Functionalized Chromans and Isochromans via a Diastereoselective Pd(0)-Catalyzed Carboiodination

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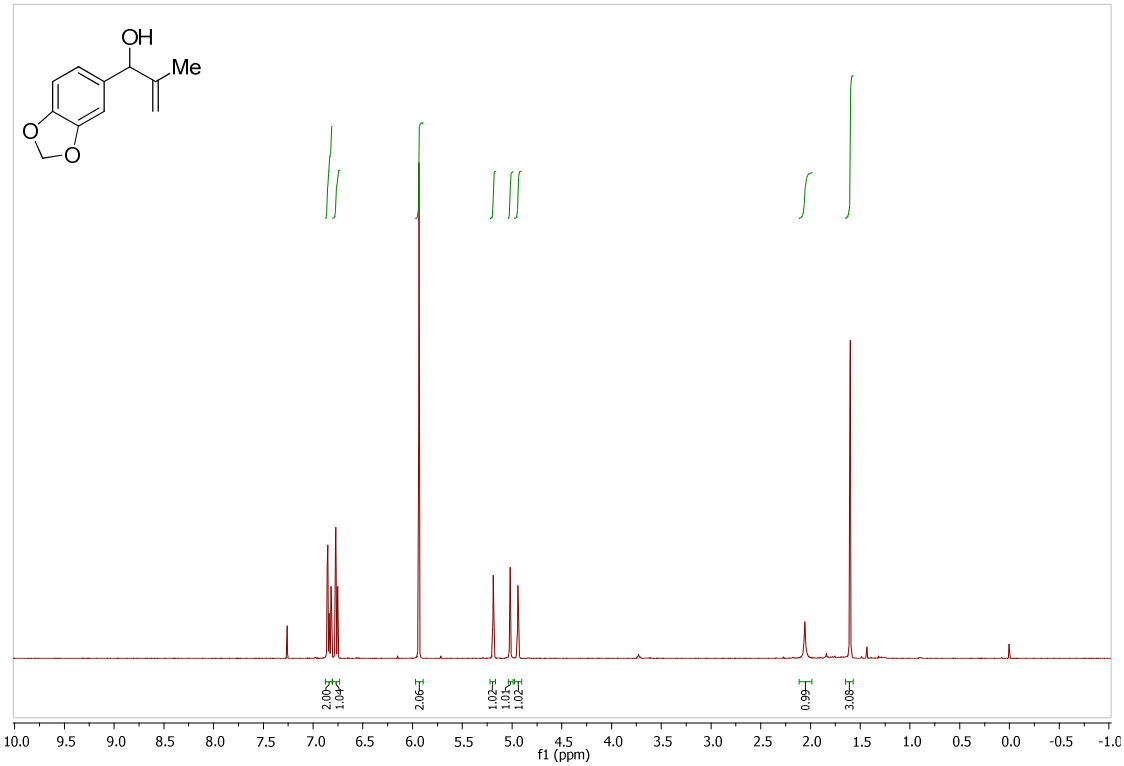
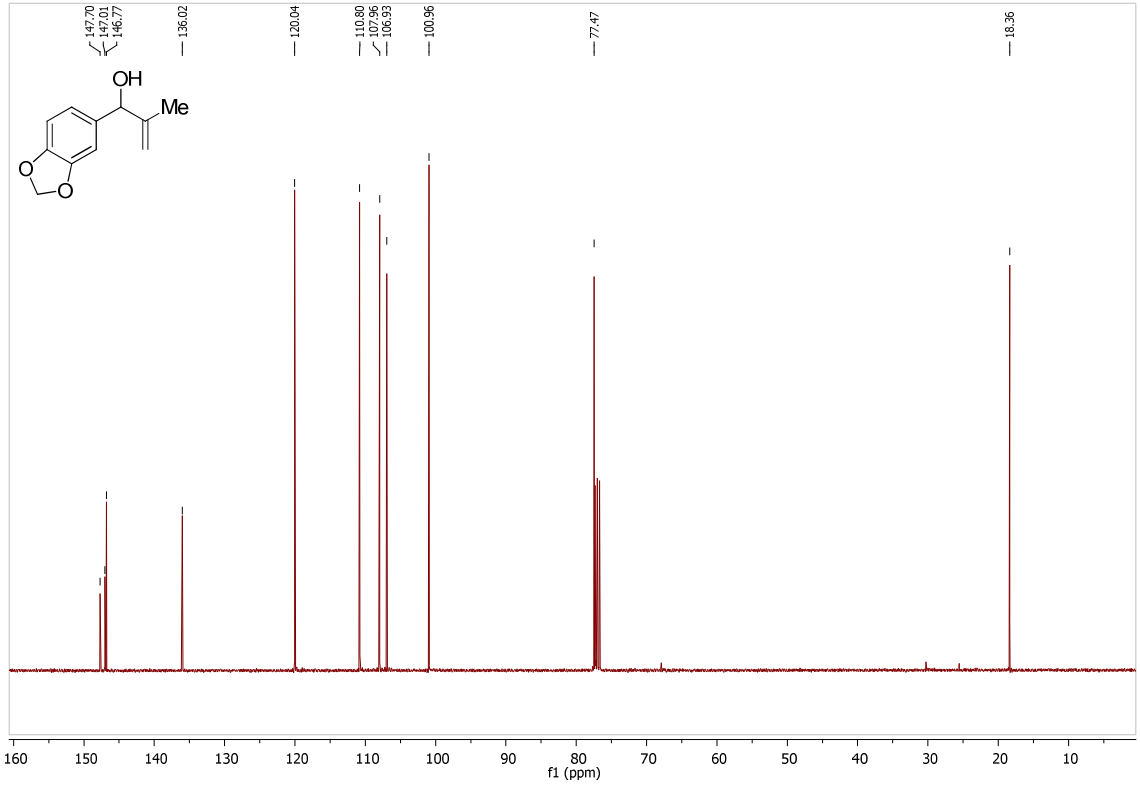
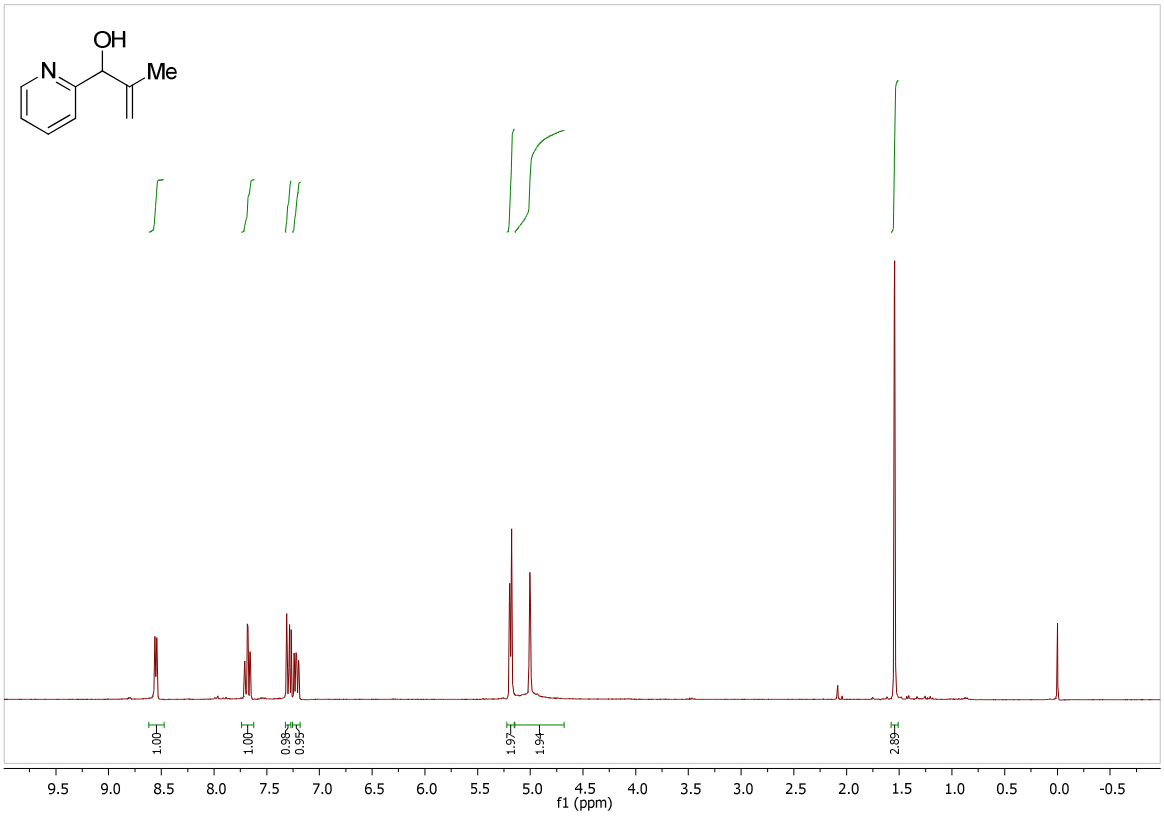
Toronto, Ontario, M5S 3H6, Canada

Supporting Information: Spectra

1. ^{1}H and ^{13}C NMR Spectra of New Compounds



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N
Me
1.00
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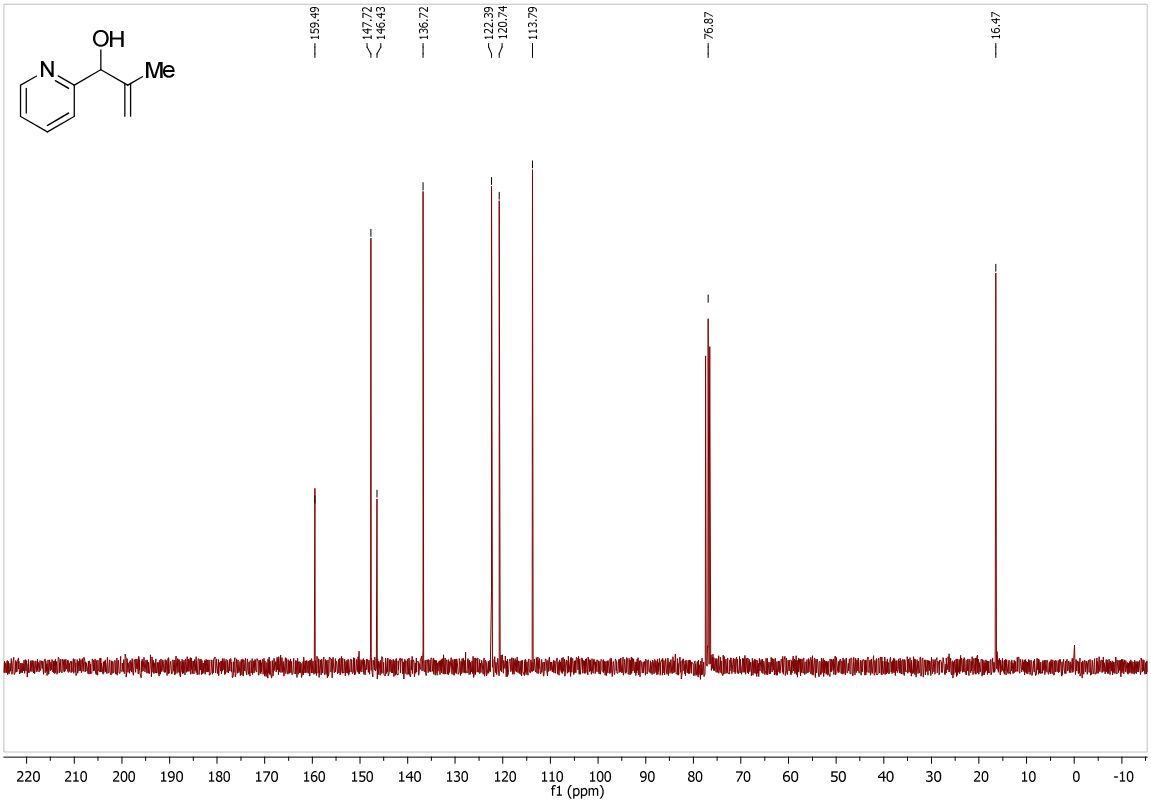
0.99
1.97
1.94
2.89
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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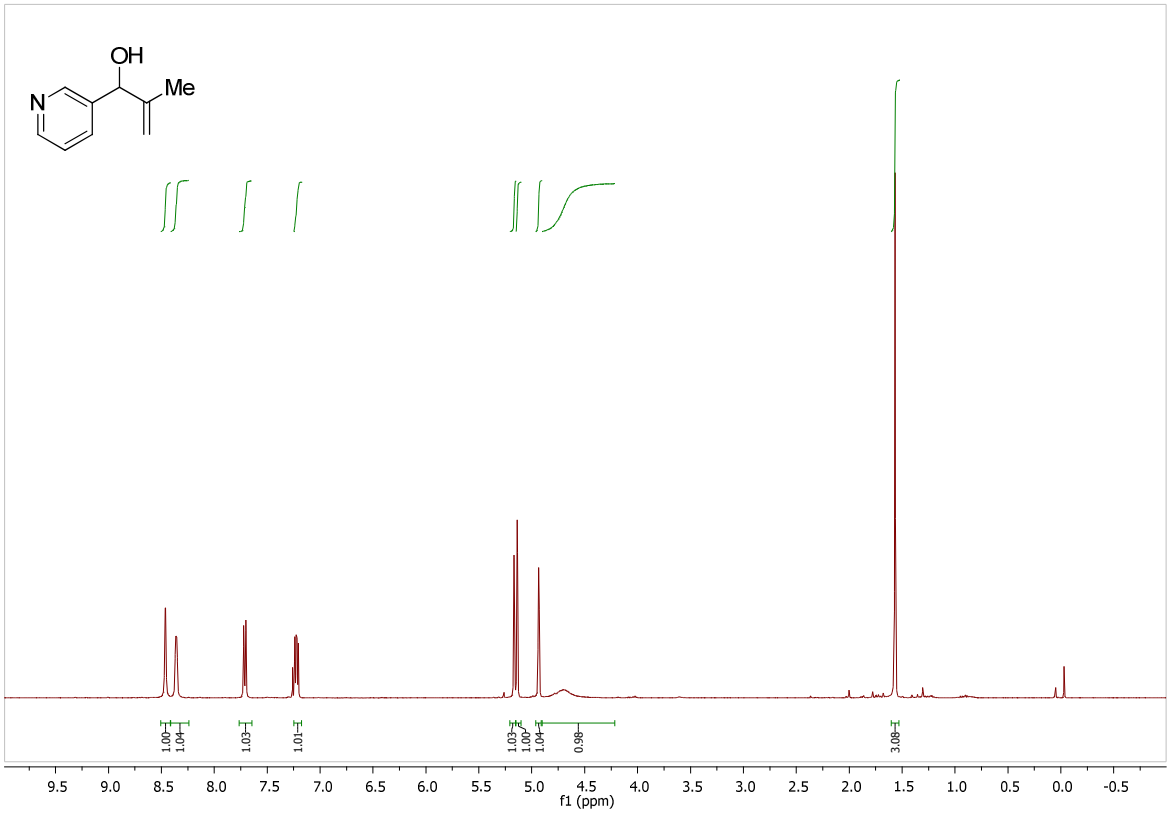
N
Me
159.49
147.72
146.43
136.72
122.39
120.74
113.79
76.87
16.47
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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Me
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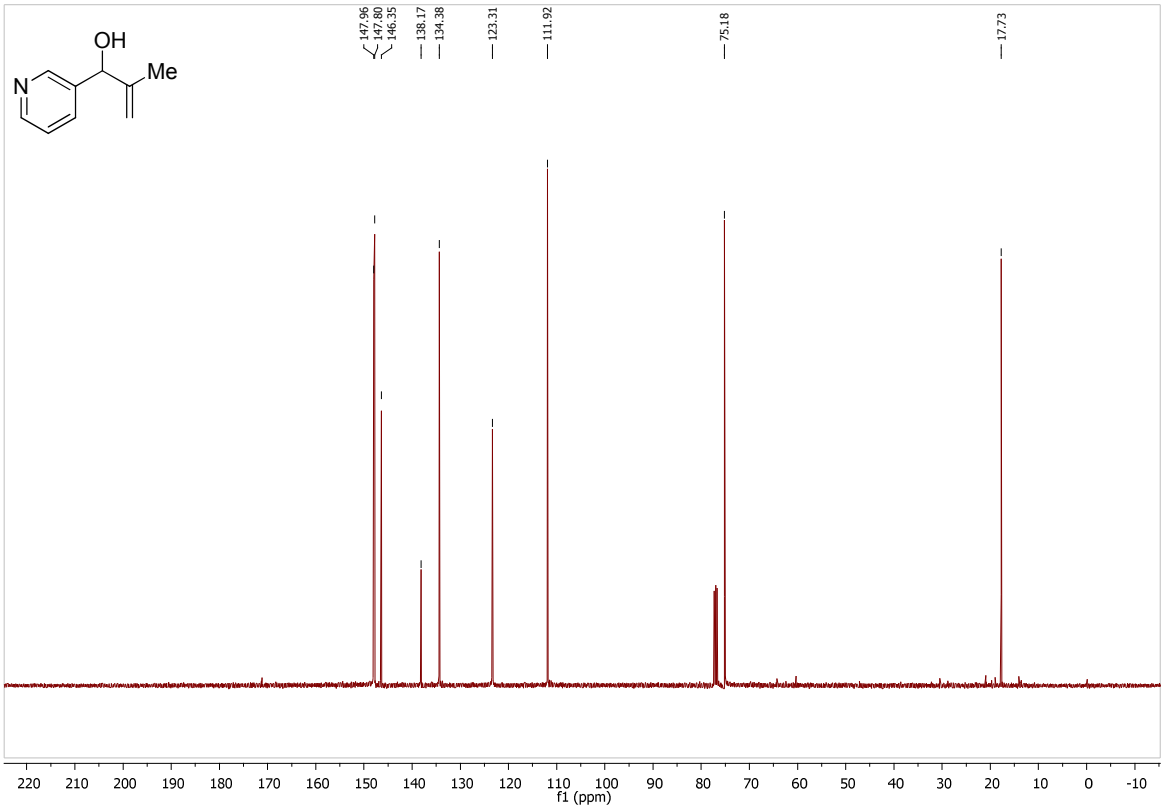
1.03
1.01
1.03
1.00
1.04
0.98
3.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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Me
N
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146.35
138.17
134.38
123.31
111.92
75.18
17.73
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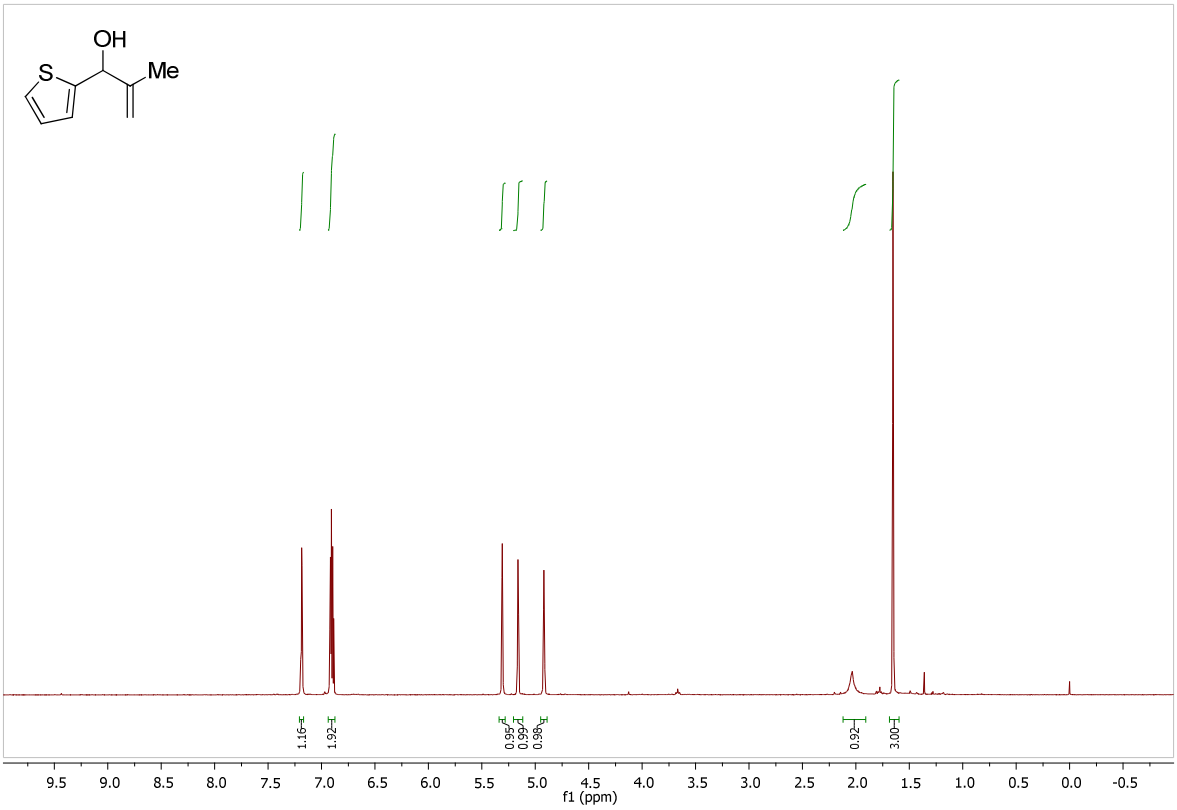
f1 (ppm)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S
Me
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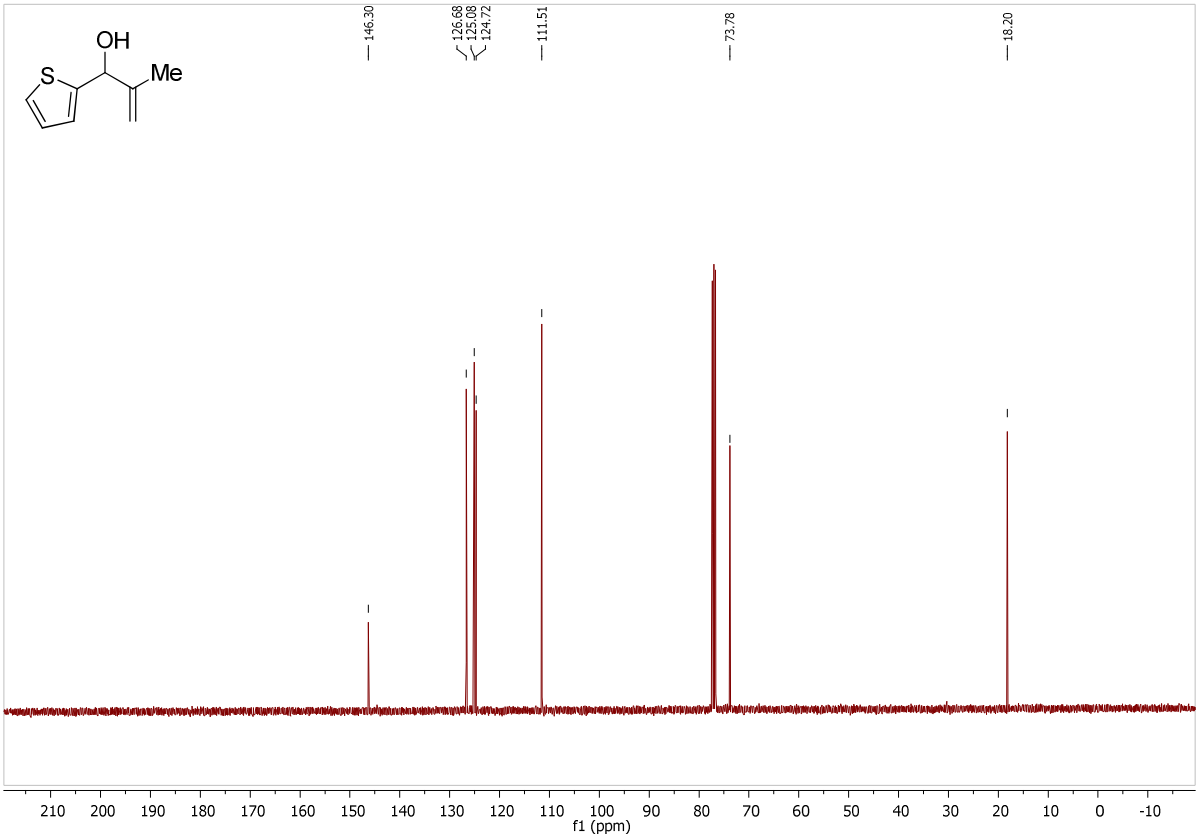
1.92
0.95
0.99
0.98
0.92
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


OH
S
Me
146.30
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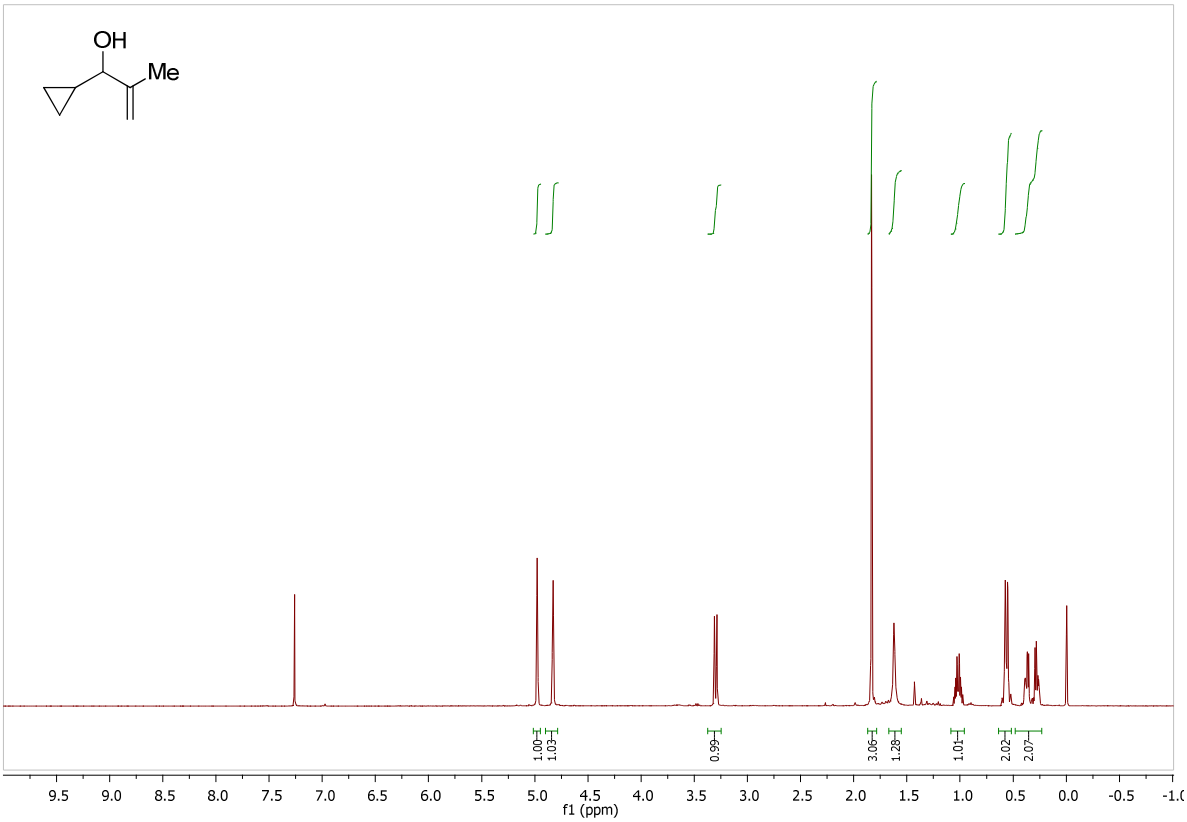
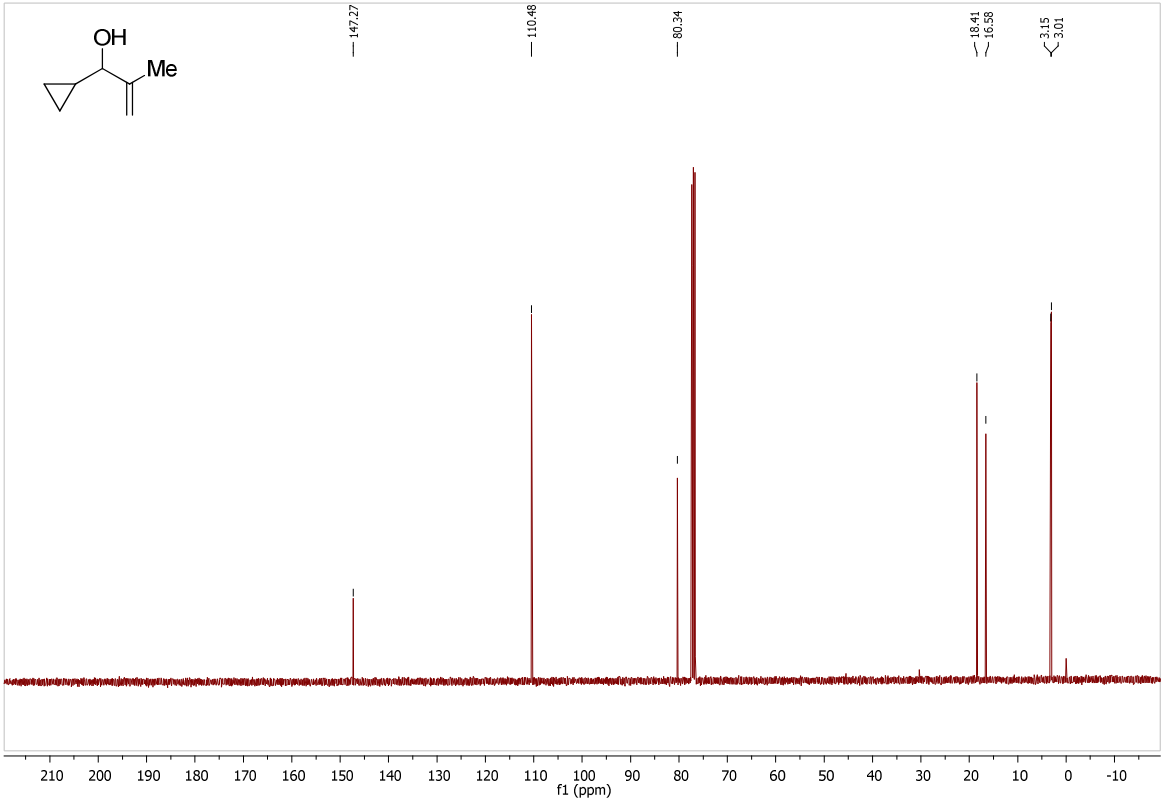
125.08
124.72
111.51
73.78
18.20
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


OH
Me
1.00
1.03
0.99
3.06
1.28
1.01
2.02
2.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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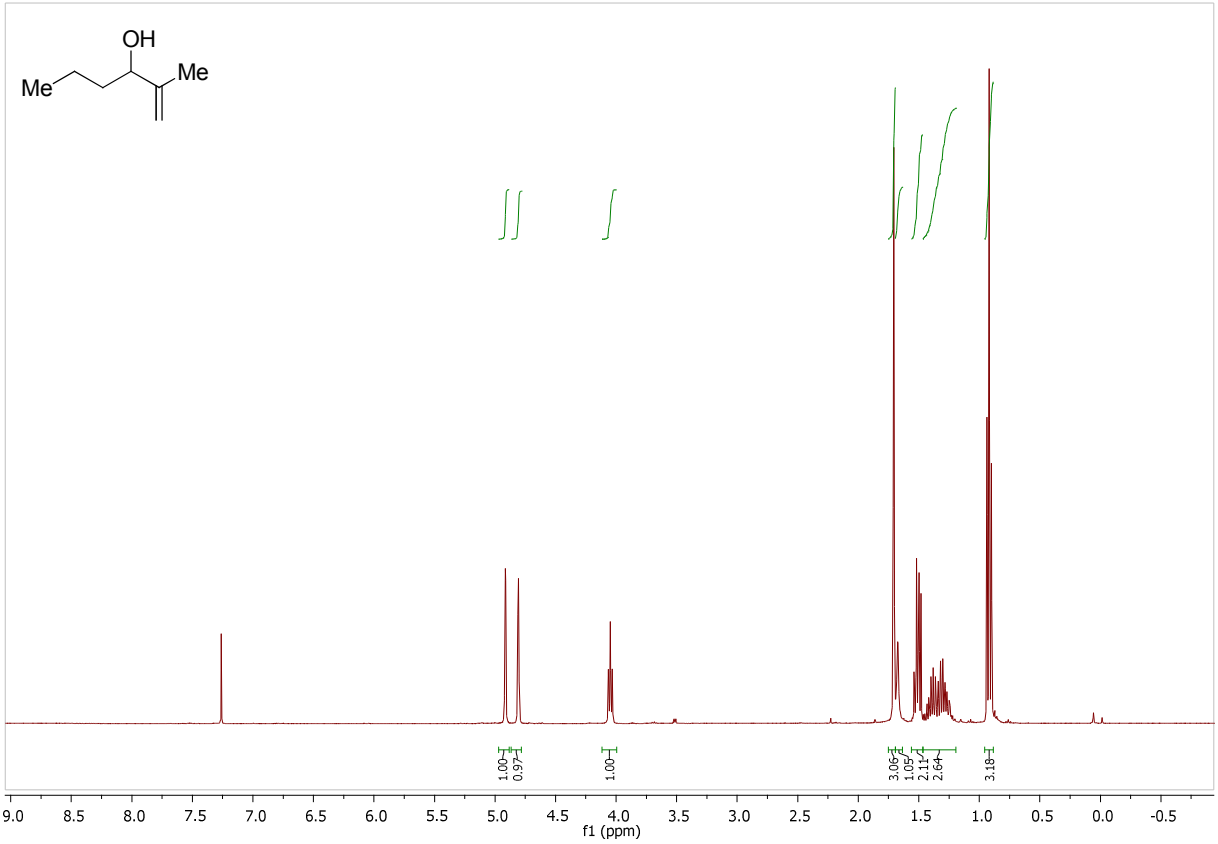
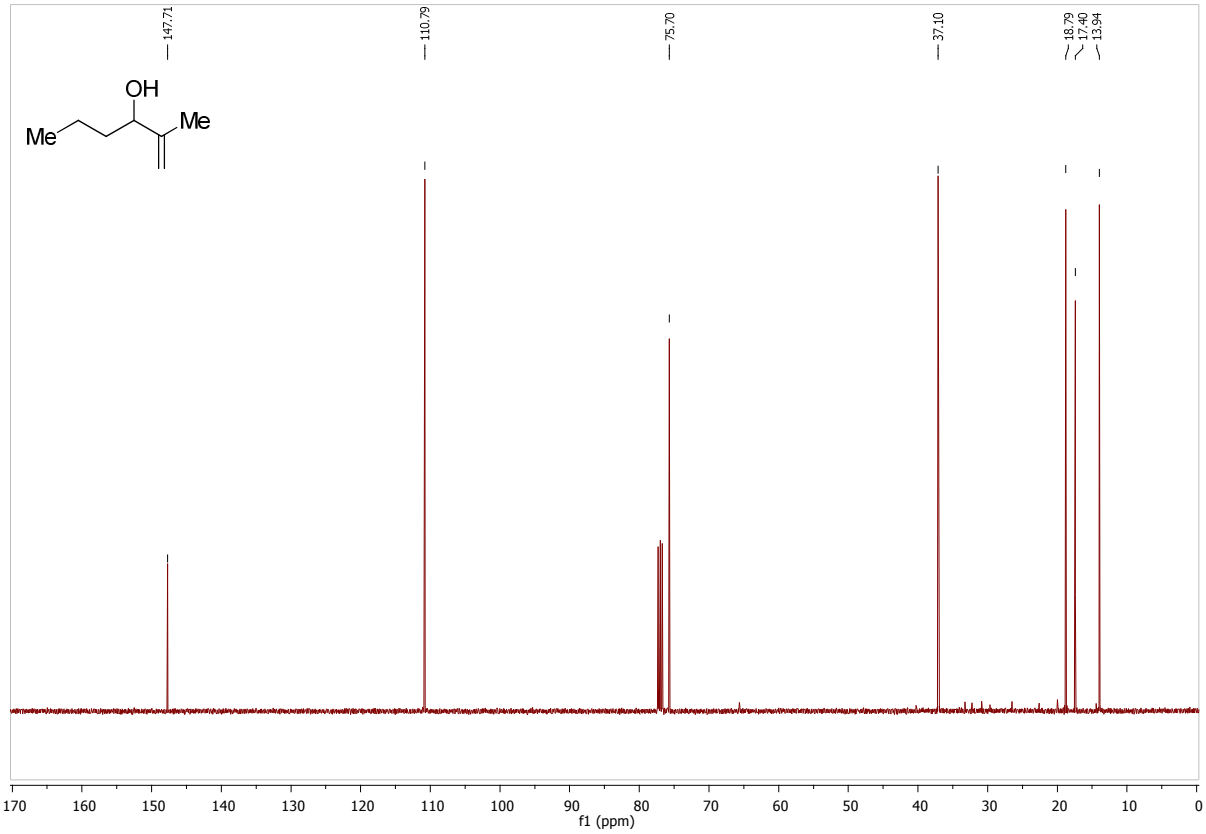
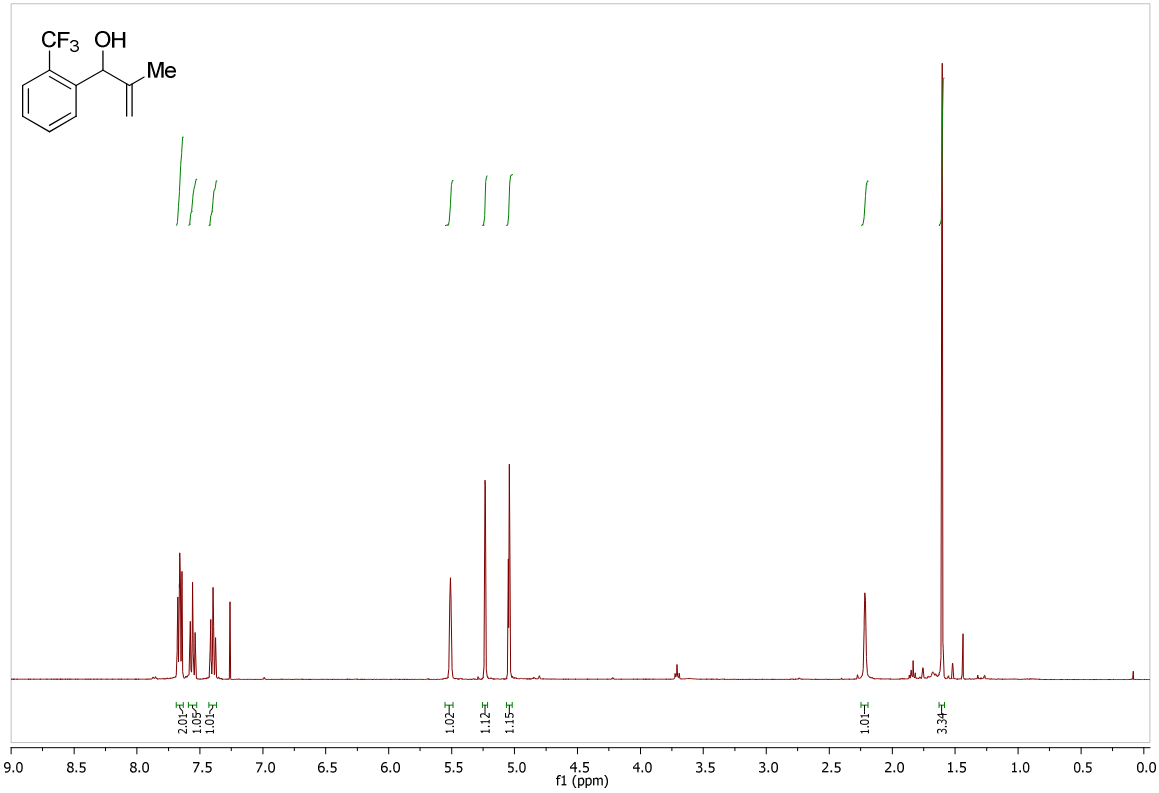
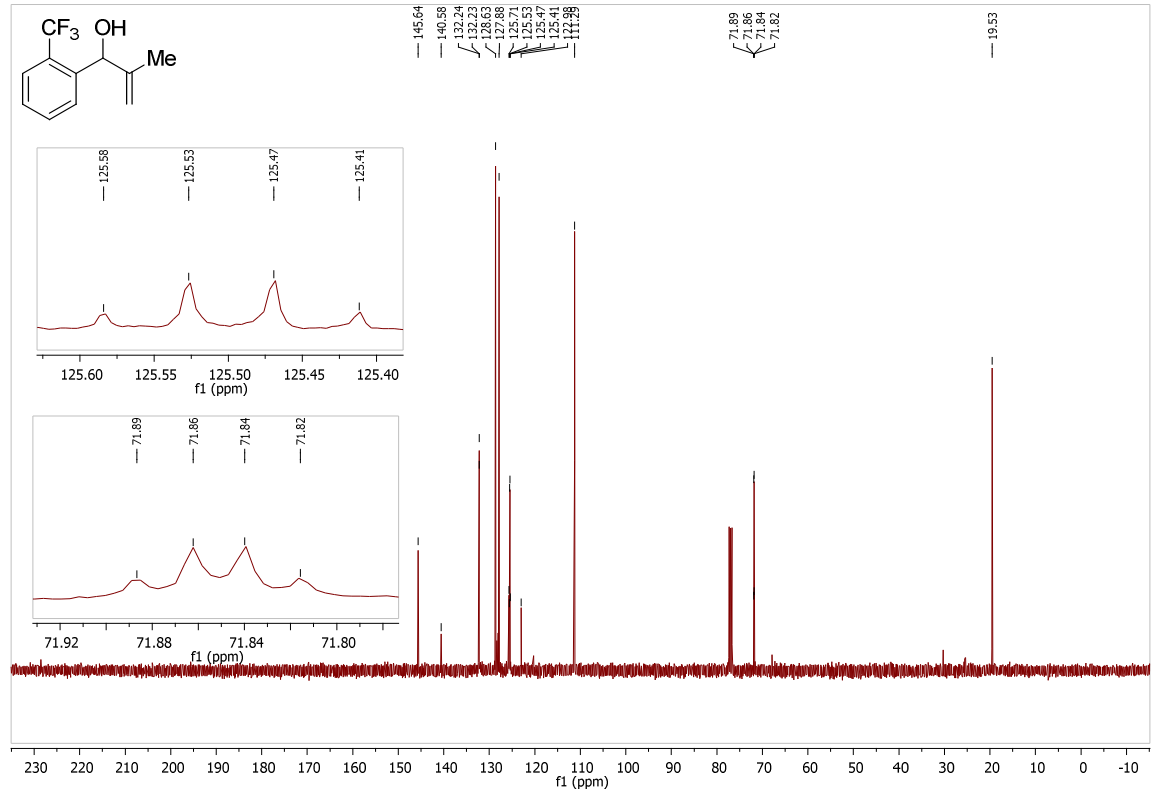
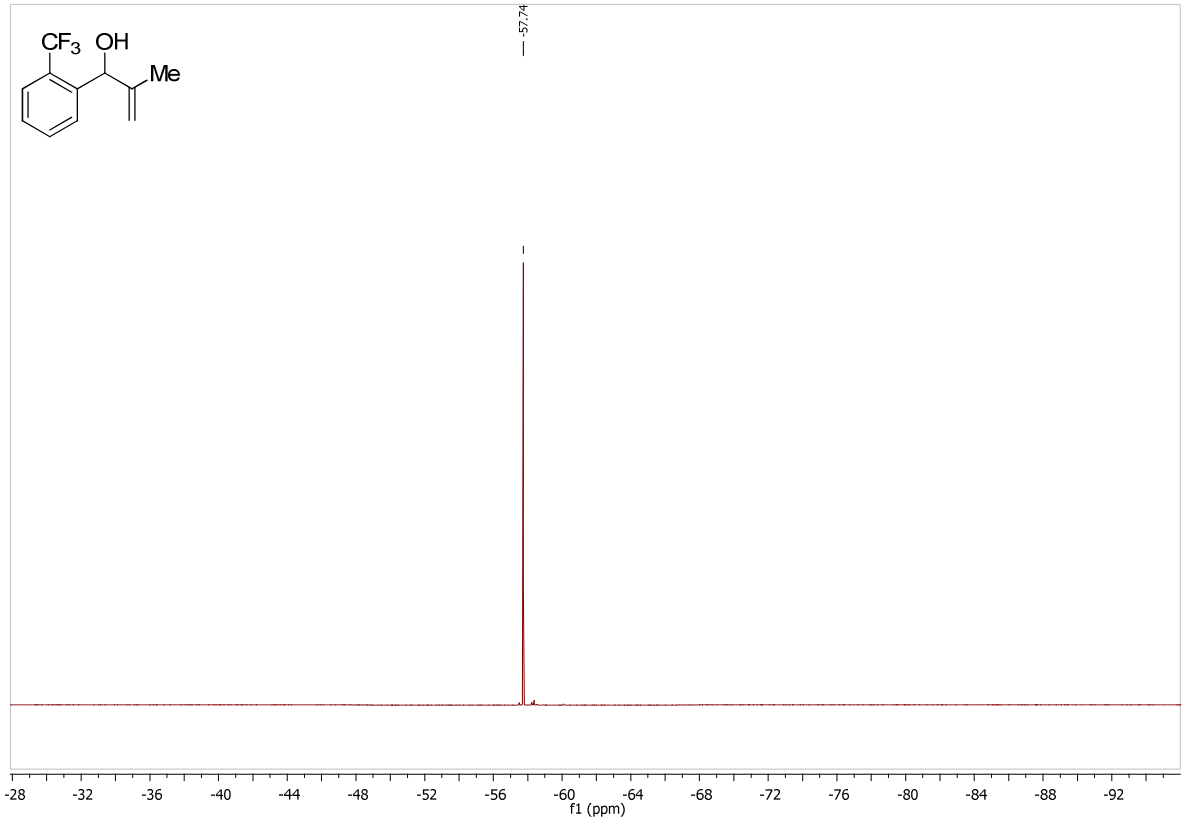
Me
147.27
110.48
80.34
18.41
16.58
3.15
3.01
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

