Electronic Supplementary Information

Copper and palladium-catalyzed sequential reactions: One-pot synthesis of isoindolo[2,1-*b*]isoquinolin-7(5*H*)-ones

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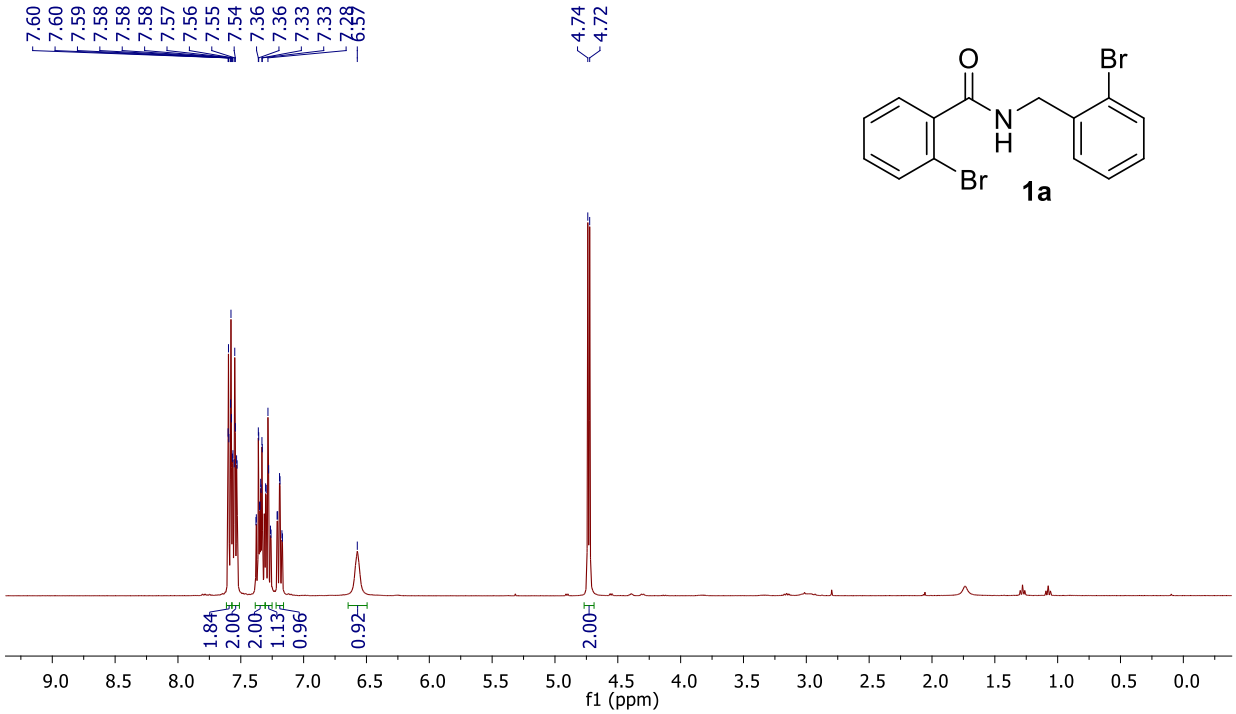
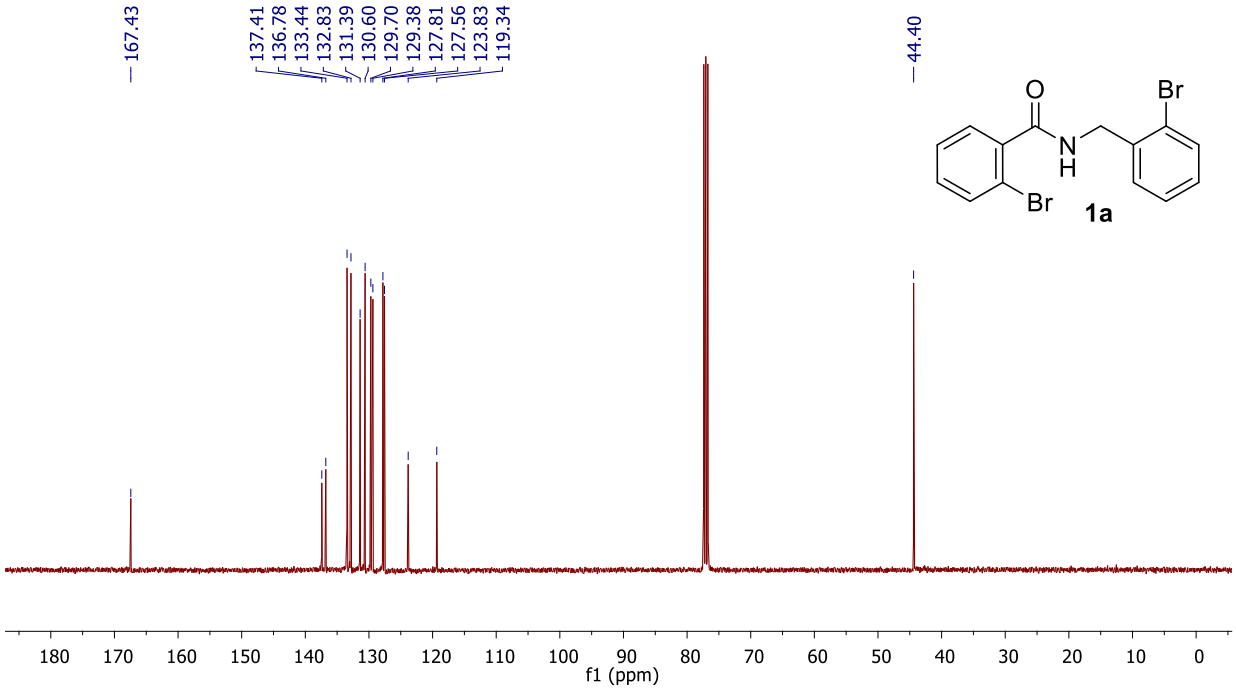
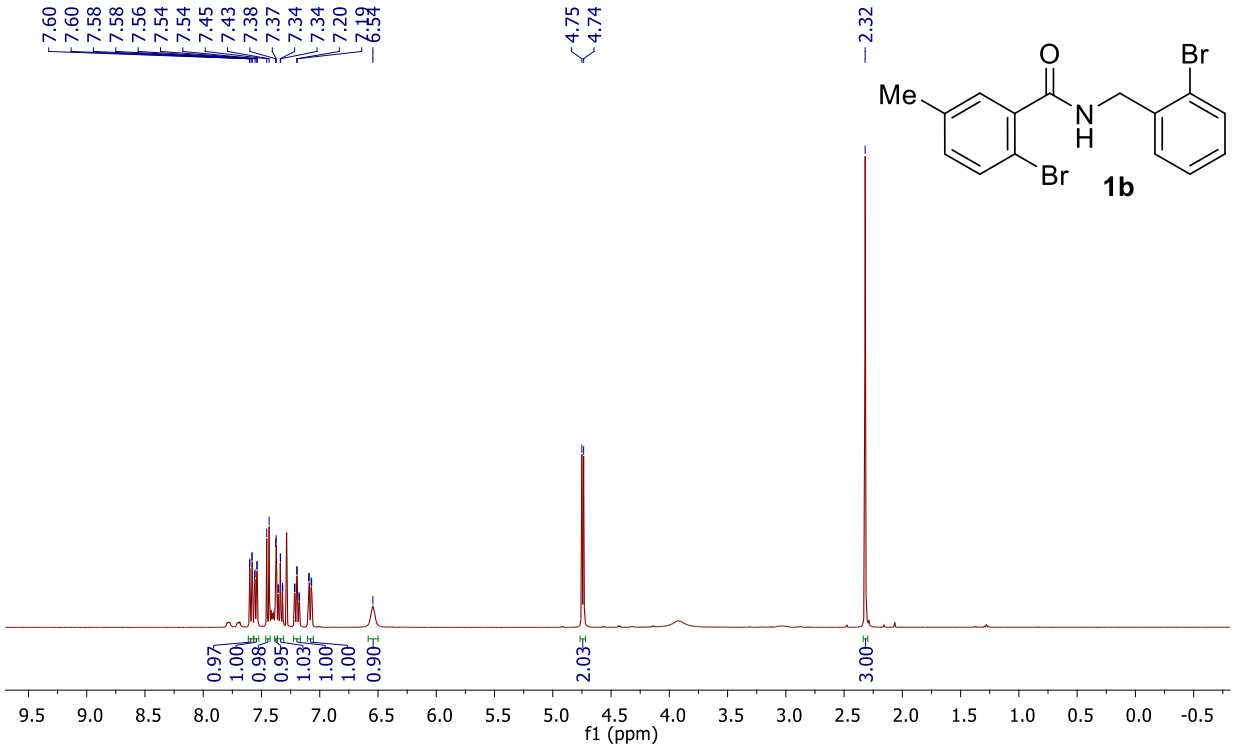
1. Copies of the ^{1}H and ^{13}C NMR spectra of 1a-g, 4aa-4gc, 5aa-5al and 6aa



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4.74
2.32
O
Br
Me
N
H
Br
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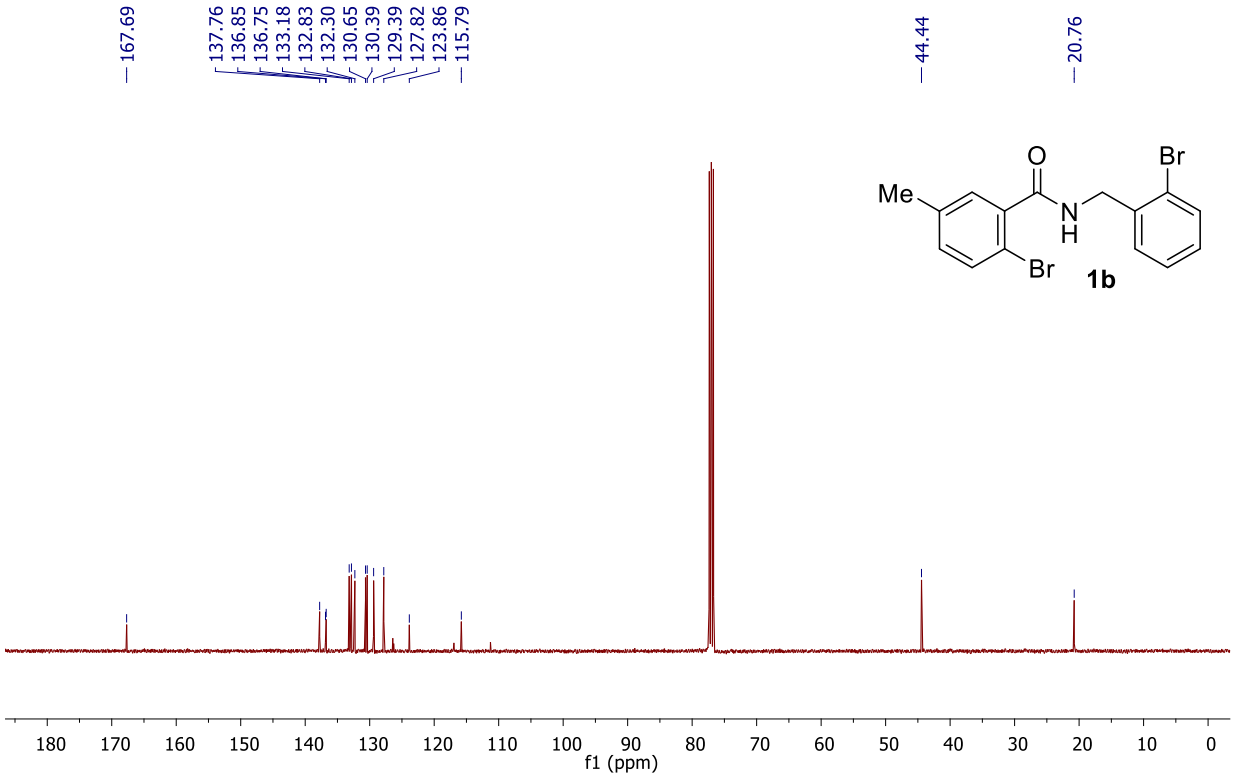
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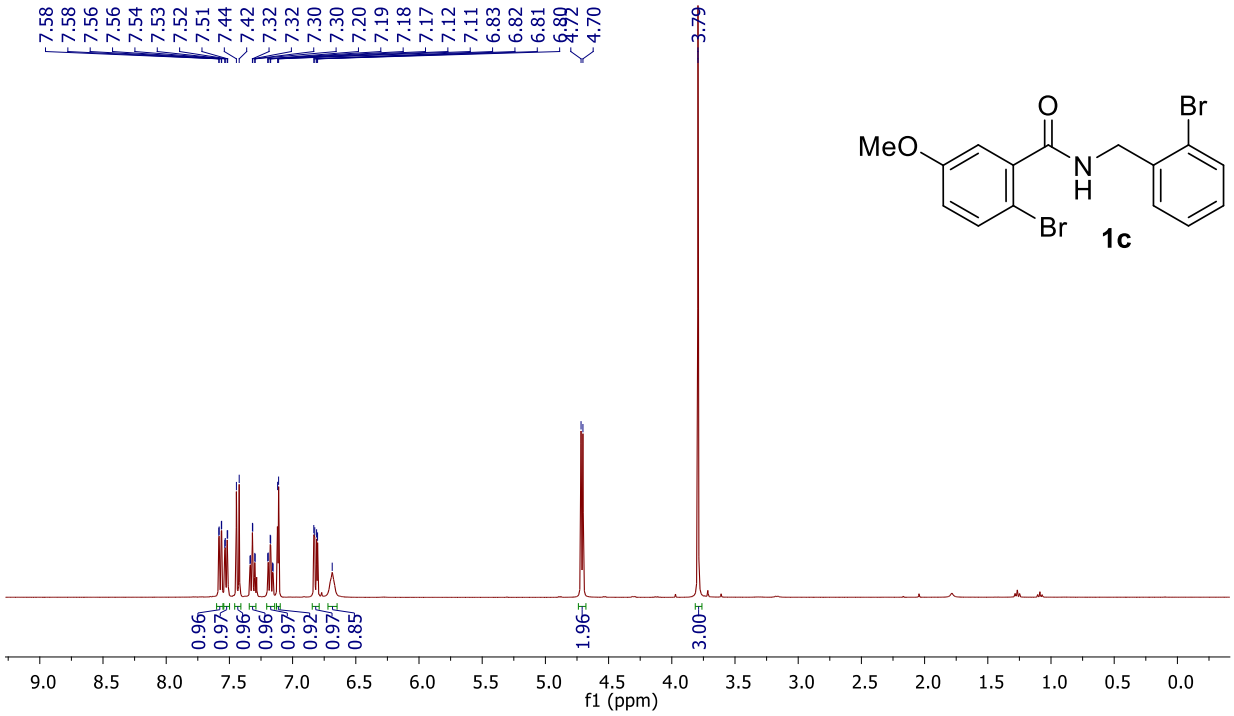
f1 (ppm)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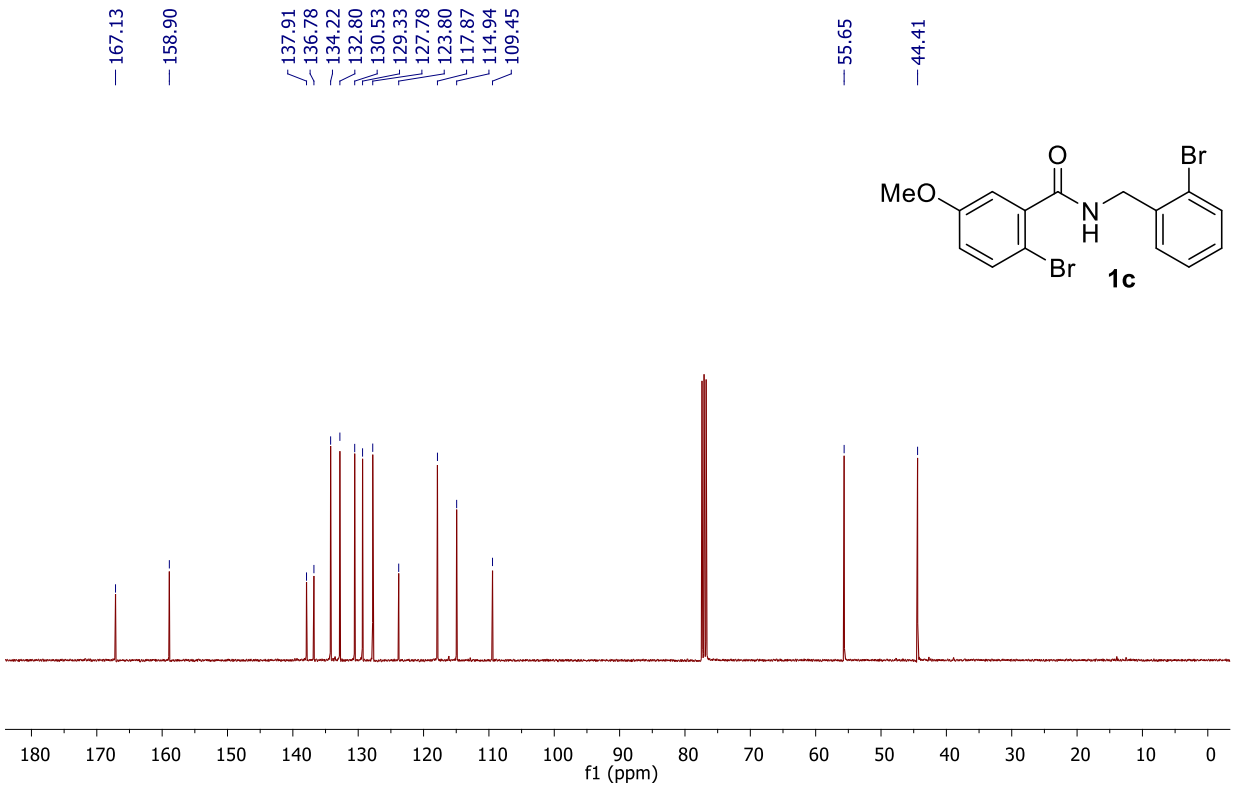
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Br
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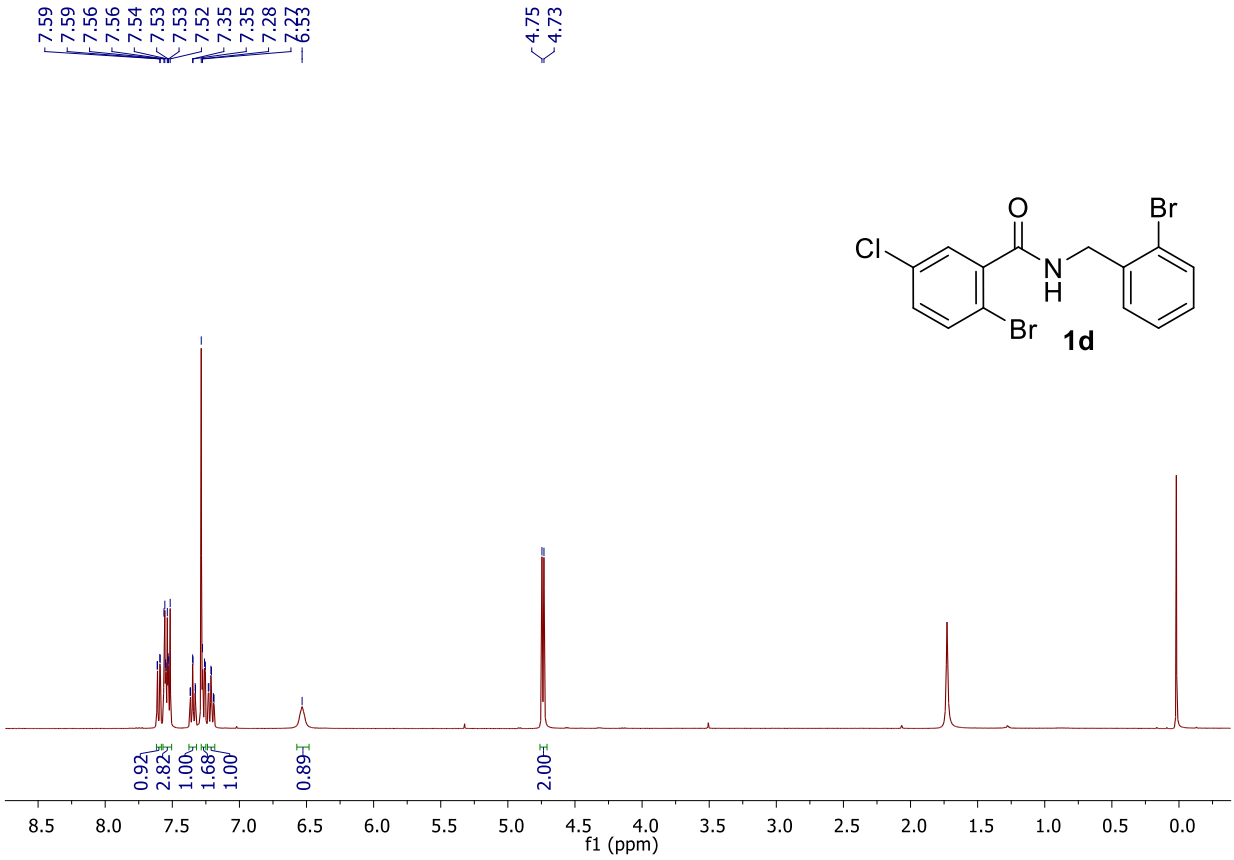
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Br
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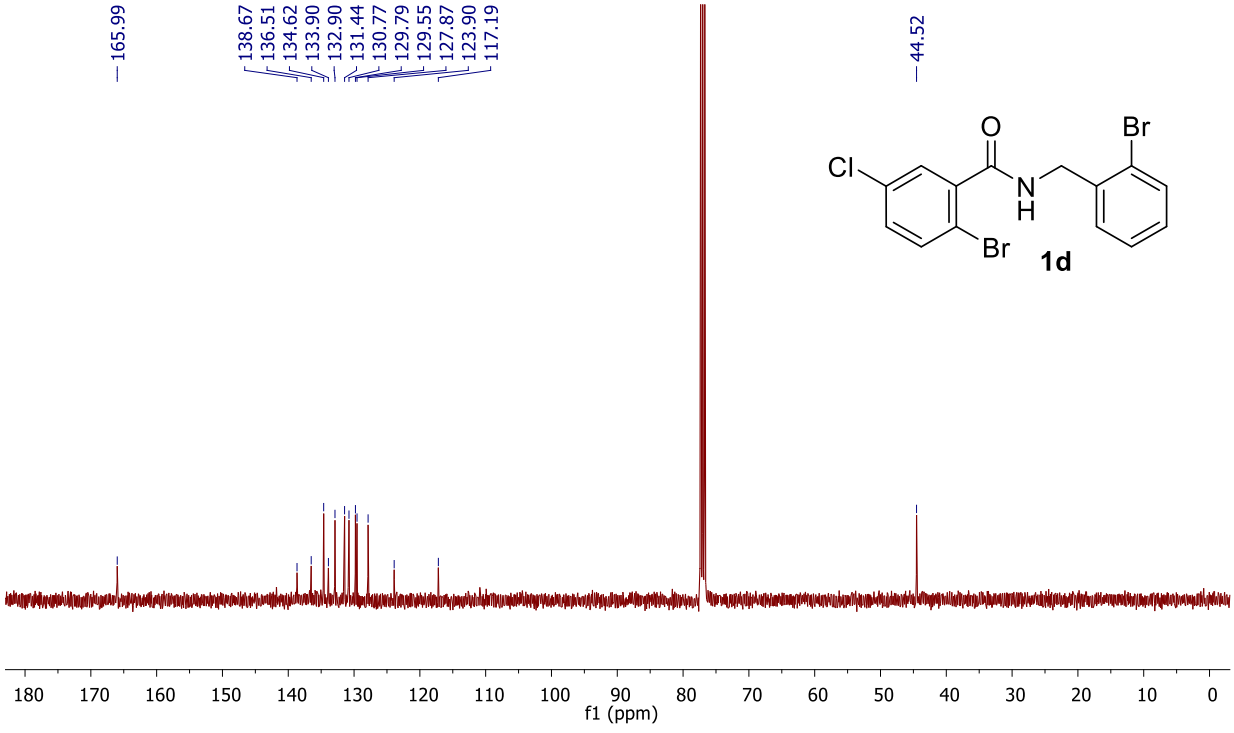
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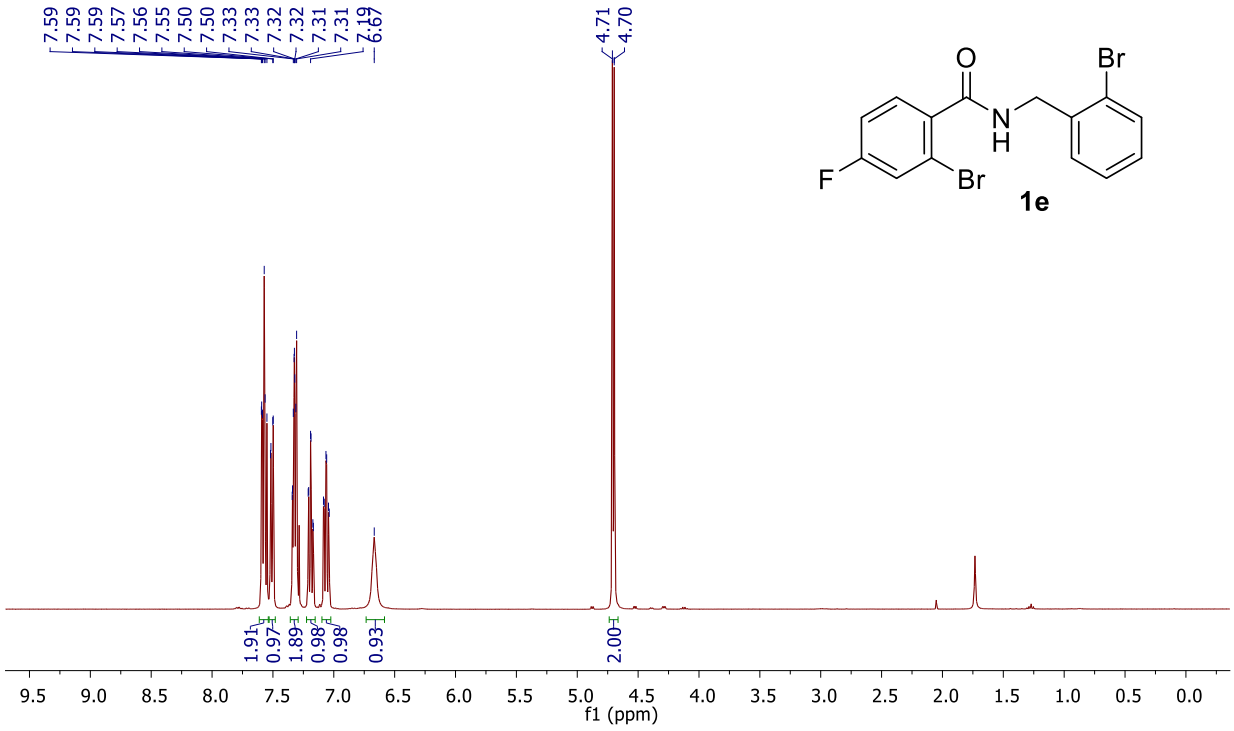
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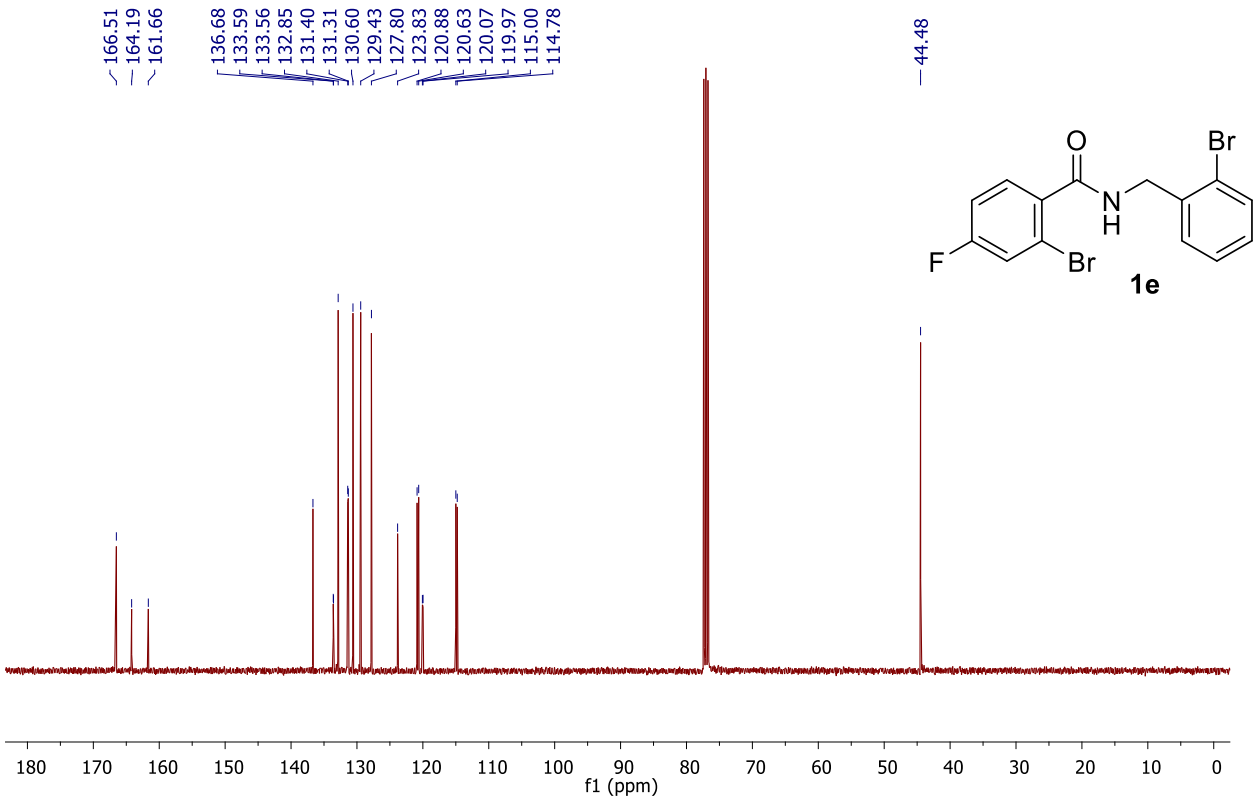
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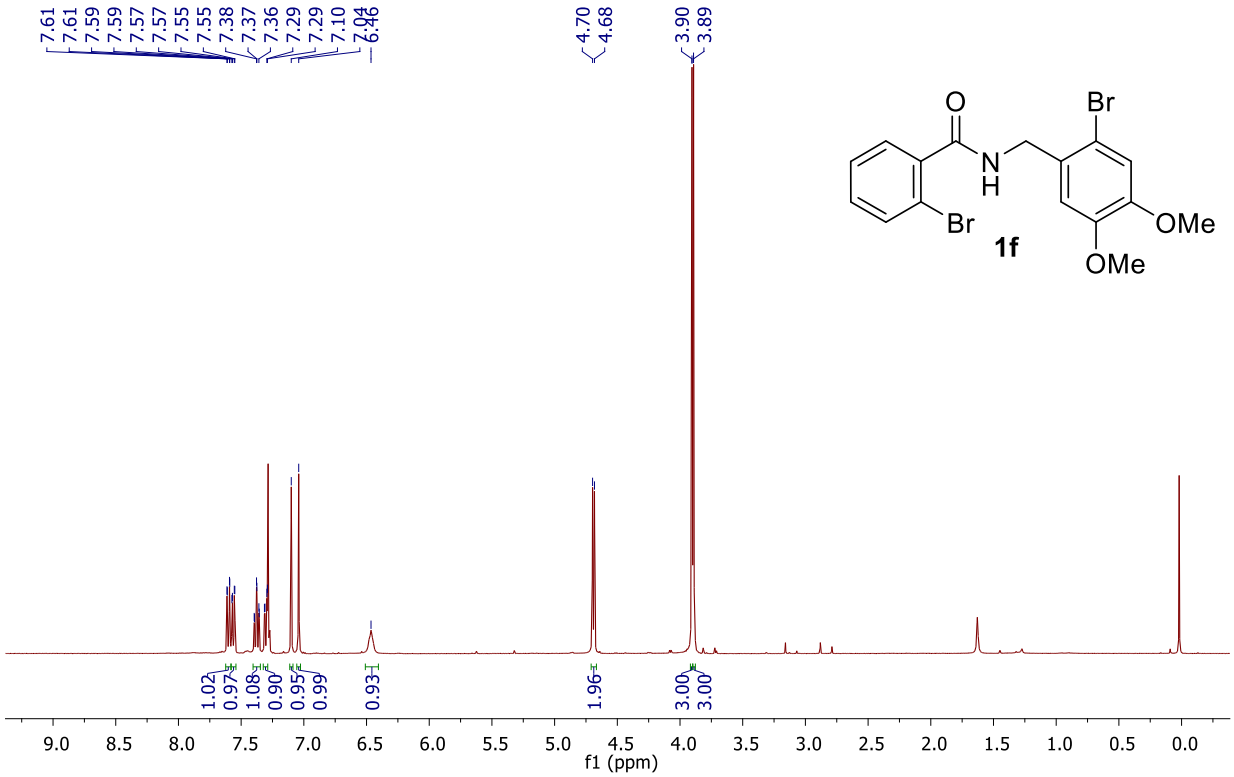
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4.68
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3.89
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Br
N
H
Br
OMe
OMe
1f
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0.97
1.08
0.90
0.95
0.99
0.93
1.96
3.00
3.00
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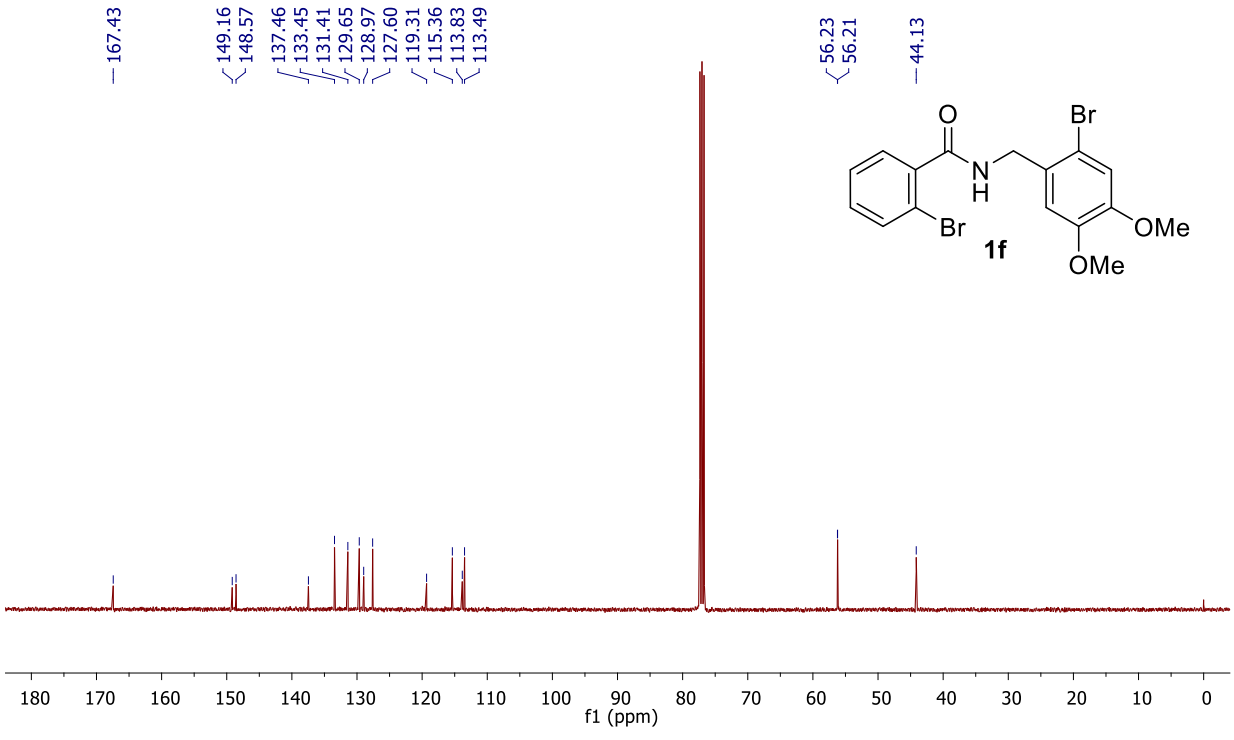
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OMe
OMe
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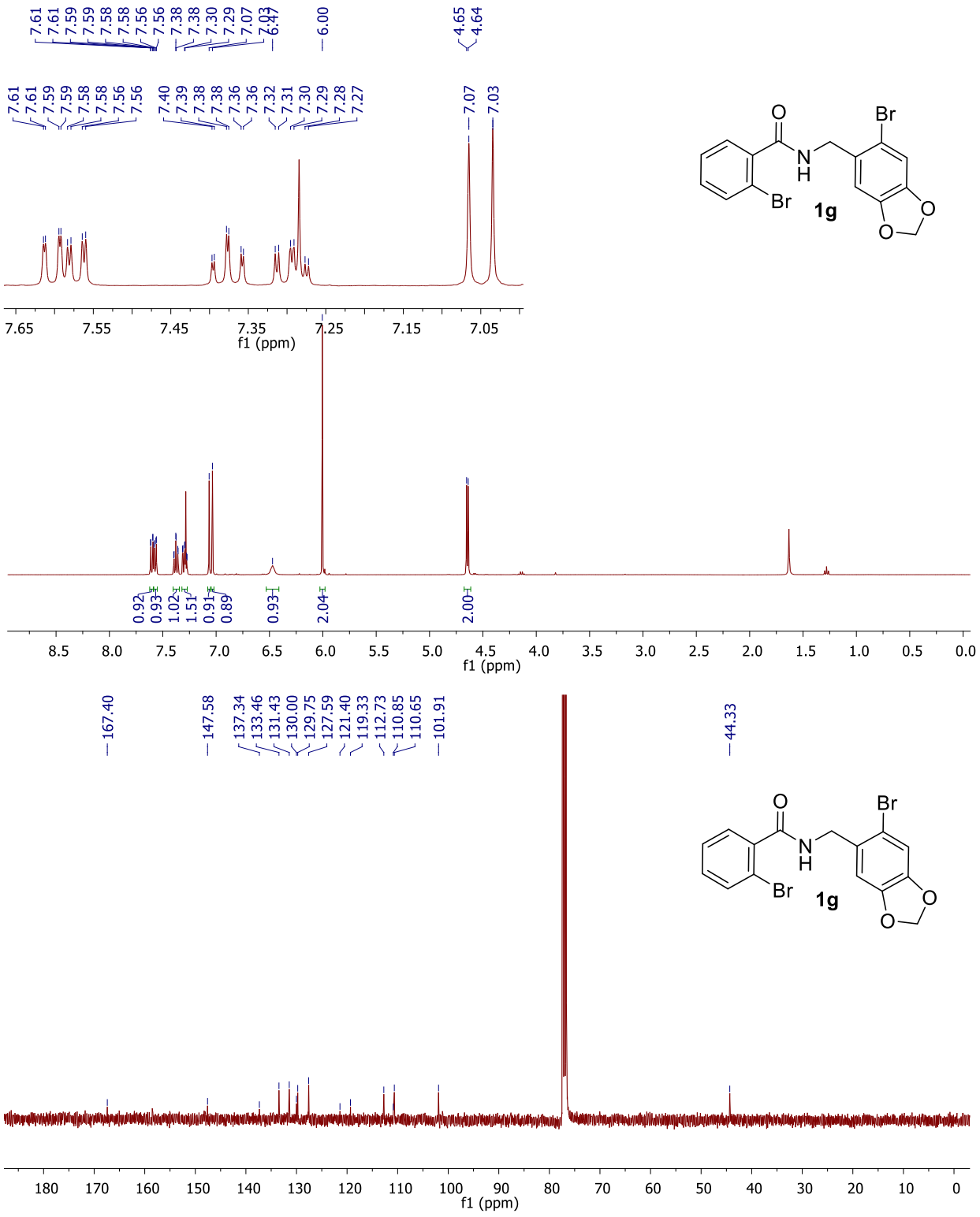
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f1 (ppm)
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0.89
0.93
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H
Br
Br
O
O
1g
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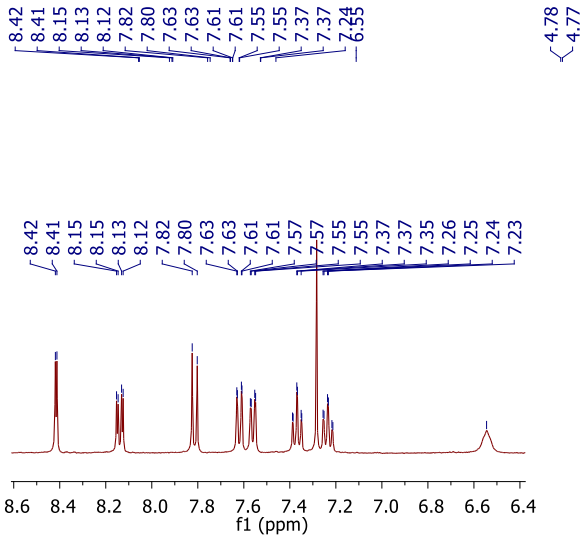
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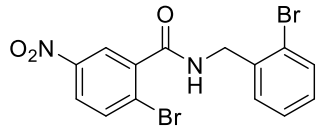
f1 (ppm)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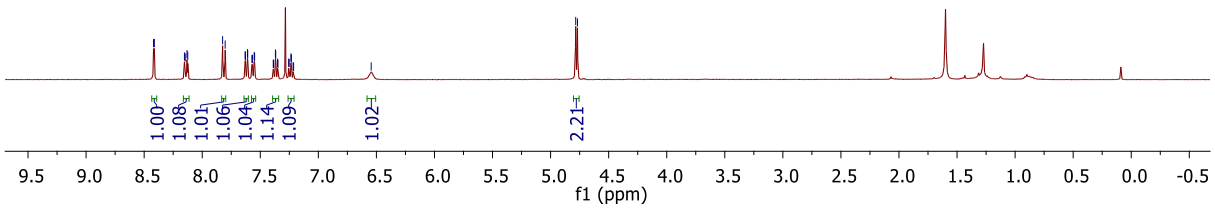
O2N
N
H
Br

1h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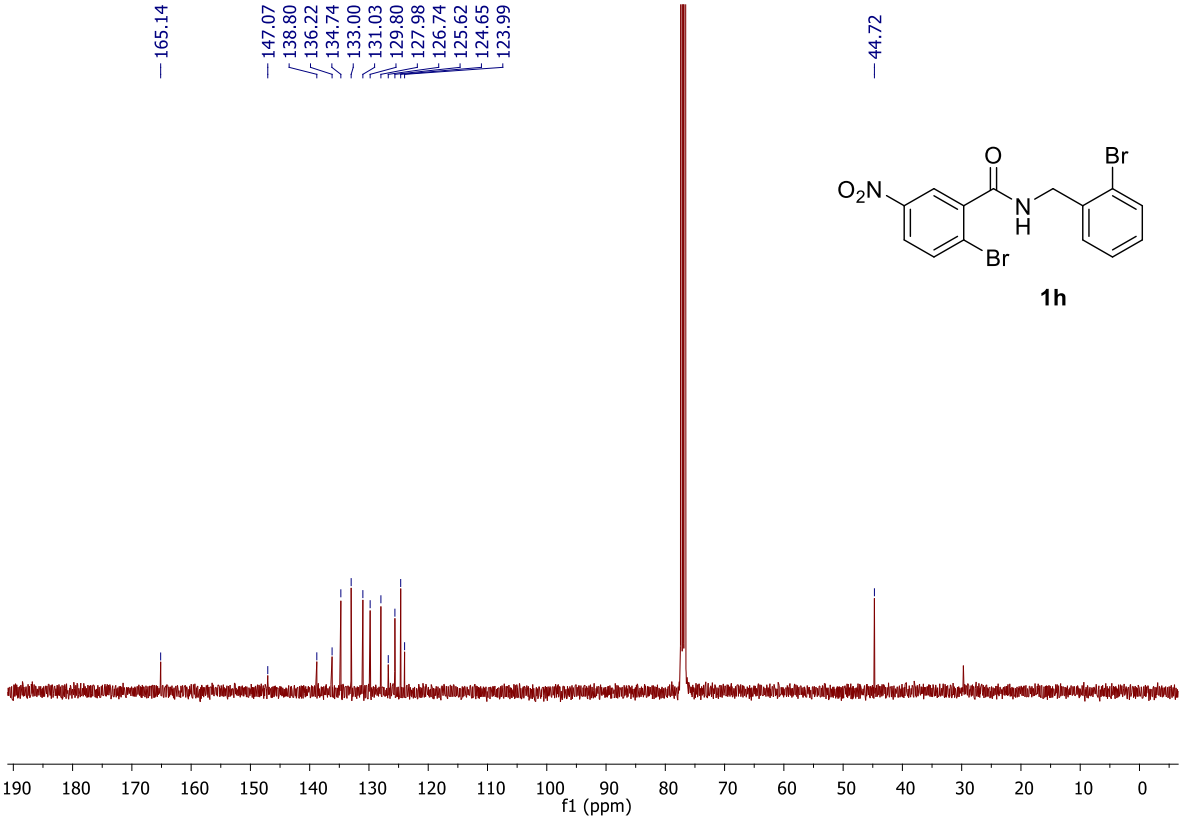
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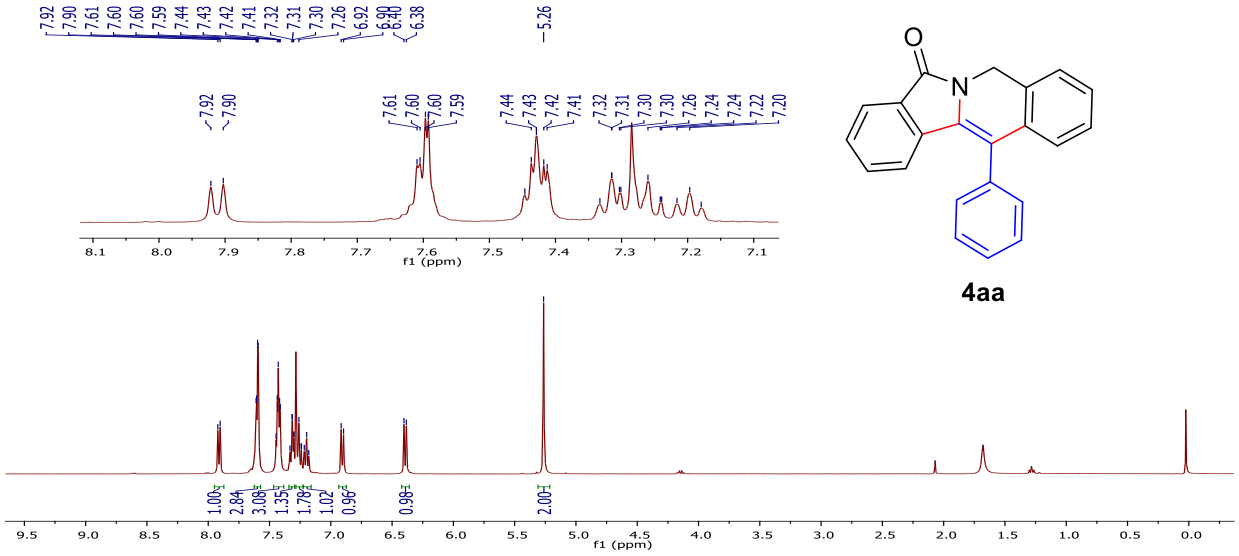
f1 (ppm)

