Activation of Enamine by Photoexcited Organo Catalyst Assisted Singlet Oxygen: Synthesis of Oxazoles and Quinoxalines

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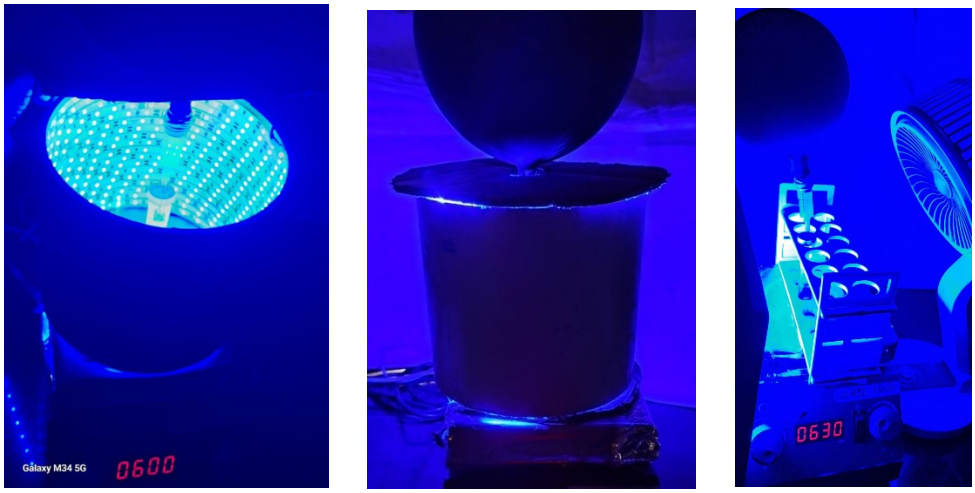


Figure S1. The photocatalytic setup: (**a**) and (**b**) reaction under light bath; (**c**) reaction with colling fan.

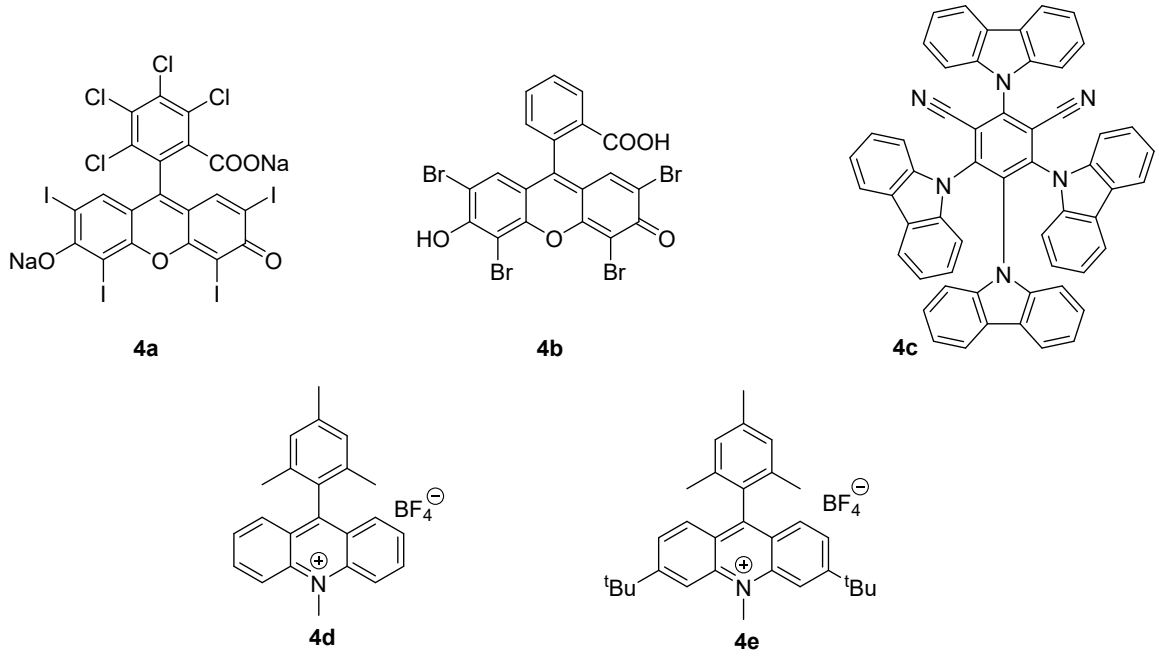


Figure S2. Chemical structure of photocatalysts used in the optimization (**4a**-**4e**):

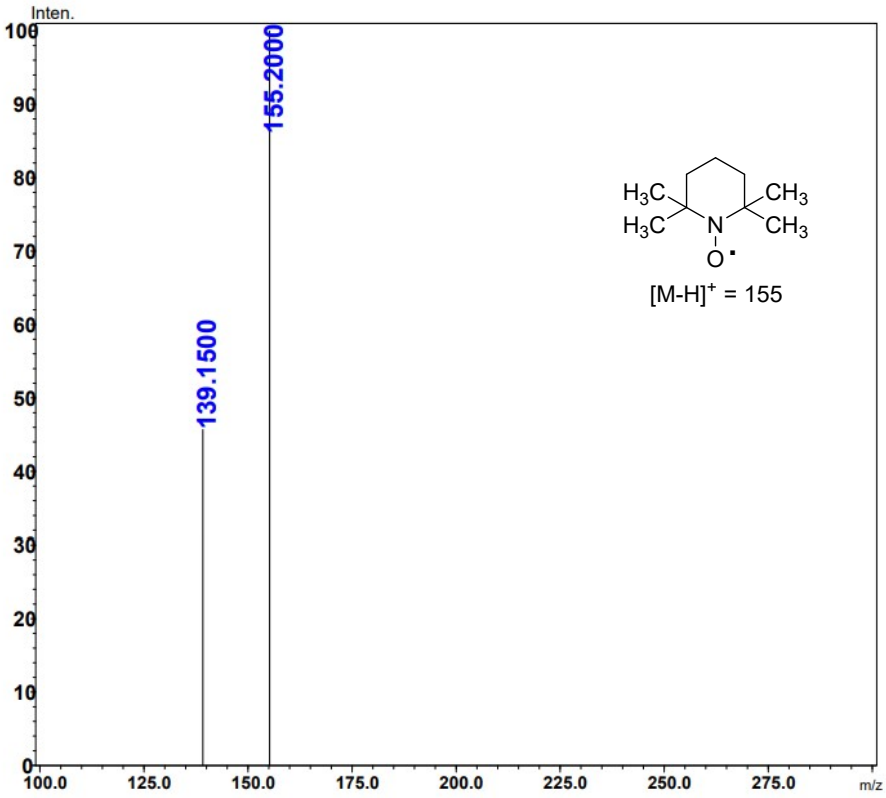


Figure S3 LCMS analysis of TEMPO formation from TEMP.

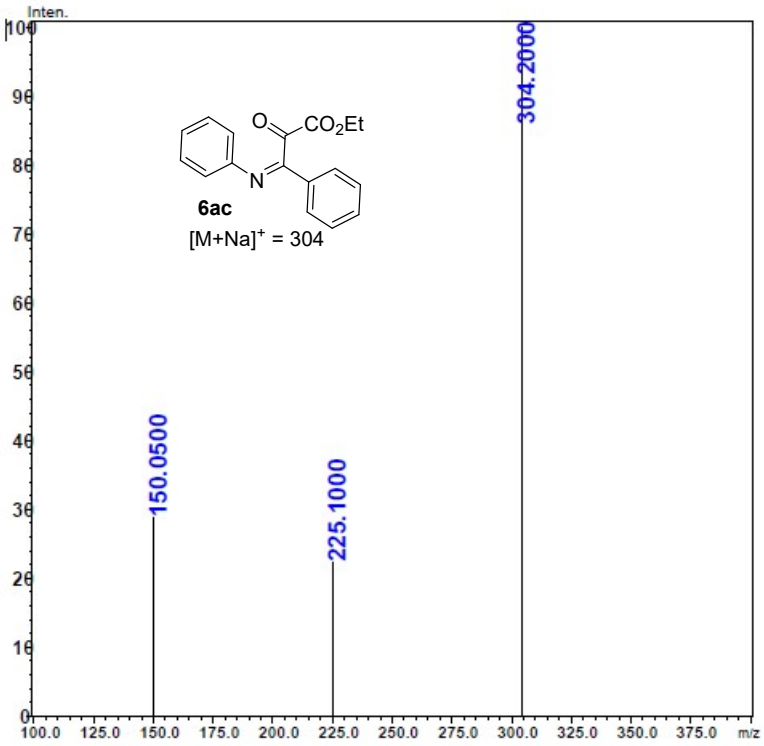
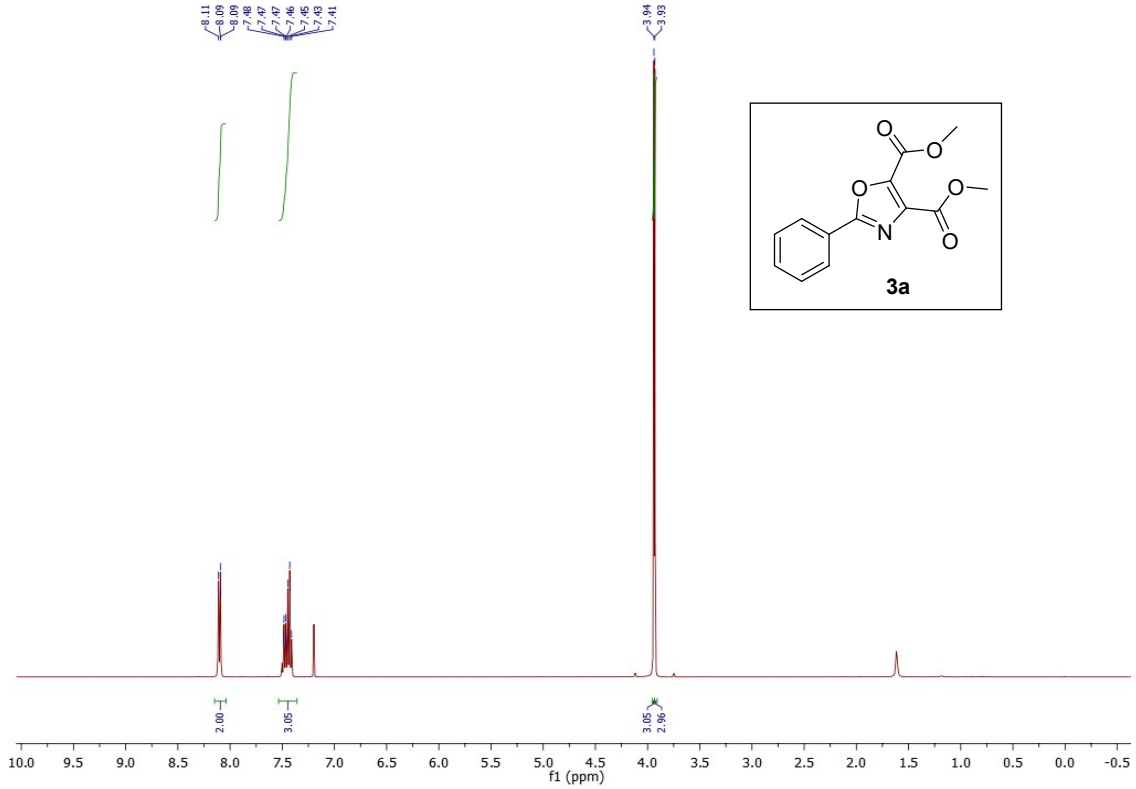
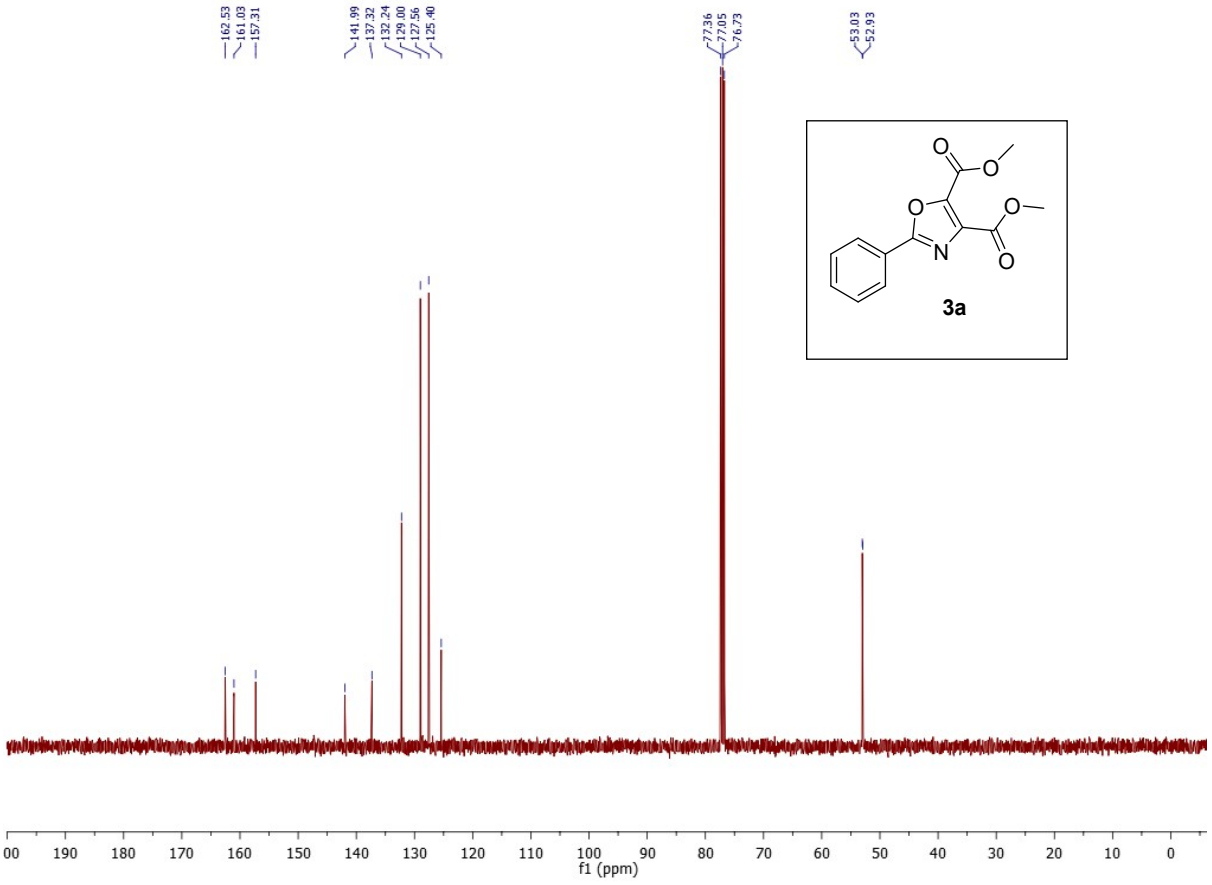
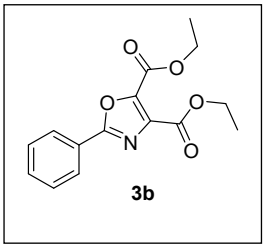


Figure S4. Mass spectrum of intermediate, **6ac**

^{1}H NMR and ^{13}C NMR Spectra:



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4.42
4.41
4.39
4.37
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1.34
1.33
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4.11
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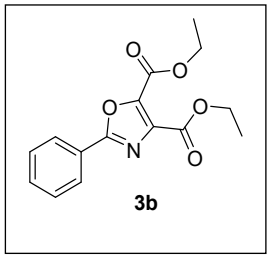
f1 (ppm)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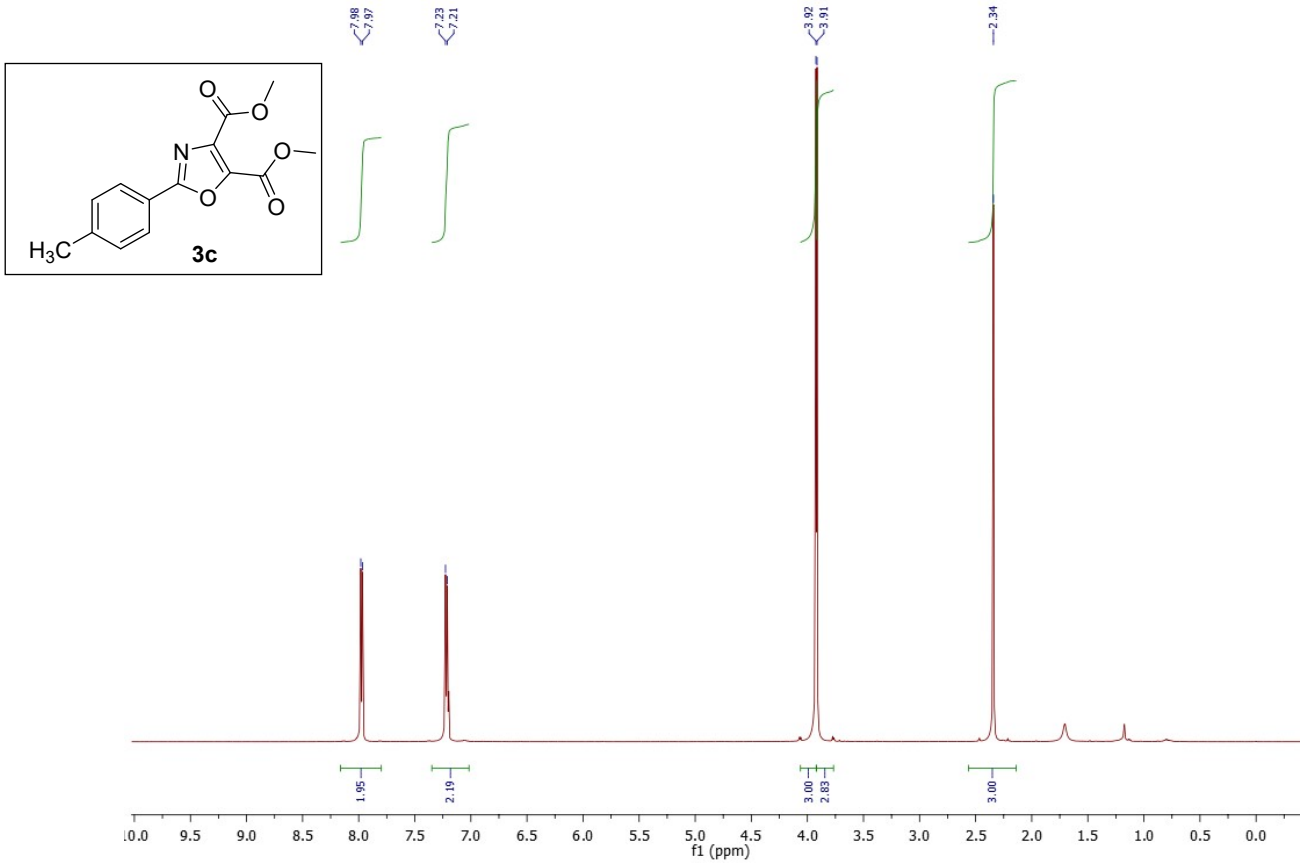
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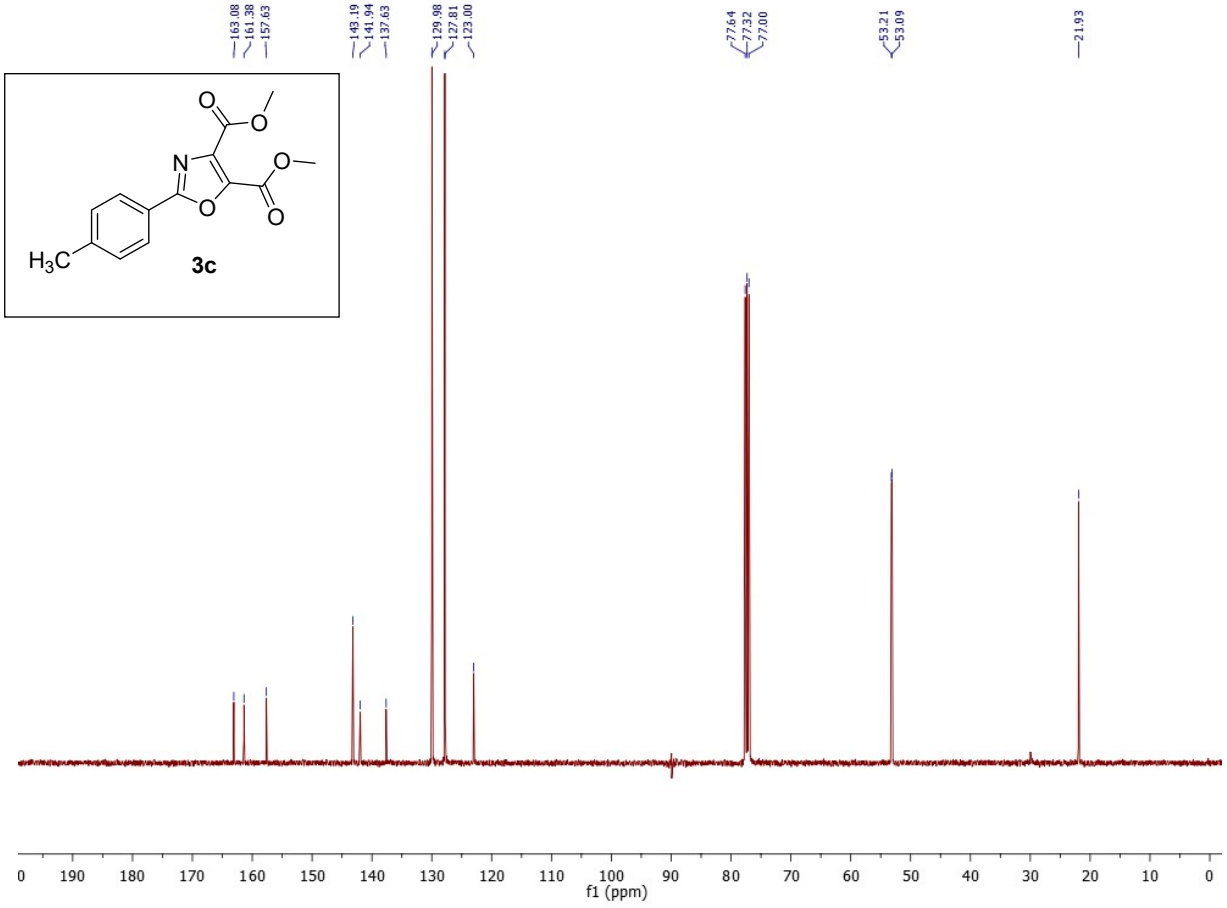
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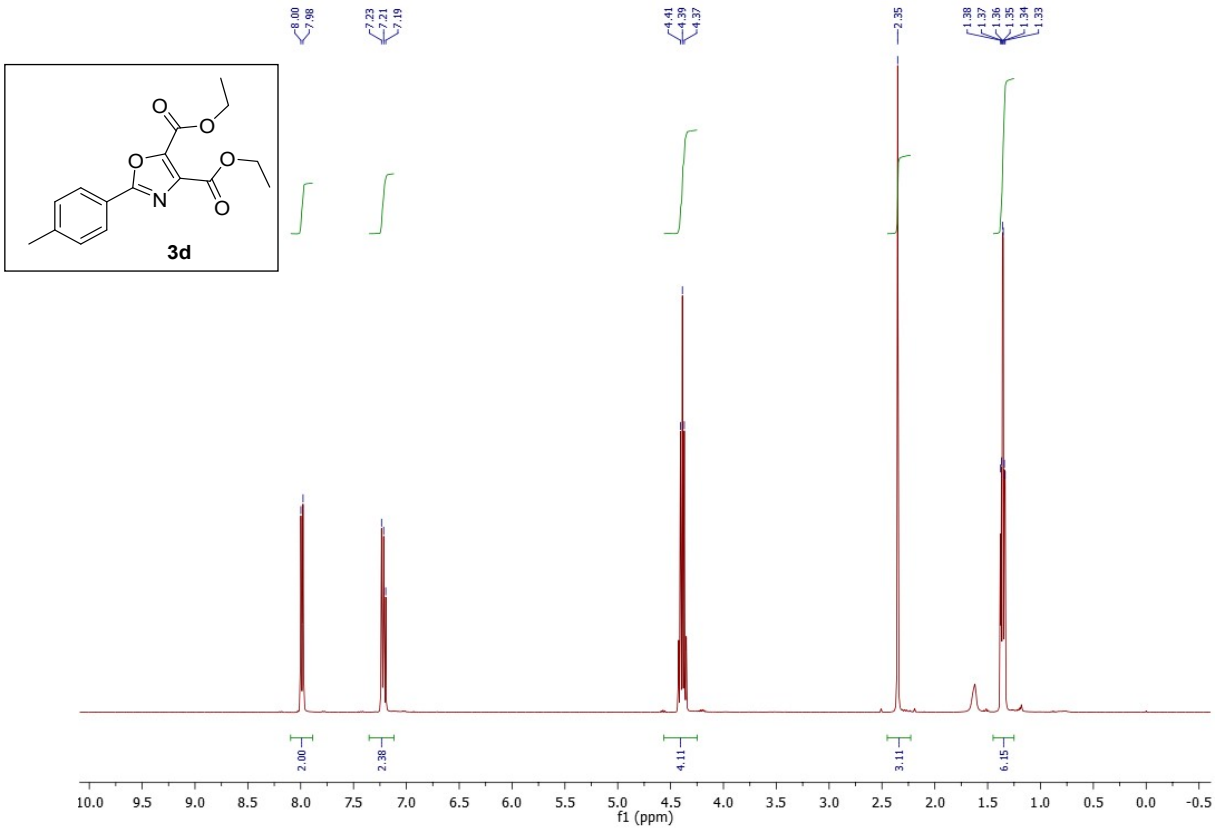
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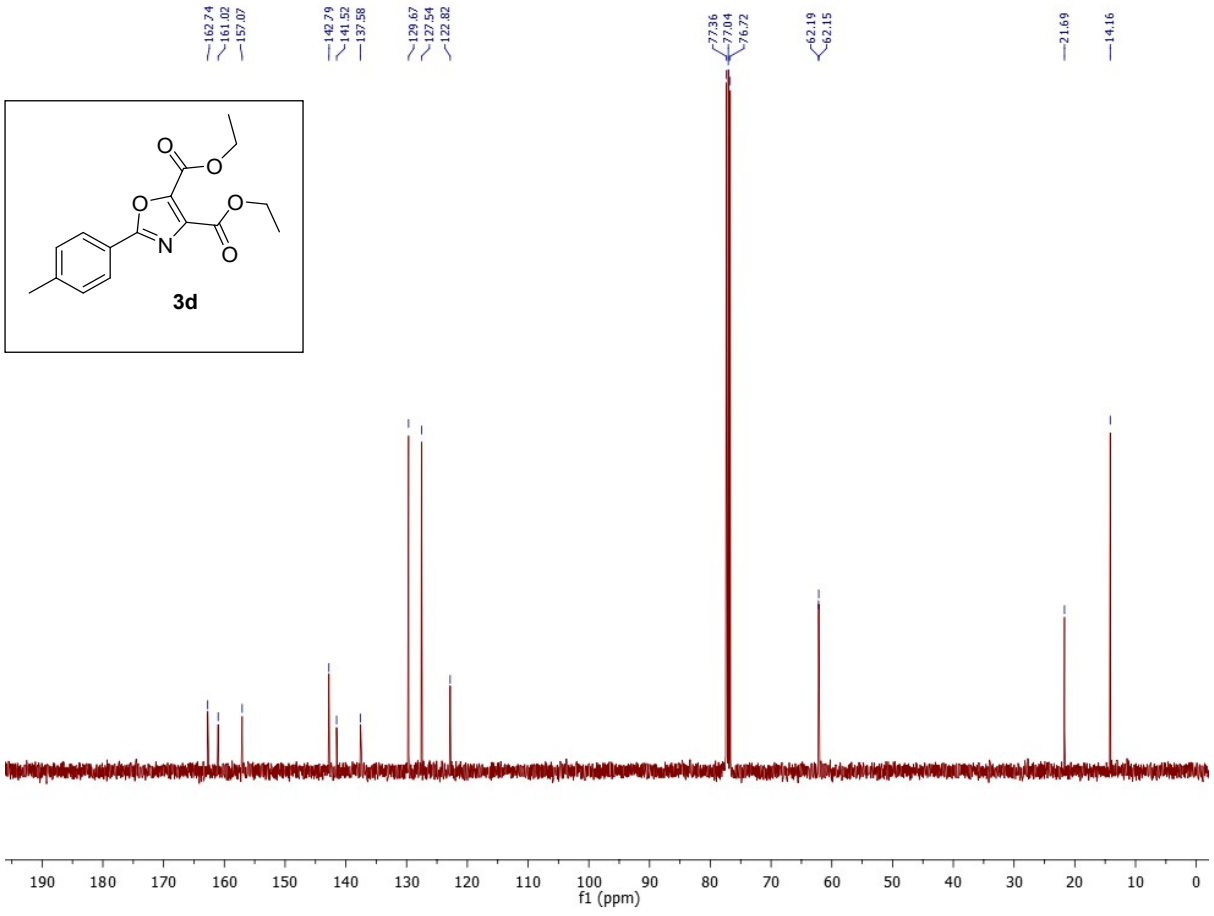
f1 (ppm)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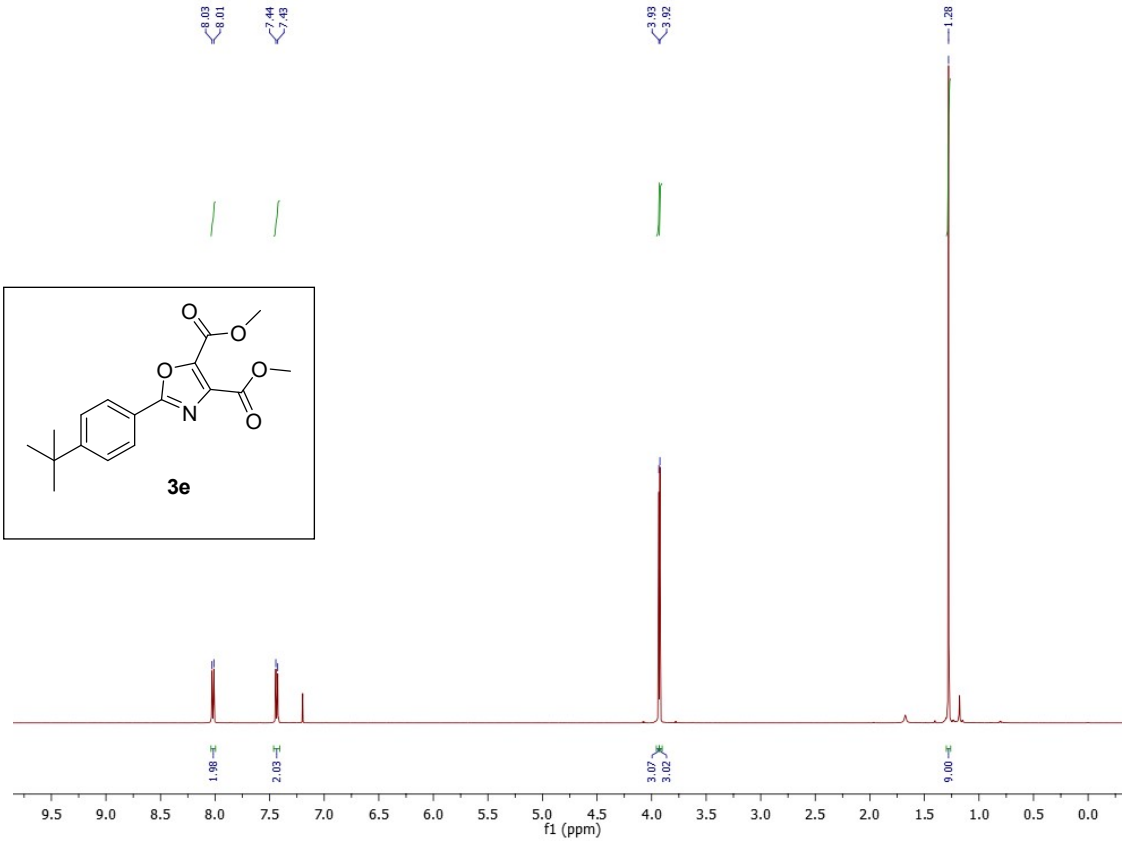
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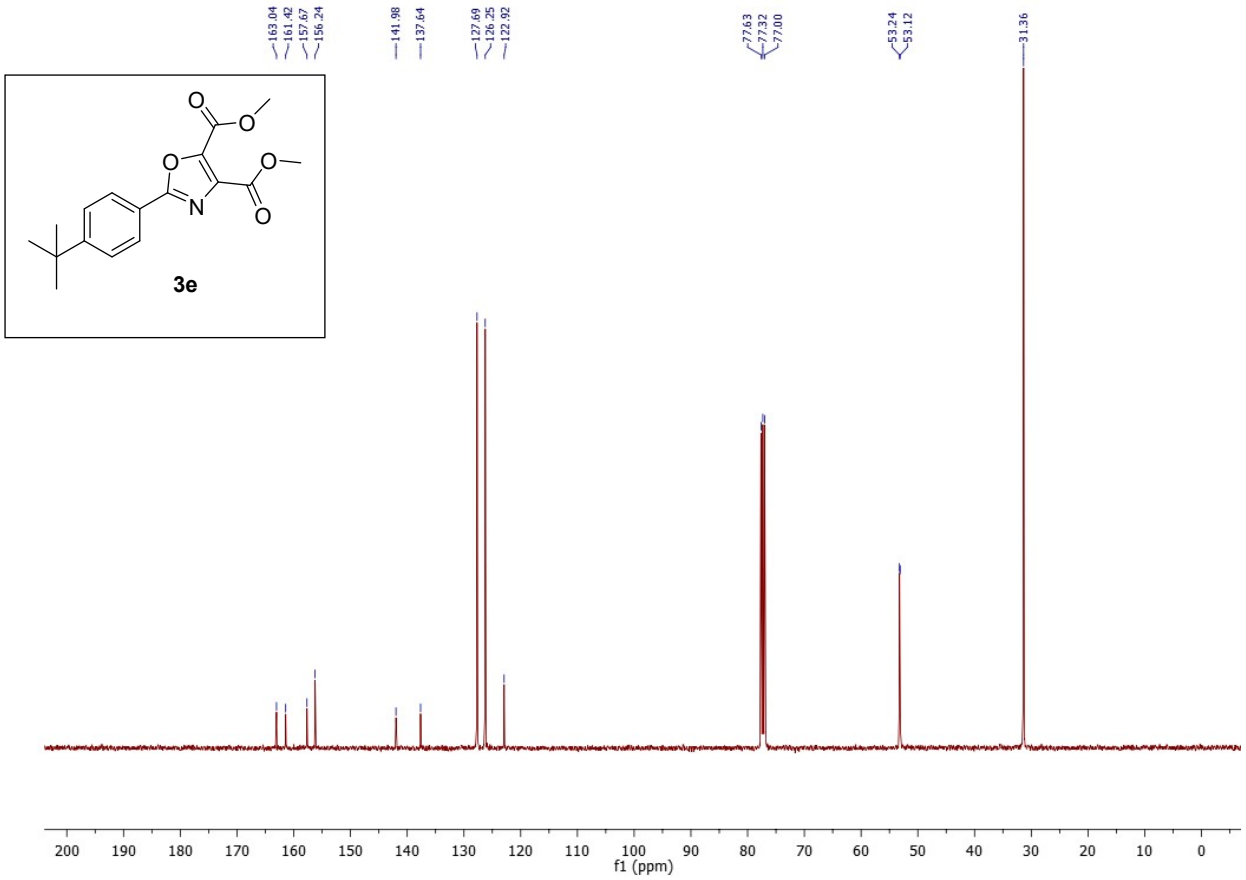
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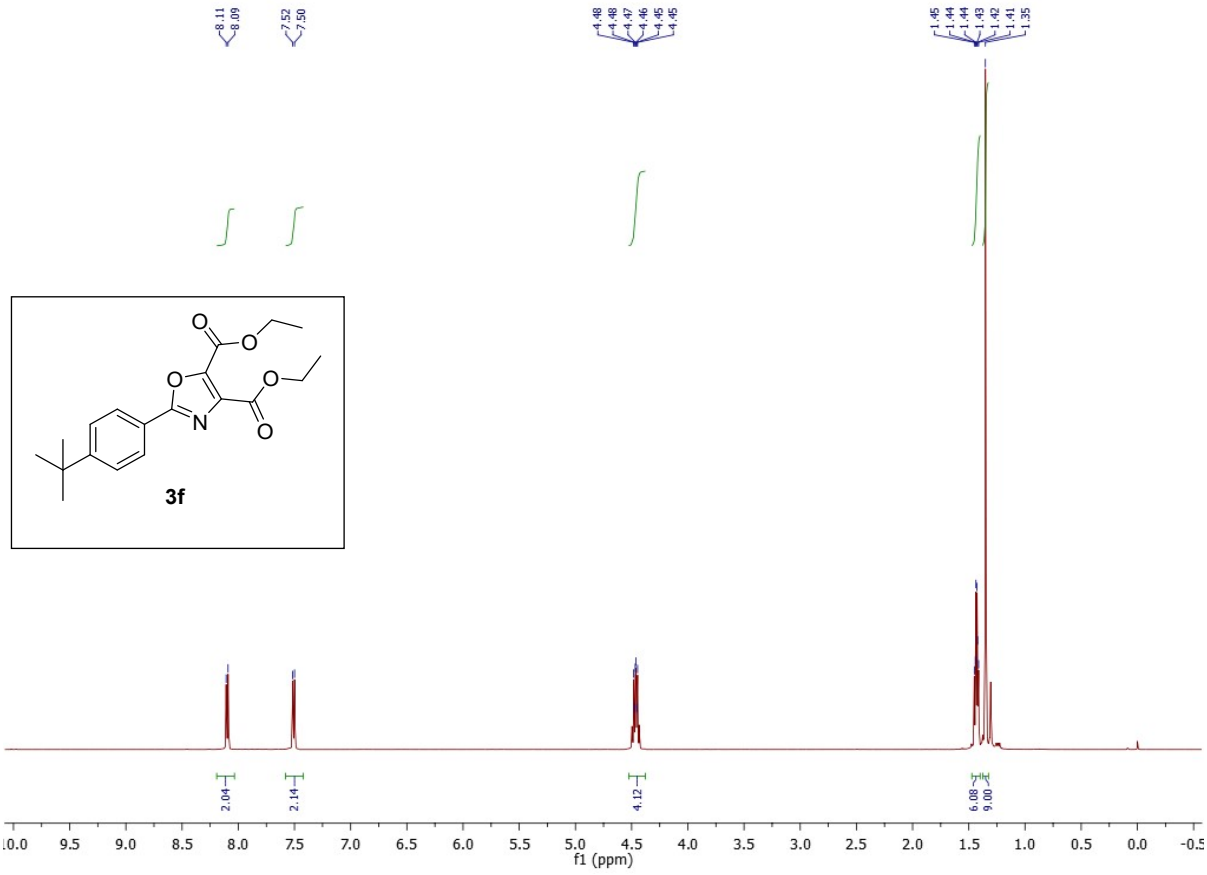
f1 (ppm)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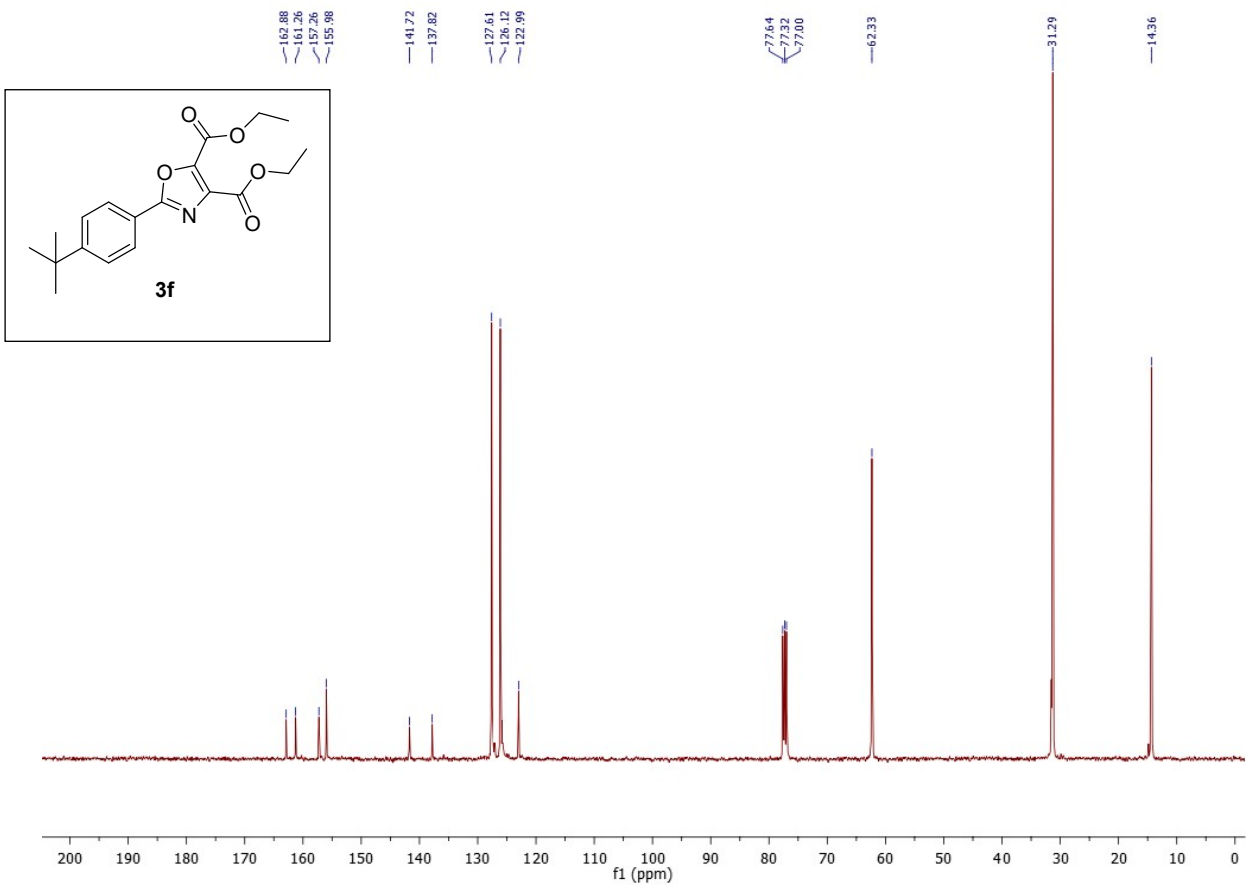
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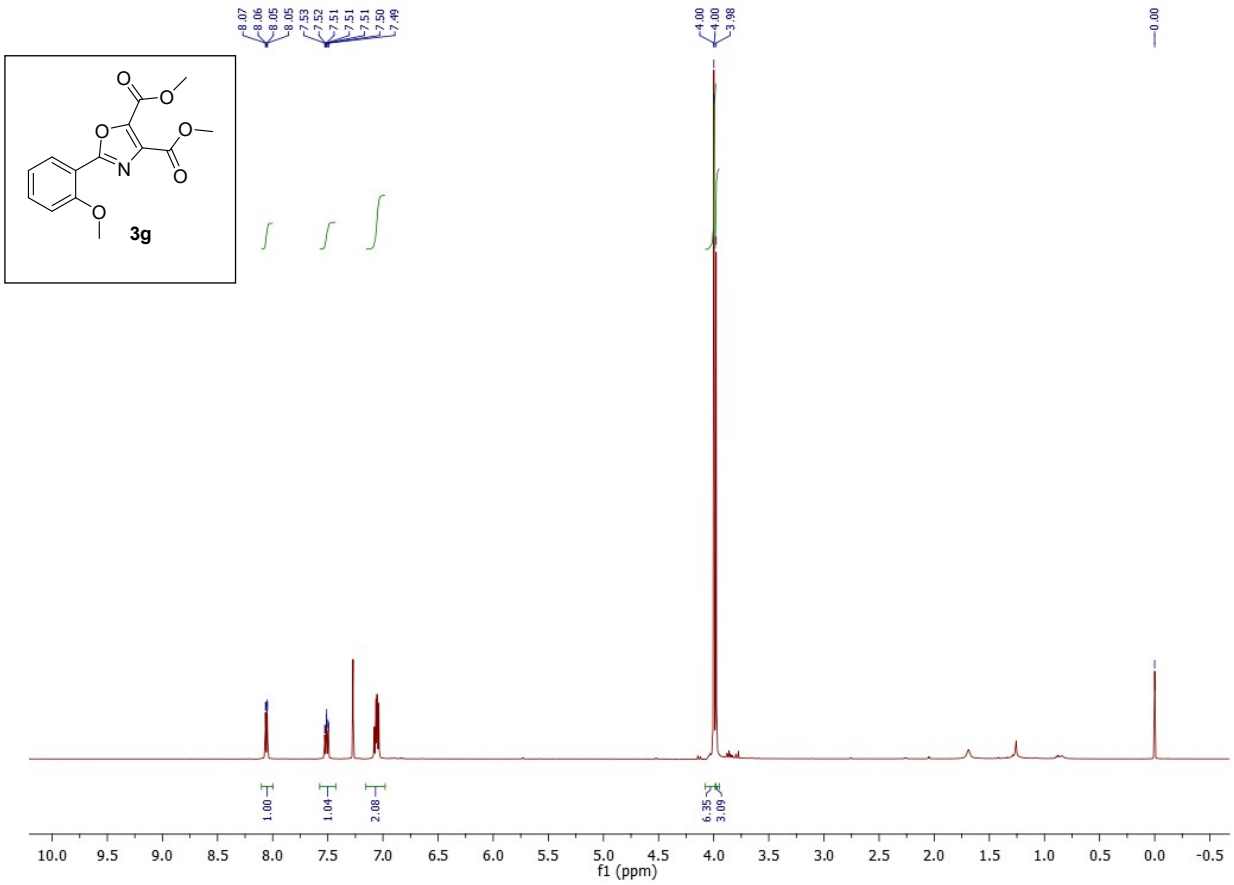
f1 (ppm)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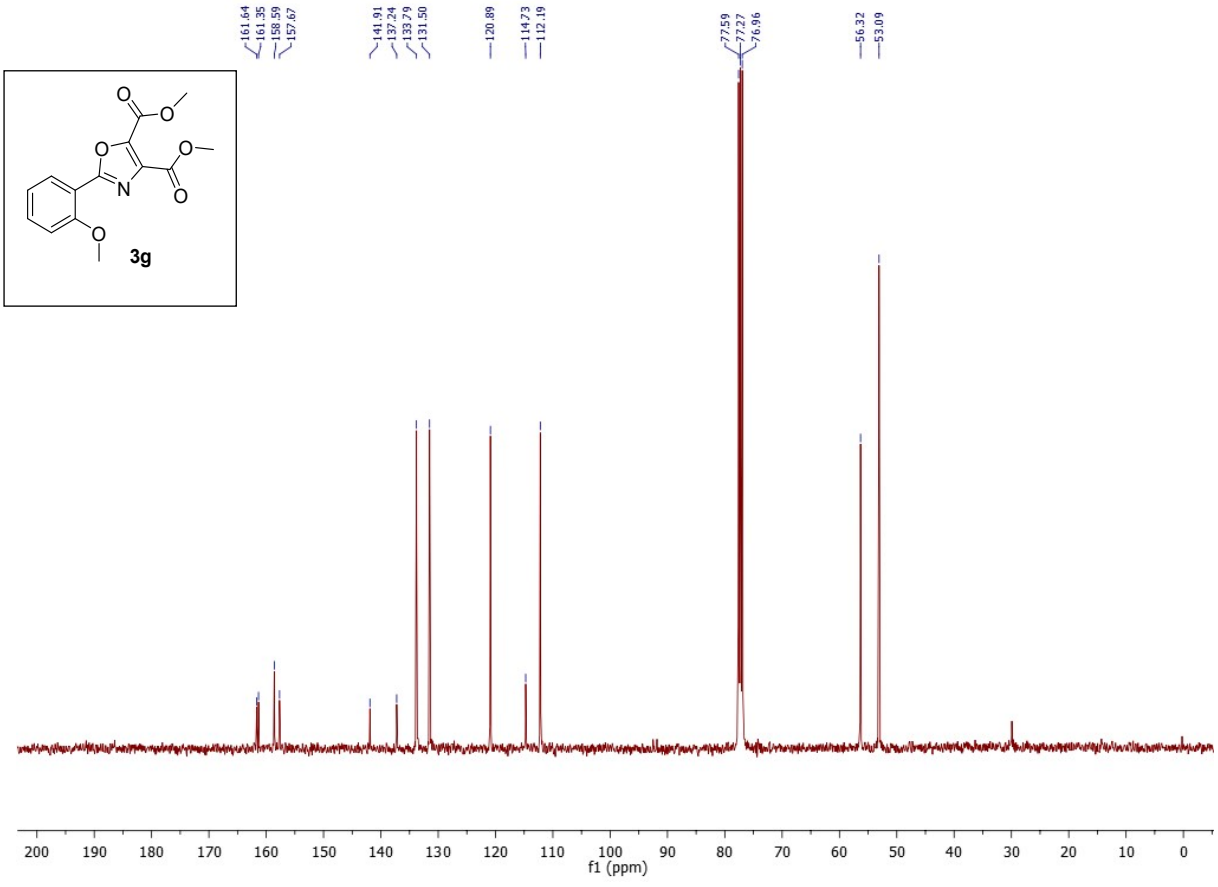
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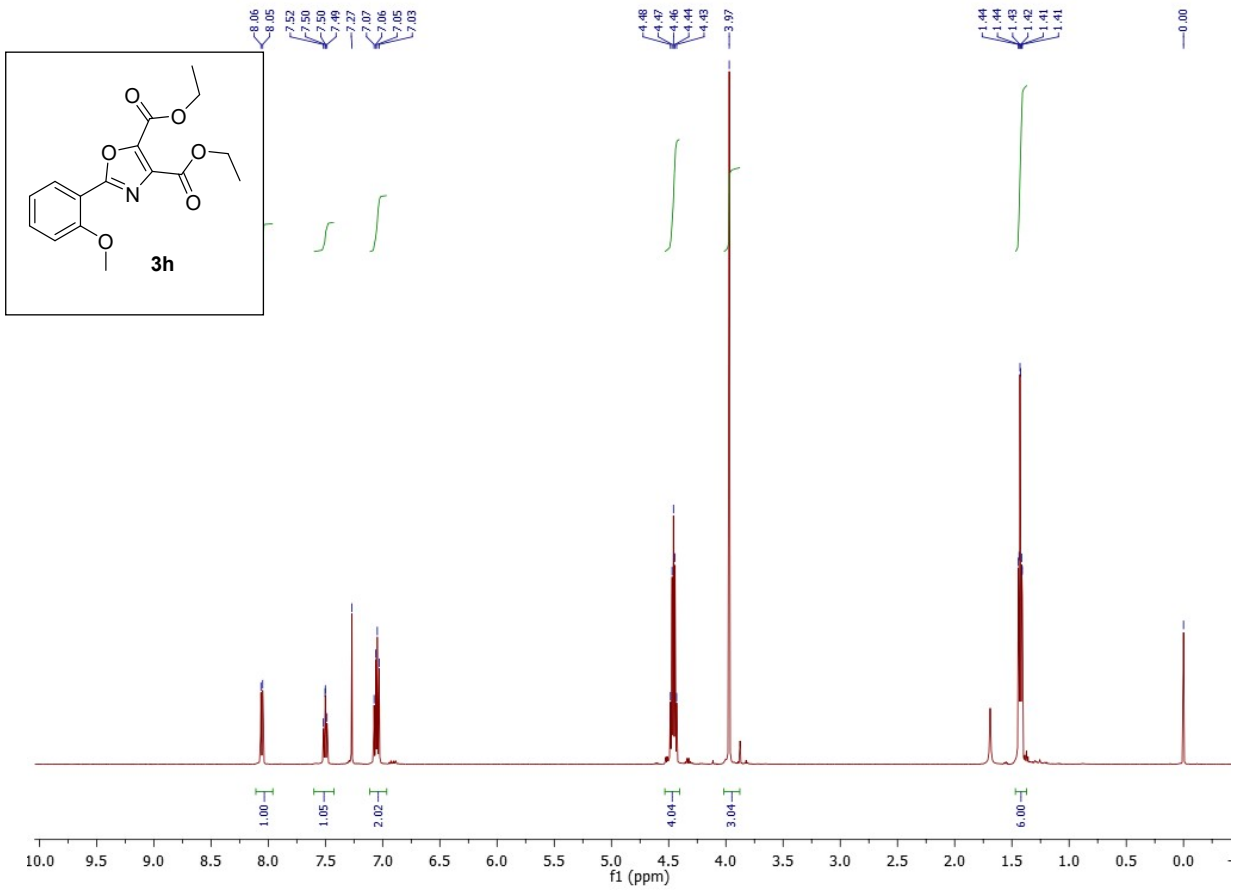
