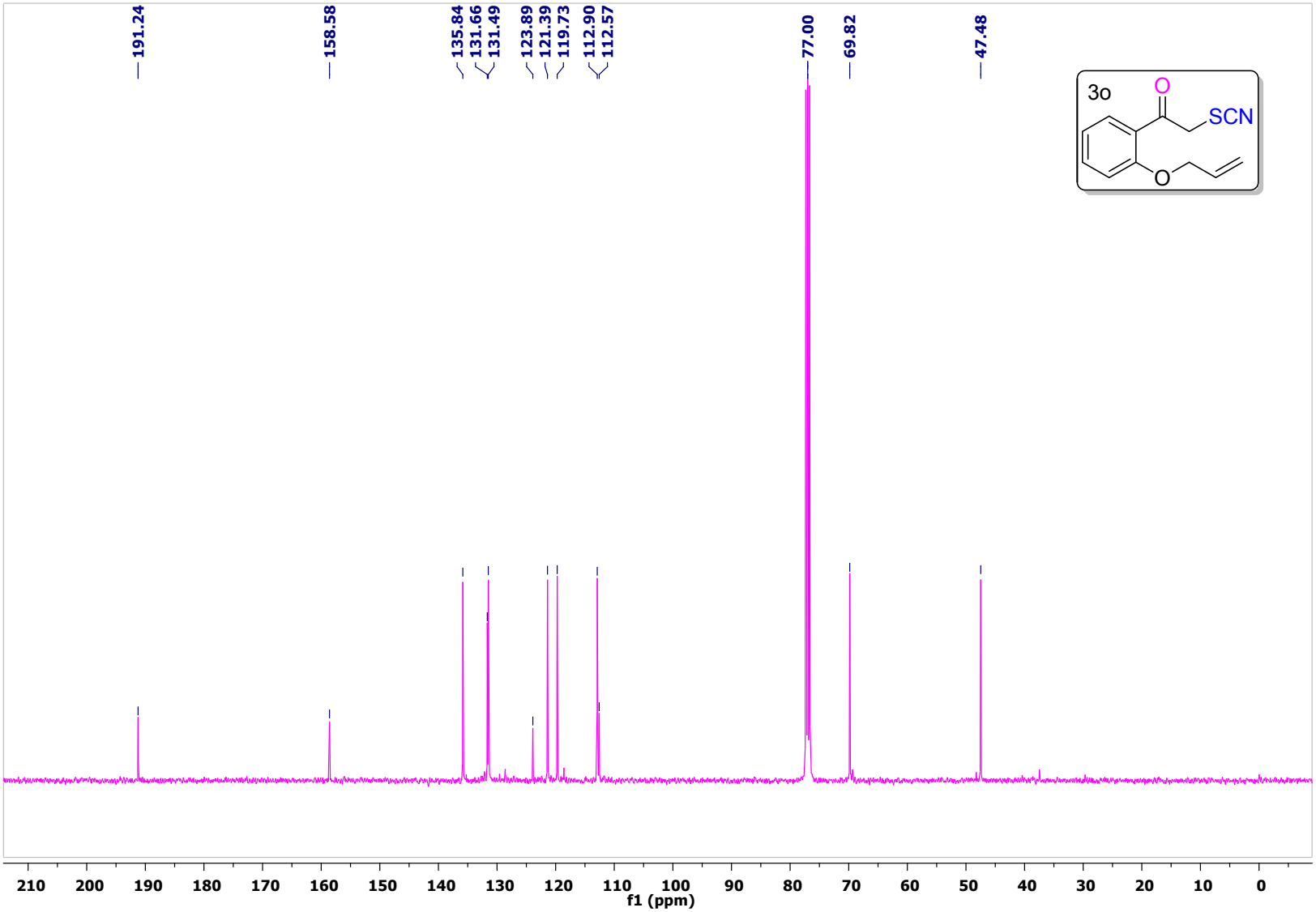
7.09
7.09
7.07
7.02
7.00
6.13
6.12
6.11
6.09
6.08
6.07
5.47
5.47
5.43
5.42
5.41
5.40
4.72
4.71
1.58
3o
O
SCN
O
1.00
1.06
1.04
1.05
1.09
2.19
4.25
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


191.24
158.58
135.84
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131.49
123.89
121.39
119.73
112.90
112.57
77.00
69.82
47.48
3o
O
SCN
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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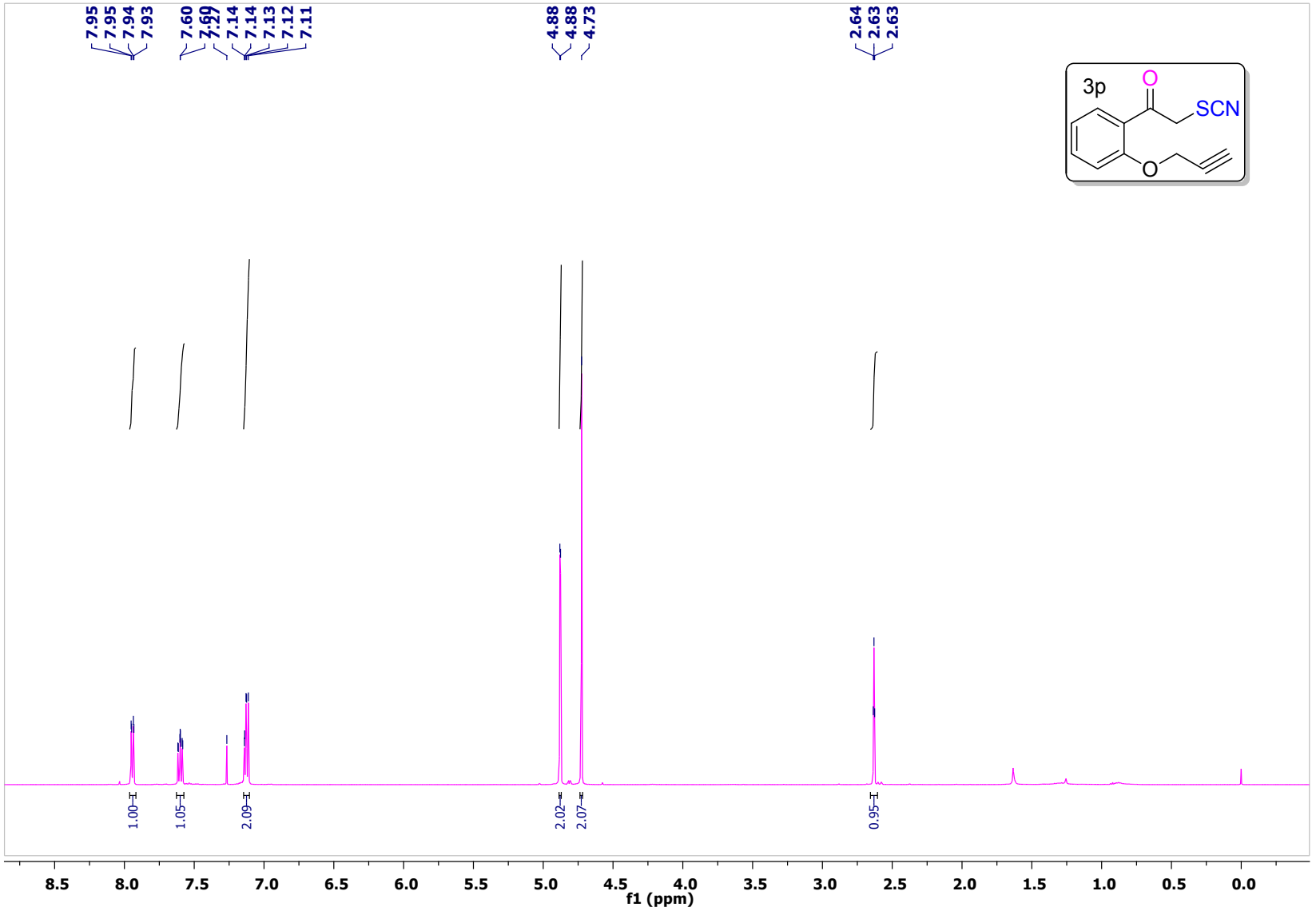
50
40
30
20
10
0
f1 (ppm)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7.95
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7.93
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7.60
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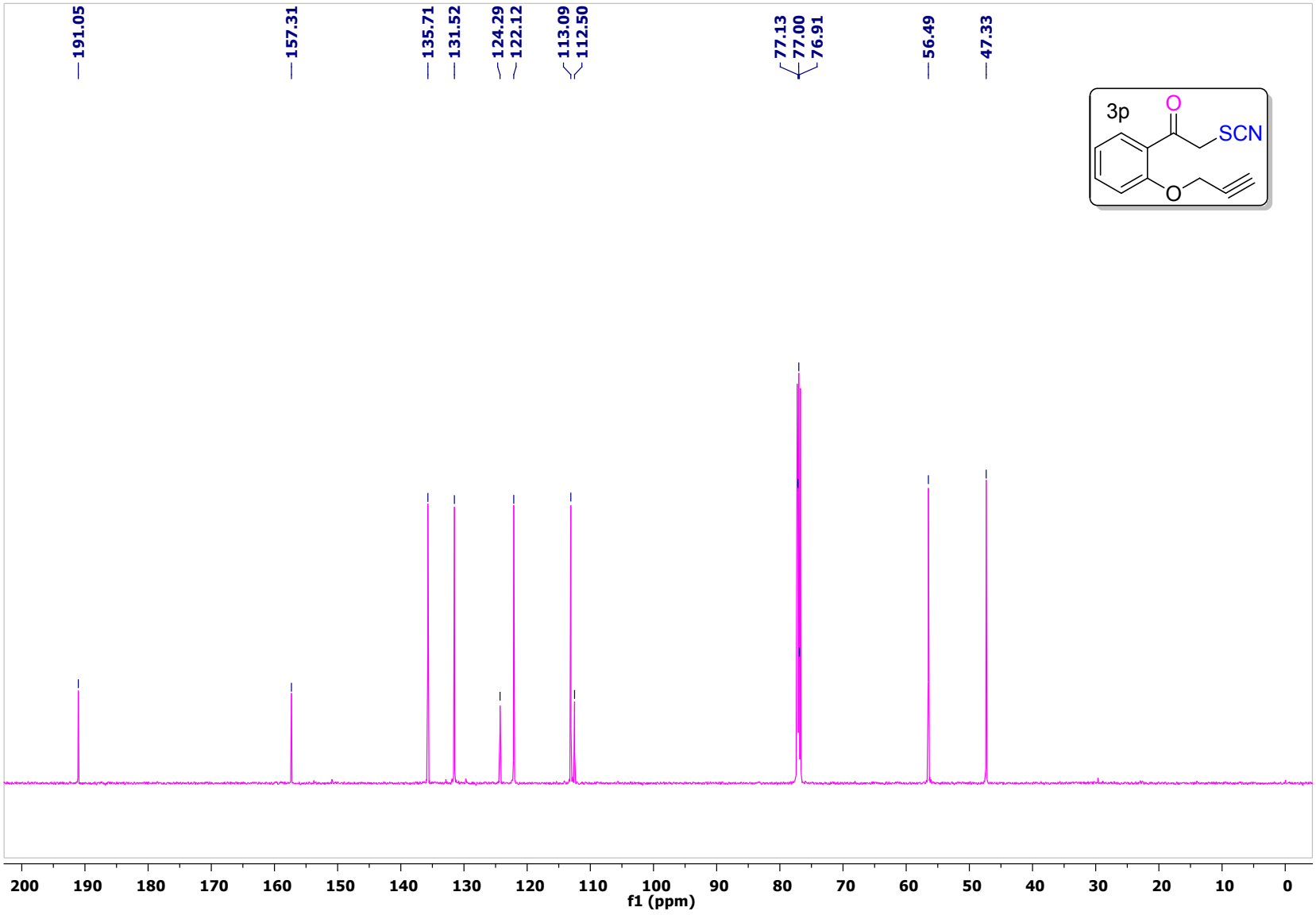
7.14
7.13
7.12
7.11
4.88
4.88
4.73
2.64
2.63
2.63
3p
O
SCN
O
1.00
1.05
2.09
2.02
2.07
0.95
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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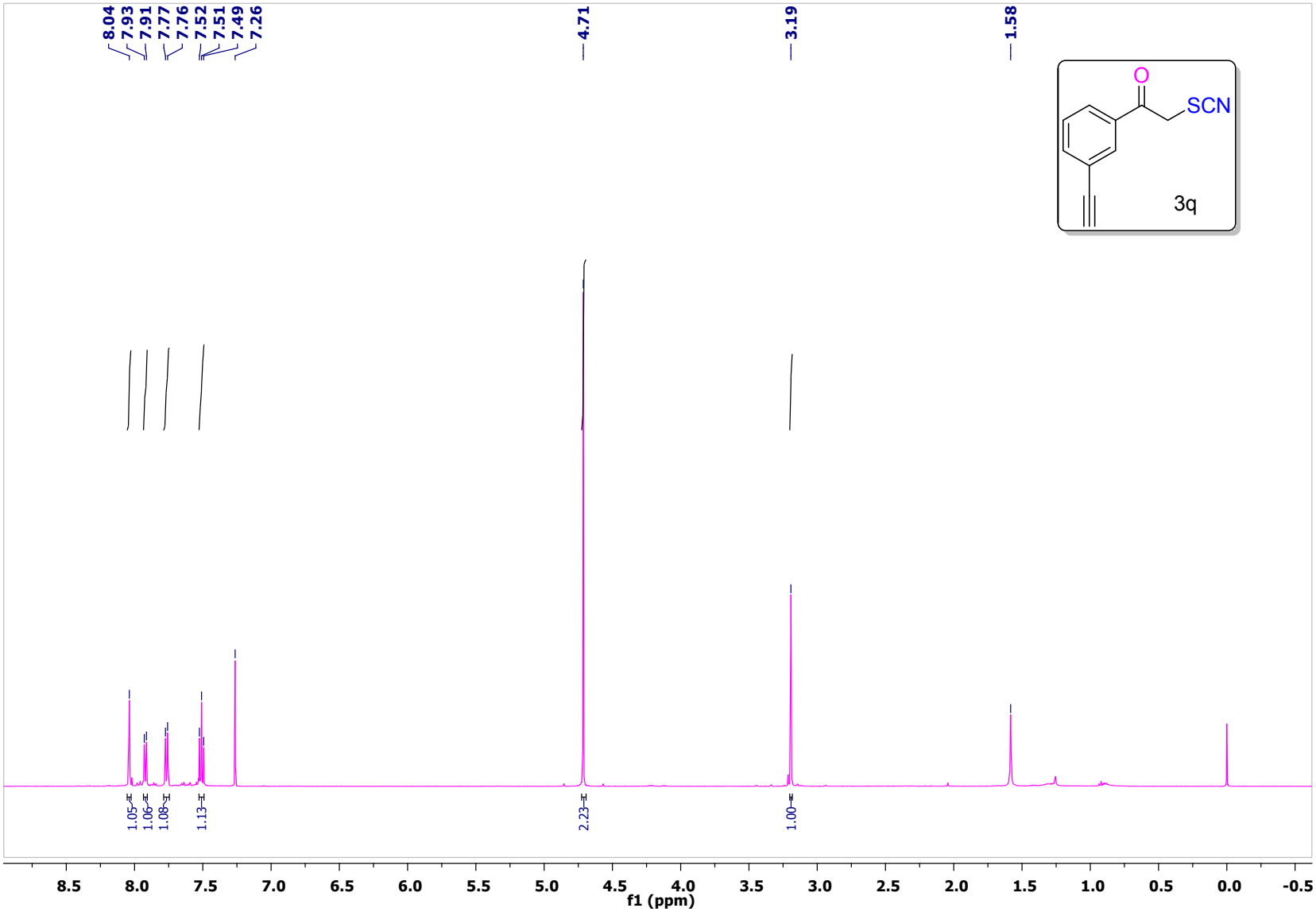
157.31
135.71
131.52
124.29
122.12
113.09
112.50
77.13
77.00
76.91
56.49
47.33
3p
O
SCN
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.04
7.93
7.91
7.77
7.76
7.52
7.51
7.49
7.26
4.71
3.19
1.58
O
SCN
3q
1.05
1.06
1.08
1.13
2.23
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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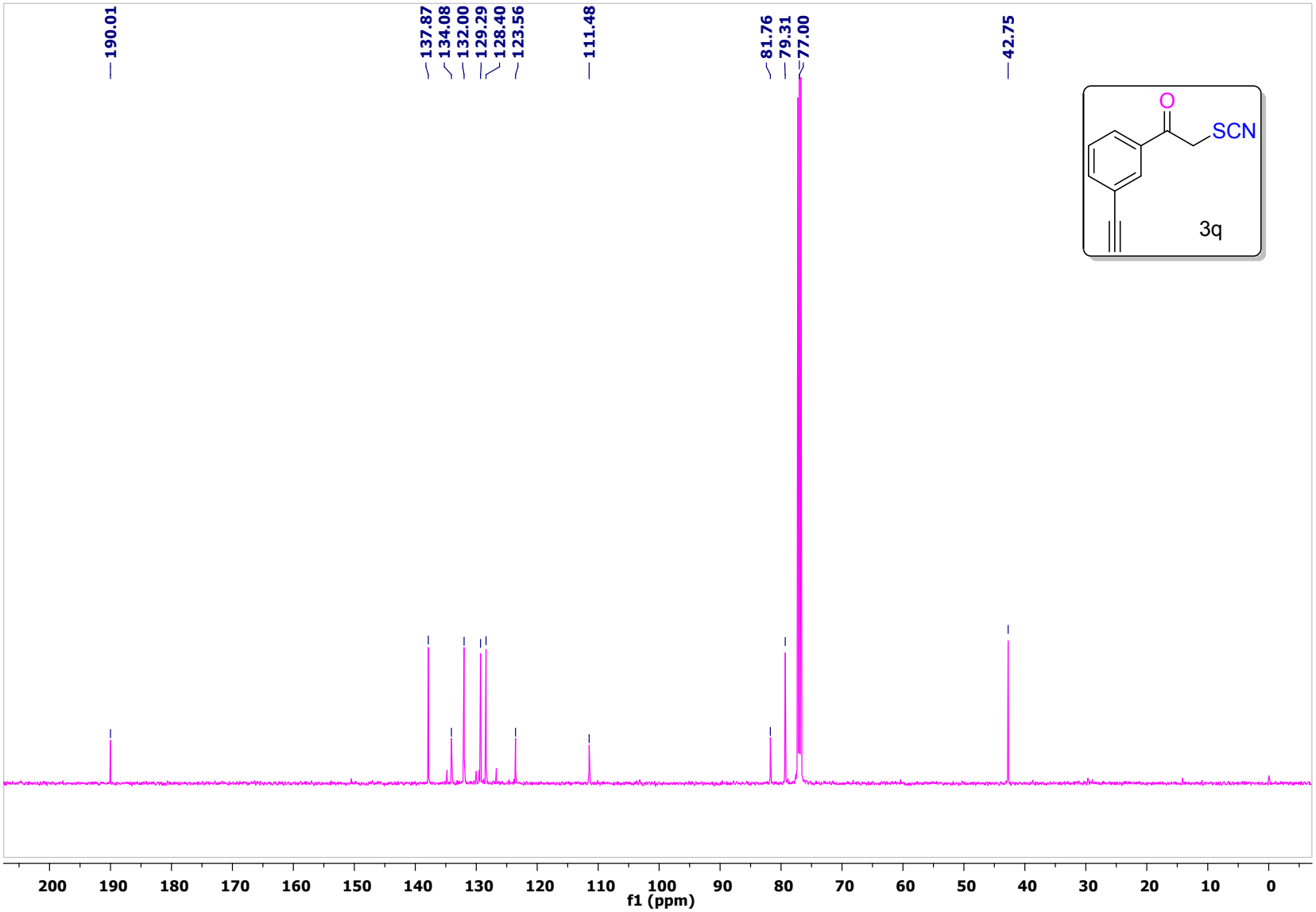
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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129.29
128.40
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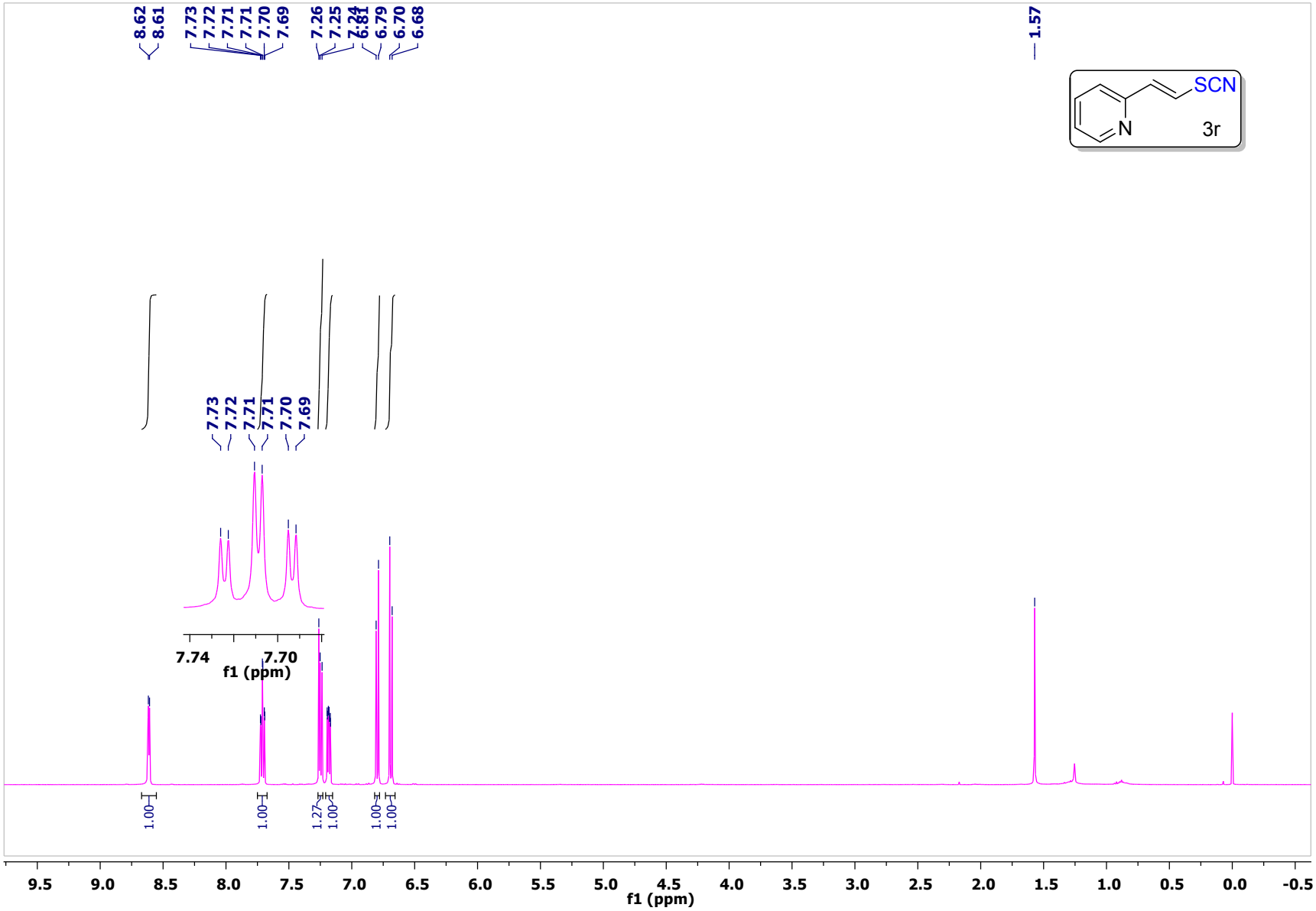
111.48
81.76
79.31
77.00
42.75
O
SCN
3q
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.62
8.61
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7.71
7.71
7.70
7.69
7.26
7.25
7.24
6.81
6.79
6.70
6.68
1.57
SCN
N
3r
7.74
7.70
f1 (ppm)
1.00
1.00
1.27
1.00
1.00
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
1.5
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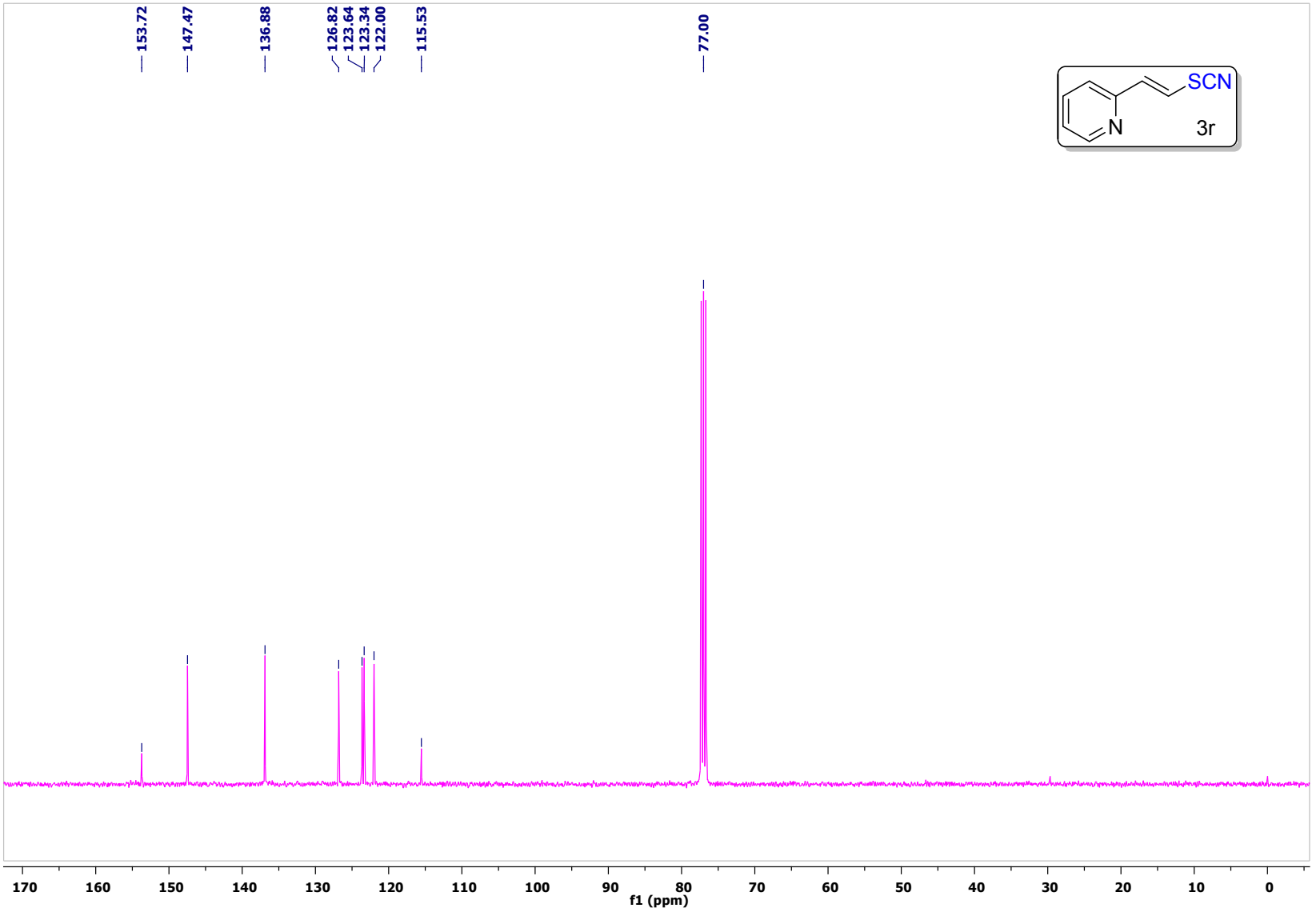
0.5
0.0
-0.5
f1 (ppm)