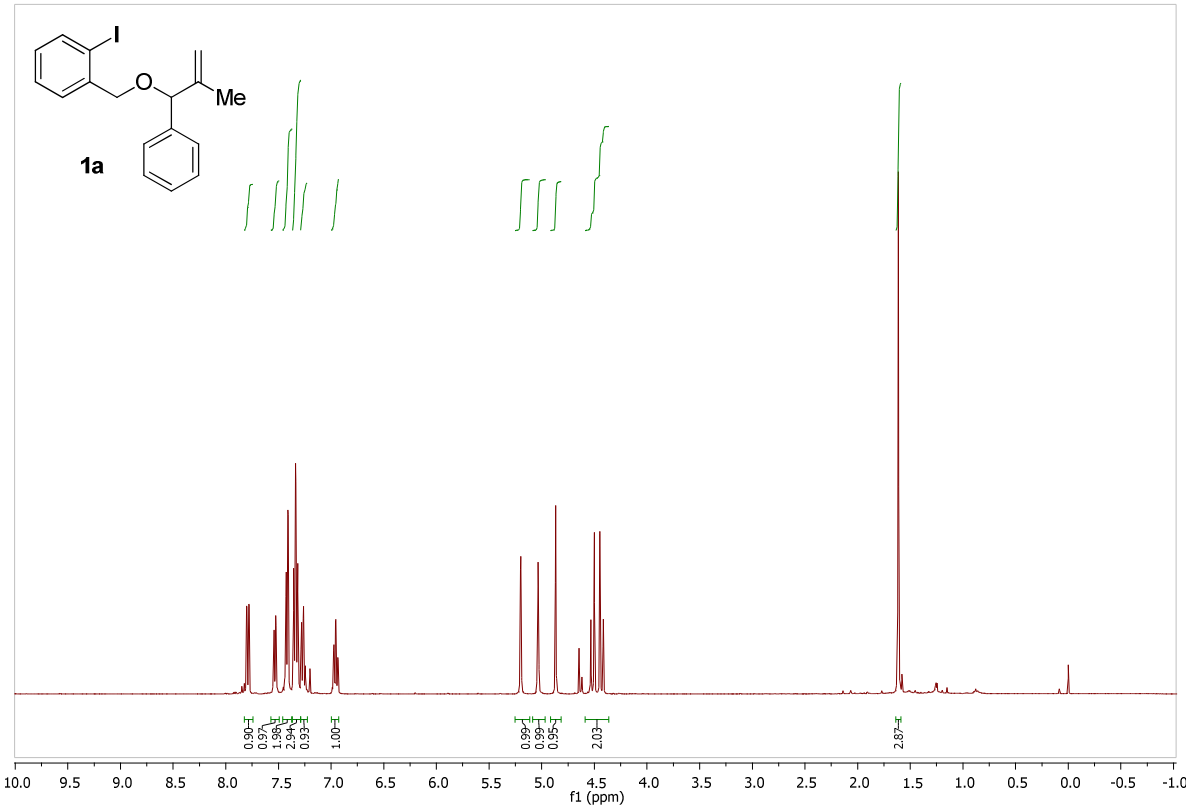

OH
Me
Me
1.00
0.97
1.00
3.06
1.05
2.11
2.64
3.18
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

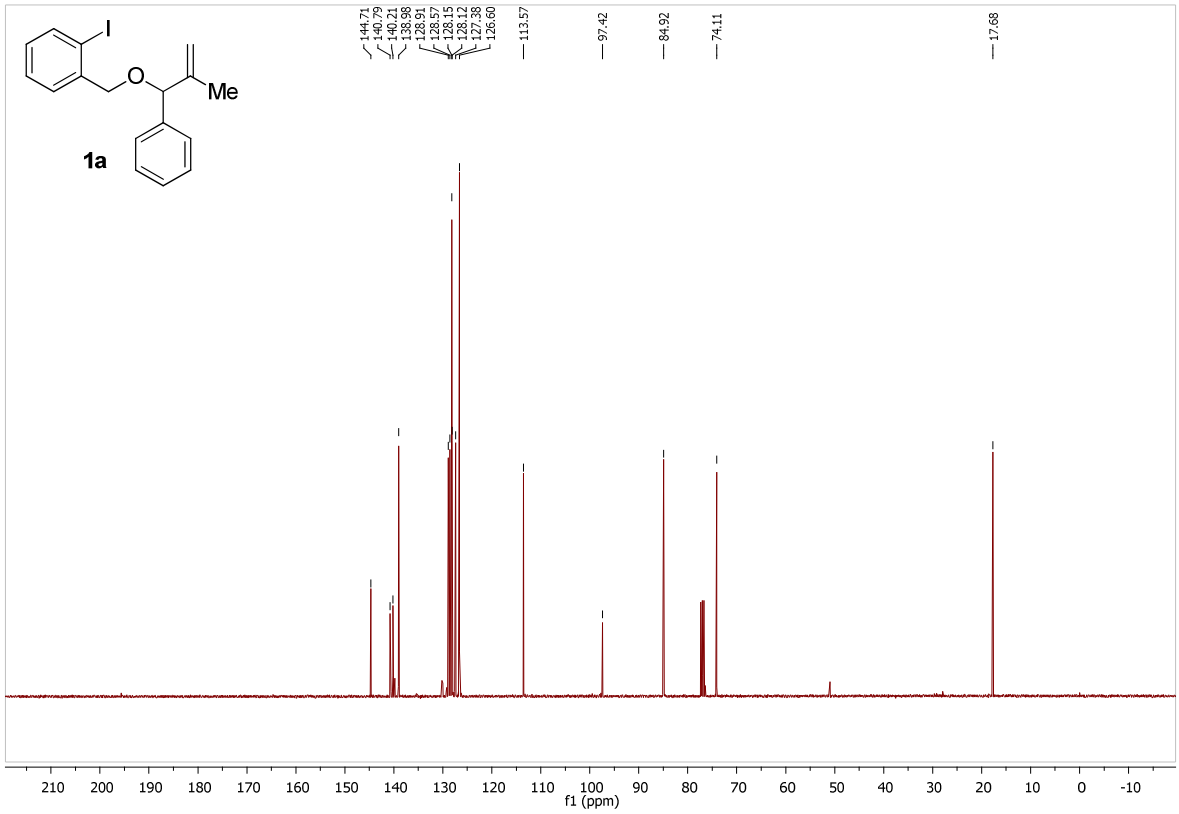

147.71
110.79
75.70
37.10
18.79
17.40
13.94
OH
Me
Me
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

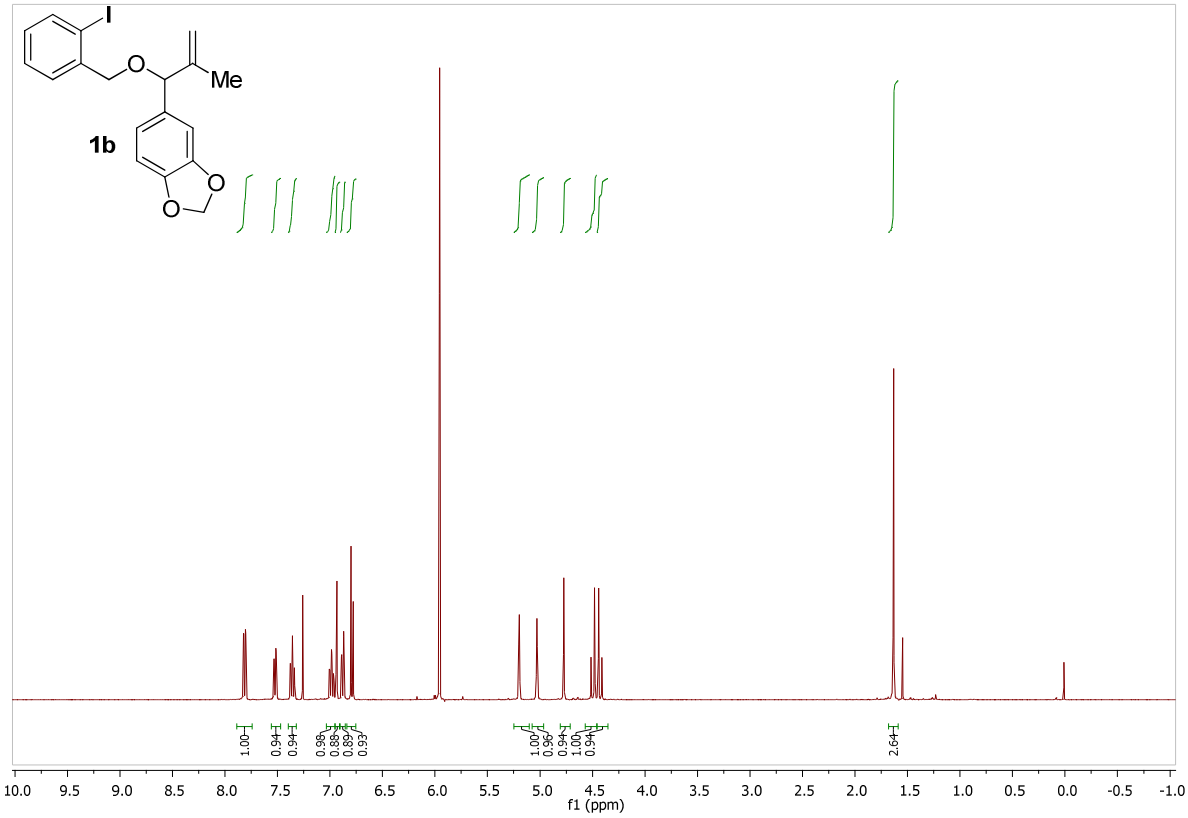

CF3 OH
Me
2.01
1.05
1.01
1.02
1.12
1.15
1.01
3.34
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

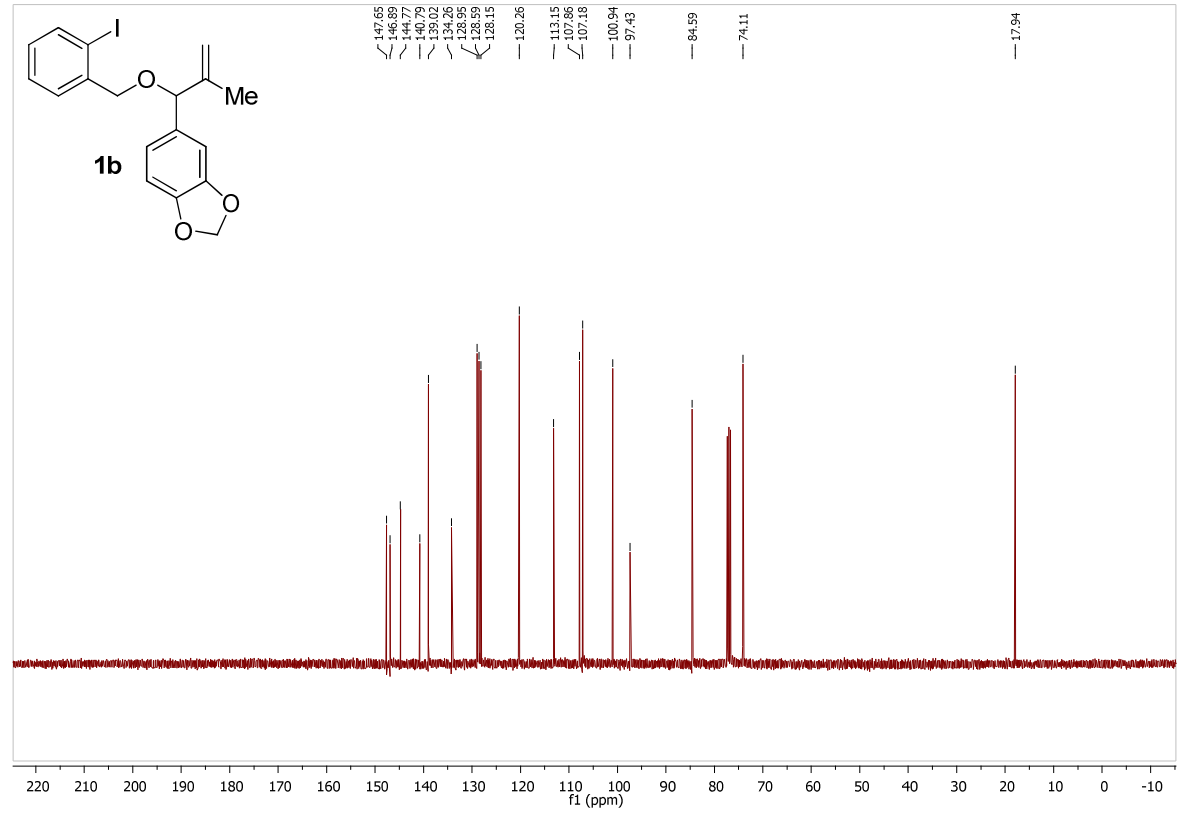

CF3 OH
Me
145.64
140.58
132.24
132.23
128.63
127.88
125.71
125.53
125.47
125.41
111.25
71.89
71.86
71.84
71.82
19.53
125.58
125.53
125.47
125.41
125.60 125.55 125.50 125.45 125.40
f1 (ppm)
71.89
71.86
71.84
71.82
71.92 71.88 71.84 71.80
f1 (ppm)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

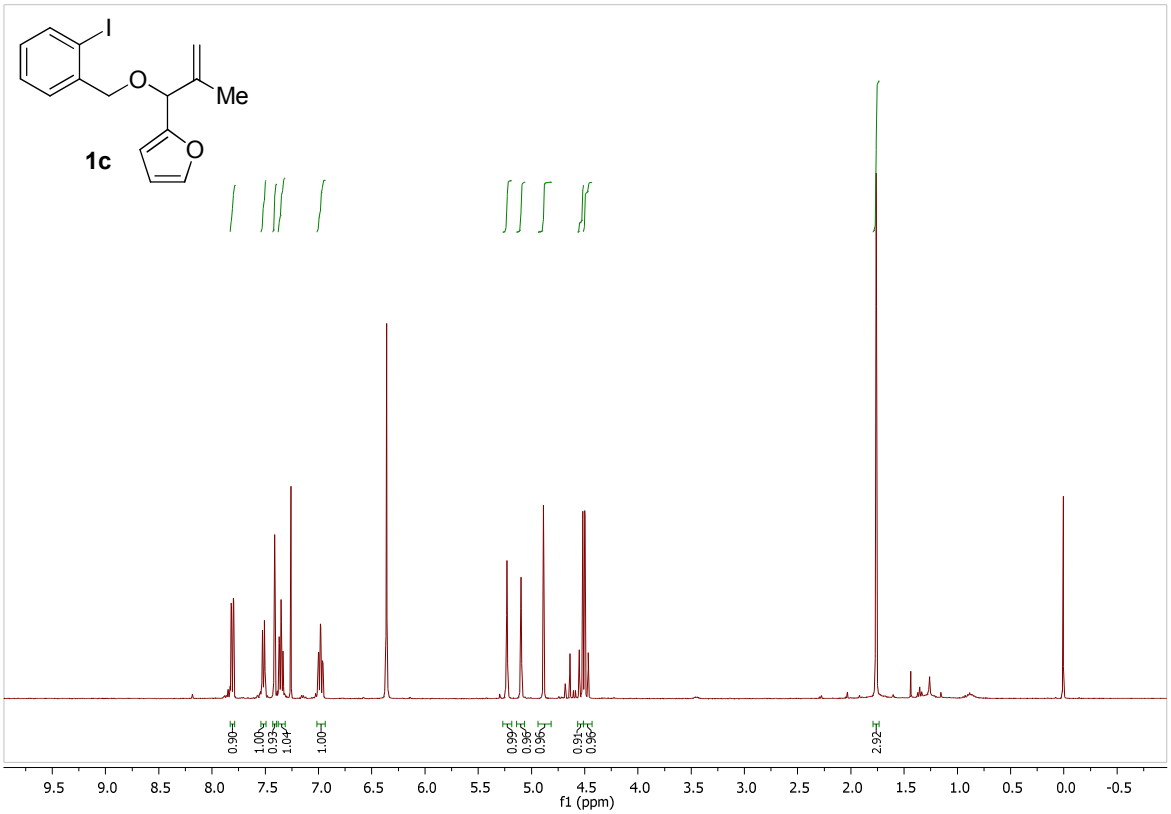

CF3
OH
Me
-57.74
-28
-32
-36
-40
-44
-48
-52
-56
-60
-64
-68
-72
-76
-80
-84
-88
-92
f1 (ppm)

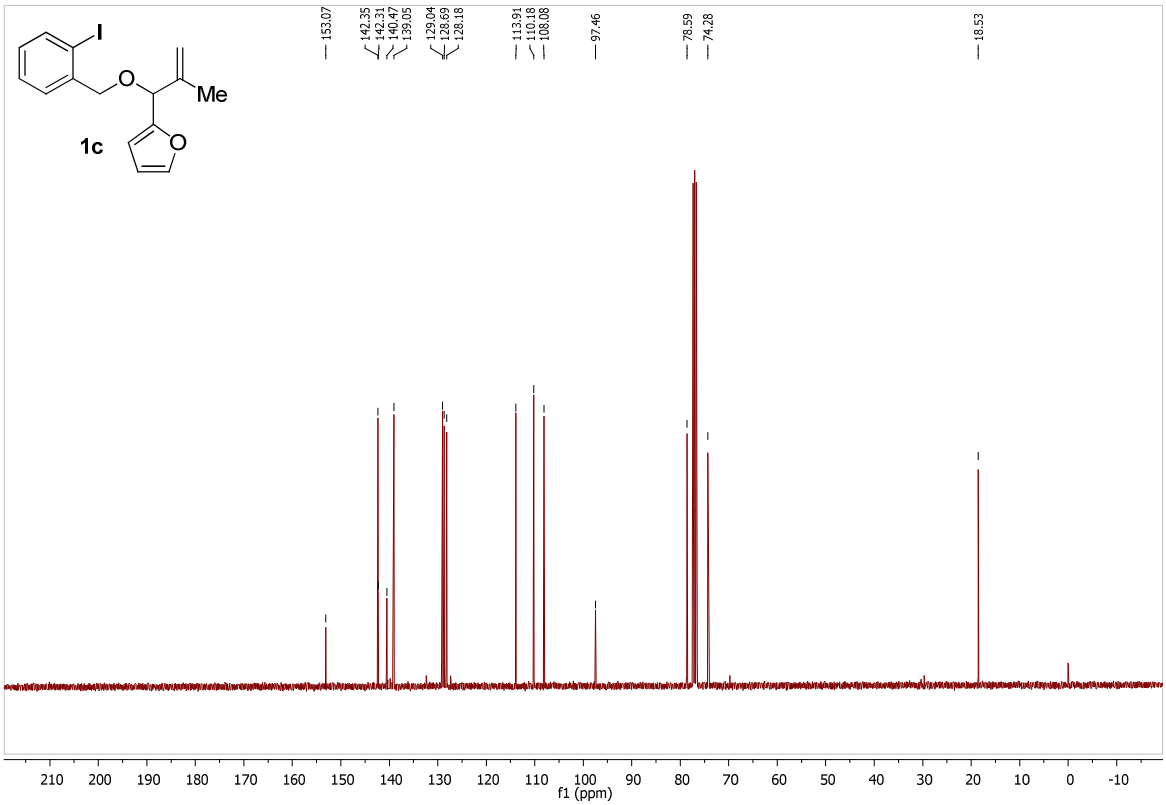

I
O
Me
1a
0.90
0.97
1.98
2.94
0.93
1.00
0.99
0.99
0.95
2.03
2.87
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


I
O
Me
1a
144.71
140.79
140.21
138.98
128.91
128.57
128.15
128.12
127.38
126.60
113.57
97.42
84.92
74.11
17.68
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)


I
O
Me
1b
O
O
1.00
0.94
0.94
0.98
0.88
0.89
0.93
1.00
0.96
0.94
1.00
0.94
2.64
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


I
O
Me
1b
O
O
147.65
146.89
144.77
140.79
139.02
134.26
128.95
128.59
128.15
120.26
113.15
107.86
107.18
100.94
97.43
84.59
74.11
17.94
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


I
O
Me
O
1c
0.90
1.00
0.98
1.04
1.00
0.99
0.98
0.96
0.91
0.96
2.92
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)


I
O
Me
O
1c
153.07
142.35
142.31
140.47
139.05
129.04
128.69
128.18
113.91
110.18
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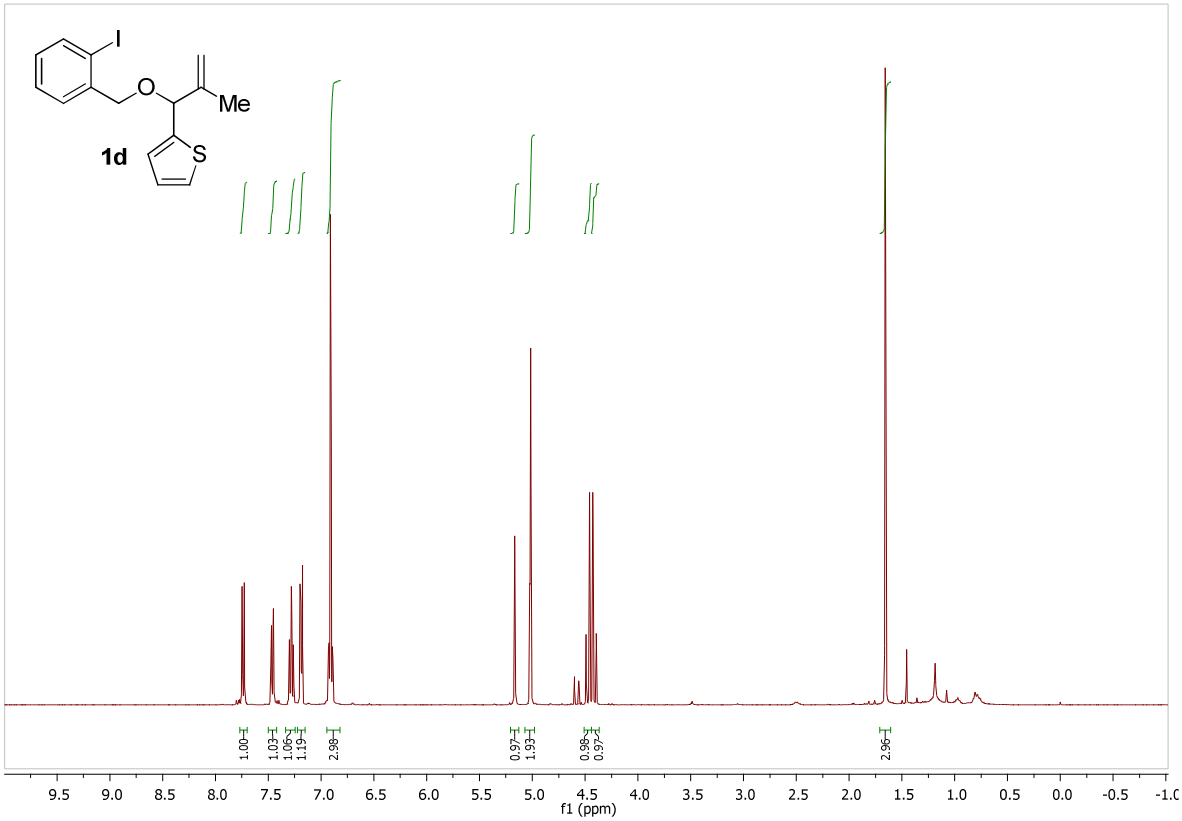
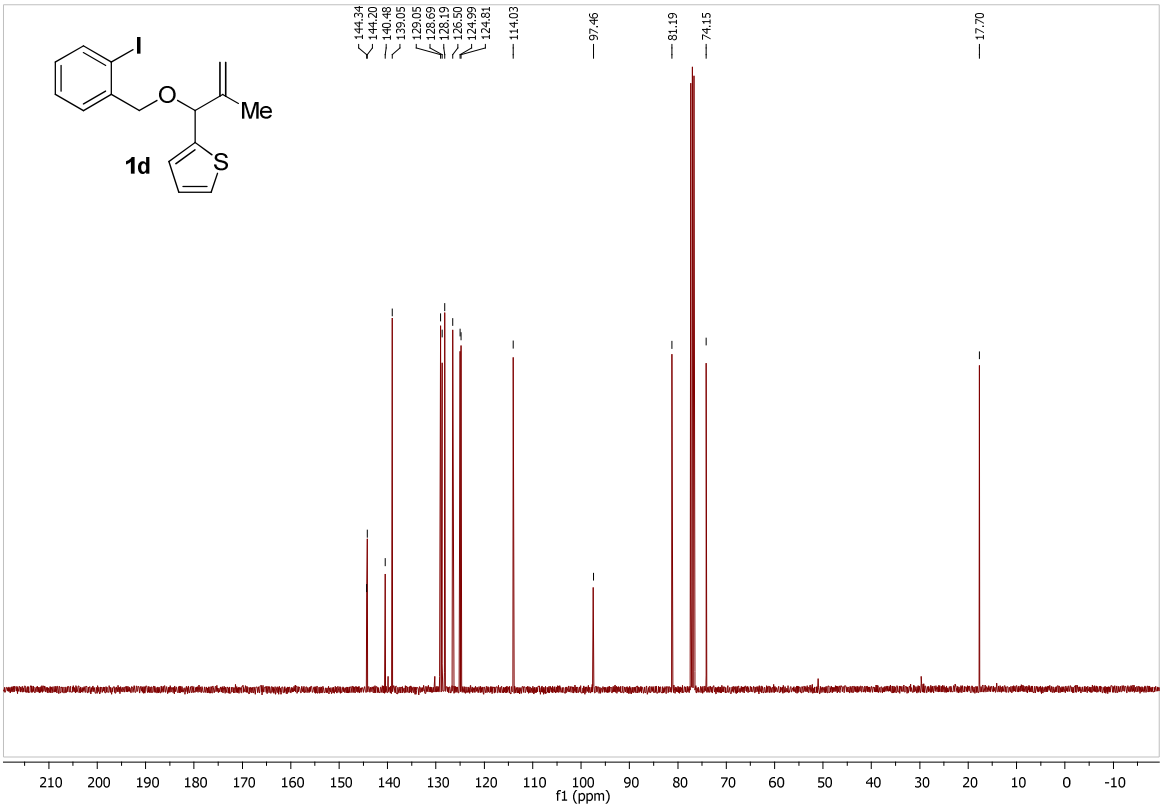
78.59
74.28
18.53
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


I
O
Me
1d
S
1.00
1.03
1.06
1.19
2.98
0.97
1.93
0.98
0.97
2.96
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)


I
O
Me
1d
S
144.34
144.20
140.48
139.05
129.05
128.69
128.19
126.50
124.99
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114.03
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81.19
74.15
17.70
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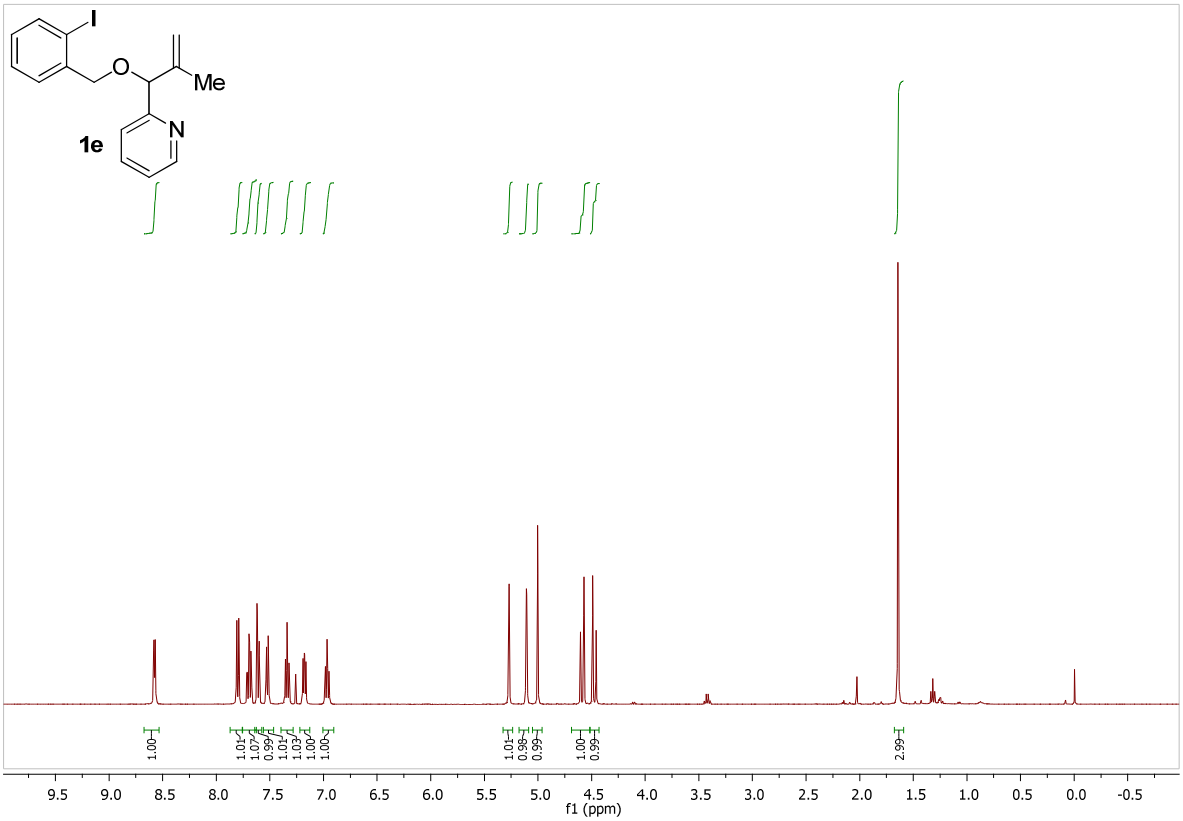
f1 (ppm)


I
O
Me
N
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1.07
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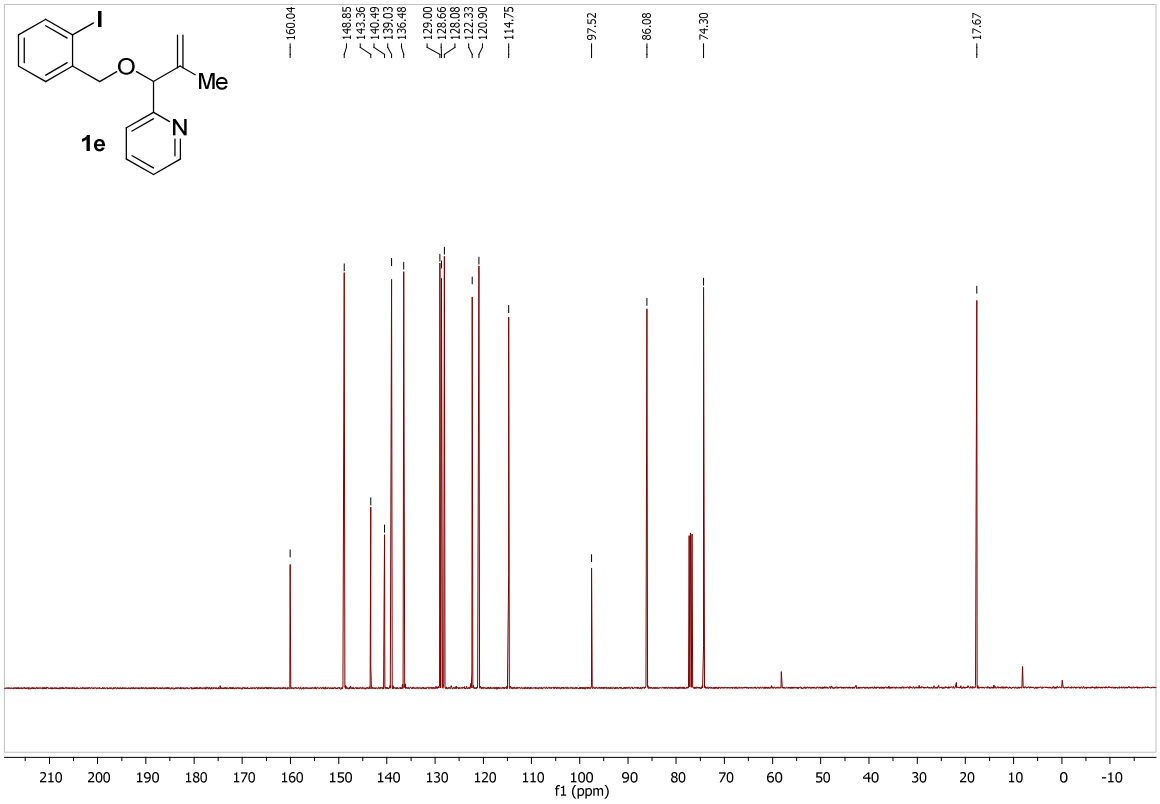
1.01
1.03
1.00
1.00
1.01
0.98
0.99
1.00
0.99
2.99
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


I
O
Me
N
1e
160.04
148.85
143.36
140.49
139.03
136.48
129.00
128.66
128.08
122.33
120.90
114.75
97.52
86.08
74.30
17.67
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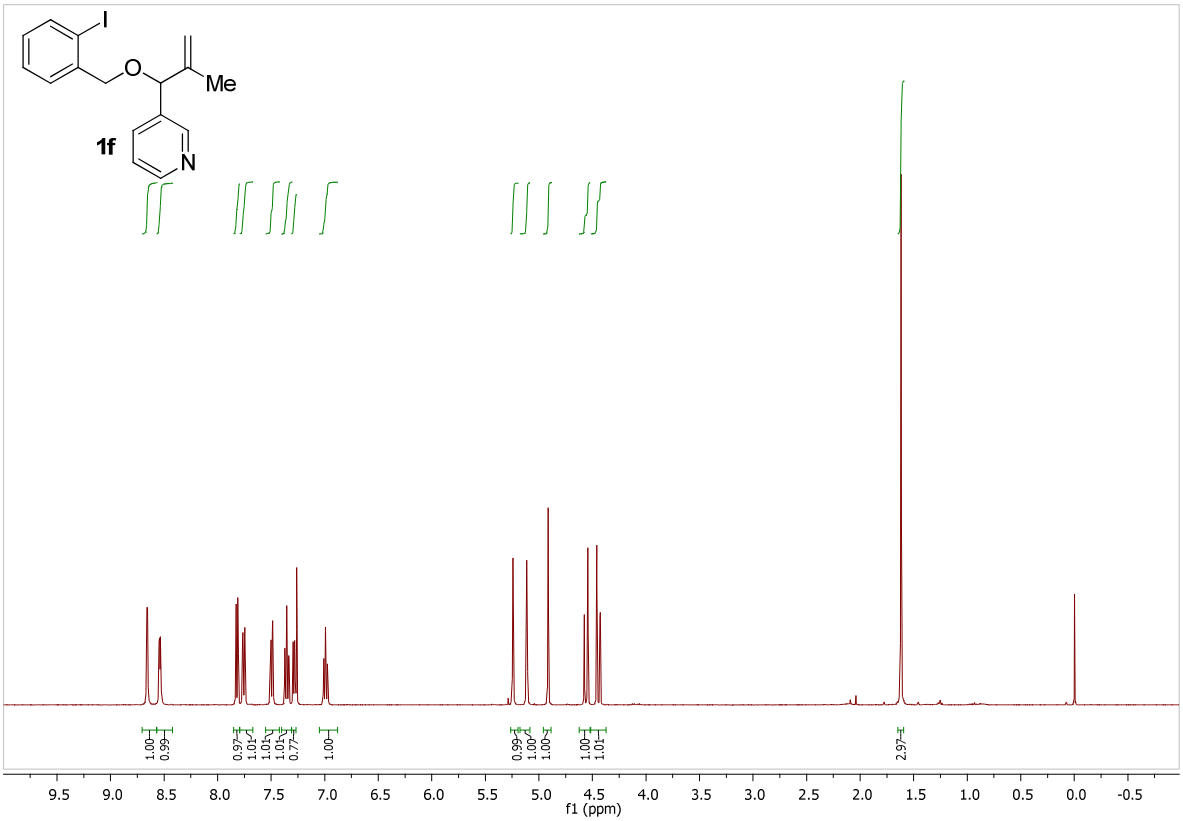
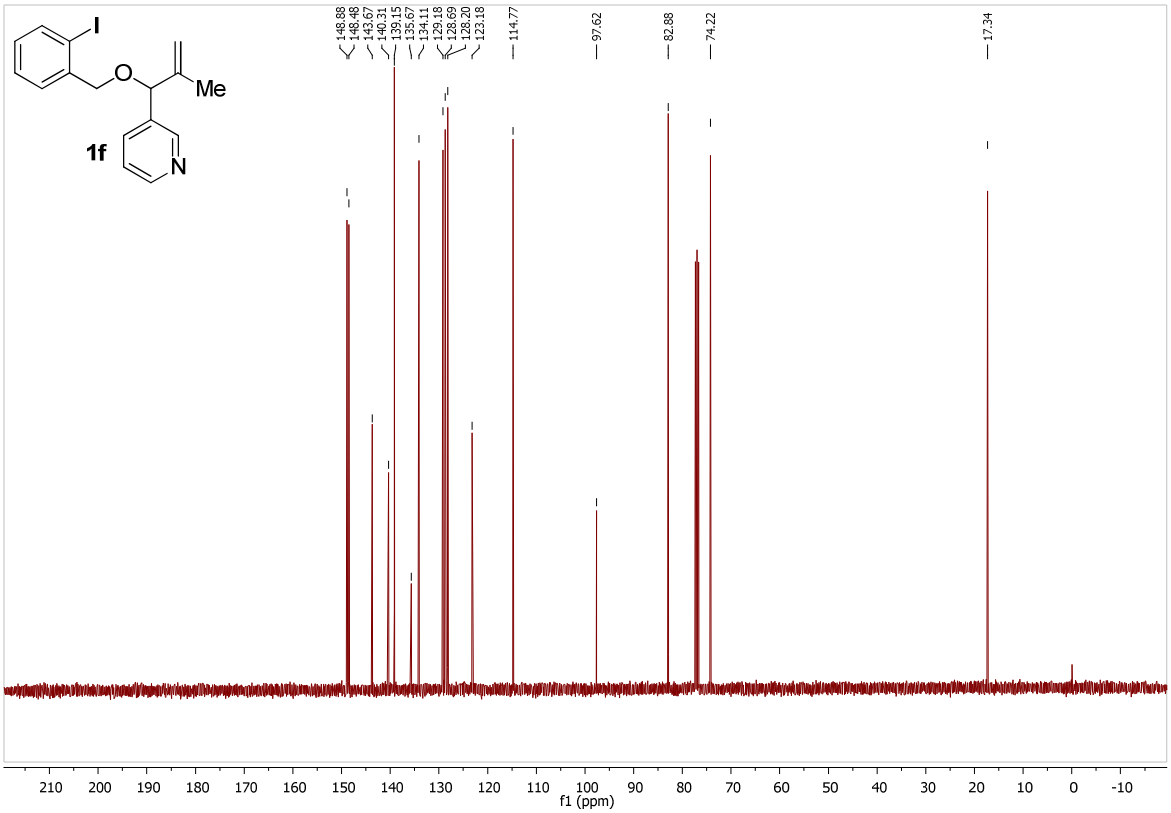
f1 (ppm)