O
Br
O2N
N
H
Br

1h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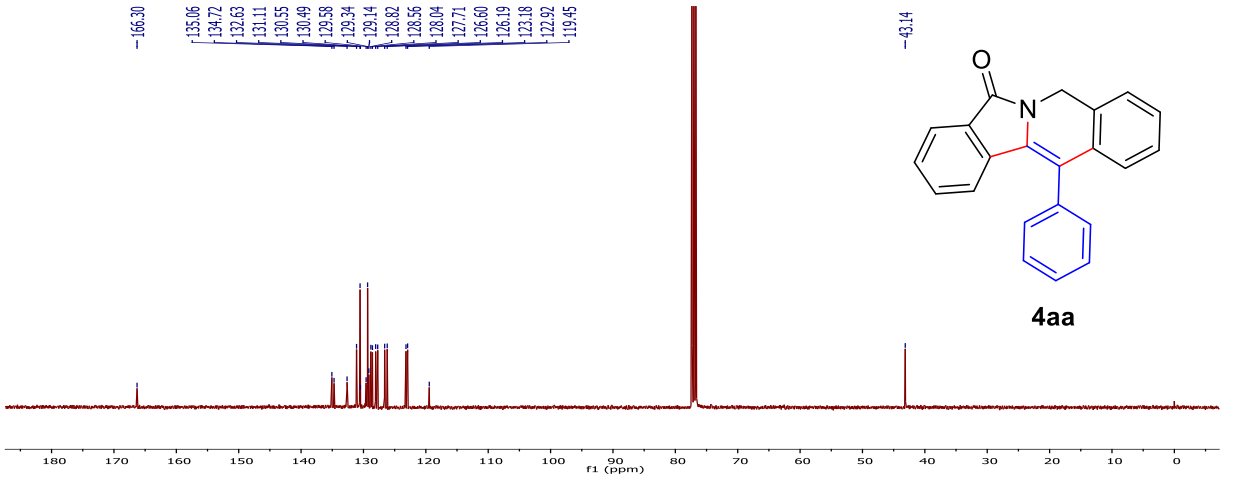
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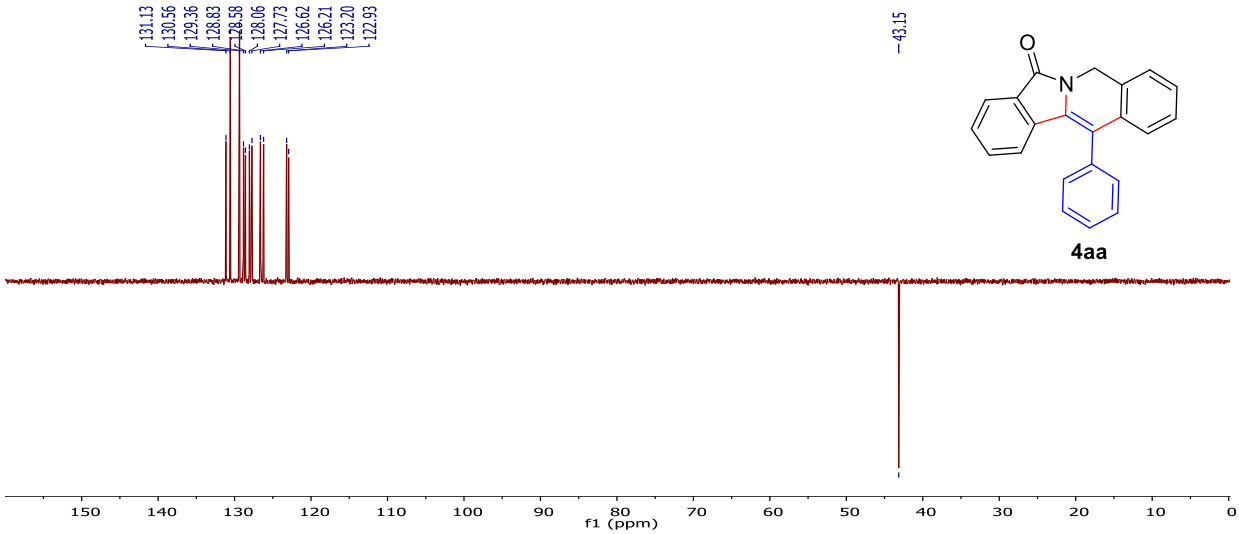
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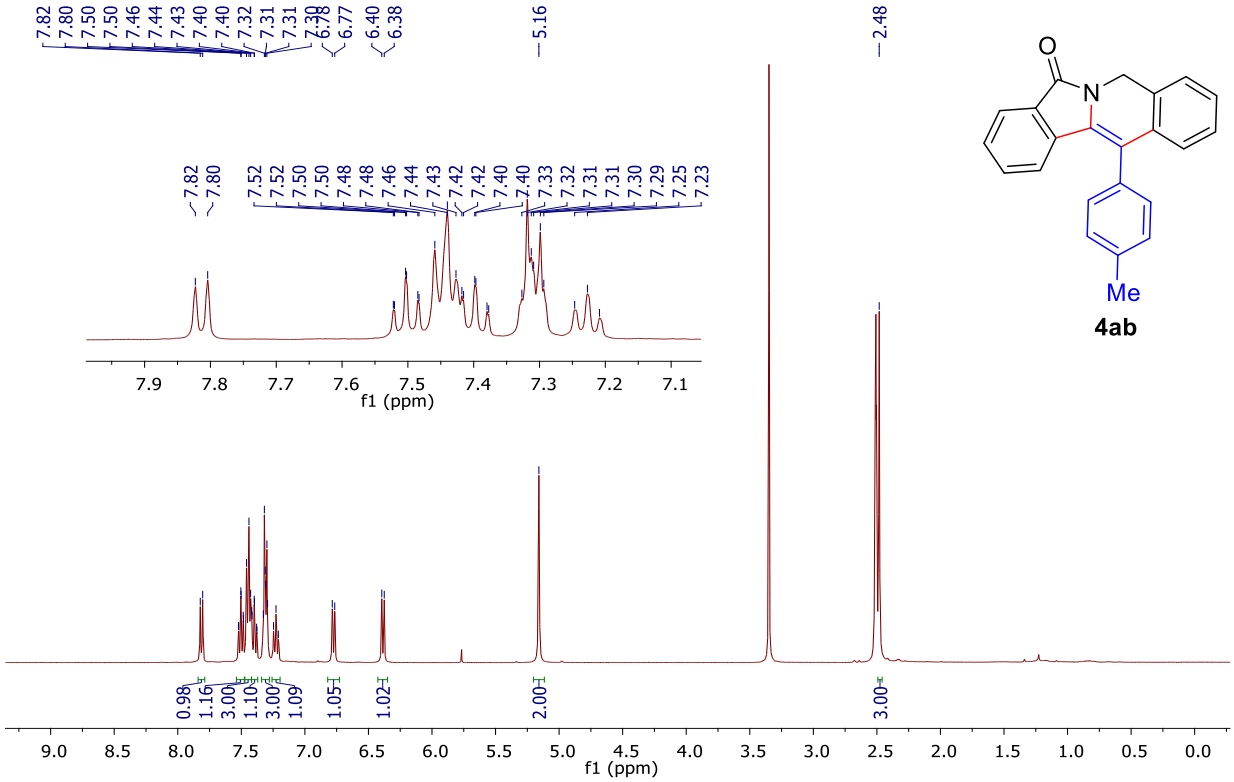
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7.29
7.25
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Me
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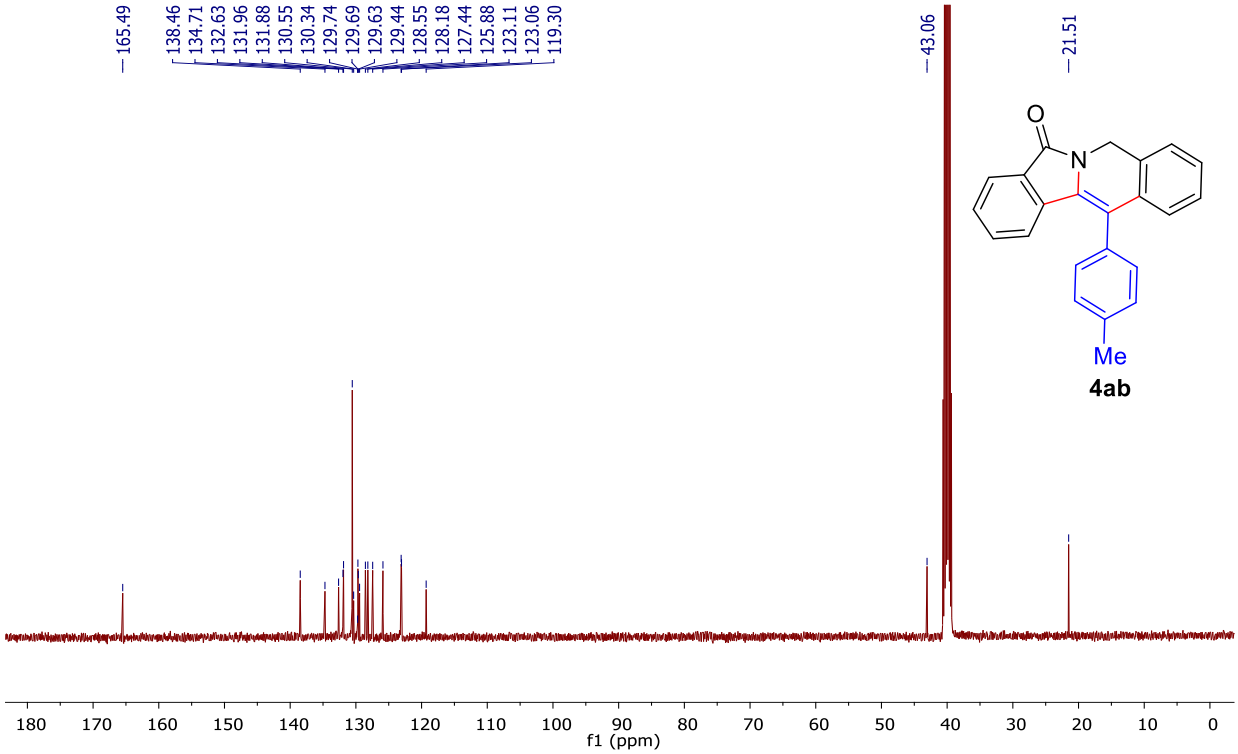
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Me
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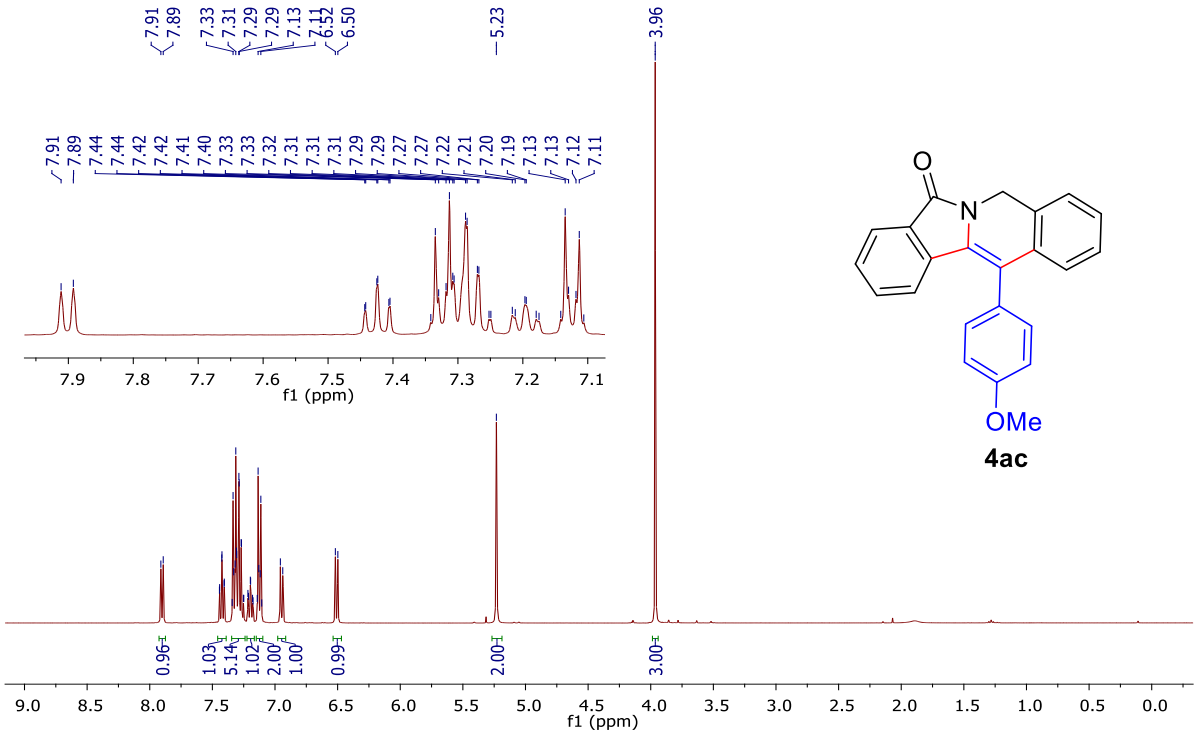
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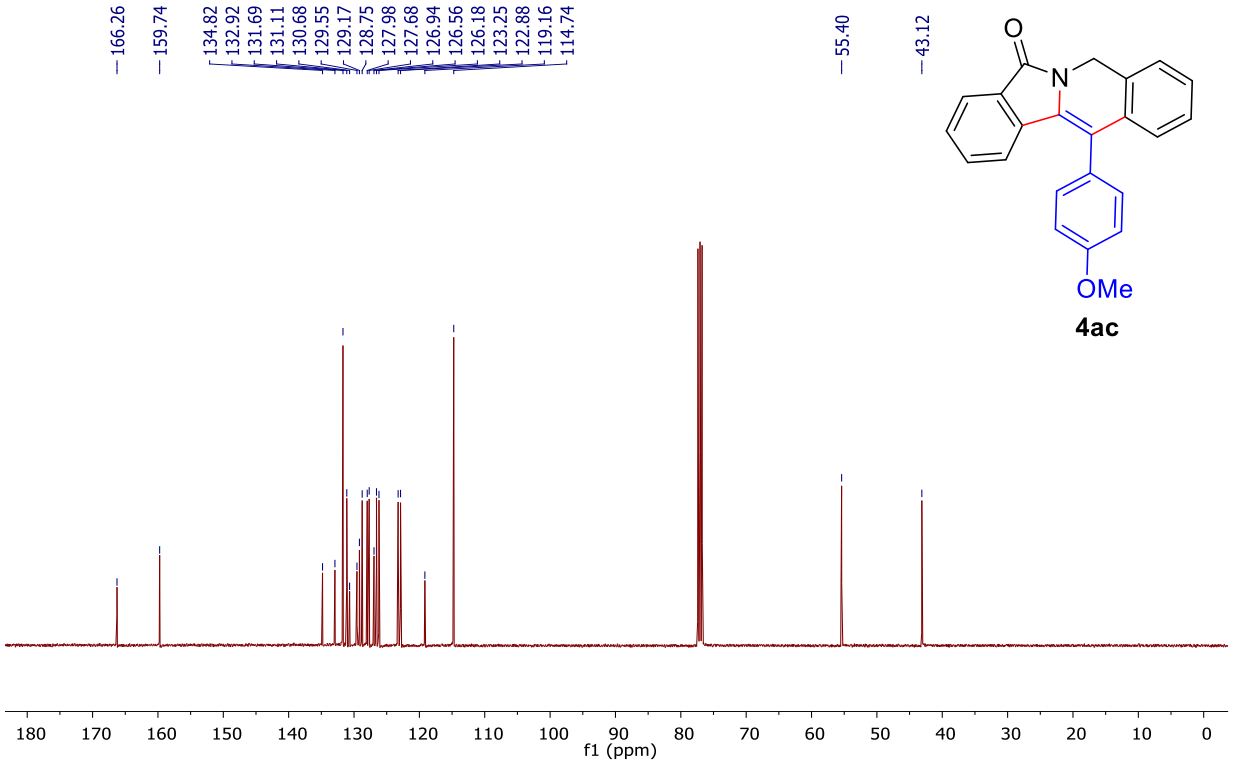
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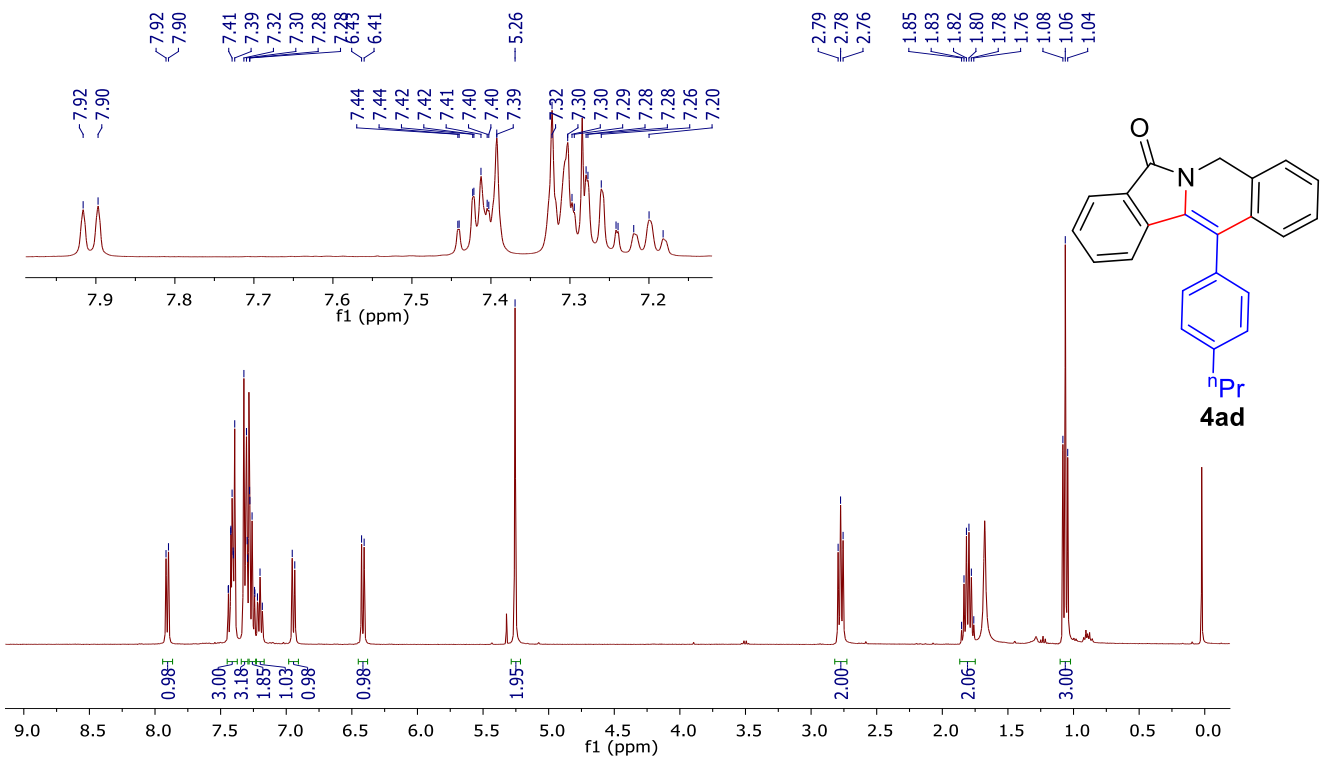
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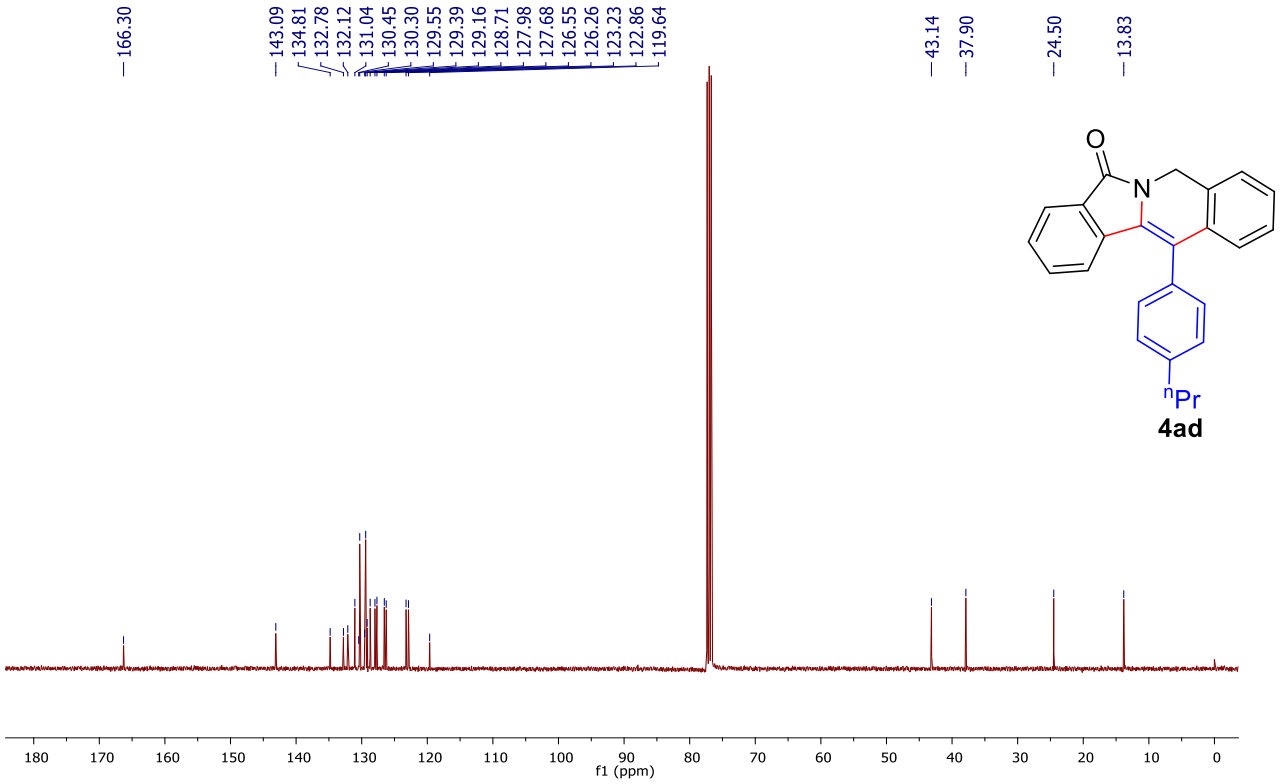
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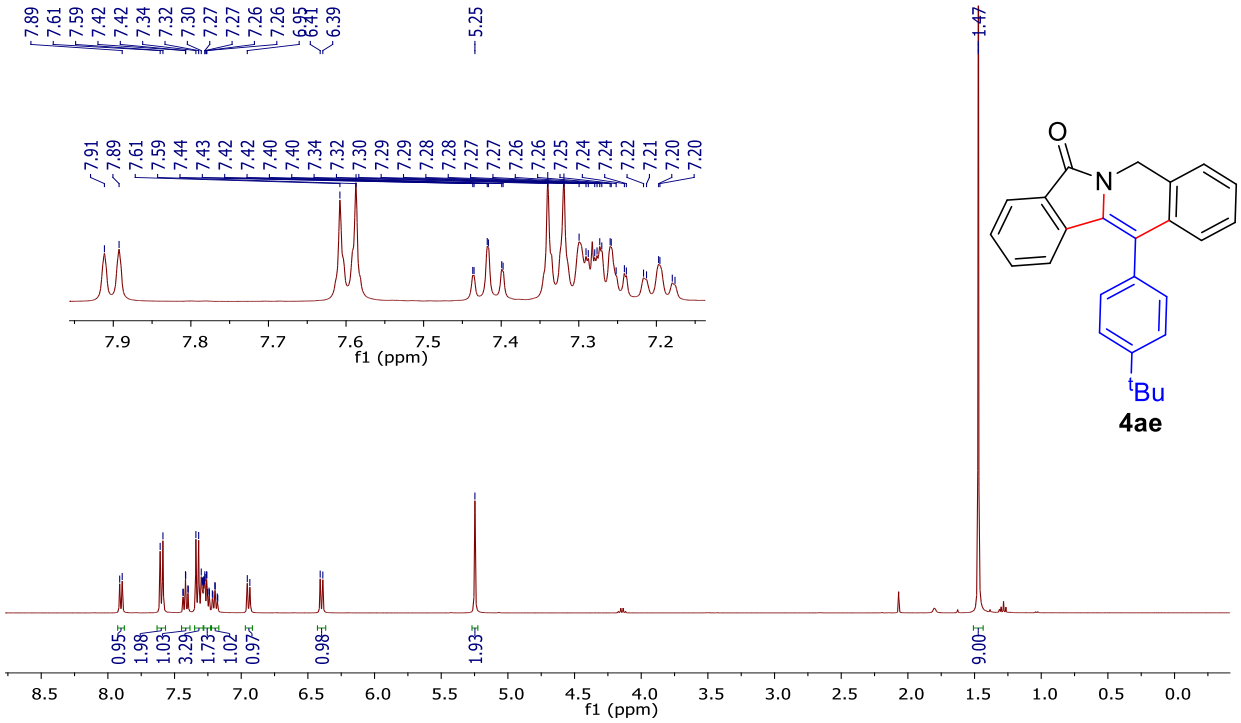
f1 (ppm)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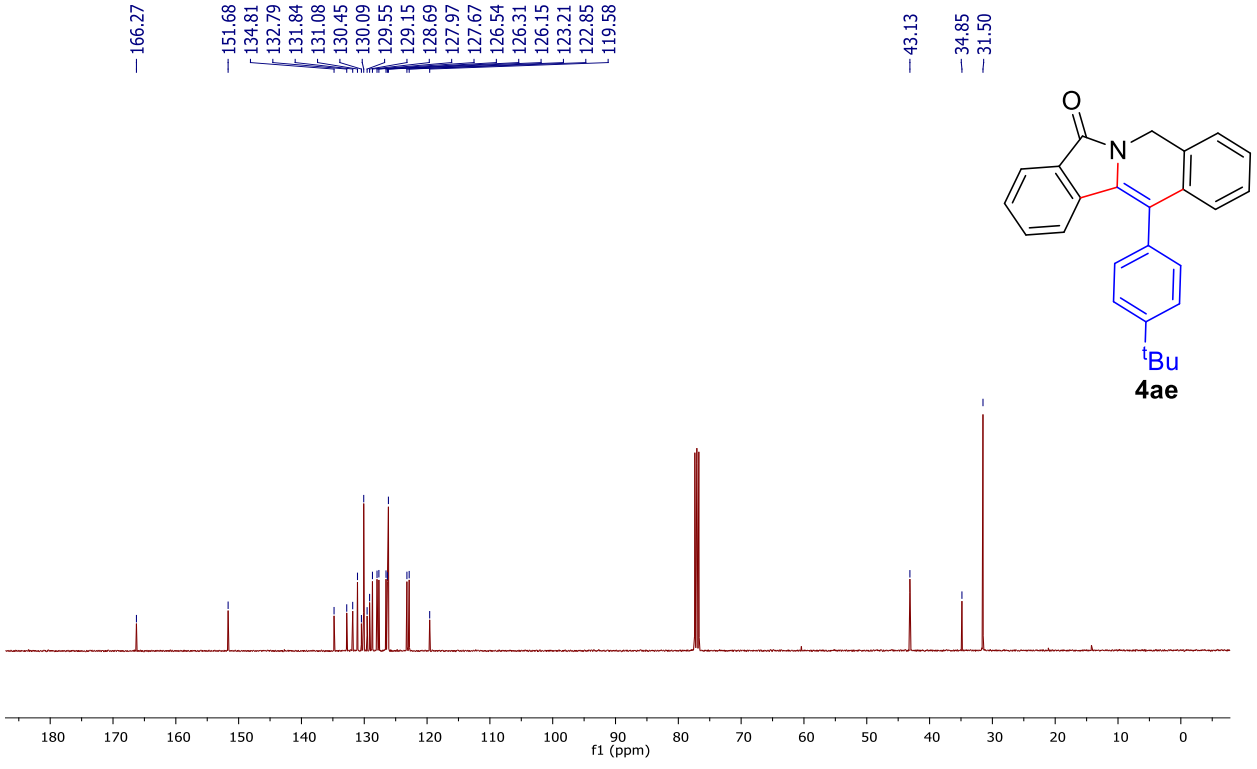
7.59
7.42
7.42
7.34
7.32
7.30
7.27
7.27
7.26
7.26
6.95
6.41
6.39
5.25
1.47
7.91
7.89
7.61
7.59
7.44
7.43
7.42
7.42
7.40
7.40
7.34
7.32
7.30
7.29
7.29
7.28
7.28
7.27
7.27
7.26
7.26
7.25
7.24
7.24
7.22
7.21
7.20
7.20
f1 (ppm)
O
N
tBu
4ae
0.95
1.98
1.03
3.29
1.73
1.02
0.97
0.98
1.93
9.00
f1 (ppm)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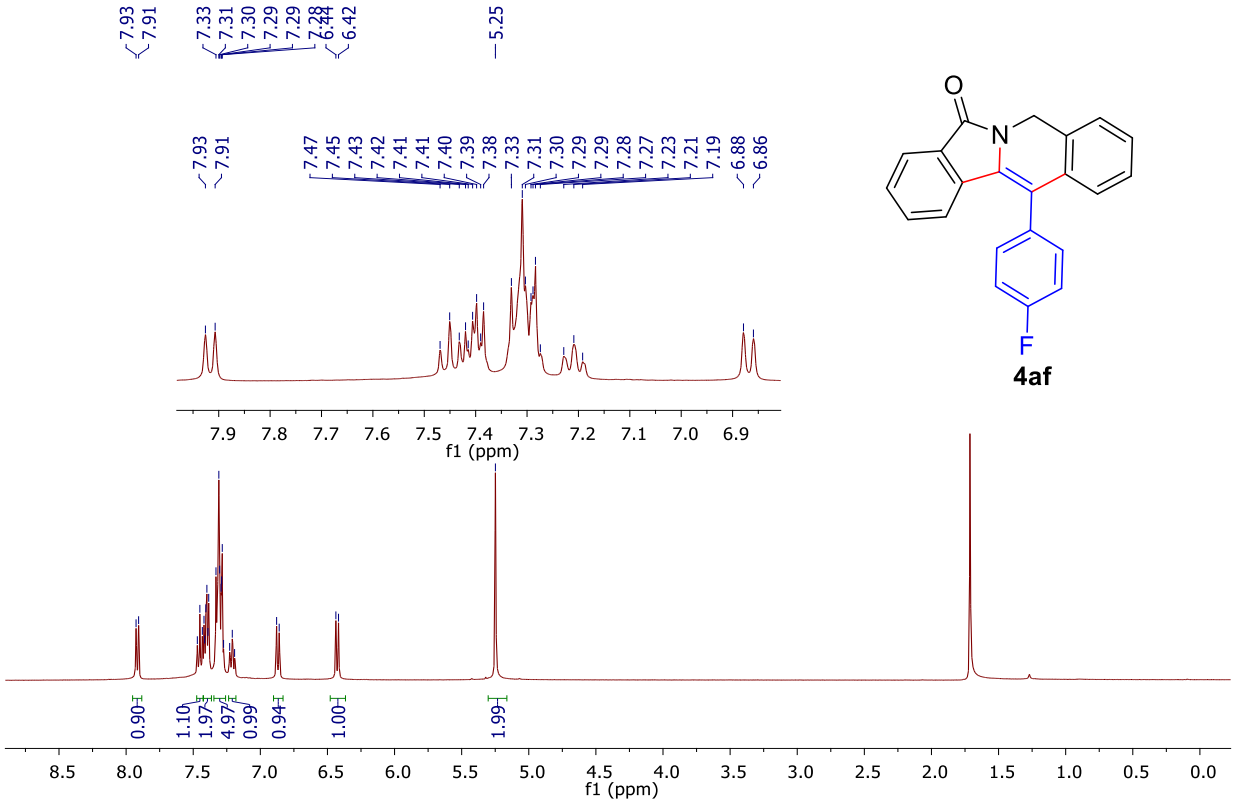
151.68
134.81
132.79
131.84
131.08
130.45
130.09
129.55
129.15
128.69
127.97
127.67
126.54
126.31
126.15
123.21
122.85
119.58
43.13
34.85
31.50
O
N
tBu
4ae
f1 (ppm)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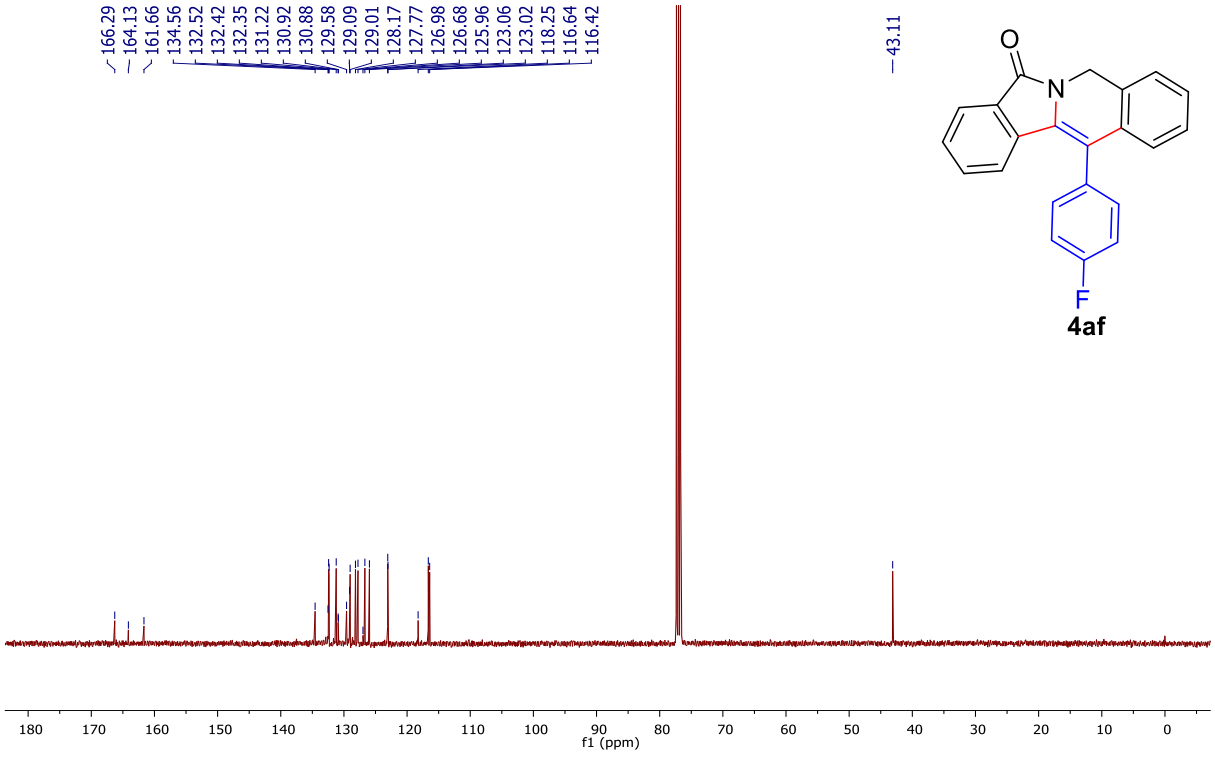
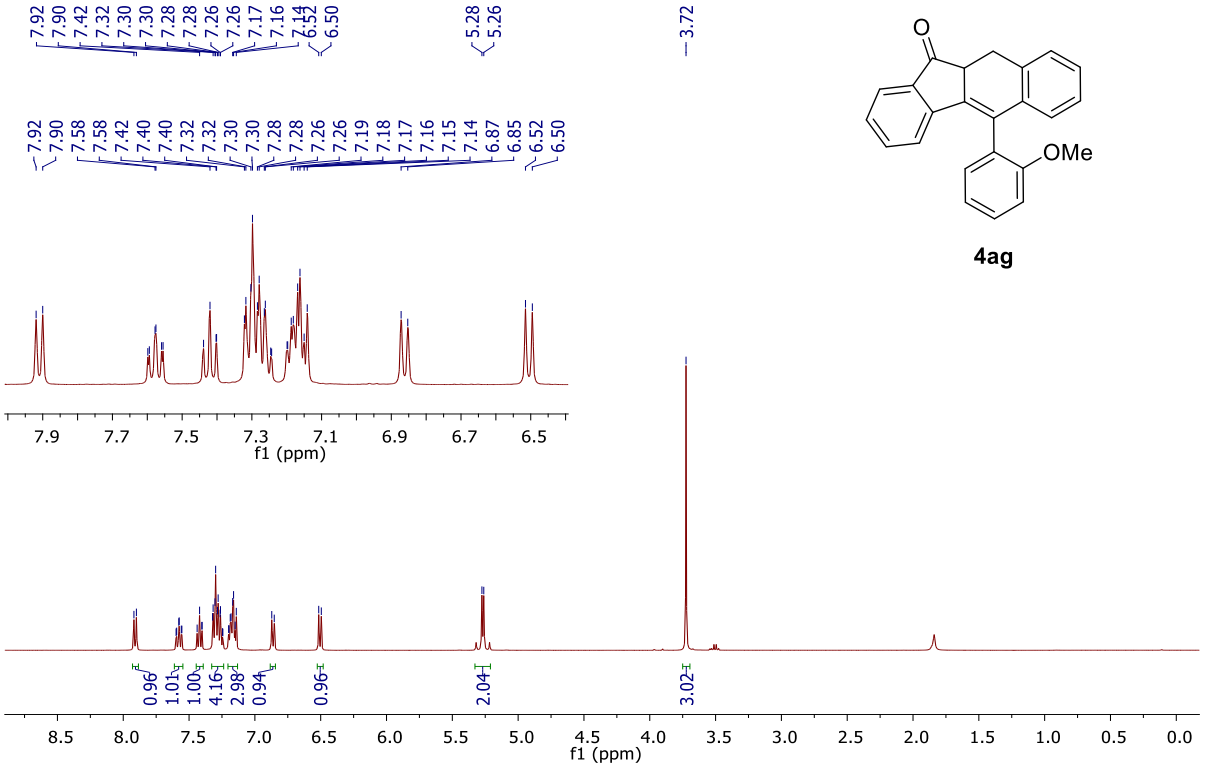
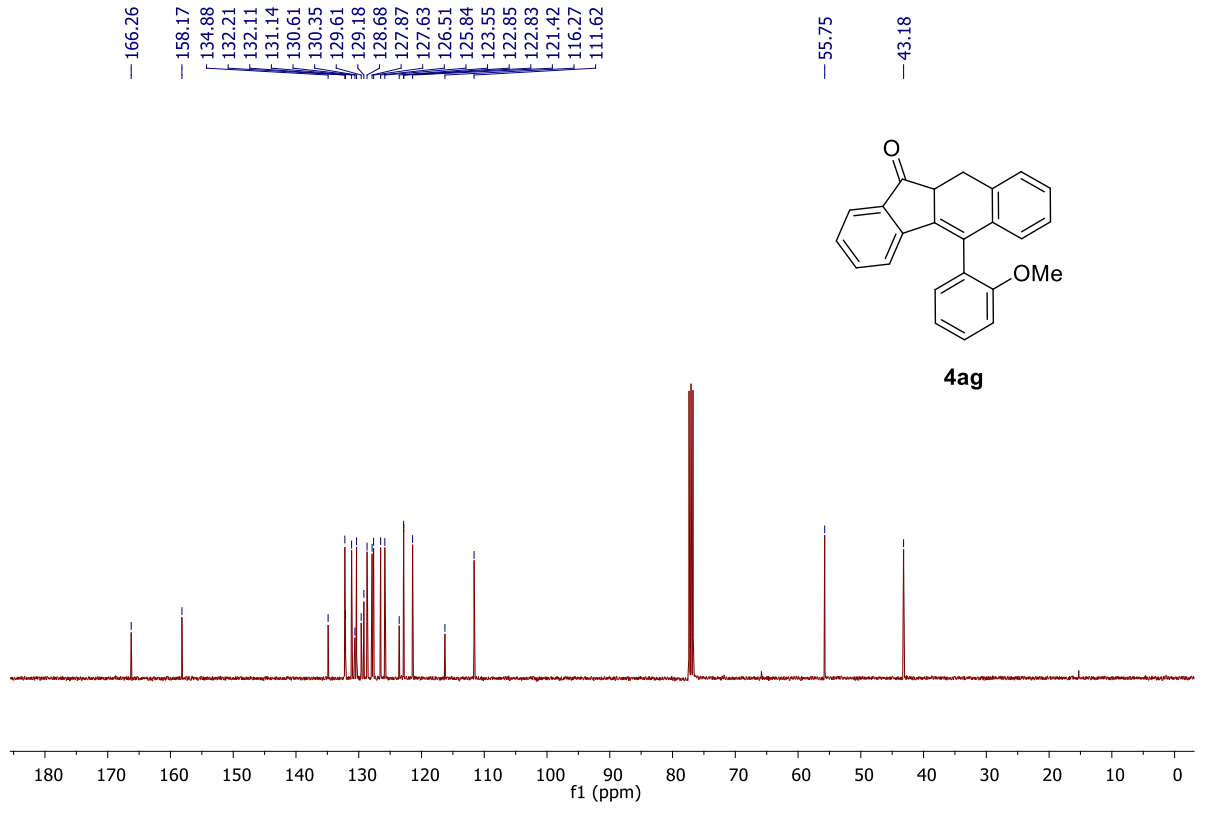
7.91
7.33
7.31
7.30
7.29
7.29
7.28
6.44
6.42
5.25
7.47
7.45
7.43
7.42
7.41
7.41
7.40
7.39
7.38
7.33
7.31
7.30
7.29
7.29
7.28
7.27
7.23
7.21
7.19
6.88
6.86
O
N
F
4af
f1 (ppm)
0.90
1.10
1.97
4.97
0.99
0.94
1.00
1.99


166.29
164.13
161.66
134.56
132.52
132.42
132.35
131.22
130.92
130.88
129.58
129.09
129.01
128.17
127.77
126.98
126.68
125.96
123.06
123.02
118.25
116.64
116.42
43.11
O
N
F
4af
f1 (ppm)


7.92
7.90
7.42
7.32
7.30
7.28
7.28
7.26
7.26
7.17
7.16
7.14
6.52
6.50
5.28
5.26
3.72
7.92
7.90
7.58
7.58
7.42
7.40
7.40
7.32
7.32
7.30
7.30
7.28
7.28
7.26
7.26
7.19
7.18
7.17
7.16
7.15
7.14
6.87
6.85
6.52
6.50
0.96
1.01
1.00
4.16
2.98
0.94
0.96
2.04
3.02
f1 (ppm)
O
OMe

4ag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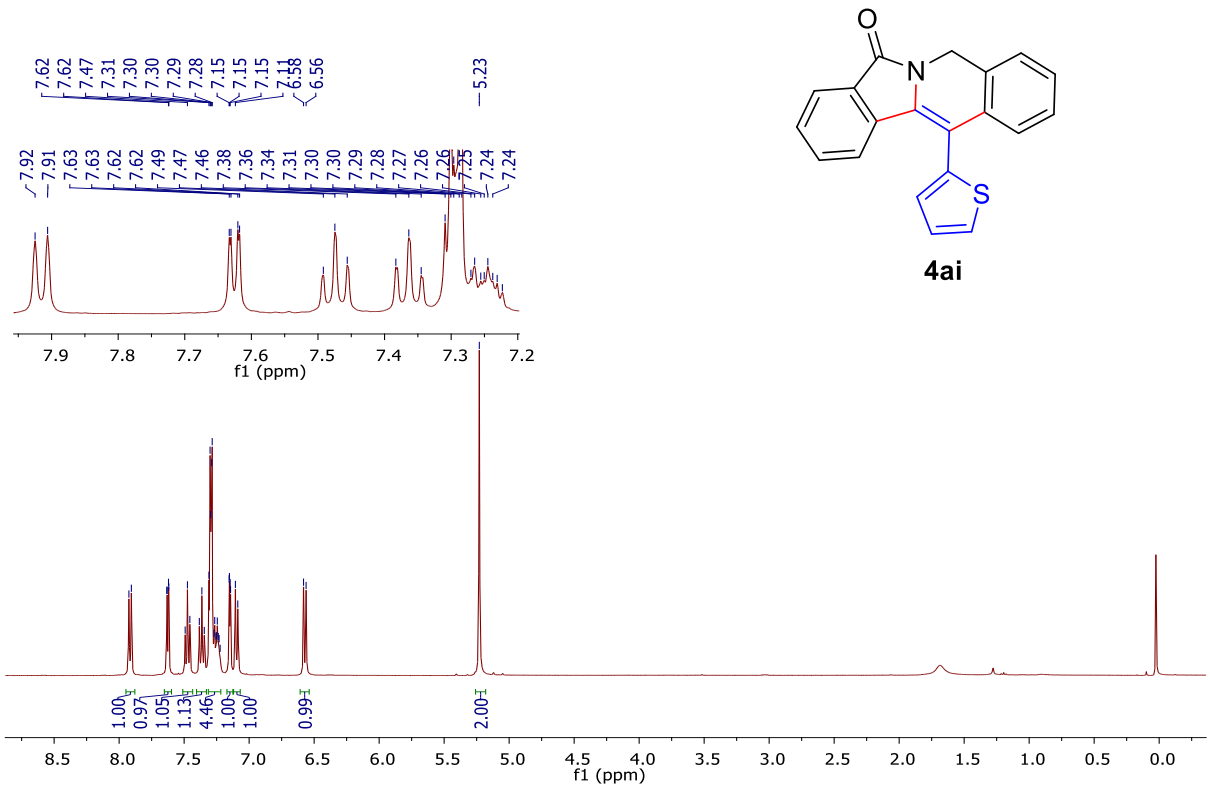
158.17
134.88
132.21
132.11
131.14
130.61
130.35
129.61
129.18
128.68
127.87
127.63
126.51
125.84
123.55
122.85
122.83
121.42
116.27
111.62
55.75
43.18
f1 (ppm)
O
OMe