f1 (ppm)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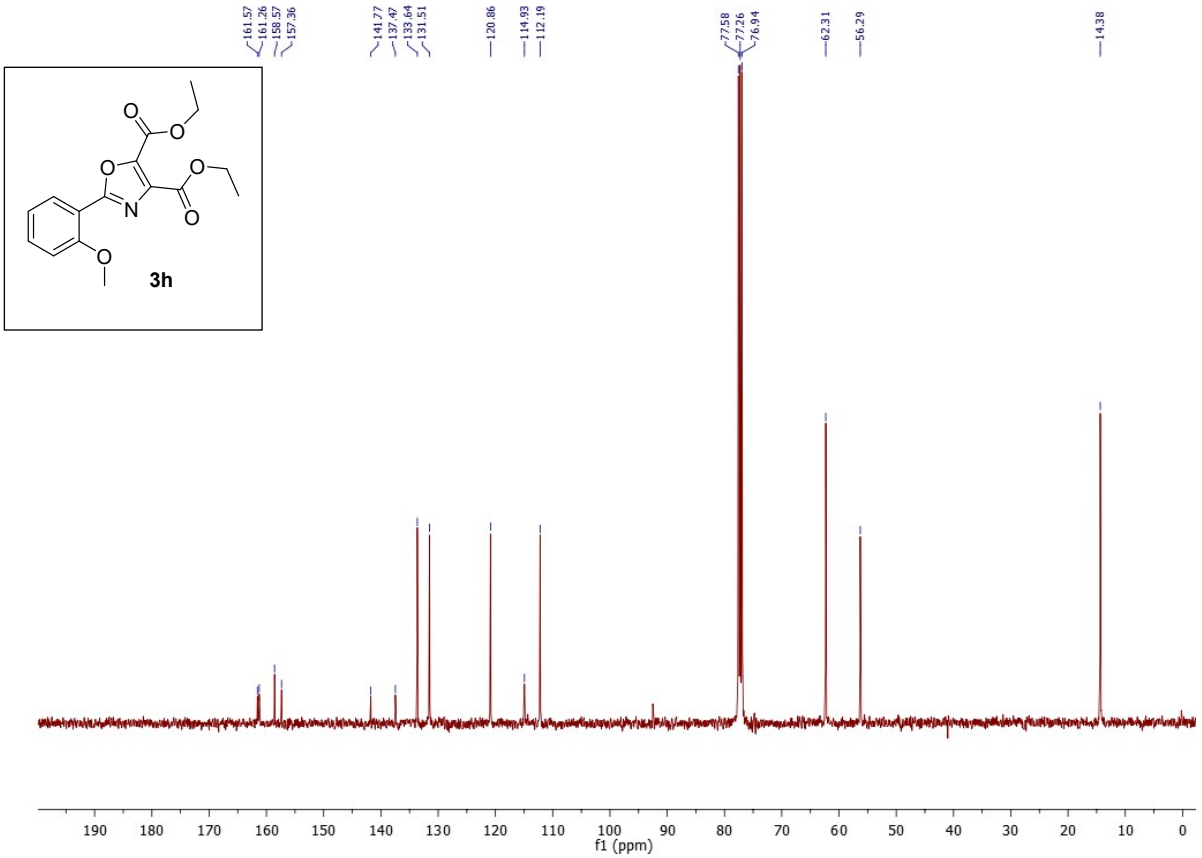
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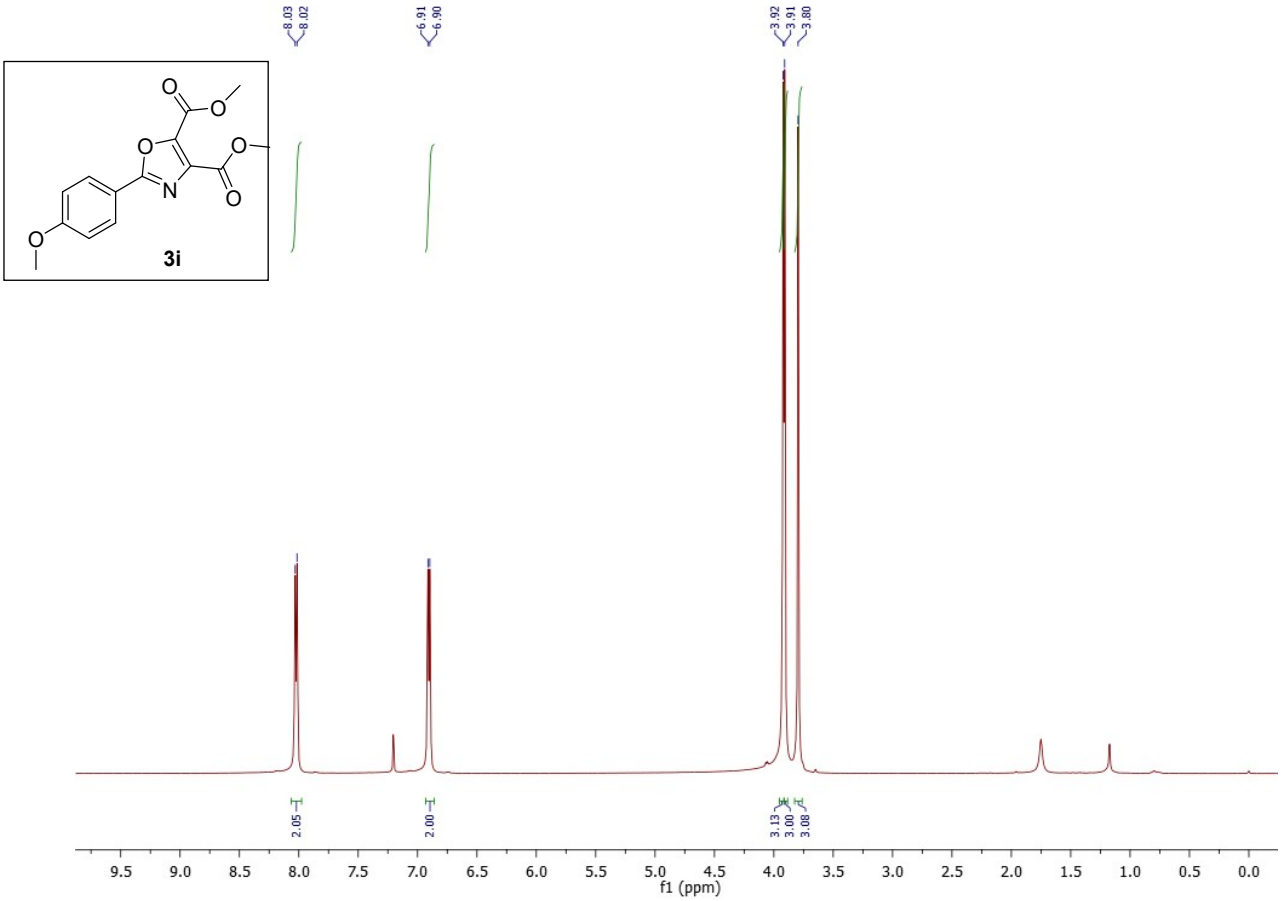
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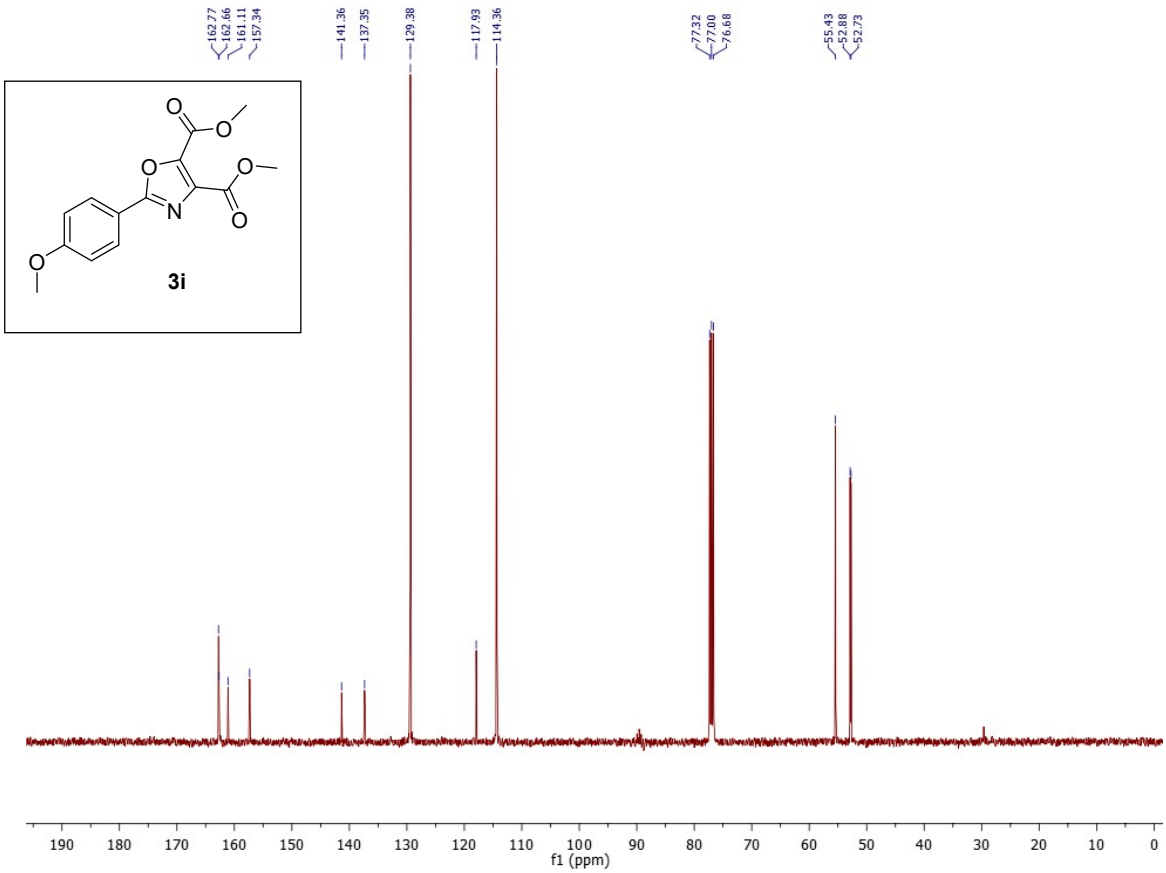
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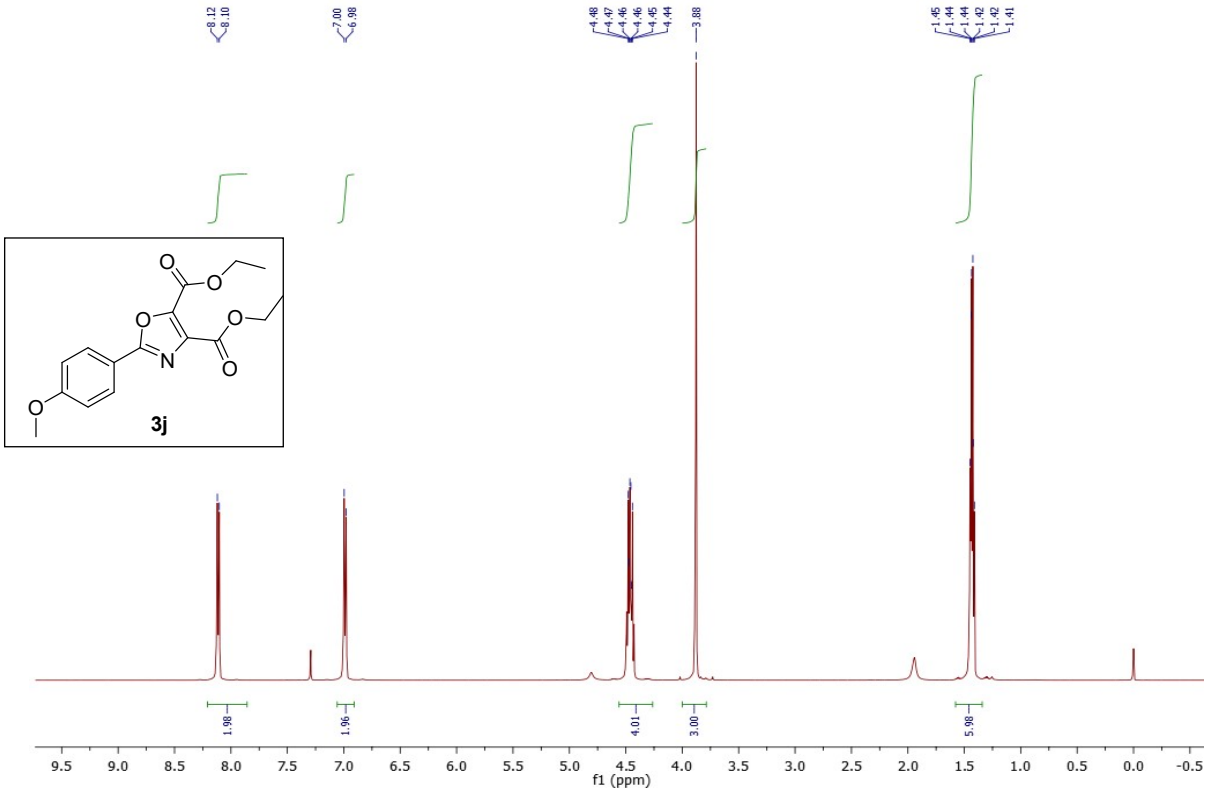
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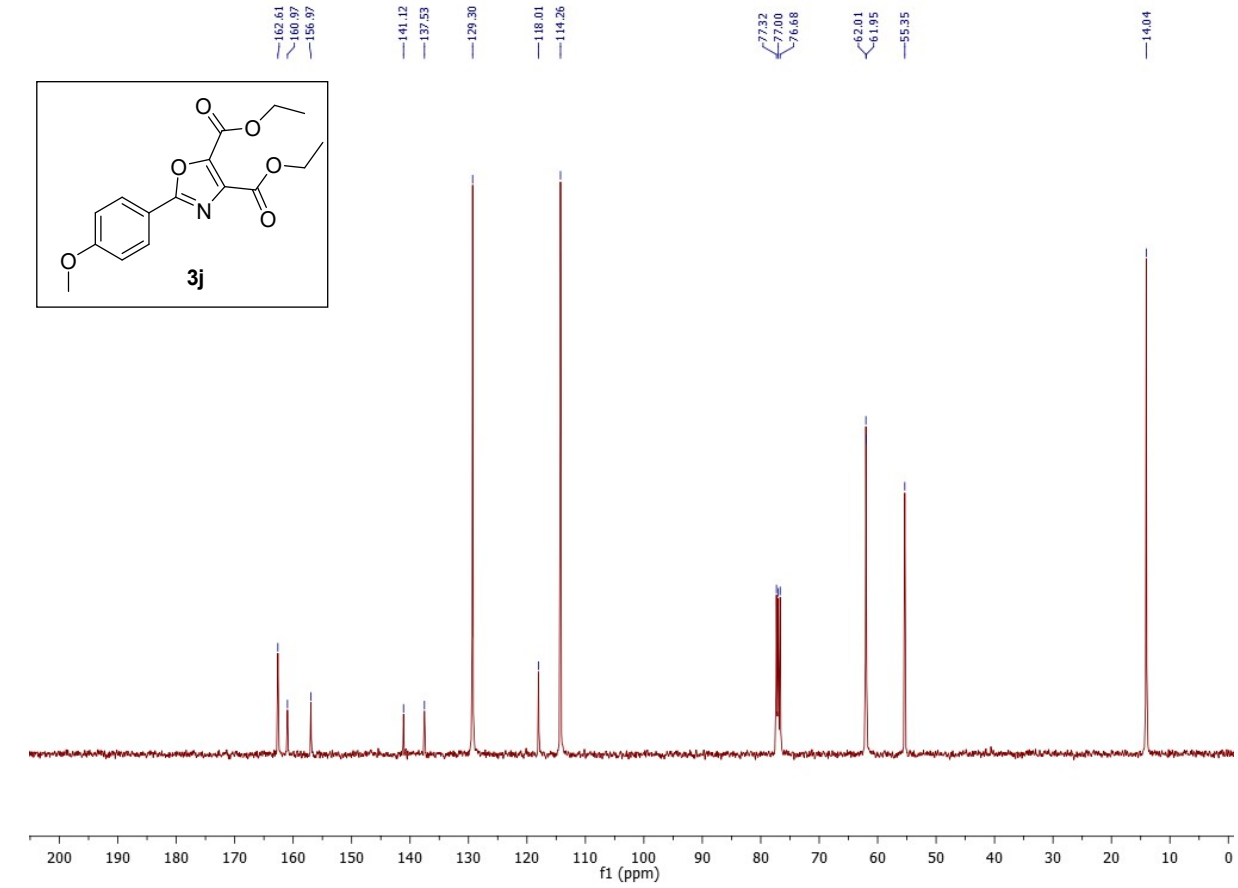
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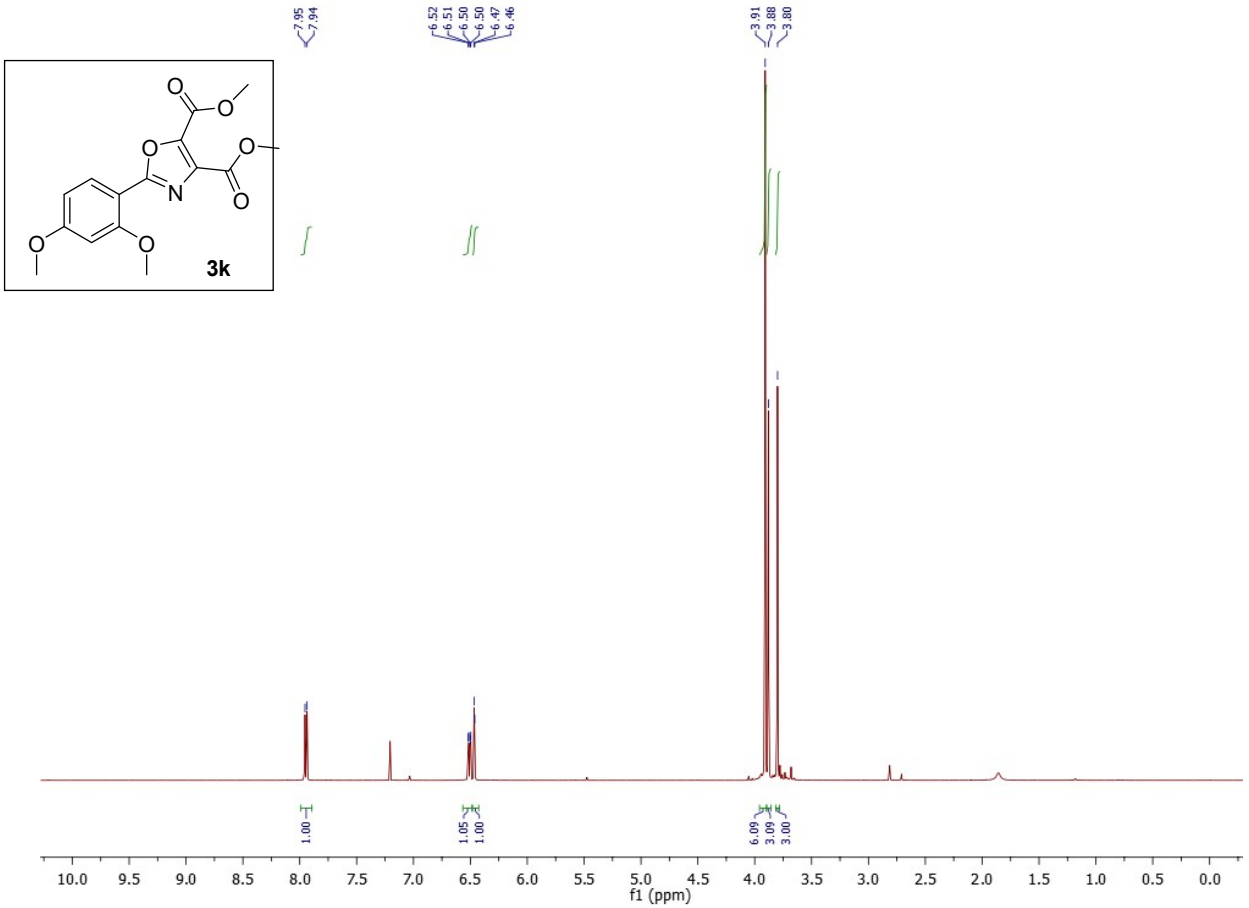
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1.00
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3.09
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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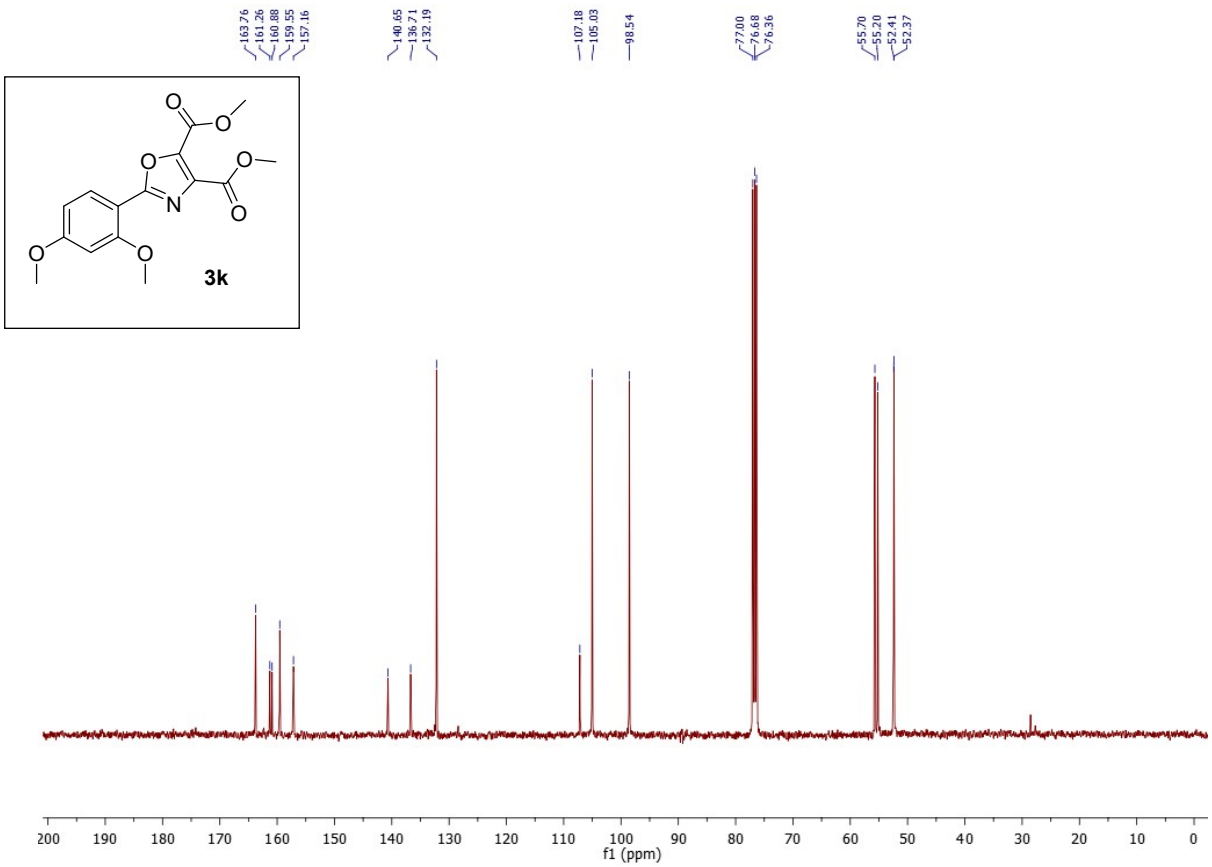
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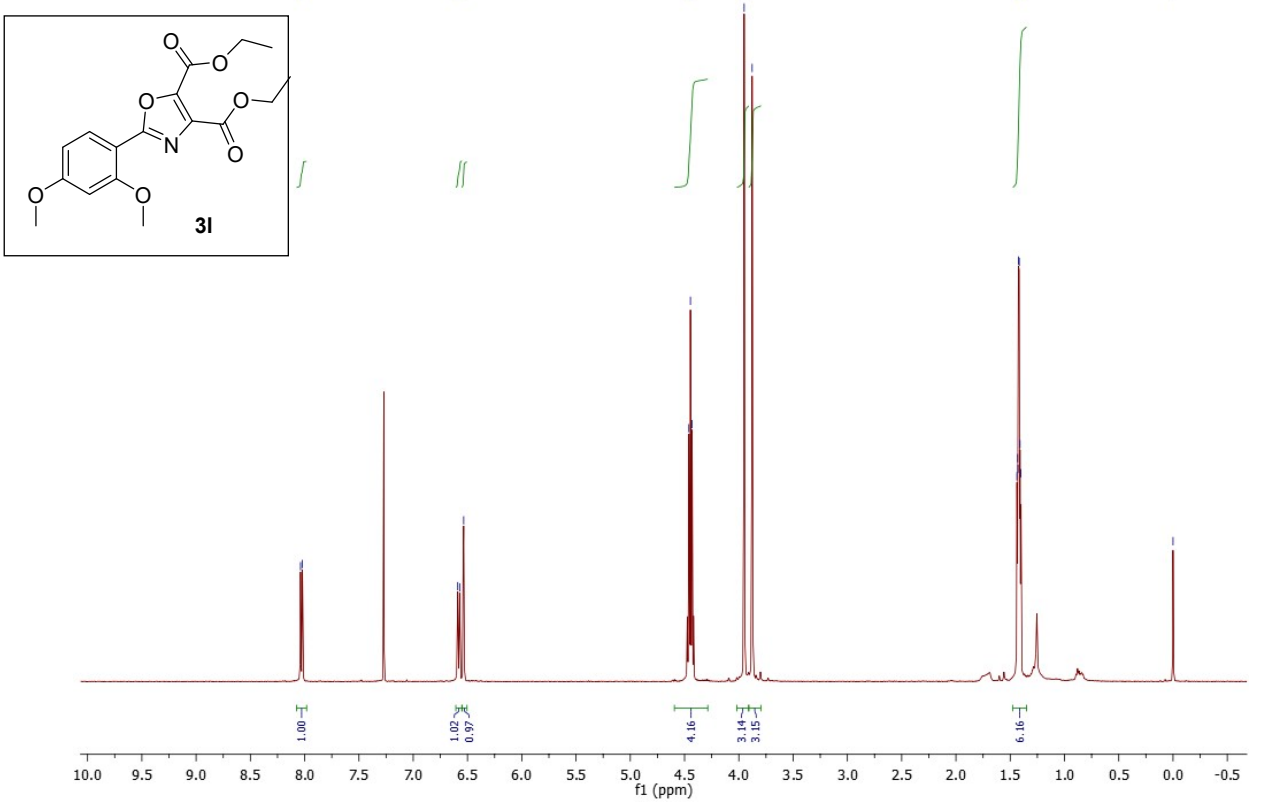
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1.43
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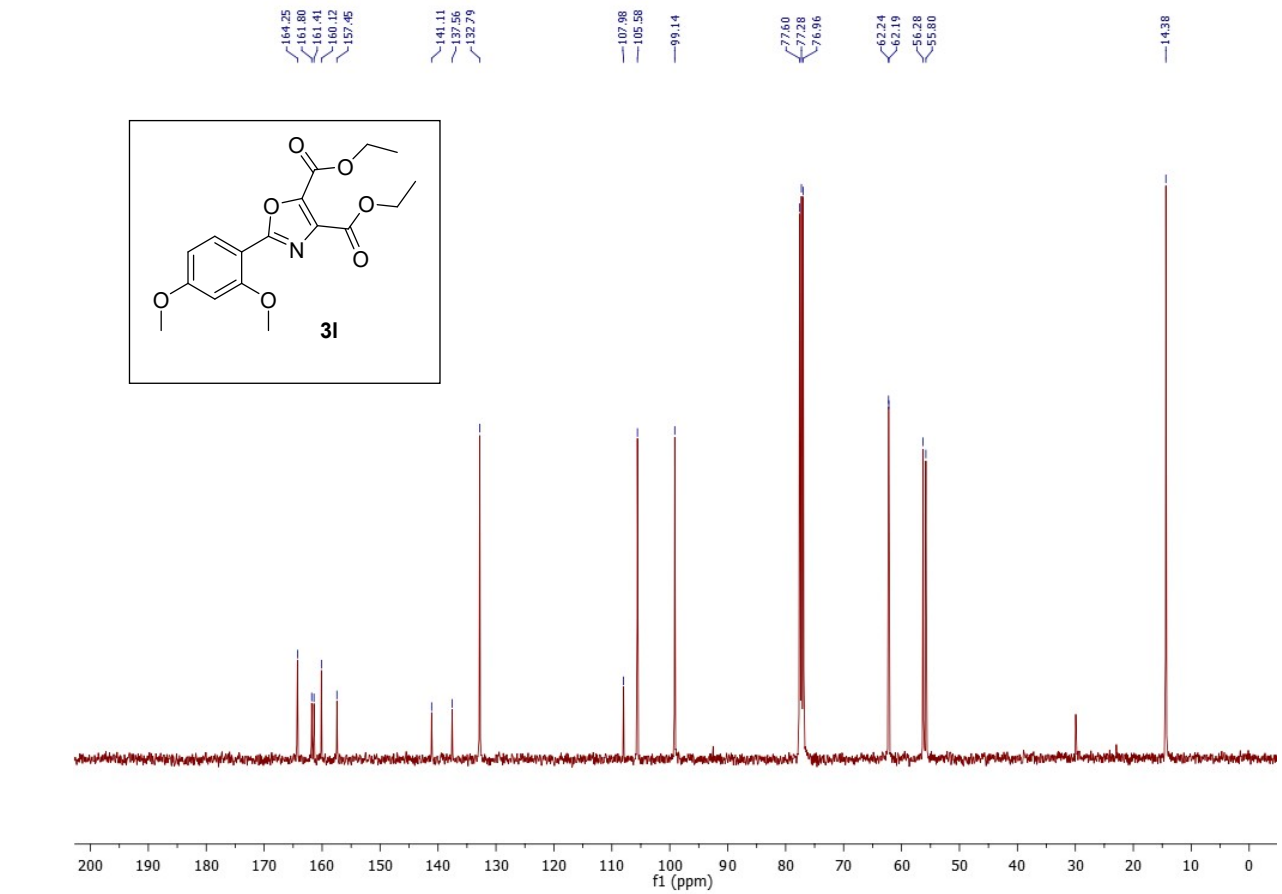
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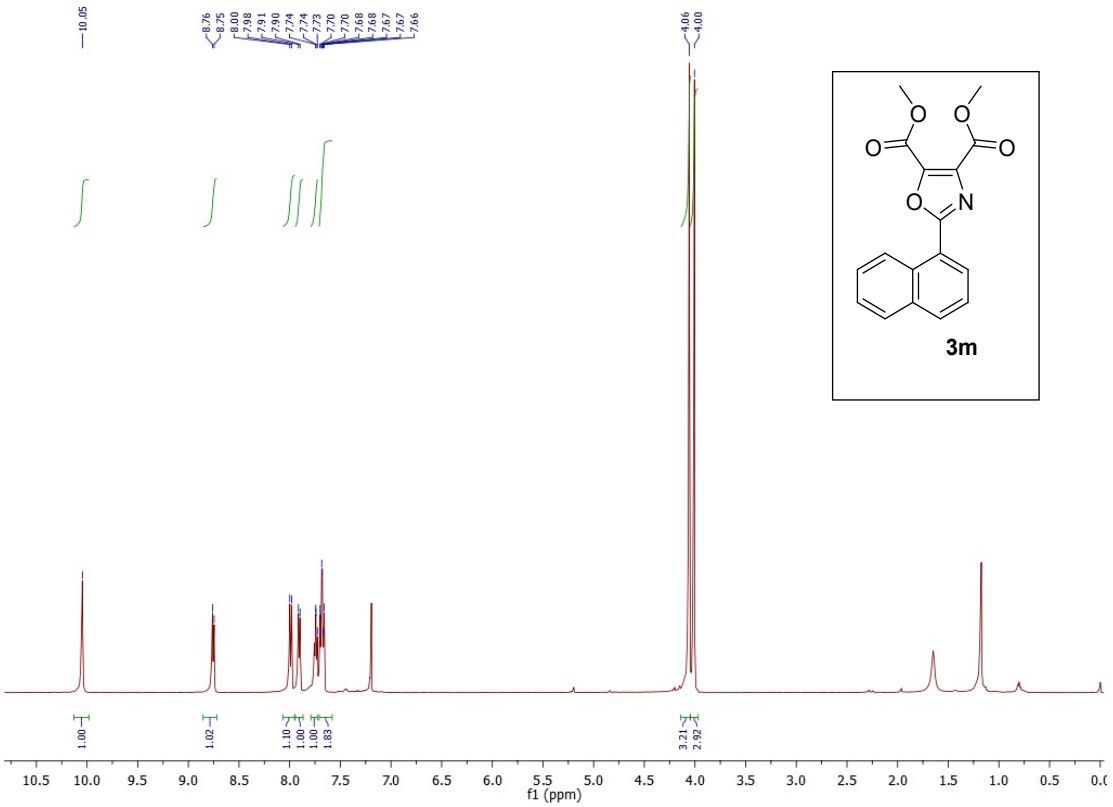
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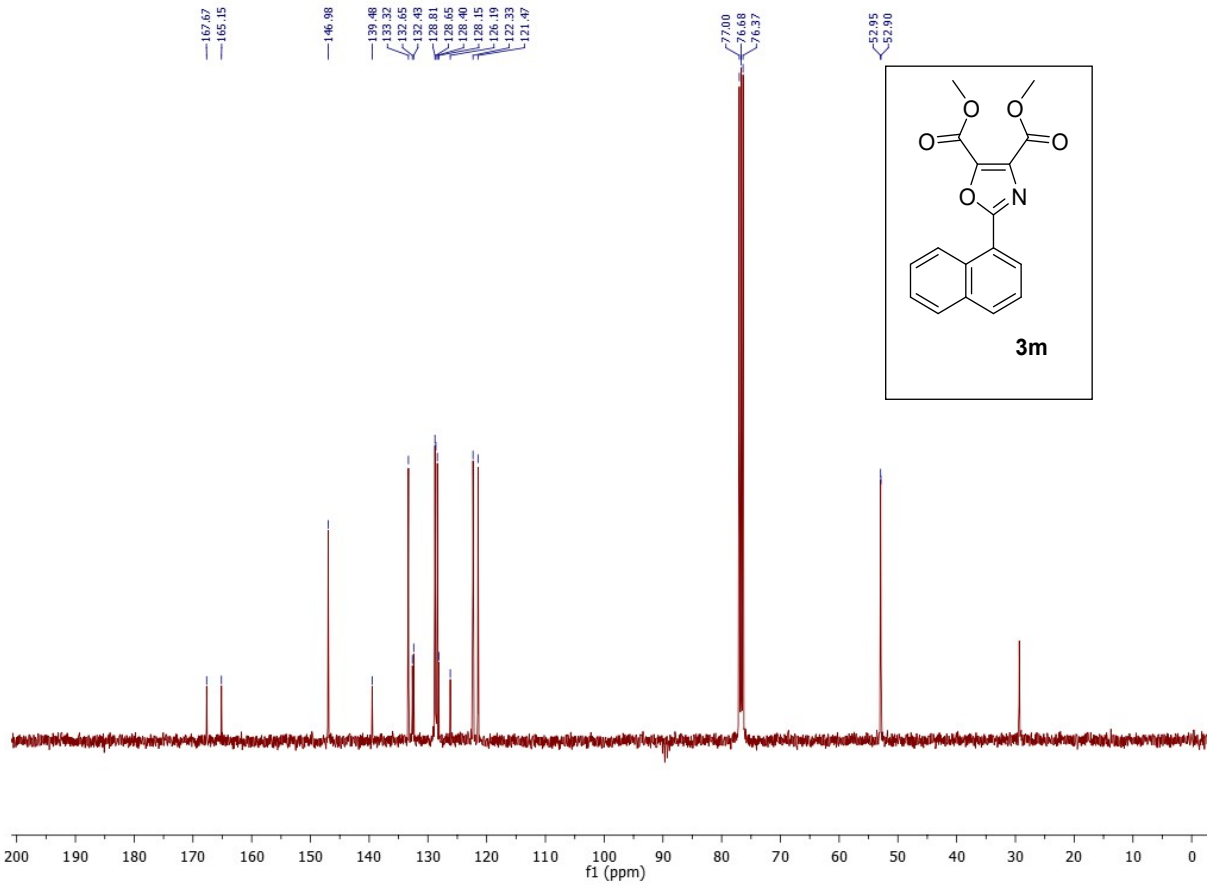
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f1 (ppm)
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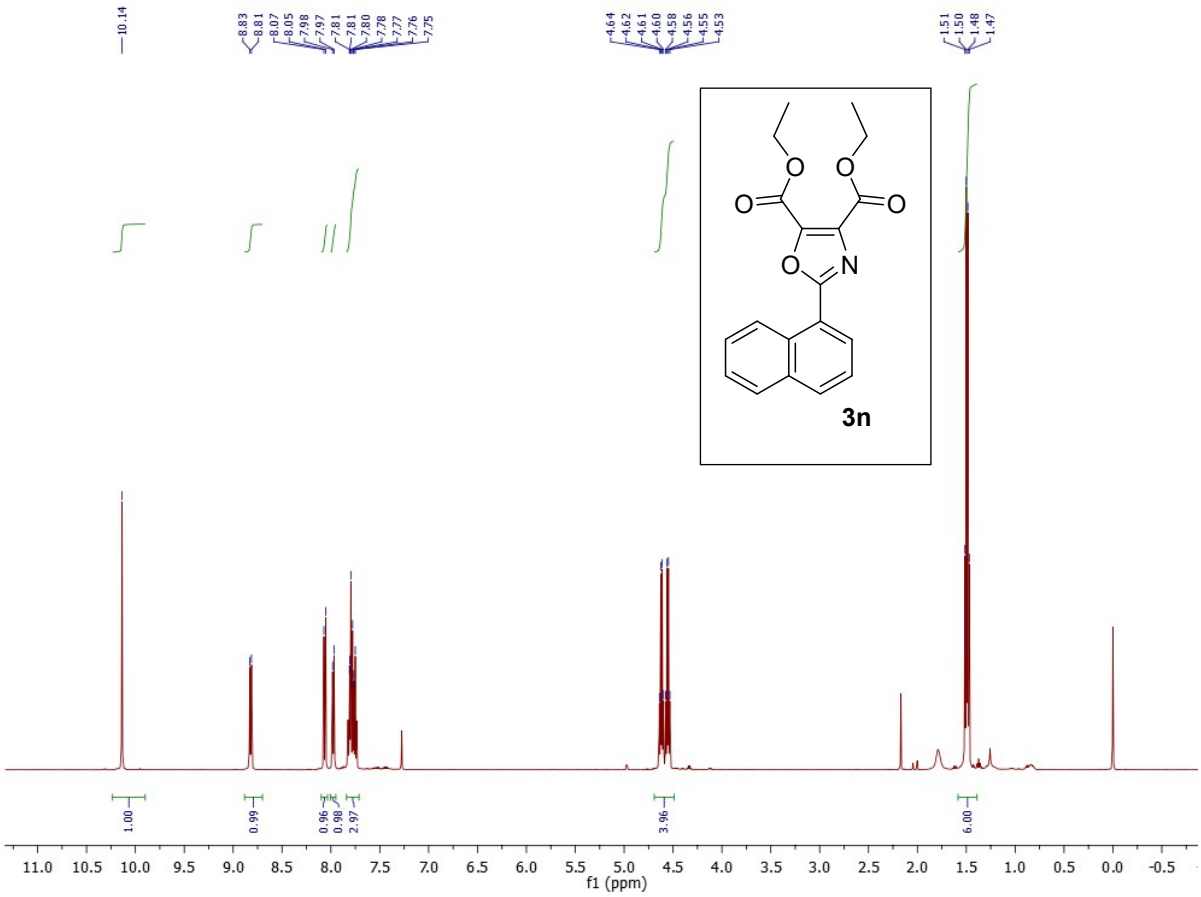
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4.62
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4.60
4.58
4.56
4.55
4.53
1.51
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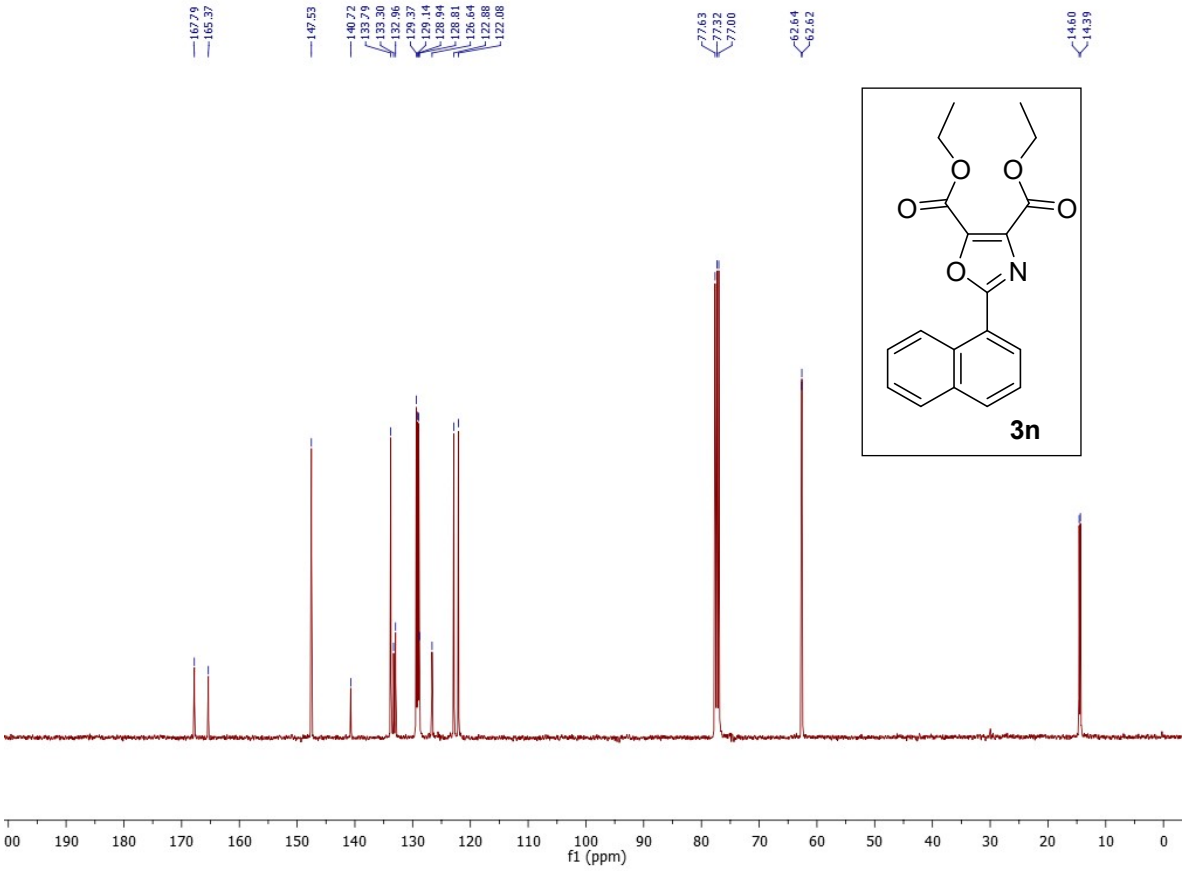
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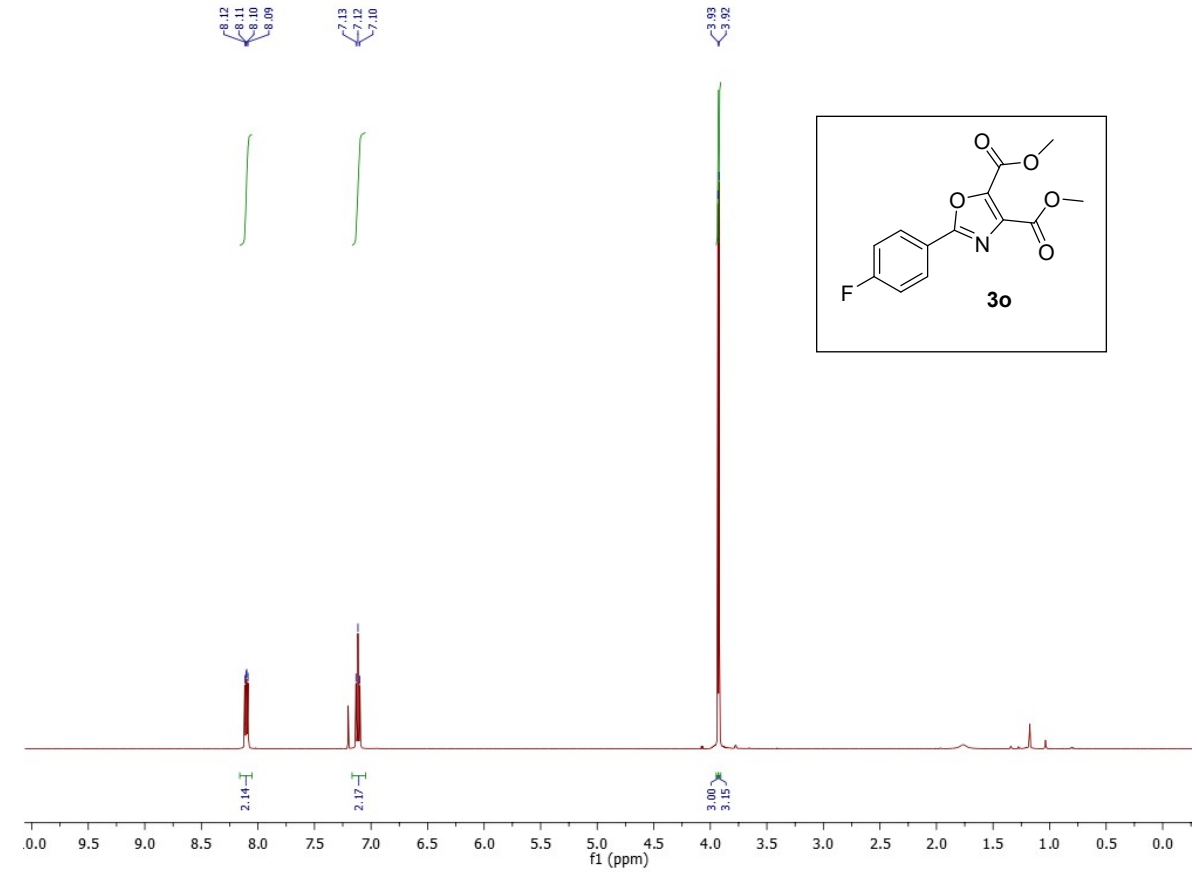
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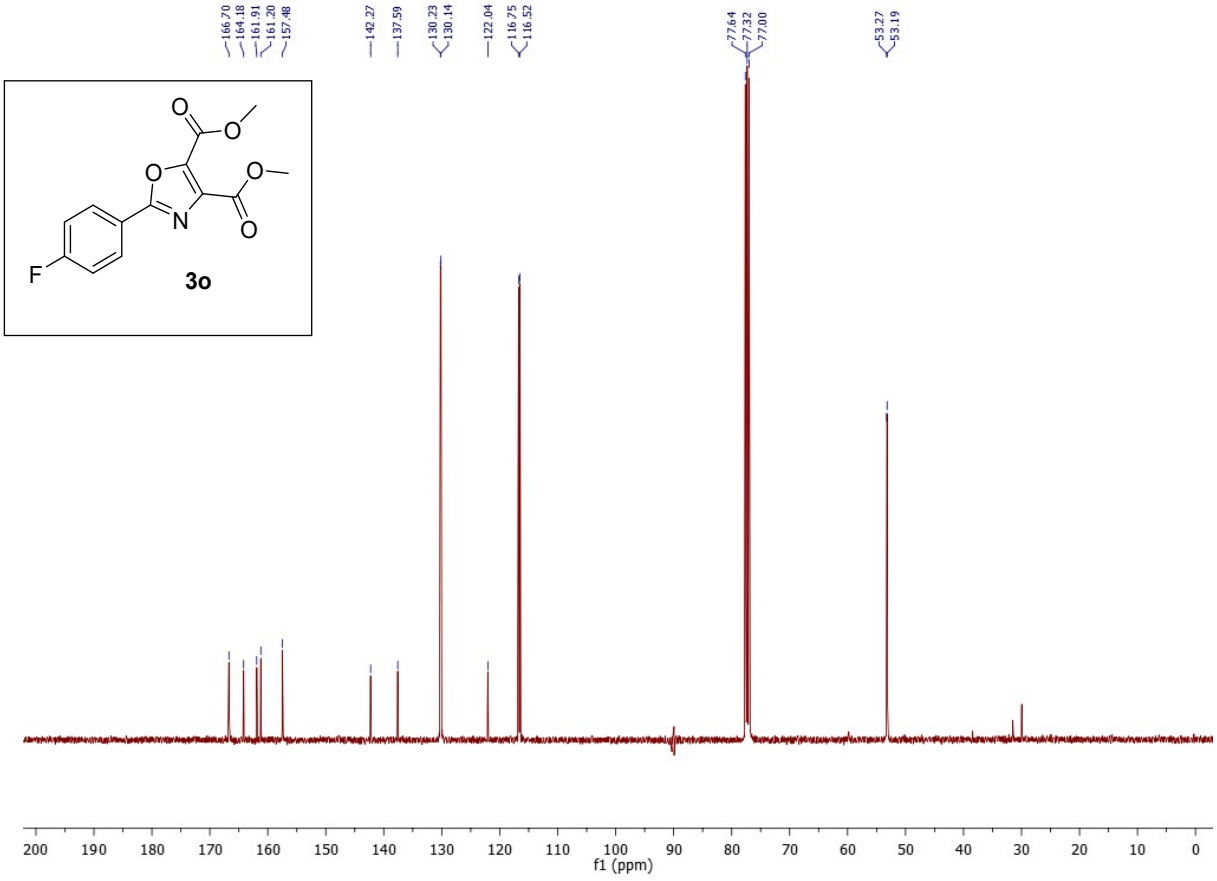
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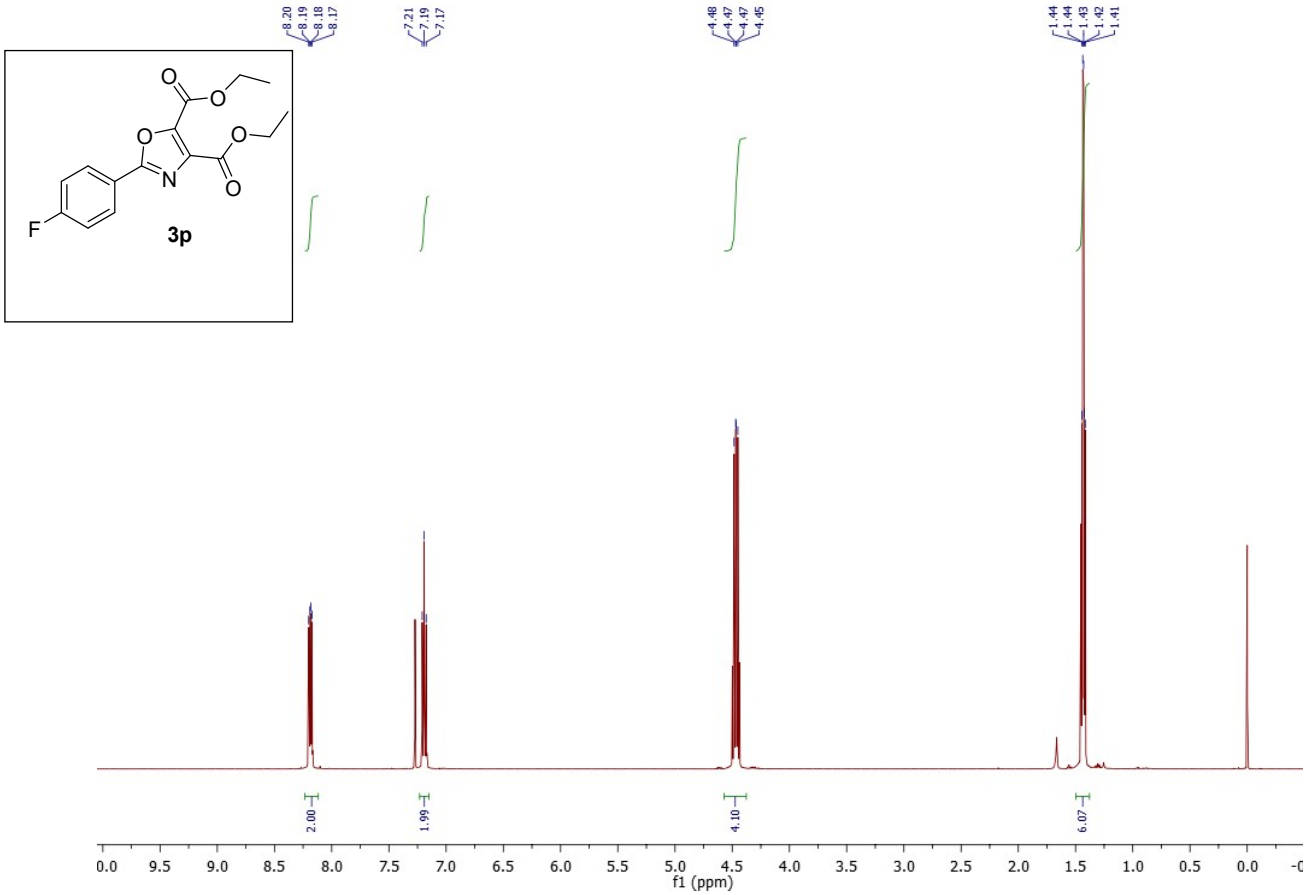
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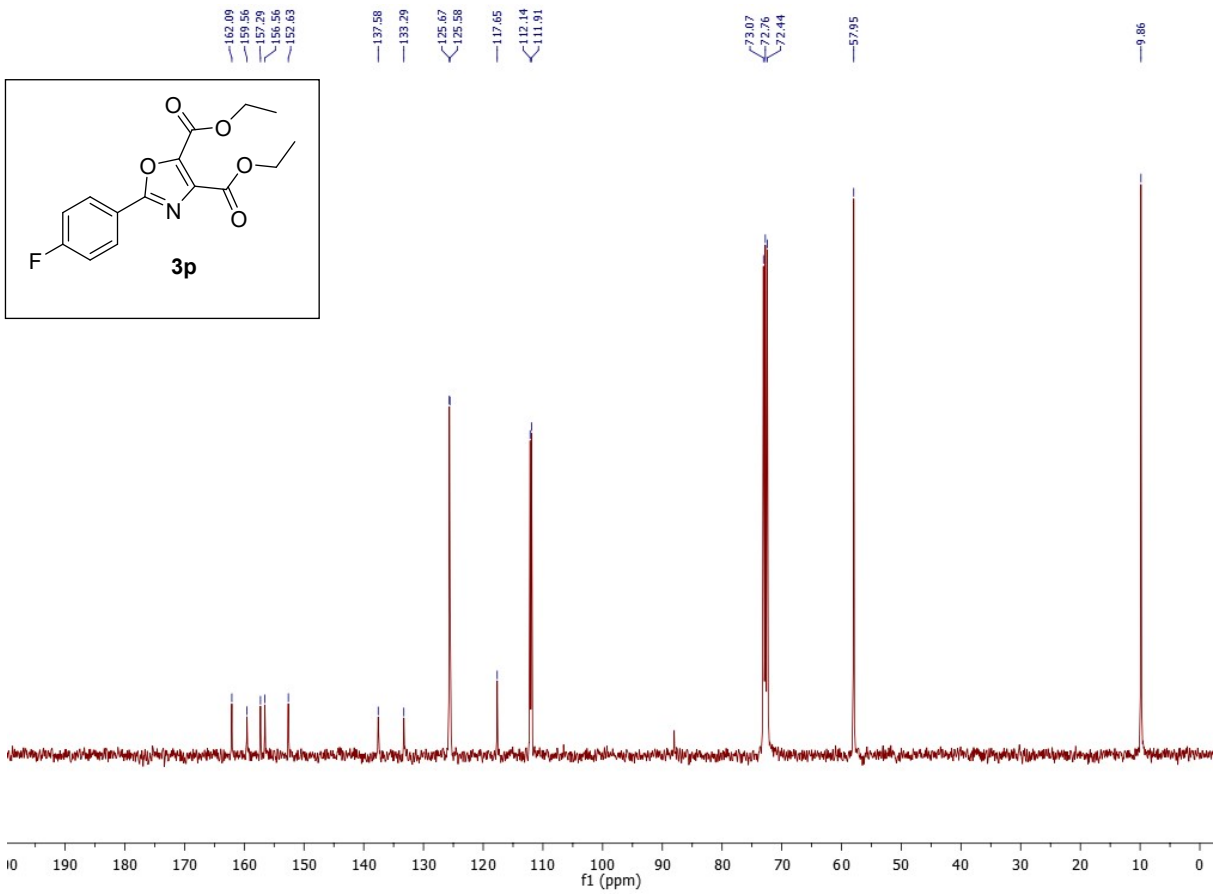
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157.29
156.56
152.63
137.58
133.29
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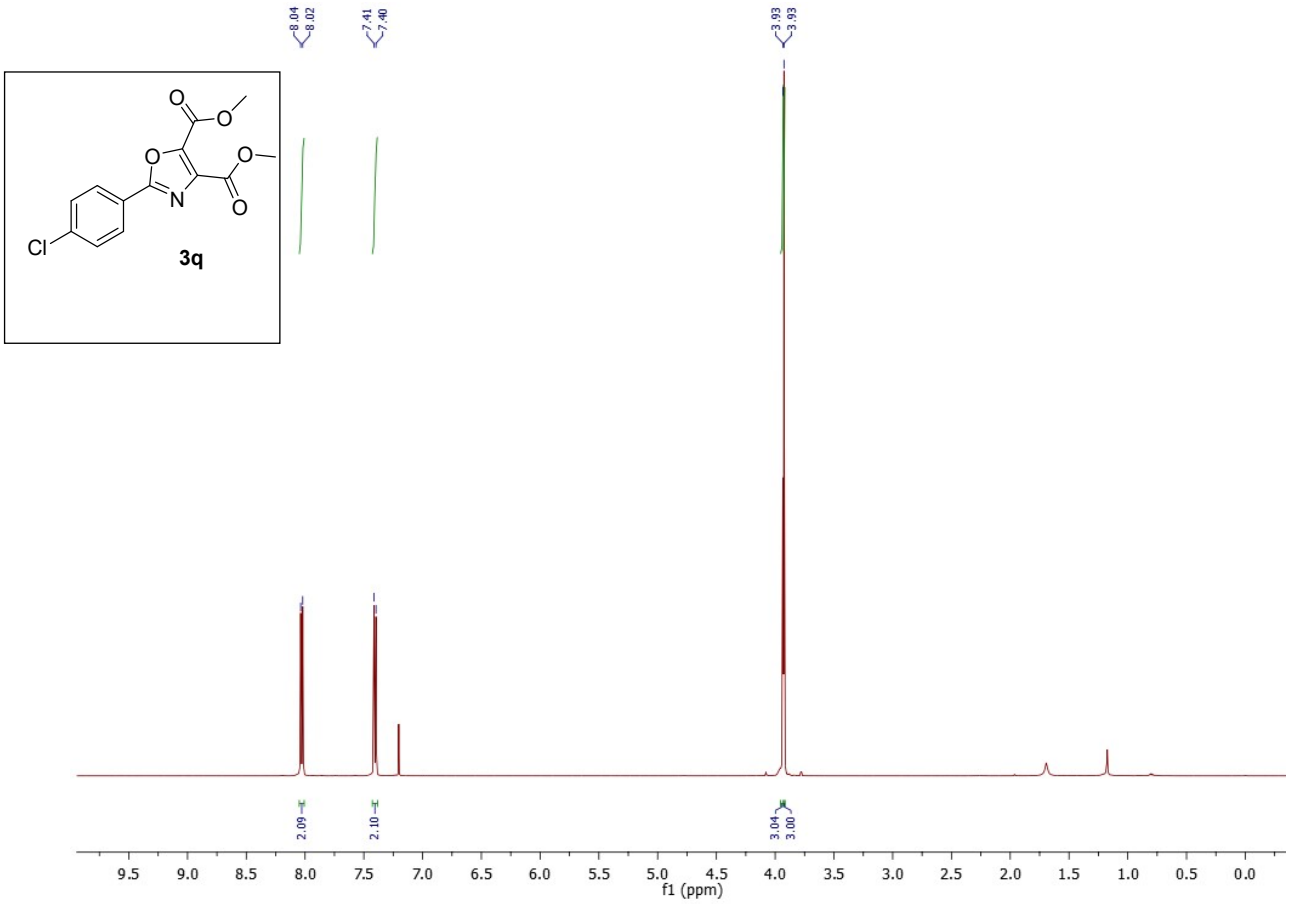
125.58
117.65
112.14
111.91
73.07
72.76
72.44
57.95
9.86
f1 (ppm)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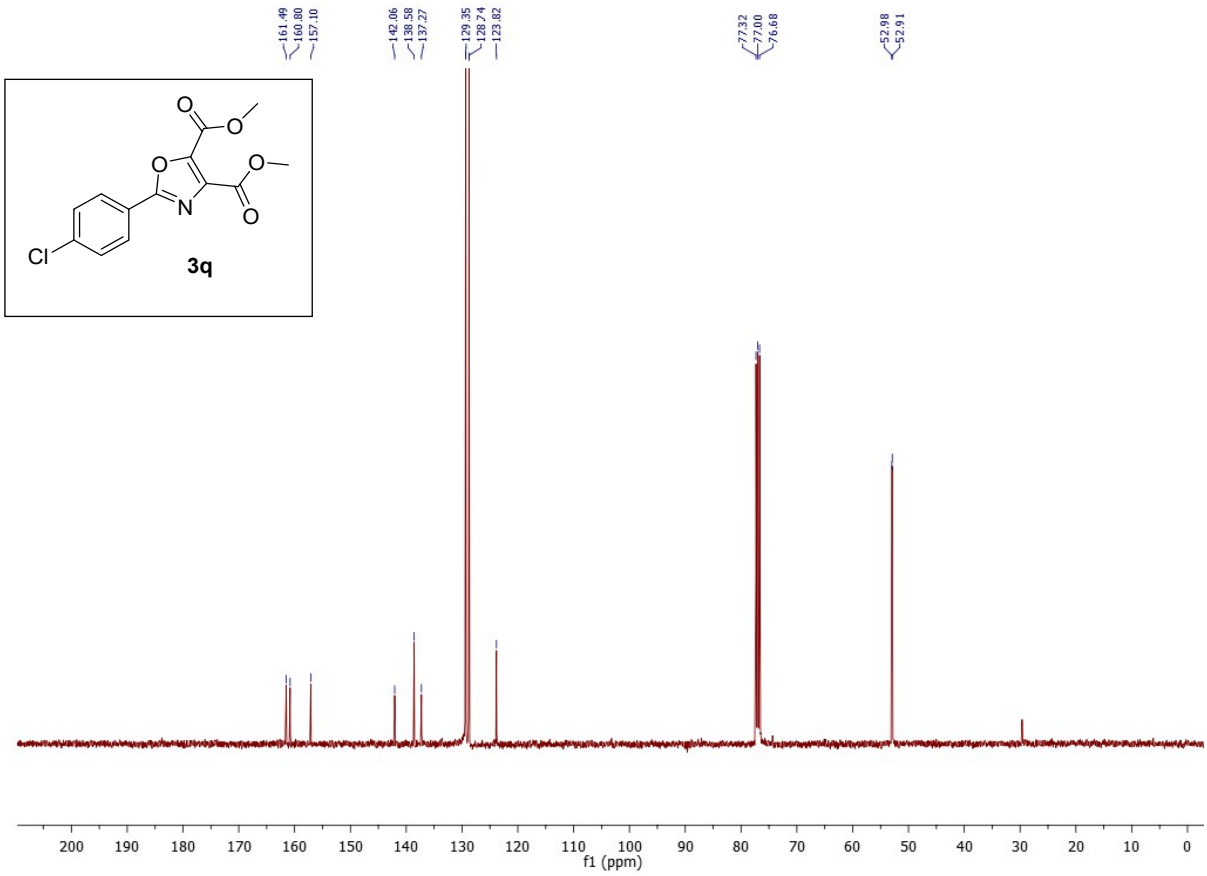
8.02
7.41
7.40
3.93
3.93
3q
2.09
2.10
3.04
3.00
f1 (ppm)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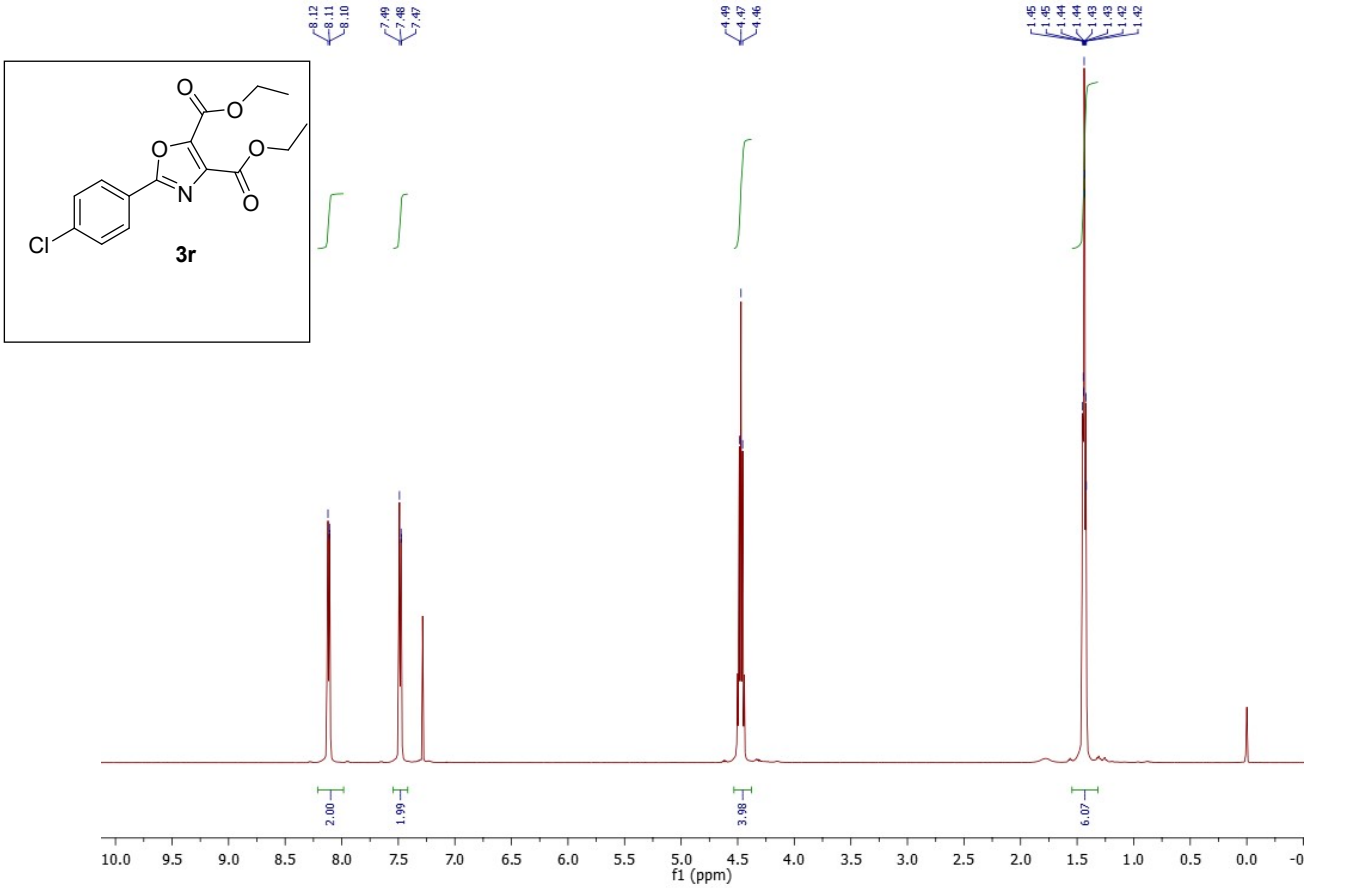
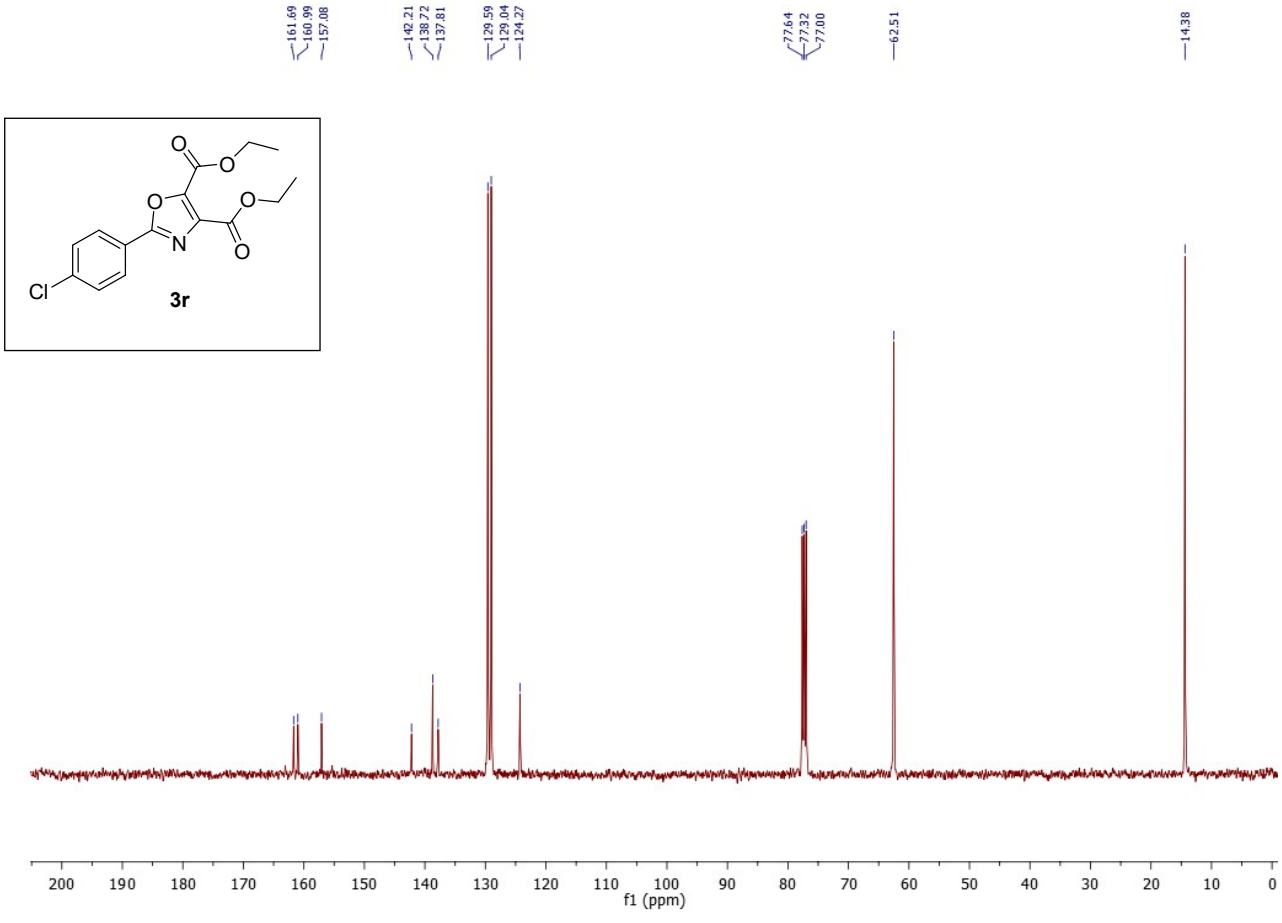
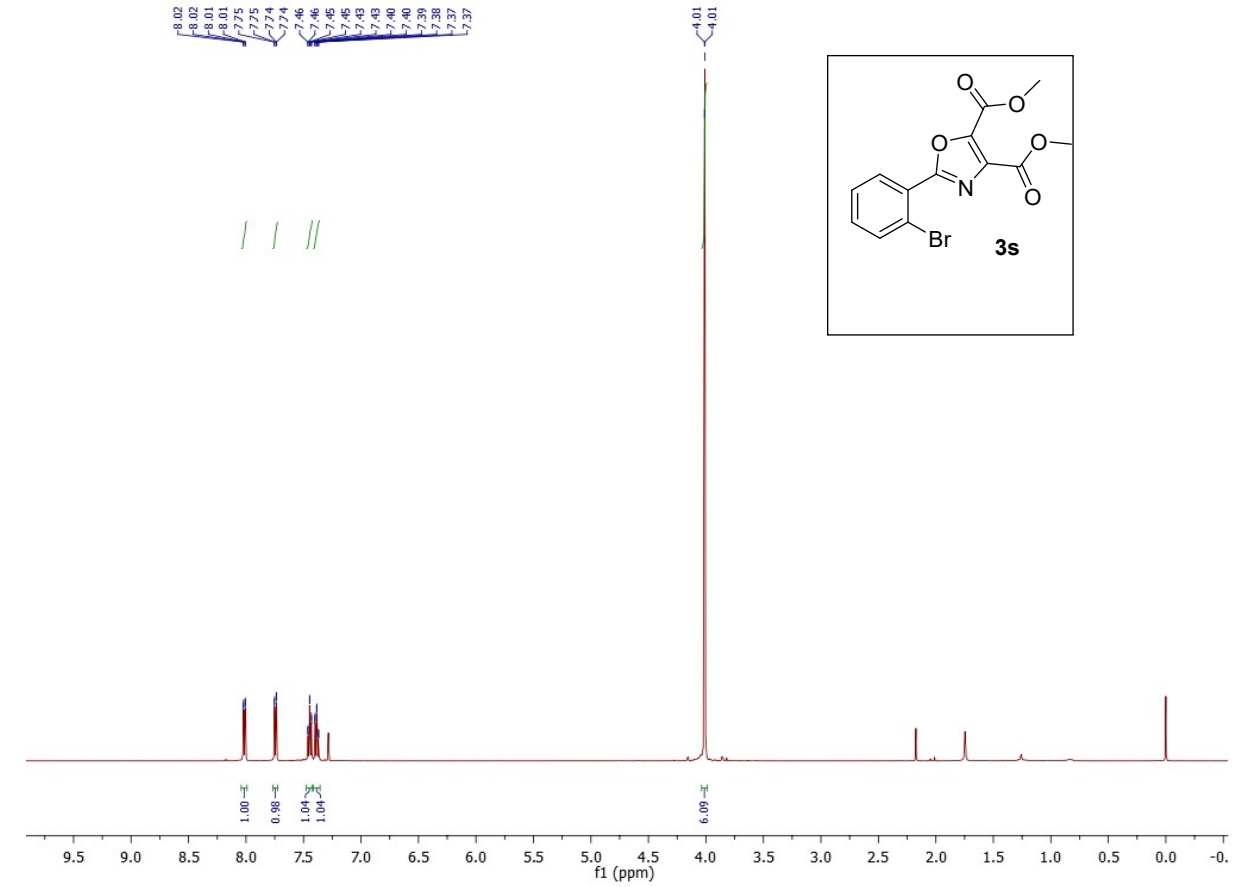
160.80
157.10
142.06
138.58
137.27
129.35
128.74
123.82
77.32
77.00
76.68
52.98
52.91
3q
f1 (ppm)