I
O
Me
1f
N
1.00
0.99
0.97
1.01
1.01
1.01
0.77
1.00
0.99
1.00
1.00
1.00
1.01
2.97
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)


I
O
Me
1f
N
148.88
148.48
143.67
140.31
139.15
135.67
134.11
129.18
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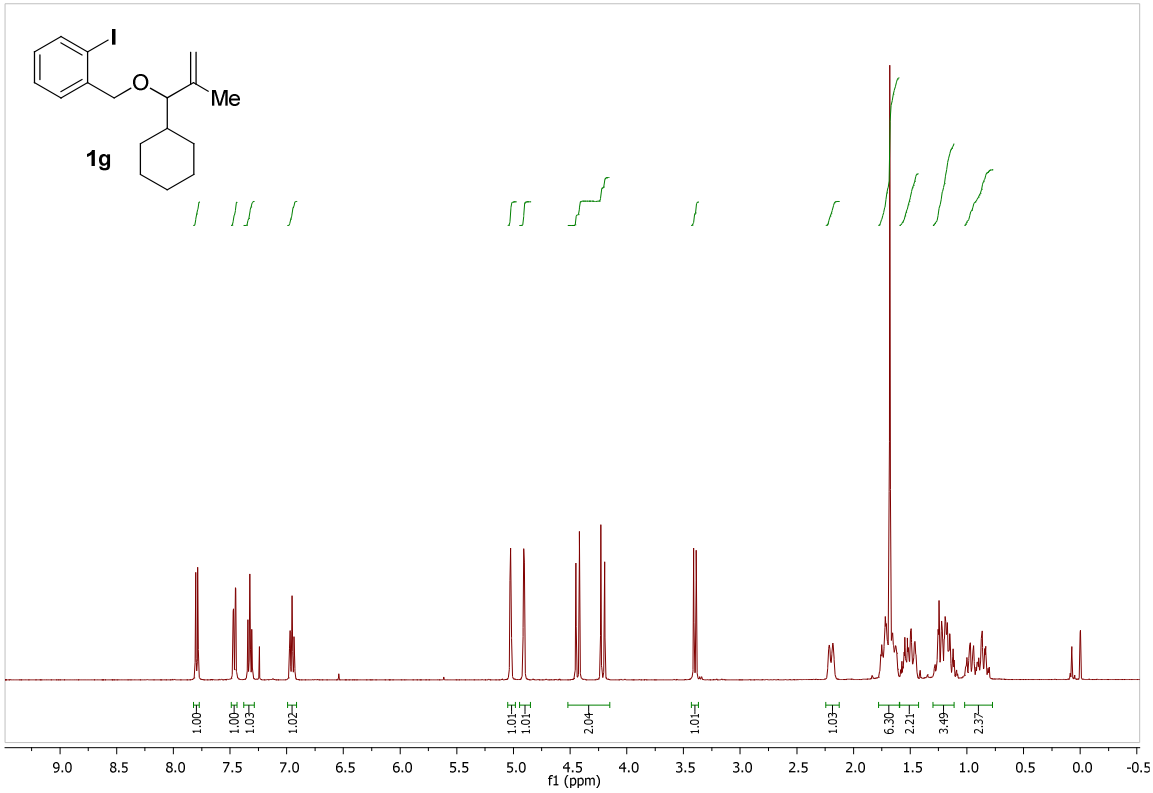
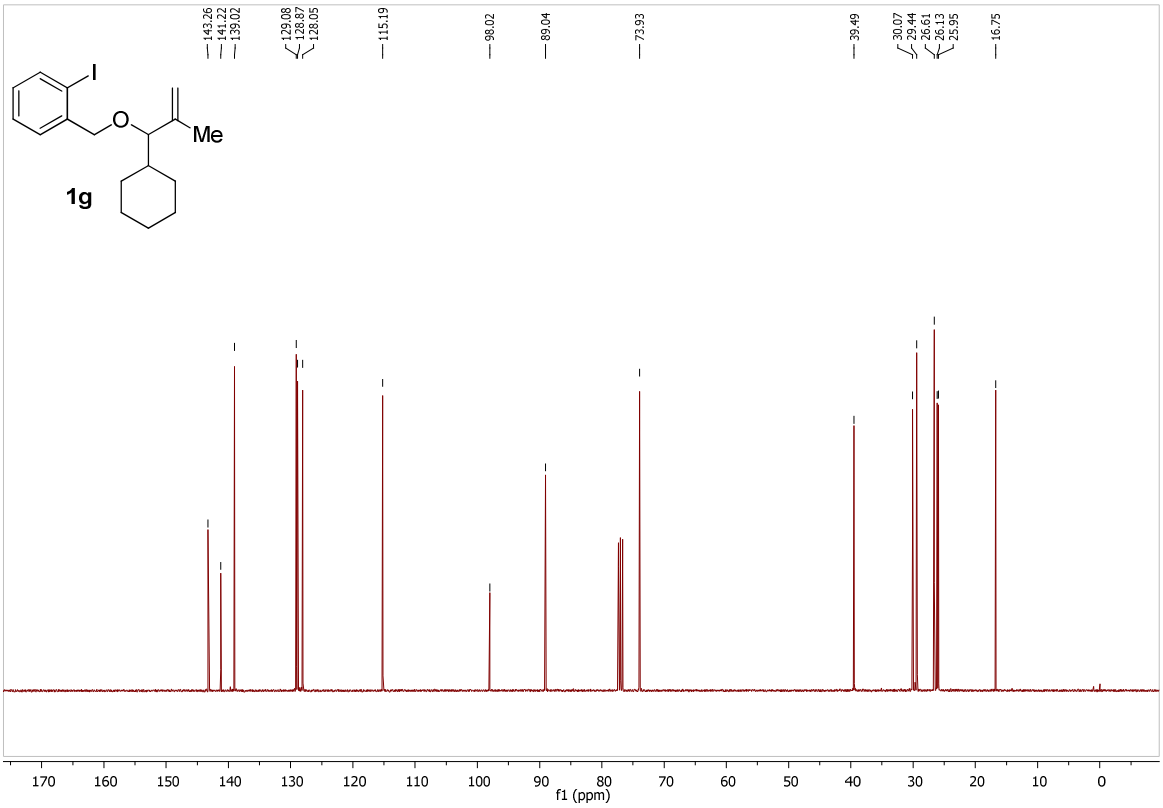
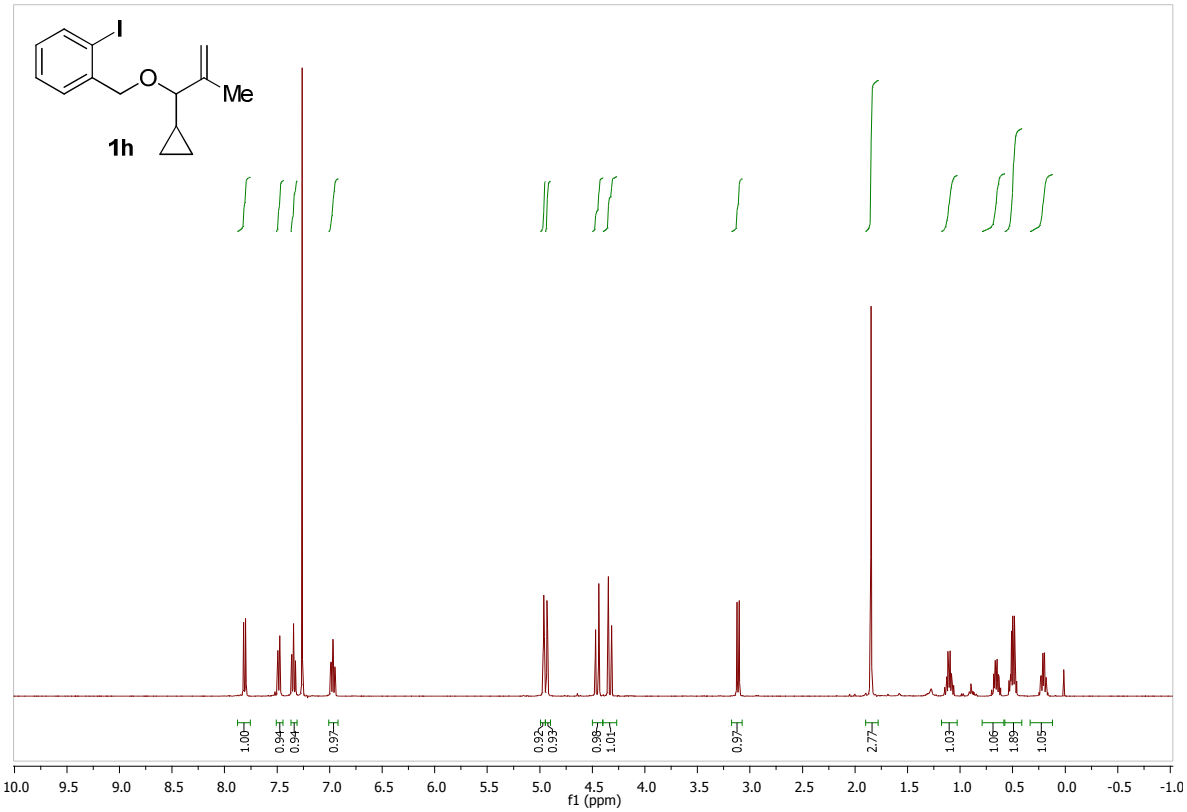
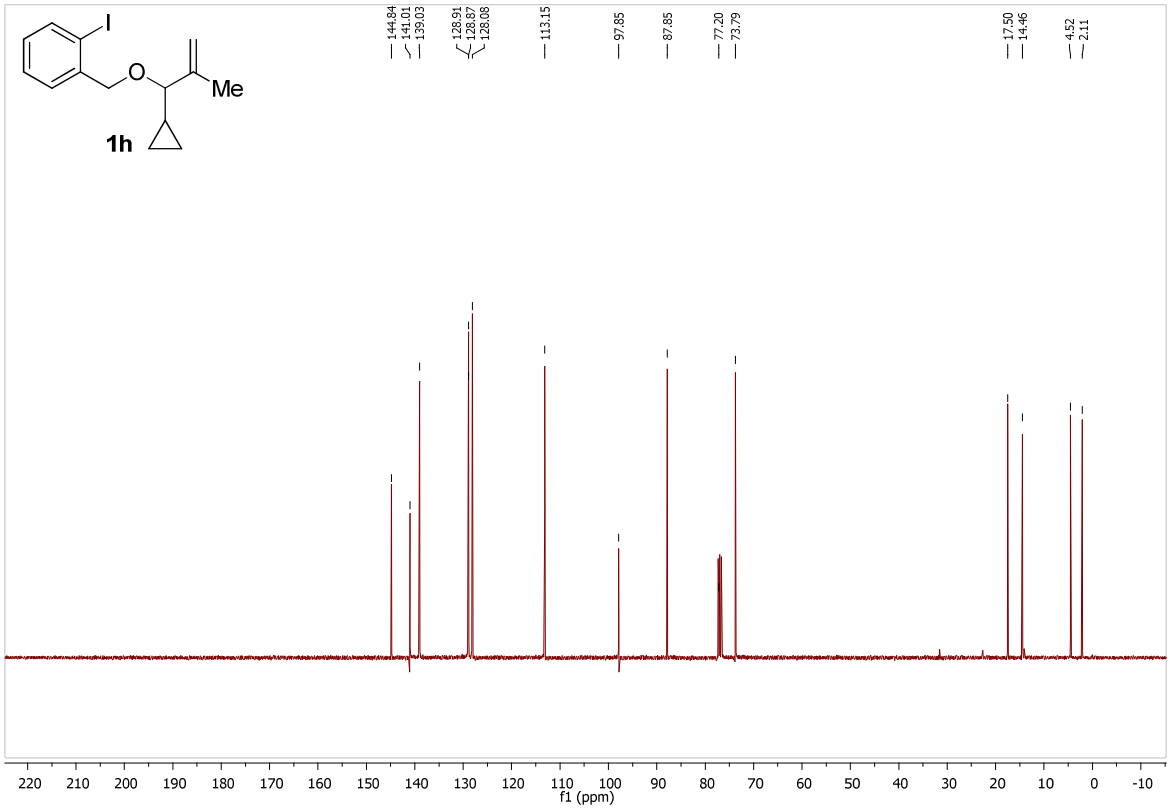
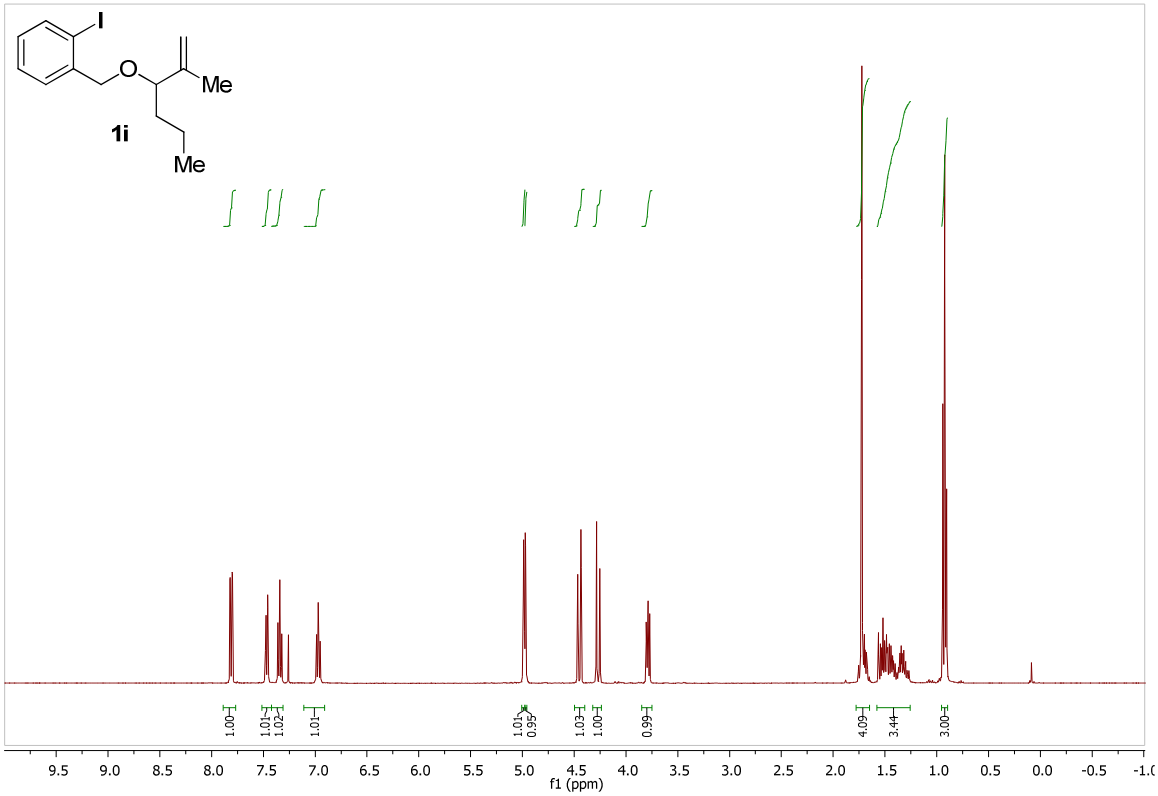
128.20
123.18
114.77
97.62
82.88
74.22
17.34
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

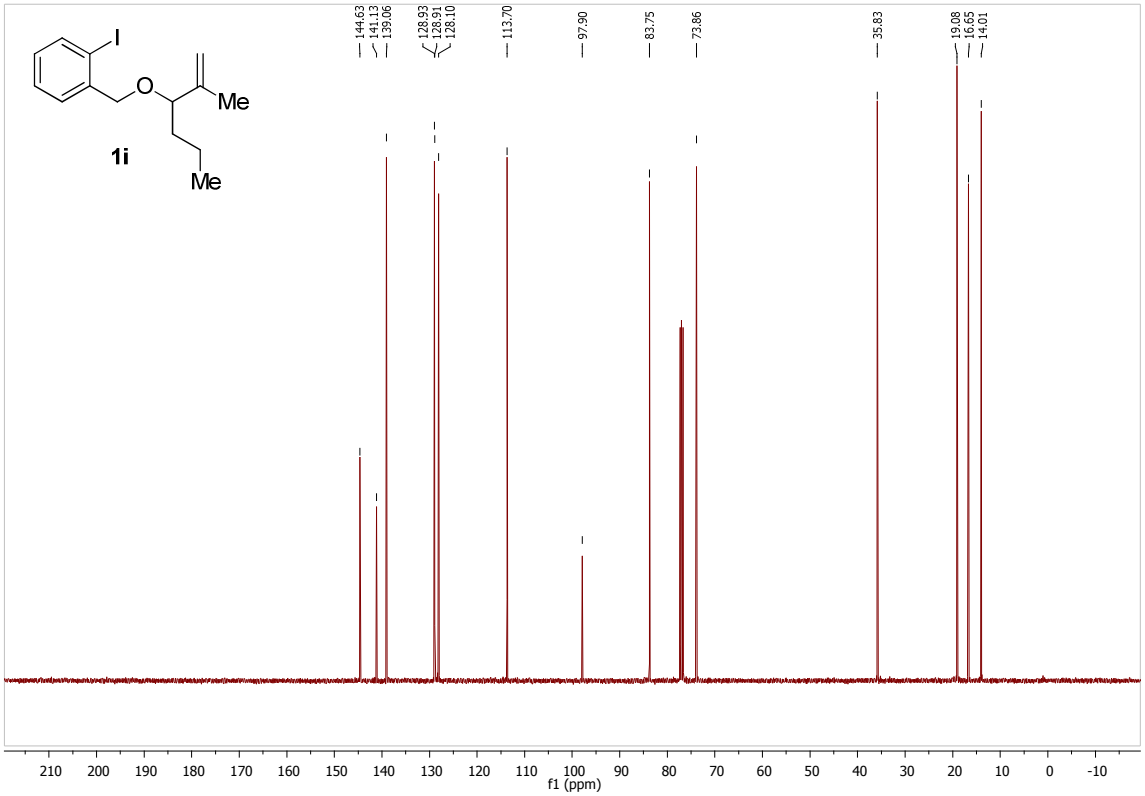

I
O
Me
1g
1.00
1.00
1.03
1.02
1.01
1.01
2.04
1.01
1.03
6.30
2.21
3.49
2.37
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

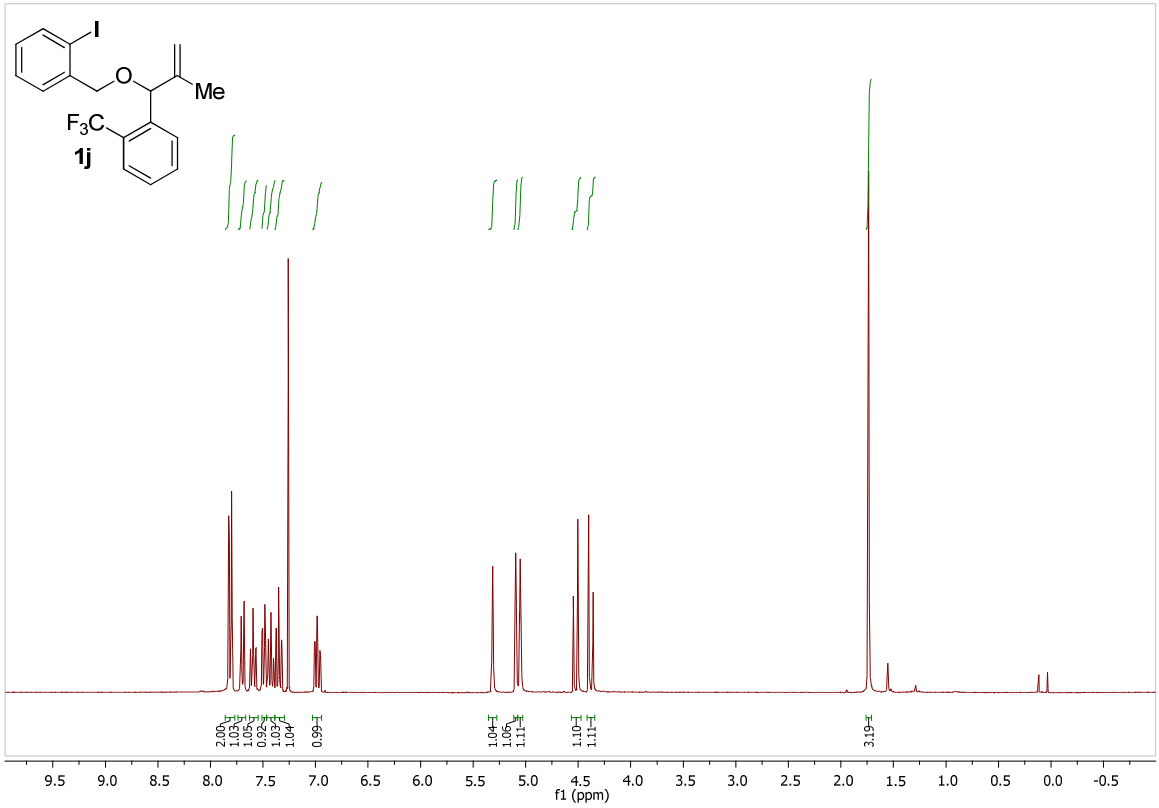

143.26
141.22
139.02
129.08
128.87
128.05
115.19
98.02
89.04
73.93
39.49
30.07
29.44
26.61
26.13
25.95
16.75
I
O
Me
1g
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

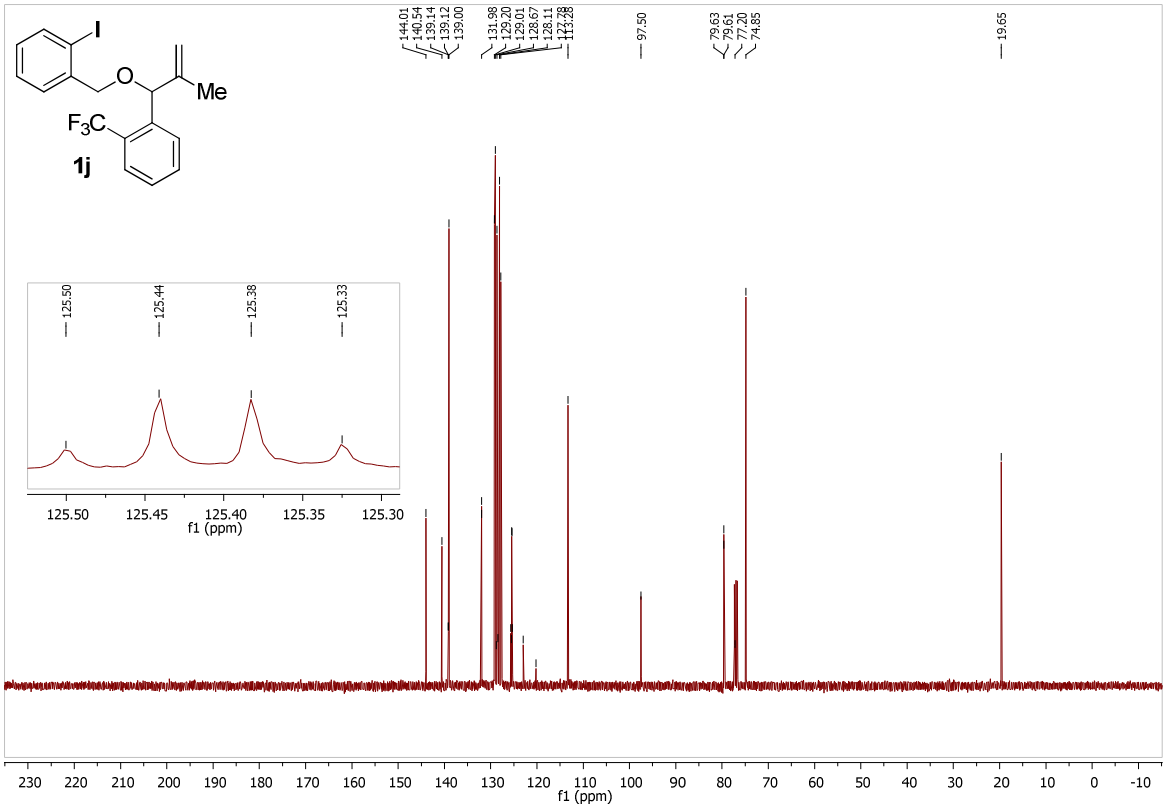

I
O
Me
1h
1.00
0.94
0.94
0.97
0.92
0.93
0.98
1.01
0.97
2.77
1.03
1.06
1.89
1.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

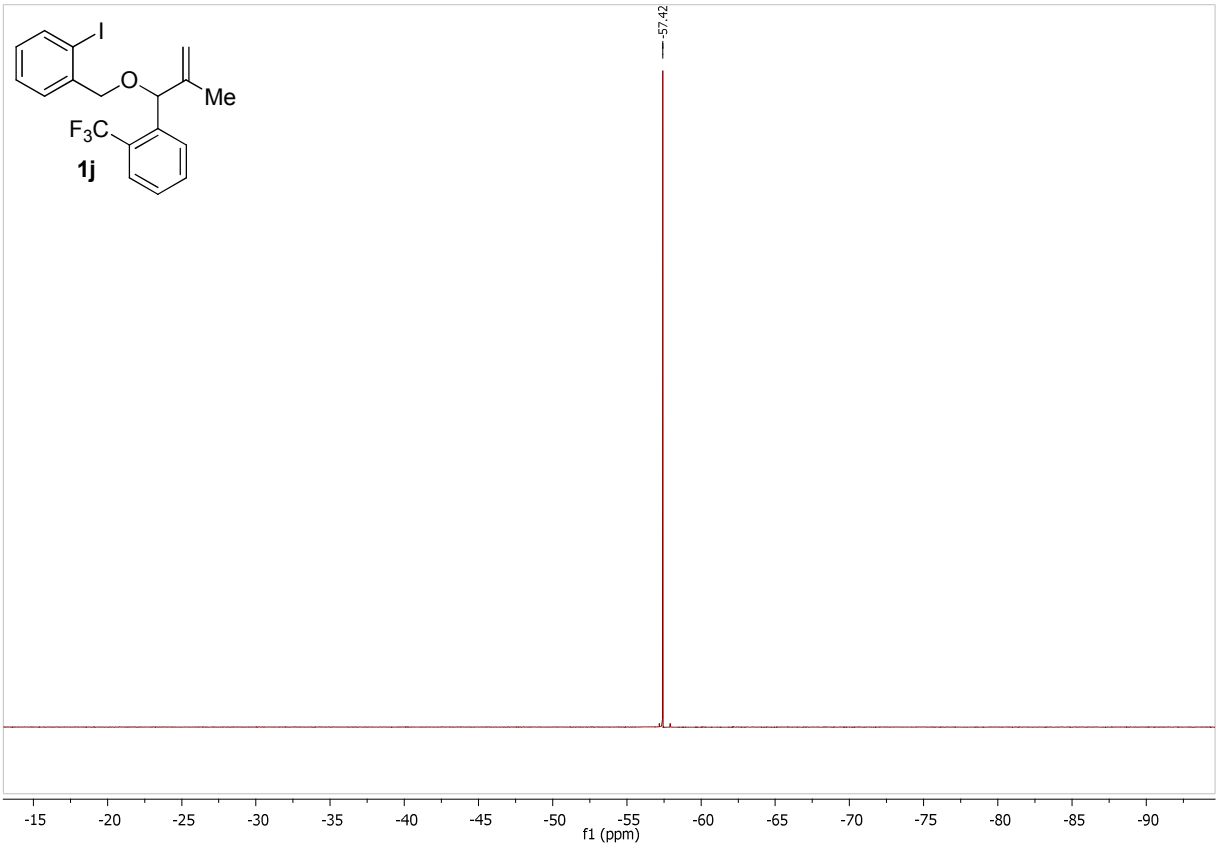

I
O
Me
1h
144.84
141.01
139.03
128.91
128.87
128.08
113.15
97.85
87.85
77.20
73.79
17.50
14.46
4.52
2.11
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

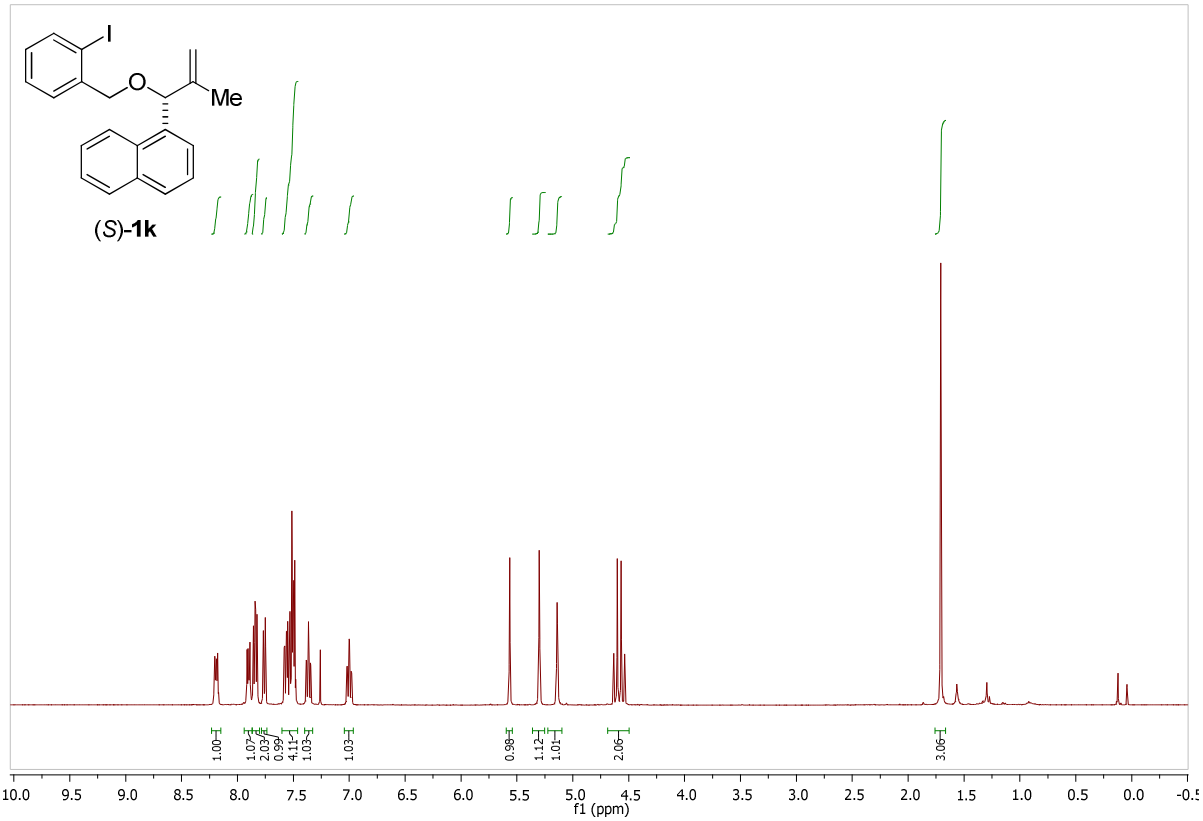

I
O
Me
1i
Me
1.00
1.01
1.02
1.01
1.01
0.99
1.03
1.00
0.99
4.09
3.44
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

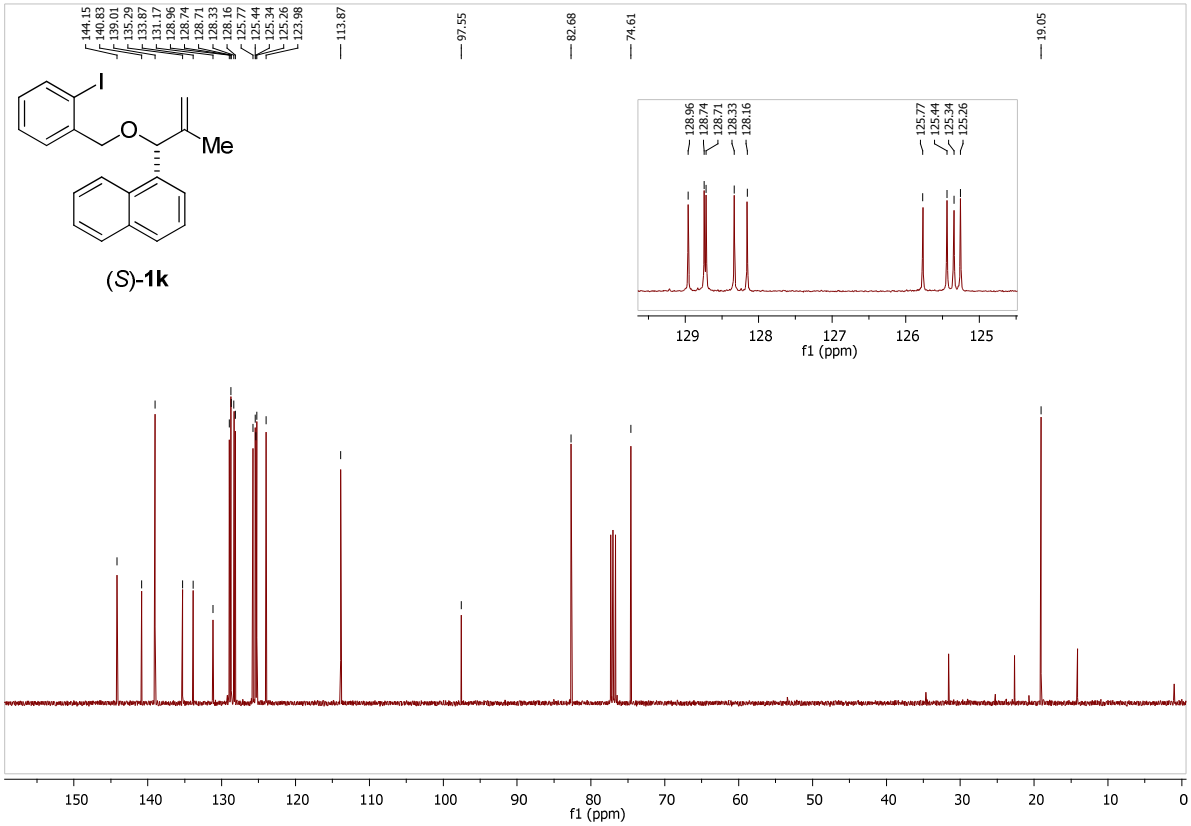

I
O
Me
1i
Me
144.63
141.13
139.06
128.93
128.91
128.10
113.70
97.90
83.75
73.86
35.83
19.08
16.65
14.01
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

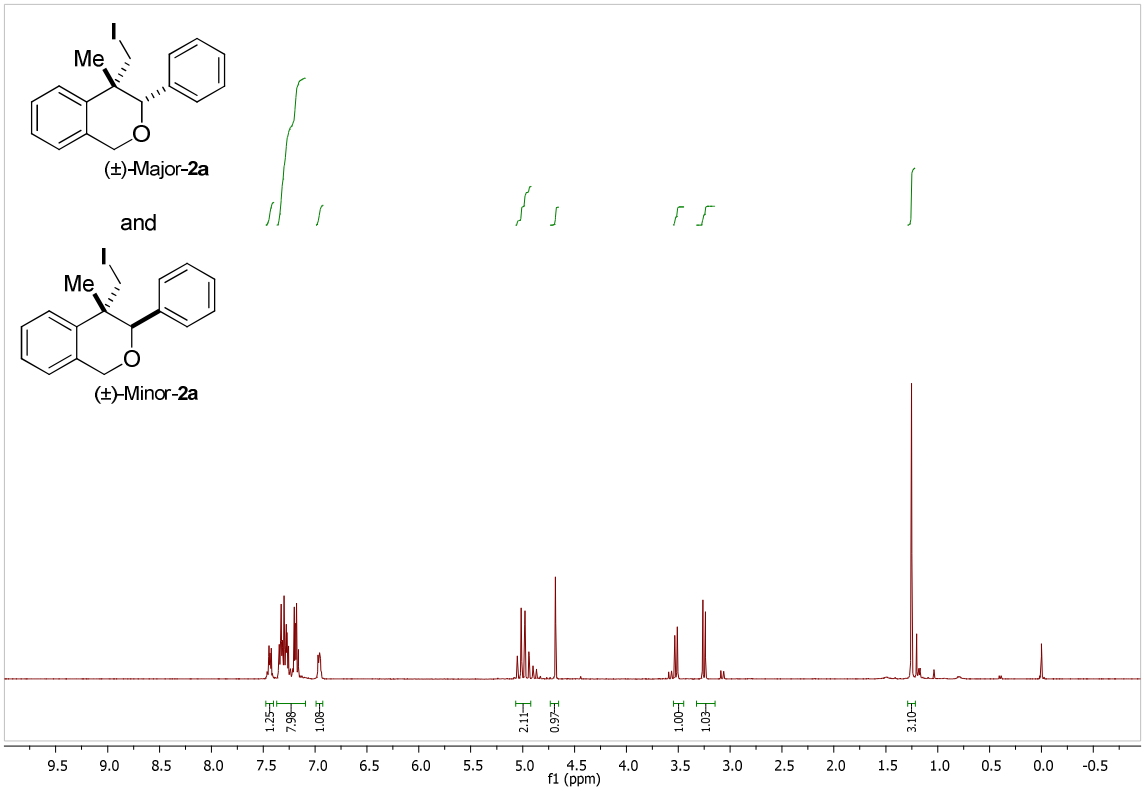

I
O
Me
F3C
1j
2.00
1.03
1.05
0.92
1.03
1.04
0.99
1.04
1.06
1.11
1.10
1.11
3.19
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