153.72
147.47
136.88
126.82
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123.34
122.00
115.53
77.00
SCN
N
3r
170
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150
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130
120
110
100
90
80
70
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50
40
30
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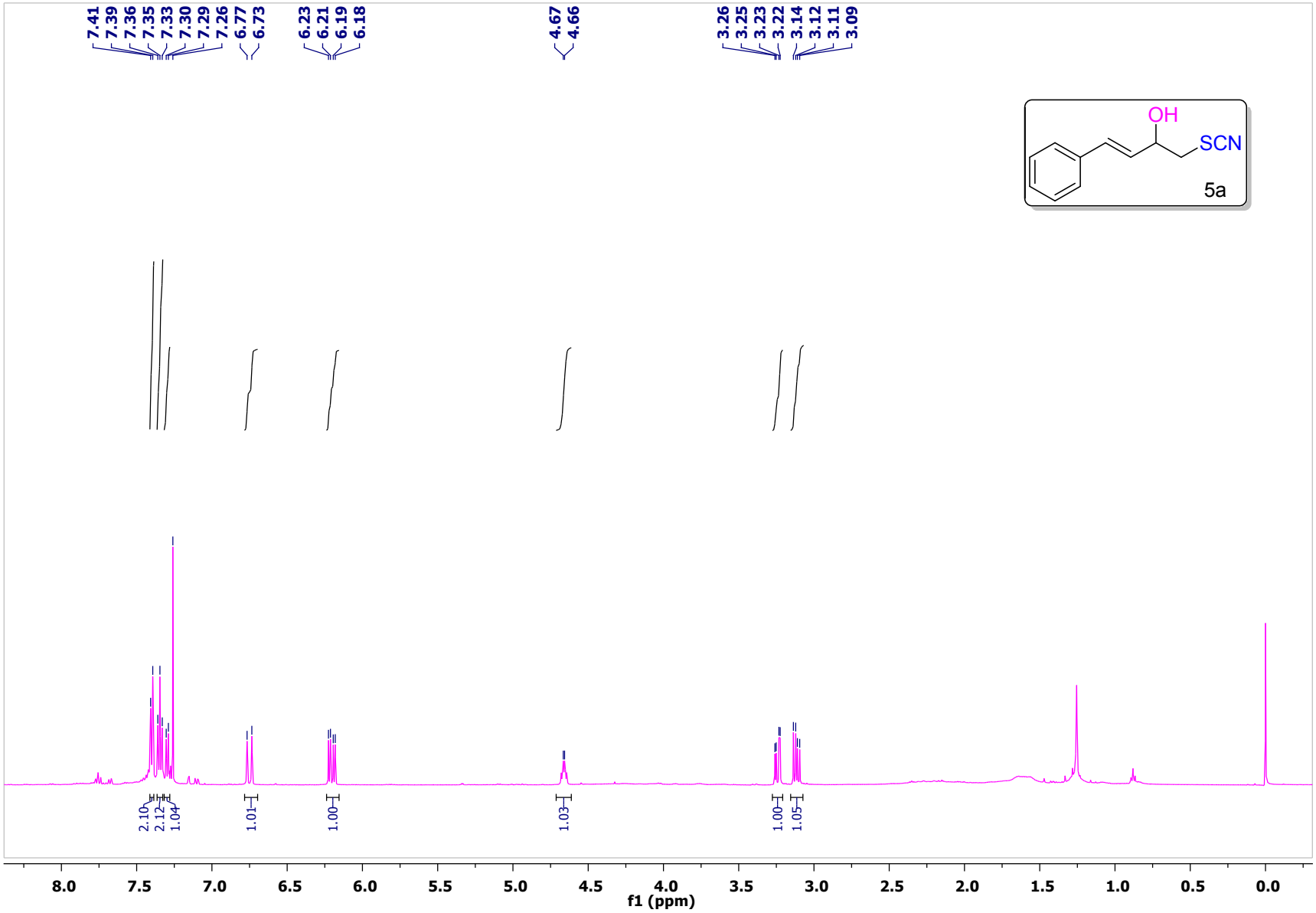
0
f1 (ppm)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7.26
6.77
6.73
6.23
6.21
6.19
6.18
4.67
4.66
3.26
3.25
3.23
3.22
3.14
3.12
3.11
3.09
OH
SCN
5a
2.10
2.12
1.04
1.01
1.00
1.03
1.00
1.05
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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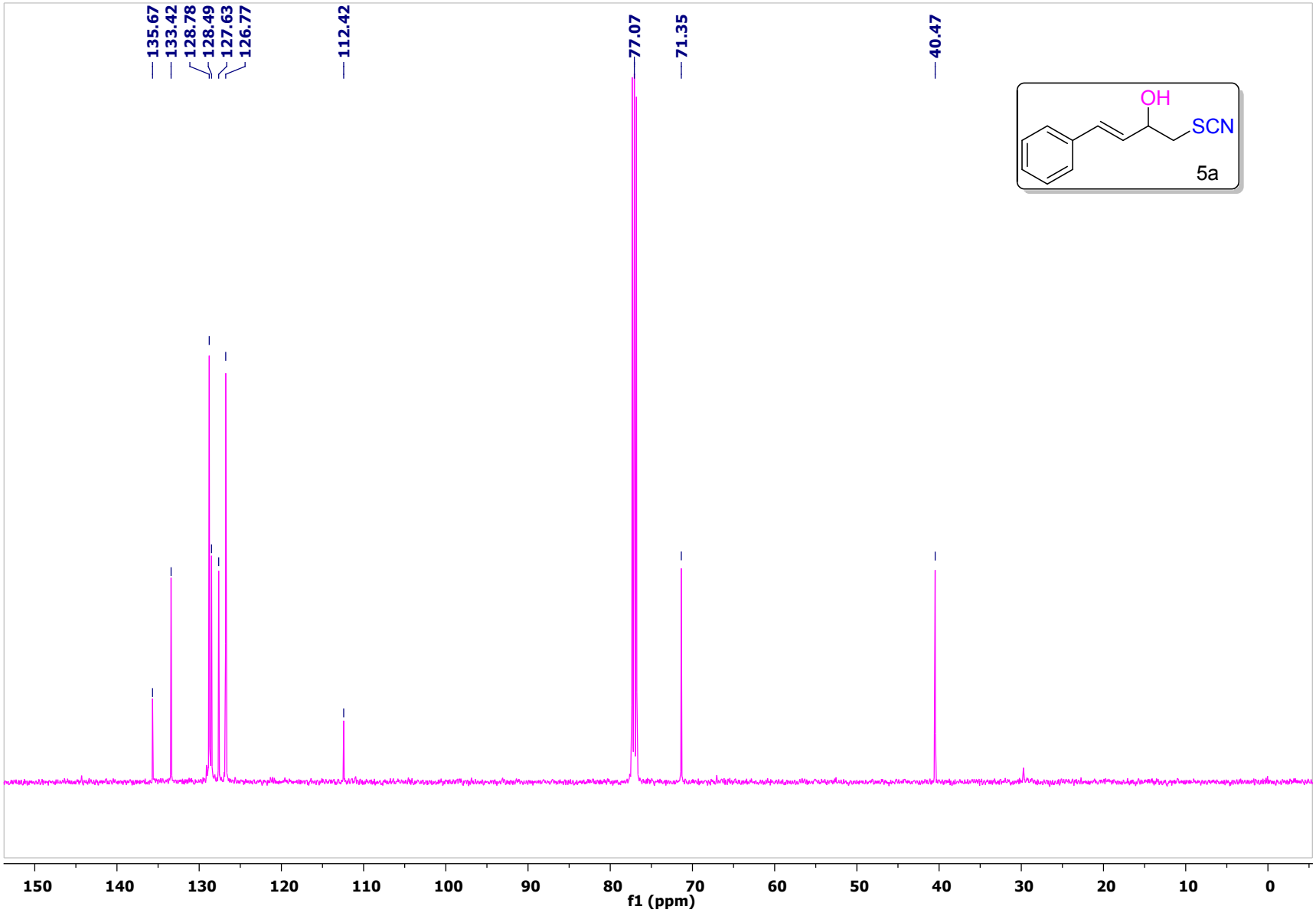
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.49
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126.77
112.42
77.07
71.35
40.47
OH
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130
120
110
100
90
80
70
60
50
40
30
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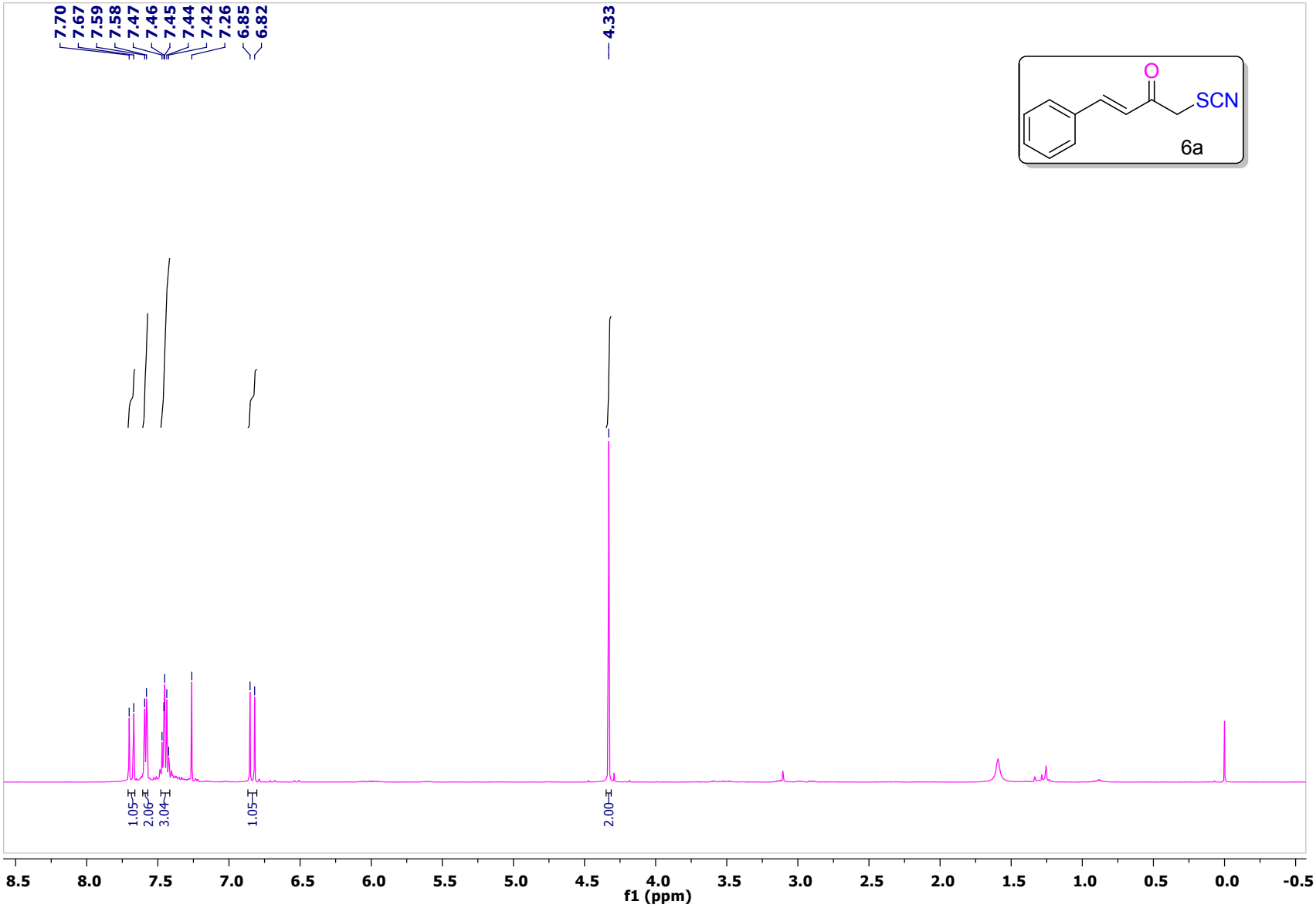
10
0
f1 (ppm)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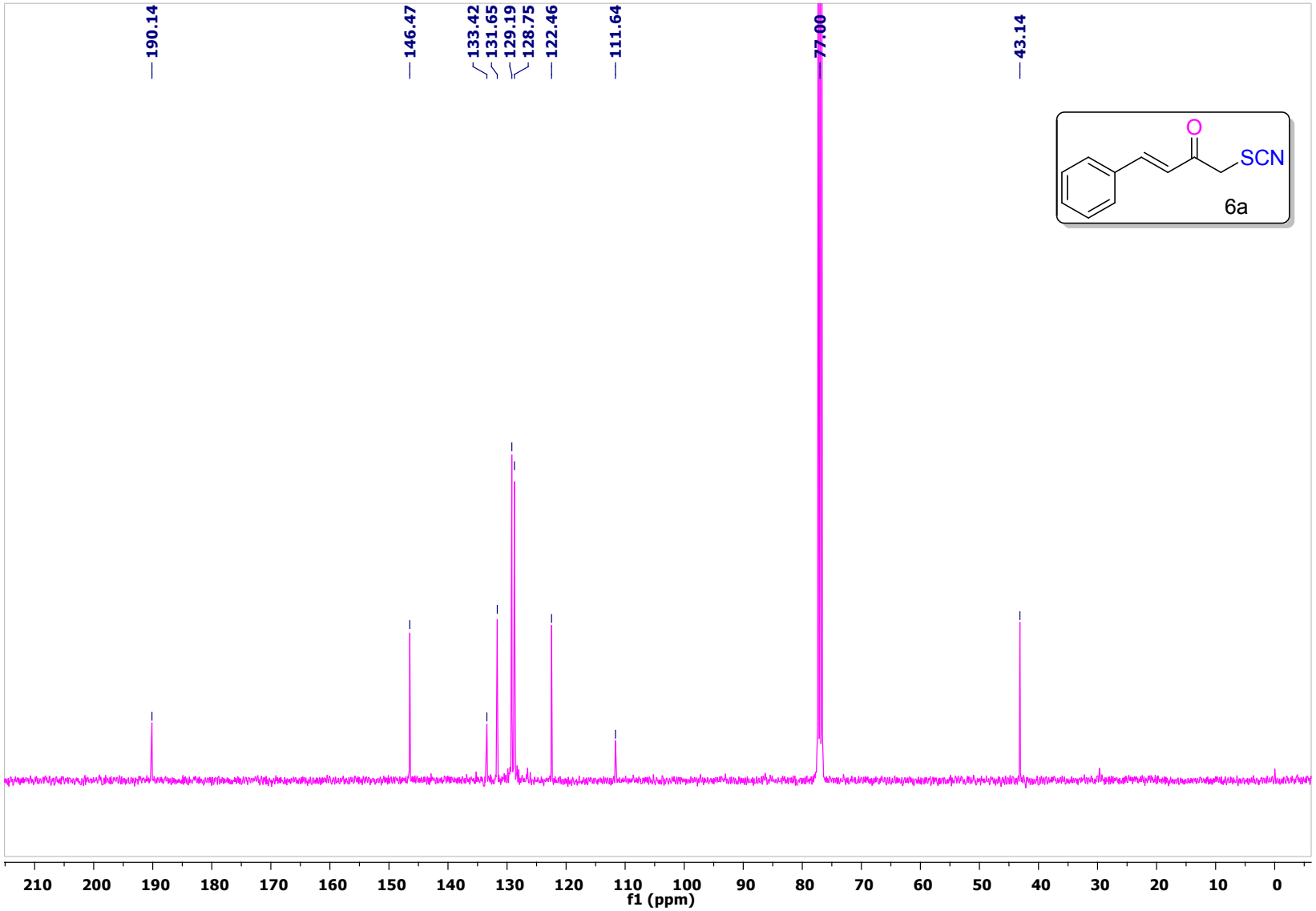
7.46
7.45
7.44
7.42
7.26
6.85
6.82
4.33
O
SCN
6a
1.05
2.06
3.04
1.05
2.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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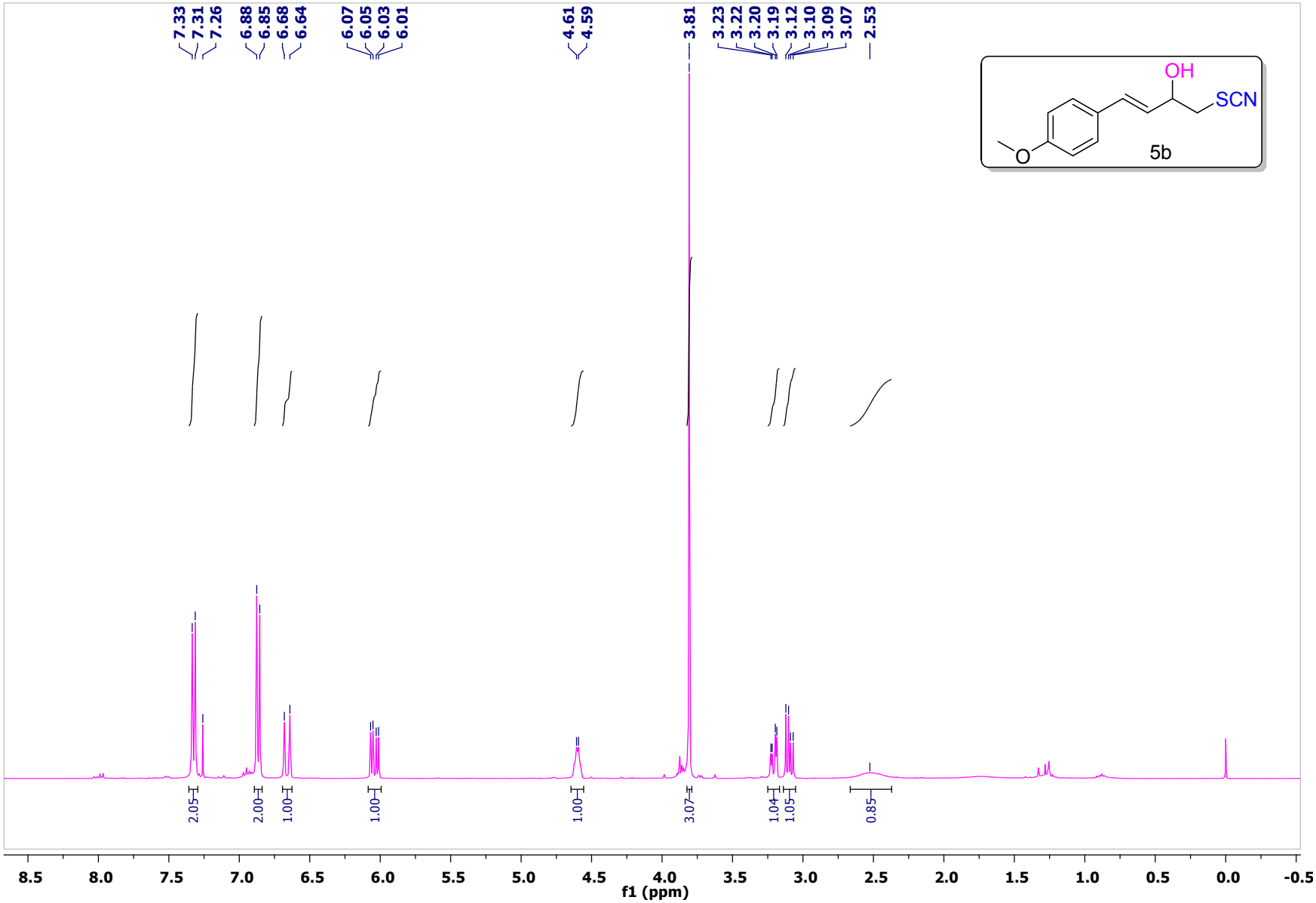
133.42
131.65
129.19
128.75
122.46
111.64
77.00
43.14
O
SCN
6a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.31
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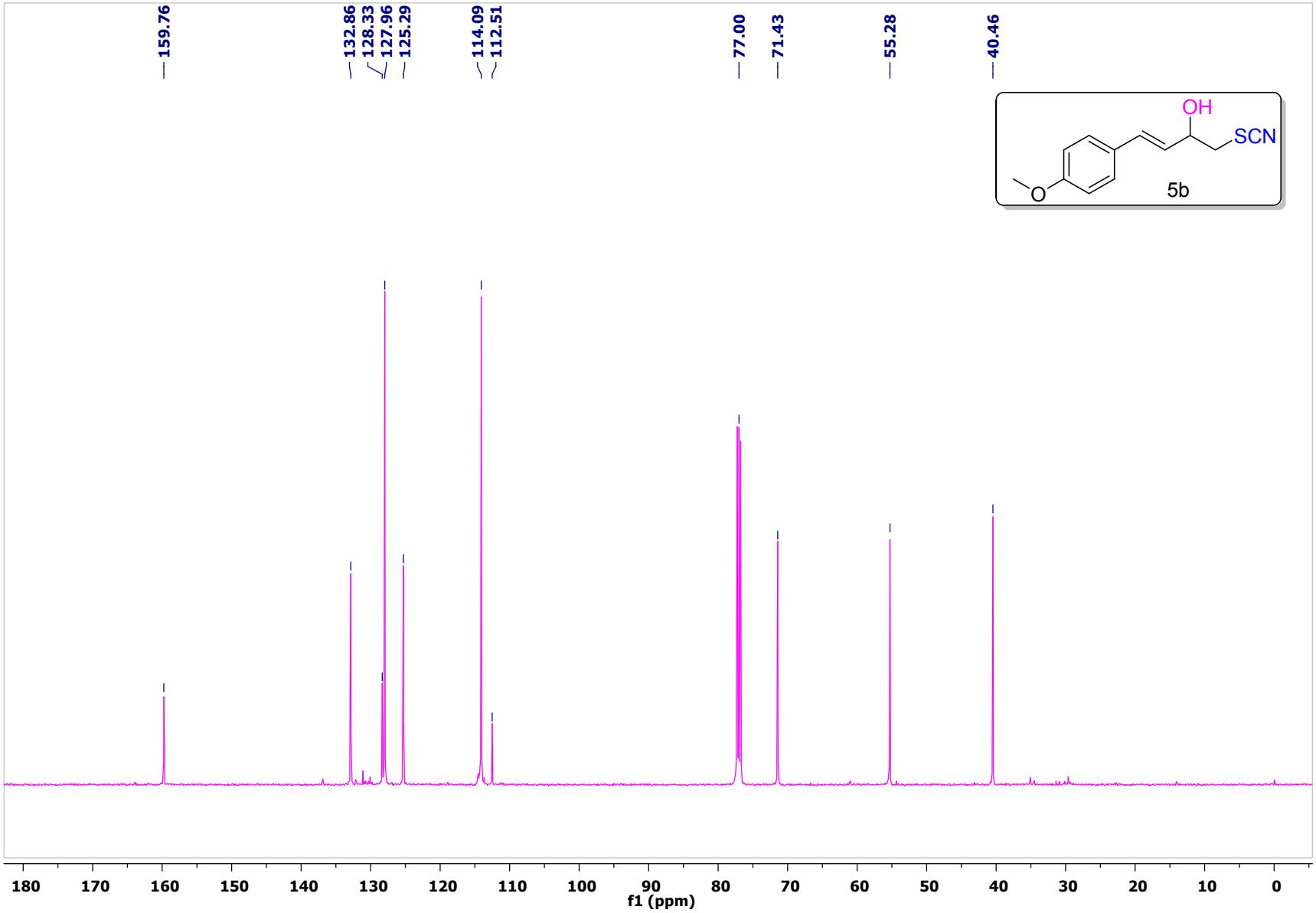
6.88
6.85
6.68
6.64
6.07
6.05
6.03
6.01
4.61
4.59
3.81
3.23
3.22
3.20
3.19
3.12
3.10
3.09
3.07
2.53
OH
SCN
O
5b
2.05
2.00
1.00
1.00
1.00
3.07
1.04
1.05
0.85
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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114.09
112.51
77.00
71.43
55.28
40.46
OH
SCN
O
5b
180
170
160
150
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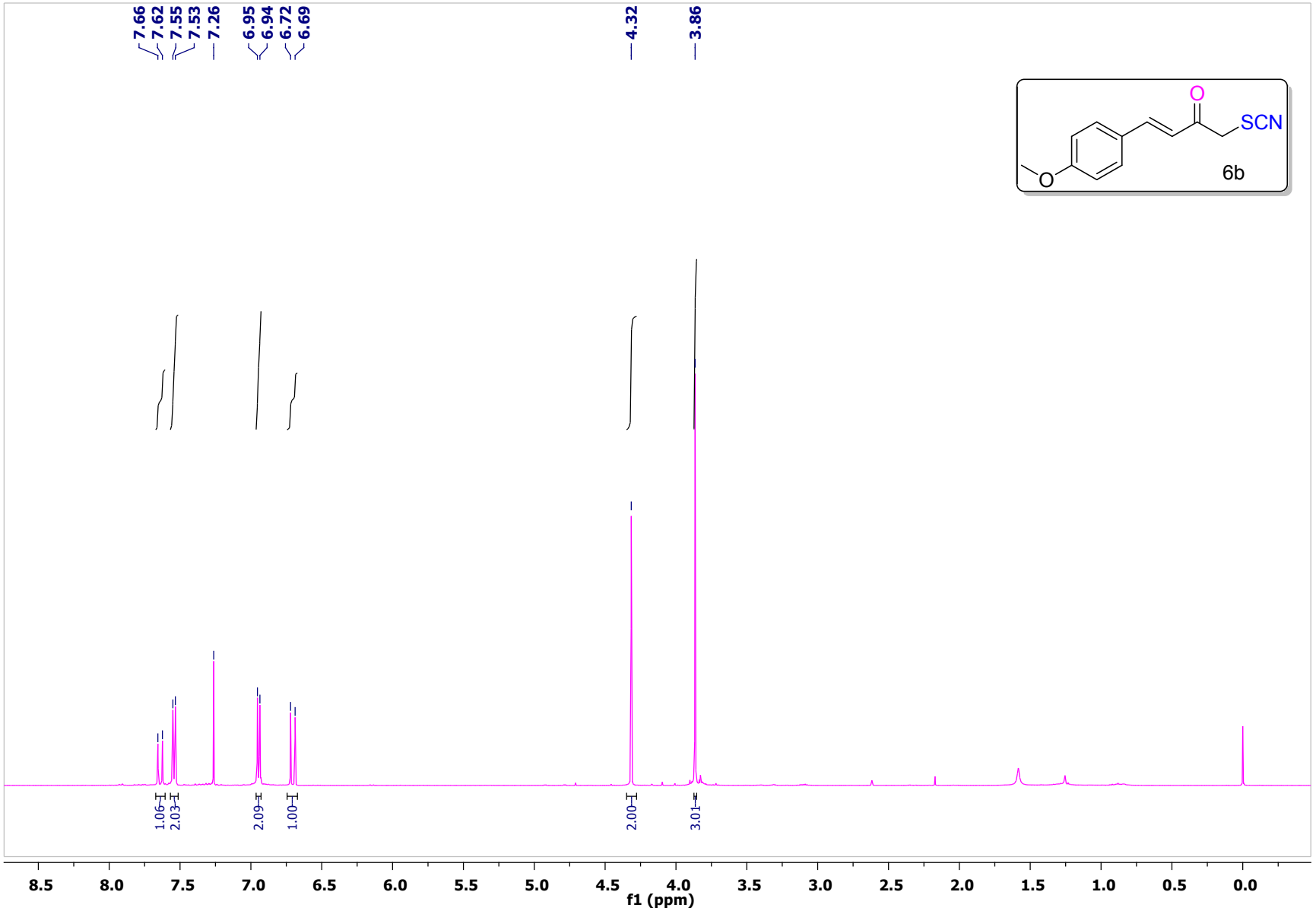
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.62
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7.53
7.26
6.95
6.94
6.72
6.69
4.32
3.86
O
SCN
O
6b
1.06
2.03
2.09
1.00
2.00
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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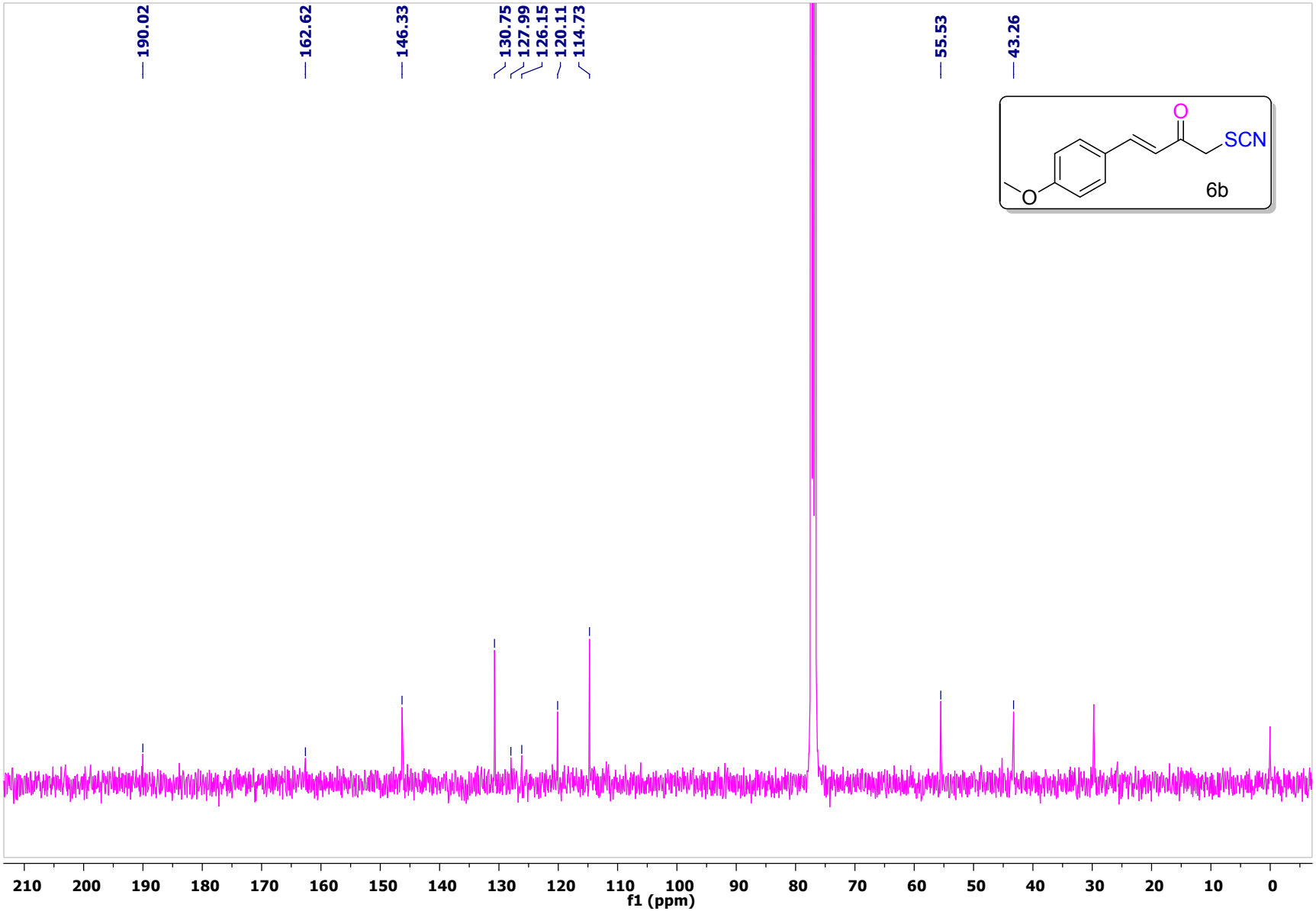
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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126.15
120.11
114.73
55.53
43.26
O
SCN
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6b
210
200
190
180
170
160
150
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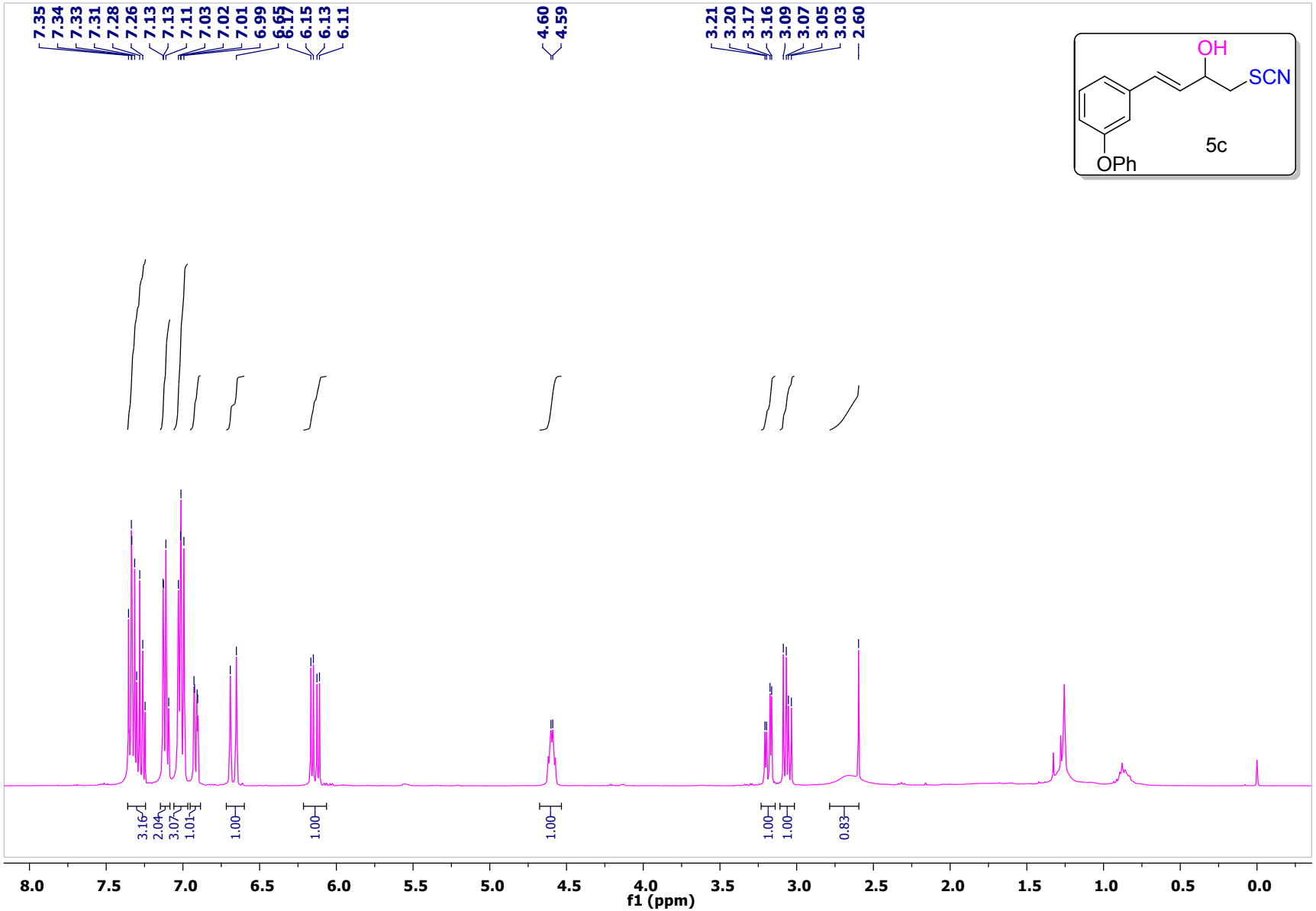
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.13
7.13
7.11
7.03
7.02
7.01
6.99
6.15
6.13
6.11
4.60
4.59
3.21
3.20
3.17
3.16
3.09
3.07
3.05
3.03
2.60
OH
SCN
OPh
5c
3.16
2.04
3.07
1.01
1.00
1.00
1.00
1.00
1.00
0.83
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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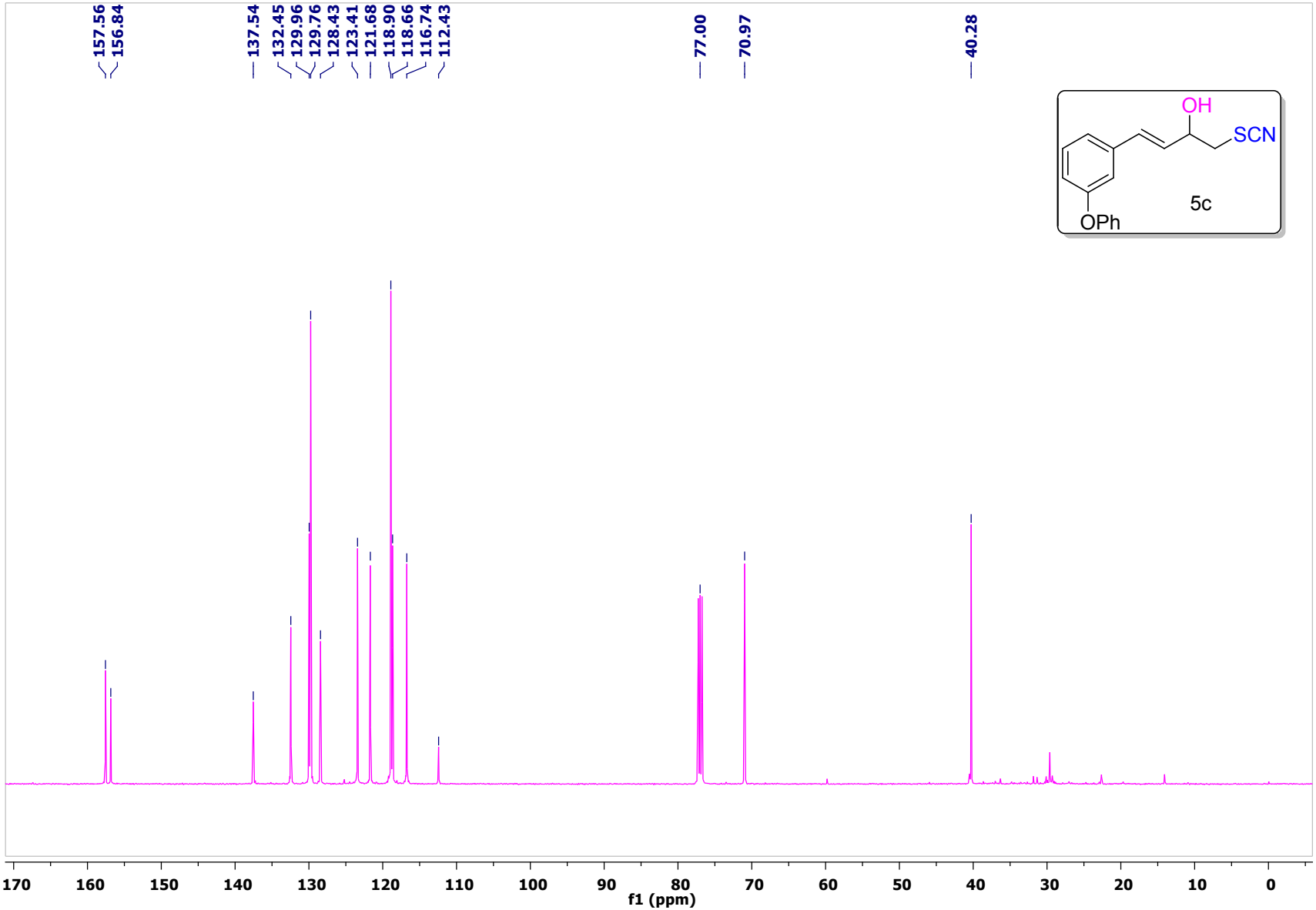
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.76
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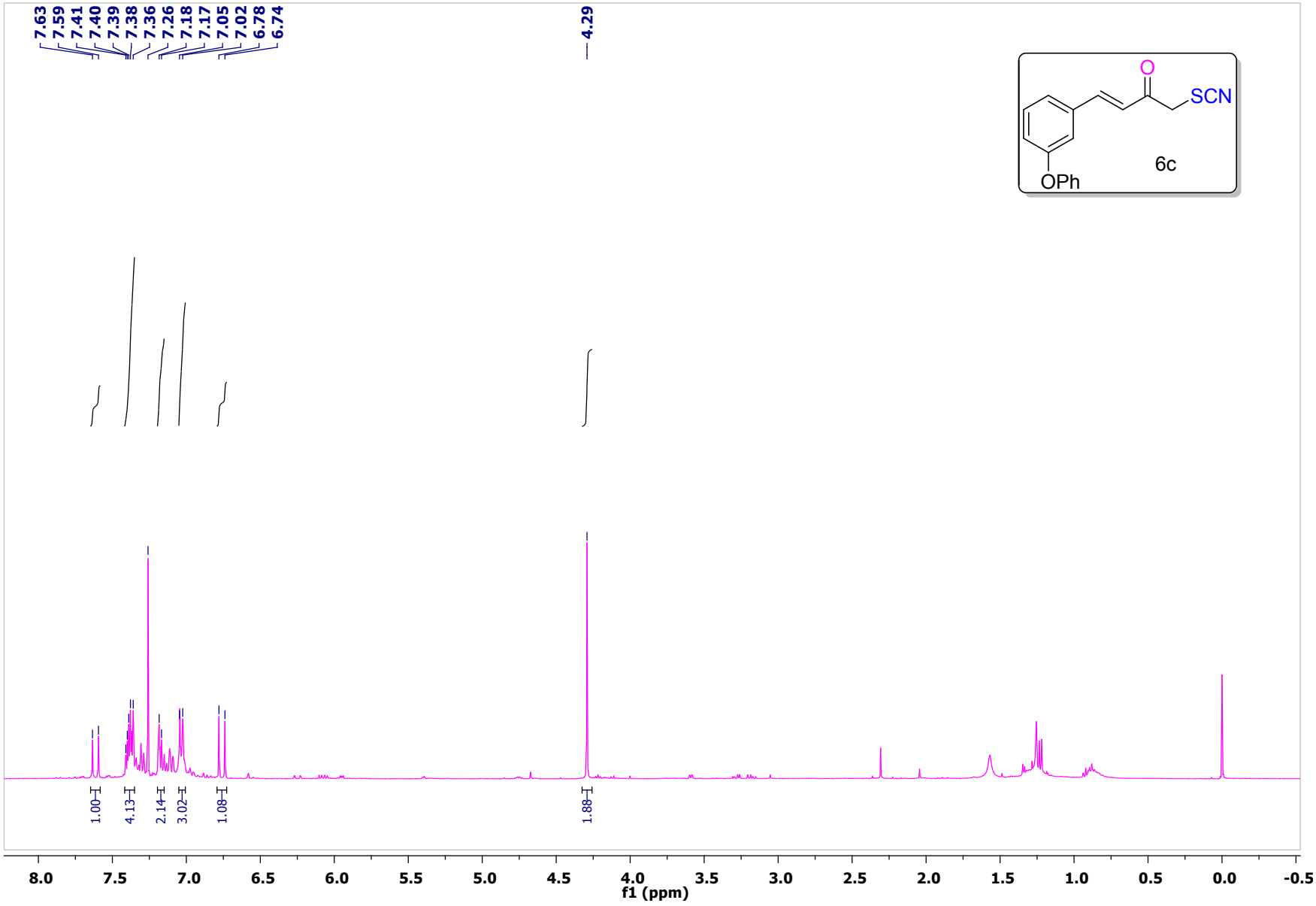
123.41
121.68
118.90
118.66
116.74
112.43
77.00
70.97
40.28
OH
SCN
OPh
5c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.02
6.78
6.74
4.29
O
SCN
OPh
6c
1.00
4.13
2.14
3.02
1.08
1.88
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