3r
8.12
8.11
8.10
7.49
7.48
7.47
4.49
4.47
4.46
1.45
1.45
1.44
1.44
1.43
1.43
1.42
1.42
2.00
1.99
3.98
6.07
f1 (ppm)


3r
161.69
160.99
157.08
142.21
138.72
137.81
129.59
129.04
124.27
77.64
77.32
77.00
62.51
14.38
f1 (ppm)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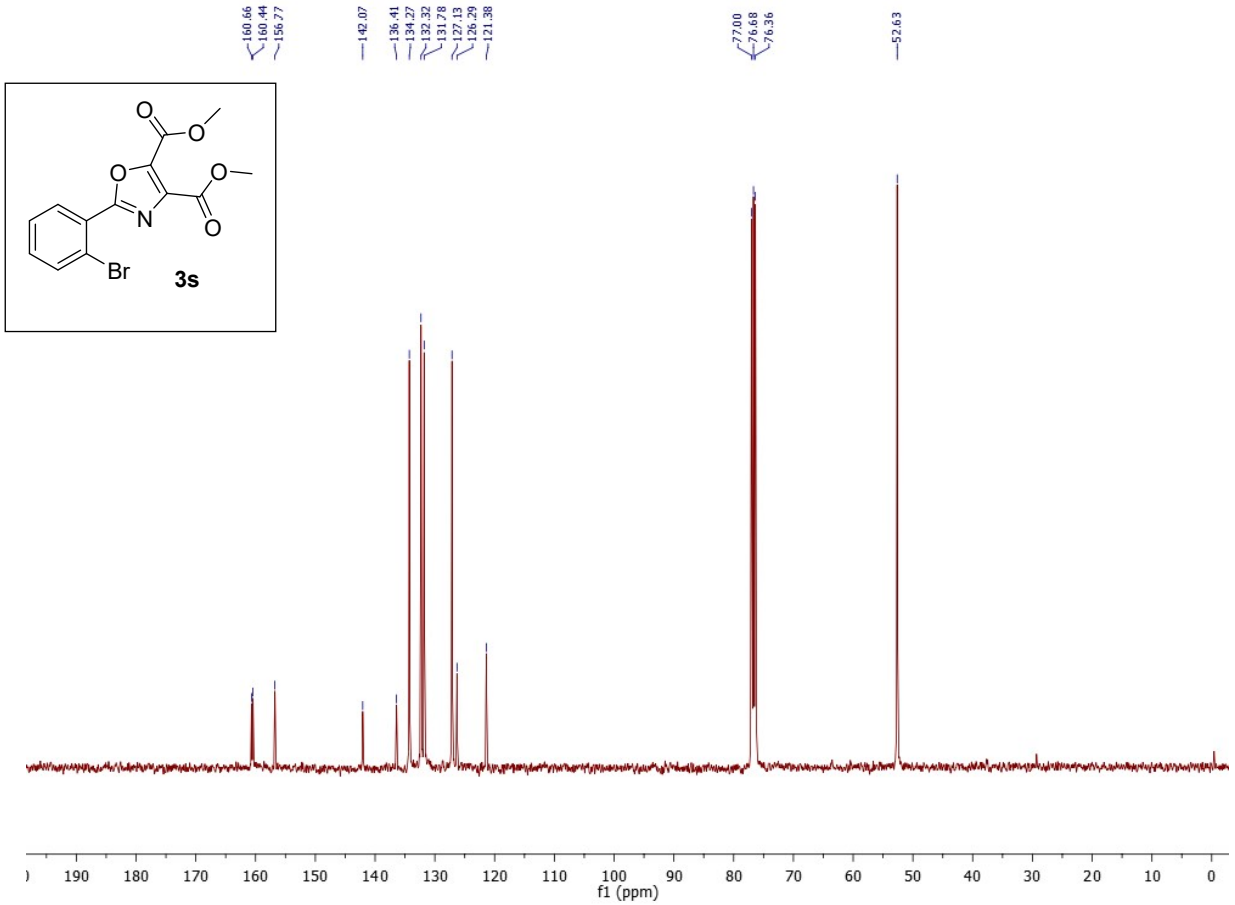
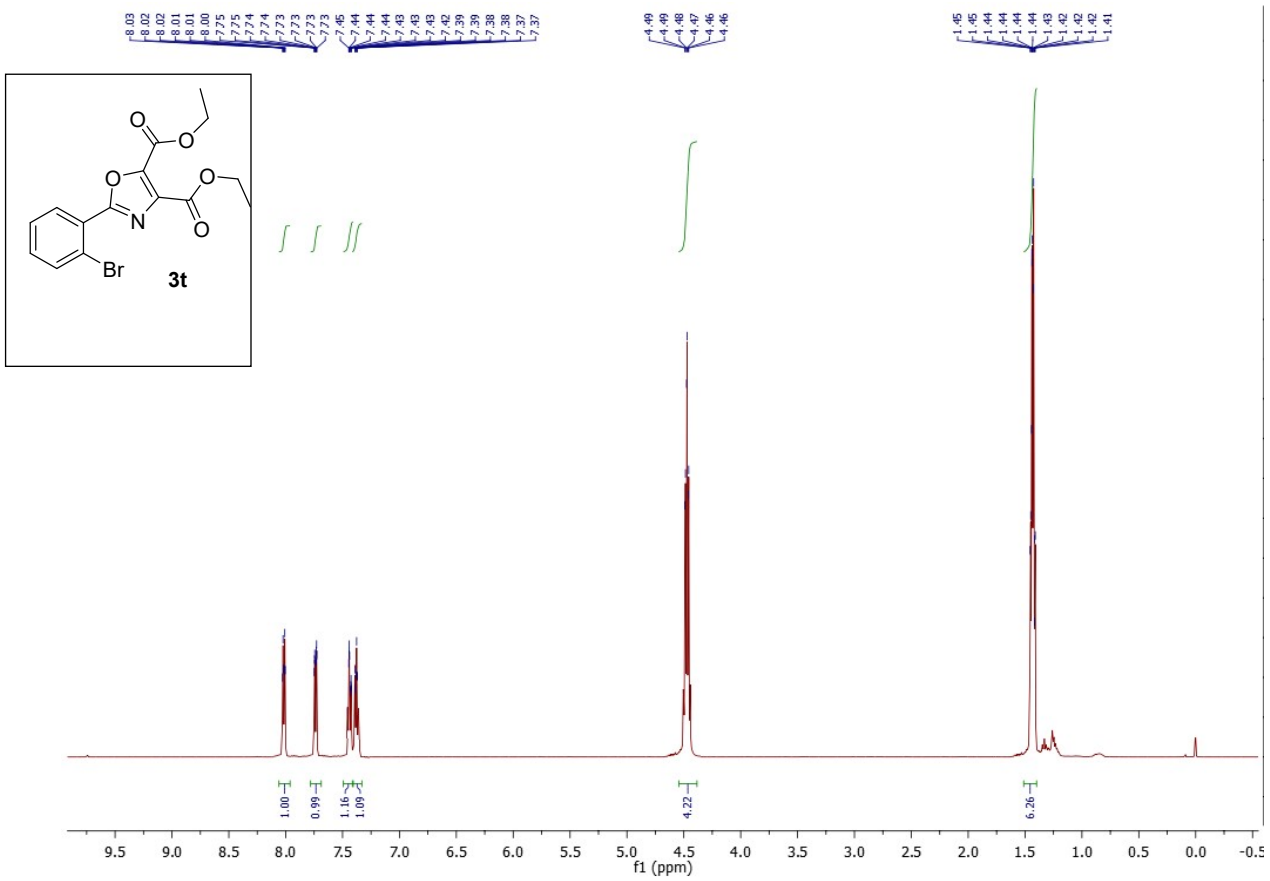
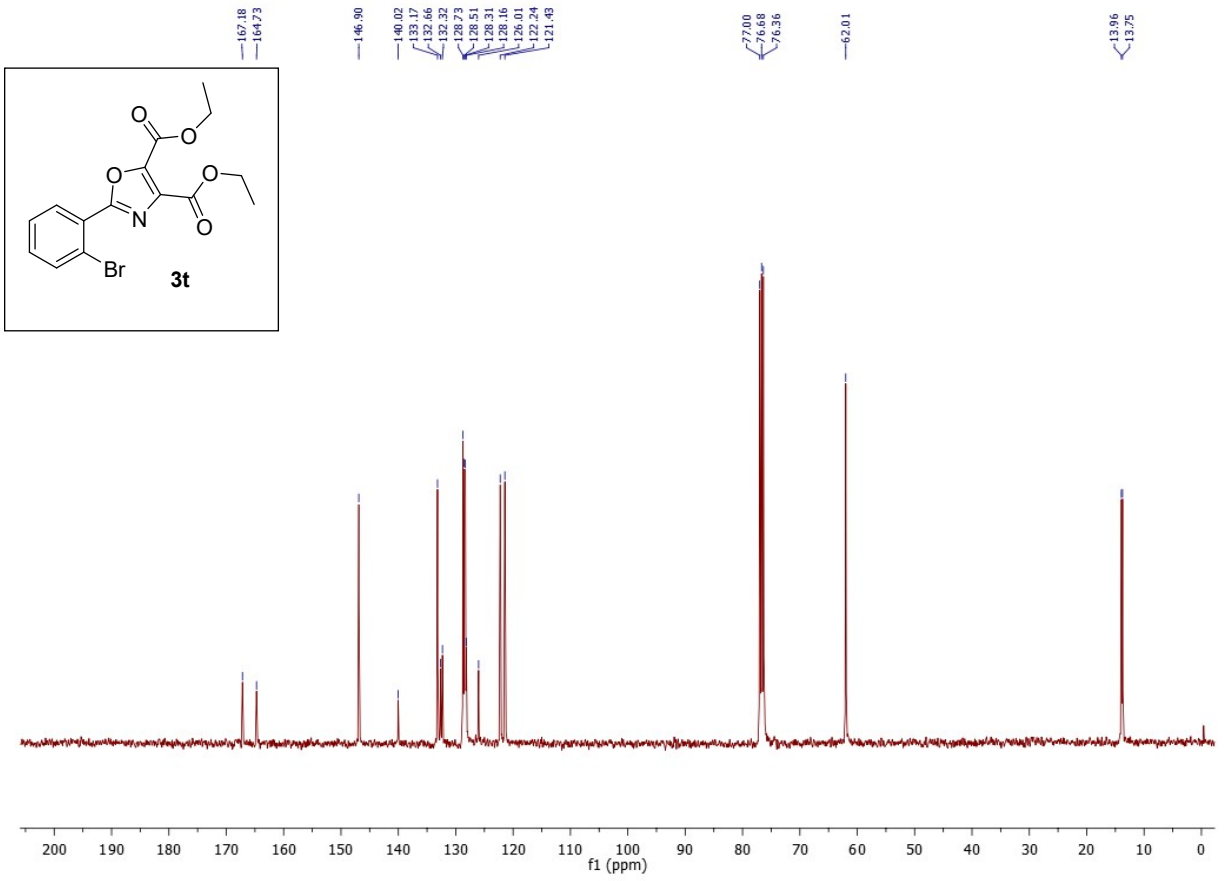
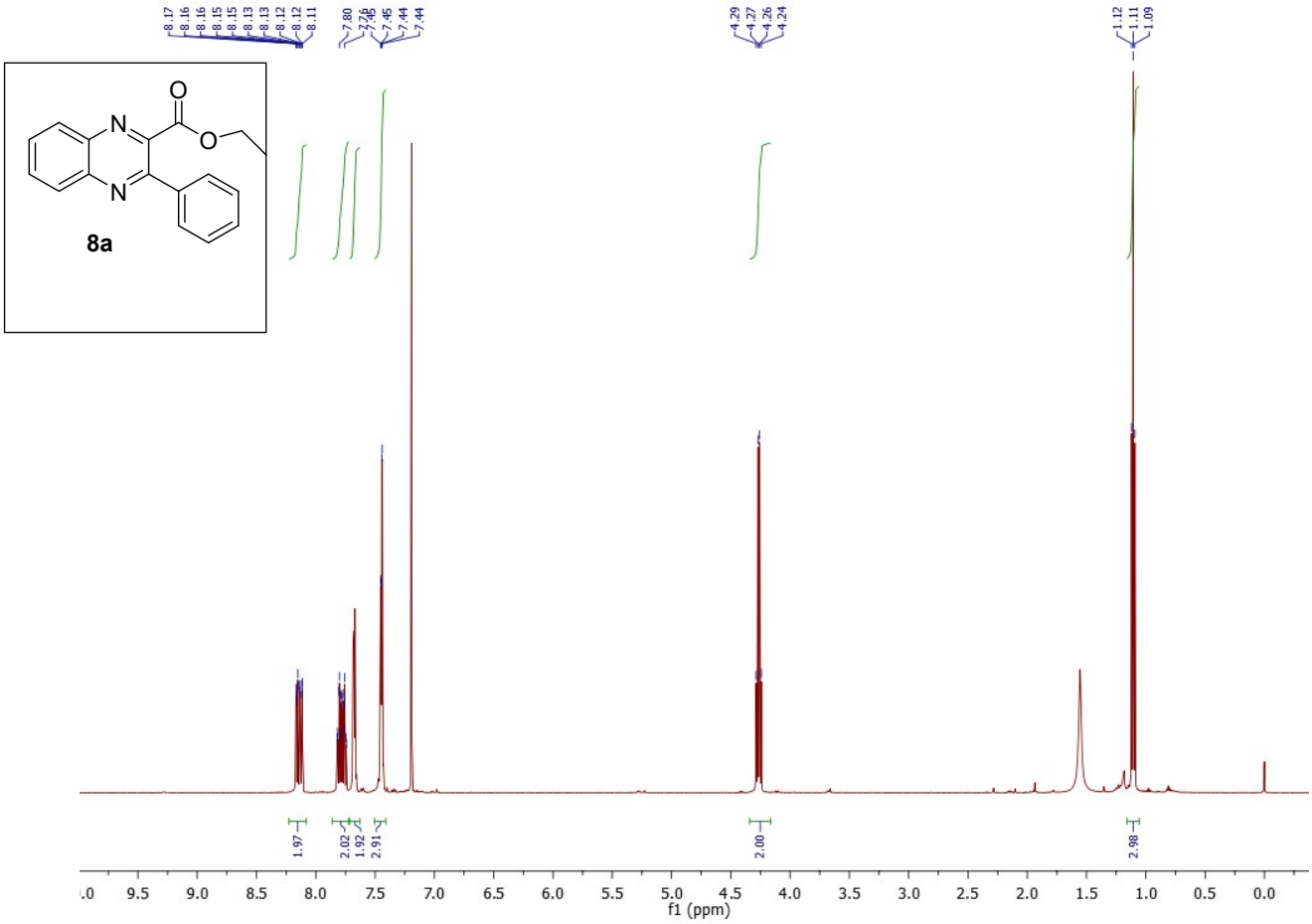
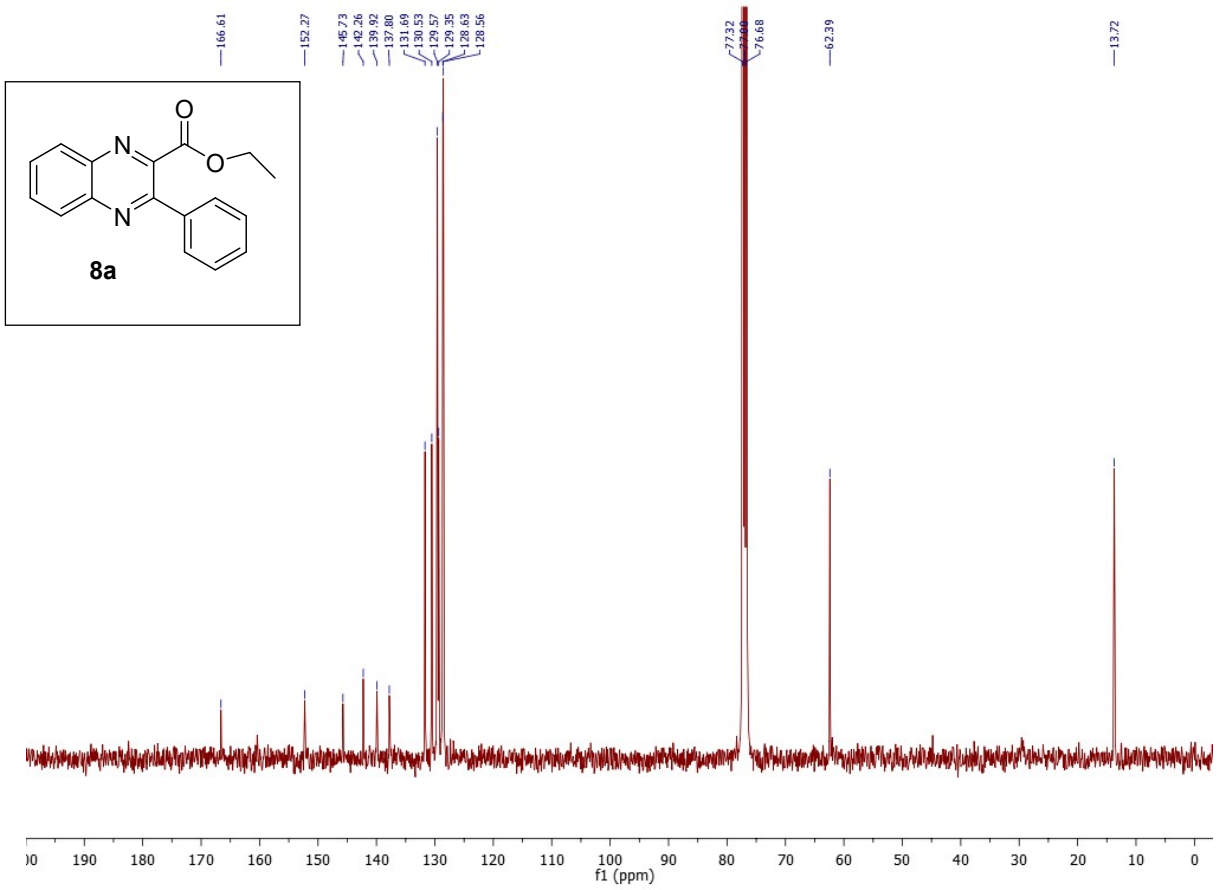
8.02
8.01
8.01
7.75
7.75
7.74
7.74
7.46
7.46
7.45
7.45
7.43
7.43
7.40
7.40
7.39
7.38
7.37
7.37
4.01
4.01
1.00
0.98
1.04
1.04
6.09
f1 (ppm)
3s


160.66
160.44
156.77
142.07
136.41
134.27
132.32
131.78
127.13
126.29
121.38
77.00
76.68
76.36
52.63
f1 (ppm)
3s


3t
f1 (ppm)


3t
f1 (ppm)


8.17
8.16
8.16
8.15
8.15
8.13
8.13
8.12
8.12
8.11
7.80
7.78
7.45
7.44
7.44
4.29
4.27
4.26
4.24
1.12
1.11
1.09
O
N
O
N
8a
1.97
2.02
1.92
2.91
2.00
2.98
f1 (ppm)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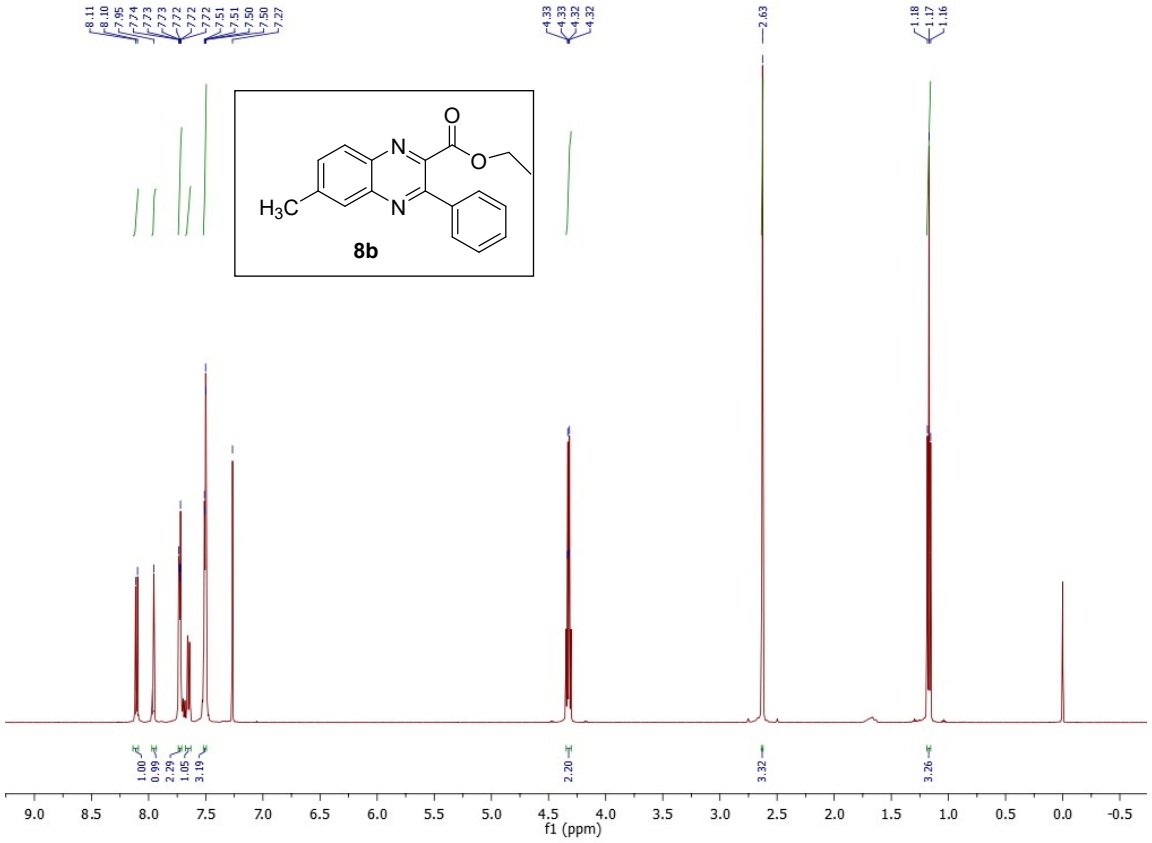
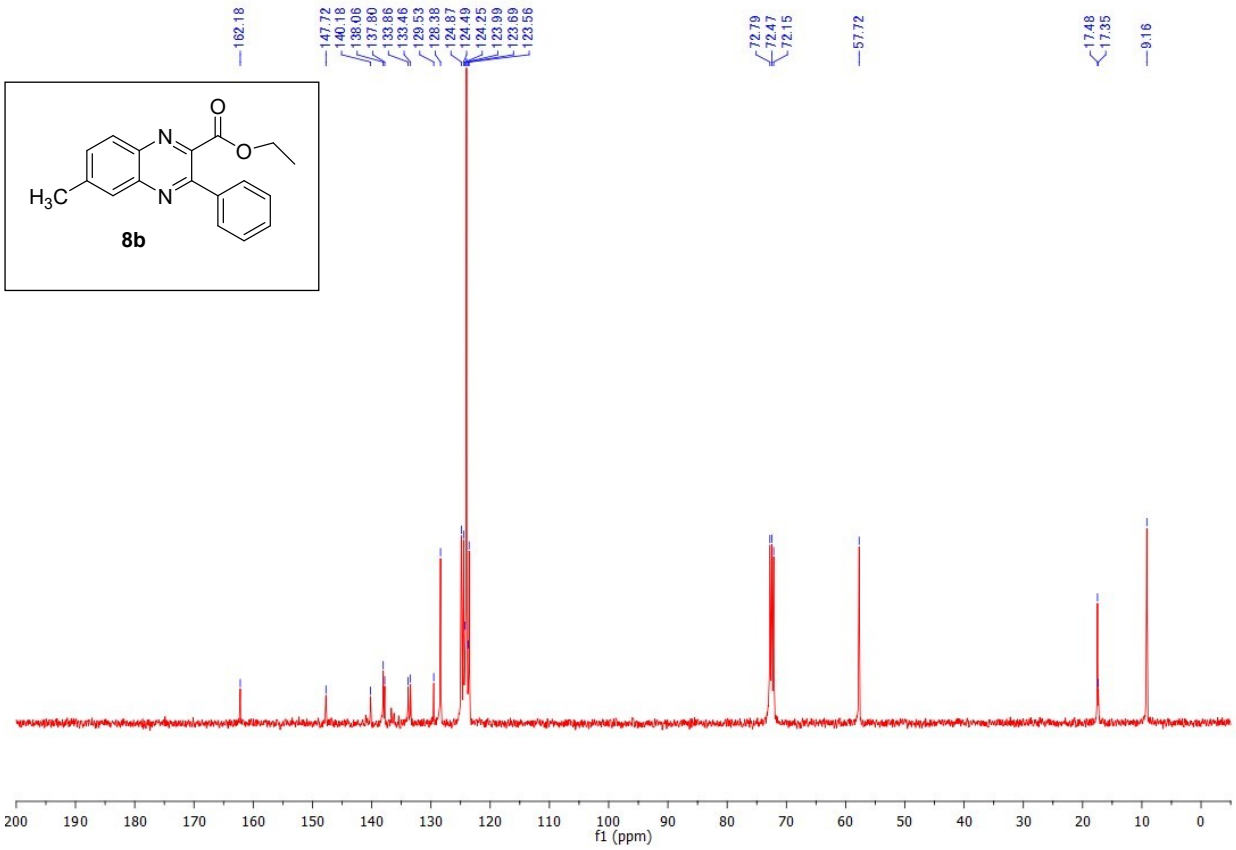
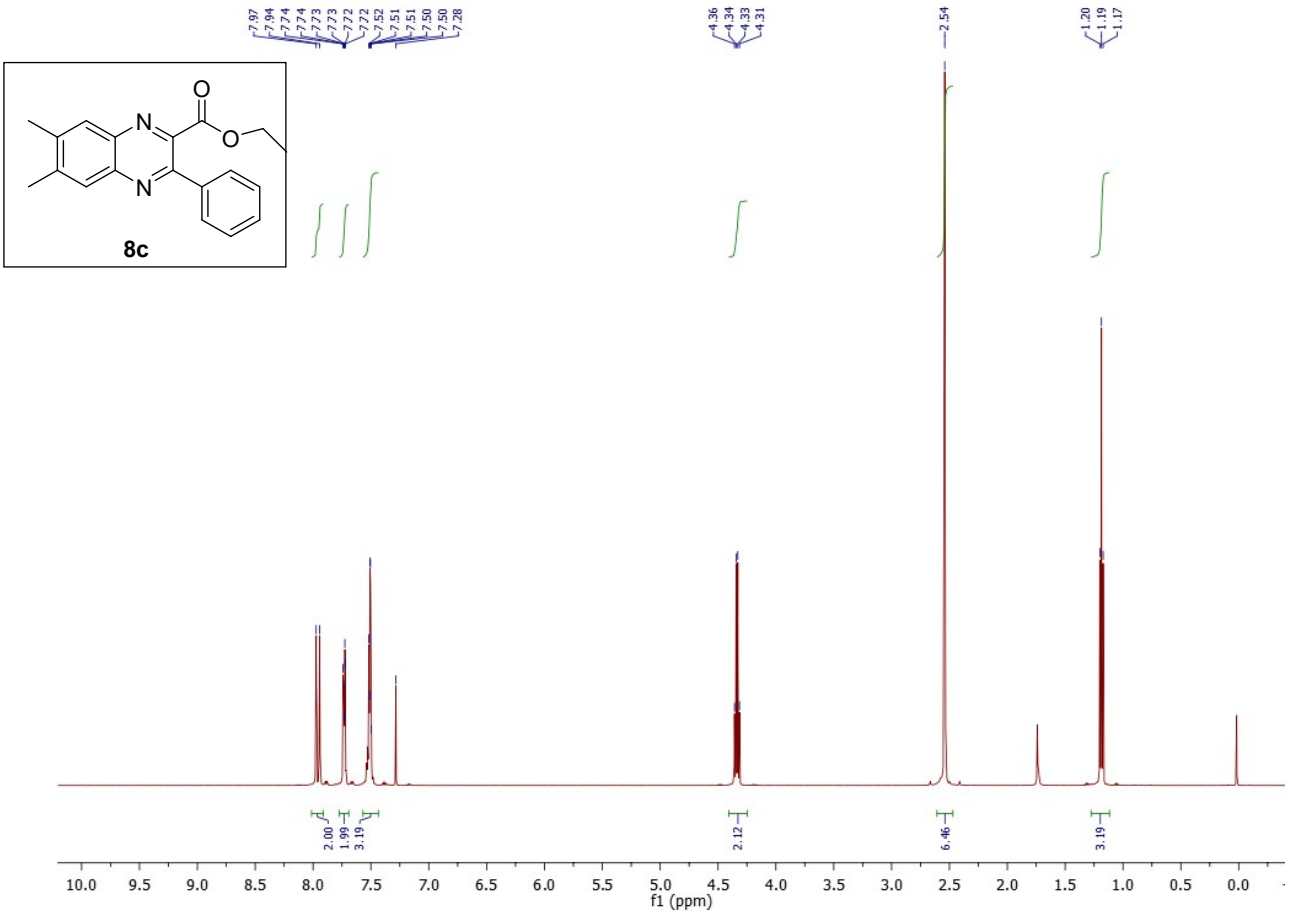
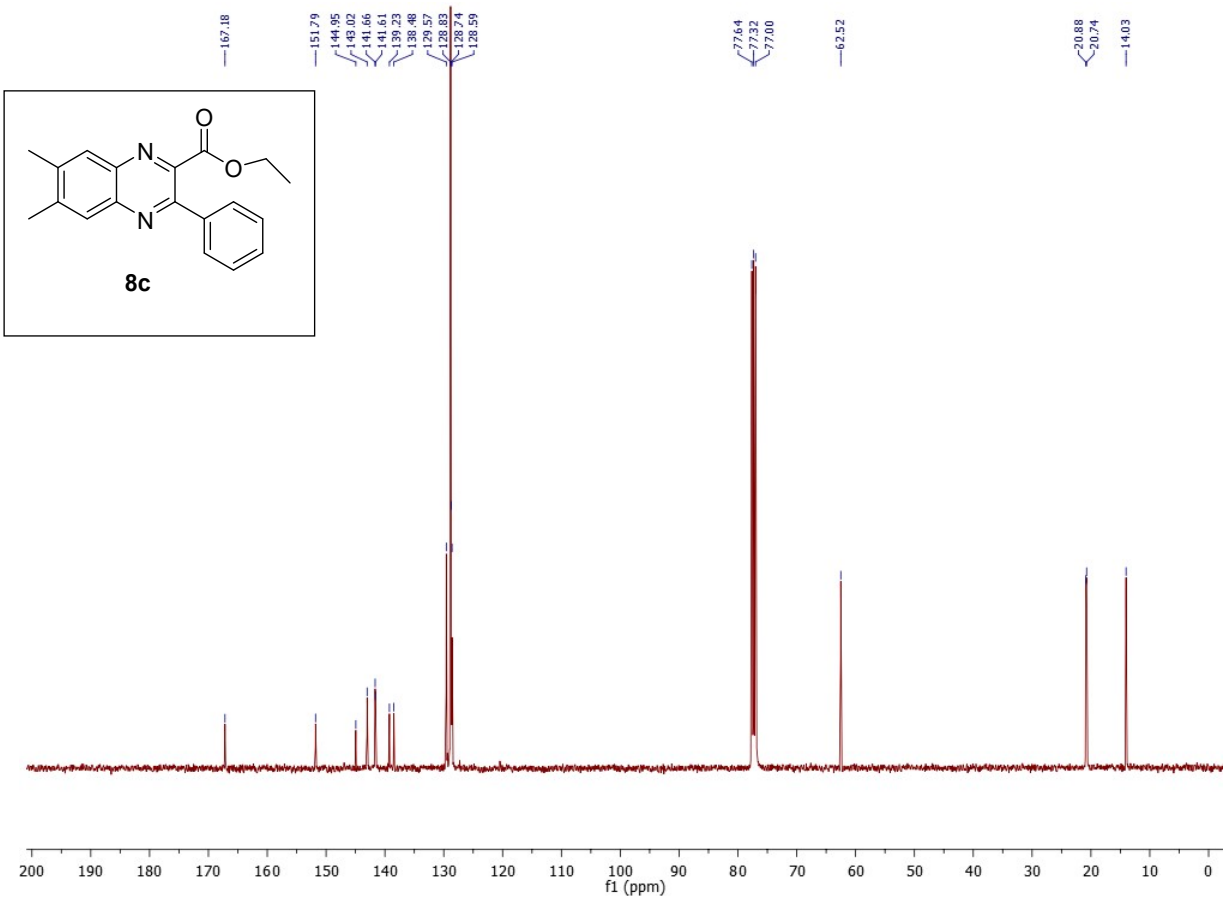
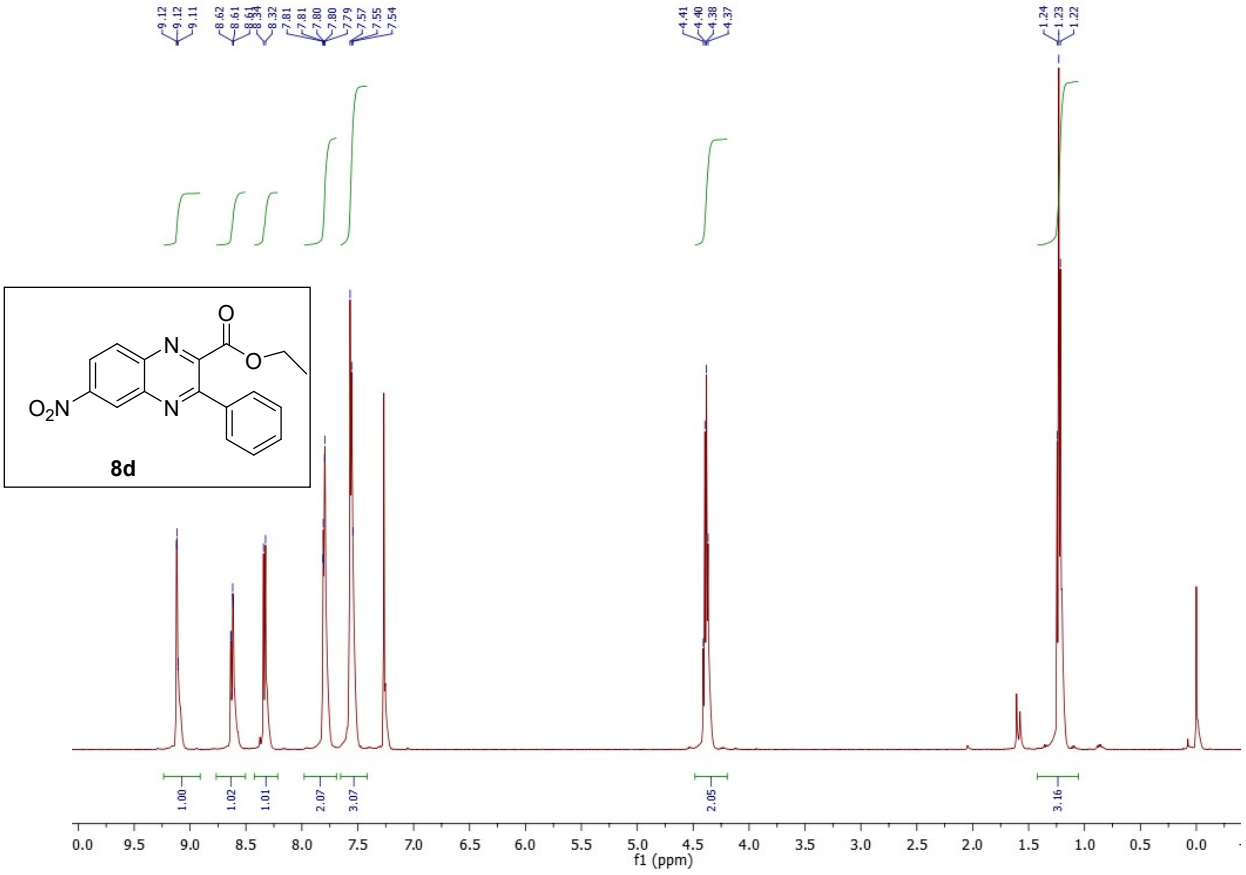
152.27
145.73
142.26
139.92
137.80
131.69
130.53
129.57
129.35
128.63
128.56
77.32
76.68
62.39
13.72
O
N
O
N
8a
f1 (ppm)

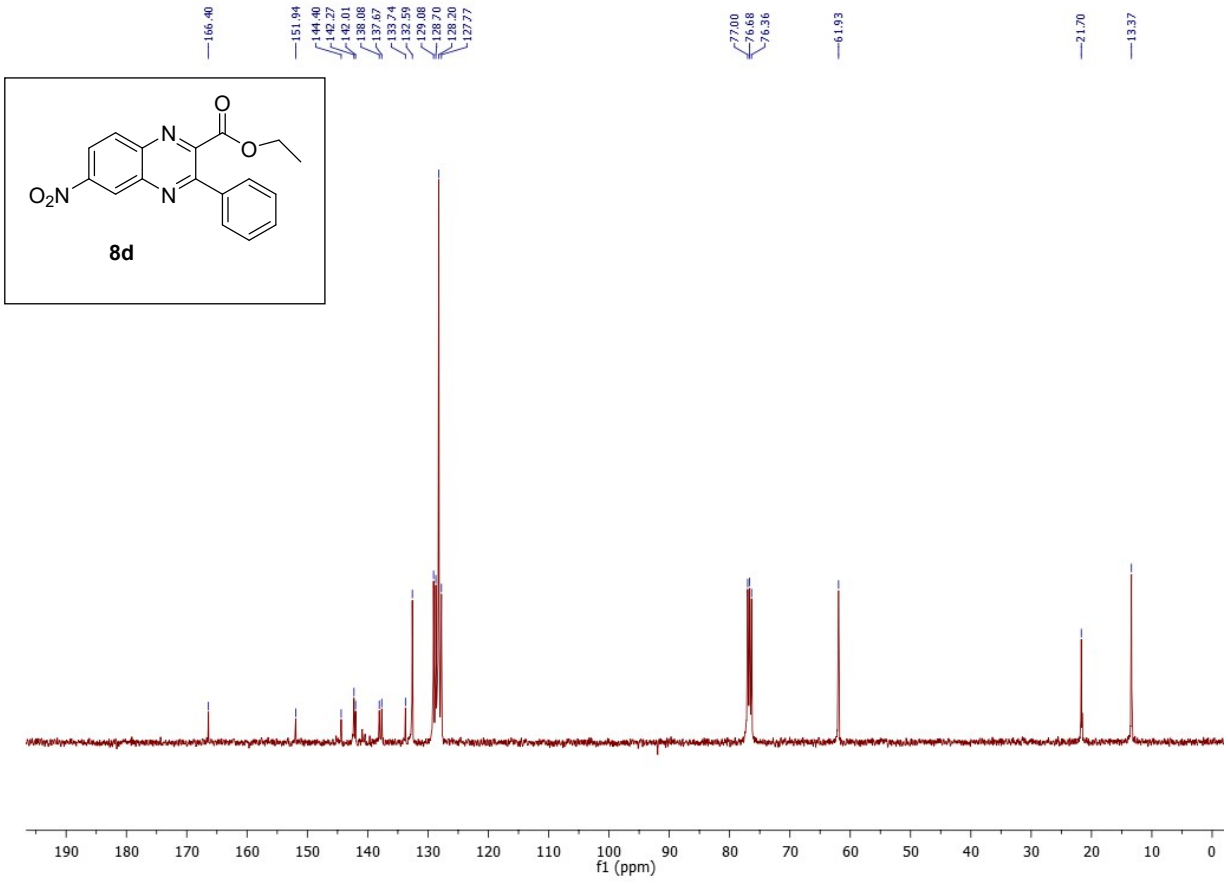

8.11
8.10
7.95
7.74
7.73
7.73
7.72
7.72
7.72
7.72
7.51
7.51
7.50
7.50
7.27
4.33
4.33
4.32
4.32
2.63
1.18
1.17
1.16
O
N
O
H3C
N
8b
1.00
0.99
2.29
1.05
3.19
2.20
3.32
3.26
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


162.18
147.72
140.18
138.06
137.80
133.86
133.46
129.53
128.38
124.87
124.49
124.25
123.99
123.69
123.56
72.79
72.47
72.15
57.72
17.48
17.35
9.16
O
N
O
H3C
N
8b
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8c
7.97
7.94
7.74
7.74
7.73
7.73
7.72
7.72
7.52
7.51
7.51
7.50
7.50
7.28
4.36
4.34
4.33
4.31
2.54
1.20
1.19
1.17
2.00
1.99
3.19
2.12
6.46
3.19
f1 (ppm)


8c
167.18
151.79
144.95
143.02
141.66
141.61
139.23
138.48
129.57
128.83
128.74
128.59
77.64
77.32
77.00
62.52
20.88
20.74
14.03
f1 (ppm)


9.12
9.12
9.11
8.62
8.61
8.34
8.32
7.81
7.81
7.80
7.80
7.79
7.57
7.55
7.54
4.41
4.40
4.38
4.37
1.24
1.23
1.22
O
N
O
O2N
N
8d
1.00
1.02
1.01
2.07
3.07
2.05
3.16
0.0
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)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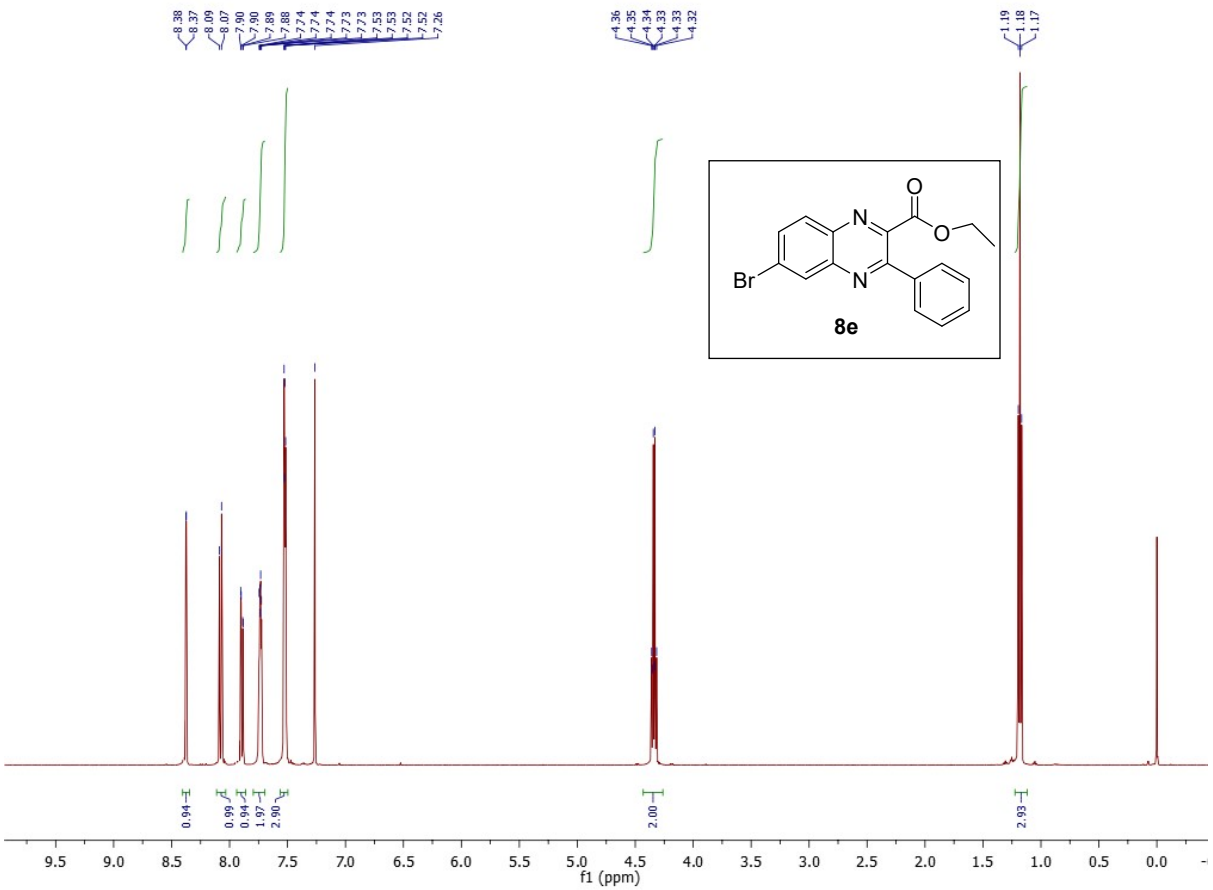
151.94
144.40
142.27
142.01
139.08
137.67
133.74
132.59
129.08
128.70
128.20
127.77
77.00
76.68
76.36
61.93
21.70
13.37
O
N
O
O2N
N
8d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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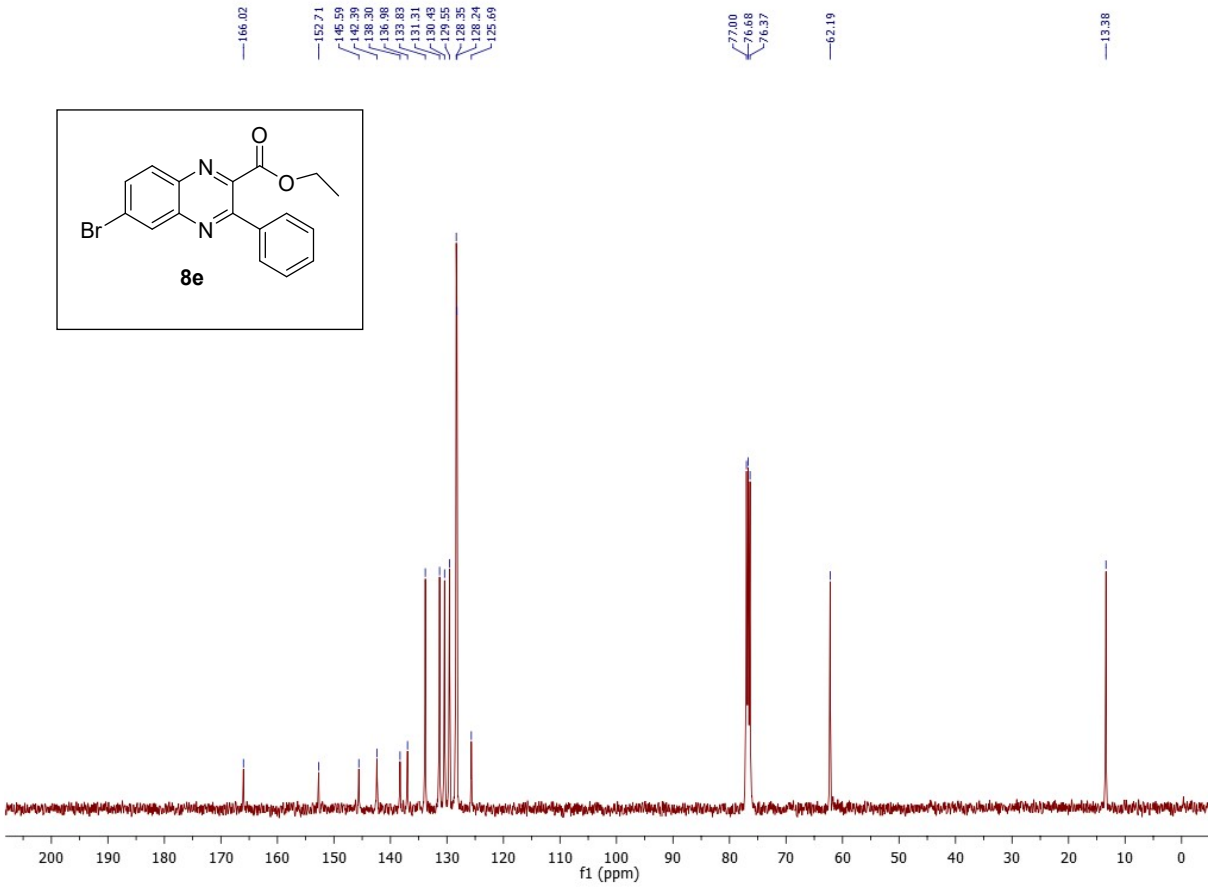
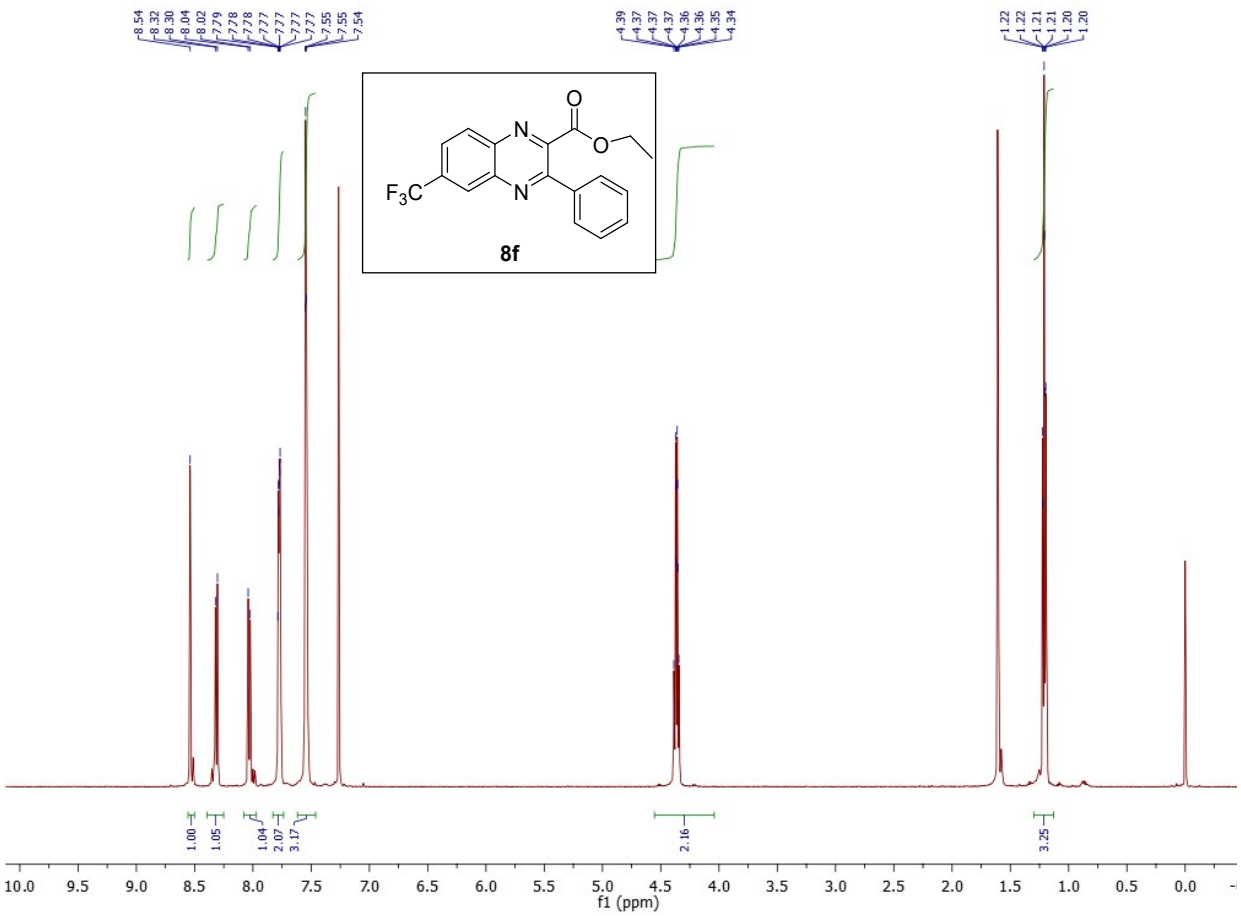
8.37
8.09
8.07
7.90
7.90
7.89
7.88
7.74
7.74
7.74
7.73
7.73
7.53
7.53
7.52
7.52
7.26
4.36
4.35
4.34
4.33
4.33
4.32
1.19
1.18
1.17
O
N
O
Br
N
8e
0.94
0.99
0.94
1.97
2.90
2.00
2.93
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


166.02
152.71
145.59
142.39
138.30
136.98
133.83
131.31
130.48
129.55
128.35
128.24
125.69
77.00
76.68
76.37
62.19
13.38
O
N
O
Br
N
8e
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.54
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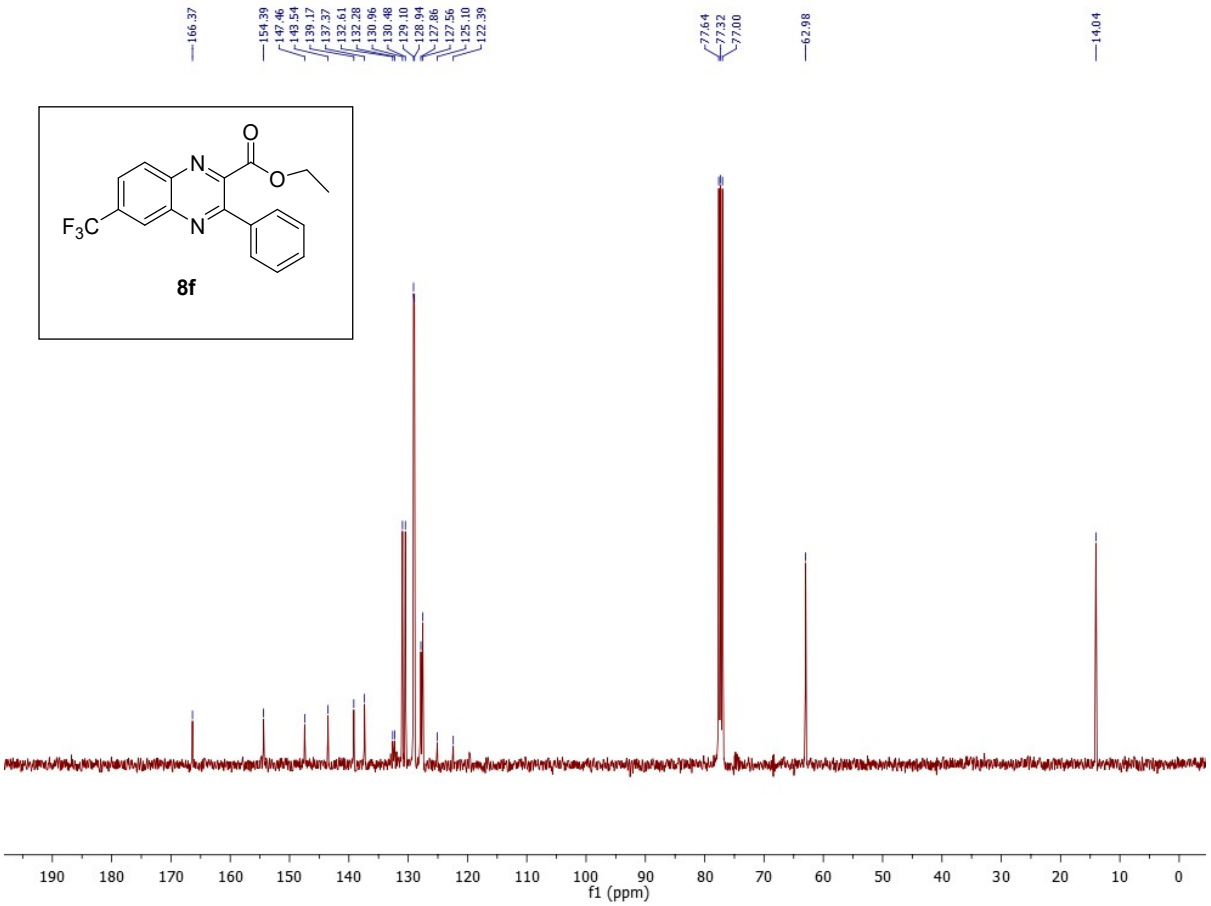
8.30
8.04
8.02
7.79
7.78
7.78
7.77
7.77
7.77
7.77
7.55
7.55
7.54
4.39
4.37
4.37
4.37
4.36
4.36
4.35
4.34
1.22
1.22
1.21
1.21
1.20
1.20
O
N
O
F3C
N
8f
1.00
1.05
1.04
2.07
3.17
2.16
3.25
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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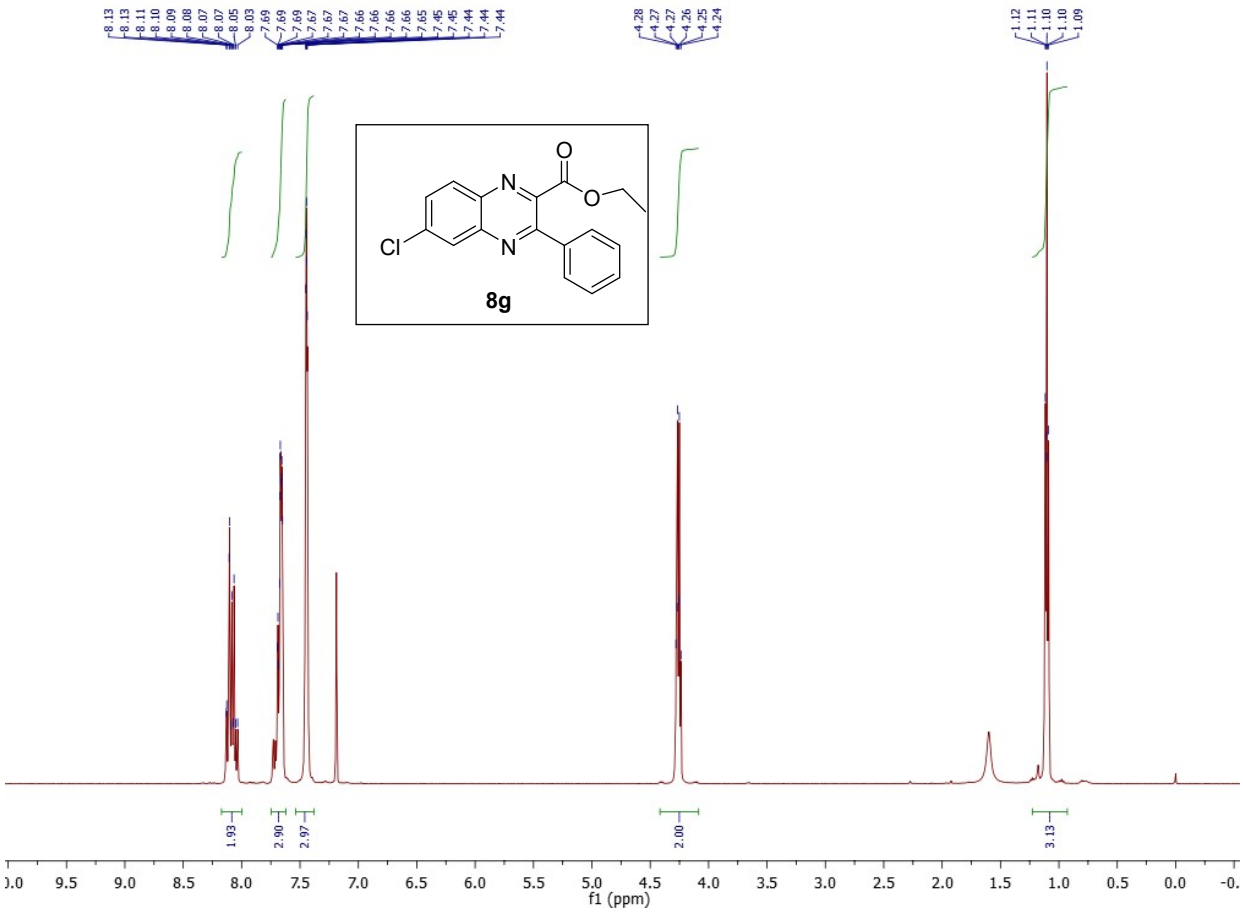
154.39
147.46
143.54
139.17
137.37
132.61
132.28
130.96
130.48
129.10
128.94
127.86
127.56
125.10
122.39
77.64
77.32
77.00
62.98
14.04
O
N
O
F3C
N
8f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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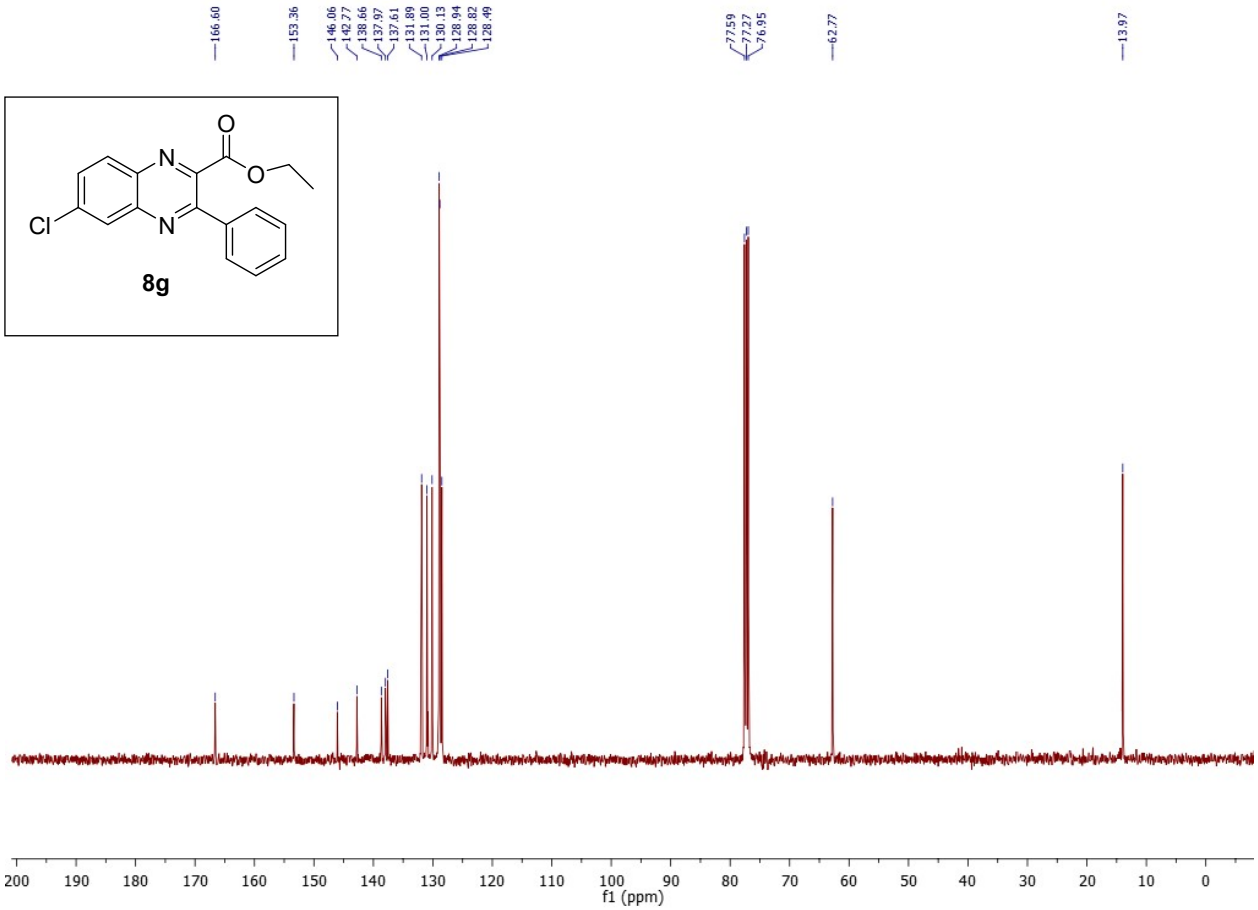
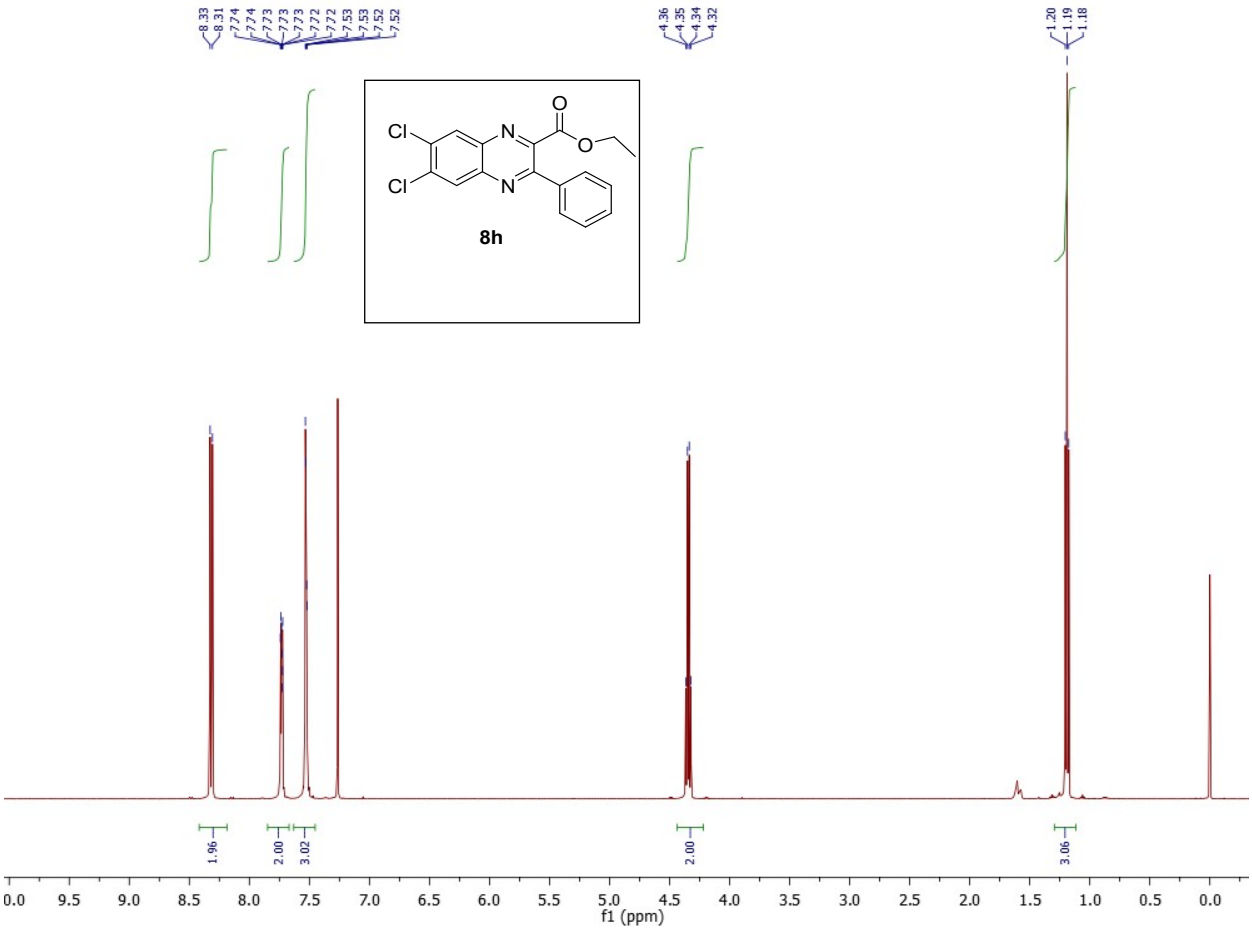
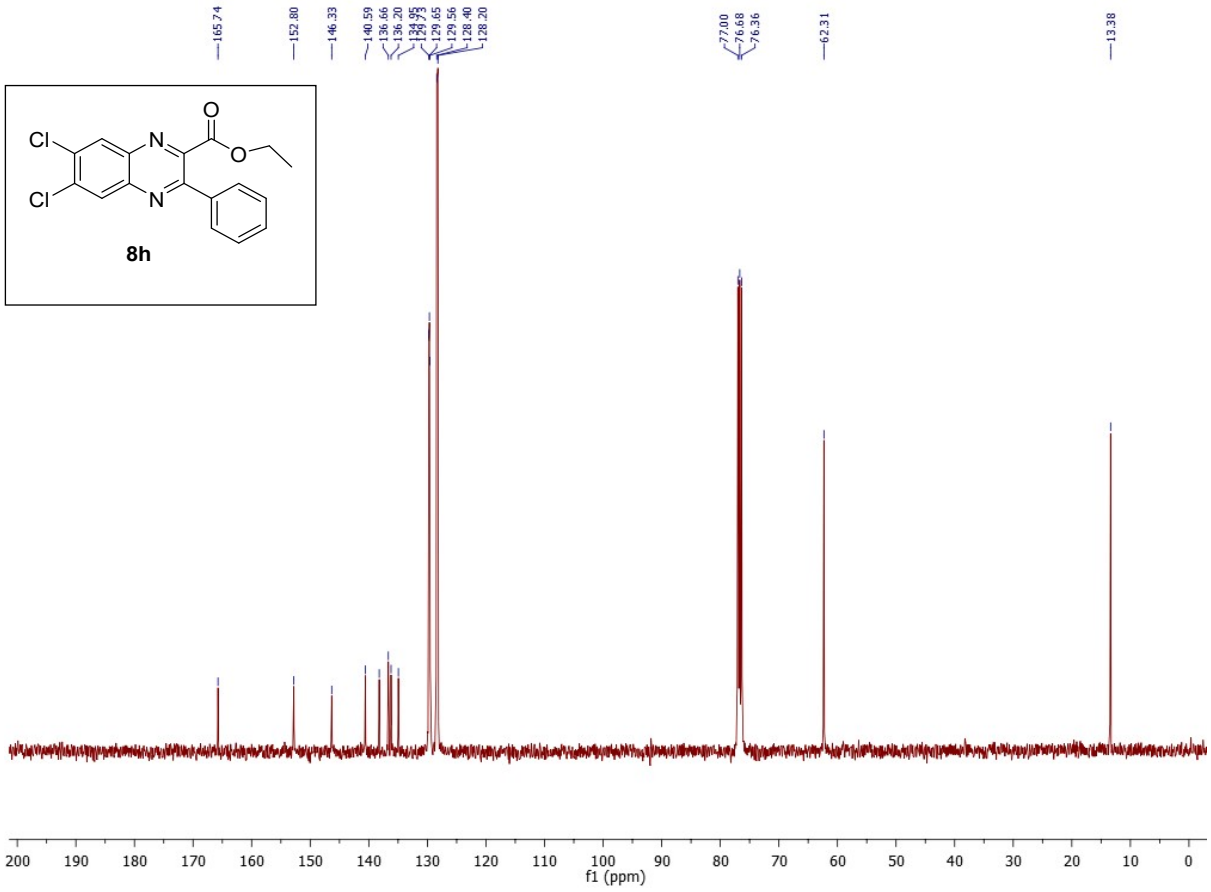
8.13
8.11
8.10
8.09
8.08
8.07
8.07
8.05
8.03
7.69
7.69
7.69
7.67
7.67
7.67
7.66
7.66
7.66
7.66
7.65
7.45
7.45
7.44
7.44
7.44
4.28
4.27
4.27
4.26
4.25
4.24
1.12
1.11
1.10
1.10
1.09
O
N
O
Cl
N
8g
1.93
2.90
2.97
2.00
3.13
f1 (ppm)


166.60
153.36
146.06
142.77
138.66
137.97
137.61
131.89
131.00
130.13
128.94
128.82
128.49
77.59
77.27
76.95
62.77
13.97
O
N
O
Cl
N
8g
f1 (ppm)


8.33
8.31
7.74
7.74
7.73
7.73
7.73
7.72
7.72
7.53
7.53
7.52
7.52
4.36
4.35
4.34
4.32
1.20
1.19
1.18
Cl
Cl
N
N
O
O
8h
1.96
2.00
3.02
2.00
3.06
f1 (ppm)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152.80
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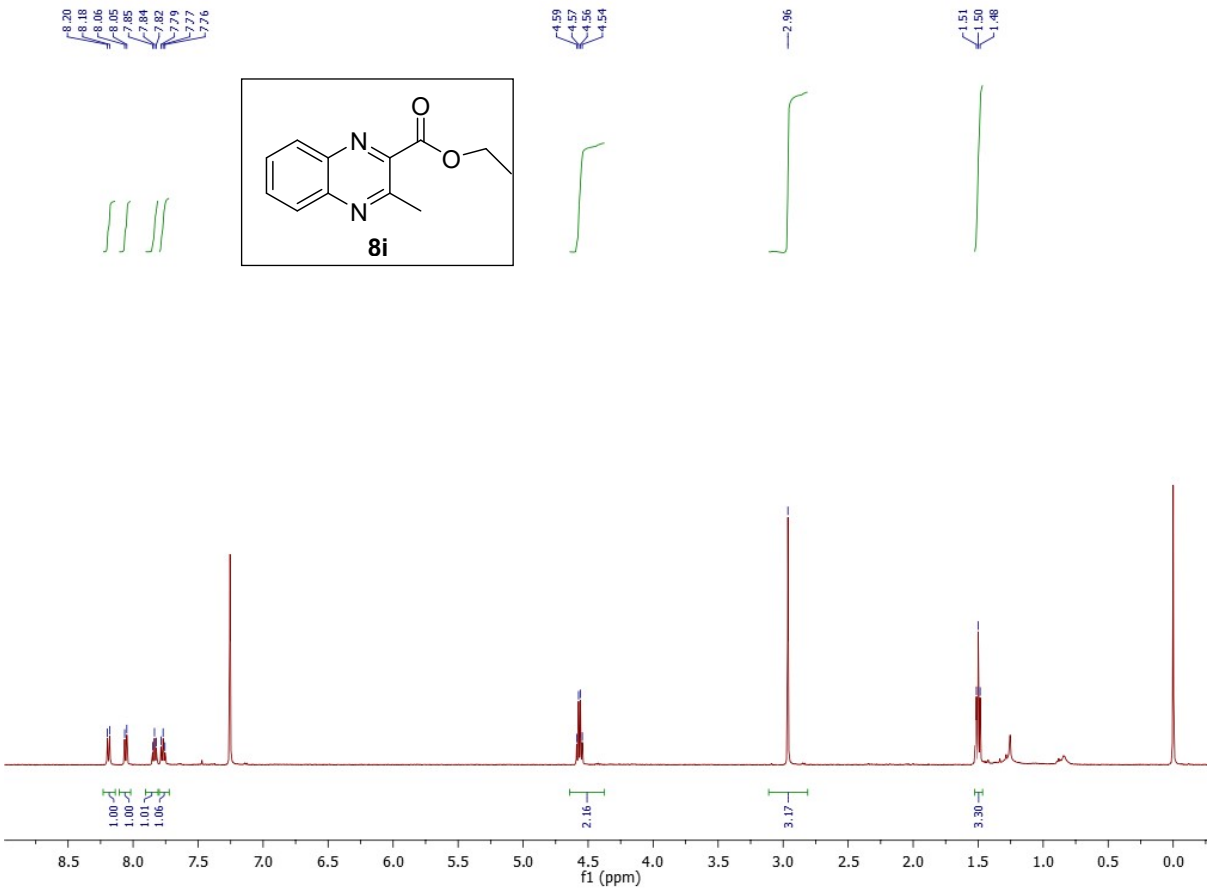
140.59
136.66
136.20
134.95
129.73
129.65
129.56
128.40
128.20
77.00
76.68
76.36
62.31
13.38
Cl
Cl
N
N
O
O
8h
f1 (ppm)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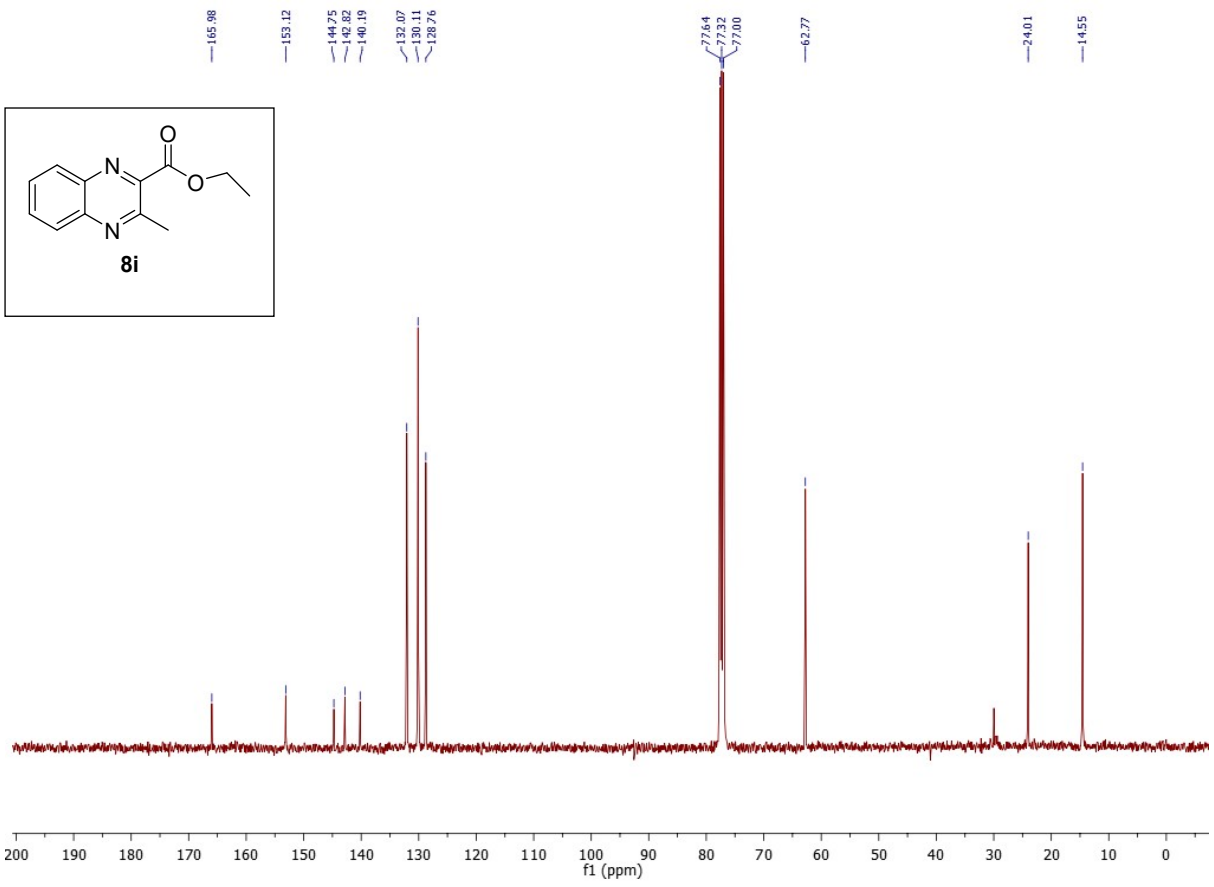
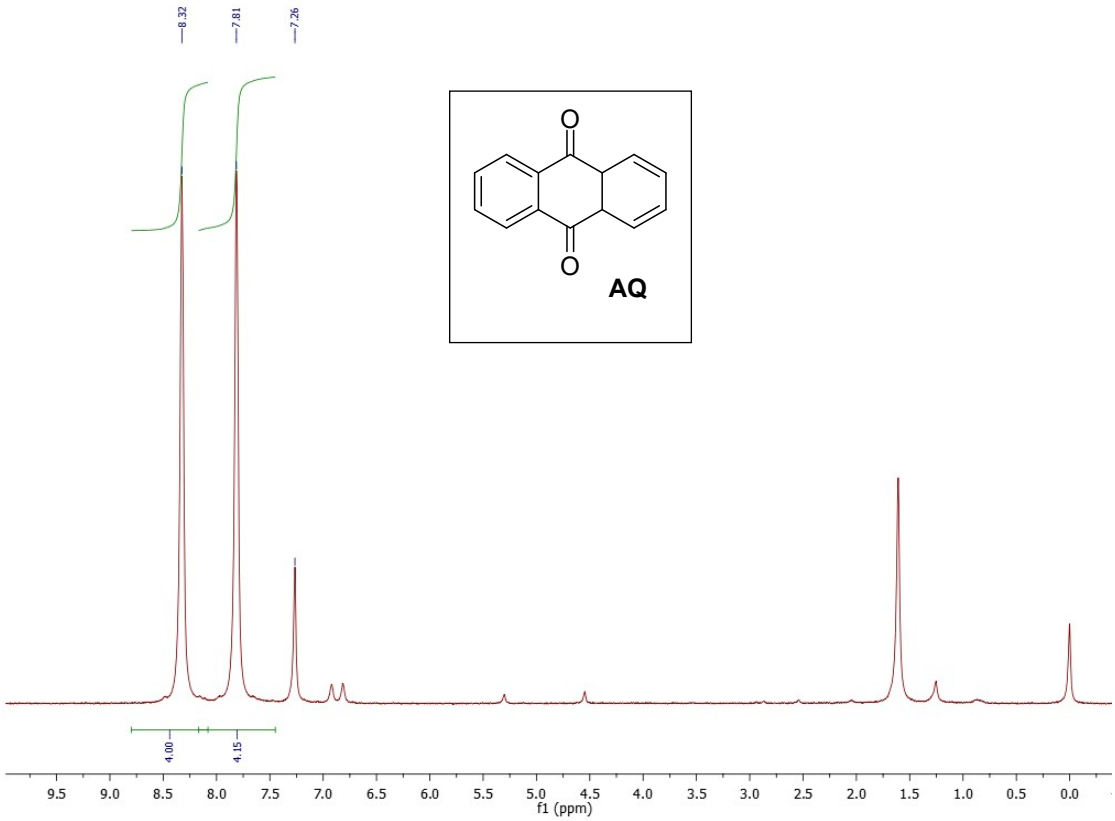
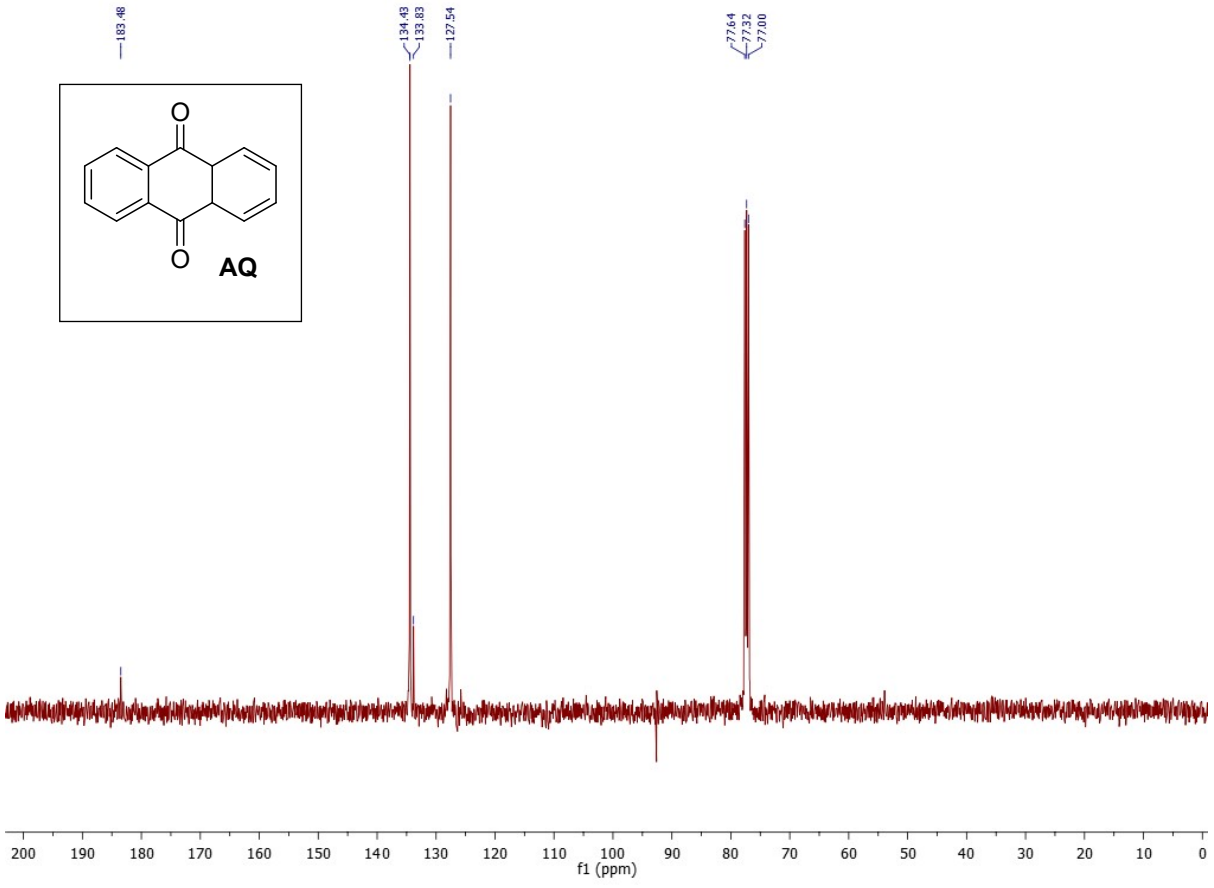
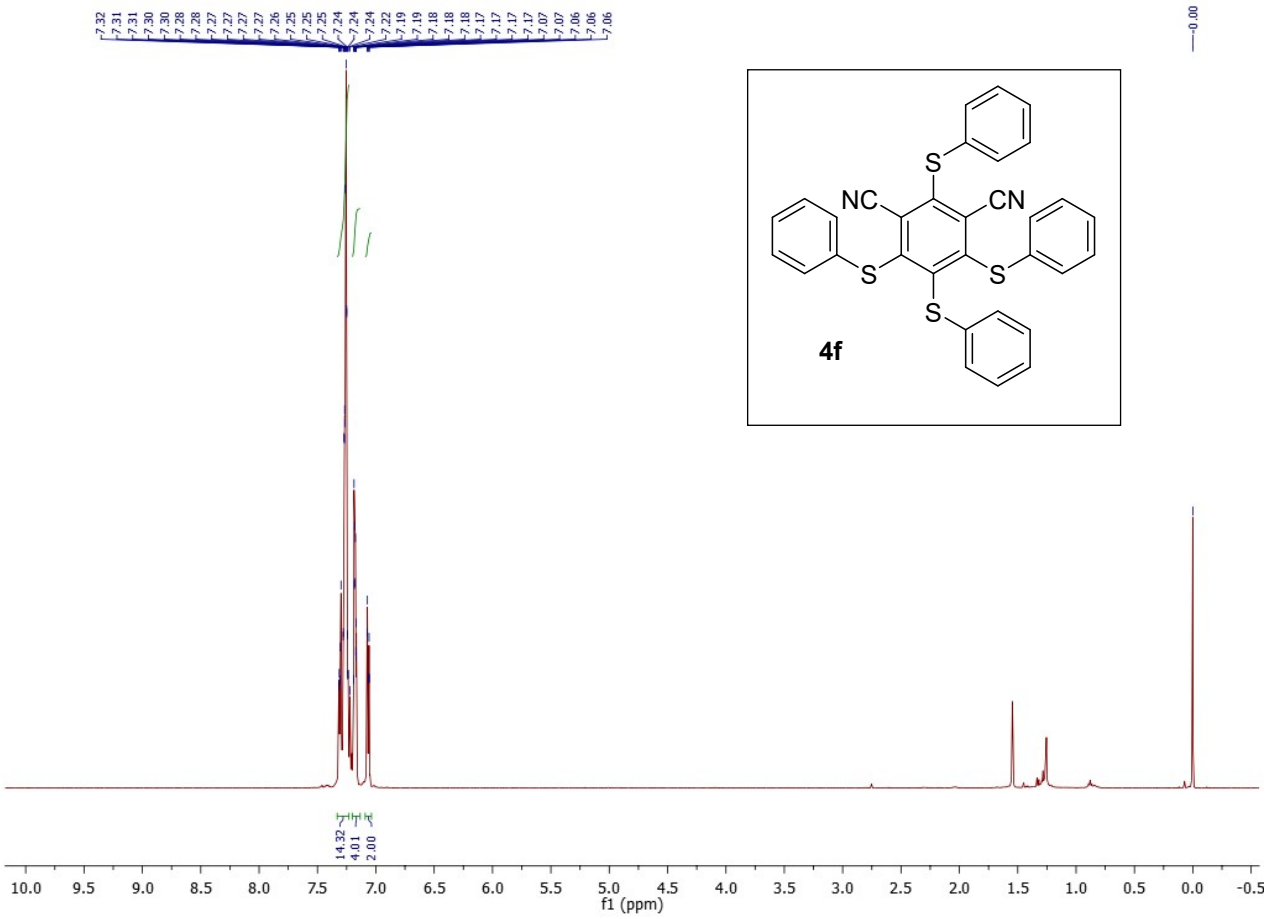
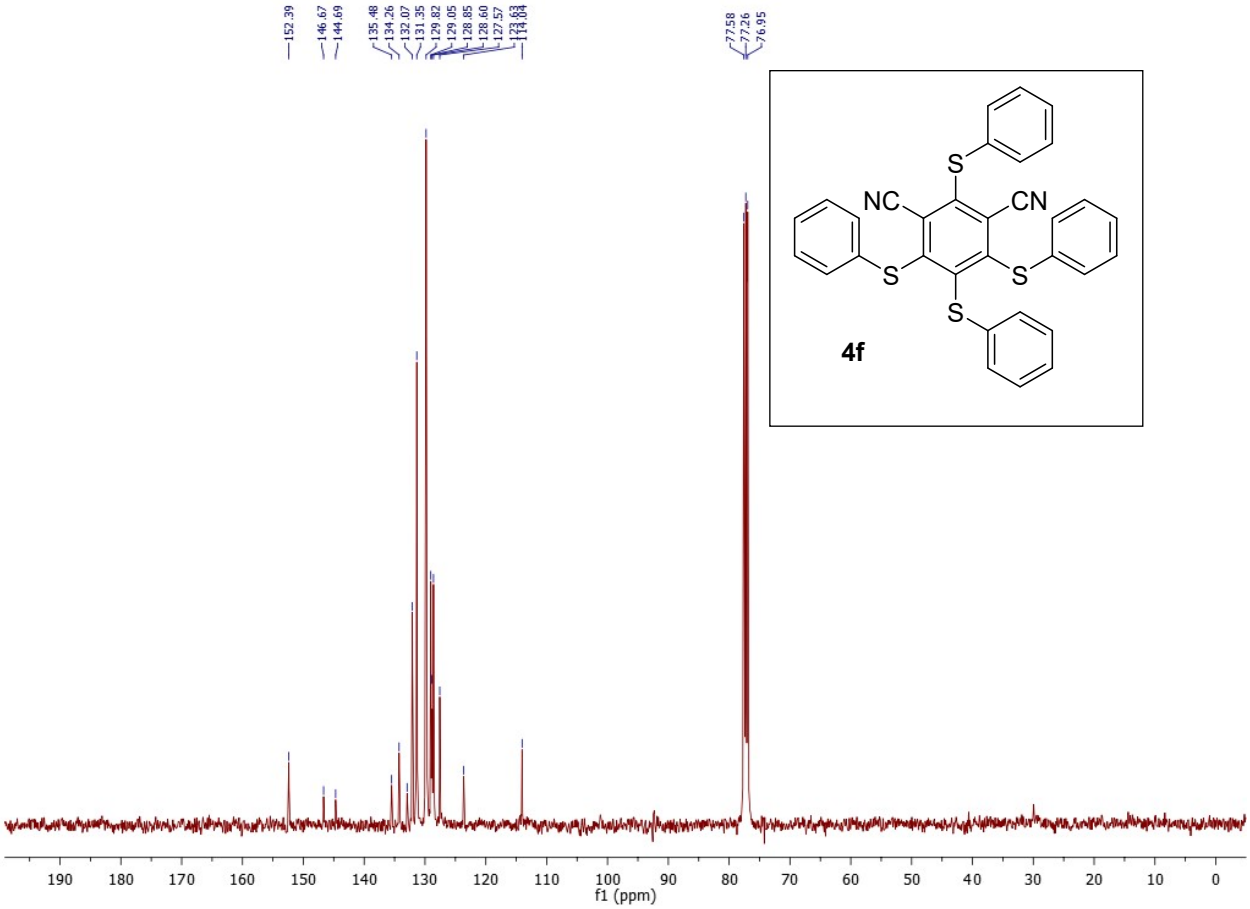
8.18
8.06
8.05
7.85
7.84
7.82
7.79
7.77
7.76
4.59
4.57
4.56
4.54
2.96
1.51
1.50
1.48
O
N
O
N
8i
1.00
1.00
1.01
1.06
2.16
3.17
3.30
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

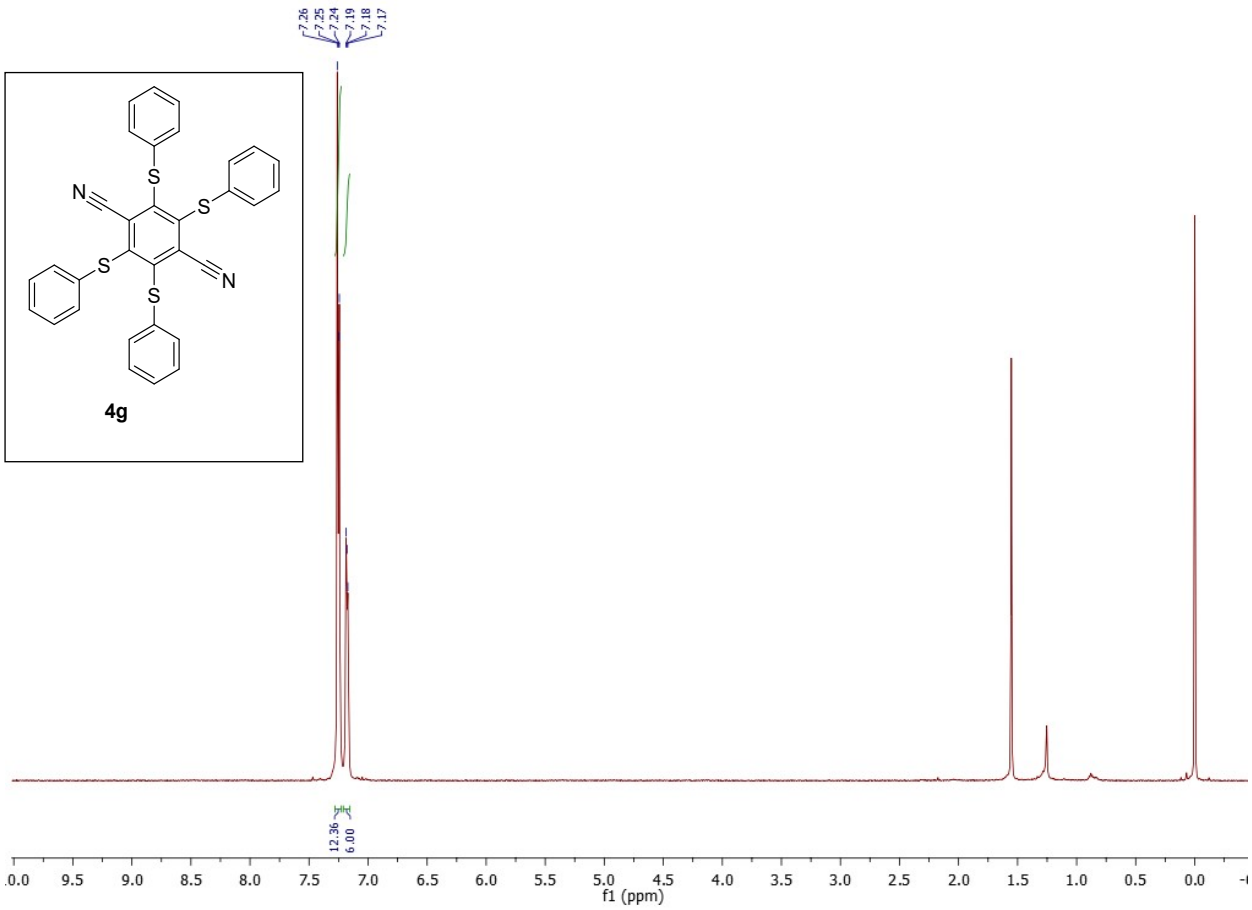

165.98
153.12
144.75
142.82
140.19
132.07
130.11
128.76
77.64
77.32
77.00
62.77
24.01
14.55
O
N
O
N
8i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

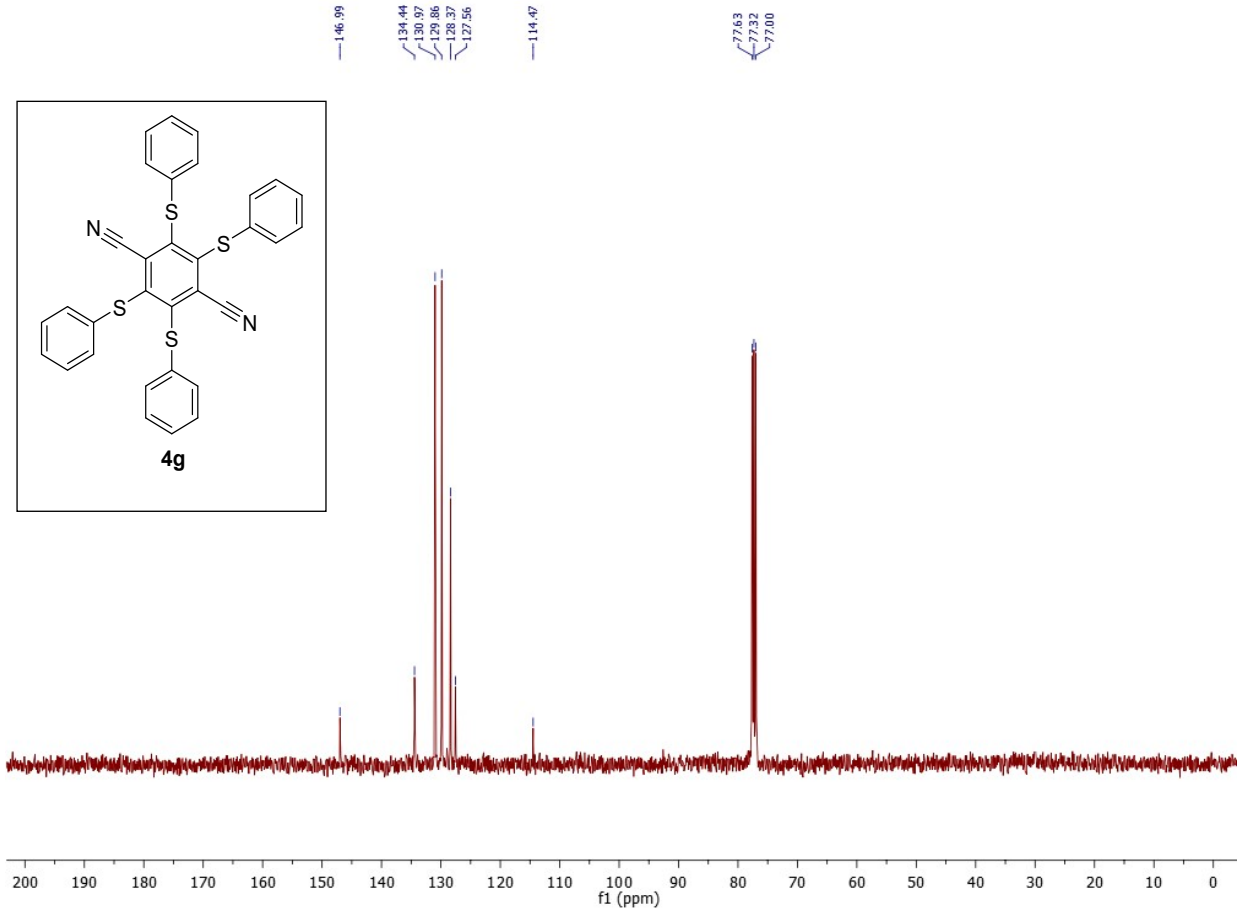

8.32
7.81
7.26
O
O
AQ
4.00
4.15
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


183.48
134.43
133.83
127.54
77.64
77.32
77.00
O
O
AQ
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


NC
CN
S
S
S
S
4f
f1 (ppm)


NC
CN
S
S
S
S
4f
f1 (ppm)


7.26
7.25
7.24
7.19
7.18
7.17
4g
12.36
6.00
f1 (ppm)


146.99
134.44
130.97
129.86
128.37
127.56
114.47
77.63
77.32
77.00
4g
f1 (ppm)