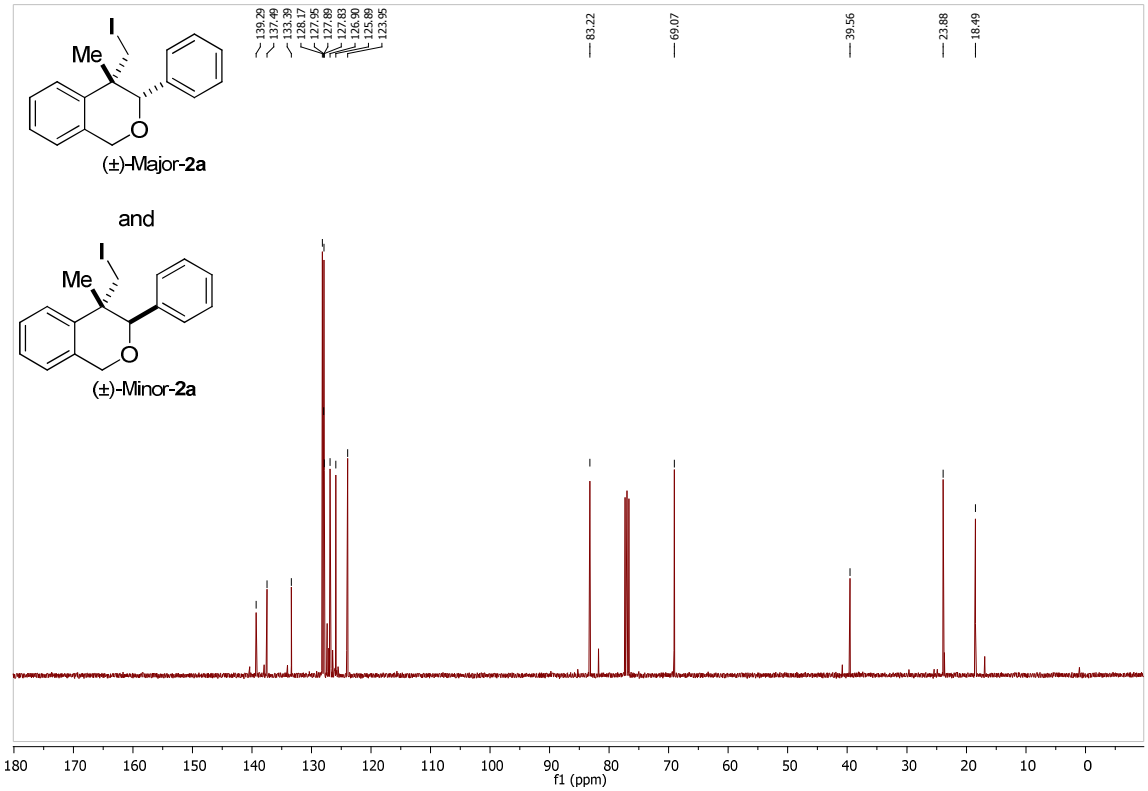

I
O
Me
F3C
1j
144.01
140.54
139.14
139.12
139.00
131.98
129.20
129.01
128.67
128.11
127.28
113.28
97.50
79.63
79.61
77.20
74.85
19.65
125.50
125.44
125.38
125.33
125.50 125.45 125.40 125.35 125.30
f1 (ppm)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

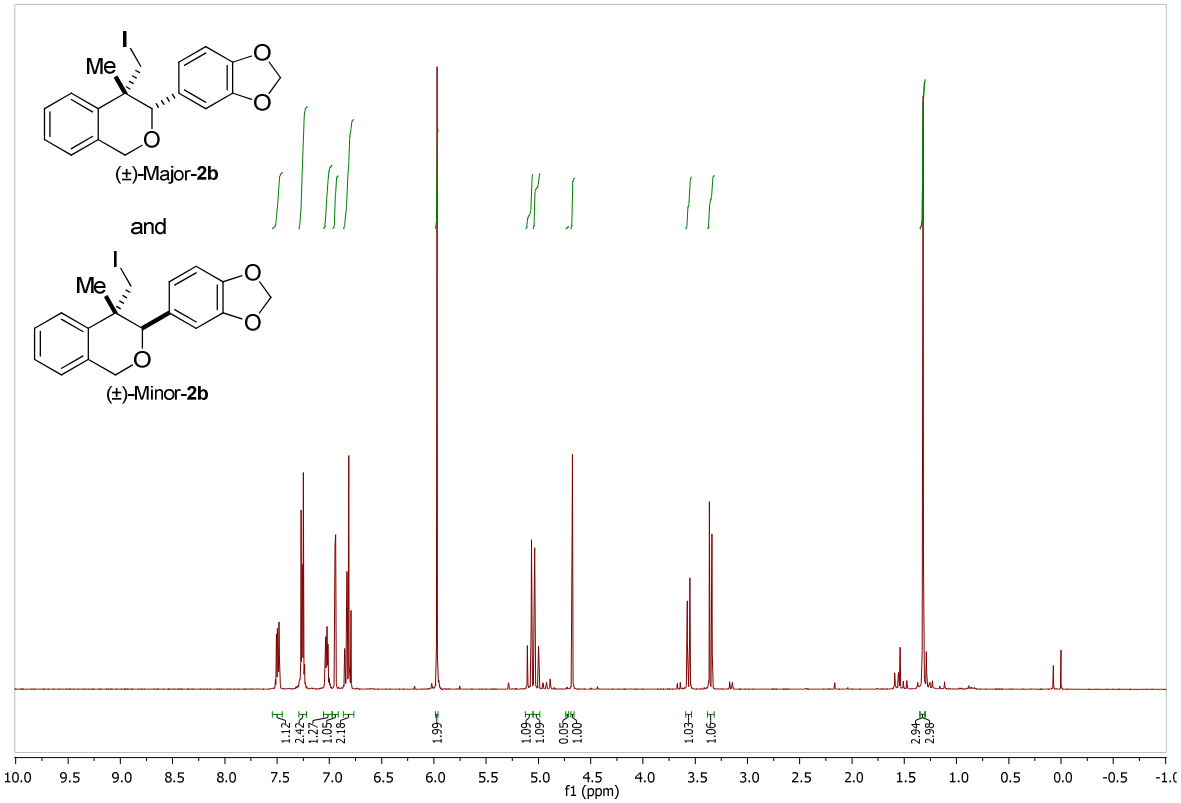

I
O
Me
F3C
1j
-57.42
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
f1 (ppm)

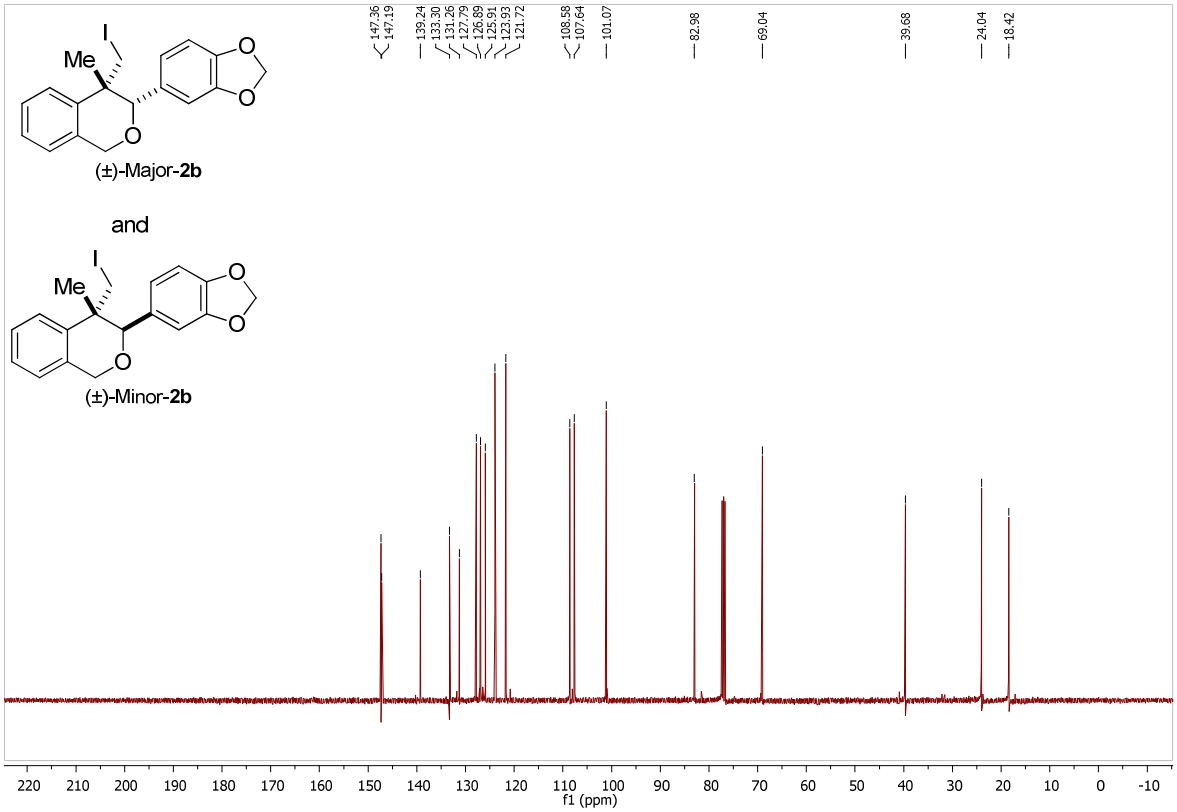

I
O
Me
(S)-1k
1.00
1.07
2.03
0.99
4.11
1.03
1.03
0.98
1.12
1.01
2.06
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

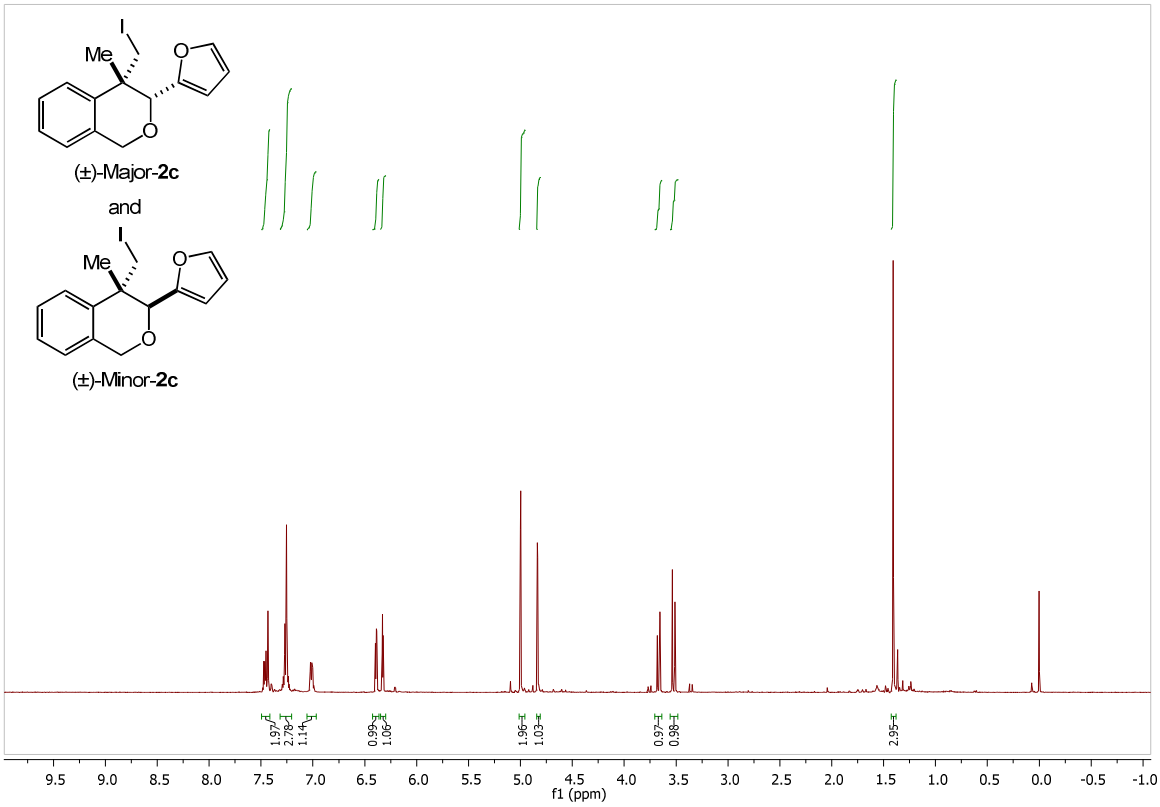

144.15
140.83
139.01
135.29
133.87
131.17
128.96
128.74
128.71
128.33
128.16
125.77
125.44
125.34
125.26
123.98
113.87
97.55
82.68
74.61
19.05
I
O
Me
(S)-1k
128.96
128.74
128.71
128.33
128.16
125.77
125.44
125.34
125.26
129 128 127 126 125
f1 (ppm)
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

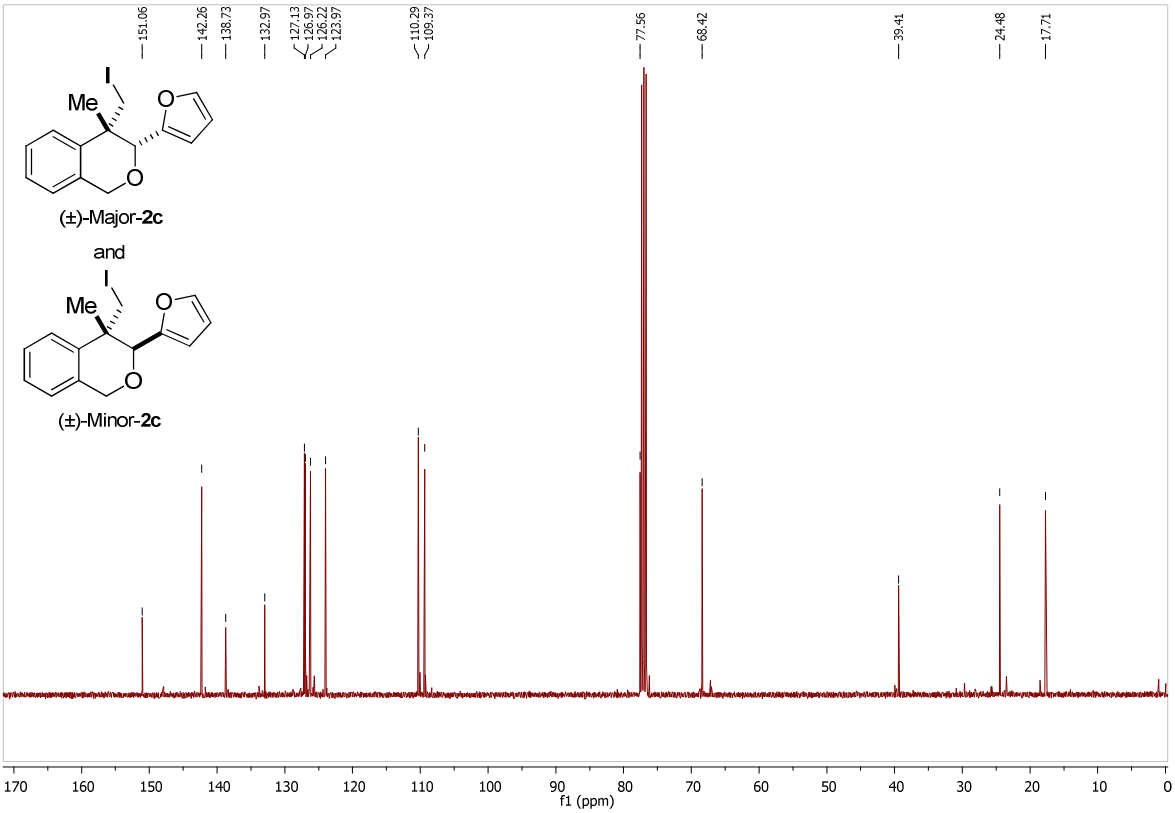

Me
I
O
(±)-Major-2a
and
Me
I
O
(±)-Minor-2a
1.25
7.98
1.09
2.11
0.97
1.00
1.03
3.10
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

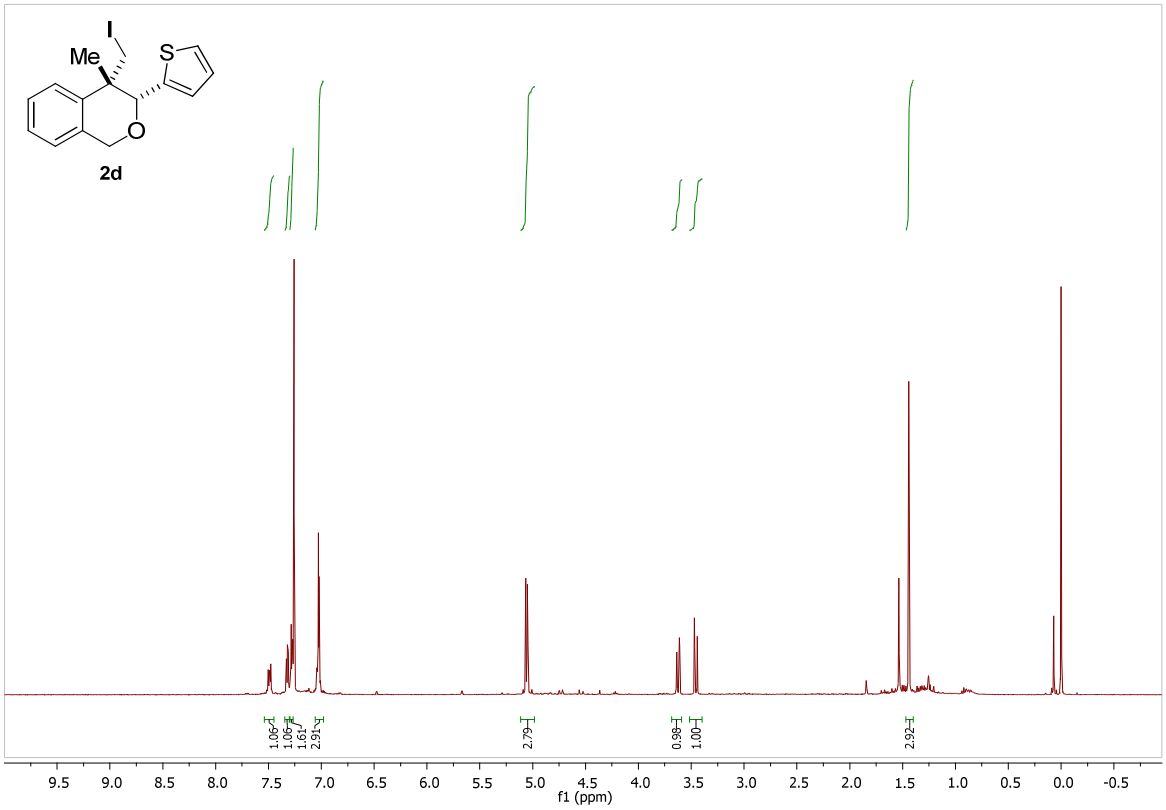

Me
I
O
(±)-Major-2a
and
Me
I
O
(±)-Minor-2a
139.29
137.49
133.39
128.17
127.95
127.89
127.83
126.90
125.89
123.95
83.22
69.07
39.56
23.88
18.49
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

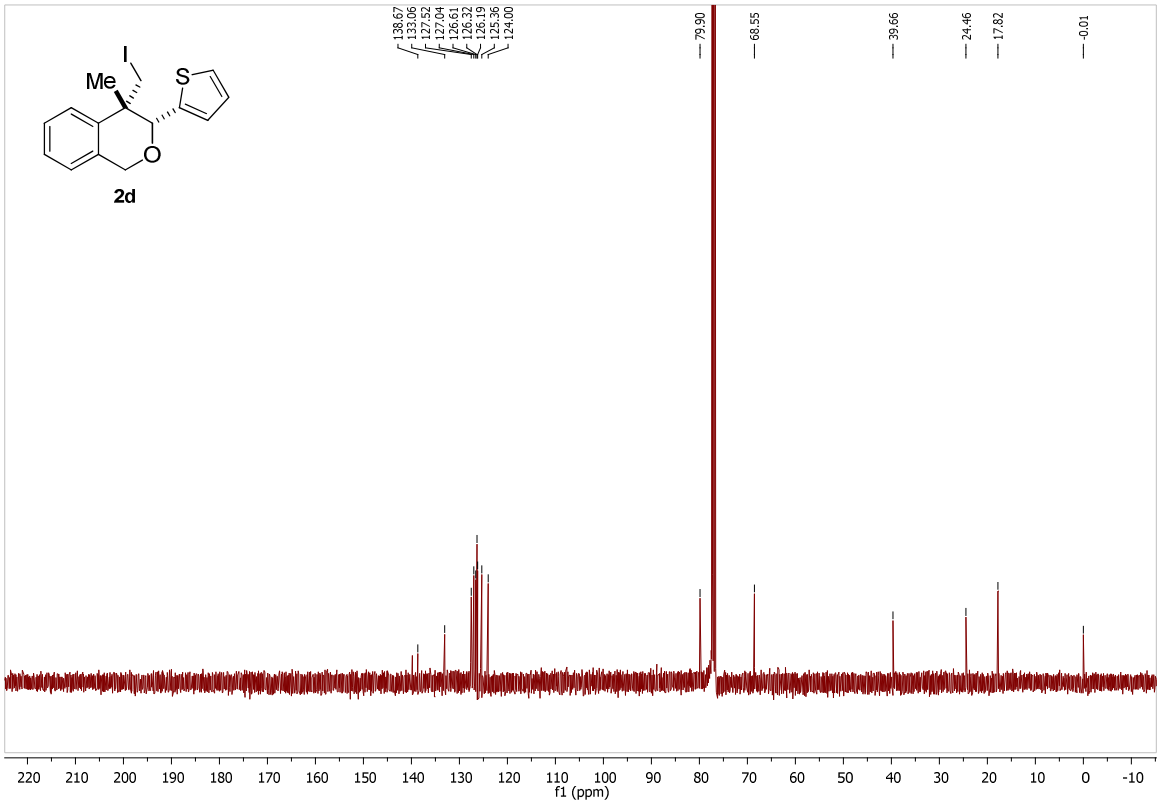

(±)-Major-2b
and
(±)-Minor-2b
1.12
2.42
1.27
1.05
2.18
1.99
1.09
1.09
0.05
1.00
1.03
1.06
2.94
2.98
f1 (ppm)

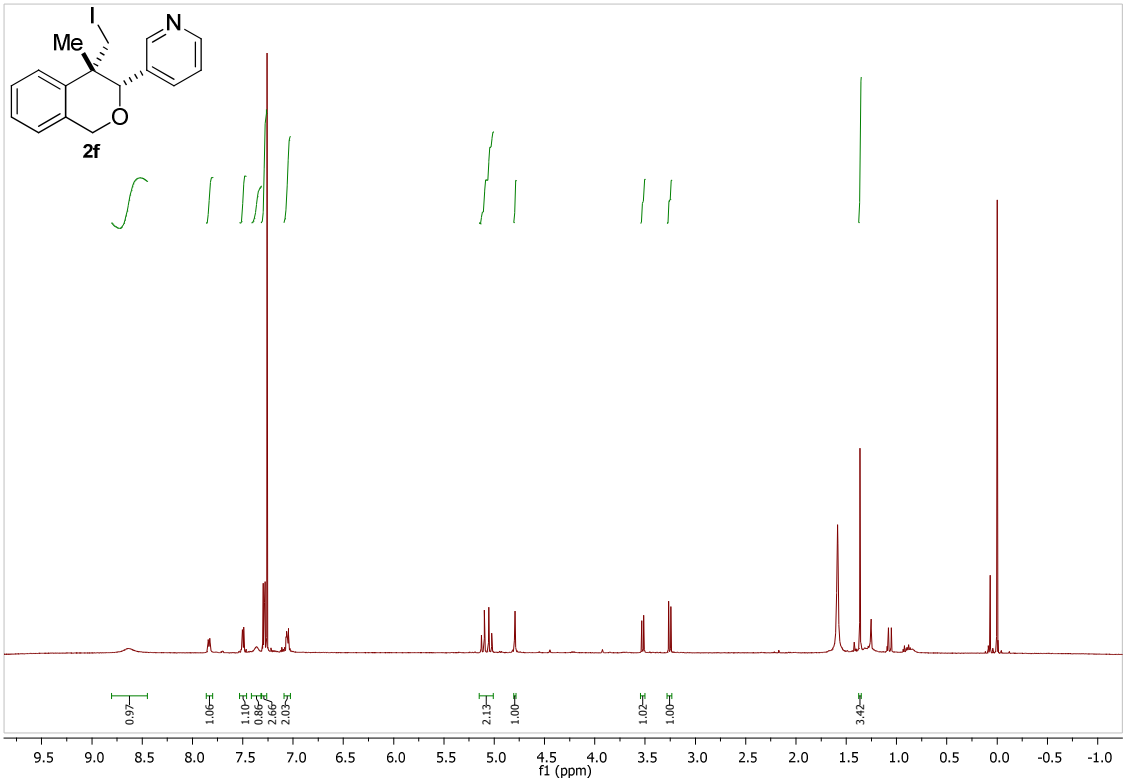

(±)-Major-2b
and
(±)-Minor-2b
147.36
147.19
139.24
133.30
131.26
127.79
126.89
125.91
123.93
121.72
108.58
107.64
101.07
82.98
69.04
39.68
24.04
18.42
f1 (ppm)

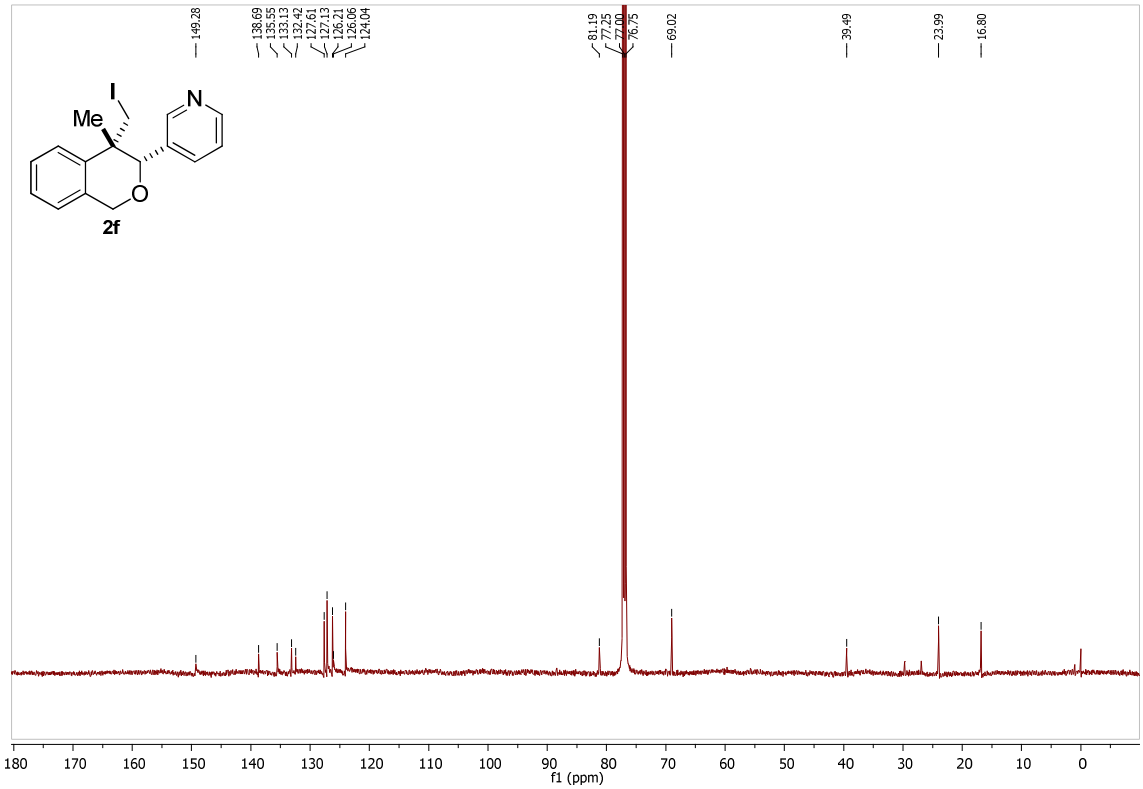

(±)-Major-2c
and
(±)-Minor-2c
1.97
2.78
1.14
0.99
1.06
1.96
1.03
0.97
0.98
2.95
f1 (ppm)

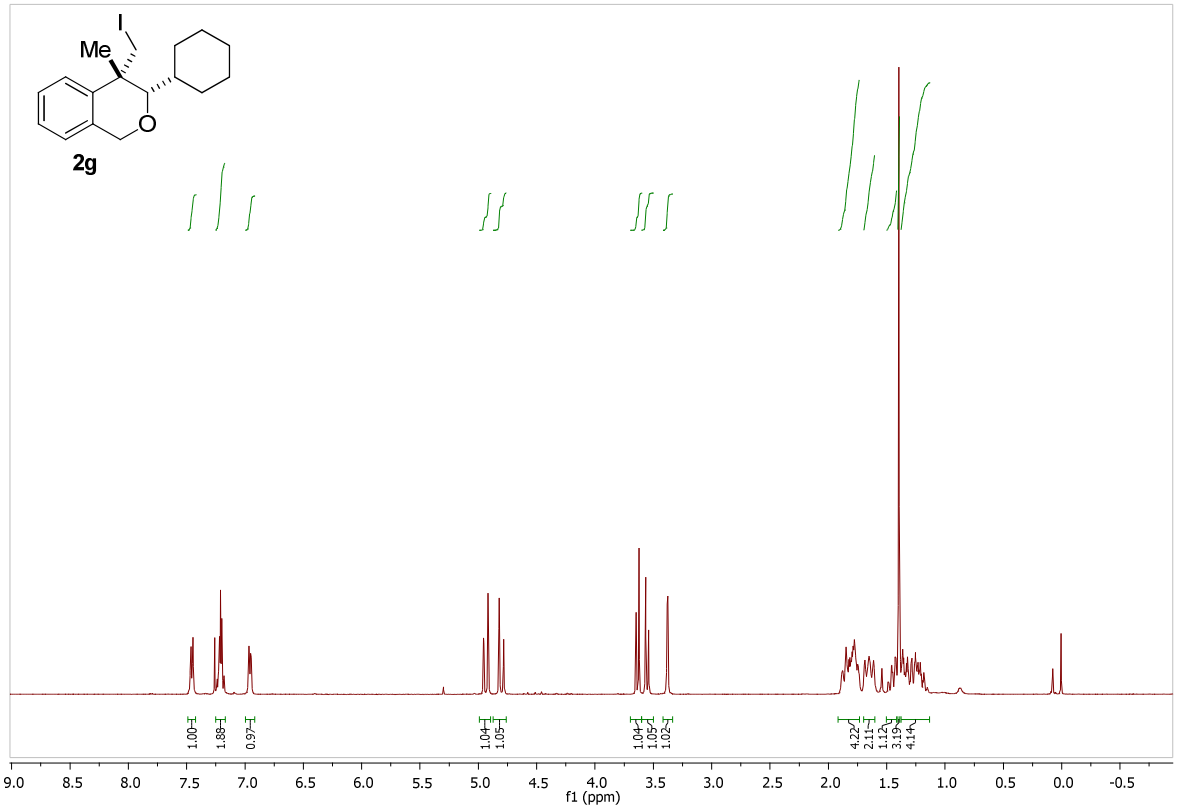

151.06
142.26
138.73
132.97
127.13
126.97
126.22
123.97
110.29
109.37
77.56
68.42
39.41
24.48
17.71
(±)-Major-2c
and
(±)-Minor-2c
f1 (ppm)

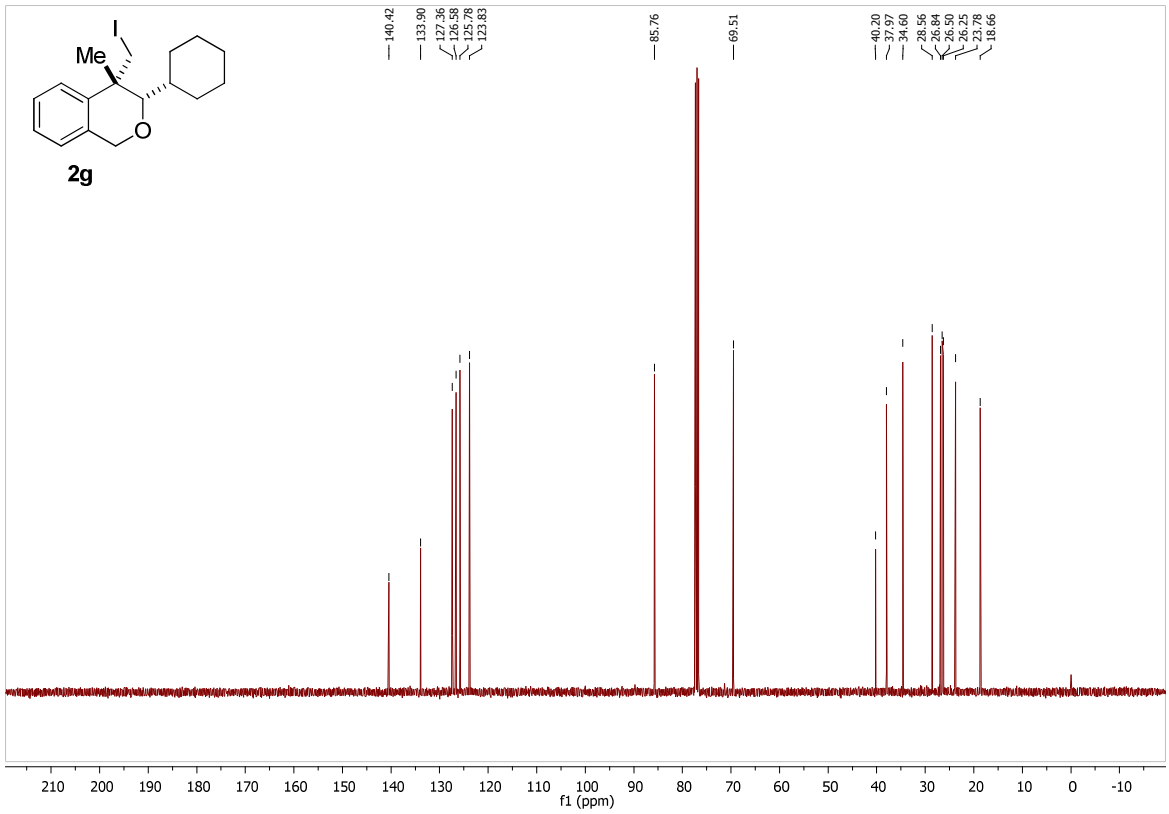

I
Me
S
O
2d
1.06
1.06
1.61
2.91
2.79
0.98
1.00
2.92
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

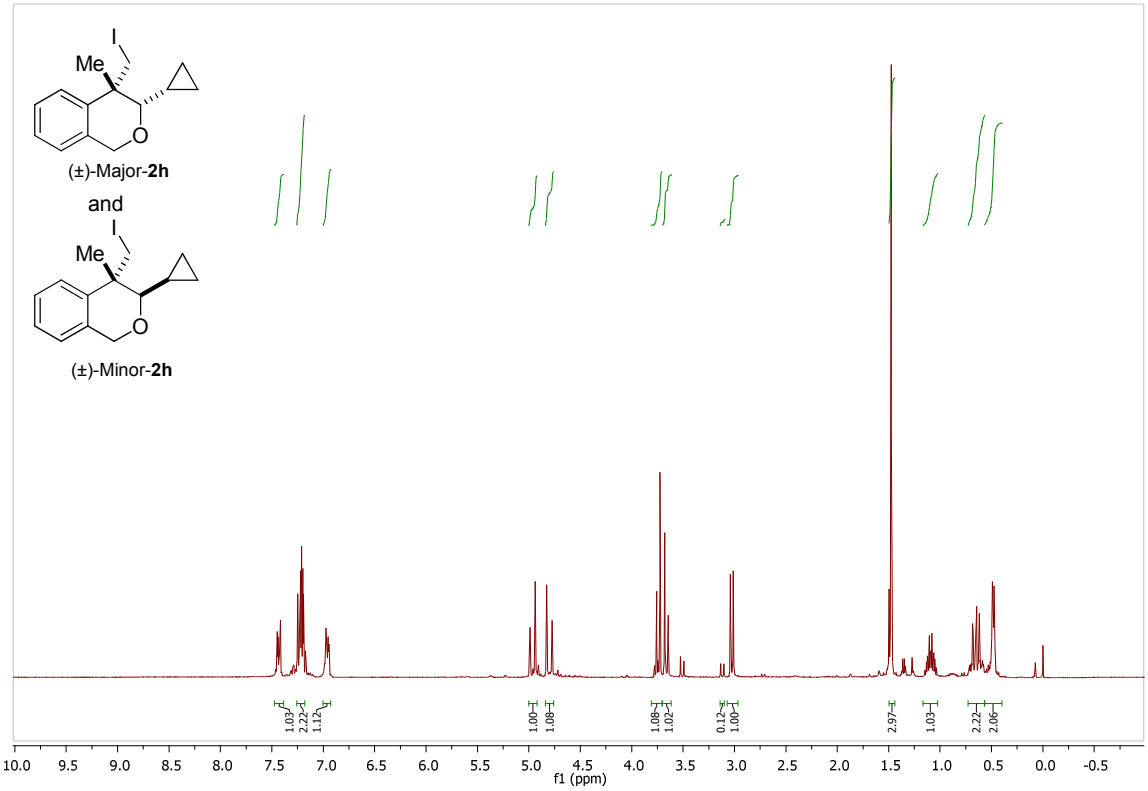

I
Me
S
O
2d
138.67
133.06
127.52
127.04
126.61
126.32
126.19
125.36
124.00
79.90
68.55
39.66
24.46
17.82
-0.01
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

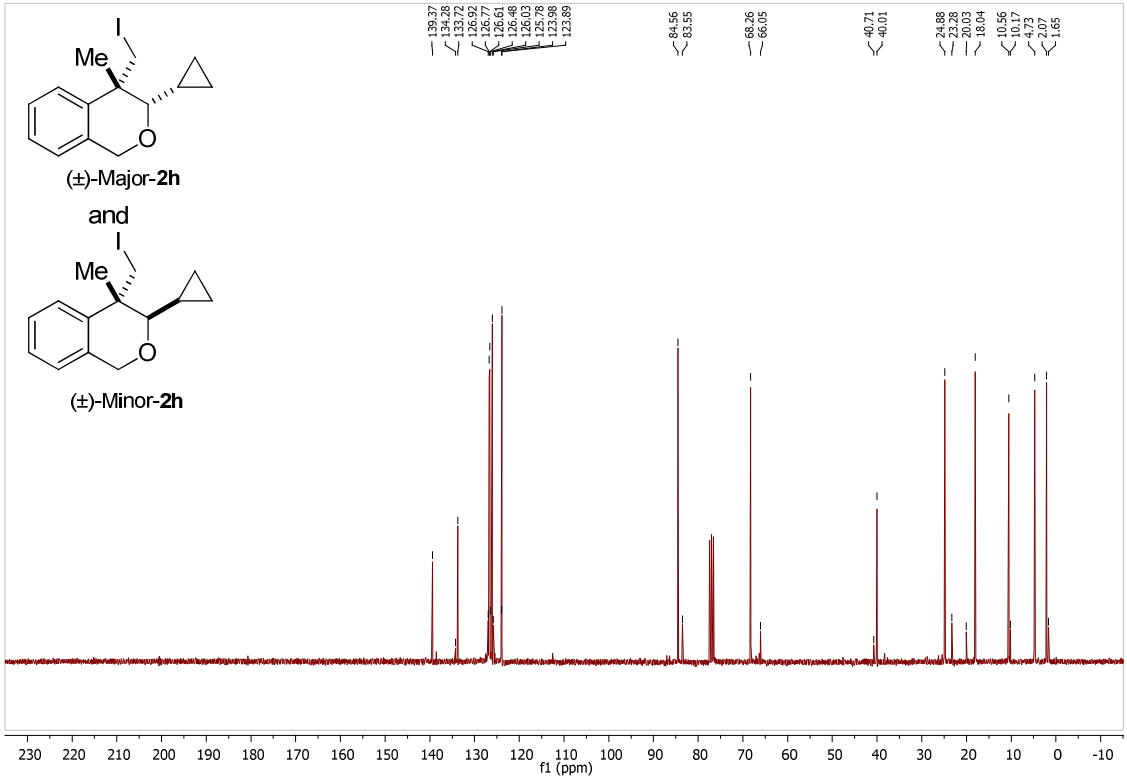

I
Me
N
O
2f
0.97
1.06
1.10
0.86
2.66
2.03
2.13
1.00
1.02
1.00
3.42
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

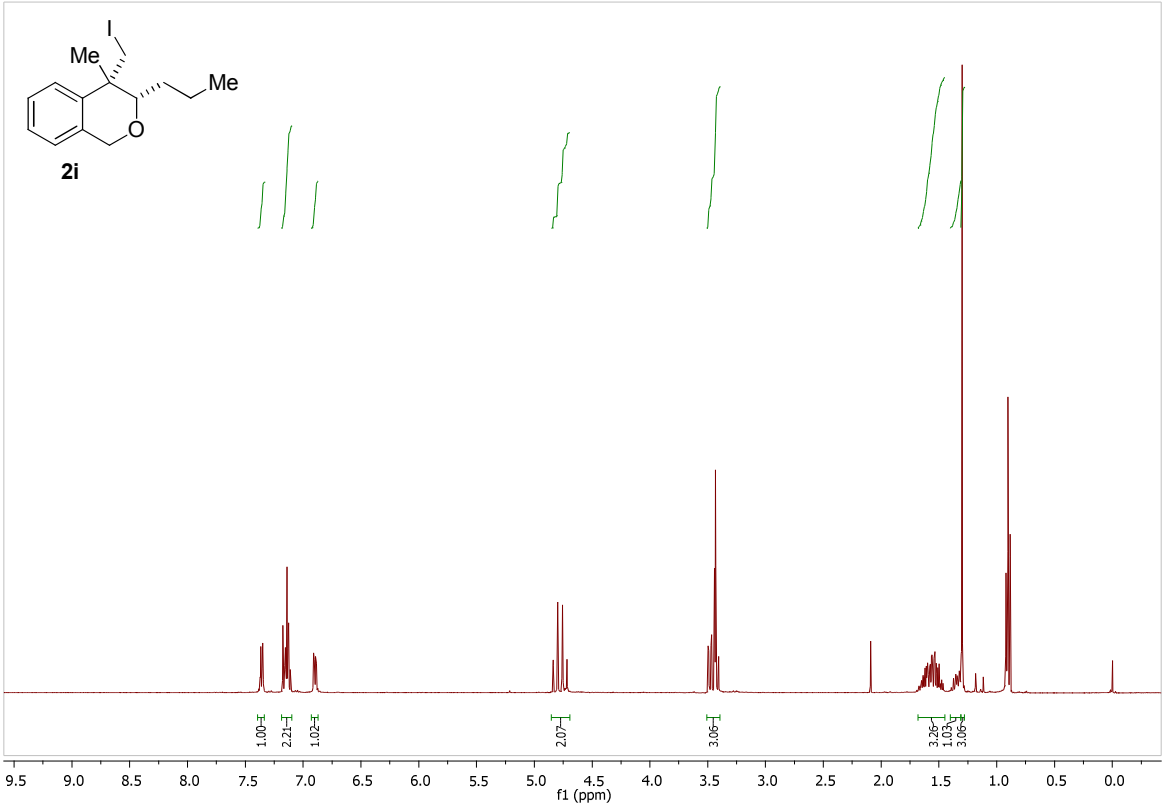

149.28
138.69
135.55
133.13
132.42
127.61
127.13
126.21
126.06
124.04
81.19
77.25
77.00
76.75
69.02
39.49
23.99
16.80
I
Me
N
O
2f
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