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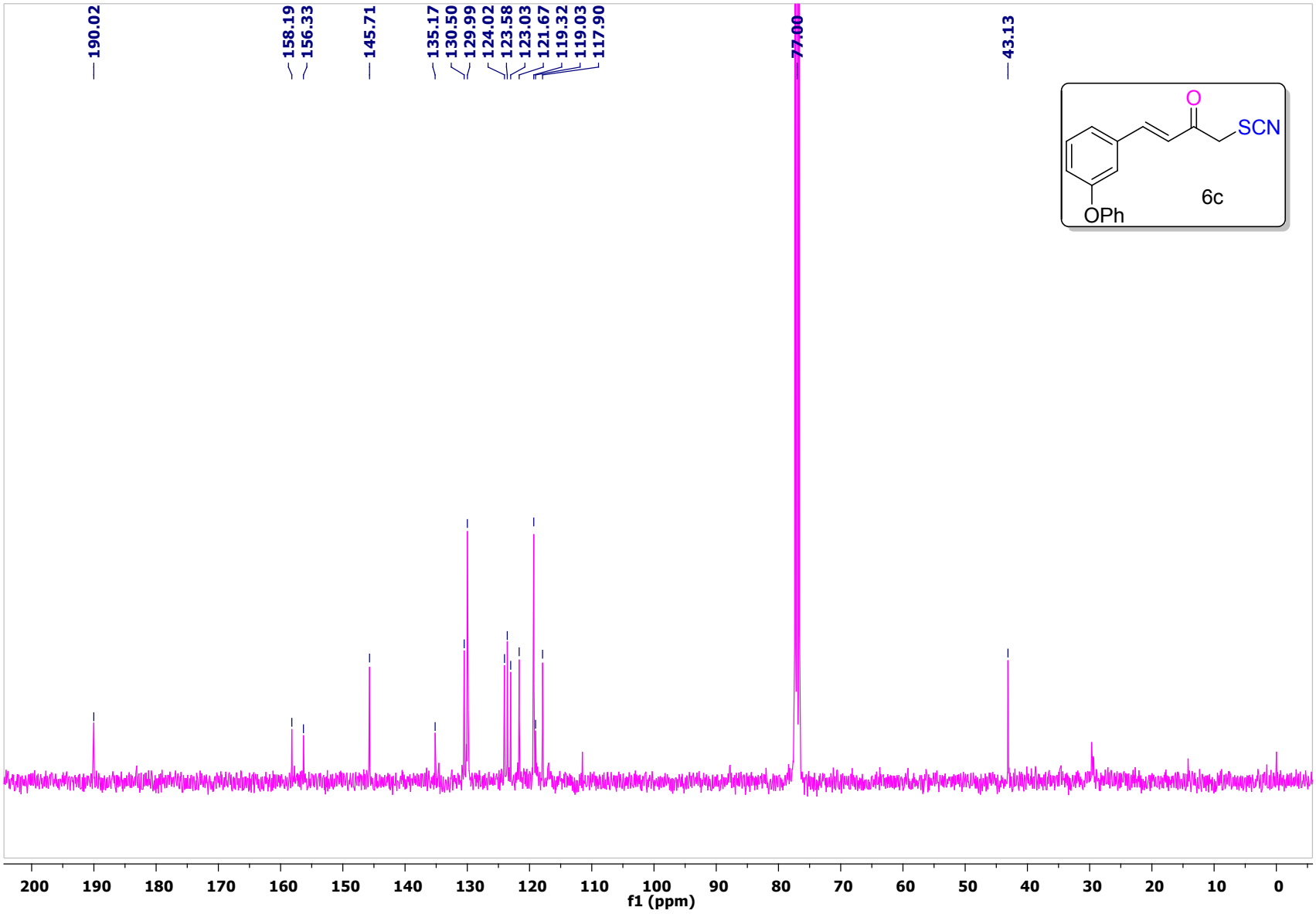
f1 (ppm)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130.50
129.99
124.02
123.58
123.03
121.67
119.32
119.03
117.90
77.00
43.13
O
SCN
OPh
6c
200
190
180
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90
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70
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40
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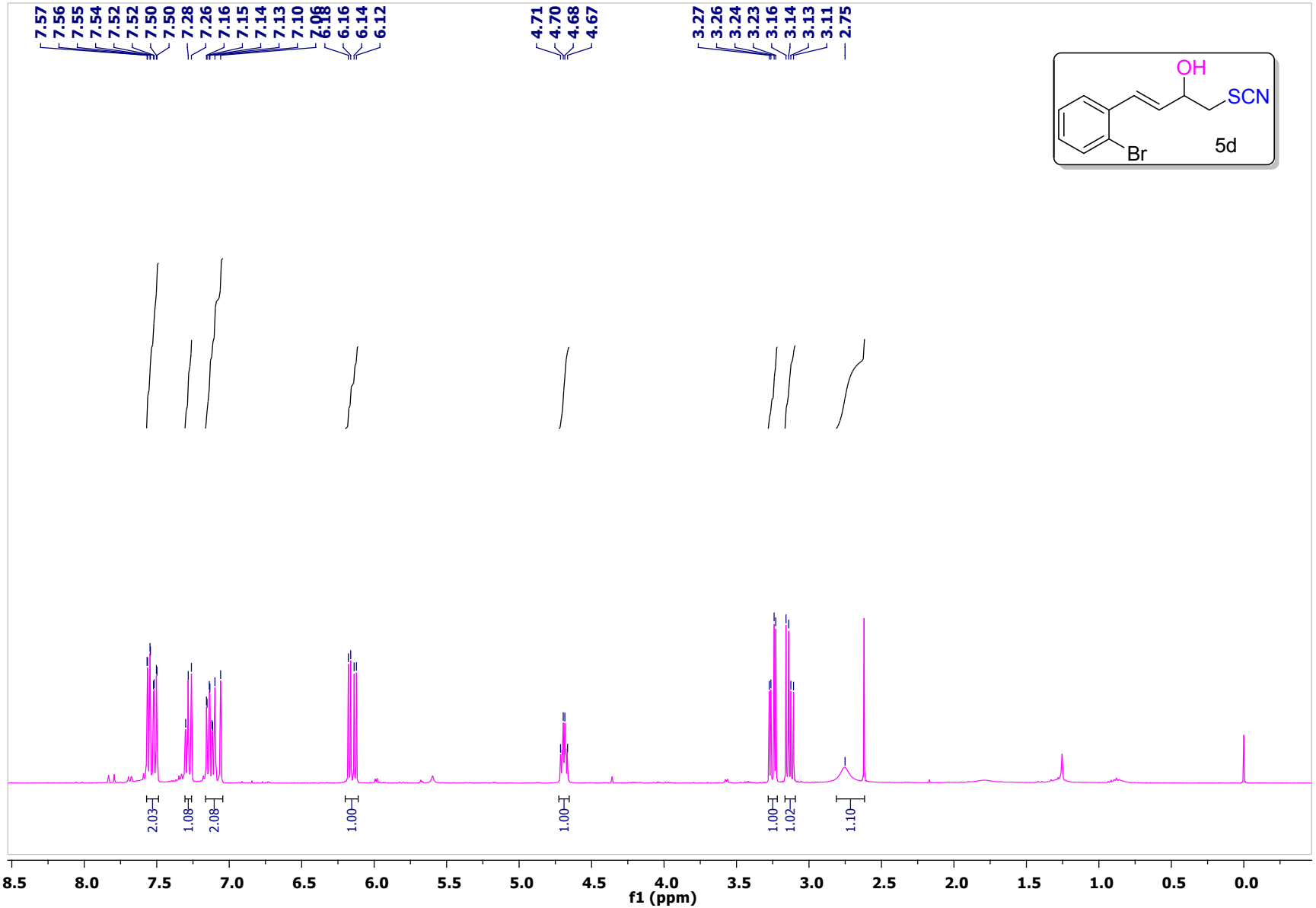
f1 (ppm)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7.14
7.13
7.10
7.06
6.18
6.16
6.14
6.12
4.71
4.70
4.68
4.67
3.27
3.26
3.24
3.23
3.16
3.14
3.13
3.11
2.75
OH
SCN
Br
5d
2.03
1.08
2.08
1.00
1.00
1.00
1.02
1.10
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
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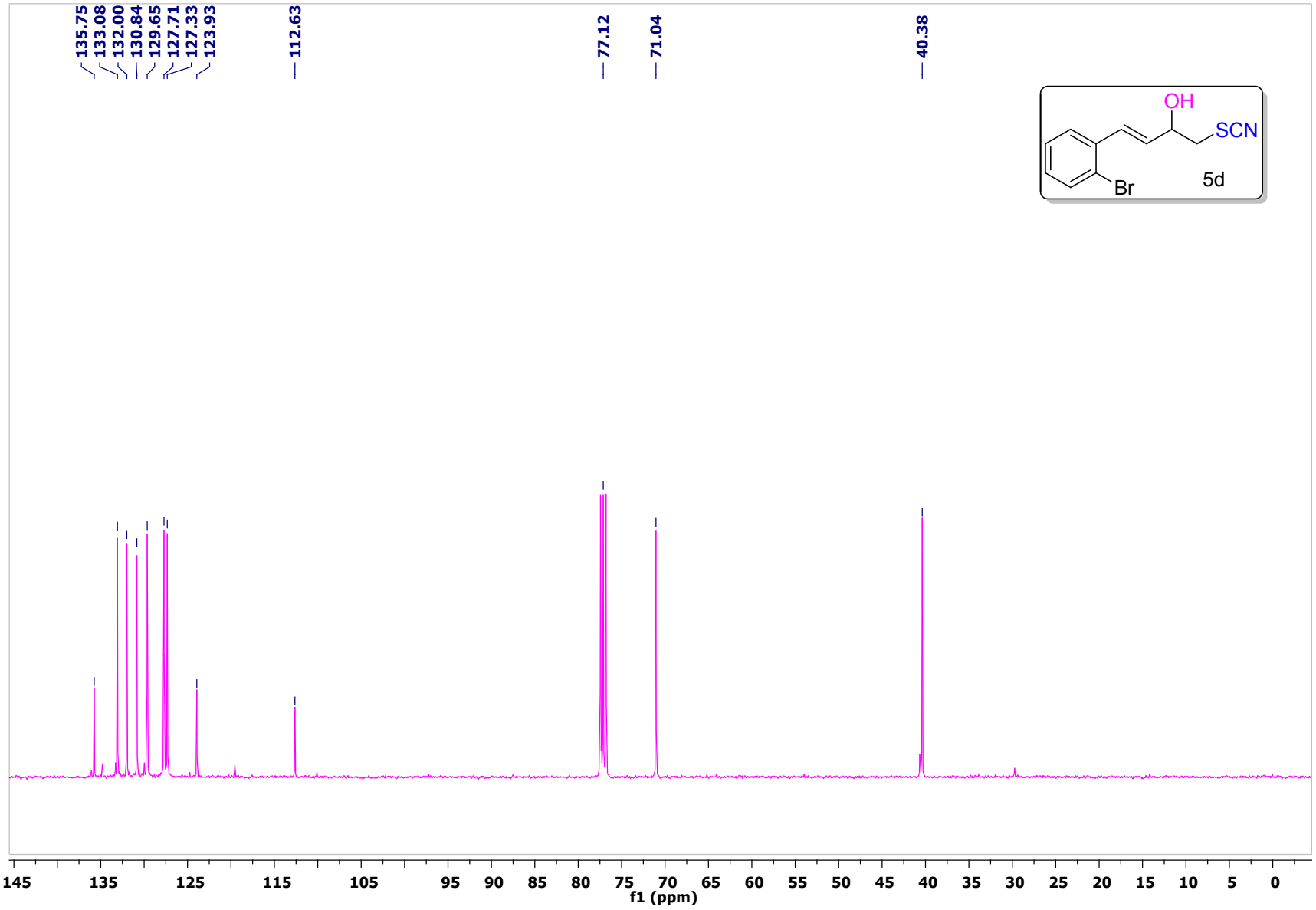
0.0
f1 (ppm)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123.93
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77.12
71.04
40.38
OH
SCN
Br
5d
145
135
125
115
105
95
90
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45
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25
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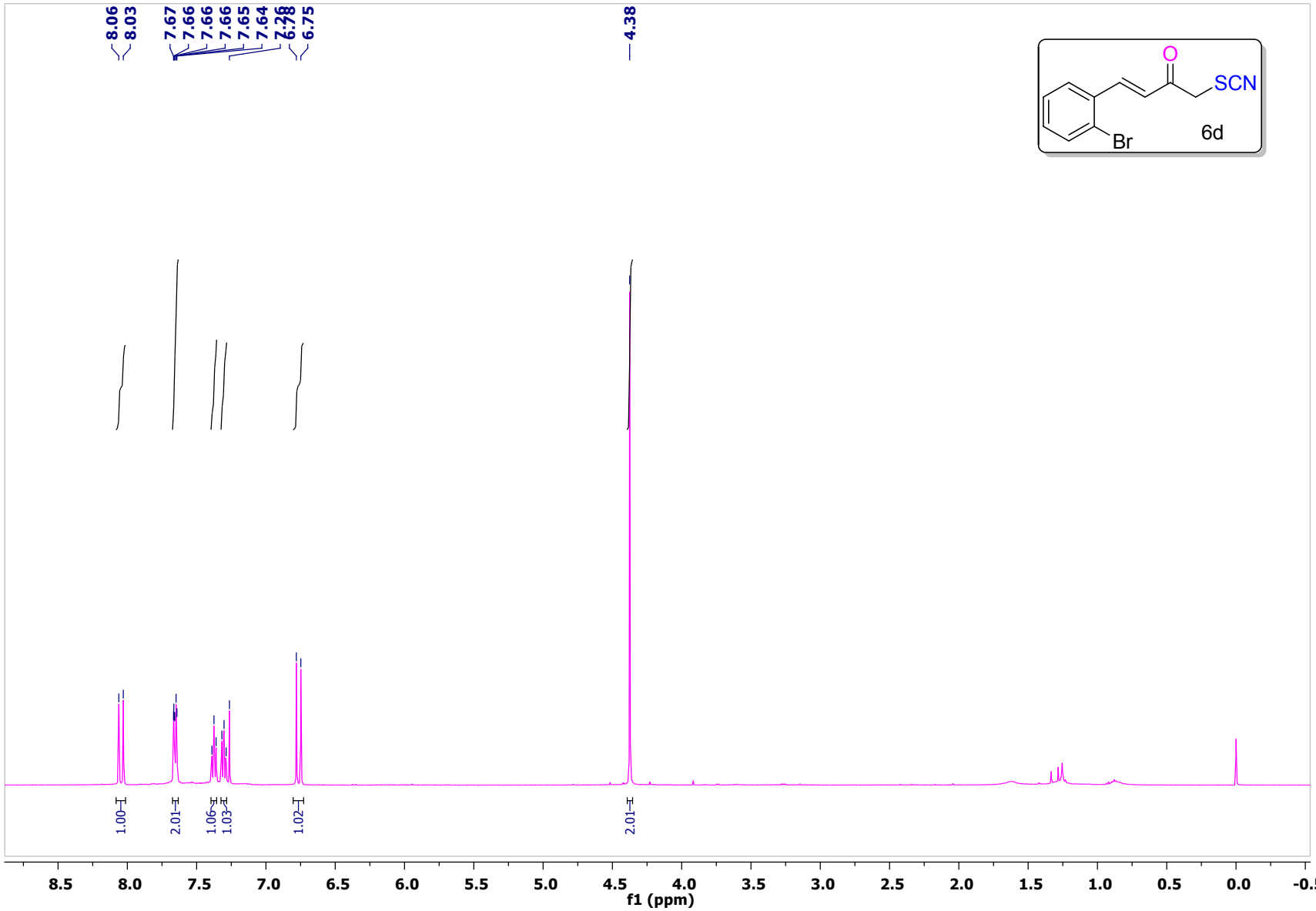
f1 (ppm)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7.66
7.66
7.65
7.64
7.28
6.78
6.75
4.38
O
SCN
Br
6d
1.00
2.01
1.06
1.03
1.02
2.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.5
2.0
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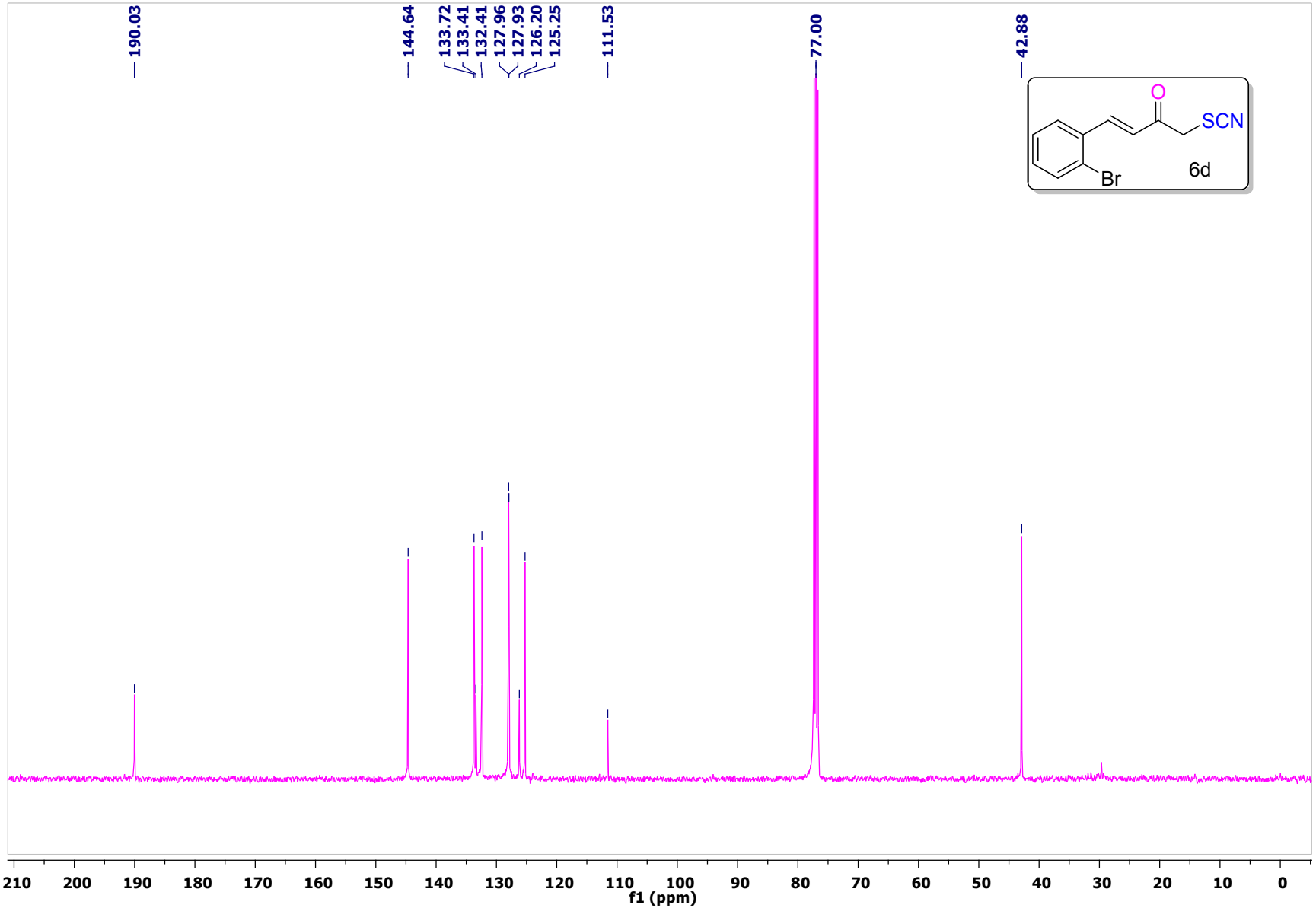
f1 (ppm)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126.20
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111.53
77.00
42.88
O
SCN
Br
6d
210
200
190
180
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110
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90
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50
40
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10
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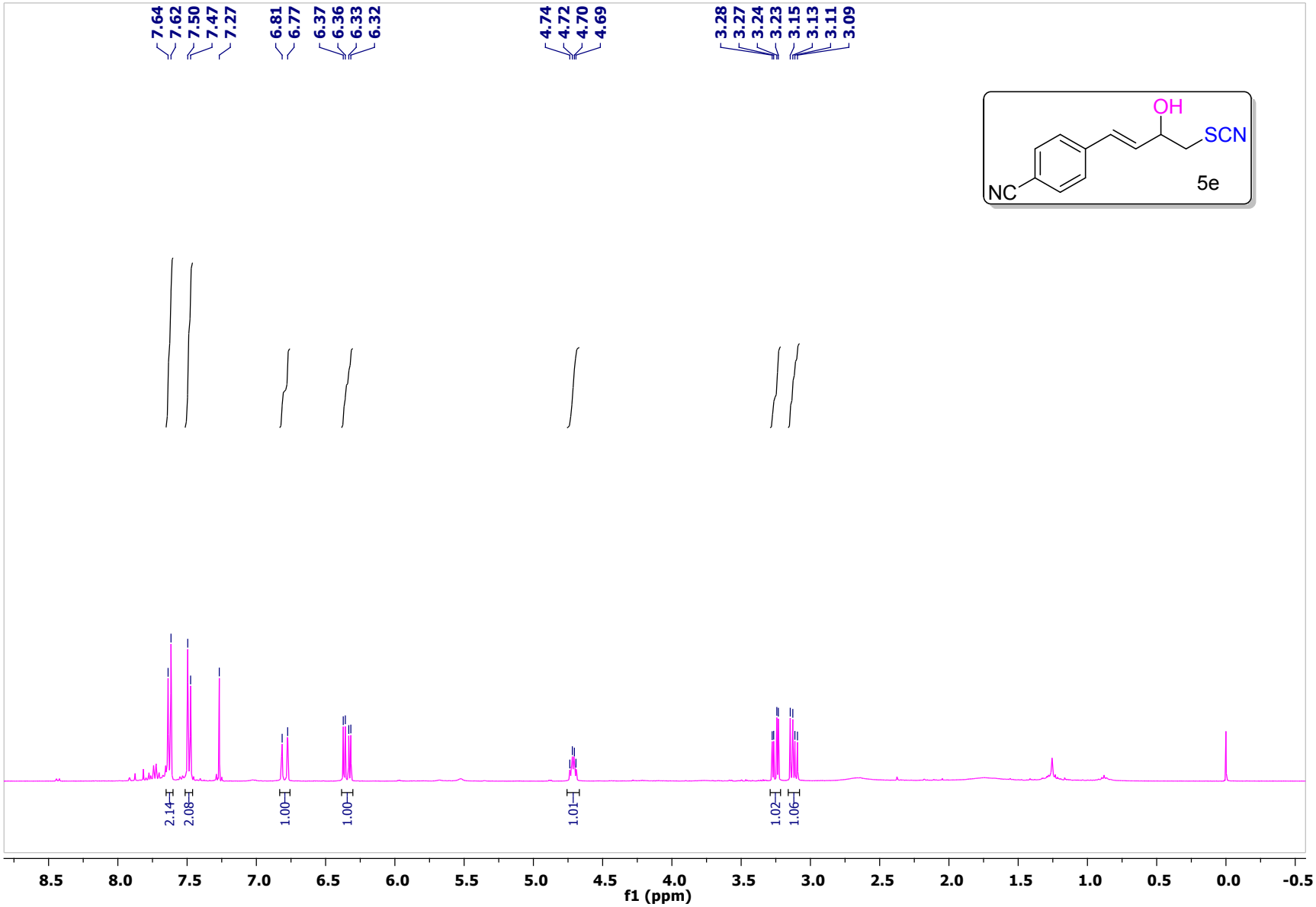
f1 (ppm)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6.37
6.36
6.33
6.32
4.74
4.72
4.70
4.69
3.28
3.27
3.24
3.23
3.15
3.13
3.11
3.09
OH
SCN
NC
5e
2.14
2.08
1.00
1.00
1.01
1.02
1.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
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1.0
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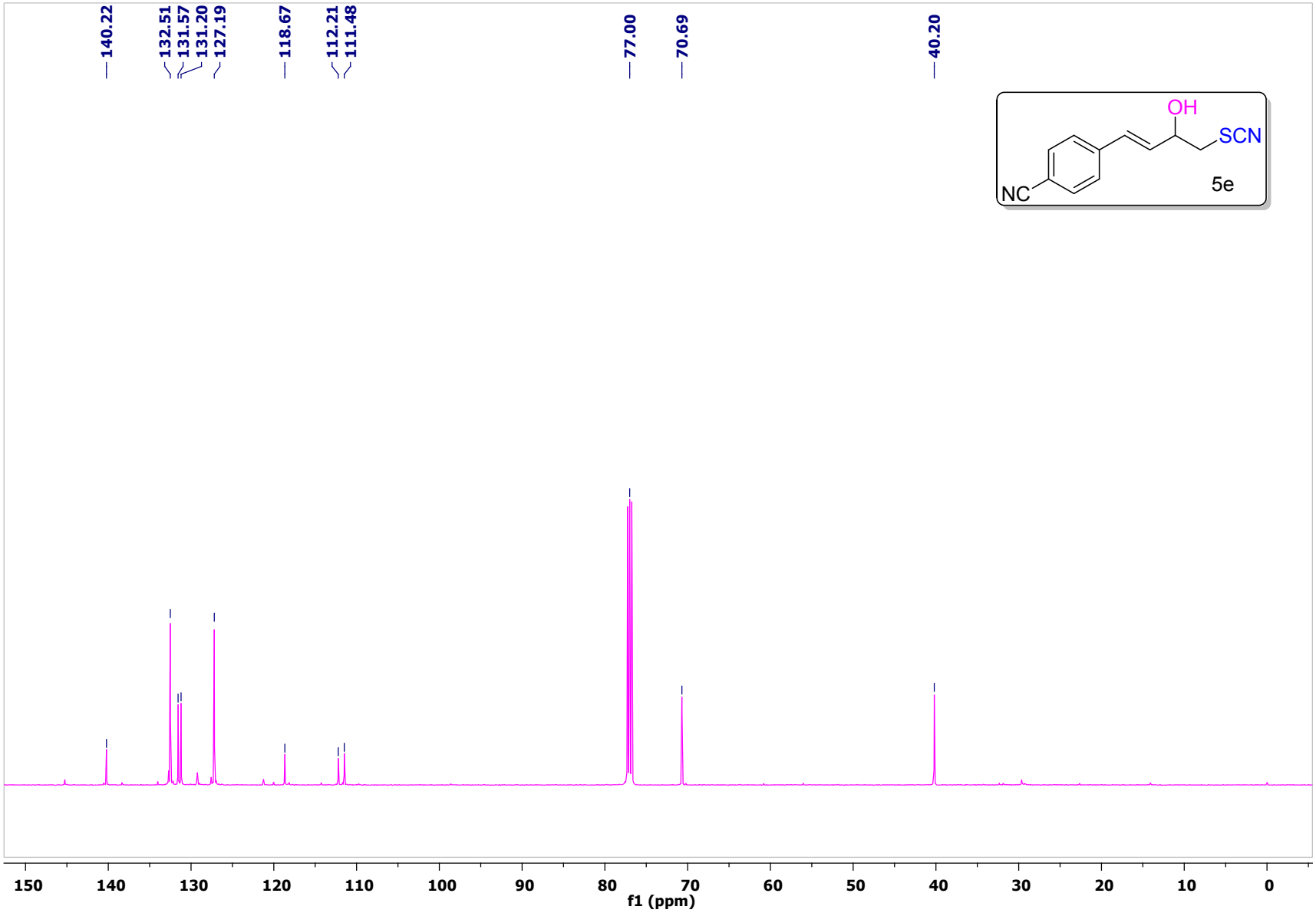
-0.5
f1 (ppm)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132.51
131.57
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118.67
112.21
111.48
77.00
70.69
40.20
OH
SCN
NC
5e
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130
120
110
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90
80
70
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50
40
30
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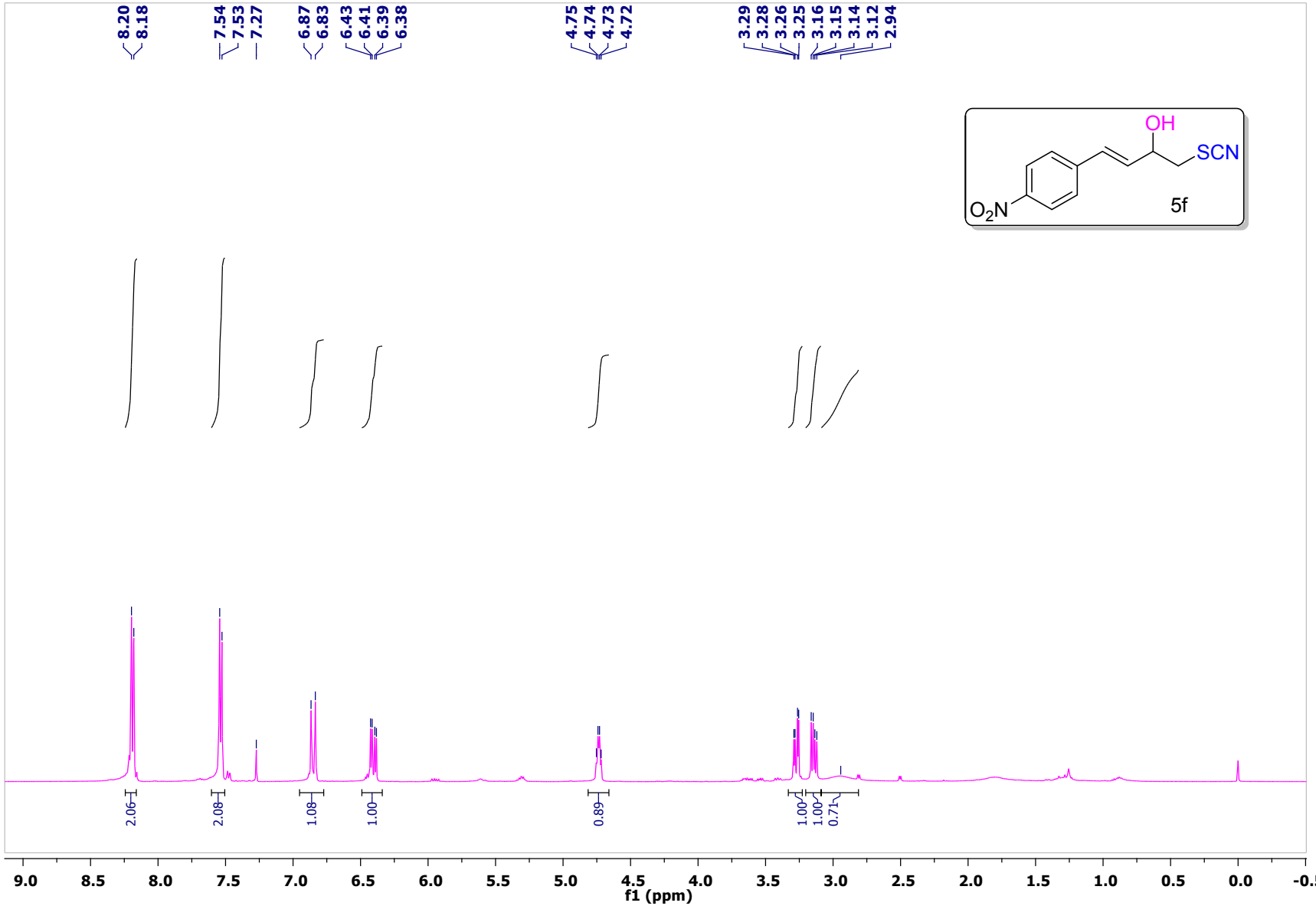
10
0
f1 (ppm)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6.43
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6.39
6.38
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4.72
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3.28
3.26
3.25
3.16
3.15
3.14
3.12
2.94
OH
SCN
O2N
5f
2.06
2.08
1.08
1.00
0.89
1.00
1.00
0.71
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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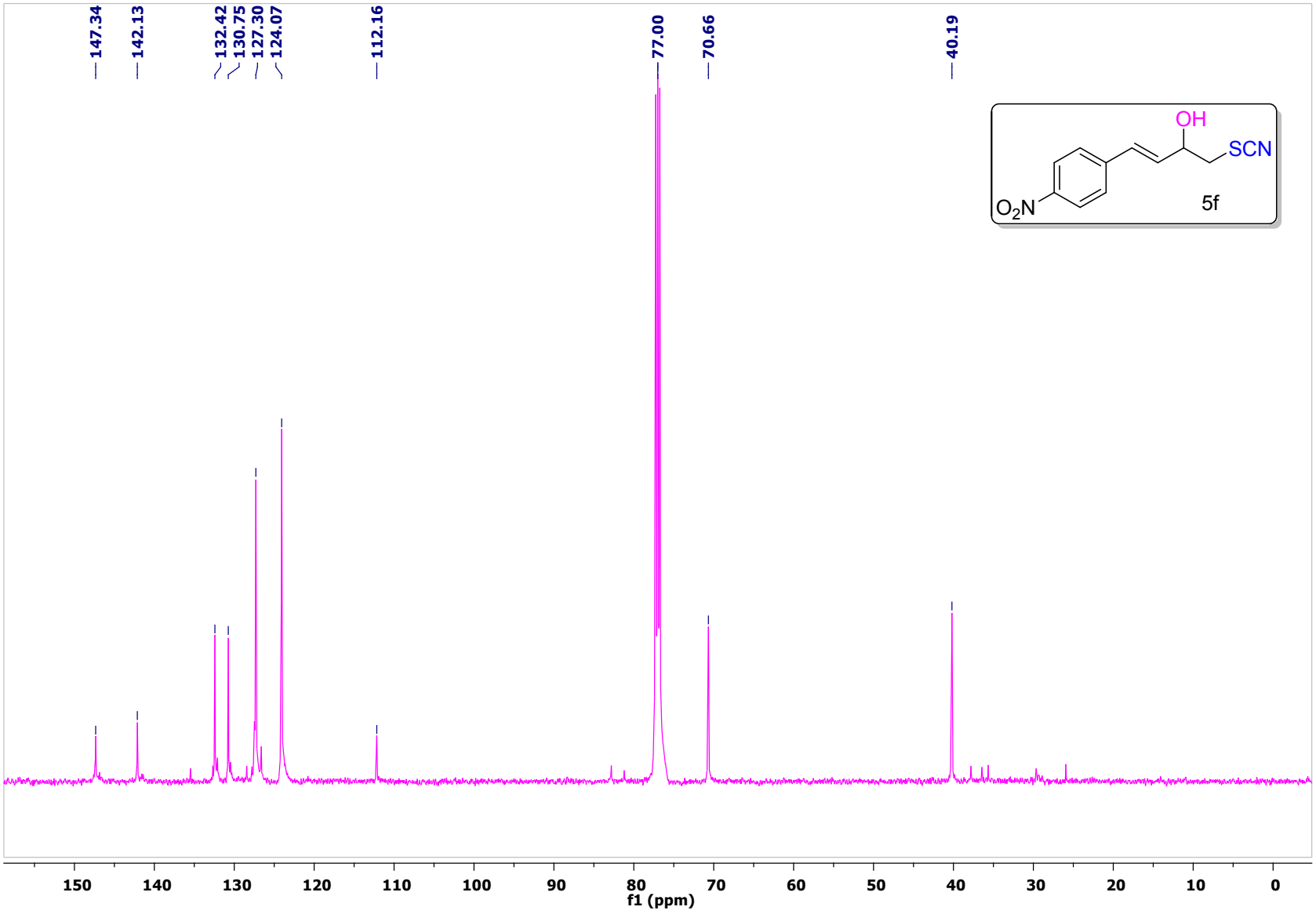