4ag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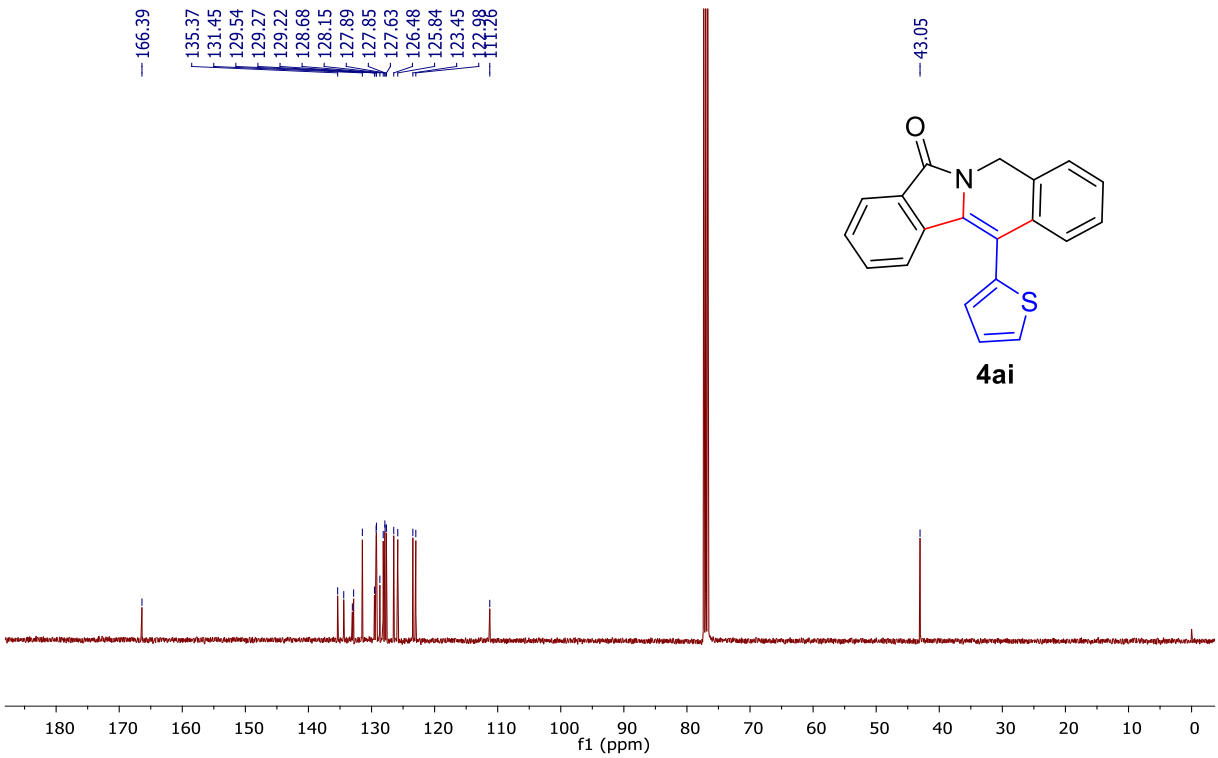
7.62
7.47
7.31
7.30
7.30
7.29
7.28
7.15
7.15
7.15
7.11
6.58
6.56
5.23
7.92
7.91
7.63
7.63
7.62
7.62
7.49
7.47
7.46
7.38
7.36
7.34
7.31
7.30
7.30
7.29
7.28
7.27
7.26
7.26
7.25
7.24
7.24
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
f1 (ppm)
1.00
0.97
1.05
1.13
4.46
1.00
1.00
0.99
2.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
O
N
S
4ai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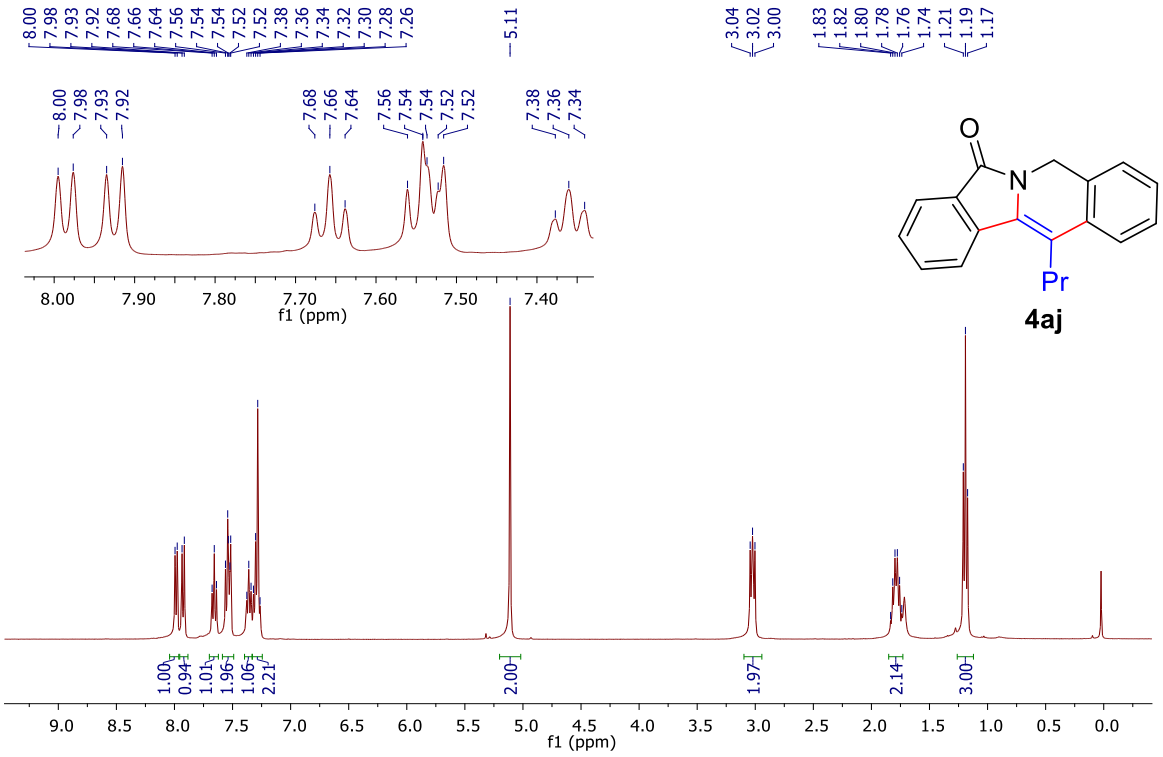
135.37
131.45
129.54
129.27
129.22
128.68
128.15
127.89
127.85
127.63
126.48
125.84
123.45
122.98
111.26
43.05
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
N
S
4ai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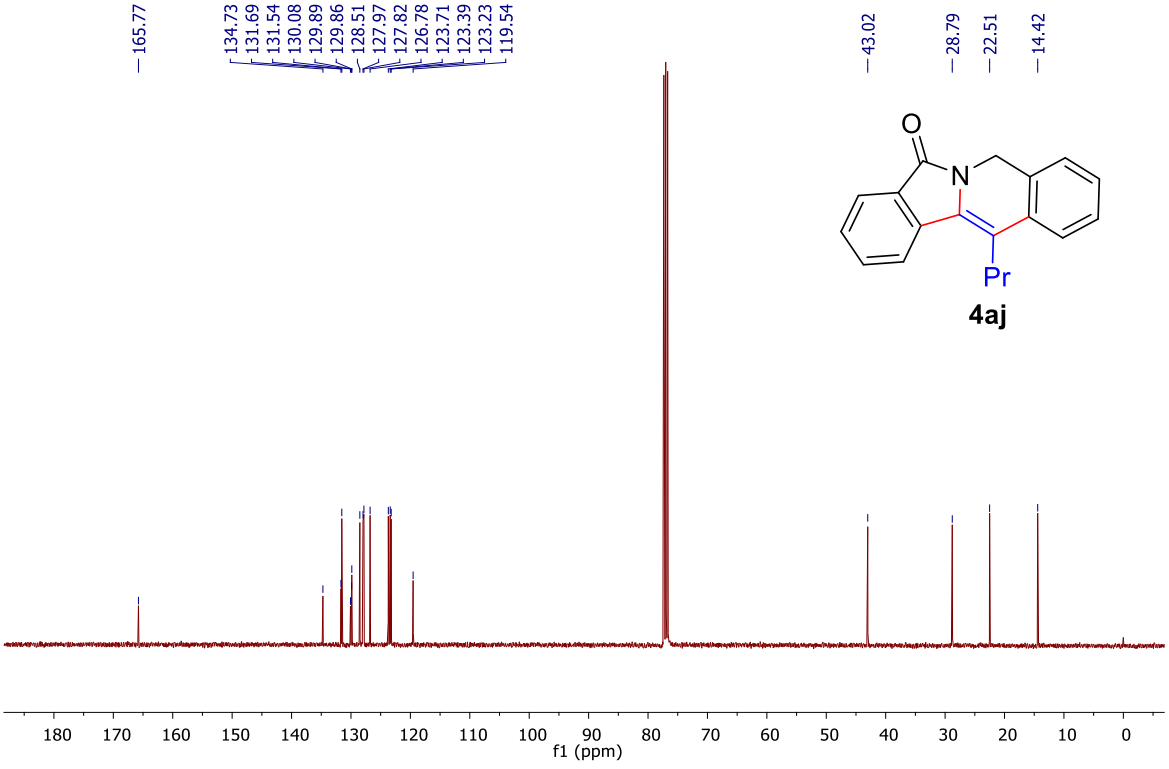
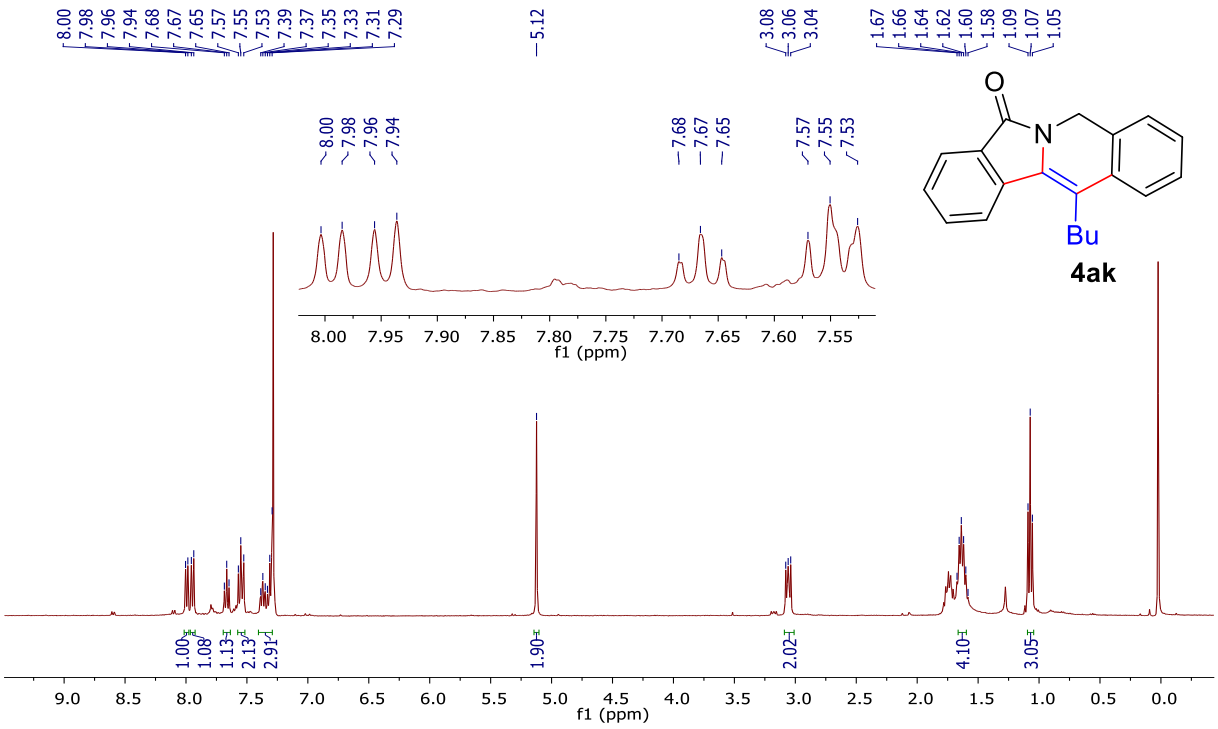
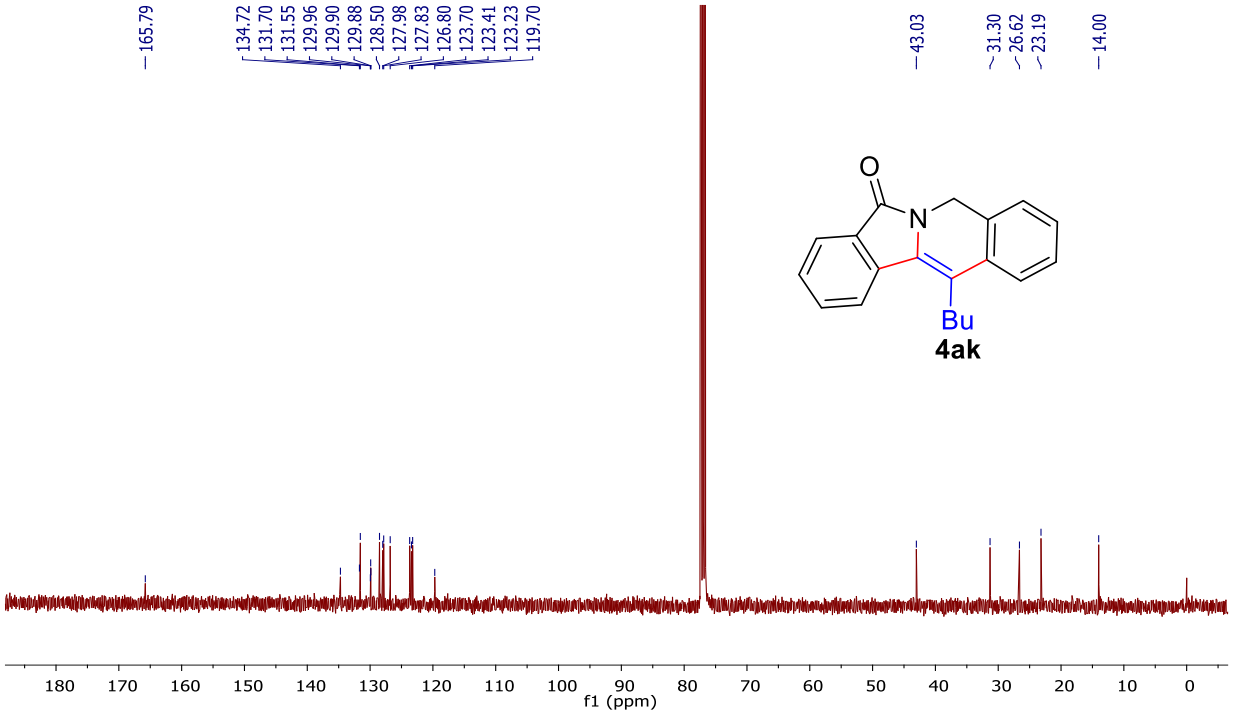
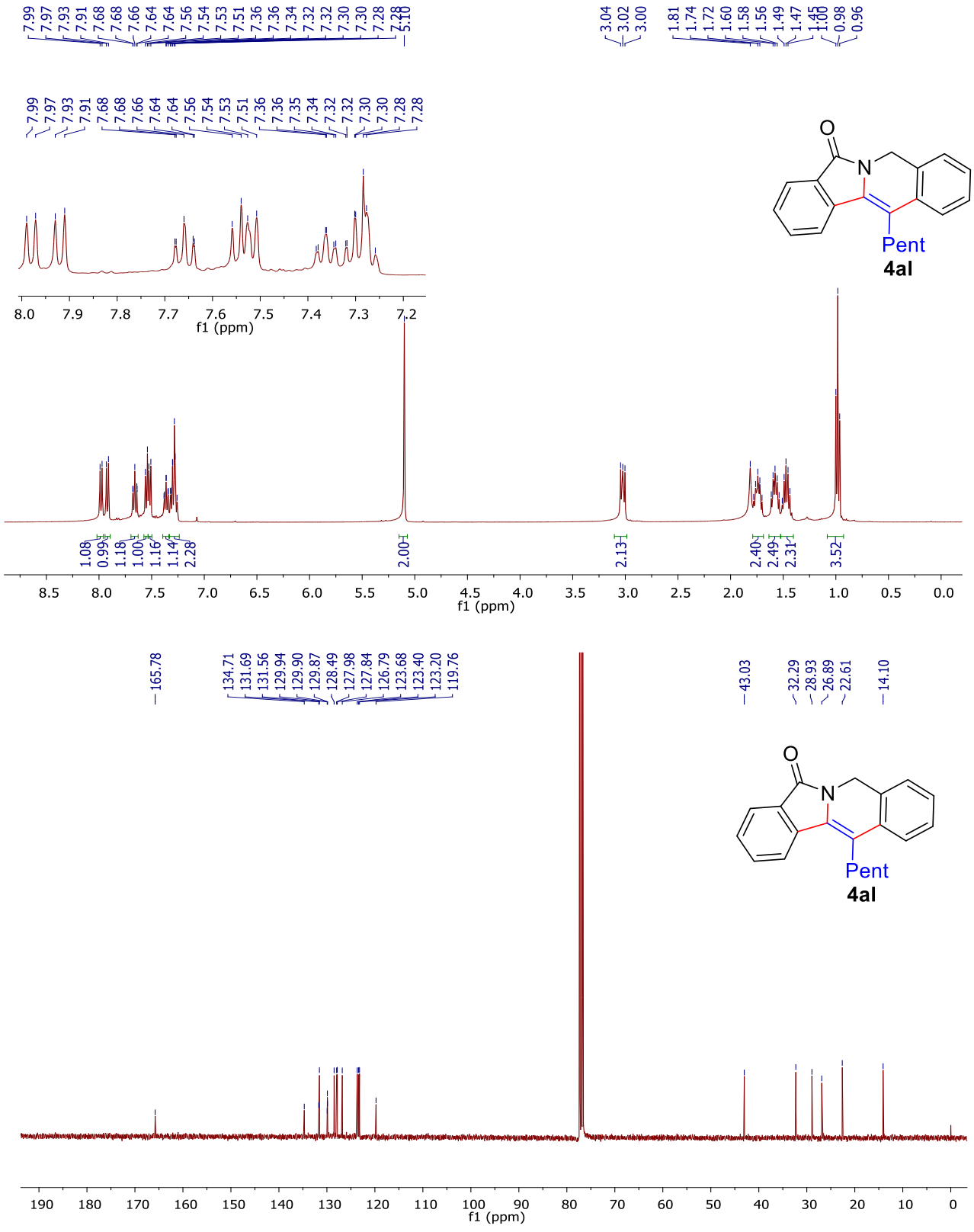
7.98
7.93
7.92
7.68
7.66
7.64
7.56
7.54
7.54
7.52
7.52
7.38
7.36
7.34
7.32
7.30
7.28
7.26
5.11
3.04
3.02
3.00
1.83
1.82
1.80
1.78
1.76
1.74
1.21
1.19
1.17
f1 (ppm)
1.00
0.94
1.01
1.96
1.06
2.21
2.00
1.97
2.14
3.00
O
N
Pr
4aj


165.77
134.73
131.69
131.54
130.08
129.89
129.86
128.51
127.97
127.82
126.78
123.71
123.39
123.23
119.54
43.02
28.79
22.51
14.42
f1 (ppm)
O
N
Pr
4aj


8.00
7.98
7.96
7.94
7.68
7.67
7.65
7.57
7.55
7.53
7.39
7.37
7.35
7.33
7.31
7.29
5.12
3.08
3.06
3.04
1.67
1.66
1.64
1.62
1.60
1.58
1.09
1.07
1.05
O
N
Bu
4ak
f1 (ppm)
1.00
1.08
1.13
2.13
2.91
1.90
2.02
4.10
3.05


165.79
134.72
131.70
131.55
129.96
129.90
129.88
128.50
127.98
127.83
126.80
123.70
123.41
123.23
119.70
43.03
31.30
26.62
23.19
14.00
O
N
Bu
4ak
f1 (ppm)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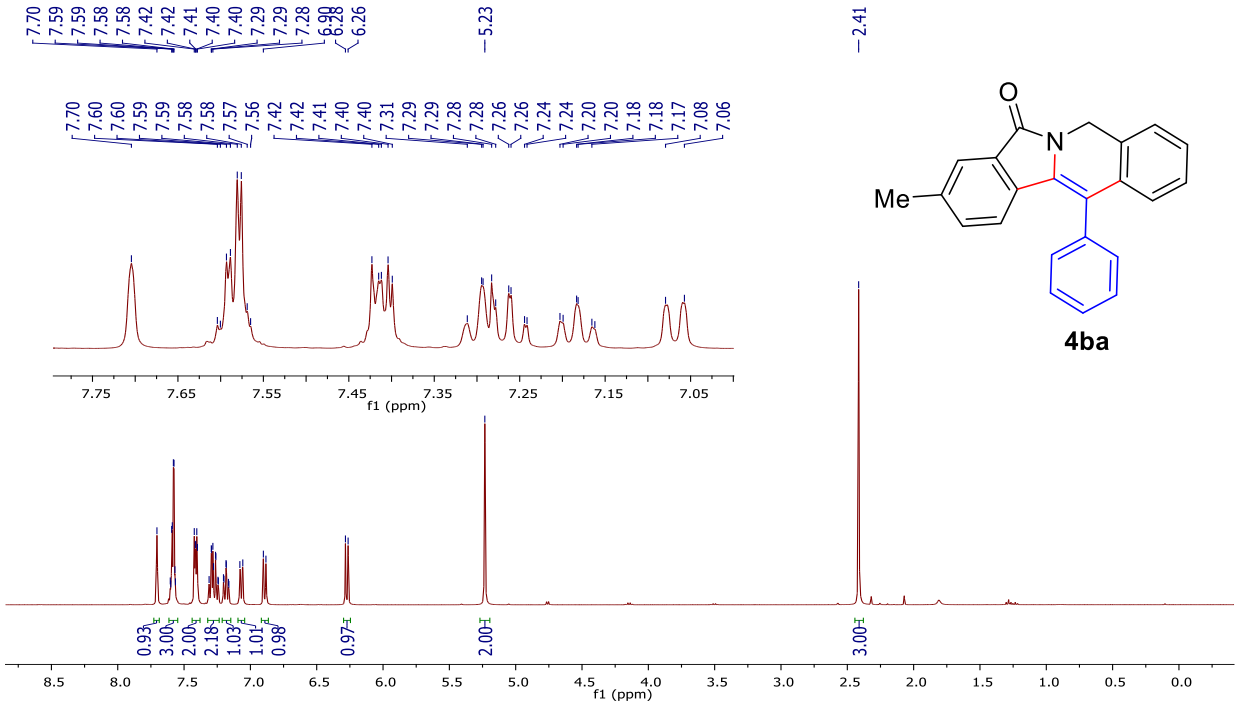
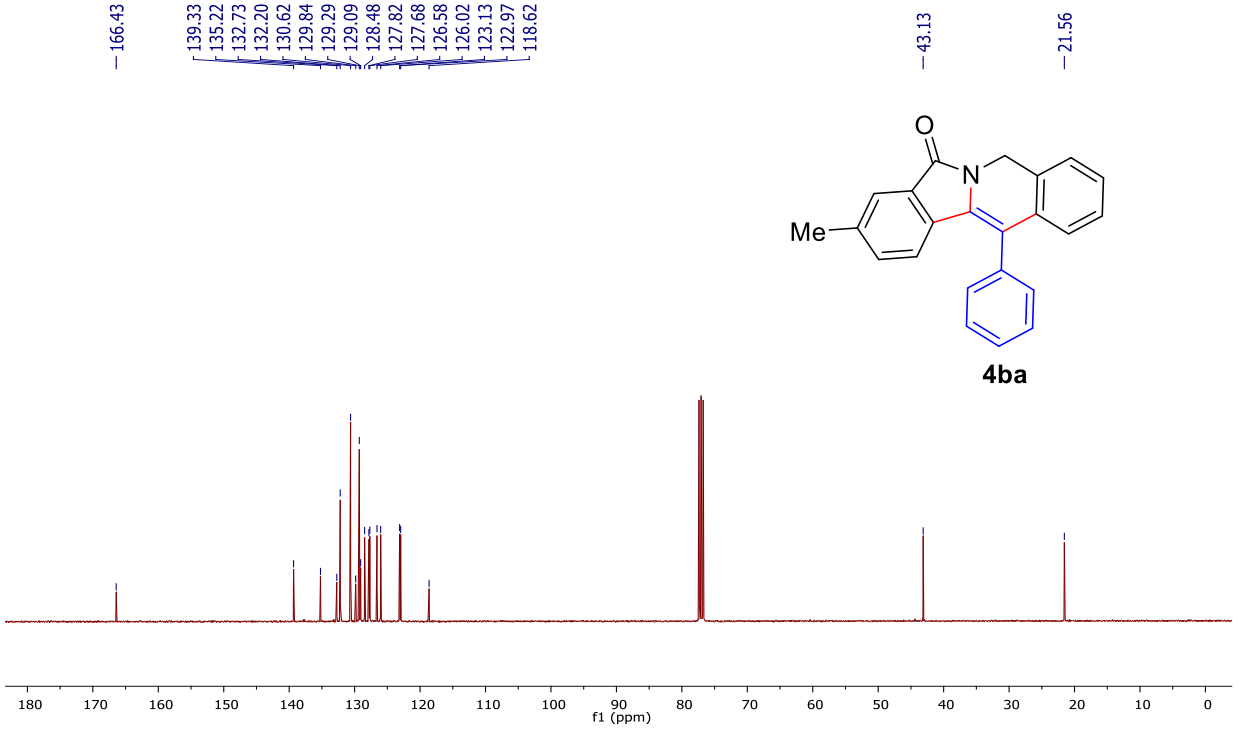
7.97
7.93
7.91
7.68
7.68
7.66
7.64
7.64
7.56
7.54
7.53
7.51
7.36
7.36
7.34
7.32
7.32
7.30
7.30
7.28
7.28
5.10
3.04
3.02
3.00
1.81
1.74
1.72
1.60
1.58
1.56
1.49
1.47
1.45
1.00
0.98
0.96
O
N
Pent
4al
f1 (ppm)
1.08
0.99
1.18
1.00
1.16
1.14
2.28
2.00
2.13
2.40
2.49
2.31
3.52
165.78
134.71
131.69
131.56
129.94
129.90
129.87
128.49
127.98
127.84
126.79
123.68
123.40
123.20
119.76
43.03
32.29
28.93
26.89
22.61
14.10


7.70
7.59
7.59
7.58
7.58
7.42
7.42
7.41
7.40
7.40
7.29
7.29
7.28
6.90
6.28
6.26
5.23
2.41
7.70
7.60
7.60
7.59
7.59
7.58
7.58
7.57
7.56
7.42
7.42
7.41
7.40
7.40
7.31
7.29
7.29
7.28
7.28
7.26
7.26
7.24
7.24
7.20
7.20
7.18
7.18
7.17
7.08
7.06
7.75
7.65
7.55
7.45
7.35
7.25
7.15
7.05
f1 (ppm)
O
N
Me
4ba
0.93
3.00
2.00
2.18
1.03
1.01
0.98
0.97
2.00
3.00
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
f1 (ppm)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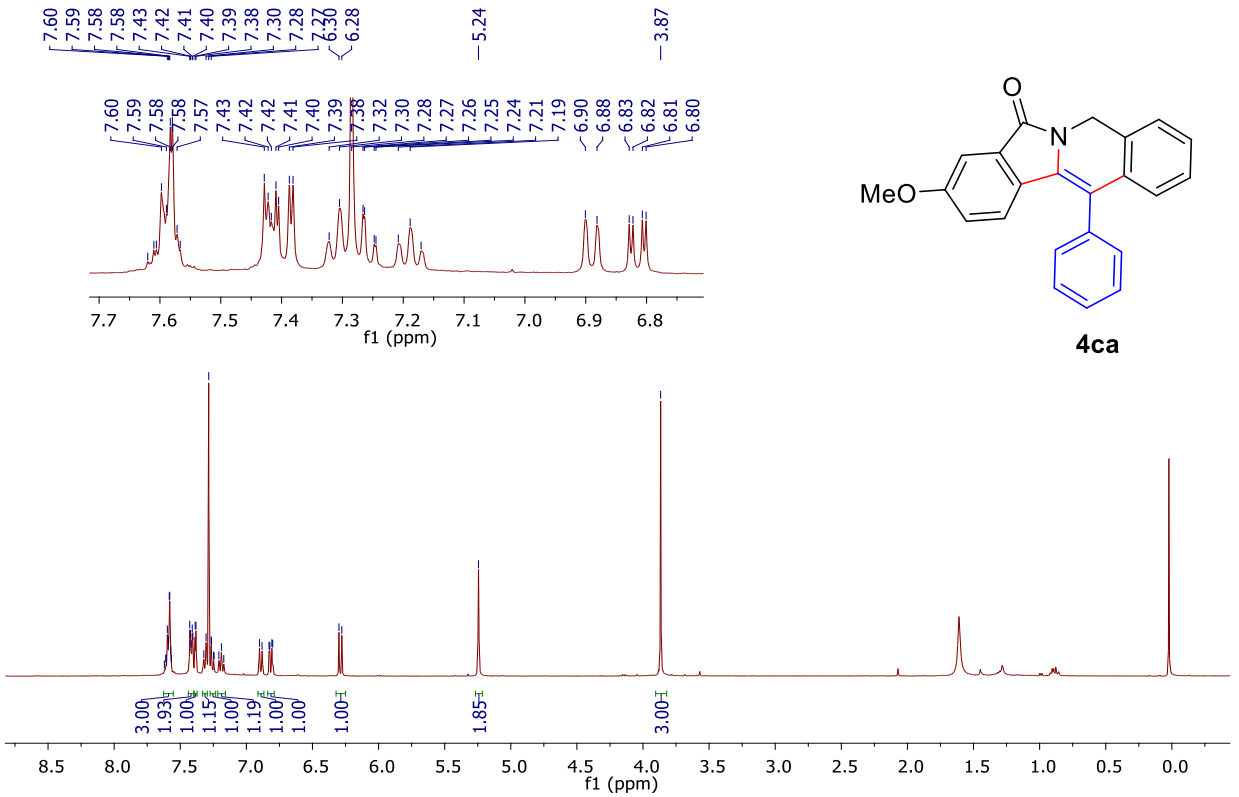
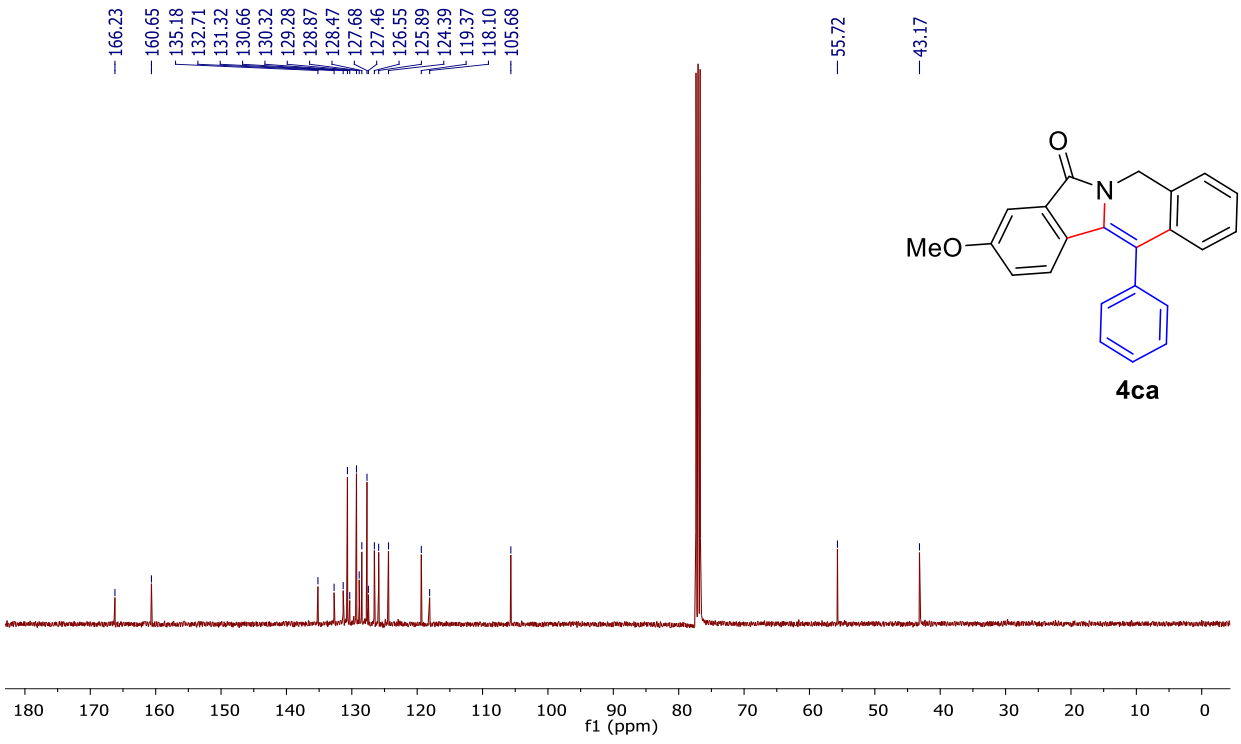
139.33
135.22
132.73
132.20
130.62
129.84
129.29
129.09
128.48
127.82
127.68
126.58
126.02
123.13
122.97
118.62
43.13
21.56
O
N
Me
4ba
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.60
7.59
7.58
7.58
7.43
7.42
7.41
7.40
7.39
7.38
7.30
7.28
7.27
6.30
6.28
5.24
3.87
7.60
7.59
7.58
7.58
7.57
7.43
7.42
7.42
7.41
7.40
7.39
7.38
7.32
7.30
7.28
7.27
7.26
7.25
7.24
7.21
7.19
6.90
6.88
6.83
6.82
6.81
6.80
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)
O
N
MeO
4ca
3.00
1.93
1.00
1.15
1.00
1.19
1.00
1.00
1.00
1.85
3.00
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
f1 (ppm)


166.23
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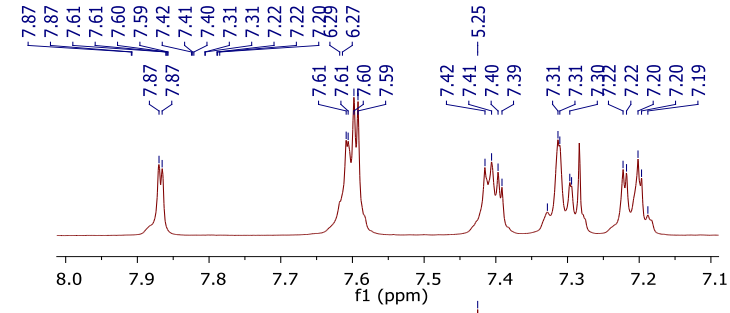
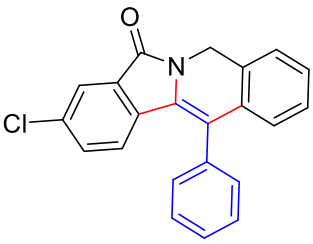
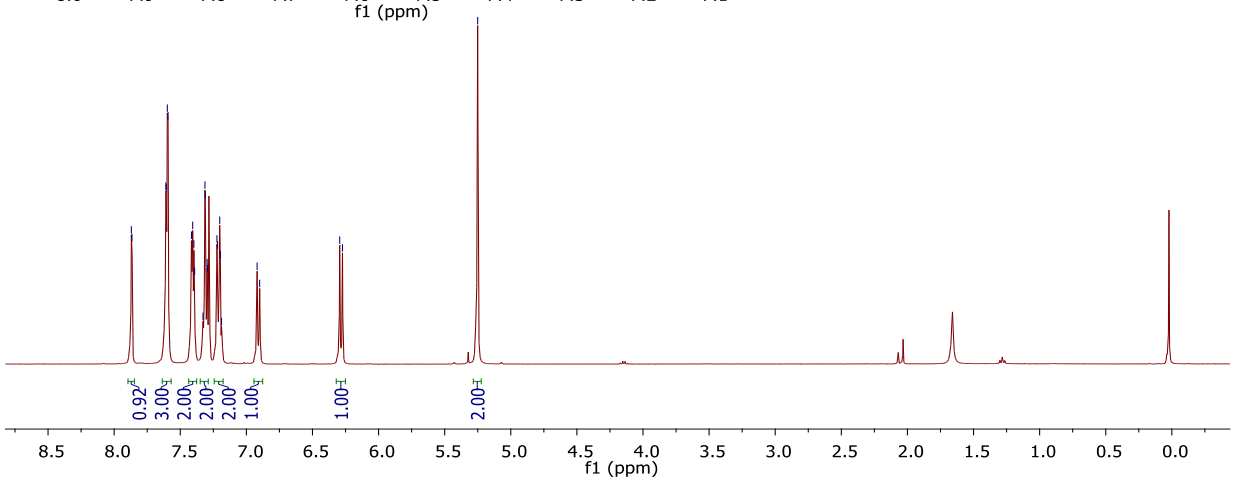
132.71
131.32
130.66
130.32
129.28
128.87
128.47
127.68
127.46
126.55
125.89
124.39
119.37
118.10
105.68
55.72
43.17
O
N
MeO
4ca
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.87
7.87
7.61
7.61
7.60
7.59
7.42
7.41
7.40
7.31
7.31
7.22
7.22
6.29
6.27
5.25
7.87
7.87
7.61
7.61
7.60
7.59
7.42
7.41
7.40
7.39
7.31
7.31
7.22
7.22
7.20
7.20
7.19
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)


O
N
Cl

4da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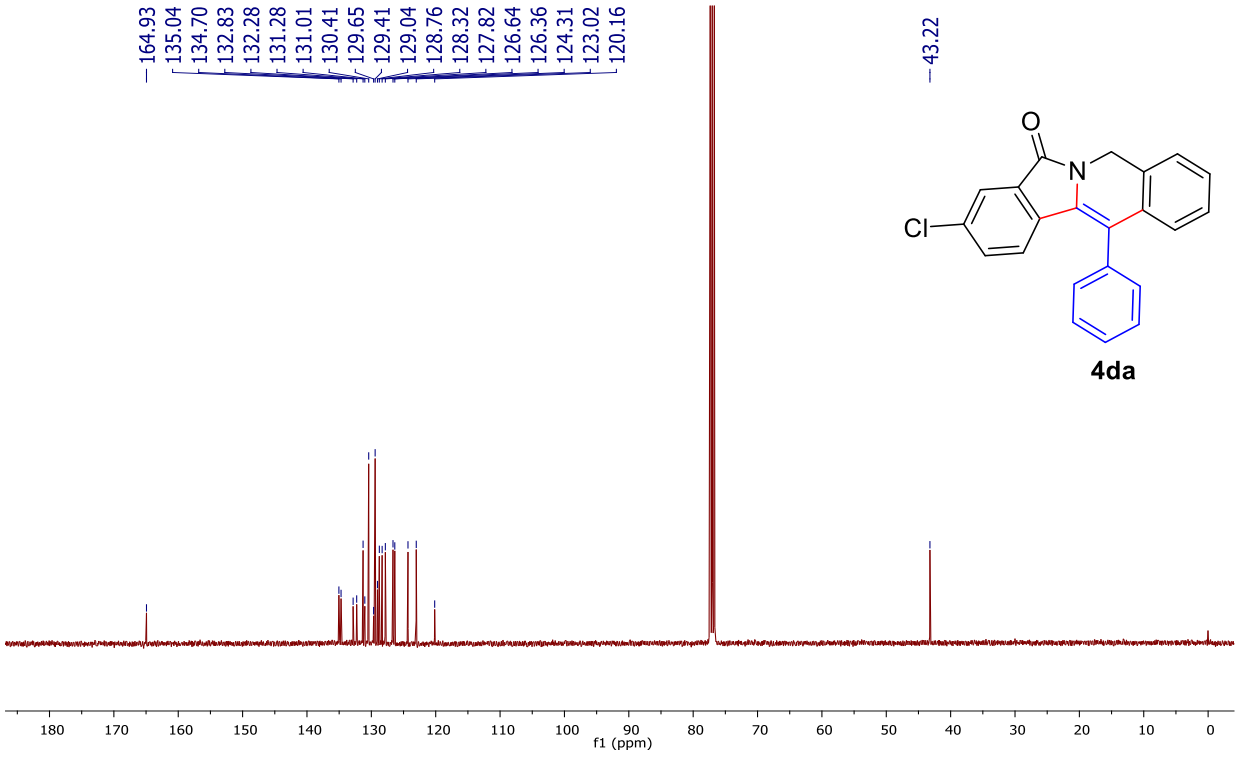
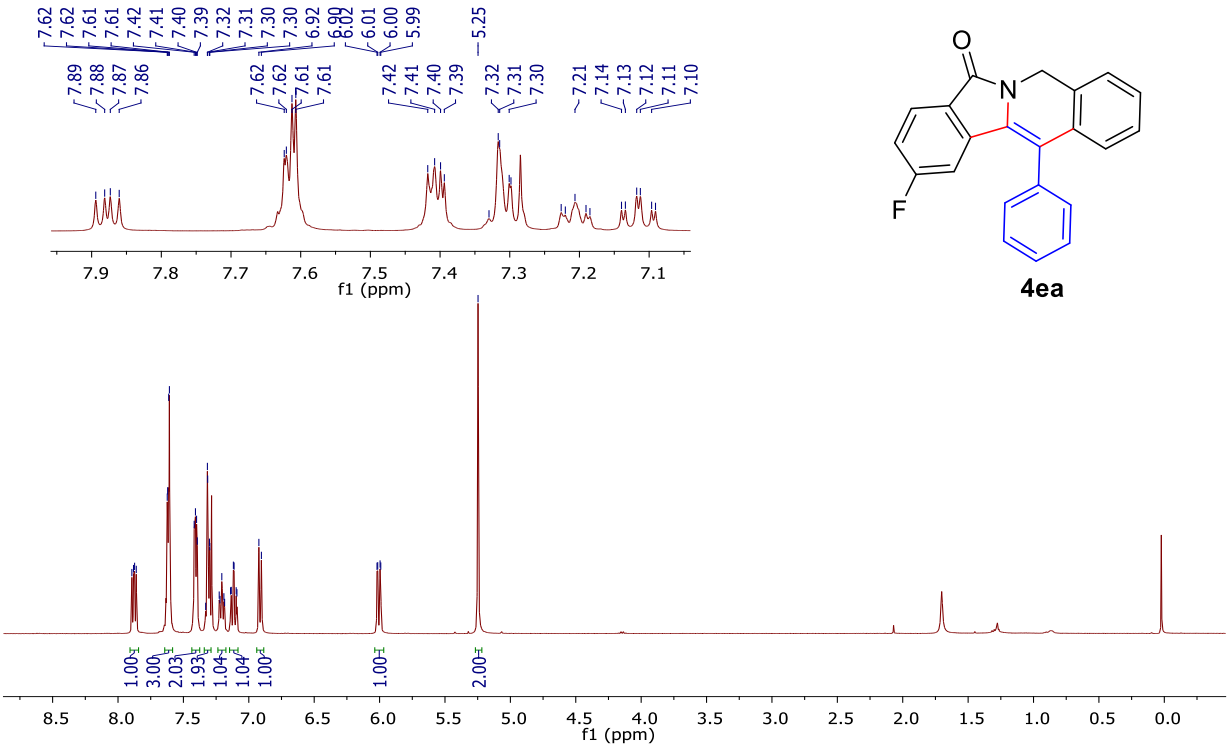
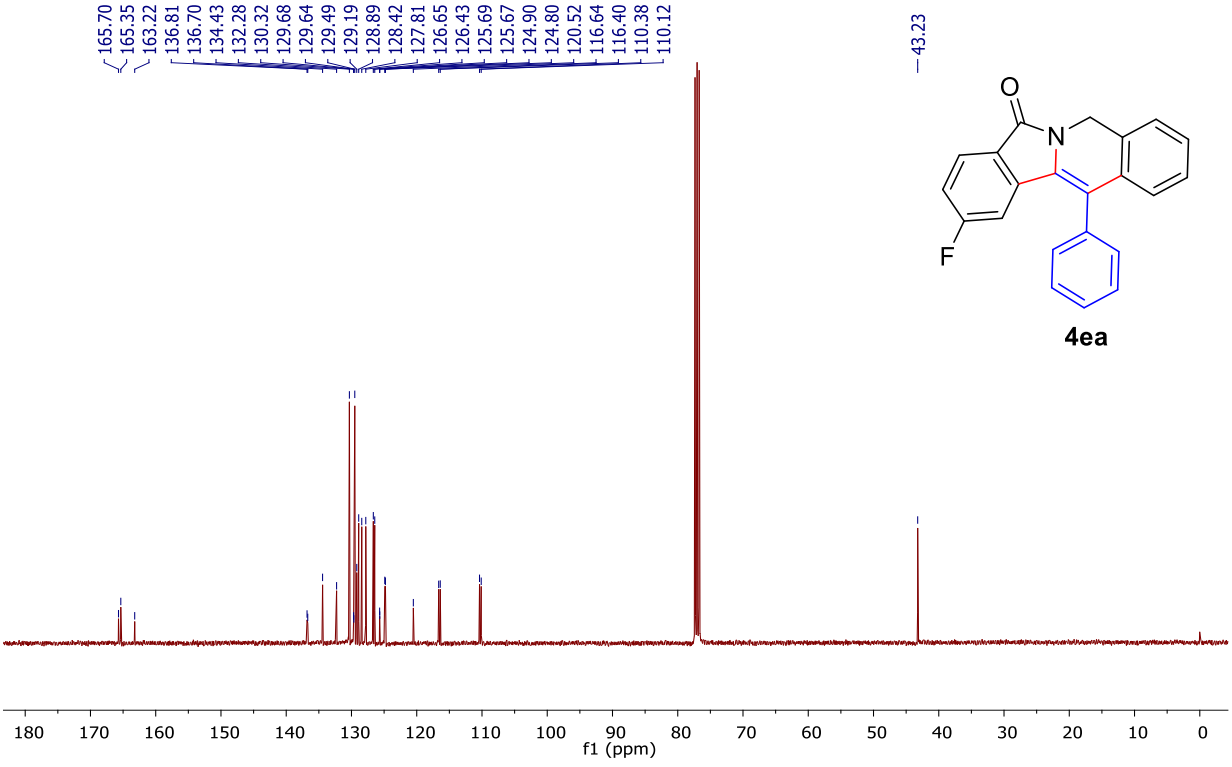
3.00
2.00
2.00
2.00
1.00
1.00
2.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

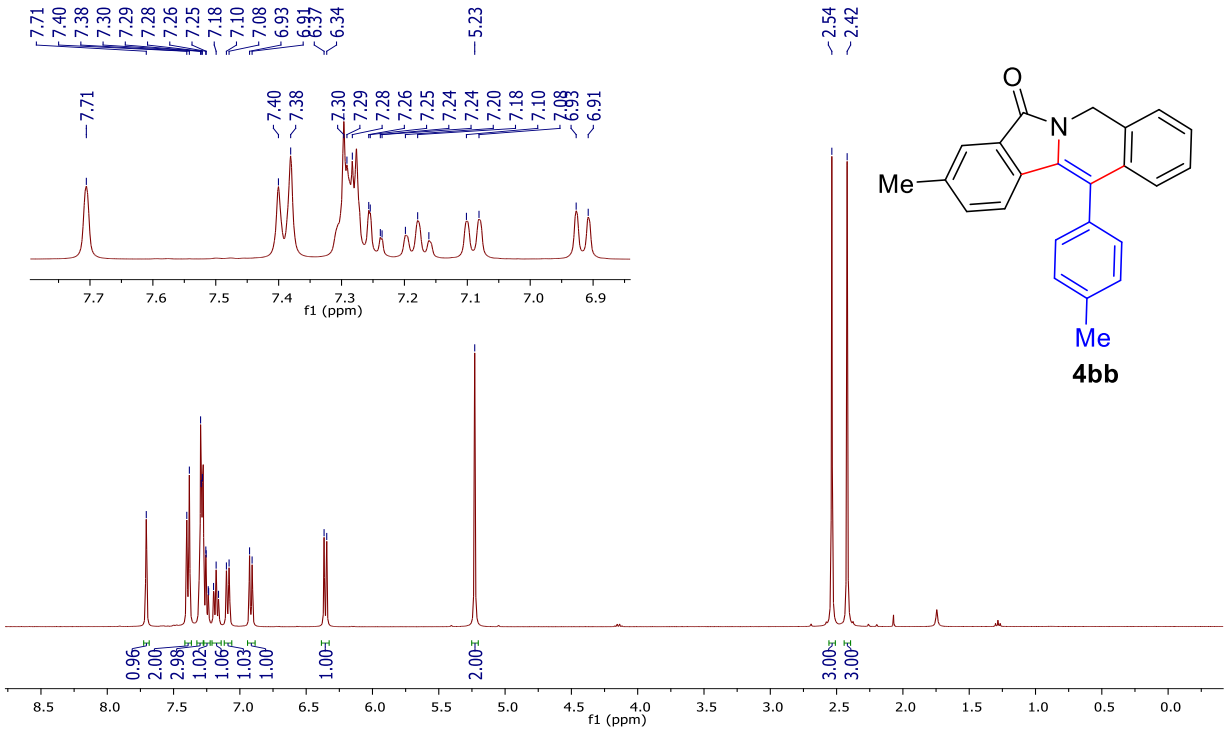

164.93
135.04
134.70
132.83
132.28
131.28
131.01
130.41
129.65
129.41
129.04
128.76
128.32
127.82
126.64
126.36
124.31
123.02
120.16
43.22
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

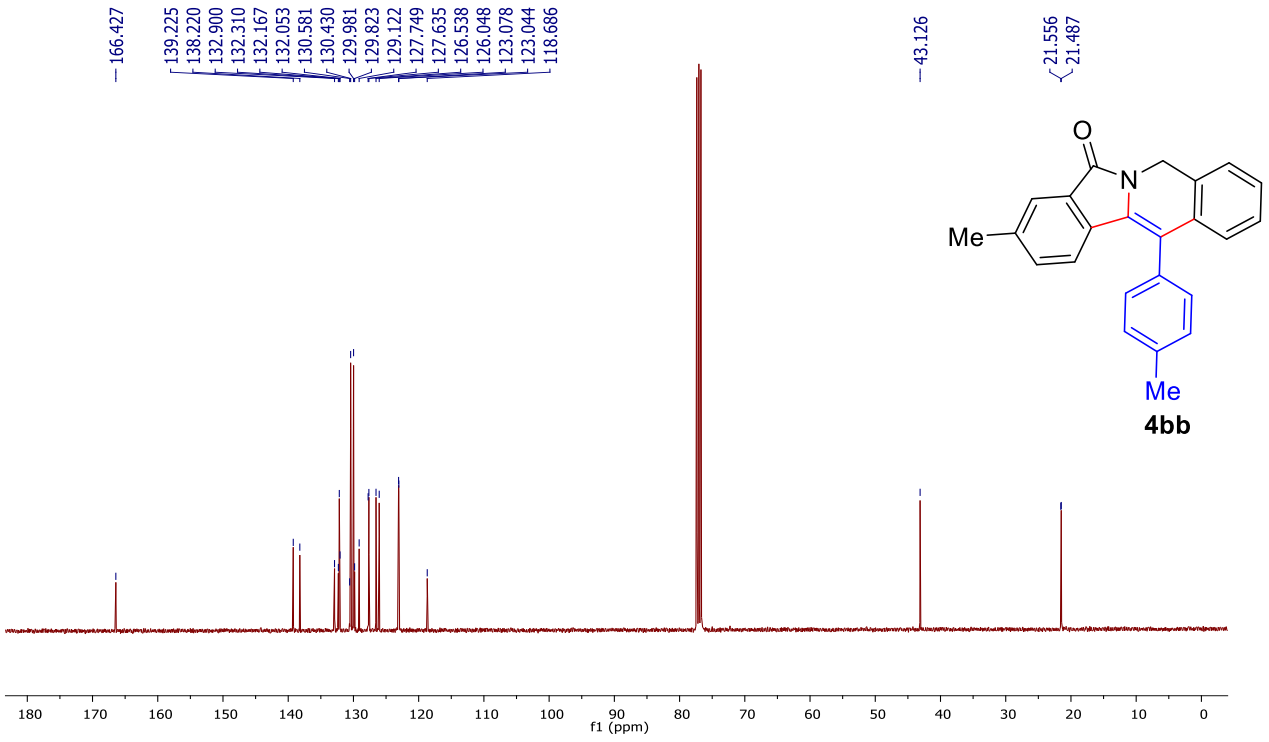
O
N
Cl

4da


7.62
7.62
7.61
7.61
7.42
7.41
7.40
7.39
7.32
7.31
7.30
7.30
6.92
6.90
6.02
6.01
6.00
5.99
5.25
7.89
7.88
7.87
7.86
7.62
7.62
7.61
7.61
7.42
7.41
7.40
7.39
7.32
7.31
7.30
7.21
7.14
7.13
7.12
7.11
7.10
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
O
N
F
4ea
1.00
3.00
2.03
1.93
1.04
1.04
1.00
1.00
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
f1 (ppm)


165.70
165.35
163.22
136.81
136.70
134.43
132.28
130.32
129.68
129.64
129.49
129.19
128.89
128.42
127.81
126.65
126.43
125.69
125.67
124.90
124.80
120.52
116.64
116.40
110.38
110.12
43.23
O
N
F
4ea
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.71
7.40
7.38
7.30
7.29
7.28
7.26
7.25
7.18
7.10
7.08
6.93
6.91
6.37
6.34
5.23
2.54
2.42
O
N
Me
Me
4bb
f1 (ppm)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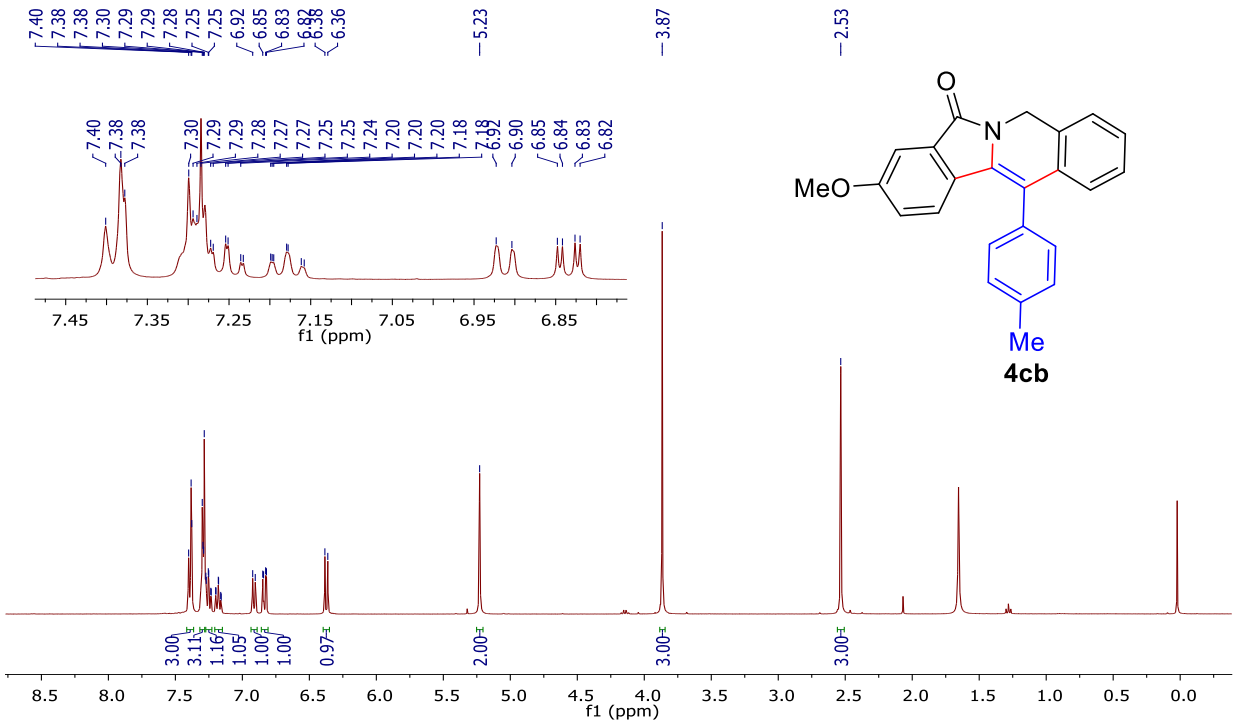
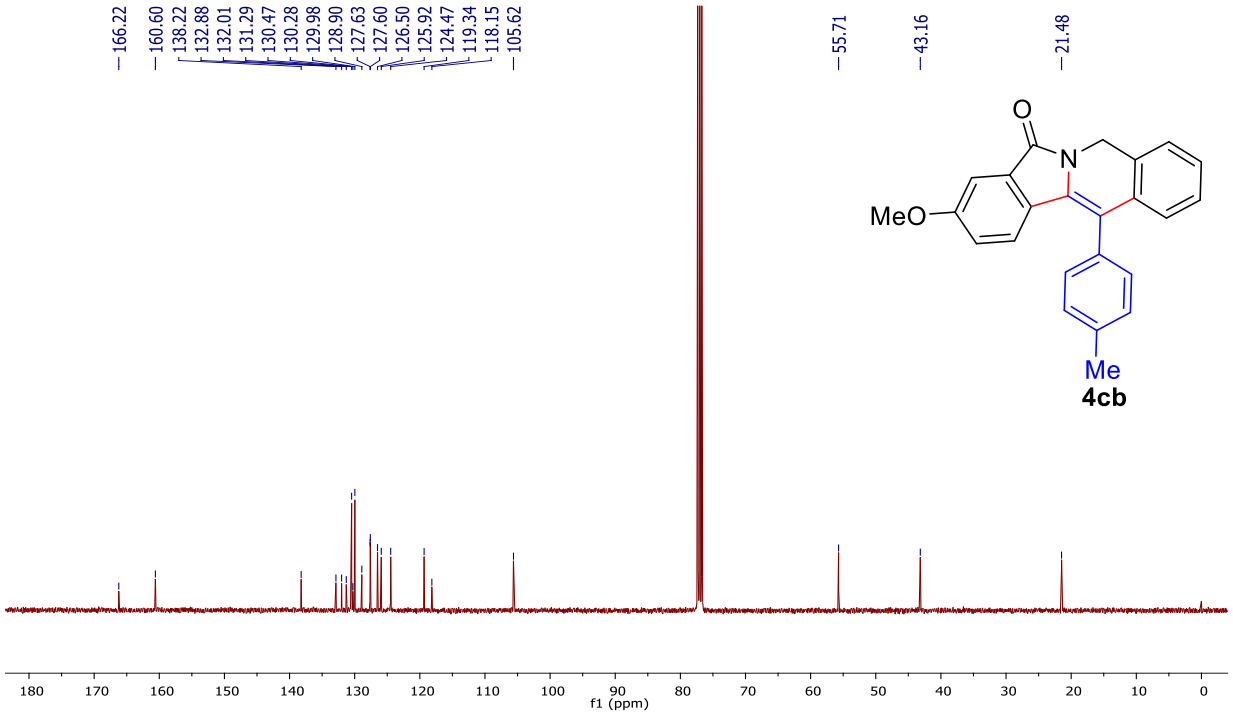
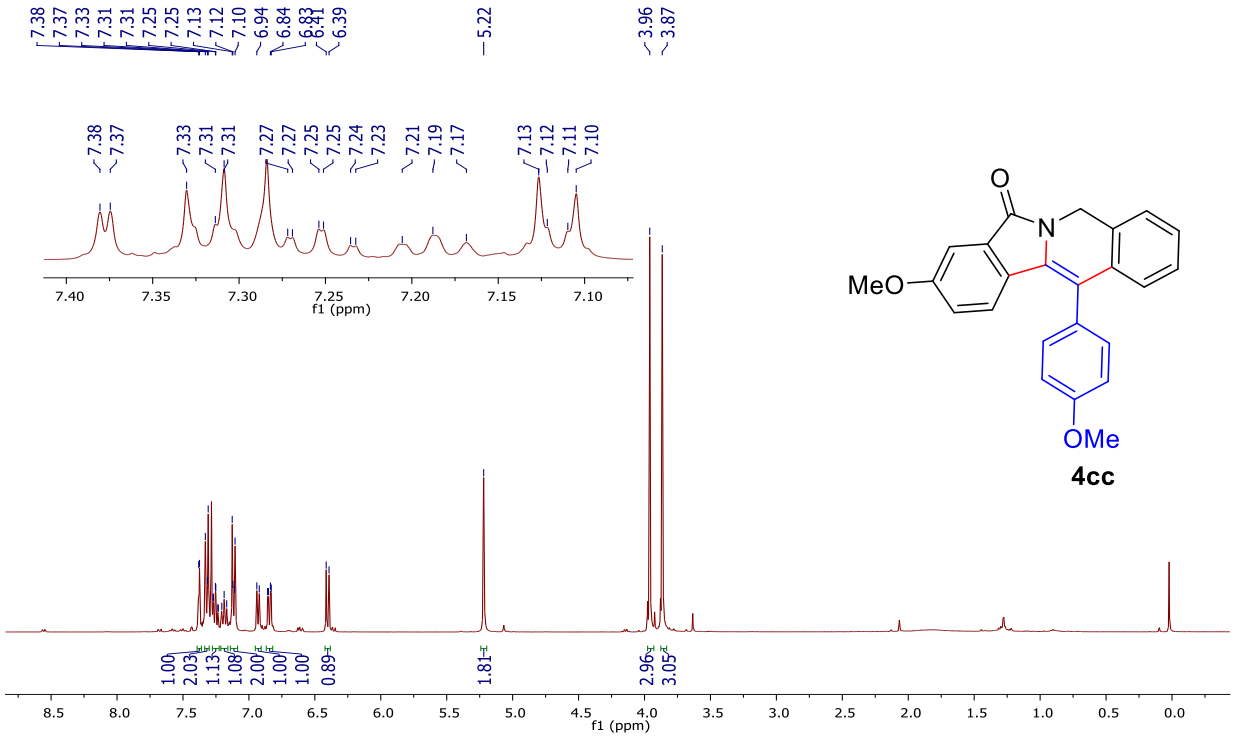
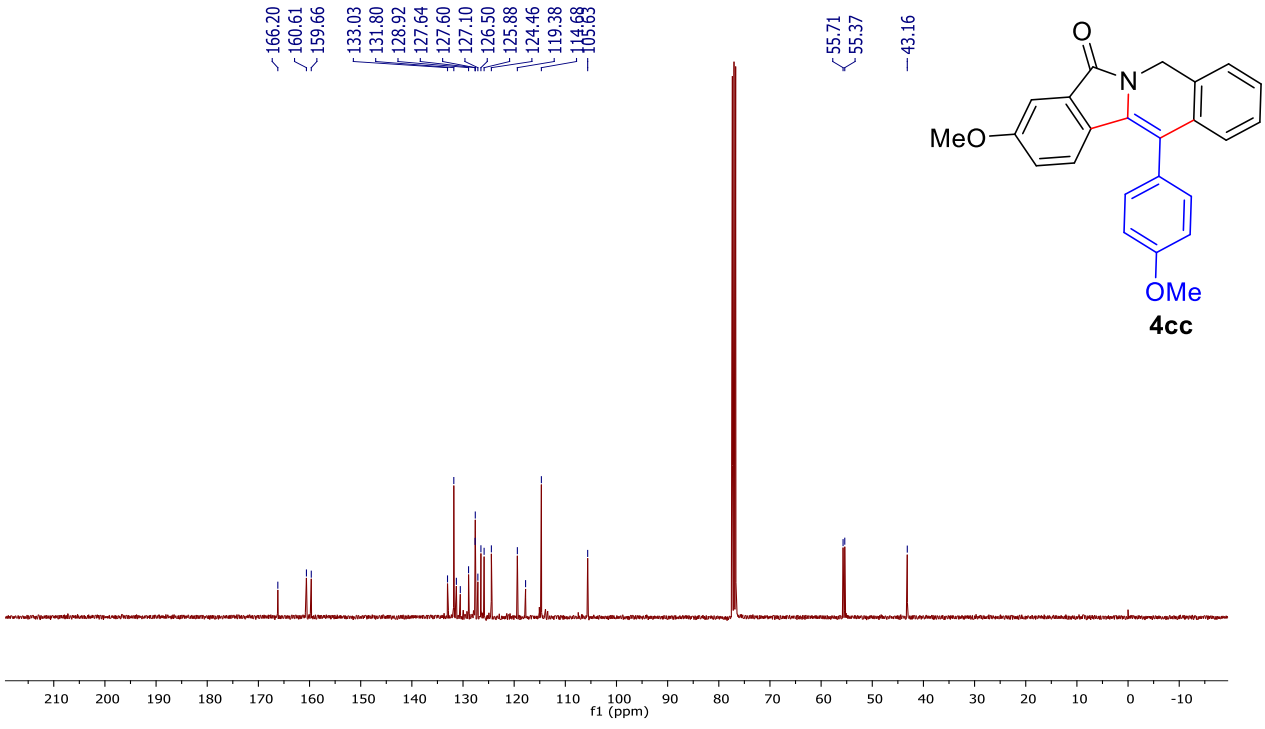
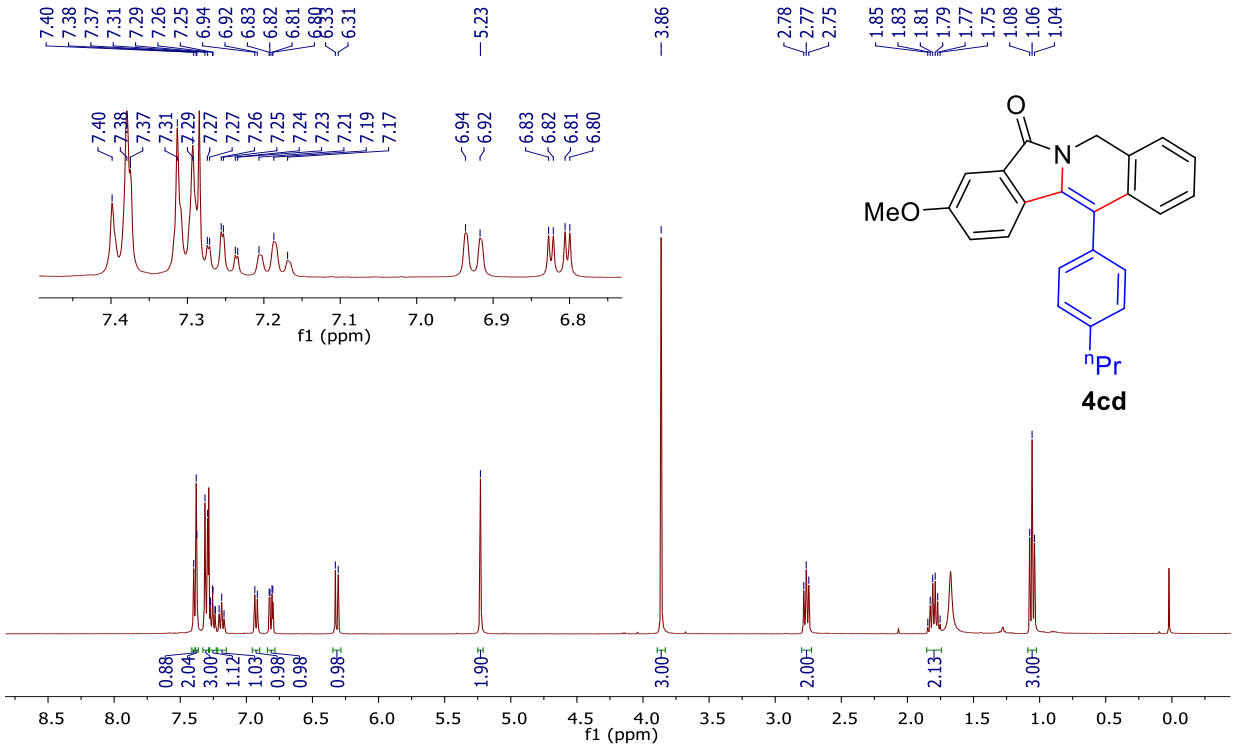
139.225
138.220
132.900
132.310
132.167
132.053
130.581
130.430
129.981
129.823
129.122
127.749
127.635
126.538
126.048
123.078
123.044
118.686
43.126
21.556
21.487
O
N
Me
Me
4bb
f1 (ppm)

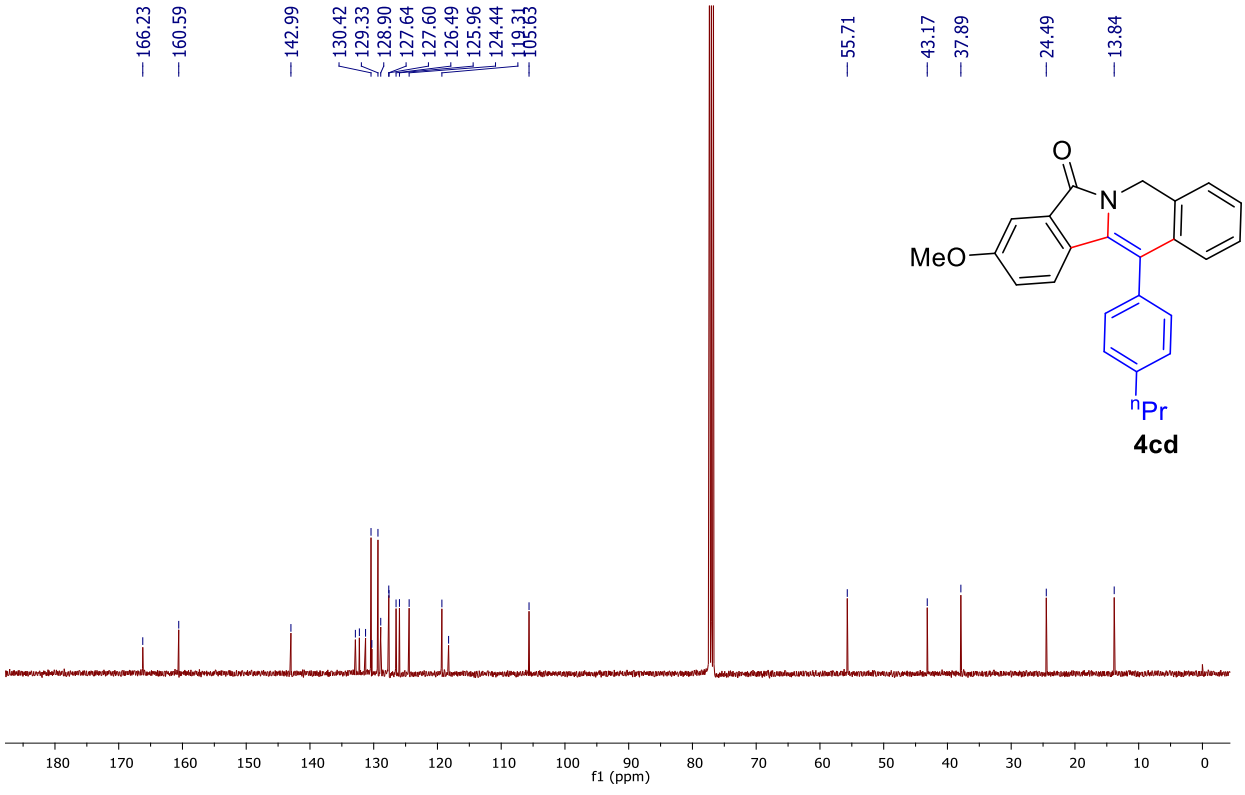

7.40
7.38
7.38
7.30
7.29
7.29
7.28
7.25
7.25
6.92
6.85
6.83
6.82
6.38
6.36
5.23
3.87
2.53
7.45
7.35
7.25
7.15
7.05
6.95
6.85
f1 (ppm)
O
N
MeO
Me
4cb
3.00
3.11
1.16
1.05
1.00
1.00
0.97
2.00
3.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

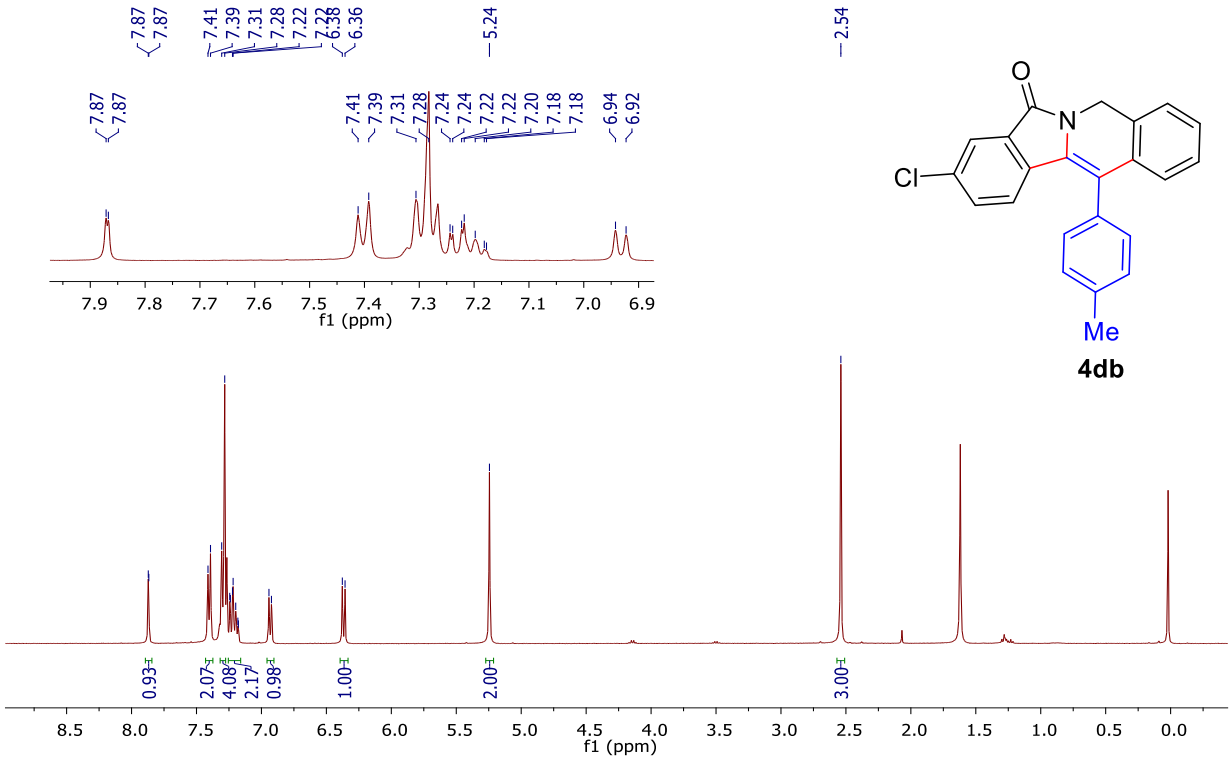

166.22
160.60
138.22
132.88
132.01
131.29
130.47
130.28
129.98
128.90
127.63
127.60
126.50
125.92
124.47
119.34
118.15
105.62
55.71
43.16
21.48
O
N
MeO
Me
4cb
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

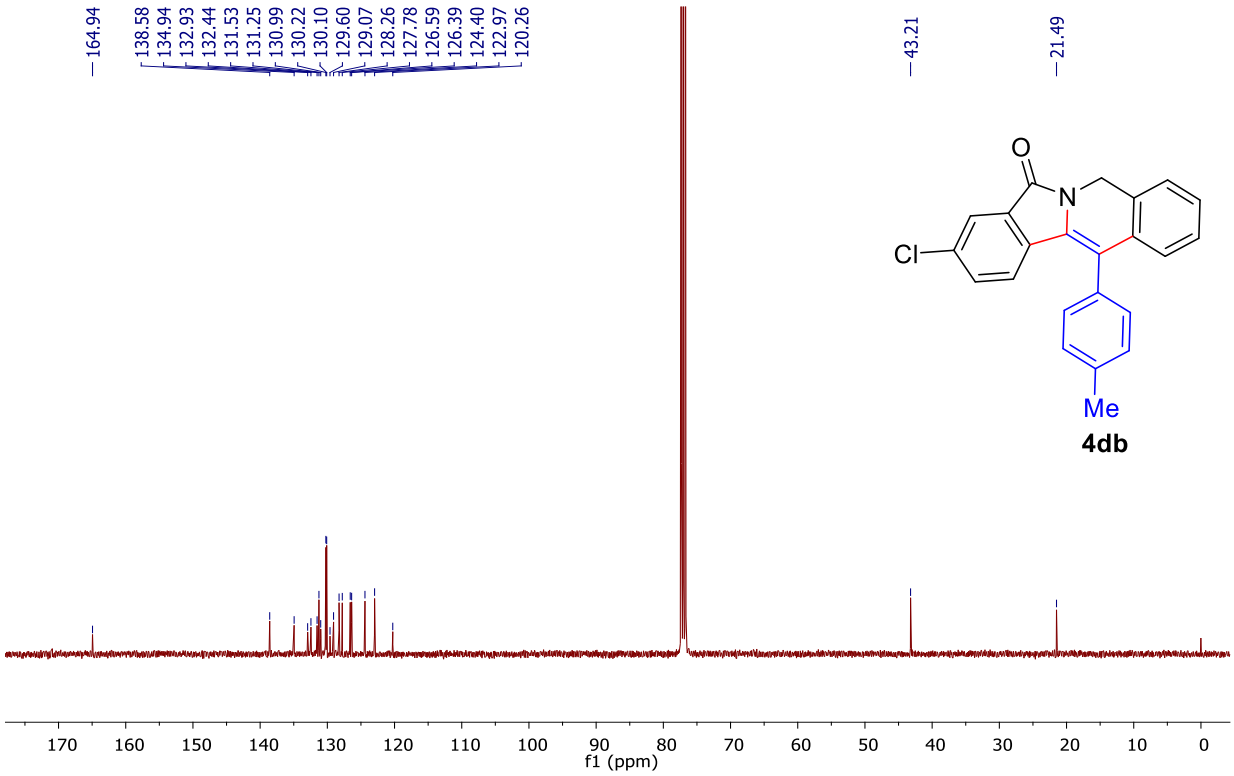

7.38
7.37
7.33
7.31
7.31
7.25
7.25
7.13
7.12
7.10
6.94
6.84
6.41
6.39
5.22
3.96
3.87
7.40
7.35
7.30
7.25
7.20
7.15
7.10
f1 (ppm)
1.00
2.03
1.13
1.08
2.00
1.00
1.00
0.89
1.81
2.96
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
O
N
MeO
OMe
4cc

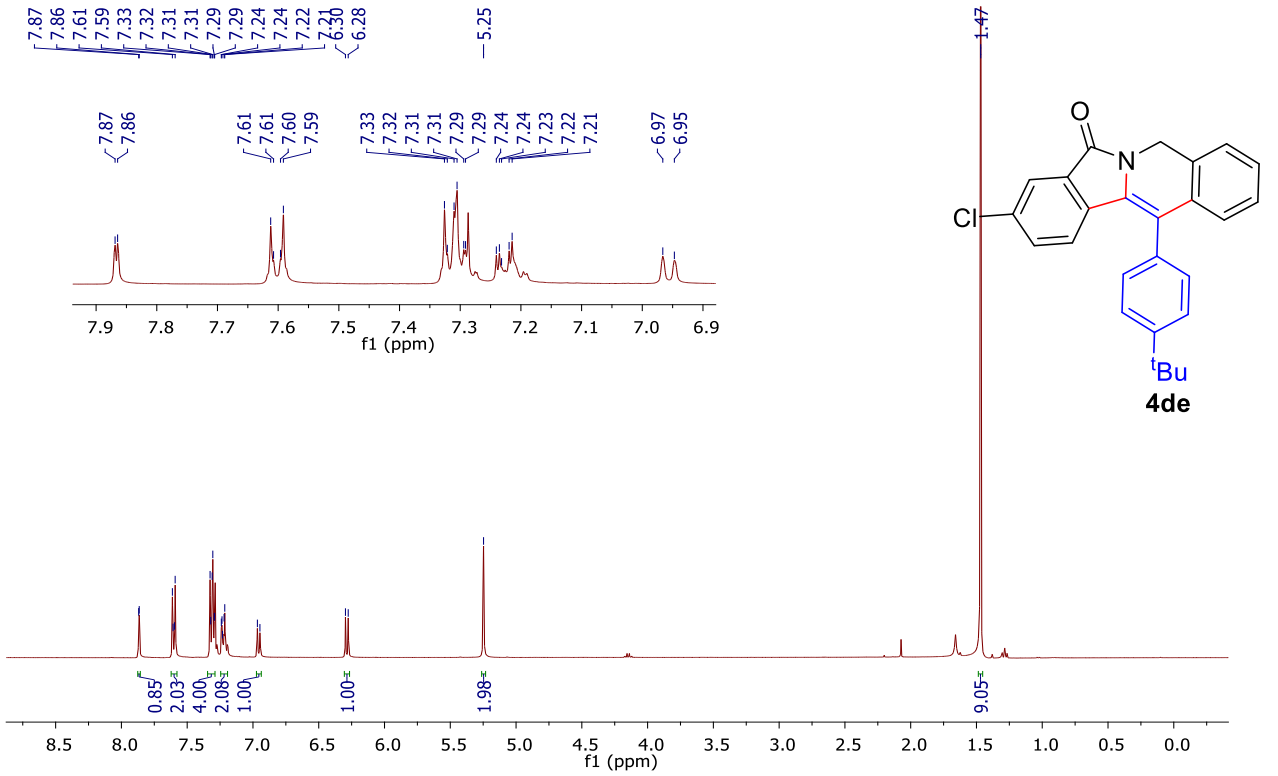

166.20
160.61
159.66
133.03
131.80
128.92
127.64
127.60
127.10
126.50
125.88
124.46
119.38
114.68
105.83
55.71
55.37
43.16
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
O
N
MeO
OMe
4cc

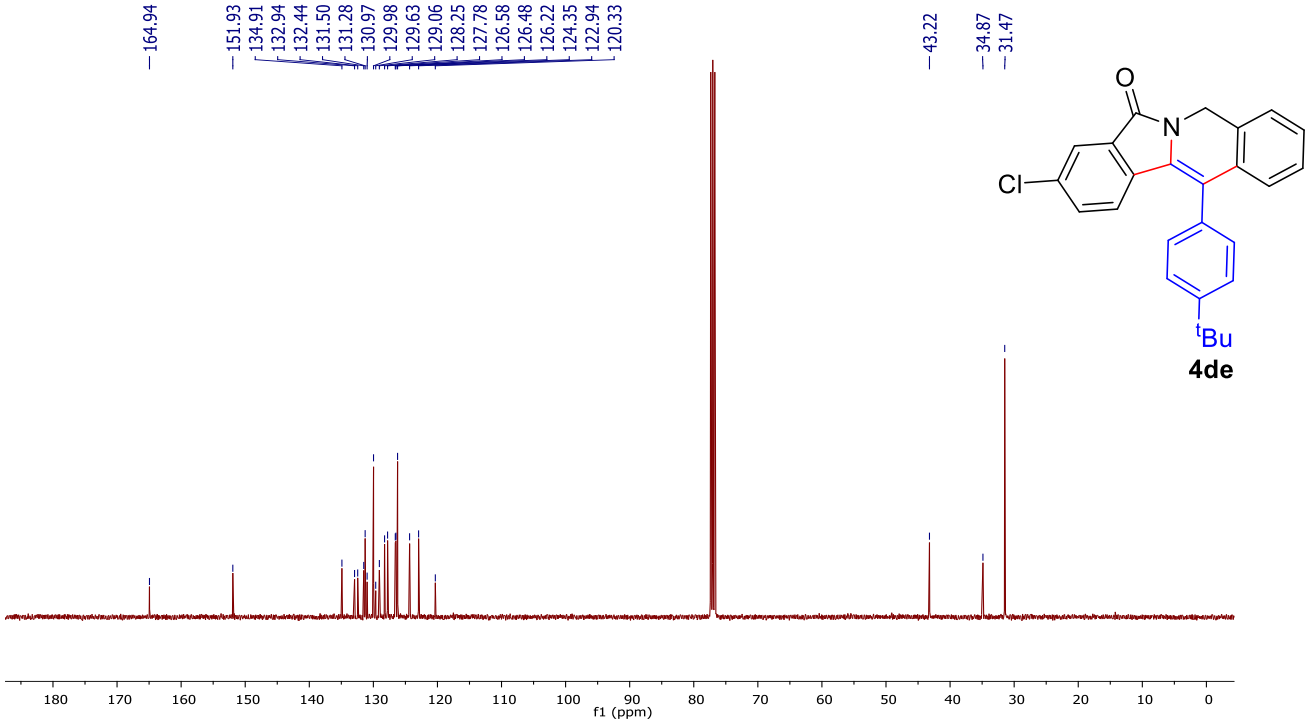

7.40
7.38
7.37
7.31
7.29
7.26
7.25
6.94
6.92
6.83
6.82
6.81
6.80
6.33
6.31
5.23
3.86
2.78
2.77
2.75
1.85
1.83
1.81
1.79
1.77
1.75
1.08
1.06
1.04
7.4
7.3
7.2
7.1
7.0
6.9
6.8
f1 (ppm)
O
N
MeO
nPr
4cd
0.88
2.04
3.00
1.12
1.03
0.98
0.98
0.98
1.90
3.00
2.00
2.13
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

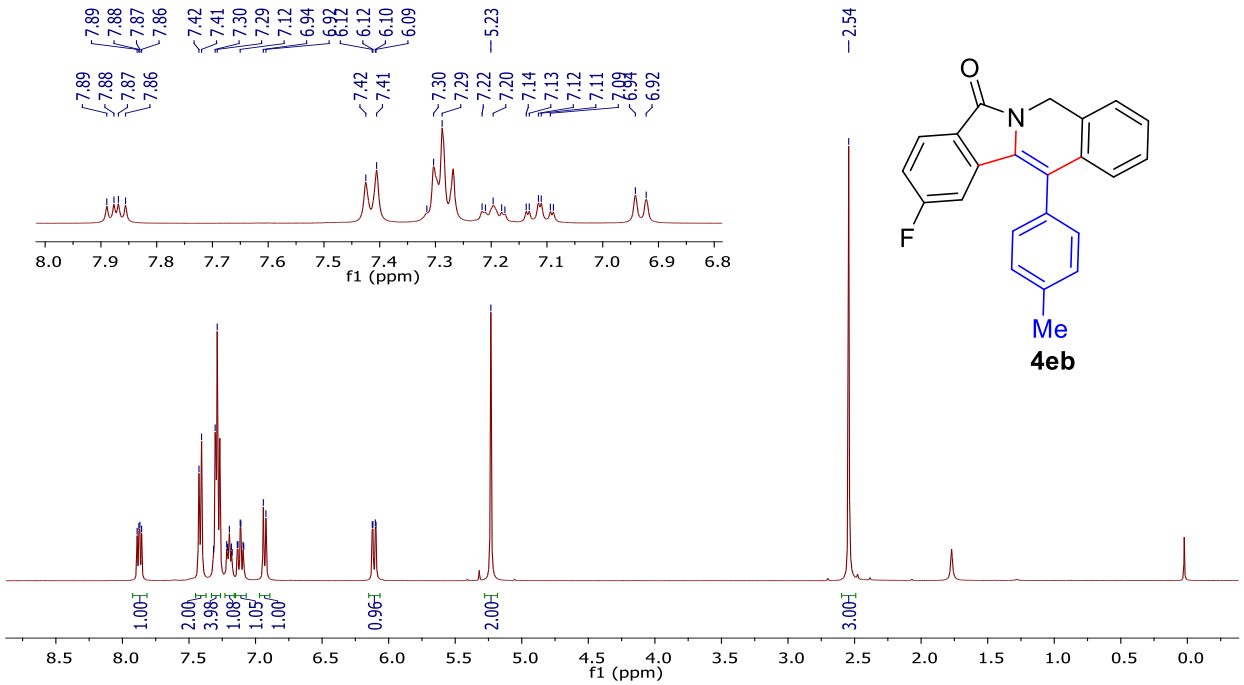

166.23
160.59
142.99
130.42
129.33
128.90
127.64
127.60
126.49
125.96
124.44
119.31
105.83
55.71
43.17
37.89
24.49
13.84
O
N
MeO
nPr
4cd
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

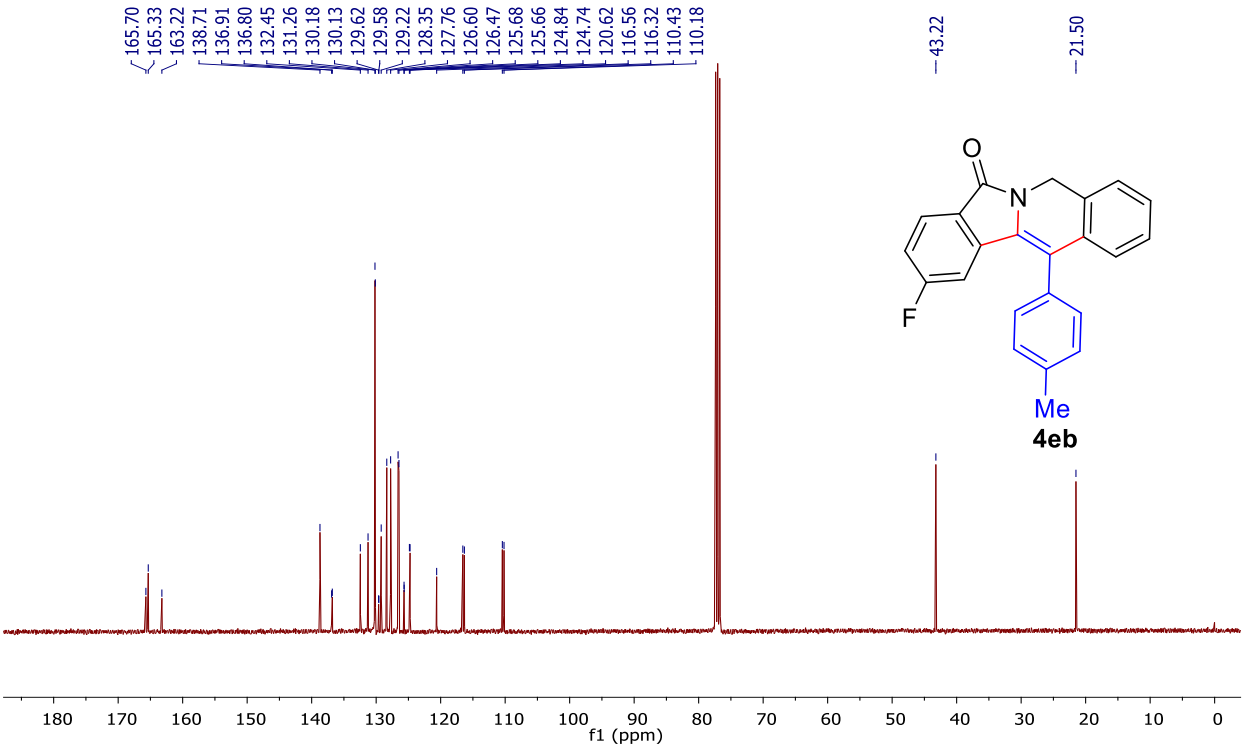

7.87
7.87
7.41
7.39
7.31
7.28
7.22
6.38
6.36
5.24
2.54
7.87
7.87
7.41
7.39
7.31
7.28
7.24
7.24
7.22
7.22
7.20
7.18
7.18
6.94
6.92
f1 (ppm)
O
N
Cl
Me
4db
0.93
2.07
4.08
2.17
0.98
1.00
2.00
3.00
f1 (ppm)

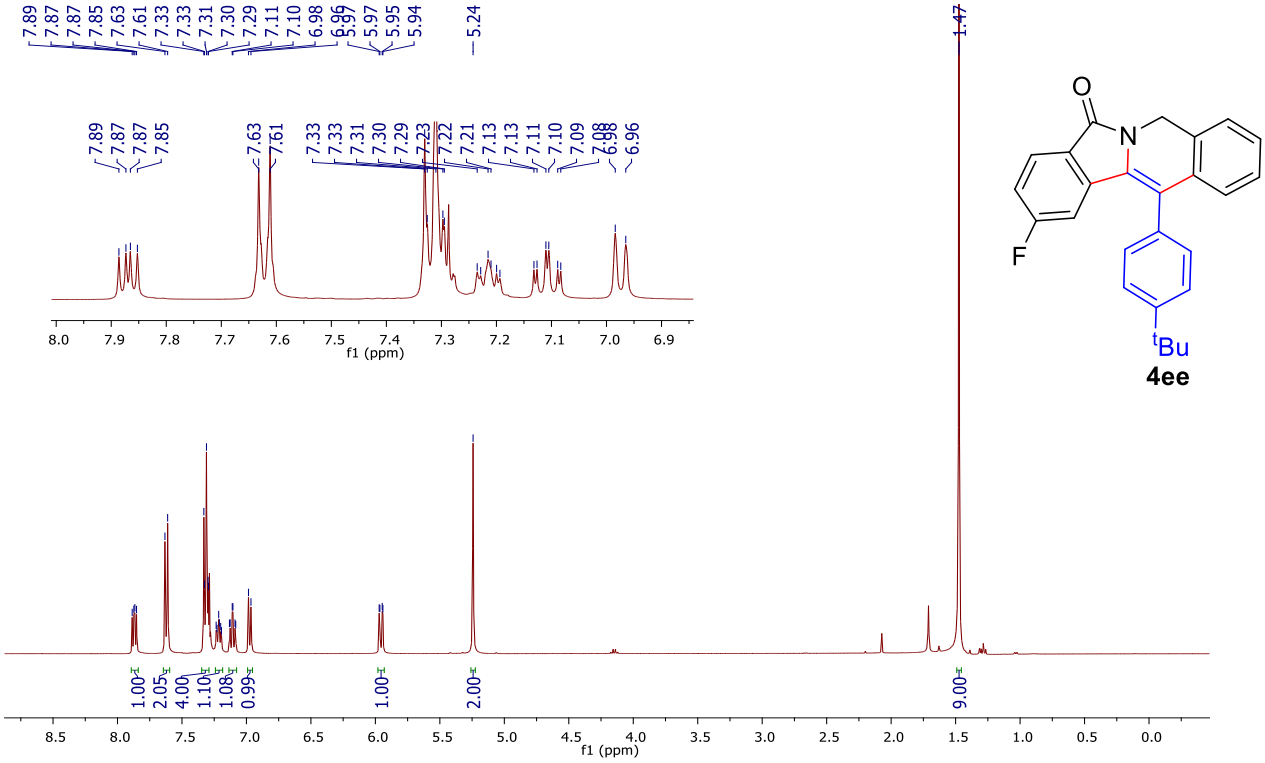

164.94
138.58
134.94
132.93
132.44
131.53
131.25
130.99
130.22
130.10
129.60
129.07
128.26
127.78
126.59
126.39
124.40
122.97
120.26
43.21
21.49
f1 (ppm)
O
N
Cl
Me
4db

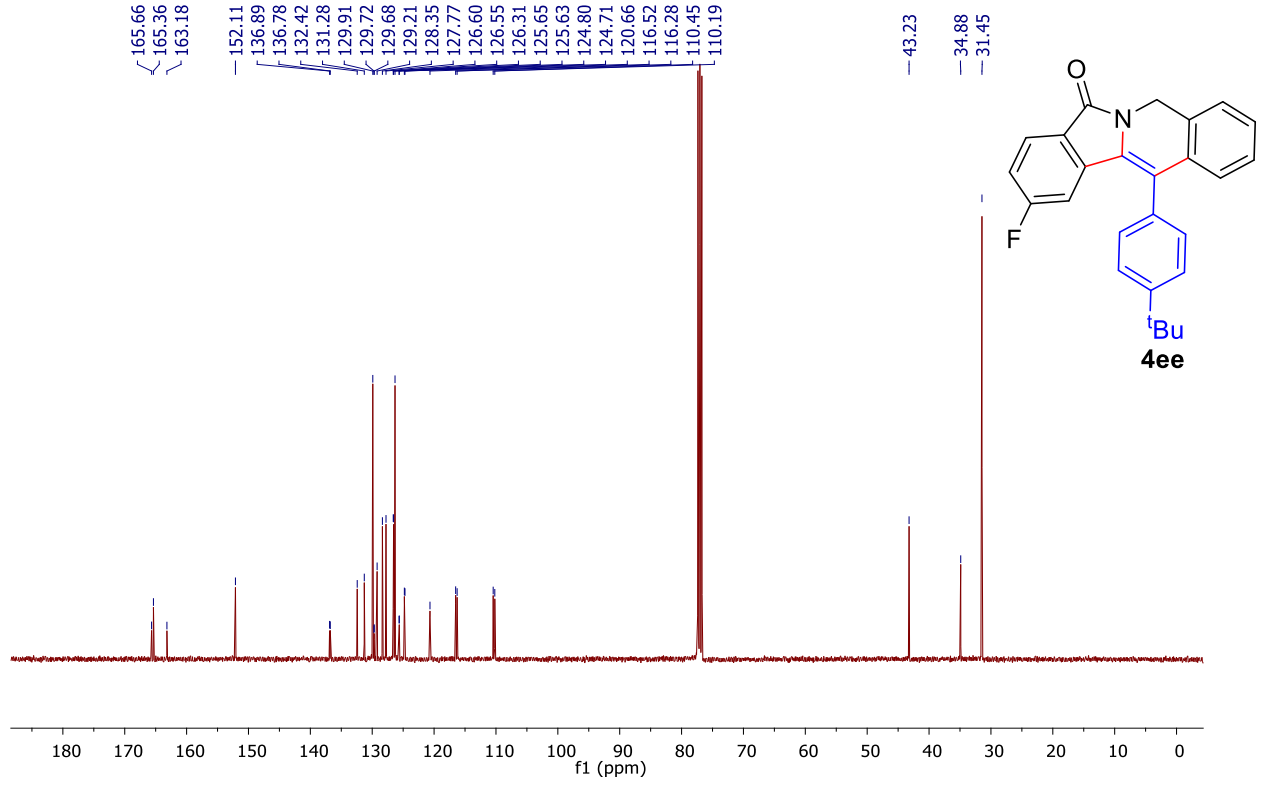

7.87
7.86
7.61
7.59
7.33
7.32
7.31
7.31
7.29
7.29
7.24
7.24
7.22
7.21
6.30
6.28
5.25
1.47
f1 (ppm)
0.85
2.03
4.00
2.08
1.00
1.00
1.98
9.05
Cl
O
N
tBu
4de

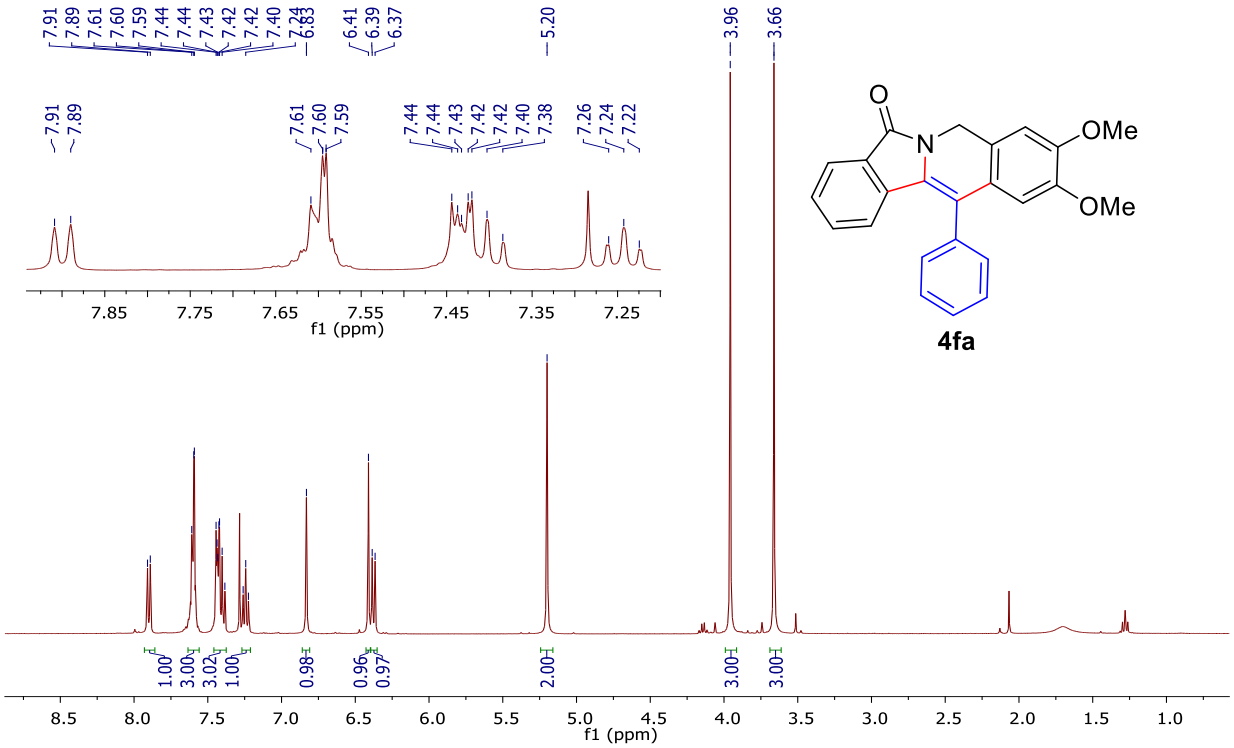

164.94
151.93
134.91
132.94
132.44
131.50
131.28
130.97
129.98
129.63
129.06
128.25
127.78
126.58
126.48
126.22
124.35
122.94
120.33
43.22
34.87
31.47
f1 (ppm)
Cl
O
N
tBu
4de


7.89
7.88
7.87
7.86
7.42
7.41
7.30
7.29
7.12
6.94
6.92
6.12
6.10
6.09
5.23
2.54
7.22
7.20
7.14
7.13
7.12
7.11
7.09
6.94
6.92
f1 (ppm)
1.00
2.00
3.98
1.08
1.05
1.00
0.96
2.00
3.00
O
N
F
Me
4eb


165.70
165.33
163.22
138.71
136.91
136.80
132.45
131.26
130.18
130.13
129.62
129.58
129.22
128.35
127.76
126.60
126.47
125.68
125.66
124.84
124.74
120.62
116.56
116.32
110.43
110.18
43.22
21.50
f1 (ppm)
O
N
F
Me
4eb


7.89
7.87
7.87
7.85
7.63
7.61
7.33
7.33
7.31
7.30
7.29
7.11
7.10
6.98
6.96
5.97
5.95
5.94
5.24
1.47
f1 (ppm)
1.00
2.05
4.00
1.10
1.08
0.99
1.00
2.00
9.00
O
N
F
tBu
4ee


165.66
165.36
163.18
152.11
136.89
136.78
132.42
131.28
129.91
129.72
129.68
129.21
128.35
127.77
126.60
126.55
126.31
125.65
125.63
124.80
124.71
120.66
116.52
116.28
110.45
110.19
43.23
34.88
31.45
f1 (ppm)
O
N
F
tBu
4ee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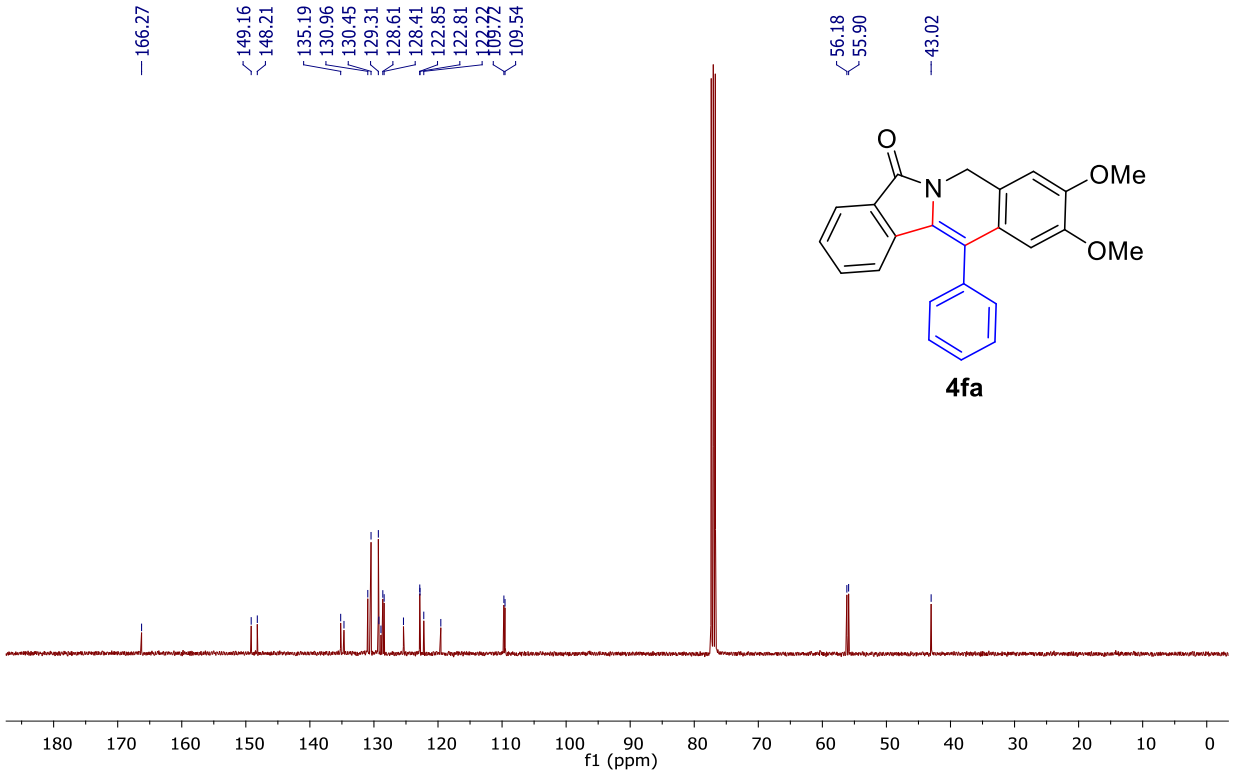
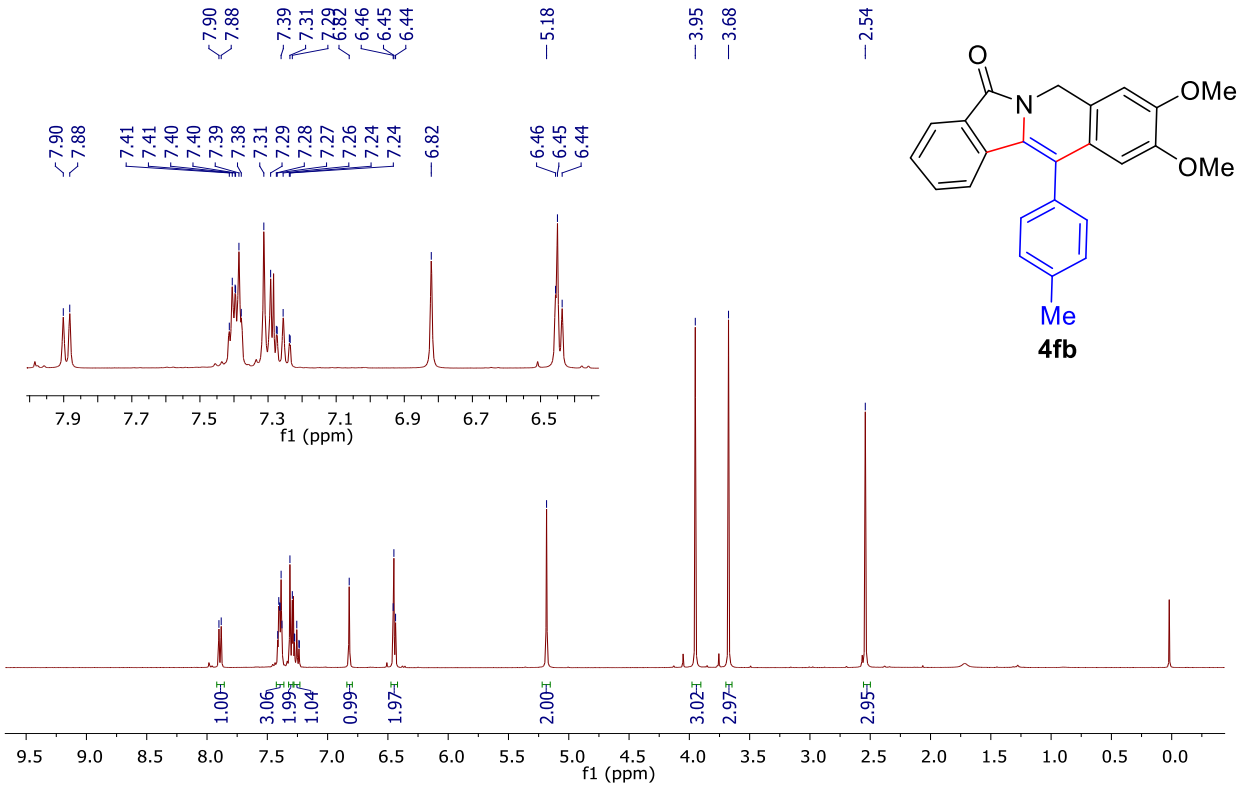
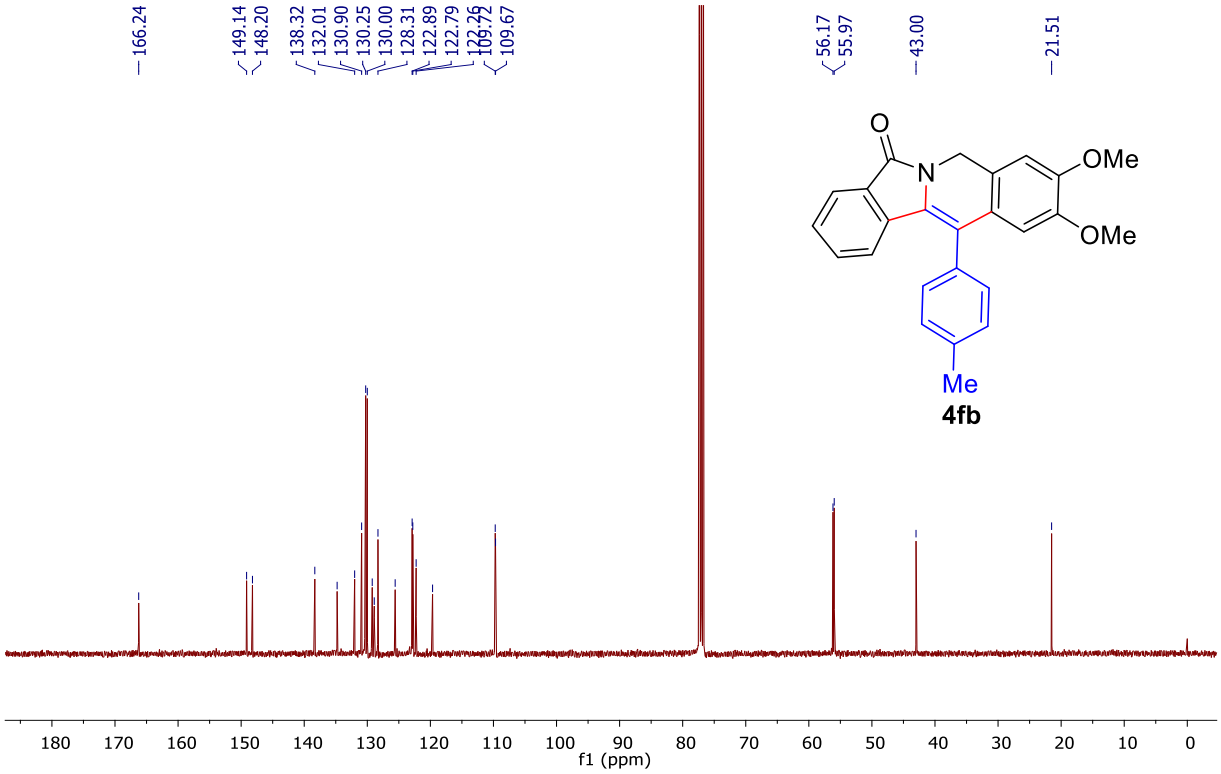
7.89
7.61
7.60
7.59
7.44
7.44
7.43
7.42
7.42
7.40
6.41
6.39
6.37
5.20
3.96
3.66
7.85
7.75
7.65
7.55
7.45
7.35
7.25
f1 (ppm)
1.00
3.00
3.02
1.00
0.98
0.96
0.97
2.00
3.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)
O
N
OMe
OMe

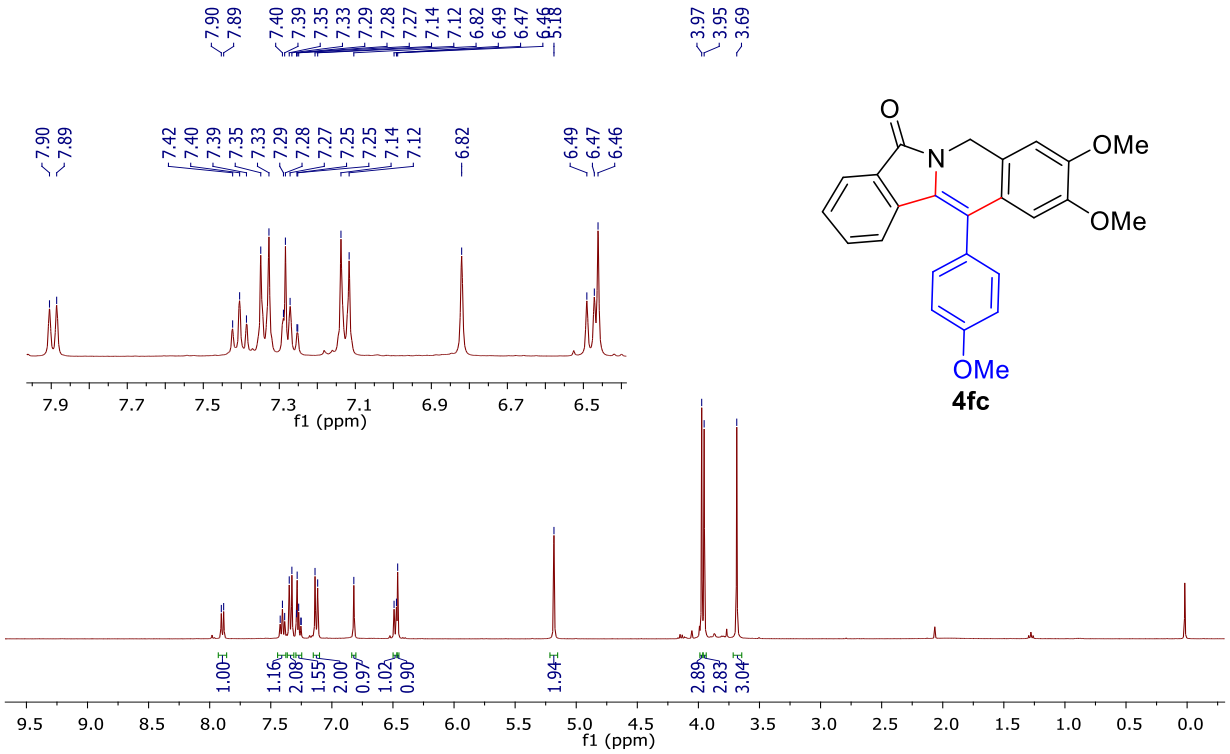
4fa

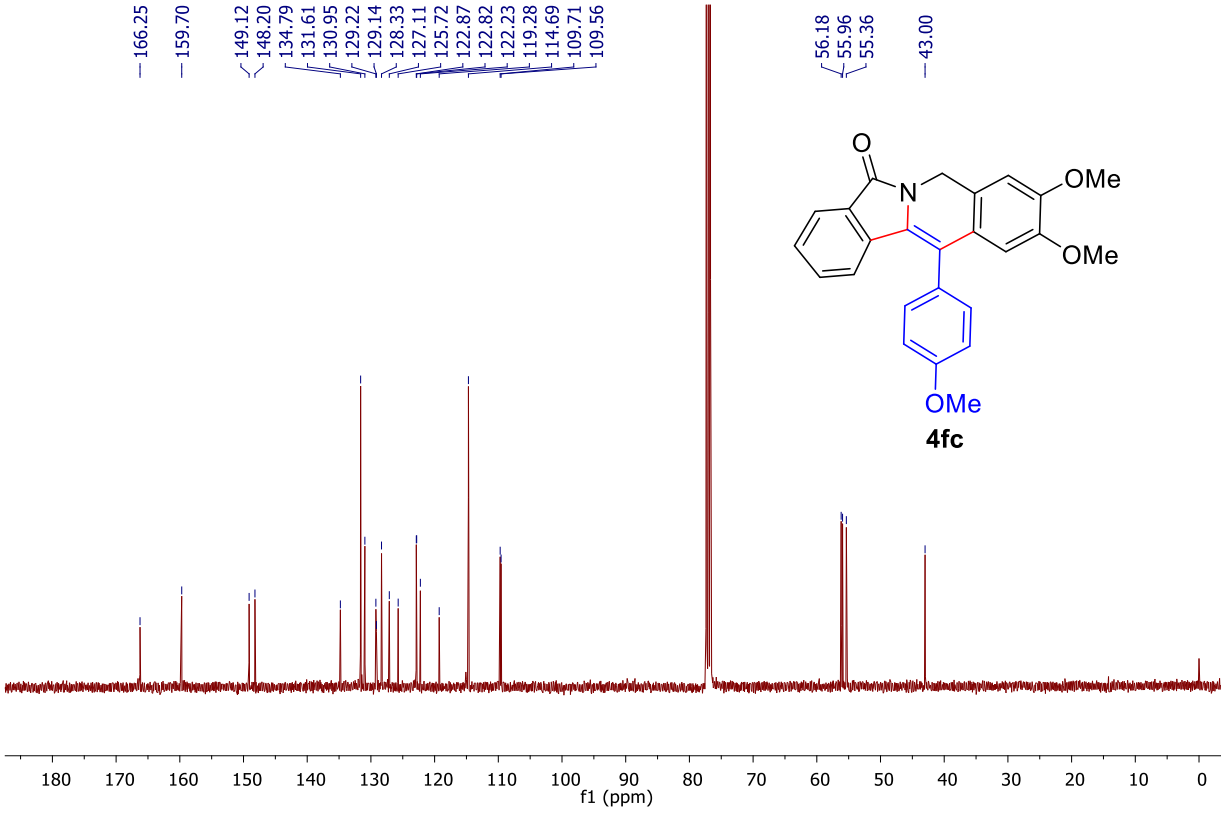

166.27
149.16
148.21
135.19
130.96
130.45
129.31
128.61
128.41
122.85
122.81
122.22
109.72
109.54
56.18
55.90
43.02
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
N
OMe
OMe

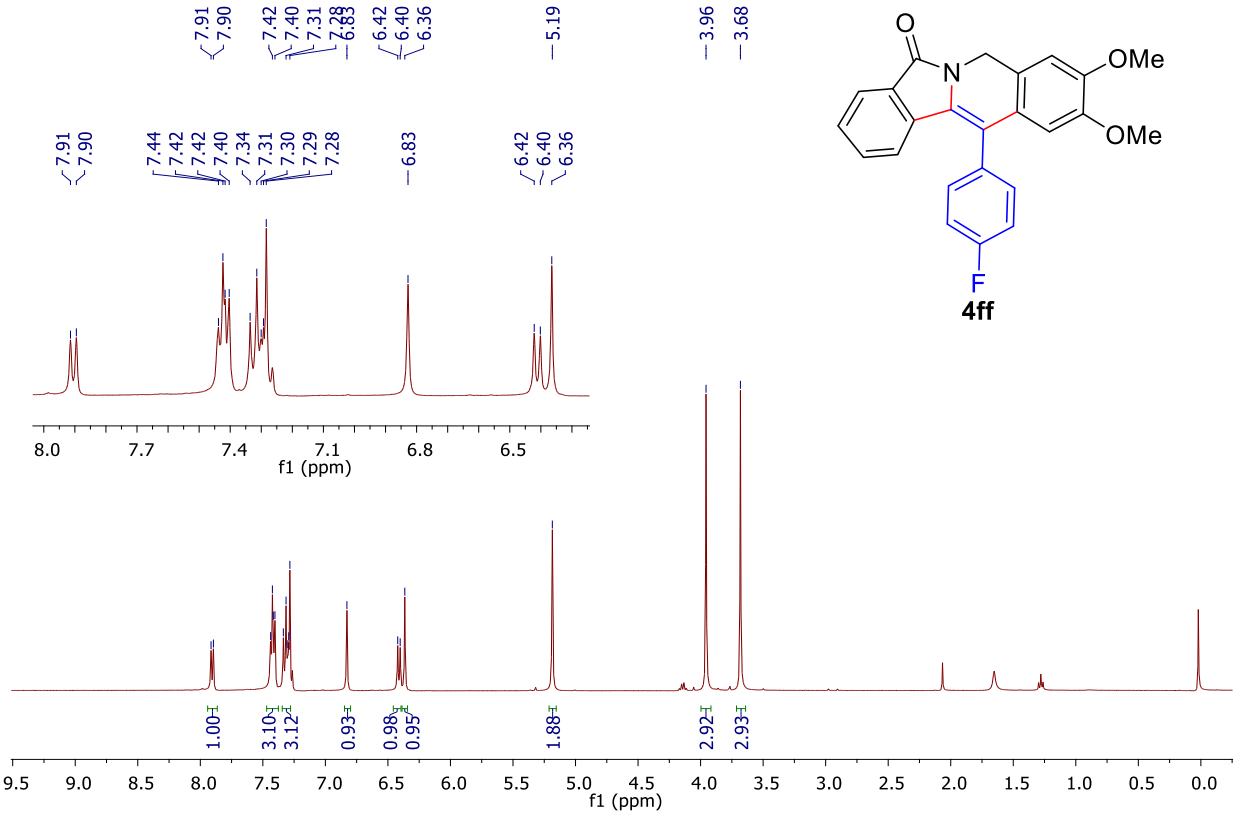
4fa

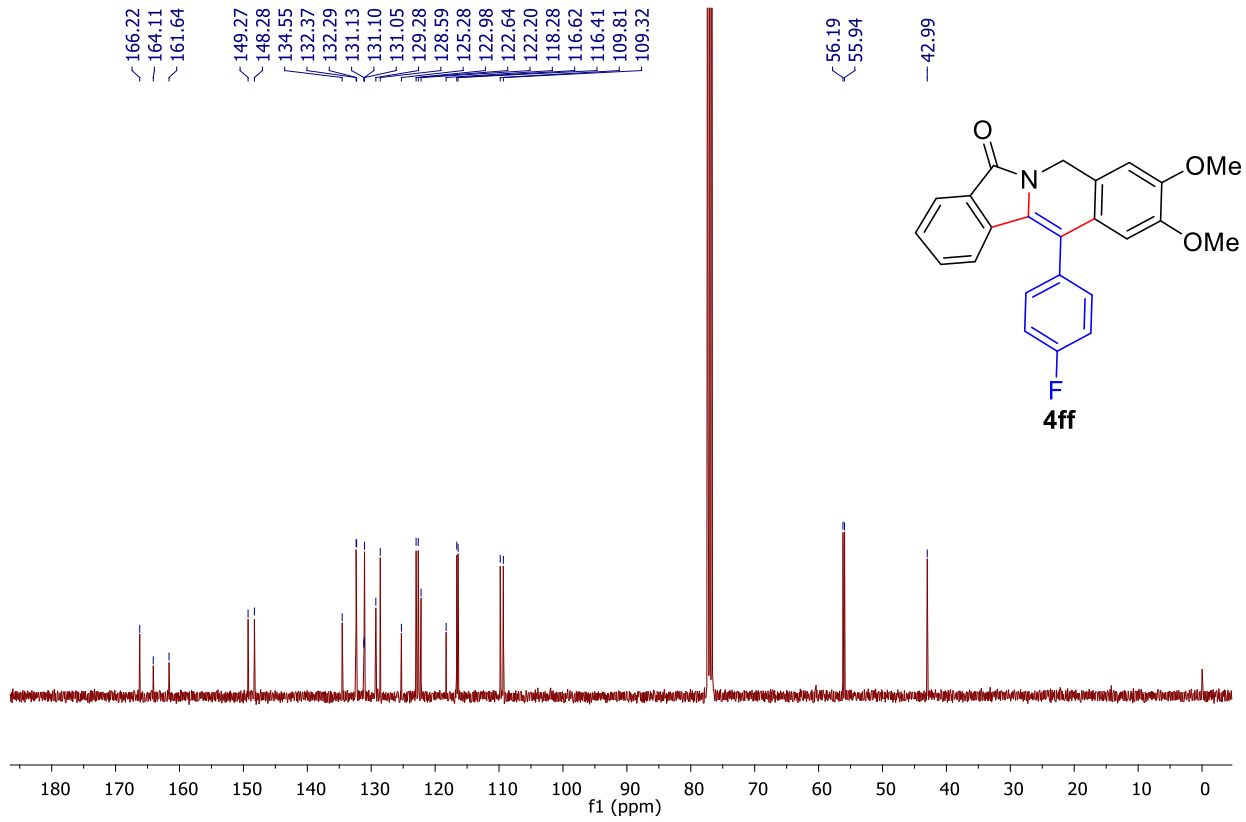

7.90
7.88
7.39
7.31
7.29
6.82
6.46
6.45
6.44
5.18
3.95
3.68
2.54
7.41
7.40
7.38
7.27
7.26
7.24
f1 (ppm)
1.00
3.06
1.99
1.04
0.99
1.97
2.00
3.02
2.97
2.95
O
N
OMe
OMe
Me
4fb

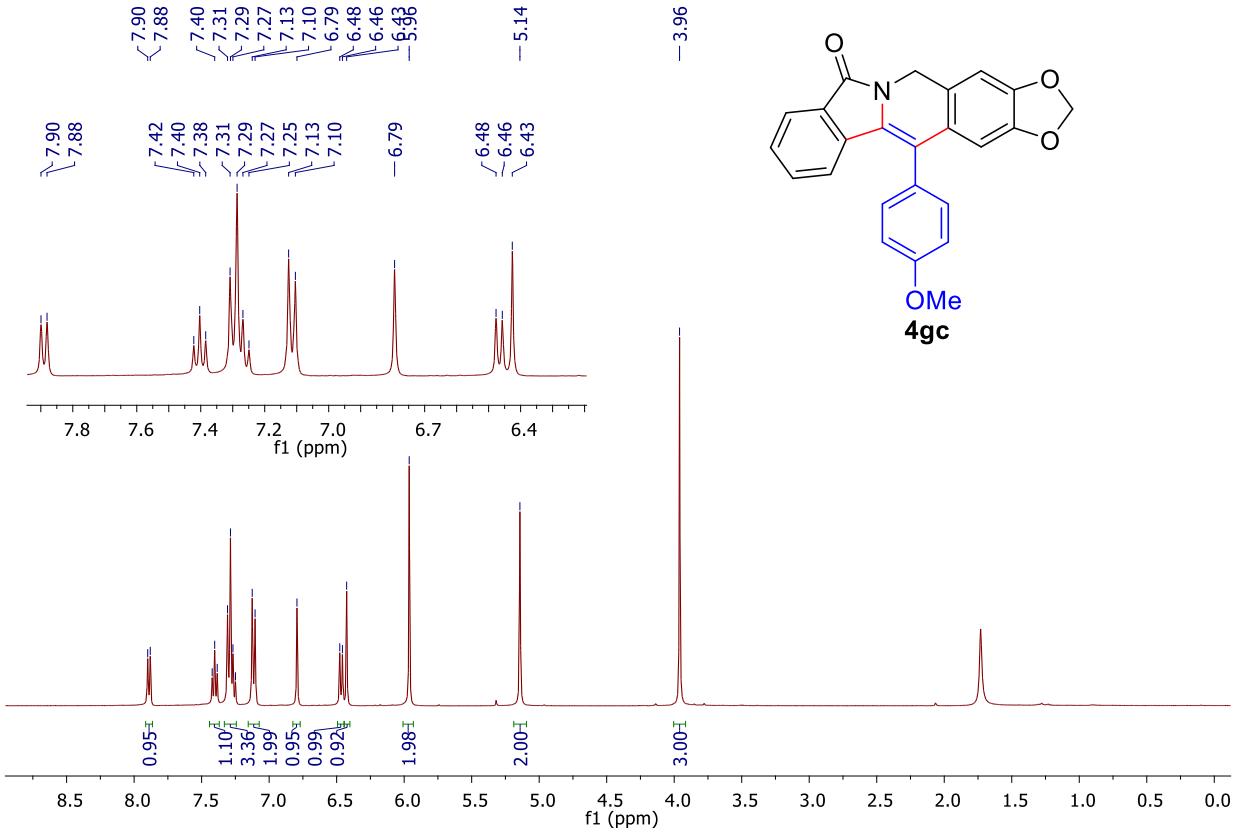

166.24
149.14
148.20
138.32
132.01
130.90
130.25
130.00
128.31
122.89
122.79
109.72
109.67
56.17
55.97
43.00
21.51
f1 (ppm)
O
N
OMe
OMe
Me
4fb

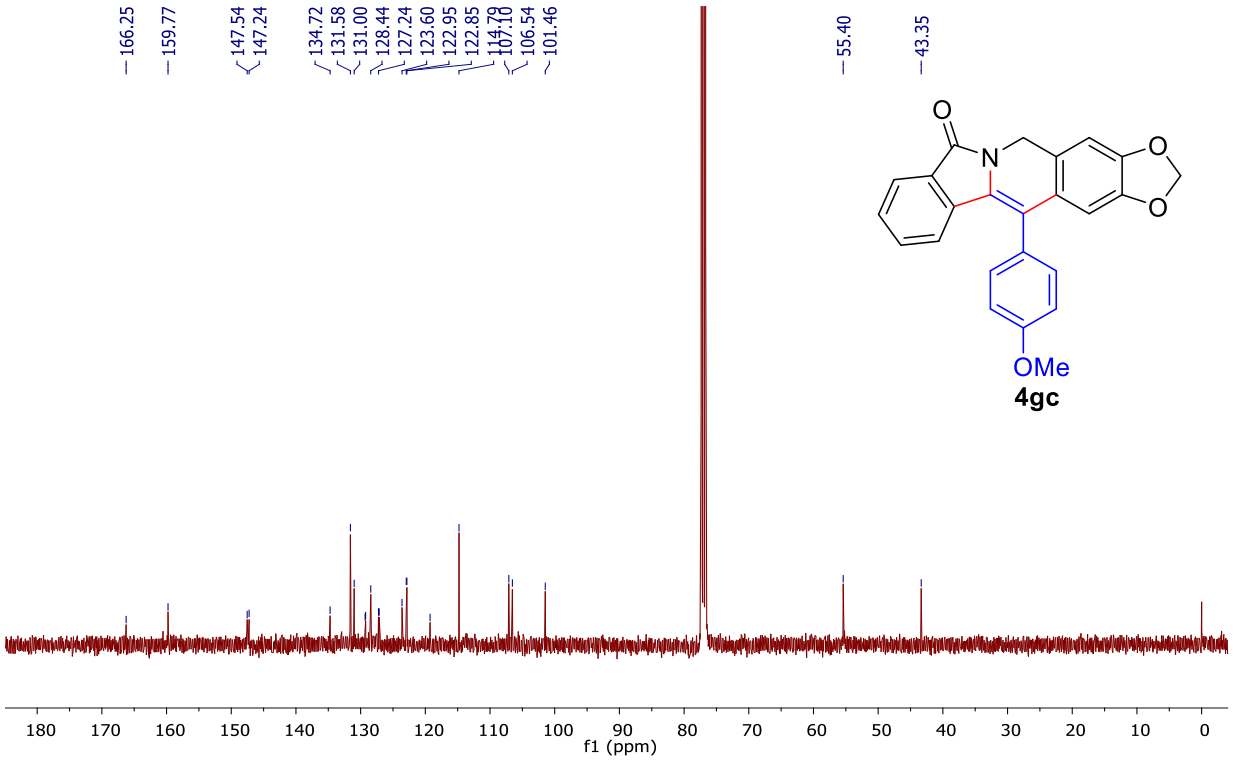

7.90
7.89
7.40
7.39
7.35
7.33
7.29
7.28
7.27
7.14
7.12
6.82
6.49
6.47
6.46
5.18
3.97
3.95
3.69
7.42
7.40
7.39
7.35
7.33
7.29
7.28
7.27
7.25
7.25
7.14
7.12
6.82
6.49
6.47
6.46
7.9
7.7
7.5
7.3
7.1
6.9
6.7
6.5
f1 (ppm)
O
N
OMe
OMe
OMe
4fc
1.00
1.16
2.08
1.55
2.00
0.97
1.02
0.90
1.94
2.89
2.83
3.04
9.5
9.0
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)

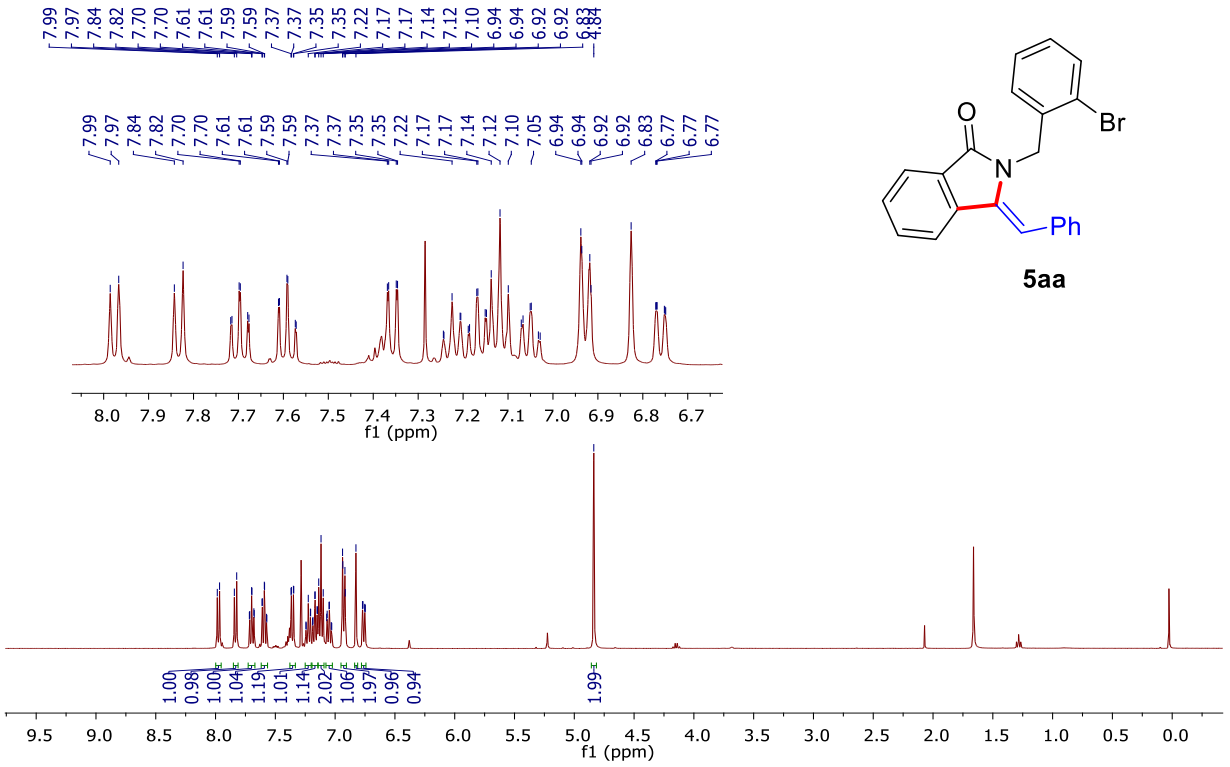

166.25
159.70
149.12
148.20
134.79
131.61
130.95
129.22
129.14
128.33
127.11
125.72
122.87
122.82
122.23
119.28
114.69
109.71
109.56
56.18
55.96
55.36
43.00
O
N
OMe
OMe
OMe
4fc
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.91
7.90
7.42
7.40
7.31
6.83
6.42
6.40
6.36
5.19
3.96
3.68
7.44
7.34
7.30
7.29
7.28
1.00
3.10
3.12
0.93
0.98
0.95
1.88
2.92
2.93
f1 (ppm)
O
N
OMe
OMe
F
4ff


166.22
164.11
161.64
149.27
148.28
134.55
132.37
132.29
131.13
131.10
131.05
129.28
128.59
125.28
122.98
122.64
122.20
118.28
116.62
116.41
109.81
109.32
56.19
55.94
42.99
f1 (ppm)
O
N
OMe
OMe
F
4ff

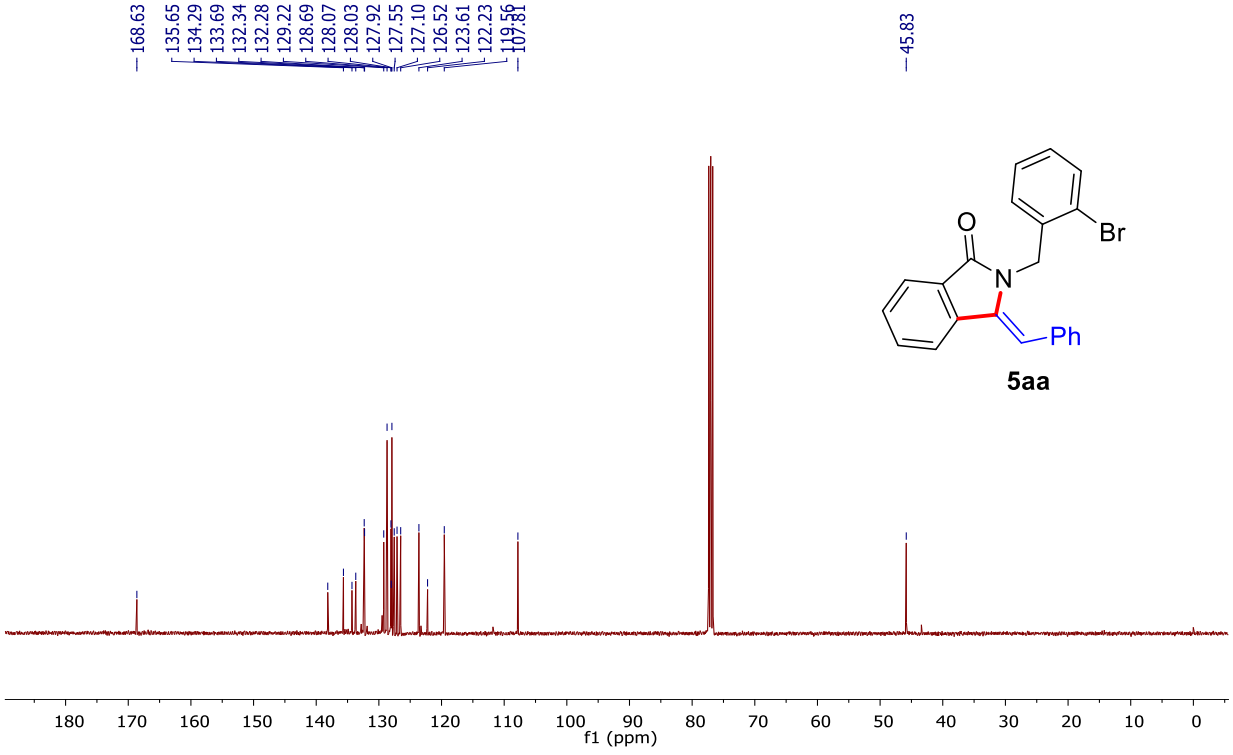

7.90
7.88
7.40
7.31
7.29
7.27
7.13
7.10
6.79
6.48
6.46
6.43
5.98
5.14
3.96
7.42
7.38
7.25
f1 (ppm)
0.95
1.10
3.36
1.99
0.95
0.99
0.92
1.98
2.00
3.00
OMe
4gc


166.25
159.77
147.54
147.24
134.72
131.58
131.00
128.44
127.24
123.60
122.95
122.85
114.79
107.10
106.54
101.46
55.40
43.35
f1 (ppm)
OMe
4gc


7.99
7.97
7.84
7.82
7.70
7.70
7.61
7.61
7.59
7.59
7.37
7.37
7.35
7.35
7.22
7.17
7.17
7.14
7.12
7.10
6.94
6.94
6.92
6.83
4.84
7.05
6.77
6.77
6.77
f1 (ppm)
1.00
0.98
1.00
1.04
1.19
1.01
1.14
2.02
1.06
1.97
0.96
0.94
1.99
f1 (ppm)

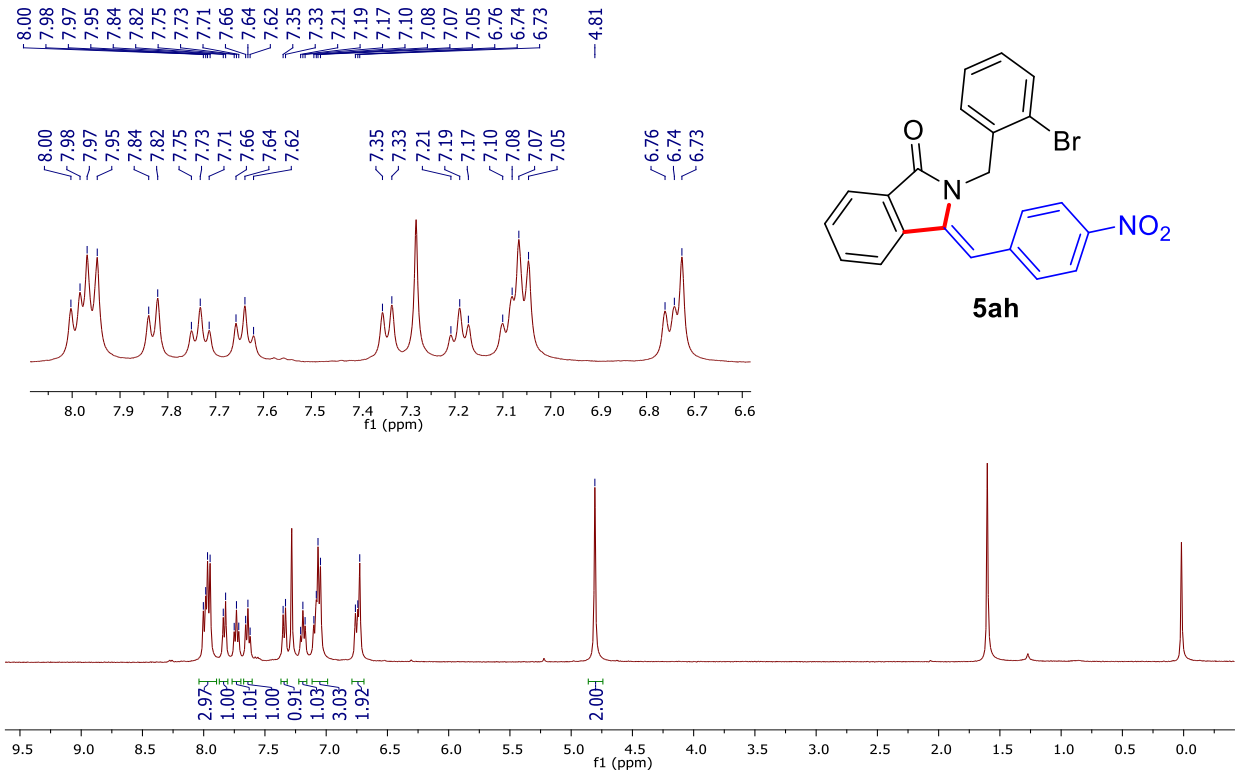
O
N
Br
Ph

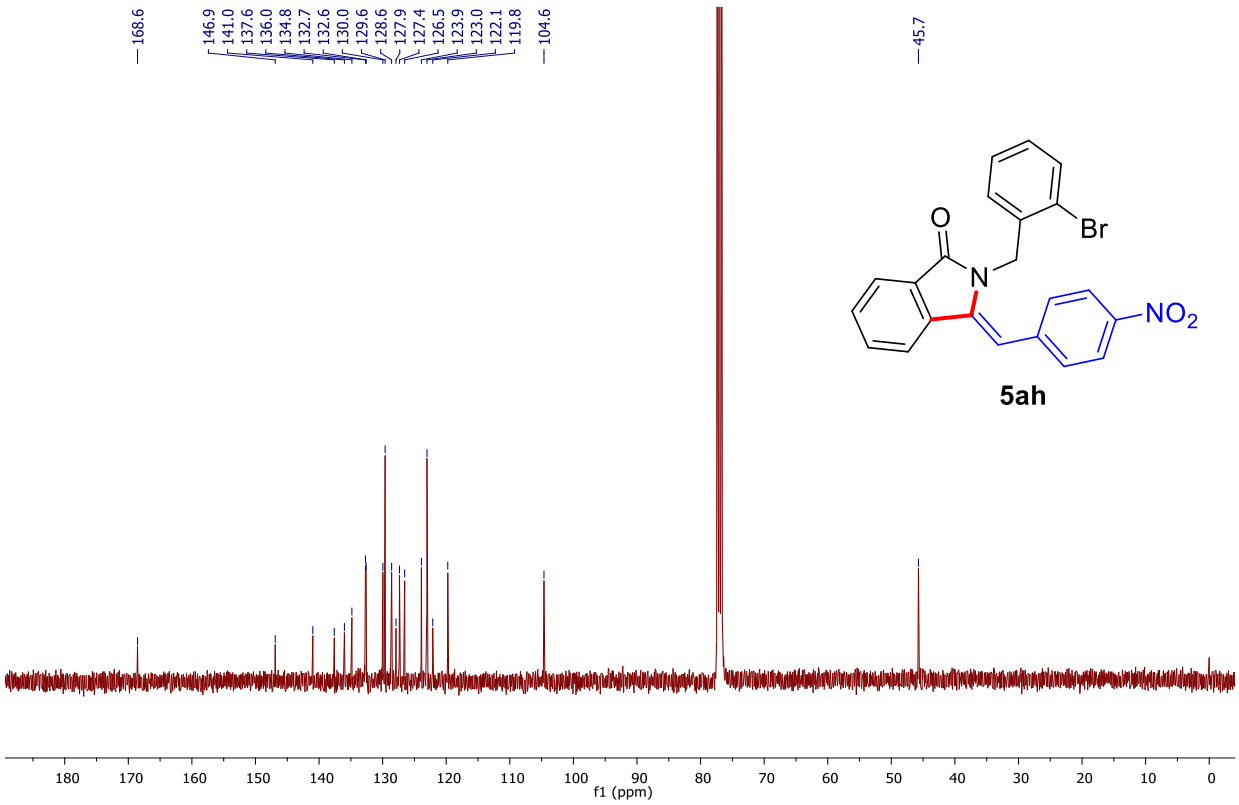
5aa

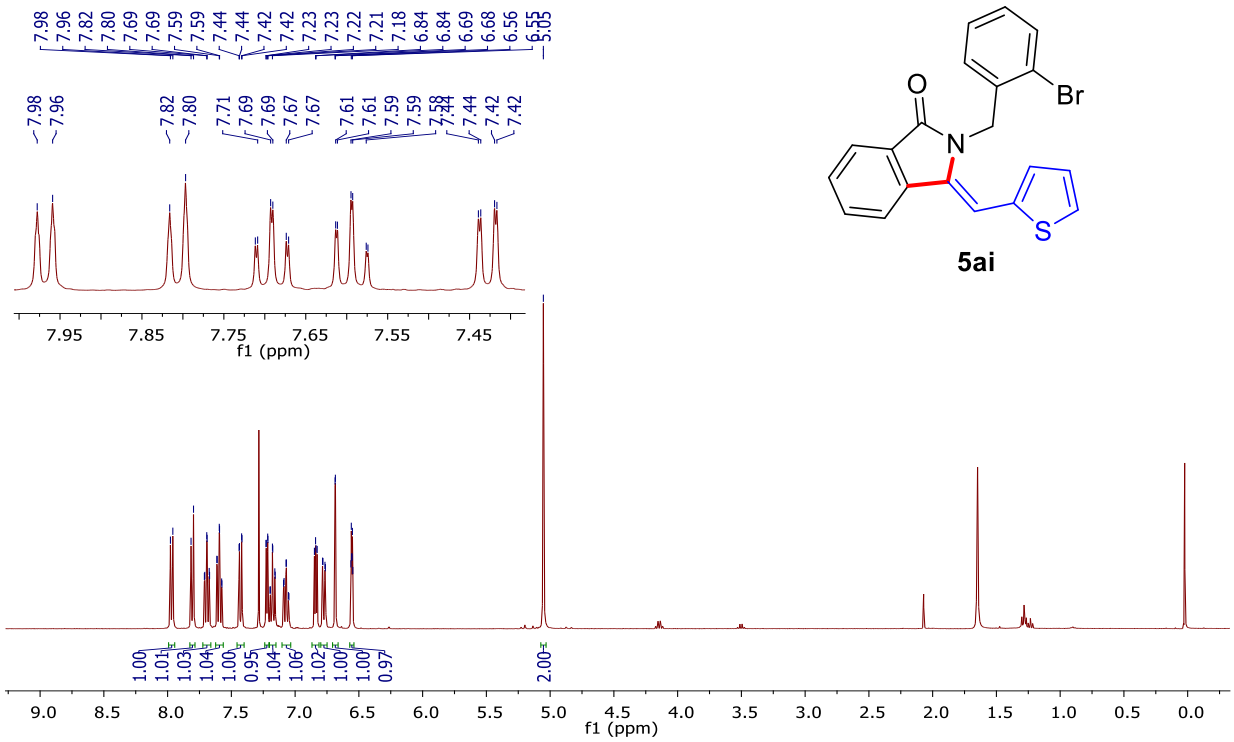

168.63
135.65
134.29
133.69
132.34
132.28
129.22
128.69
128.07
128.03
127.92
127.55
127.10
126.52
123.61
122.23
119.56
107.81
45.83
f1 (ppm)

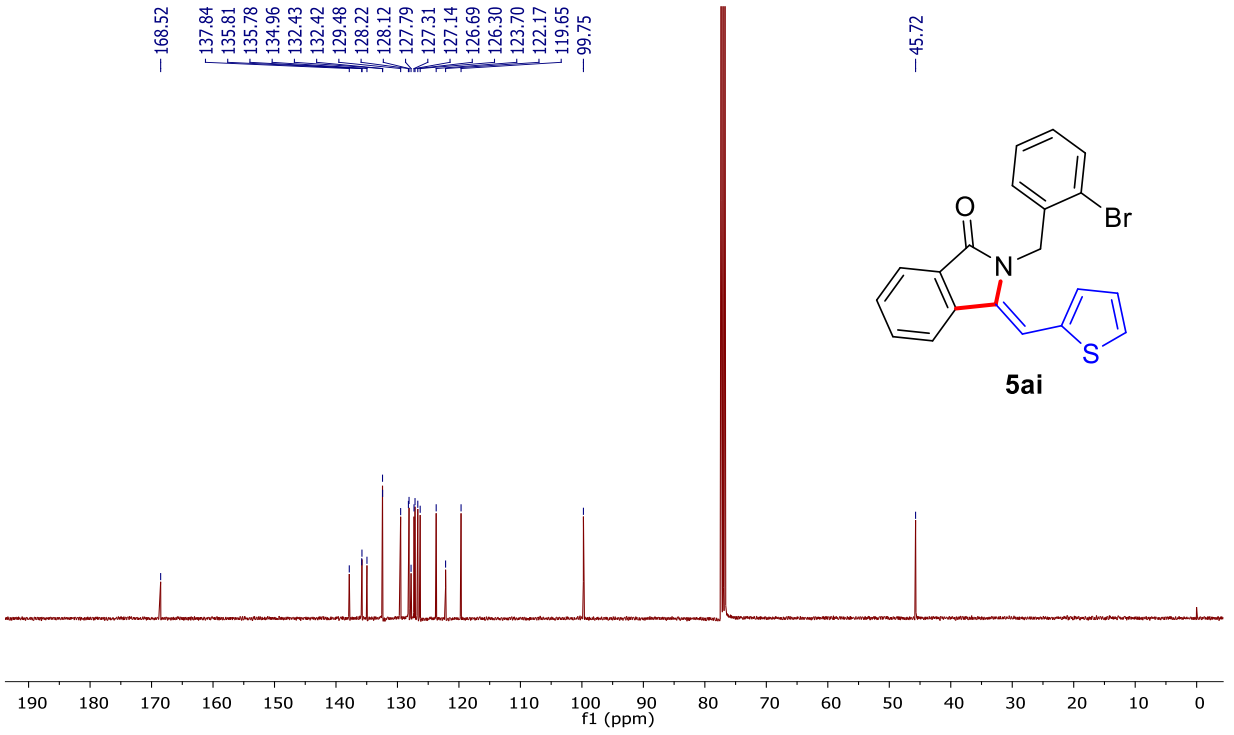
O
N
Br
Ph

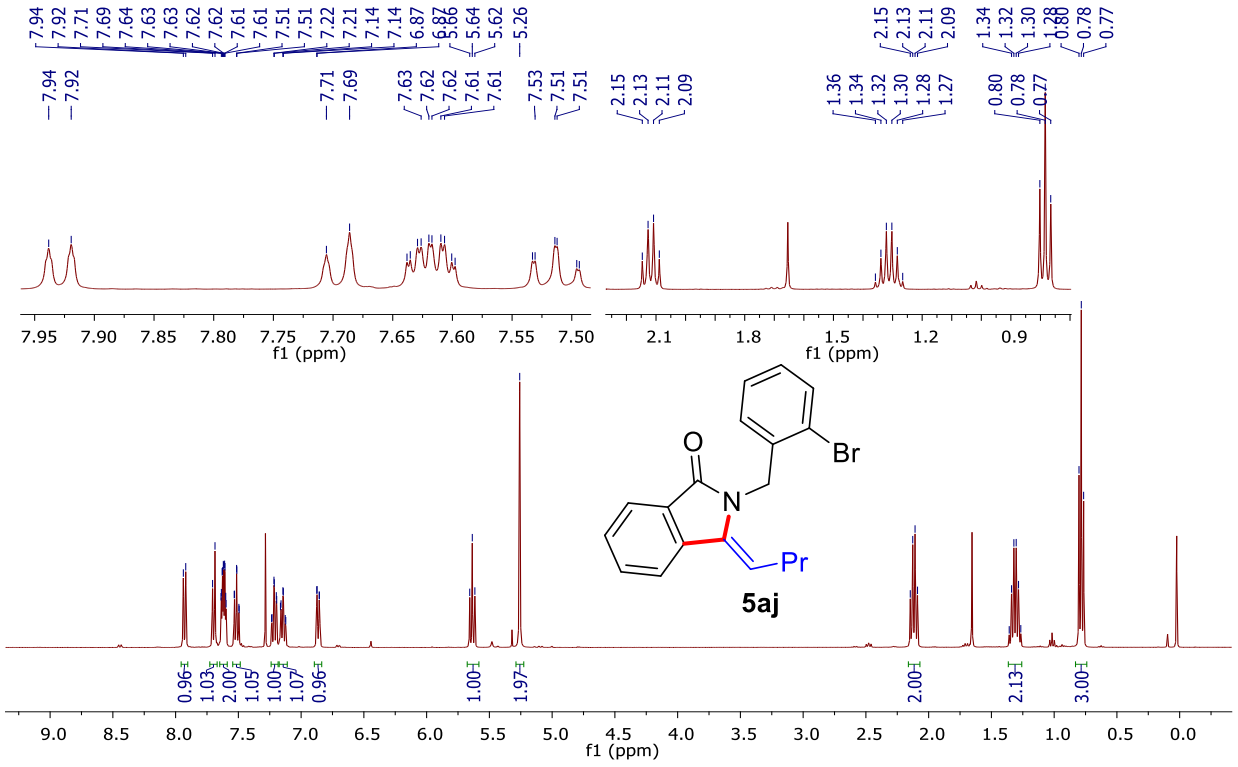
5aa

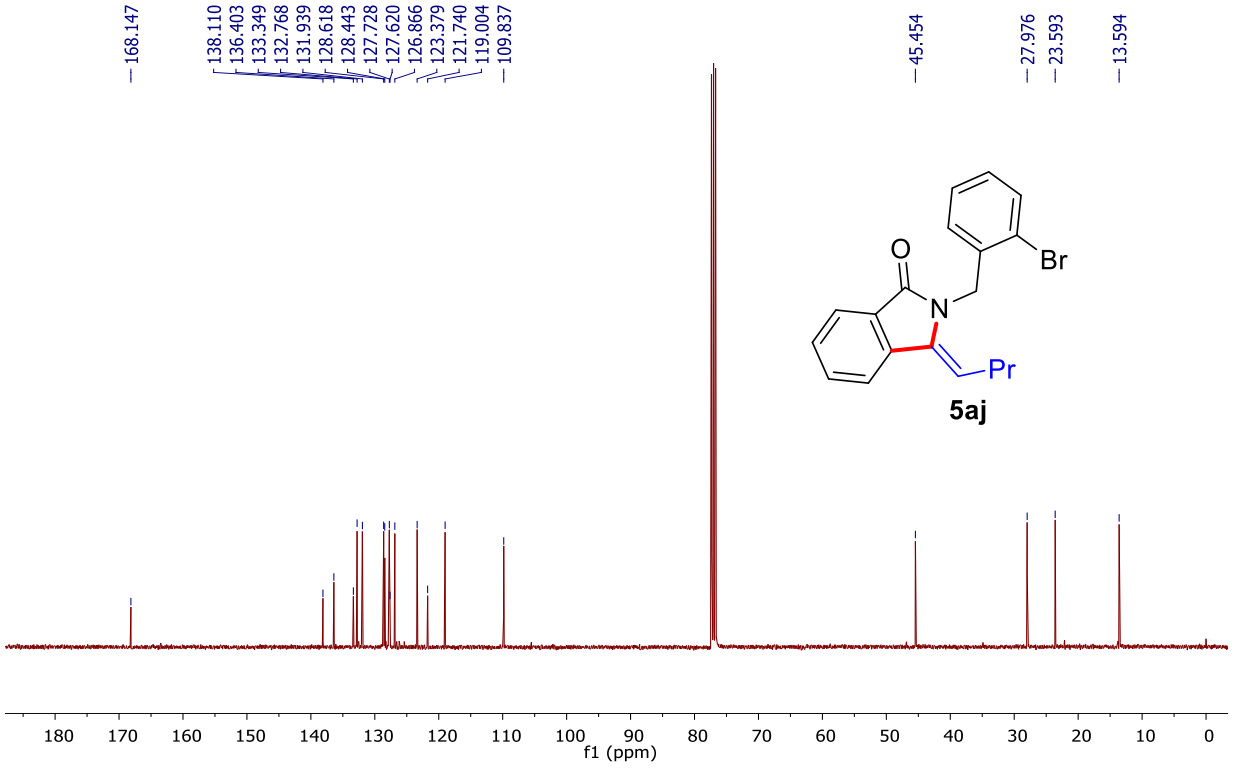

8.00
7.98
7.97
7.95
7.84
7.82
7.75
7.73
7.71
7.66
7.64
7.62
7.35
7.33
7.21
7.19
7.17
7.10
7.08
7.07
7.05
6.76
6.74
6.73
4.81
f1 (ppm)
O
N
Br
NO2
5ah
2.97
1.00
1.01
1.00
0.91
1.03
3.03
1.92
2.00

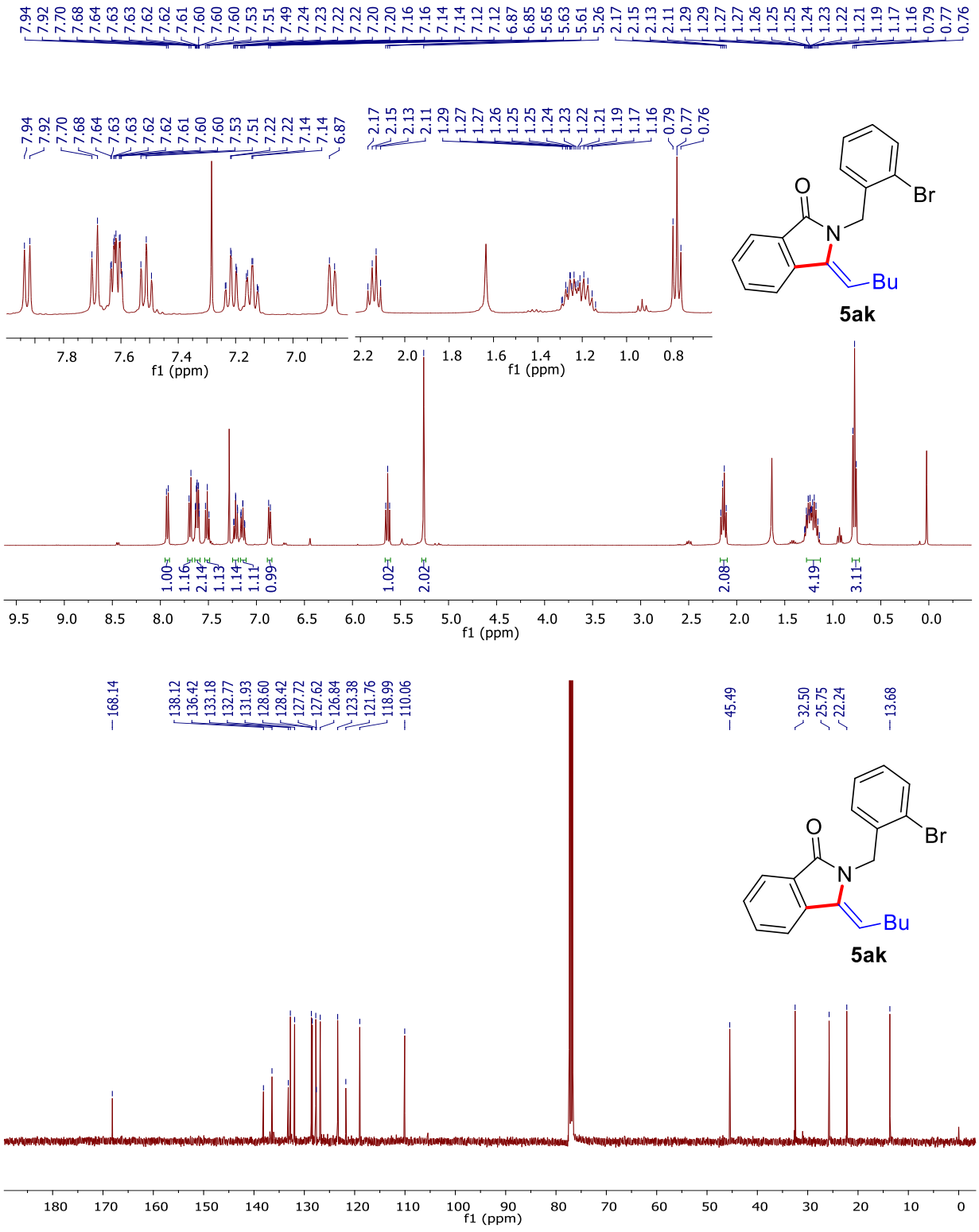

168.6
146.9
141.0
137.6
136.0
134.8
132.7
132.6
130.0
129.6
128.6
127.9
127.4
126.5
123.9
123.0
122.1
119.8
104.6
45.7
f1 (ppm)
O
N
Br
NO2
5ah

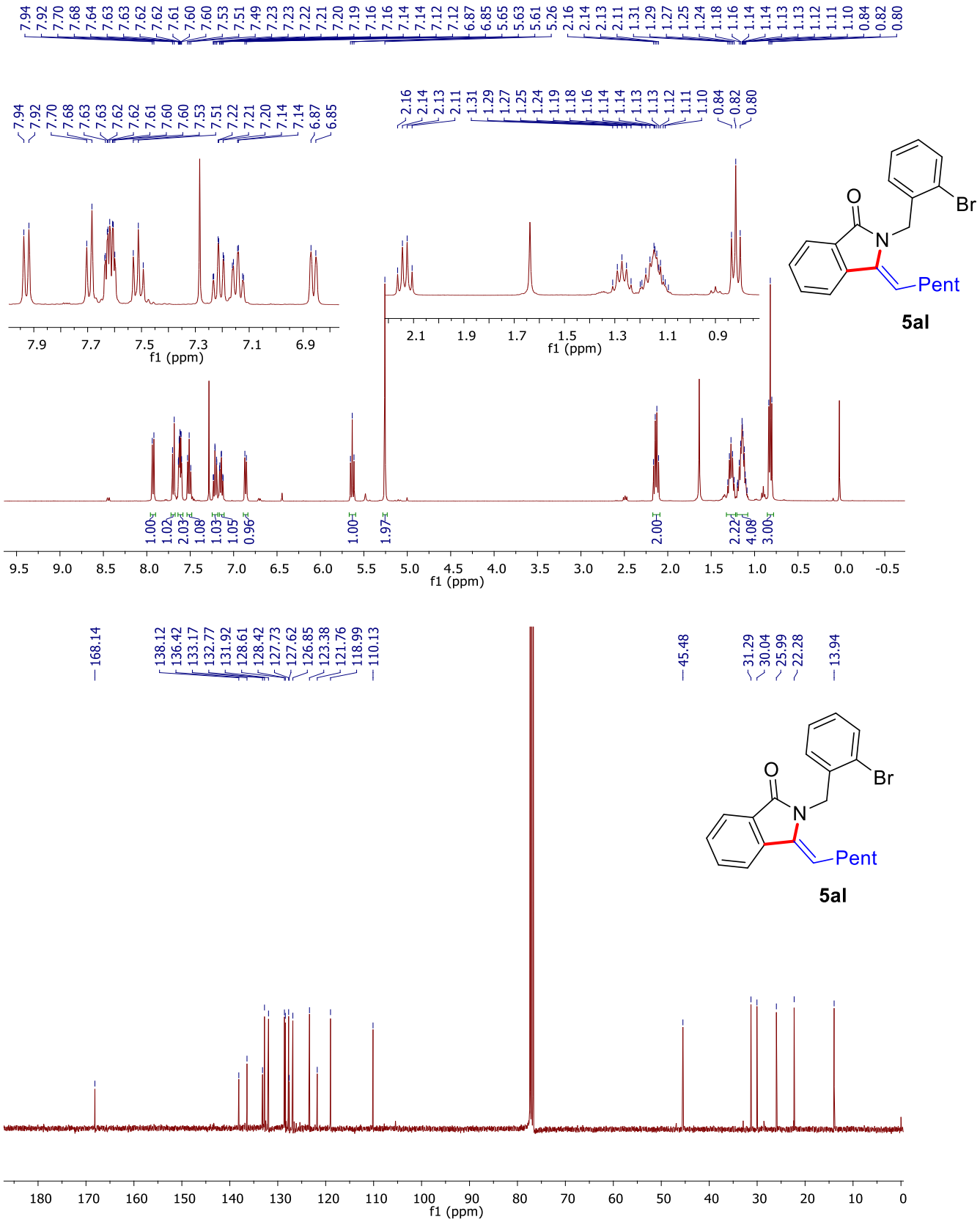

7.98
7.96
7.82
7.80
7.69
7.69
7.59
7.59
7.44
7.44
7.42
7.42
7.23
7.23
7.22
7.21
7.18
6.84
6.84
6.69
6.68
6.56
6.55
5.05
7.95
7.85
7.75
7.65
7.55
7.45
f1 (ppm)
1.00
1.01
1.03
1.04
1.00
0.95
1.04
1.06
1.02
1.00
1.00
0.97
2.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
O
Br
N
S
5ai

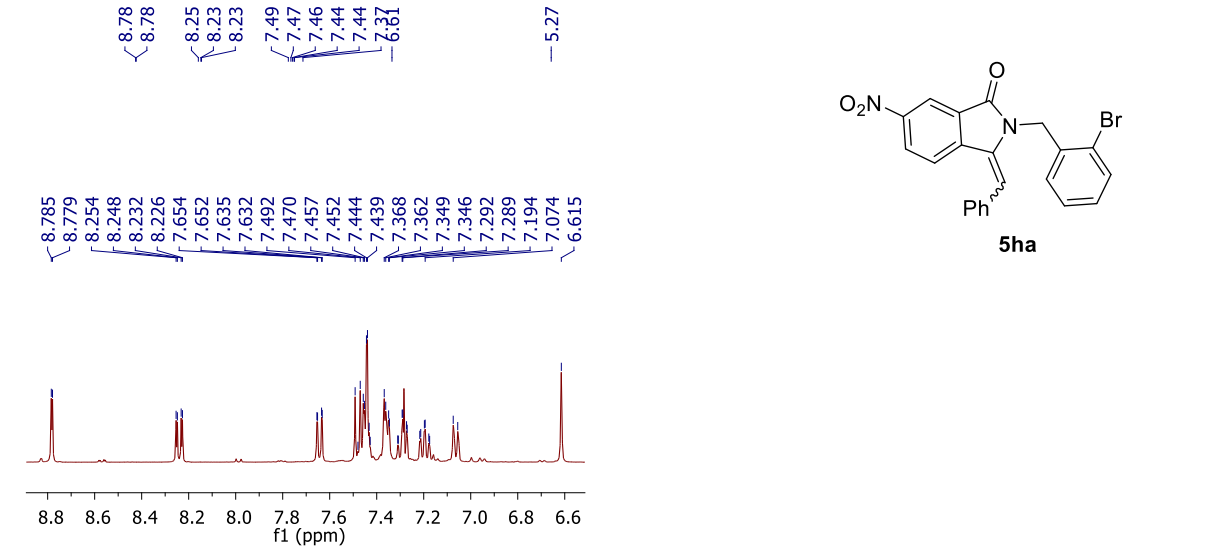

168.52
137.84
135.81
135.78
134.96
132.43
132.42
129.48
128.22
128.12
127.79
127.31
127.14
126.69
126.30
123.70
122.17
119.65
99.75
45.72
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
Br
N
S
5ai

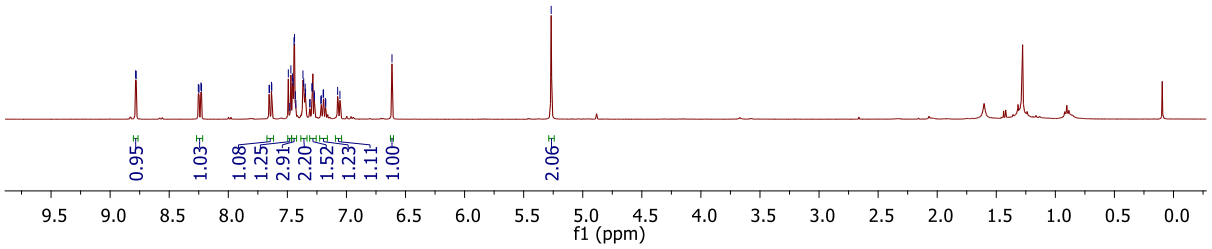

7.94
7.92
7.71
7.69
7.64
7.63
7.63
7.62
7.62
7.61
7.61
7.51
7.51
7.22
7.21
7.14
6.87
5.64
5.62
5.26
2.15
2.13
2.11
2.09
1.34
1.32
1.30
1.28
0.80
0.78
0.77
f1 (ppm)
Br
O
N
Pr
5aj
0.96
1.03
2.00
1.05
1.00
1.07
0.96
1.00
1.97
2.00
2.13
3.00

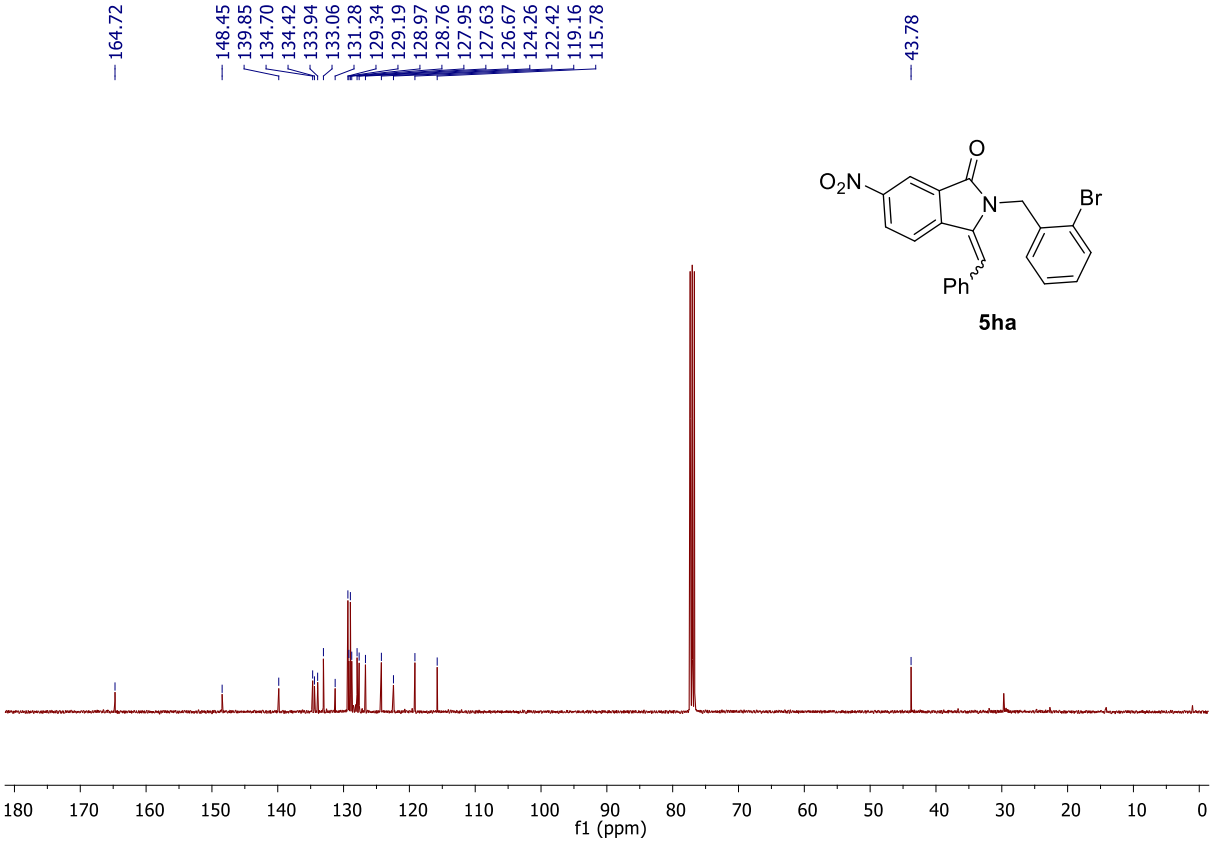

168.147
138.110
136.403
133.349
132.768
131.939
128.618
128.443
127.728
127.620
126.866
123.379
121.740
119.004
109.837
45.454
27.976
23.593
13.594
f1 (ppm)
Br
O
N
Pr
5aj

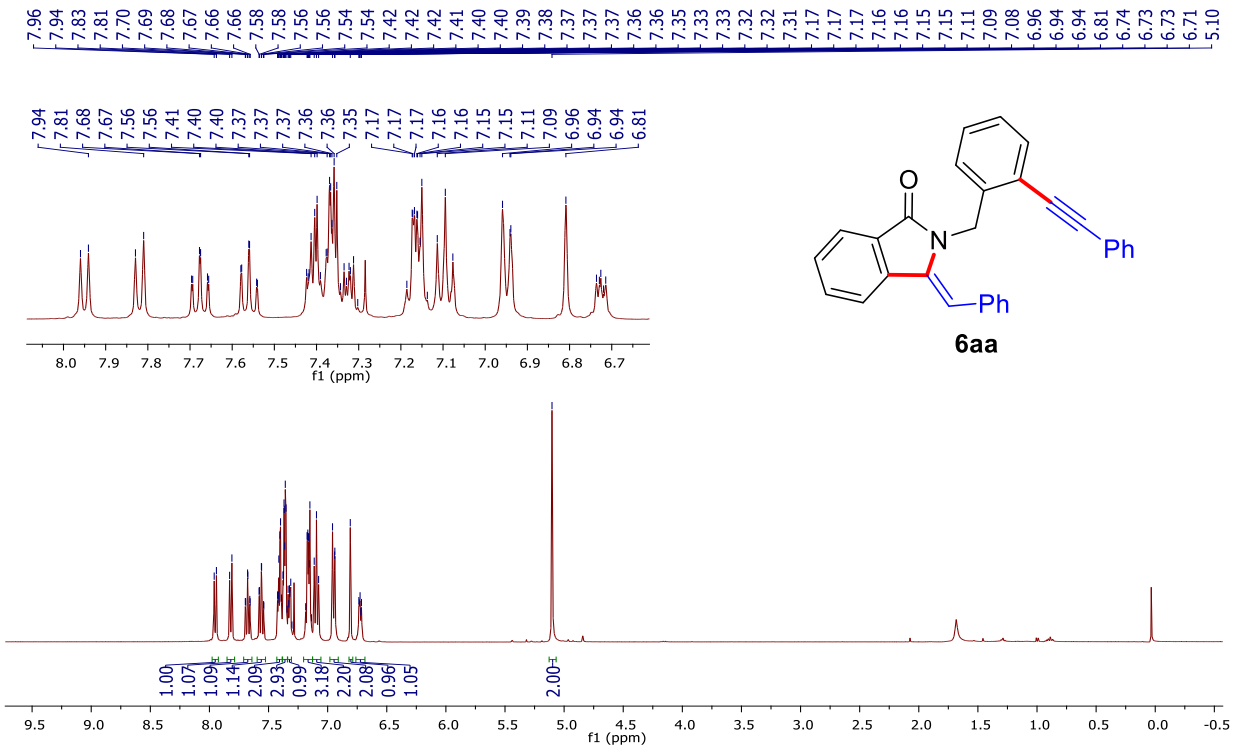

7.94 7.92 7.70 7.68 7.64 7.63 7.63 7.62 7.62 7.61 7.60 7.60 7.60 7.53 7.51 7.49 7.24 7.23 7.22 7.22 7.20 7.20 7.16 7.16 7.14 7.14 7.12 7.12 6.87 6.85 5.65 5.63 5.61 5.26 2.17 2.15 2.13 2.11 1.29 1.29 1.27 1.27 1.26 1.25 1.25 1.24 1.23 1.22 1.21 1.19 1.17 1.16 0.79 0.77 0.76
7.94 7.92 7.70 7.68 7.64 7.63 7.63 7.62 7.62 7.61 7.60 7.60 7.53 7.51 7.22 7.22 7.14 7.14 6.87
2.17 2.15 2.13 2.11 1.29 1.27 1.27 1.26 1.25 1.25 1.24 1.23 1.22 1.21 1.19 1.17 1.16 0.79 0.77 0.76
O
N
Br
Bu
5ak
f1 (ppm)
1.00 1.16 2.14 1.13 1.14 1.11 0.99 1.02 2.02 2.08 4.19 3.11
f1 (ppm)
168.14 138.12 136.42 133.18 132.77 131.93 128.60 128.42 127.72 127.62 126.84 123.38 121.76 118.99 110.06 45.49 32.50 25.75 22.24 13.68
O
N
Br
Bu
5ak
f1 (ppm)


7.94 7.92 7.70 7.68 7.64 7.63 7.63 7.62 7.62 7.61 7.60 7.60 7.53 7.51 7.49 7.23 7.23 7.22 7.21 7.20 7.19 7.16 7.16 7.14 7.14 7.12 7.12 6.87 6.85 5.65 5.63 5.61 5.26 2.16 2.14 2.13 2.11 1.31 1.29 1.27 1.25 1.24 1.18 1.16 1.14 1.14 1.13 1.13 1.12 1.11 1.10 0.84 0.82 0.80
f1 (ppm)
1.00 1.02 2.03 1.08 1.03 1.05 0.96 1.00 1.97 2.00 2.22 4.08 3.00
O
N
Br
Pent
5al
168.14 138.12 136.42 133.17 132.77 131.92 128.61 128.42 127.73 127.62 126.85 123.38 121.76 118.99 110.13 45.48 31.29 30.04 25.99 22.28 13.94

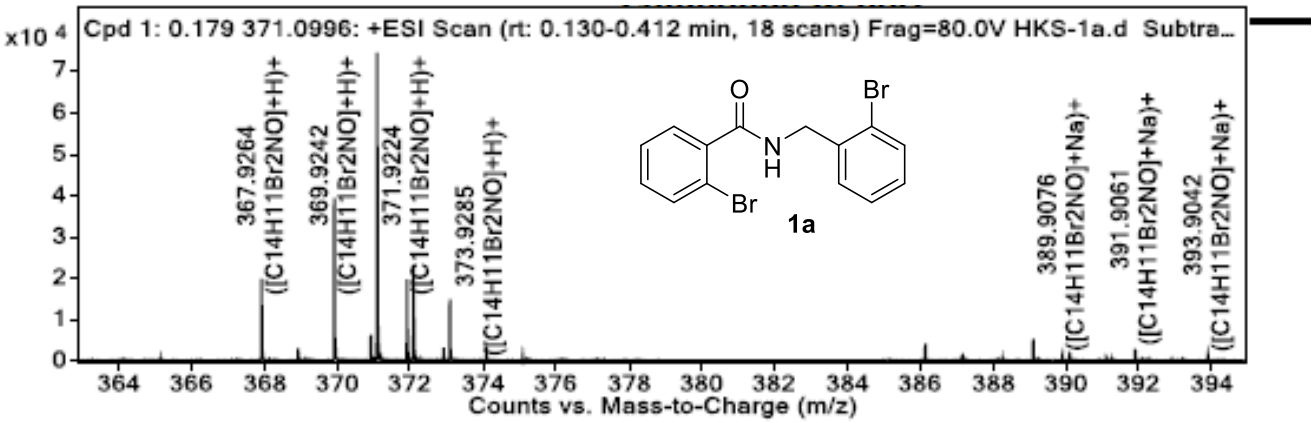

8.78
8.78
8.25
8.23
8.23
7.49
7.47
7.46
7.44
7.44
7.37
6.81
5.27
8.785
8.779
8.254
8.248
8.232
8.226
7.654
7.652
7.635
7.632
7.492
7.470
7.457
7.452
7.444
7.439
7.368
7.362
7.349
7.346
7.292
7.289
7.194
7.074
6.615
8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6
f1 (ppm)
O
O2N
N
Br
Ph
5ha

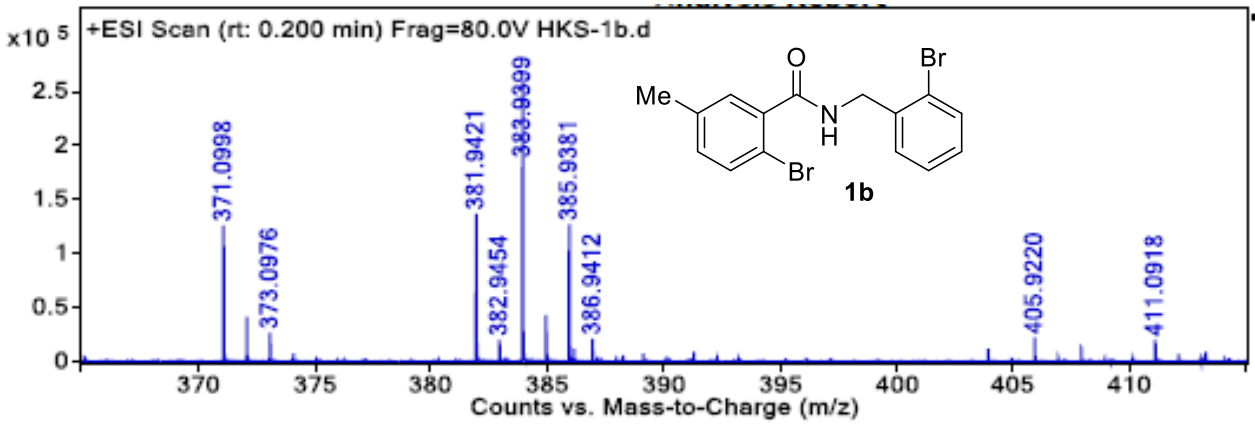

0.95
1.03
1.08
1.25
2.91
2.20
1.52
1.23
1.11
1.00
2.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

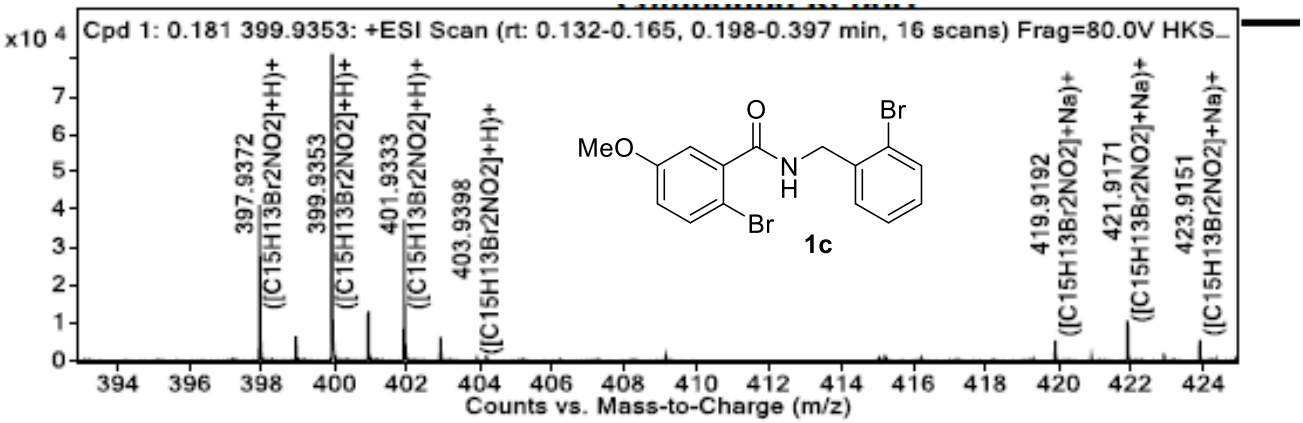

164.72
148.45
139.85
134.70
134.42
133.94
133.06
131.28
129.34
129.19
128.97
128.76
127.95
127.63
126.67
124.26
122.42
119.16
115.78
43.78
O
O2N
N
Br
Ph
5ha
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

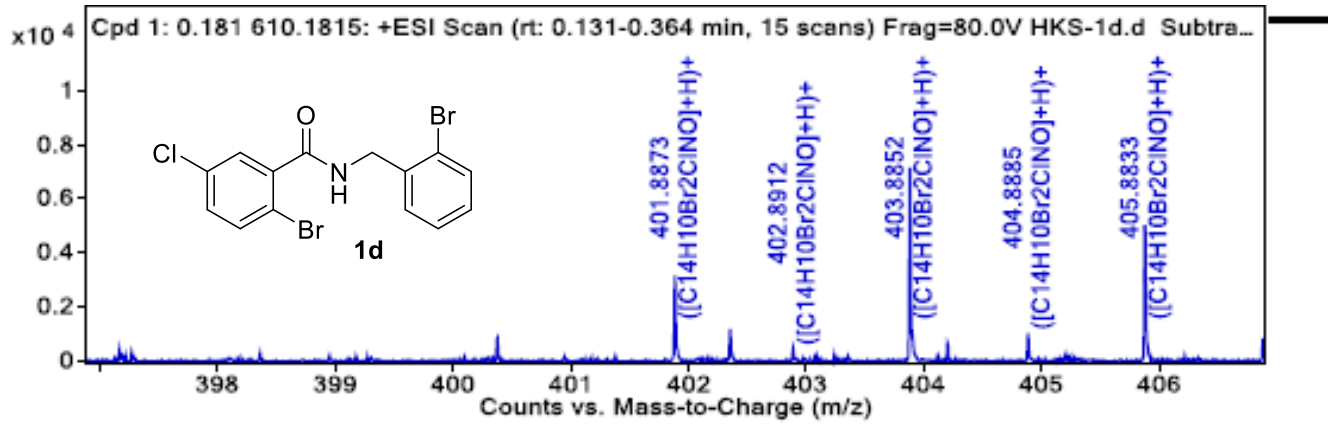

7.96 7.94 7.83 7.81 7.70 7.69 7.68 7.67 7.66 7.66 7.58 7.58 7.56 7.56 7.54 7.54 7.42 7.42 7.42 7.41 7.40 7.40 7.39 7.38 7.37 7.37 7.37 7.36 7.36 7.35 7.33 7.33 7.32 7.32 7.31 7.17 7.17 7.17 7.16 7.16 7.15 7.15 7.11 7.09 7.08 6.96 6.94 6.94 6.81 6.74 6.73 6.73 6.71 5.10
7.94 7.81 7.68 7.67 7.56 7.56 7.41 7.40 7.40 7.37 7.37 7.37 7.36 7.36 7.35 7.17 7.17 7.17 7.16 7.16 7.15 7.15 7.11 7.09 6.96 6.94 6.94 6.81
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
f1 (ppm)
O
N
Ph
Ph
6aa
1.00 1.07 1.09 1.14 2.09 2.93 0.99 3.18 2.20 2.08 0.96 1.05 2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
168.84 138.41 133.97 132.15 131.79 131.42 129.09 128.77 128.25 128.19 128.13 127.86 127.40 126.36 124.87 123.58 119.50 107.82 94.59 86.55 44.30
O
N
Ph
Ph
6aa
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

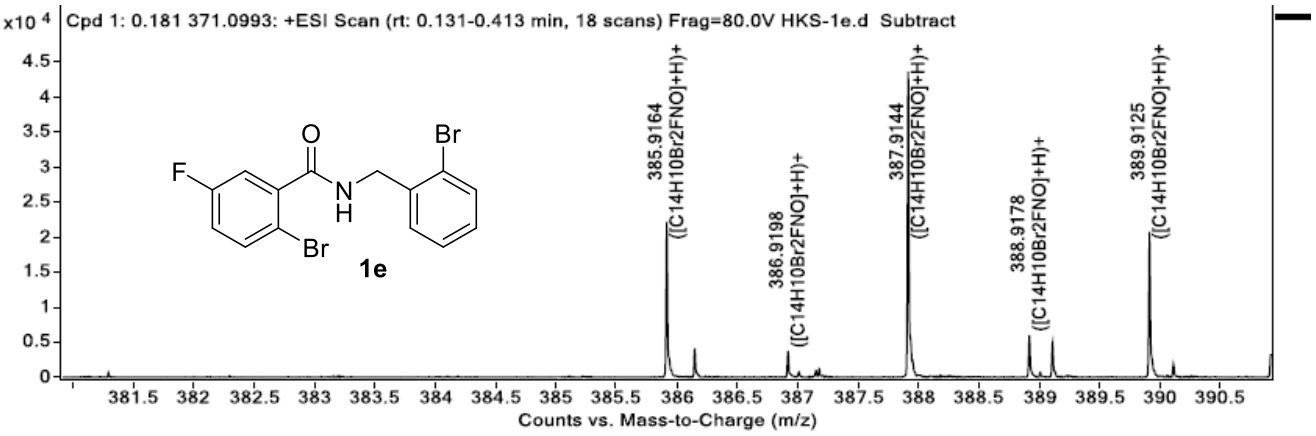
2. Copies of HRMS spectra of 1a-h, 4aa-4gc, 5aa-5ak and 6aa

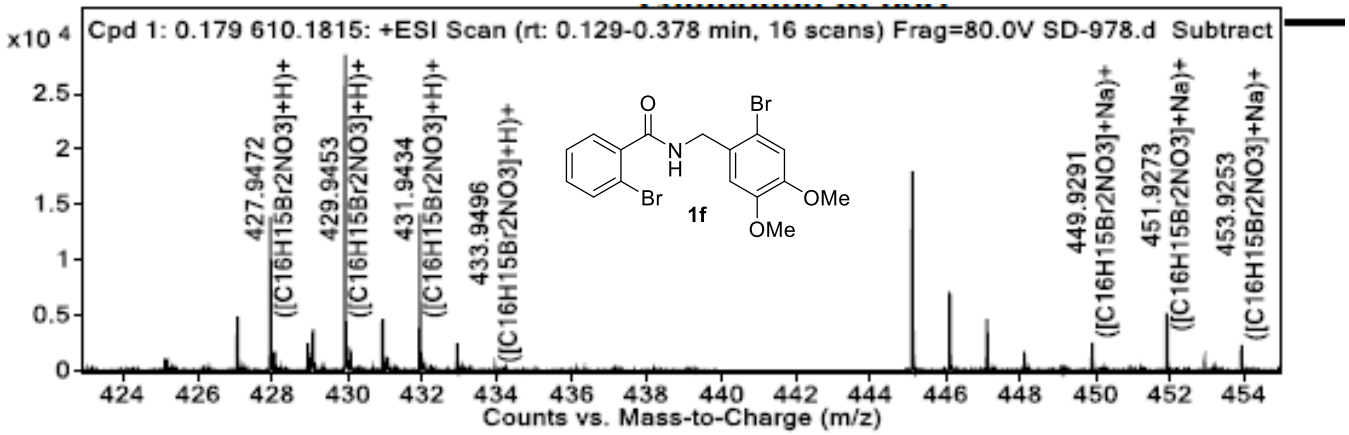


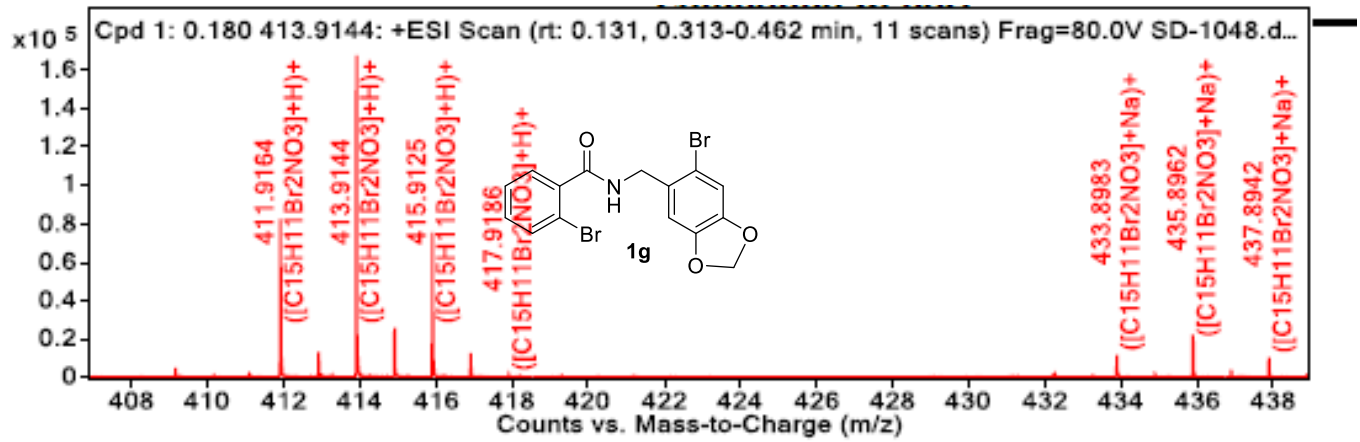


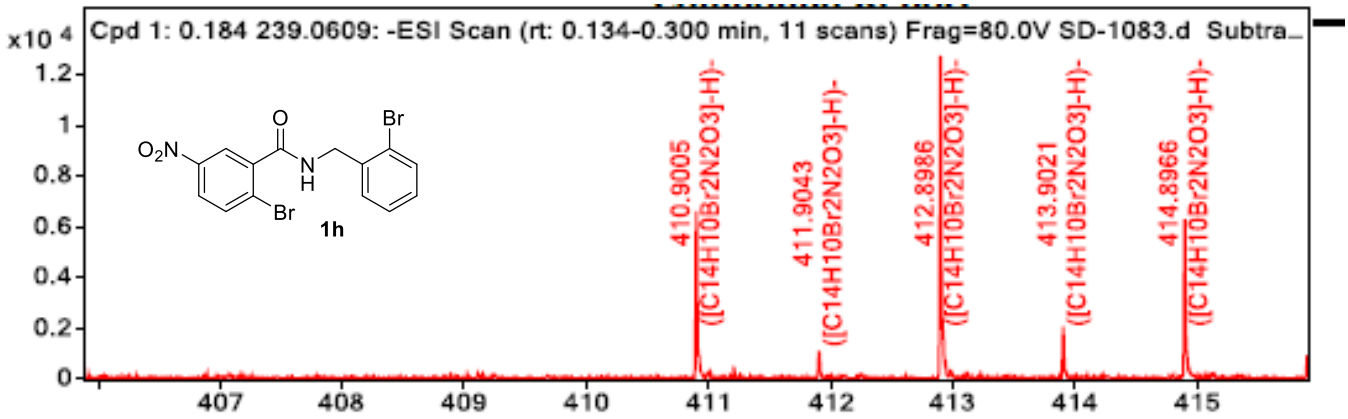


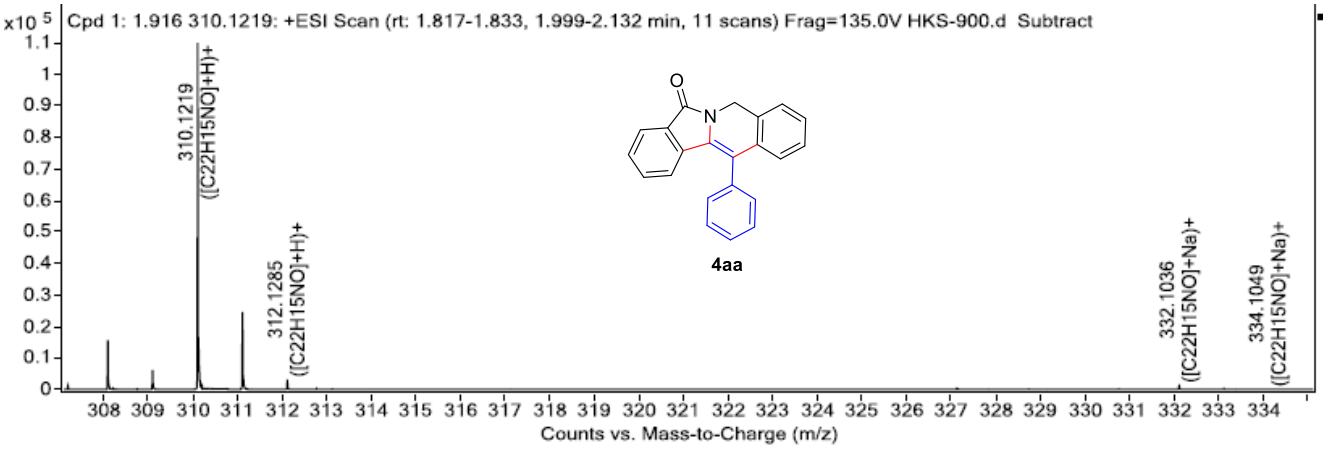

Cpd 1: 0.181 610.1815: +ESI Scan (rt: 0.131-0.364 min, 15 scans) Frag=80.0V HKS-1d.d Subtra...
x10 4
1
0.8
0.6
0.4
0.2
0
Cl
O
N
H
Br
Br
1d
401.8873
([C14H10Br2ClNO]+H)+
402.8912
([C14H10Br2ClNO]+H)+
403.8852
([C14H10Br2ClNO]+H)+
404.8885
([C14H10Br2ClNO]+H)+
405.8833
([C14H10Br2ClNO]+H)+
398
399
400
401
402
403
404
405
406
Counts vs. Mass-to-Charge (m/z)

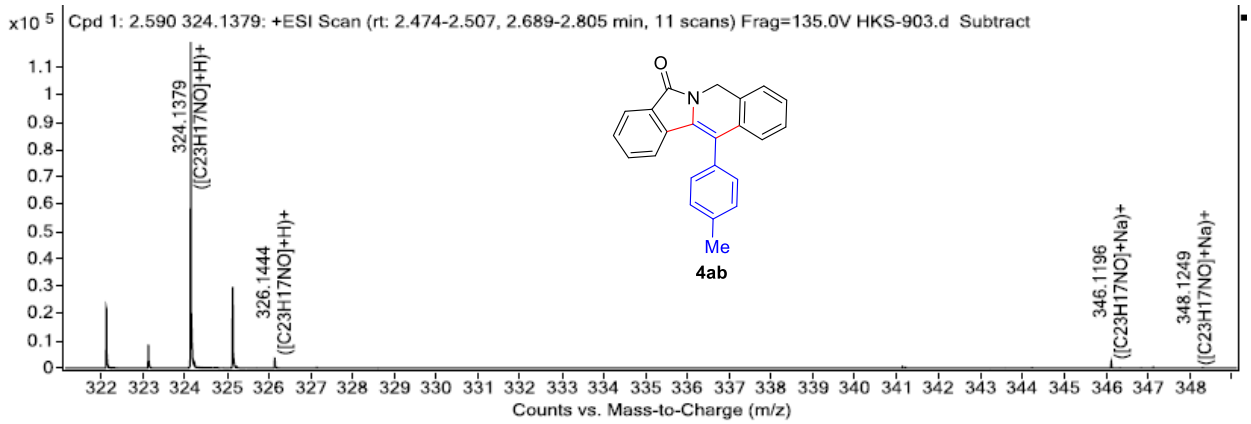

Cpd 1: 0.181 371.0993: +ESI Scan (rt: 0.131-0.413 min, 18 scans) Frag=80.0V HKS-1e.d Subtract
x10 4
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
F
O
N
H
Br
Br
1e
385.9164
([C14H10Br2FNO]+H)+
386.9198
([C14H10Br2FNO]+H)+
387.9144
([C14H10Br2FNO]+H)+
388.9178
([C14H10Br2FNO]+H)+
389.9125
([C14H10Br2FNO]+H)+
381.5
382
382.5
383
383.5
384
384.5
385
385.5
386
386.5
387
387.5
388
388.5
389
389.5
390
390.5
Counts vs. Mass-to-Charge (m/z)

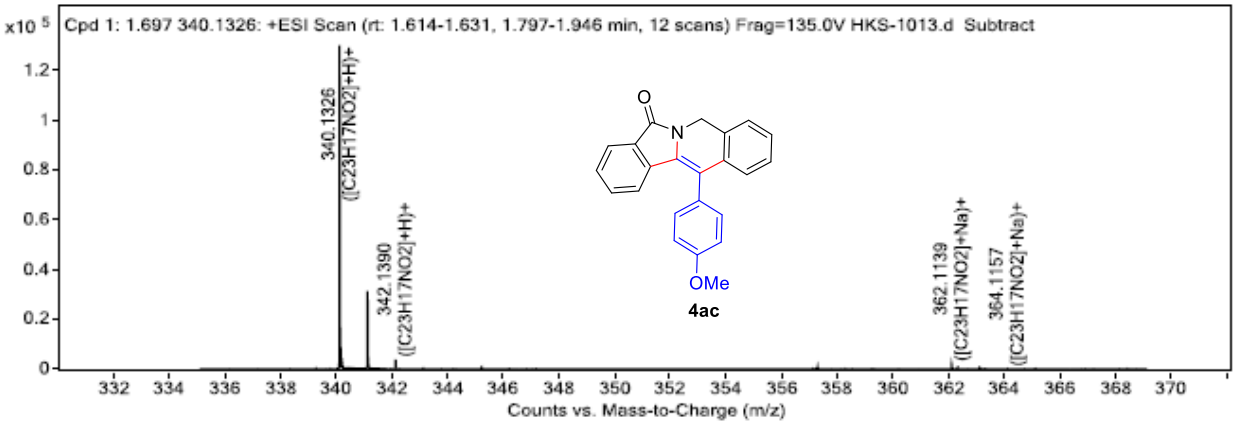

Cpd 1: 0.179 610.1815: +ESI Scan (rt: 0.129-0.378 min, 16 scans) Frag=80.0V SD-978.d Subtract
x10 4
2.5
2
1.5
1
0.5
0
427.9472
([C16H15Br2NO3]+H)+
429.9453
([C16H15Br2NO3]+H)+
431.9434
([C16H15Br2NO3]+H)+
433.9496
([C16H15Br2NO3]+H)+
O
N
H
Br
Br
OMe
OMe
1f
449.9291
([C16H15Br2NO3]+Na)+
451.9273
([C16H15Br2NO3]+Na)+
453.9253
([C16H15Br2NO3]+Na)+
424
426
428
430
432
434
436
438
440
442
444
446
448
450
452
454
Counts vs. Mass-to-Charge (m/z)

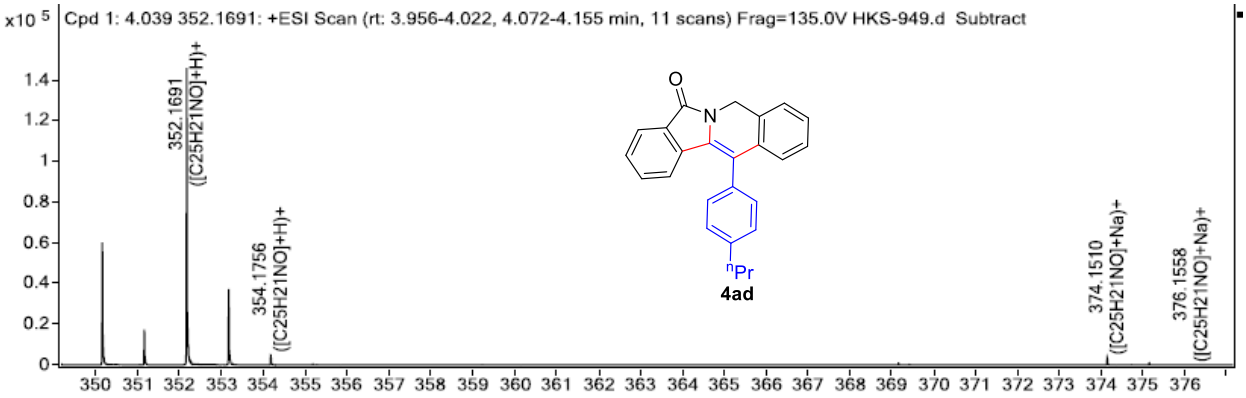

Cpd 1: 0.180 413.9144: +ESI Scan (rt: 0.131, 0.313-0.462 min, 11 scans) Frag=80.0V SD-1048.d...
x10 5
411.9164 ([C15H11Br2NO3]+H)+
413.9144 ([C15H11Br2NO3]+H)+
415.9125 ([C15H11Br2NO3]+H)+
417.9186 ([C15H11Br2NO3]+H)+
433.8983 ([C15H11Br2NO3]+Na)+
435.8962 ([C15H11Br2NO3]+Na)+
437.8942 ([C15H11Br2NO3]+Na)+
1g
Counts vs. Mass-to-Charge (m/z)

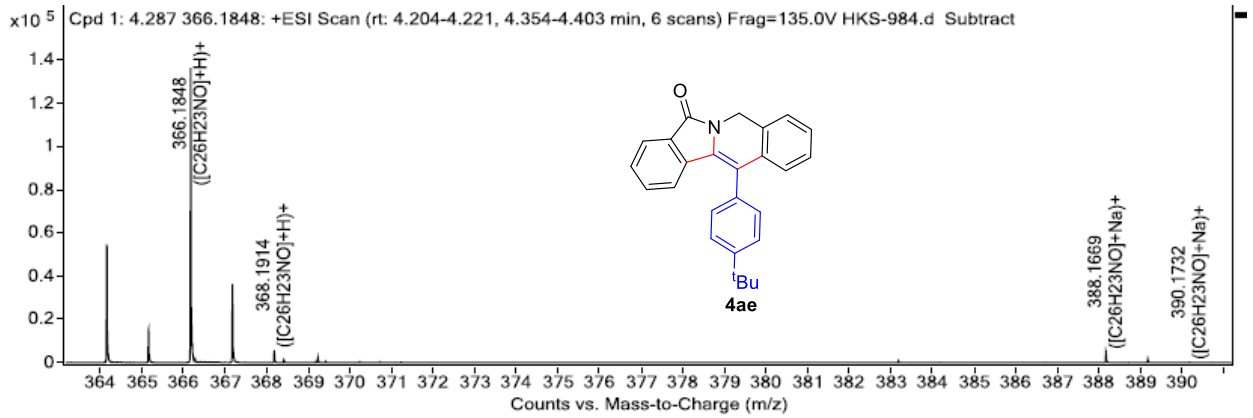

Cpd 1: 0.184 239.0609: -ESI Scan (rt: 0.134-0.300 min, 11 scans) Frag=80.0V SD-1083.d Subtra...
x10 4
410.9005 ([C14H10Br2N2O3]-H)-
411.9043 ([C14H10Br2N2O3]-H)-
412.8986 ([C14H10Br2N2O3]-H)-
413.9021 ([C14H10Br2N2O3]-H)-
414.8966 ([C14H10Br2N2O3]-H)-
1h

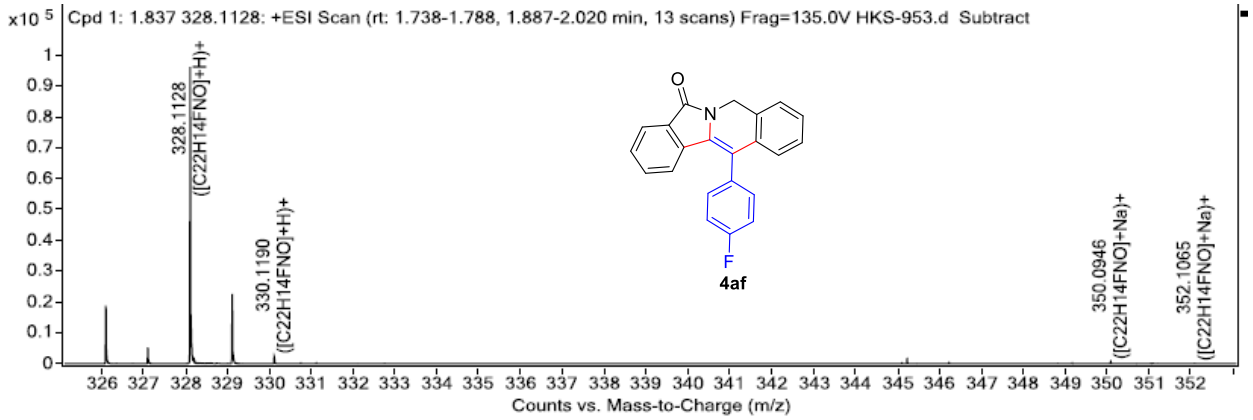

Cpd 1: 1.916 310.1219: +ESI Scan (rt: 1.817-1.833, 1.999-2.132 min, 11 scans) Frag=135.0V HKS-900.d Subtract
x10 5
310.1219 ([C22H15NO]+H)+
312.1285 ([C22H15NO]+H)+
332.1036 ([C22H15NO]+Na)+
334.1049 ([C22H15NO]+Na)+
4aa
Counts vs. Mass-to-Charge (m/z)

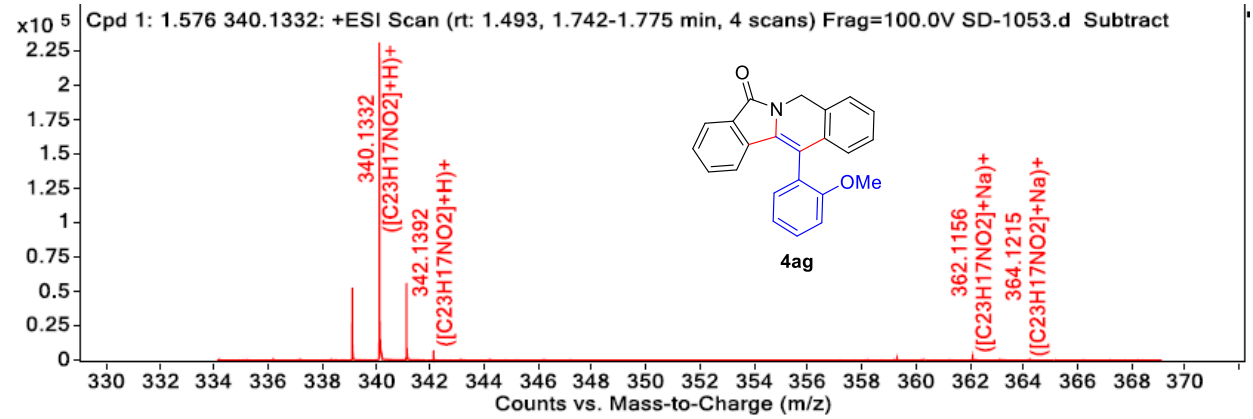

x10 5
Cpd 1: 2.590 324.1379: +ESI Scan (rt: 2.474-2.507, 2.689-2.805 min, 11 scans) Frag=135.0V HKS-903.d Subtract
324.1379
([C23H17NO]+H)+
326.1444
([C23H17NO]+H)+
346.1196
([C23H17NO]+Na)+
348.1249
([C23H17NO]+Na)+
Me
4ab
Counts vs. Mass-to-Charge (m/z)

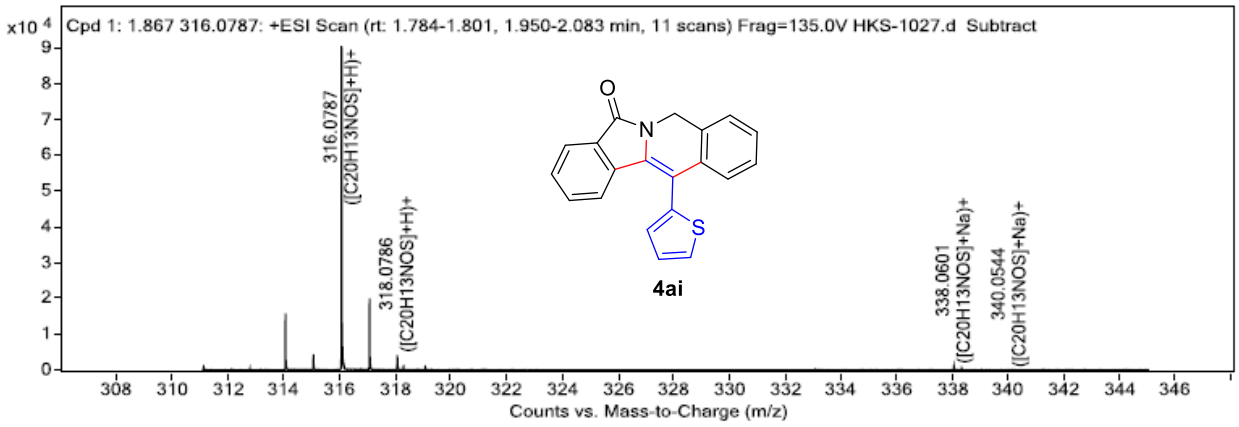

x10 5
Cpd 1: 1.697 340.1326: +ESI Scan (rt: 1.614-1.631, 1.797-1.946 min, 12 scans) Frag=135.0V HKS-1013.d Subtract
340.1326
([C23H17NO2]+H)+
342.1390
([C23H17NO2]+H)+
362.1139
([C23H17NO2]+Na)+
364.1157
([C23H17NO2]+Na)+
OMe
4ac
Counts vs. Mass-to-Charge (m/z)

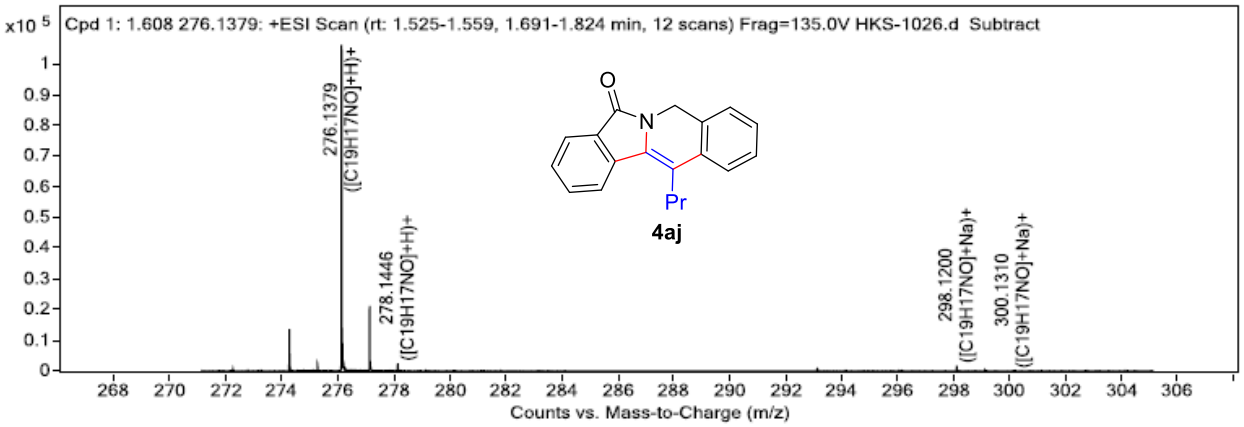

x10 5
Cpd 1: 4.039 352.1691: +ESI Scan (rt: 3.956-4.022, 4.072-4.155 min, 11 scans) Frag=135.0V HKS-949.d Subtract
352.1691
([C25H21NO]+H)+
354.1756
([C25H21NO]+H)+
374.1510
([C25H21NO]+Na)+
376.1558
([C25H21NO]+Na)+
nPr
4ad

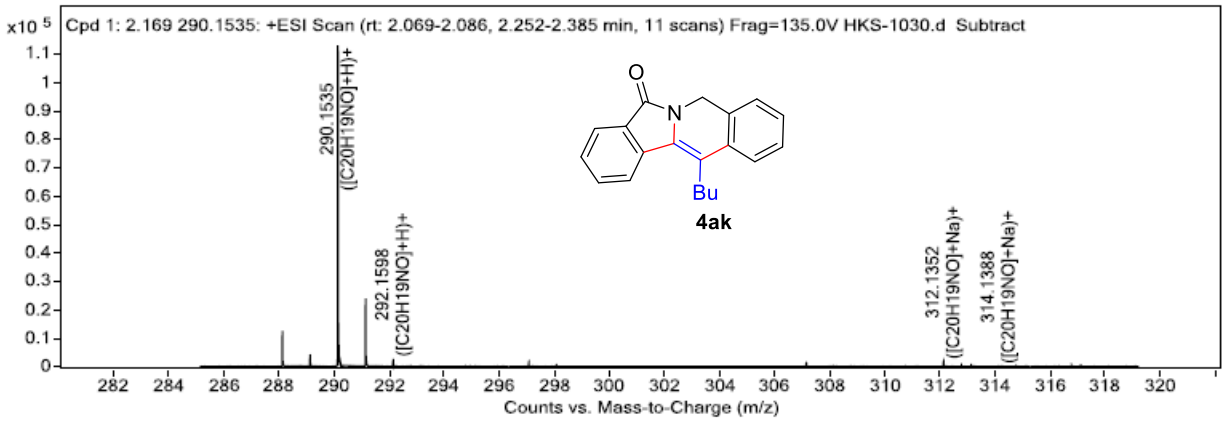

x10 5
Cpd 1: 4.287 366.1848: +ESI Scan (rt: 4.204-4.221, 4.354-4.403 min, 6 scans) Frag=135.0V HKS-984.d Subtract
366.1848
([C26H23NO]+H)+
368.1914
([C26H23NO]+H)+
388.1669
([C26H23NO]+Na)+
390.1732
([C26H23NO]+Na)+
tBu
4ae
Counts vs. Mass-to-Charge (m/z)

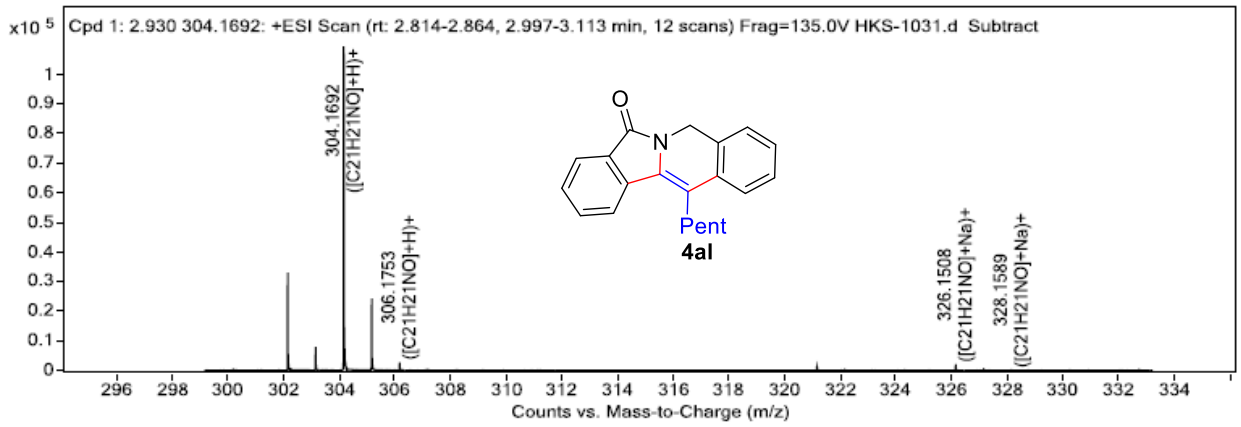

x10 5
Cpd 1: 1.837 328.1128: +ESI Scan (rt: 1.738-1.788, 1.887-2.020 min, 13 scans) Frag=135.0V HKS-953.d Subtract
328.1128
([C22H14FNO]+H)+
330.1190
([C22H14FNO]+H)+
350.0946
([C22H14FNO]+Na)+
352.1065
([C22H14FNO]+Na)+
F
4af
Counts vs. Mass-to-Charge (m/z)

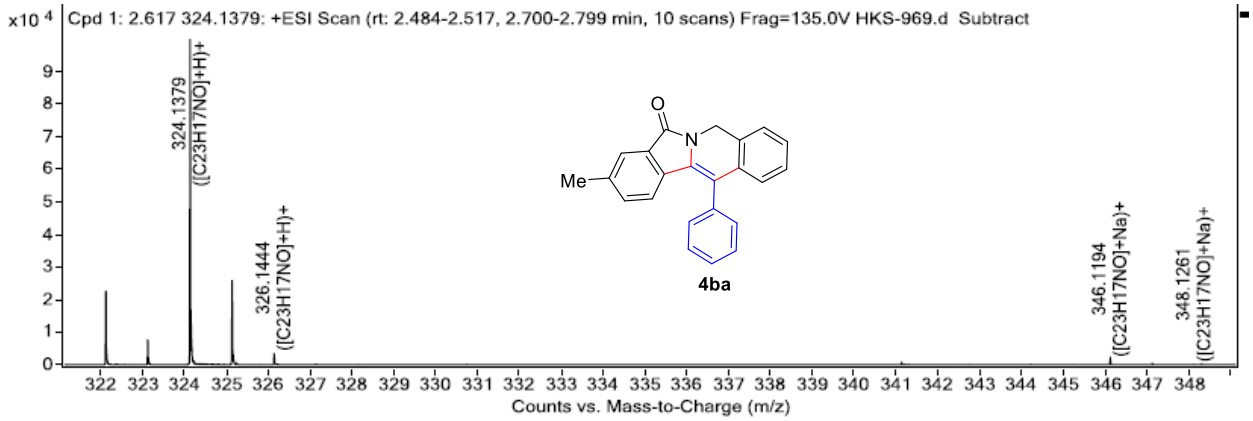

x10 5
Cpd 1: 1.576 340.1332: +ESI Scan (rt: 1.493, 1.742-1.775 min, 4 scans) Frag=100.0V SD-1053.d Subtract
340.1332
([C23H17NO2]+H)+
342.1392
([C23H17NO2]+H)+
362.1156
([C23H17NO2]+Na)+
364.1215
([C23H17NO2]+Na)+
OMe
4ag
Counts vs. Mass-to-Charge (m/z)

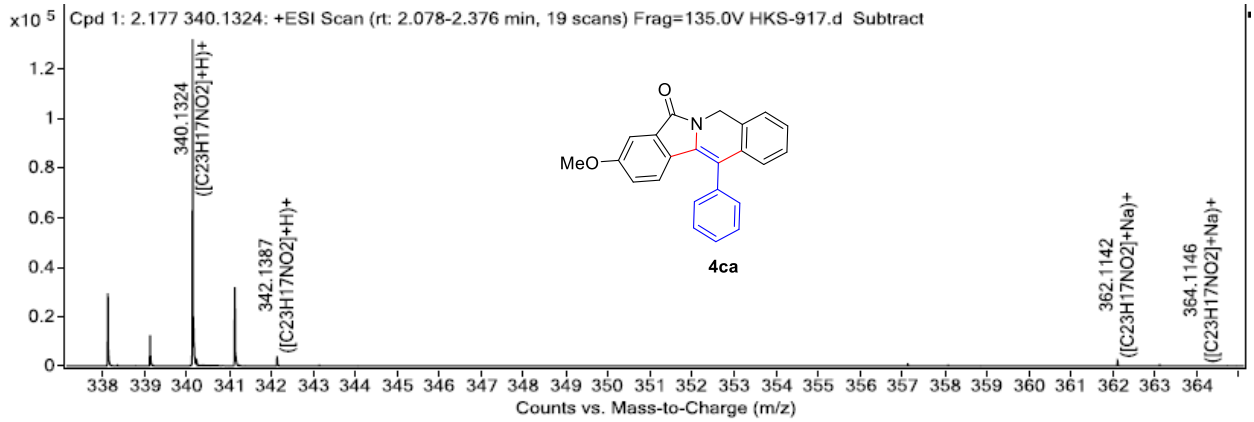

Cpd 1: 1.867 316.0787: +ESI Scan (rt: 1.784-1.801, 1.950-2.083 min, 11 scans) Frag=135.0V HKS-1027.d Subtract
x10 4
316.0787
([C20H13NOS]+H)+
318.0786
([C20H13NOS]+H)+
338.0601
([C20H13NOS]+Na)+
340.0544
([C20H13NOS]+Na)+
O
N
S
4ai
Counts vs. Mass-to-Charge (m/z)

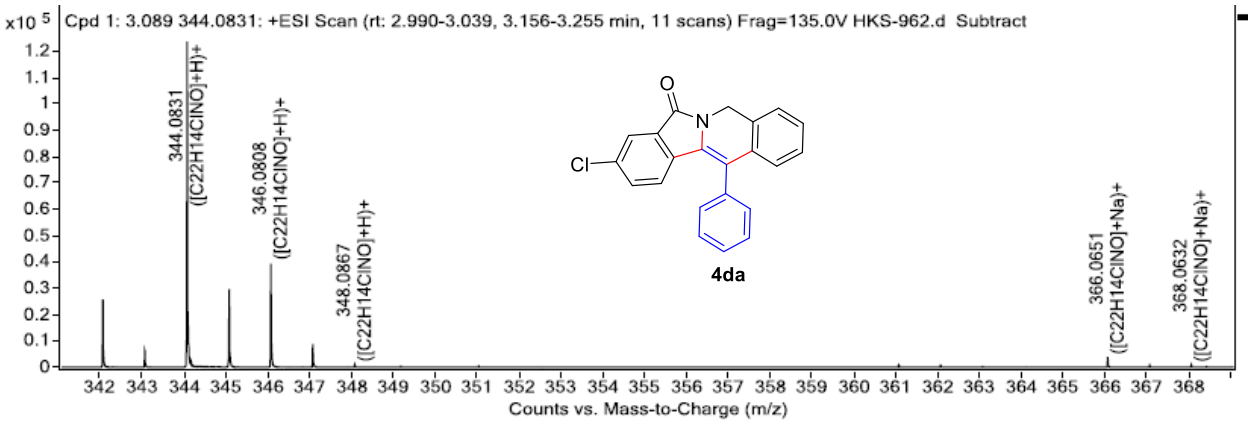

Cpd 1: 1.608 276.1379: +ESI Scan (rt: 1.525-1.559, 1.691-1.824 min, 12 scans) Frag=135.0V HKS-1026.d Subtract
x10 5
276.1379
([C19H17NO]+H)+
278.1446
([C19H17NO]+H)+
298.1200
([C19H17NO]+Na)+
300.1310
([C19H17NO]+Na)+
O
N
Pr
4aj
Counts vs. Mass-to-Charge (m/z)

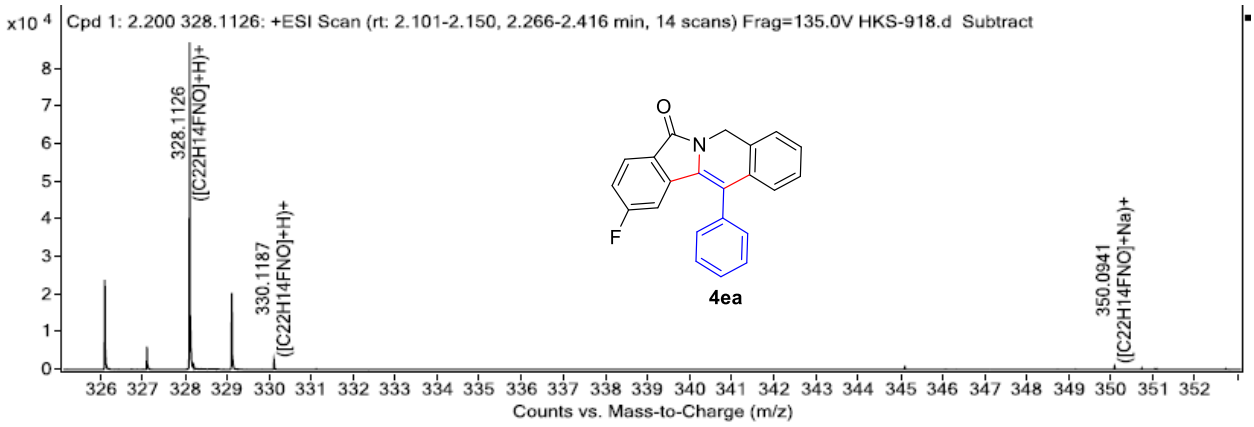

Cpd 1: 2.169 290.1535: +ESI Scan (rt: 2.069-2.086, 2.252-2.385 min, 11 scans) Frag=135.0V HKS-1030.d Subtract
x10 5
290.1535
([C20H19NO]+H)+
292.1598
([C20H19NO]+H)+
312.1352
([C20H19NO]+Na)+
314.1388
([C20H19NO]+Na)+
O
N
Bu
4ak
Counts vs. Mass-to-Charge (m/z)

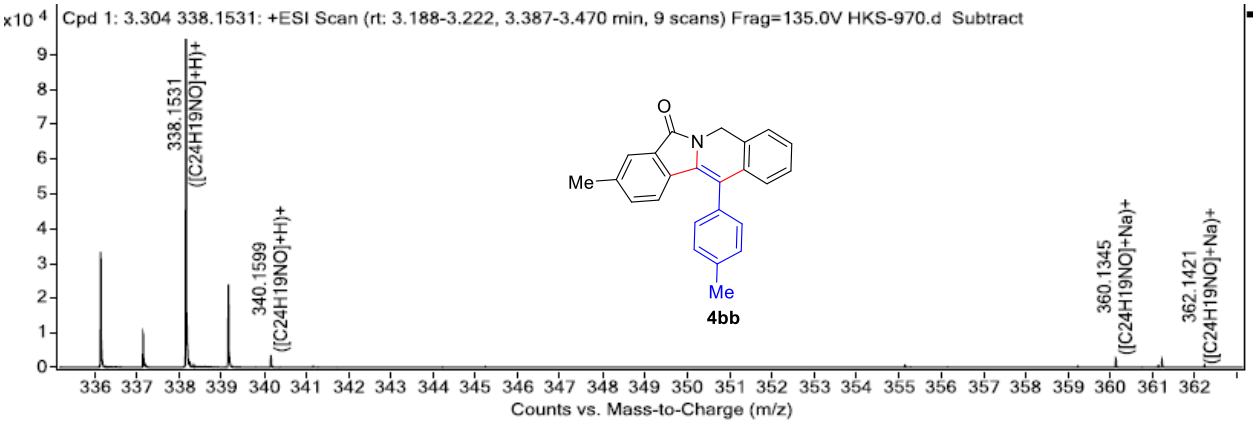

Cpd 1: 2.930 304.1692: +ESI Scan (rt: 2.814-2.864, 2.997-3.113 min, 12 scans) Frag=135.0V HKS-1031.d Subtract
x10 5
304.1692
([C21H21NO]+H)+
306.1753
([C21H21NO]+H)+
326.1508
([C21H21NO]+Na)+
328.1589
([C21H21NO]+Na)+
Pent
4al
Counts vs. Mass-to-Charge (m/z)

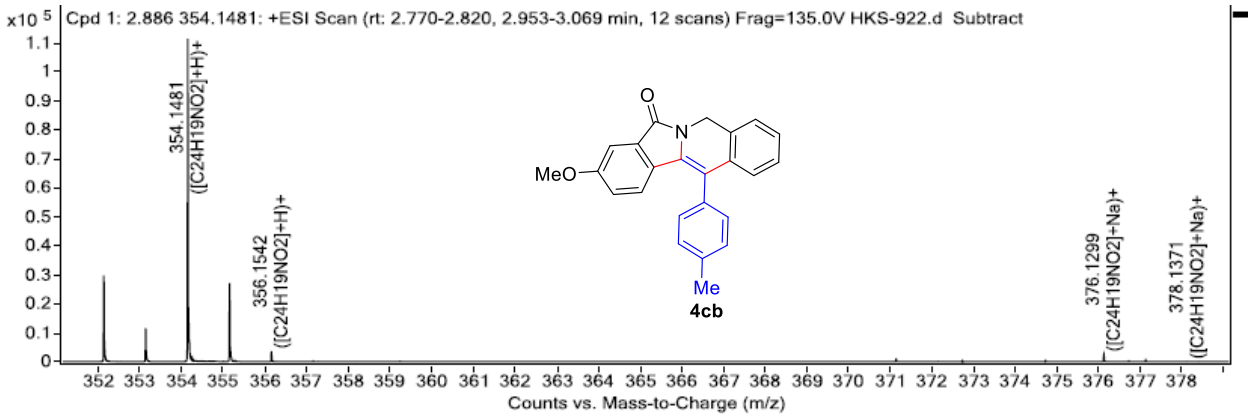

Cpd 1: 2.617 324.1379: +ESI Scan (rt: 2.484-2.517, 2.700-2.799 min, 10 scans) Frag=135.0V HKS-969.d Subtract
x10 4
324.1379
([C23H17NO]+H)+
326.1444
([C23H17NO]+H)+
346.1194
([C23H17NO]+Na)+
348.1261
([C23H17NO]+Na)+
Me
4ba
Counts vs. Mass-to-Charge (m/z)

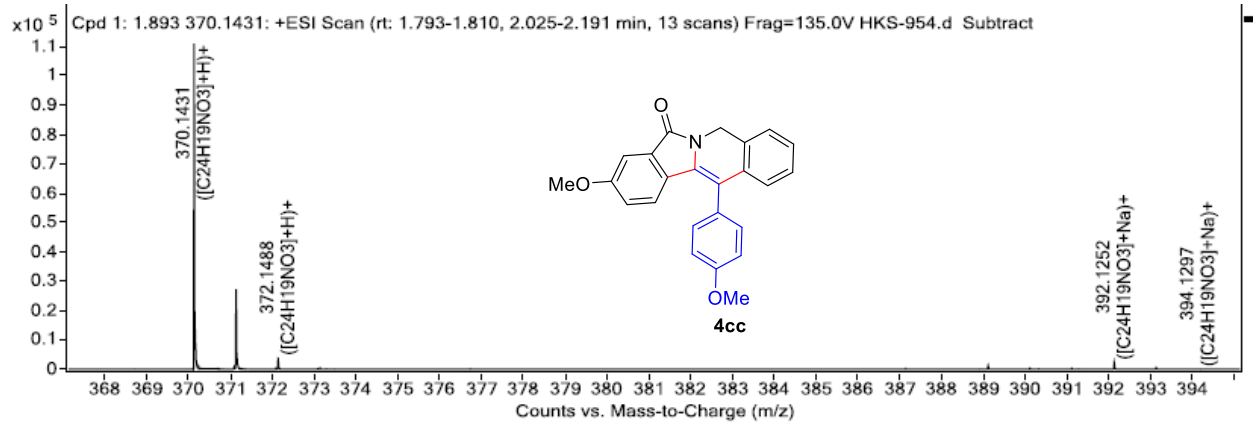

Cpd 1: 2.177 340.1324: +ESI Scan (rt: 2.078-2.376 min, 19 scans) Frag=135.0V HKS-917.d Subtract
x10 5
340.1324
([C23H17NO2]+H)+
342.1387
([C23H17NO2]+H)+
362.1142
([C23H17NO2]+Na)+
364.1146
([C23H17NO2]+Na)+
MeO
4ca
Counts vs. Mass-to-Charge (m/z)

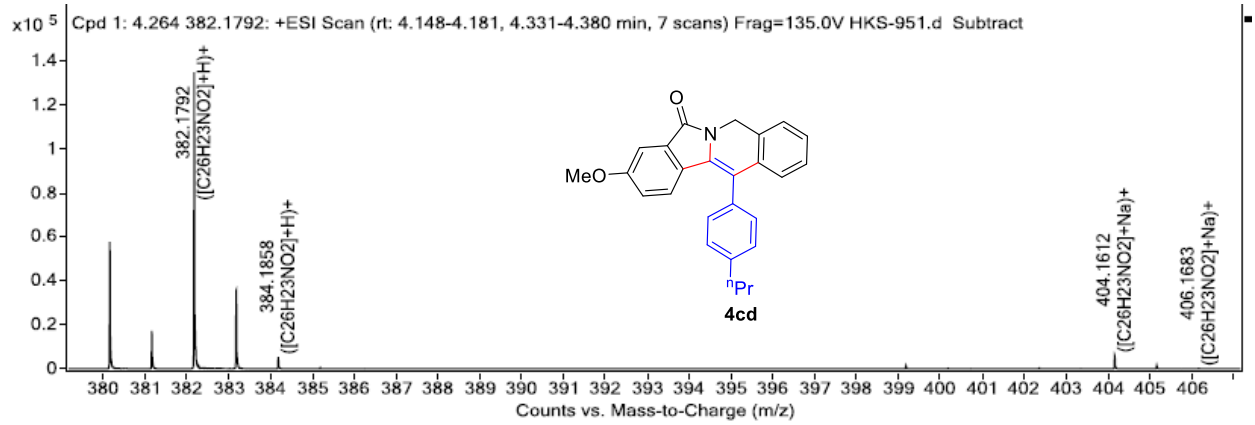

x10 5
Cpd 1: 3.089 344.0831: +ESI Scan (rt: 2.990-3.039, 3.156-3.255 min, 11 scans) Frag=135.0V HKS-962.d Subtract
344.0831
([C22H14ClNO]+H)+
346.0808
([C22H14ClNO]+H)+
348.0867
([C22H14ClNO]+H)+
366.0651
([C22H14ClNO]+Na)+
368.0632
([C22H14ClNO]+Na)+
Cl
O
N
4da
Counts vs. Mass-to-Charge (m/z)

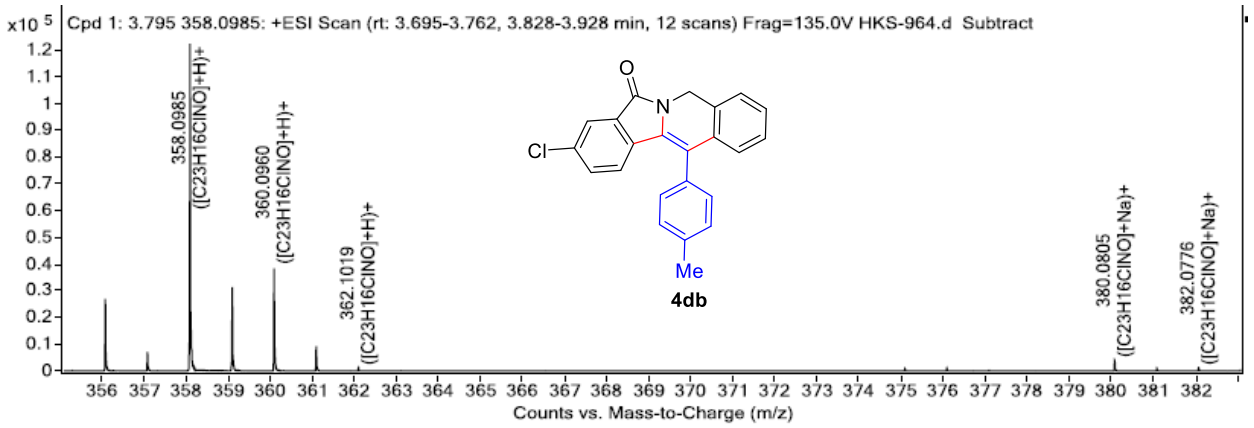

x10 4
Cpd 1: 2.200 328.1126: +ESI Scan (rt: 2.101-2.150, 2.266-2.416 min, 14 scans) Frag=135.0V HKS-918.d Subtract
328.1126
([C22H14FNO]+H)+
330.1187
([C22H14FNO]+H)+
350.0941
([C22H14FNO]+Na)+
F
O
N
4ea
Counts vs. Mass-to-Charge (m/z)

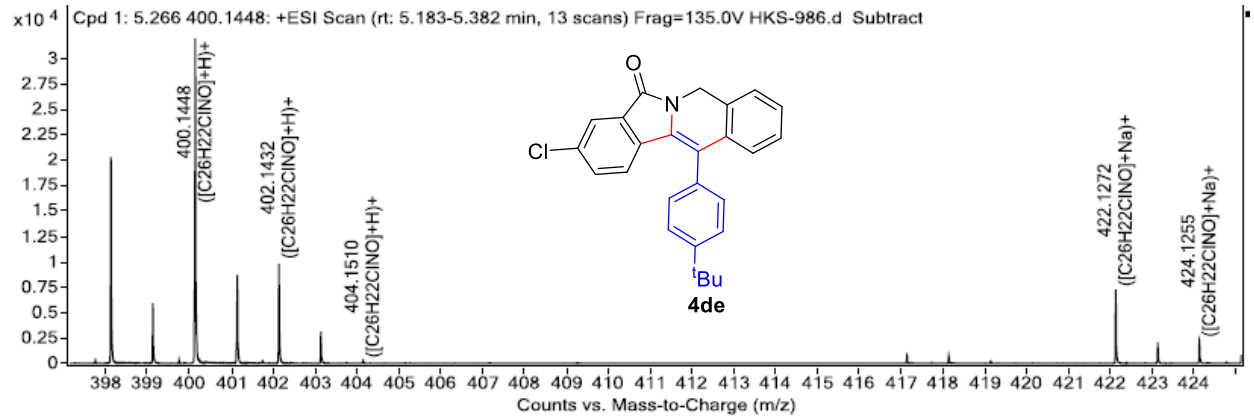

x10 4
Cpd 1: 3.304 338.1531: +ESI Scan (rt: 3.188-3.222, 3.387-3.470 min, 9 scans) Frag=135.0V HKS-970.d Subtract
338.1531
([C24H19NO]+H)+
340.1599
([C24H19NO]+H)+
360.1345
([C24H19NO]+Na)+
362.1421
([C24H19NO]+Na)+
Me
Me
O
N
4bb
Counts vs. Mass-to-Charge (m/z)

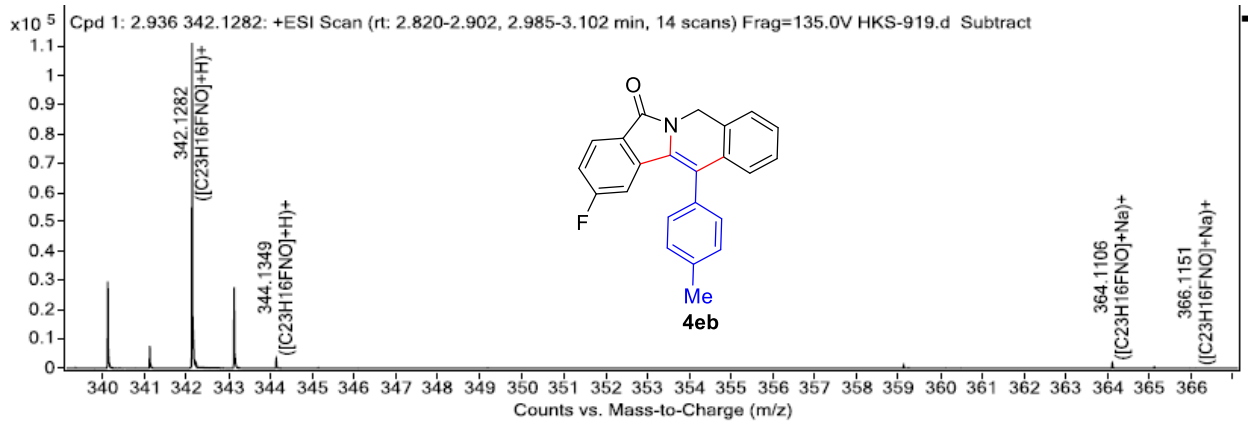

x10 5
Cpd 1: 2.886 354.1481: +ESI Scan (rt: 2.770-2.820, 2.953-3.069 min, 12 scans) Frag=135.0V HKS-922.d Subtract
354.1481
([C24H19NO2]+H)+
356.1542
([C24H19NO2]+H)+
376.1299
([C24H19NO2]+Na)+
378.1371
([C24H19NO2]+Na)+
MeO
Me
4cb
Counts vs. Mass-to-Charge (m/z)

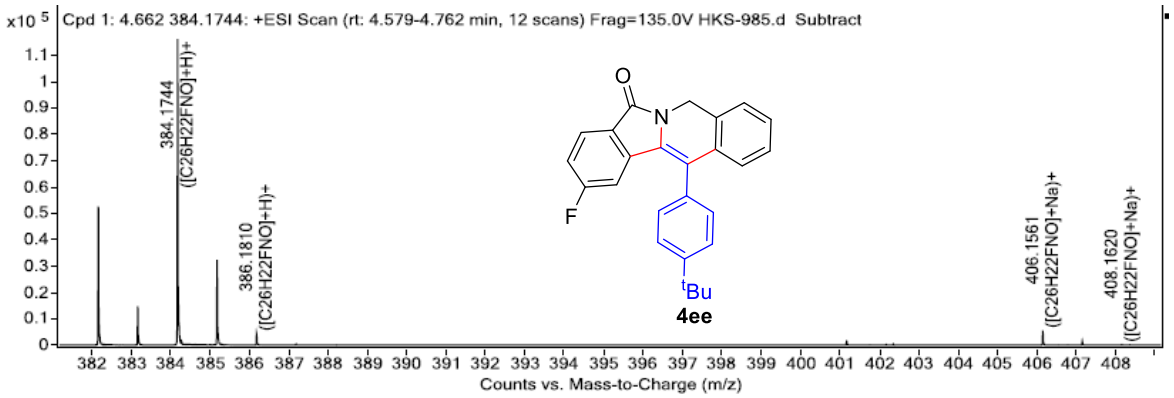

x10 5
Cpd 1: 1.893 370.1431: +ESI Scan (rt: 1.793-1.810, 2.025-2.191 min, 13 scans) Frag=135.0V HKS-954.d Subtract
370.1431
([C24H19NO3]+H)+
372.1488
([C24H19NO3]+H)+
392.1252
([C24H19NO3]+Na)+
394.1297
([C24H19NO3]+Na)+
MeO
OMe
4cc
Counts vs. Mass-to-Charge (m/z)

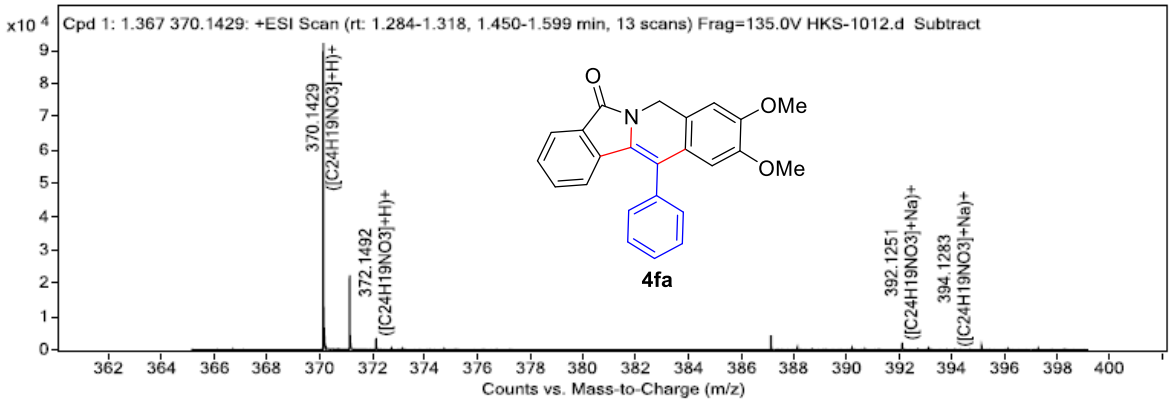

x10 5
Cpd 1: 4.264 382.1792: +ESI Scan (rt: 4.148-4.181, 4.331-4.380 min, 7 scans) Frag=135.0V HKS-951.d Subtract
382.1792
([C26H23NO2]+H)+
384.1858
([C26H23NO2]+H)+
404.1612
([C26H23NO2]+Na)+
406.1683
([C26H23NO2]+Na)+
MeO
nPr
4cd
Counts vs. Mass-to-Charge (m/z)

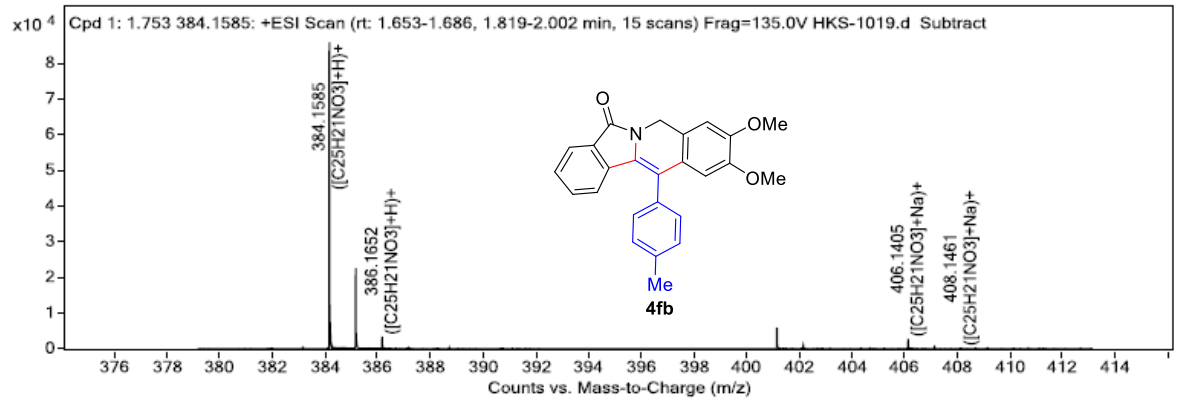

x10 5
Cpd 1: 3.795 358.0985: +ESI Scan (rt: 3.695-3.762, 3.828-3.928 min, 12 scans) Frag=135.0V HKS-964.d Subtract
358.0985 ([C23H16ClNO]+H)+
360.0960 ([C23H16ClNO]+H)+
362.1019 ([C23H16ClNO]+H)+
380.0805 ([C23H16ClNO]+Na)+
382.0776 ([C23H16ClNO]+Na)+
Cl
O
N
Me
4db
Counts vs. Mass-to-Charge (m/z)

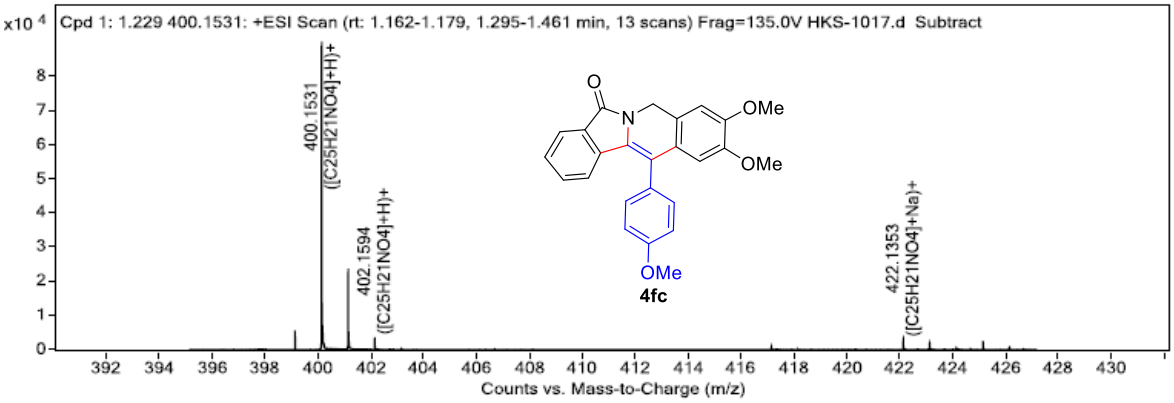

x10 4
Cpd 1: 5.266 400.1448: +ESI Scan (rt: 5.183-5.382 min, 13 scans) Frag=135.0V HKS-986.d Subtract
400.1448 ([C26H22ClNO]+H)+
402.1432 ([C26H22ClNO]+H)+
404.1510 ([C26H22ClNO]+H)+
422.1272 ([C26H22ClNO]+Na)+
424.1255 ([C26H22ClNO]+Na)+
Cl
O
N
tBu
4de
Counts vs. Mass-to-Charge (m/z)

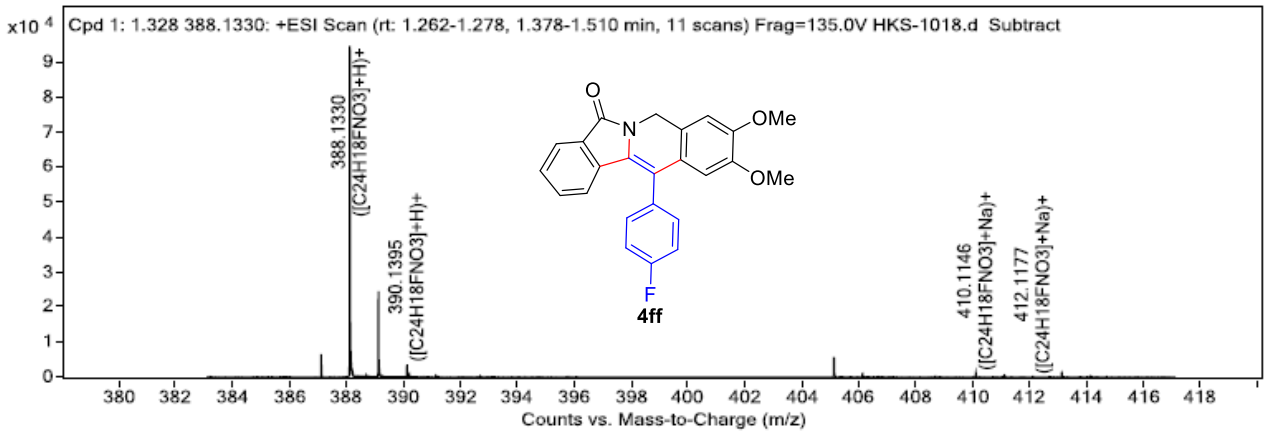

x10 5
Cpd 1: 2.936 342.1282: +ESI Scan (rt: 2.820-2.902, 2.985-3.102 min, 14 scans) Frag=135.0V HKS-919.d Subtract
342.1282 ([C23H16FNO]+H)+
344.1349 ([C23H16FNO]+H)+
364.1106 ([C23H16FNO]+Na)+
366.1151 ([C23H16FNO]+Na)+
F
O
N
Me
4eb
Counts vs. Mass-to-Charge (m/z)

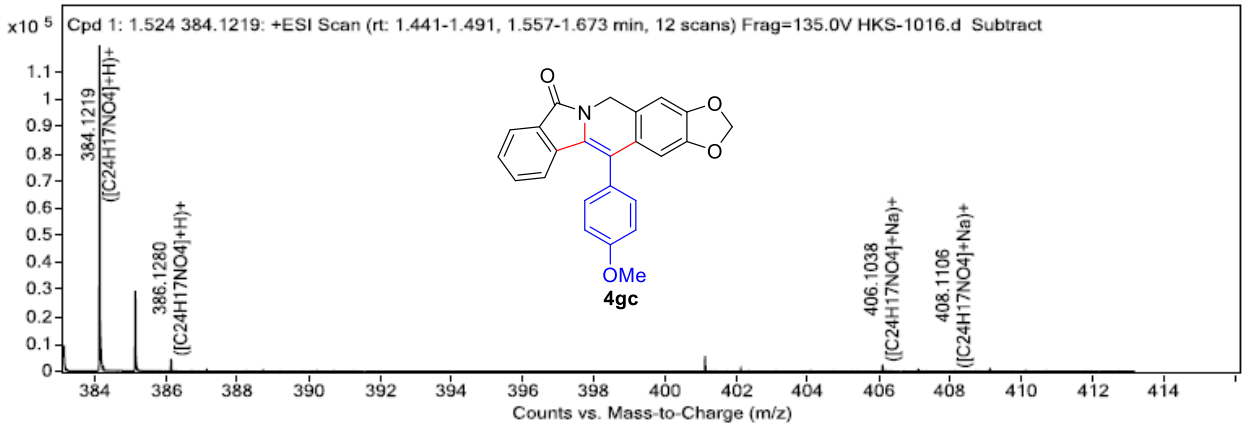

x10 5
Cpd 1: 4.662 384.1744: +ESI Scan (rt: 4.579-4.762 min, 12 scans) Frag=135.0V HKS-985.d Subtract
384.1744
([C26H22FNO]+H)+
386.1810
([C26H22FNO]+H)+
406.1561
([C26H22FNO]+Na)+
408.1620
([C26H22FNO]+Na)+
O
N
F
tBu
4ee
Counts vs. Mass-to-Charge (m/z)

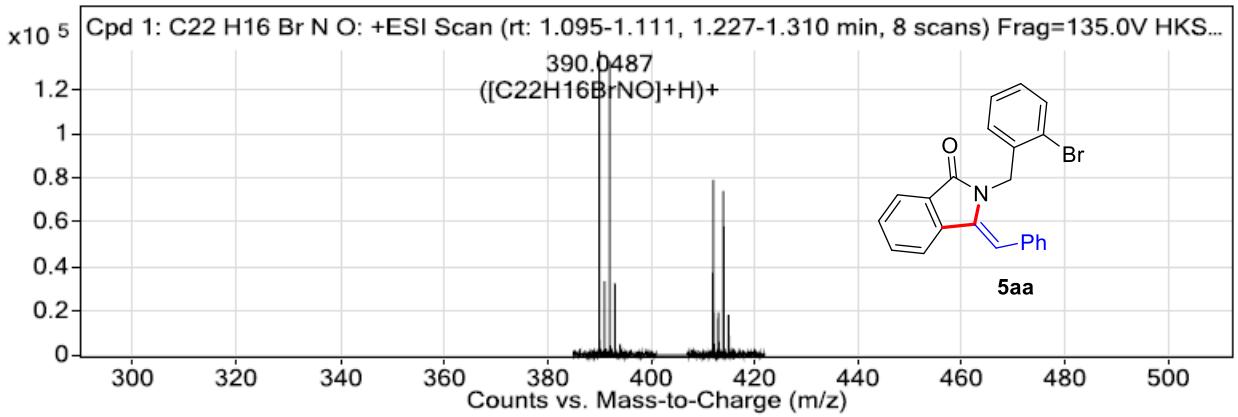

x10 4
Cpd 1: 1.367 370.1429: +ESI Scan (rt: 1.284-1.318, 1.450-1.599 min, 13 scans) Frag=135.0V HKS-1012.d Subtract
370.1429
([C24H19NO3]+H)+
372.1492
([C24H19NO3]+H)+
392.1251
([C24H19NO3]+Na)+
394.1283
([C24H19NO3]+Na)+
O
N
OMe
OMe
4fa
Counts vs. Mass-to-Charge (m/z)

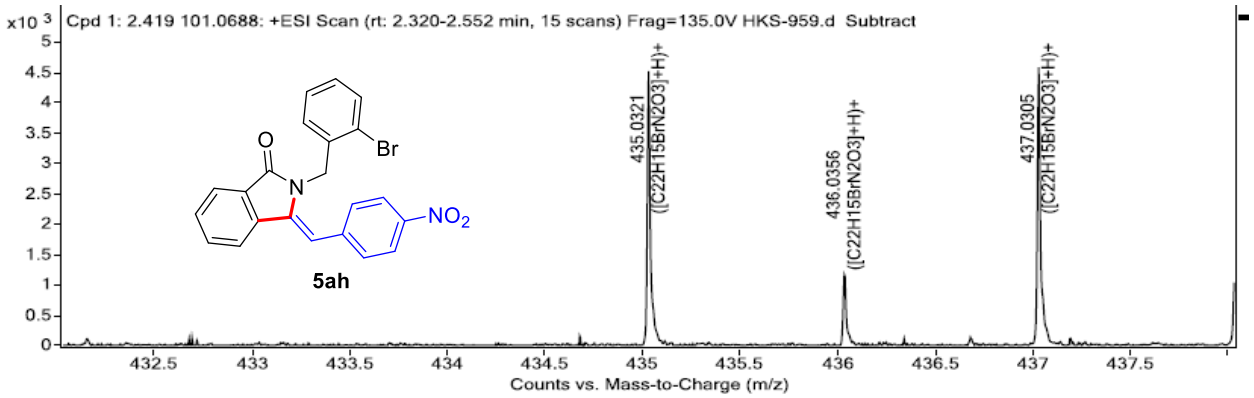

x10 4
Cpd 1: 1.753 384.1585: +ESI Scan (rt: 1.653-1.686, 1.819-2.002 min, 15 scans) Frag=135.0V HKS-1019.d Subtract
384.1585
([C25H21NO3]+H)+
386.1652
([C25H21NO3]+H)+
406.1405
([C25H21NO3]+Na)+
408.1461
([C25H21NO3]+Na)+
O
N
OMe
OMe
Me
4fb
Counts vs. Mass-to-Charge (m/z)

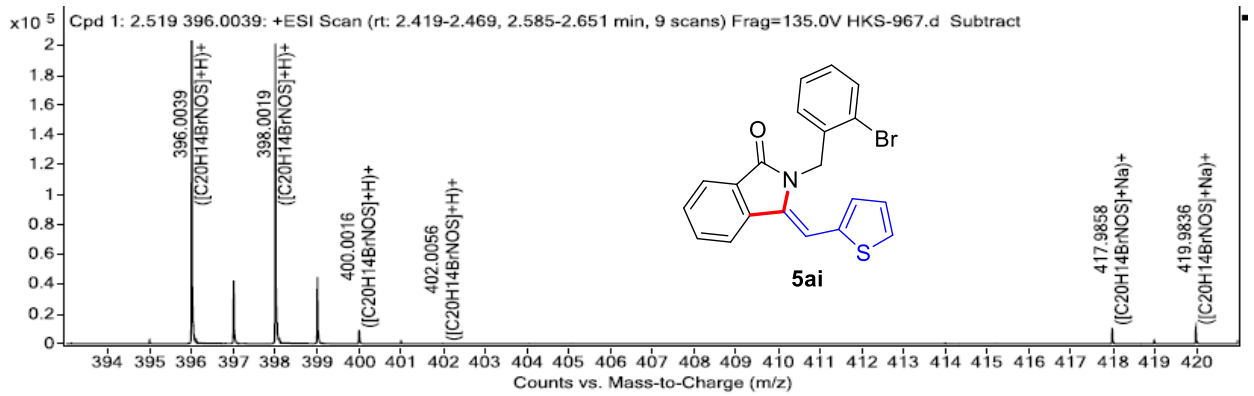

x10 4
Cpd 1: 1.229 400.1531: +ESI Scan (rt: 1.162-1.179, 1.295-1.461 min, 13 scans) Frag=135.0V HKS-1017.d Subtract
400.1531
([C25H21NO4]+H)+
402.1594
([C25H21NO4]+H)+
422.1353
([C25H21NO4]+Na)+
O
N
OMe
OMe
OMe
4fc
Counts vs. Mass-to-Charge (m/z)

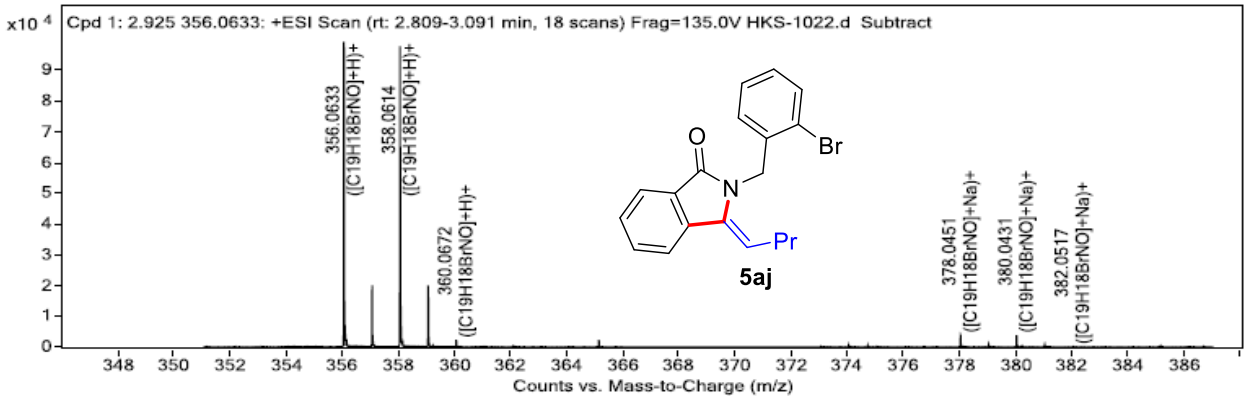

Cpd 1: 1.328 388.1330: +ESI Scan (rt: 1.262-1.278, 1.378-1.510 min, 11 scans) Frag=135.0V HKS-1018.d Subtract
x10 4
388.1330
([C24H18FNO3]+H)+
390.1395
([C24H18FNO3]+H)+
410.1146
([C24H18FNO3]+Na)+
412.1177
([C24H18FNO3]+Na)+
OMe
OMe
F
4ff
Counts vs. Mass-to-Charge (m/z)

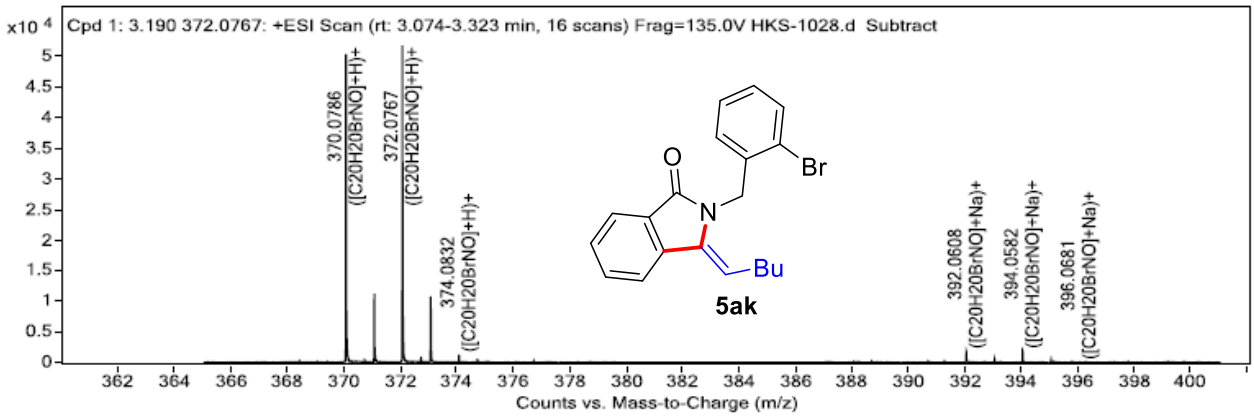

Cpd 1: 1.524 384.1219: +ESI Scan (rt: 1.441-1.491, 1.557-1.673 min, 12 scans) Frag=135.0V HKS-1016.d Subtract
x10 5
384.1219
([C24H17NO4]+H)+
386.1280
([C24H17NO4]+H)+
406.1038
([C24H17NO4]+Na)+
408.1106
([C24H17NO4]+Na)+
OMe
4gc
Counts vs. Mass-to-Charge (m/z)

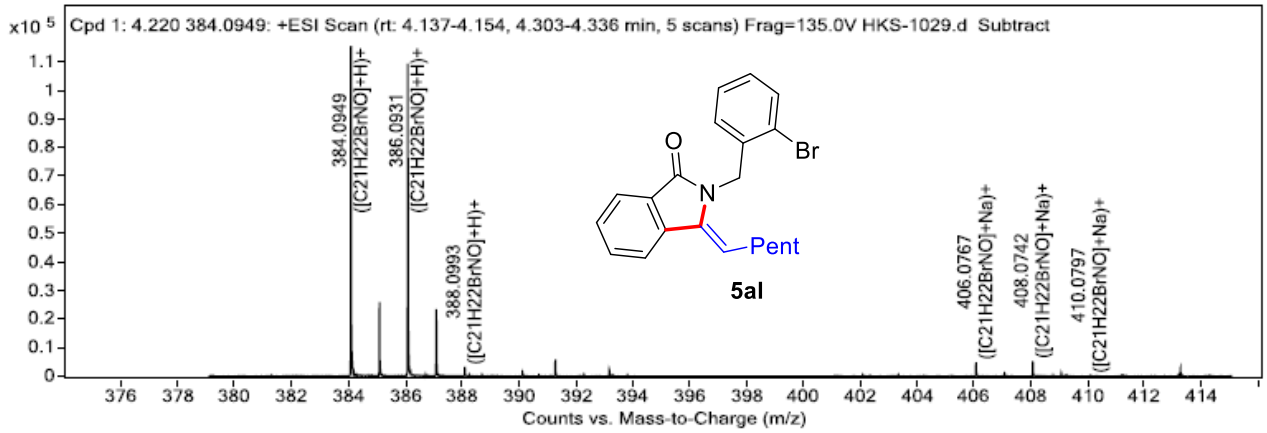

Cpd 1: C22 H16 Br N O: +ESI Scan (rt: 1.095-1.111, 1.227-1.310 min, 8 scans) Frag=135.0V HKS...
x10 5
390.0487
([C22H16BrNO]+H)+
Br
Ph
5aa
Counts vs. Mass-to-Charge (m/z)

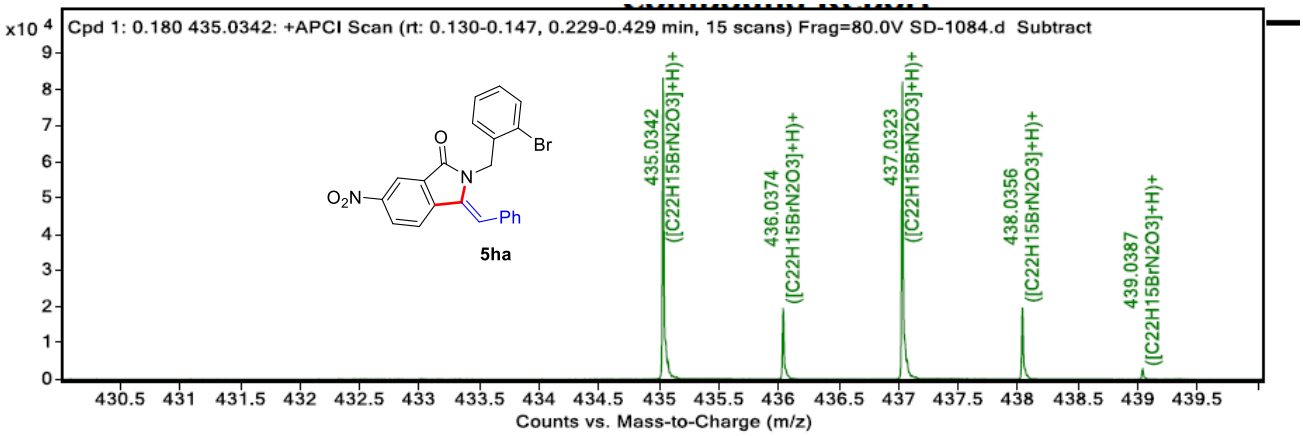

Cpd 1: 2.419 101.0688: +ESI Scan (rt: 2.320-2.552 min, 15 scans) Frag=135.0V HKS-959.d Subtract
x10 3
435.0321 ([C22H15BrN2O3]+H)+
436.0356 ([C22H15BrN2O3]+H)+
437.0305 ([C22H15BrN2O3]+H)+
Br
O
N
NO2
5ah
Counts vs. Mass-to-Charge (m/z)

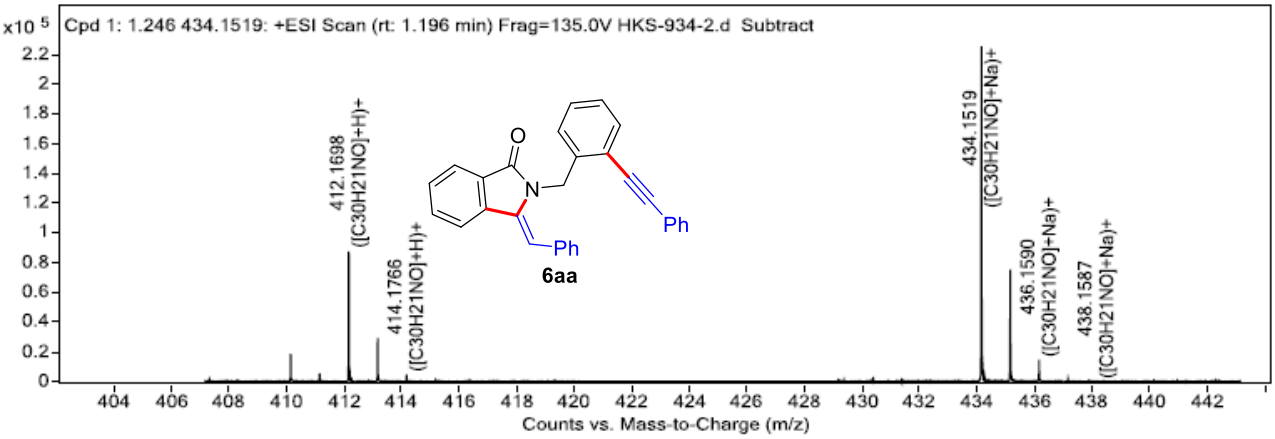

Cpd 1: 2.519 396.0039: +ESI Scan (rt: 2.419-2.469, 2.585-2.651 min, 9 scans) Frag=135.0V HKS-967.d Subtract
x10 5
396.0039 ([C20H14BrNOS]+H)+
398.0019 ([C20H14BrNOS]+H)+
400.0016 ([C20H14BrNOS]+H)+
402.0056 ([C20H14BrNOS]+H)+
417.9858 ([C20H14BrNOS]+Na)+
419.9836 ([C20H14BrNOS]+Na)+
Br
O
N
S
5ai
Counts vs. Mass-to-Charge (m/z)


Cpd 1: 2.925 356.0633: +ESI Scan (rt: 2.809-3.091 min, 18 scans) Frag=135.0V HKS-1022.d Subtract
x10 4
356.0633 ([C19H18BrNO]+H)+
358.0614 ([C19H18BrNO]+H)+
360.0672 ([C19H18BrNO]+H)+
378.0451 ([C19H18BrNO]+Na)+
380.0431 ([C19H18BrNO]+Na)+
382.0517 ([C19H18BrNO]+Na)+
Br
O
N
Pr
5aj
Counts vs. Mass-to-Charge (m/z)


Cpd 1: 3.190 372.0767: +ESI Scan (rt: 3.074-3.323 min, 16 scans) Frag=135.0V HKS-1028.d Subtract
x10 4
370.0786 ([C20H20BrNO]+H)+
372.0767 ([C20H20BrNO]+H)+
374.0832 ([C20H20BrNO]+H)+
392.0608 ([C20H20BrNO]+Na)+
394.0582 ([C20H20BrNO]+Na)+
396.0681 ([C20H20BrNO]+Na)+
Br
O
N
Bu
5ak
Counts vs. Mass-to-Charge (m/z)


Cpd 1: 4.220 384.0949: +ESI Scan (rt: 4.137-4.154, 4.303-4.336 min, 5 scans) Frag=135.0V HKS-1029.d Subtract
x10 5
384.0949 ([C21H22BrNO]+H)+
386.0931 ([C21H22BrNO]+H)+
388.0993 ([C21H22BrNO]+H)+
406.0767 ([C21H22BrNO]+Na)+
408.0742 ([C21H22BrNO]+Na)+
410.0797 ([C21H22BrNO]+Na)+
Br
O
N
Pent
5al
Counts vs. Mass-to-Charge (m/z)


Cpd 1: 0.180 435.0342: +APCI Scan (rt: 0.130-0.147, 0.229-0.429 min, 15 scans) Frag=80.0V SD-1084.d Subtract
x10 4
435.0342 ([C22H15BrN2O3]+H)+
436.0374 ([C22H15BrN2O3]+H)+
437.0323 ([C22H15BrN2O3]+H)+
438.0356 ([C22H15BrN2O3]+H)+
439.0387 ([C22H15BrN2O3]+H)+
Br
O
N
O2N
Ph
5ha
Counts vs. Mass-to-Charge (m/z)


Cpd 1: 1.246 434.1519: +ESI Scan (rt: 1.196 min) Frag=135.0V HKS-934-2.d Subtract
x10 5
412.1698 ([C30H21NO]+H)+
414.1766 ([C30H21NO]+H)+
434.1519 ([C30H21NO]+Na)+
436.1590 ([C30H21NO]+Na)+
438.1587 ([C30H21NO]+Na)+
O
N
Ph
Ph
6aa
Counts vs. Mass-to-Charge (m/z)

3. Single crystal X-ray data for 4aa, 5aa and 6aa.

Table S1 Crystal data and structure refinement for 4aa.

Identification code	exp_140-HKS-900
Empirical formula	$C_{22}H_{15}NO$
Formula weight	309.35
Temperature/K	93(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.6454(10)
b/Å	15.8564(11)
c/Å	9.6081(10)
α/°	90
β/°	112.912(12)
γ/°	90
Volume/Å^3	1493.9(3)
Z	4
ρ_{calc}g/cm^3	1.375
μ/mm^{-1}	0.084
F(000)	648.0
Crystal size/mm^3	0.5 × 0.5 × 0.3
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	10.05 to 57.916
Index ranges	$-11 \le h \le 14$, $-18 \le k \le 21$, $-12 \le l \le 12$
Reflections collected	10300
Independent reflections	3477 [R_{int} = 0.0492, R_{sigma} = 0.0255]
Data/restraints/parameters	3477/0/217
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0855, wR_2 = 0.2156
Final R indexes [all data]	R_1 = 0.0885, wR_2 = 0.2174
Largest diff. peak/hole / e Å^{-3}	1.60/-0.40

Table S2 Crystal data and structure refinement for 5aa

Identification code	exp_189-HKS-934-1
Empirical formula	$C_{22}H_{16}BrNO$
Formula weight	390.27
Temperature/K	93(2)
Crystal system	triclinic
Space group	P-1
a/Å	8.7437(4)
b/Å	9.0981(5)
c/Å	11.3532(6)
α/°	89.931(4)
β/°	69.876(5)
γ/°	83.515(4)
Volume/Å^3	841.91(8)
Z	2
ρ_{calc}g/cm^3	1.539
μ/mm^{-1}	2.450
F(000)	396.0
Crystal size/mm^3	0.11 × 0.08 × 0.06
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	7.124 to 59.814
Index ranges	$-12 \leq h \leq 10$, $-12 \leq k \leq 11$, $-15 \leq l \leq 15$
Reflections collected	12080
Independent reflections	4229 [R_{int} = 0.0664, R_{sigma} = 0.0706]
Data/restraints/parameters	4229/0/226
Goodness-of-fit on F^2	0.989
Final R indexes [I>=2σ (I)]	R_1 = 0.0469, wR_2 = 0.0969
Final R indexes [all data]	R_1 = 0.0723, wR_2 = 0.1055
Largest diff. peak/hole / e Å^{-3}	0.91/-0.56

Table S3 Crystal data and structure refinement for 6aa.

Identification code	exp-188-HKS-934-2
Empirical formula	$C_{30}H_{21}NO$
Formula weight	411.48
Temperature/K	93(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.9969(4)
b/Å	14.8584(3)
c/Å	10.6249(3)
α/°	90
β/°	110.575(3)
γ/°	90
Volume/Å^3	2216.53(11)
Z	4
ρ_{calc}g/cm^3	1.233
μ/mm^{-1}	0.575
F(000)	864.0
Crystal size/mm^3	0.1 × 0.1 × 0.06
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.664 to 148.818
Index ranges	-13 ≤ h ≤ 18, -12 ≤ k ≤ 18, -12 ≤ l ≤ 12
Reflections collected	7754
Independent reflections	3961 [R_{int} = 0.0186, R_{sigma} = 0.0195]
Data/restraints/parameters	3961/0/290
Goodness-of-fit on F^2	1.024
Final R indexes [I>=2σ (I)]	R_1 = 0.0379, wR_2 = 0.0994
Final R indexes [all data]	R_1 = 0.0395, wR_2 = 0.1006
Largest diff. peak/hole / e Å^{-3}	0.43/-0.17