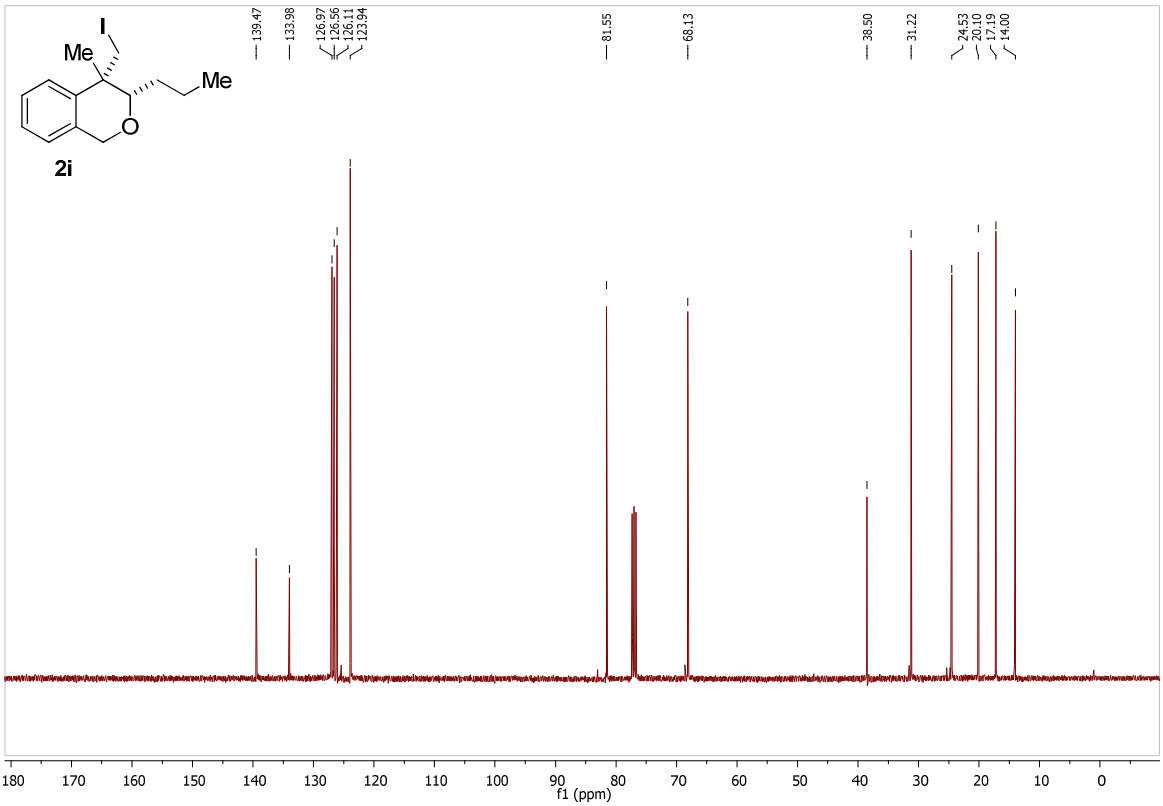

I
Me
O
2g
1.00
1.89
0.97
1.04
1.05
1.04
1.05
1.02
4.22
2.11
1.12
3.19
4.14
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

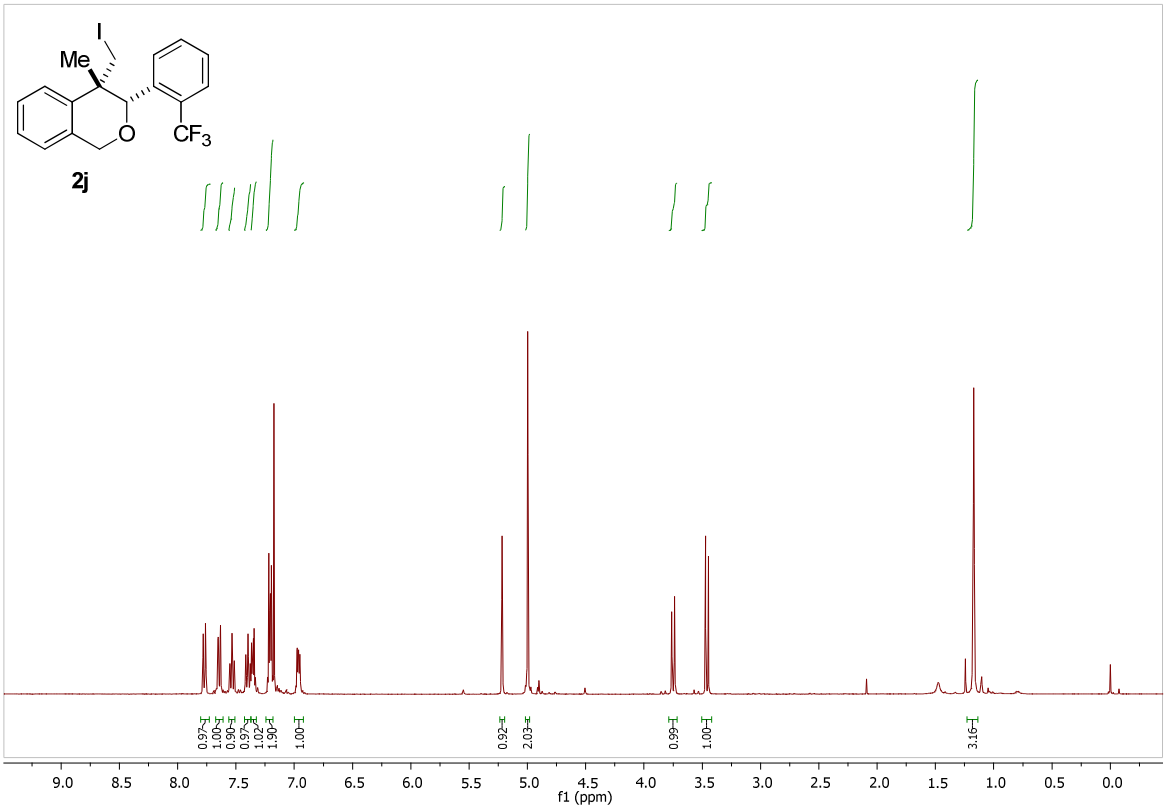

I
Me
O
2g
140.42
133.90
127.36
126.58
125.78
123.83
85.76
69.51
40.20
37.97
34.60
28.56
26.84
26.50
26.25
23.78
18.66
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

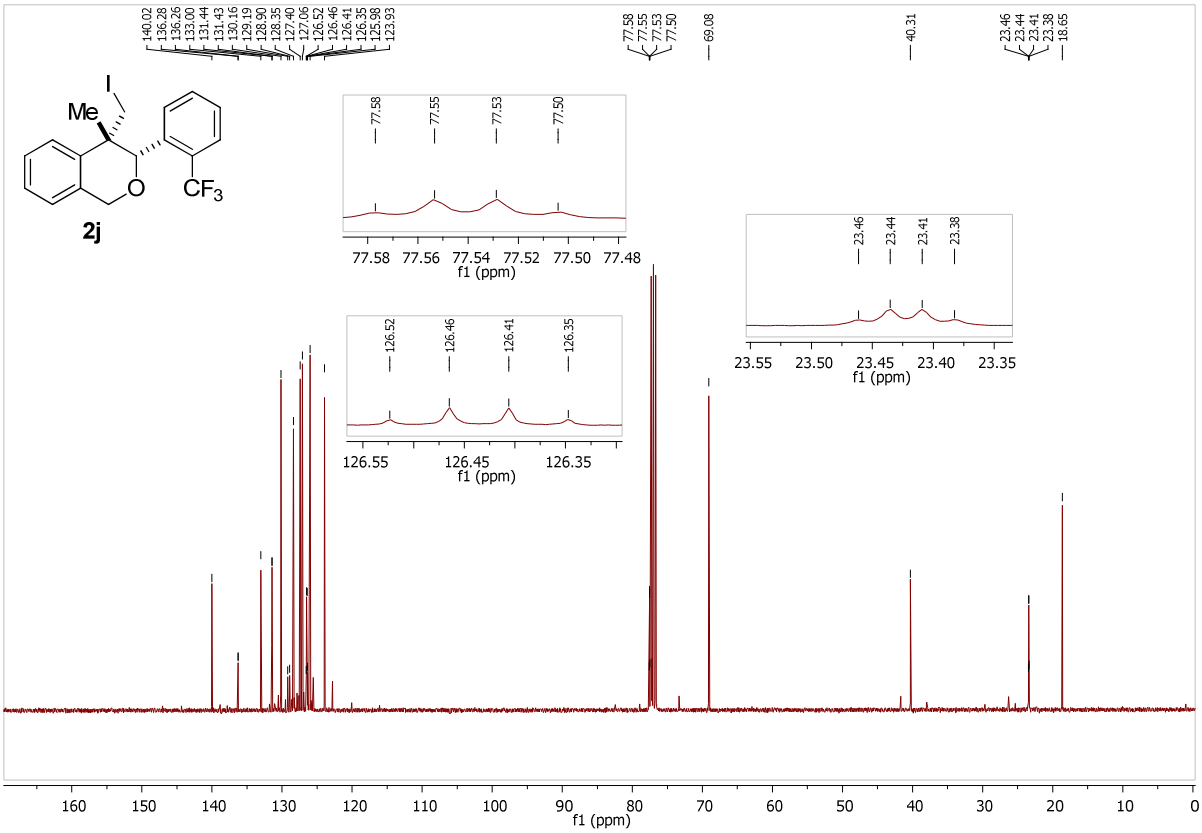

(±)-Major-2h
and
(±)-Minor-2h
1.03
2.22
1.12
1.00
1.08
1.08
1.02
0.12
1.00
2.97
1.03
2.22
2.06
f1 (ppm)

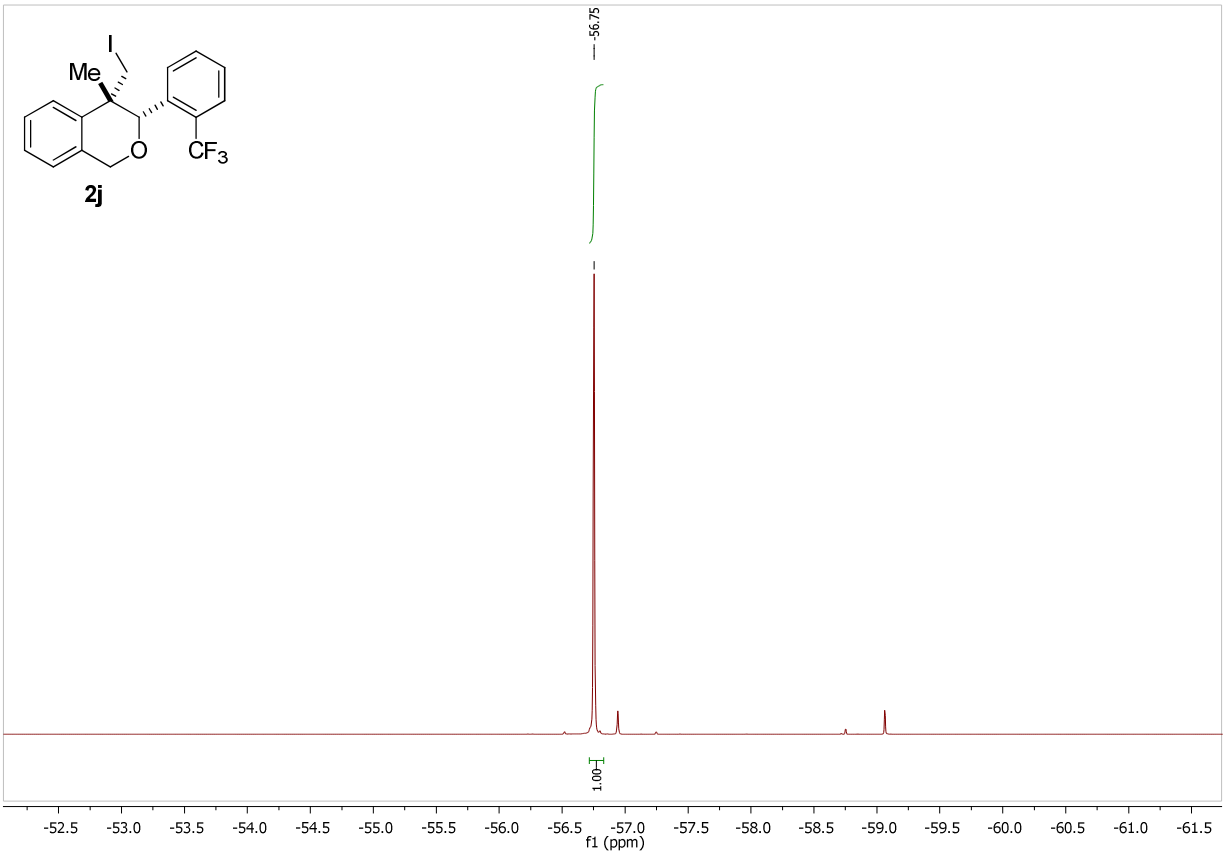

(±)-Major-2h
and
(±)-Minor-2h
139.37
134.28
133.72
126.92
126.77
126.61
126.48
126.03
125.78
123.98
123.89
84.56
83.55
68.26
66.05
40.71
40.01
24.88
23.28
20.03
18.04
10.56
10.17
4.73
2.07
1.65
f1 (ppm)

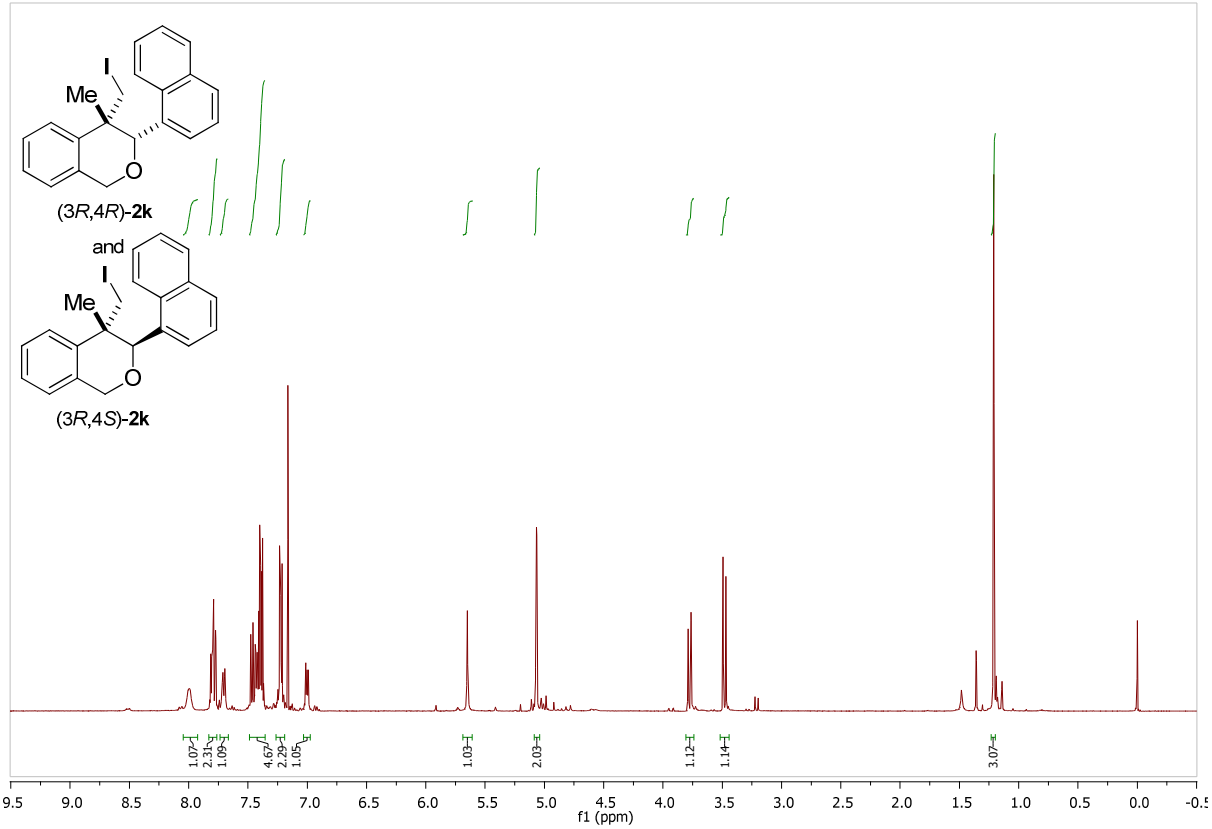

I
Me
Me
O
2i
1.00
2.21
1.02
2.07
3.06
3.26
1.03
3.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

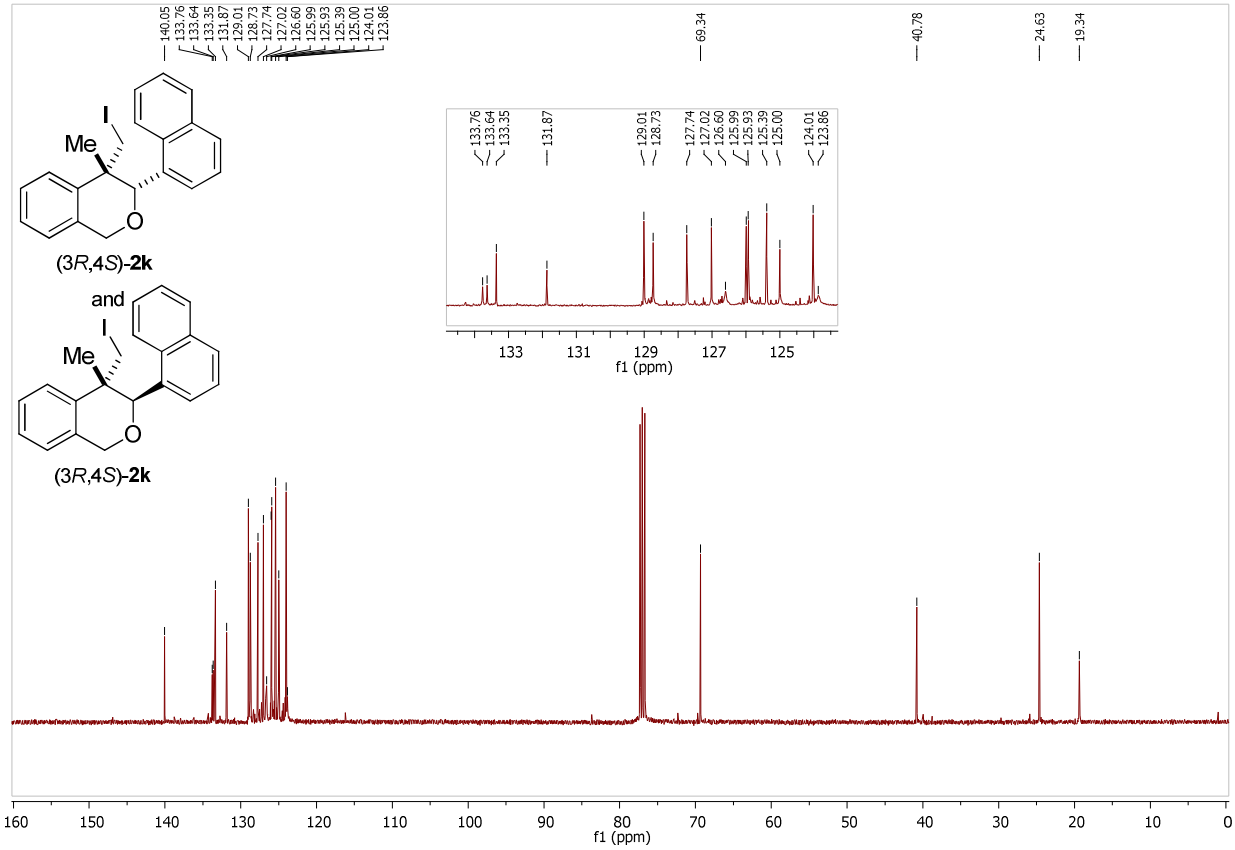

I
Me
Me
O
2i
139.47
133.98
126.97
126.56
126.11
123.94
81.55
68.13
38.50
31.22
24.53
20.10
17.19
14.00
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

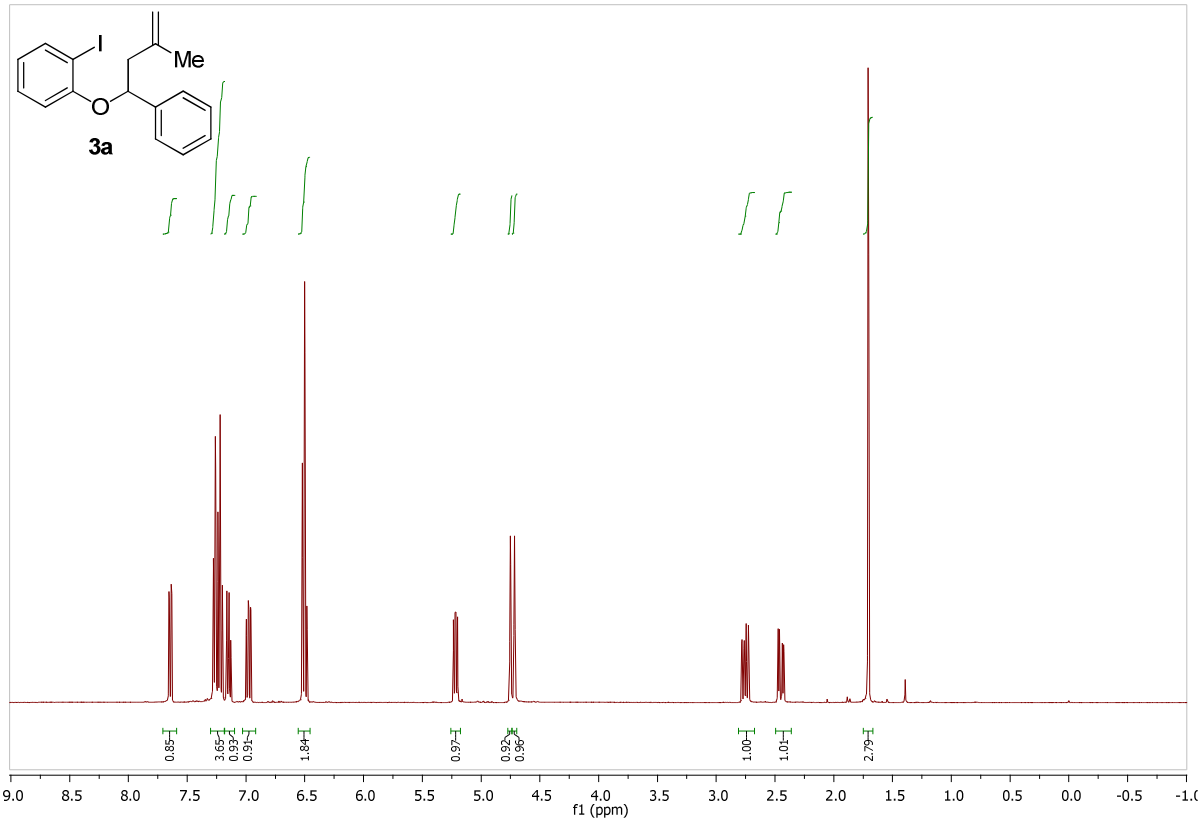

I
Me
O
CF3
2j
0.97
1.00
0.90
0.97
1.02
1.90
1.00
0.92
2.03
0.99
1.00
3.16
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

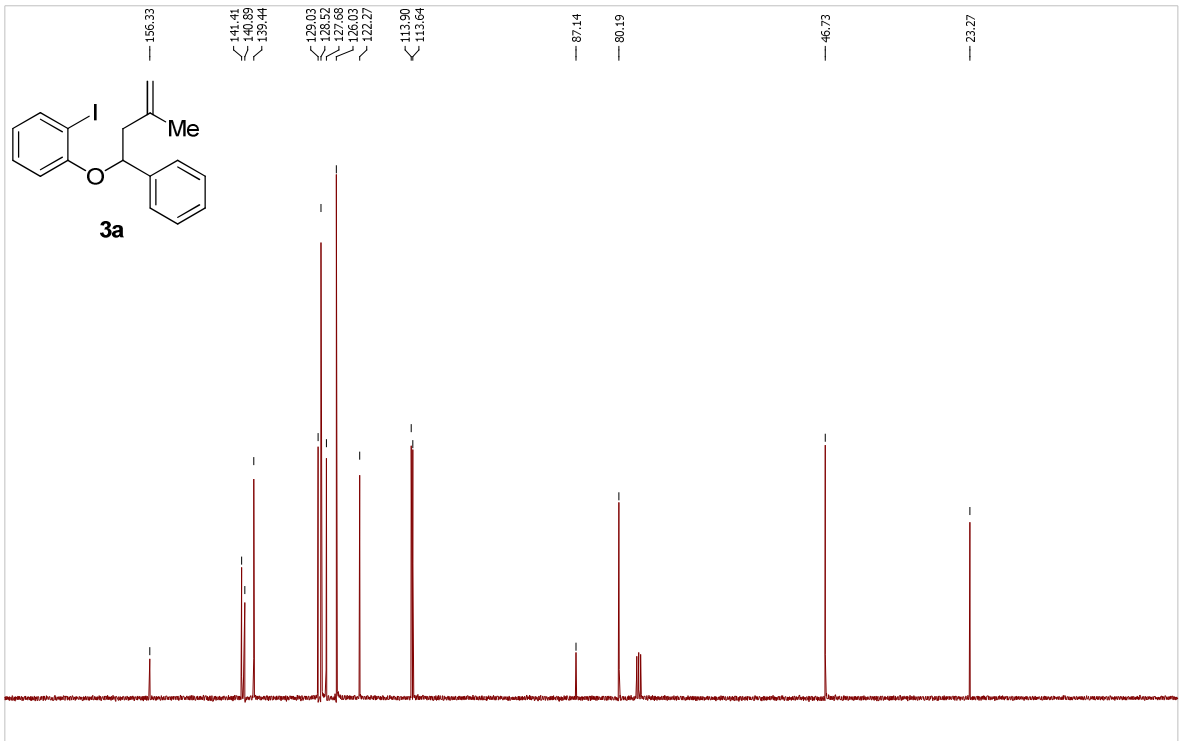

140.02
136.28
136.26
133.00
131.44
131.43
130.16
129.19
128.90
128.35
127.40
127.06
126.52
126.46
126.41
126.35
125.98
123.93
77.58
77.55
77.53
77.50
69.08
40.31
23.46
23.44
23.41
23.38
18.65
I
Me
O
CF3
2j
77.58 77.56 77.54 77.52 77.50 77.48
f1 (ppm)
126.52
126.46
126.41
126.35
126.55 126.45 126.35
f1 (ppm)
23.46
23.44
23.41
23.38
23.55 23.50 23.45 23.40 23.35
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

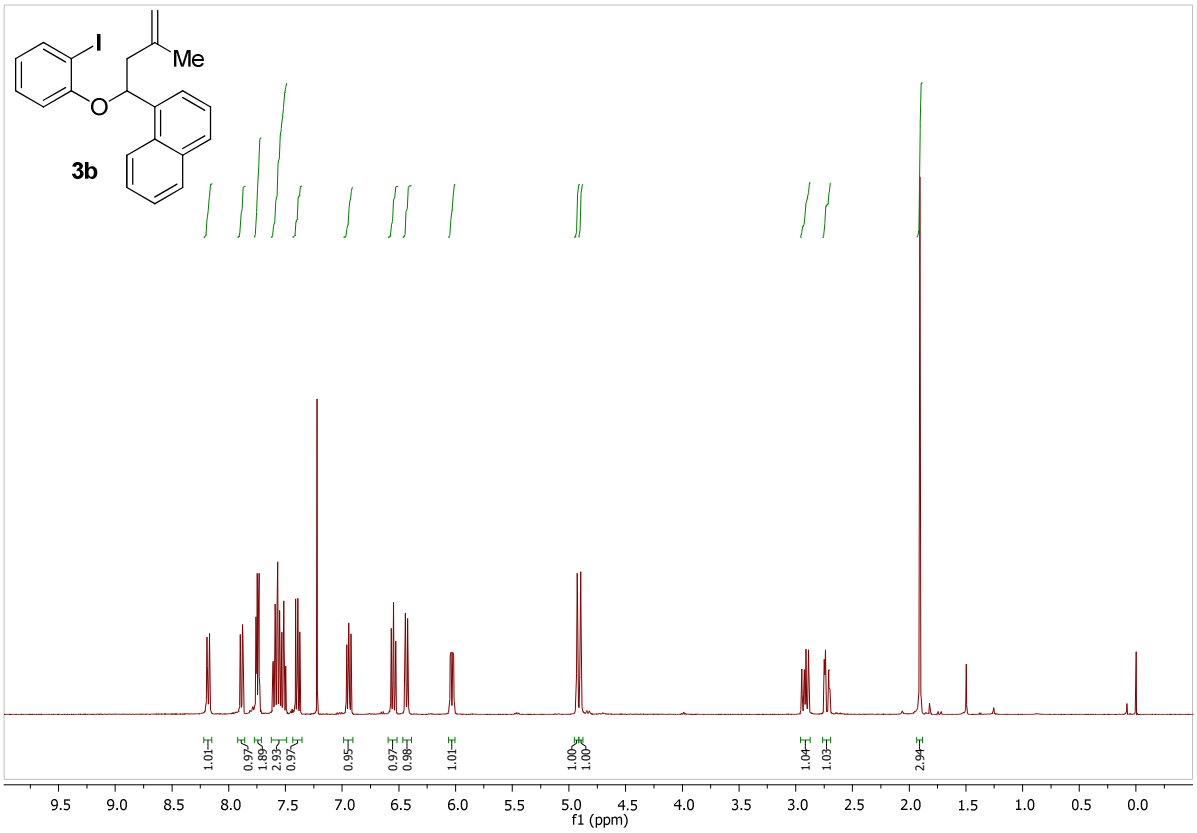

I
Me
O
CF3
2j
-56.75
1.00
-52.5
-53.0
-53.5
-54.0
-54.5
-55.0
-55.5
-56.0
-56.5
-57.0
-57.5
-58.0
-58.5
-59.0
-59.5
-60.0
-60.5
-61.0
-61.5
f1 (ppm)

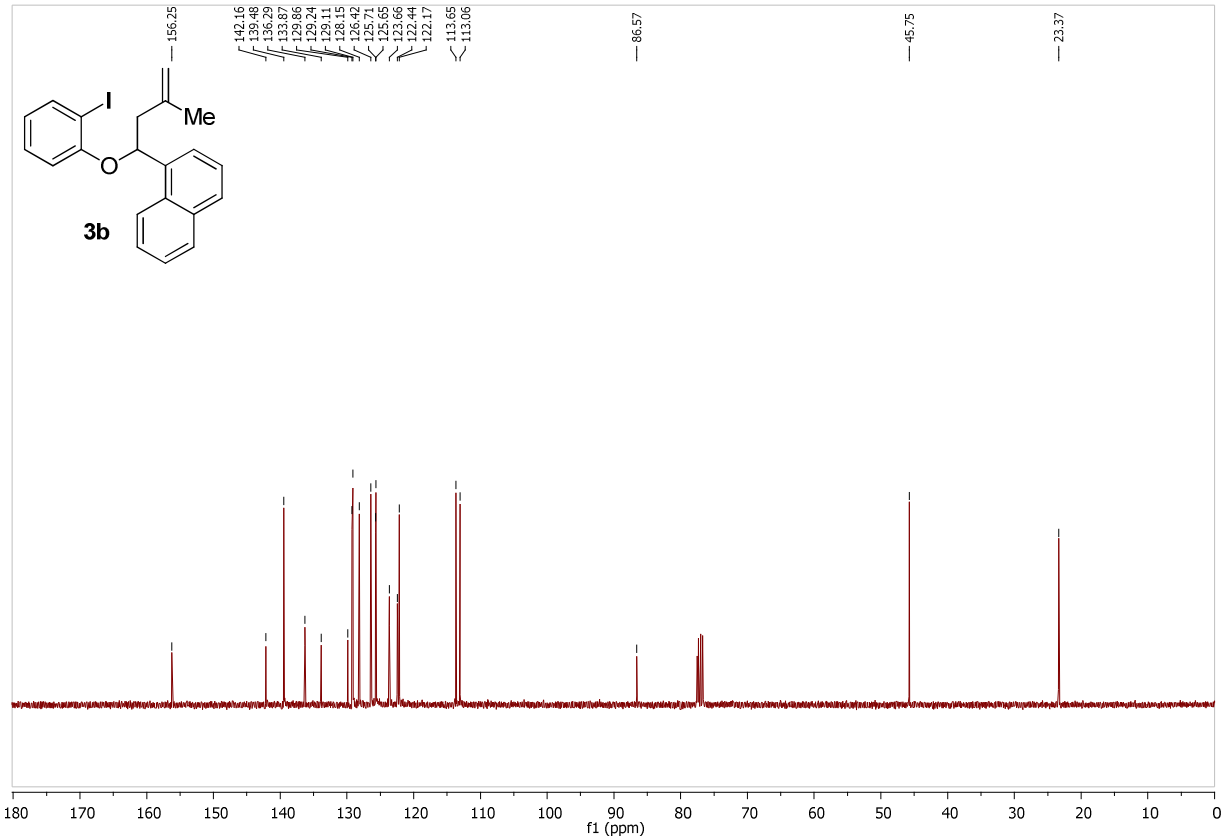

I
Me
O
(3R,4R)-2k
and
I
Me
O
(3R,4S)-2k
1.07
2.31
1.09
4.67
2.29
1.05
1.03
2.03
1.12
1.14
3.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


140.05
133.76
133.64
133.35
131.87
129.01
128.73
127.74
127.02
126.60
125.99
125.93
125.39
125.00
124.01
123.86
69.34
40.78
24.63
19.34
I
Me
O
(3R,4S)-2k
and
I
Me
O
(3R,4S)-2k
133 131 129 127 125
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


I
Me
O
3a
0.85
3.65
0.93
0.91
1.84
0.97
0.92
0.96
1.00
1.01
2.79
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)


156.33
141.41
140.89
139.44
129.03
128.52
127.68
126.03
122.27
113.90
113.64
87.14
80.19
46.73
23.27
I
Me
O
3a