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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142.13
132.42
130.75
127.30
124.07
112.16
77.00
70.66
40.19
OH
SCN
O2N
5f
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130
120
110
100
90
80
70
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50
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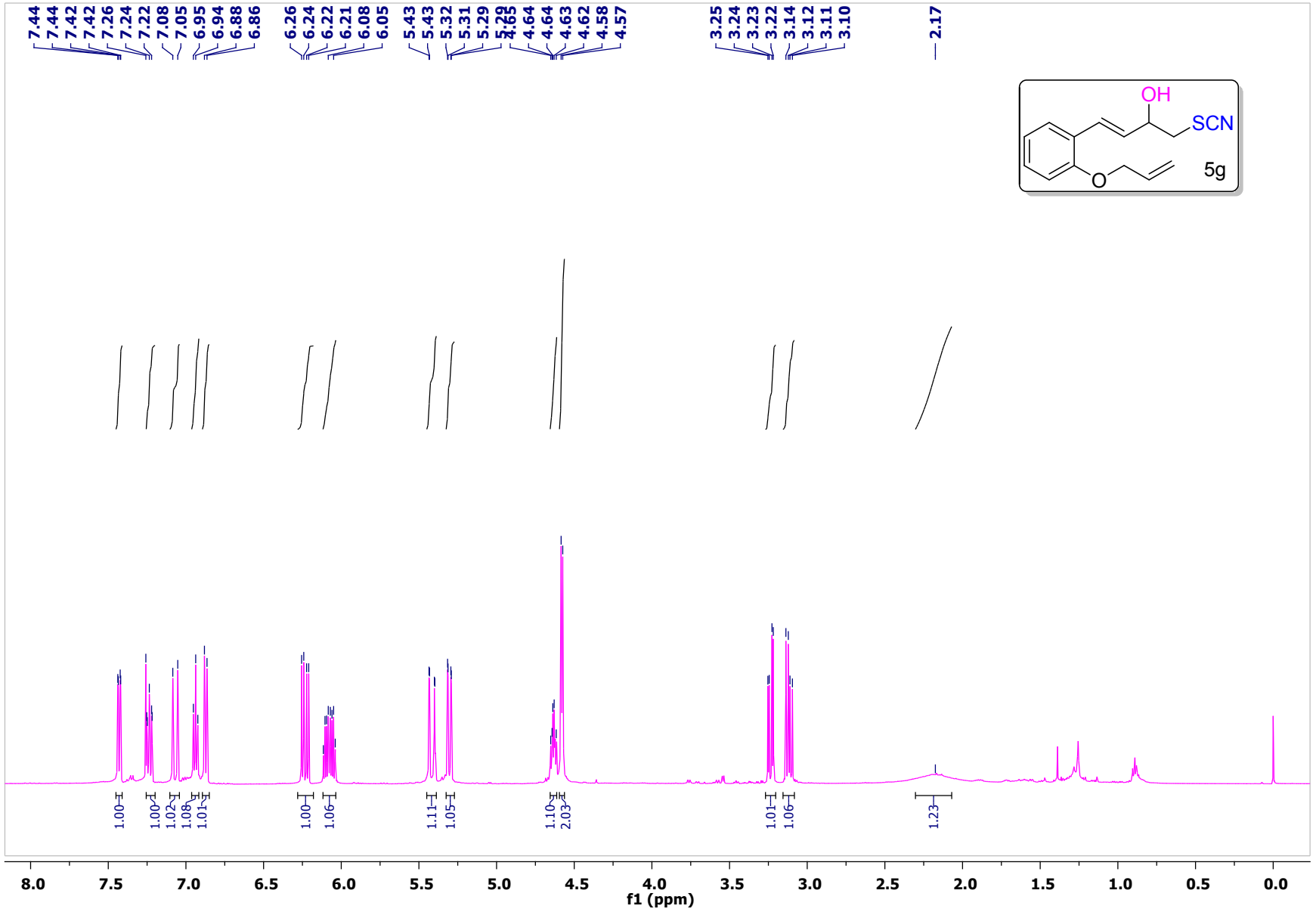
30
20
10
0
f1 (ppm)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7.24
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7.08
7.05
6.95
6.94
6.88
6.86
6.26
6.24
6.22
6.21
6.08
6.05
5.43
5.43
5.32
5.31
5.29
4.65
4.64
4.64
4.63
4.62
4.58
4.57
3.25
3.24
3.23
3.22
3.14
3.12
3.11
3.10
2.17
OH
SCN
O
5g
1.00
1.00
1.02
1.08
1.01
1.00
1.06
1.11
1.05
1.10
2.03
1.01
1.06
1.23
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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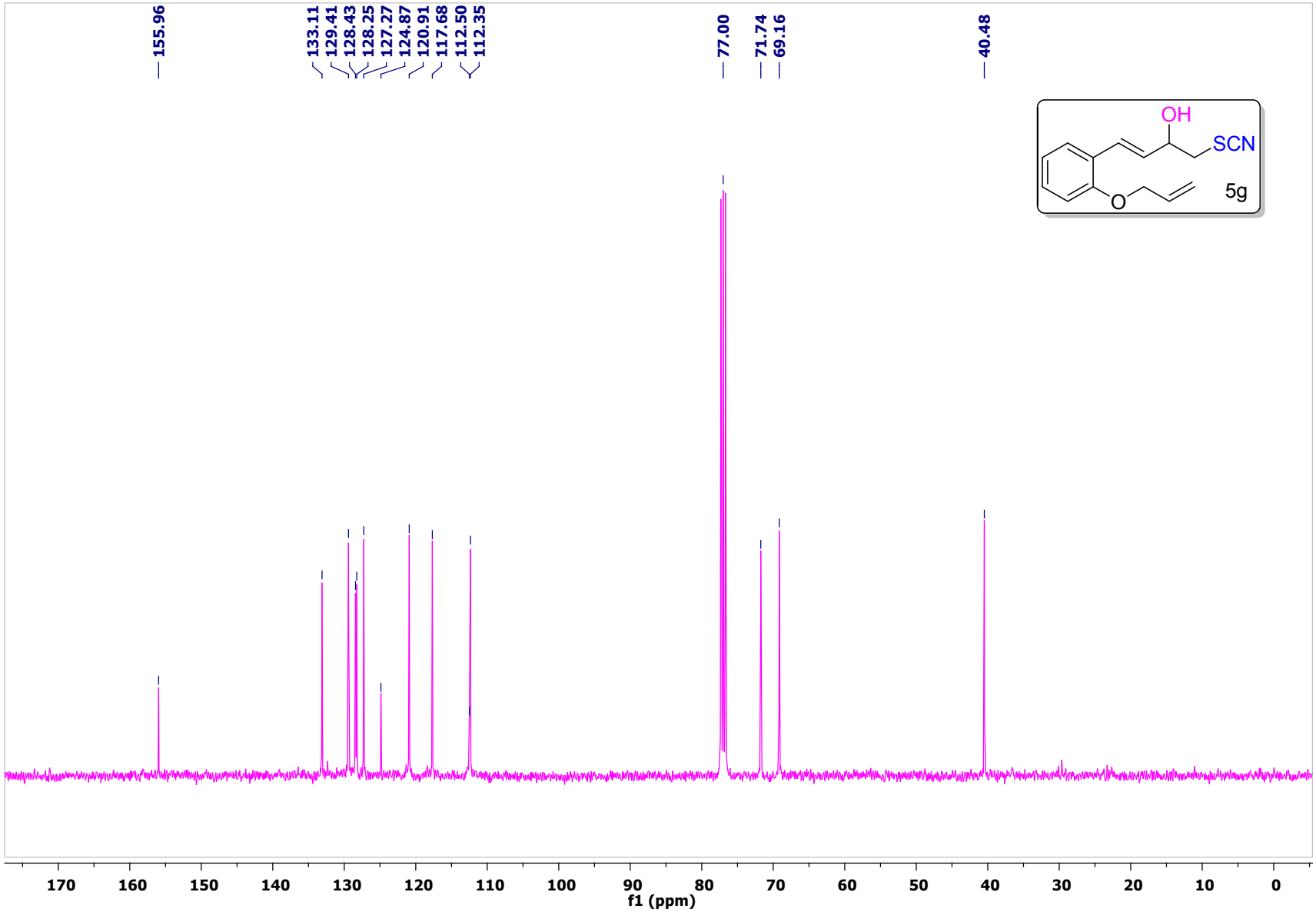
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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124.87
120.91
117.68
112.50
112.35
77.00
71.74
69.16
40.48
OH
SCN
O
5g
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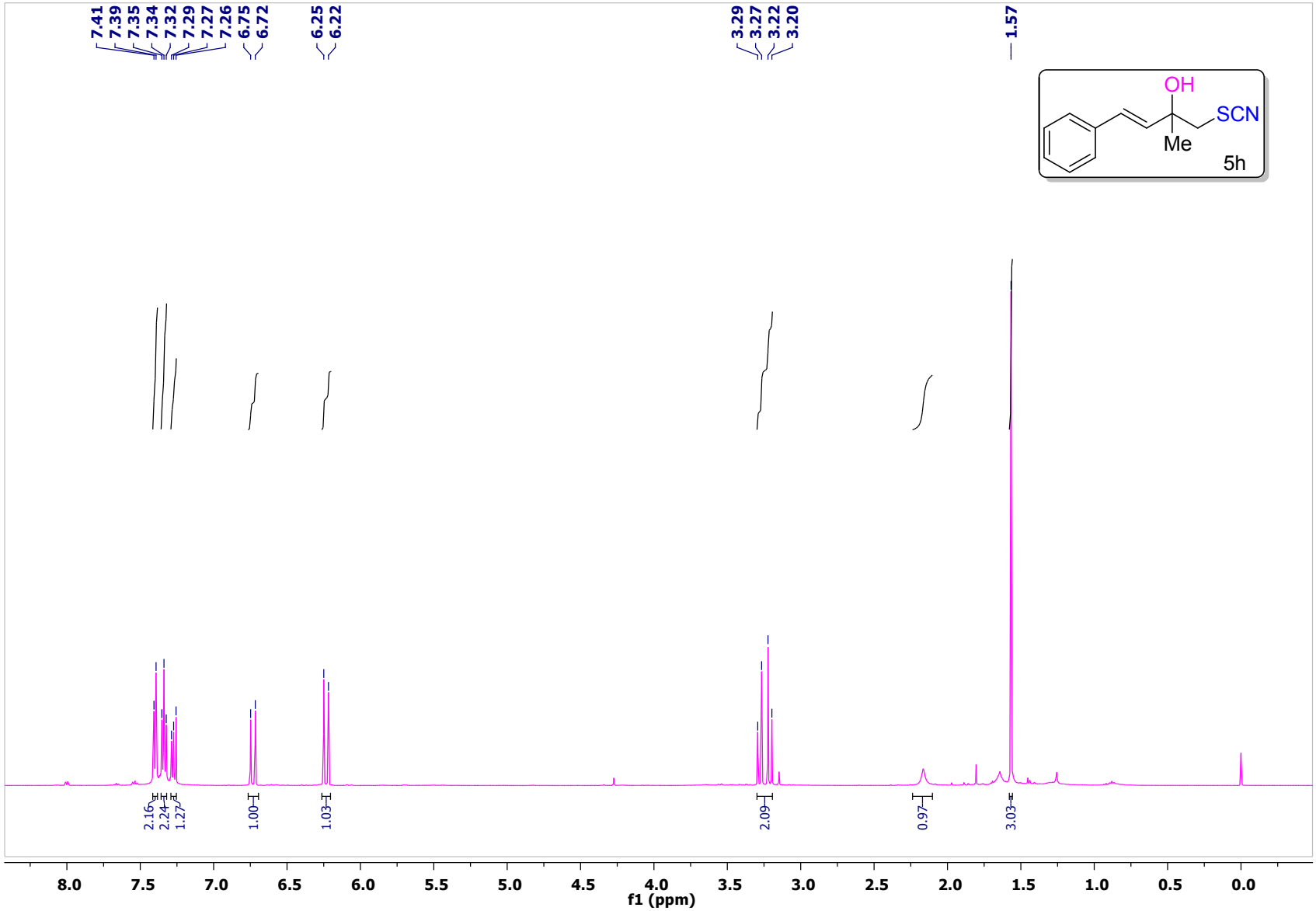
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.26
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6.72
6.25
6.22
3.29
3.27
3.22
3.20
1.57
OH
SCN
Me
5h
2.16
2.24
1.27
1.00
1.03
2.09
0.97
3.03
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
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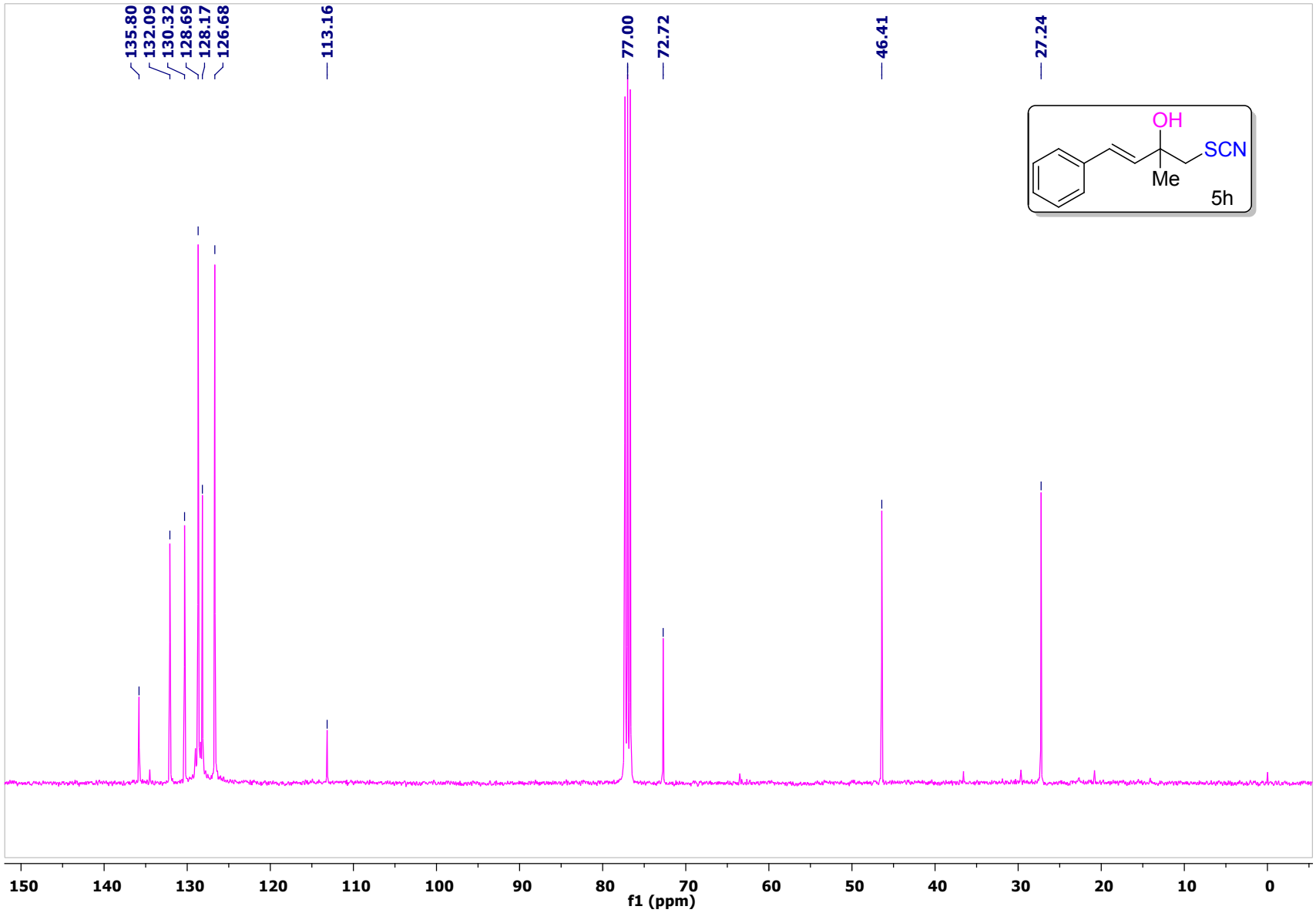
0.0
f1 (ppm)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132.09
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128.17
126.68
113.16
77.00
72.72
46.41
27.24
OH
SCN
Me
5h
150
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130
120
110
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90
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70
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50
40
30
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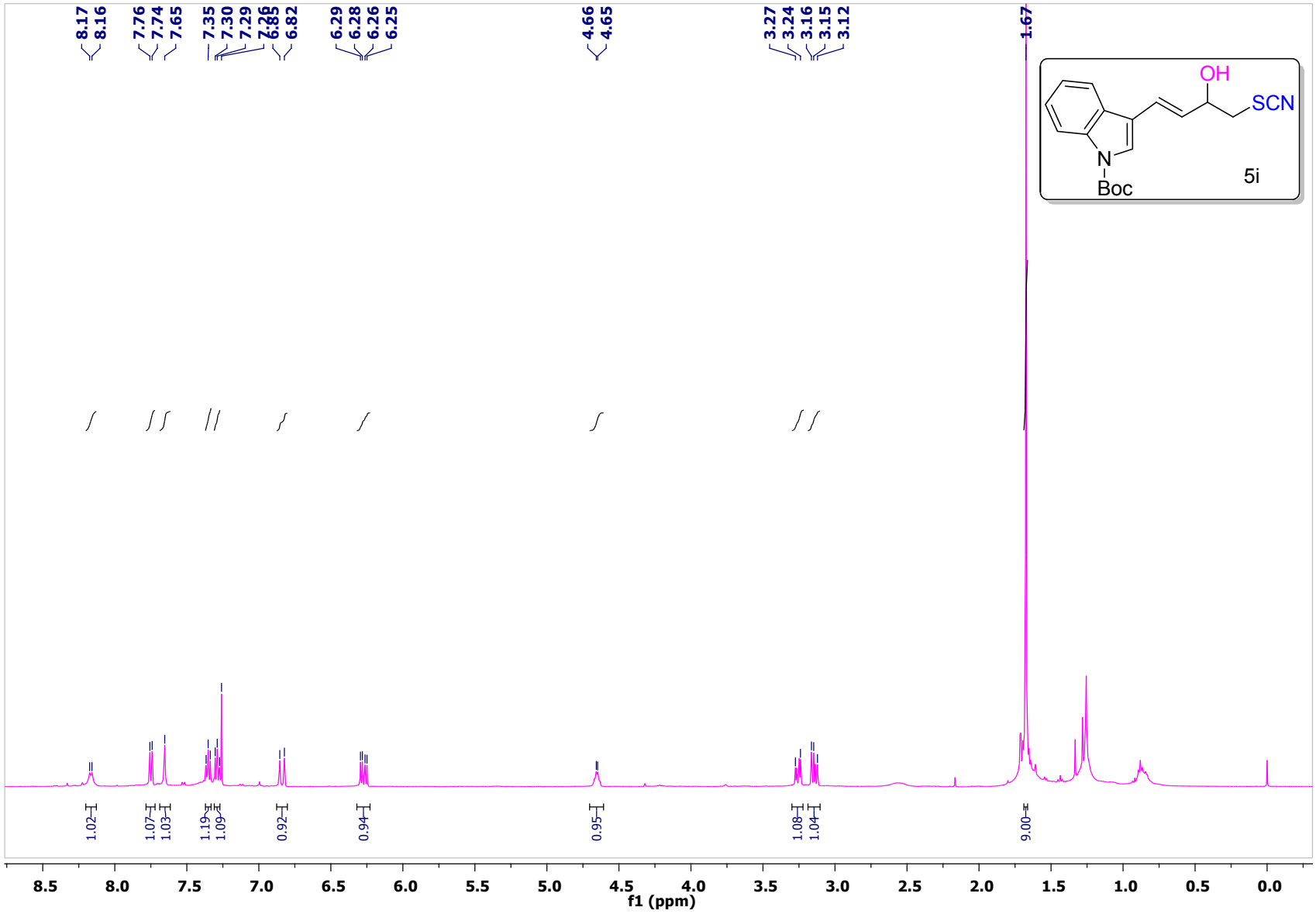
10
0
f1 (ppm)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6.29
6.28
6.26
6.25
4.66
4.65
3.27
3.24
3.16
3.15
3.12
1.67
OH
SCN
N
Boc
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1.02
1.07
1.03
1.19
1.09
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0.94
0.95
1.08
1.04
9.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
1.5
1.0
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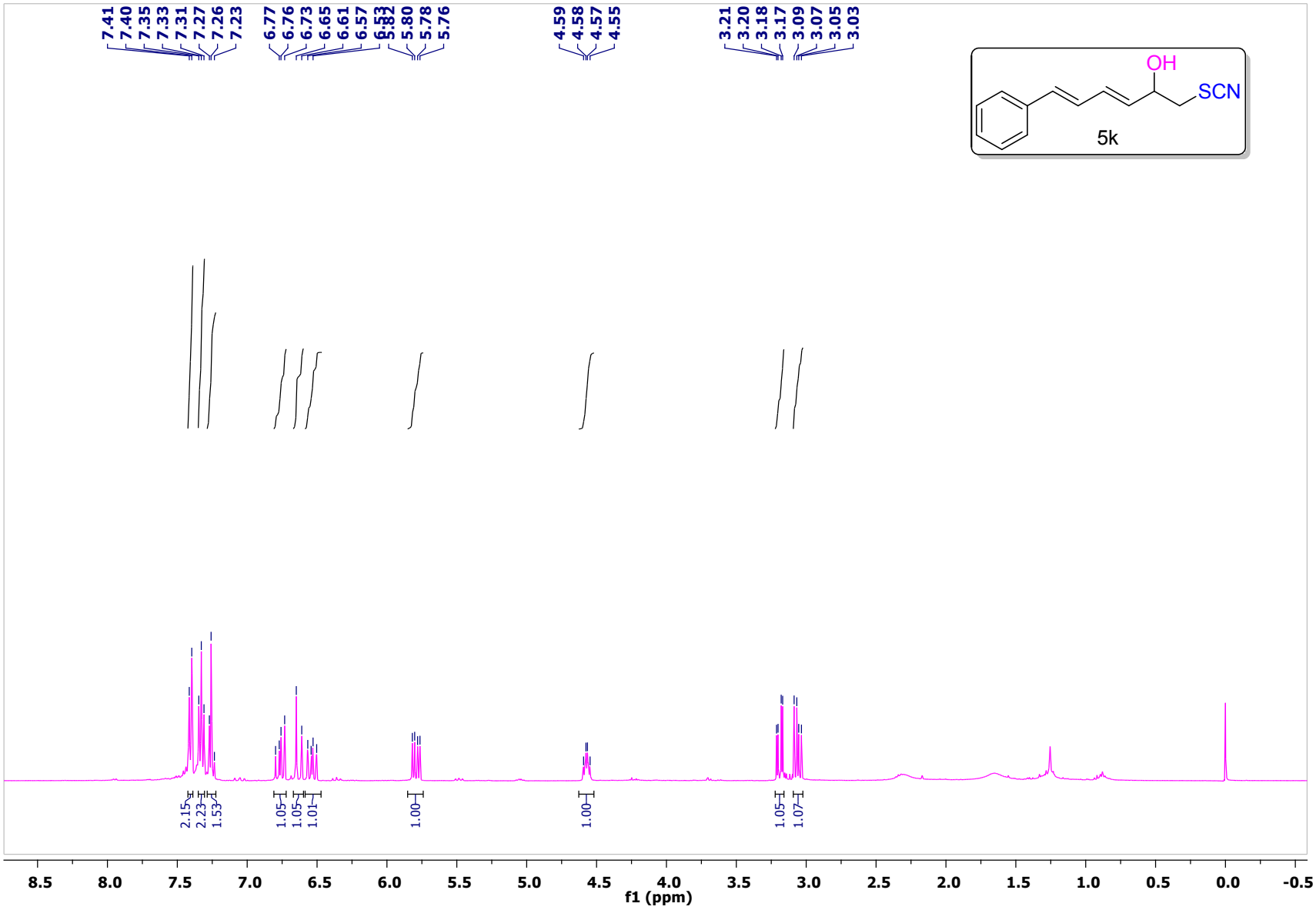
0.0
f1 (ppm)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7.27
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7.23
6.77
6.76
6.73
6.65
6.61
6.57
6.53
5.82
5.80
5.78
5.76
4.59
4.58
4.57
4.55
3.21
3.20
3.18
3.17
3.09
3.07
3.05
3.03
OH
SCN
5k
2.15
2.23
1.53
1.05
1.05
1.01
1.00
1.00
1.05
1.07
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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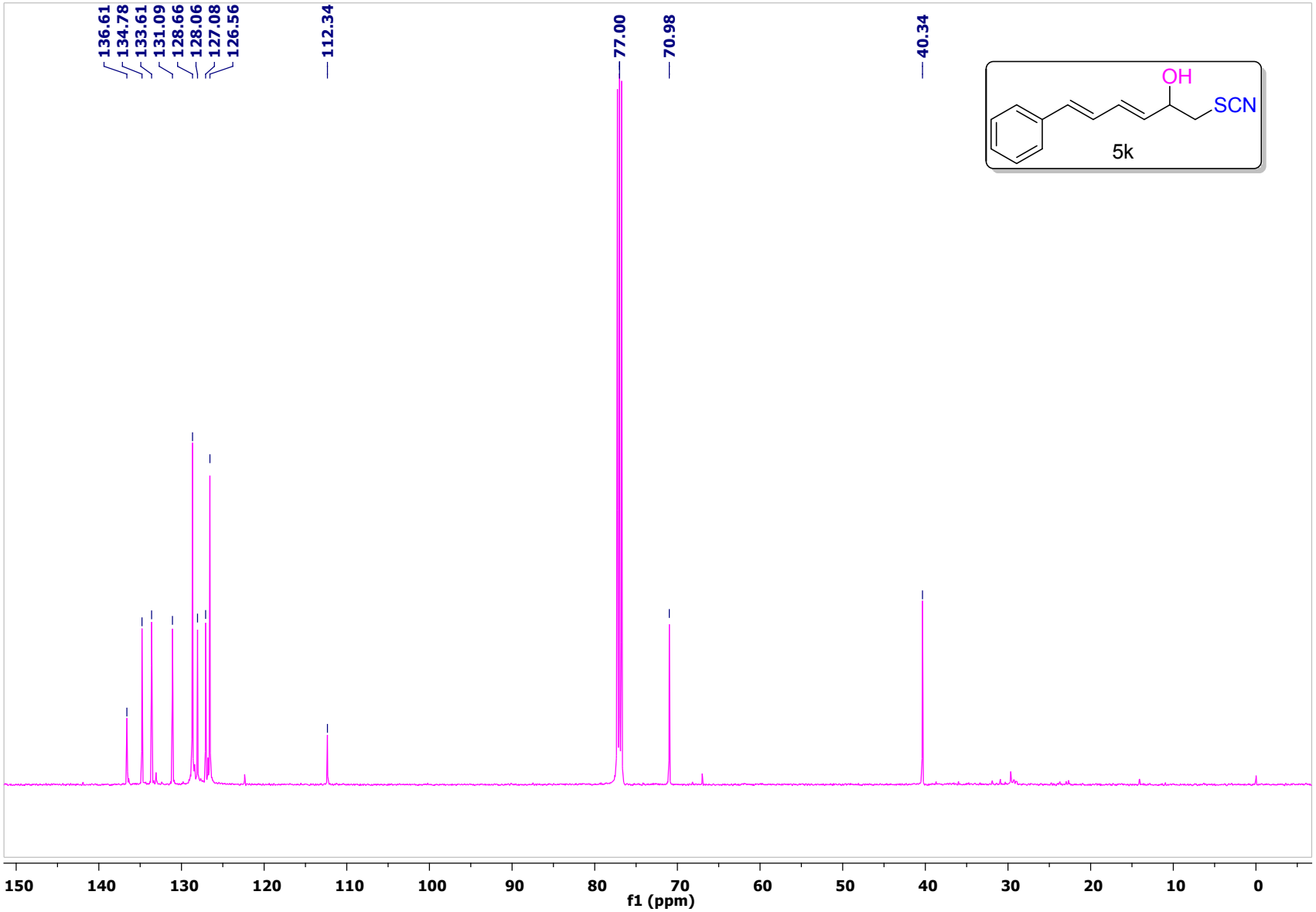
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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133.61
131.09
128.66
128.06
127.08
126.56
112.34
77.00
70.98
40.34
OH
SCN
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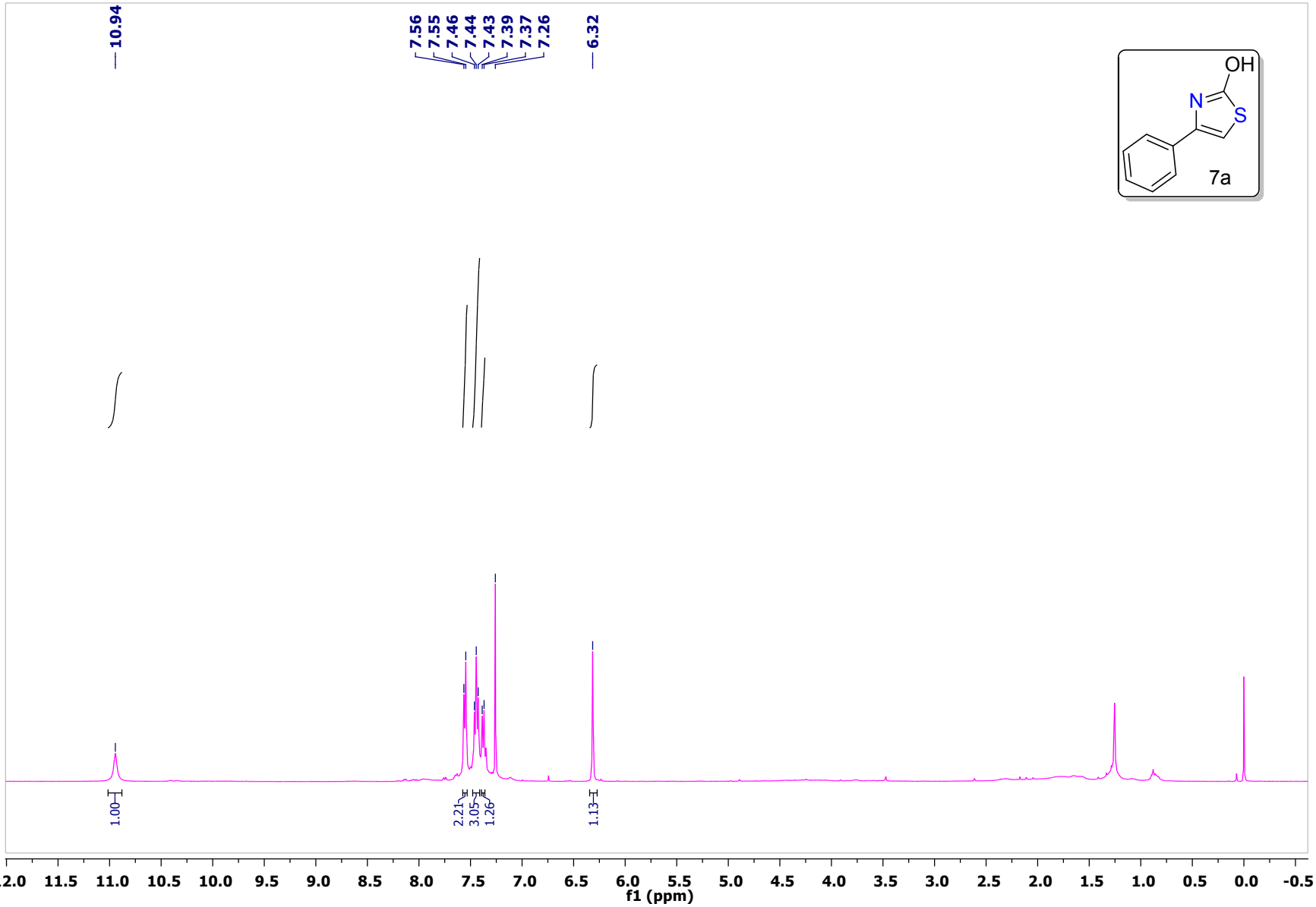
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.46
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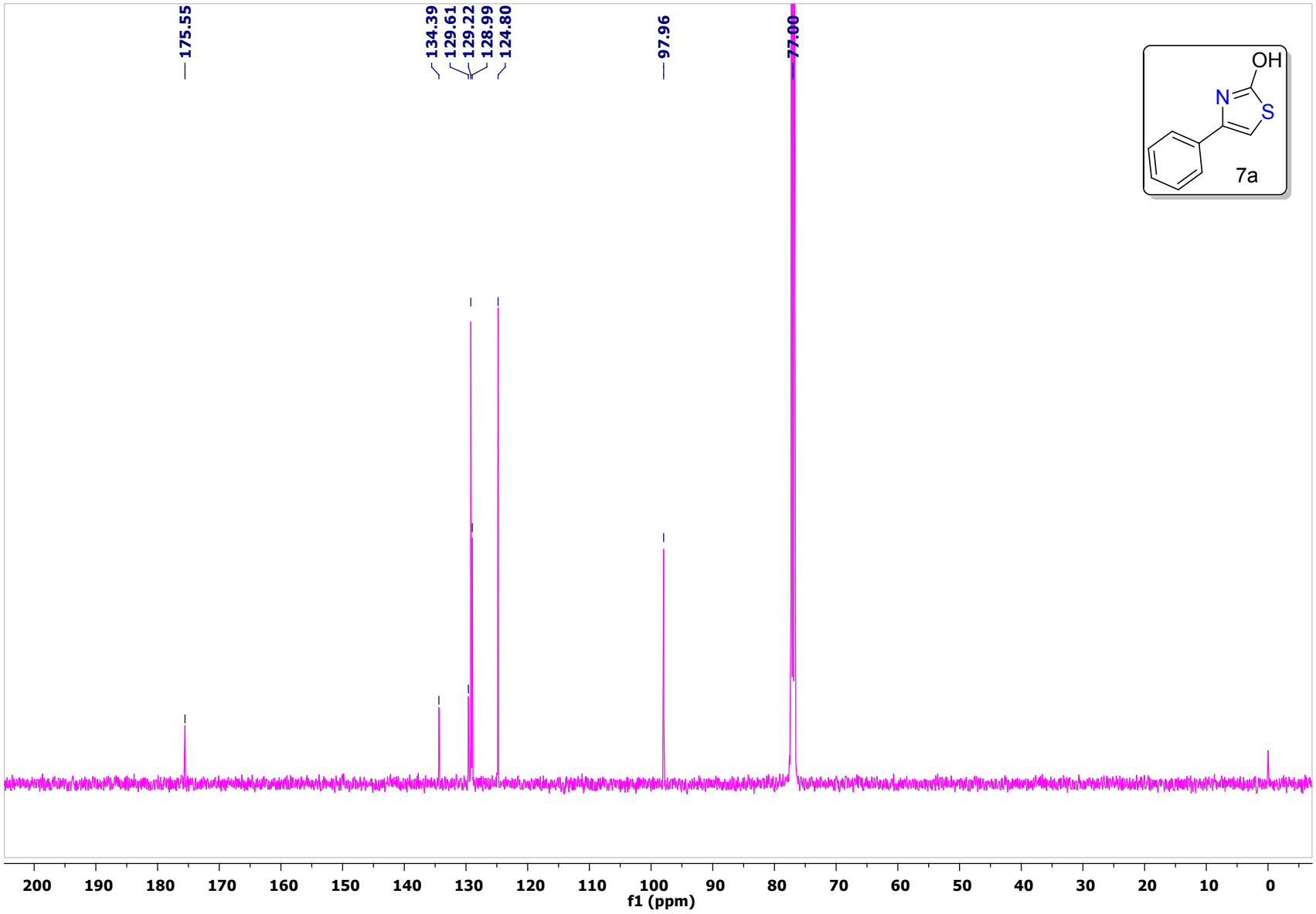
7.43
7.39
7.37
7.26
6.32
OH
N
S
7a
1.00
2.21
3.05
1.26
1.13
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


