Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Site-selective gold(I) catalyzed synthesis of 1,3-dioxin-3 ones via cascade reaction

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[c] CITACA - Clúster de Investigación y Transferencia Agroalimentaria del Campus Auga, Universidad de Vigo, 32004-Ourense, Spain.

[d] CINMPIS, via Selmi 2, 40126, Bologna, Italy.

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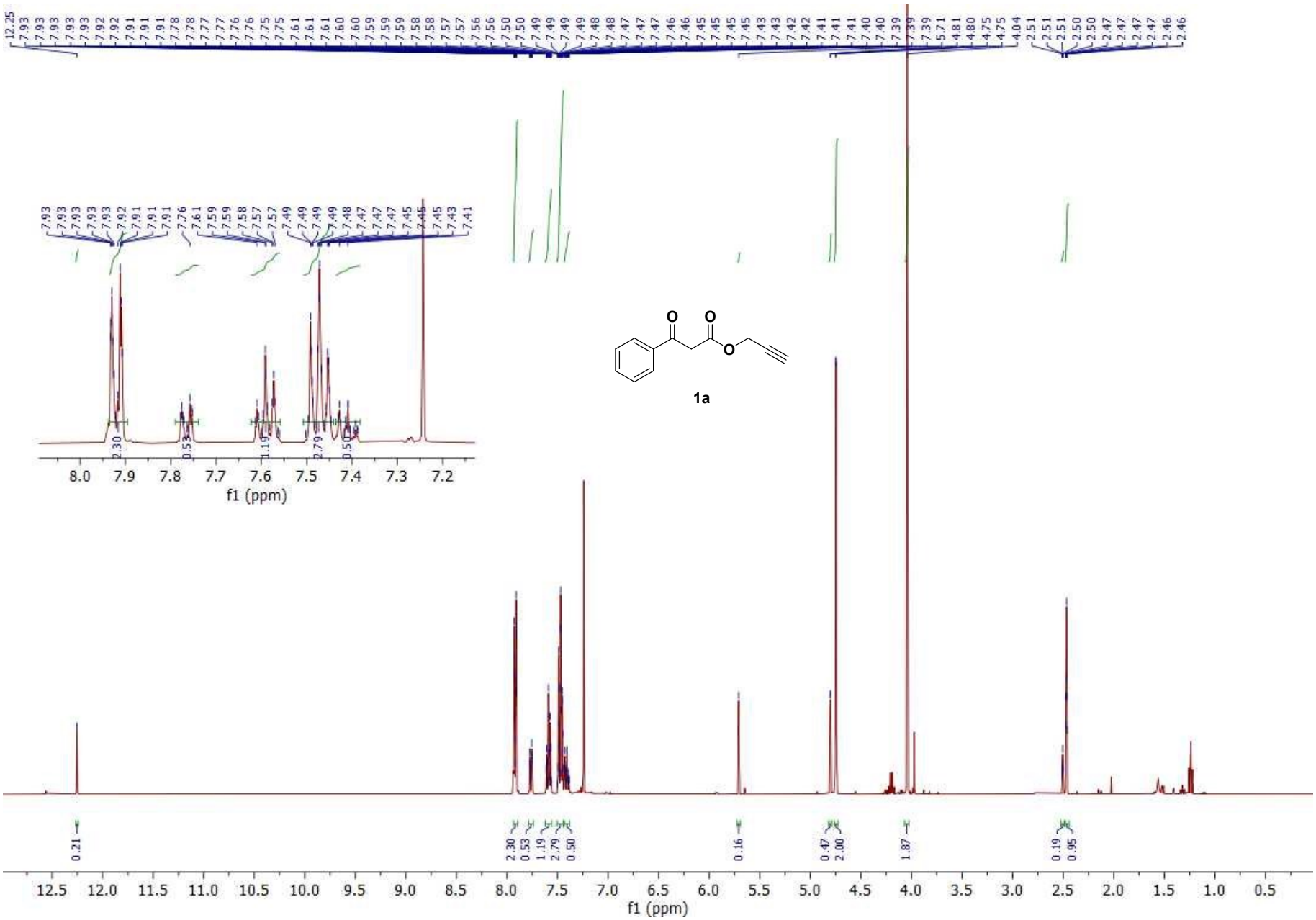
NMR spectra **1a-u** S2

NMR spectra **2a-u** S45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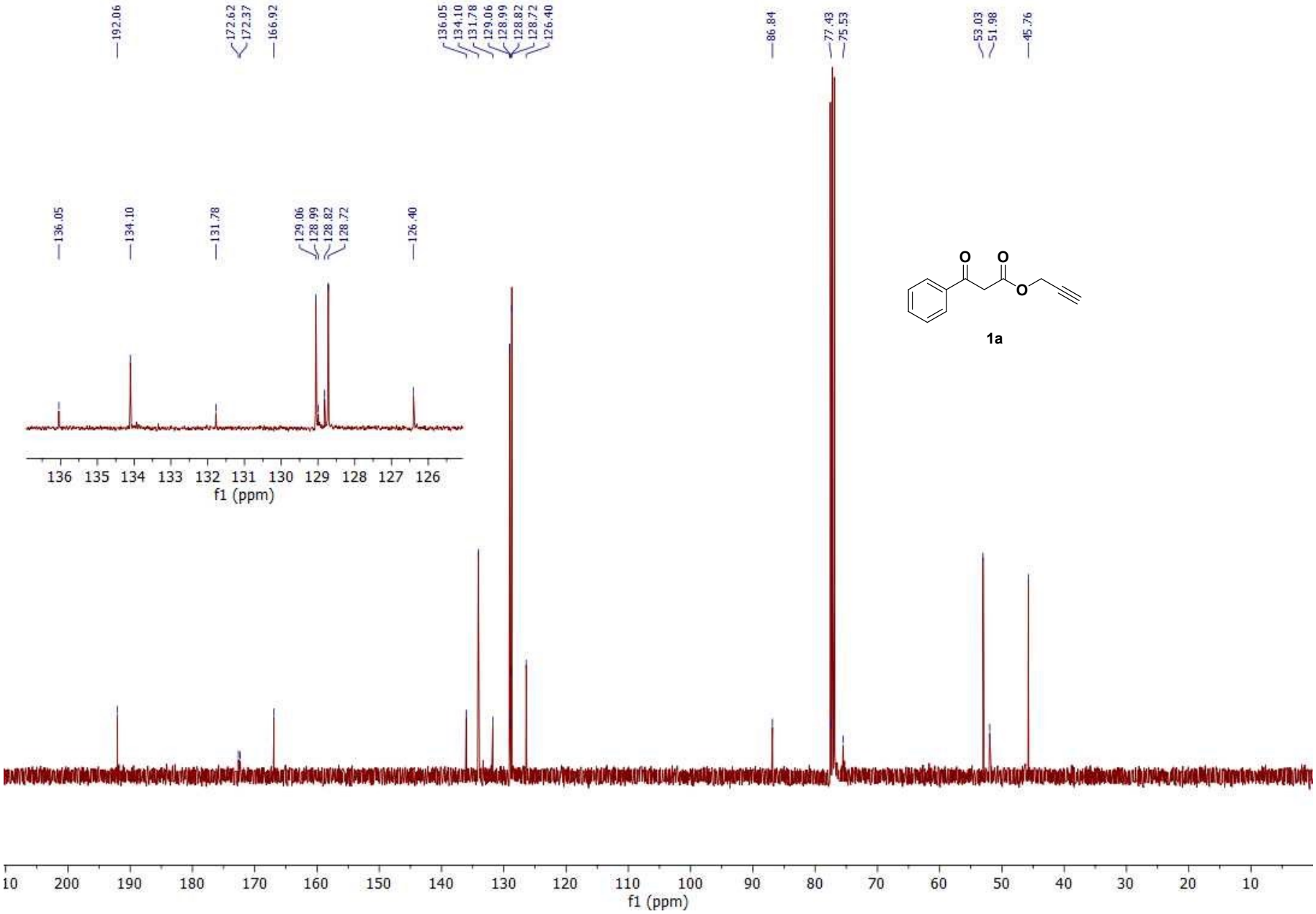
f1 (ppm)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77.43
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53.03
51.98
45.76
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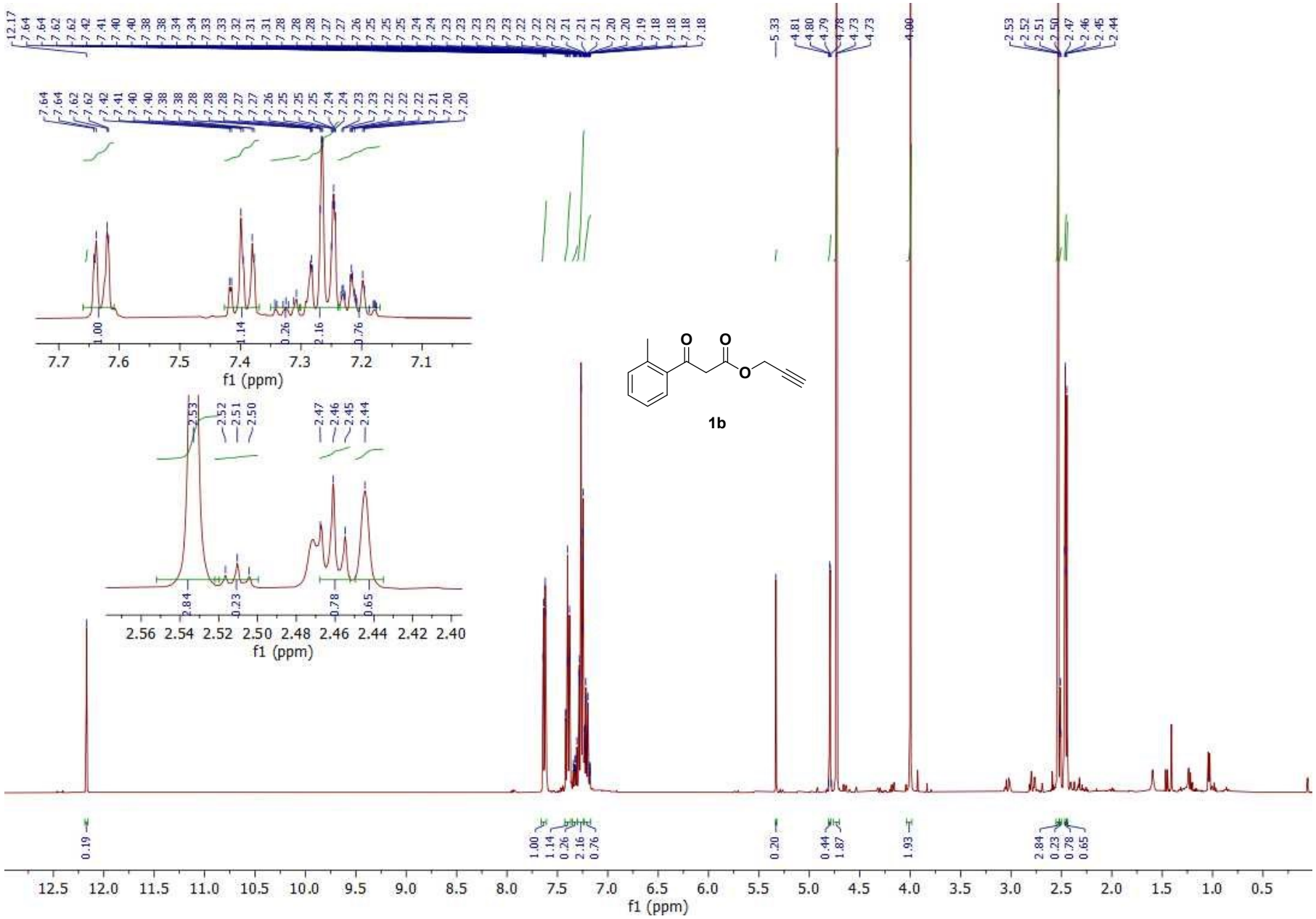
O
1a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7.31
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7.27
7.26
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7.25
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7.22
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7.19
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7.18
7.18
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4.80
4.79
4.78
4.73
4.73
4.00
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2.50
2.47
2.46
2.45
2.44
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7.6
7.5
7.4
7.3
7.2
7.1
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0.23
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0.65
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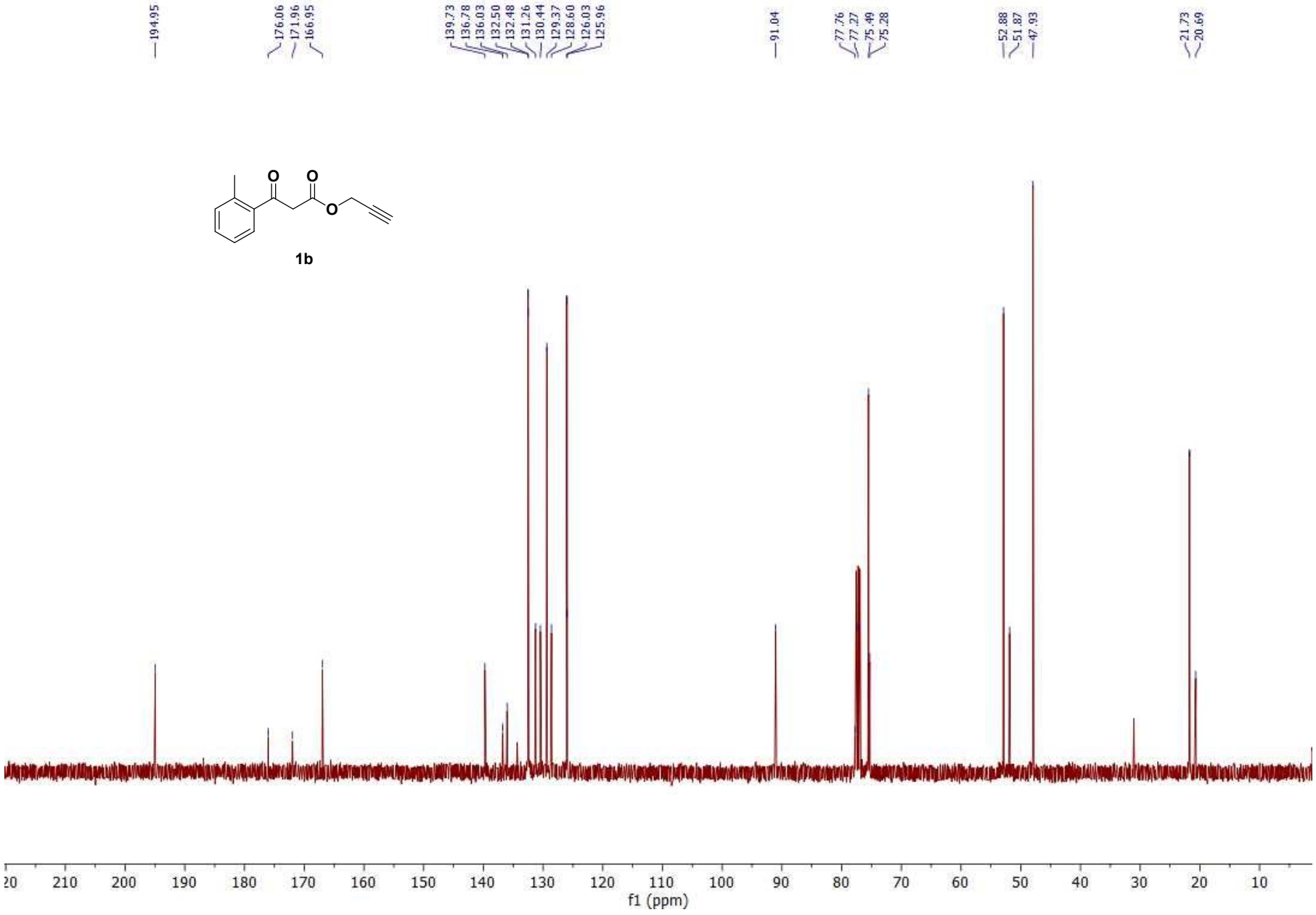
f1 (ppm)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O
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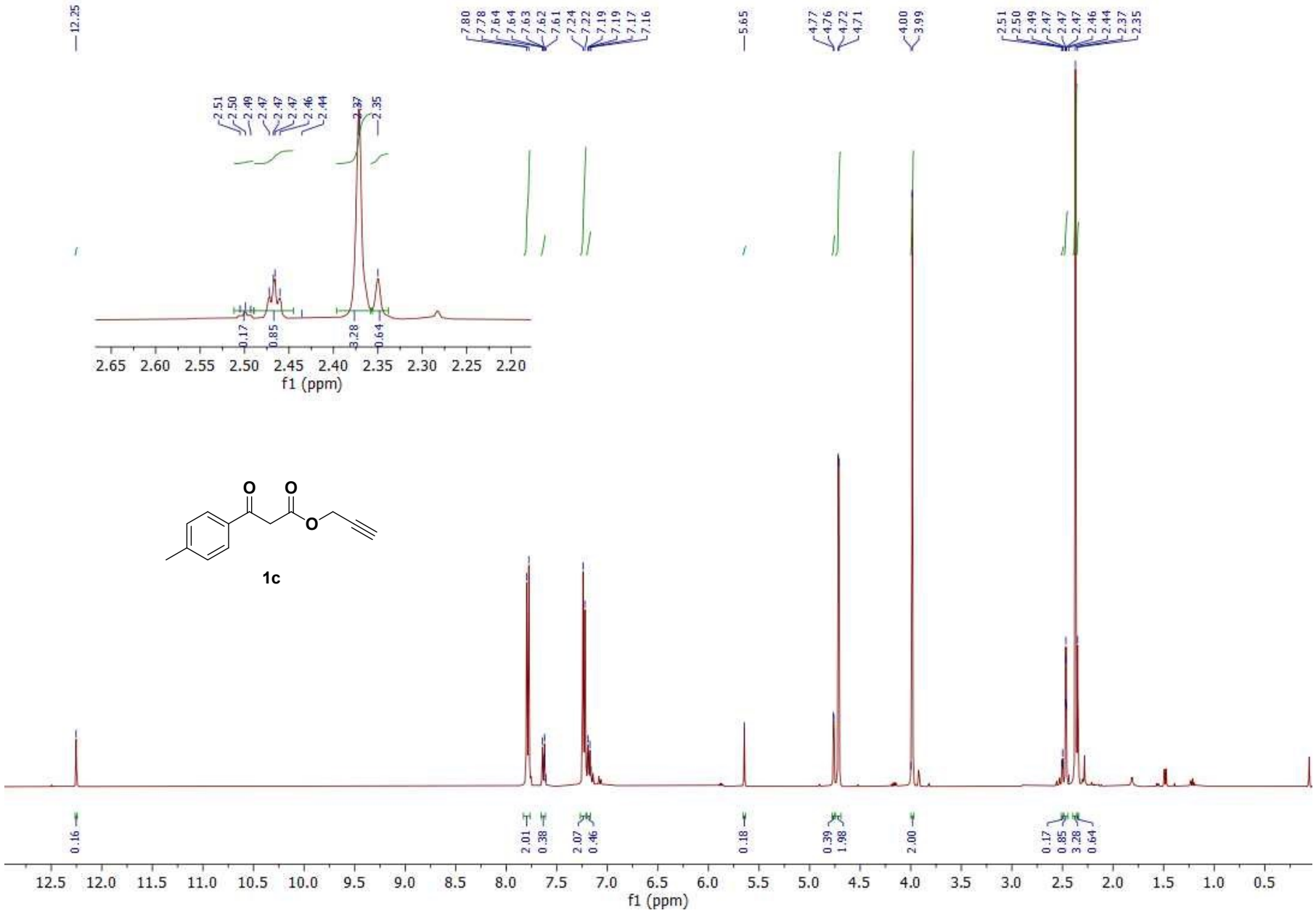
f1 (ppm)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5.65
4.77
4.76
4.72
4.71
4.00
3.99
2.51
2.50
2.49
2.47
2.47
2.47
2.46
2.44
2.37
2.35
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3.28
0.64
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O
O
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0.38
2.07
0.46
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0.39
1.98
2.00
0.17
0.85
3.28
0.64
12.5 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
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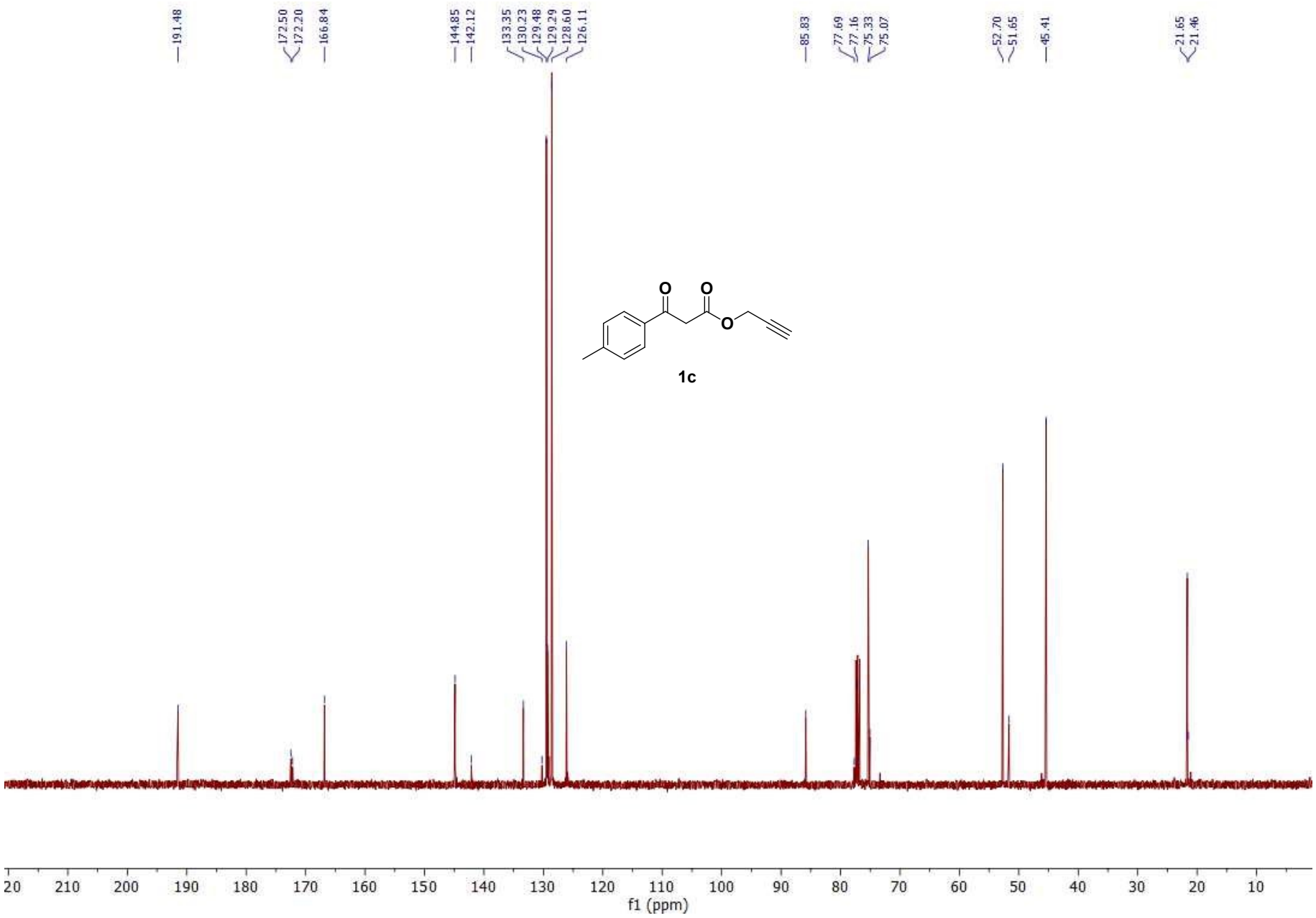
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75.33
75.07
52.70
51.65
45.41
21.65
21.46
O
O
O
1c
20
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200
190
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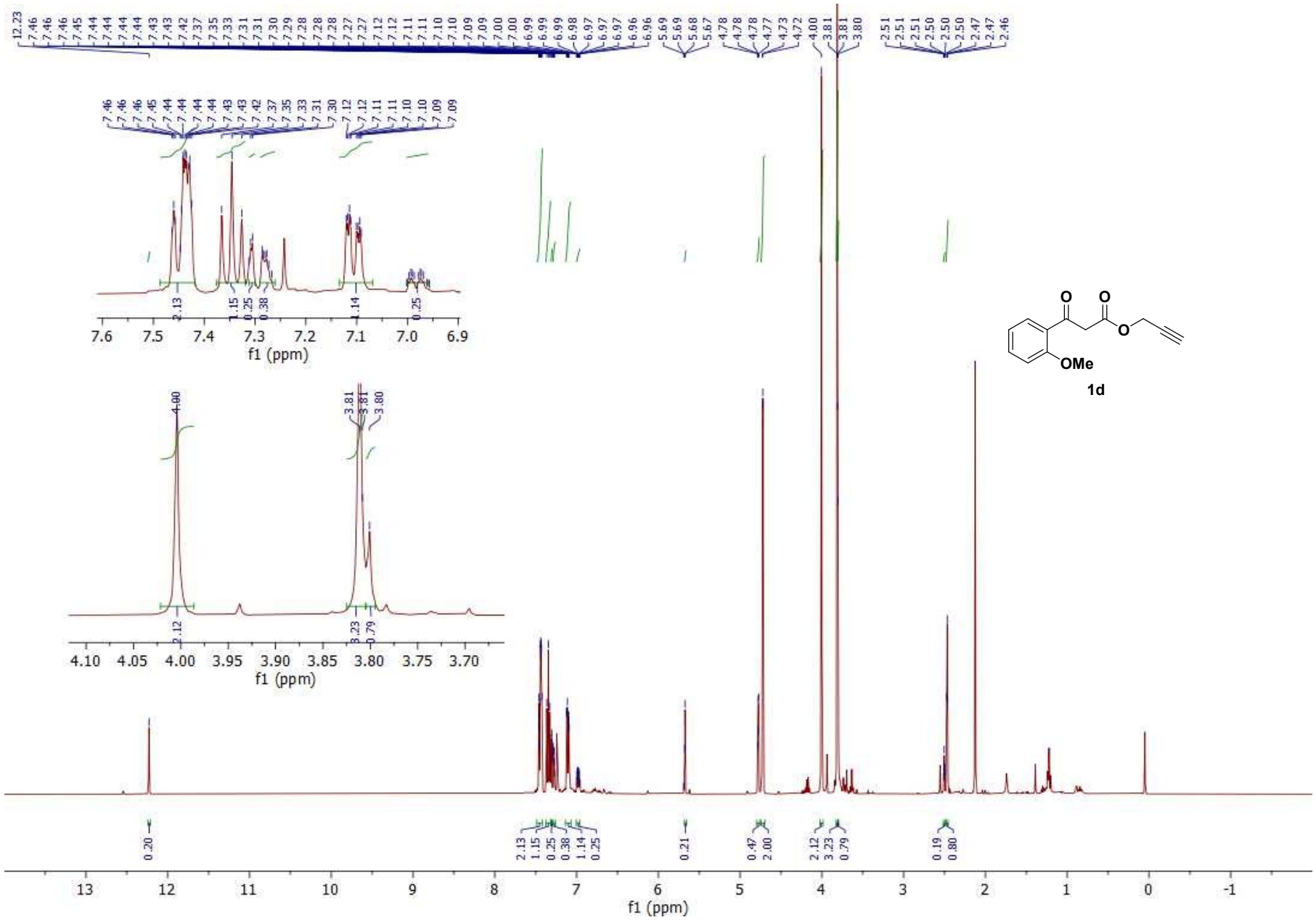
f1 (ppm)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7.11
7.11
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7.10
7.09
7.09
7.00
7.00
6.99
6.99
6.99
6.98
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3.80
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2.51
2.51
2.50
2.50
2.50
2.47
2.47
2.46
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1.15
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1.14
0.25
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
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3.81
3.80
2.12
3.23
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4.10
4.05
4.00
3.95
3.90
3.85
3.80
3.75
3.70
f1 (ppm)
O
O
O
OMe
1d
0.20
2.13
1.15
0.25
0.38
1.14
0.25
0.21
0.47
2.00
2.12
3.23
0.79
0.19
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8
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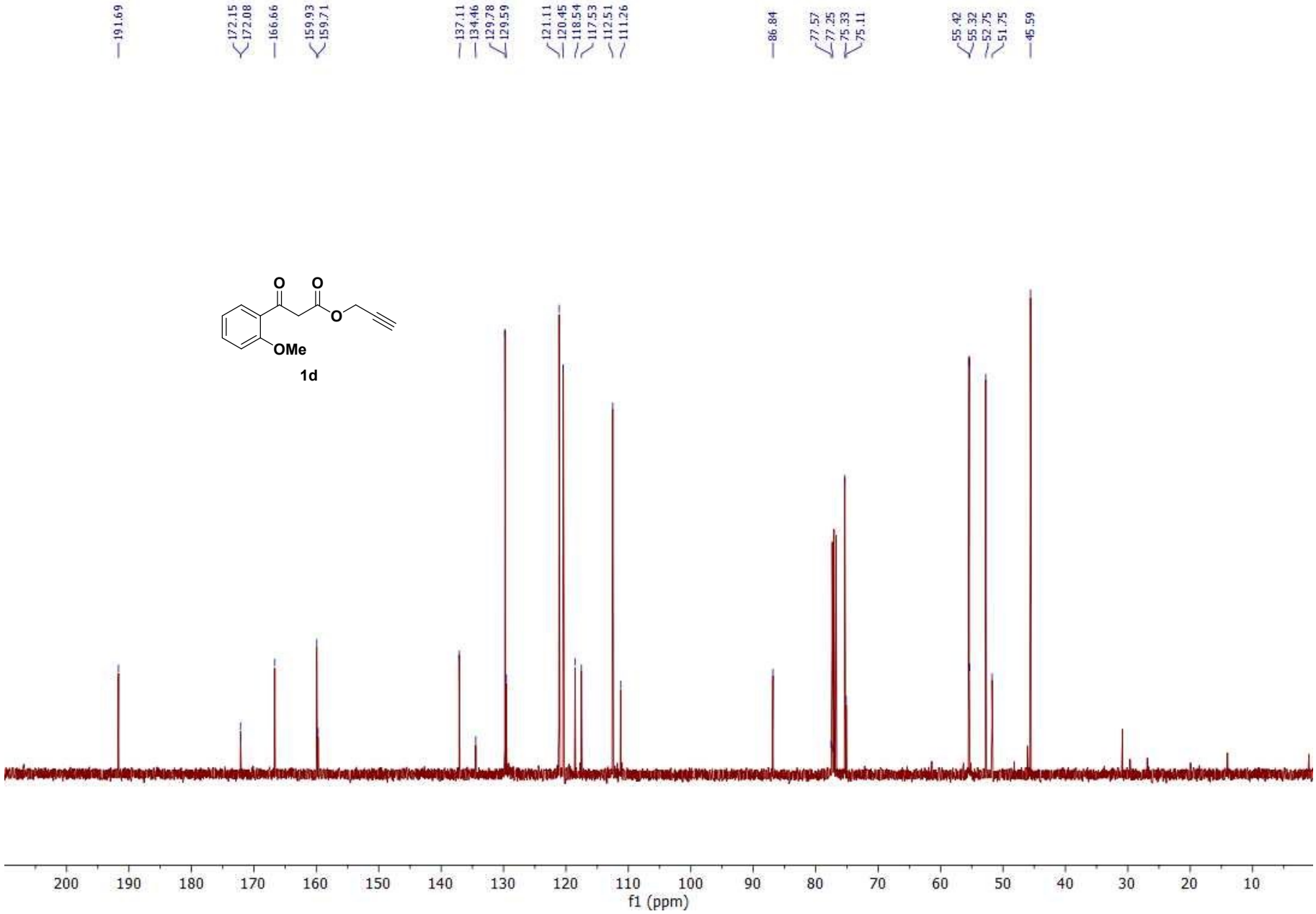
3
2
1
0
-1
f1 (ppm)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86.84
77.57
77.25
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75.11
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55.32
52.75
51.75
45.59
O
O
O
OMe
1d
200
190
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20
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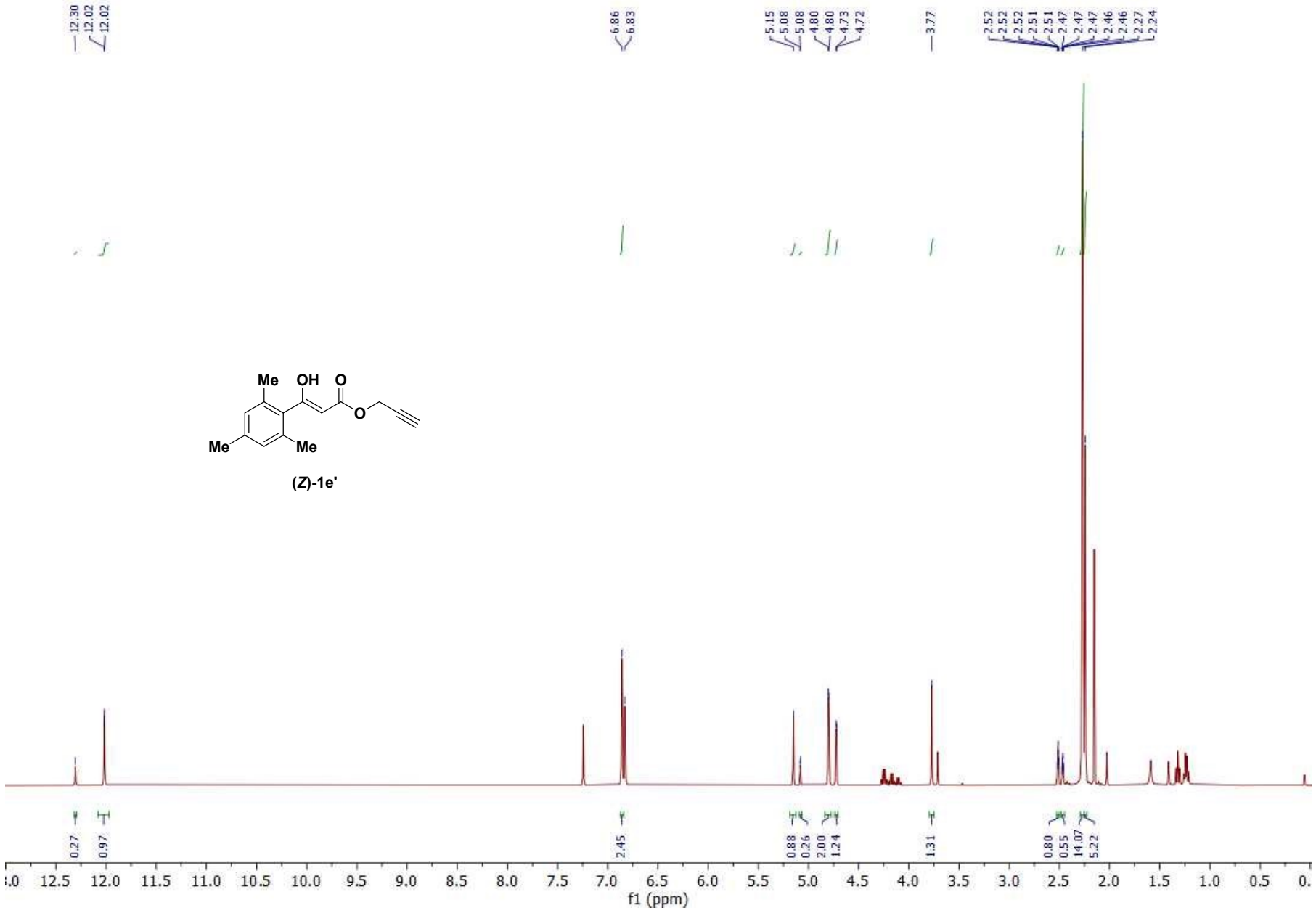
f1 (ppm)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2.47
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O
O
Me
Me
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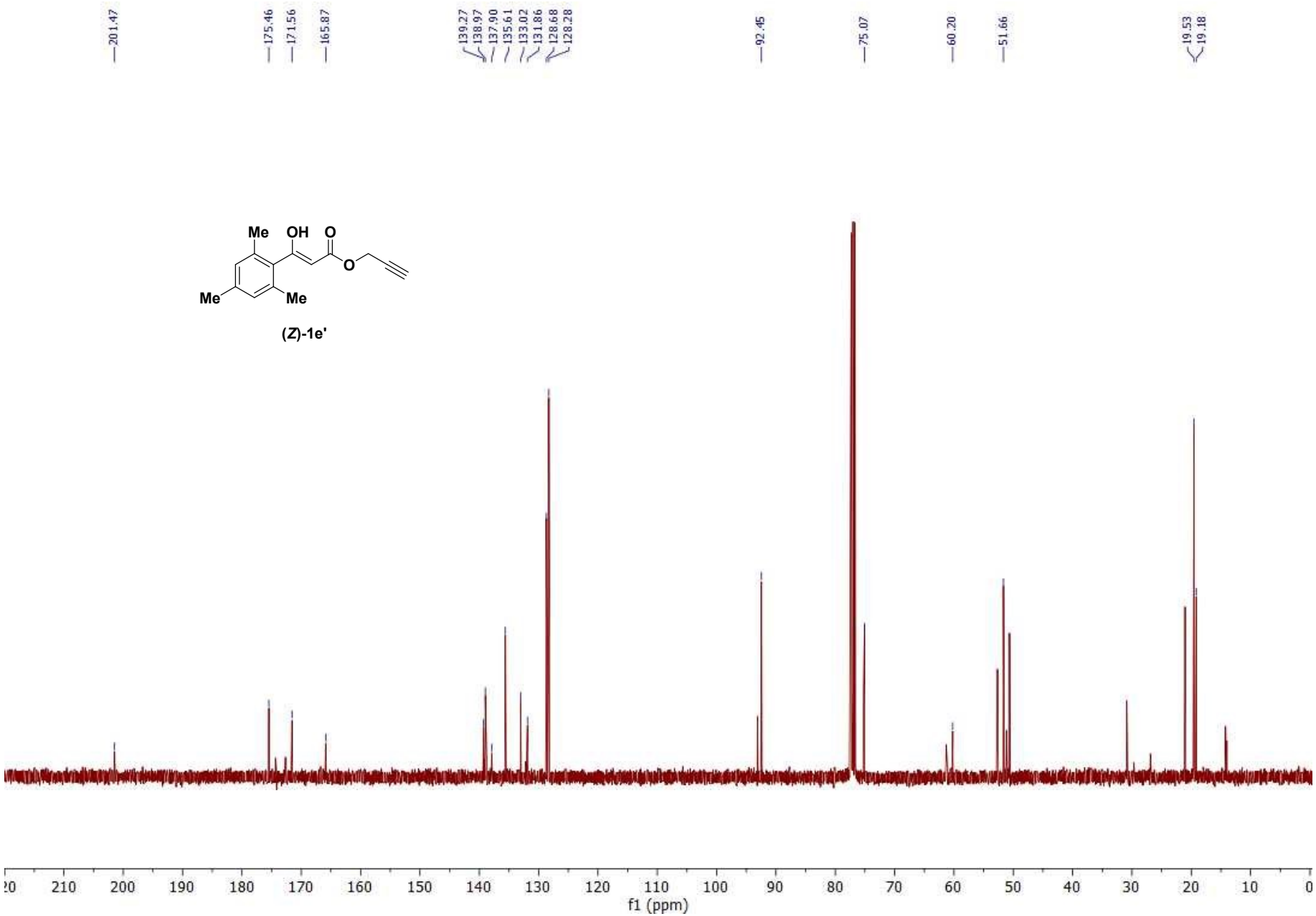
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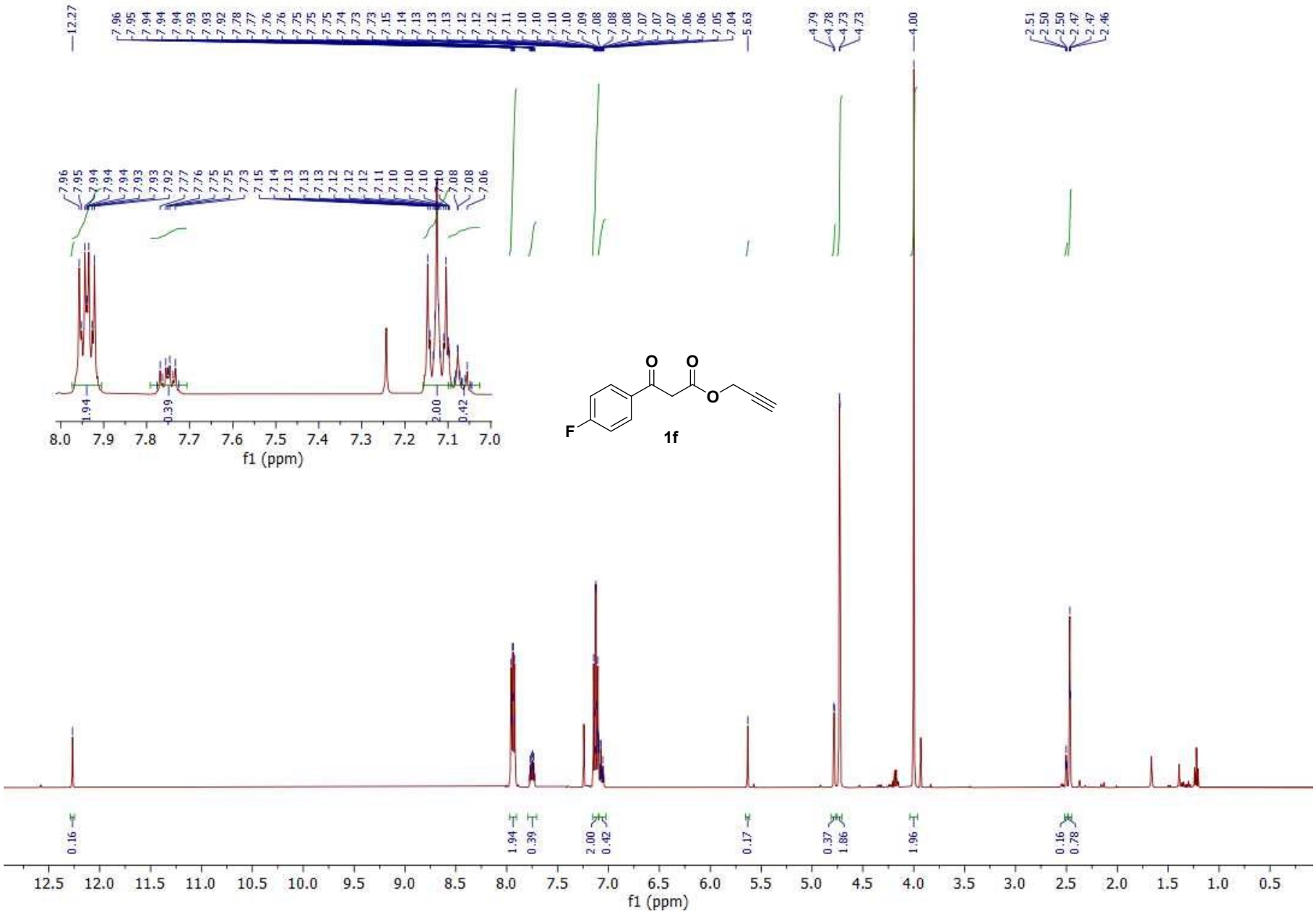
O
O
Me
Me
(Z)-1e'
f1 (ppm)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5.63
4.79 4.78 4.73 4.73
4.00
2.51 2.50 2.50 2.47 2.47 2.46
1.94 0.39 2.00 0.42
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
O O O F
1f
0.16 1.94 0.39 2.00 0.42 0.17 0.37 1.86 1.96 0.16 0.78
12.5 12.0 11.5 11.0 10.5 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
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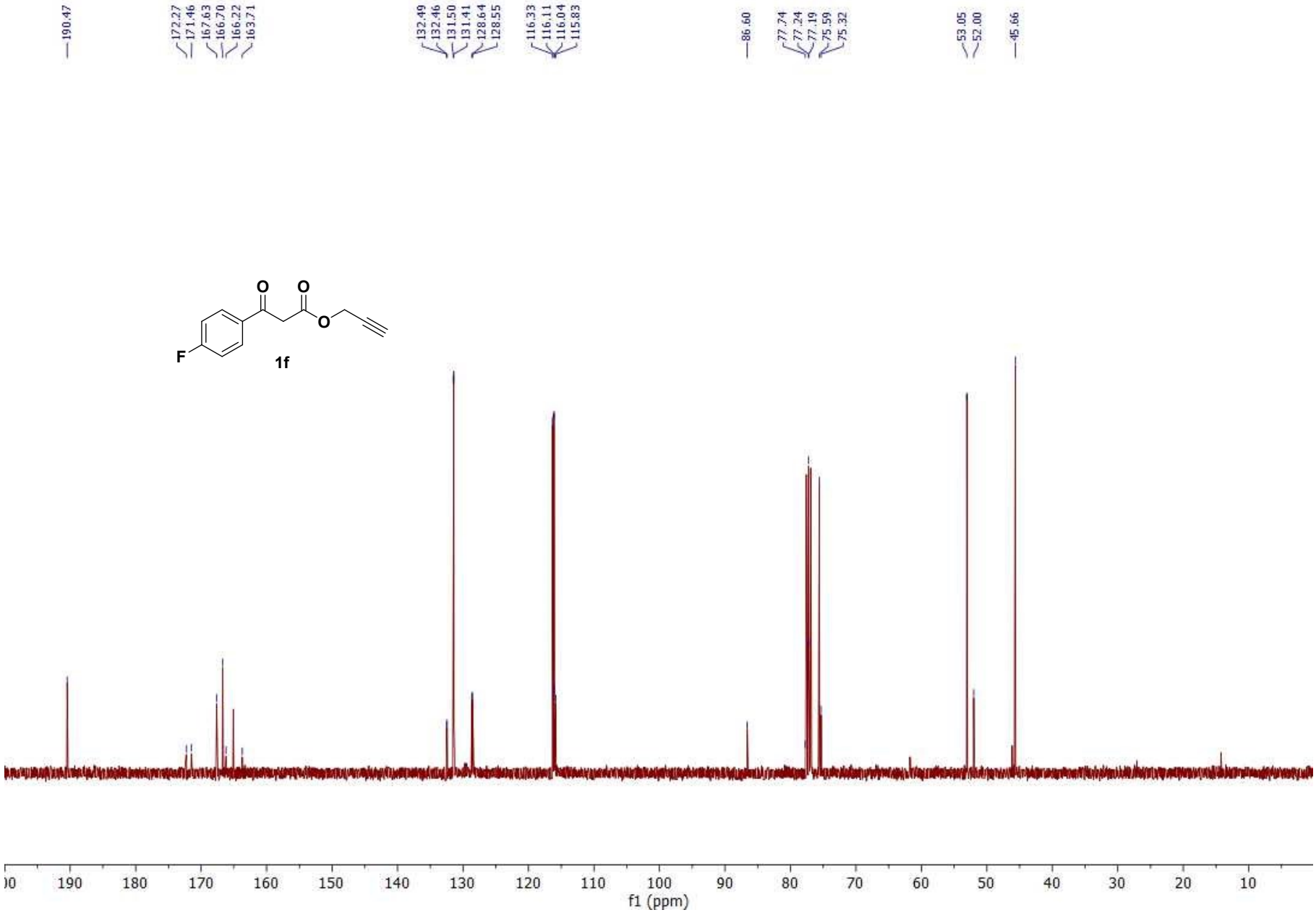
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45.66
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O
O
F
1f
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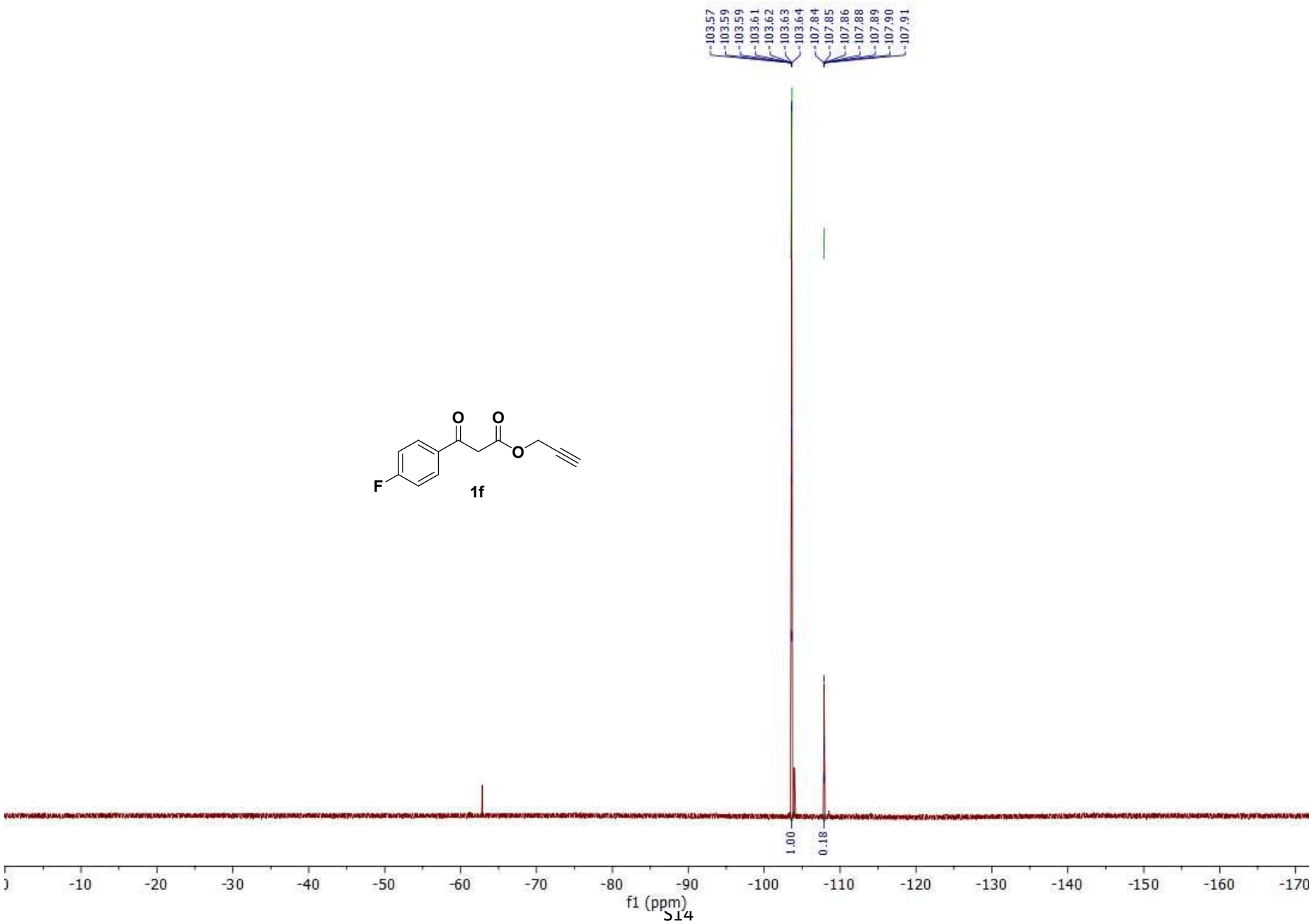
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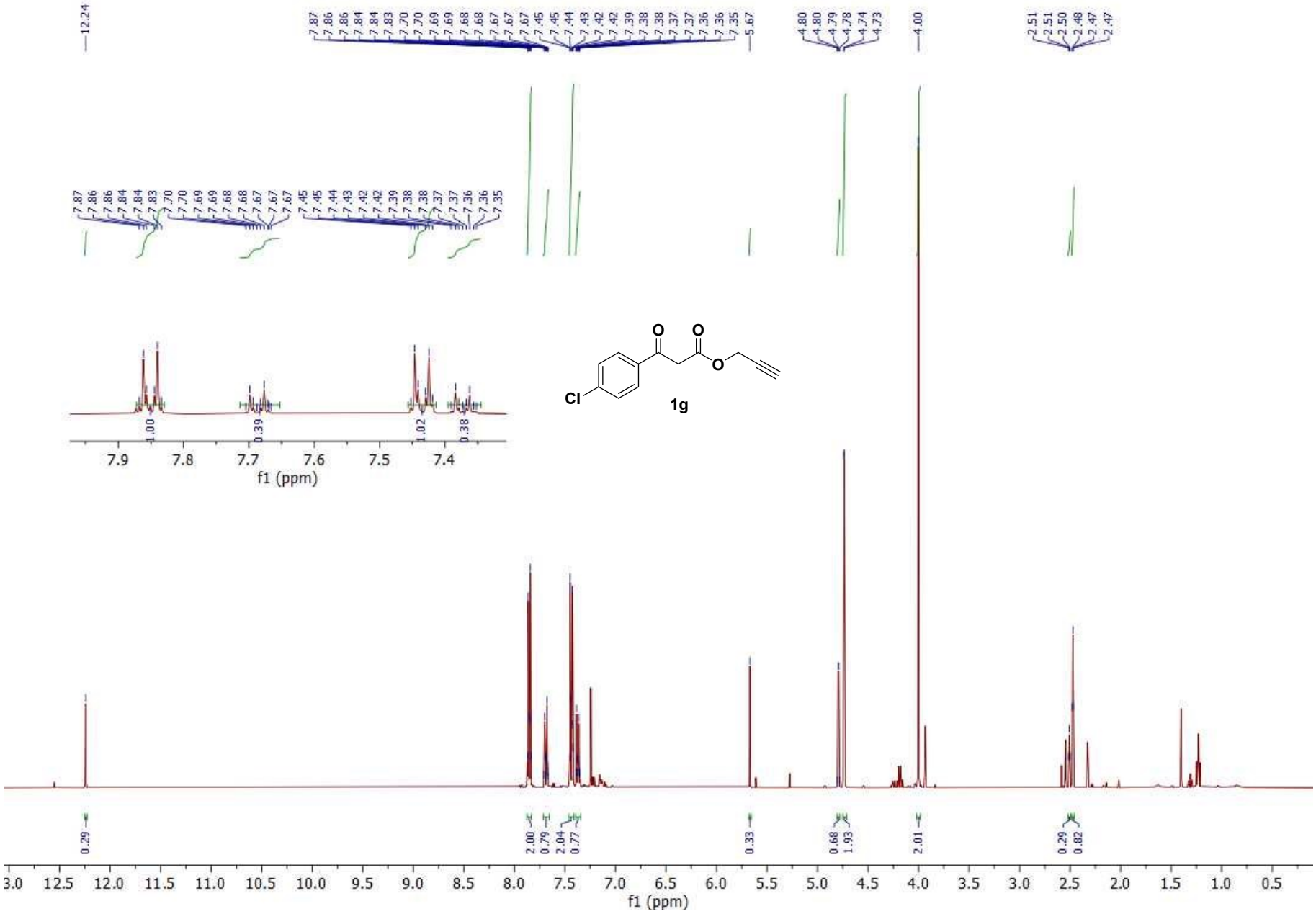
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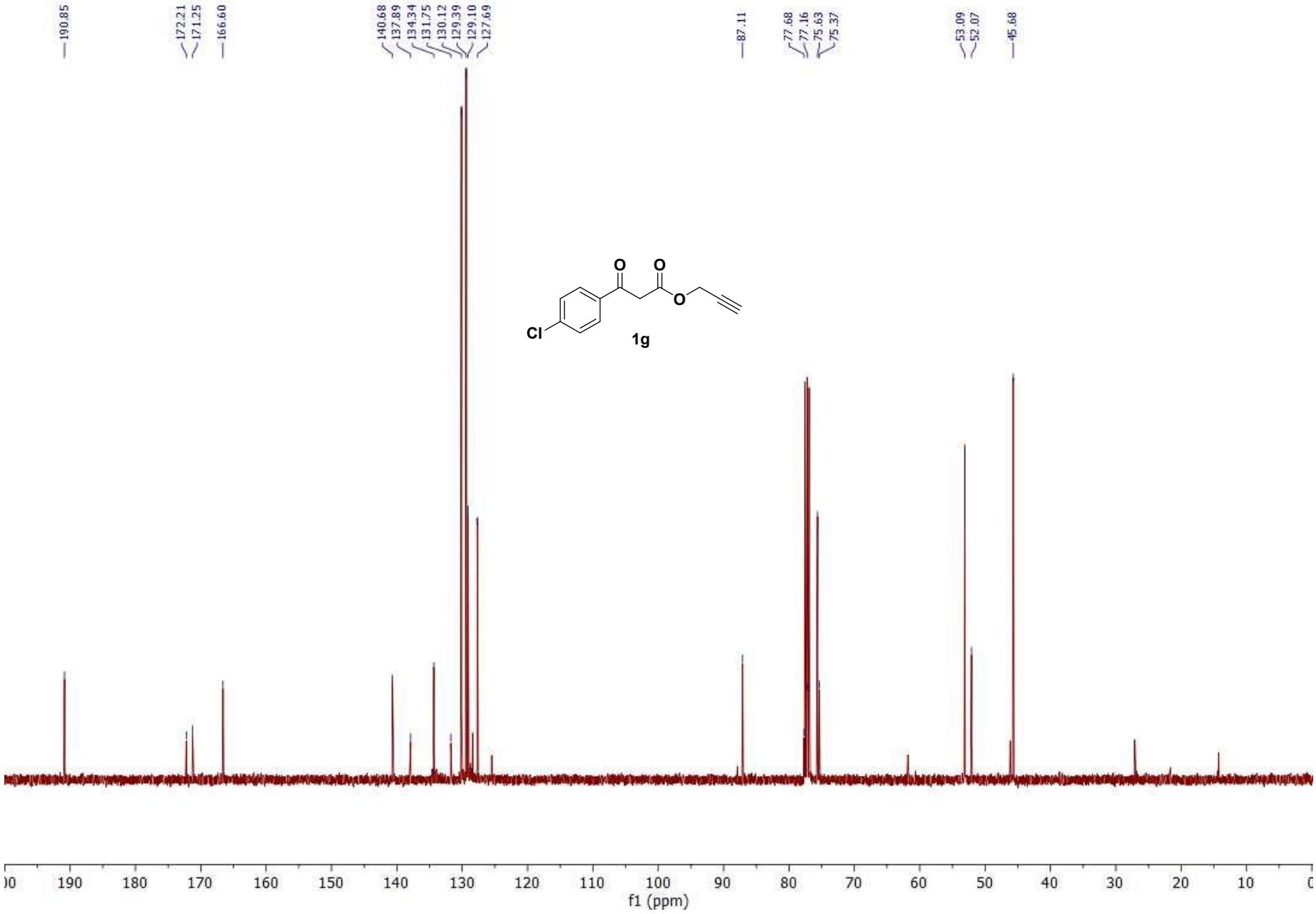
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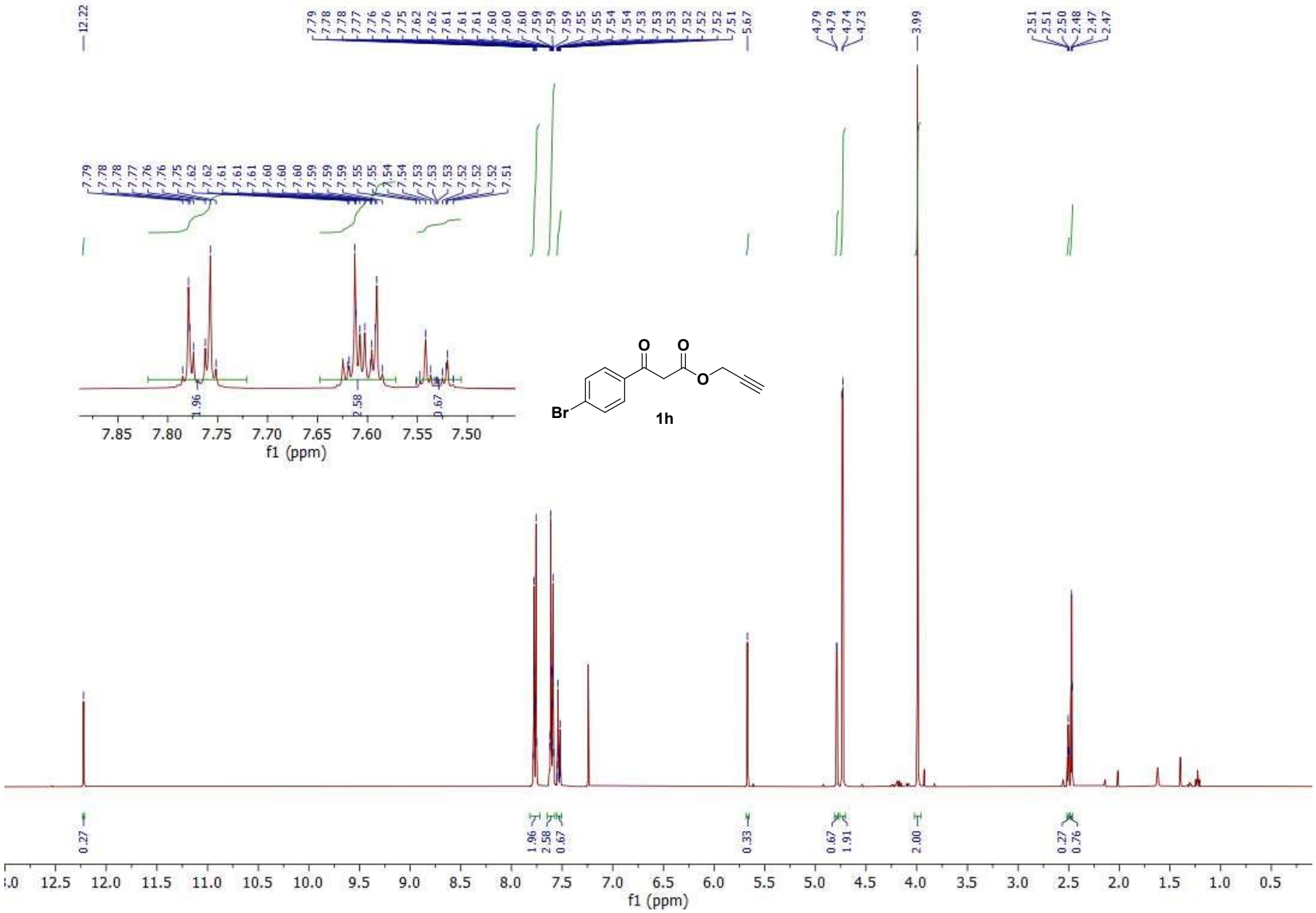
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7.50
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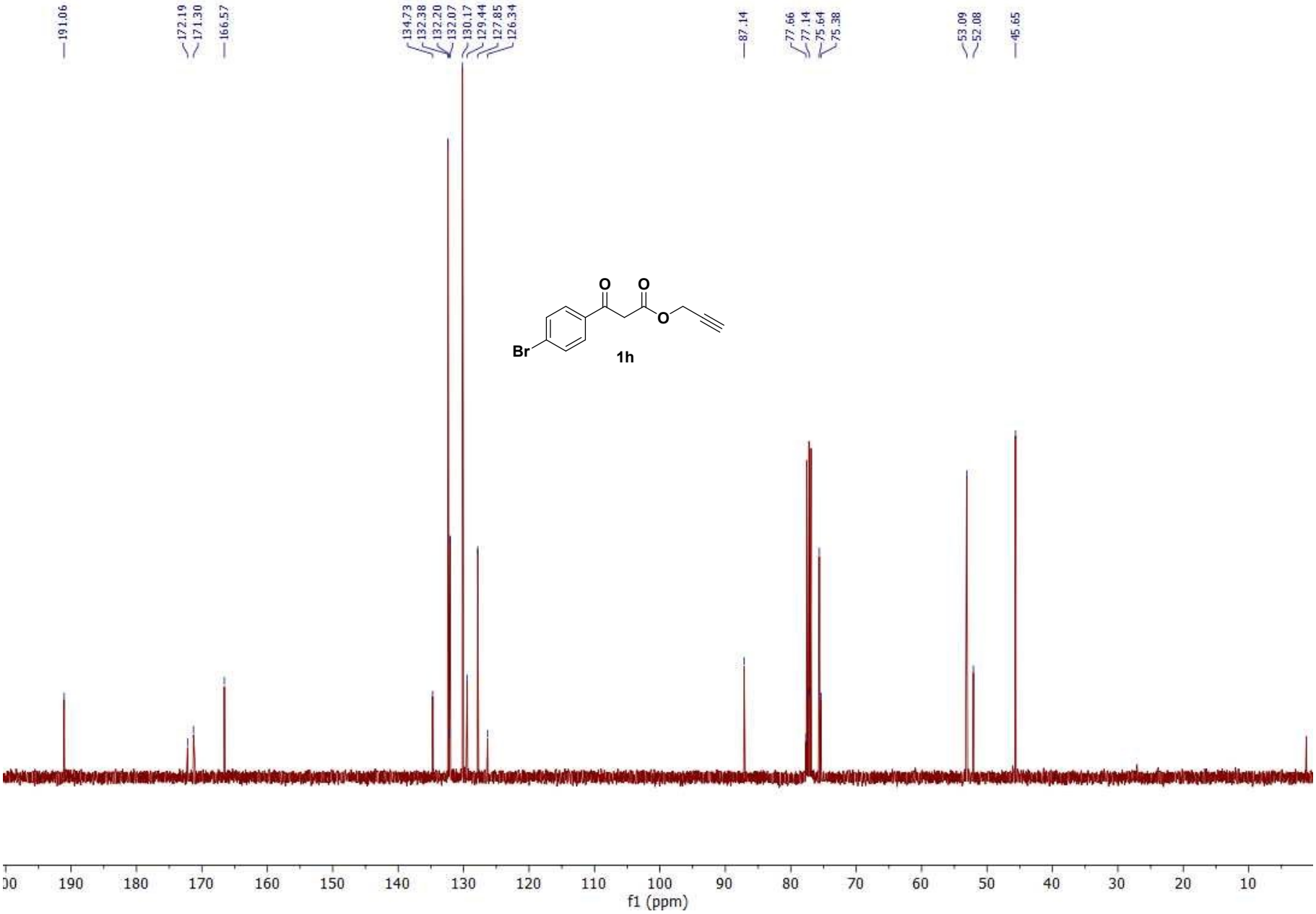
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O
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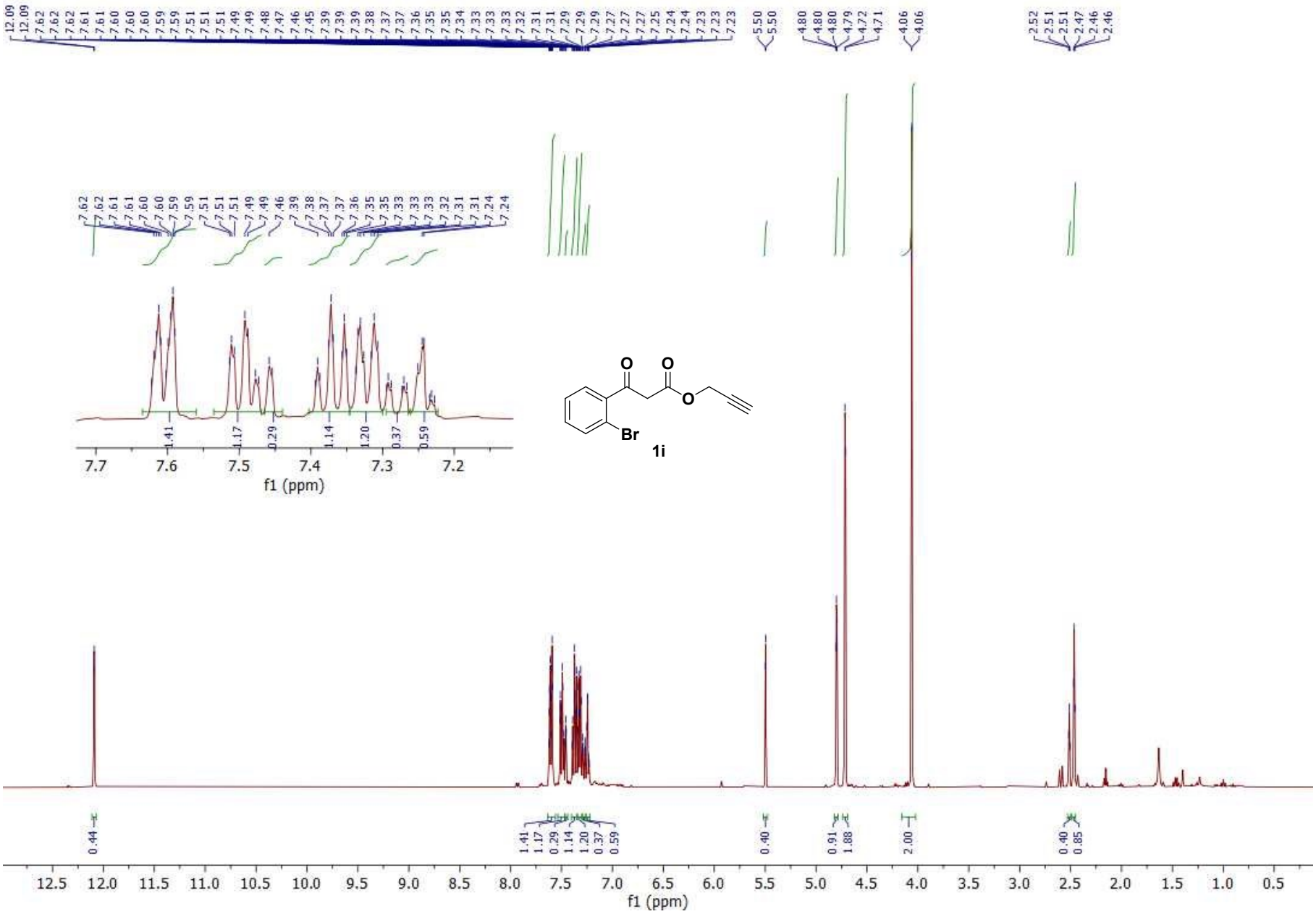
Br
1h
f1 (ppm)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4.79
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4.71
4.06
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O
Br
1i
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1.17
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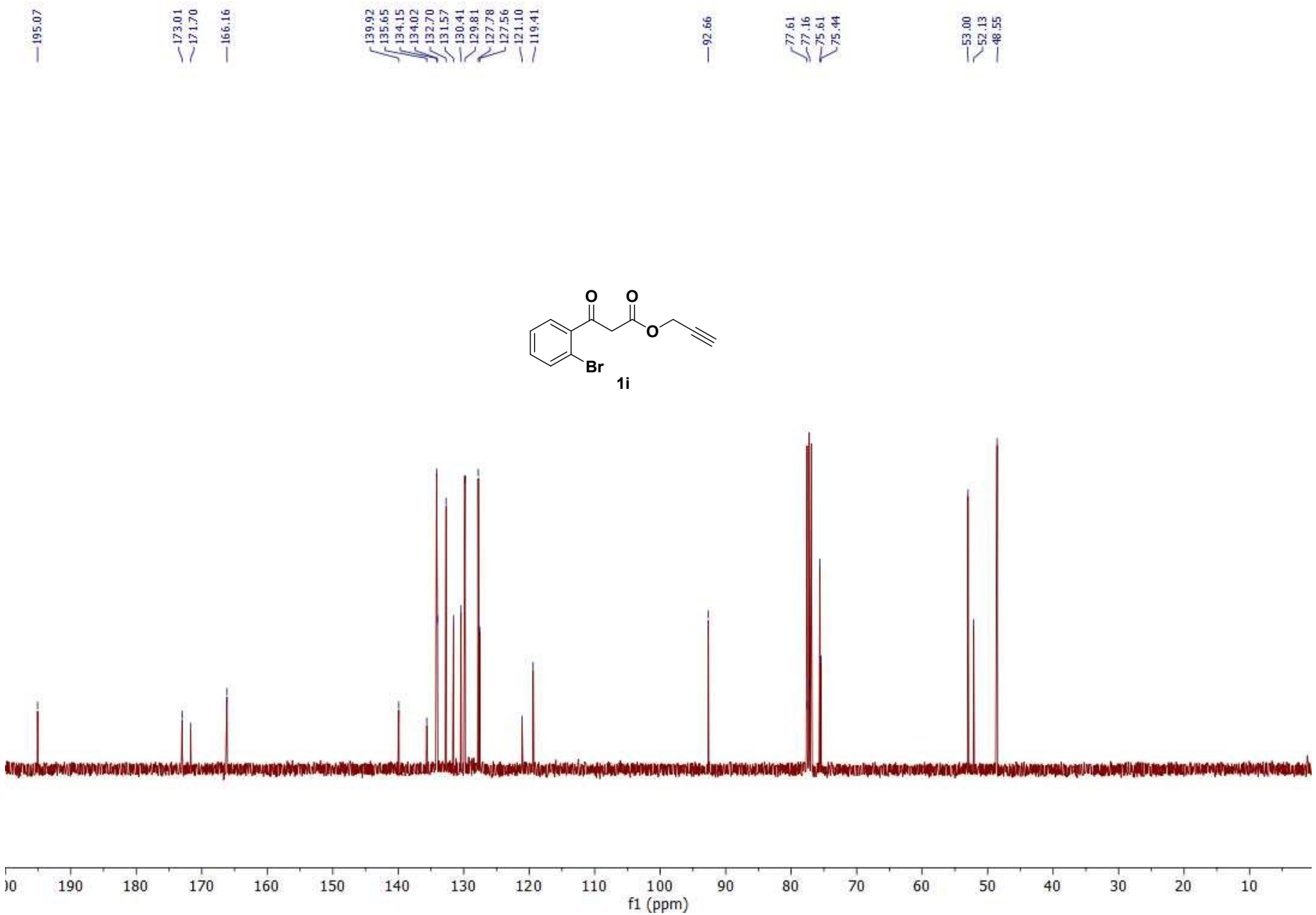
f1 (ppm)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129.81
127.78
127.56
121.10
119.41
92.66
77.61
77.16
75.61
75.44
53.00
52.13
48.55
O
O
O
Br
1i
190
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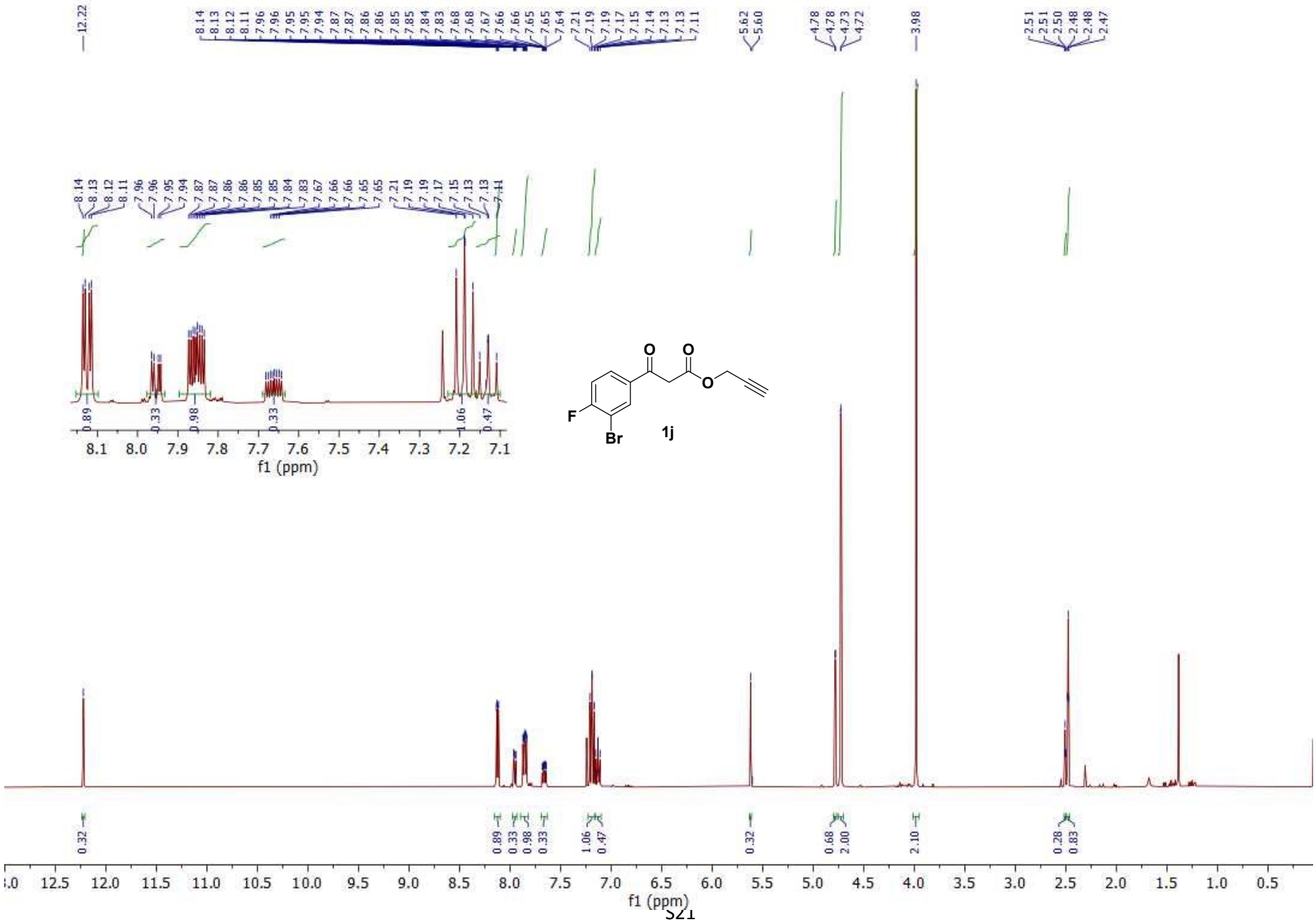
f1 (ppm)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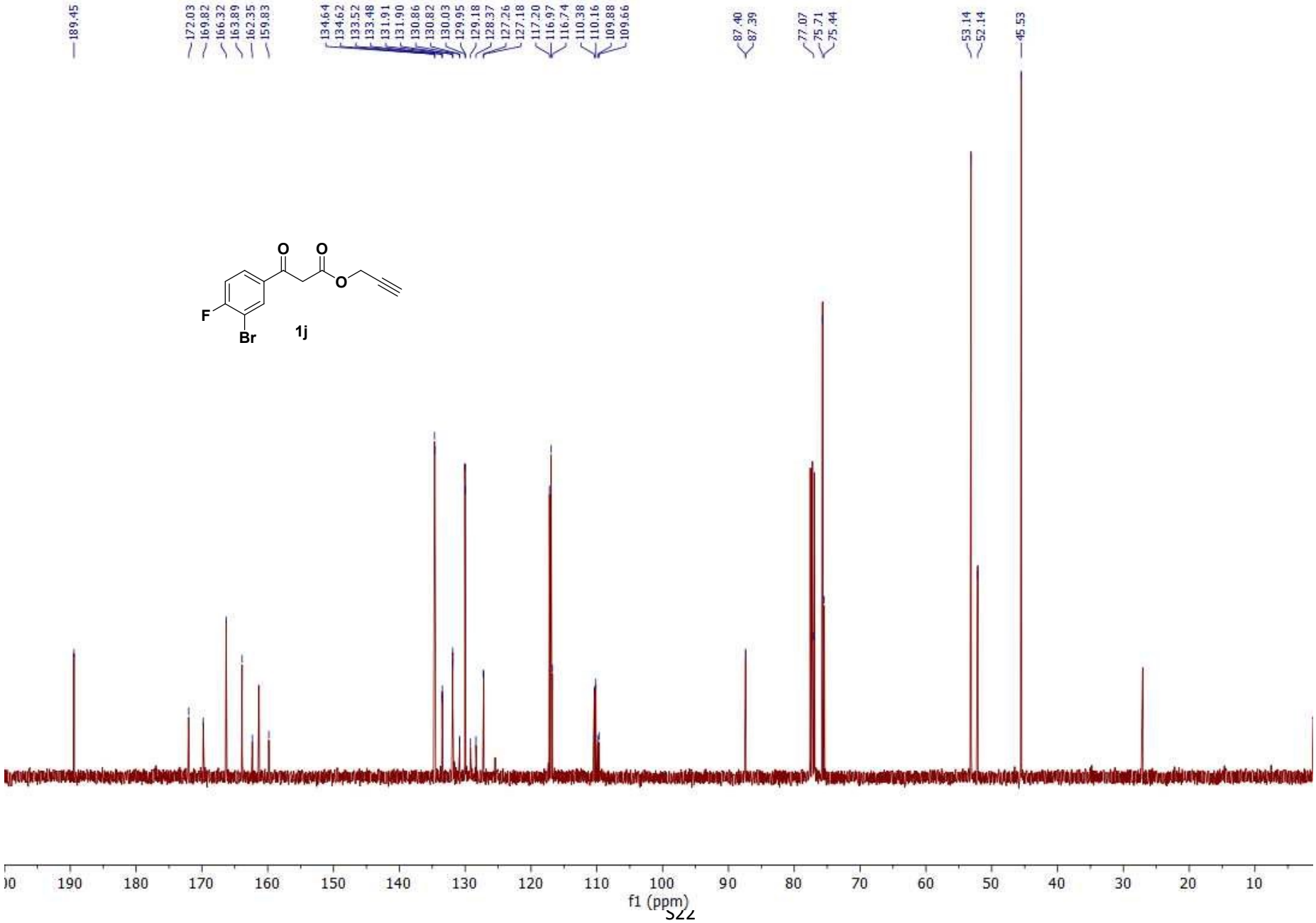
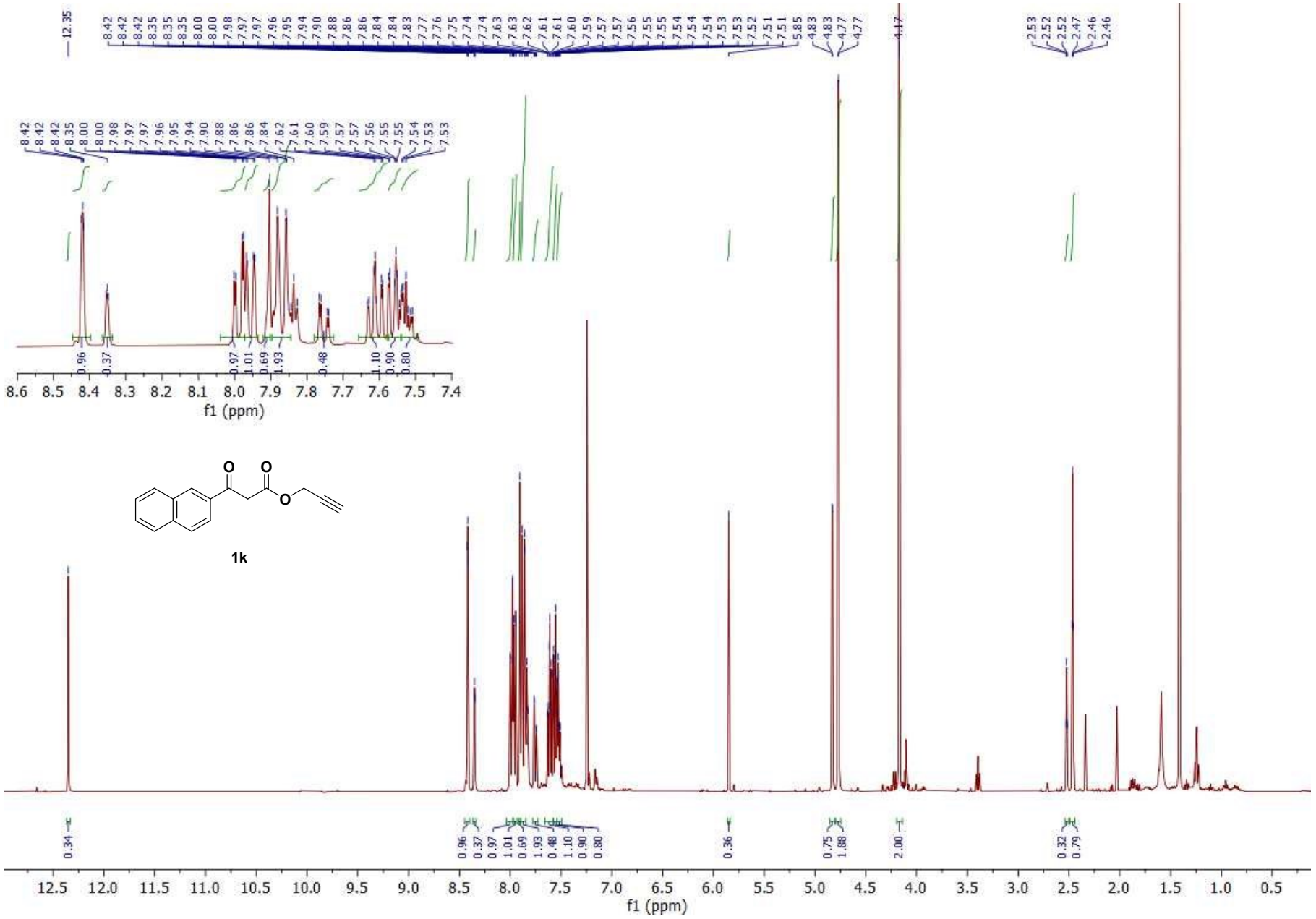
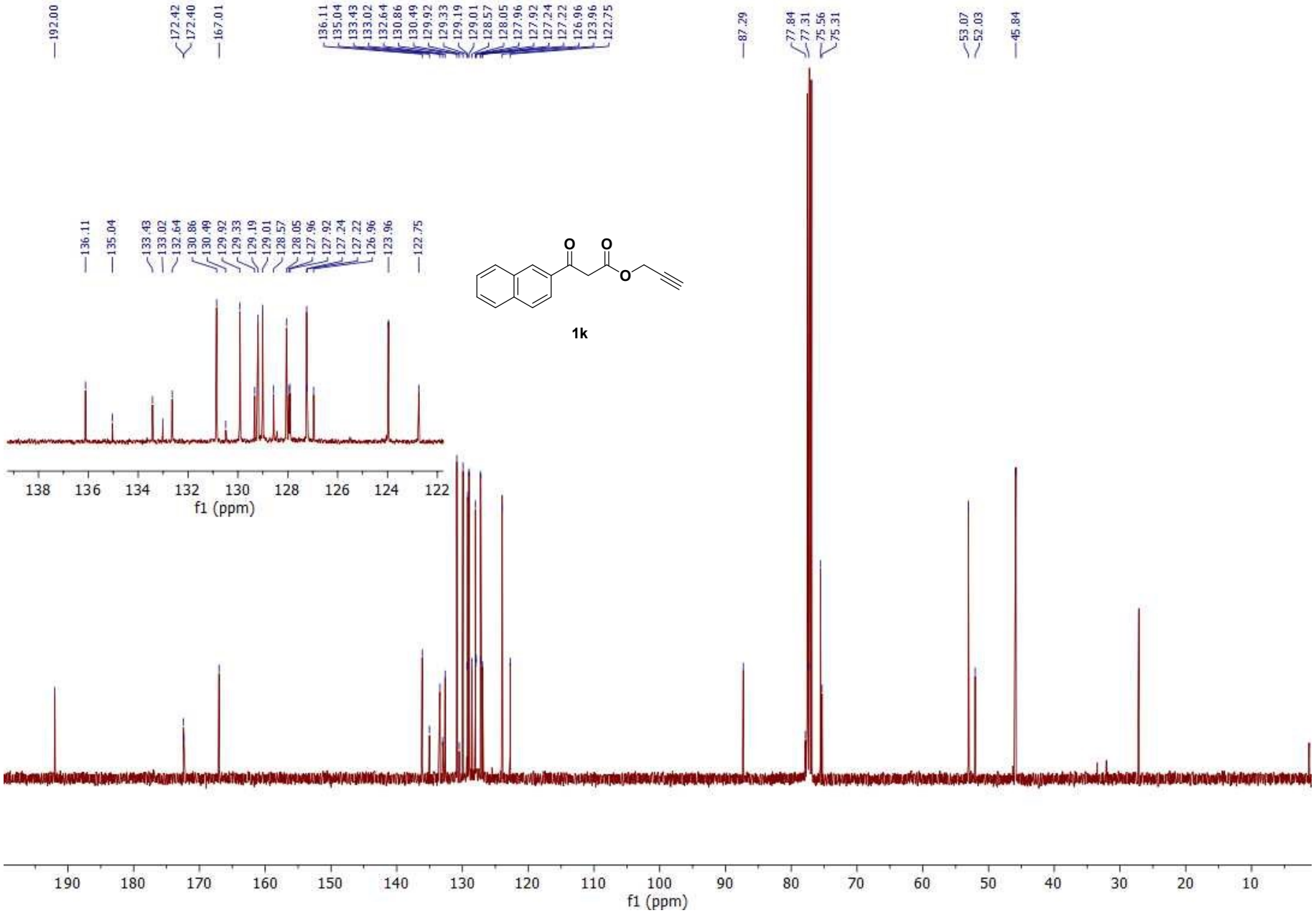
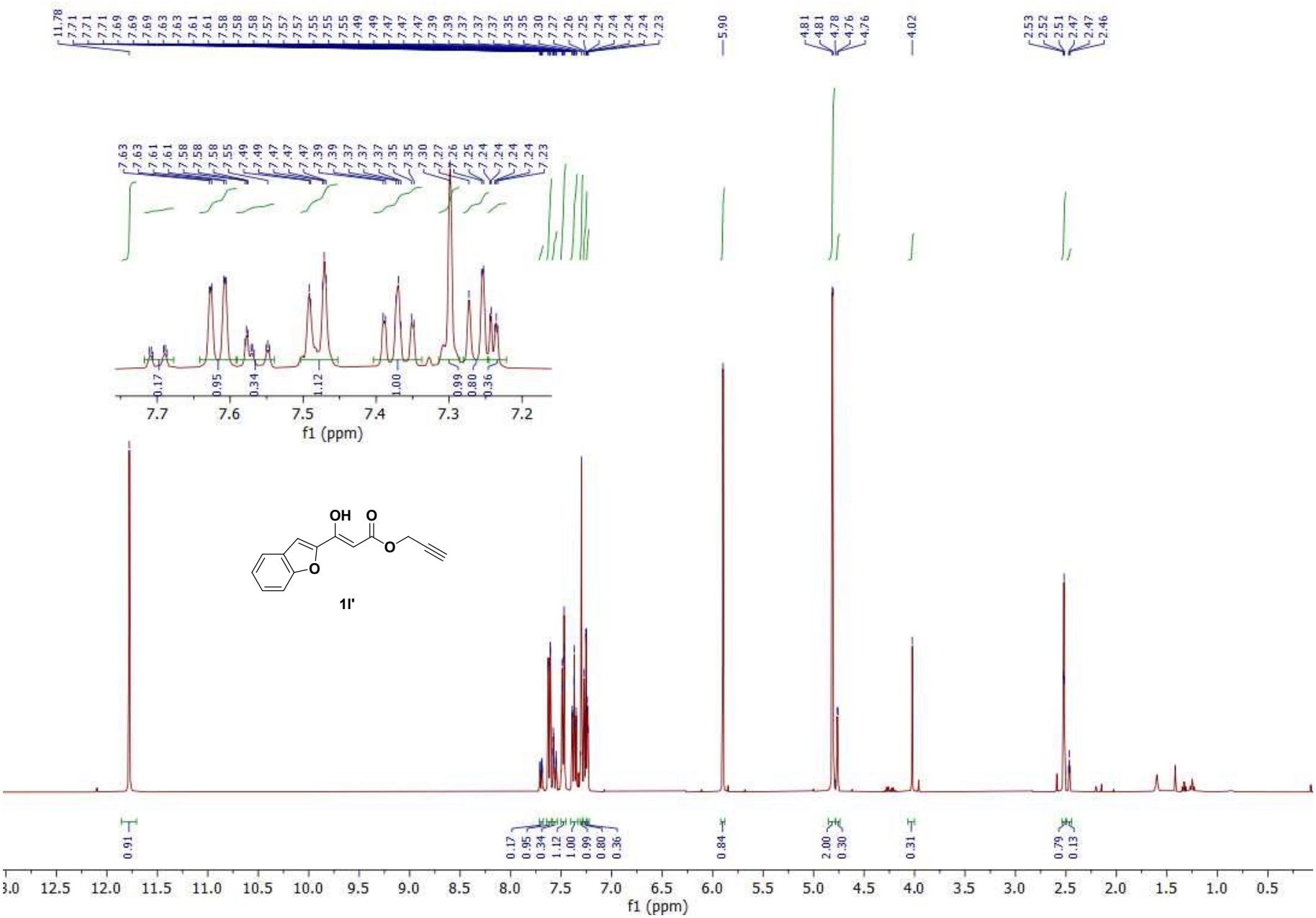
5.62 5.60
4.78 4.78 4.73 4.72
3.98
2.51 2.51 2.50 2.48 2.48 2.47
0.89 0.33 0.98 0.33 1.06 0.47
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
O O O
F Br
1j
0.32 0.89 0.33 0.98 0.33 1.06 0.47 0.32 0.68 2.00 2.10 0.28 0.83
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

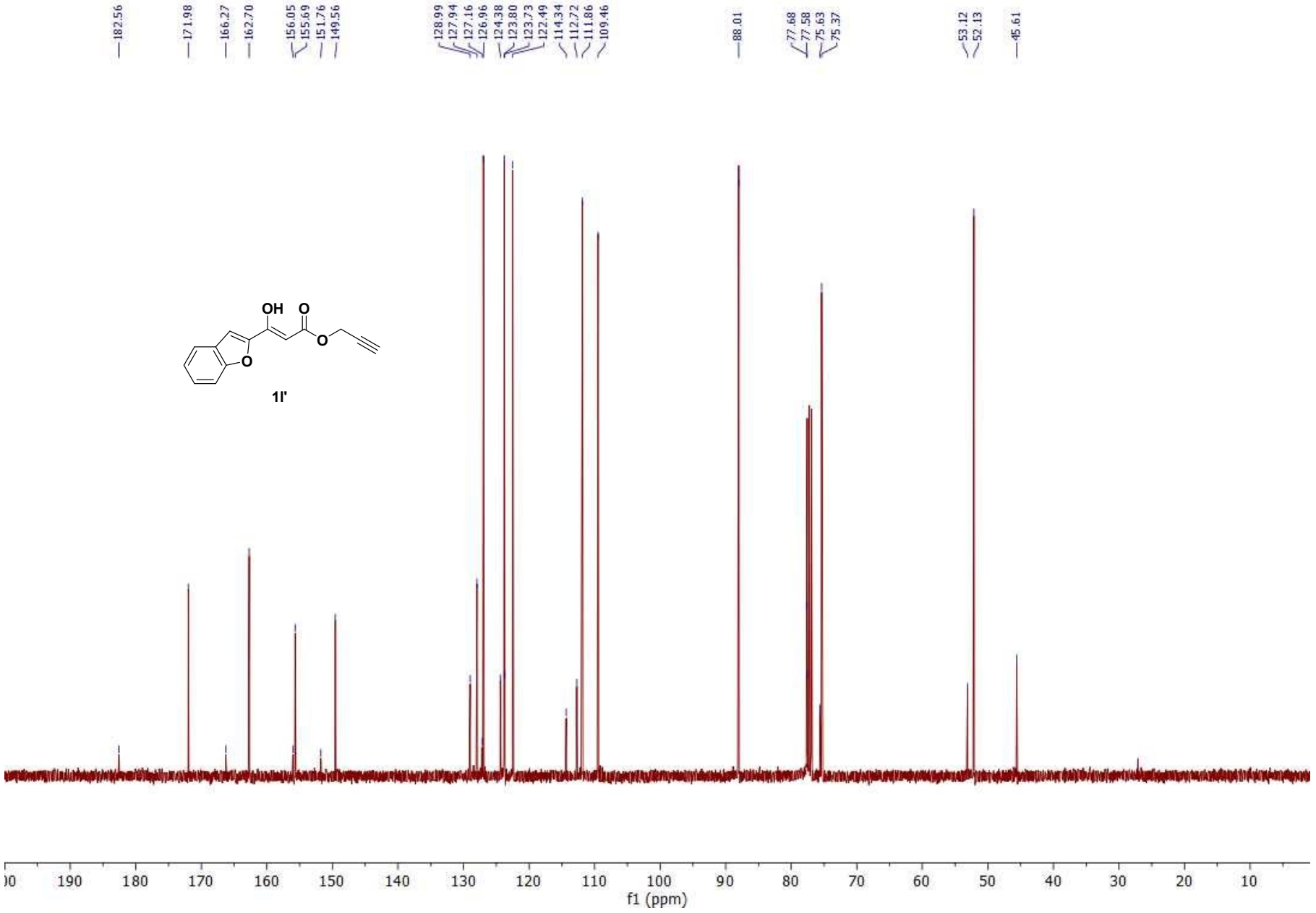

189.45
172.03
169.82
166.32
163.89
162.35
159.83
134.64
134.62
133.52
133.48
131.91
131.90
130.86
130.82
130.03
129.95
129.18
128.37
127.26
127.18
117.20
116.97
116.74
110.38
110.16
109.88
109.66
87.40
87.39
77.07
75.71
75.44
53.14
52.14
45.53
O
O
O
F
Br
1j
f1 (ppm)

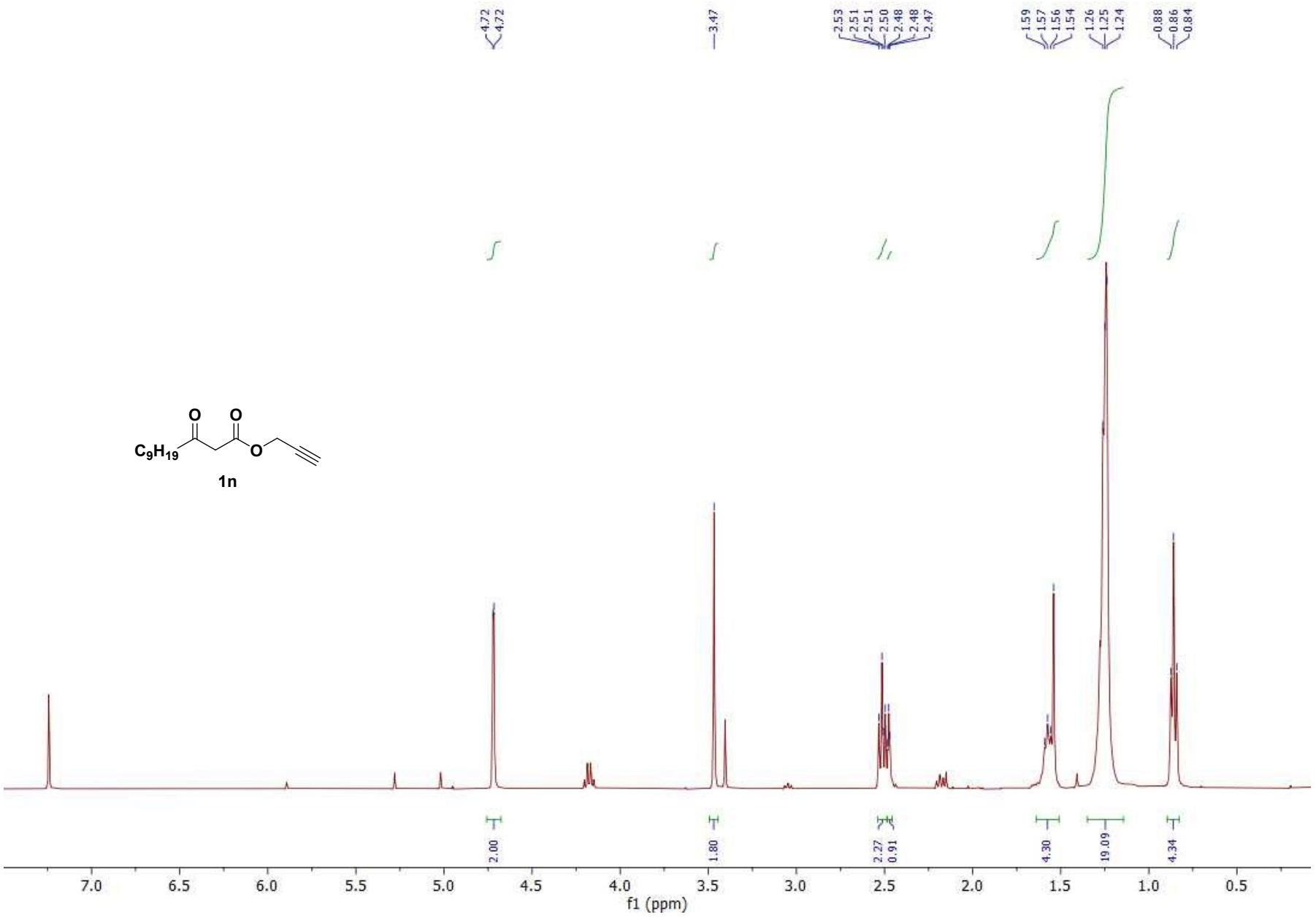


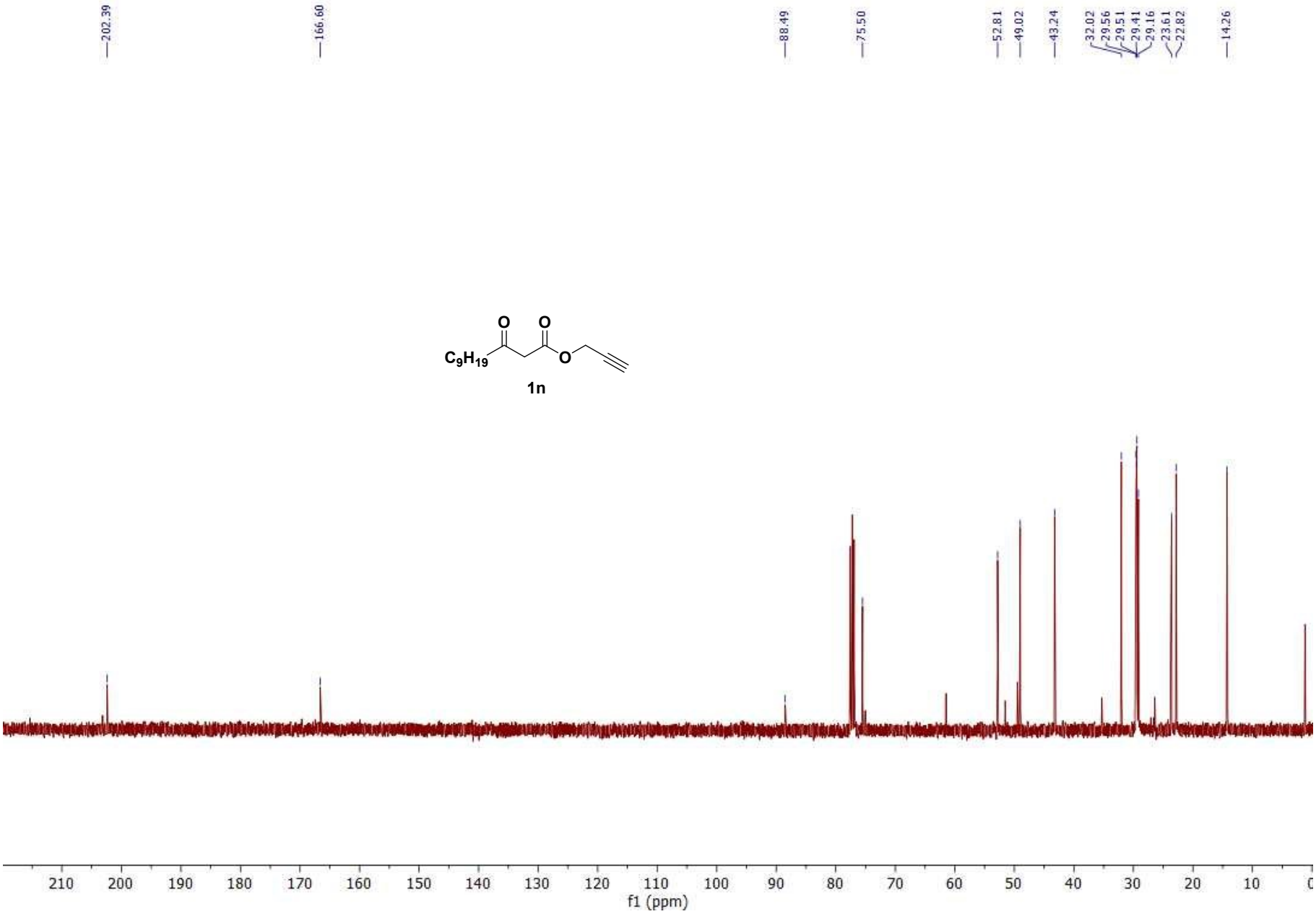
1k

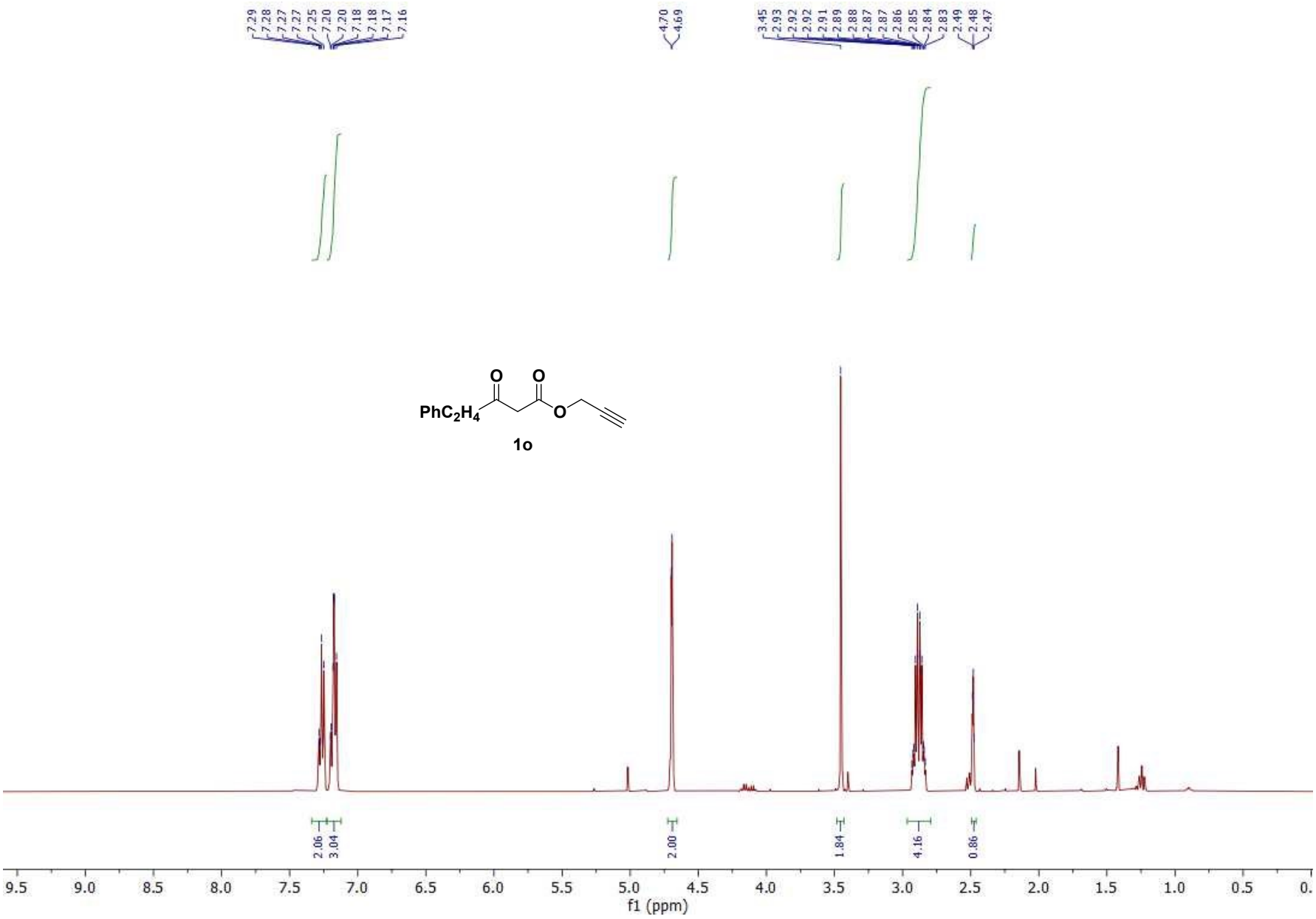

192.00
172.42
172.40
167.01
136.11
135.04
133.43
133.02
132.64
130.86
130.49
129.92
129.33
129.19
129.01
128.57
128.05
127.96
127.92
127.24
127.22
126.96
123.96
122.75
87.29
77.84
77.31
75.56
75.31
53.07
52.03
45.84
O
O
O
1k
f1 (ppm)
f1 (ppm)

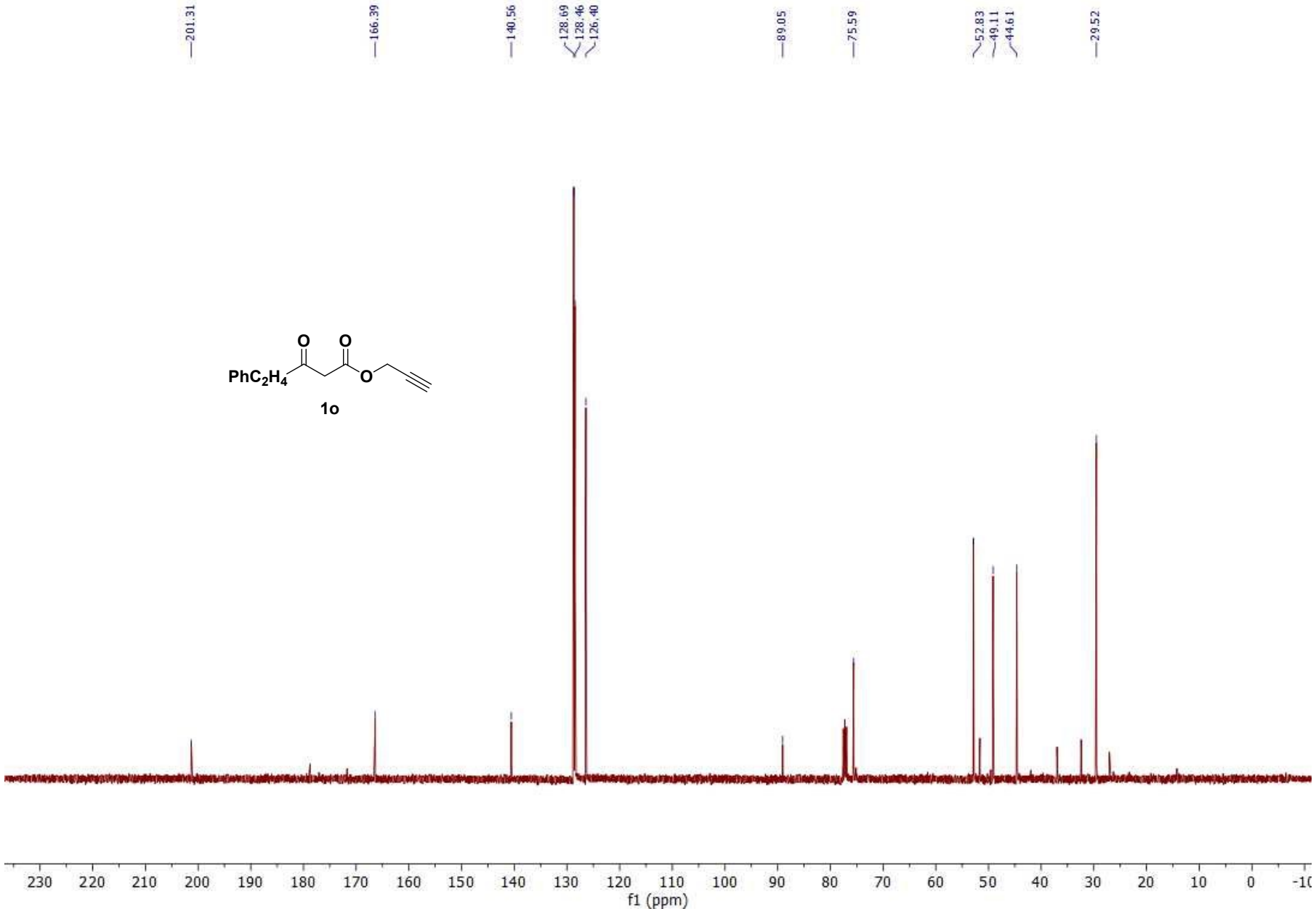

OH
O
O
O
1l'
f1 (ppm)

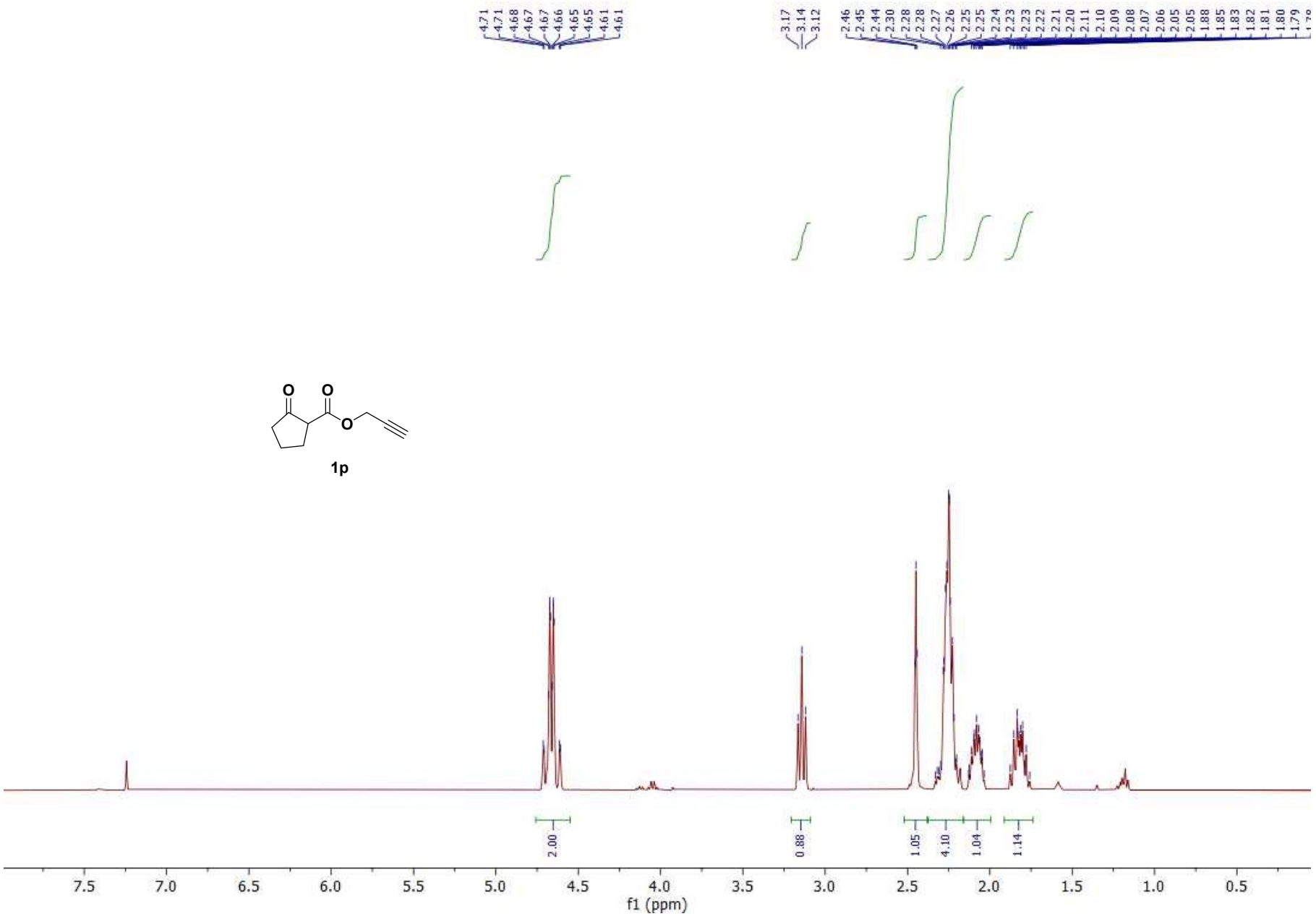

182.56
171.98
166.27
162.70
156.05
155.69
151.76
149.56
128.99
127.94
127.16
126.96
124.38
123.80
123.73
122.49
114.34
112.72
111.86
109.46
88.01
77.68
77.58
75.63
75.37
53.12
52.13
45.61
OH
O
O
O
1l'
f1 (ppm)

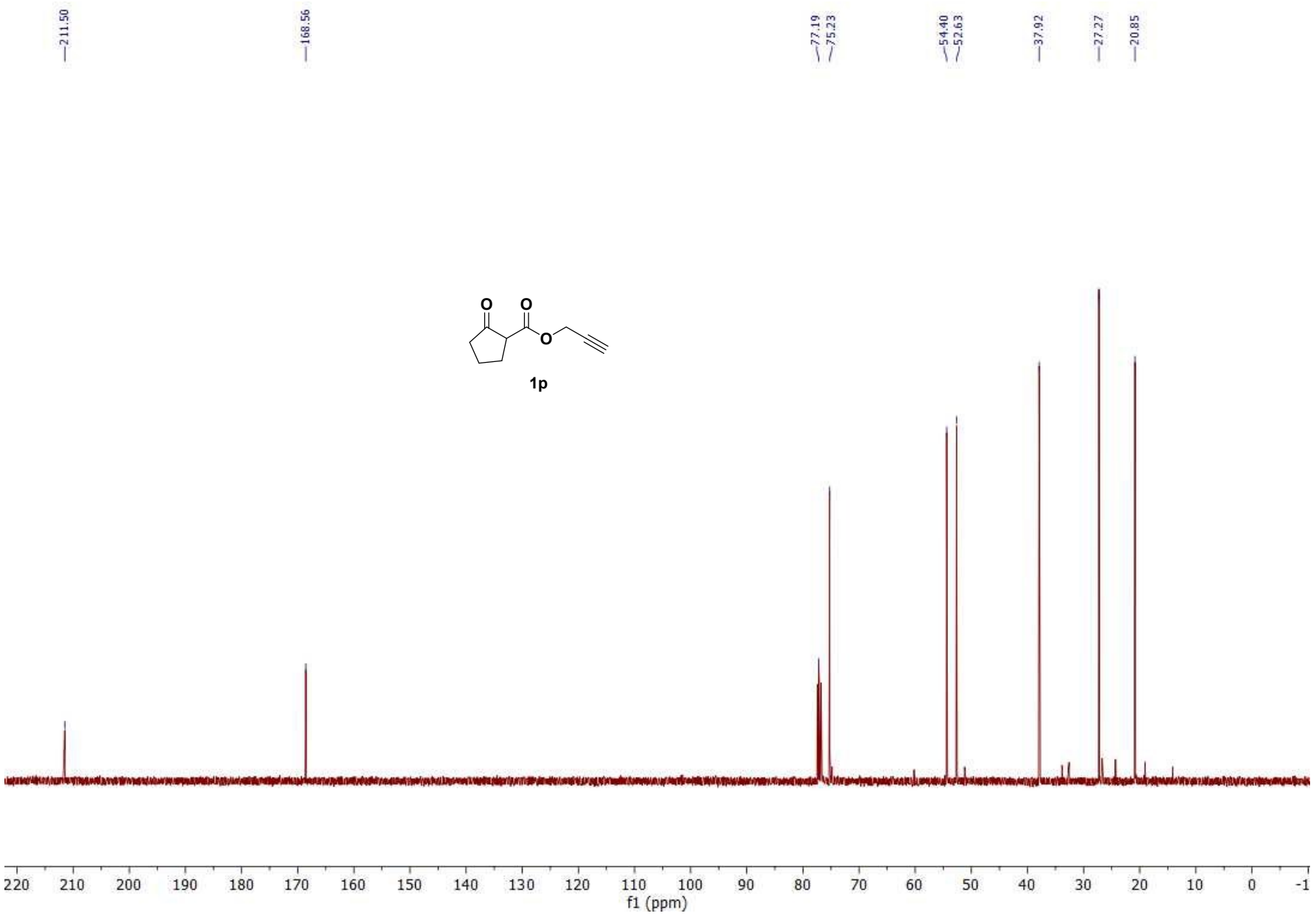

4.72
4.72
3.47
2.53
2.51
2.51
2.50
2.48
2.48
2.47
1.59
1.57
1.56
1.54
1.26
1.25
1.24
0.88
0.86
0.84
O
O
O
C9H19
1n
2.00
1.80
2.27
0.91
4.30
19.09
4.34
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

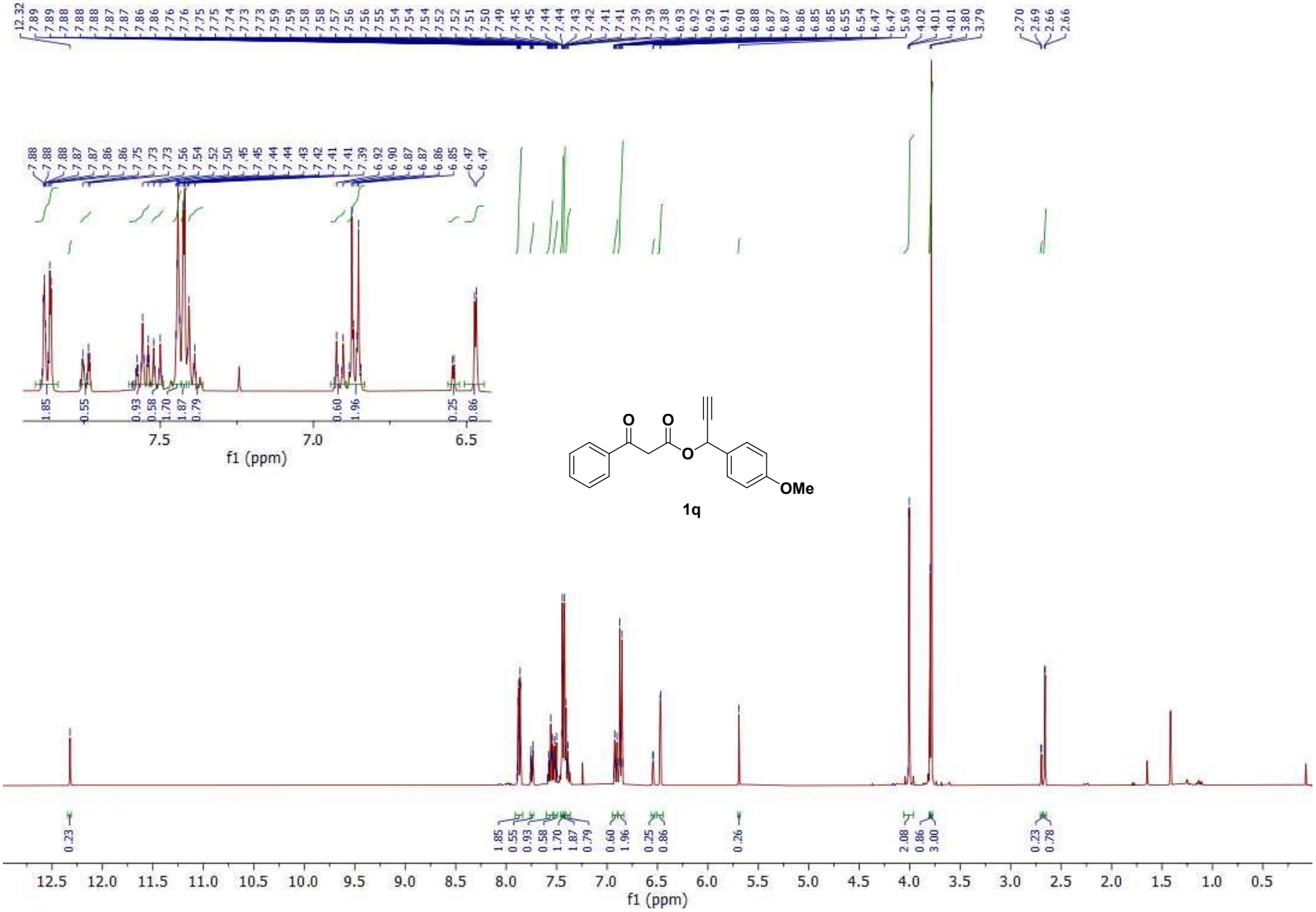

202.39
166.60
88.49
75.50
52.81
49.02
43.24
32.02
29.56
29.51
29.41
29.16
23.61
22.82
14.26
O
O
C9H19
O
1n
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

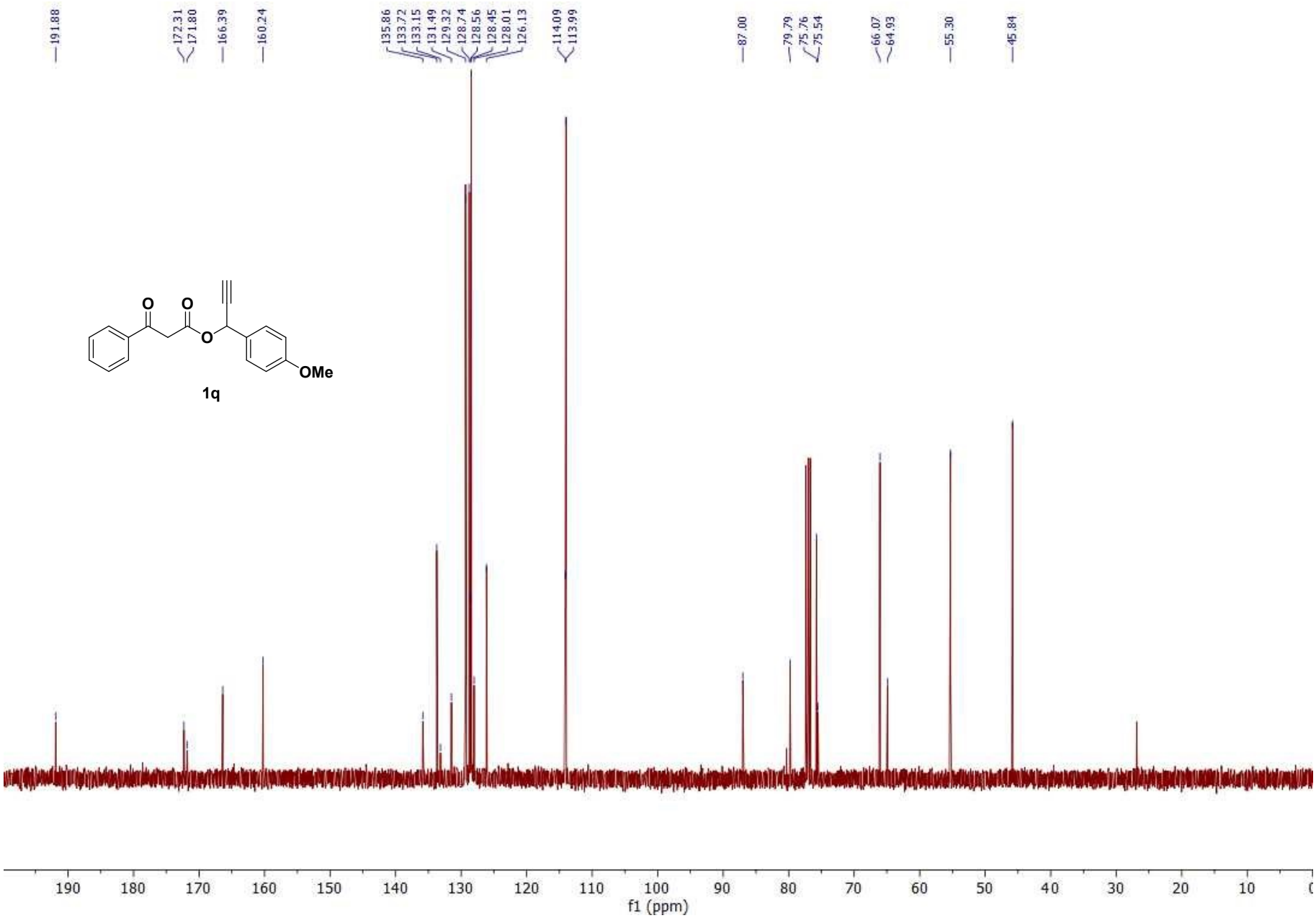

7.29
7.28
7.27
7.27
7.25
7.20
7.20
7.18
7.18
7.17
7.16
4.70
4.69
3.45
2.93
2.92
2.92
2.91
2.89
2.88
2.87
2.87
2.86
2.85
2.84
2.83
2.49
2.48
2.47
O
O
PhC2H4
O
1o
2.06
3.04
2.00
1.84
4.16
0.86
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

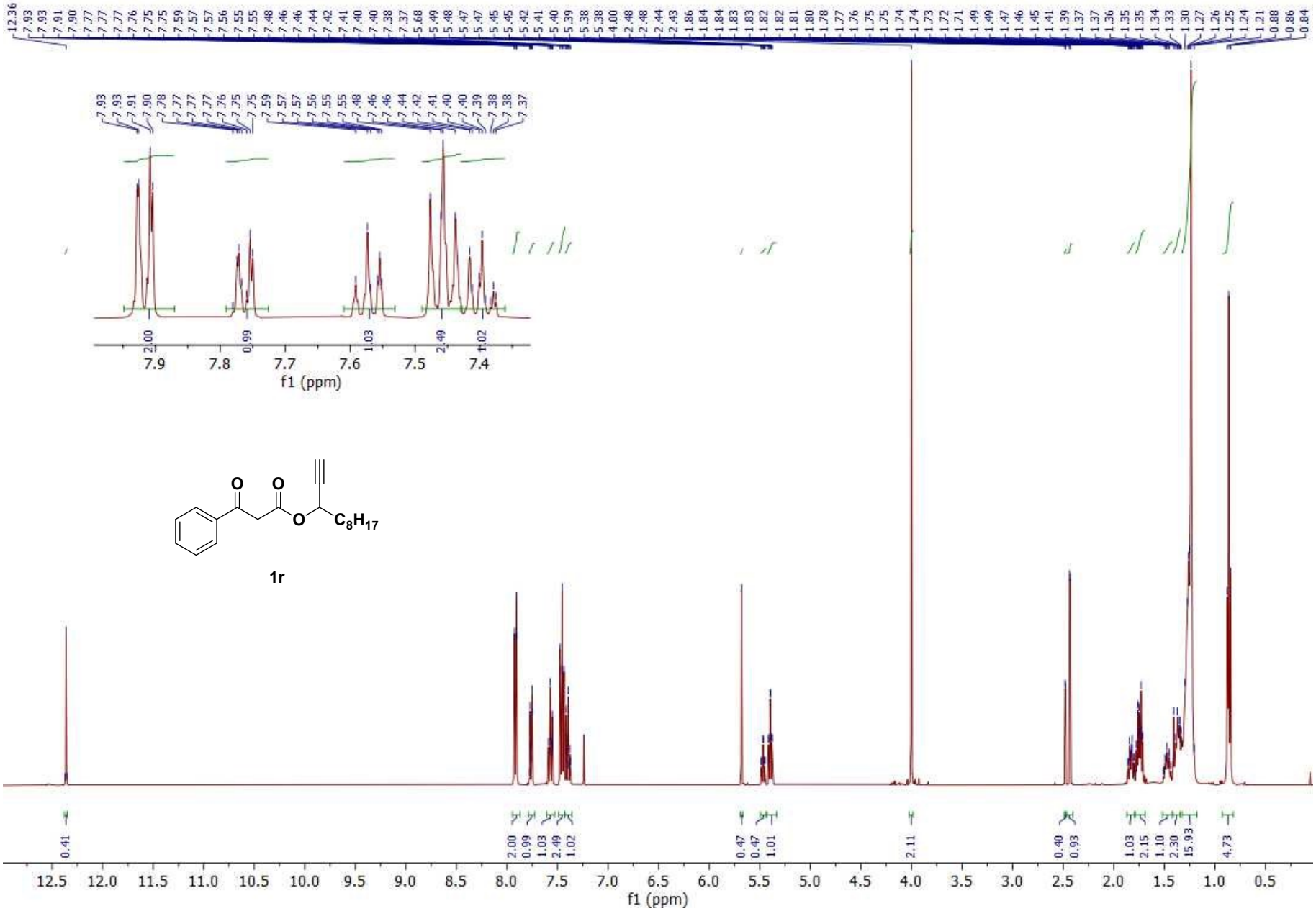

201.31
166.39
140.56
128.69
128.46
126.40
89.05
75.59
52.83
49.11
44.61
29.52
O
O
PhC2H4
O
1o
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


4.71
4.71
4.68
4.67
4.67
4.66
4.65
4.65
4.61
4.61
3.17
3.14
3.12
2.46
2.45
2.44
2.30
2.28
2.28
2.27
2.26
2.25
2.25
2.24
2.23
2.23
2.22
2.21
2.20
2.11
2.10
2.09
2.08
2.07
2.06
2.05
2.05
1.88
1.85
1.83
1.82
1.81
1.80
1.79
O
O
O
1p
2.00
0.88
1.05
4.10
1.04
1.14
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
f1 (ppm)

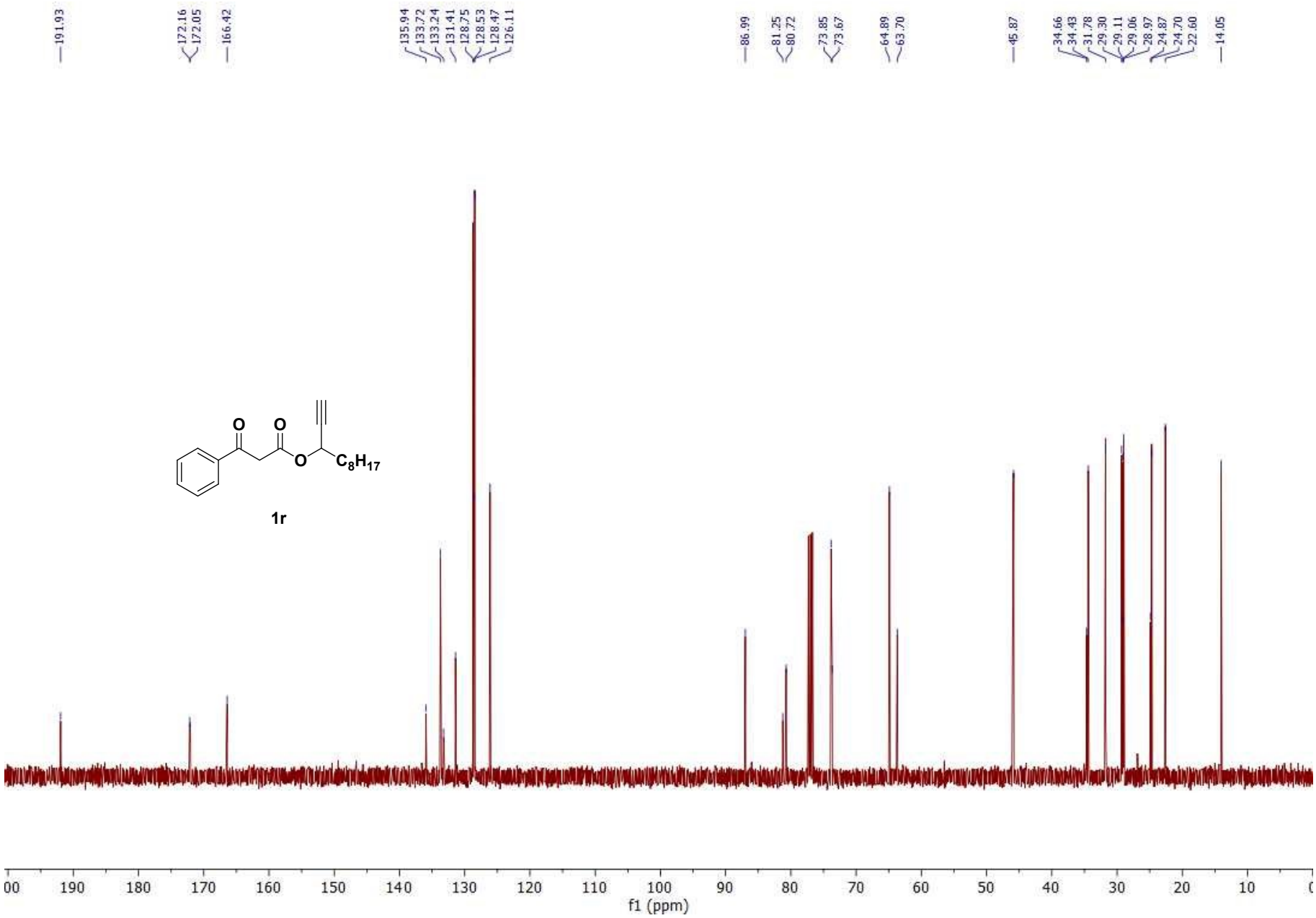

211.50
168.56
77.19
75.23
54.40
52.63
37.92
27.27
20.85
O
O
O
1p
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

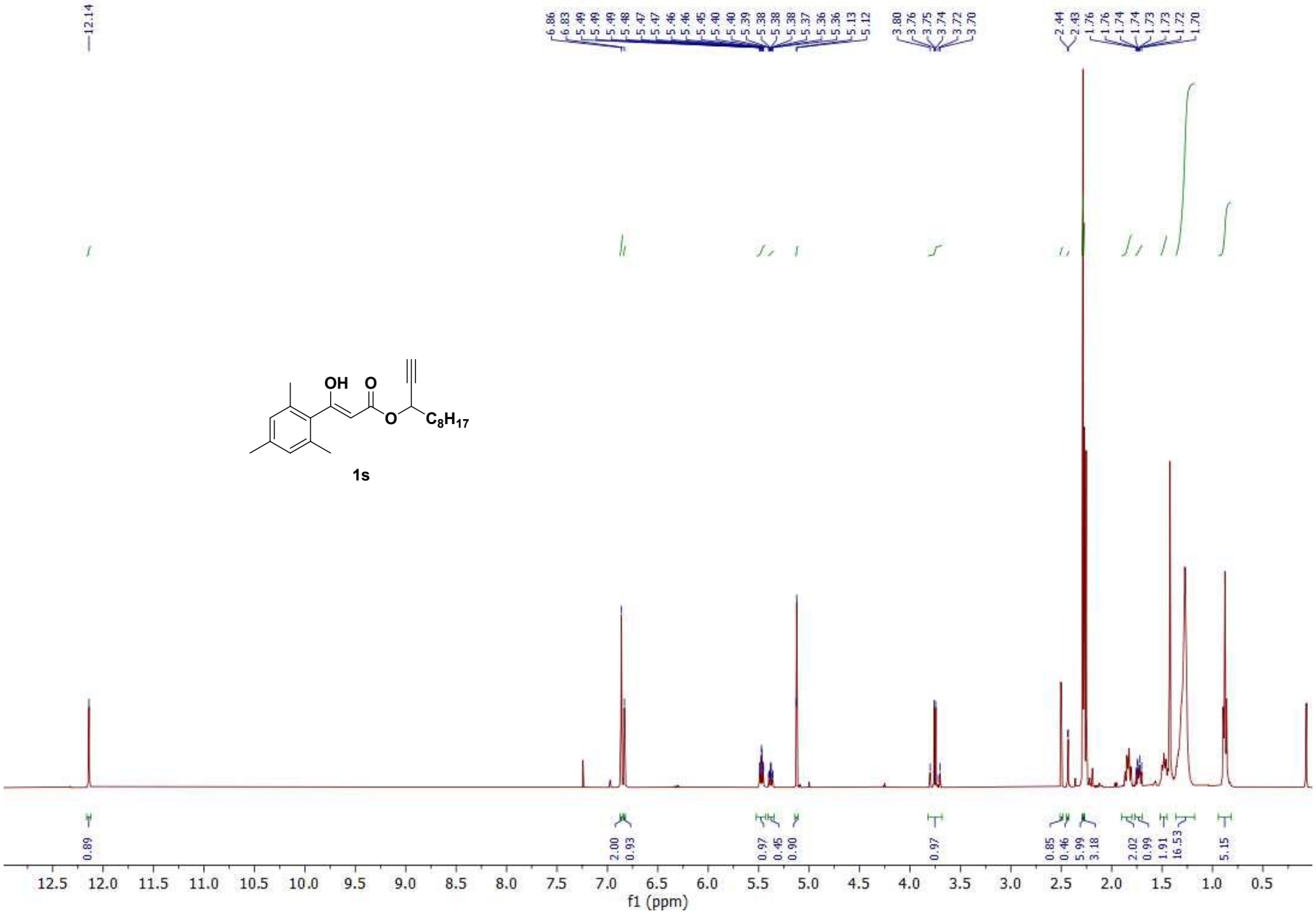

12.32
7.89
7.88
7.87
7.86
7.76
7.75
7.74
7.73
7.59
7.58
7.57
7.56
7.55
7.54
7.52
7.51
7.50
7.49
7.45
7.44
7.43
7.42
7.41
7.39
7.38
6.93
6.92
6.91
6.90
6.88
6.87
6.86
6.85
6.55
6.54
6.47
5.69
4.02
4.01
3.80
3.79
2.70
2.69
2.66
2.66
1.85
0.55
0.93
0.58
1.70
1.87
0.79
0.60
1.96
0.25
0.86
0.26
2.08
0.86
3.00
0.23
0.78
7.5
7.0
6.5
f1 (ppm)
O
O
O
OMe
1q
0.23
12.5
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
f1 (ppm)

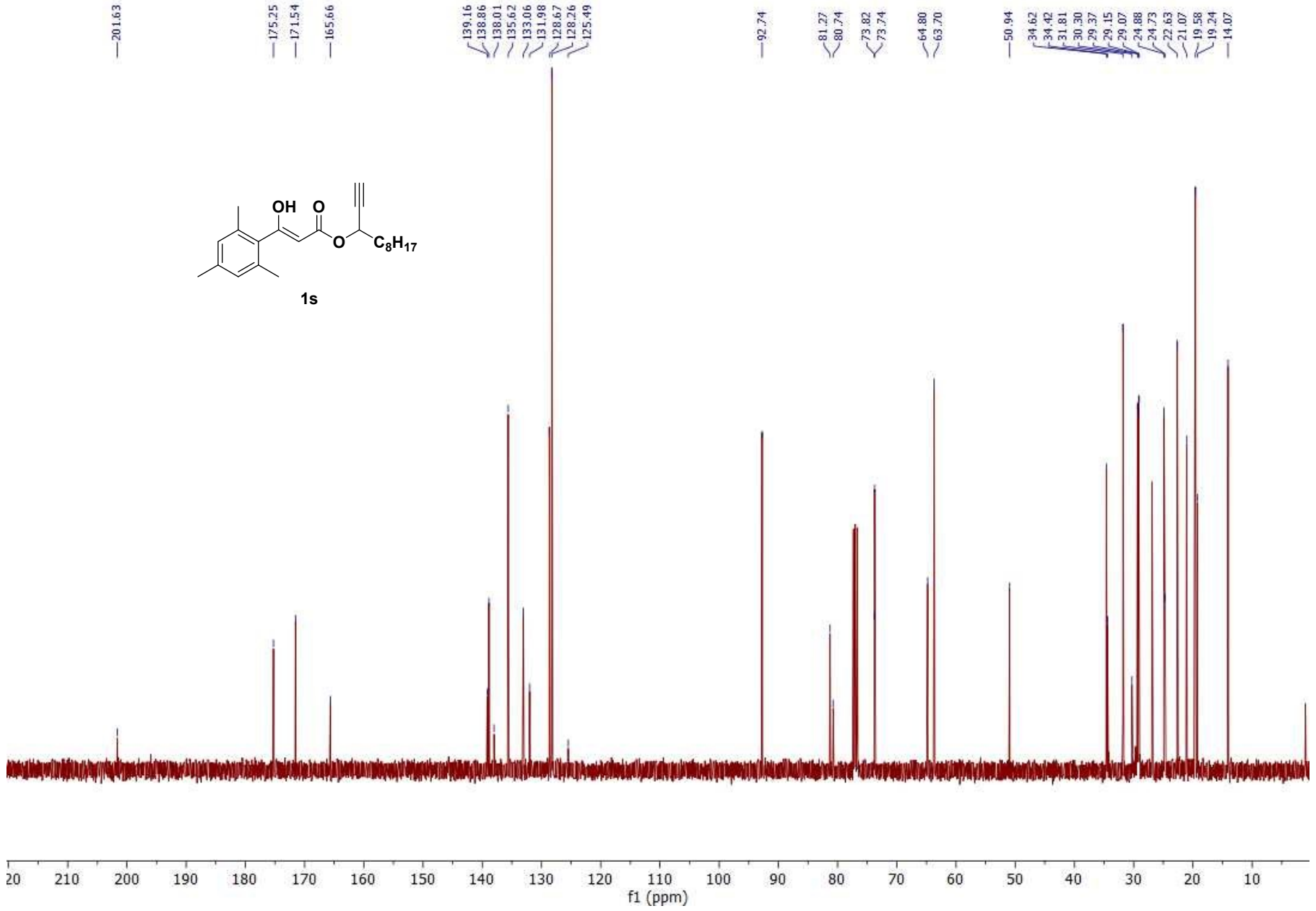

191.88
172.31
171.80
166.39
160.24
135.86
133.72
133.15
131.49
129.32
128.74
128.56
128.45
128.01
126.13
114.09
113.99
87.00
79.79
75.76
75.54
66.07
64.93
55.30
45.84
O
O
O
OMe
1q
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

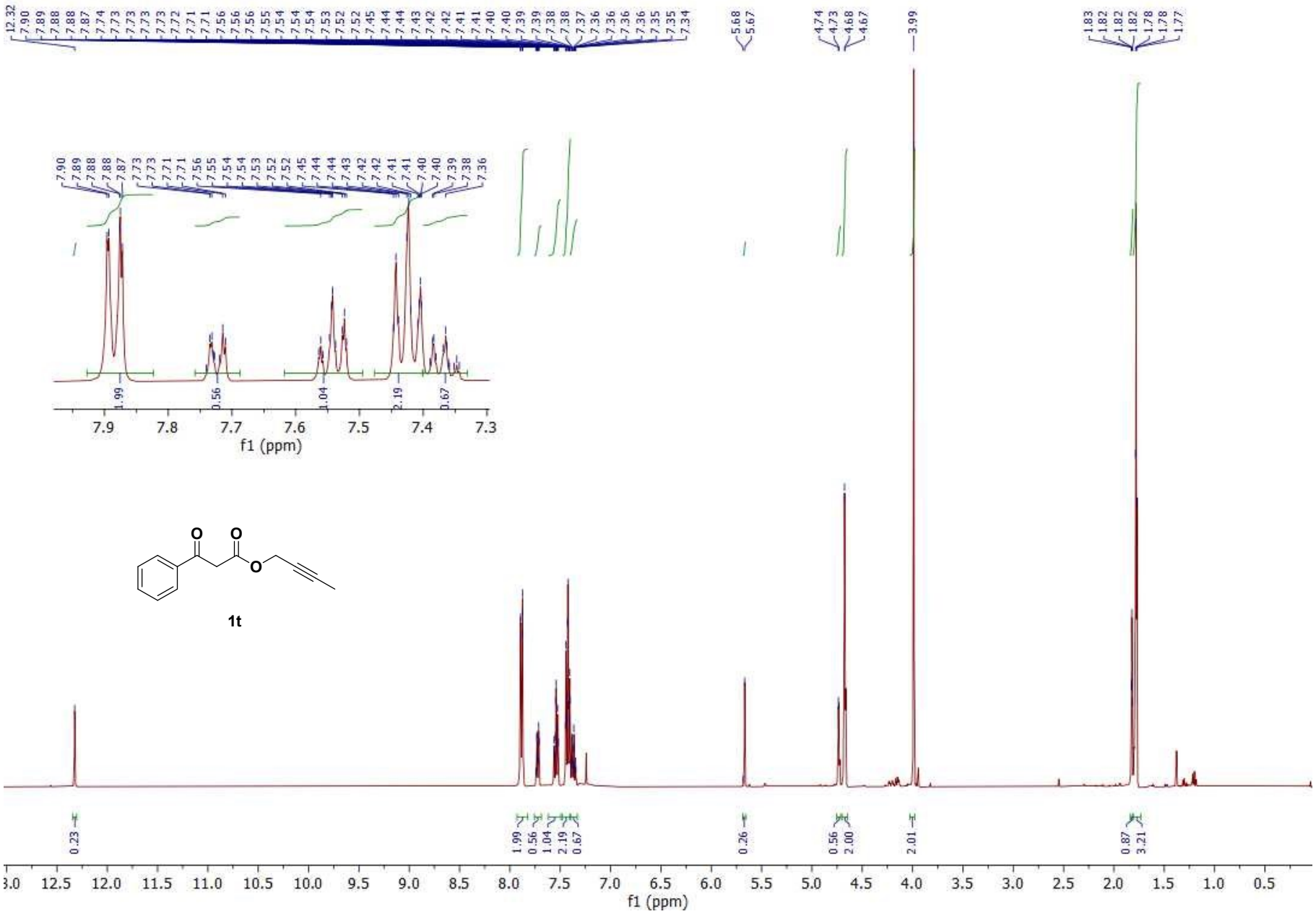


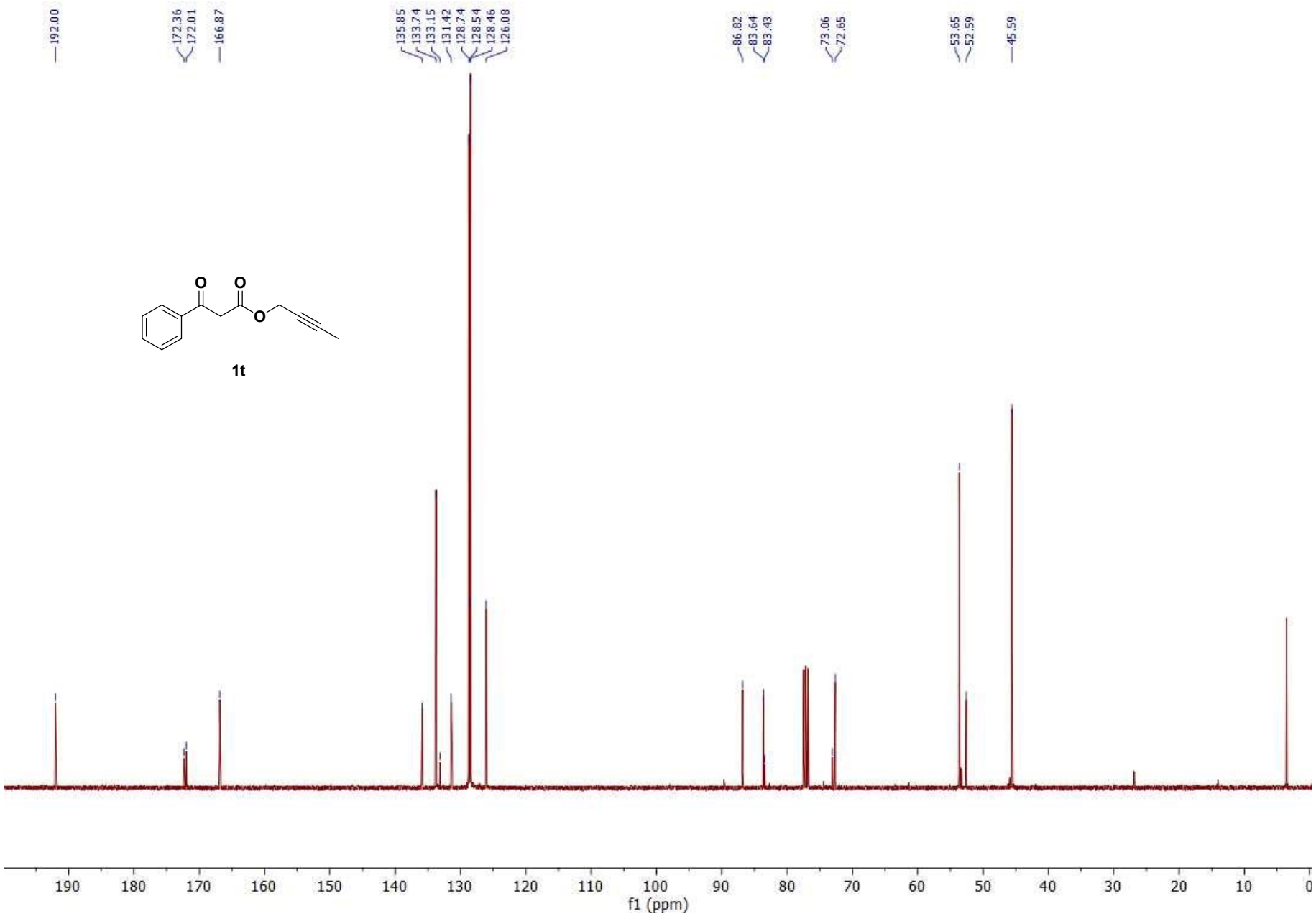
1r

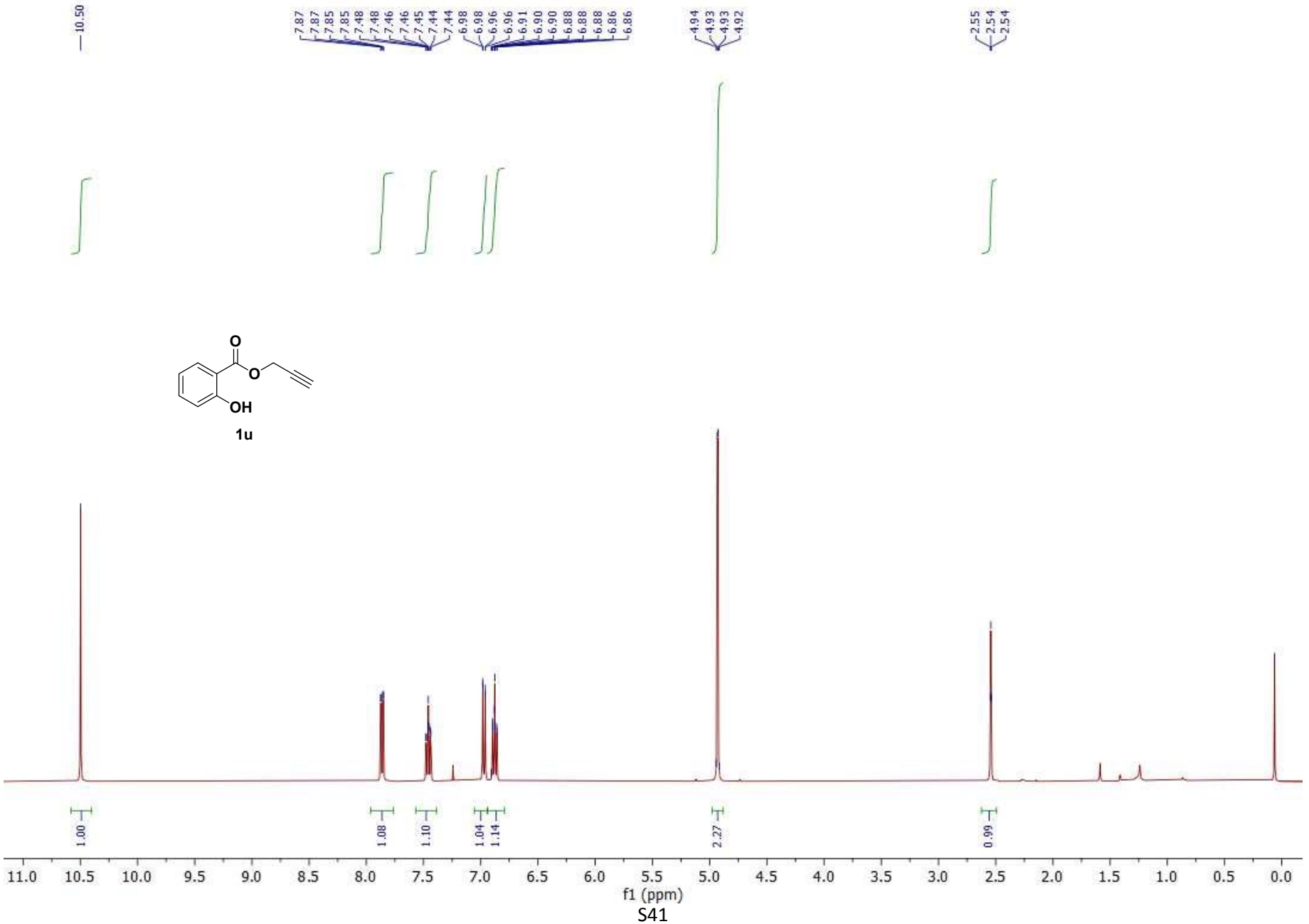

191.93
172.16
172.05
166.42
135.94
133.72
133.24
131.41
128.75
128.53
128.47
126.11
86.99
81.25
80.72
73.85
73.67
64.89
63.70
45.87
34.66
34.43
31.78
29.30
29.11
29.06
28.97
24.87
24.70
22.60
14.05
O
O
O
C8H17
1r
f1 (ppm)


12.14
6.86
6.83
5.49
5.49
5.49
5.48
5.47
5.47
5.46
5.46
5.45
5.40
5.40
5.39
5.38
5.38
5.38
5.37
5.36
5.36
5.13
5.12
3.80
3.76
3.75
3.74
3.72
3.70
2.44
2.43
1.76
1.76
1.74
1.74
1.73
1.73
1.72
1.70
OH
O
O
C8H17
1s
0.89
2.00
0.93
0.97
0.45
0.90
0.97
0.85
0.46
5.99
3.18
2.02
0.99
1.91
16.53
5.15
12.5
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
f1 (ppm)


201.63
175.25
171.54
165.66
139.16
138.86
138.01
135.62
133.06
131.98
128.67
128.26
125.49
92.74
81.27
80.74
73.82
73.74
64.80
63.70
50.94
34.62
34.42
31.81
30.30
29.37
29.15
29.07
24.88
24.73
22.63
21.07
19.58
19.24
14.07
OH
O
O
C8H17
1s
f1 (ppm)


12.32
7.90
7.89
7.88
7.88
7.87
7.74
7.73
7.73
7.73
7.72
7.71
7.71
7.56
7.56
7.55
7.54
7.54
7.53
7.52
7.52
7.45
7.44
7.44
7.43
7.42
7.42
7.41
7.41
7.40
7.40
7.39
7.39
7.38
7.38
7.37
7.36
7.36
7.36
7.35
7.34
5.68
5.67
4.74
4.73
4.68
4.67
3.99
1.83
1.82
1.82
1.82
1.78
1.78
1.77
1.99
0.56
1.04
2.19
0.67
f1 (ppm)
O
O
O
1t
0.23
1.99
0.56
1.04
2.19
0.67
0.26
0.56
2.00
2.01
0.87
3.21
f1 (ppm)


192.00
172.36
172.01
166.87
135.85
133.74
133.15
131.42
128.74
128.54
128.46
126.08
86.82
83.64
83.43
73.06
72.65
53.65
52.59
45.59
O
O
O
1t
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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7.87
7.87
7.85
7.85
7.48
7.48
7.46
7.46
7.45
7.44
7.44
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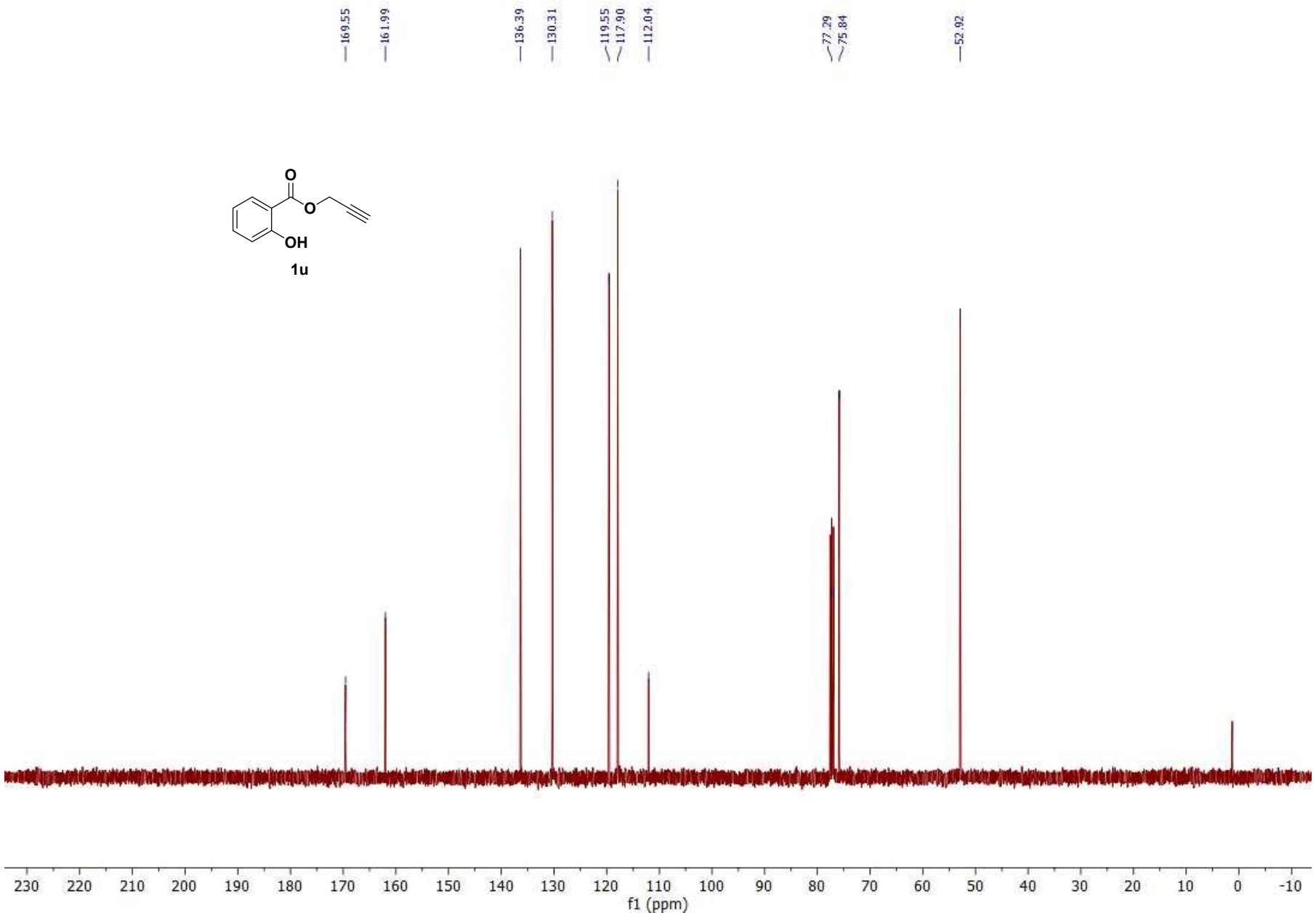
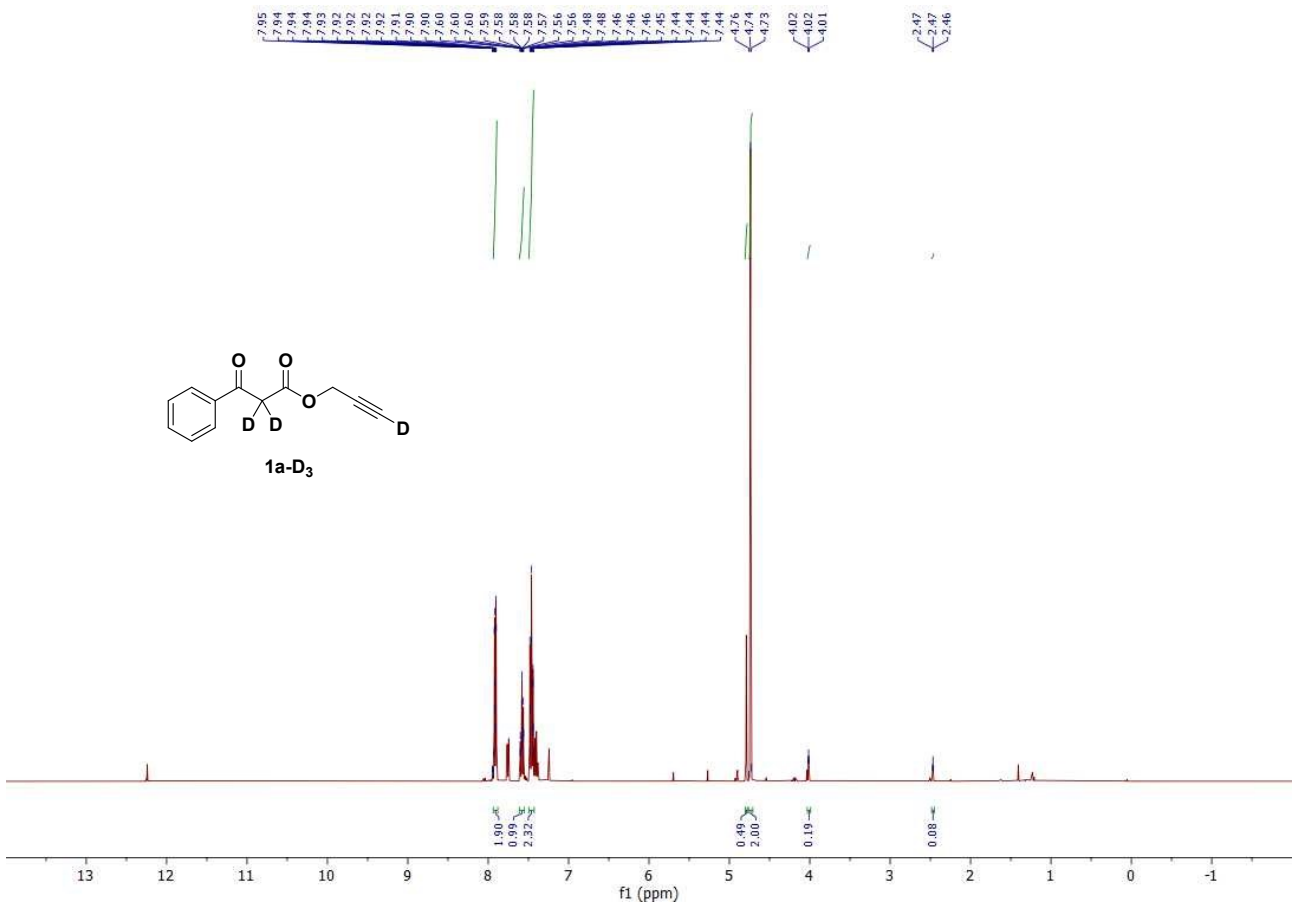
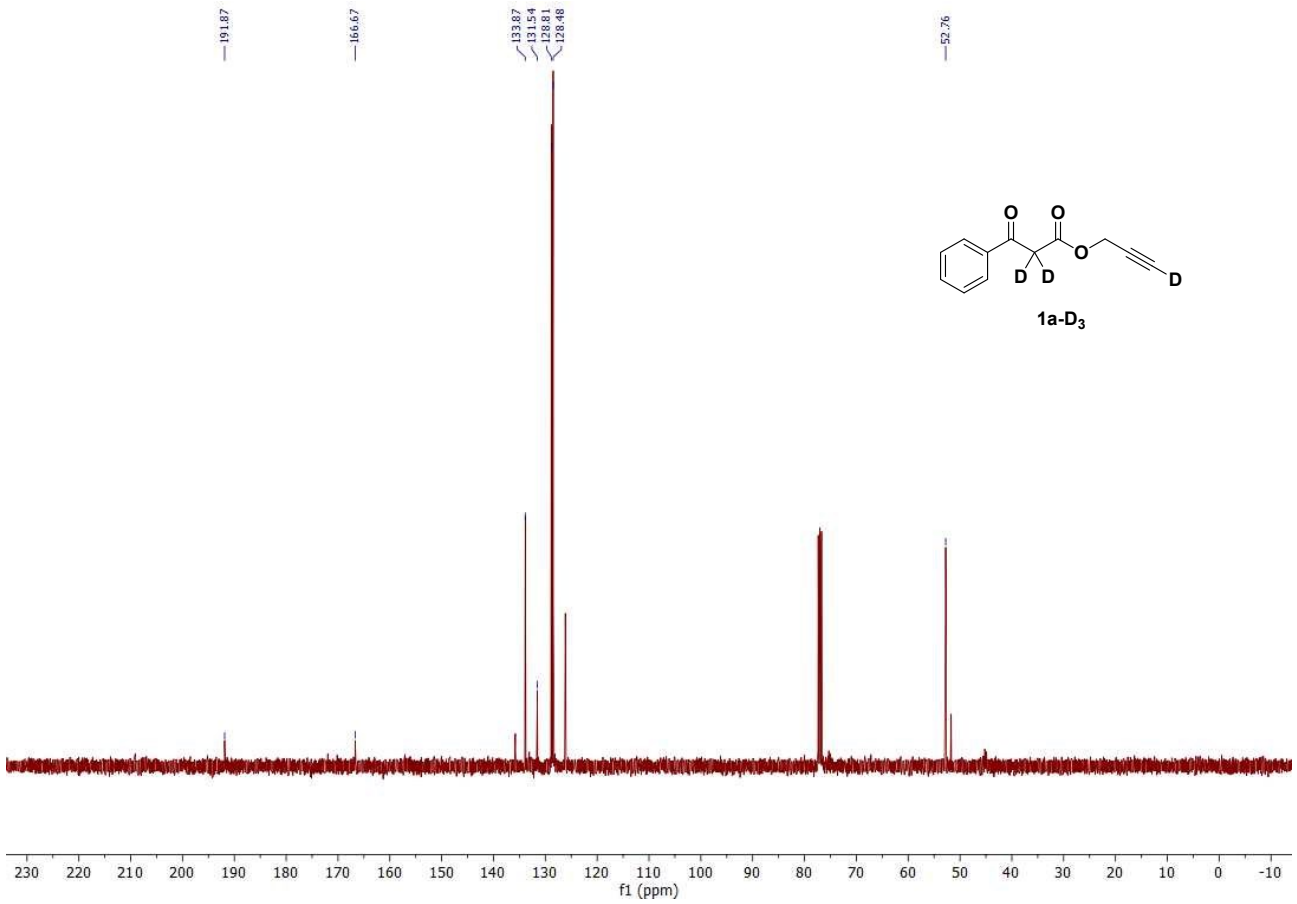
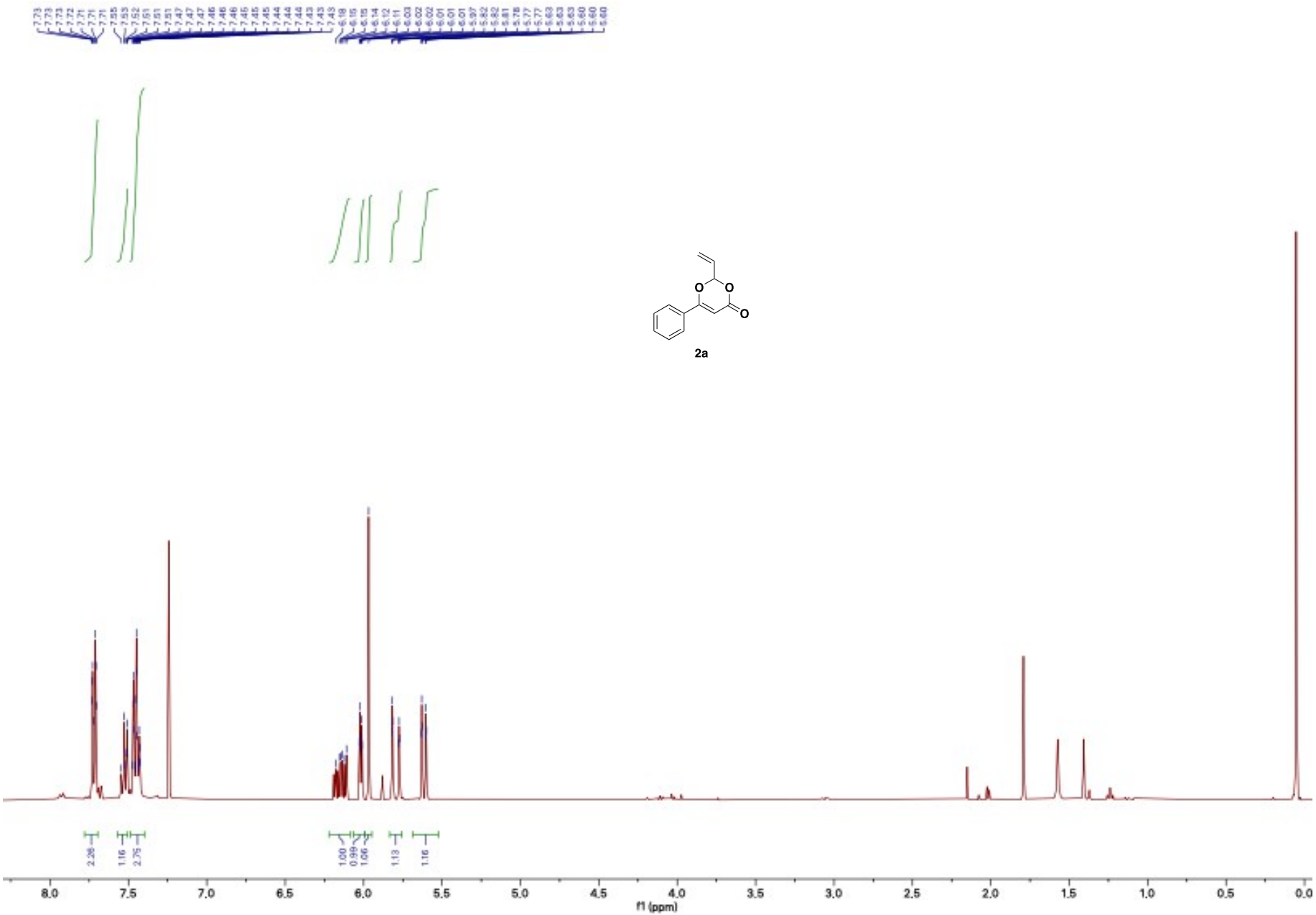
6.98
6.96
6.96
6.91
6.90
6.90
6.88
6.88
6.88
6.86
6.86
4.94
4.93
4.93
4.92
2.55
2.54
2.54
O
O
OH
1u
1.00
1.08
1.10
1.04
1.14
2.27
0.99
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

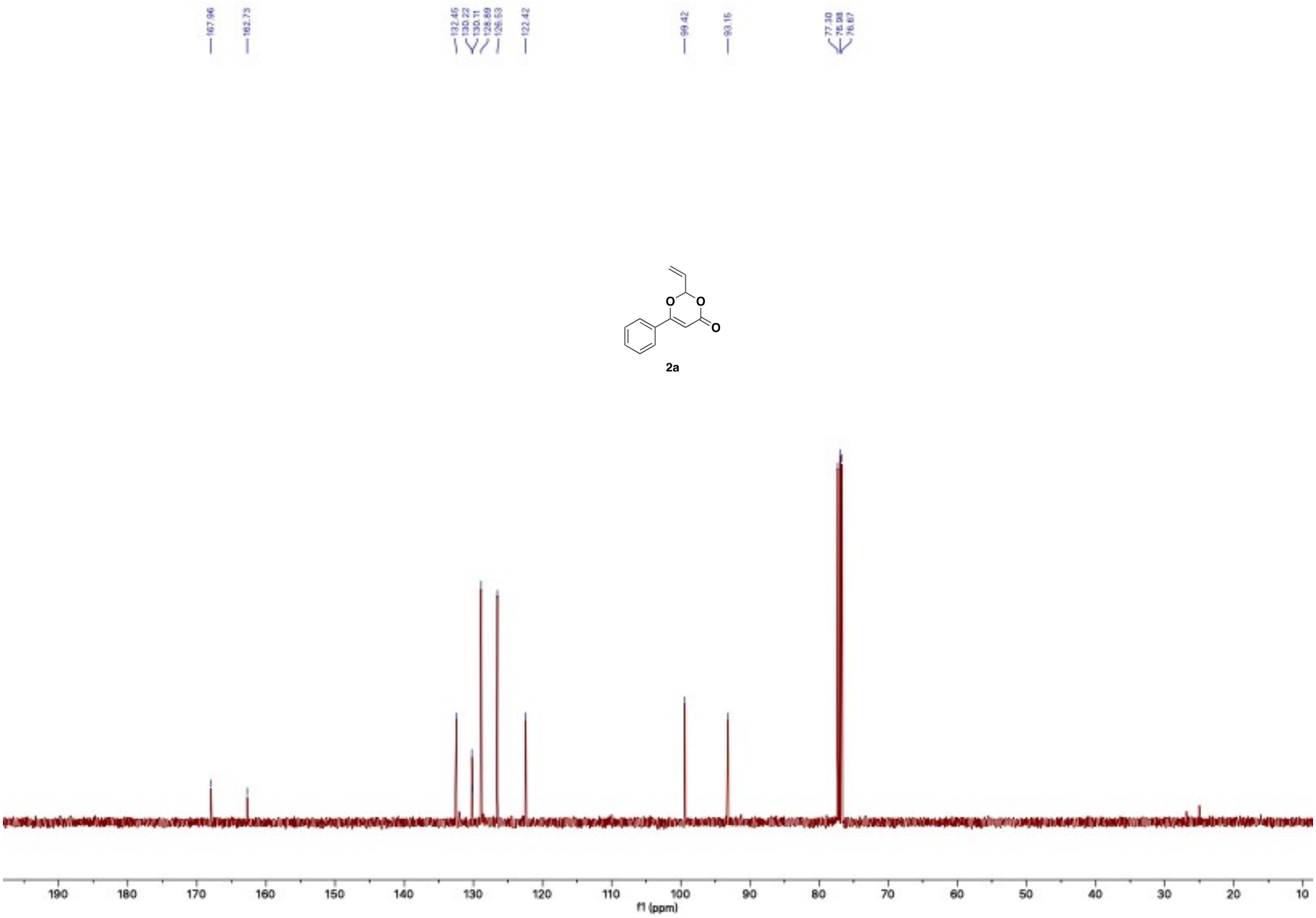

169.55
161.99
136.39
130.31
119.55
117.90
112.04
77.29
75.84
52.92
O
O
OH
1u
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

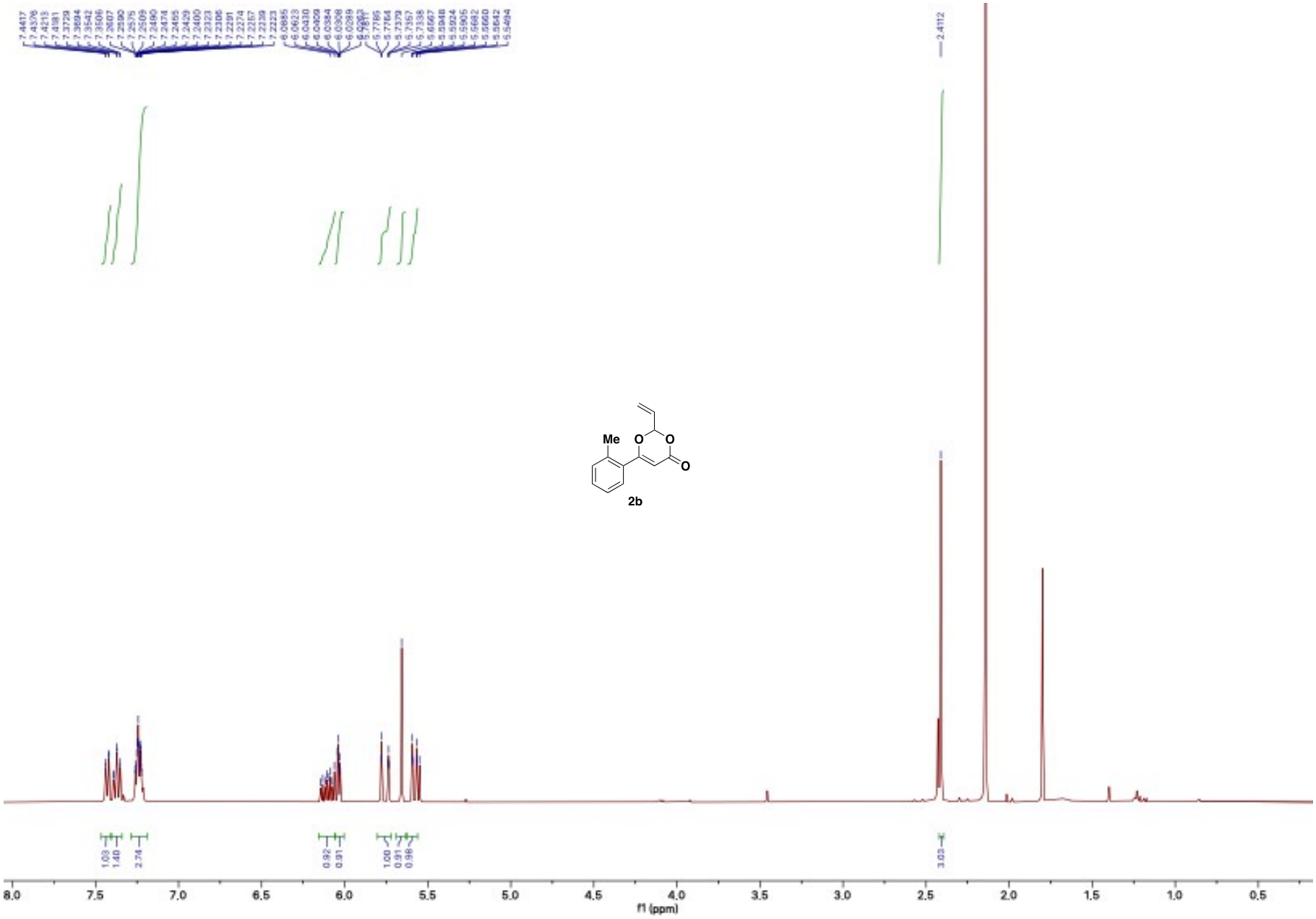

7.95
7.94
7.94
7.94
7.93
7.92
7.92
7.92
7.92
7.91
7.90
7.90
7.90
7.60
7.60
7.60
7.59
7.58
7.58
7.58
7.57
7.56
7.56
7.48
7.48
7.46
7.46
7.46
7.45
7.44
7.44
7.44
7.44
4.76
4.74
4.73
4.02
4.02
4.01
2.47
2.47
2.46
O
O
O
D
D
D
1a-D3
1.90
0.99
2.32
0.49
2.00
0.19
0.08
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

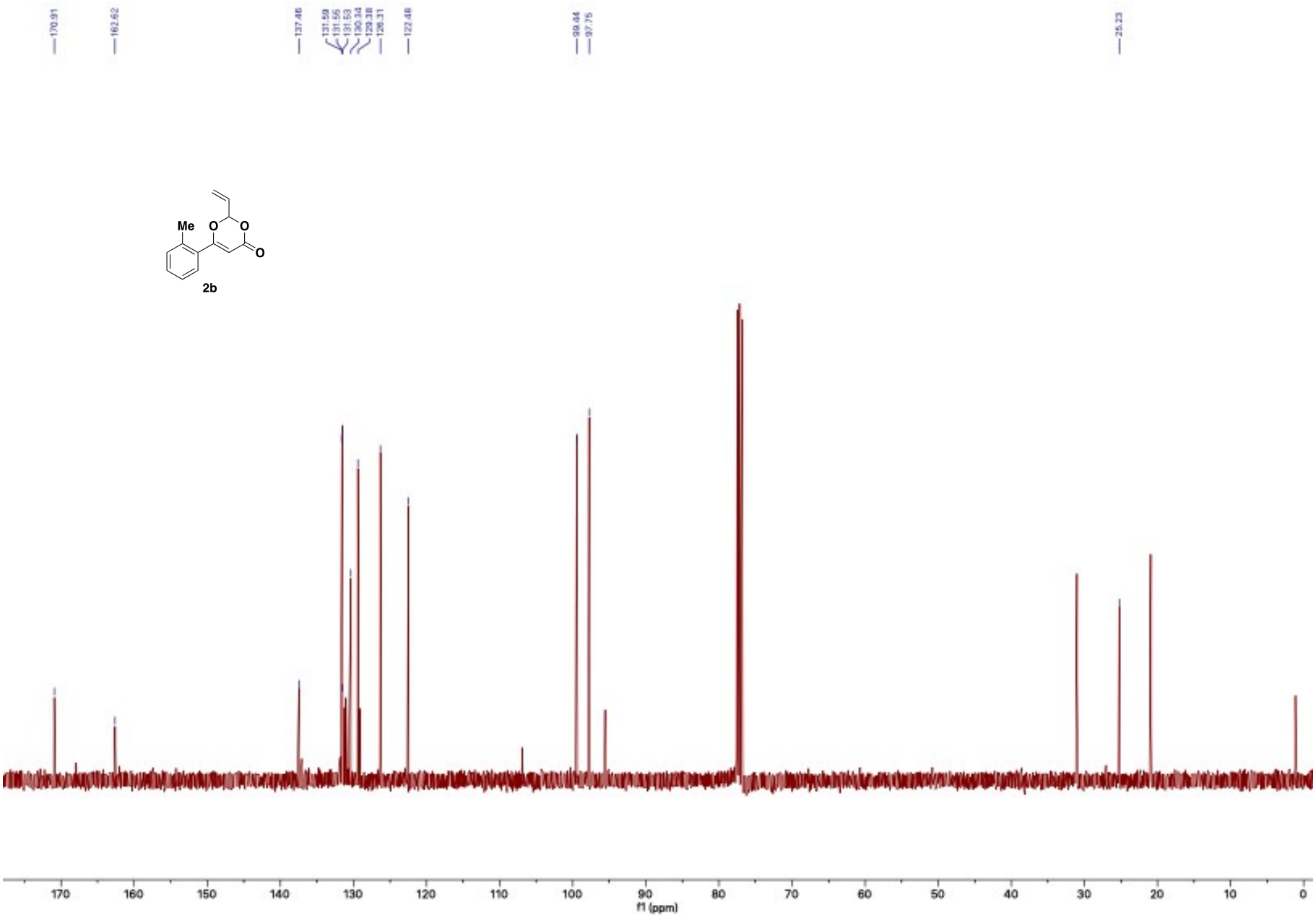

191.87
166.67
133.87
131.54
128.81
128.48
52.76
O
O
O
D
D
D
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

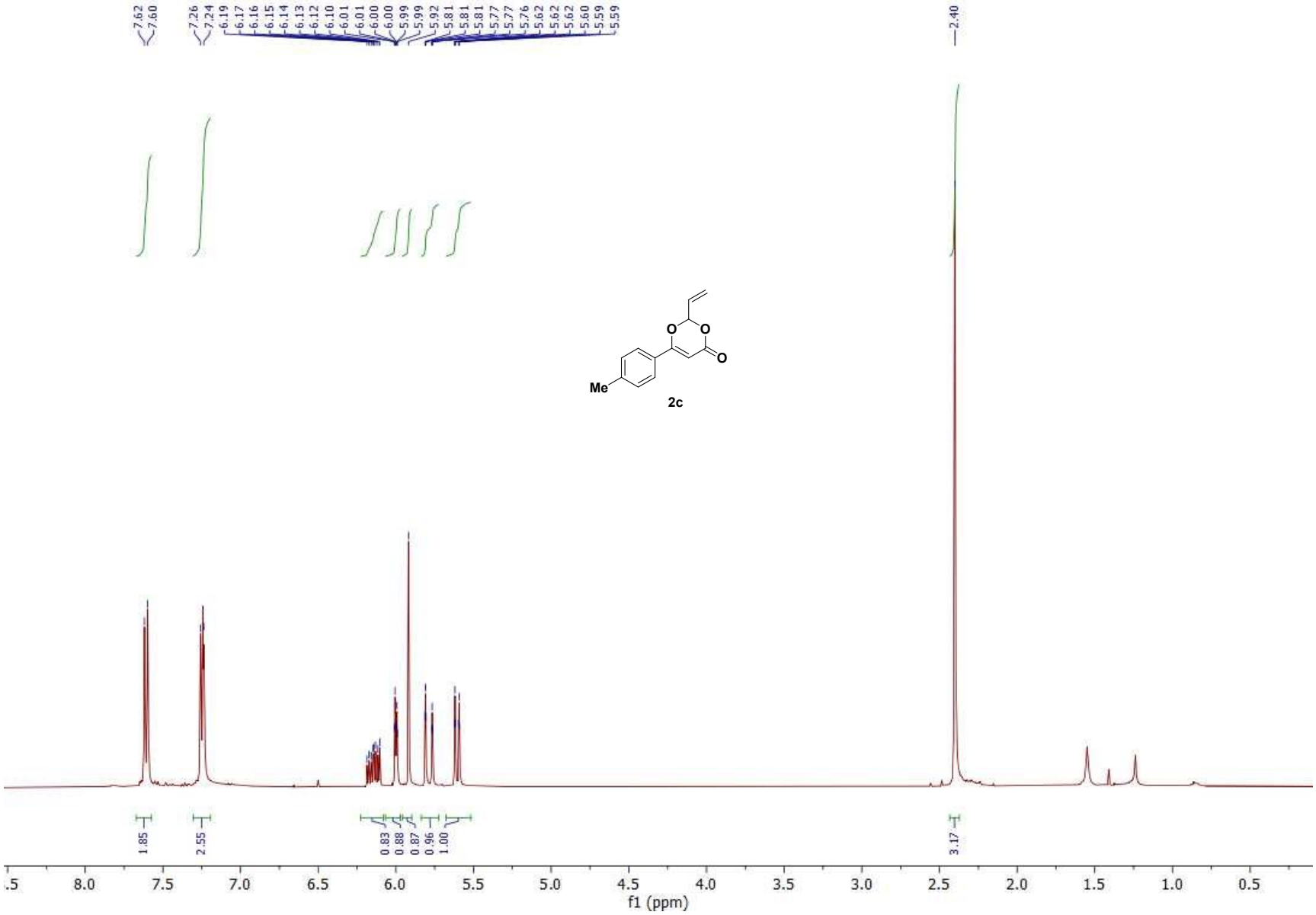
1a-D_3

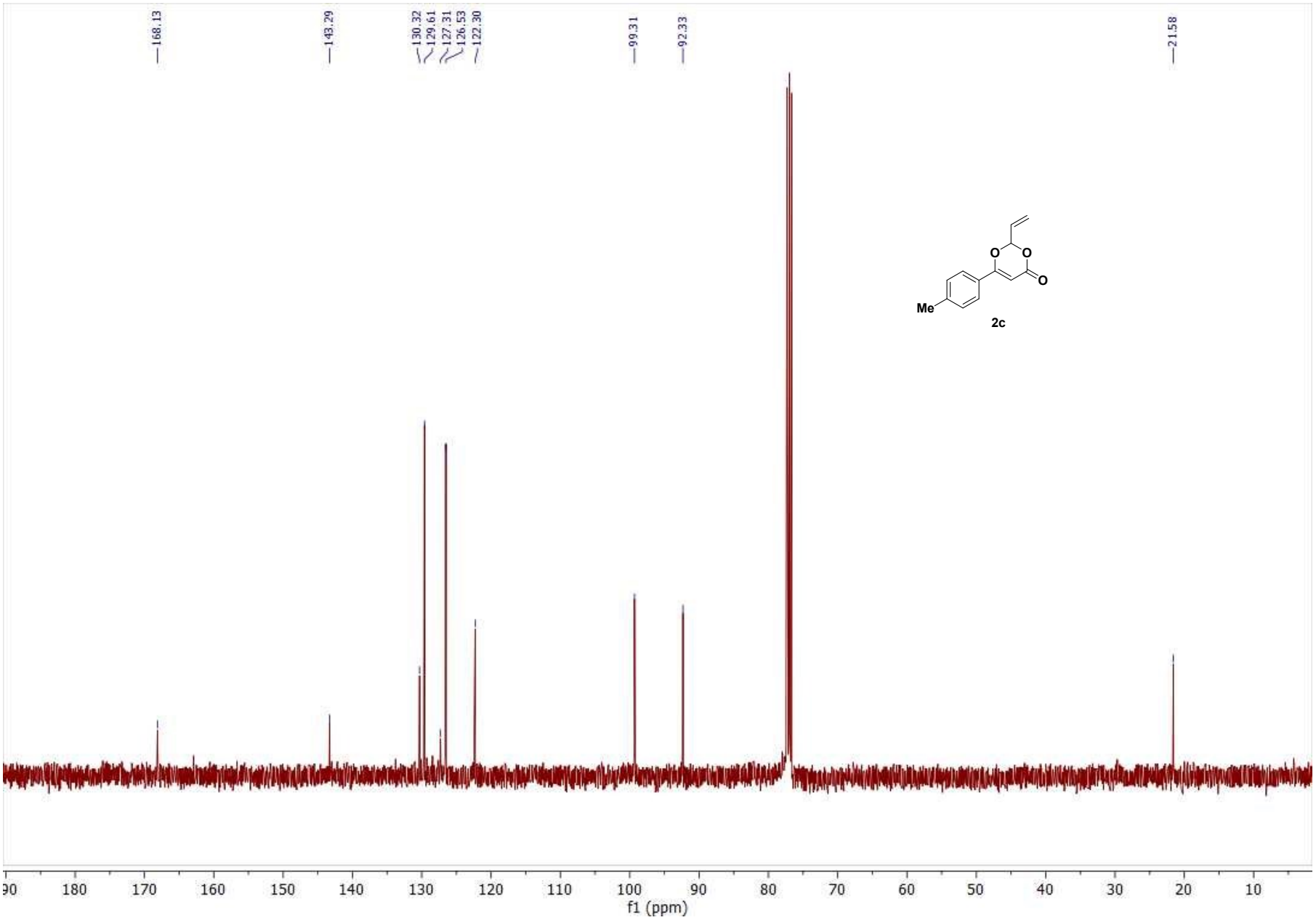

7.73
7.73
7.73
7.72
7.71
7.71
7.55
7.53
7.52
7.51
7.51
7.51
7.47
7.47
7.47
7.46
7.46
7.46
7.45
7.45
7.45
7.44
7.44
7.44
7.43
7.43
7.43
6.18
6.15
6.15
6.14
6.12
6.11
6.03
6.02
6.02
6.01
6.01
6.01
5.97
5.82
5.82
5.81
5.78
5.77
5.77
5.63
5.63
5.63
5.60
5.60
5.60
O
O
O
2a
2.26
1.16
2.75
1.00
0.99
1.06
1.13
1.16
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)

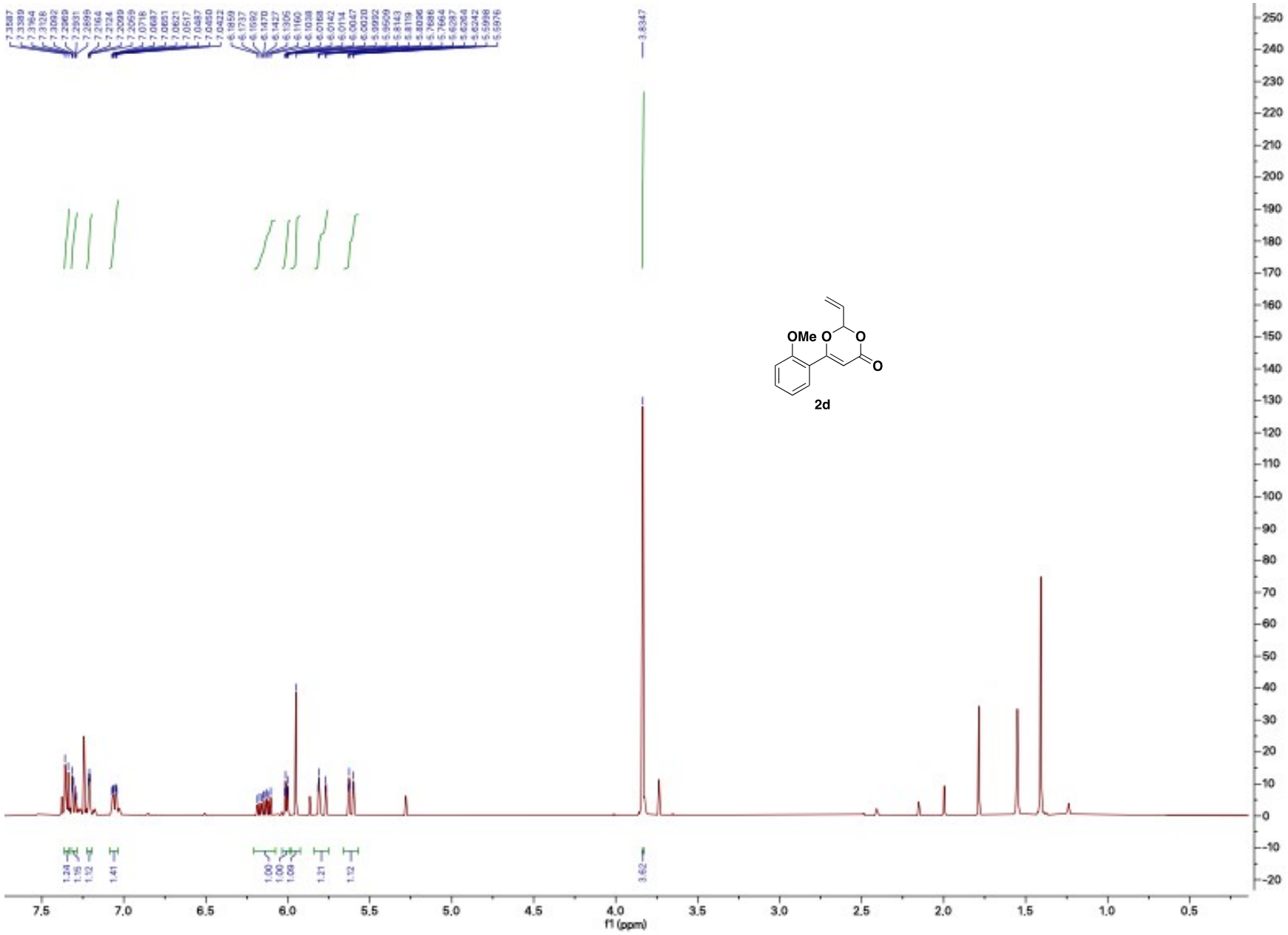

167.96
162.73
132.45
130.22
130.11
128.89
126.53
122.42
99.42
93.15
77.30
76.98
76.67
O
O
O
2a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

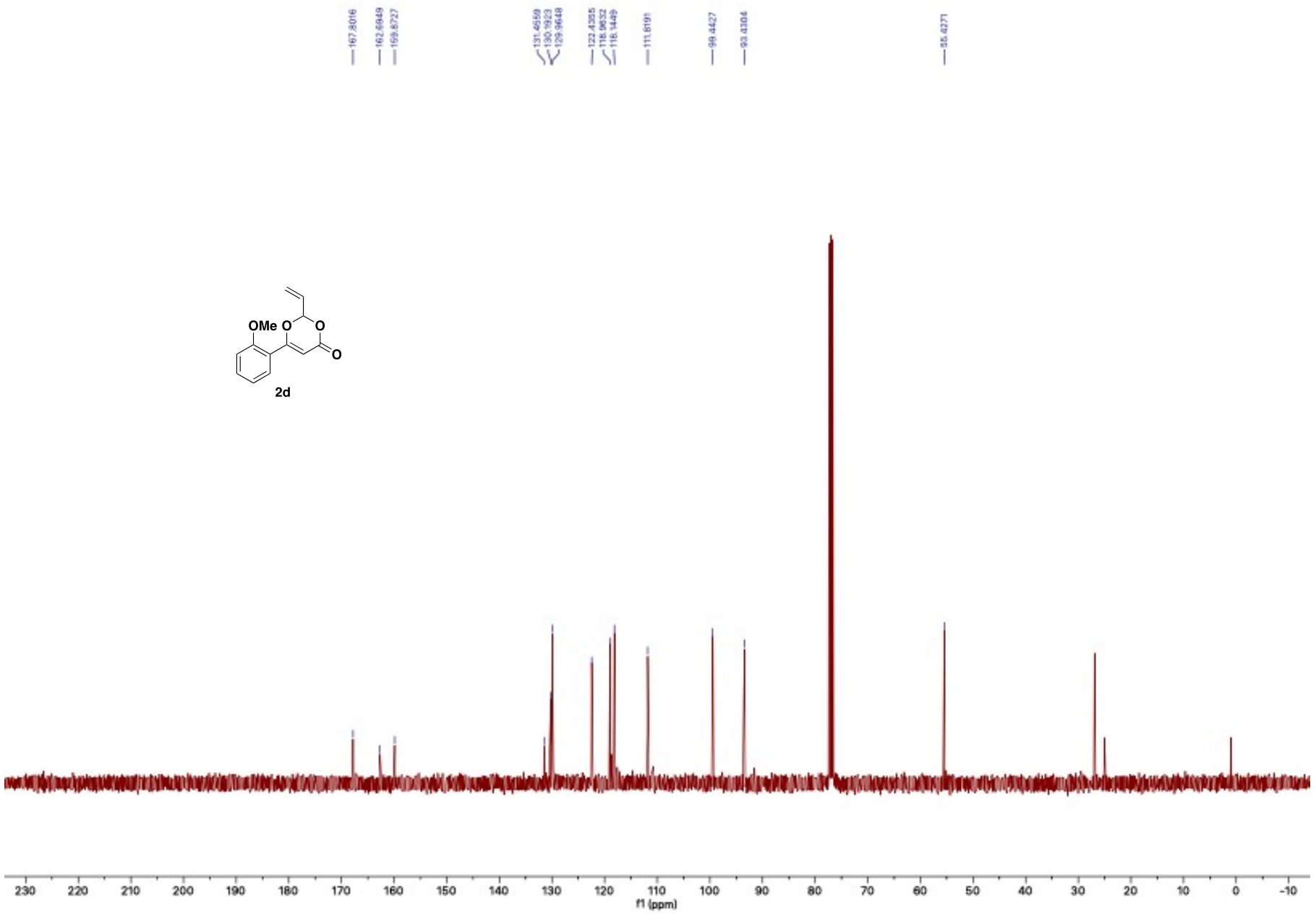

Me
O
O
O
2b
f1 (ppm)


170.91
162.62
137.46
131.59
131.55
131.53
130.34
129.38
126.31
122.48
99.64
97.75
25.23
Me
O
O
O
2b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.62
7.60
7.26
7.24
6.19
6.17
6.16
6.15
6.14
6.13
6.12
6.10
6.01
6.01
6.00
6.00
5.99
5.99
5.92
5.81
5.81
5.81
5.77
5.77
5.76
5.62
5.62
5.62
5.60
5.59
5.59
2.40
O
O
O
Me
2c
1.85
2.55
0.83
0.88
0.87
0.96
1.00
3.17
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
f1 (ppm)


168.13
143.29
130.32
129.61
127.31
126.53
122.30
99.31
92.33
21.58
O
O
O
Me
2c
f1 (ppm)


OMe
O
O
O
2d
f1 (ppm)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159.8727
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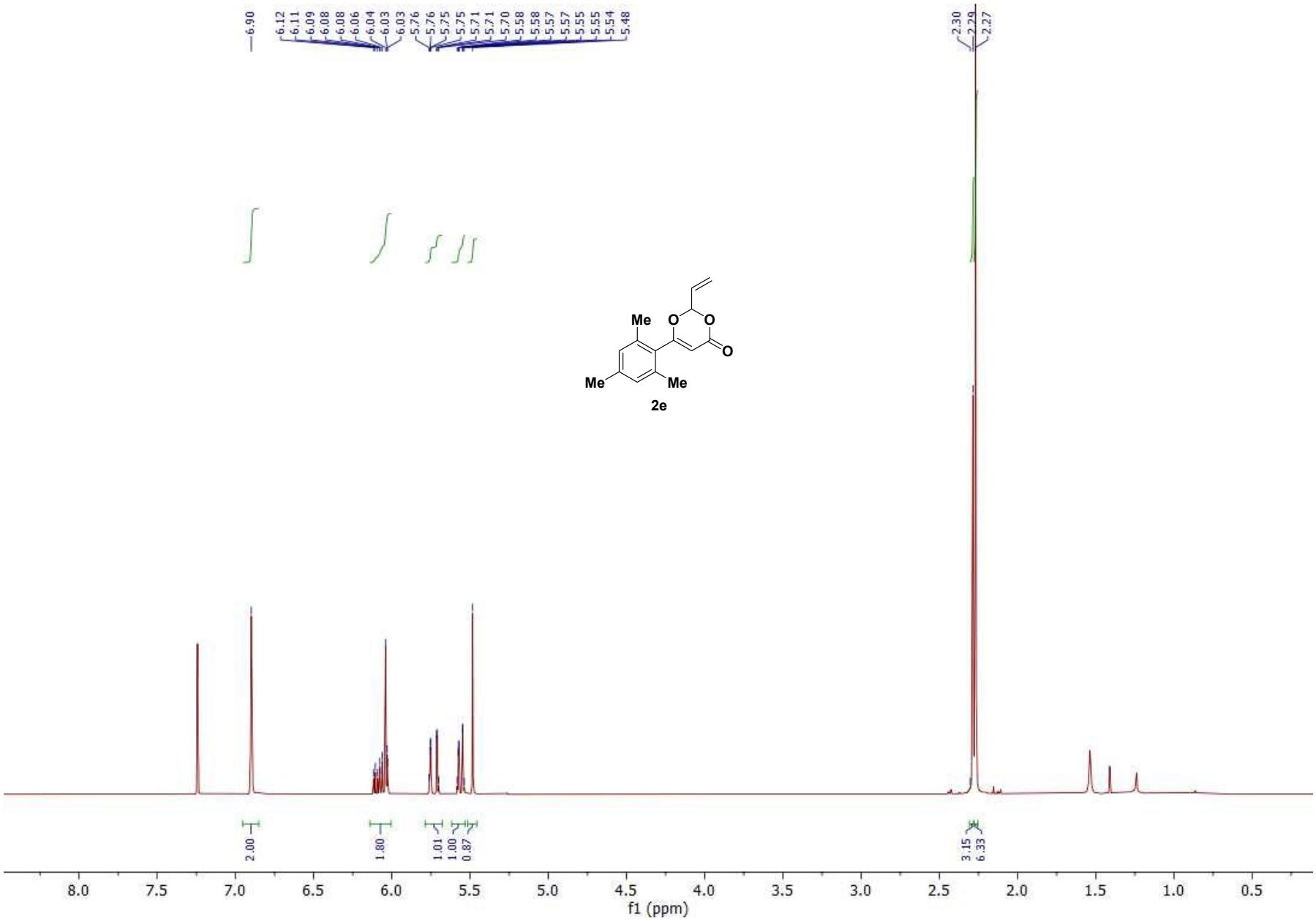
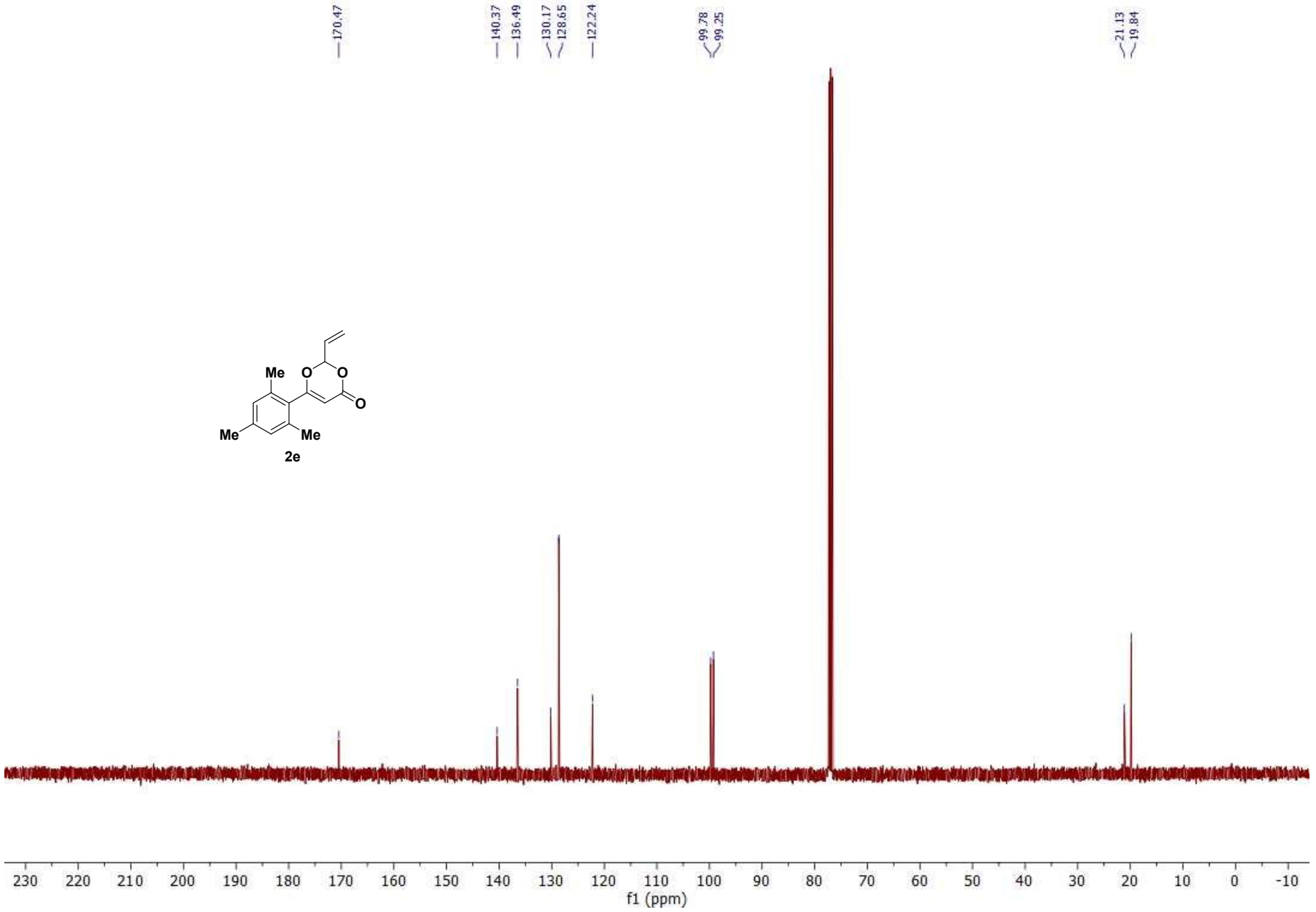
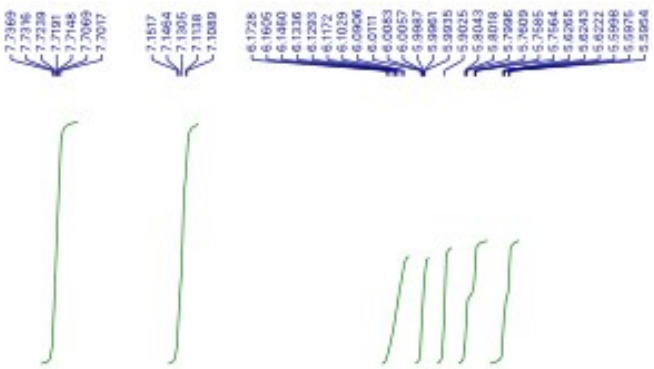
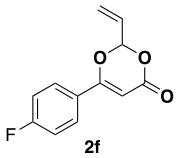
130.1923
129.9648
123.4355
118.9832
118.1449
111.8191
99.4427
93.4304
55.6271
OMe
O
O
O
2d
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

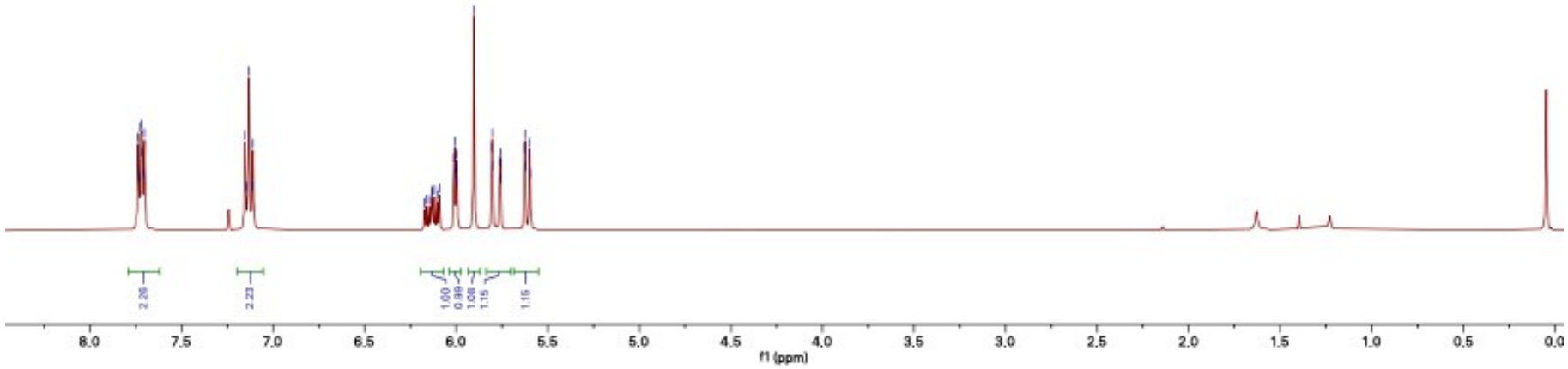

6.90
6.12
6.11
6.09
6.08
6.08
6.06
6.04
6.03
6.03
5.76
5.76
5.75
5.75
5.71
5.71
5.70
5.58
5.58
5.57
5.57
5.55
5.55
5.54
5.48
2.30
2.29
2.27
Me
O
O
O
Me
Me
2e
2.00
1.80
1.01
1.00
0.87
3.15
6.33
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

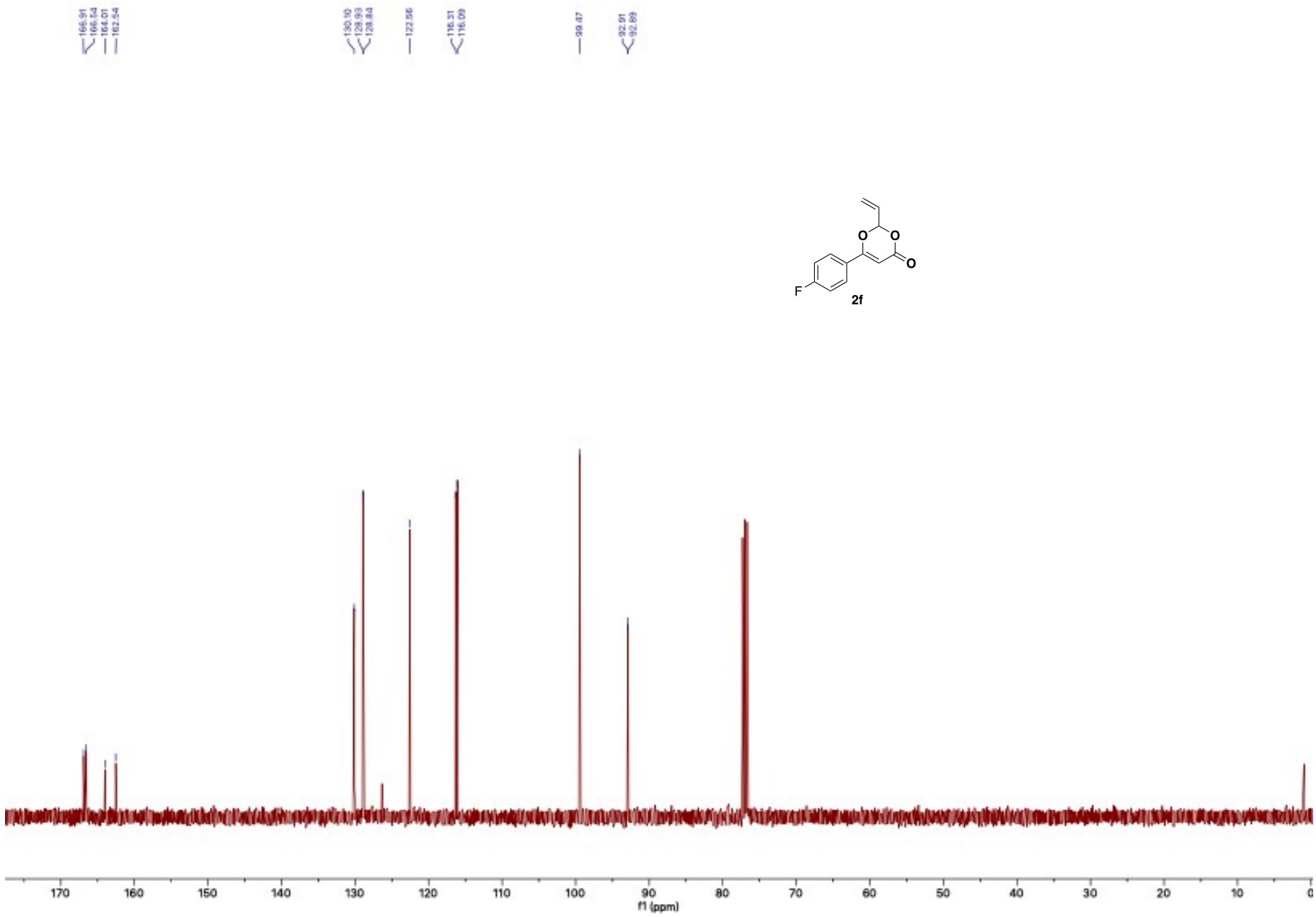

170.47
140.37
136.49
130.17
128.65
122.24
99.78
99.25
21.13
19.84
Me
O
O
O
Me
Me
2e
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

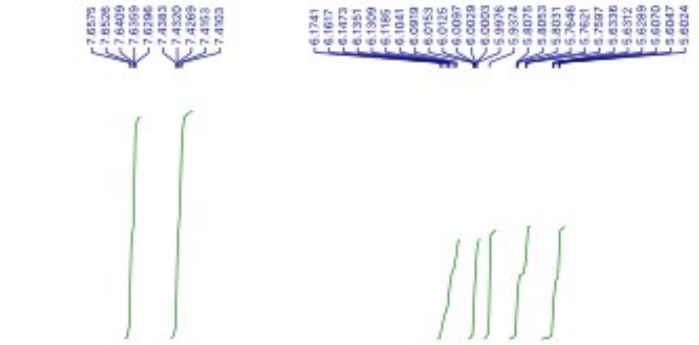


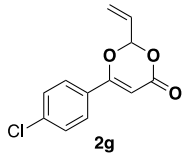


2f

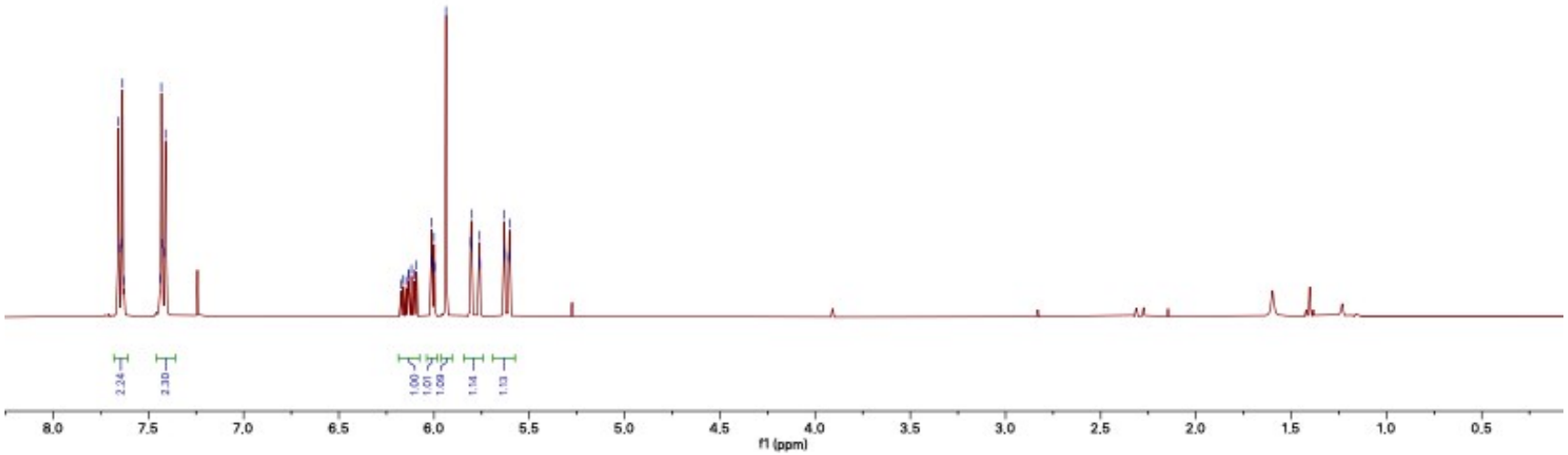

2.26
2.23
1.00
0.99
1.08
1.15
1.16
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

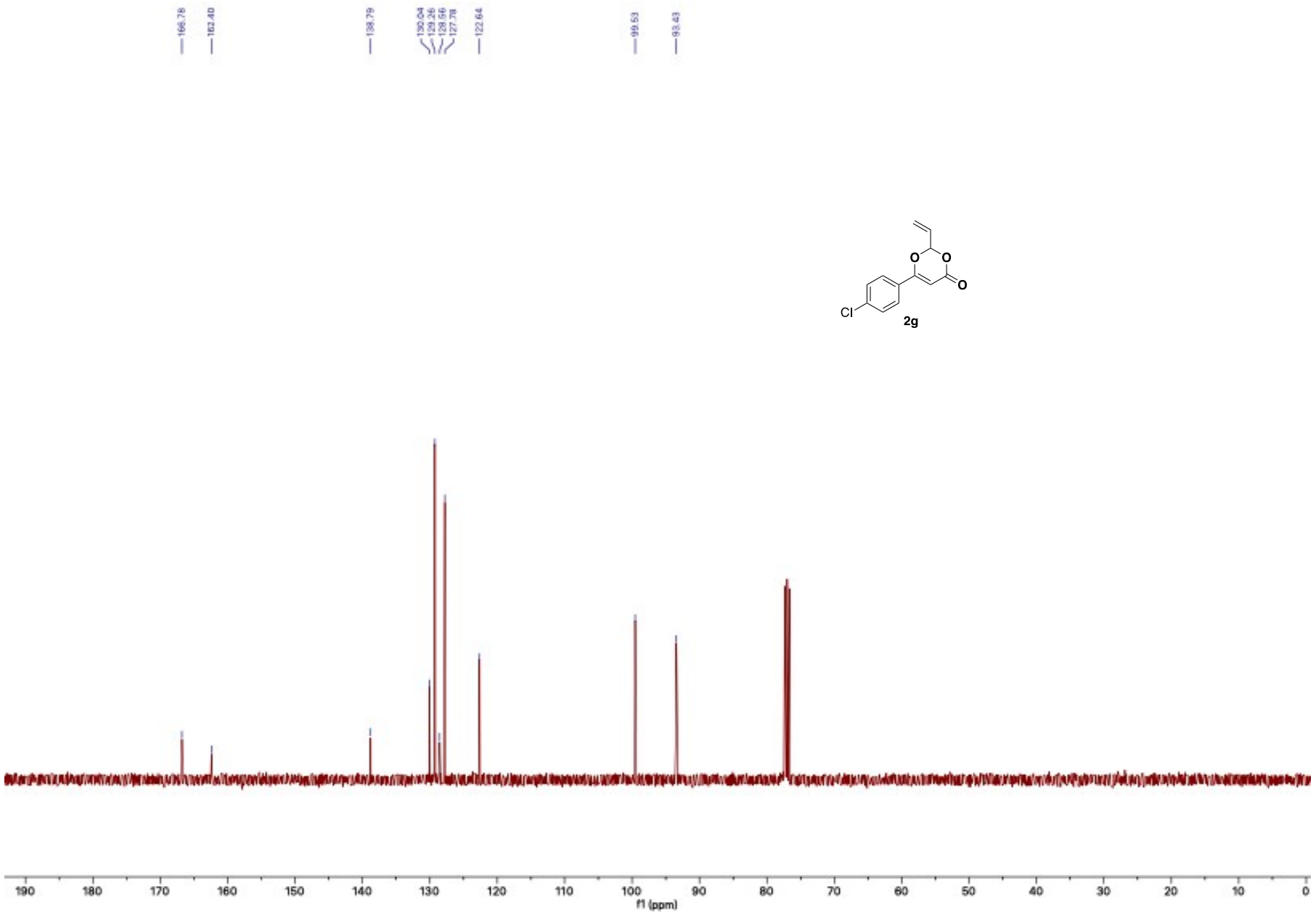

166.91
166.54
164.01
162.54
130.10
128.93
128.84
123.56
116.31
116.09
99.47
92.91
92.89
F
2f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

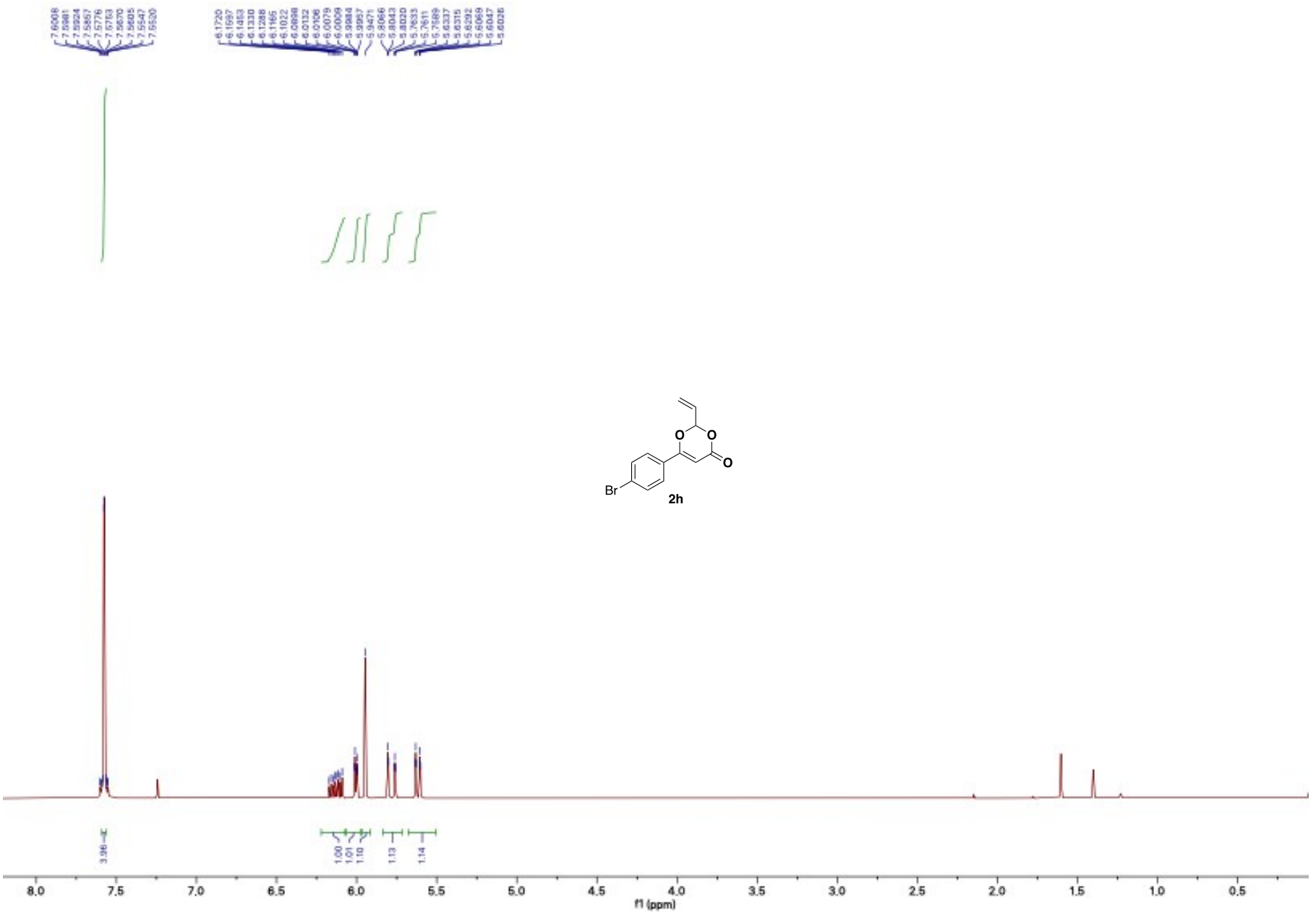


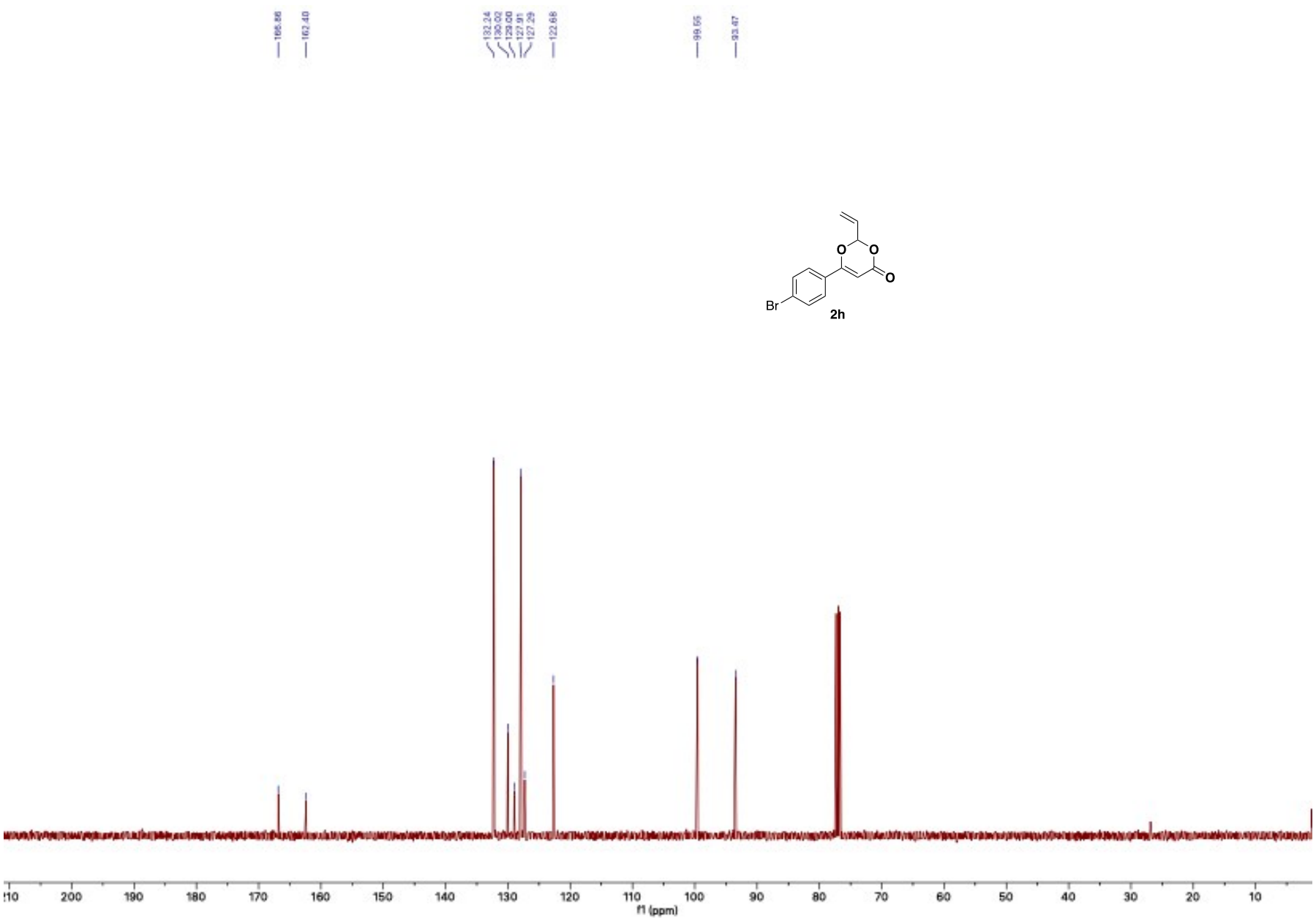

O
O
O
Cl

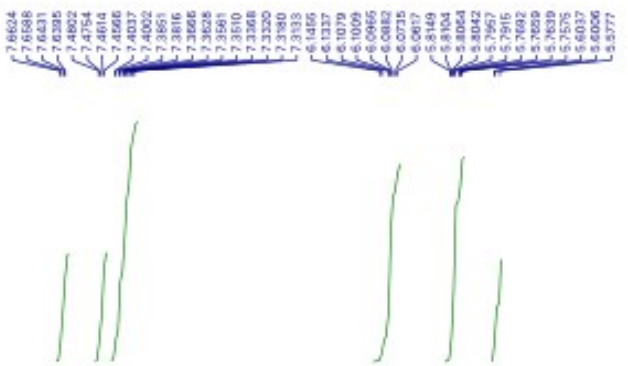
2g

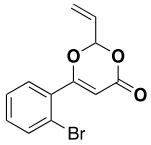

2.24
2.30
1.00
1.01
1.09
1.14
1.13
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


166.78
162.40
138.79
130.64
129.26
128.56
127.78
122.64
99.53
93.43
O
O
O
Cl
2g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

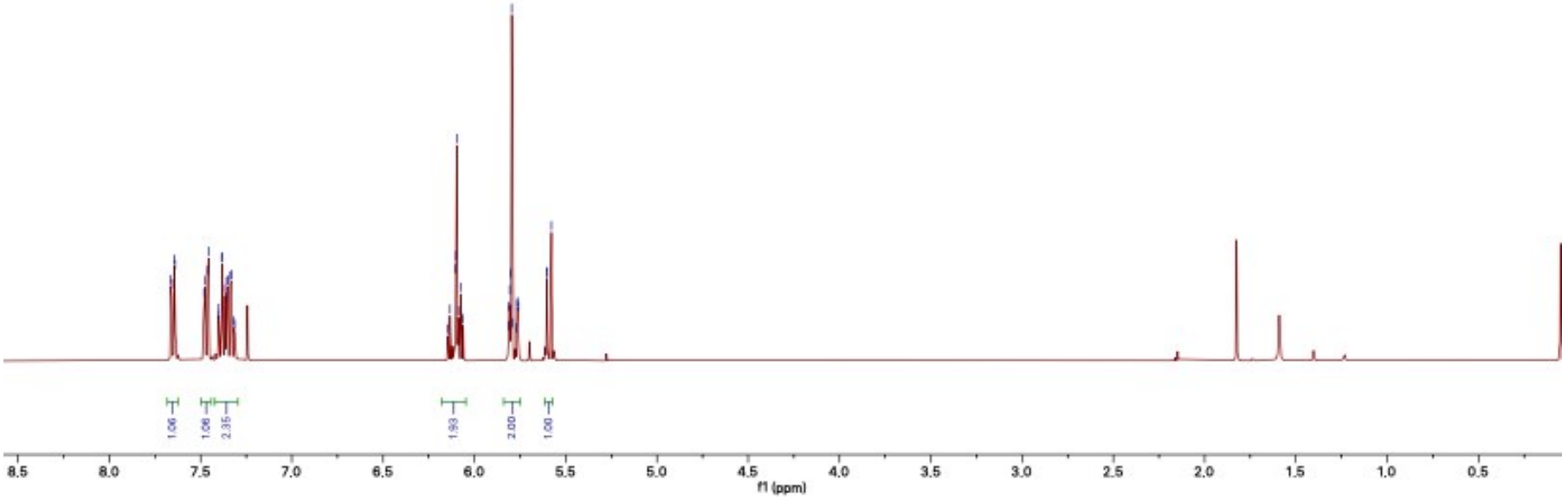

7.6008
7.5981
7.5924
7.5857
7.5776
7.5763
7.5670
7.5605
7.5547
7.5520
6.1720
6.1697
6.1453
6.1330
6.1288
6.1165
6.1022
6.0898
6.0132
6.0106
6.0079
6.0059
5.9844
5.9957
5.9471
5.8066
5.8043
5.8020
5.7833
5.7611
5.7589
5.6337
5.6315
5.6292
5.6069
5.6047
5.6026
Br
O
O
O
2h
3.96
1.00
1.01
1.10
1.13
1.14
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
f1 (ppm)

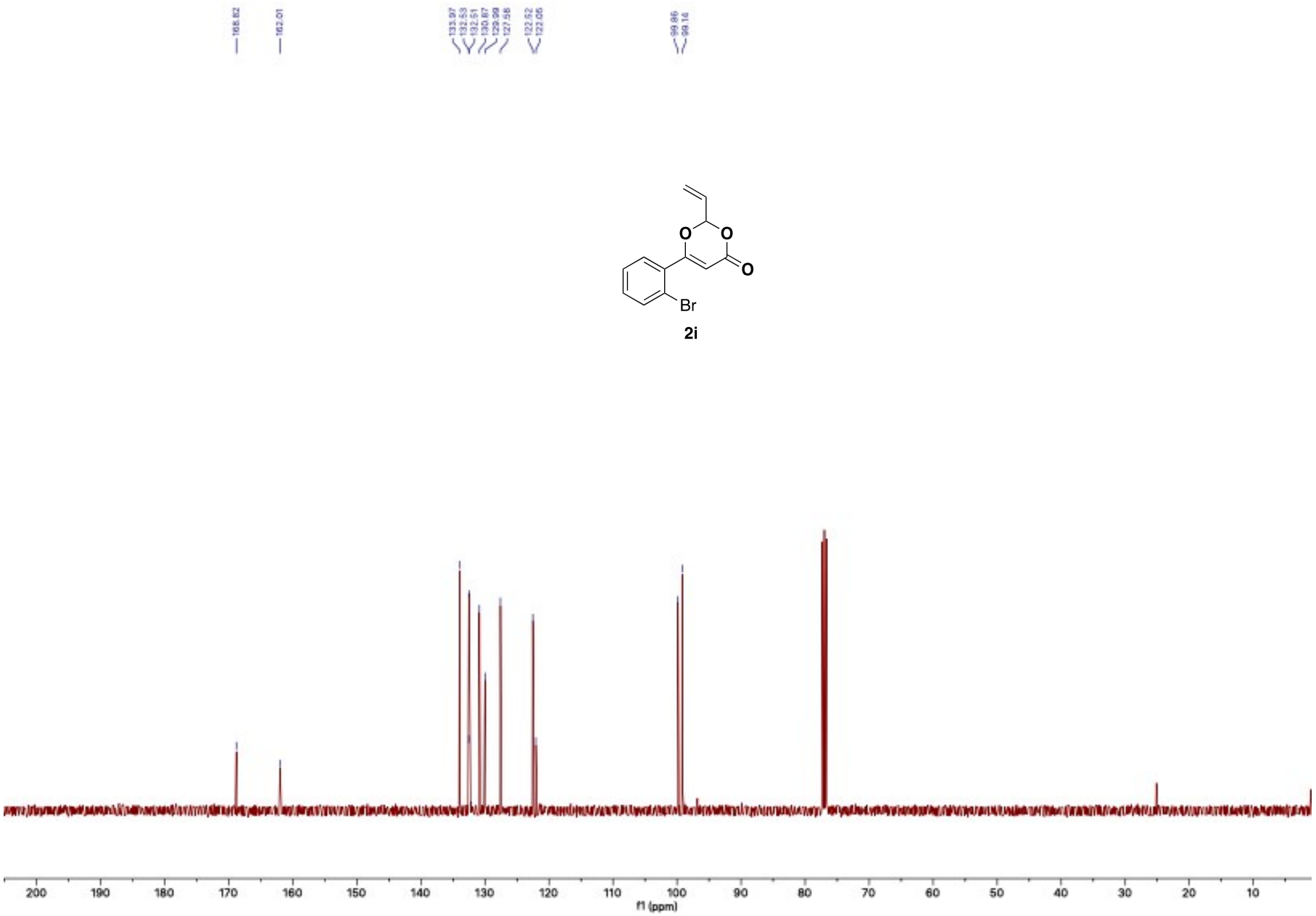

165.86
162.40
132.24
130.02
129.00
127.91
127.29
122.68
99.55
93.47
Br
2h
f1 (ppm)

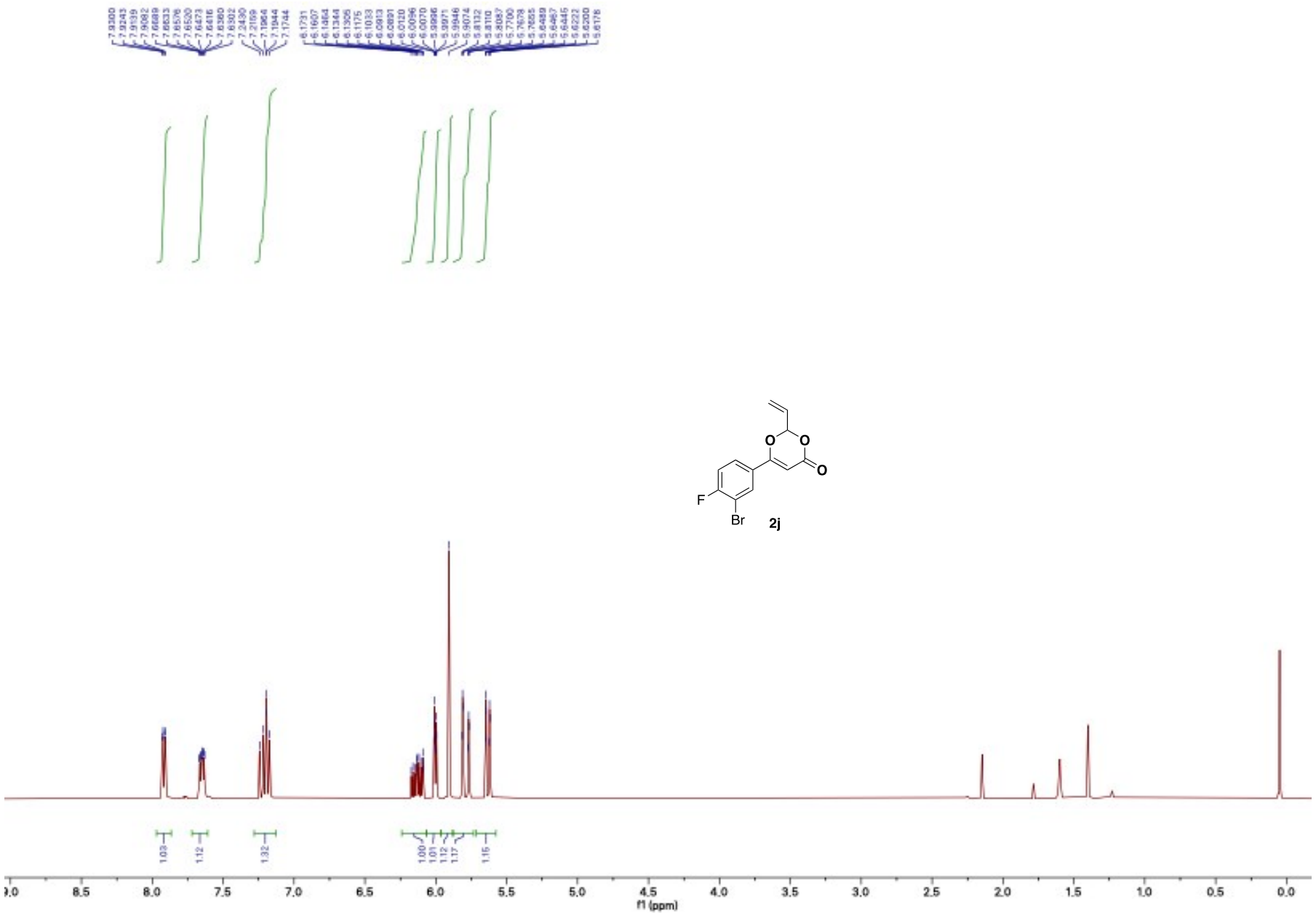


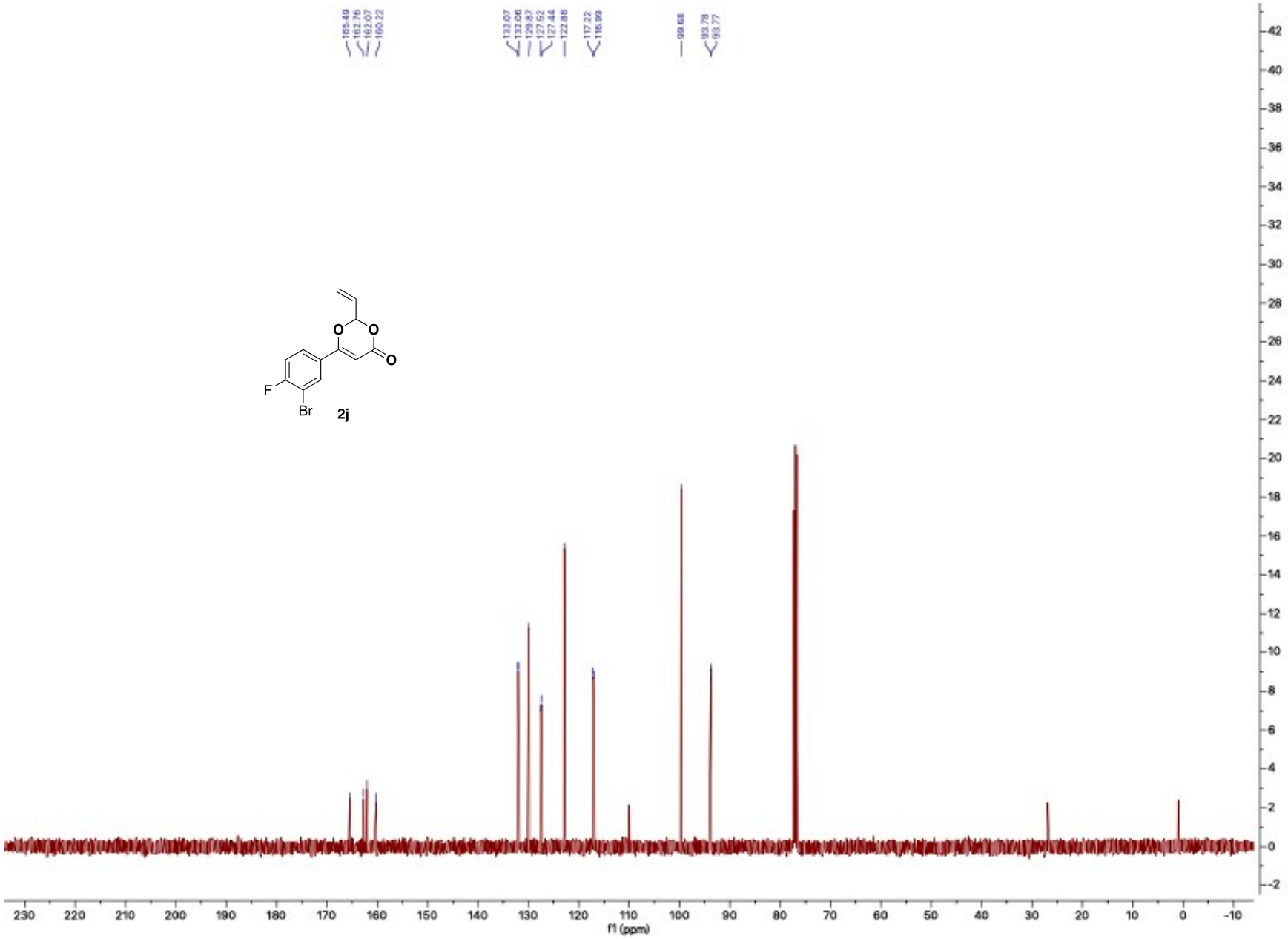


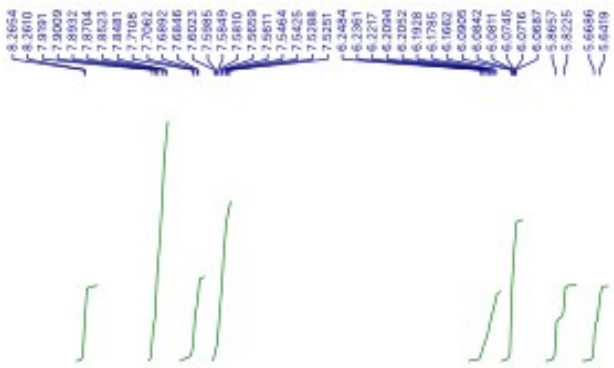
2i

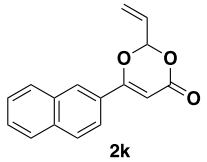

1.00
1.06
2.35
1.93
2.00
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


168.82
162.01
133.97
132.53
132.51
130.67
129.99
127.58
122.52
122.05
99.86
99.16
O
O
O
Br
2i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

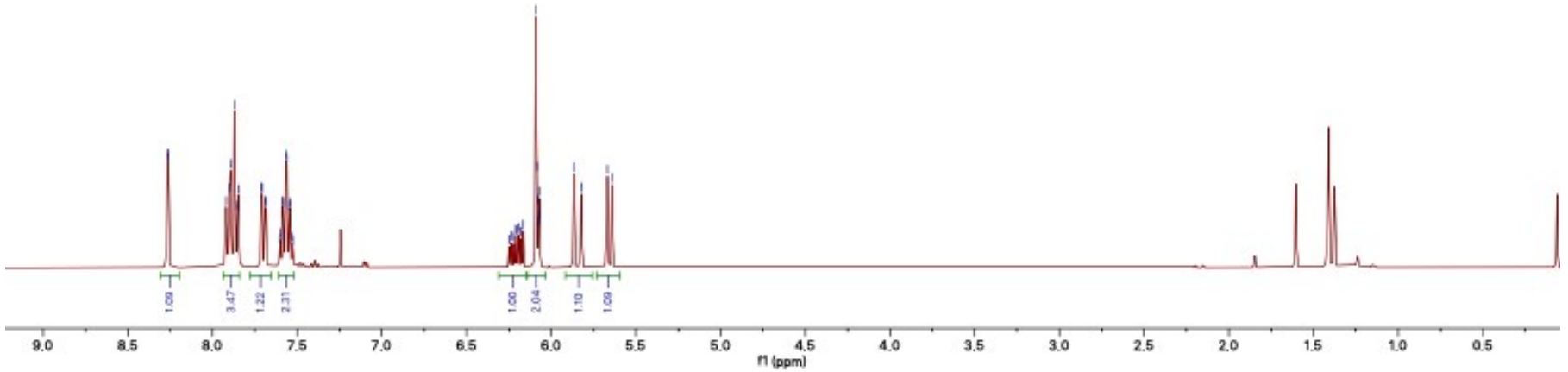

F
Br
O
O
O
2j
1.03
1.12
1.32
1.00
1.01
1.12
1.17
1.16
f1 (ppm)


165.49
162.76
162.07
160.22
133.07
133.06
129.87
127.52
127.44
122.88
117.22
116.99
99.68
93.78
93.77
F
Br
O
O
O
2j
f1 (ppm)





2k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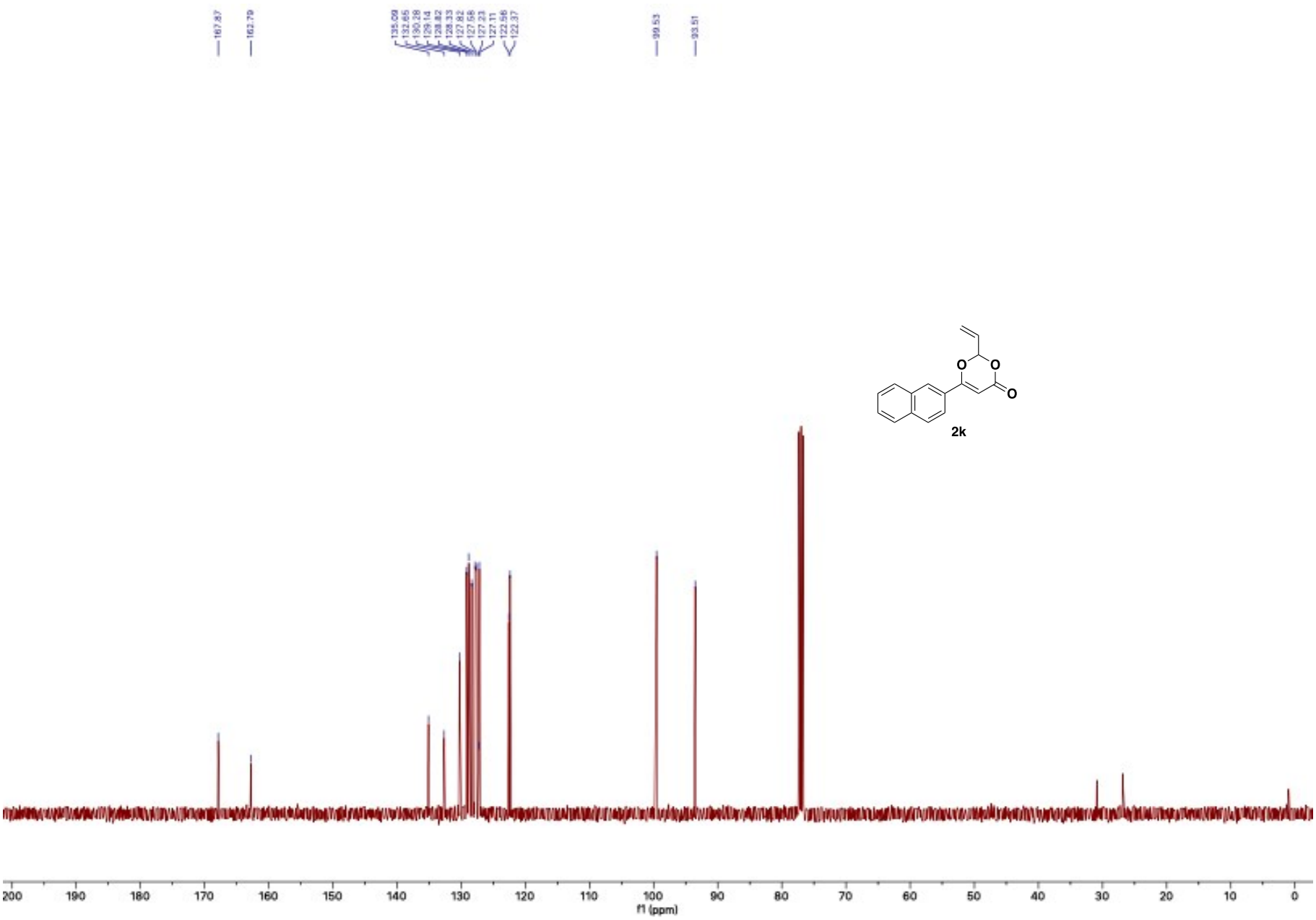
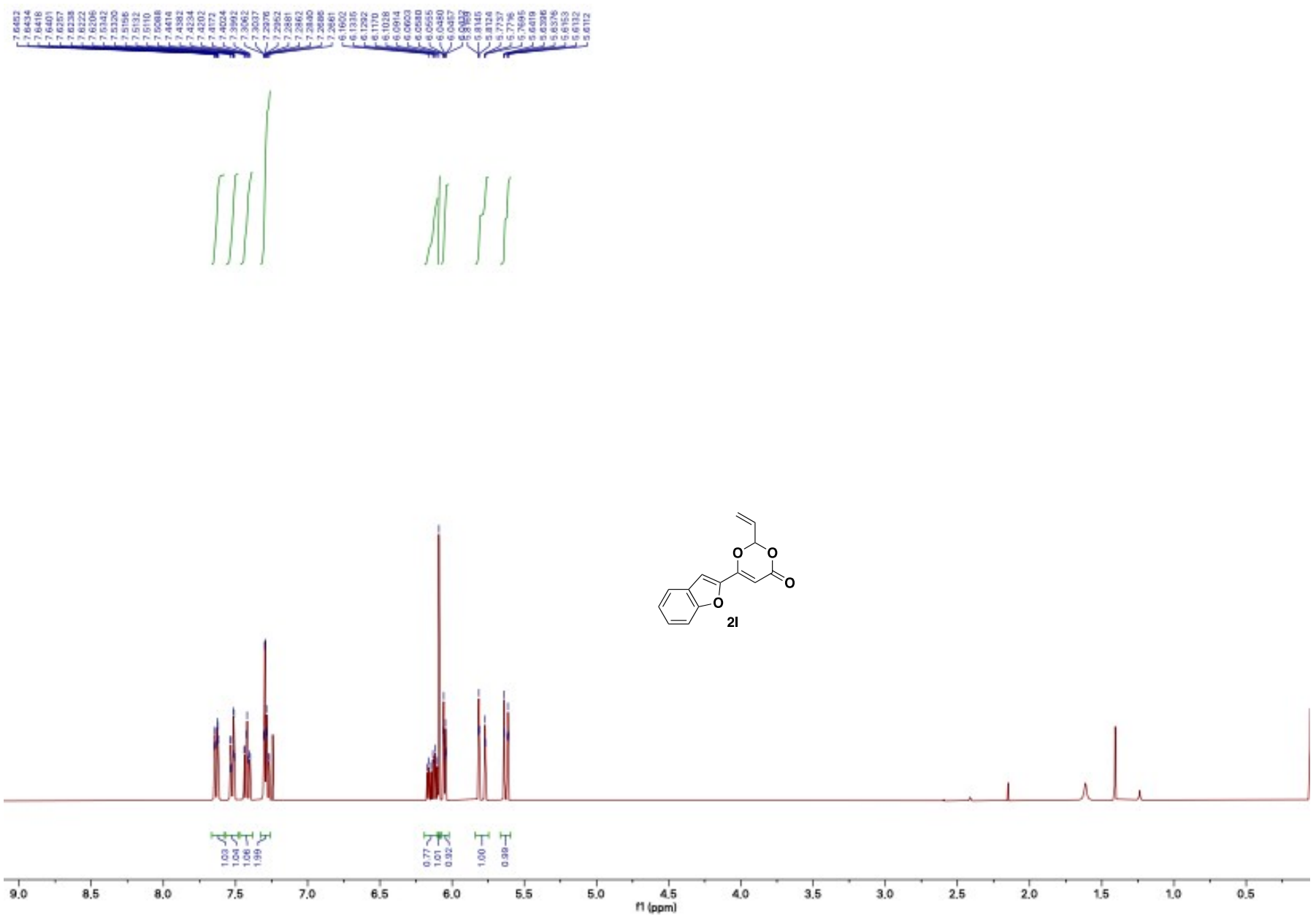
3.47
1.22
2.31
1.00
2.04
1.10
1.09
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


167.87
162.79
135.09
133.65
130.28
129.14
128.82
128.33
127.82
127.58
127.23
127.11
122.56
122.37
99.53
93.51
O
O
O
2k
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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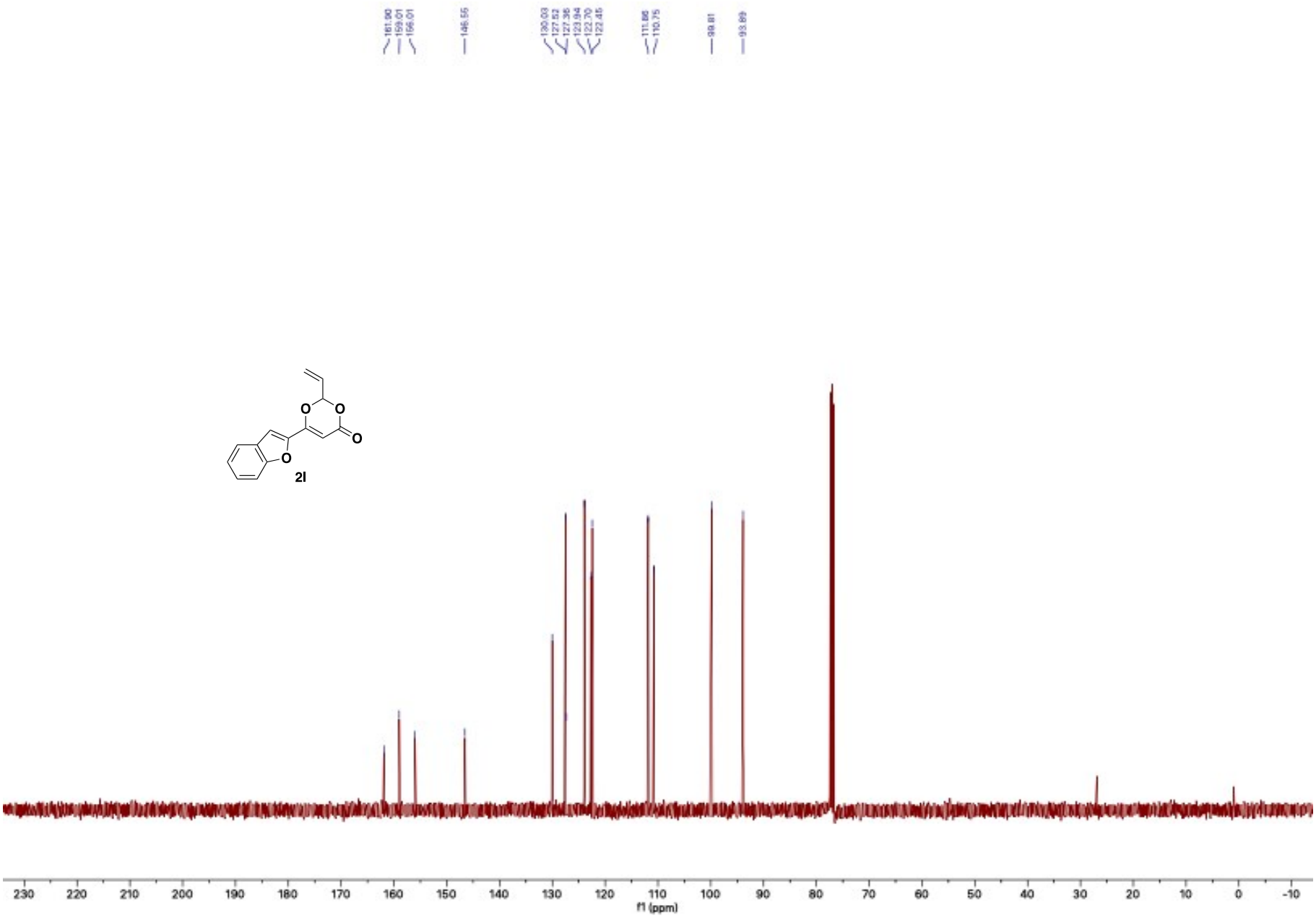
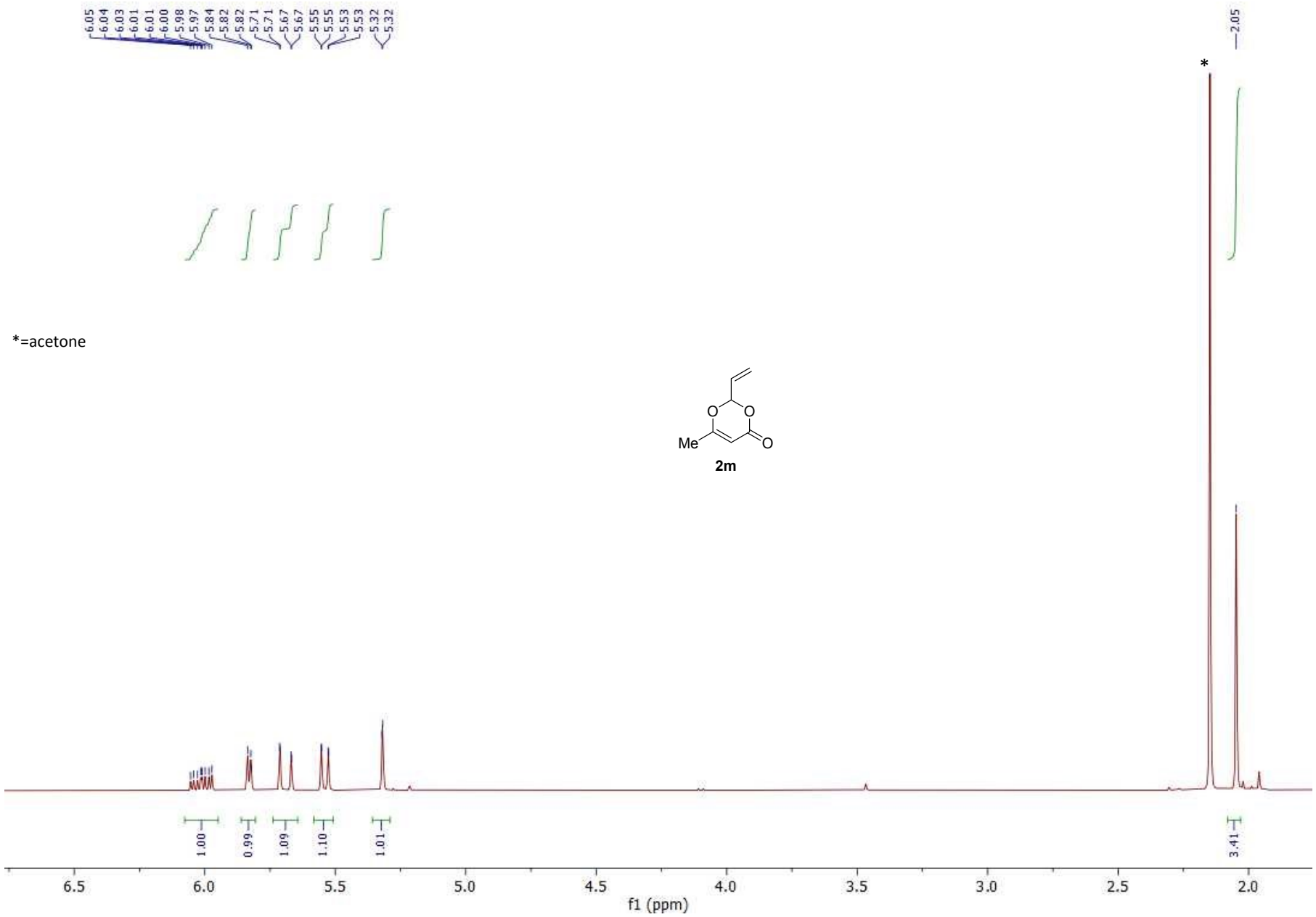
7.6418
7.6401
7.6257
7.6238
7.6222
7.6206
7.6342
7.5320
7.5156
7.5132
7.5110
7.5088
7.4414
7.4382
7.4234
7.4202
7.4172
7.4024
7.3992
7.3062
7.3037
7.2376
7.2952
7.2881
7.2862
7.2840
7.2688
7.2661
6.1662
6.1335
6.1292
6.1170
6.1028
6.0914
6.0803
6.0580
6.0565
6.0480
6.0457
5.8145
5.8124
5.7737
5.7716
5.7695
5.6419
5.6396
5.6376
5.6153
5.6132
5.6112
O
O
O
O
2l
1.03
1.04
1.06
1.99
0.77
1.01
0.92
1.00
0.99
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
f1 (ppm)


161.90
159.01
156.01
145.55
130.03
127.53
127.36
123.94
122.70
122.45
111.86
110.75
99.81
93.89
2l
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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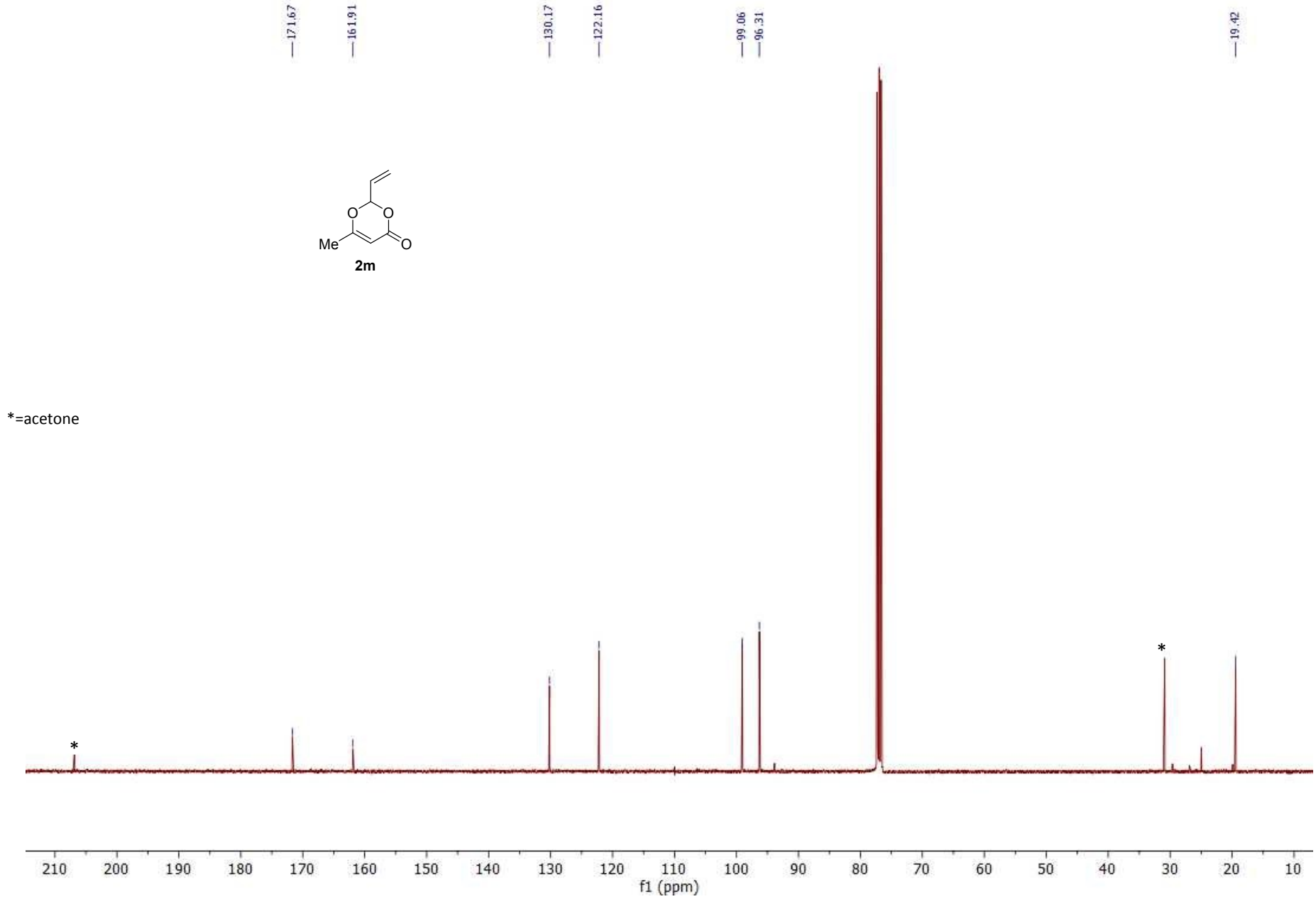
6.04
6.03
6.01
6.01
6.00
5.98
5.97
5.84
5.82
5.82
5.71
5.71
5.67
5.67
5.55
5.55
5.53
5.53
5.32
5.32
2.05
*
1.00
0.99
1.09
1.10
1.01
3.41
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)

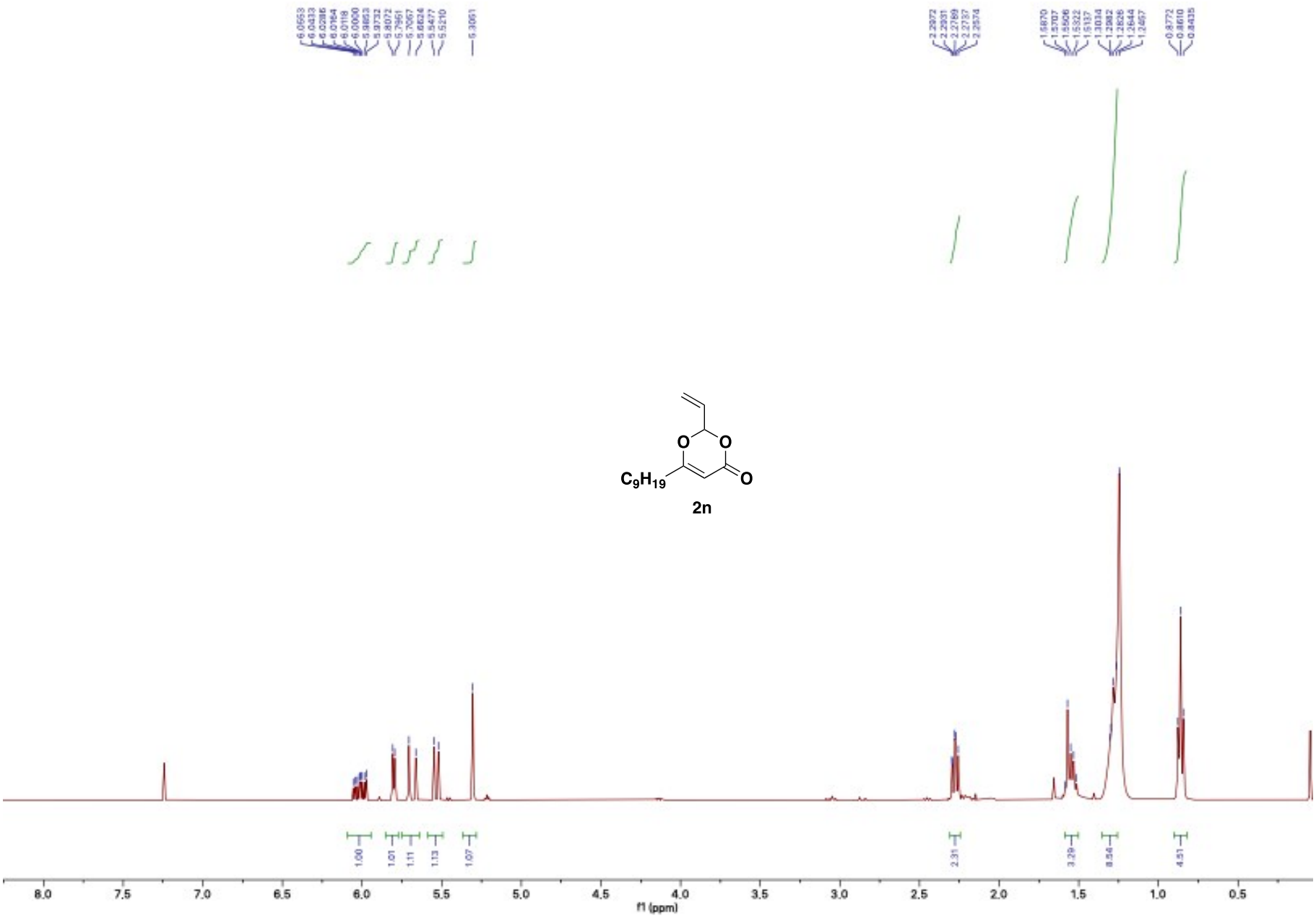
*=acetone

O
O
Me
O

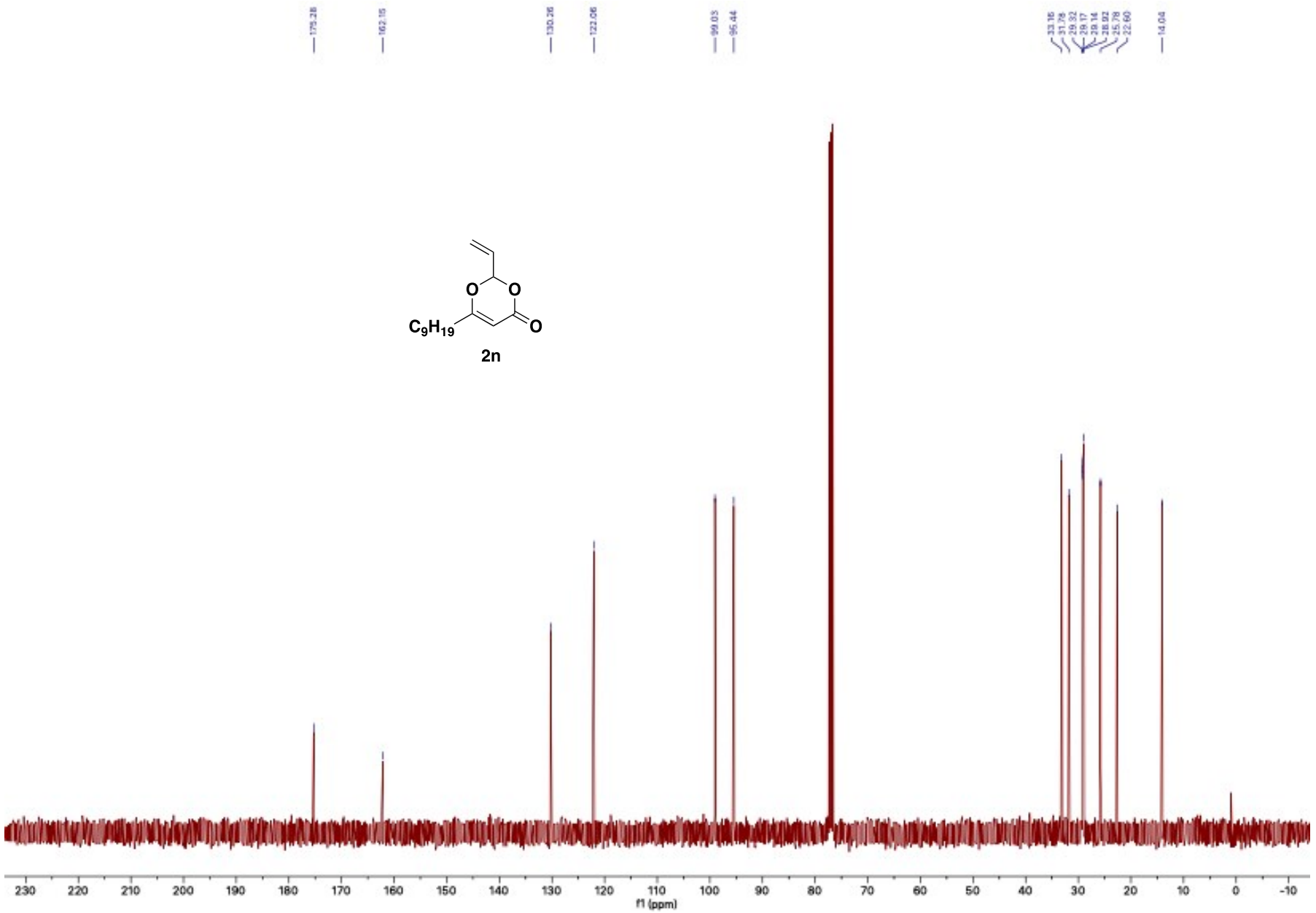
2m

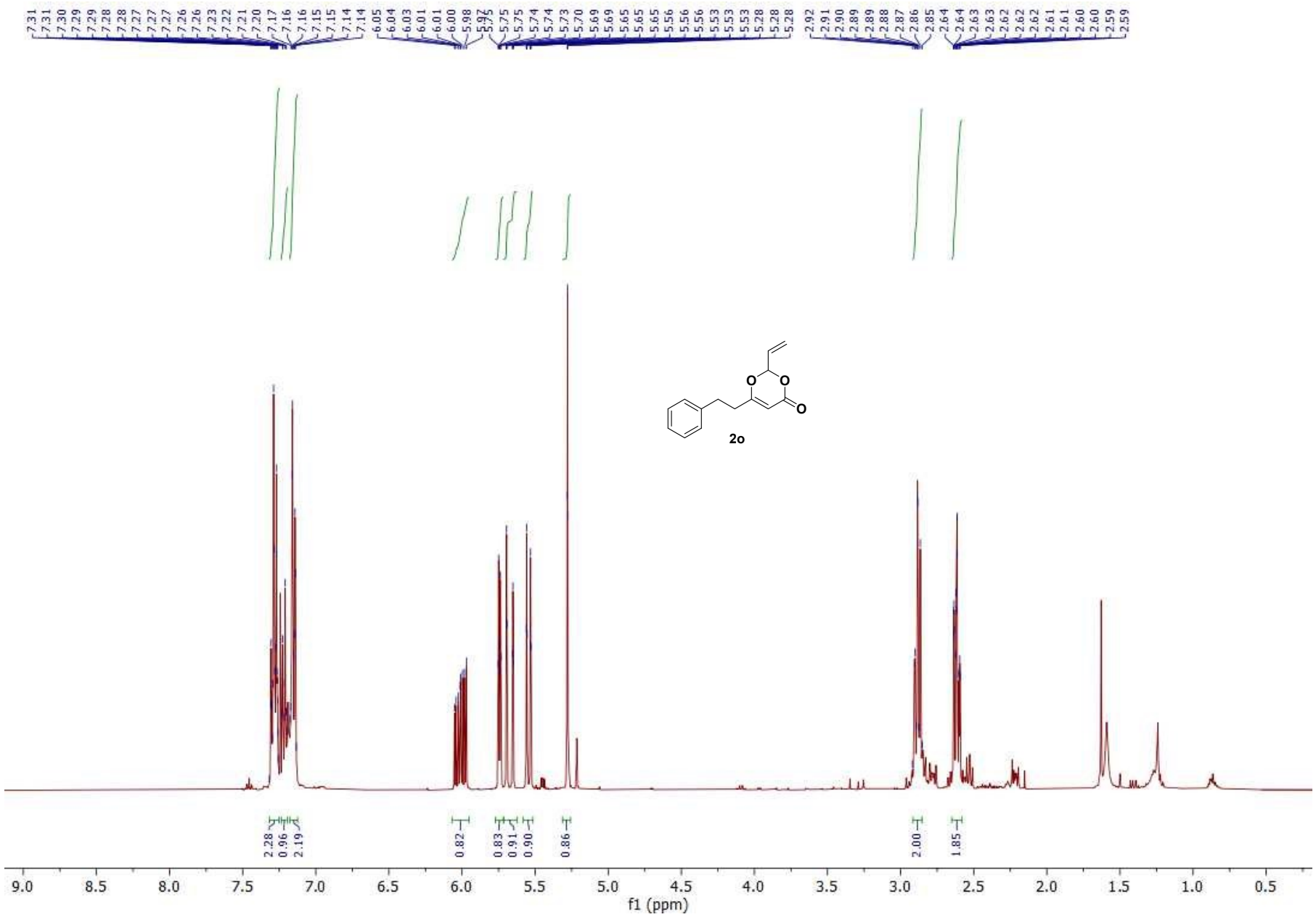

171.67
161.91
130.17
122.16
99.06
96.31
19.42
O
O
Me
O
2m
*
*
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

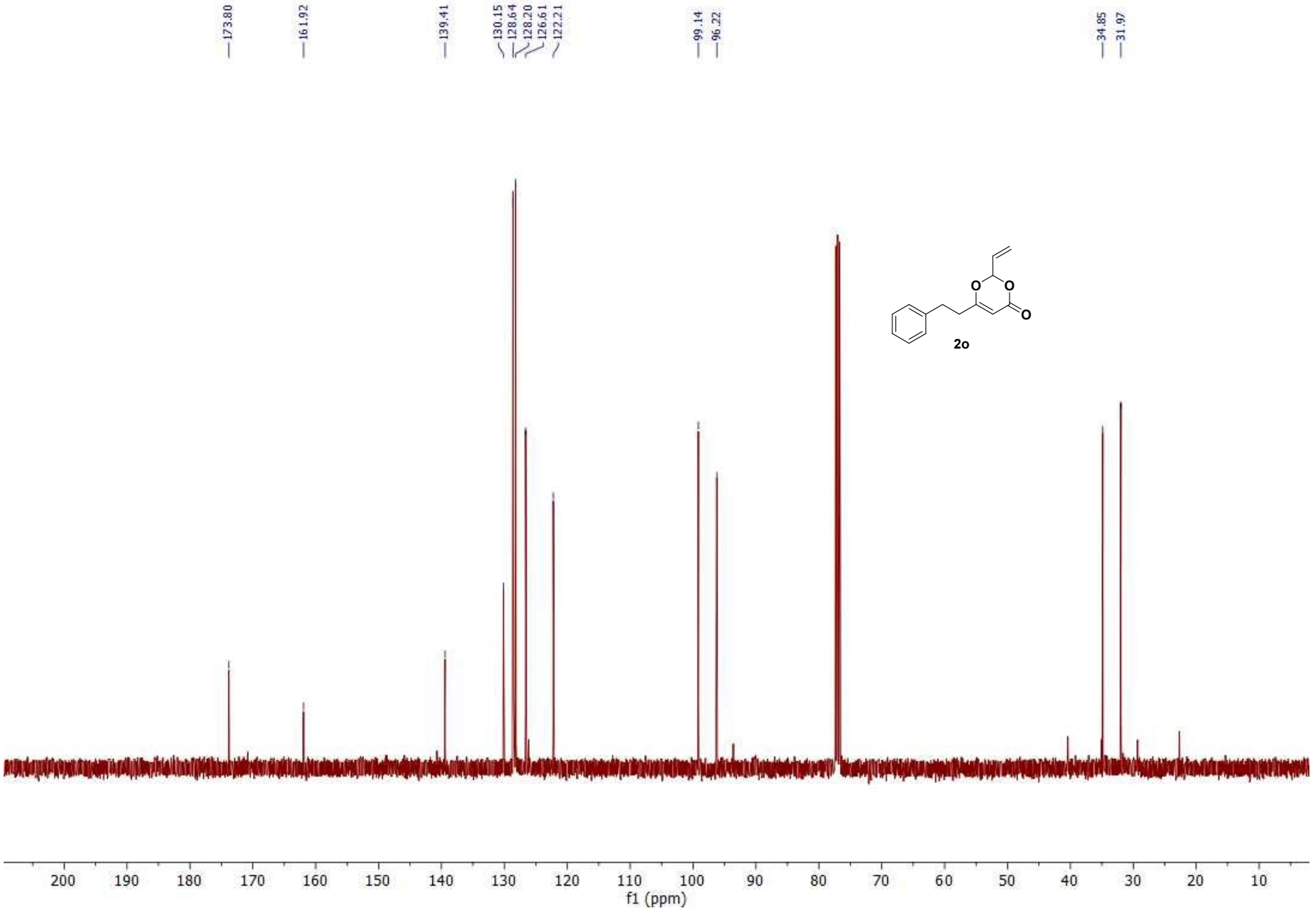
*=acetone

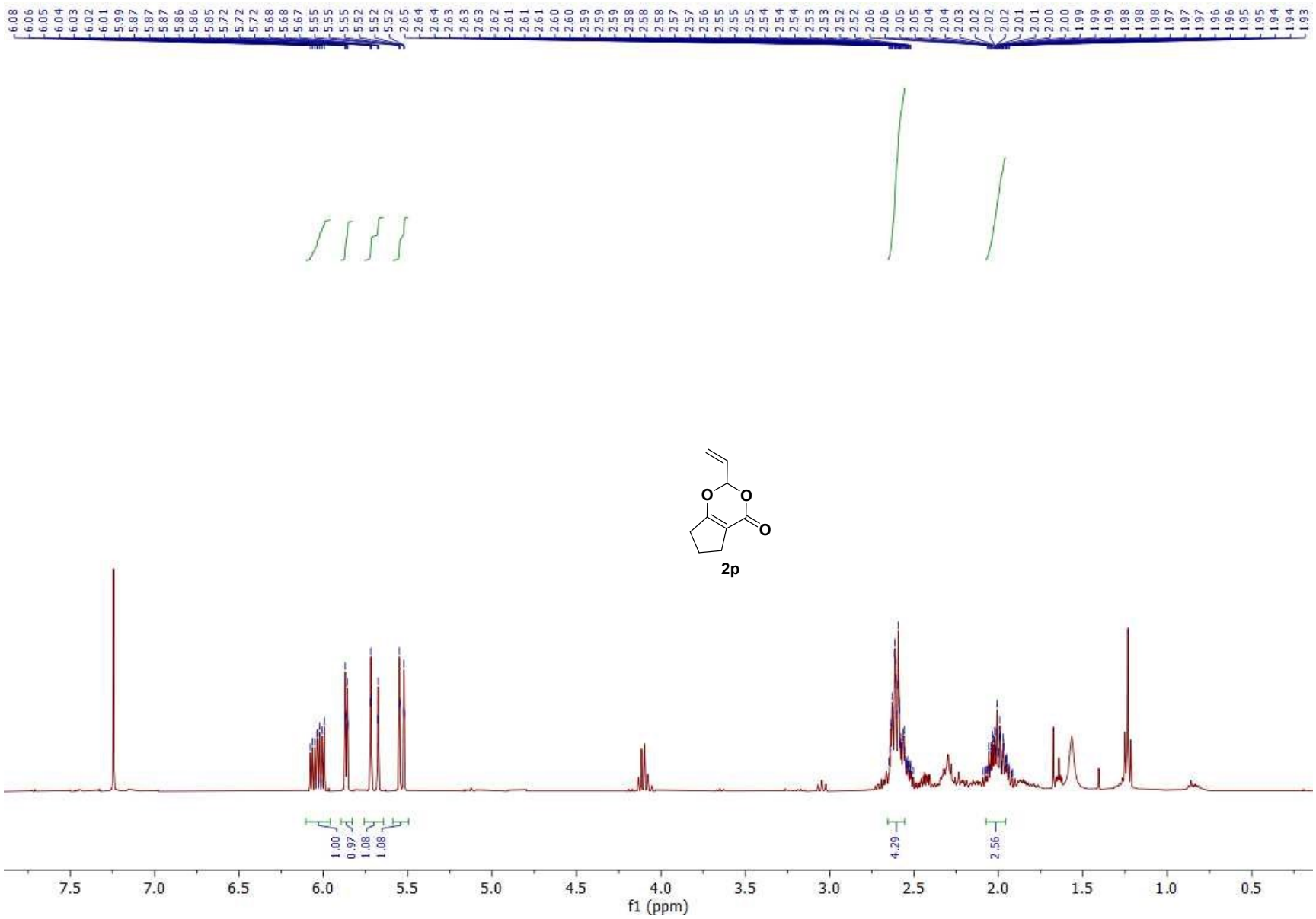

6.0553
6.0433
6.0286
6.0164
6.0119
6.0000
5.9863
5.9732
5.8072
5.7961
5.7067
5.6624
5.5477
5.5210
5.3061
2.2972
2.2931
2.2789
2.2737
2.2574
1.5870
1.5707
1.5506
1.5322
1.5137
1.3034
1.2882
1.2826
1.2644
1.2457
0.8772
0.8610
0.8435
O
O
O
C9H19
1.00
1.01
1.11
1.13
1.07
2.31
3.29
8.54
4.51
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

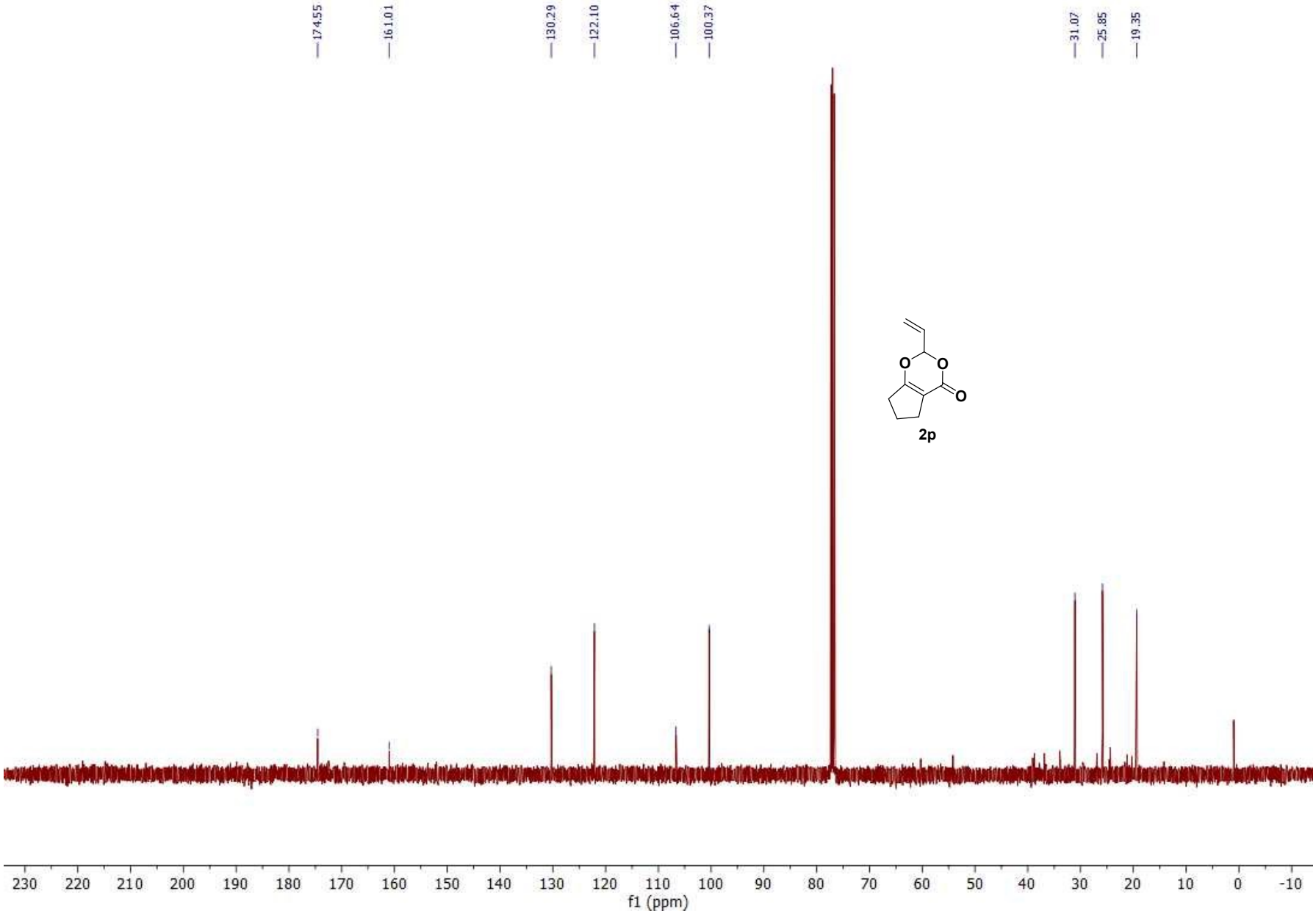
2n

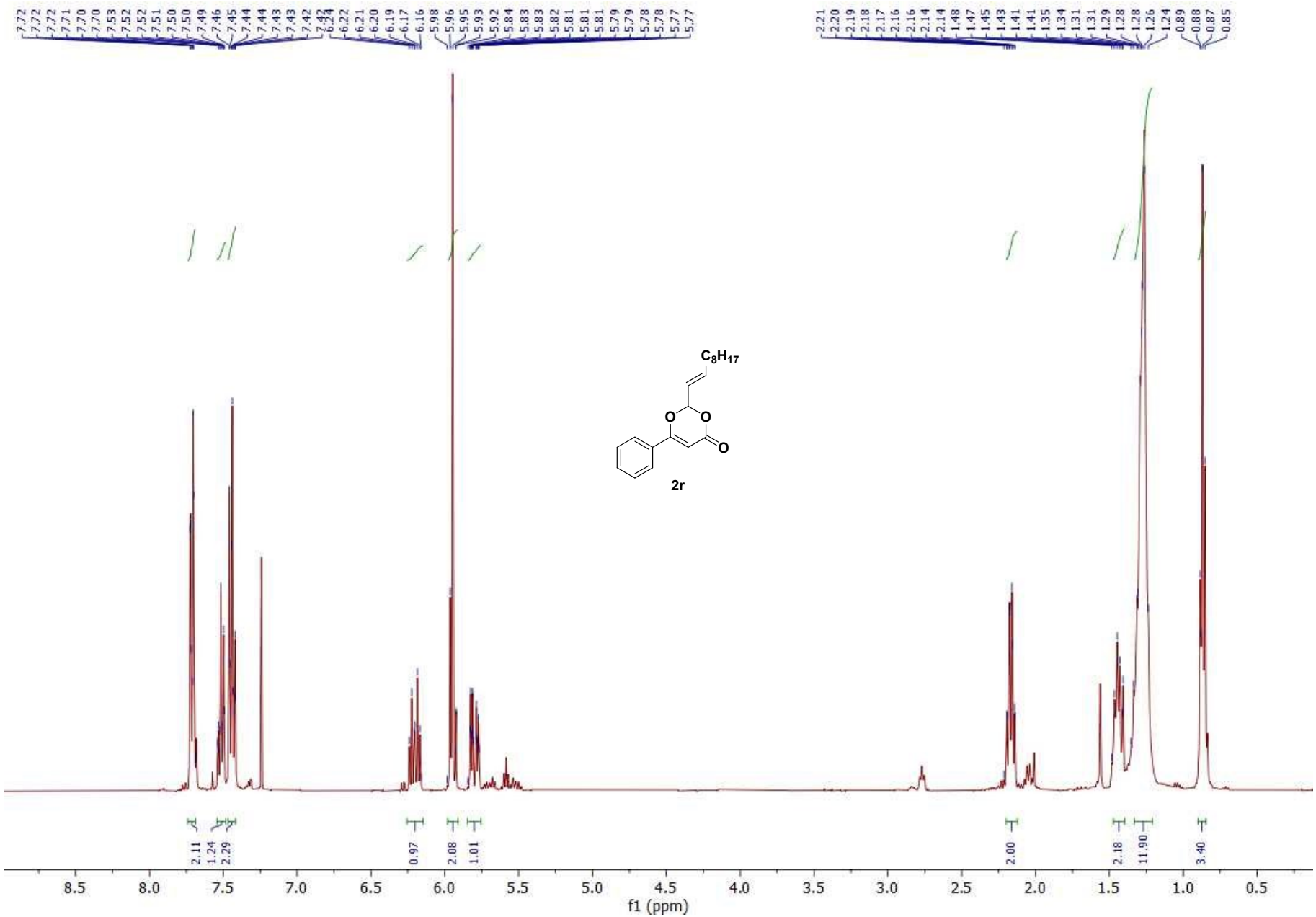

175.28
162.15
130.26
122.06
99.03
95.44
33.16
31.78
29.32
29.17
29.14
28.92
25.79
22.60
14.04
O
O
O
C_9H_{19}
2n
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

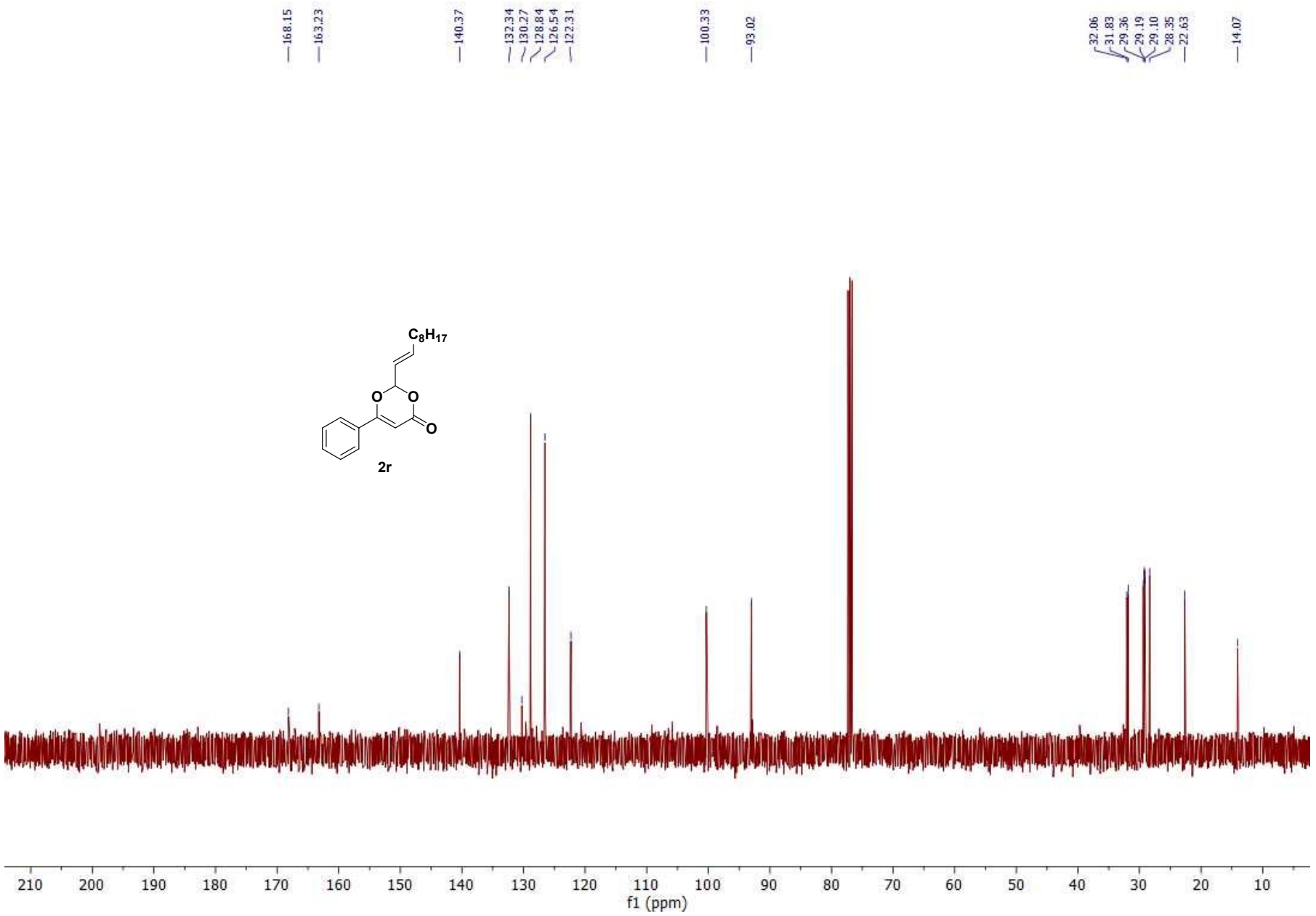

7.31 7.31 7.30 7.29 7.29 7.28 7.27 7.27 7.26 7.26 7.23 7.22 7.21 7.20 7.17 7.16 7.16 7.15 7.15 7.14 7.14
6.05 6.04 6.03 6.01 6.01 6.00 5.98 5.97 5.75 5.75 5.74 5.74 5.73 5.70 5.69 5.69 5.65 5.65 5.56 5.56 5.56 5.53 5.53 5.28 5.28
2.92 2.91 2.90 2.89 2.89 2.88 2.87 2.86 2.85 2.64 2.64 2.63 2.63 2.62 2.62 2.61 2.61 2.60 2.60 2.59 2.59
O
O
O
2o
2.28
0.96
2.19
0.82
0.83
0.91
0.90
0.86
2.00
1.85
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
f1 (ppm)

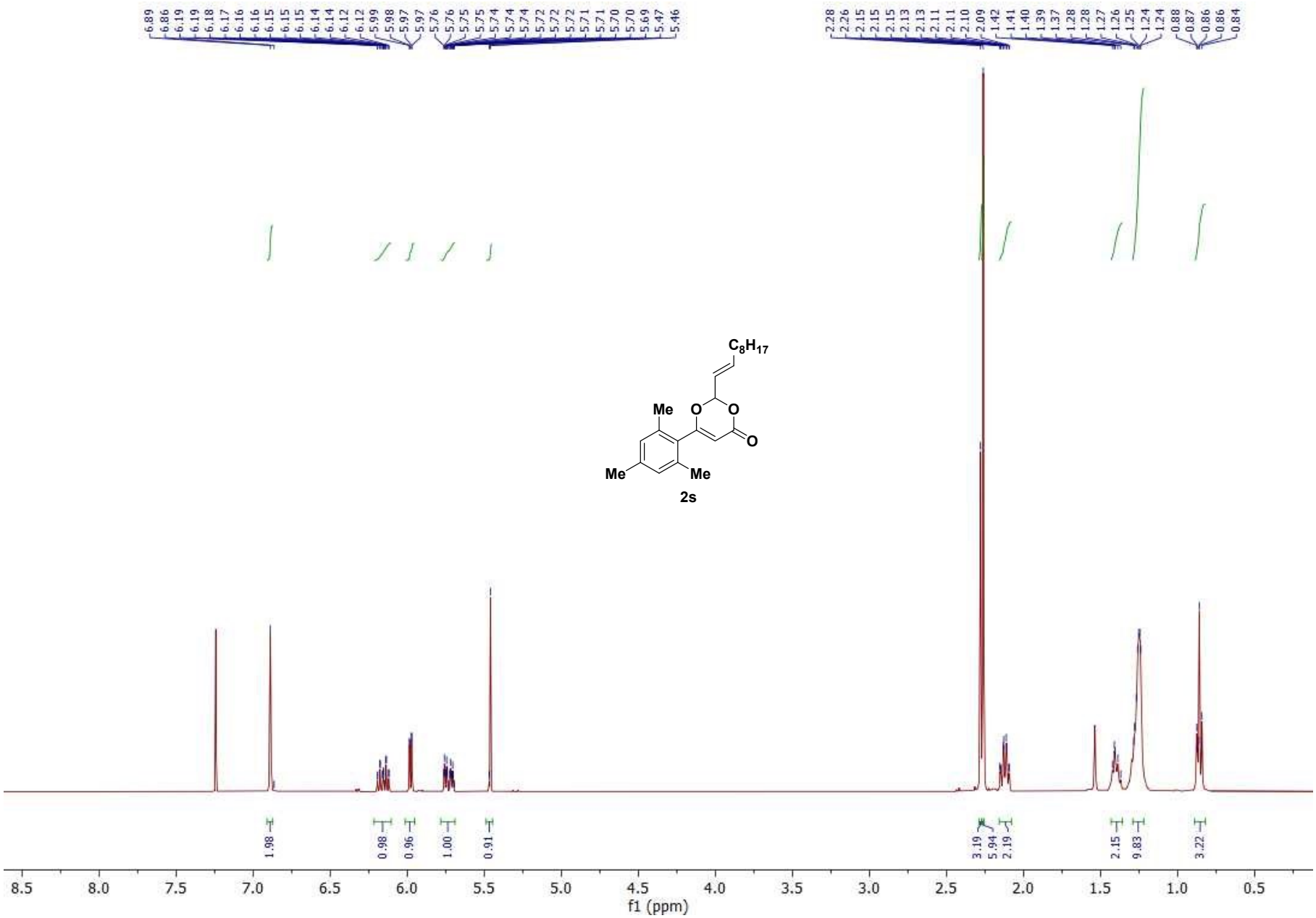

173.80
161.92
139.41
130.15
128.64
128.20
126.61
122.21
99.14
96.22
34.85
31.97
O
O
O
2o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

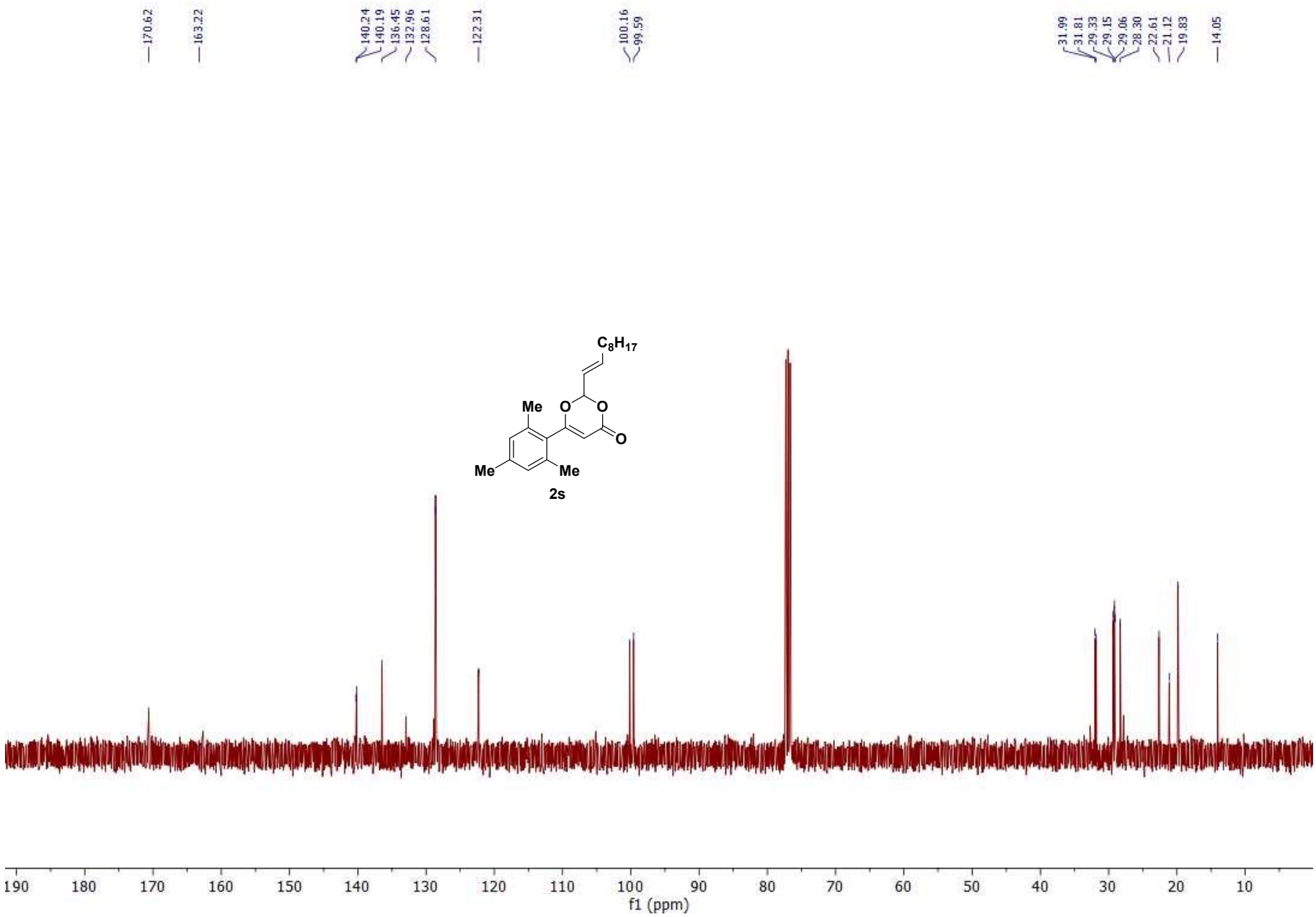

6.08 6.06 6.05 6.04 6.03 6.02 6.01 5.99 5.87 5.87 5.87 5.86 5.86 5.85 5.72 5.72 5.72 5.68 5.68 5.67 5.55 5.55 5.55 5.52 5.52 5.52 2.65 2.64 2.64 2.63 2.63 2.63 2.62 2.61 2.61 2.61 2.60 2.60 2.59 2.59 2.59 2.58 2.58 2.58 2.57 2.57 2.56 2.55 2.55 2.55 2.54 2.54 2.53 2.52 2.52 2.06 2.06 2.05 2.05 2.04 2.04 2.03 2.02 2.02 2.02 2.01 2.01 2.00 2.00 1.99 1.99 1.99 1.98 1.98 1.98 1.97 1.97 1.97 1.96 1.96 1.95 1.95 1.94 1.94 1.93
O
O
O
2p
1.00
0.97
1.08
1.08
4.29
2.56
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
f1 (ppm)

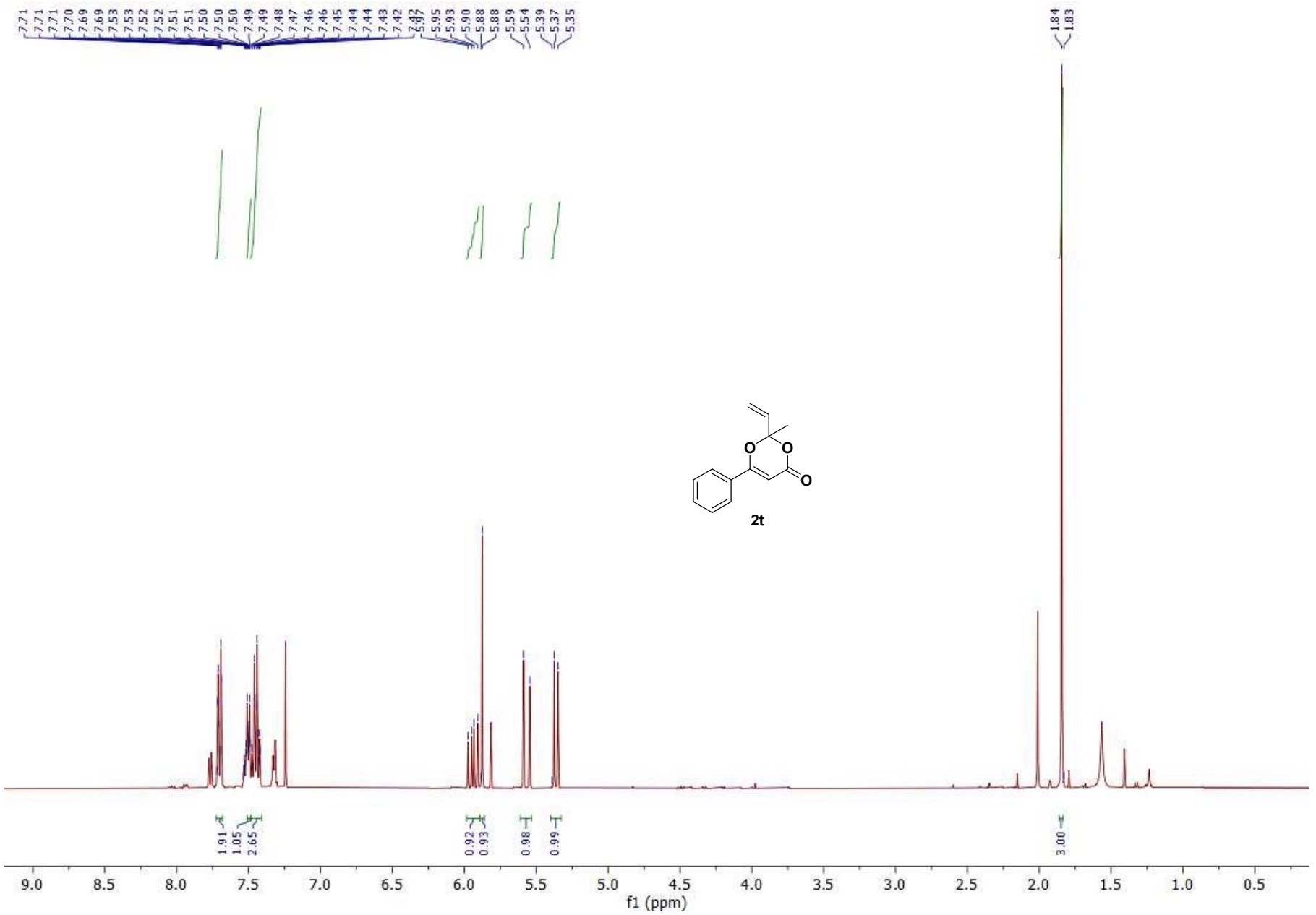

174.55
161.01
130.29
122.10
106.64
100.37
31.07
25.85
19.35
O
O
O
2p
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

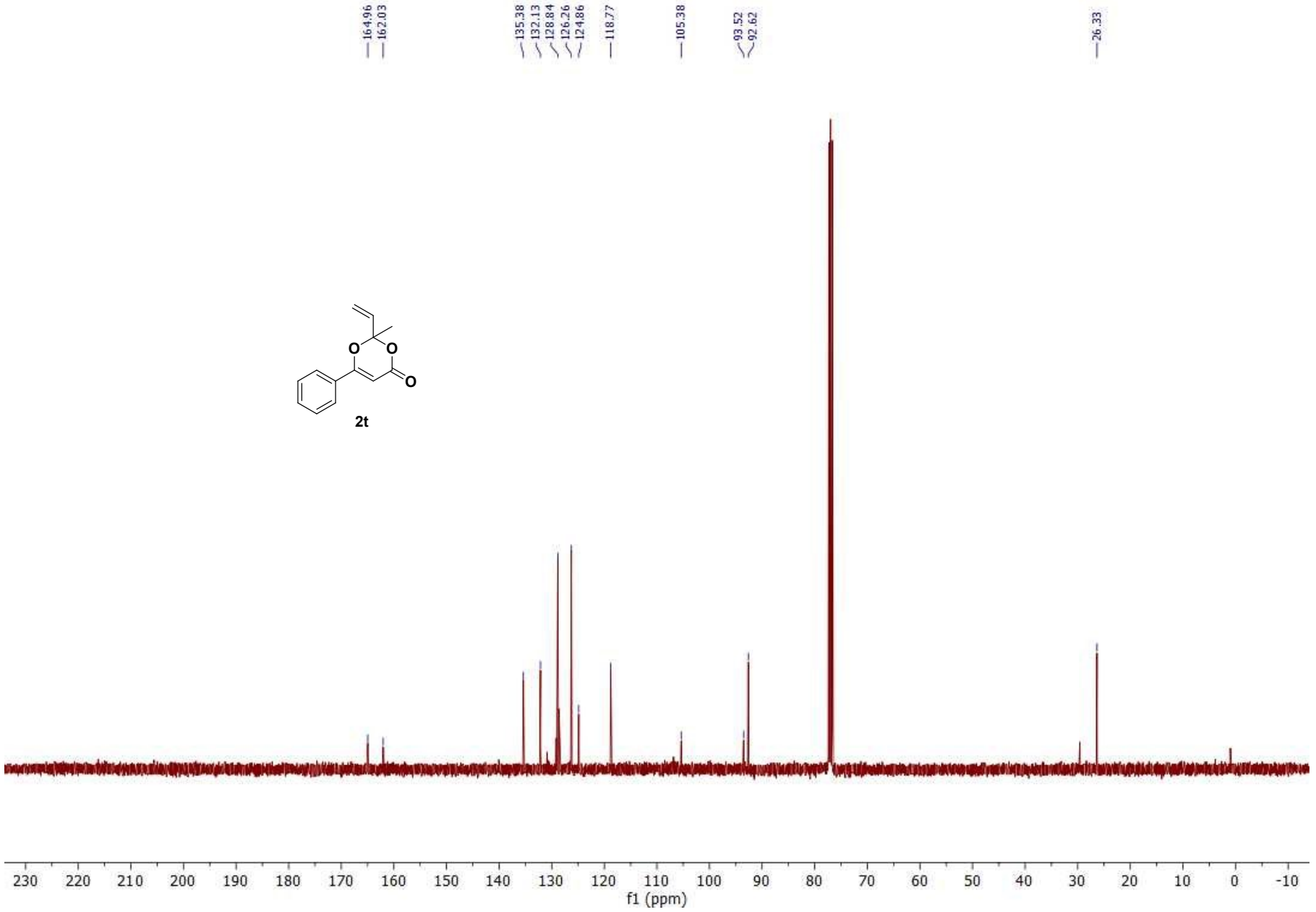

7.72 7.72 7.72 7.71 7.70 7.70 7.53 7.52 7.52 7.51 7.50 7.50 7.49 7.46 7.45 7.44 7.44 7.43 7.43 7.42 6.22 6.21 6.20 6.19 6.17 6.16 5.98 5.96 5.95 5.93 5.92 5.84 5.83 5.83 5.82 5.81 5.81 5.81 5.79 5.79 5.78 5.78 5.77 5.77
2.21 2.20 2.19 2.18 2.17 2.16 2.16 2.14 2.14 1.48 1.47 1.45 1.43 1.41 1.41 1.35 1.34 1.31 1.31 1.29 1.28 1.28 1.26 1.24 0.89 0.88 0.87 0.85
C8H17
O
O
O
2r
2.11 1.24 2.29 0.97 2.08 1.01 2.00 2.18 11.90 3.40
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
f1 (ppm)

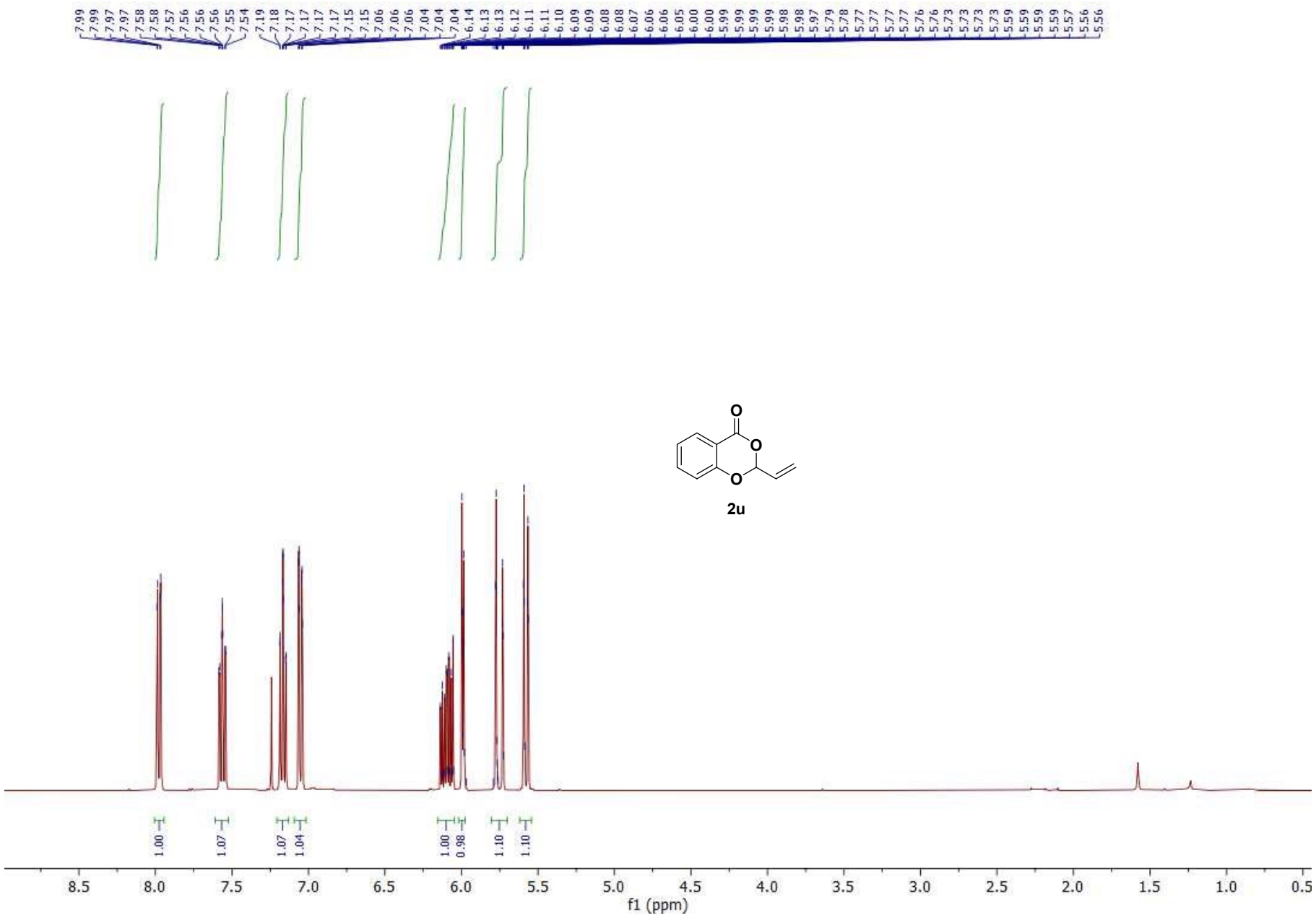

168.15
163.23
140.37
132.34
130.27
128.84
126.54
122.31
100.33
93.02
32.06
31.83
29.36
29.19
29.10
28.35
22.63
14.07
C8H17
O
O
O
2r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

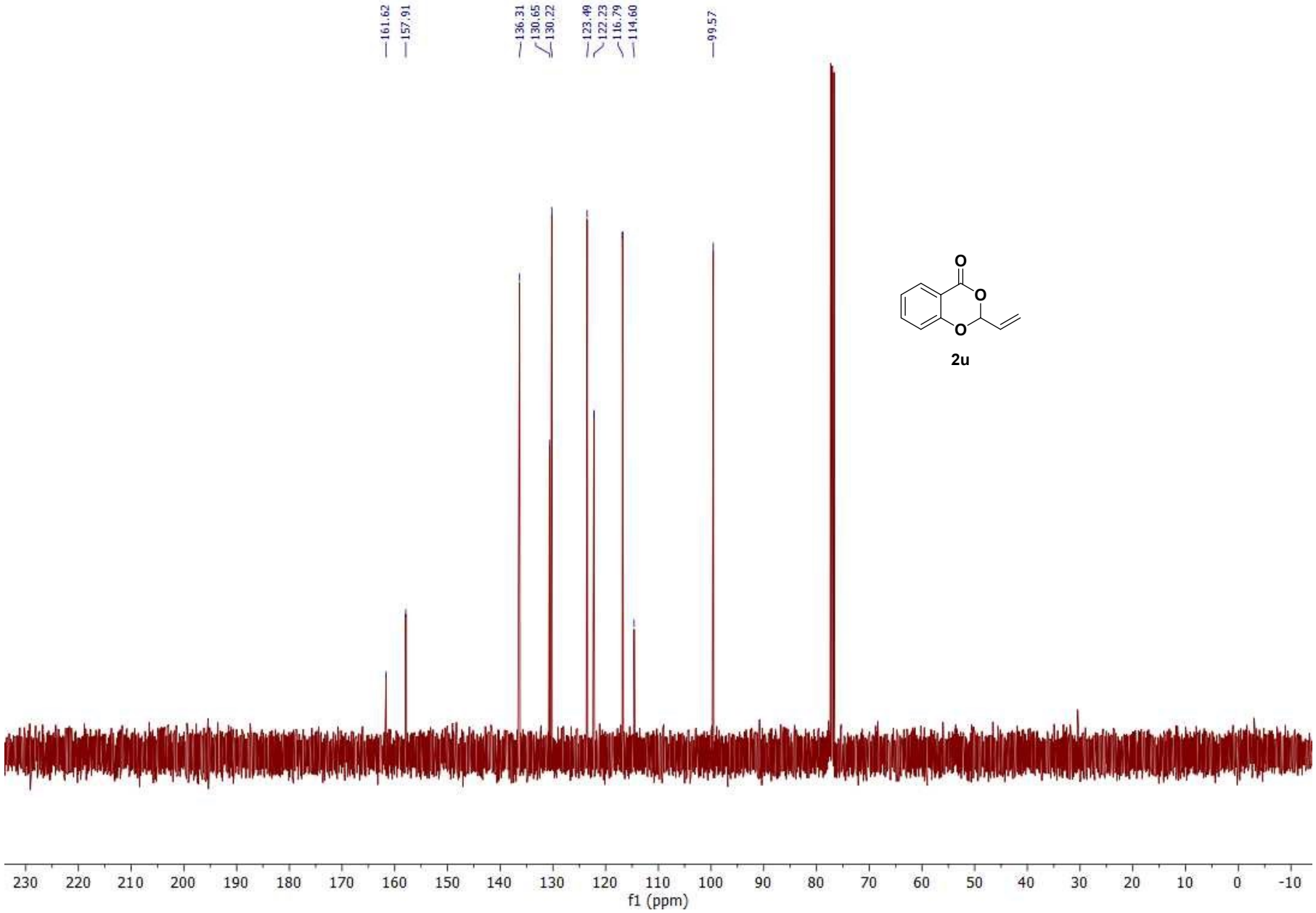

6.89 6.86 6.19 6.19 6.18 6.17 6.16 6.16 6.15 6.15 6.15 6.14 6.14 6.12 6.12 5.99 5.98 5.97 5.97 5.76 5.76 5.75 5.75 5.74 5.74 5.74 5.72 5.72 5.72 5.71 5.71 5.70 5.70 5.69 5.47 5.46
2.28 2.26 2.15 2.15 2.15 2.13 2.13 2.11 2.11 2.10 2.09 1.42 1.41 1.40 1.39 1.37 1.28 1.28 1.27 1.26 1.25 1.24 1.24 0.88 0.87 0.86 0.86 0.84
C8H17
Me
O
O
O
Me
Me
2s
1.98
0.98
0.96
1.00
0.91
3.19
5.94
2.19
2.15
9.83
3.22
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
f1 (ppm)

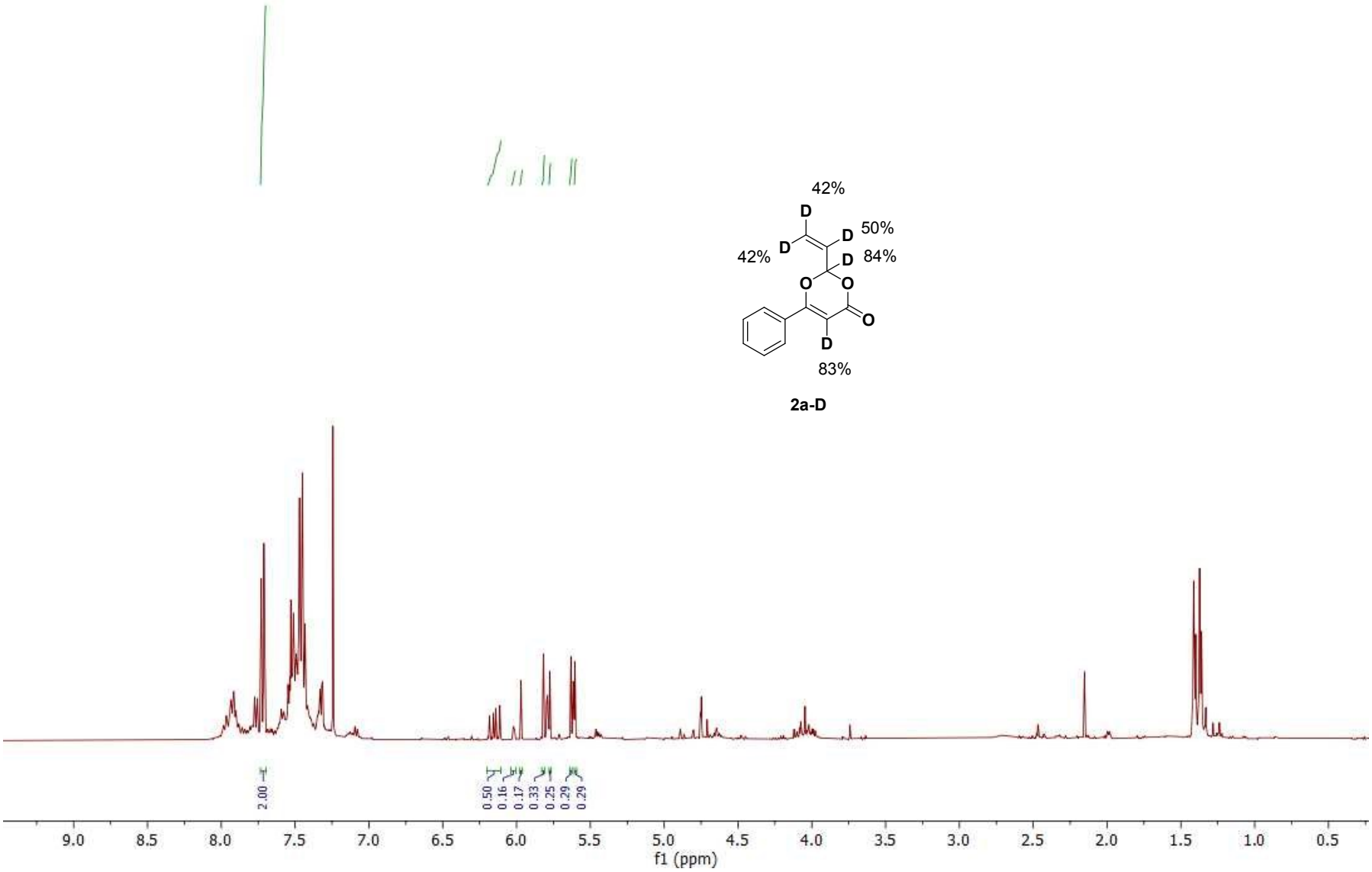

170.62
163.22
140.24
140.19
136.45
132.96
128.61
122.31
100.16
99.59
31.99
31.81
29.33
29.15
29.06
28.30
22.61
21.12
19.83
14.05
C8H17
Me
O
O
O
Me
Me
2s
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.71
7.71
7.71
7.70
7.69
7.69
7.53
7.52
7.52
7.51
7.51
7.50
7.50
7.50
7.49
7.49
7.48
7.47
7.46
7.46
7.45
7.44
7.44
7.43
7.42
5.95
5.93
5.90
5.88
5.88
5.59
5.54
5.39
5.37
5.35
1.84
1.83
O
O
O
2t
1.91
1.05
2.65
0.92
0.93
0.98
0.99
3.00
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
f1 (ppm)


164.96
162.03
135.38
132.13
128.84
126.26
124.86
118.77
105.38
93.52
92.62
26.33
O
O
O
2t
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.99 7.99 7.97 7.97 7.58 7.58 7.57 7.56 7.56 7.56 7.55 7.54 7.19 7.18 7.17 7.17 7.17 7.17 7.15 7.06 7.06 7.06 7.04 7.04 7.04 6.14 6.13 6.13 6.12 6.11 6.11 6.10 6.09 6.09 6.08 6.08 6.07 6.06 6.06 6.05 6.00 6.00 5.99 5.99 5.99 5.99 5.98 5.98 5.97 5.79 5.78 5.77 5.77 5.77 5.77 5.76 5.76 5.73 5.73 5.73 5.59 5.59 5.59 5.59 5.57 5.56 5.56
O
O
O
2u
1.00 1.07 1.07 1.04 1.00 0.98 1.10 1.10
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
f1 (ppm)


161.62
157.91
136.31
130.65
130.22
123.49
122.23
116.79
114.60
99.57
O
O
O
2u
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


42%
D
D
50%
D
42%
D
84%
O
O
O
D
83%
2a-D
2.00
0.50
0.16
0.17
0.33
0.25
0.29
0.29
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
f1 (ppm)