Supporting Information

$FeCl_3$ and Ether Mediated Direct Intramolecular Acylation of Esters and its Application in Efficient Preparation of Xanthone and Chromone Derivatives

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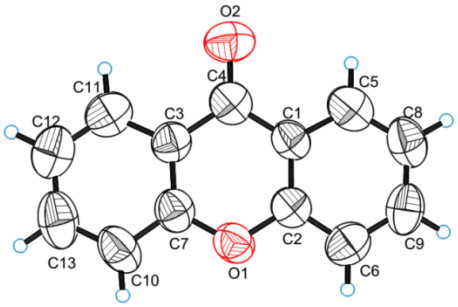

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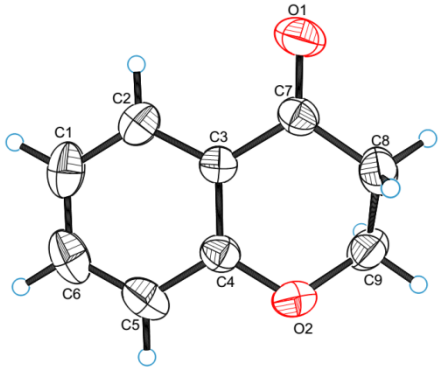

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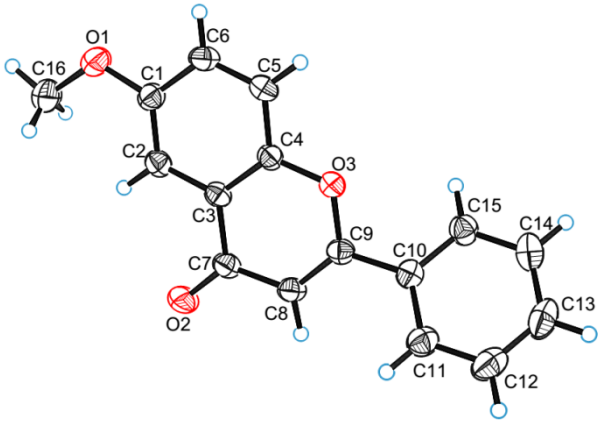


4d

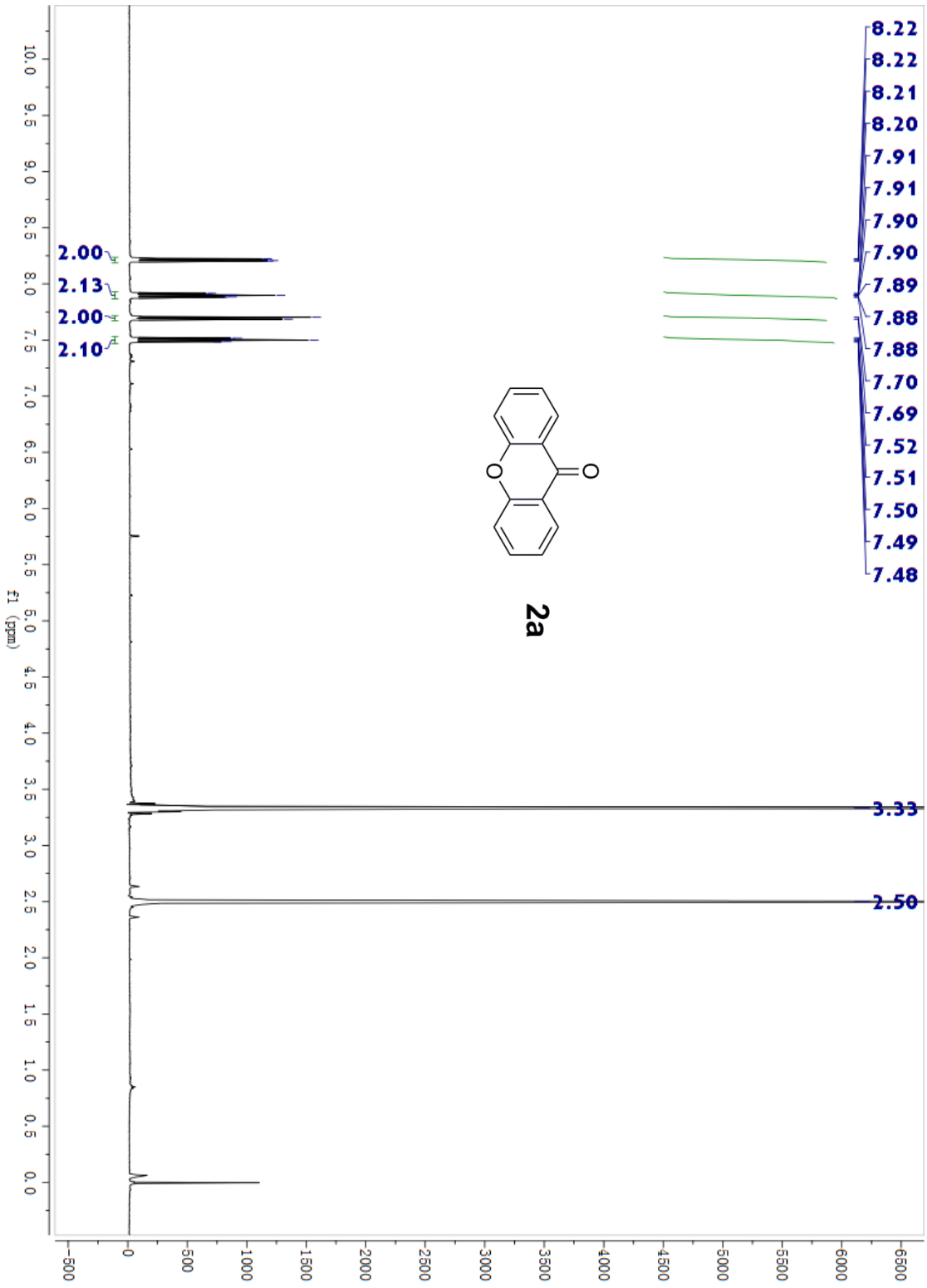
Fig. S1 Molecular structure of **2a**, **4a**, **4d**[1]

Reference

[1] CCDC 982623 (**2a**). Crystal data for compound **2a**: $C_{13}H_8O_2$, M = 196.19, orthorhombic, a=4.8978(14) Å, α = 90°, b = 13.654(5) Å, β = 90°, c = 14.129(5) Å, γ = 90°, V = 944.9(6) Å3, T = 291(2) K, space group = $P2_12_12_1$, Z = 4, number of reflections = 7057, independent reflections = 1762, [R_{int}= 0.0655], final R indices[I >= 2δ(I)] R_1 = 0.1100, wR_2 = 0.1685, R indices (all data) R_1 = 0.1625, wR_2 = 0.1900.

CCDC 982620 (**4a**). Crystal data for compound **4a**: $C_9H_8O_2$, M =148.15, monoclinic, a = 8.6255(4) Å, α = 90°, b= 6.6197(3) Å, β = 90.297(4)°, c = 13.1658(7) Å, γ = 90°, V = 751.73(6) Å3, T = 291(2) K, space group = P21/n, Z= 4, number of reflections = 6402, independent reflections = 1528, [R_{int}= 0.0201], final R indices[I >=2δ(I)] R_1 = 0.0396, wR_2= 0.1031, R indices (all data) R_1 = 0.0525, wR_2 = 0.1130.