175.55
134.39
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129.22
128.99
124.80
97.96
77.00
OH
N
S
7a
200
190
180
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150
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130
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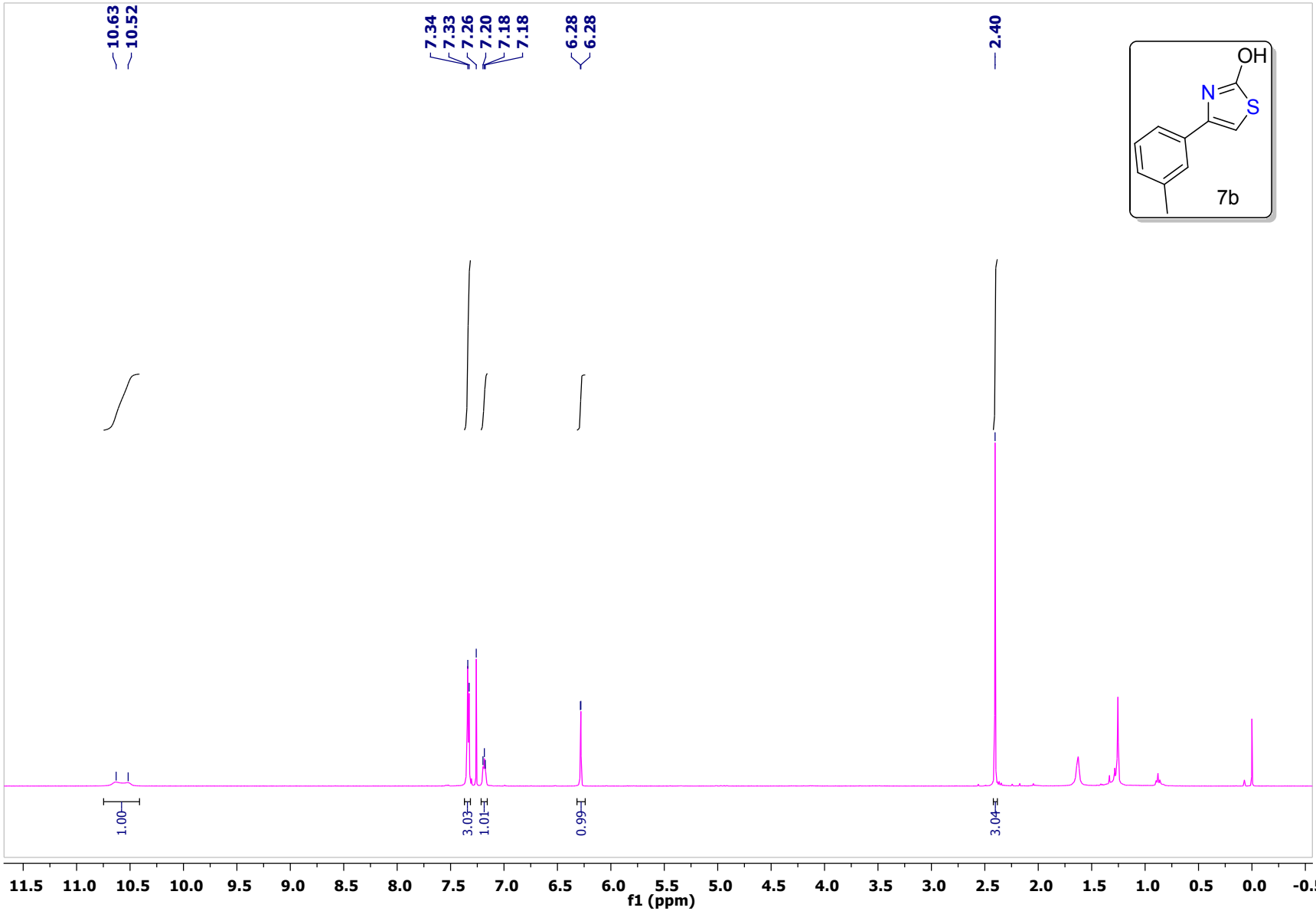
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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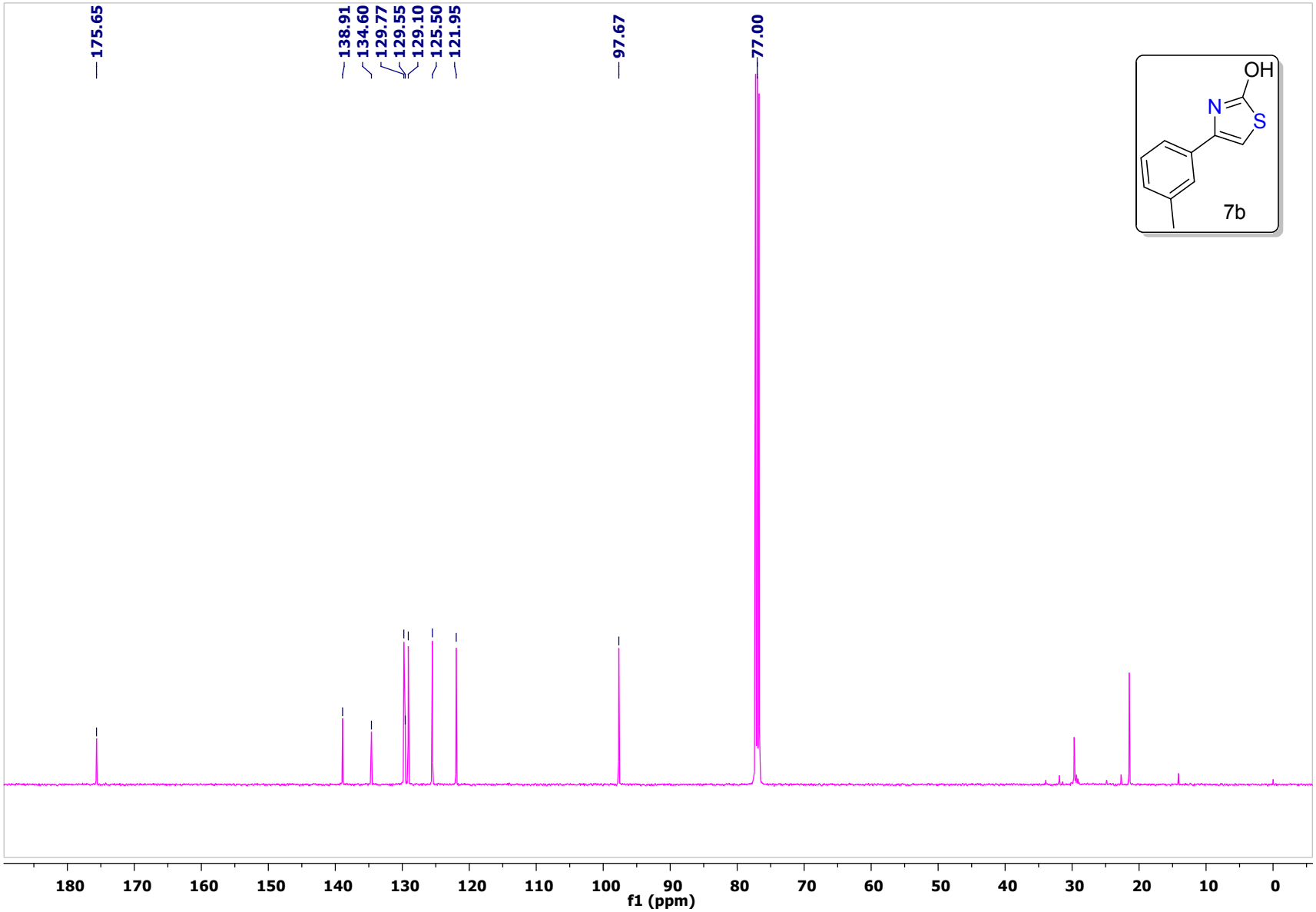
7.18
6.28
6.28
2.40
OH
N
S
7b
1.00
3.03
1.01
0.99
3.04
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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138.91
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129.55
129.10
125.50
121.95
97.67
77.00
OH
N
S
7b
180
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150
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130
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110
100
90
80
70
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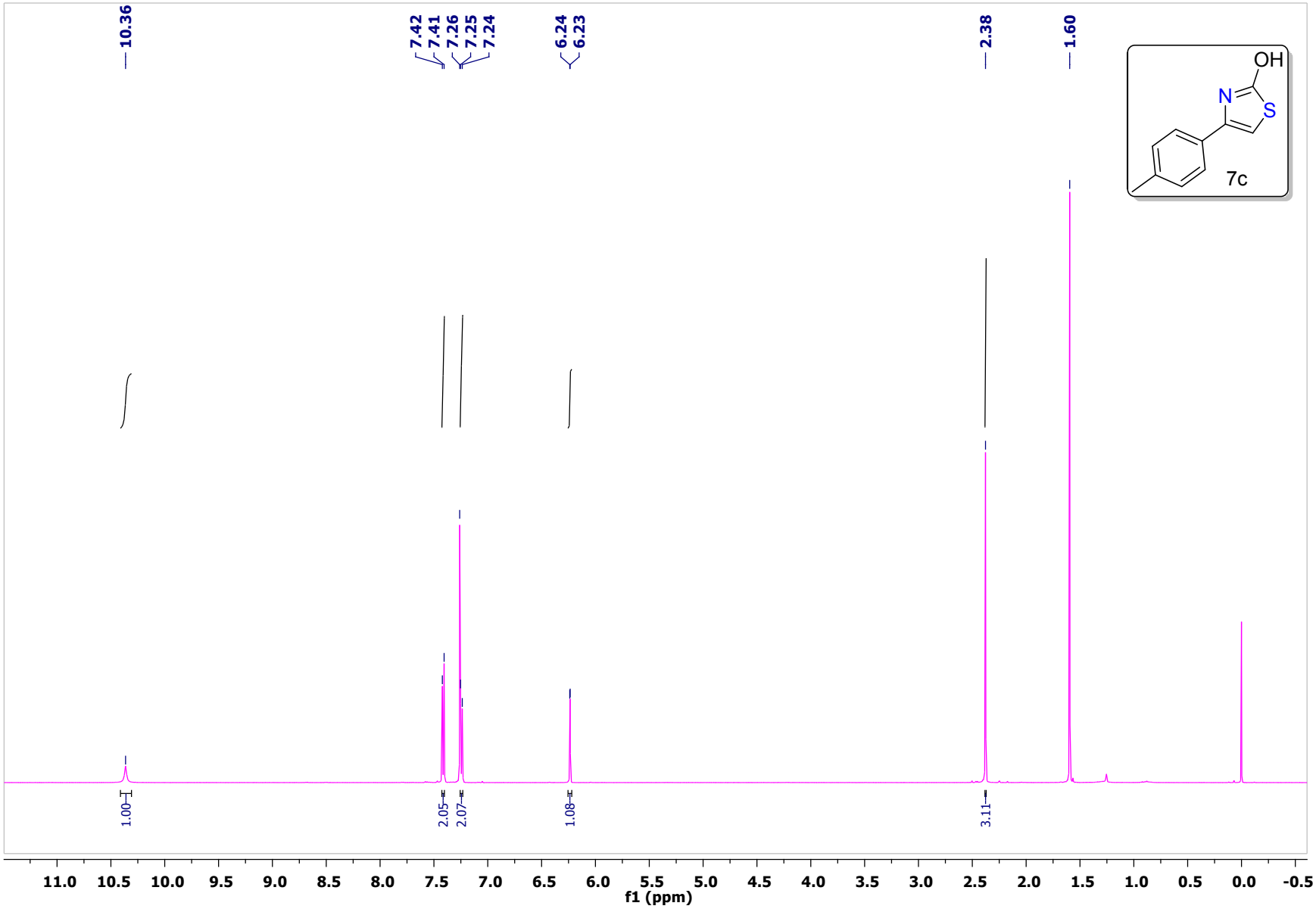
50
40
30
20
10
0
f1 (ppm)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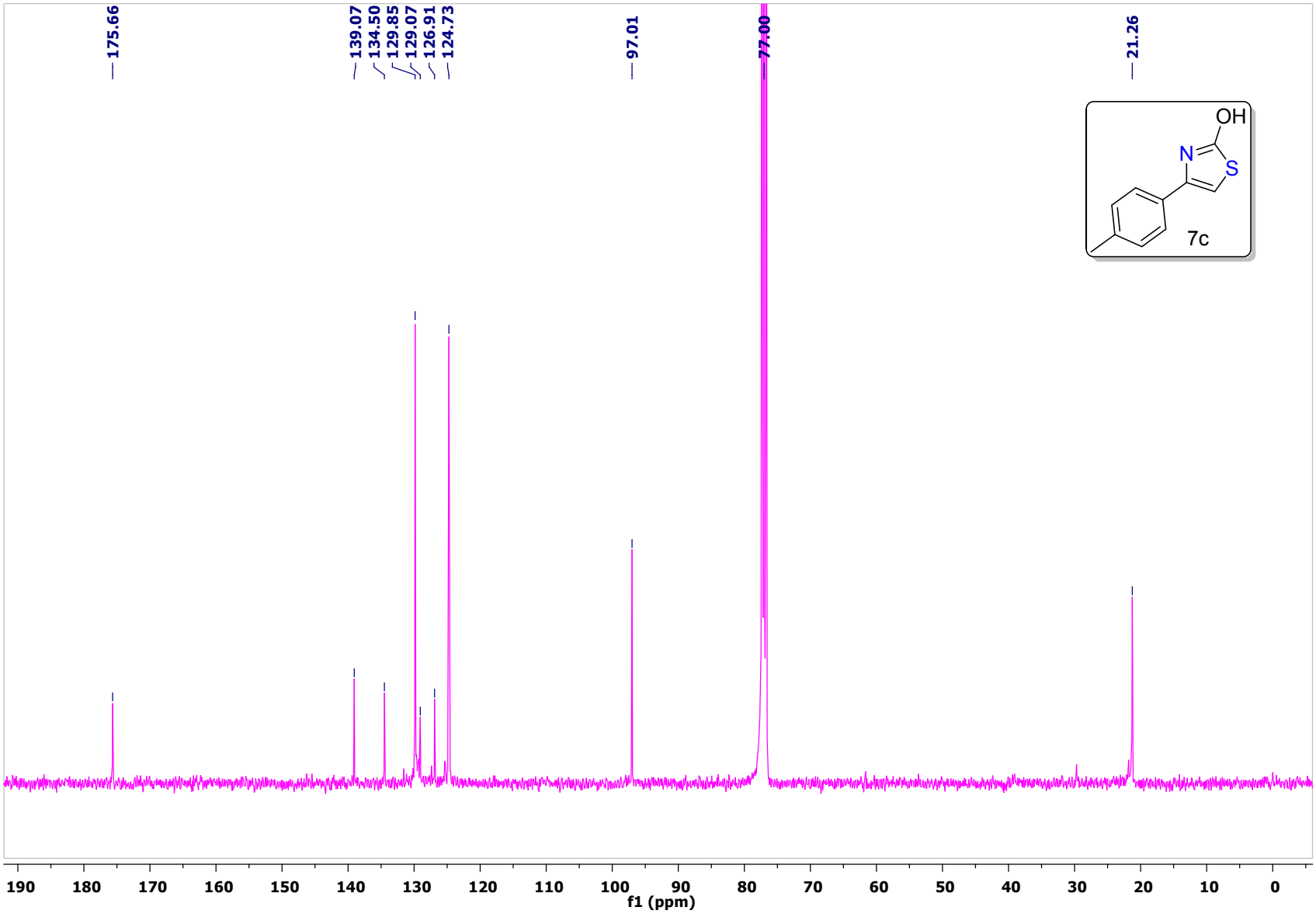
7.26
7.25
7.24
6.24
6.23
2.38
1.60
OH
N
S
7c
1.00
2.05
2.07
1.08
3.11
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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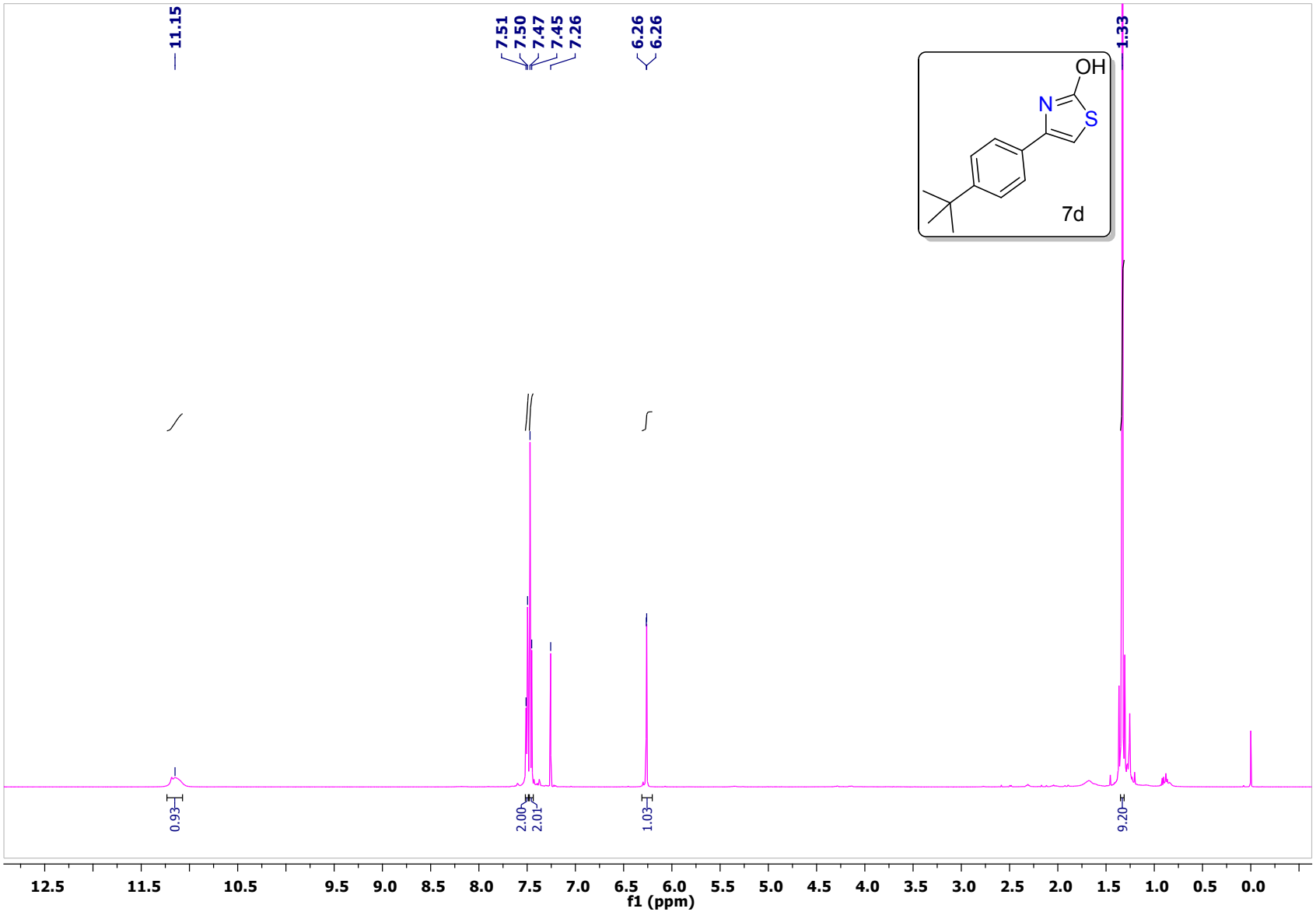
129.85
129.07
126.91
124.73
97.01
77.00
21.26
OH
N
S
7c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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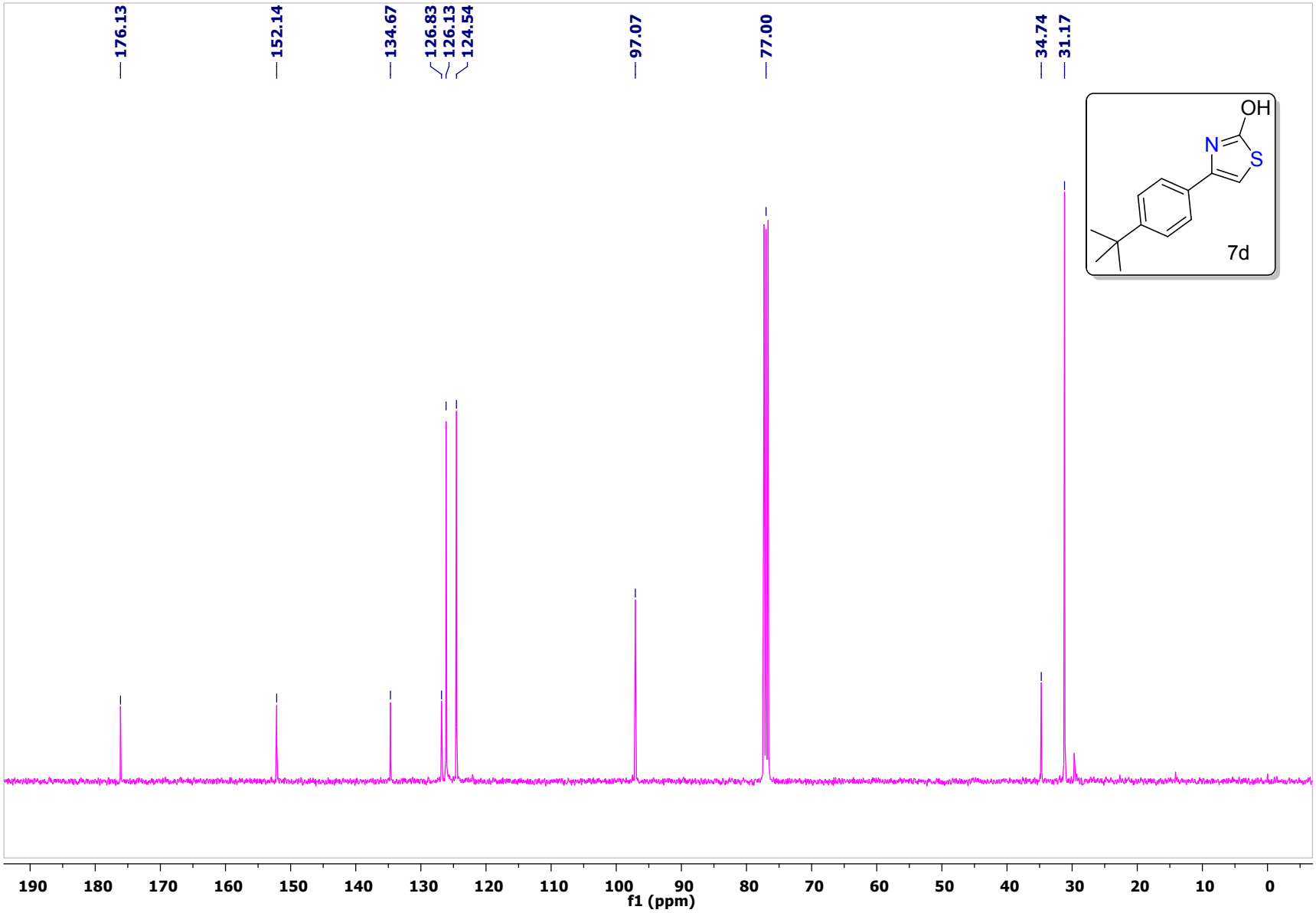
7.45
7.26
6.26
6.26
1.33
OH
N
S
7d
0.93
2.00
2.01
1.03
9.20
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


176.13
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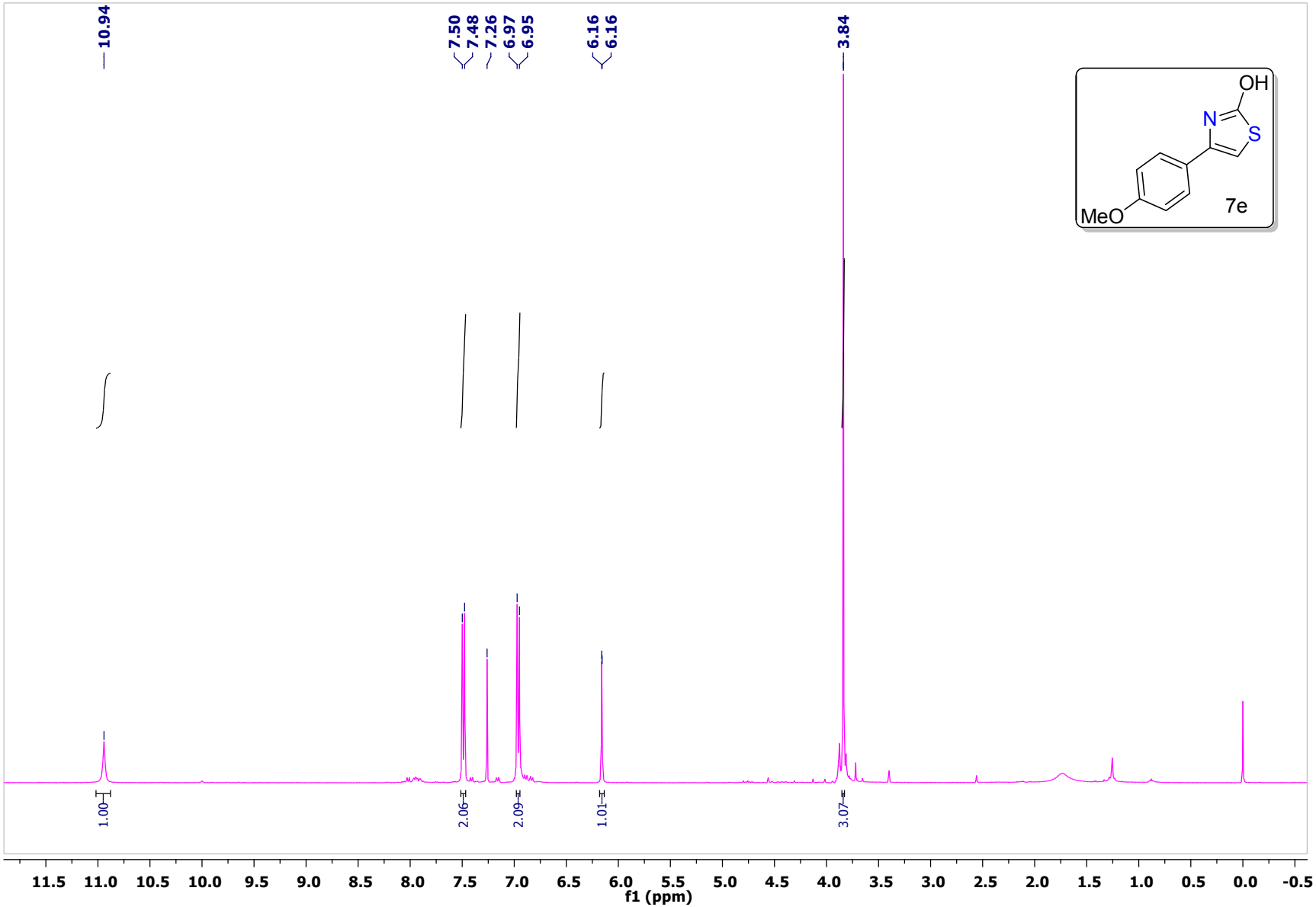
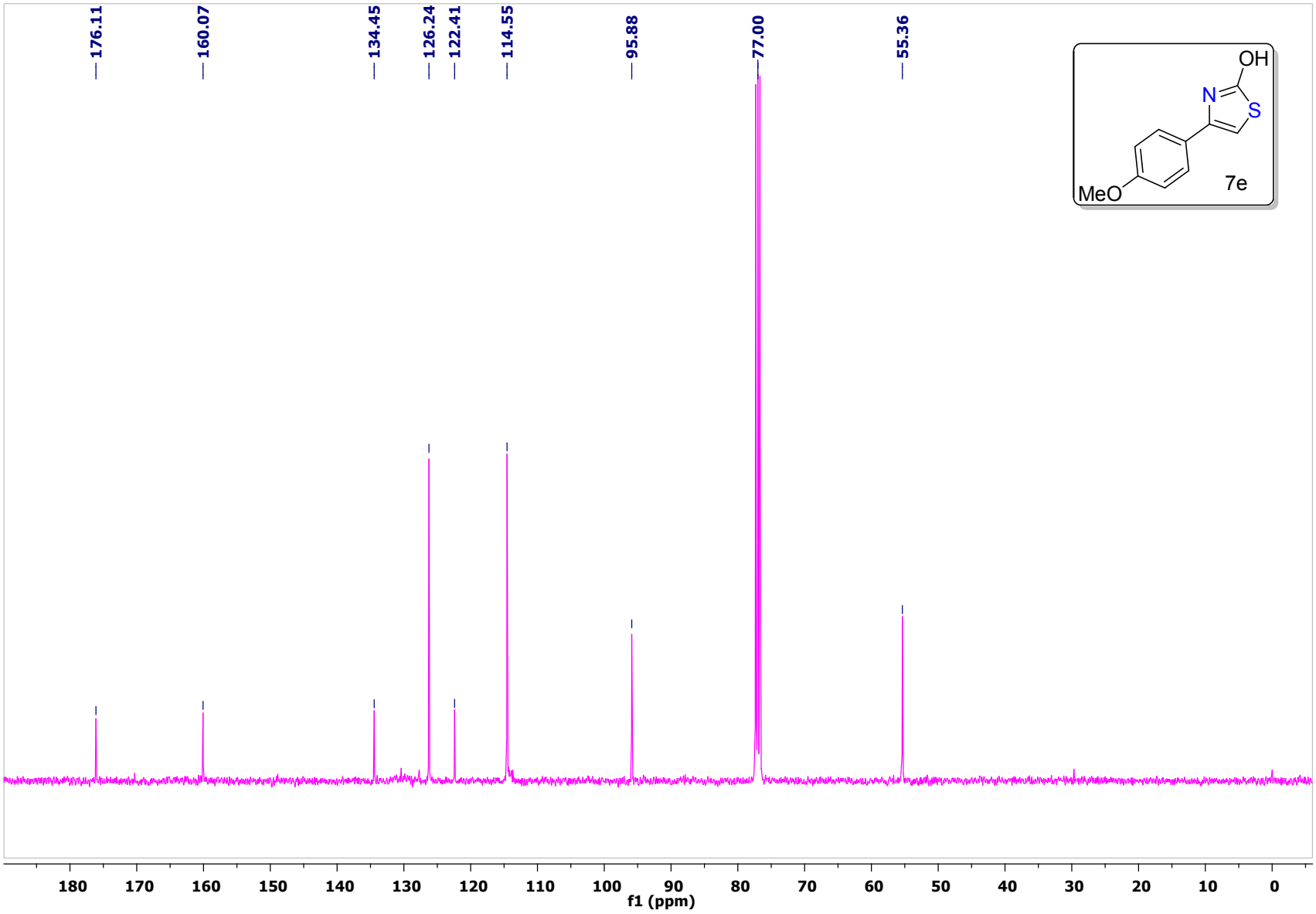
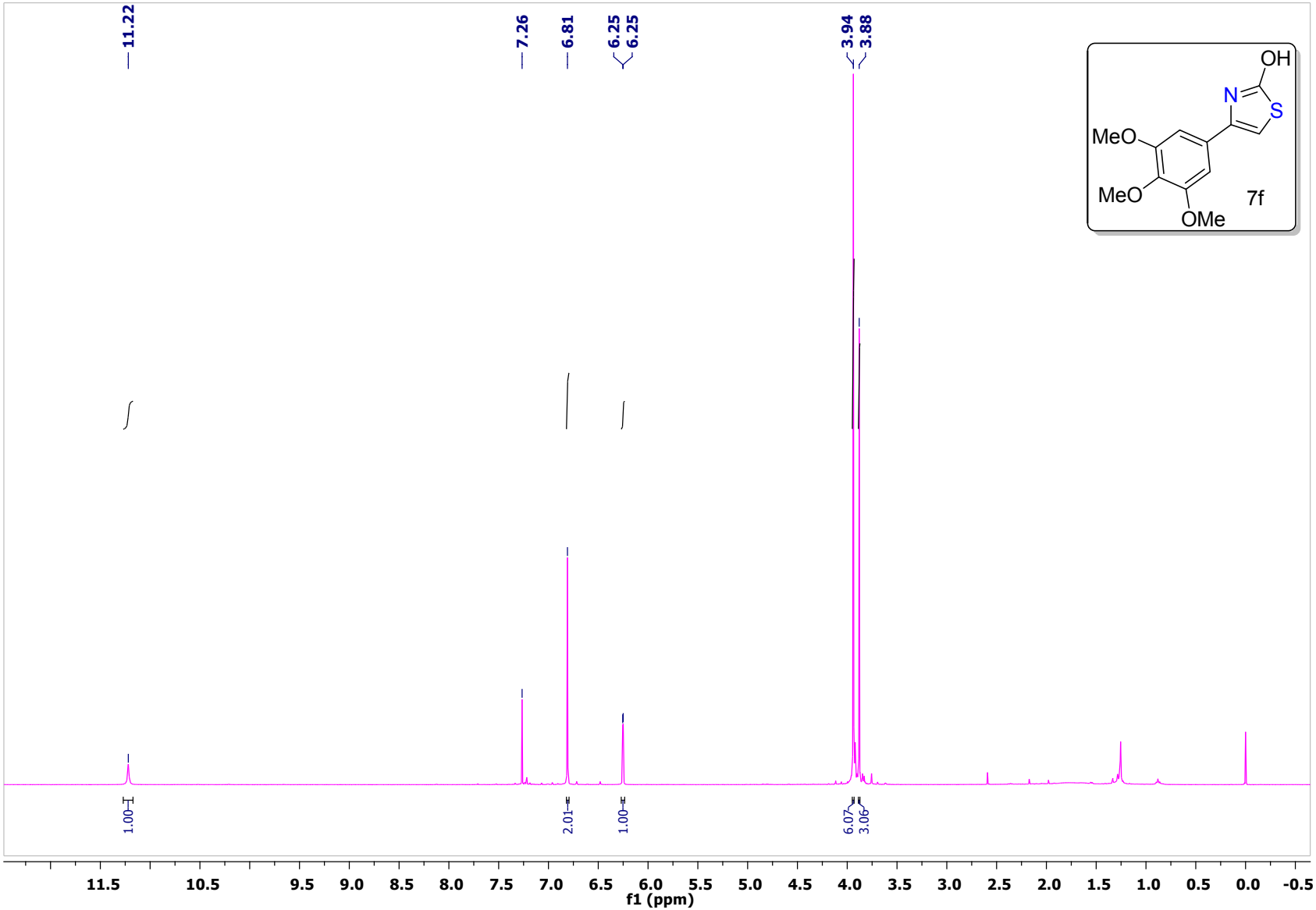
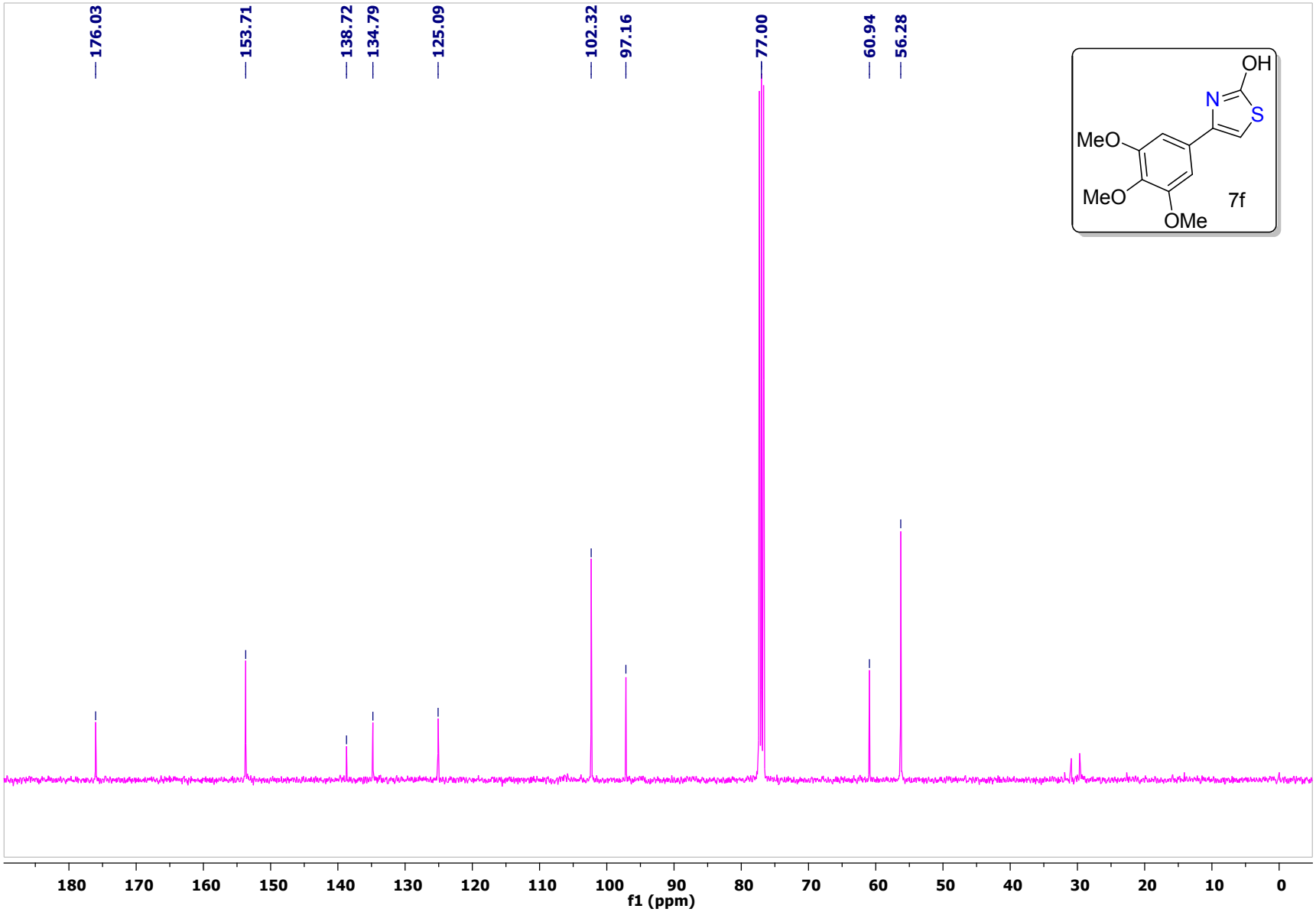
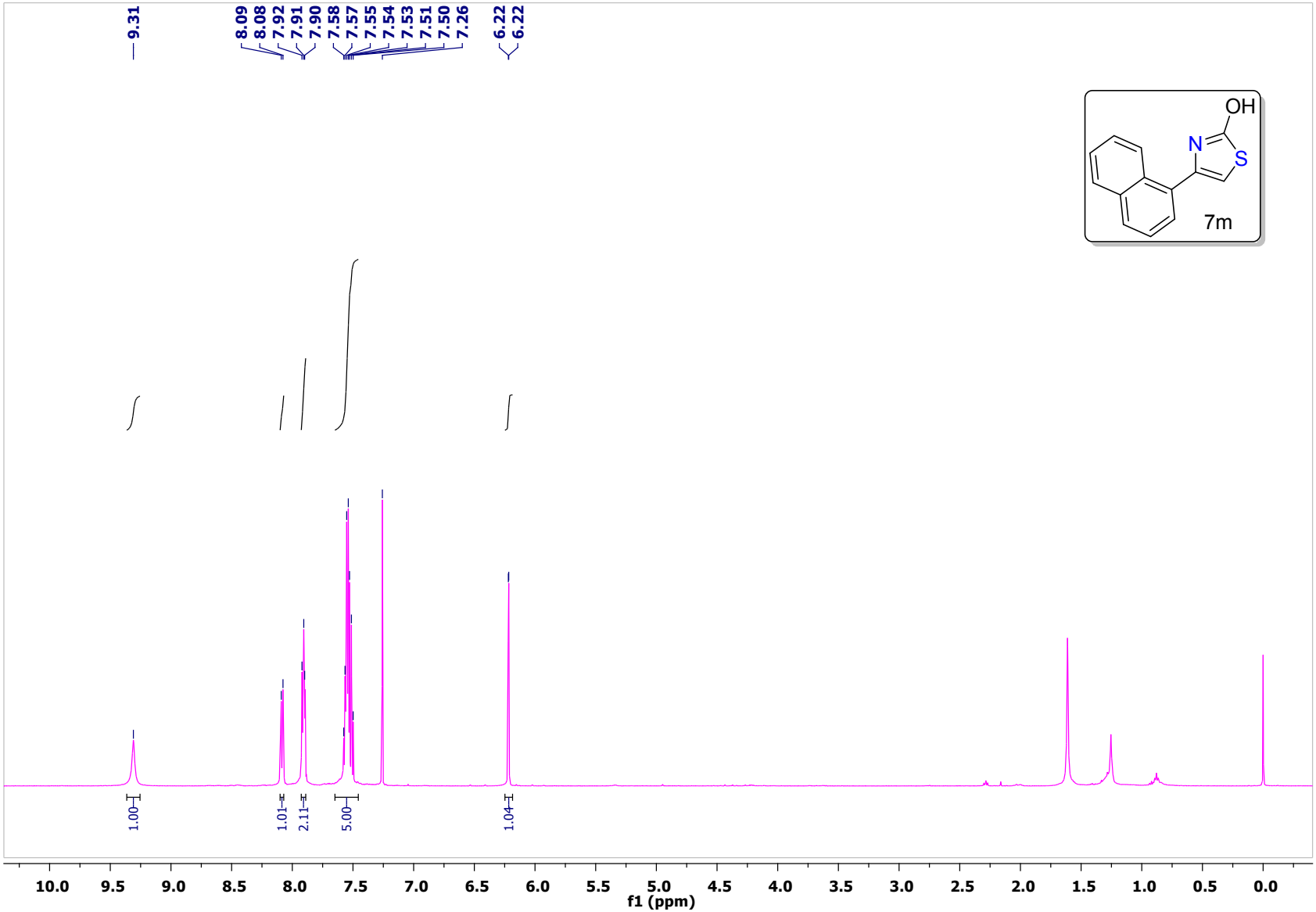
126.13
124.54
97.07
77.00
34.74
31.17
OH
N
S
7d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