I
Me
O
3b
1.01
0.97
1.89
2.93
0.97
0.95
0.97
0.98
1.01
1.00
1.00
1.04
1.03
2.94
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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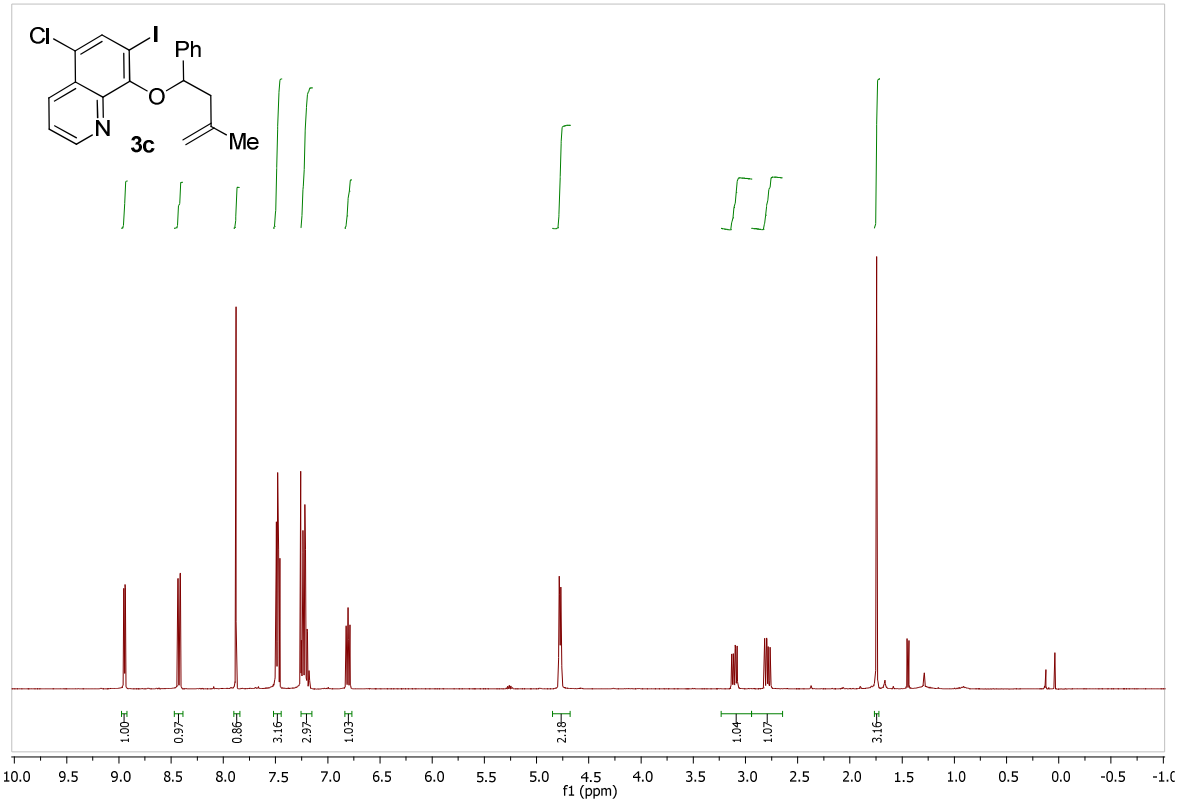
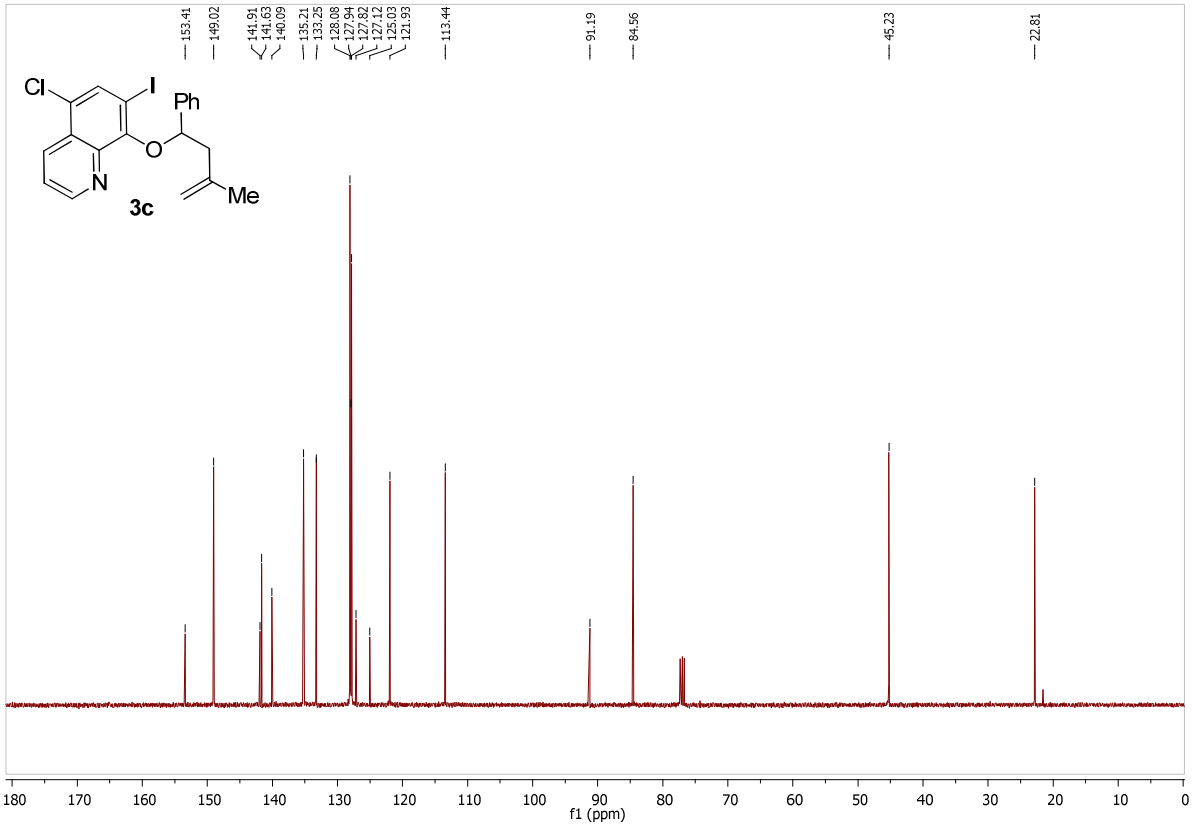
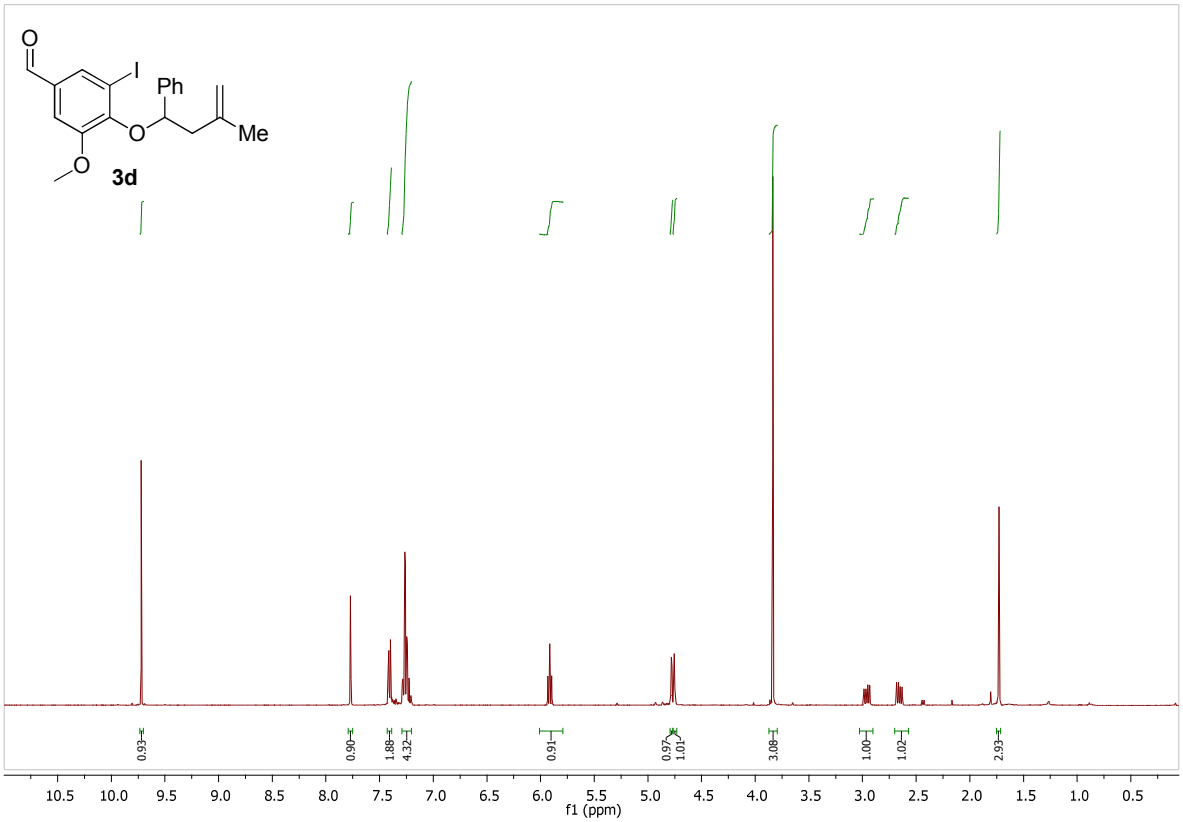
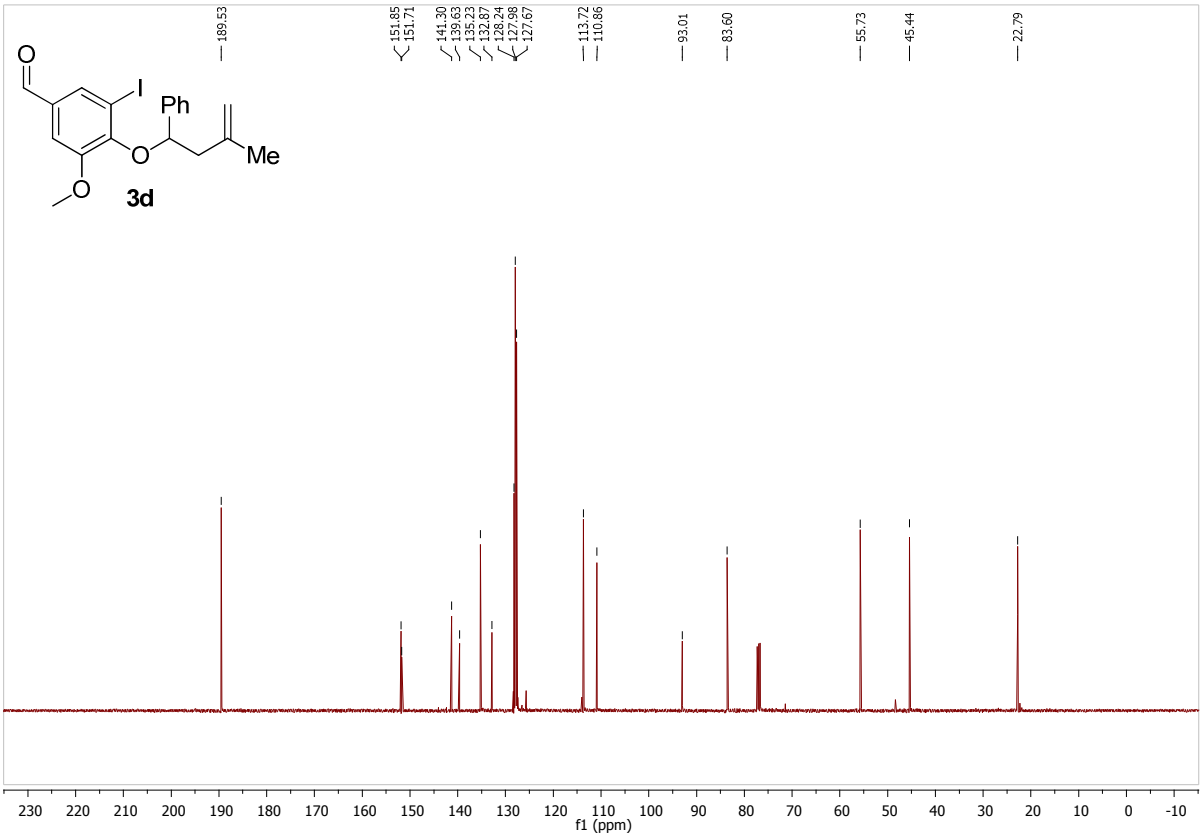
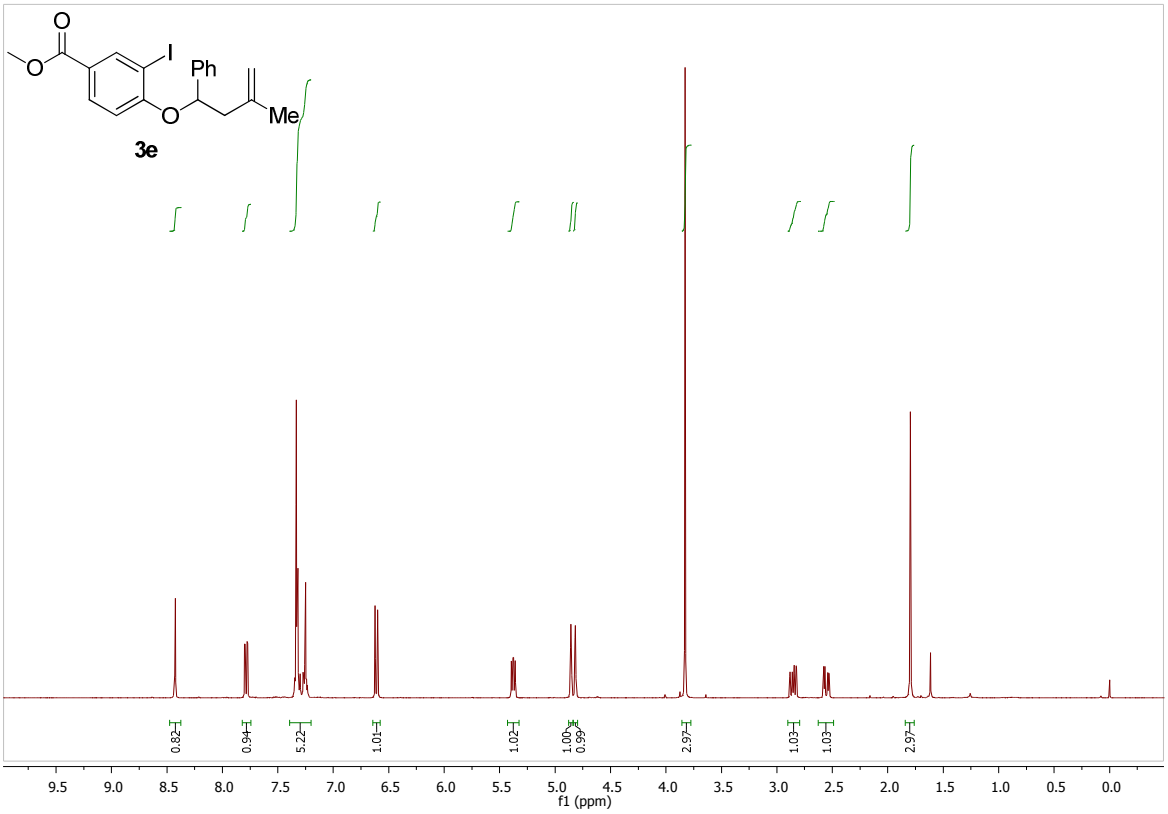
142.16
139.48
136.29
133.87
129.86
129.24
129.11
128.15
126.42
125.71
125.65
123.66
122.44
122.17
113.65
113.06
86.57
45.75
23.37
I
Me
O
3b
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

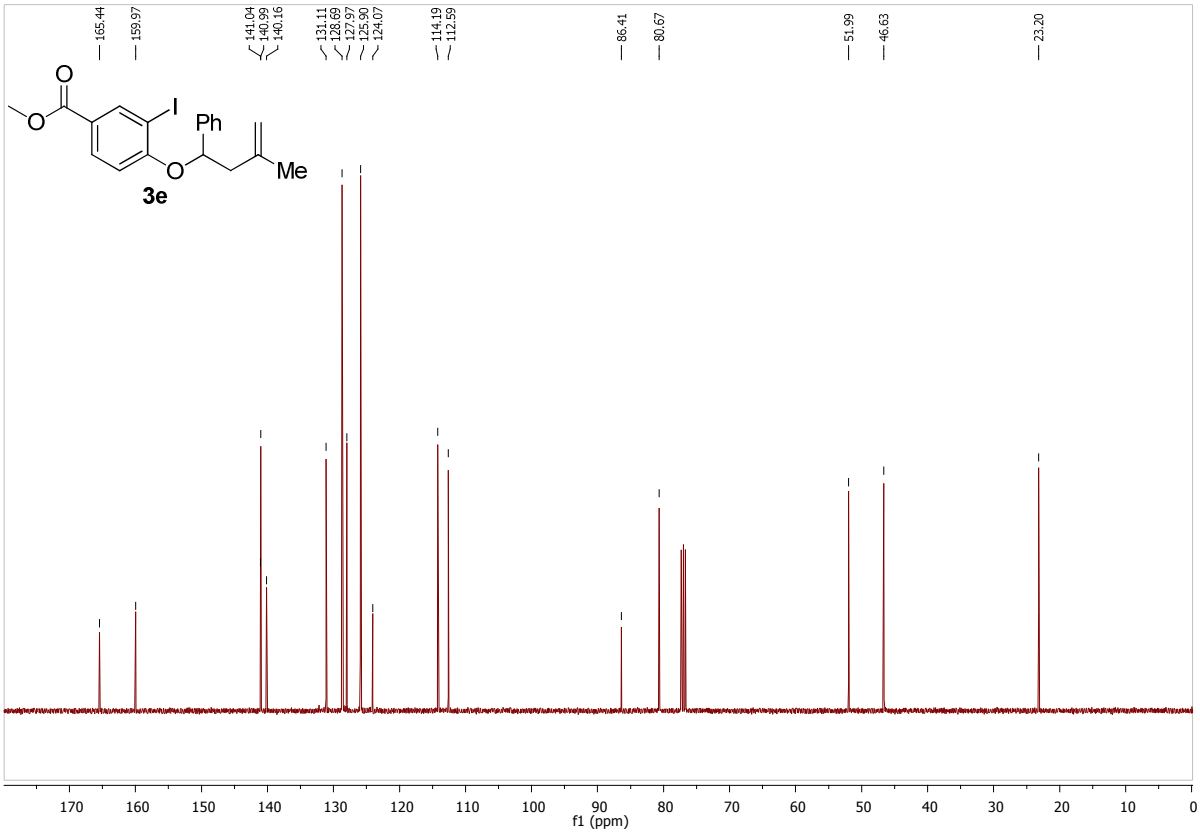

Cl
I
Ph
O
N
3c
Me
1.00
0.97
0.86
3.16
2.97
1.03
2.18
1.04
1.07
3.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

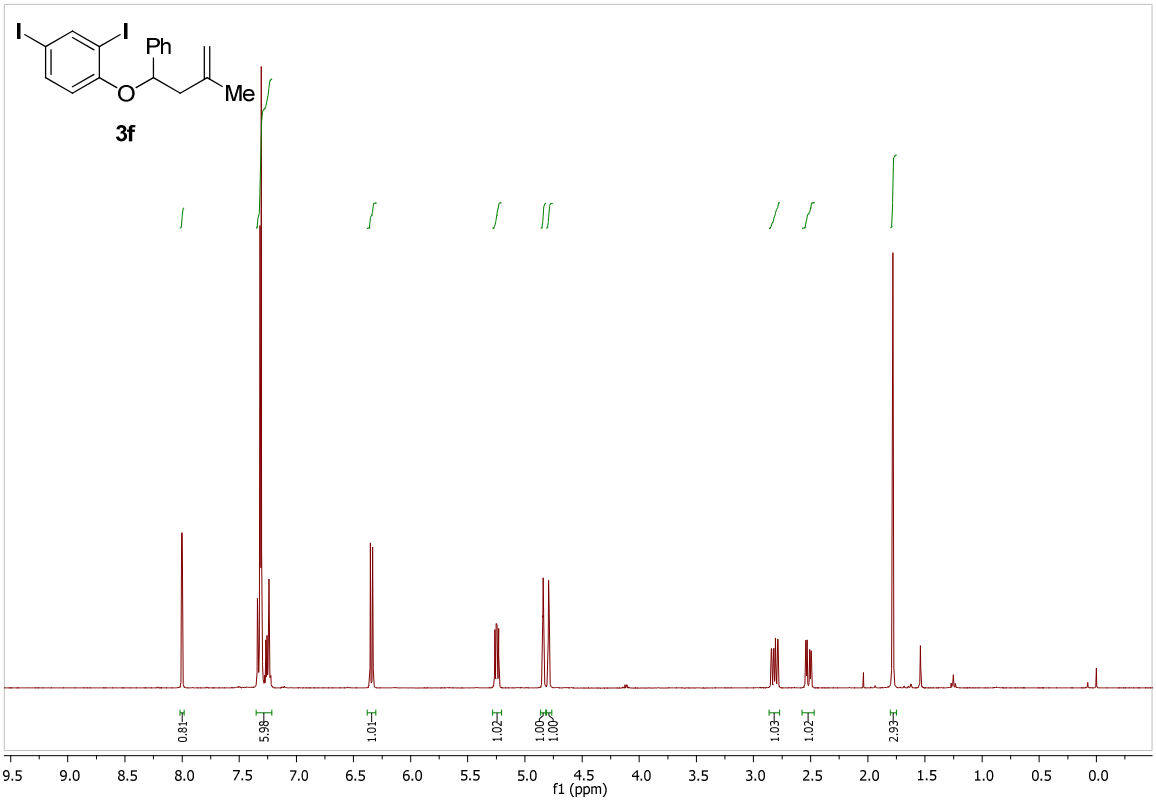

153.41
149.02
141.91
141.63
140.09
135.21
133.25
128.08
127.94
127.82
127.12
125.03
121.93
113.44
91.19
84.56
45.23
22.81
Cl
I
Ph
O
N
3c
Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

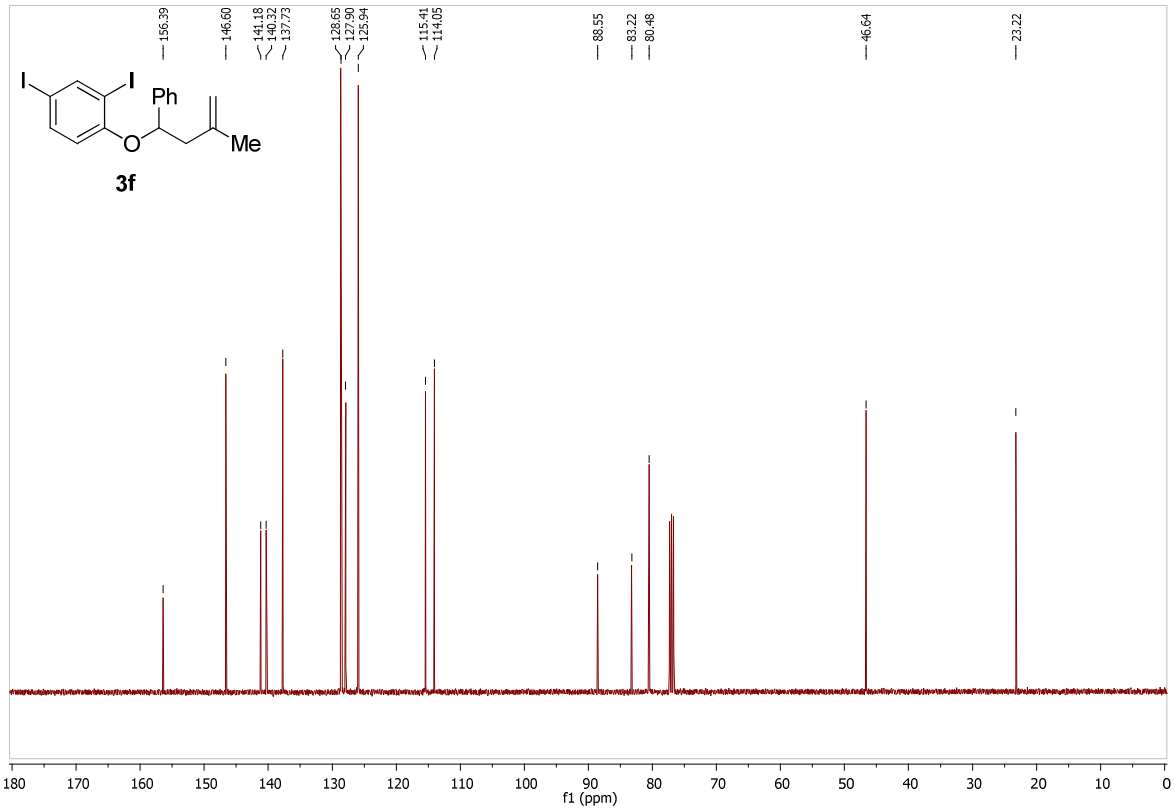

O
I
Ph
O
Me
O
3d
0.93
0.90
1.88
4.32
0.91
0.97
1.01
3.08
1.00
1.02
2.93
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

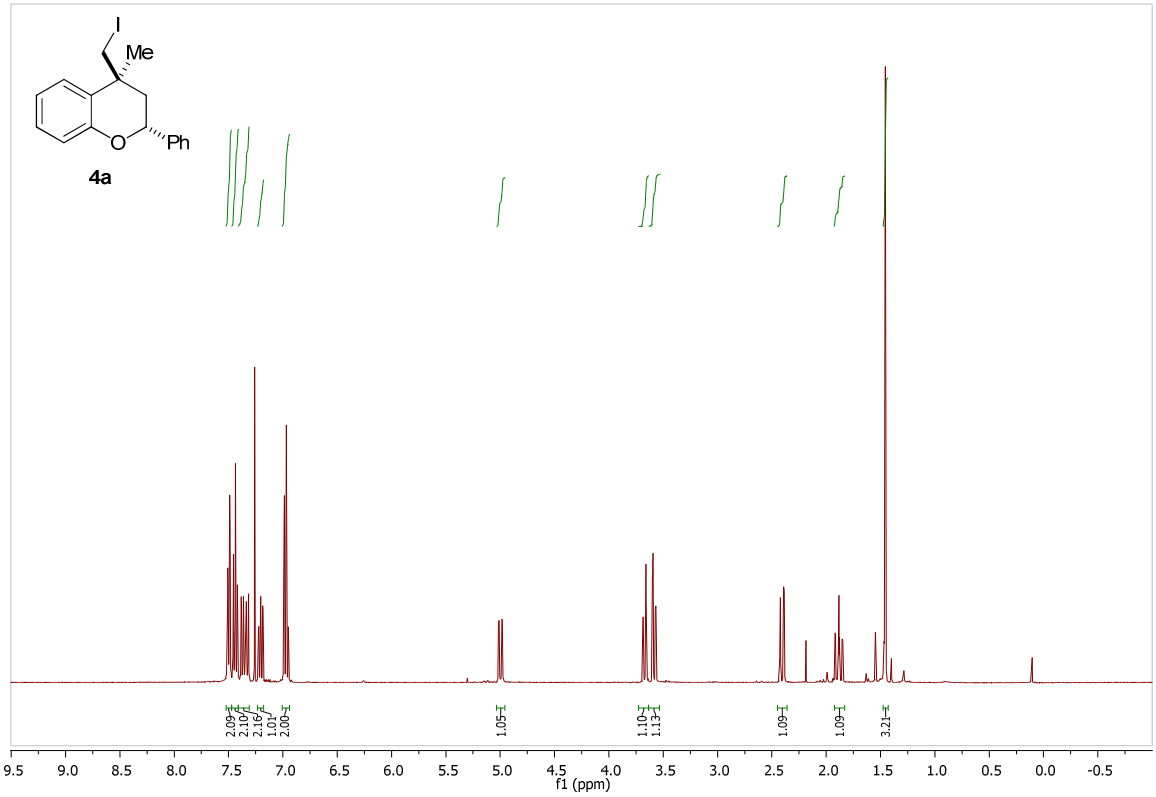

189.53
151.85
151.71
141.30
139.63
135.23
132.87
128.24
127.98
127.67
113.72
110.86
93.01
83.60
55.73
45.44
22.79
O
I
Ph
O
Me
O
3d
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

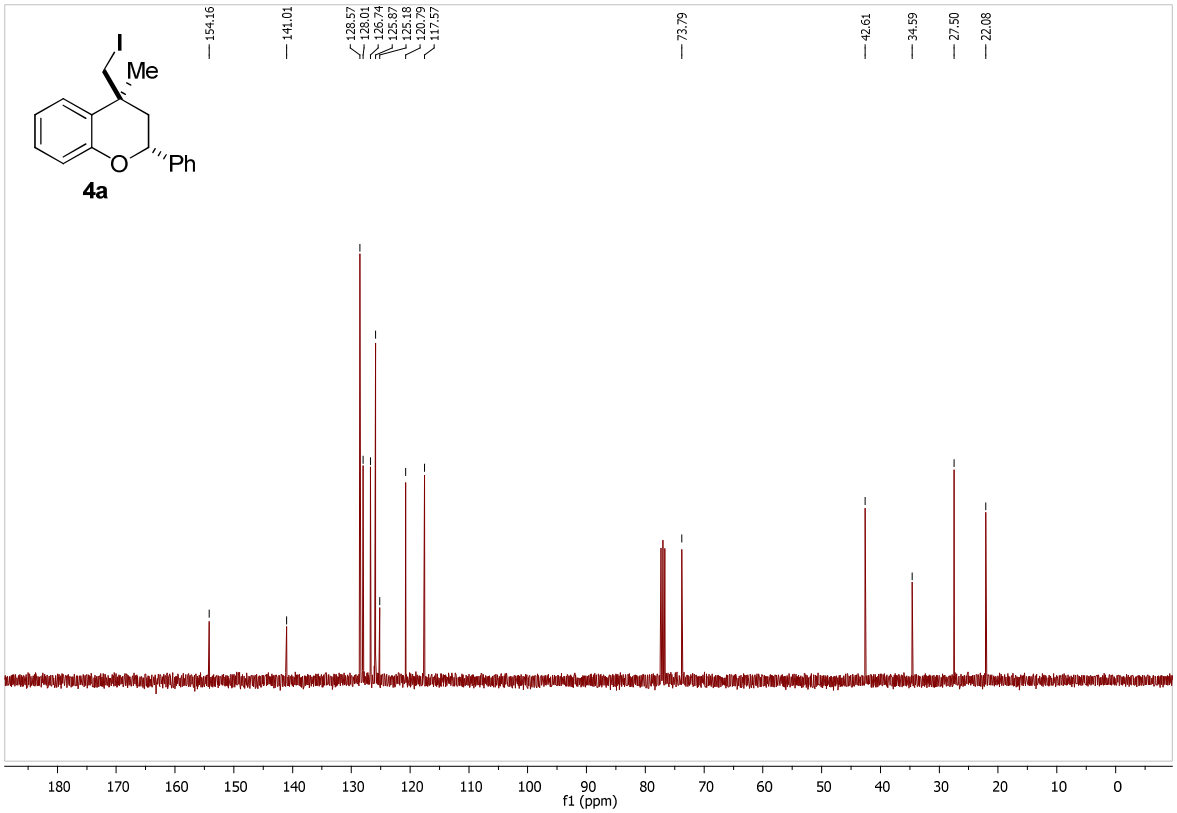

3e
0.82
0.94
5.22
1.01
1.02
1.00
0.99
2.97
1.03
1.03
2.97
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


165.44
159.97
141.04
140.99
140.16
131.11
128.69
127.97
125.90
124.07
114.19
112.59
86.41
80.67
51.99
46.63
23.20
3e
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

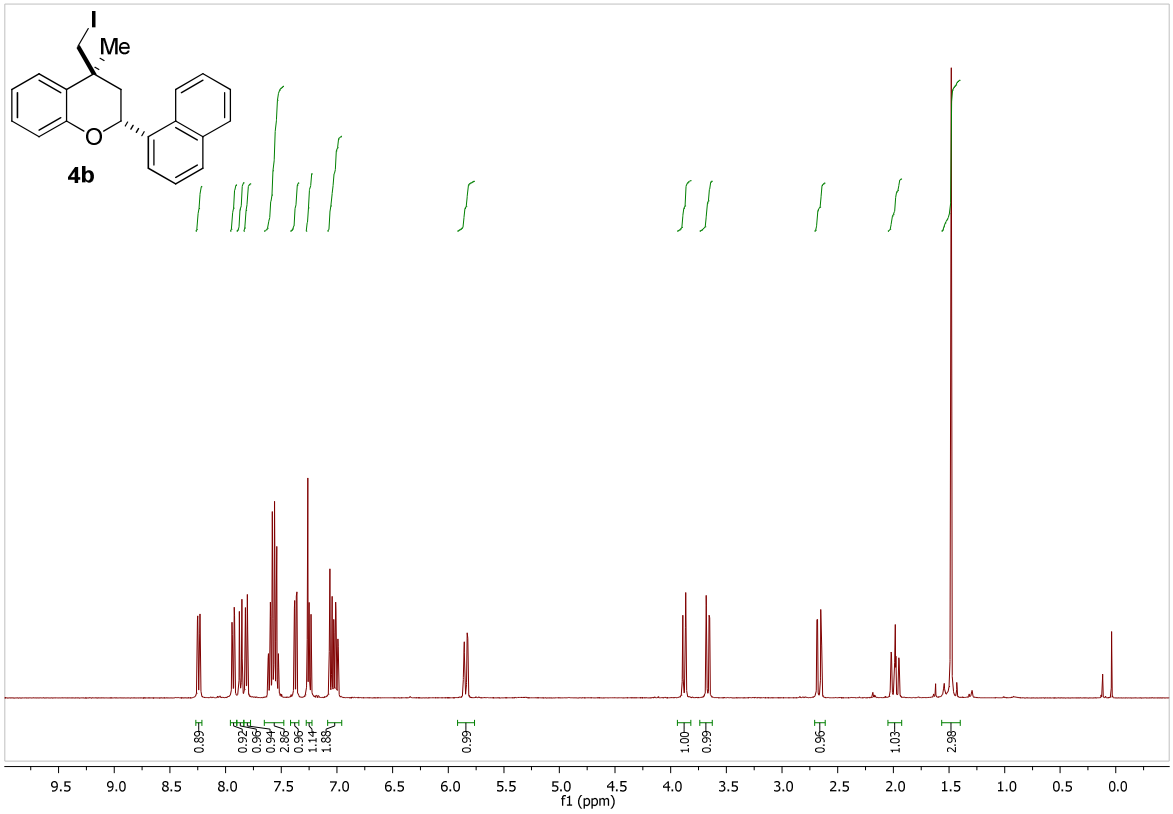

I
I
Ph
O
Me
3f
0.81
5.98
1.01
1.02
1.00
1.00
1.03
1.02
2.93
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

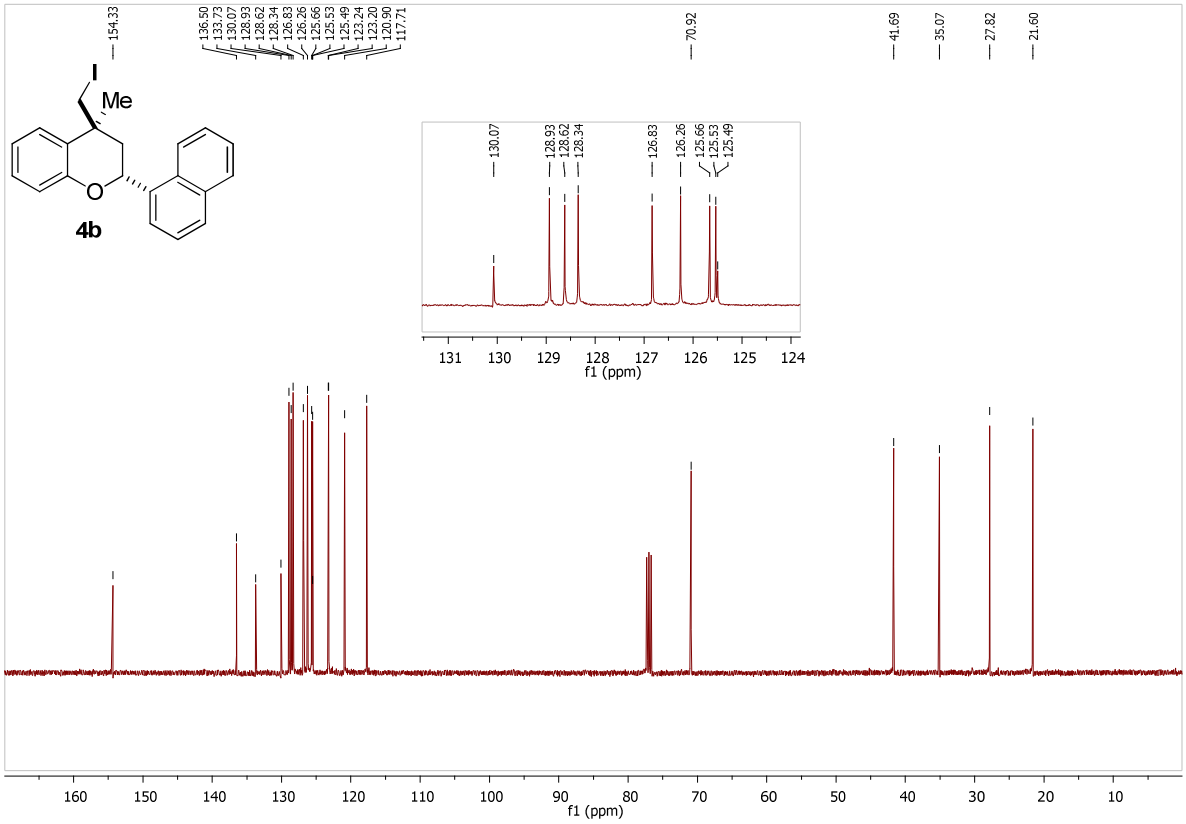

156.39
146.60
141.18
140.32
137.73
128.65
127.90
125.94
115.41
114.05
88.55
83.22
80.48
46.64
23.22
I
I
Ph
O
Me
3f
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

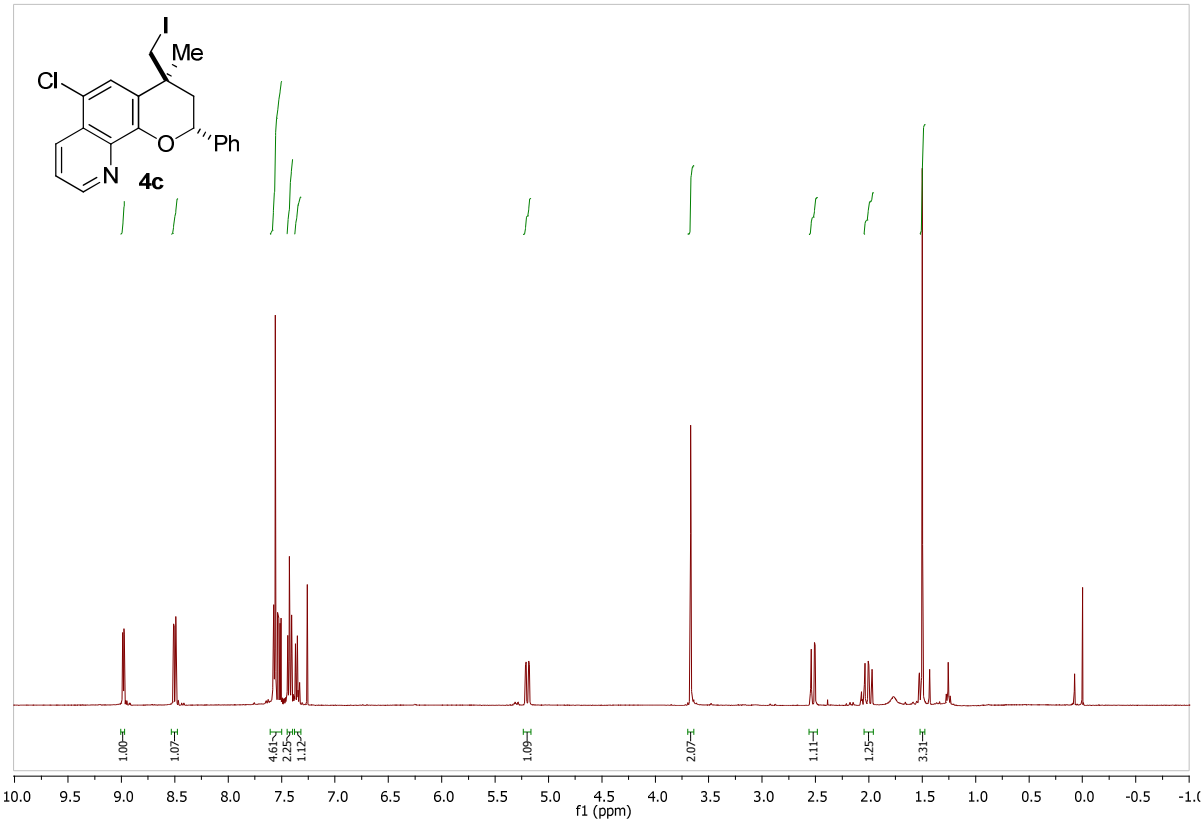

I
Me
Ph
O
4a
2.09
2.10
2.16
1.01
2.00
1.05
1.10
1.13
1.09
1.09
3.21
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

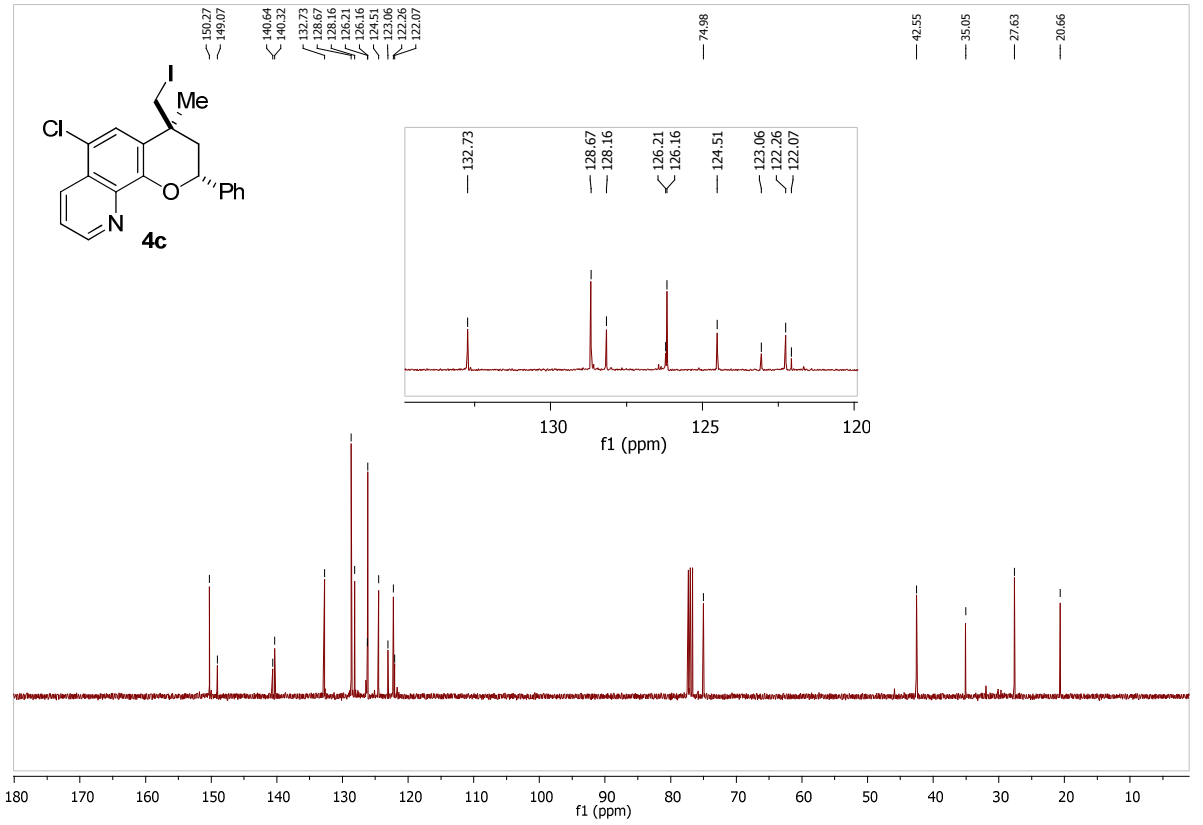

154.16
141.01
128.57
128.01
126.74
125.87
125.18
120.79
117.57
73.79
42.61
34.59
27.50
22.08
I
Me
Ph
O
4a
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

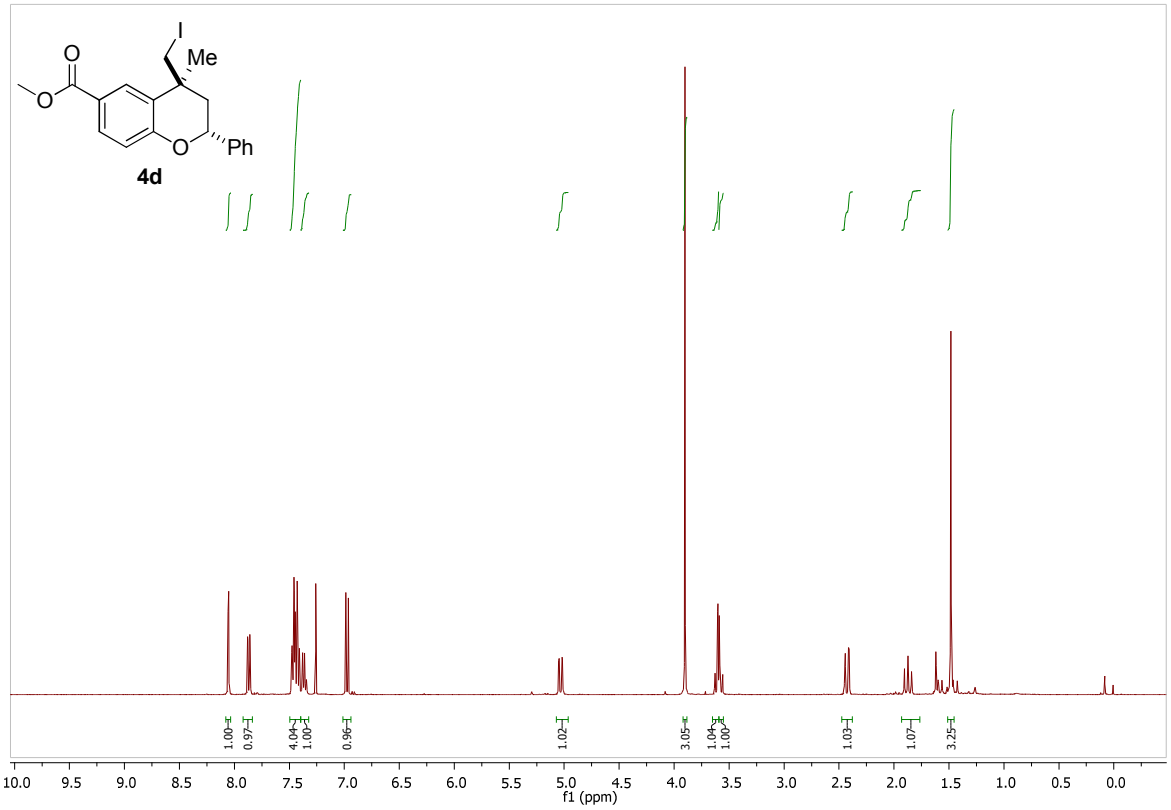
NOE
NOE
NOE
Me
H
H
H
O
Ph
f2 (ppm)
f1 (ppm)