CCDC 982630 (**4d**). Crystal data for compound **4d**: $C_{16}H_{12}O_3$, M=252.26, orthorhombic, a = 13.5324(8) Å, α = 90°, b = 7.0687(4) Å, β = 90°, c = 25.6858(17) Å, γ = 90°, V = 2457.0(3) Å3, T = 290(2) K, space group = Pbca, Z = 8, number of reflections = 9593, independent reflections = 2871, [R_{int} = 0.0274], final R indices [I >= 2δ(I)] R_1= 0.0465, wR_2= 0.1021, R indices (all data) R_1= 0.0736, wR_2= 0.1163.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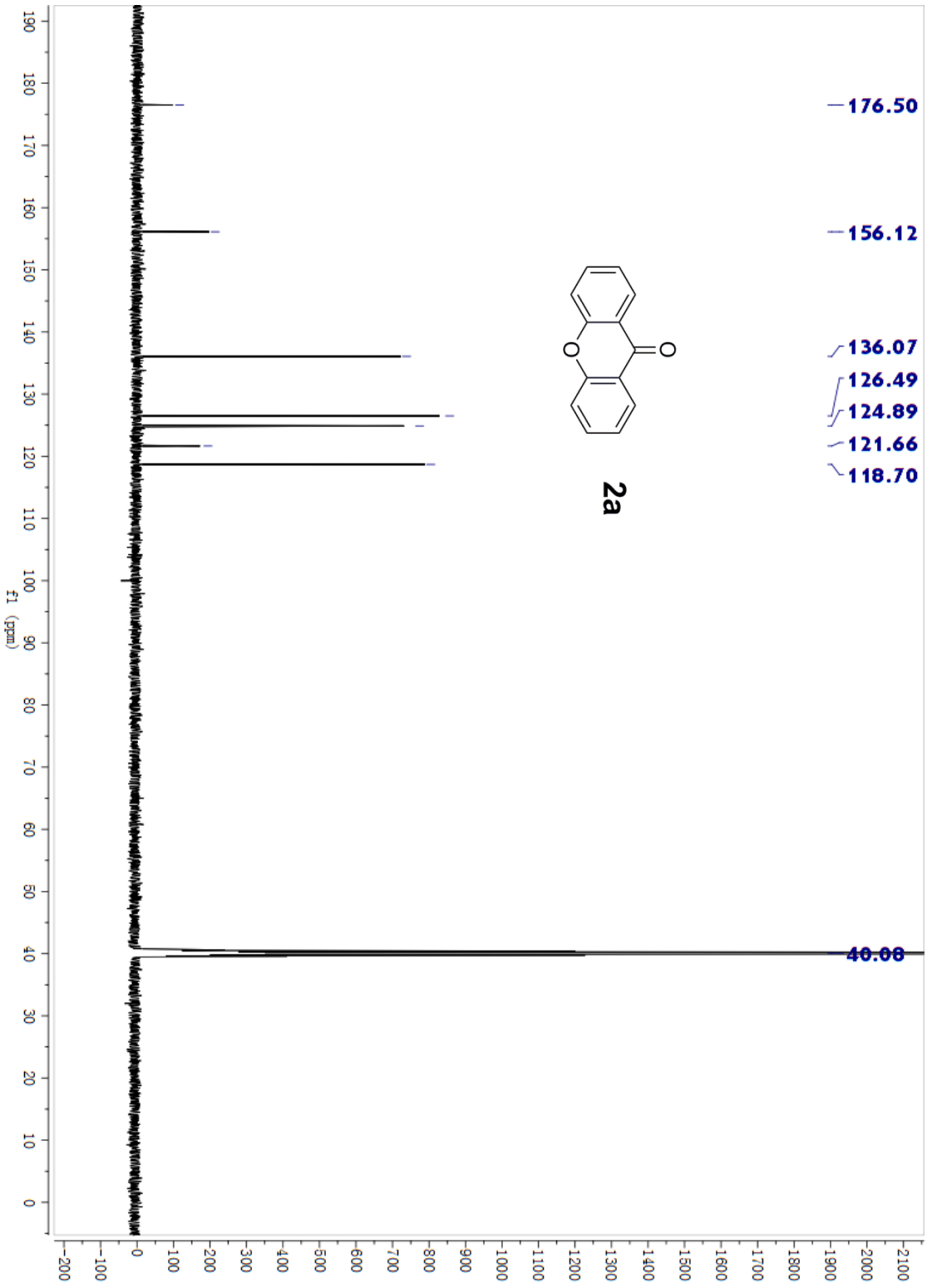
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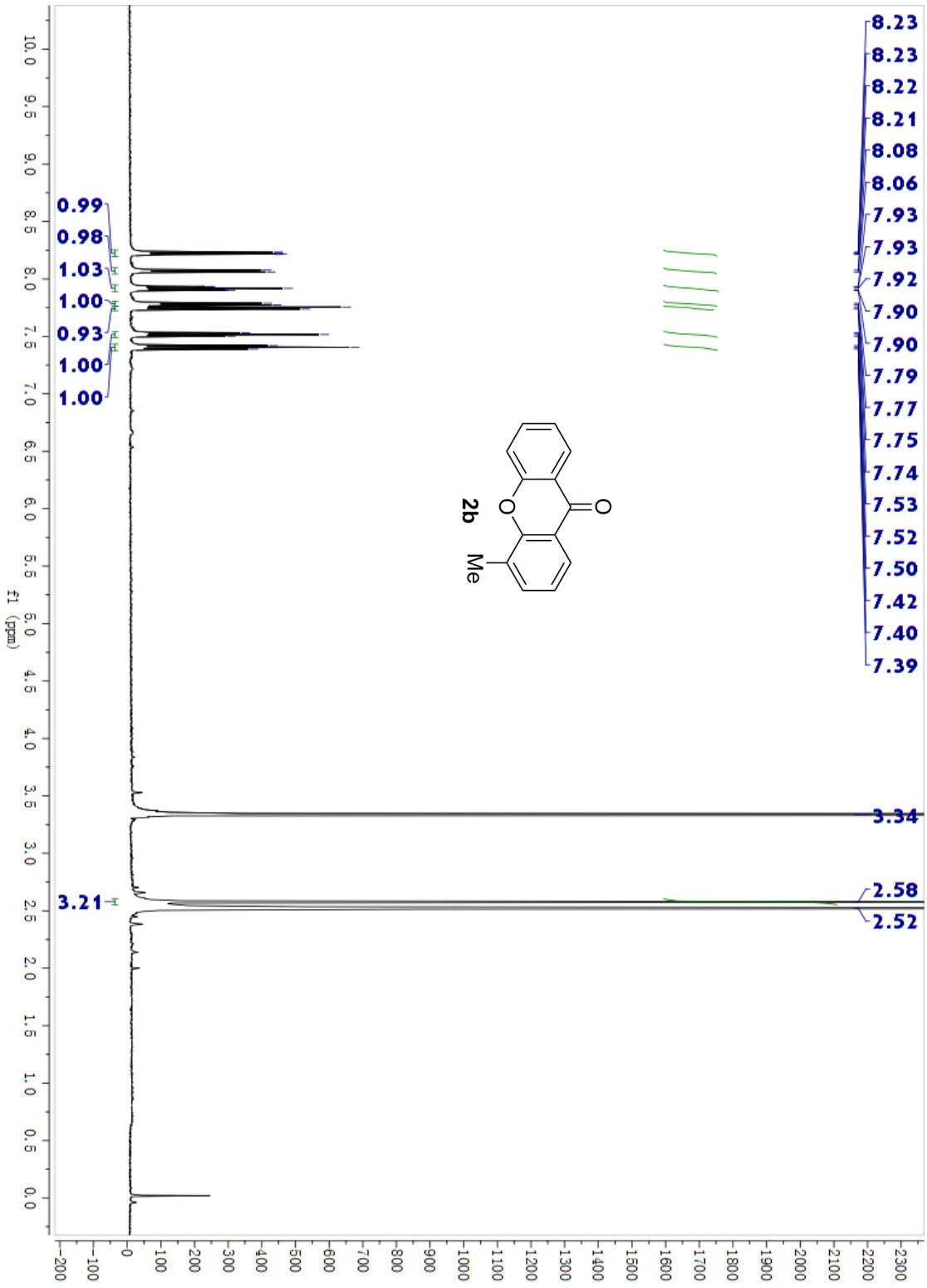
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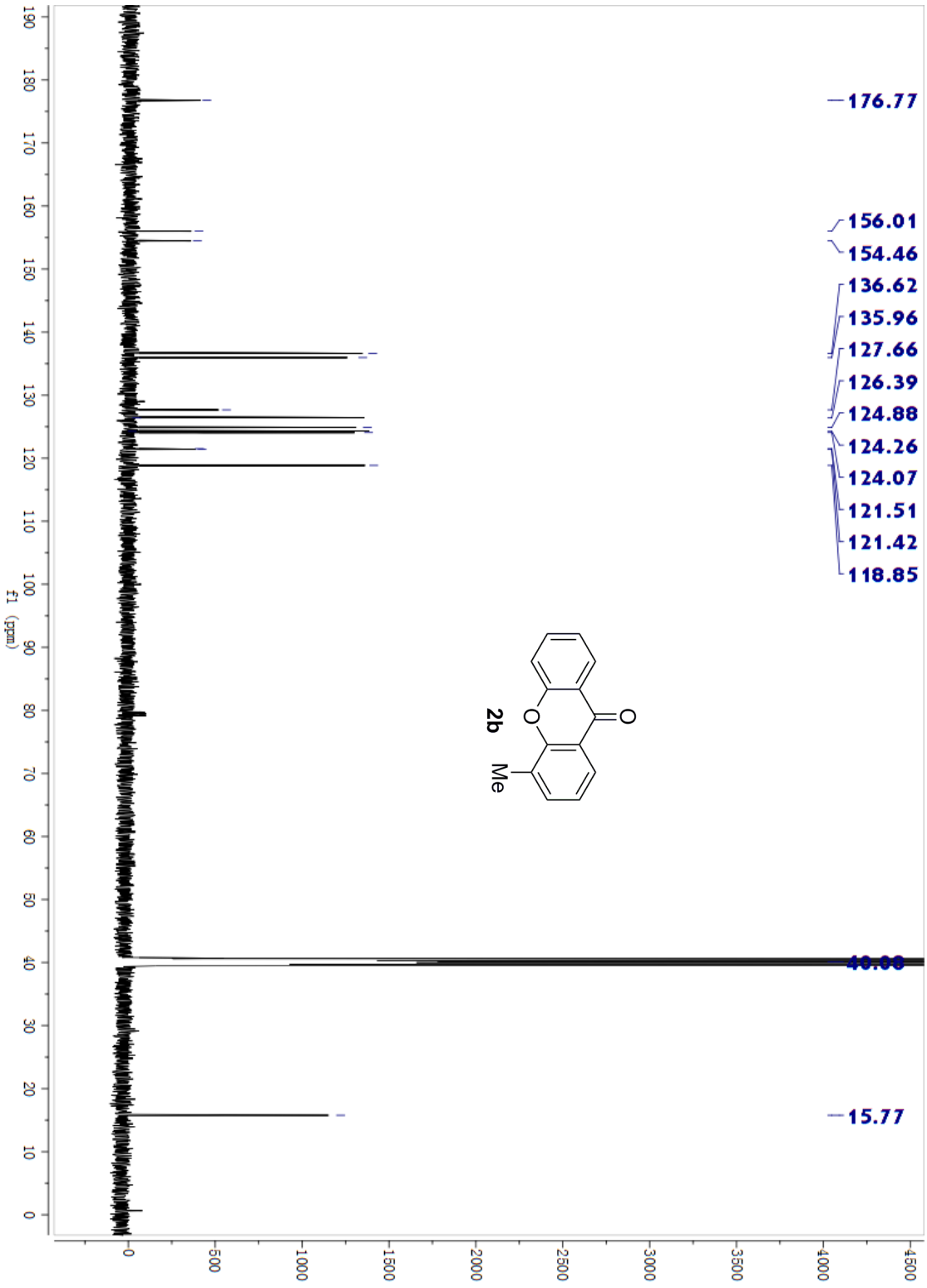
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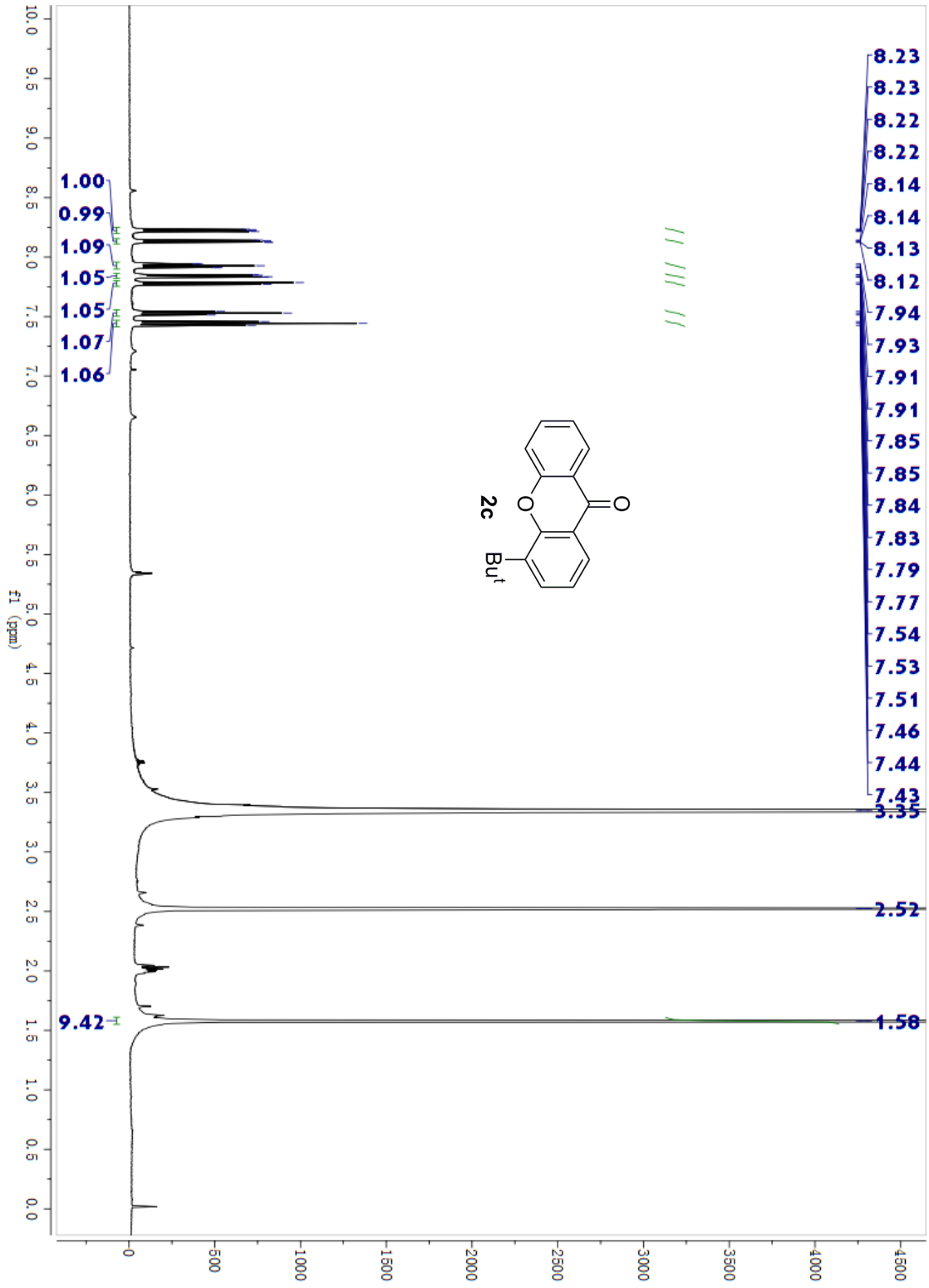
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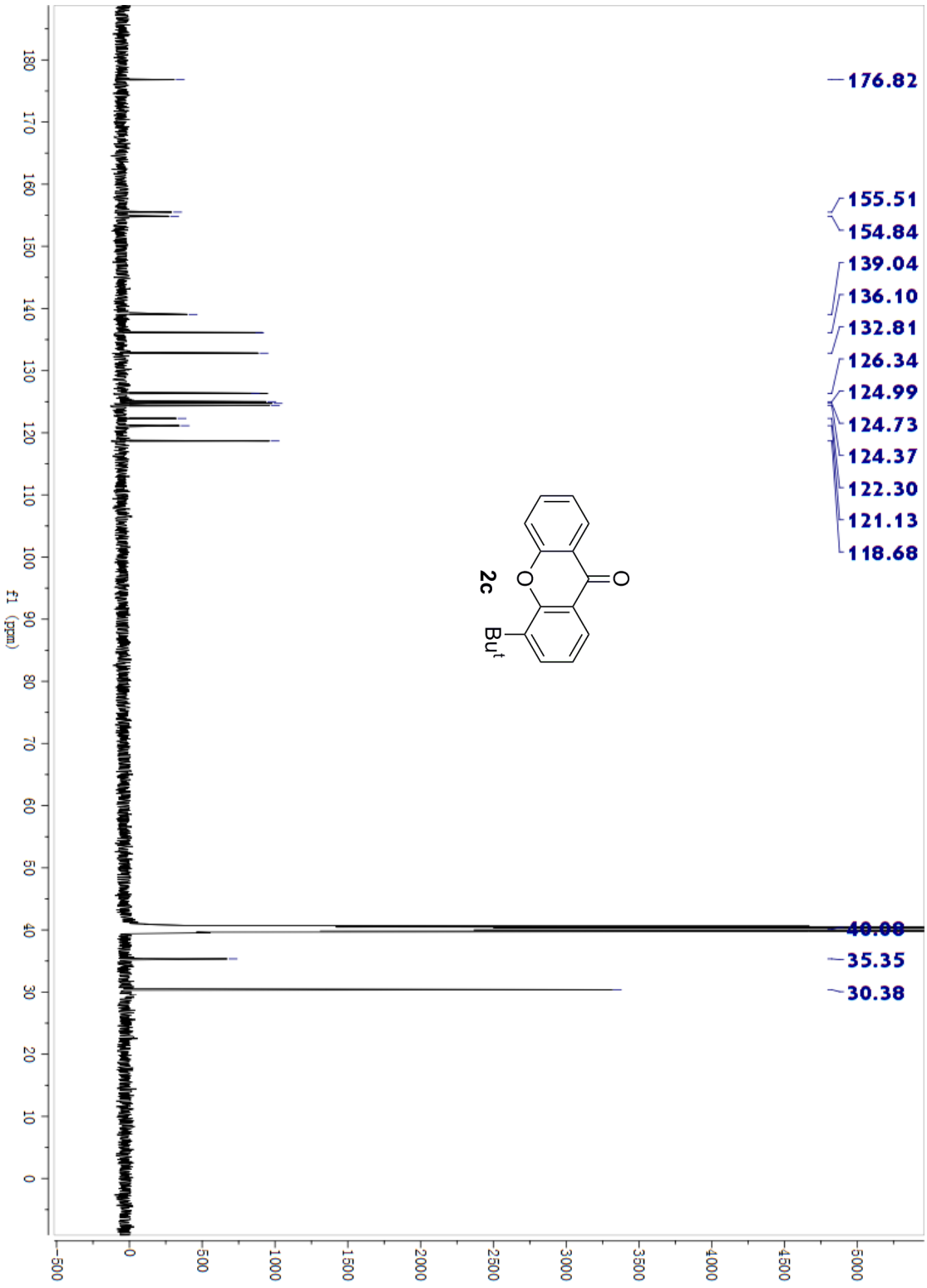
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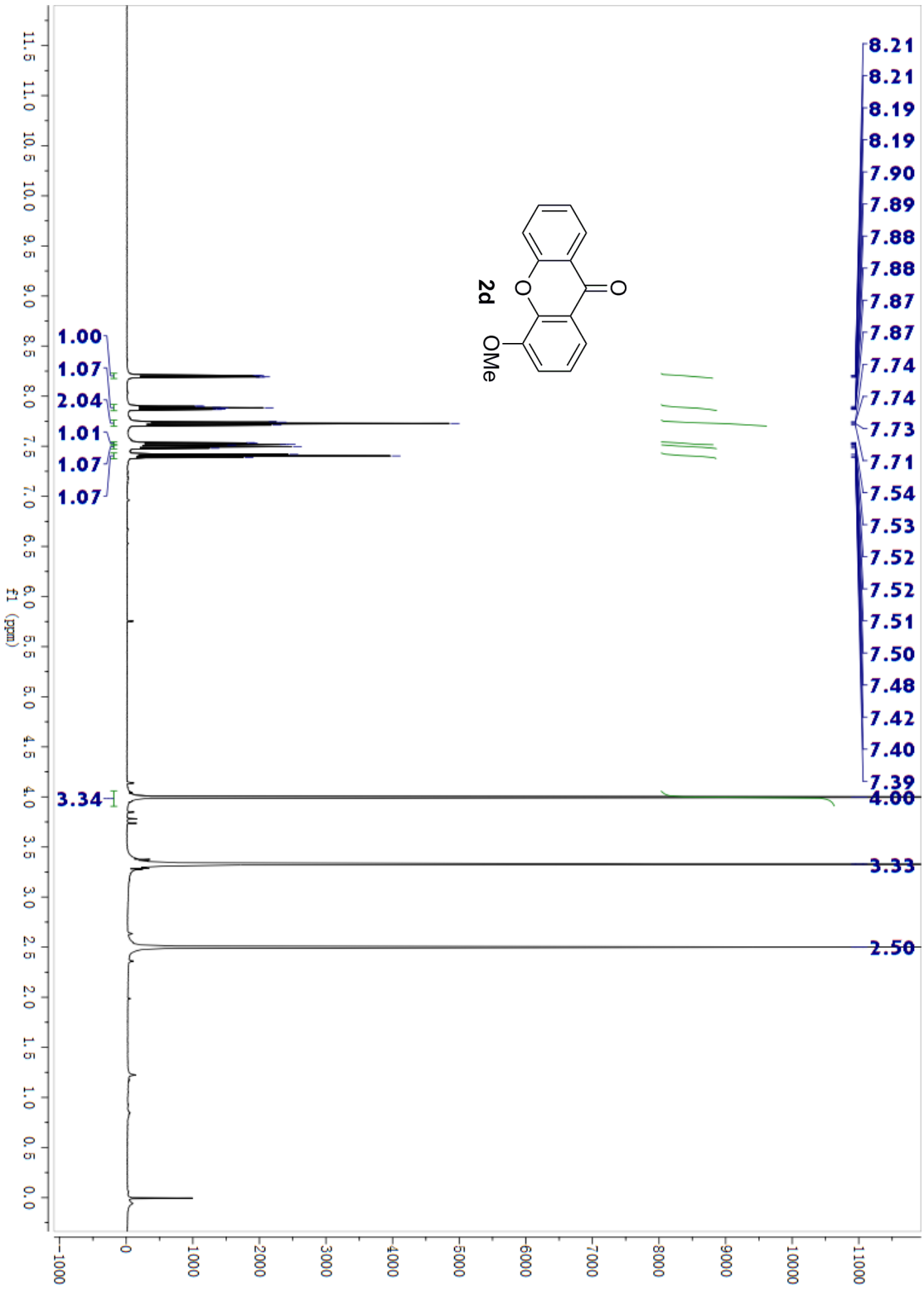
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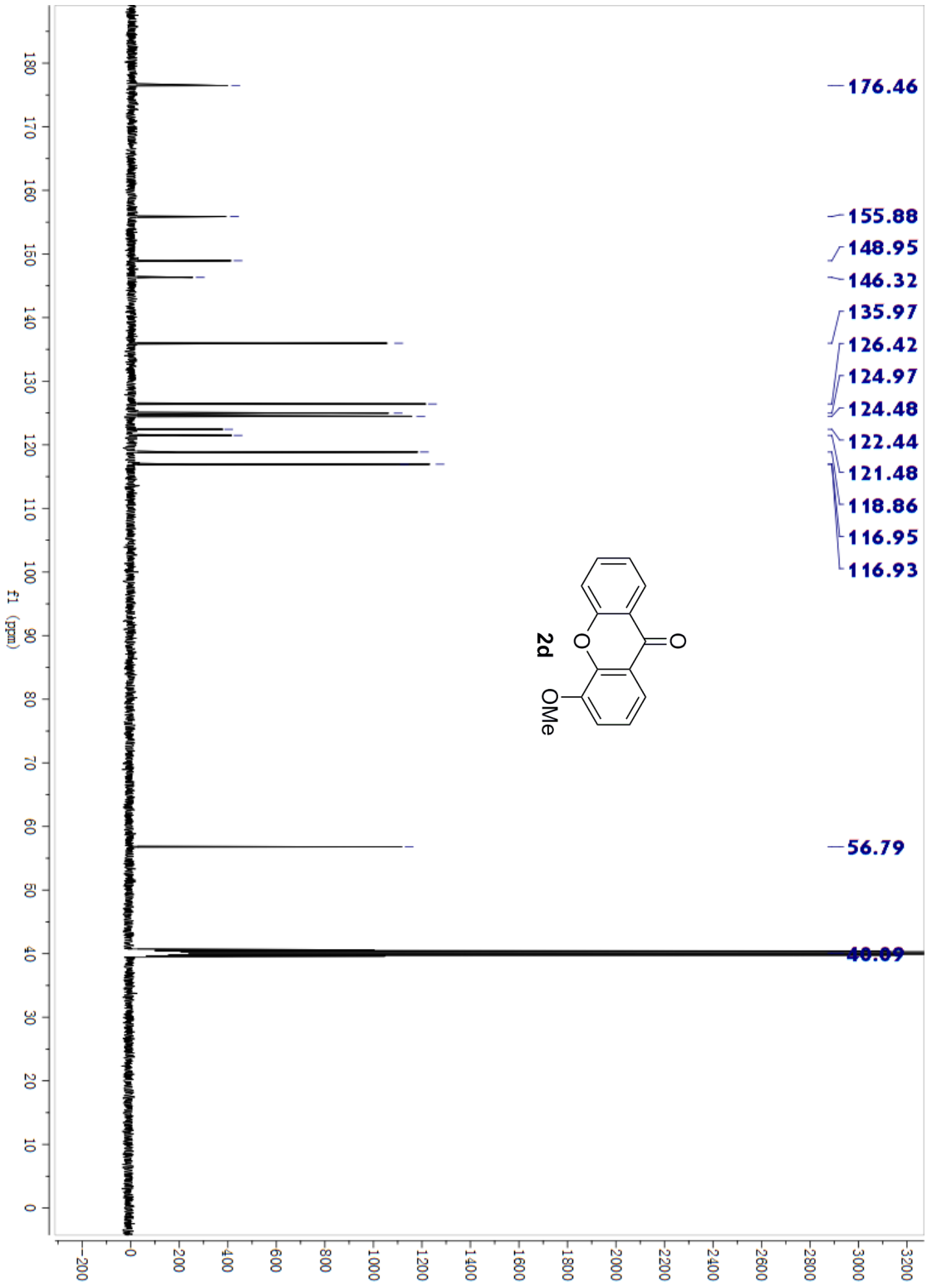
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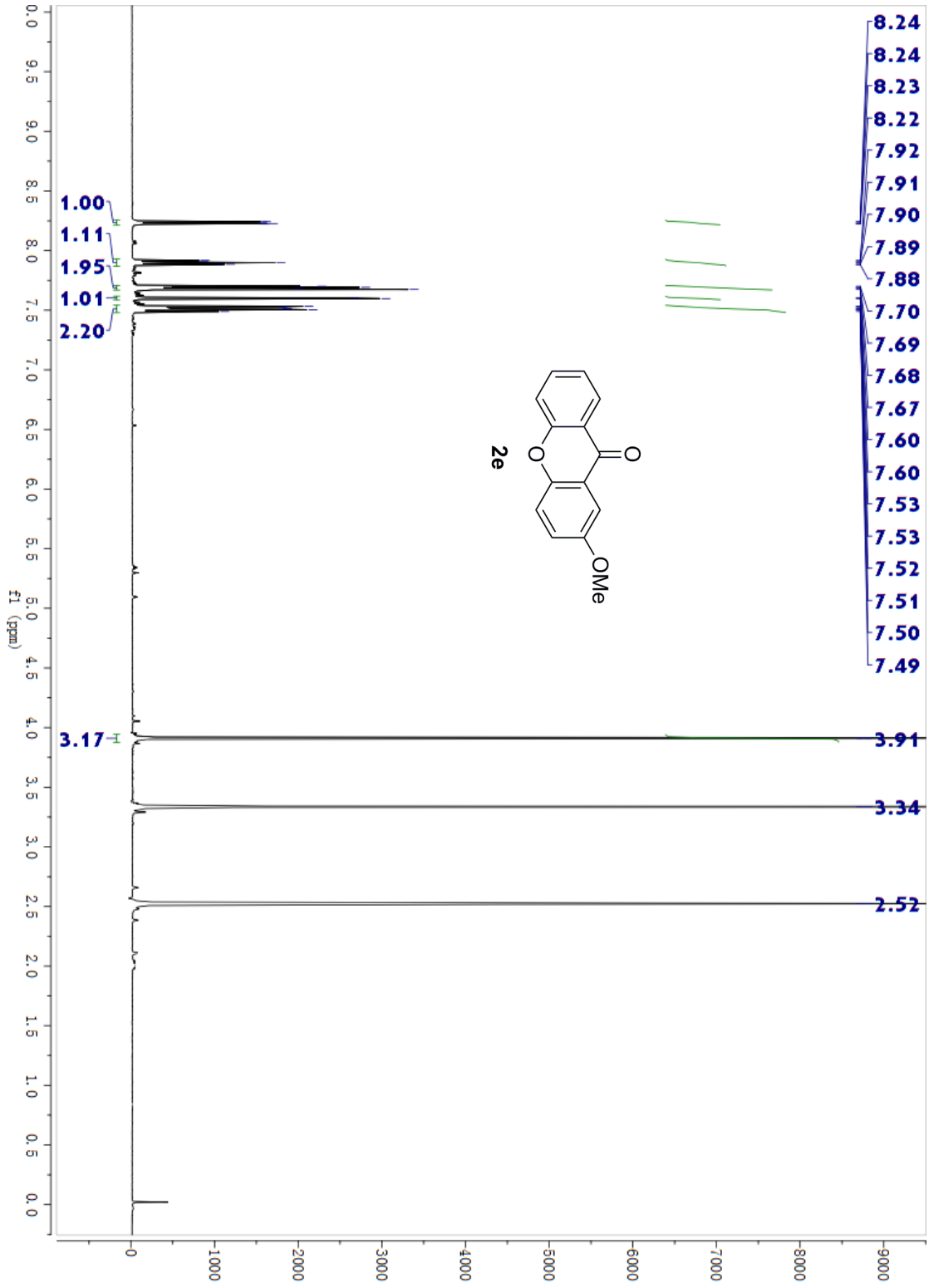
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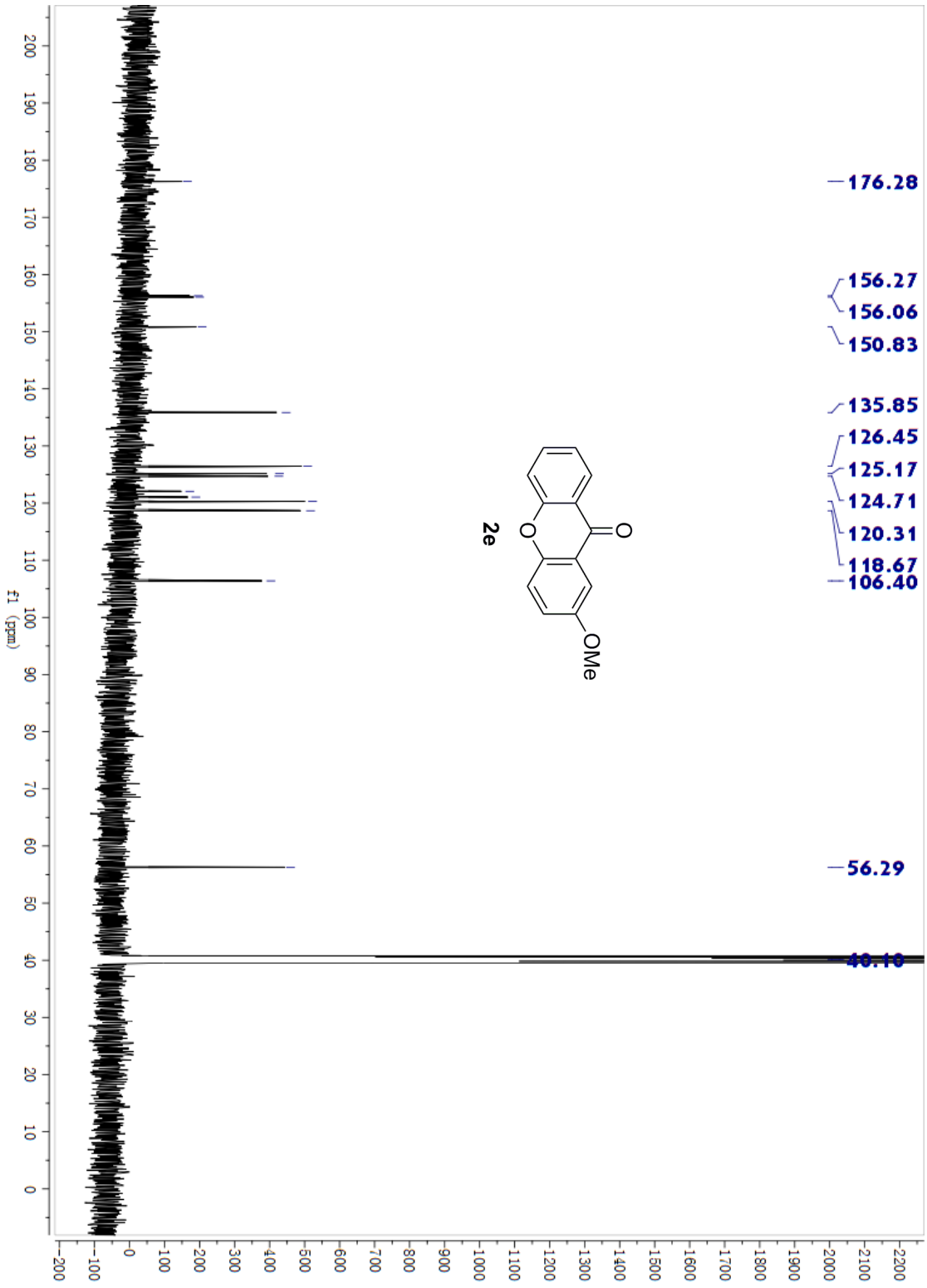
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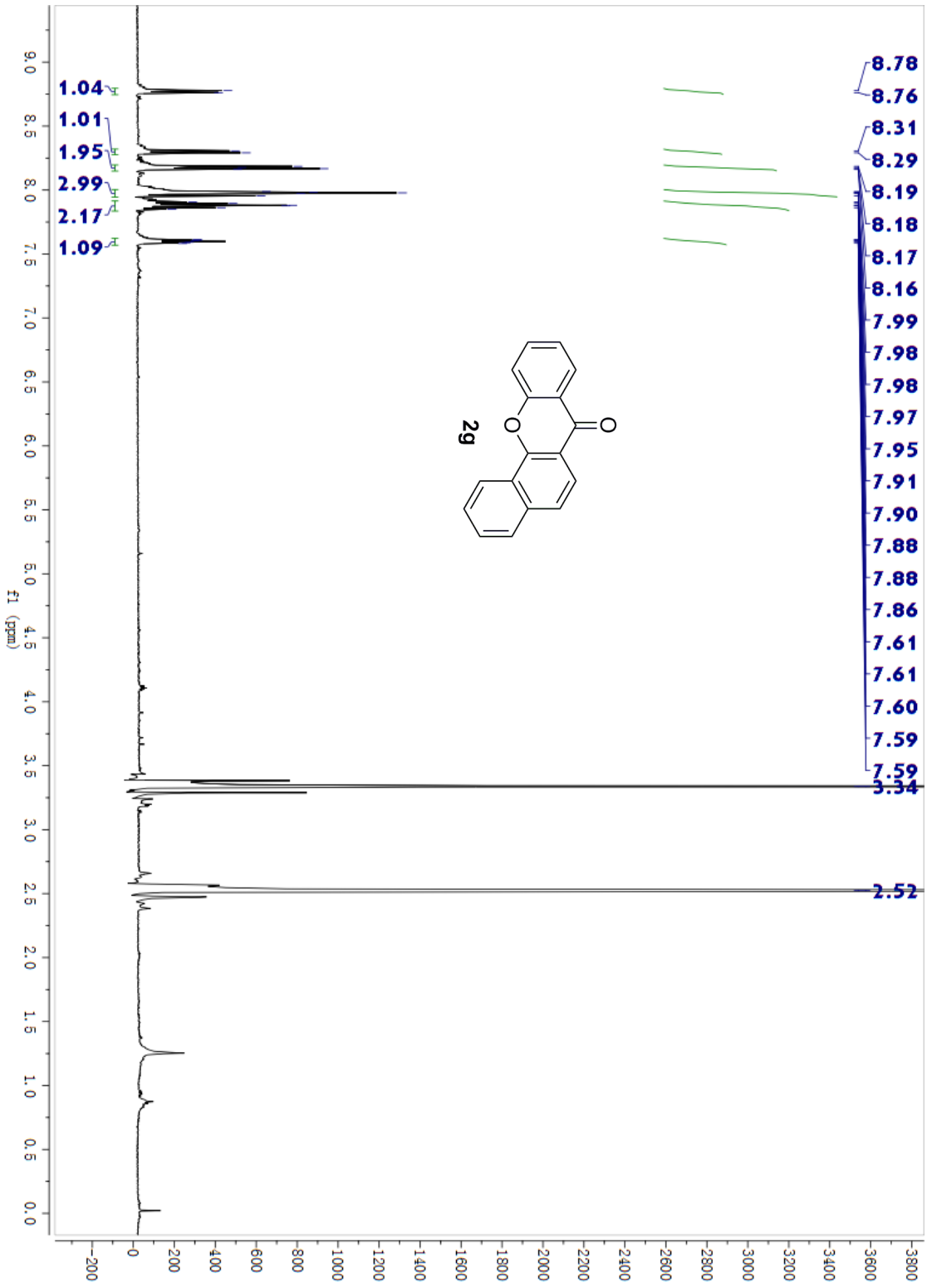
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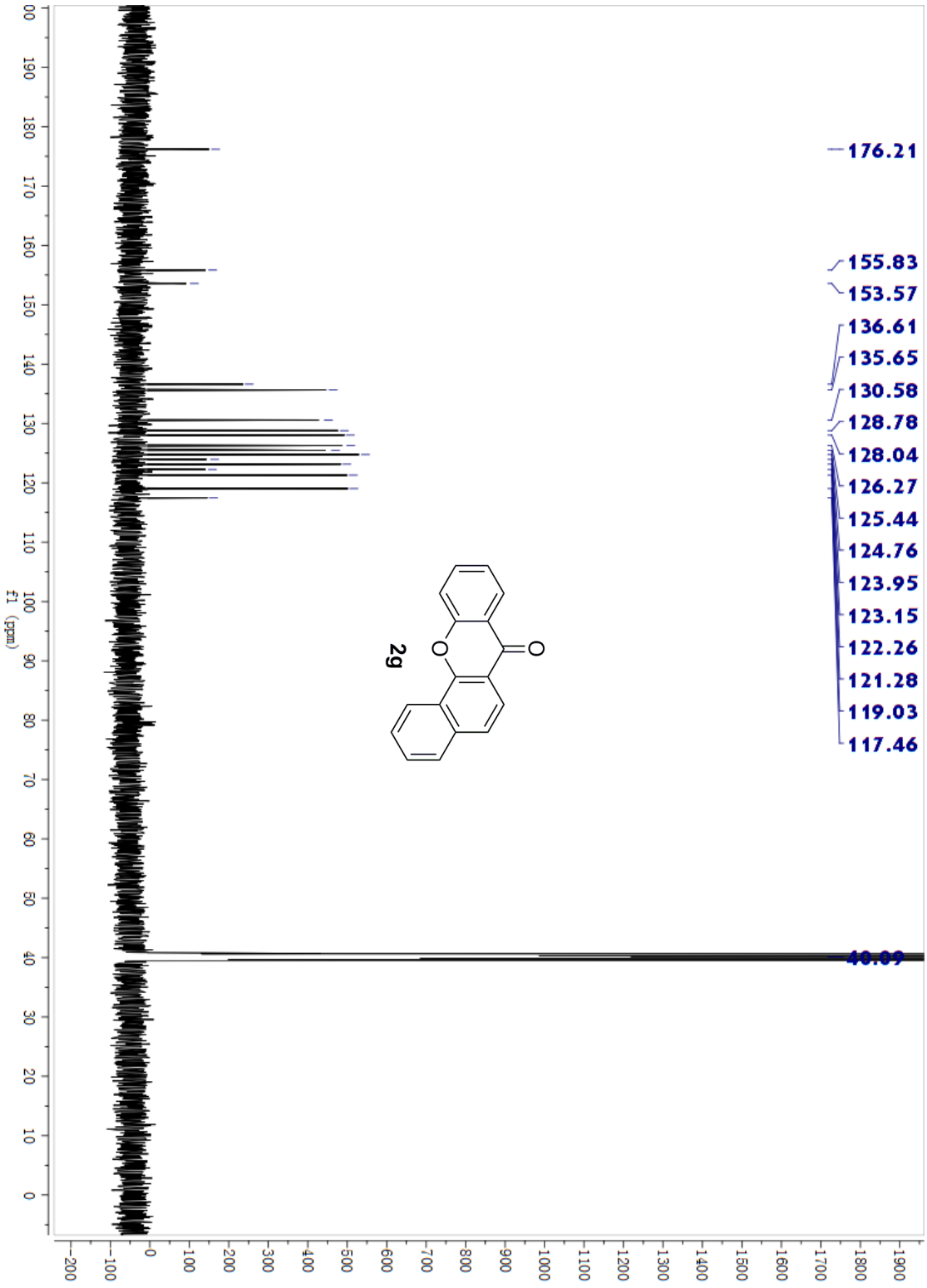
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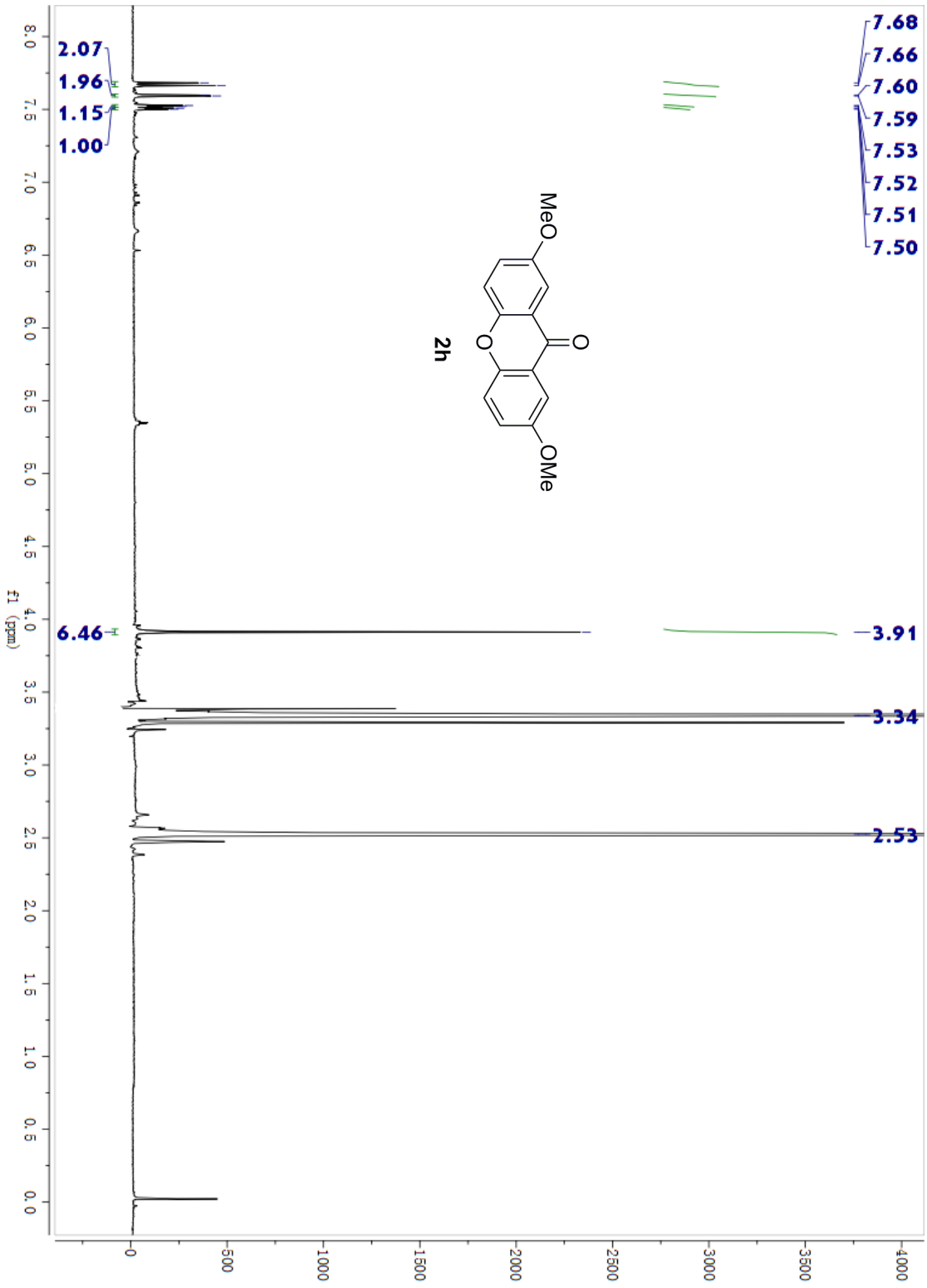
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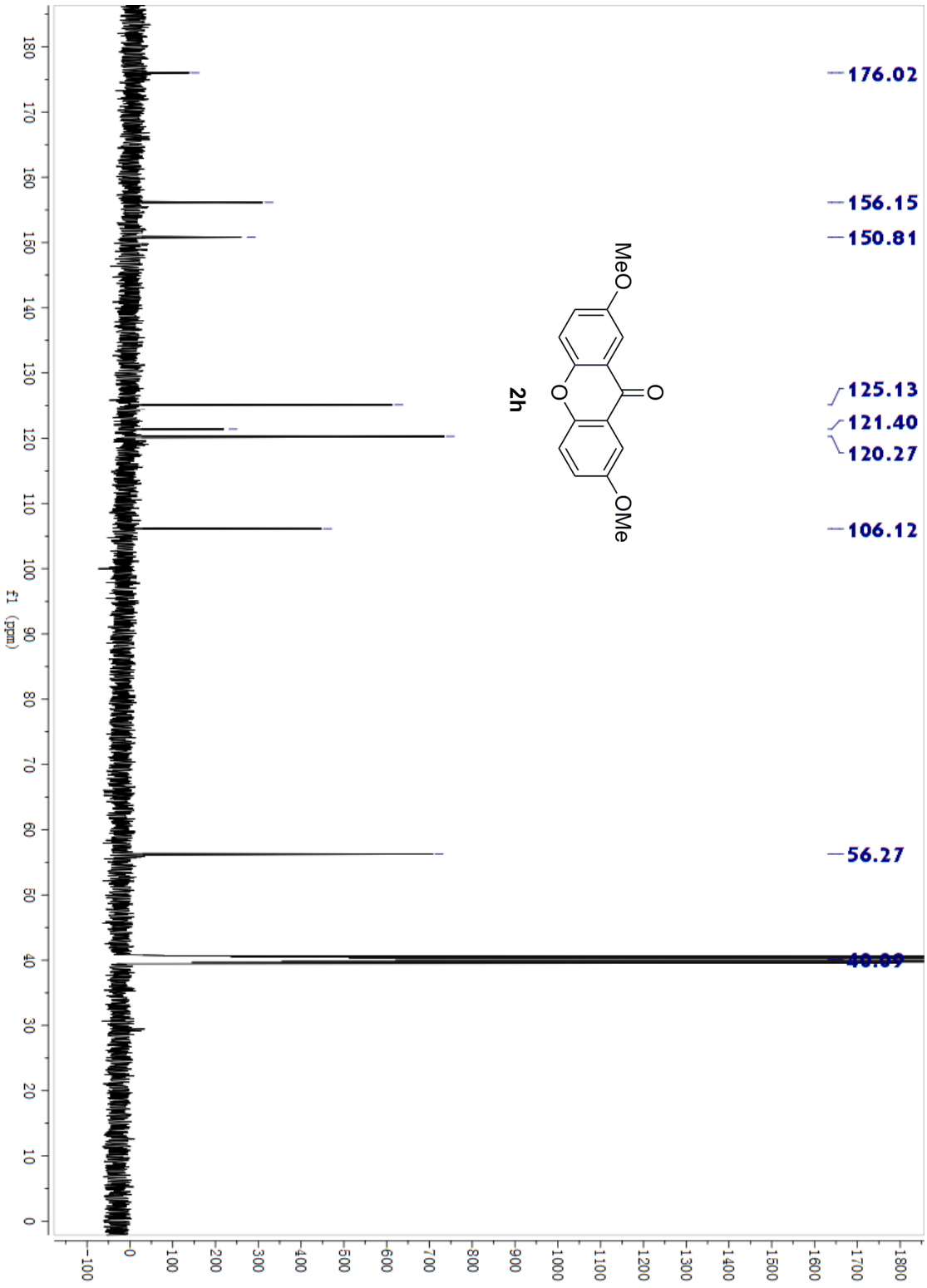
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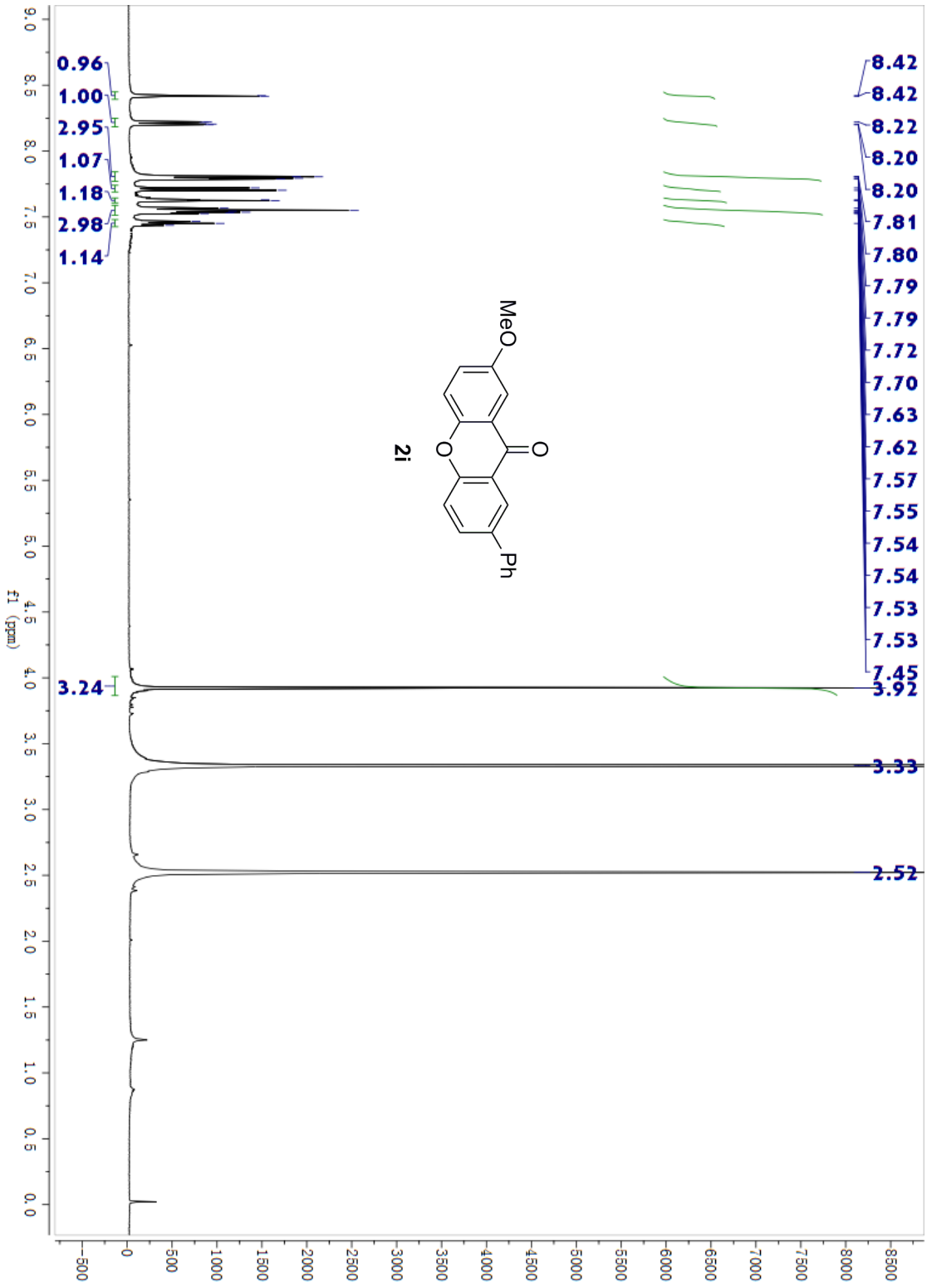
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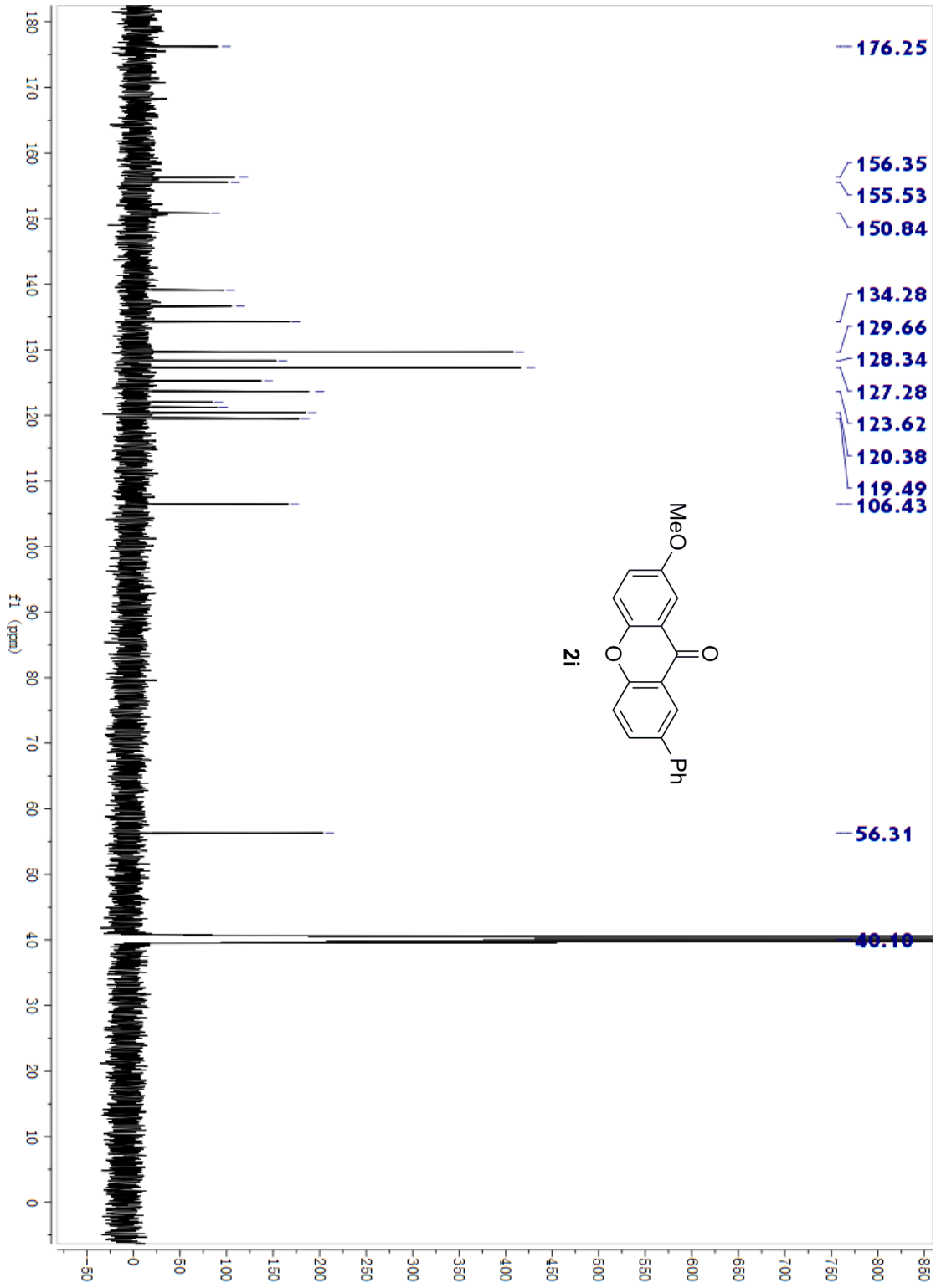
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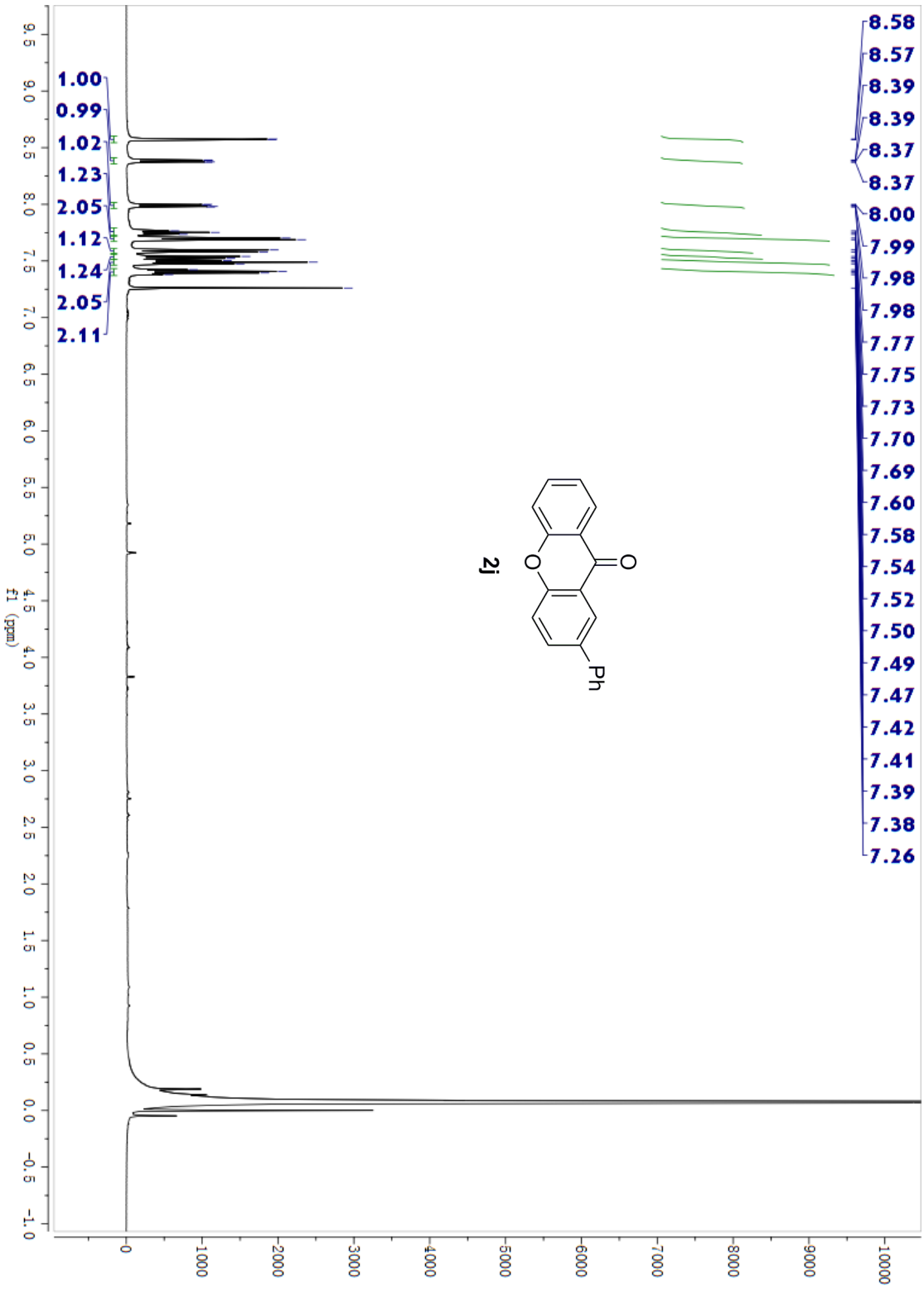
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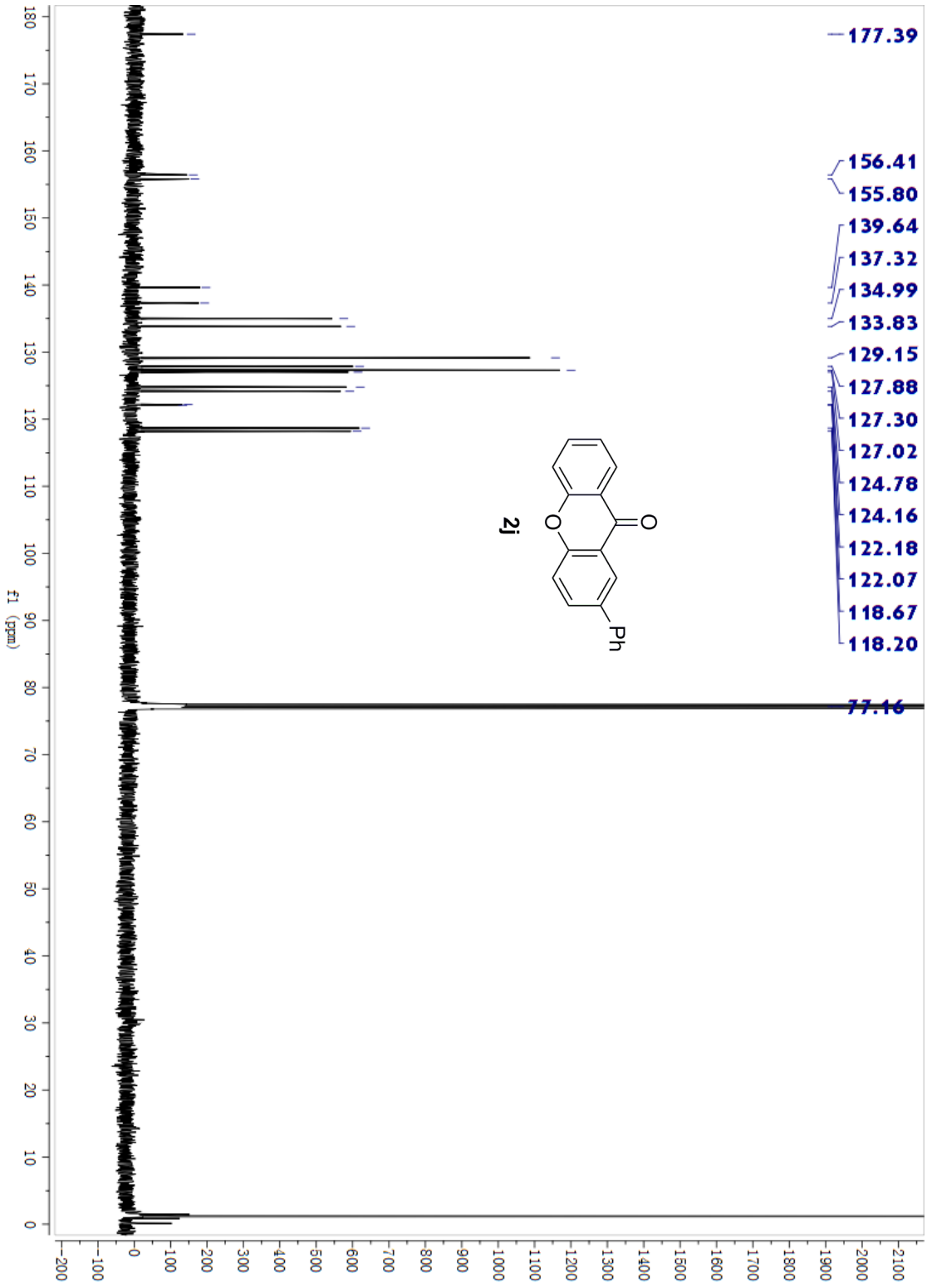
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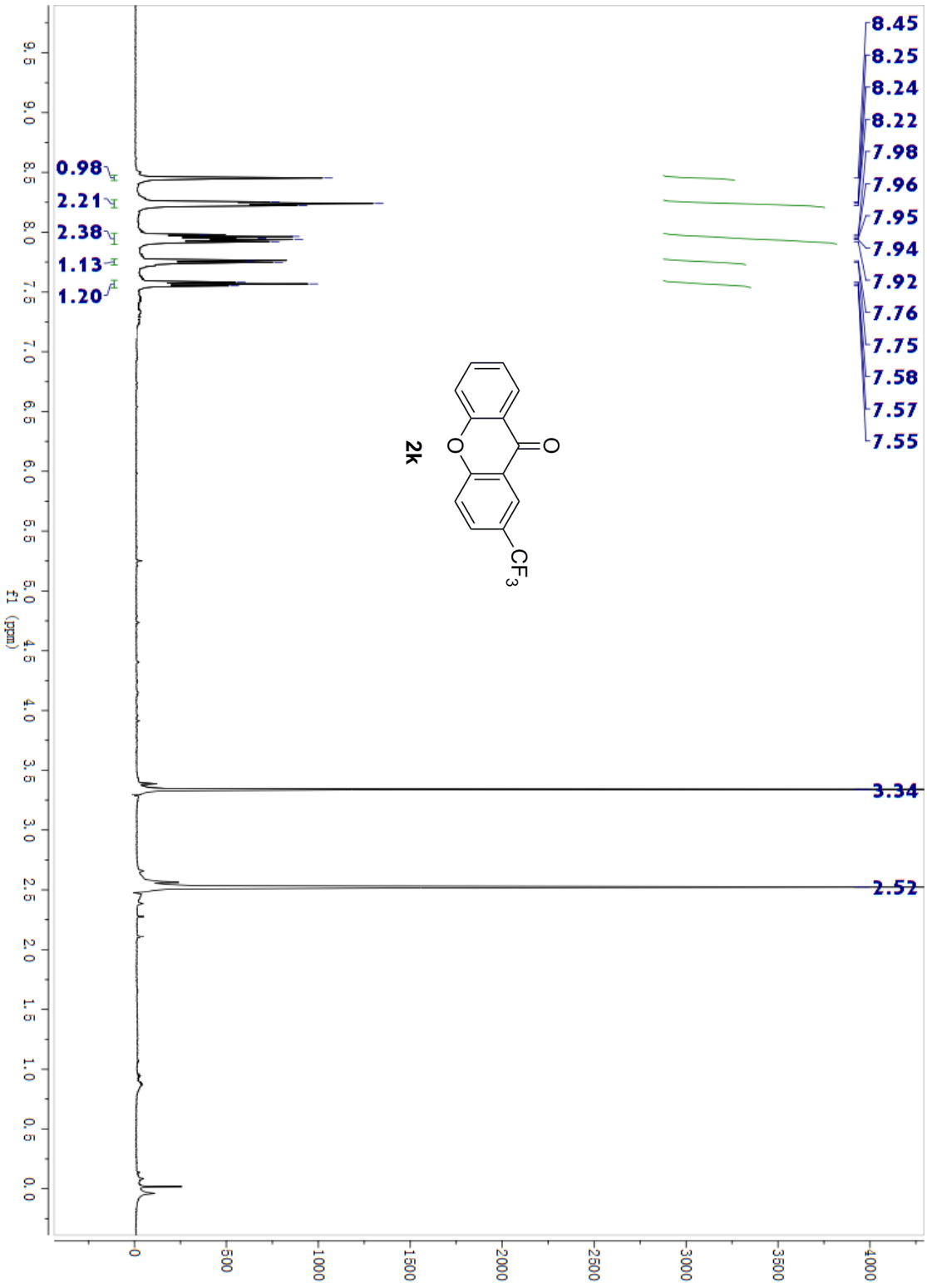
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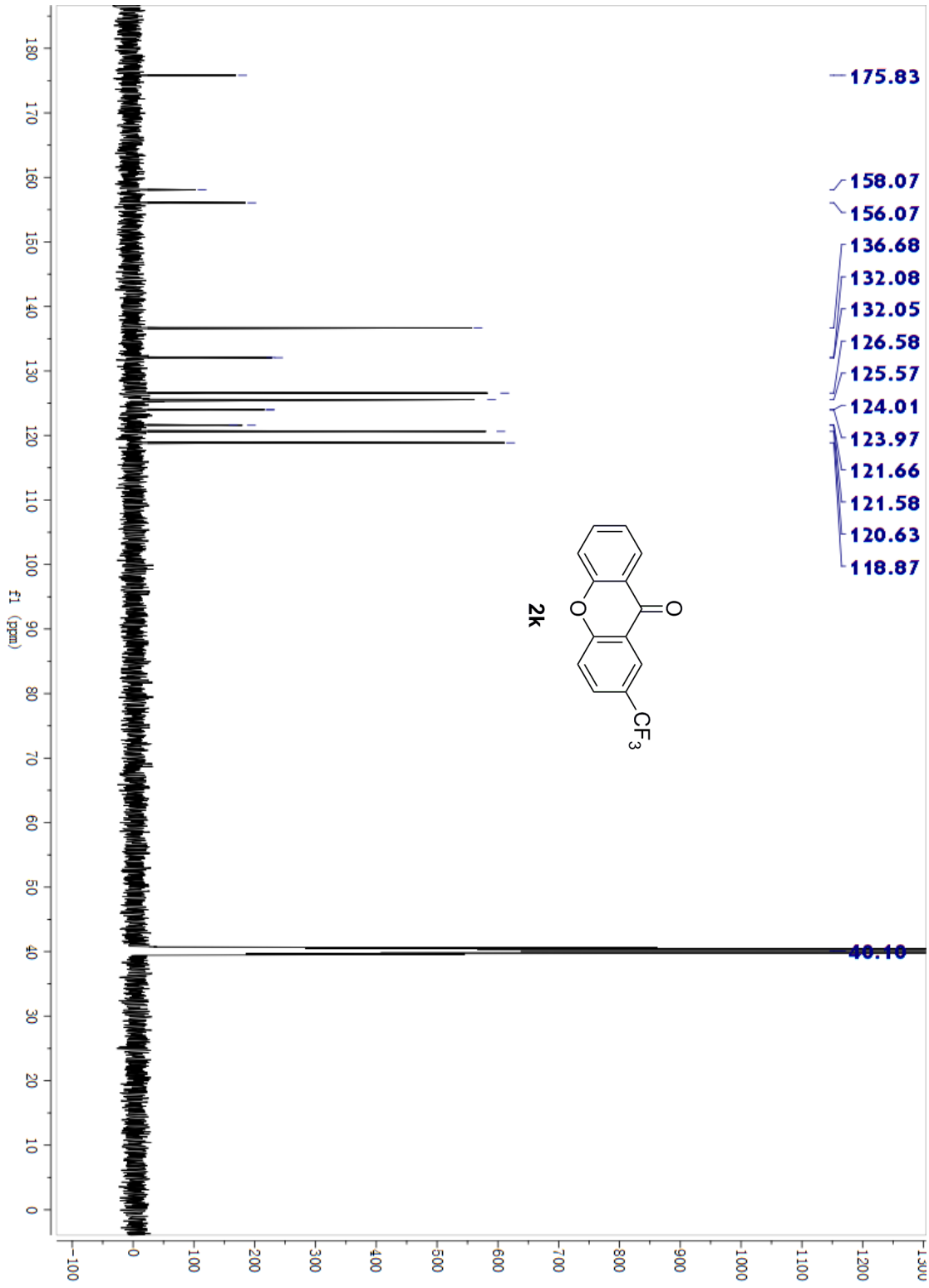
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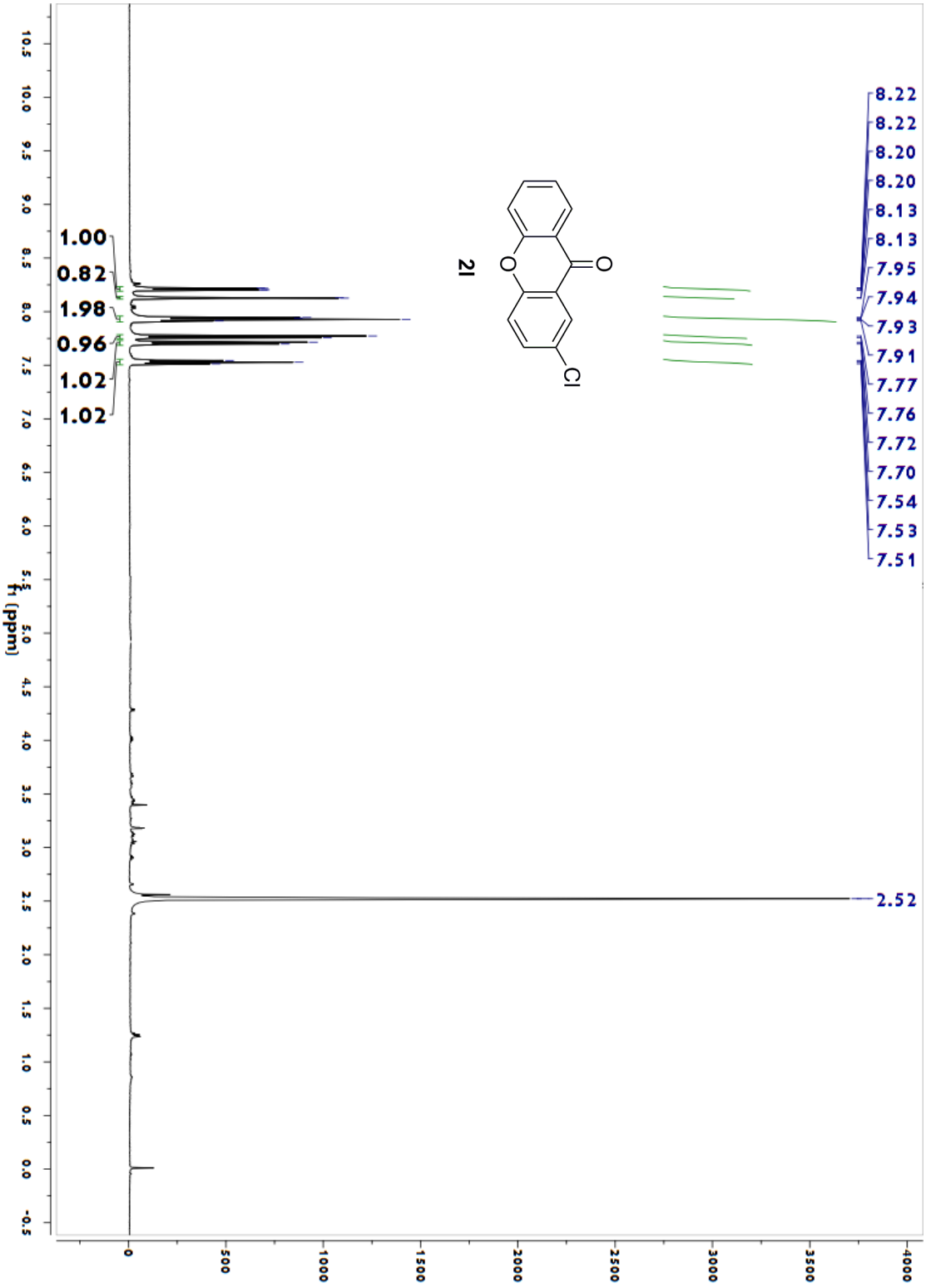
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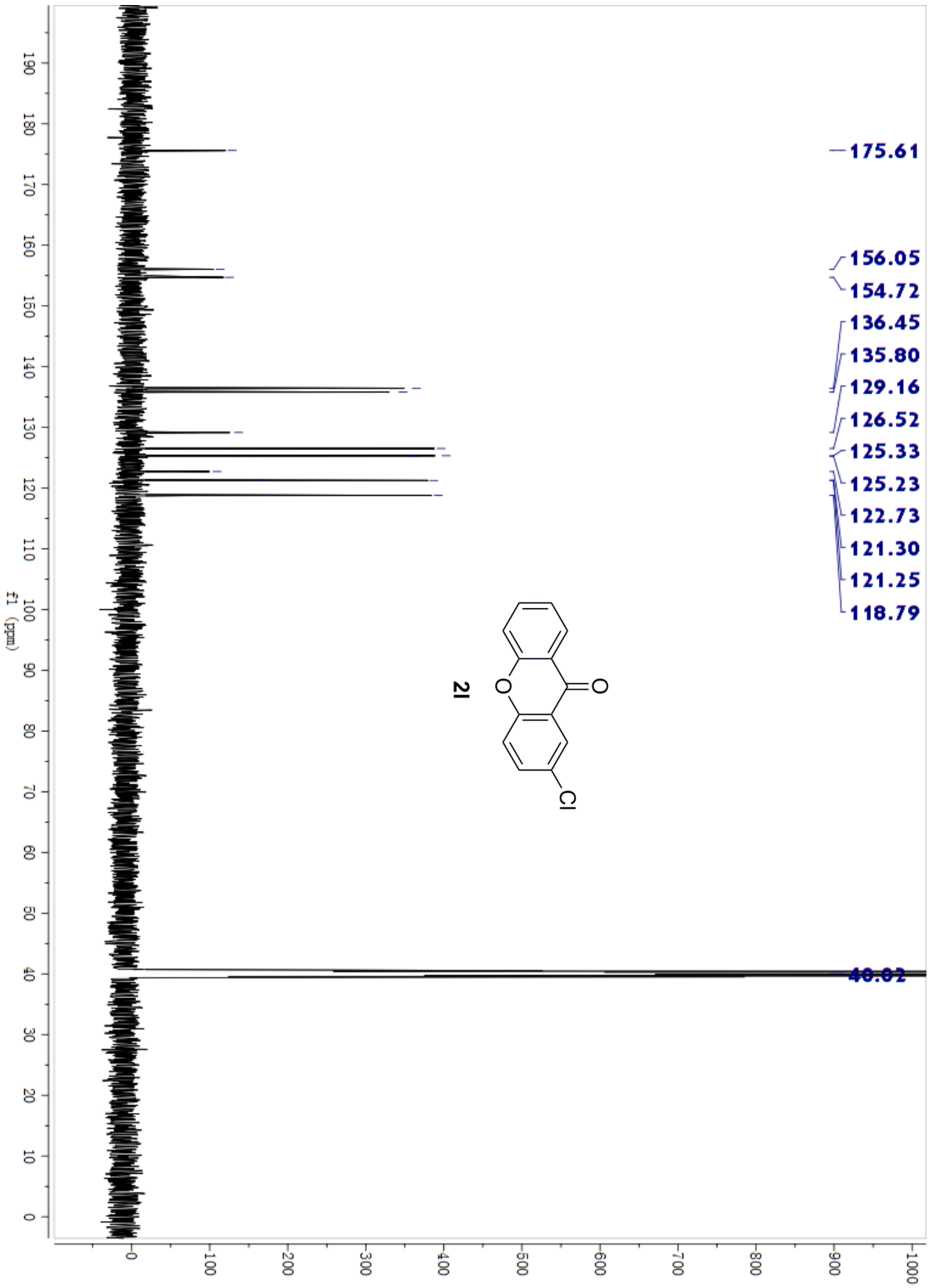
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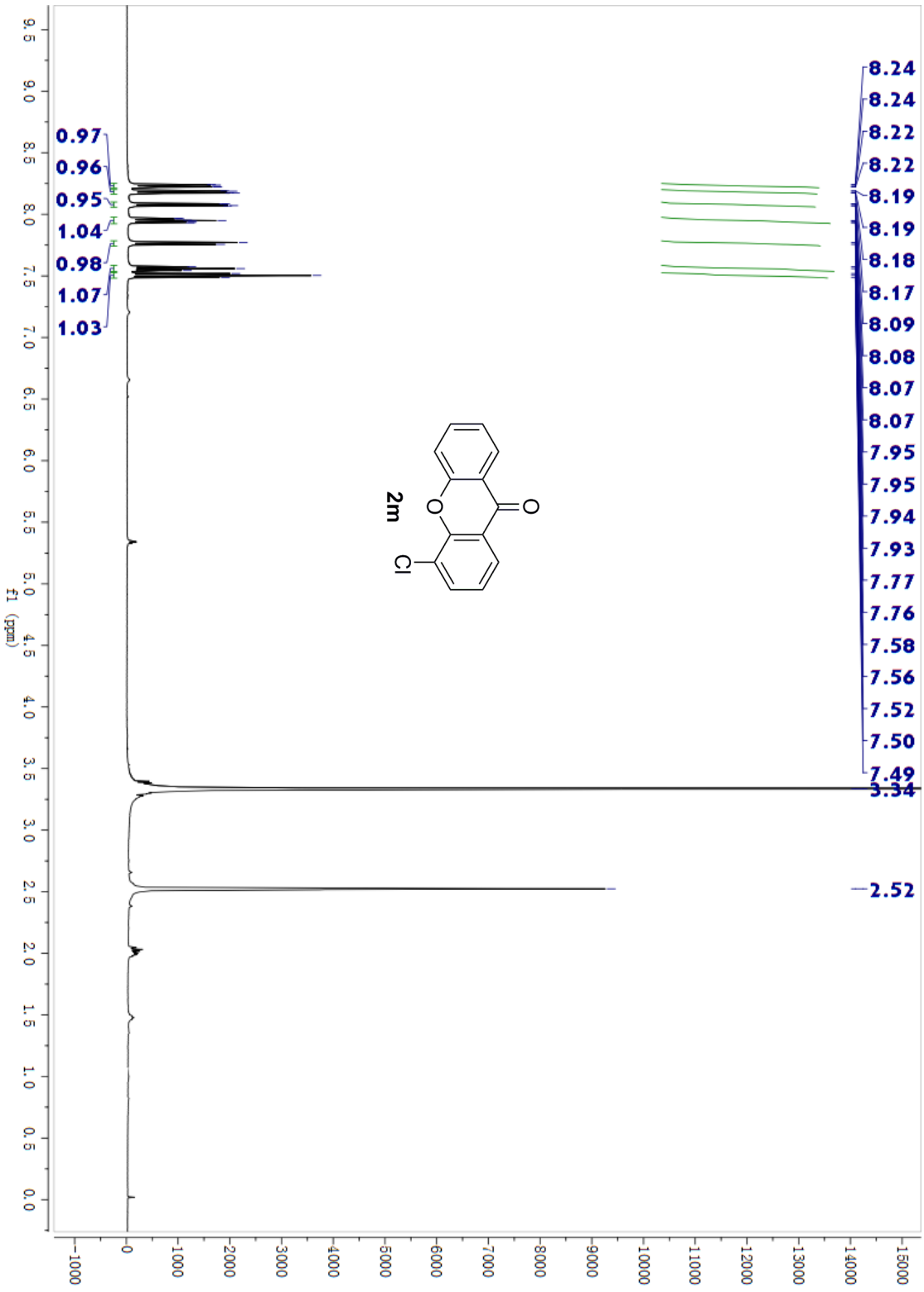
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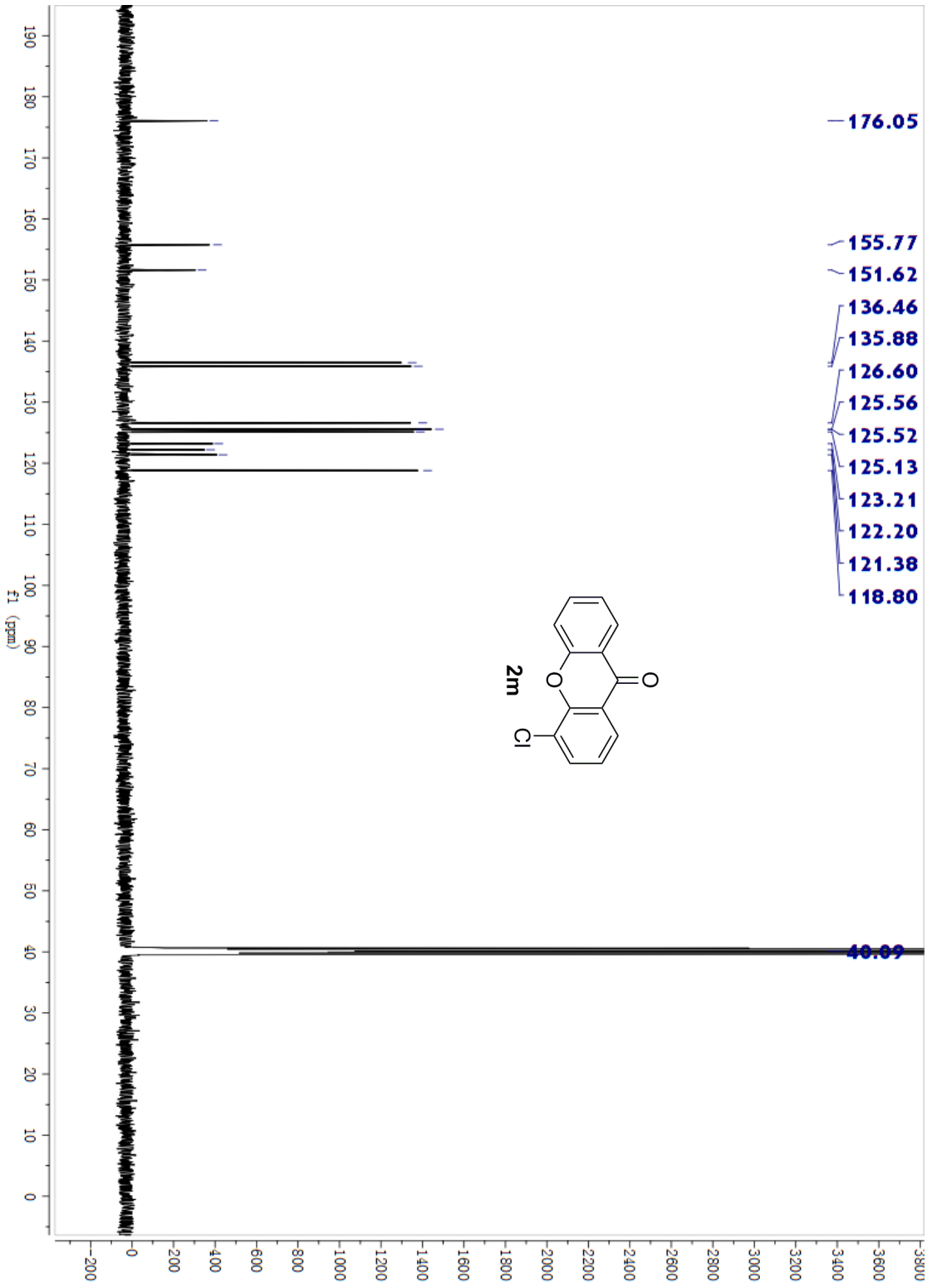
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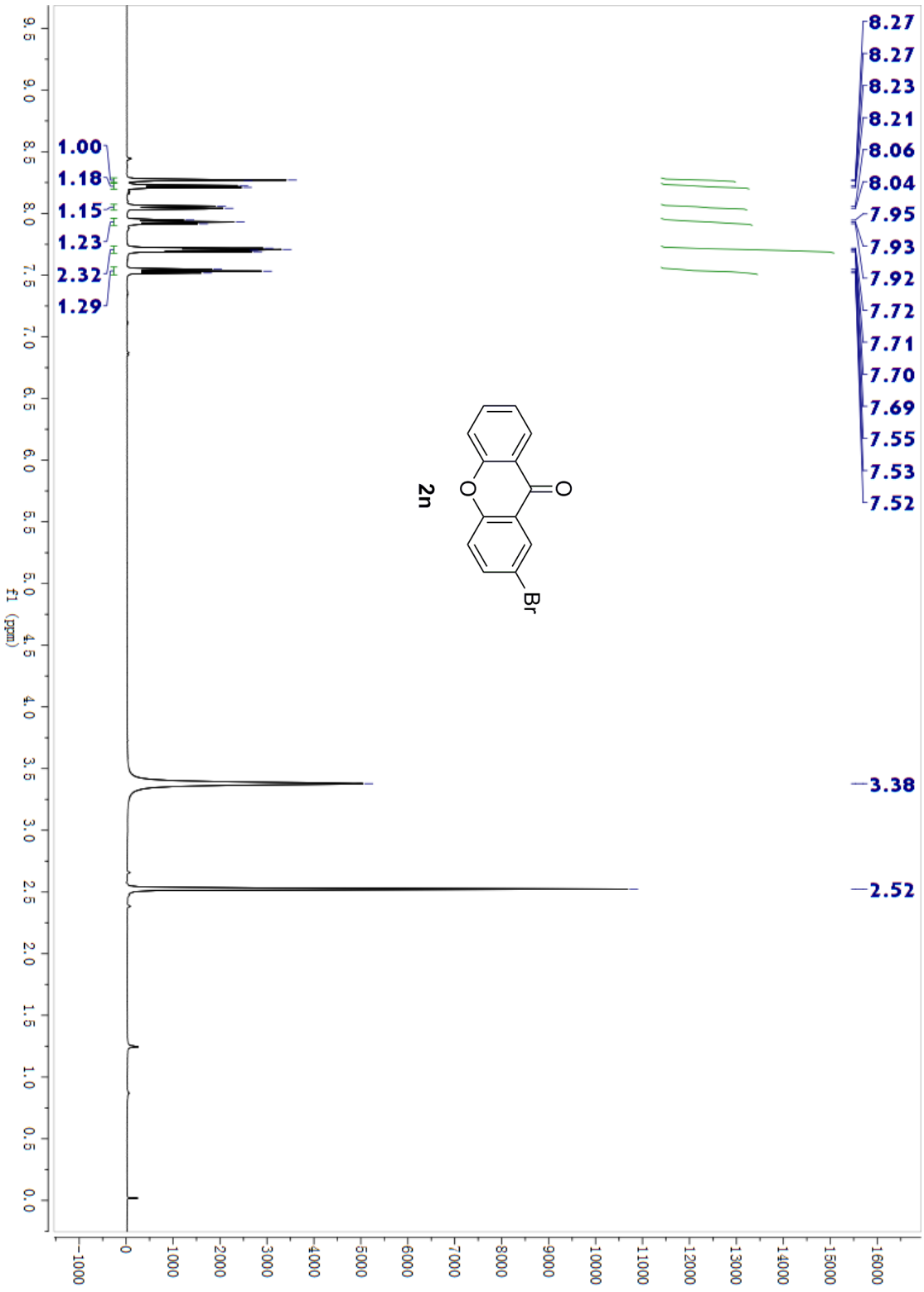
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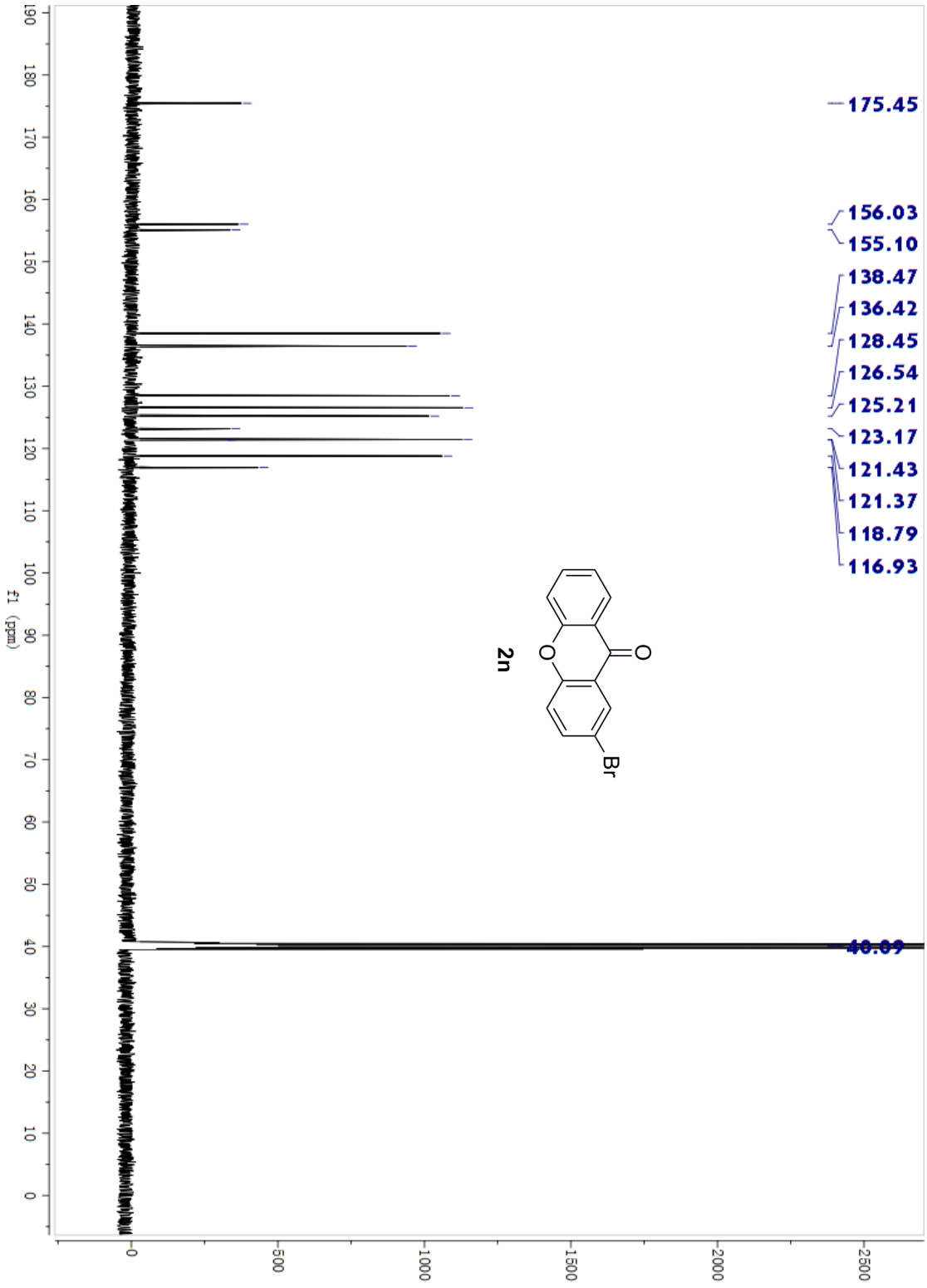
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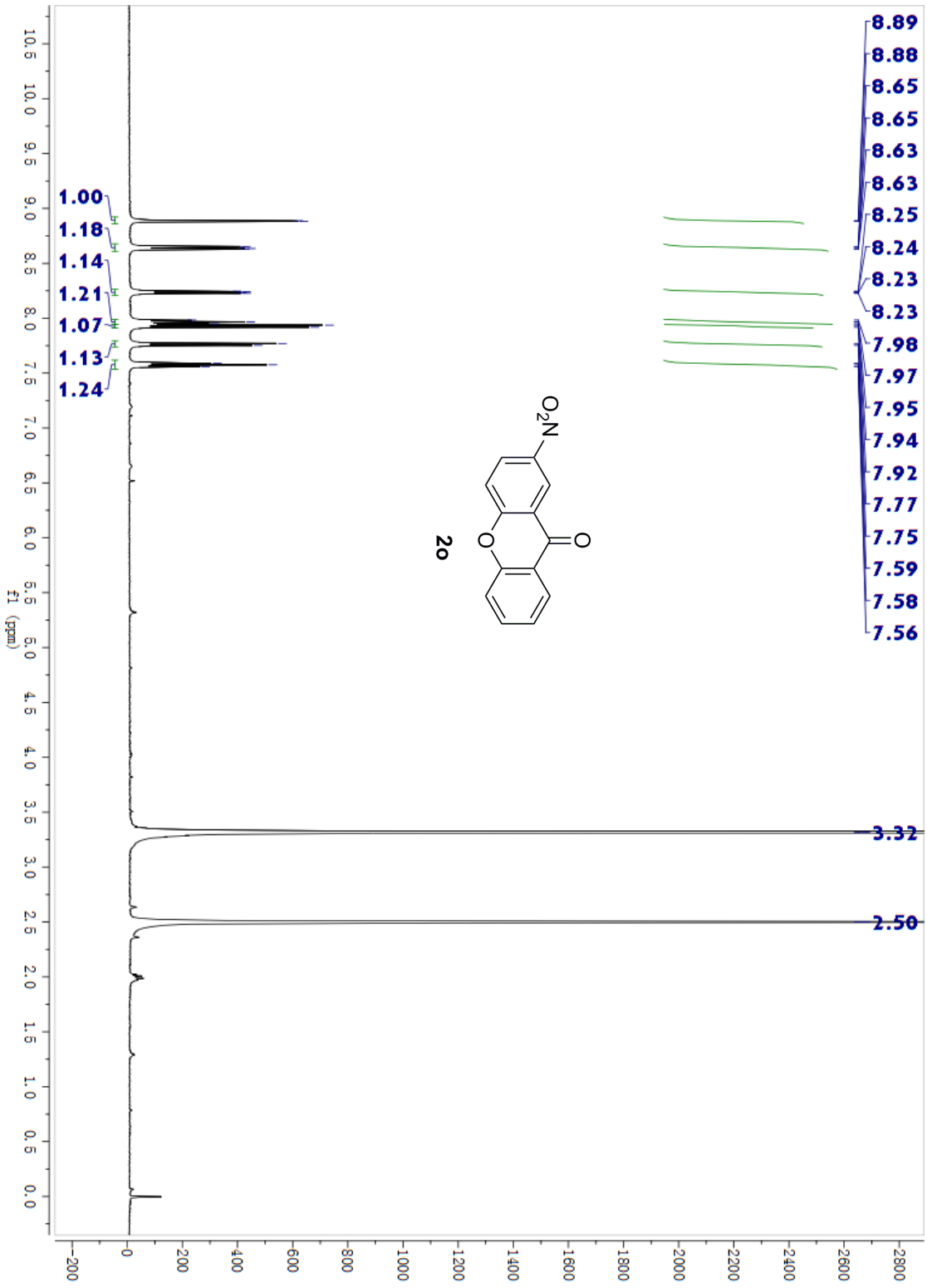
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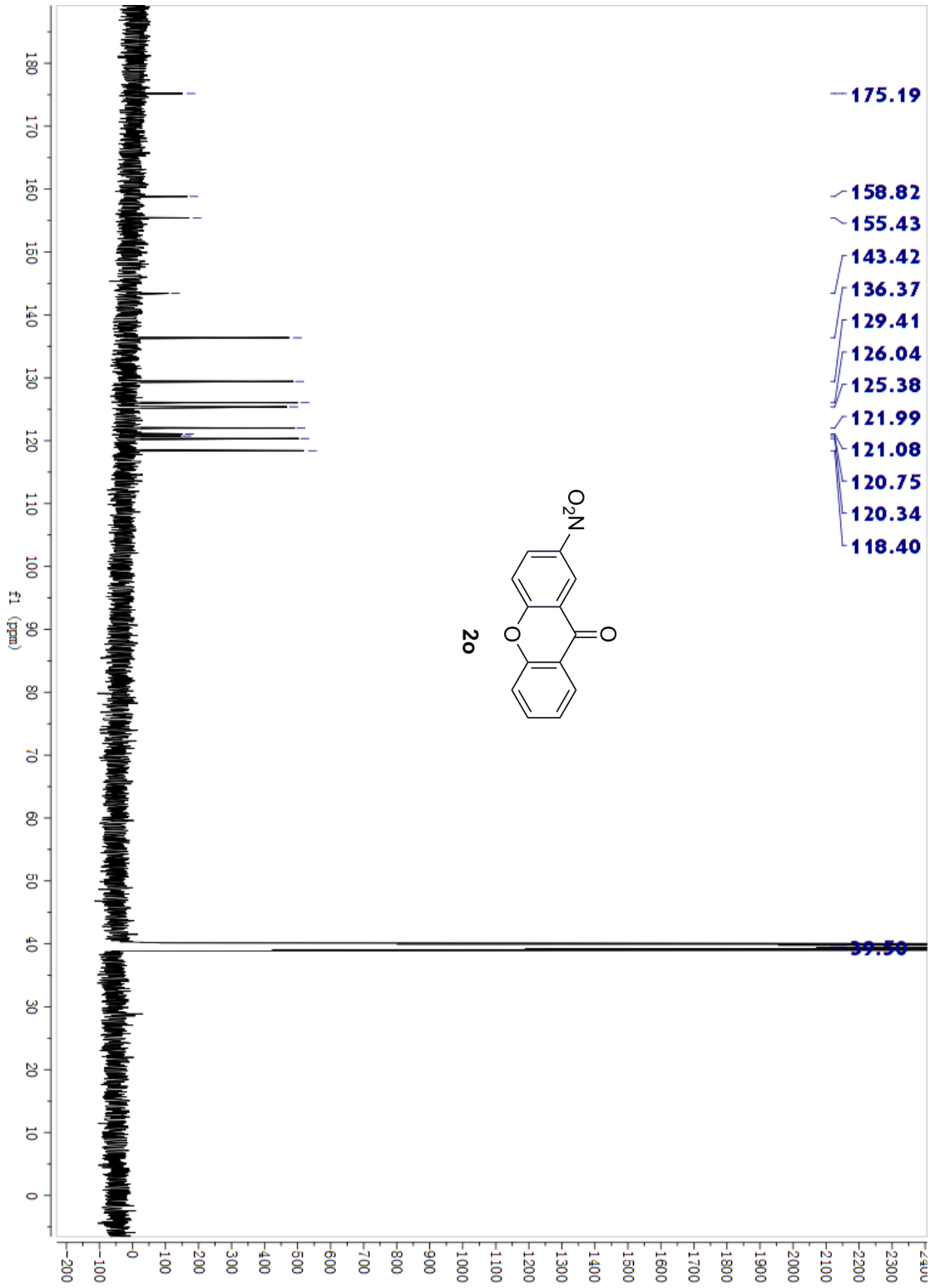
f1 (ppm)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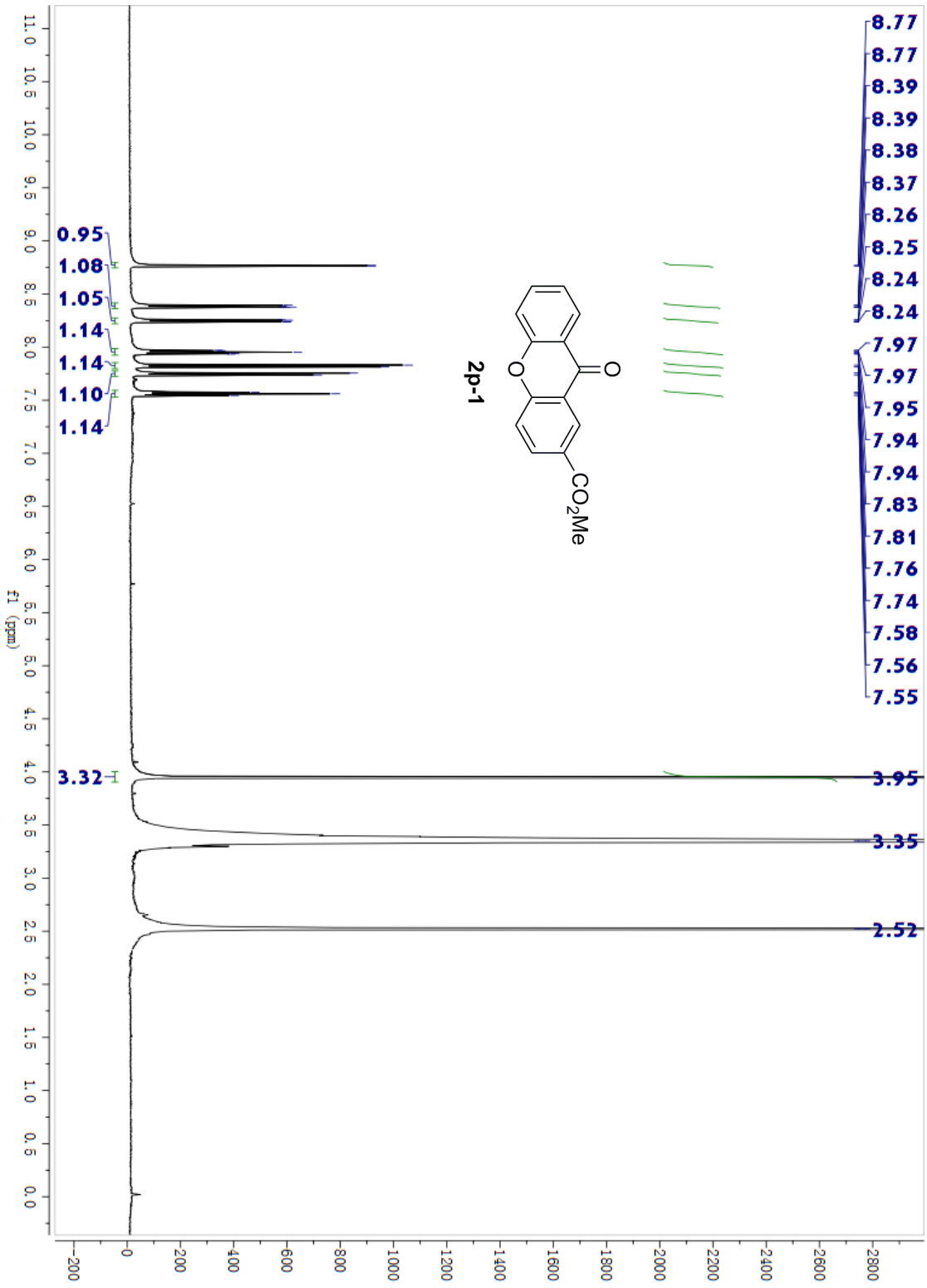
158.82
155.43
143.42
136.37
129.41
126.04
125.38
121.99
121.08
120.75
120.34
118.40
39.50
O2N
O
O
2o
f1 (ppm)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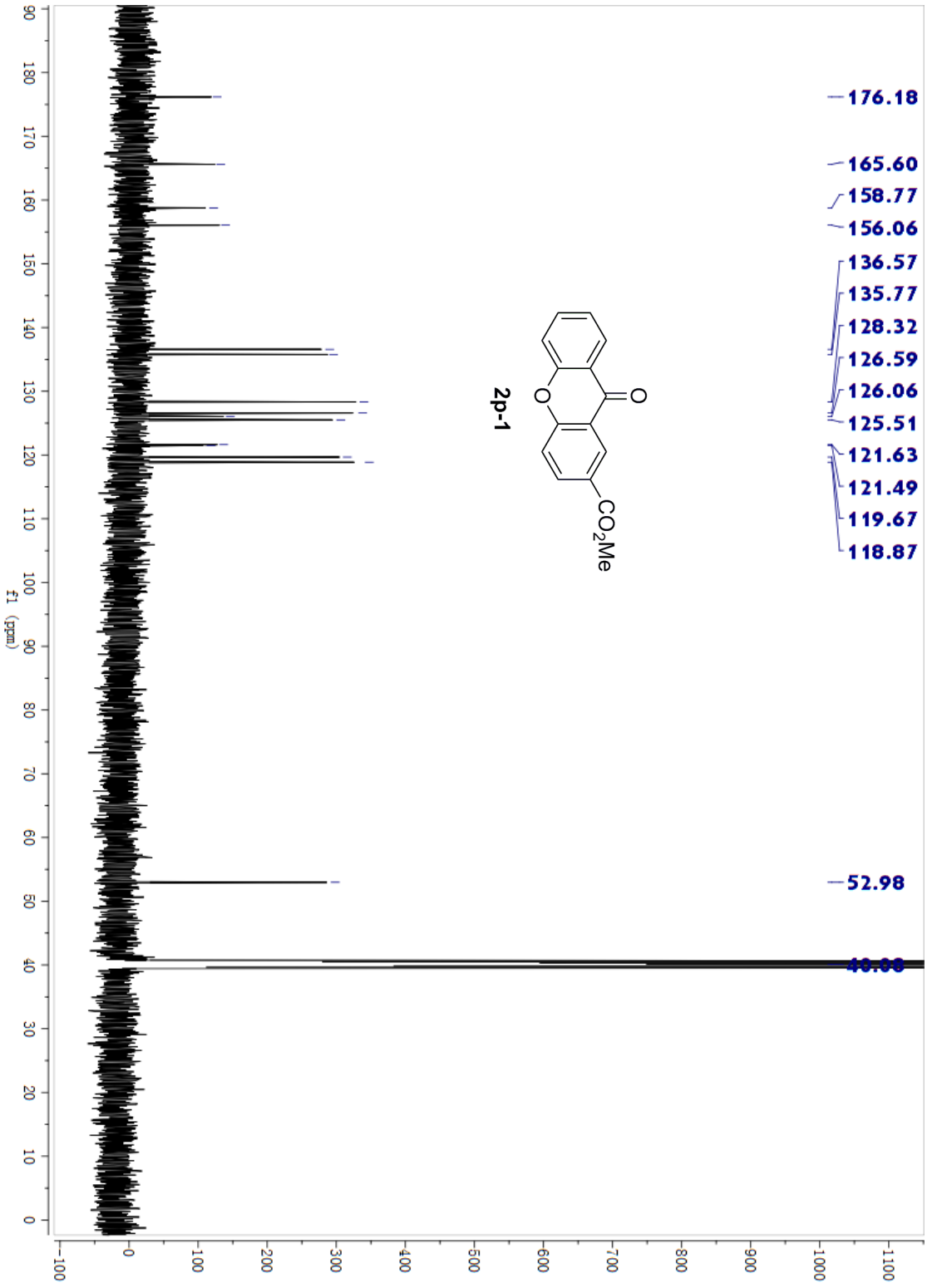
8.77
8.39
8.39
8.38
8.37
8.26
8.25
8.24
8.24
7.97
7.97
7.95
7.94
7.94
7.83
7.81
7.76
7.74
7.58
7.56
7.55
0.95
1.08
1.05
1.14
1.14
1.10
1.14
3.32
3.95
3.35
2.52
2p-1
O
O
CO2Me
f1 (ppm)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165.60
158.77
156.06
136.57
135.77
128.32
126.59
126.06
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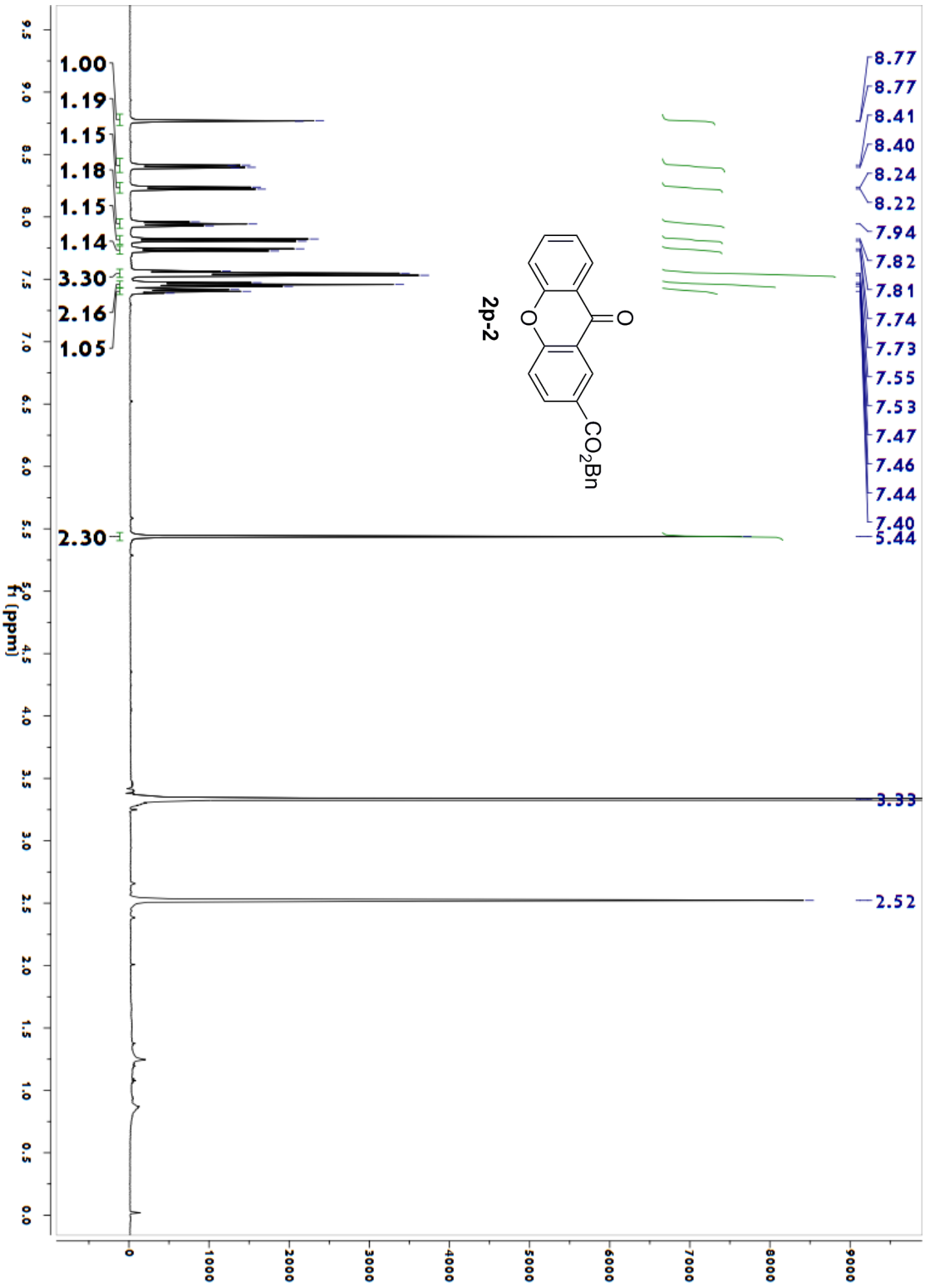
121.63
121.49
119.67
118.87
52.98
2p-1
O
O
CO2Me
f1 (ppm)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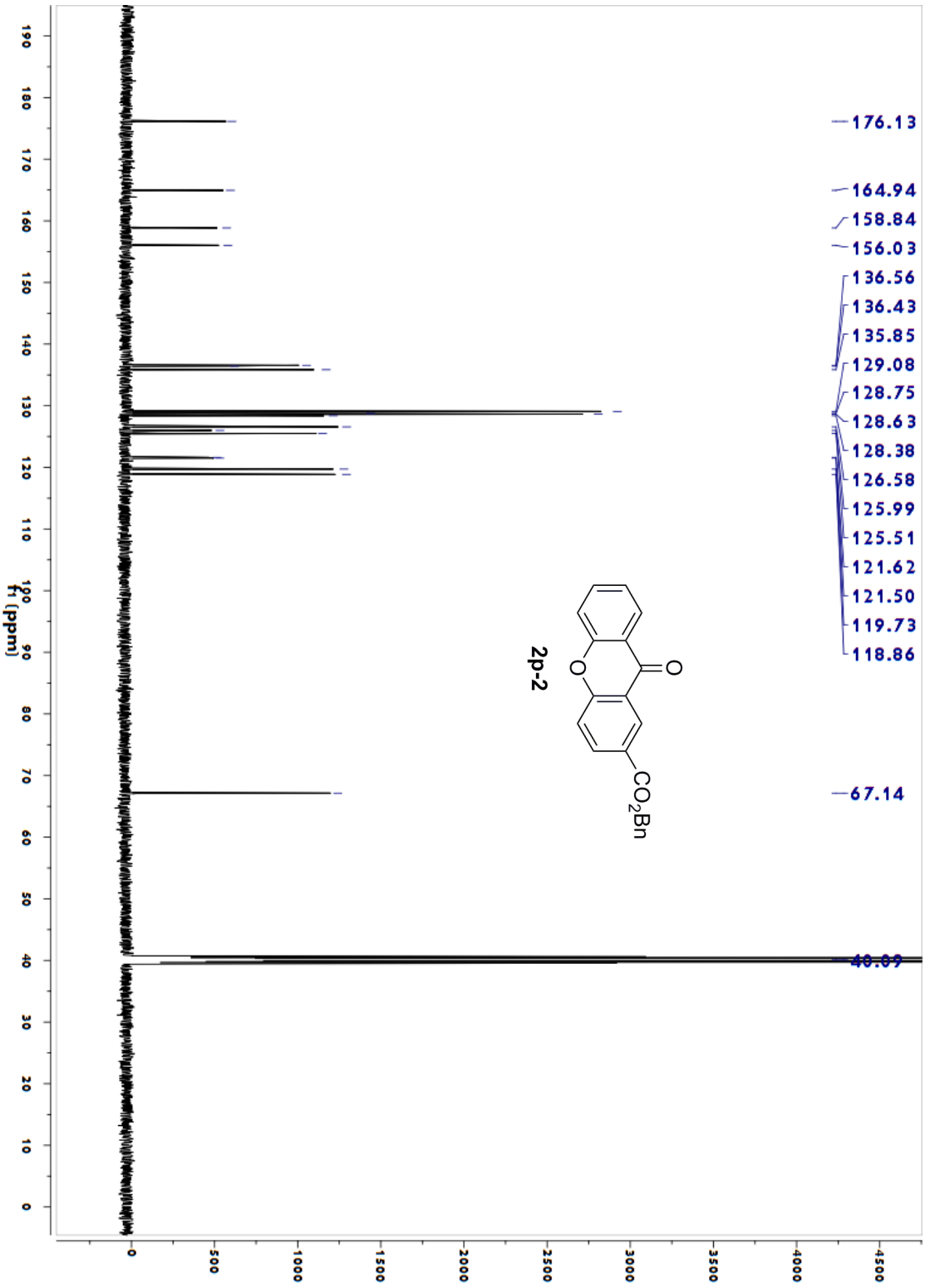
1.19
1.15
1.18
1.15
1.14
3.30
2.16
1.05
2.30
3.33
2.52
8.77
8.77
8.41
8.40
8.24
8.22
7.94
7.82
7.81
7.74
7.73
7.55
7.53
7.47
7.46
7.44
7.40
5.44
2p-2
O
O
CO2Bn
f1 (ppm)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164.94
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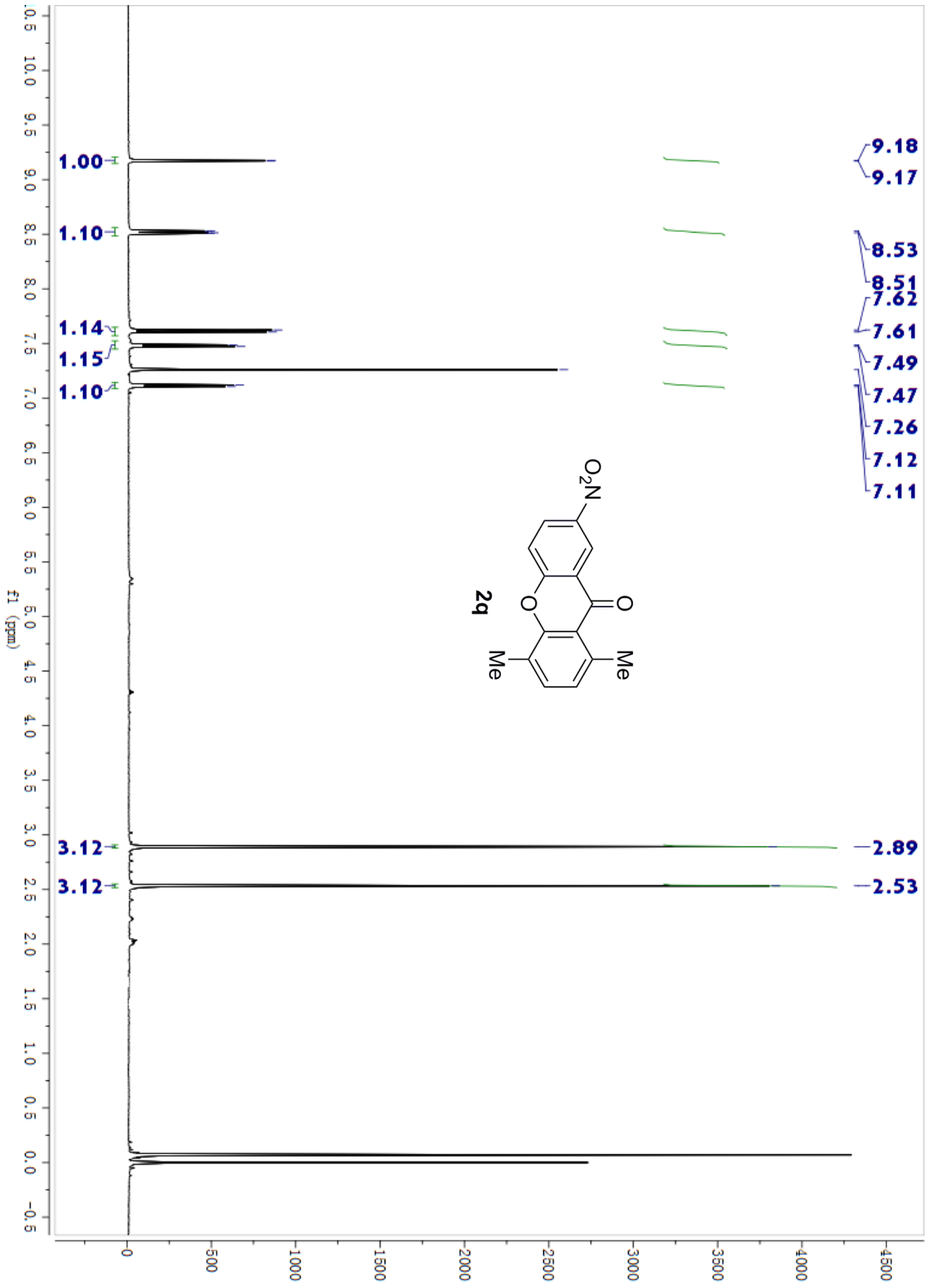
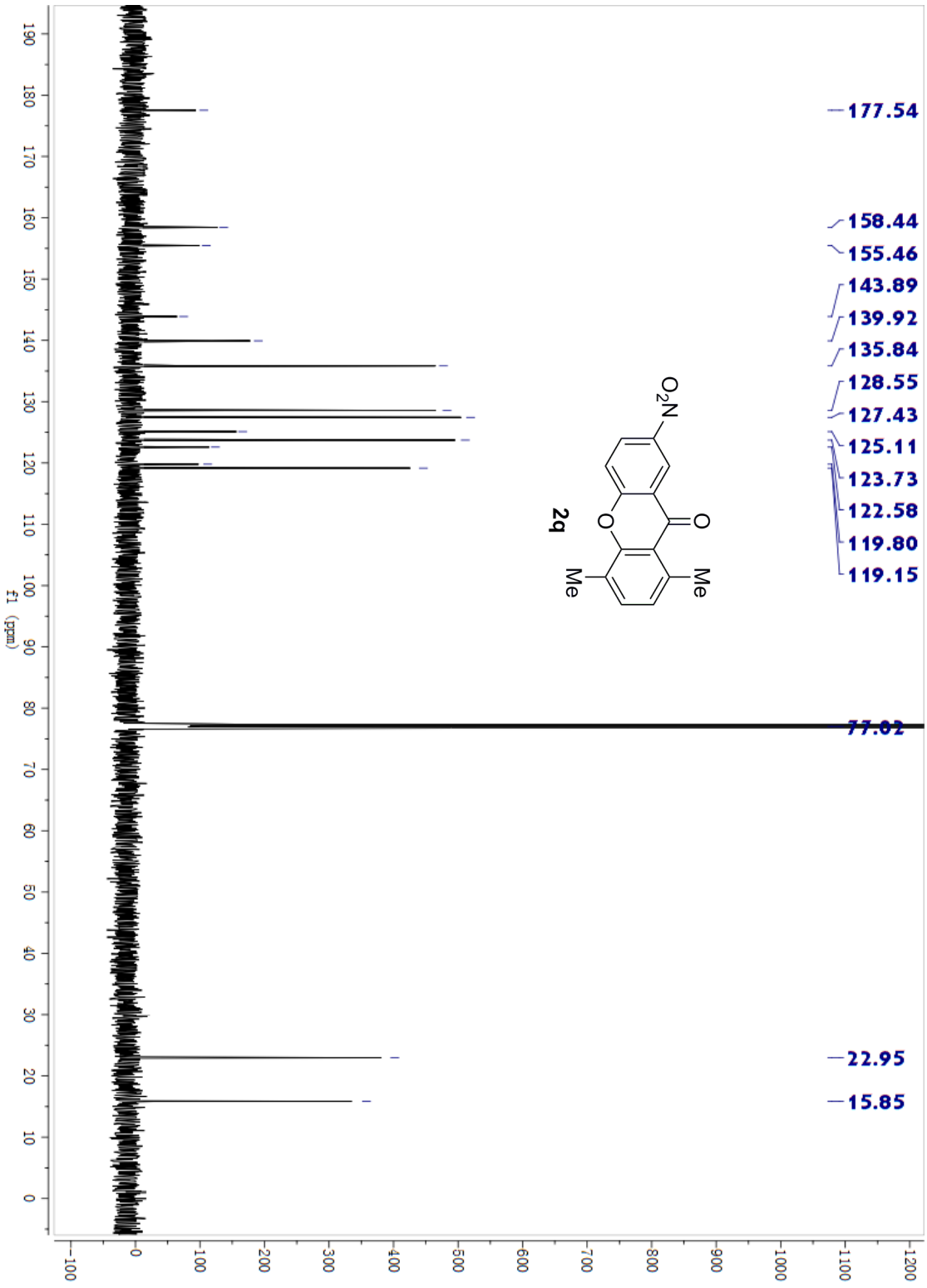
136.56
136.43
135.85
129.08
128.75
128.63
128.38
126.58
125.99
125.51
121.62
121.50
119.73
118.86
67.14
40.09
2p-2
O
O
CO2Bn
f1 (ppm)


9.18
9.17
8.53
8.51
7.62
7.61
7.49
7.47
7.26
7.12
7.11
2.89
2.53
1.00
1.10
1.14
1.15
1.10
3.12
3.12
O2N
O
O
Me
Me
2q
f1 (ppm)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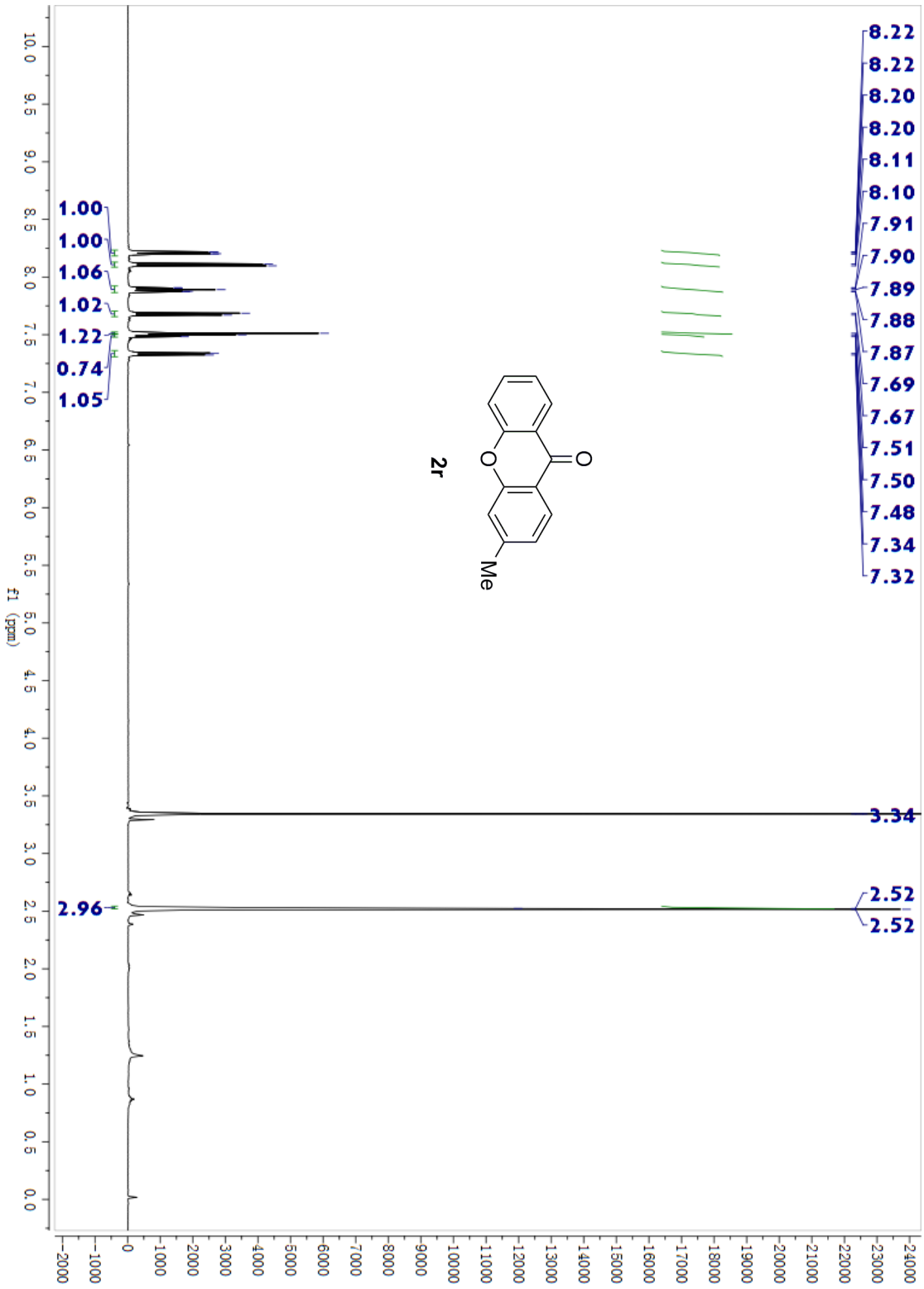
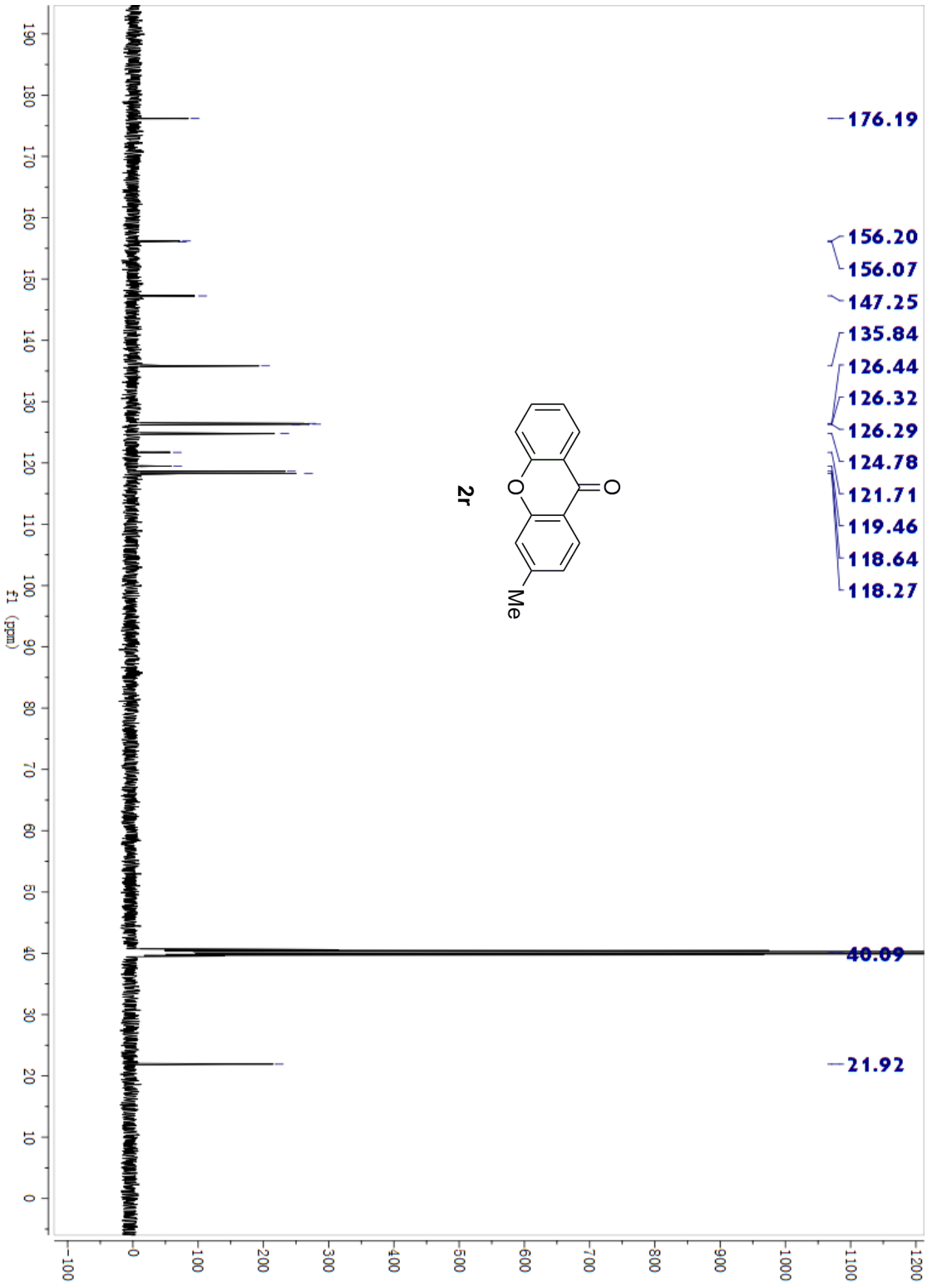
158.44
155.46
143.89
139.92
135.84
128.55
127.43
125.11
123.73
122.58
119.80
119.15
77.02
22.95
15.85
2q
O2N
Me
Me
O
O
f1 (ppm)


8.22
8.22
8.20
8.20
8.11
8.10
7.91
7.90
7.89
7.88
7.87
7.69
7.67
7.51
7.50
7.48
7.34
7.32
1.00
1.00
1.06
1.02
1.22
0.74
1.05
3.34
2.96
2.52
2.52
2r
O
O
Me
f1 (ppm)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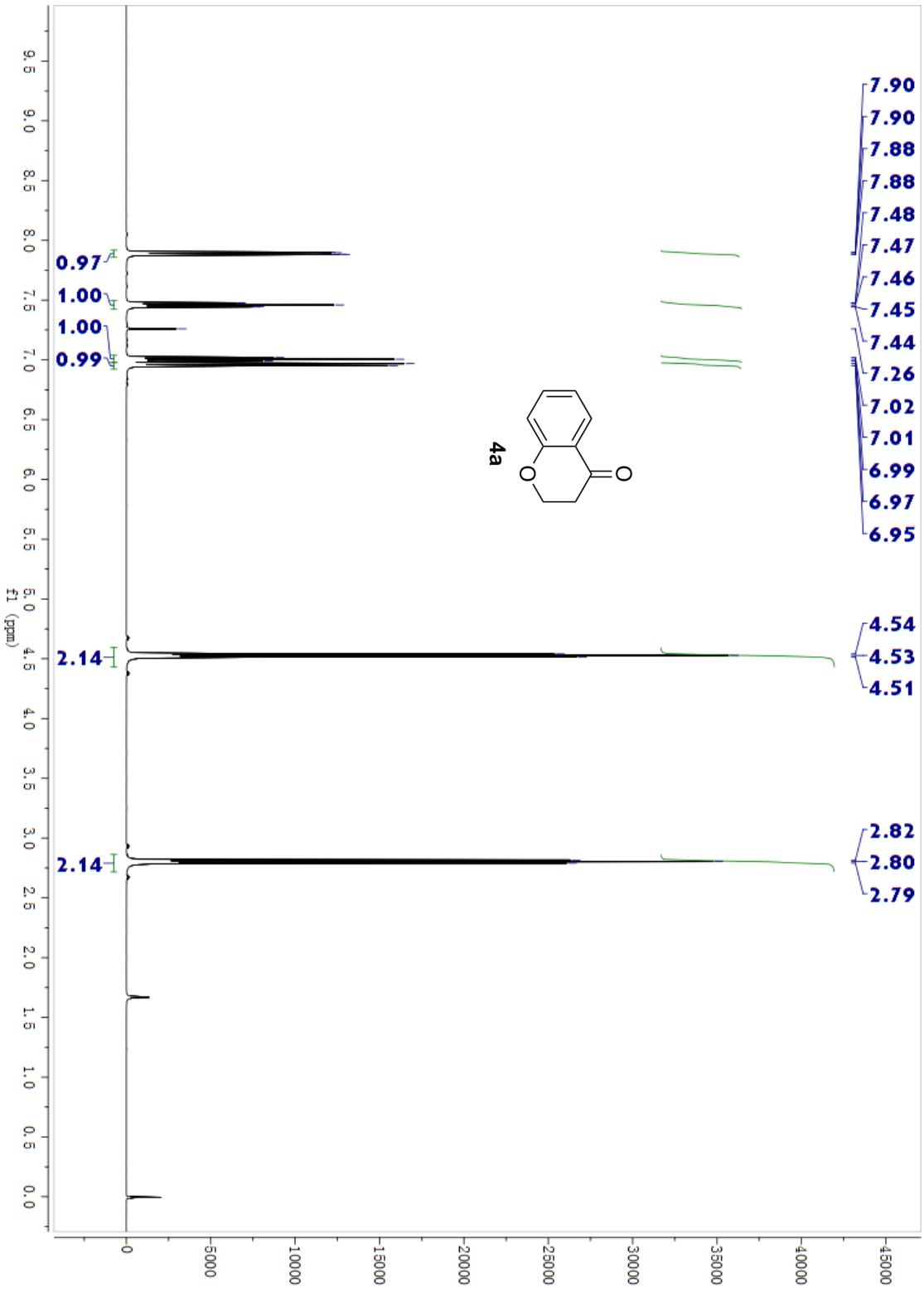
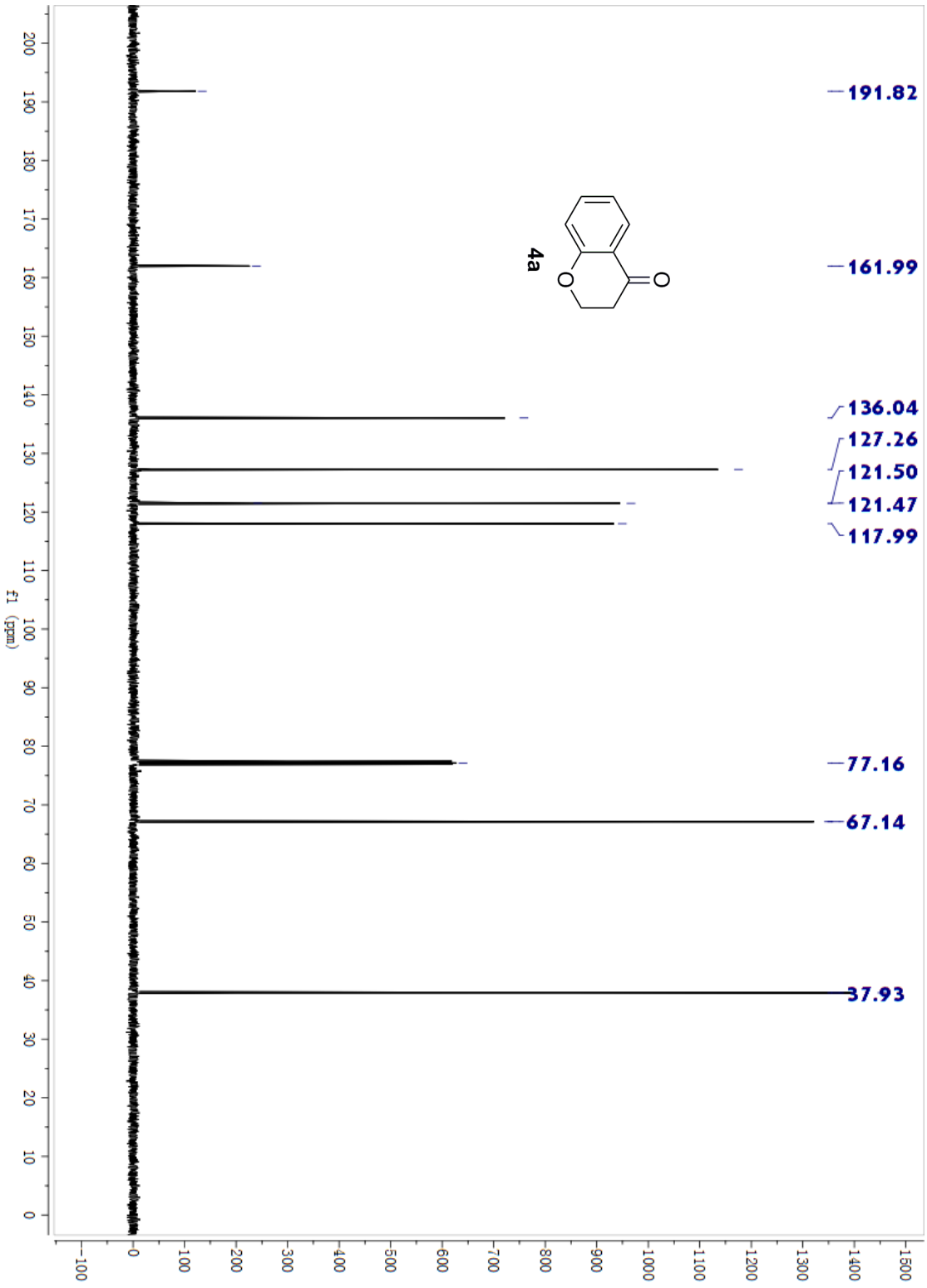
156.20
156.07
147.25
135.84
126.44
126.32
126.29
124.78
121.71
119.46
118.64
118.27
40.09
21.92
2r
O
O
Me
f1 (ppm)


7.90
7.90
7.88
7.88
7.48
7.47
7.46
7.45
7.44
7.26
7.02
7.01
6.99
6.97
6.95
4.54
4.53
4.51
2.82
2.80
2.79
0.97
1.00
1.00
0.99
2.14
2.14
4a
f1 (ppm)


191.82
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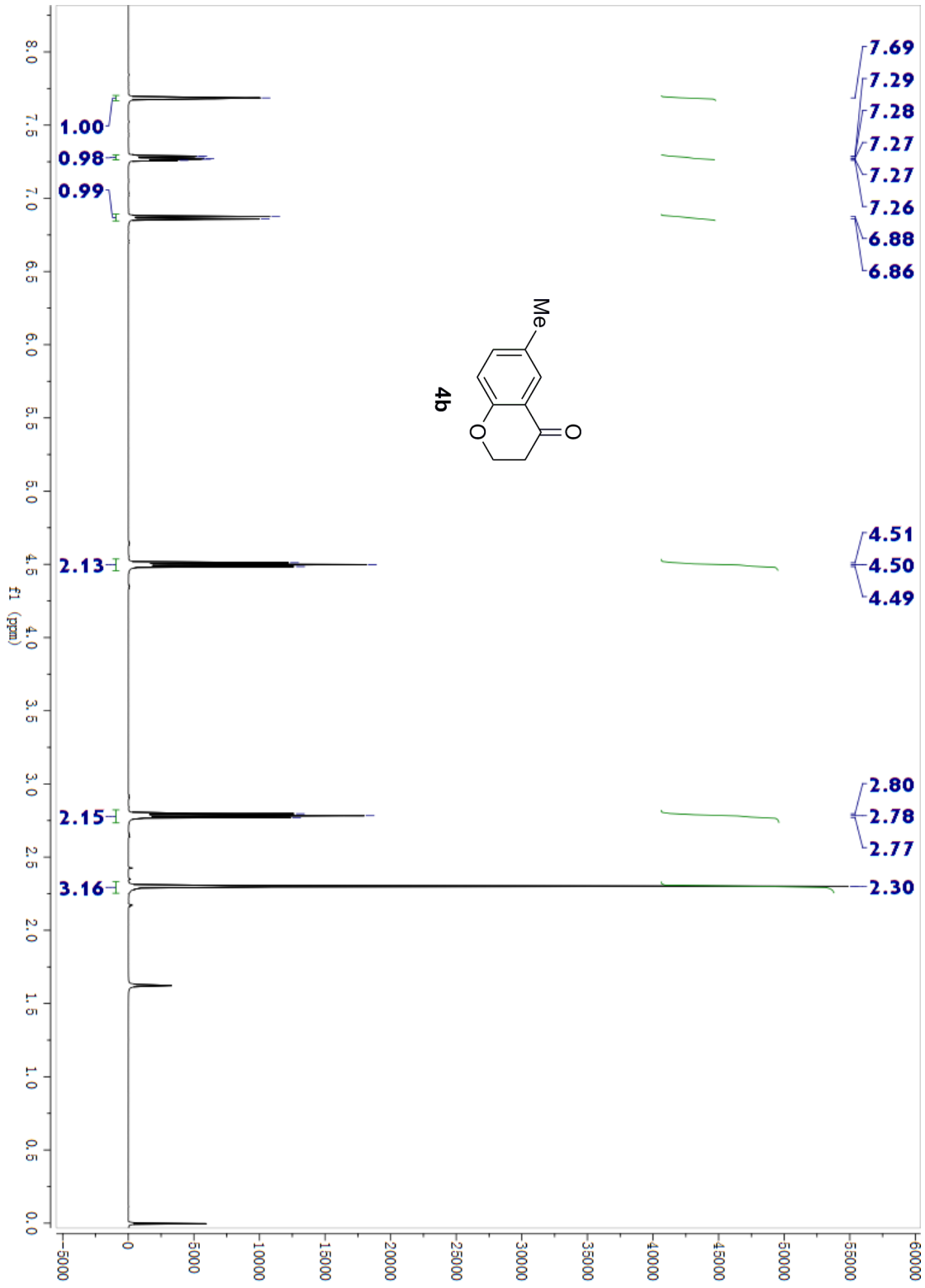
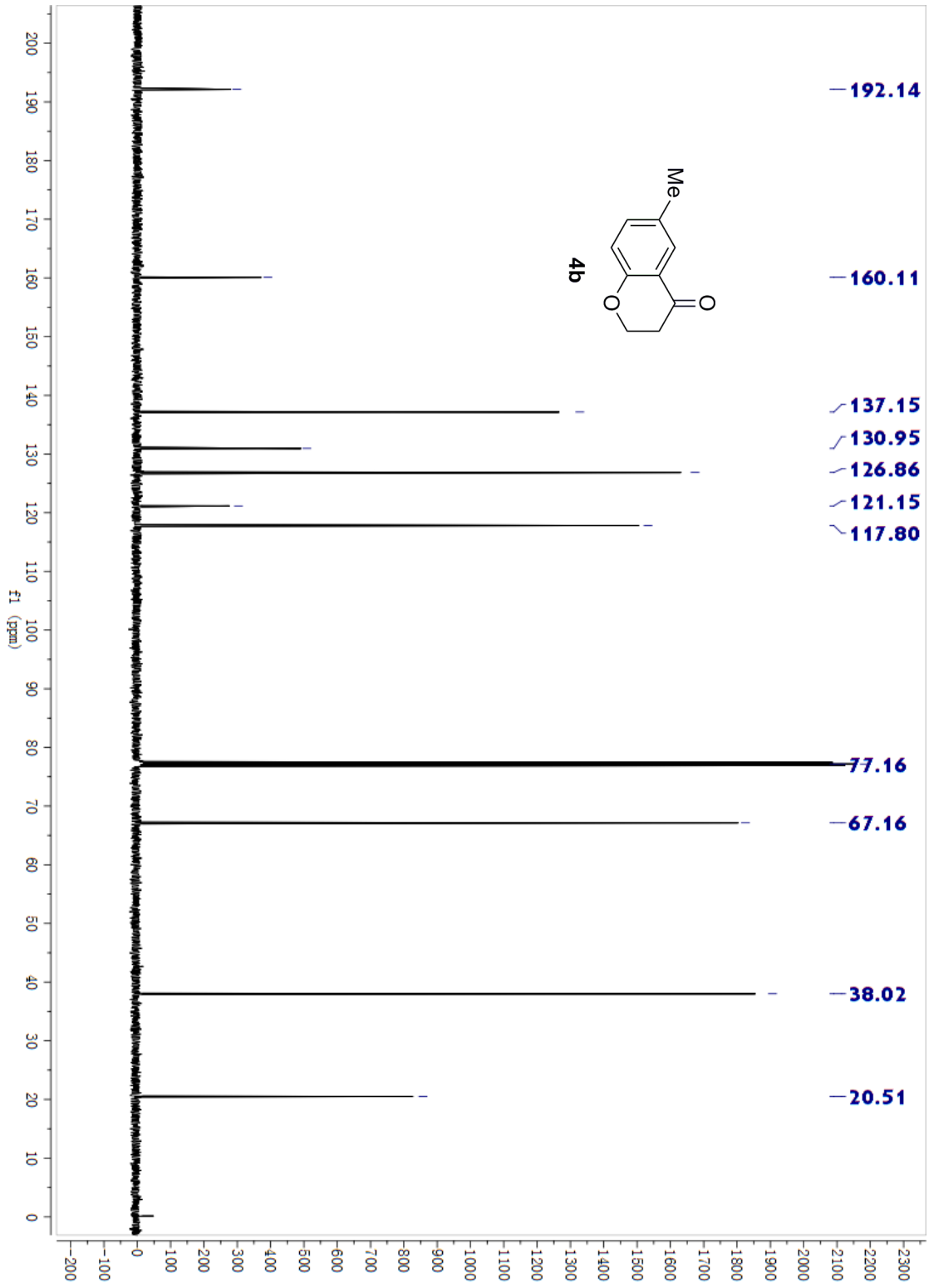
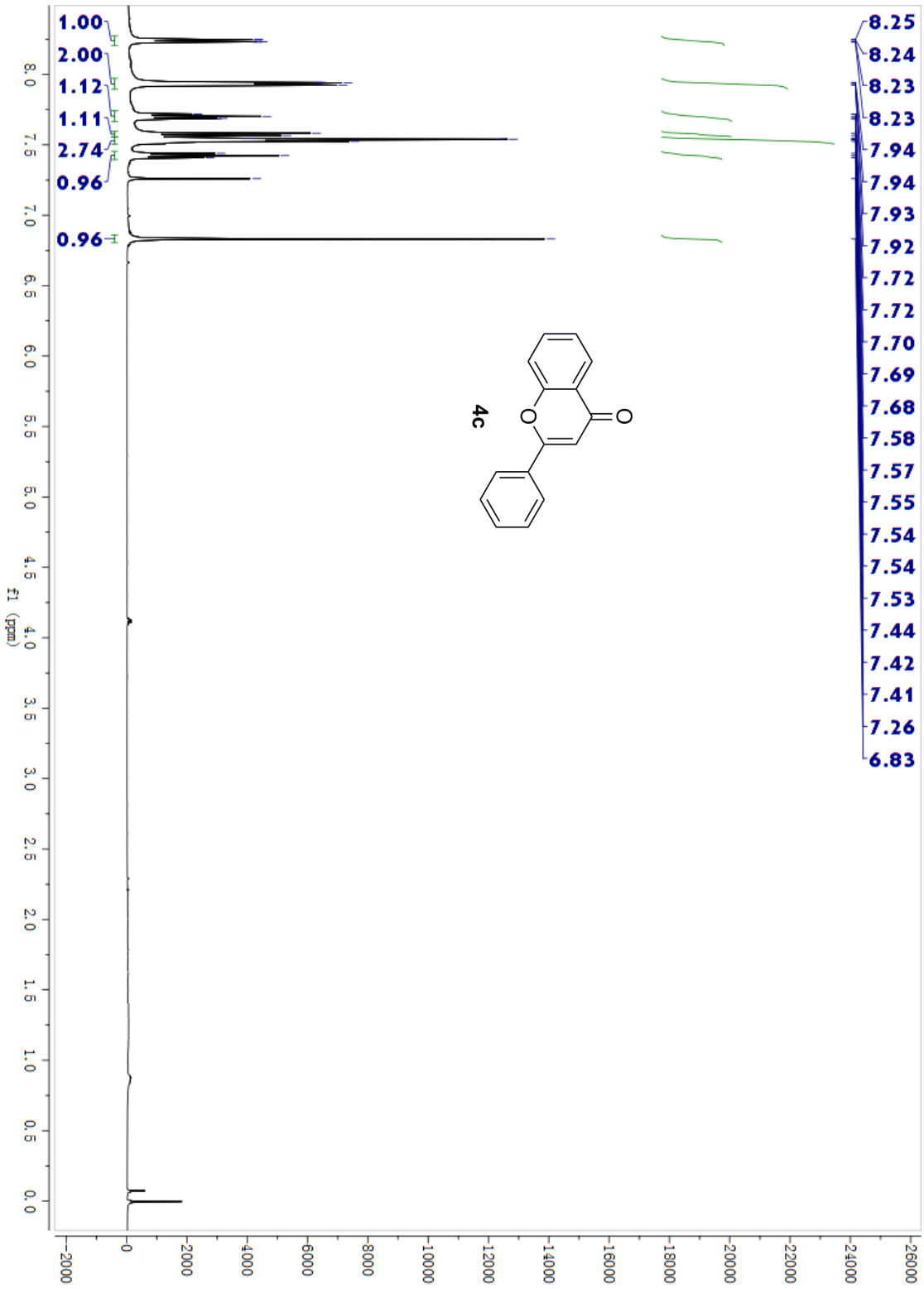
136.04
127.26
121.50
121.47
117.99
77.16
67.14
37.93
4a
f1 (ppm)


7.69
7.29
7.28
7.27
7.27
7.26
6.88
6.86
4.51
4.50
4.49
2.80
2.78
2.77
2.30
1.00
0.98
0.99
2.13
2.15
3.16
Me
O
O
4b
f1 (ppm)


192.14
160.11
137.15
130.95
126.86
121.15
117.80
77.16
67.16
38.02
20.51
4b
Me
O
O
f1 (ppm)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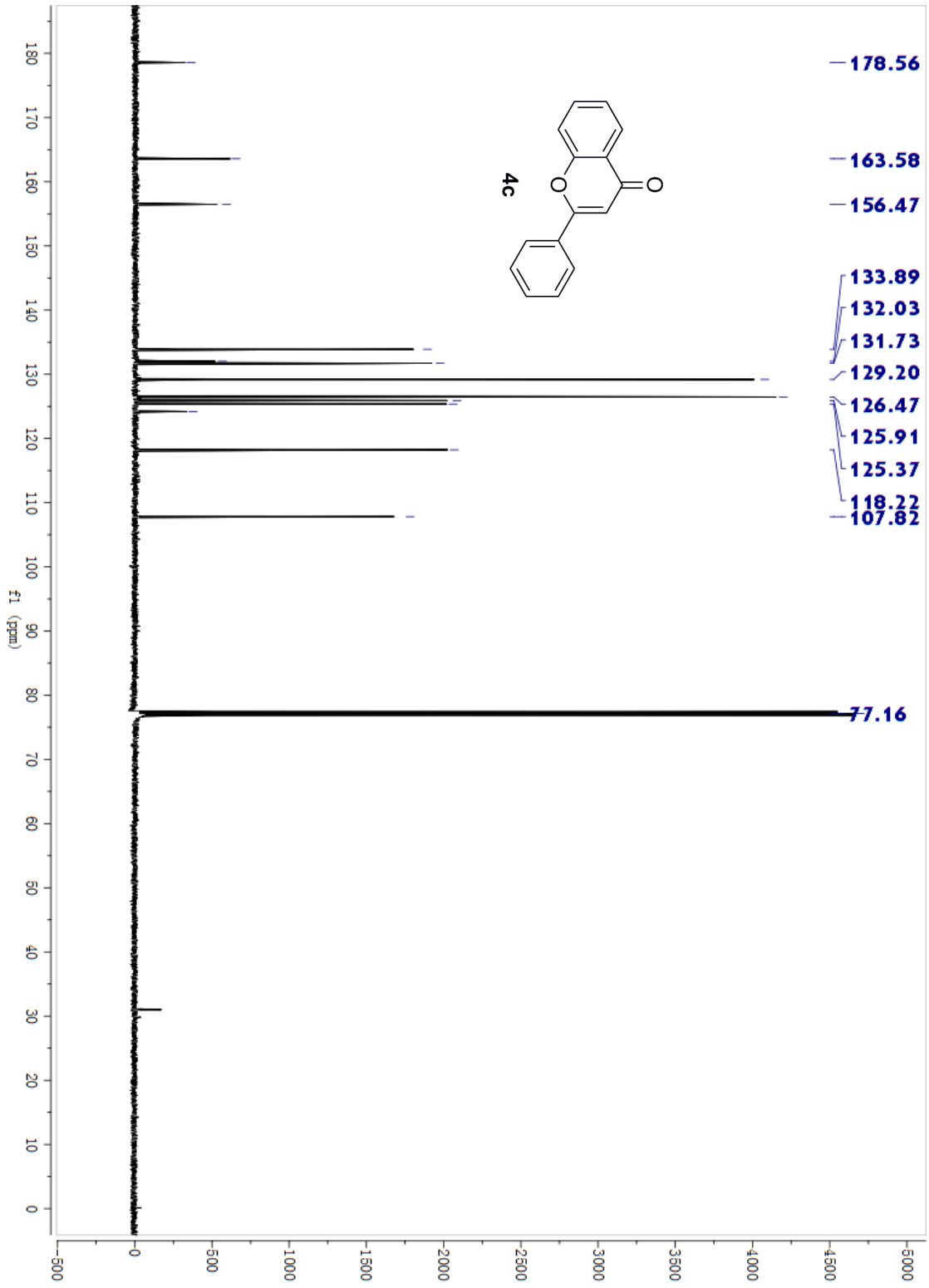
2.00
1.12
1.11
2.74
0.96
0.96
8.25
8.24
8.23
8.23
7.94
7.94
7.93
7.92
7.72
7.72
7.70
7.69
7.68
7.58
7.57
7.55
7.54
7.54
7.53
7.44
7.42
7.41
7.26
6.83
4c
O
O
f1 (ppm)


178.56
163.58
156.47
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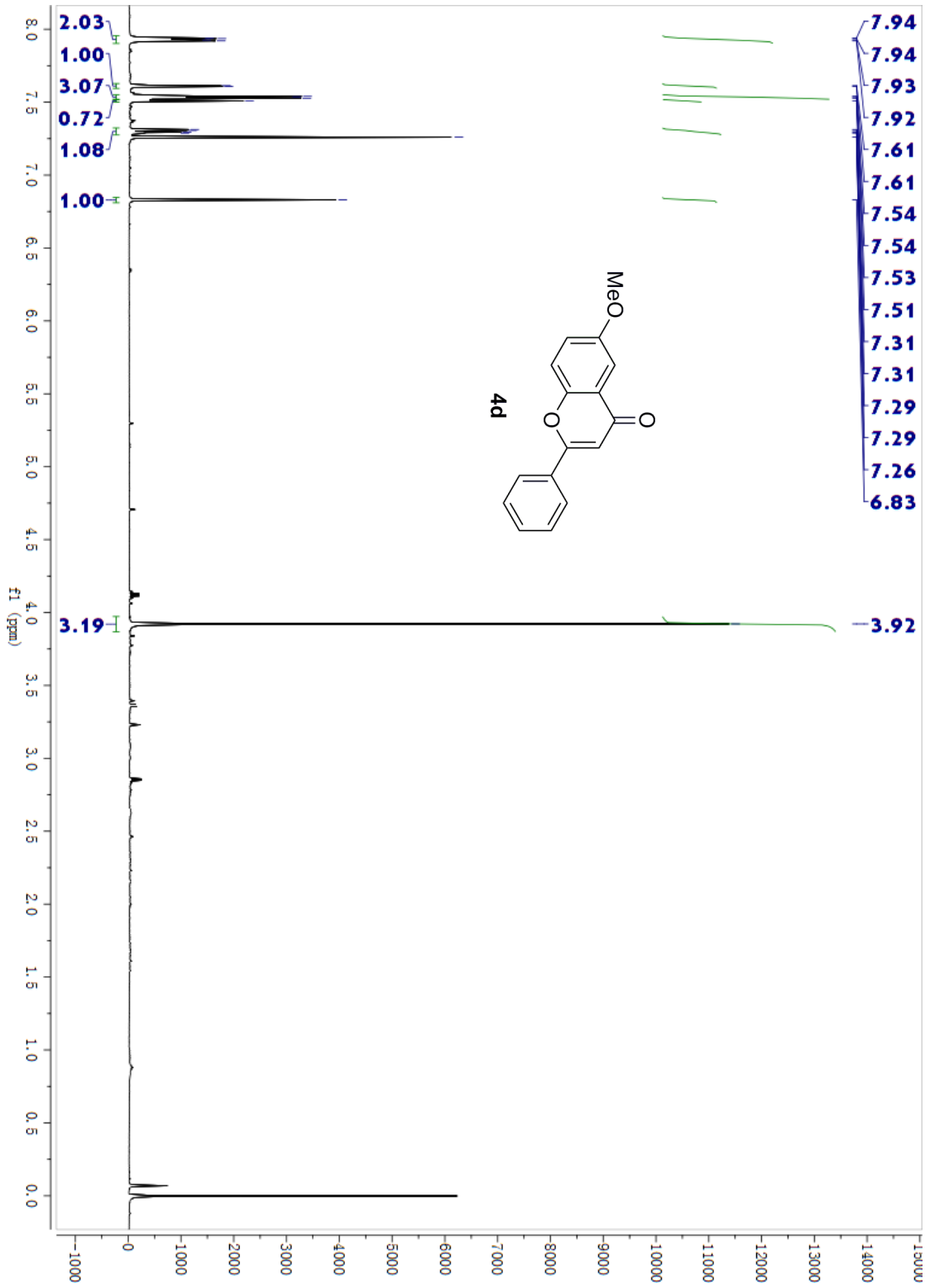
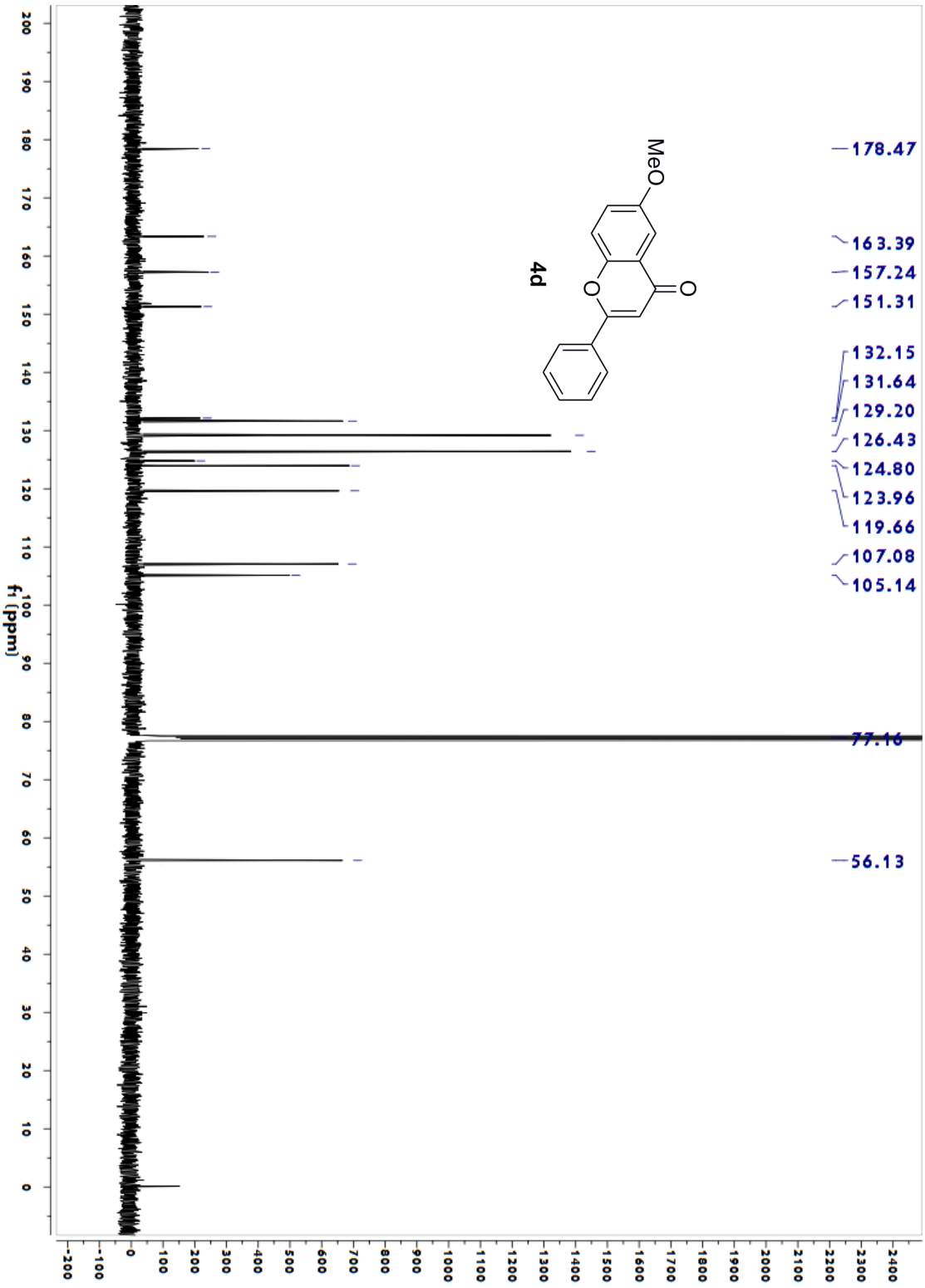
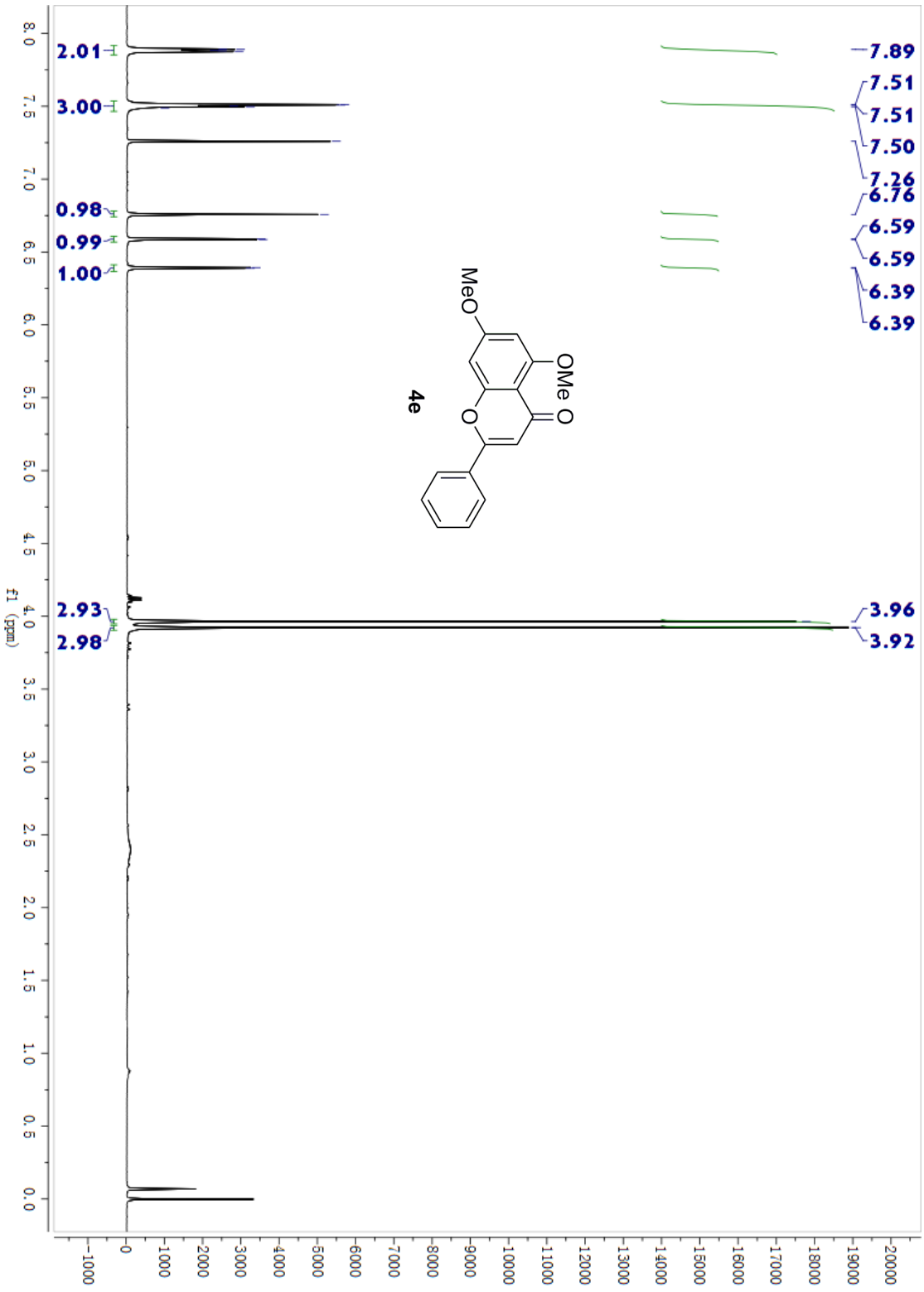
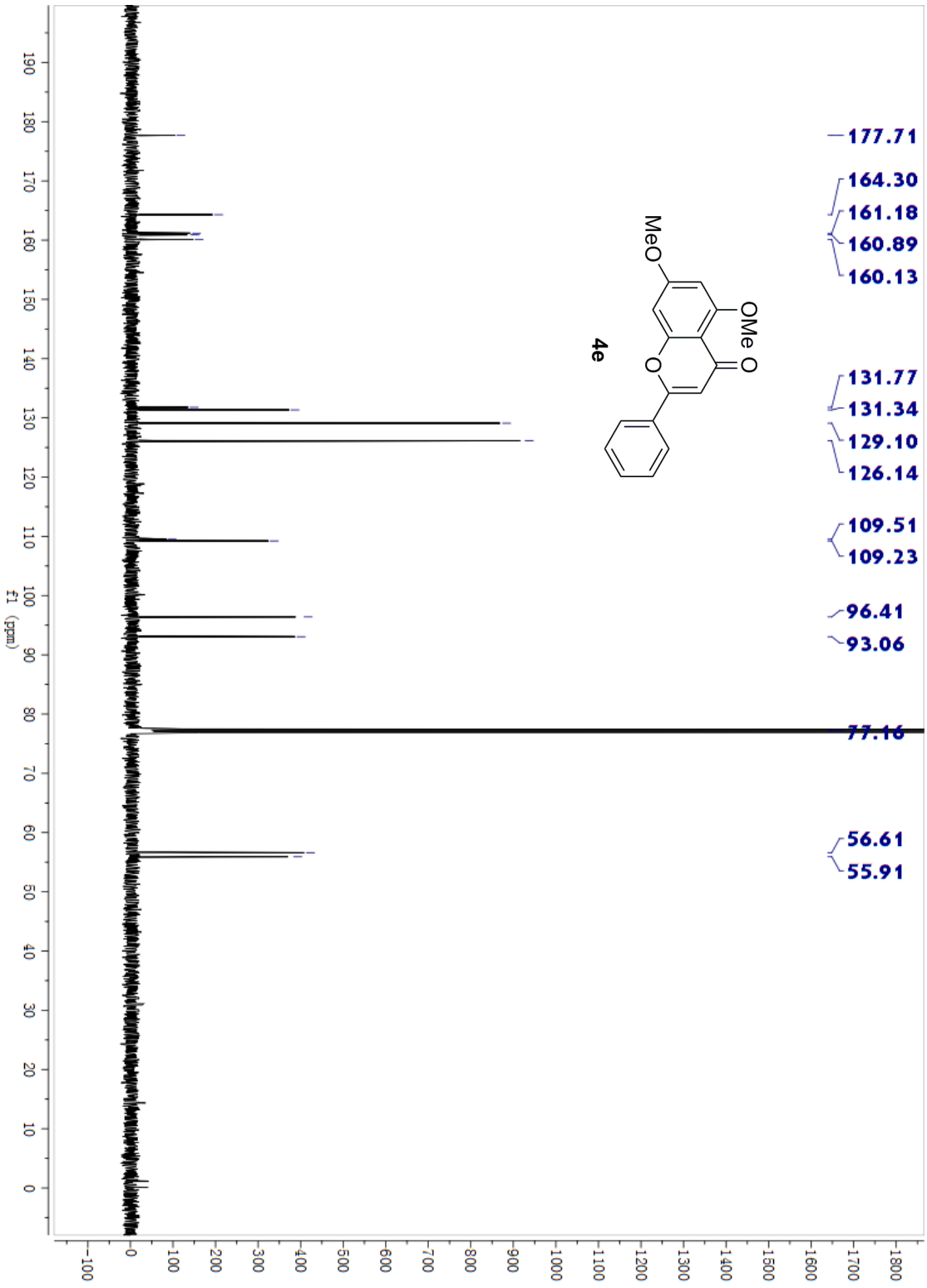
132.03
131.73
129.20
126.47
125.91
125.37
118.22
107.82
77.16
4c
f1 (ppm)


2.03
1.00
3.07
0.72
1.08
1.00
3.19
7.94
7.94
7.93
7.92
7.61
7.61
7.54
7.54
7.53
7.51
7.31
7.31
7.29
7.29
7.26
6.83
3.92
MeO
O
O
4d
f1 (ppm)


MeO
O
O
4d
178.47
163.39
157.24
151.31
132.15
131.64
129.20
126.43
124.80
123.96
119.66
107.08
105.14
77.16
56.13
f1 (ppm)


2.01
3.00
0.98
0.99
1.00
2.93
2.98
7.89
7.51
7.51
7.50
7.26
6.76
6.59
6.59
6.39
6.39
3.96
3.92
MeO
OMe
O
O
4e
f1 (ppm)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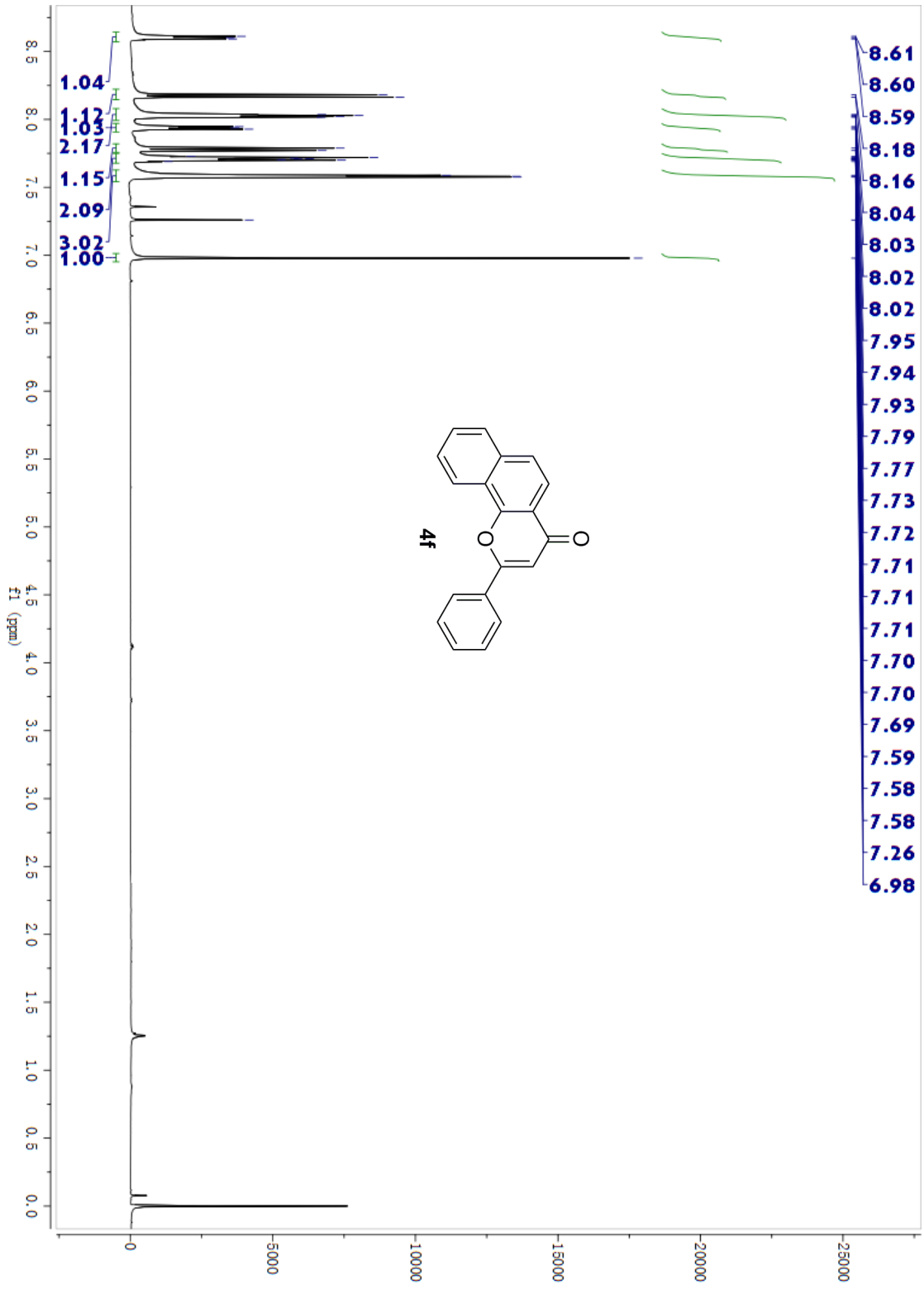
160.89
160.13
131.77
131.34
129.10
126.14
109.51
109.23
96.41
93.06
77.16
56.61
55.91
MeO
OMe O
O
4e
f1 (ppm)


1.04
1.12
1.03
2.17
1.15
2.09
3.02
1.00
8.61
8.60
8.59
8.18
8.16
8.04
8.03
8.02
8.02
7.95
7.94
7.93
7.79
7.77
7.73
7.72
7.71
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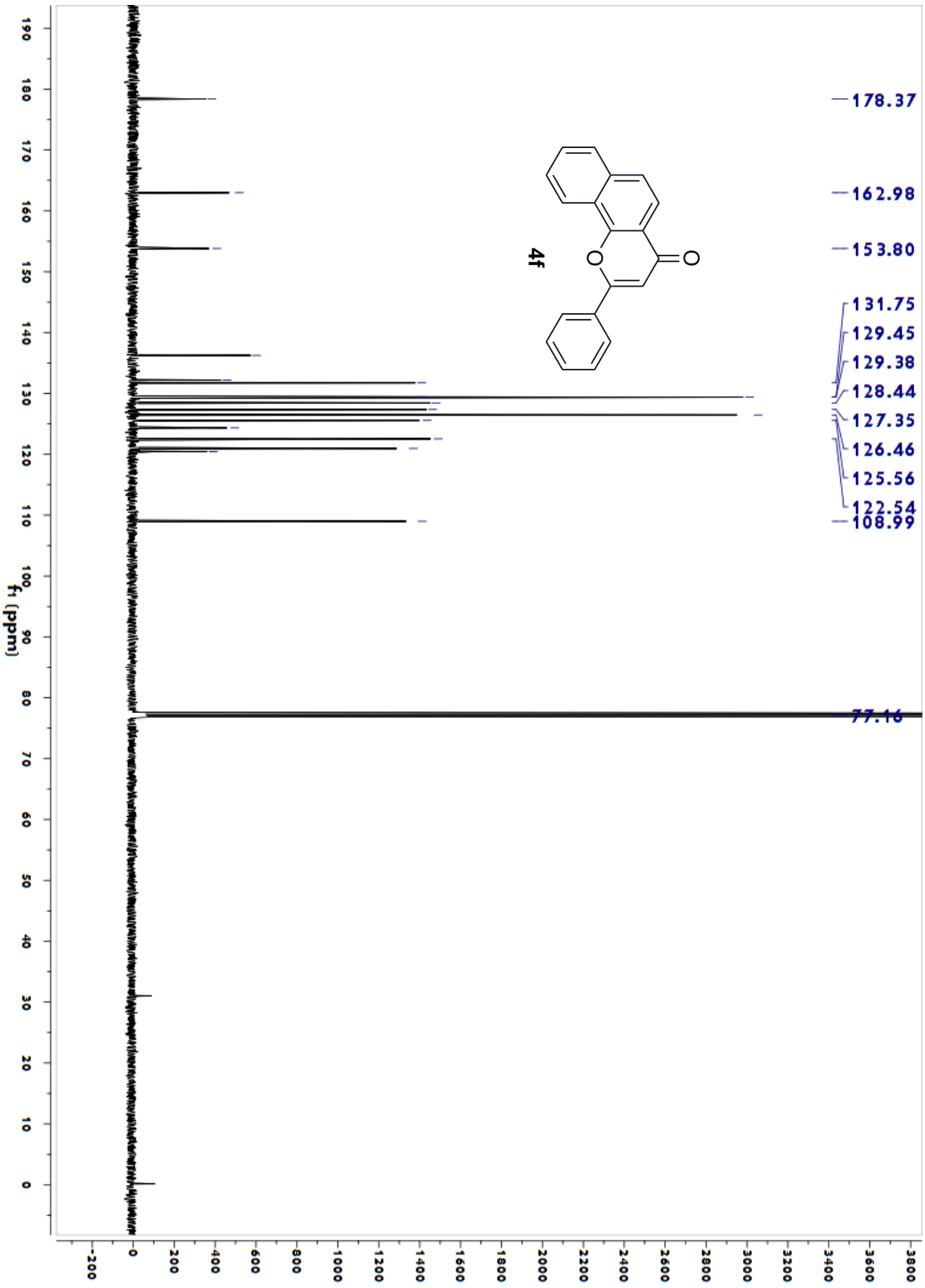
7.58
7.26
6.98
4f
f1 (ppm)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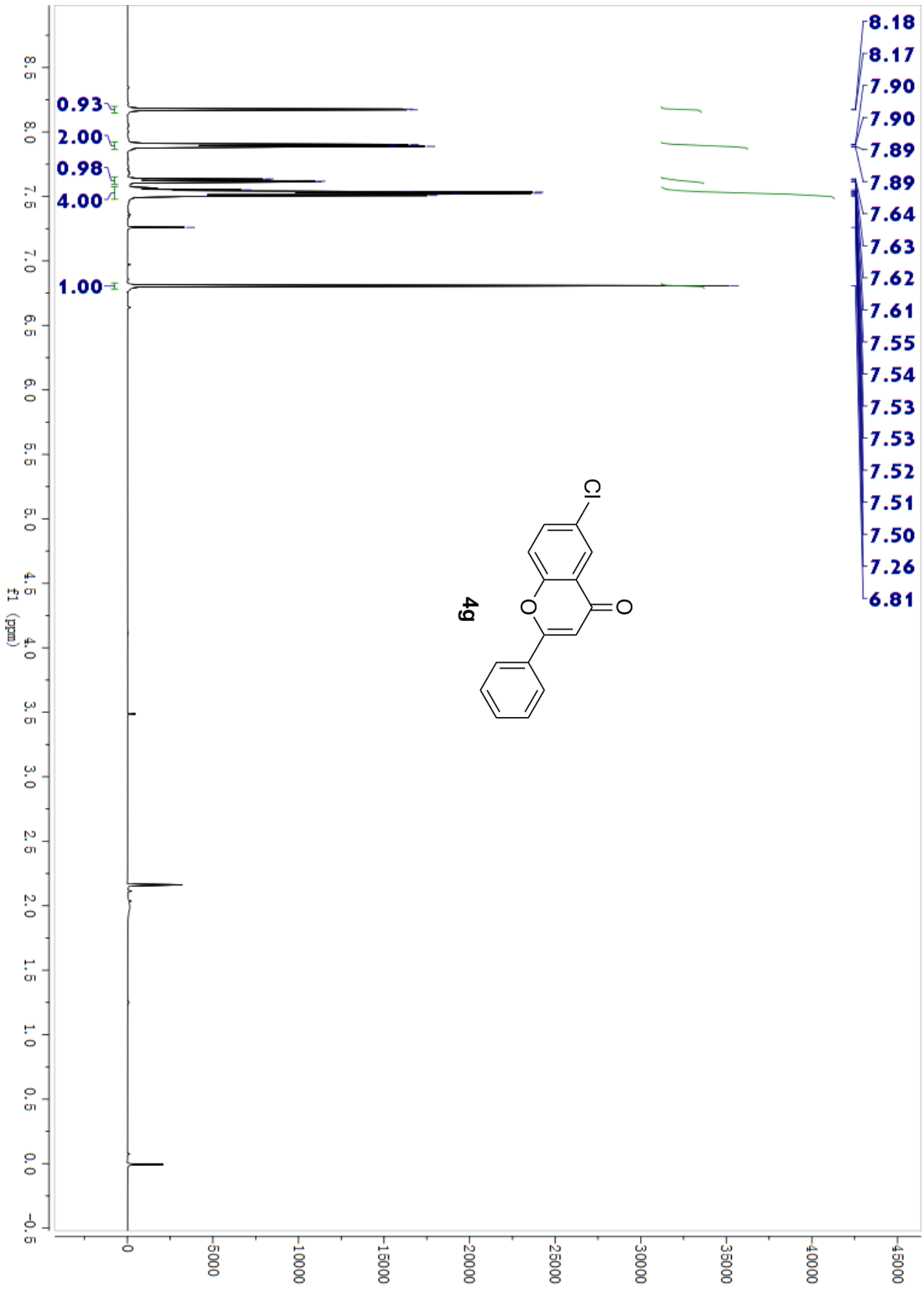
128.44
127.35
126.46
125.56
122.54
108.99
77.16
4f
f1 (ppm)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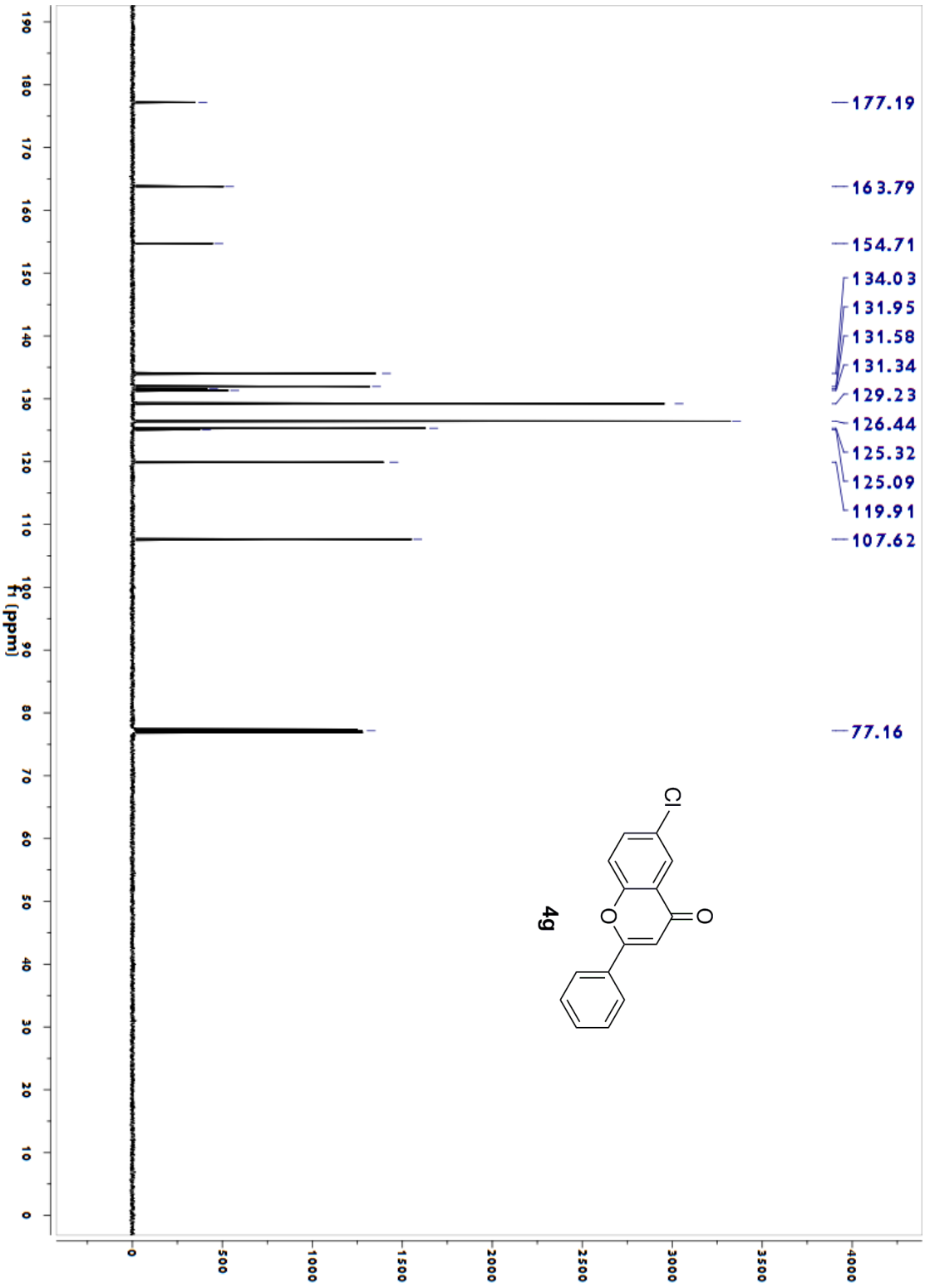
8.17
7.90
7.90
7.89
7.89
7.64
7.63
7.62
7.61
7.55
7.54
7.53
7.53
7.52
7.51
7.50
7.26
6.81
0.93
2.00
0.98
4.00
1.00
Cl
O
O
4g
f1 (ppm)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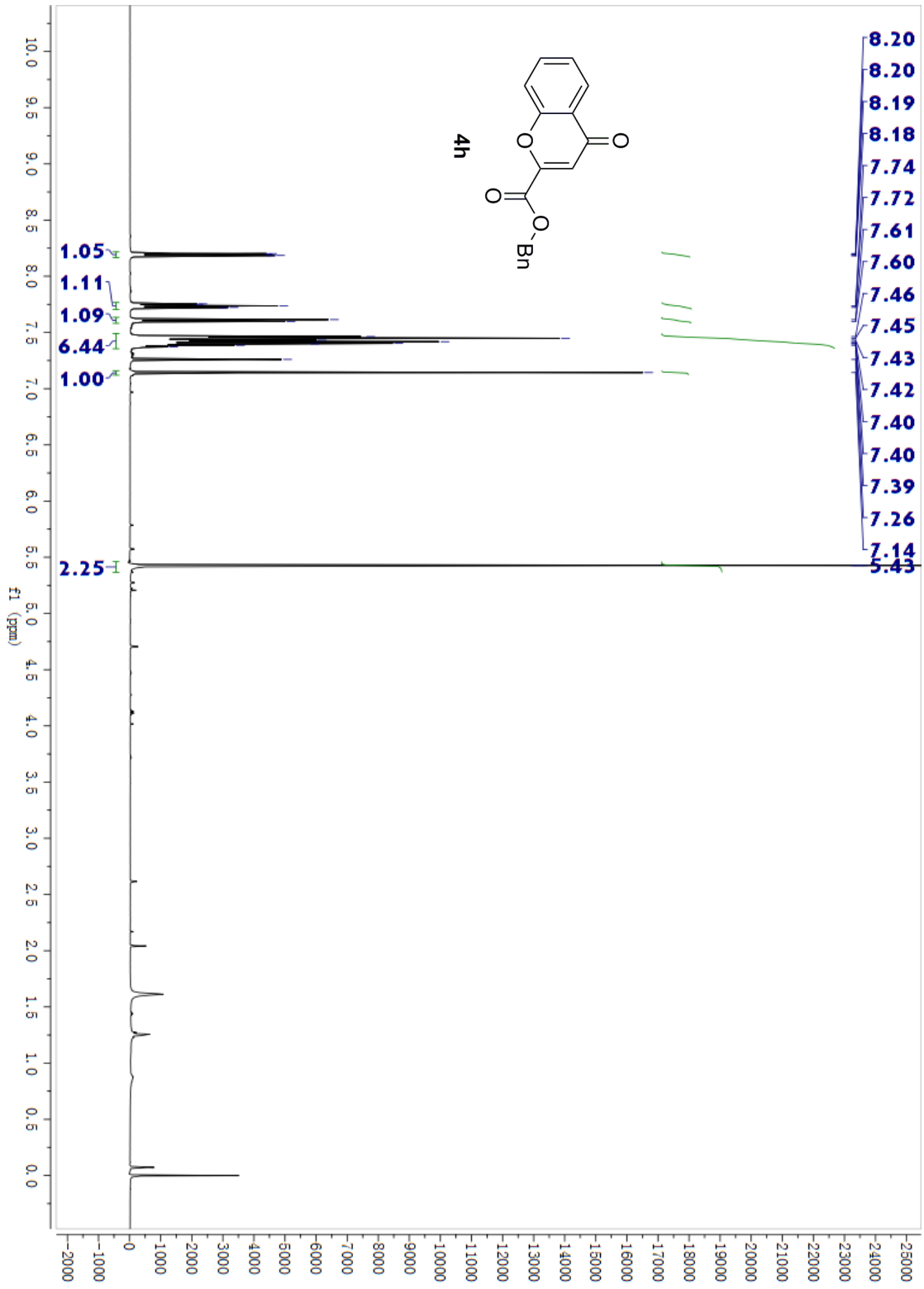
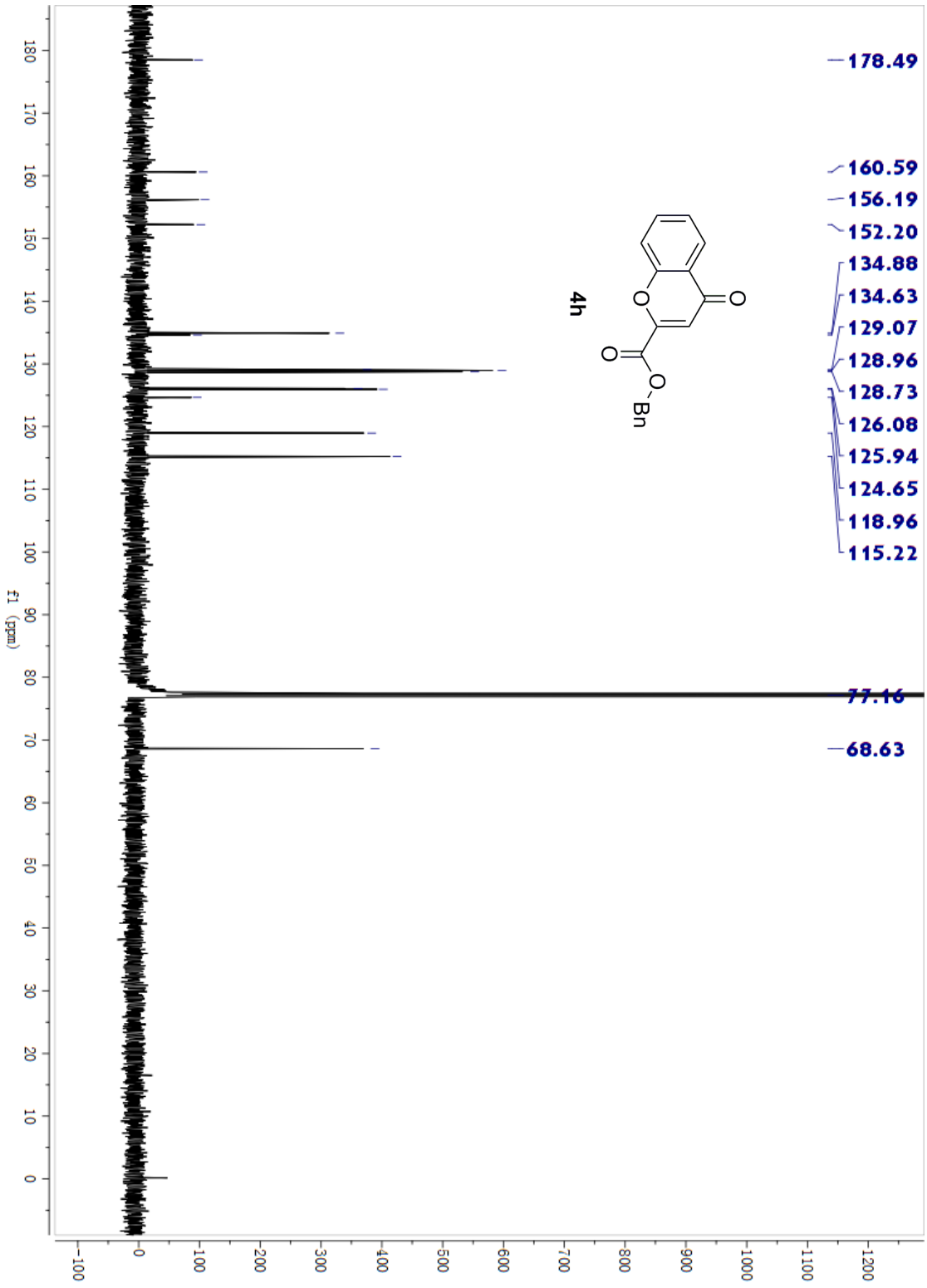
154.71
134.03
131.95
131.58
131.34
129.23
126.44
125.32
125.09
119.91
107.62
77.16
f1 (ppm)
Cl
O
O
4g


4h
O
O
O
O
Bn
8.20
8.20
8.19
8.18
7.74
7.72
7.61
7.60
7.46
7.45
7.43
7.42
7.40
7.40
7.39
7.26
7.14
5.43
1.05
1.11
1.09
6.44
1.00
2.25
f1 (ppm)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152.20
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134.63
129.07
128.96
128.73
126.08
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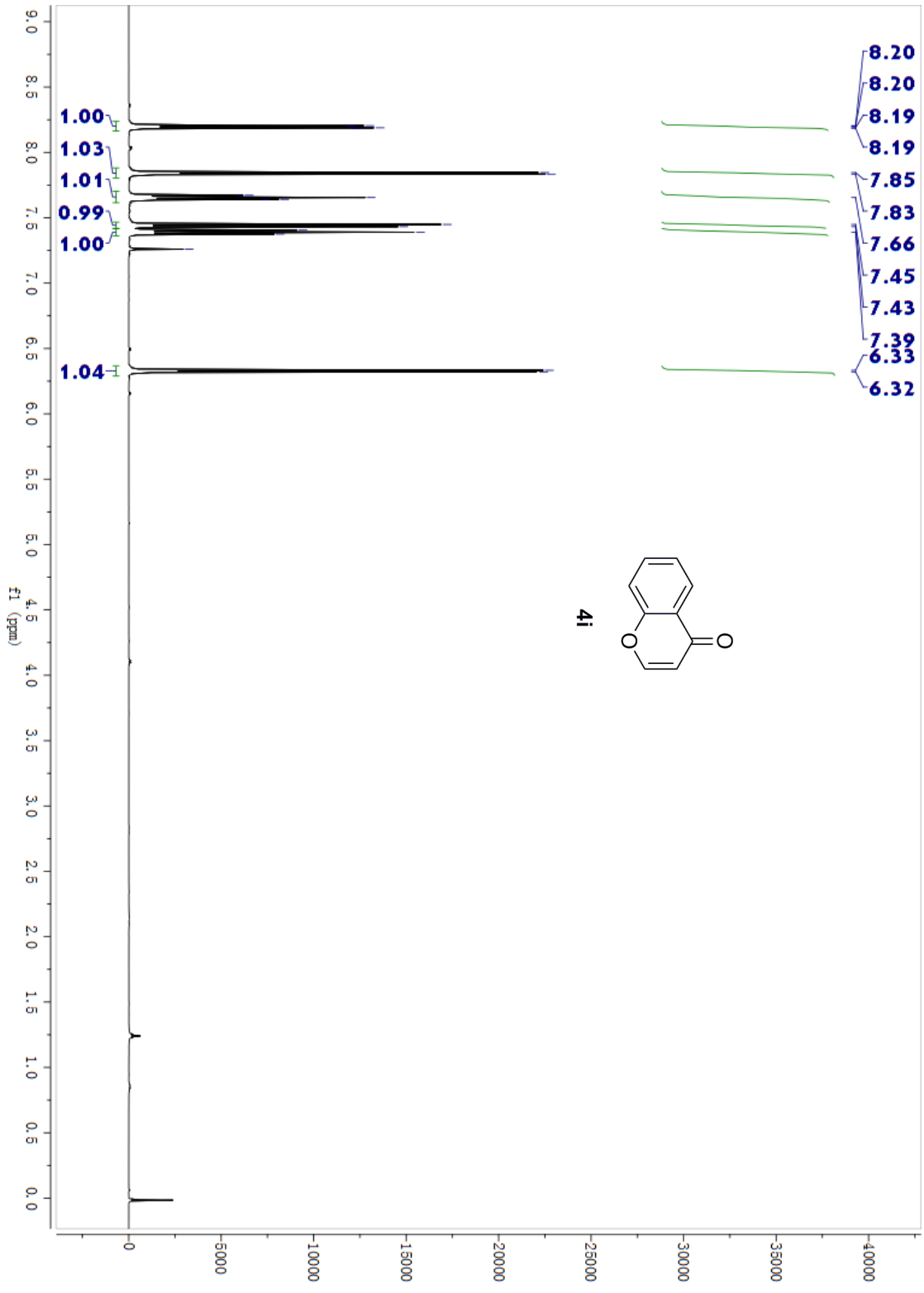
124.65
118.96
115.22
77.16
68.63
4h
O
O
O
O
Bn
f1 (ppm)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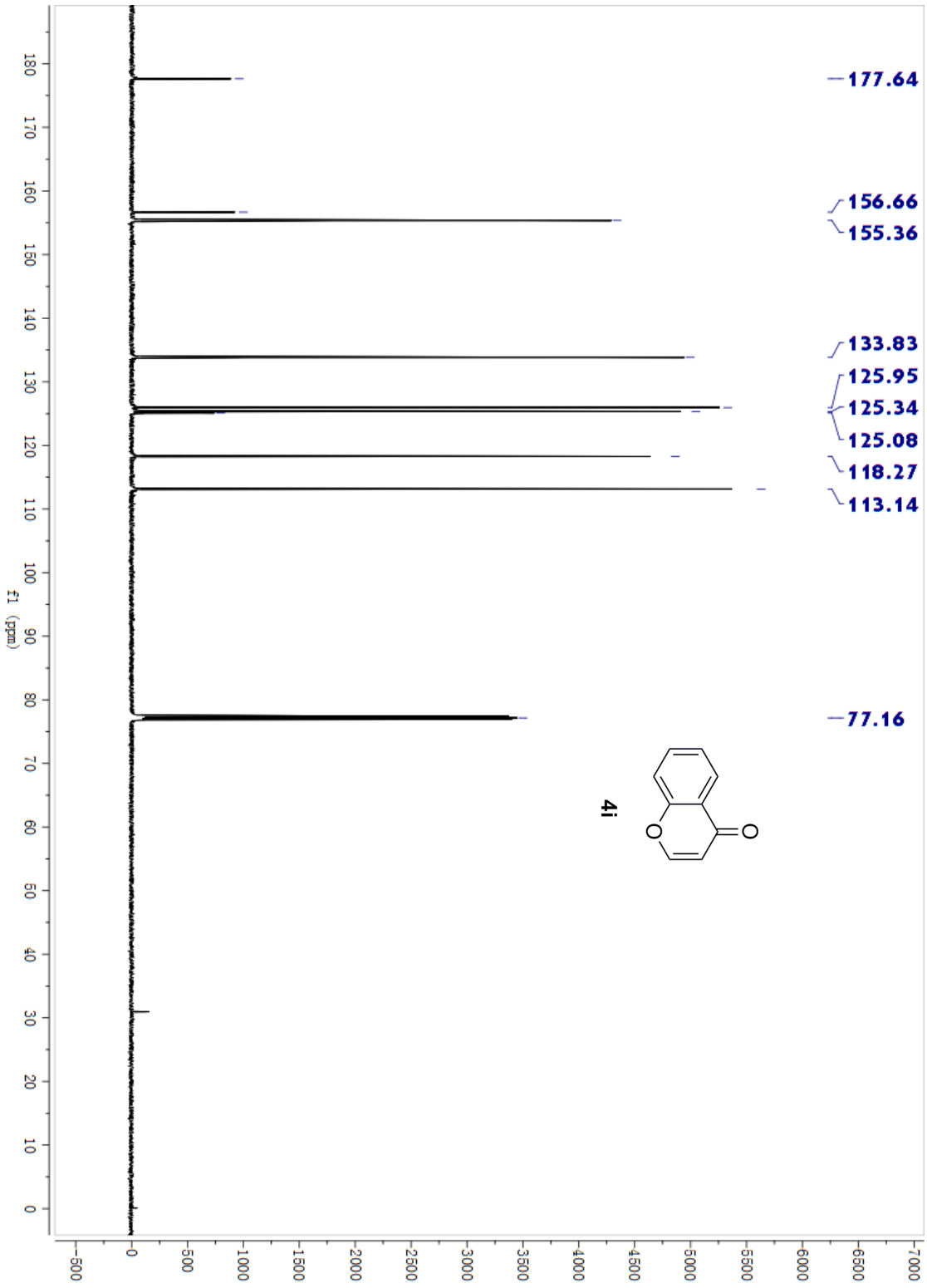
8.20
8.19
8.19
7.85
7.83
7.66
7.45
7.43
7.39
6.33
6.32
1.00
1.03
1.01
0.99
1.00
1.04
4i
f1 (ppm)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133.83
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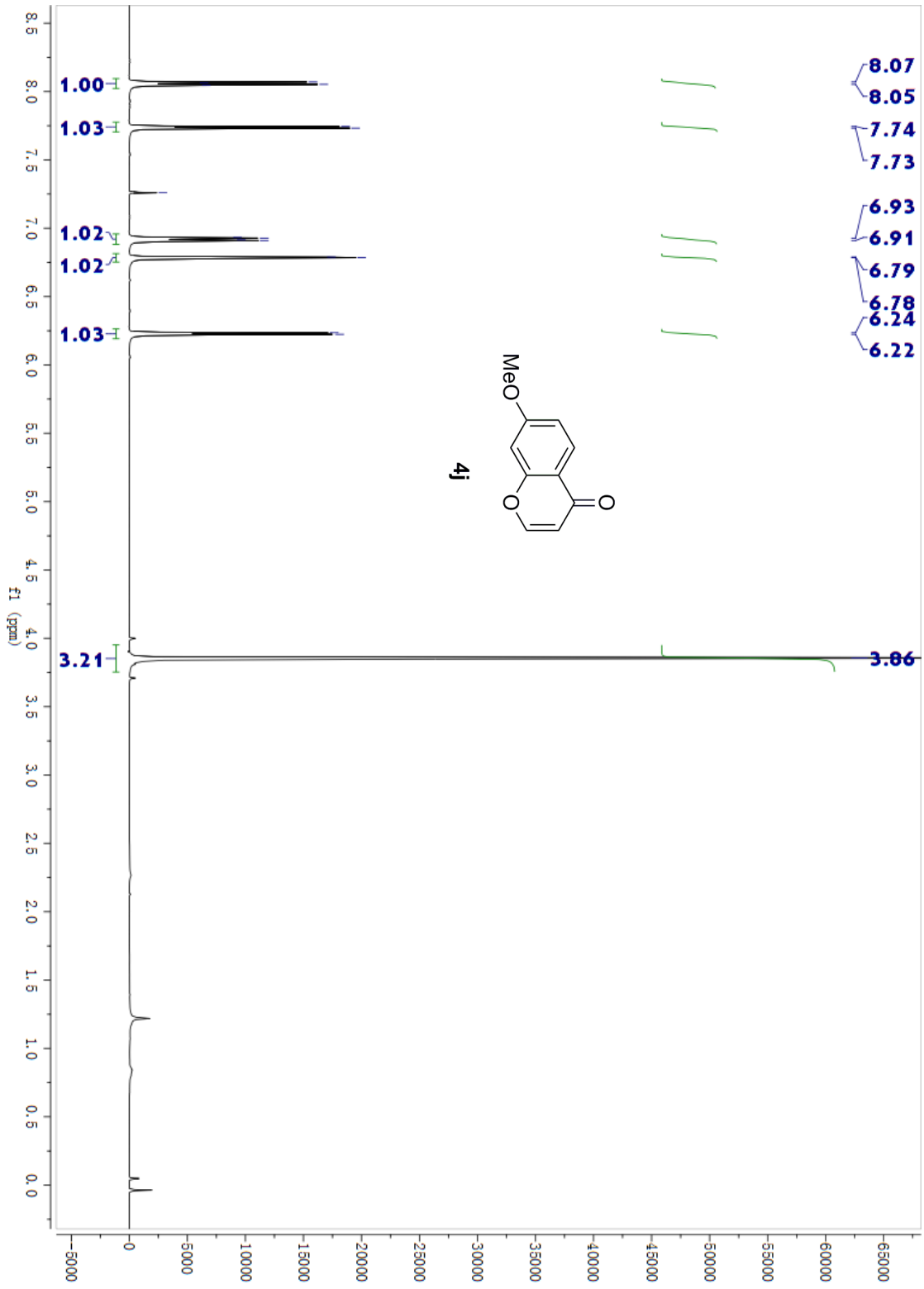
125.34
125.08
118.27
113.14
77.16
4i
f1 (ppm)


8.07
8.05
7.74
7.73
6.93
6.91
6.79
6.78
6.24
6.22
3.86
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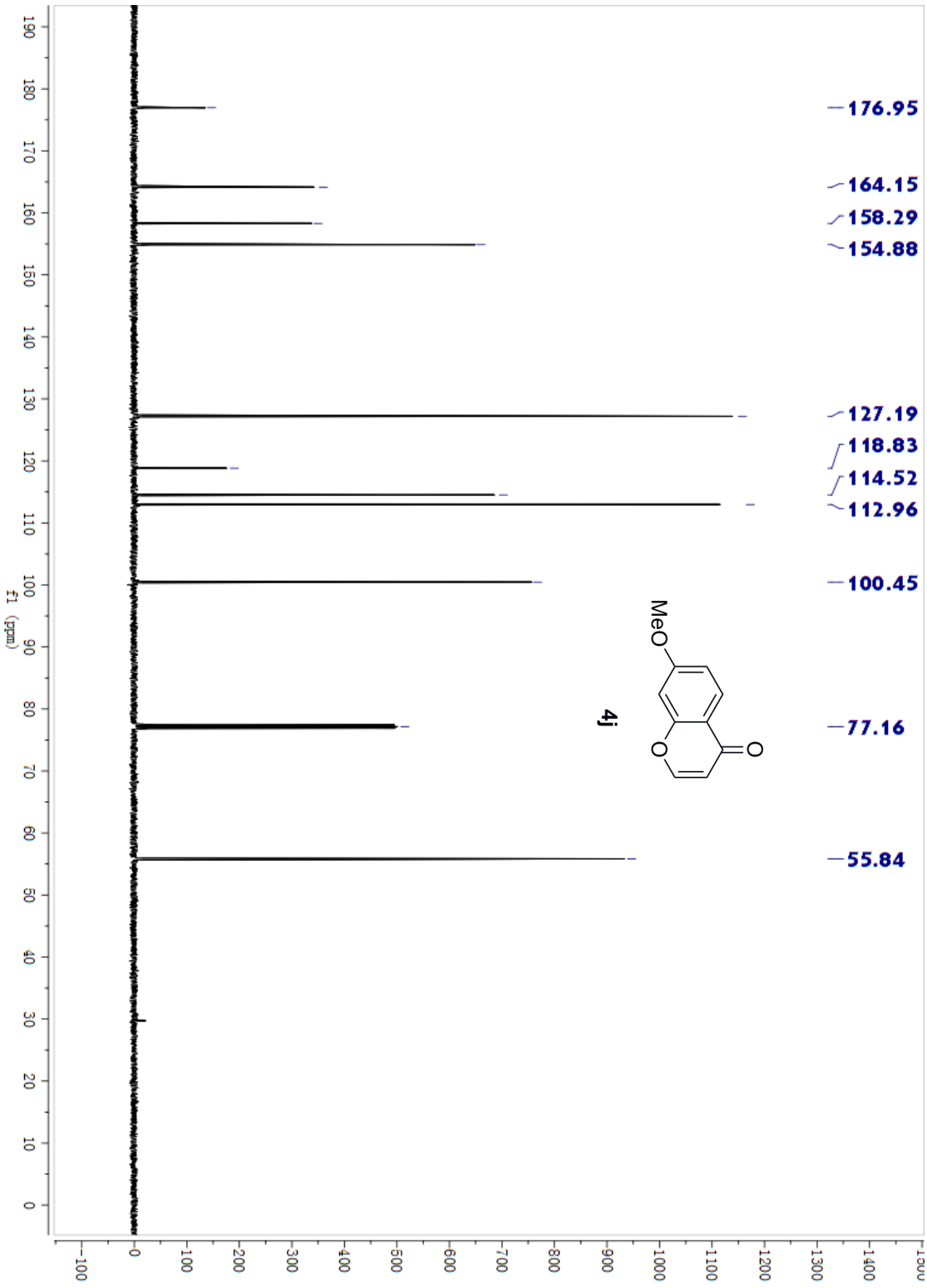
1.03
1.02
1.02
1.03
3.21
MeO
O
O
4j
f1 (ppm)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164.15
158.29
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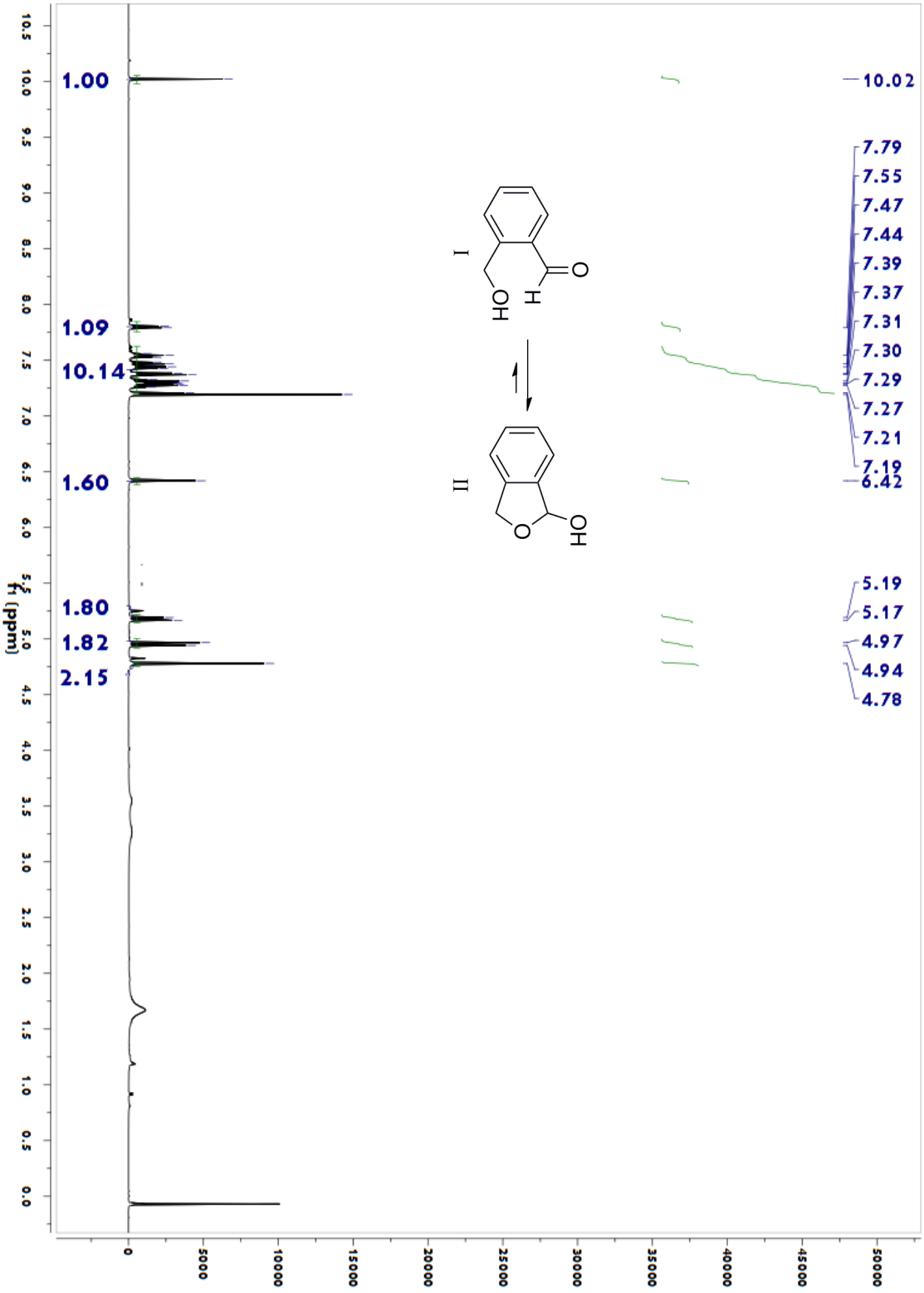
127.19
118.83
114.52
112.96
100.45
77.16
55.84
MeO
O
O
4j
f1 (ppm)


1.00
1.09
10.14
1.60
1.80
1.82
2.15
10.02
7.79
7.55
7.47
7.44
7.39
7.37
7.31
7.30
7.29
7.27
7.21
7.19
6.42
5.19
5.17
4.97
4.94
4.78
I
II
HO
O
H
O
OH
f1 (ppm)