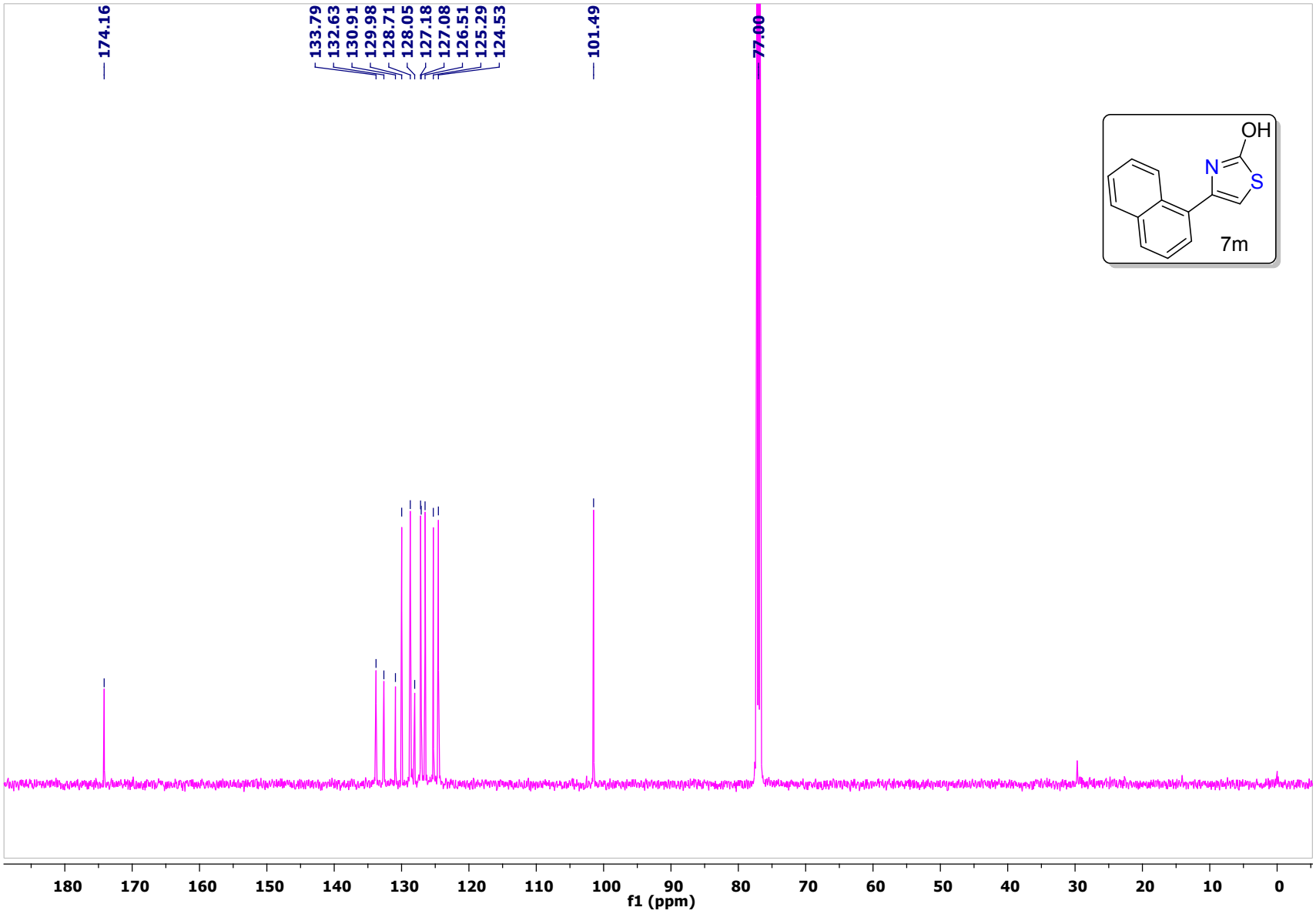

10.94
7.50
7.48
7.26
6.97
6.95
6.16
6.16
3.84
OH
N
S
MeO
7e
1.00
2.06
2.09
1.01
3.07
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

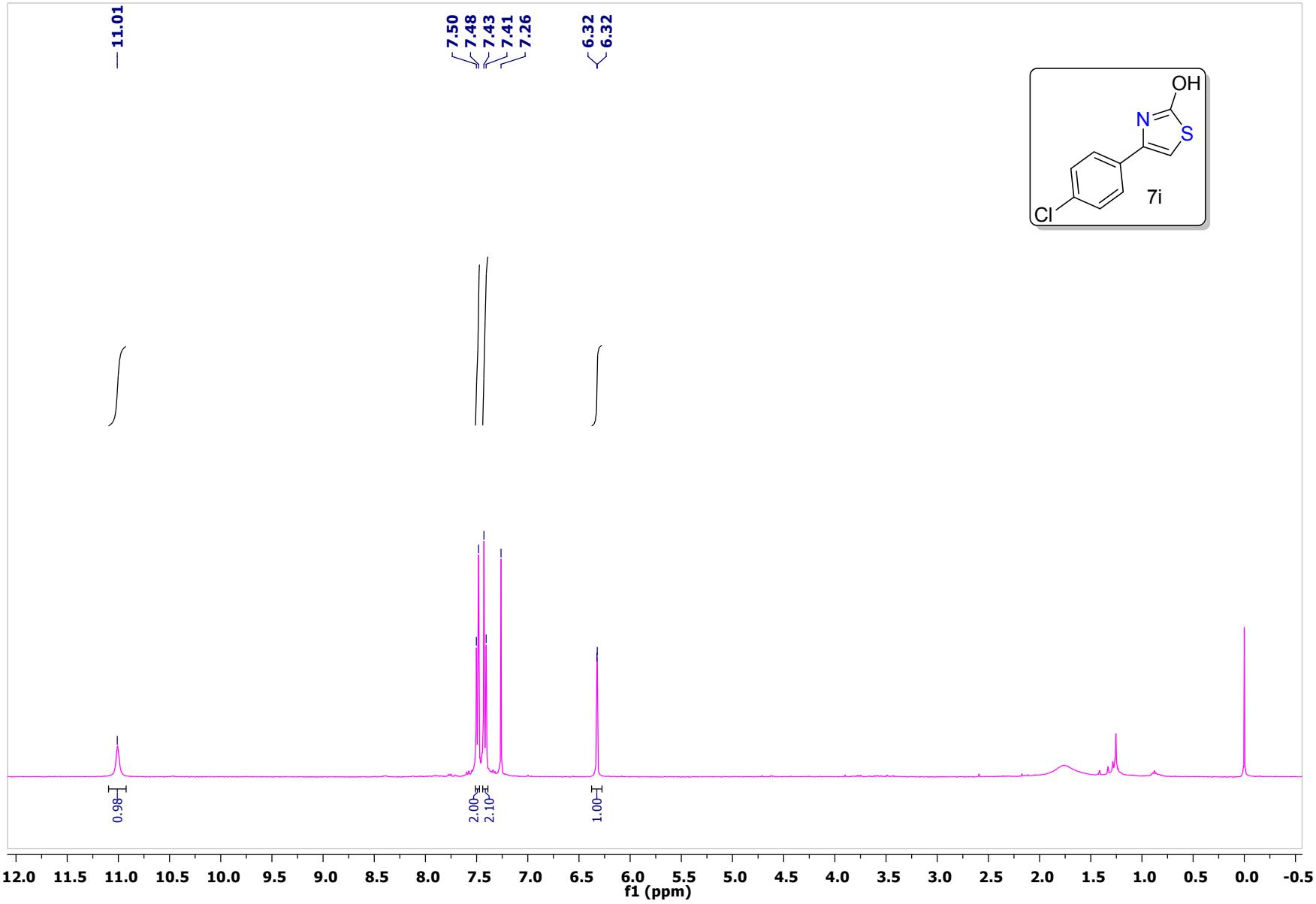

176.11
160.07
134.45
126.24
122.41
114.55
95.88
77.00
55.36
OH
N
S
MeO
7e
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

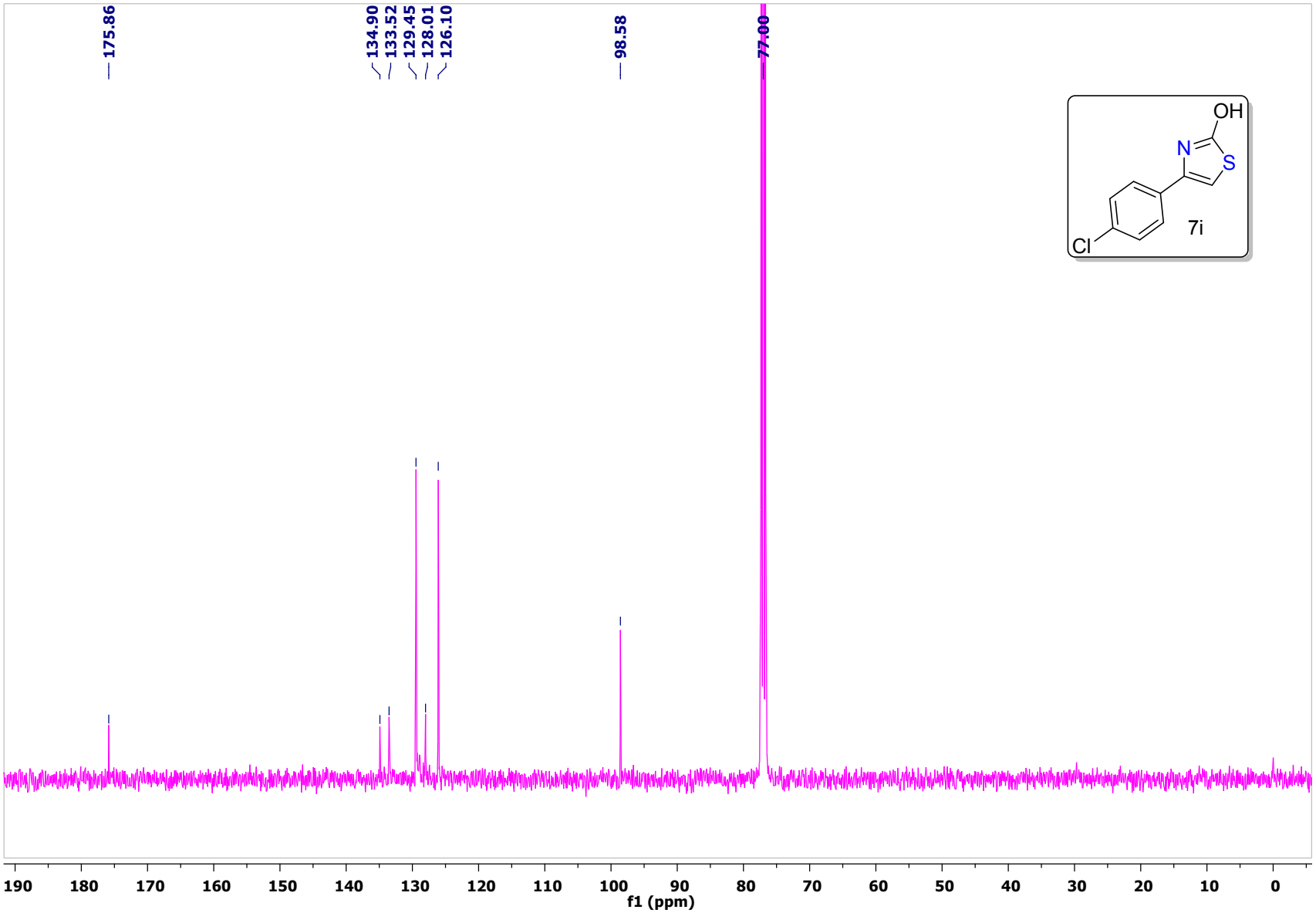

11.22
7.26
6.81
6.25
6.25
3.94
3.88
OH
N
S
MeO
MeO
OMe
7f
1.00
2.01
1.00
6.07
3.06
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

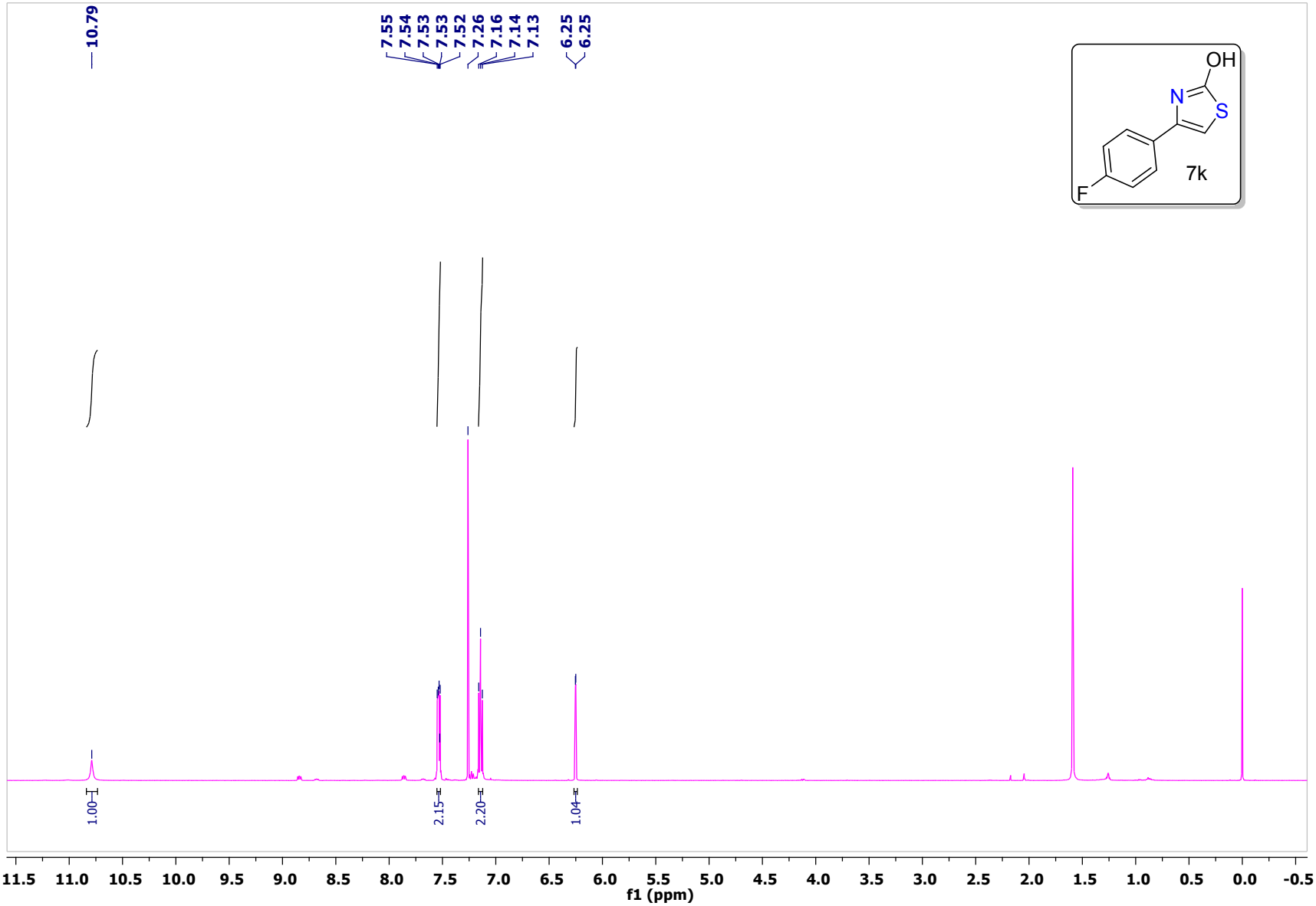

176.03
153.71
138.72
134.79
125.09
102.32
97.16
77.00
60.94
56.28
OH
N
S
MeO
MeO
OMe
7f
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

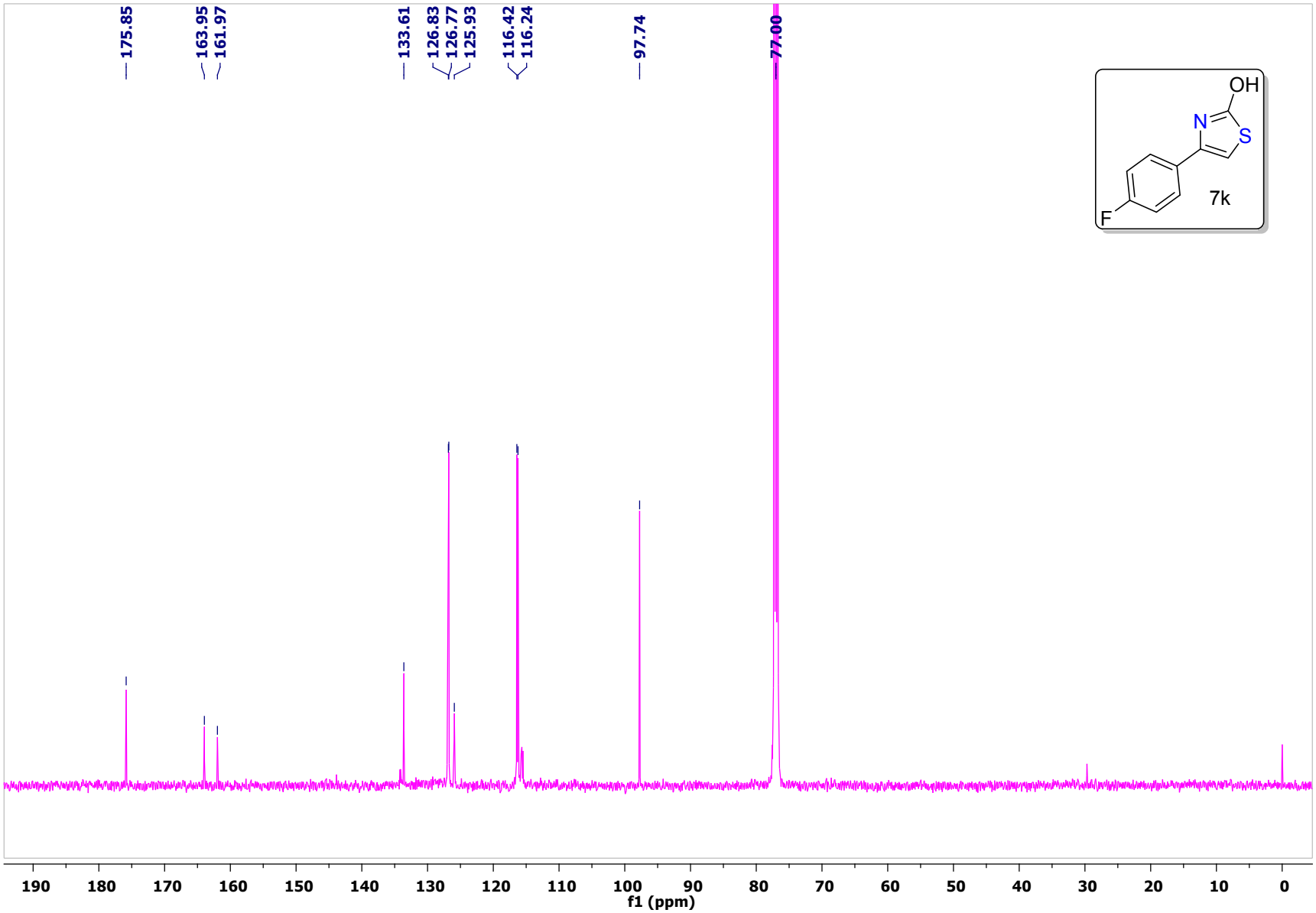

9.31
8.09
8.08
7.92
7.91
7.90
7.58
7.57
7.55
7.54
7.53
7.51
7.50
7.26
6.22
6.22
OH
N
S
7m
1.00
1.01
2.11
5.00
1.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

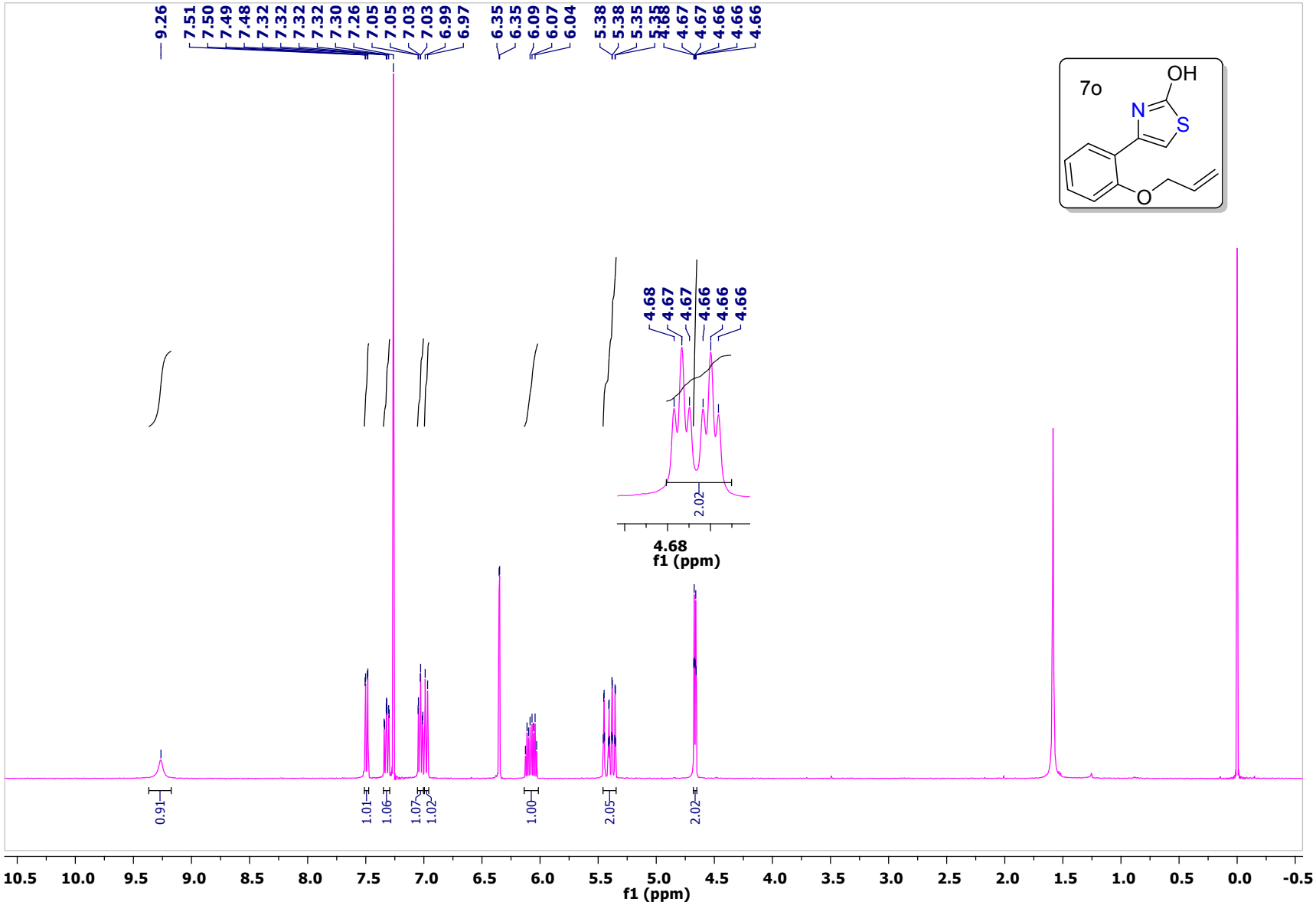

174.16
133.79
132.63
130.91
129.98
128.71
128.05
127.18
127.08
126.51
125.29
124.53
101.49
77.00
OH
N
S
7m
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

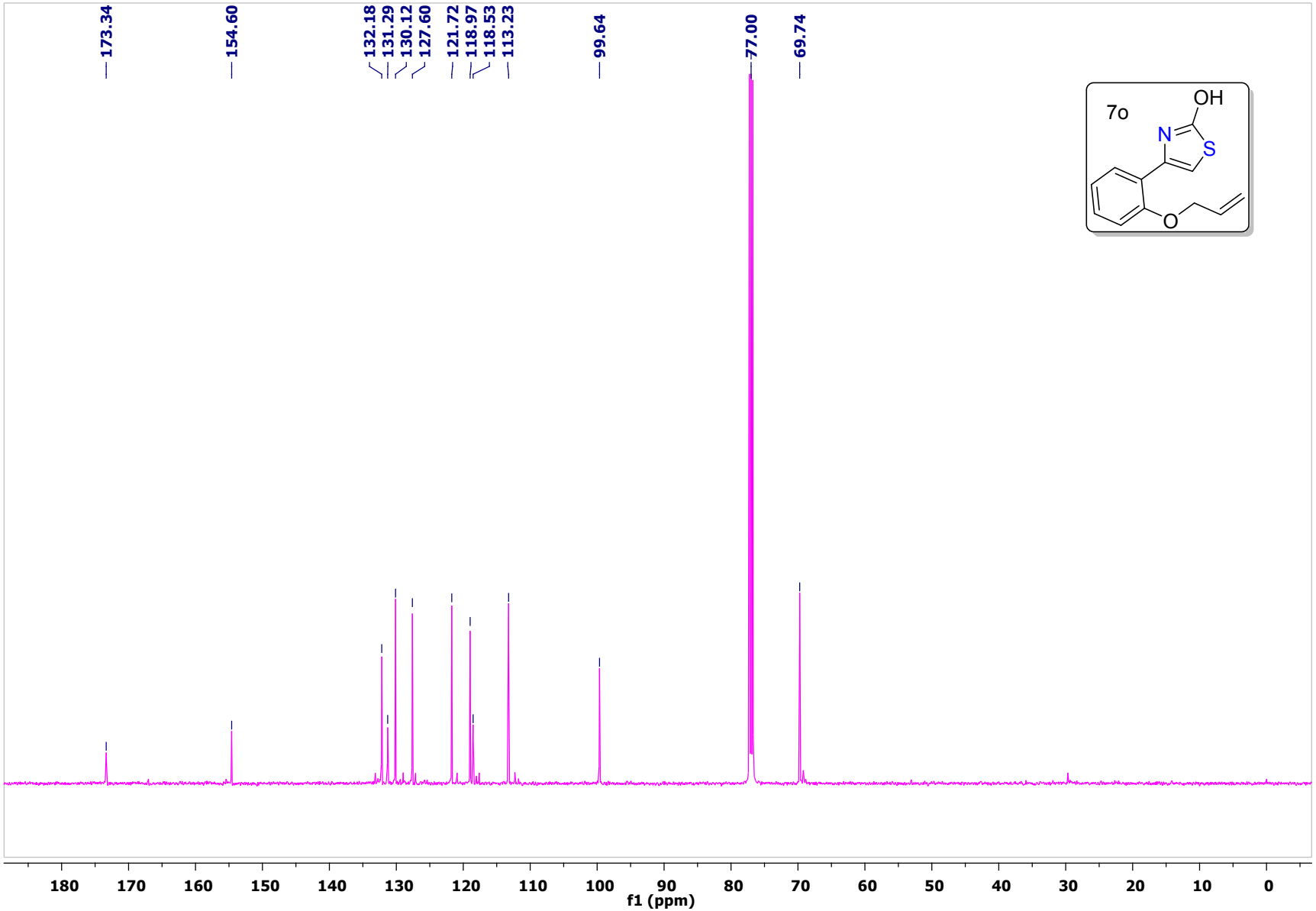

11.01
7.50
7.48
7.43
7.41
7.26
6.32
6.32
OH
N
S
Cl
7i
0.98
2.00
2.10
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

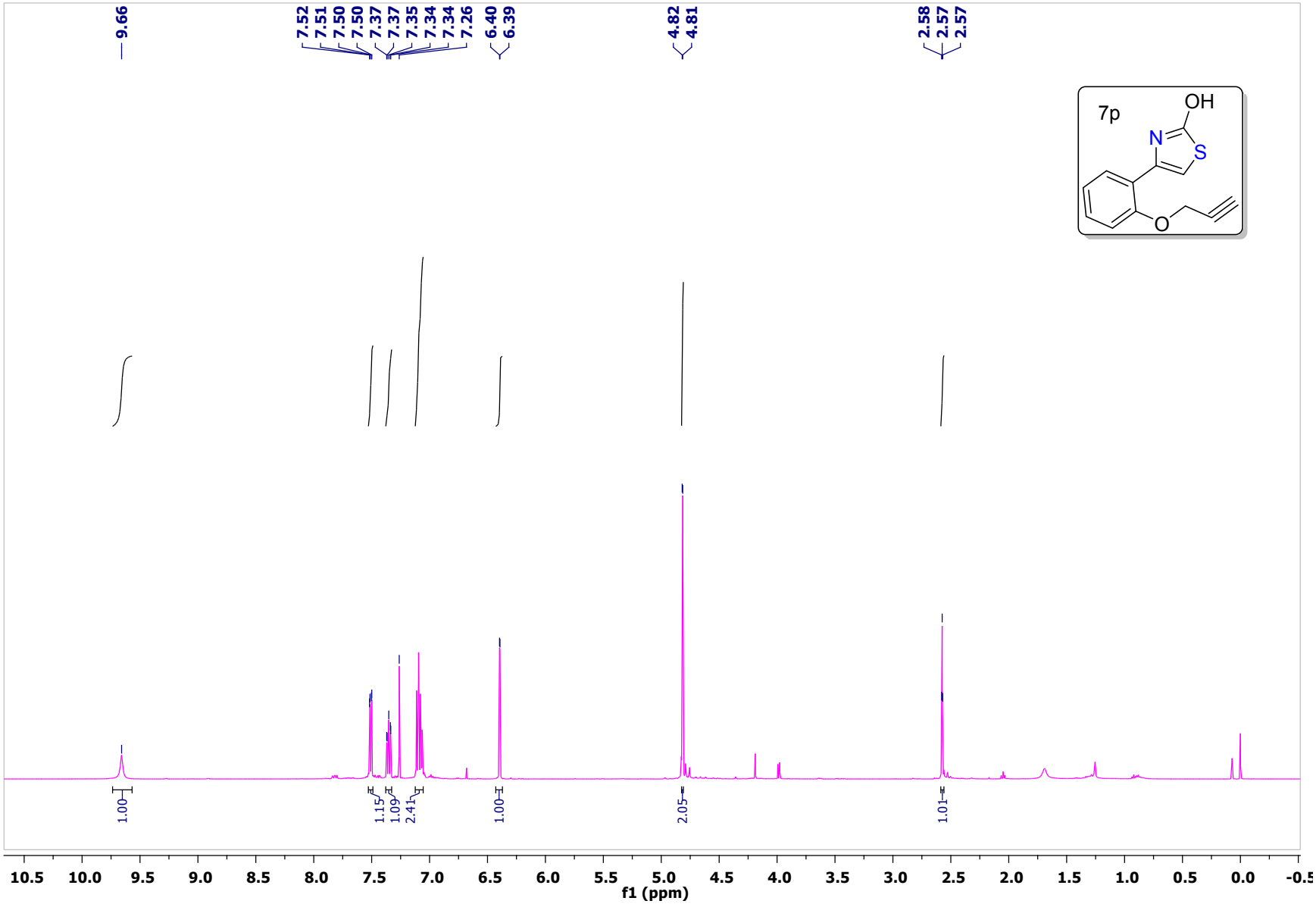

175.86
134.90
133.52
129.45
128.01
126.10
98.58
77.00
OH
N
S
Cl
7i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

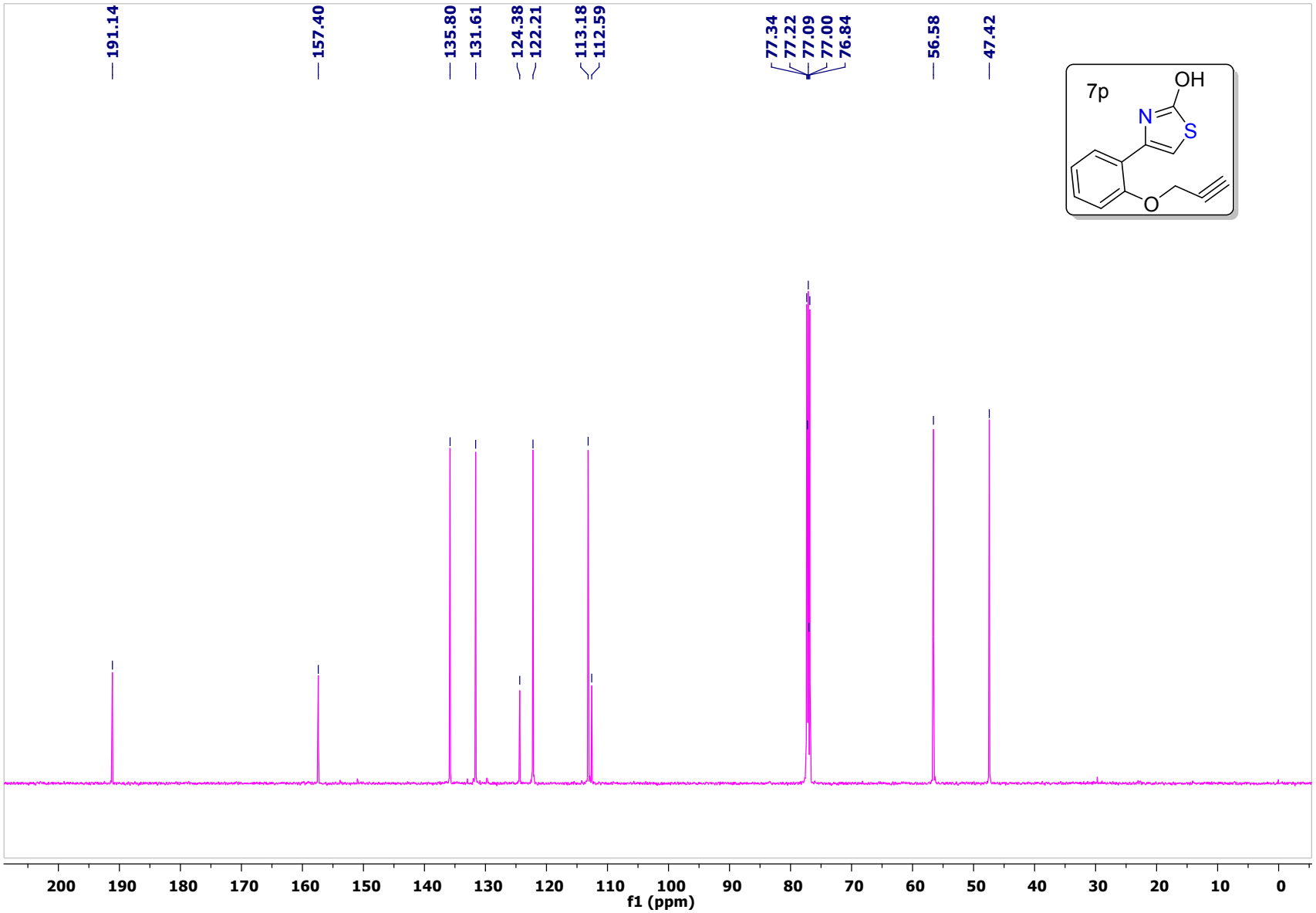

10.79
7.55
7.54
7.53
7.53
7.52
7.26
7.16
7.14
7.13
6.25
6.25
OH
N
S
F
7k
1.00
2.15
2.20
1.04
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


175.85
163.95
161.97
133.61
126.83
126.77
125.93
116.42
116.24
97.74
77.00
OH
N
S
F
7k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.26
7.51
7.50
7.49
7.48
7.32
7.32
7.32
7.32
7.30
7.26
7.05
7.05
7.03
7.03
6.99
6.97
6.35
6.35
6.09
6.07
6.04
5.38
5.38
5.35
5.35
4.68
4.67
4.67
4.66
4.66
4.66
4.66
7o
OH
N
S
O
2.02
4.68
f1 (ppm)
0.91
1.01
1.06
1.07
1.02
1.00
2.05
2.02
10.5
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
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


173.34
154.60
132.18
131.29
130.12
127.60
121.72
118.97
118.53
113.23
99.64
77.00
69.74
7o
OH
N
S
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.66
7.52
7.51
7.50
7.50
7.37
7.37
7.35
7.34
7.34
7.26
6.40
6.39
4.82
4.81
2.58
2.57
2.57
7p
OH
N
S
O
1.00
1.15
1.09
2.41
1.00
2.05
1.01
10.5
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
1.5
1.0
0.5
0.0
f1 (ppm)


191.14
157.40
135.80
131.61
124.38
122.21
113.18
112.59
77.34
77.22
77.09
77.00
76.84
56.58
47.42
7p
OH
N
S
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)