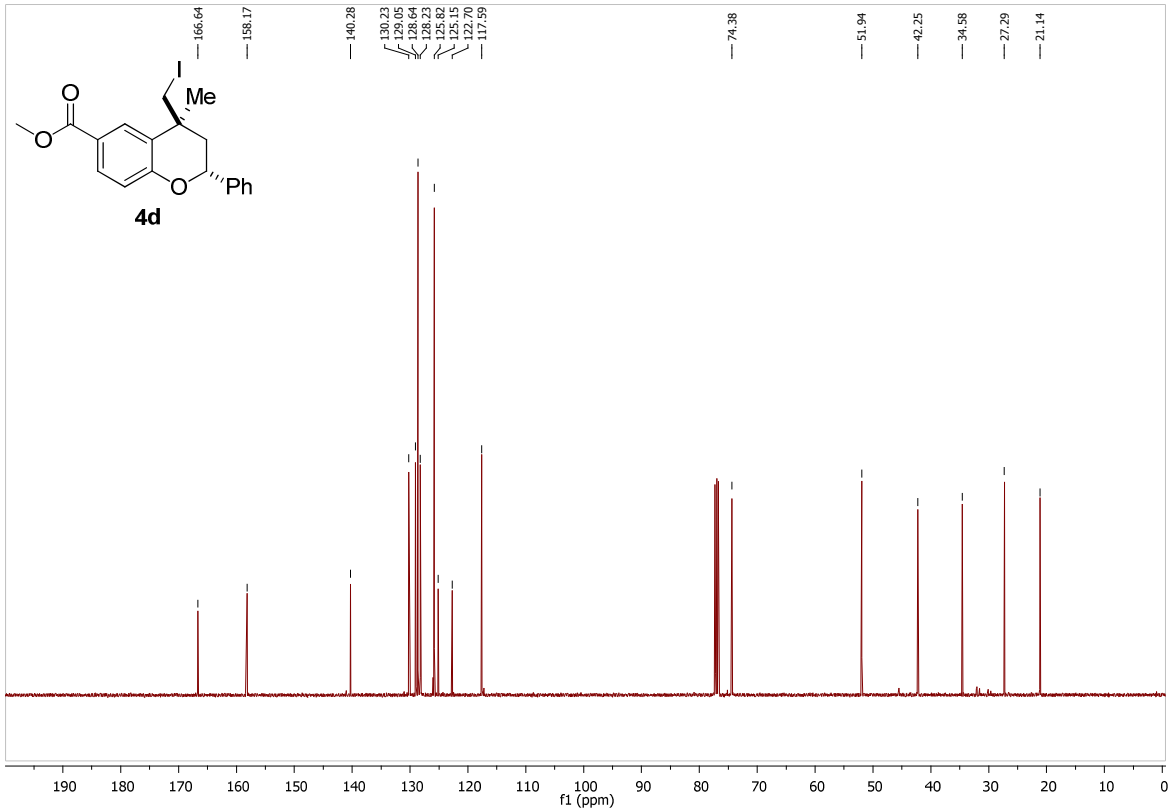

I
Me
O
4b
0.89
0.92
0.95
0.94
2.86
0.96
1.14
1.88
0.99
1.00
0.99
0.96
1.03
2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

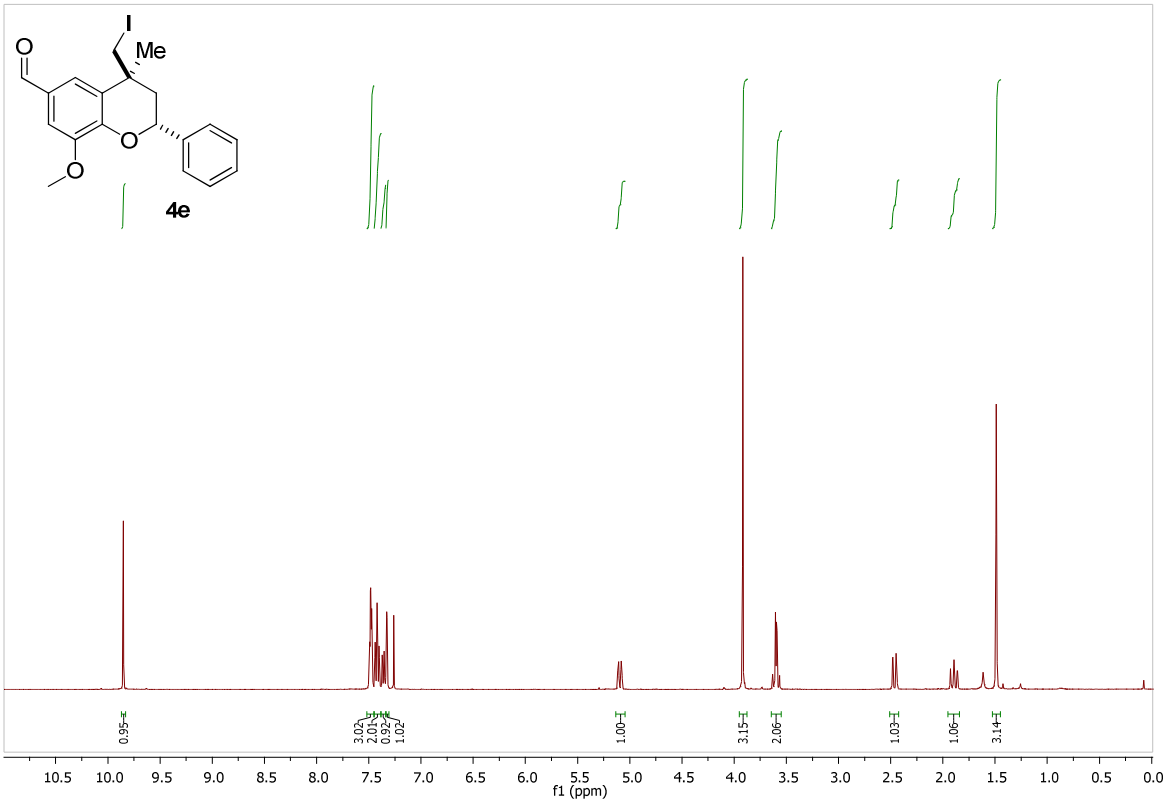

154.33
136.50
133.73
130.07
128.93
128.62
128.34
126.83
126.26
125.66
125.53
125.49
123.24
123.20
120.90
117.71
70.92
41.69
35.07
27.82
21.60
I
Me
O
4b
130.07
128.93
128.62
128.34
126.83
126.26
125.66
125.53
125.49
131 130 129 128 127 126 125 124
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


I
Me
Cl
O
Ph
N
4c
1.00
1.07
4.61
2.25
1.12
1.09
2.07
1.11
1.25
3.31
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


150.27
149.07
140.64
140.32
132.73
128.67
128.16
126.21
126.16
124.51
123.06
122.26
122.07
74.98
42.55
35.05
27.63
20.66
I
Me
Cl
O
Ph
N
4c
132.73
128.67
128.16
126.21
126.16
124.51
123.06
122.26
122.07
130 125 120
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


4d
1.00
0.97
4.04
1.00
0.96
1.02
3.05
1.04
1.00
1.03
1.07
3.25
f1 (ppm)


166.64
158.17
140.28
130.23
129.05
128.64
128.23
125.82
125.15
122.70
117.59
74.38
51.94
42.25
34.58
27.29
21.14
4d
f1 (ppm)


4e
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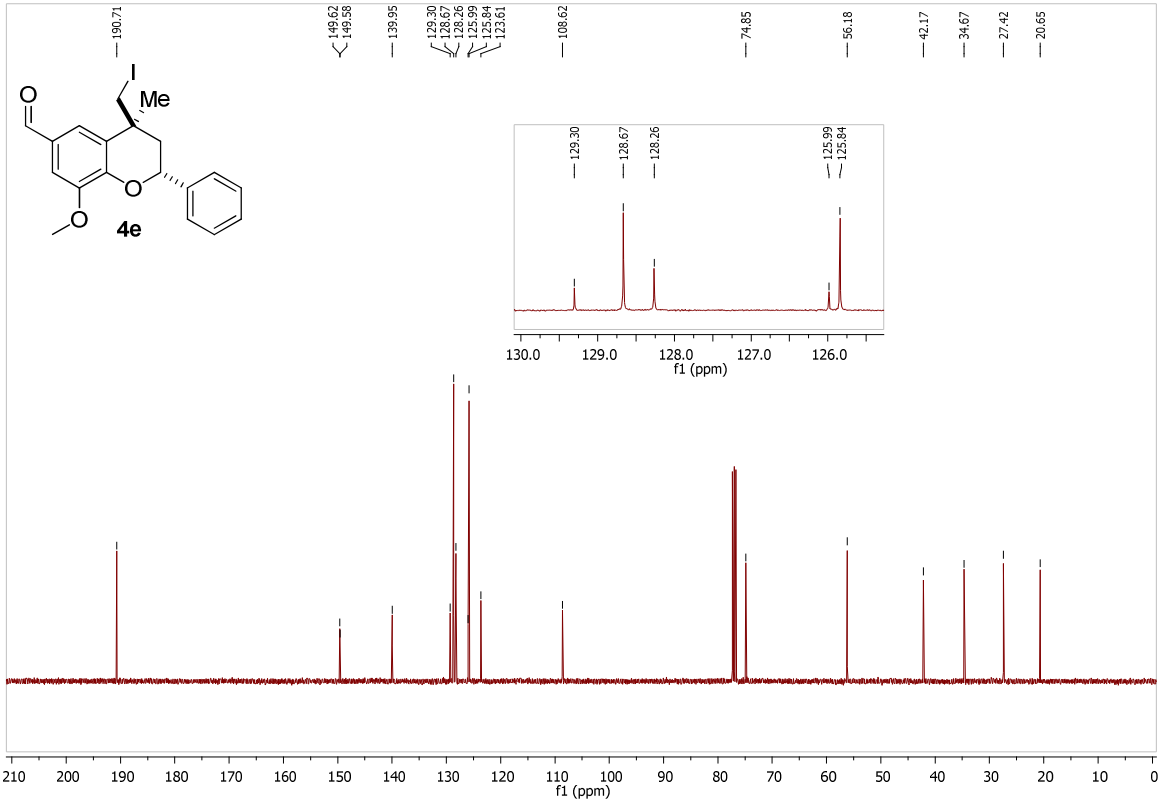
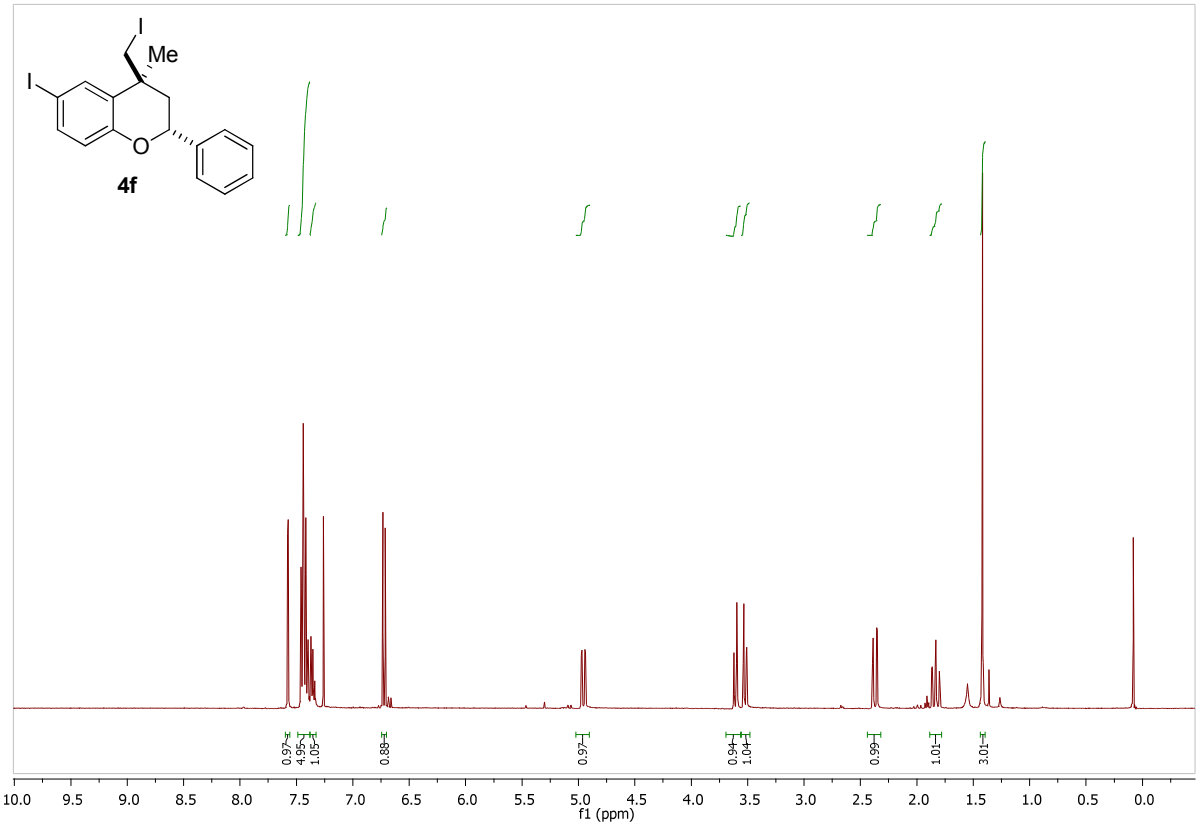
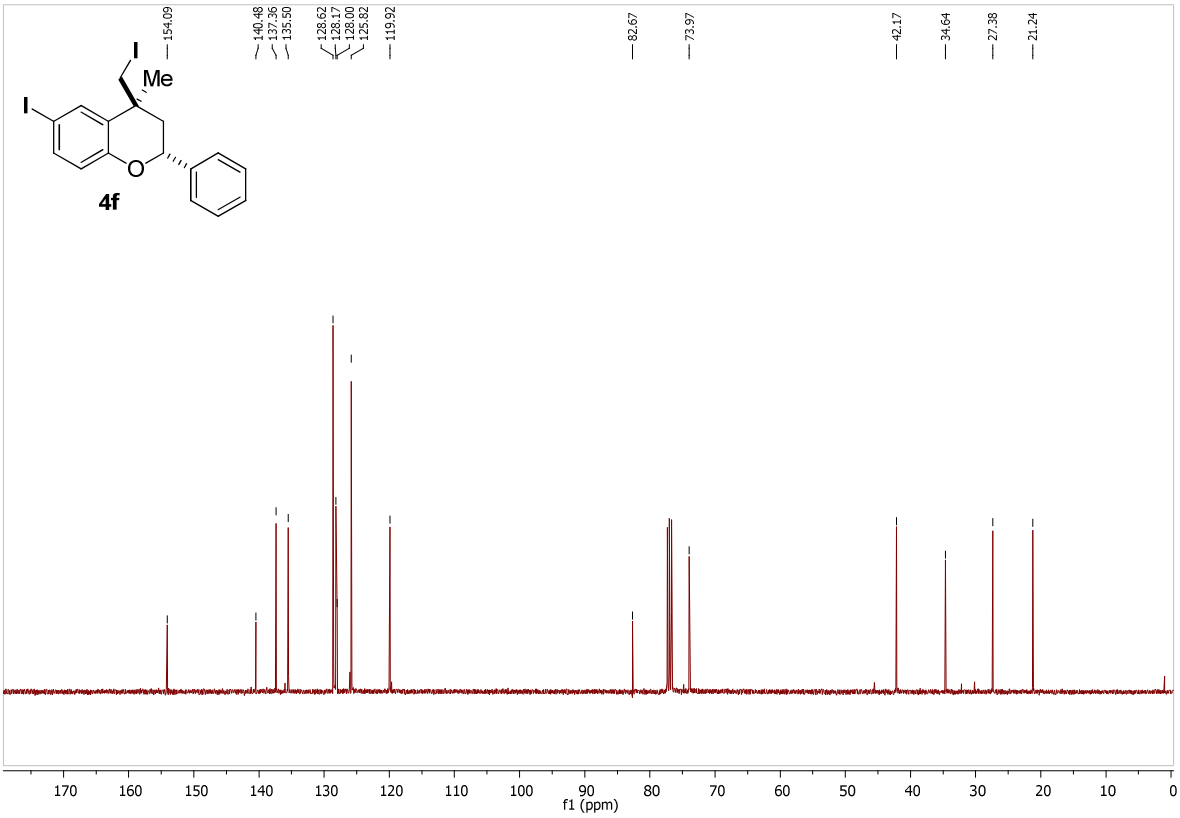
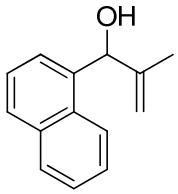
3.02
2.01
0.92
1.02
1.00
3.15
2.06
1.03
1.06
3.14
f1 (ppm)


190.71
149.62
149.58
139.95
129.30
128.67
128.26
125.99
125.84
123.61
108.62
74.85
56.18
42.17
34.67
27.42
20.65
4e
f1 (ppm)


I
Me
I
O
4f
0.97
4.95
1.05
0.88
0.97
0.94
1.04
0.99
1.01
3.01
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)

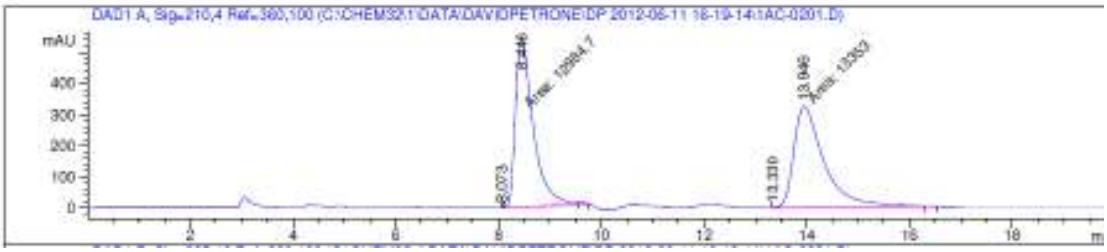

154.09
140.48
137.36
135.50
128.62
128.17
128.00
125.82
119.92
82.67
73.97
42.17
34.64
27.38
21.24
I
Me
I
O
4f
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

2. HPLC traces and data




```
Data File C:\CHEM32\1\DATA\DAVIDPETRONE\DP 2012-06-11 16-19-14\1AC-0201.D
Sample Name: DP-2-29-p
    ==================================================================
    Acq. Operator   : DaveP                          Seq. Line :   2
    Acq. Instrument : HPLC_3                          Location : P1-A-03
    Injection Date  : 6/11/2012 4:40:14 PM                 Inj :   1
                                                     Inj Volume : 5 µl
    Acq. Method     : C:\Chem32\1\DATA\DAVIDPETRONE\DP 2012-06-11 16-19-14\DP-COL2-90-10-HEX-IPA.M
    Last changed    : 6/11/2012 4:18:40 PM by DaveP
    Analysis Method : C:\CHEM32\1\DATA\DAVIDPETRONE\DP 2012-06-11 16-19-14\1AC-0201.D\DA.M (DP-COL2-
                      90-10-HEX-IPA.M)
    Last changed    : 6/11/2012 4:18:40 PM by DaveP
    Method Info     : 0.8 ml/min 90:10 IPrOH:Hexanes

    ==================================================================
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=360,100

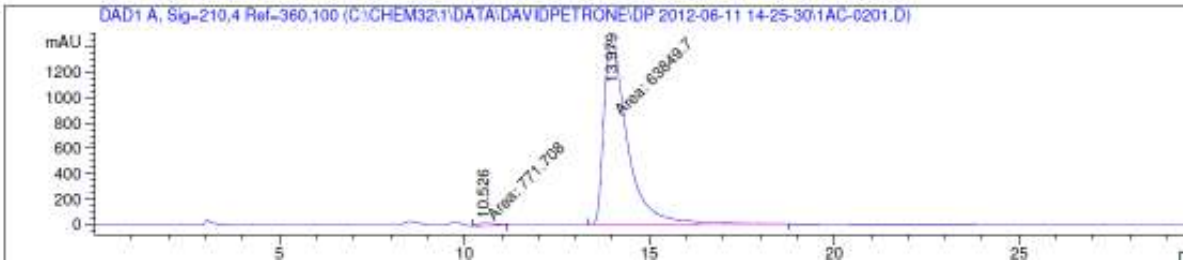
    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   8.073 BB R 2.34e-3   83.63090 1.99840e-15  0.3163
       2   8.446 MM T  0.4050 1.29847e4   534.35358  49.1040
       3  13.330 VB R 9.89e-4   21.89771    4.08024   0.0828
       4  13.946 MM T  0.7246 1.33530e4   325.97153  50.4969

    Totals :                  2.64432e4   864.40534
```

Data File C:\CHEM32\1\DATA\DAVIDPETRONE\DP 2012-06-11 14-25-30\1AC-0201.D
Sample Name: DP-2-32-p

```
==================================================================
Acq. Operator   : DaveP                          Seq. Line :  2
Acq. Instrument : HPLC_3                          Location : P1-A-03
Injection Date  : 6/11/2012 2:56:31 PM                Inj :  1
                                               Inj Volume : 5 µl
Acq. Method     : C:\Chem32\1\DATA\DAVIDPETRONE\DP 2012-06-11 14-25-30\DP-COL2-90-10-HEX-IPA.M
Last changed    : 6/11/2012 2:20:42 PM by lei
Analysis Method : C:\CHEM32\1\DATA\DAVIDPETRONE\DP 2012-06-11 14-25-30\1AC-0201.D\DA.M (DP-COL2-
                  90-10-HEX-IPA.M)
Last changed    : 6/11/2012 2:20:42 PM by lei
Method Info     : 0.8 ml/min 90:10 IPrOH:Hexanes

------------------------------------------------------------------
```



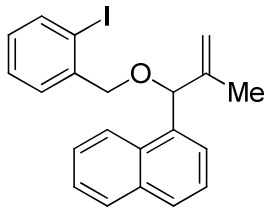

```
==================================================================
                          Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.526 MM T  0.6155  771.70764   20.89733   1.1942
   2  13.979 MM T  0.7431 6.38497e4  1432.03906  98.8058

Totals :                  6.46214e4  1452.93639
```



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Acq. Instrument : HPLC_3                           Location : P1-B-01
Injection Date  : 6/26/2012 12:30:25 PM                  Inj :   1
                                                 Inj Volume : 5 µl
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Last changed    : 6/26/2012 11:58:53 AM by Dave P
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                  DAVEP.M)
Last changed    : 6/26/2012 6:55:47 PM by tao
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Signal 4: DAD1 D, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.264	MM T	0.2571	392.68115	30.80783	48.8878
2	5.553	MM T	0.2771	410.54892	24.69442	51.1122
Totals :				803.23007	55.50225	

==========

*** End of Report ***

```
Data File C:\CHEM32\1\DATA\DAVIDPETRONE\DAVEP1 2012-06-26 14-06-30\DP000002.D
Sample Name: DP-2-33-p-chiral
    ==================================================================
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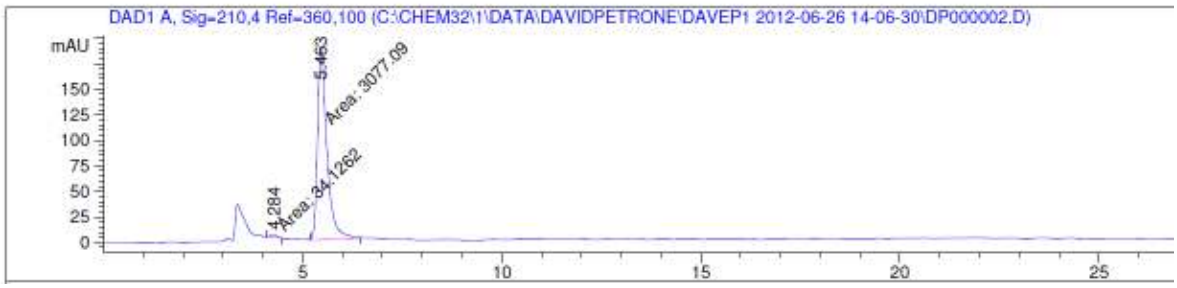
    Acq. Instrument : HPLC_3                           Location : P1-B-01
    Injection Date  : 6/26/2012 2:37:30 PM                 Inj :   1
                                                     Inj Volume : 5 µl
    Acq. Method     : C:\Chem32\1\DATA\DAVIDPETRONE\DAVEP1 2012-06-26 14-06-30\DAVEP.M
    Last changed    : 6/26/2012 11:58:53 AM by Dave P
    Analysis Method : C:\CHEM32\1\DATA\DAVIDPETRONE\DAVEP1 2012-06-26 14-06-30\DP000002.D\DA.
                      DAVEP.M)
    Last changed    : 6/26/2012 7:01:44 PM by tao
    ==================================================================
```

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    ------------------------------------------------------------------
                              Area Percent Report
    ------------------------------------------------------------------

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    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.284 MM T  0.2267   34.12615    2.50888   1.0969
       2   5.463 MM T  0.2709 3077.09351  189.33217  98.9031

    Totals :                   3111.21966  191.84105
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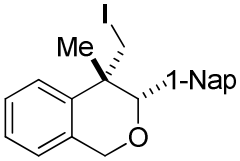

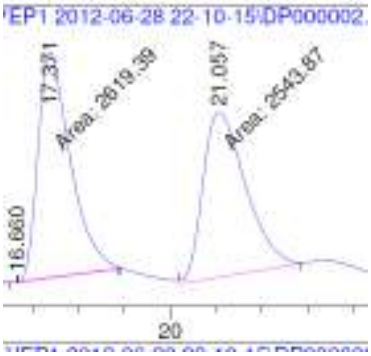


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---------------------------------------------------------------------
                          Area Percent Report
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Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   3.111 BV    0.1288   20.13337    2.42698   0.2712
   2   3.341 VB    0.2633  711.21185   35.87396   9.5784
   3   7.226 BB    0.3215  310.36649   14.62775   4.1799
   4   9.162 BB    0.3851  287.60553   10.85482   3.8734
   5  11.181 BB    0.4703  305.97168    9.33692   4.1207
   6  14.114 BV    0.5231  307.32156    8.27854   4.1389
   7  15.498 VB    0.5834  285.34576    6.61370   3.8429
   8  16.660 BB R 9.33e-3   33.95815 1.33227e-15  0.4573
   9  17.371 MM T  0.8151 2619.39160   53.56079  35.2772
  10  21.057 MM T  1.0775 2543.87158   39.34771  34.2601

Totals :                  7425.17757  180.92118
```

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   Acq. Instrument  : HPLC_3                           Location : P1-C-01
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                                                     Inj Volume : 5 µl
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   Analysis Method  : C:\CHEM32\1\DATA\DAVIDPETRONE\DAVEP1 2012-06-29 09-02-54\DP000002.D\DA.M
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   Last changed     : 6/28/2012 10:01:28 PM by Dave P
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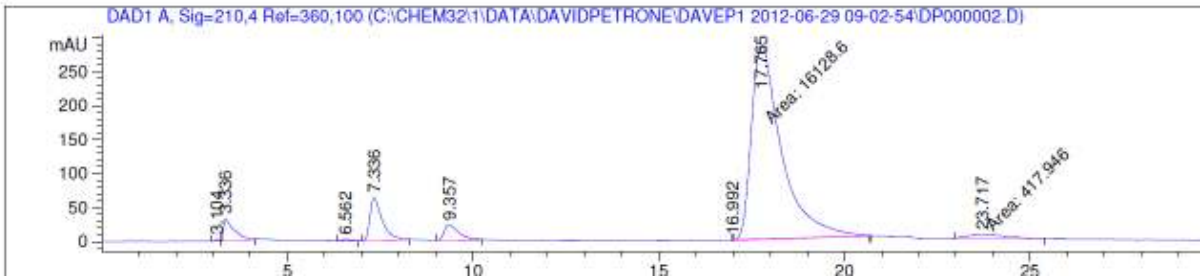


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==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   3.104 BV    0.1250   20.15257    2.42457   0.1041
   2   3.336 VB    0.2561  623.21399   32.15690   3.2178
   3   6.562 BB    0.2402   32.31733    1.88335   0.1669
   4   7.336 BB    0.3395 1436.50671   62.66233   7.4171
   5   9.357 BB    0.4038  612.41504   22.47936   3.1621
   6  16.992 BB R 4.92e-3   96.40501 1.73390e-2   0.4978
   7  17.765 MM T  0.9400 1.61286e4   285.95746  83.2764
   8  23.717 MM T  1.2249  417.94617    5.68684   2.1580

Totals :                  1.93676e4   413.26815
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3. X-ray crystallographic structures and data

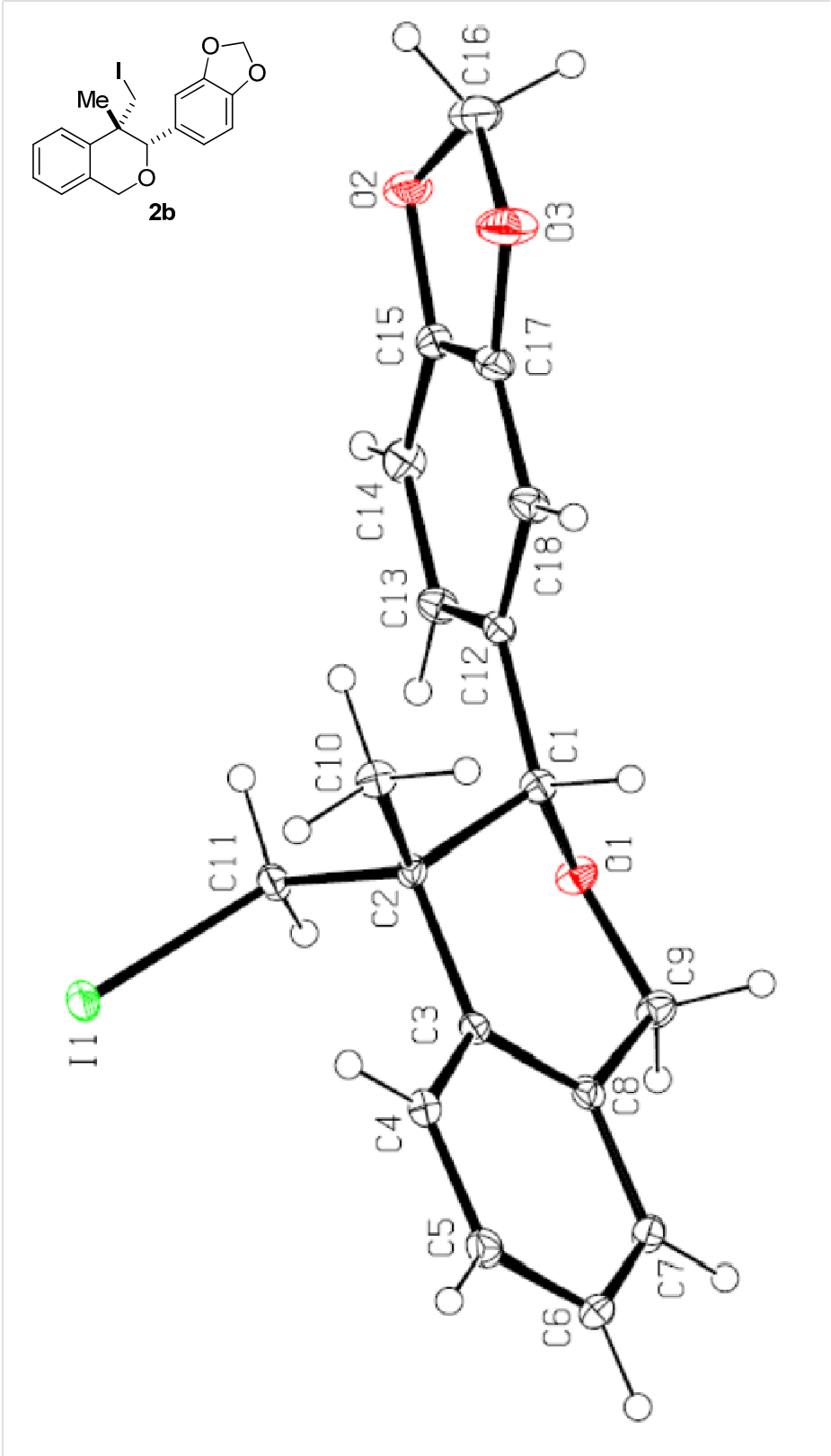

Table 1. Crystal data and structure refinement for d12115.

Identification code	d12115	
Empirical formula	C18 H17 I O3	
Formula weight	408.22	
Temperature	147(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P c a 21	
Unit cell dimensions	a = 14.2621(4) Å	α= 90°.
	b = 16.5312(6) Å	β= 90°.
	c = 6.6380(2) Å	γ = 90°.
Volume	1565.04(9) $Å^3$	
Z	4	
Density (calculated)	1.733 Mg/m^3	
Absorption coefficient	2.056 mm^{-1}	
F(000)	808	
Crystal size	0.16 x 0.14 x 0.04 mm^3	
Theta range for data collection	1.23 to 30.57°.	
Index ranges	-18<=h<=20, -23<=k<=23, -8<=l<=9	
Reflections collected	17169	
Independent reflections	4630 [R(int) = 0.0388]	
Completeness to theta = 30.57°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.7011	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4630 / 1 / 200	
Goodness-of-fit on F^2	1.014	
Final R indices [I>2sigma(I)]	R1 = 0.0252, wR2 = 0.0473	
R indices (all data)	R1 = 0.0355, wR2 = 0.0505	
Absolute structure parameter	-0.013(16)	
Largest diff. peak and hole	0.422 and -0.417 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d12115. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	-1560(1)	8103(1)	7539(1)	24(1)
O(1)	1408(1)	7771(1)	11138(3)	19(1)
O(2)	1173(1)	4002(1)	10531(3)	30(1)
O(3)	1923(1)	4452(1)	7645(5)	37(1)
C(1)	1390(2)	7362(2)	9228(4)	16(1)
C(2)	596(2)	7741(1)	7905(3)	14(1)
C(3)	819(1)	8652(1)	7721(5)	14(1)
C(4)	522(2)	9105(2)	6052(4)	19(1)
C(5)	747(2)	9920(2)	5878(4)	22(1)
C(6)	1272(2)	10296(1)	7355(7)	24(1)
C(7)	1576(2)	9856(2)	9011(4)	20(1)
C(8)	1350(2)	9032(2)	9197(4)	17(1)
C(9)	1755(2)	8577(2)	10959(4)	20(1)
C(10)	602(2)	7330(2)	5849(4)	19(1)
C(11)	-339(2)	7597(2)	8998(4)	18(1)
C(12)	1298(2)	6463(2)	9654(4)	16(1)
C(13)	839(2)	6188(2)	11362(4)	20(1)
C(14)	766(2)	5362(2)	11820(4)	23(1)
C(15)	1167(2)	4836(2)	10464(4)	21(1)
C(16)	1775(2)	3761(2)	8916(5)	33(1)
C(17)	1619(2)	5104(2)	8767(4)	23(1)
C(18)	1710(2)	5910(2)	8302(4)	20(1)

Table 3. Bond lengths [Å] and angles [°] for d12115.

I(1)-C(11)	2.160(2)
O(1)-C(9)	1.426(3)
O(1)-C(1)	1.437(3)
O(2)-C(15)	1.379(3)
O(2)-C(16)	1.431(4)
O(3)-C(17)	1.380(3)
O(3)-C(16)	1.436(4)
C(1)-C(12)	1.518(3)
C(1)-C(2)	1.565(3)
C(1)-H(1A)	1.0000
C(2)-C(10)	1.525(3)
C(2)-C(11)	1.536(3)
C(2)-C(3)	1.545(3)
C(3)-C(8)	1.389(4)
C(3)-C(4)	1.402(4)
C(4)-C(5)	1.389(3)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.382(5)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.387(5)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.405(4)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.506(4)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.386(3)
C(12)-C(18)	1.410(3)
C(13)-C(14)	1.403(4)

C(13)-H(13A)	0.9500
C(14)-C(15)	1.377(4)
C(14)-H(14A)	0.9500
C(15)-C(17)	1.372(4)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.374(4)
C(18)-H(18A)	0.9500

C(9)-O(1)-C(1)	111.84(18)
C(15)-O(2)-C(16)	105.0(2)
C(17)-O(3)-C(16)	105.0(3)
O(1)-C(1)-C(12)	107.30(19)
O(1)-C(1)-C(2)	108.59(19)
C(12)-C(1)-C(2)	115.70(19)
O(1)-C(1)-H(1A)	108.3
C(12)-C(1)-H(1A)	108.3
C(2)-C(1)-H(1A)	108.3
C(10)-C(2)-C(11)	111.0(2)
C(10)-C(2)-C(3)	111.3(2)
C(11)-C(2)-C(3)	111.55(19)
C(10)-C(2)-C(1)	108.60(19)
C(11)-C(2)-C(1)	107.57(18)
C(3)-C(2)-C(1)	106.60(18)
C(8)-C(3)-C(4)	118.7(2)
C(8)-C(3)-C(2)	119.8(2)
C(4)-C(3)-C(2)	121.4(2)
C(5)-C(4)-C(3)	120.9(2)
C(5)-C(4)-H(4A)	119.5
C(3)-C(4)-H(4A)	119.5
C(6)-C(5)-C(4)	120.1(3)
C(6)-C(5)-H(5A)	119.9
C(4)-C(5)-H(5A)	119.9
C(5)-C(6)-C(7)	119.8(2)
C(5)-C(6)-H(6A)	120.1
C(7)-C(6)-H(6A)	120.1

C(6)-C(7)-C(8)	120.4(2)
C(6)-C(7)-H(7A)	119.8
C(8)-C(7)-H(7A)	119.8
C(3)-C(8)-C(7)	120.1(2)
C(3)-C(8)-C(9)	122.1(2)
C(7)-C(8)-C(9)	117.7(2)
O(1)-C(9)-C(8)	113.5(2)
O(1)-C(9)-H(9A)	108.9
C(8)-C(9)-H(9A)	108.9
O(1)-C(9)-H(9B)	108.9
C(8)-C(9)-H(9B)	108.9
H(9A)-C(9)-H(9B)	107.7
C(2)-C(10)-H(10A)	109.5
C(2)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(2)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(2)-C(11)-I(1)	115.32(15)
C(2)-C(11)-H(11A)	108.4
I(1)-C(11)-H(11A)	108.4
C(2)-C(11)-H(11B)	108.4
I(1)-C(11)-H(11B)	108.4
H(11A)-C(11)-H(11B)	107.5
C(13)-C(12)-C(18)	120.3(2)
C(13)-C(12)-C(1)	121.0(2)
C(18)-C(12)-C(1)	118.7(2)
C(12)-C(13)-C(14)	122.1(2)
C(12)-C(13)-H(13A)	118.9
C(14)-C(13)-H(13A)	118.9
C(15)-C(14)-C(13)	116.3(2)
C(15)-C(14)-H(14A)	121.9
C(13)-C(14)-H(14A)	121.9
C(17)-C(15)-C(14)	121.9(2)
C(17)-C(15)-O(2)	110.3(2)
C(14)-C(15)-O(2)	127.8(2)

O(2)-C(16)-O(3)	107.9(2)
O(2)-C(16)-H(16A)	110.1
O(3)-C(16)-H(16A)	110.1
O(2)-C(16)-H(16B)	110.1
O(3)-C(16)-H(16B)	110.1
H(16A)-C(16)-H(16B)	108.4
C(15)-C(17)-C(18)	122.8(2)
C(15)-C(17)-O(3)	109.8(2)
C(18)-C(17)-O(3)	127.4(3)
C(17)-C(18)-C(12)	116.6(2)
C(17)-C(18)-H(18A)	121.7
C(12)-C(18)-H(18A)	121.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for d12115. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(1)	13(1)	21(1)	38(1)	5(1)	-3(1)	0(1)
O(1)	24(1)	19(1)	14(1)	-1(1)	-4(1)	-2(1)
O(2)	30(1)	16(1)	46(1)	3(1)	9(1)	-1(1)
O(3)	46(1)	19(1)	47(1)	-3(2)	22(2)	4(1)
C(1)	18(1)	18(1)	13(1)	-3(1)	1(1)	1(1)
C(2)	13(1)	16(1)	14(2)	-2(1)	-2(1)	-1(1)
C(3)	12(1)	15(1)	17(1)	3(1)	1(1)	1(1)
C(4)	14(1)	20(1)	22(1)	0(1)	-2(1)	0(1)
C(5)	17(1)	19(1)	29(1)	7(1)	1(1)	1(1)
C(6)	18(1)	15(1)	39(2)	3(2)	1(2)	-3(1)
C(7)	15(1)	20(1)	26(1)	-5(1)	1(1)	-2(1)
C(8)	14(1)	18(1)	18(1)	-4(1)	2(1)	3(1)
C(9)	24(1)	19(1)	18(1)	-2(1)	-3(1)	-2(1)
C(10)	22(1)	19(1)	15(1)	-1(1)	2(1)	0(1)
C(11)	14(1)	19(1)	21(1)	4(1)	1(1)	2(1)
C(12)	14(1)	16(1)	19(1)	1(1)	0(1)	2(1)
C(13)	21(1)	19(1)	18(1)	0(1)	3(1)	3(1)
C(14)	24(1)	25(1)	20(1)	4(1)	5(1)	-1(1)
C(15)	18(1)	16(1)	28(1)	4(1)	-1(1)	-1(1)
C(16)	38(2)	19(1)	44(2)	-2(1)	3(2)	2(1)
C(17)	21(1)	19(1)	29(1)	-3(1)	5(1)	4(1)
C(18)	20(1)	20(1)	22(1)	2(1)	7(1)	4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for d12115.

	x	y	z	U(eq)
H(1A)	2004	7457	8539	19
H(4A)	163	8851	5027	22
H(5A)	539	10219	4740	26
H(6A)	1425	10853	7237	29
H(7A)	1938	10114	10026	24
H(9A)	2445	8558	10818	24
H(9B)	1609	8876	12213	24
H(10A)	107	7561	5004	28
H(10B)	492	6748	6018	28
H(10C)	1212	7415	5202	28
H(11A)	-293	7829	10370	21
H(11B)	-433	7007	9144	21
H(13A)	565	6572	12252	23
H(14A)	456	5177	13000	28
H(16A)	1482	3317	8137	40
H(16B)	2381	3565	9456	40
H(18A)	2033	6085	7130	25

Table 6. Torsion angles [°] for d12115.

C(9)-O(1)-C(1)-C(12)	163.36(19)
C(9)-O(1)-C(1)-C(2)	-70.9(2)
O(1)-C(1)-C(2)-C(10)	177.81(19)
C(12)-C(1)-C(2)-C(10)	-61.5(3)
O(1)-C(1)-C(2)-C(11)	-61.9(2)
C(12)-C(1)-C(2)-C(11)	58.7(2)
O(1)-C(1)-C(2)-C(3)	57.8(2)
C(12)-C(1)-C(2)-C(3)	178.5(2)
C(10)-C(2)-C(3)-C(8)	-143.4(2)
C(11)-C(2)-C(3)-C(8)	92.0(3)
C(1)-C(2)-C(3)-C(8)	-25.2(3)
C(10)-C(2)-C(3)-C(4)	34.4(3)
C(11)-C(2)-C(3)-C(4)	-90.2(3)
C(1)-C(2)-C(3)-C(4)	152.7(2)
C(8)-C(3)-C(4)-C(5)	-0.5(4)
C(2)-C(3)-C(4)-C(5)	-178.4(2)
C(3)-C(4)-C(5)-C(6)	0.2(4)
C(4)-C(5)-C(6)-C(7)	0.1(4)
C(5)-C(6)-C(7)-C(8)	-0.1(4)
C(4)-C(3)-C(8)-C(7)	0.5(4)
C(2)-C(3)-C(8)-C(7)	178.4(2)
C(4)-C(3)-C(8)-C(9)	-175.6(2)
C(2)-C(3)-C(8)-C(9)	2.3(4)
C(6)-C(7)-C(8)-C(3)	-0.2(4)
C(6)-C(7)-C(8)-C(9)	176.0(2)
C(1)-O(1)-C(9)-C(8)	44.7(3)
C(3)-C(8)-C(9)-O(1)	-10.2(3)
C(7)-C(8)-C(9)-O(1)	173.7(2)
C(10)-C(2)-C(11)-I(1)	-63.4(2)
C(3)-C(2)-C(11)-I(1)	61.3(2)
C(1)-C(2)-C(11)-I(1)	177.85(15)
O(1)-C(1)-C(12)-C(13)	29.5(3)
C(2)-C(1)-C(12)-C(13)	-91.8(3)
O(1)-C(1)-C(12)-C(18)	-148.9(2)

C(2)-C(1)-C(12)-C(18)	89.7(3)
C(18)-C(12)-C(13)-C(14)	0.1(4)
C(1)-C(12)-C(13)-C(14)	-178.3(2)
C(12)-C(13)-C(14)-C(15)	-0.7(4)
C(13)-C(14)-C(15)-C(17)	0.4(4)
C(13)-C(14)-C(15)-O(2)	-178.2(3)
C(16)-O(2)-C(15)-C(17)	8.1(3)
C(16)-O(2)-C(15)-C(14)	-173.2(3)
C(15)-O(2)-C(16)-O(3)	-14.0(3)
C(17)-O(3)-C(16)-O(2)	14.6(3)
C(14)-C(15)-C(17)-C(18)	0.4(4)
O(2)-C(15)-C(17)-C(18)	179.2(2)
C(14)-C(15)-C(17)-O(3)	-177.8(3)
O(2)-C(15)-C(17)-O(3)	1.0(3)
C(16)-O(3)-C(17)-C(15)	-9.7(3)
C(16)-O(3)-C(17)-C(18)	172.2(3)
C(15)-C(17)-C(18)-C(12)	-0.9(4)
O(3)-C(17)-C(18)-C(12)	177.0(3)
C(13)-C(12)-C(18)-C(17)	0.6(4)
C(1)-C(12)-C(18)-C(17)	179.1(2)

Symmetry transformations used to generate equivalent atoms:

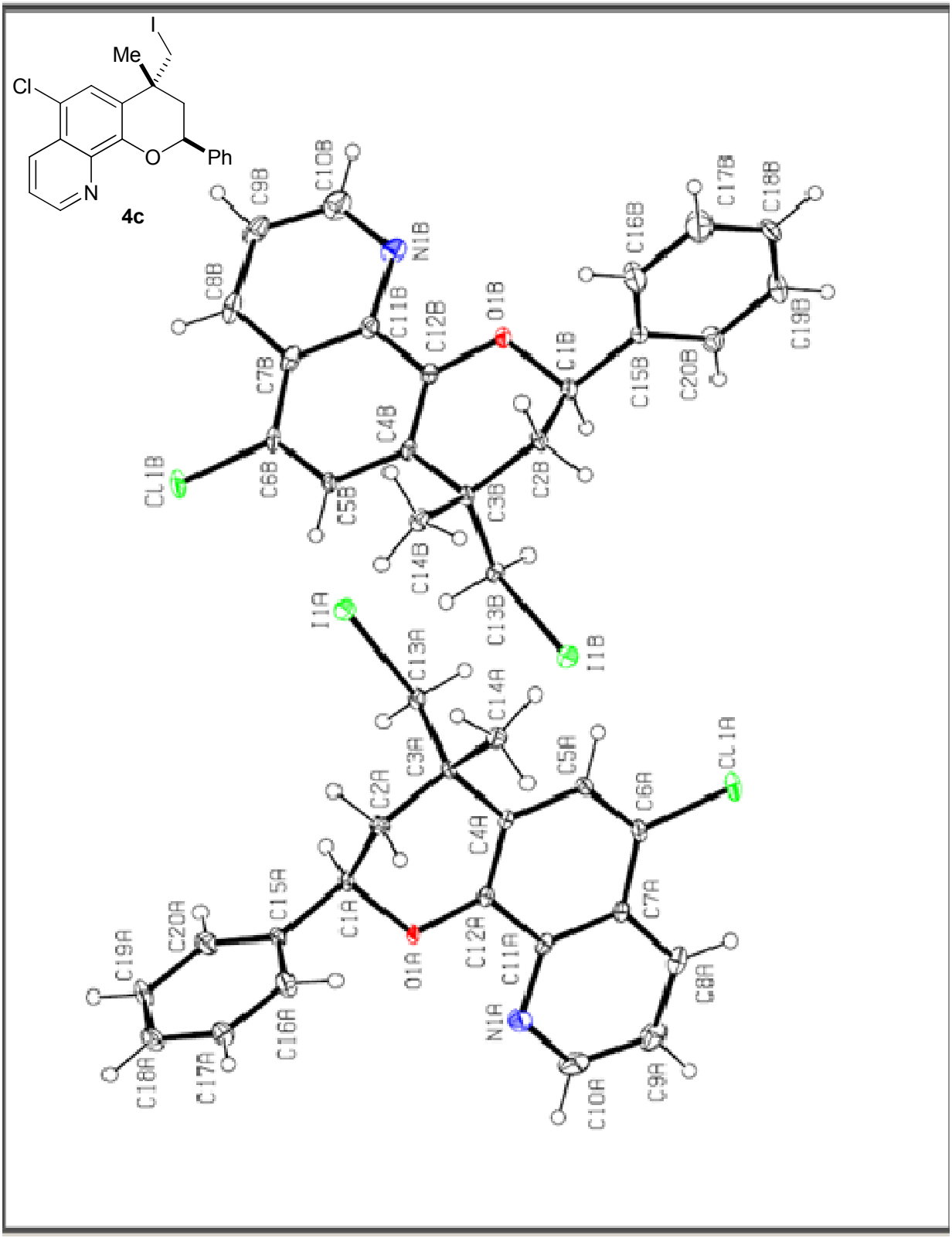
I
Me
Cl
O
Ph
N
4c
C10B
C9B
N1B
C8B
C11B
C12B
O1B
C1B
C16B
C17B
C18B
C19B
C20B
C15B
C7B
C4B
C6B
C5B
C3B
C2B
CL1B
C14B
C13B
I1B
I1A
C13A
C14A
C3A
C2A
C5A
C6A
CL1A
C4A
C7A
C8A
C1A
C15A
C20A
C19A
C18A
C17A
C16A
O1A
C12A
C11A
N1A
C10A
C9A

Table 1. Crystal data and structure refinement for d12196.

Identification code	d12196	
Empirical formula	C20 H17 Cl I N O	
Formula weight	449.70	
Temperature	147(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.3159(14) Å	α= 91.746(3)°.
	b = 11.7847(18) Å	β= 99.673(4)°.
	c = 15.718(2) Å	γ = 90.051(4)°.
Volume	1700.2(4) $Å^3$	
Z	4	
Density (calculated)	1.757 Mg/m^3	
Absorption coefficient	2.047 mm^{-1}	
F(000)	888	
Crystal size	0.25 x 0.14 x 0.13 mm^3	
Theta range for data collection	1.31 to 27.68°.	
Index ranges	-12<=h<=11, -15<=k<=15, -20<=l<=20	
Reflections collected	24722	
Independent reflections	7601 [R(int) = 0.0305]	
Completeness to theta = 25.00°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.6247	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7601 / 0 / 435	
Goodness-of-fit on F^2	1.074	
Final R indices [I>2sigma(I)]	R1 = 0.0445, wR2 = 0.1161	
R indices (all data)	R1 = 0.0546, wR2 = 0.1188	
Largest diff. peak and hole	2.791 and -1.118 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d12196. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1B)	6805(1)	6073(1)	5344(1)	22(1)
Cl(1B)	3329(2)	11234(1)	3324(1)	29(1)
O(1B)	4281(4)	6674(3)	1915(2)	18(1)
N(1B)	2598(4)	8077(4)	922(3)	23(1)
C(1B)	4941(5)	5819(4)	2497(3)	19(1)
C(2B)	6299(5)	6300(4)	3062(3)	16(1)
C(3B)	5969(5)	7326(4)	3607(3)	15(1)
C(4B)	4834(5)	8068(4)	3077(3)	14(1)
C(5B)	4554(5)	9174(4)	3389(3)	16(1)
C(6B)	3653(5)	9898(4)	2894(3)	19(1)
C(7B)	2997(5)	9593(4)	2040(3)	20(1)
C(8B)	2158(5)	10333(5)	1460(4)	25(1)
C(9B)	1657(6)	9937(5)	640(4)	33(1)
C(10B)	1861(6)	8813(5)	408(4)	32(1)
C(11B)	3210(5)	8475(4)	1734(3)	19(1)
C(12B)	4131(5)	7713(4)	2271(3)	16(1)
C(13B)	5322(5)	6980(4)	4397(3)	17(1)
C(14B)	7381(5)	8016(4)	3895(3)	20(1)
C(15B)	5210(6)	4812(4)	1946(3)	20(1)
C(16B)	6208(9)	4860(6)	1386(5)	50(2)
C(17B)	6440(9)	3935(6)	873(5)	56(2)
C(18B)	5696(6)	2942(5)	913(3)	28(1)
C(19B)	4744(6)	2867(5)	1483(4)	32(1)
C(20B)	4496(6)	3792(5)	1997(4)	26(1)
I(1A)	1616(1)	8997(1)	4618(1)	22(1)
Cl(1A)	-697(1)	3730(1)	6492(1)	27(1)
O(1A)	864(4)	8282(3)	7998(2)	16(1)
N(1A)	-424(5)	6849(4)	8883(3)	25(1)
C(1A)	1238(5)	9164(4)	7440(3)	16(1)
C(2A)	2327(5)	8697(4)	6904(3)	18(1)
C(3A)	1734(5)	7688(4)	6320(3)	15(1)

C(4A)	889(5)	6910(4)	6828(3)	14(1)
C(5A)	476(5)	5806(4)	6494(3)	16(1)
C(6A)	-189(5)	5069(4)	6946(3)	18(1)
C(7A)	-507(5)	5363(4)	7768(3)	16(1)
C(8A)	-1160(5)	4623(5)	8275(4)	26(1)
C(9A)	-1422(6)	5006(5)	9052(4)	33(1)
C(10A)	-1042(6)	6119(5)	9330(4)	33(1)
C(11A)	-132(5)	6466(4)	8103(3)	17(1)
C(12A)	553(5)	7248(4)	7612(3)	15(1)
C(13A)	651(5)	8046(4)	5535(3)	17(1)
C(14A)	3024(5)	7037(4)	6046(3)	19(1)
C(15A)	1806(5)	10158(4)	8024(3)	16(1)
C(16A)	3149(6)	10115(5)	8556(3)	25(1)
C(17A)	3675(6)	11036(5)	9078(3)	26(1)
C(18A)	2867(6)	11990(5)	9092(3)	29(1)
C(19A)	1539(6)	12052(5)	8571(4)	29(1)
C(20A)	1005(6)	11131(5)	8041(3)	23(1)

Table 3. Bond lengths [Å] and angles [°] for d12196.

I(1B)-C(13B)	2.163(5)
Cl(1B)-C(6B)	1.741(5)
O(1B)-C(12B)	1.348(6)
O(1B)-C(1B)	1.449(6)
N(1B)-C(10B)	1.317(7)
N(1B)-C(11B)	1.375(6)
C(1B)-C(15B)	1.494(7)
C(1B)-C(2B)	1.517(6)
C(1B)-H(1BA)	1.0000
C(2B)-C(3B)	1.521(6)
C(2B)-H(2BA)	0.9900
C(2B)-H(2BB)	0.9900
C(3B)-C(4B)	1.525(6)
C(3B)-C(13B)	1.534(6)
C(3B)-C(14B)	1.540(6)
C(4B)-C(12B)	1.377(7)
C(4B)-C(5B)	1.419(6)
C(5B)-C(6B)	1.364(7)
C(5B)-H(5BA)	0.9500
C(6B)-C(7B)	1.414(7)
C(7B)-C(11B)	1.414(7)
C(7B)-C(8B)	1.419(7)
C(8B)-C(9B)	1.363(8)
C(8B)-H(8BA)	0.9500
C(9B)-C(10B)	1.384(9)
C(9B)-H(9BA)	0.9500
C(10B)-H(10A)	0.9500
C(11B)-C(12B)	1.435(7)
C(13B)-H(13A)	0.9900
C(13B)-H(13B)	0.9900
C(14B)-H(14A)	0.9800
C(14B)-H(14B)	0.9800
C(14B)-H(14C)	0.9800
C(15B)-C(20B)	1.384(7)

C(15B)-C(16B)	1.386(8)
C(16B)-C(17B)	1.375(9)
C(16B)-H(16A)	0.9500
C(17B)-C(18B)	1.368(9)
C(17B)-H(17A)	0.9500
C(18B)-C(19B)	1.367(8)
C(18B)-H(18A)	0.9500
C(19B)-C(20B)	1.380(8)
C(19B)-H(19A)	0.9500
C(20B)-H(20A)	0.9500
I(1A)-C(13A)	2.162(4)
Cl(1A)-C(6A)	1.743(5)
O(1A)-C(12A)	1.354(6)
O(1A)-C(1A)	1.459(5)
N(1A)-C(10A)	1.318(7)
N(1A)-C(11A)	1.363(6)
C(1A)-C(15A)	1.505(6)
C(1A)-C(2A)	1.517(7)
C(1A)-H(1AA)	1.0000
C(2A)-C(3A)	1.525(6)
C(2A)-H(2AA)	0.9900
C(2A)-H(2AB)	0.9900
C(3A)-C(13A)	1.527(6)
C(3A)-C(4A)	1.534(6)
C(3A)-C(14A)	1.541(7)
C(4A)-C(12A)	1.368(7)
C(4A)-C(5A)	1.416(6)
C(5A)-C(6A)	1.352(6)
C(5A)-H(5AA)	0.9500
C(6A)-C(7A)	1.407(7)
C(7A)-C(8A)	1.404(7)
C(7A)-C(11A)	1.409(7)
C(8A)-C(9A)	1.350(8)
C(8A)-H(8AA)	0.9500
C(9A)-C(10A)	1.396(9)
C(9A)-H(9AA)	0.9500

C(10A)-H(10B)	0.9500
C(11A)-C(12A)	1.435(6)
C(13A)-H(13C)	0.9900
C(13A)-H(13D)	0.9900
C(14A)-H(14D)	0.9800
C(14A)-H(14E)	0.9800
C(14A)-H(14F)	0.9800
C(15A)-C(20A)	1.371(7)
C(15A)-C(16A)	1.386(7)
C(16A)-C(17A)	1.378(7)
C(16A)-H(16B)	0.9500
C(17A)-C(18A)	1.355(8)
C(17A)-H(17B)	0.9500
C(18A)-C(19A)	1.368(8)
C(18A)-H(18B)	0.9500
C(19A)-C(20A)	1.387(7)
C(19A)-H(19B)	0.9500
C(20A)-H(20B)	0.9500

C(12B)-O(1B)-C(1B)	116.2(4)
C(10B)-N(1B)-C(11B)	116.7(5)
O(1B)-C(1B)-C(15B)	106.5(4)
O(1B)-C(1B)-C(2B)	109.9(4)
C(15B)-C(1B)-C(2B)	114.2(4)
O(1B)-C(1B)-H(1BA)	108.7
C(15B)-C(1B)-H(1BA)	108.7
C(2B)-C(1B)-H(1BA)	108.7
C(1B)-C(2B)-C(3B)	112.2(4)
C(1B)-C(2B)-H(2BA)	109.2
C(3B)-C(2B)-H(2BA)	109.2
C(1B)-C(2B)-H(2BB)	109.2
C(3B)-C(2B)-H(2BB)	109.2
H(2BA)-C(2B)-H(2BB)	107.9
C(2B)-C(3B)-C(4B)	109.9(4)
C(2B)-C(3B)-C(13B)	111.9(4)
C(4B)-C(3B)-C(13B)	106.4(4)

C(2B)-C(3B)-C(14B)	108.9(4)
C(4B)-C(3B)-C(14B)	109.5(4)
C(13B)-C(3B)-C(14B)	110.2(4)
C(12B)-C(4B)-C(5B)	118.8(4)
C(12B)-C(4B)-C(3B)	121.2(4)
C(5B)-C(4B)-C(3B)	119.9(4)
C(6B)-C(5B)-C(4B)	121.2(5)
C(6B)-C(5B)-H(5BA)	119.4
C(4B)-C(5B)-H(5BA)	119.4
C(5B)-C(6B)-C(7B)	121.5(5)
C(5B)-C(6B)-Cl(1B)	118.9(4)
C(7B)-C(6B)-Cl(1B)	119.6(4)
C(11B)-C(7B)-C(6B)	117.8(4)
C(11B)-C(7B)-C(8B)	117.4(5)
C(6B)-C(7B)-C(8B)	124.7(5)
C(9B)-C(8B)-C(7B)	118.2(5)
C(9B)-C(8B)-H(8BA)	120.9
C(7B)-C(8B)-H(8BA)	120.9
C(8B)-C(9B)-C(10B)	120.4(5)
C(8B)-C(9B)-H(9BA)	119.8
C(10B)-C(9B)-H(9BA)	119.8
N(1B)-C(10B)-C(9B)	124.2(5)
N(1B)-C(10B)-H(10A)	117.9
C(9B)-C(10B)-H(10A)	117.9
N(1B)-C(11B)-C(7B)	122.9(5)
N(1B)-C(11B)-C(12B)	117.3(5)
C(7B)-C(11B)-C(12B)	119.9(4)
O(1B)-C(12B)-C(4B)	124.2(4)
O(1B)-C(12B)-C(11B)	115.2(4)
C(4B)-C(12B)-C(11B)	120.5(4)
C(3B)-C(13B)-I(1B)	114.5(3)
C(3B)-C(13B)-H(13A)	108.6
I(1B)-C(13B)-H(13A)	108.6
C(3B)-C(13B)-H(13B)	108.6
I(1B)-C(13B)-H(13B)	108.6
H(13A)-C(13B)-H(13B)	107.6

C(3B)-C(14B)-H(14A)	109.5
C(3B)-C(14B)-H(14B)	109.5
H(14A)-C(14B)-H(14B)	109.5
C(3B)-C(14B)-H(14C)	109.5
H(14A)-C(14B)-H(14C)	109.5
H(14B)-C(14B)-H(14C)	109.5
C(20B)-C(15B)-C(16B)	118.0(5)
C(20B)-C(15B)-C(1B)	120.9(5)
C(16B)-C(15B)-C(1B)	121.2(5)
C(17B)-C(16B)-C(15B)	120.9(6)
C(17B)-C(16B)-H(16A)	119.5
C(15B)-C(16B)-H(16A)	119.5
C(18B)-C(17B)-C(16B)	120.4(6)
C(18B)-C(17B)-H(17A)	119.8
C(16B)-C(17B)-H(17A)	119.8
C(17B)-C(18B)-C(19B)	119.4(6)
C(17B)-C(18B)-H(18A)	120.3
C(19B)-C(18B)-H(18A)	120.3
C(18B)-C(19B)-C(20B)	120.6(5)
C(18B)-C(19B)-H(19A)	119.7
C(20B)-C(19B)-H(19A)	119.7
C(19B)-C(20B)-C(15B)	120.6(5)
C(19B)-C(20B)-H(20A)	119.7
C(15B)-C(20B)-H(20A)	119.7
C(12A)-O(1A)-C(1A)	115.7(3)
C(10A)-N(1A)-C(11A)	116.5(5)
O(1A)-C(1A)-C(15A)	106.5(4)
O(1A)-C(1A)-C(2A)	109.3(4)
C(15A)-C(1A)-C(2A)	113.7(4)
O(1A)-C(1A)-H(1AA)	109.1
C(15A)-C(1A)-H(1AA)	109.1
C(2A)-C(1A)-H(1AA)	109.1
C(1A)-C(2A)-C(3A)	112.9(4)
C(1A)-C(2A)-H(2AA)	109.0
C(3A)-C(2A)-H(2AA)	109.0
C(1A)-C(2A)-H(2AB)	109.0

C(3A)-C(2A)-H(2AB)	109.0
H(2AA)-C(2A)-H(2AB)	107.8
C(2A)-C(3A)-C(13A)	112.3(4)
C(2A)-C(3A)-C(4A)	108.6(4)
C(13A)-C(3A)-C(4A)	106.1(3)
C(2A)-C(3A)-C(14A)	108.7(4)
C(13A)-C(3A)-C(14A)	111.2(4)
C(4A)-C(3A)-C(14A)	109.7(4)
C(12A)-C(4A)-C(5A)	119.0(4)
C(12A)-C(4A)-C(3A)	121.4(4)
C(5A)-C(4A)-C(3A)	119.6(4)
C(6A)-C(5A)-C(4A)	121.5(4)
C(6A)-C(5A)-H(5AA)	119.3
C(4A)-C(5A)-H(5AA)	119.3
C(5A)-C(6A)-C(7A)	121.6(4)
C(5A)-C(6A)-Cl(1A)	119.3(4)
C(7A)-C(6A)-Cl(1A)	119.0(4)
C(8A)-C(7A)-C(6A)	124.1(5)
C(8A)-C(7A)-C(11A)	118.2(4)
C(6A)-C(7A)-C(11A)	117.7(4)
C(9A)-C(8A)-C(7A)	118.6(5)
C(9A)-C(8A)-H(8AA)	120.7
C(7A)-C(8A)-H(8AA)	120.7
C(8A)-C(9A)-C(10A)	119.6(5)
C(8A)-C(9A)-H(9AA)	120.2
C(10A)-C(9A)-H(9AA)	120.2
N(1A)-C(10A)-C(9A)	124.5(5)
N(1A)-C(10A)-H(10B)	117.8
C(9A)-C(10A)-H(10B)	117.8
N(1A)-C(11A)-C(7A)	122.5(4)
N(1A)-C(11A)-C(12A)	117.2(4)
C(7A)-C(11A)-C(12A)	120.2(4)
O(1A)-C(12A)-C(4A)	125.0(4)
O(1A)-C(12A)-C(11A)	115.0(4)
C(4A)-C(12A)-C(11A)	120.0(4)
C(3A)-C(13A)-I(1A)	114.1(3)

C(3A)-C(13A)-H(13C)	108.7
I(1A)-C(13A)-H(13C)	108.7
C(3A)-C(13A)-H(13D)	108.7
I(1A)-C(13A)-H(13D)	108.7
H(13C)-C(13A)-H(13D)	107.6
C(3A)-C(14A)-H(14D)	109.5
C(3A)-C(14A)-H(14E)	109.5
H(14D)-C(14A)-H(14E)	109.5
C(3A)-C(14A)-H(14F)	109.5
H(14D)-C(14A)-H(14F)	109.5
H(14E)-C(14A)-H(14F)	109.5
C(20A)-C(15A)-C(16A)	118.3(5)
C(20A)-C(15A)-C(1A)	120.7(4)
C(16A)-C(15A)-C(1A)	121.0(5)
C(17A)-C(16A)-C(15A)	120.7(5)
C(17A)-C(16A)-H(16B)	119.7
C(15A)-C(16A)-H(16B)	119.7
C(18A)-C(17A)-C(16A)	120.4(5)
C(18A)-C(17A)-H(17B)	119.8
C(16A)-C(17A)-H(17B)	119.8
C(17A)-C(18A)-C(19A)	119.9(5)
C(17A)-C(18A)-H(18B)	120.1
C(19A)-C(18A)-H(18B)	120.1
C(18A)-C(19A)-C(20A)	120.1(5)
C(18A)-C(19A)-H(19B)	120.0
C(20A)-C(19A)-H(19B)	120.0
C(15A)-C(20A)-C(19A)	120.6(5)
C(15A)-C(20A)-H(20B)	119.7
C(19A)-C(20A)-H(20B)	119.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for d12196. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(1B)	27(1)	18(1)	20(1)	3(1)	2(1)	3(1)
Cl(1B)	36(1)	11(1)	40(1)	-2(1)	11(1)	5(1)
O(1B)	23(2)	12(2)	20(2)	1(1)	1(1)	-2(1)
N(1B)	18(2)	26(2)	23(2)	5(2)	-5(2)	-2(2)
C(1B)	23(2)	10(2)	23(2)	2(2)	6(2)	0(2)
C(2B)	13(2)	14(2)	22(2)	-4(2)	8(2)	1(2)
C(3B)	17(2)	11(2)	16(2)	-1(2)	3(2)	-2(2)
C(4B)	14(2)	12(2)	19(2)	4(2)	6(2)	1(2)
C(5B)	20(2)	10(2)	20(2)	0(2)	8(2)	-2(2)
C(6B)	19(2)	9(2)	31(3)	3(2)	9(2)	0(2)
C(7B)	13(2)	17(3)	30(3)	10(2)	5(2)	1(2)
C(8B)	16(2)	17(3)	42(3)	11(2)	0(2)	-1(2)
C(9B)	26(3)	32(3)	37(3)	16(3)	-8(2)	-3(2)
C(10B)	26(3)	34(3)	33(3)	7(3)	-6(2)	-4(2)
C(11B)	17(2)	18(2)	23(2)	3(2)	4(2)	-5(2)
C(12B)	14(2)	11(2)	22(2)	3(2)	6(2)	-2(2)
C(13B)	16(2)	17(2)	19(2)	2(2)	4(2)	1(2)
C(14B)	18(2)	20(3)	23(2)	4(2)	2(2)	-4(2)
C(15B)	30(3)	15(2)	16(2)	0(2)	4(2)	-1(2)
C(16B)	87(5)	23(3)	52(4)	-6(3)	46(4)	-9(3)
C(17B)	90(6)	33(4)	57(5)	2(3)	47(4)	1(4)
C(18B)	39(3)	21(3)	23(3)	-9(2)	-1(2)	8(2)
C(19B)	30(3)	18(3)	47(4)	-6(3)	3(3)	-4(2)
C(20B)	26(3)	20(3)	32(3)	-2(2)	8(2)	-5(2)
I(1A)	30(1)	18(1)	19(1)	3(1)	7(1)	-3(1)
Cl(1A)	32(1)	12(1)	37(1)	-4(1)	6(1)	-7(1)
O(1A)	27(2)	8(2)	16(2)	-1(1)	10(1)	-4(1)
N(1A)	31(2)	23(2)	24(2)	-1(2)	11(2)	-2(2)
C(1A)	23(2)	9(2)	19(2)	0(2)	6(2)	-3(2)
C(2A)	21(2)	16(2)	17(2)	-2(2)	5(2)	-6(2)
C(3A)	18(2)	11(2)	16(2)	-2(2)	5(2)	-2(2)

C(4A)	14(2)	12(2)	17(2)	3(2)	2(2)	0(2)
C(5A)	17(2)	14(2)	15(2)	-2(2)	1(2)	-1(2)
C(6A)	16(2)	11(2)	24(2)	-2(2)	-2(2)	1(2)
C(7A)	14(2)	11(2)	22(2)	3(2)	1(2)	3(2)
C(8A)	21(2)	19(3)	37(3)	8(2)	3(2)	-1(2)
C(9A)	32(3)	34(3)	37(3)	12(3)	17(2)	-4(2)
C(10A)	38(3)	42(4)	25(3)	6(3)	20(2)	-4(3)
C(11A)	15(2)	17(2)	19(2)	6(2)	6(2)	0(2)
C(12A)	14(2)	12(2)	18(2)	2(2)	3(2)	-1(2)
C(13A)	20(2)	14(2)	19(2)	0(2)	7(2)	-5(2)
C(14A)	19(2)	21(3)	19(2)	1(2)	7(2)	1(2)
C(15A)	24(2)	12(2)	16(2)	-3(2)	10(2)	-8(2)
C(16A)	29(3)	17(3)	29(3)	-4(2)	4(2)	2(2)
C(17A)	27(3)	24(3)	24(3)	-4(2)	0(2)	-6(2)
C(18A)	44(3)	21(3)	22(3)	-7(2)	7(2)	-12(2)
C(19A)	41(3)	13(3)	32(3)	-7(2)	6(2)	4(2)
C(20A)	26(3)	22(3)	21(3)	-3(2)	4(2)	3(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for d12196.

	x	y	z	U(eq)
H(1BA)	4231	5598	2875	22
H(2BA)	7007	6522	2692	19
H(2BB)	6753	5704	3448	19
H(5BA)	5003	9415	3954	20
H(8BA)	1952	11084	1638	30
H(9BA)	1163	10434	226	40
H(10A)	1444	8557	-159	38
H(13A)	4453	6497	4198	21
H(13B)	4994	7673	4679	21
H(14A)	7644	8400	3398	30
H(14B)	8168	7504	4129	30
H(14C)	7230	8582	4340	30
H(16A)	6739	5542	1355	60
H(17A)	7121	3986	488	67
H(18A)	5840	2310	547	34
H(19A)	4249	2172	1526	39
H(20A)	3829	3729	2389	31
H(1AA)	337	9397	7045	20
H(2AA)	3214	8462	7296	21
H(2AB)	2608	9307	6544	21
H(5AA)	671	5579	5940	19
H(8AA)	-1413	3868	8076	31
H(9AA)	-1861	4521	9408	39
H(10B)	-1243	6367	9878	40
H(13C)	-116	8513	5737	21
H(13D)	176	7357	5237	21
H(14D)	3565	6656	6545	29
H(14E)	3670	7570	5825	29
H(14F)	2657	6469	5592	29
H(16B)	3715	9444	8561	30

H(17B)	4608	11001	9429	31
H(18B)	3224	12615	9464	35
H(19B)	981	12726	8571	34
H(20B)	75	11175	7686	28

Table 6. Torsion angles [°] for d12196.

C(12B)-O(1B)-C(1B)-C(15B)	-171.2(4)
C(12B)-O(1B)-C(1B)-C(2B)	-47.0(5)
O(1B)-C(1B)-C(2B)-C(3B)	60.1(5)
C(15B)-C(1B)-C(2B)-C(3B)	179.7(4)
C(1B)-C(2B)-C(3B)-C(4B)	-39.5(5)
C(1B)-C(2B)-C(3B)-C(13B)	78.4(5)
C(1B)-C(2B)-C(3B)-C(14B)	-159.5(4)
C(2B)-C(3B)-C(4B)-C(12B)	7.9(6)
C(13B)-C(3B)-C(4B)-C(12B)	-113.5(5)
C(14B)-C(3B)-C(4B)-C(12B)	127.5(4)
C(2B)-C(3B)-C(4B)-C(5B)	-168.1(4)
C(13B)-C(3B)-C(4B)-C(5B)	70.5(5)
C(14B)-C(3B)-C(4B)-C(5B)	-48.5(5)
C(12B)-C(4B)-C(5B)-C(6B)	-2.6(6)
C(3B)-C(4B)-C(5B)-C(6B)	173.5(4)
C(4B)-C(5B)-C(6B)-C(7B)	-2.1(7)
C(4B)-C(5B)-C(6B)-Cl(1B)	178.8(3)
C(5B)-C(6B)-C(7B)-C(11B)	5.0(7)
Cl(1B)-C(6B)-C(7B)-C(11B)	-176.0(3)
C(5B)-C(6B)-C(7B)-C(8B)	-173.9(4)
Cl(1B)-C(6B)-C(7B)-C(8B)	5.1(7)
C(11B)-C(7B)-C(8B)-C(9B)	-2.3(7)
C(6B)-C(7B)-C(8B)-C(9B)	176.7(5)
C(7B)-C(8B)-C(9B)-C(10B)	5.3(8)
C(11B)-N(1B)-C(10B)-C(9B)	-1.0(8)
C(8B)-C(9B)-C(10B)-N(1B)	-3.8(9)
C(10B)-N(1B)-C(11B)-C(7B)	4.2(7)
C(10B)-N(1B)-C(11B)-C(12B)	-174.2(4)
C(6B)-C(7B)-C(11B)-N(1B)	178.5(4)
C(8B)-C(7B)-C(11B)-N(1B)	-2.5(7)
C(6B)-C(7B)-C(11B)-C(12B)	-3.3(6)
C(8B)-C(7B)-C(11B)-C(12B)	175.8(4)
C(1B)-O(1B)-C(12B)-C(4B)	15.0(6)
C(1B)-O(1B)-C(12B)-C(11B)	-167.4(4)

C(5B)-C(4B)-C(12B)-O(1B)	-178.3(4)
C(3B)-C(4B)-C(12B)-O(1B)	5.6(7)
C(5B)-C(4B)-C(12B)-C(11B)	4.2(6)
C(3B)-C(4B)-C(12B)-C(11B)	-171.8(4)
N(1B)-C(11B)-C(12B)-O(1B)	-0.6(6)
C(7B)-C(11B)-C(12B)-O(1B)	-179.0(4)
N(1B)-C(11B)-C(12B)-C(4B)	177.1(4)
C(7B)-C(11B)-C(12B)-C(4B)	-1.3(7)
C(2B)-C(3B)-C(13B)-I(1B)	66.6(4)
C(4B)-C(3B)-C(13B)-I(1B)	-173.4(3)
C(14B)-C(3B)-C(13B)-I(1B)	-54.7(5)
O(1B)-C(1B)-C(15B)-C(20B)	-115.6(5)
C(2B)-C(1B)-C(15B)-C(20B)	122.9(5)
O(1B)-C(1B)-C(15B)-C(16B)	66.2(7)
C(2B)-C(1B)-C(15B)-C(16B)	-55.3(7)
C(20B)-C(15B)-C(16B)-C(17B)	2.4(11)
C(1B)-C(15B)-C(16B)-C(17B)	-179.3(7)
C(15B)-C(16B)-C(17B)-C(18B)	-0.6(13)
C(16B)-C(17B)-C(18B)-C(19B)	-1.6(11)
C(17B)-C(18B)-C(19B)-C(20B)	2.0(9)
C(18B)-C(19B)-C(20B)-C(15B)	-0.2(9)
C(16B)-C(15B)-C(20B)-C(19B)	-2.0(9)
C(1B)-C(15B)-C(20B)-C(19B)	179.7(5)
C(12A)-O(1A)-C(1A)-C(15A)	-169.7(4)
C(12A)-O(1A)-C(1A)-C(2A)	-46.5(5)
O(1A)-C(1A)-C(2A)-C(3A)	61.0(5)
C(15A)-C(1A)-C(2A)-C(3A)	179.7(4)
C(1A)-C(2A)-C(3A)-C(13A)	75.2(5)
C(1A)-C(2A)-C(3A)-C(4A)	-41.8(5)
C(1A)-C(2A)-C(3A)-C(14A)	-161.2(4)
C(2A)-C(3A)-C(4A)-C(12A)	10.9(6)
C(13A)-C(3A)-C(4A)-C(12A)	-110.1(5)
C(14A)-C(3A)-C(4A)-C(12A)	129.6(5)
C(2A)-C(3A)-C(4A)-C(5A)	-167.5(4)
C(13A)-C(3A)-C(4A)-C(5A)	71.5(5)
C(14A)-C(3A)-C(4A)-C(5A)	-48.8(5)

C(12A)-C(4A)-C(5A)-C(6A)	-2.6(7)
C(3A)-C(4A)-C(5A)-C(6A)	175.8(4)
C(4A)-C(5A)-C(6A)-C(7A)	0.2(7)
C(4A)-C(5A)-C(6A)-Cl(1A)	179.0(4)
C(5A)-C(6A)-C(7A)-C(8A)	-178.3(5)
Cl(1A)-C(6A)-C(7A)-C(8A)	3.0(7)
C(5A)-C(6A)-C(7A)-C(11A)	1.1(7)
Cl(1A)-C(6A)-C(7A)-C(11A)	-177.6(3)
C(6A)-C(7A)-C(8A)-C(9A)	-179.5(5)
C(11A)-C(7A)-C(8A)-C(9A)	1.1(7)
C(7A)-C(8A)-C(9A)-C(10A)	0.1(8)
C(11A)-N(1A)-C(10A)-C(9A)	-0.8(9)
C(8A)-C(9A)-C(10A)-N(1A)	-0.3(10)
C(10A)-N(1A)-C(11A)-C(7A)	2.1(7)
C(10A)-N(1A)-C(11A)-C(12A)	-179.4(5)
C(8A)-C(7A)-C(11A)-N(1A)	-2.3(7)
C(6A)-C(7A)-C(11A)-N(1A)	178.3(4)
C(8A)-C(7A)-C(11A)-C(12A)	179.3(4)
C(6A)-C(7A)-C(11A)-C(12A)	-0.1(7)
C(1A)-O(1A)-C(12A)-C(4A)	16.2(6)
C(1A)-O(1A)-C(12A)-C(11A)	-166.2(4)
C(5A)-C(4A)-C(12A)-O(1A)	-179.0(4)
C(3A)-C(4A)-C(12A)-O(1A)	2.6(7)
C(5A)-C(4A)-C(12A)-C(11A)	3.5(7)
C(3A)-C(4A)-C(12A)-C(11A)	-174.9(4)
N(1A)-C(11A)-C(12A)-O(1A)	1.5(6)
C(7A)-C(11A)-C(12A)-O(1A)	-180.0(4)
N(1A)-C(11A)-C(12A)-C(4A)	179.2(4)
C(7A)-C(11A)-C(12A)-C(4A)	-2.2(7)
C(2A)-C(3A)-C(13A)-I(1A)	68.2(4)
C(4A)-C(3A)-C(13A)-I(1A)	-173.2(3)
C(14A)-C(3A)-C(13A)-I(1A)	-53.9(5)
O(1A)-C(1A)-C(15A)-C(20A)	-109.1(5)
C(2A)-C(1A)-C(15A)-C(20A)	130.6(5)
O(1A)-C(1A)-C(15A)-C(16A)	71.1(5)
C(2A)-C(1A)-C(15A)-C(16A)	-49.3(6)

C(20A)-C(15A)-C(16A)-C(17A)	-1.1(7)
C(1A)-C(15A)-C(16A)-C(17A)	178.8(5)
C(15A)-C(16A)-C(17A)-C(18A)	1.5(8)
C(16A)-C(17A)-C(18A)-C(19A)	-1.6(8)
C(17A)-C(18A)-C(19A)-C(20A)	1.3(8)
C(16A)-C(15A)-C(20A)-C(19A)	0.8(7)
C(1A)-C(15A)-C(20A)-C(19A)	-179.1(5)
C(18A)-C(19A)-C(20A)-C(15A)	-0.9(8)

Symmetry transformations used to generate equivalent atoms: