Skeletal Diversification via Heteroatom Linkage Control: Preparation of Bicyclic and Spirocyclic Scaffolds from *N*-Substituted Homopropargyl Alcohols

Thomas O. Painter,[†] Jonathon R. Bunn,[†] Frank J. Schoenen,[‡] Justin T. Douglas,[§†] Victor W. Day,[§] Conrad Santini[†*]

[†]Center for Chemical Methodologies and Library Development, The University of Kansas, 2034 Becker Drive, Lawrence, Kansas 66047, United States

[‡]Specialized Chemistry Center, The University of Kansas, 2034 Becker Drive, Lawrence, Kansas 66047, United States

[§]The University of Kansas Molecular Structures Group, 1251 Wescoe Hall Drive, Lawrence, Kansas, 66045 United States

Supporting Information

Table of Contents

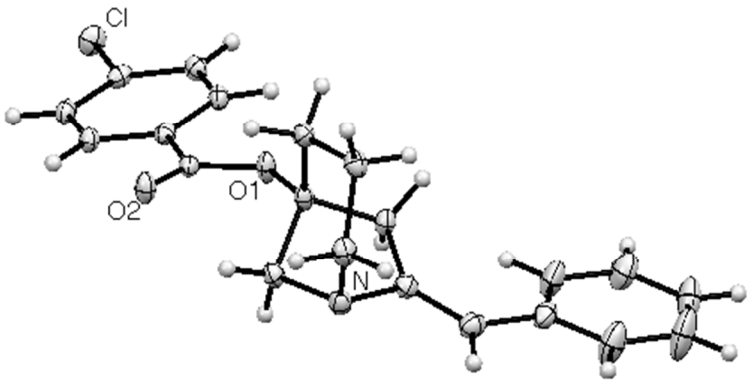


Figure S1. Structure of **10*{10,1}*** as determined by X-ray crystallography

Overall pass rate and yield trend data shown below.

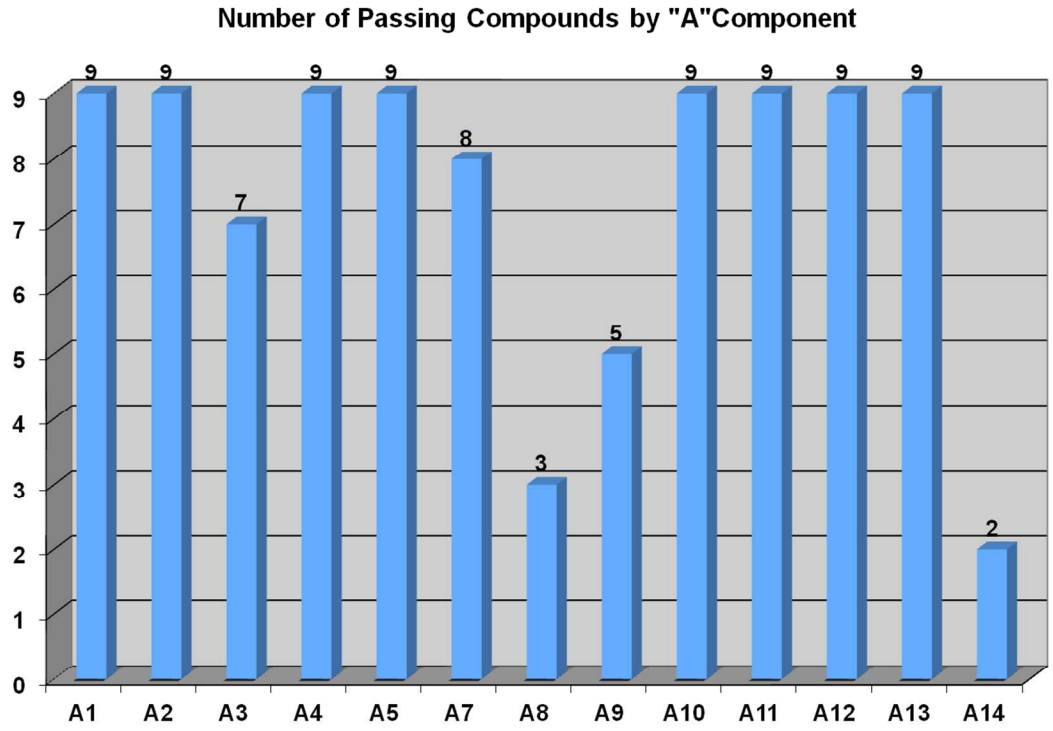
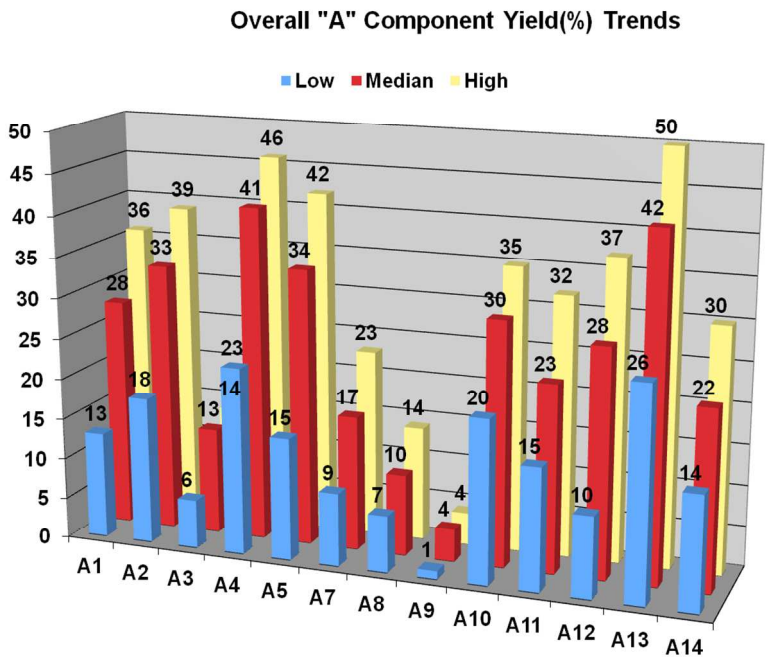
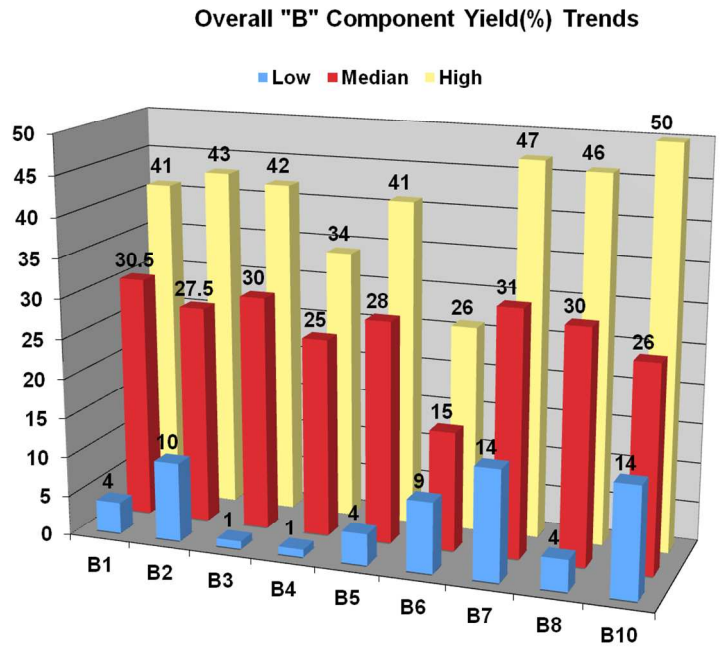


Chart S1. Number of passing compounds by "A" component

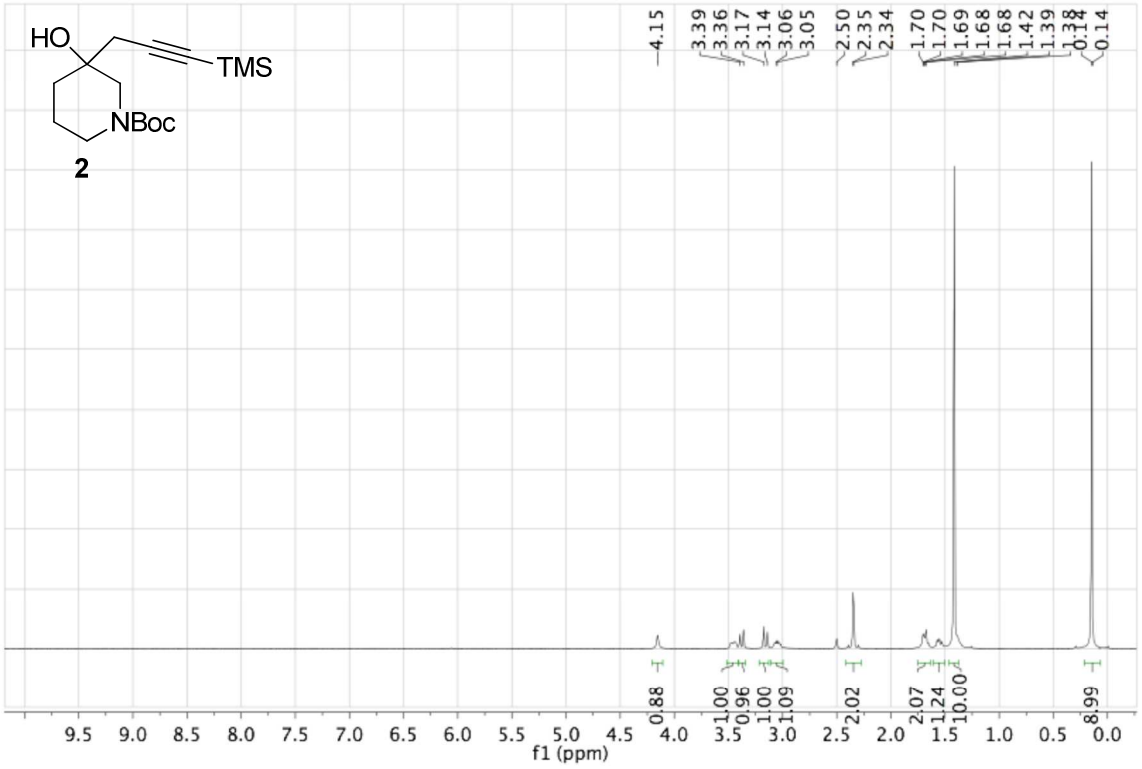


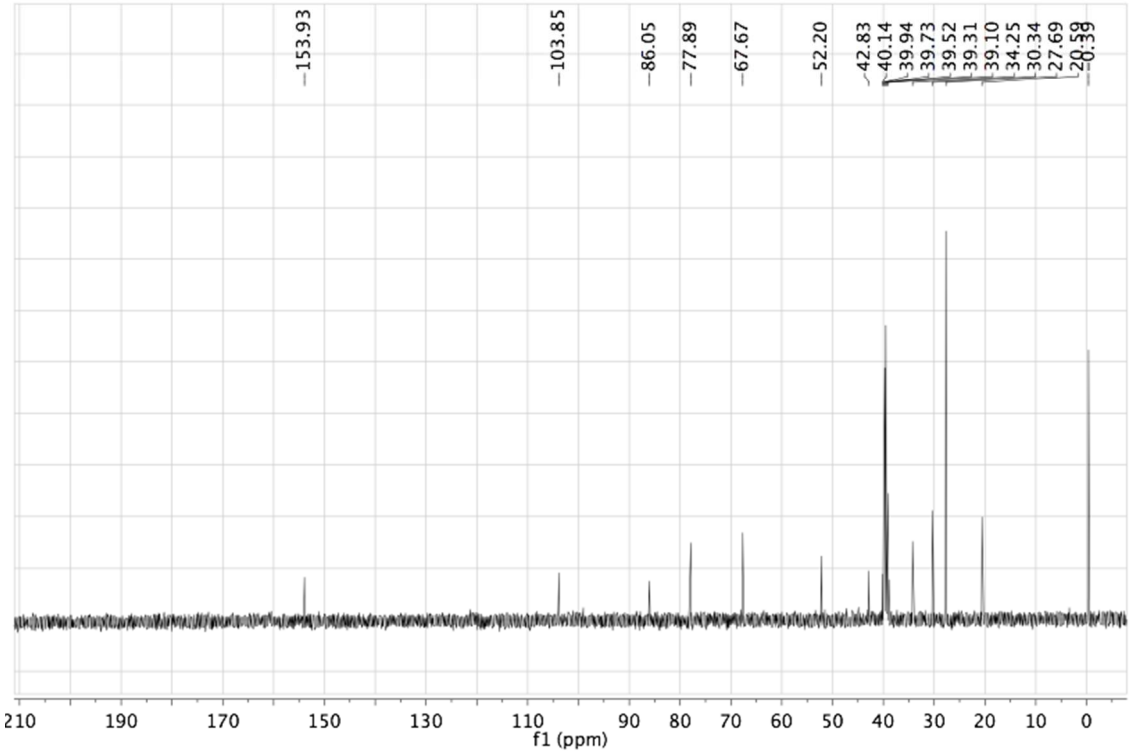


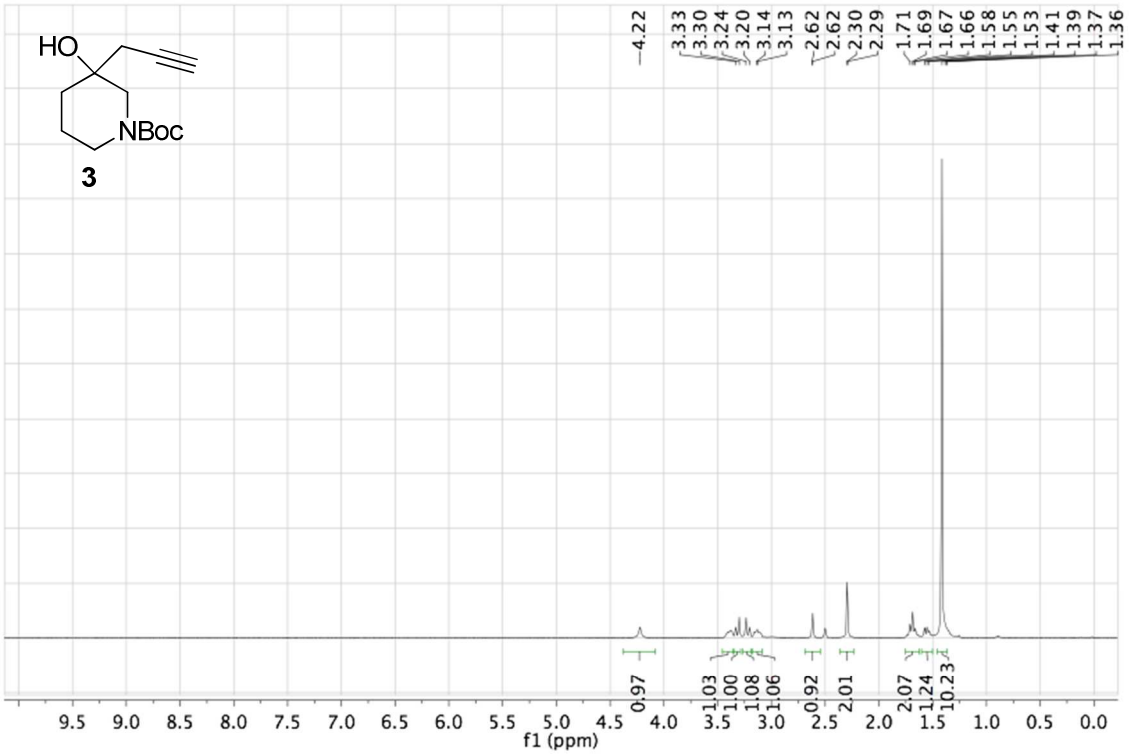
Charts S2 and S3. Yield trends of library compounds by components "A" or "B". The blue bar is the lowest yield obtained. The yellow bar is the highest yield obtained. The red bar is the median yield for each component across the range of library compounds into which they were incorporated. Based on the data, we can infer that the "A" component was more important in

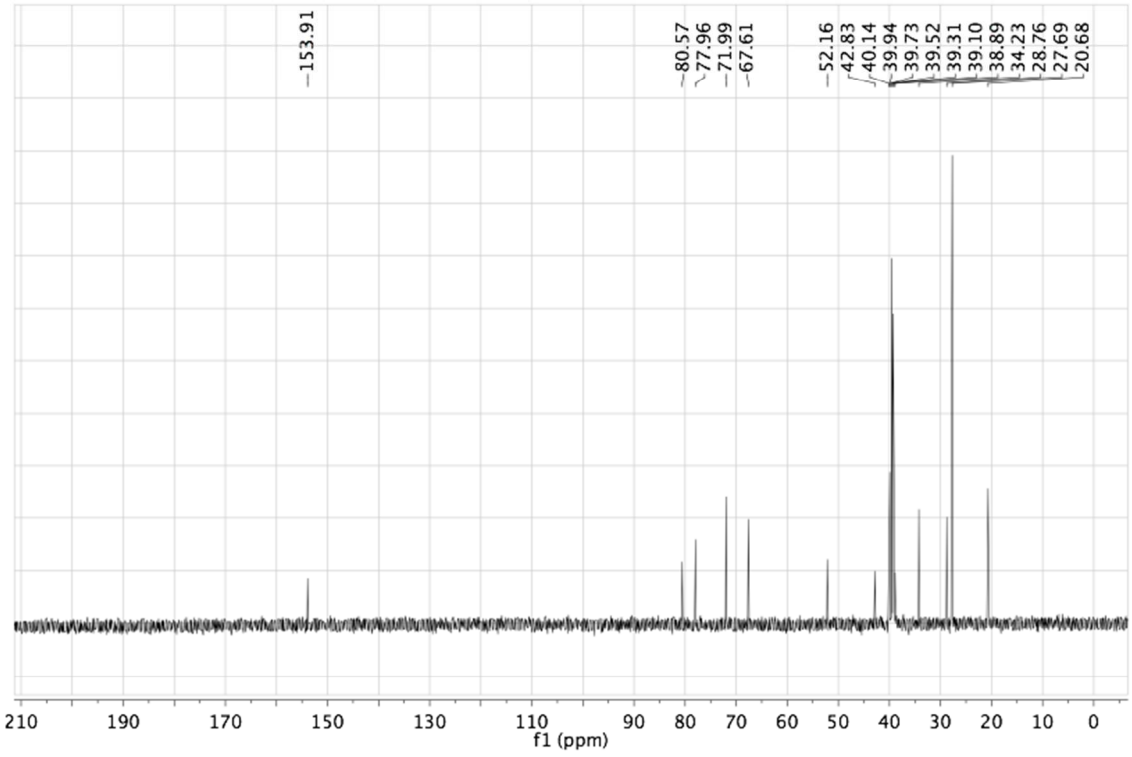
determining the yield outcome of each reaction than the "B" component due to the greater degree in yield variation. "B6" yields are lower presumably due to an extra purification step (prep TLC).

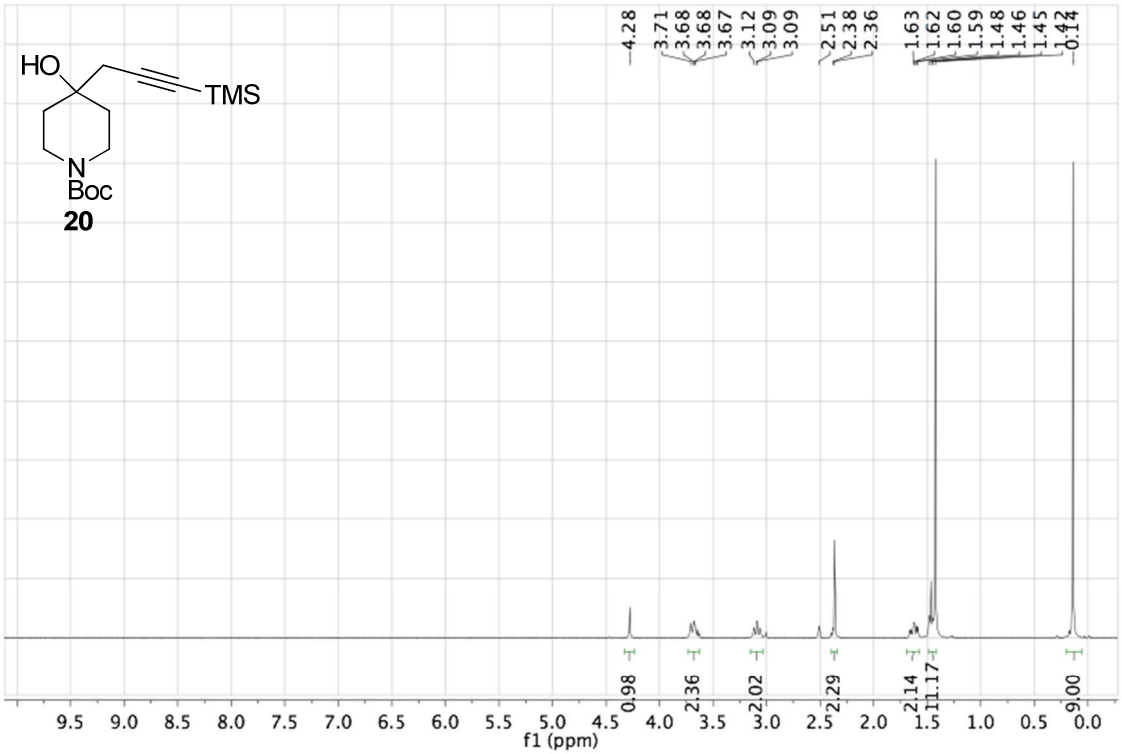
Precursor and Scaffold NMR Spectra

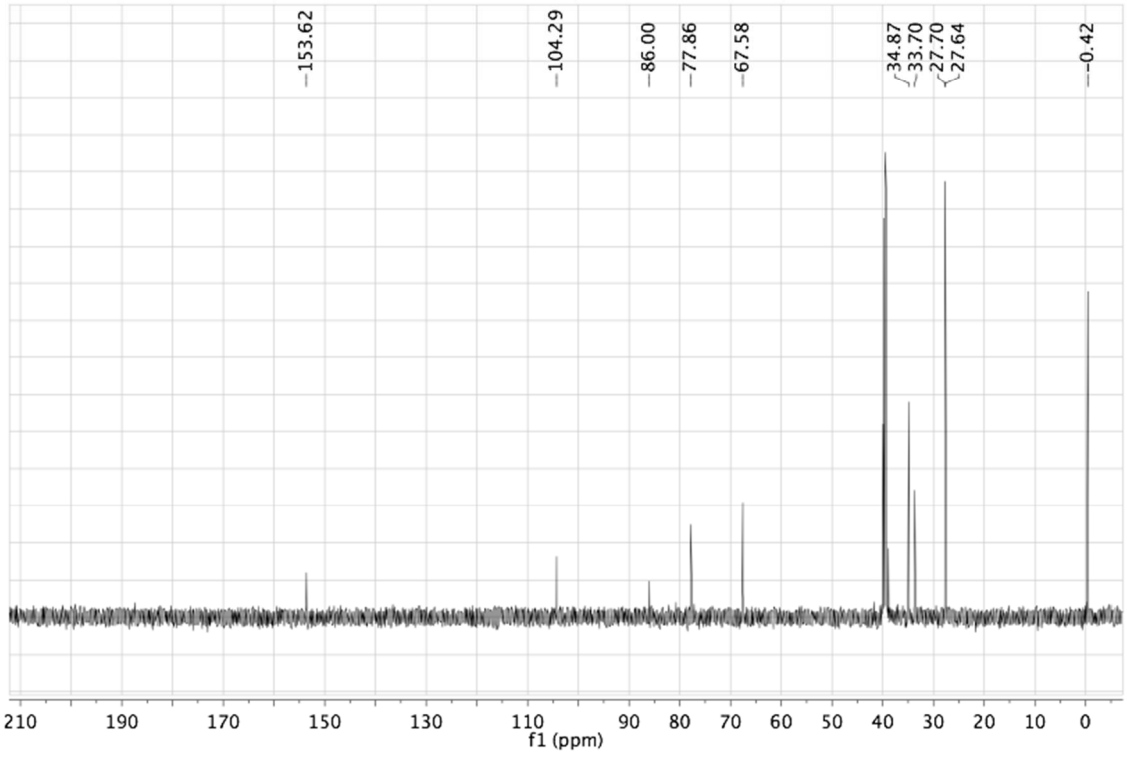


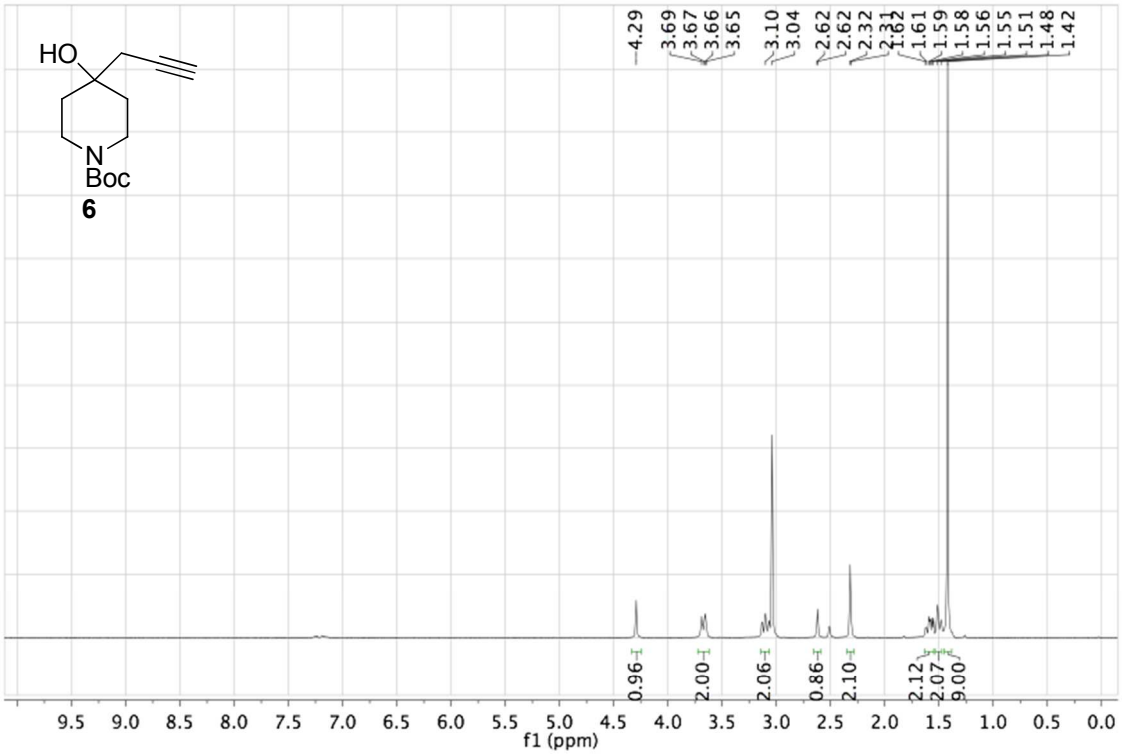


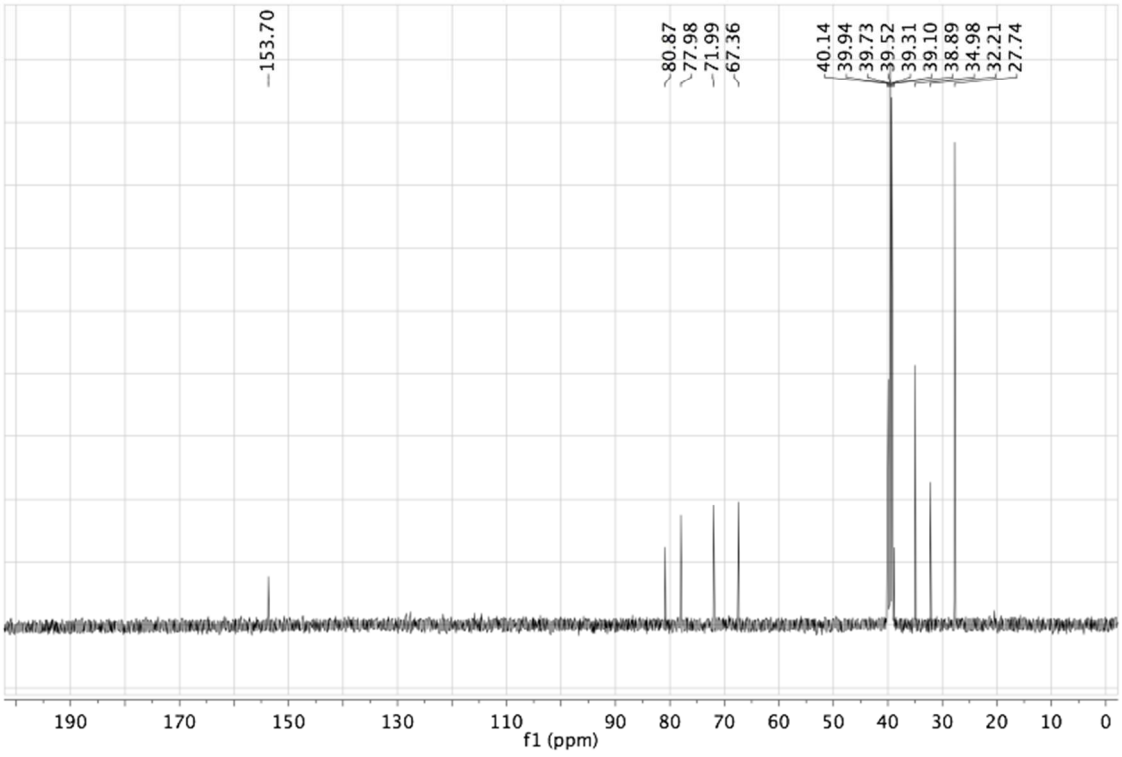

HO
NBoc
3
4.22
3.33
3.30
3.24
3.20
3.14
3.13
2.62
2.62
2.30
2.29
1.71
1.69
1.67
1.66
1.58
1.55
1.53
1.41
1.39
1.37
1.36
0.97
1.03
1.00
1.08
1.06
0.92
2.01
2.07
1.24
10.23
f1 (ppm)

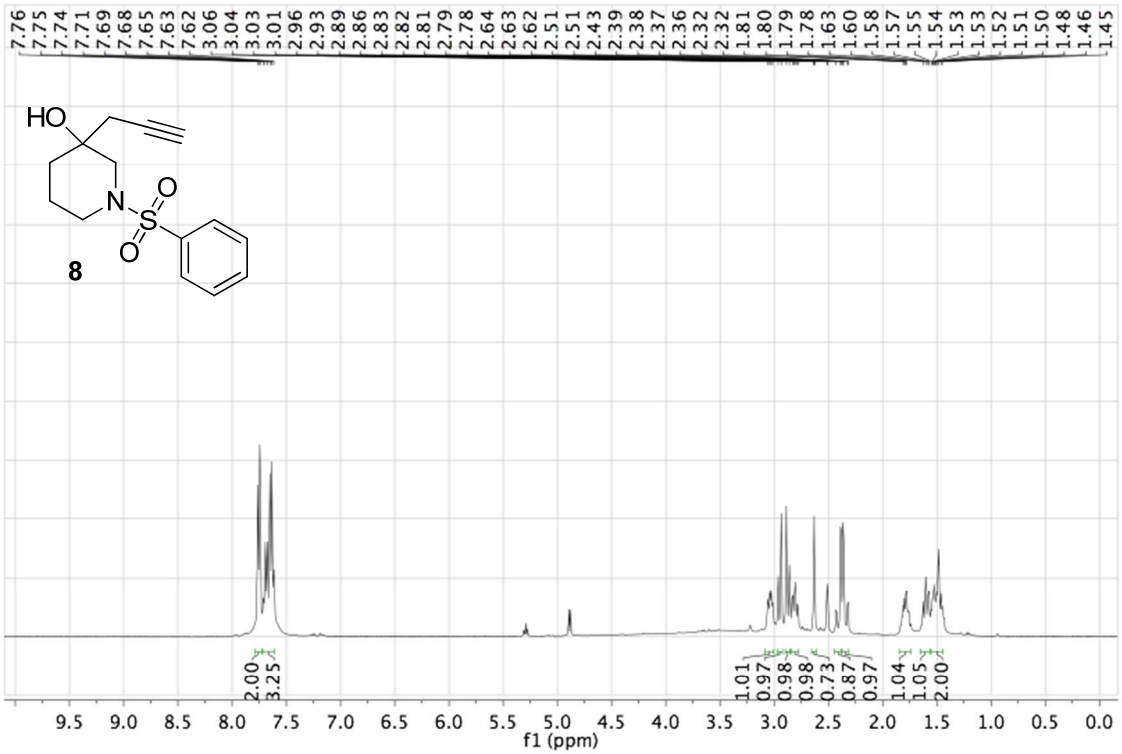

153.91
80.57
77.96
71.99
67.61
52.16
42.83
40.14
39.94
39.73
39.52
39.31
39.10
38.89
34.23
28.76
27.69
20.68
f1 (ppm)

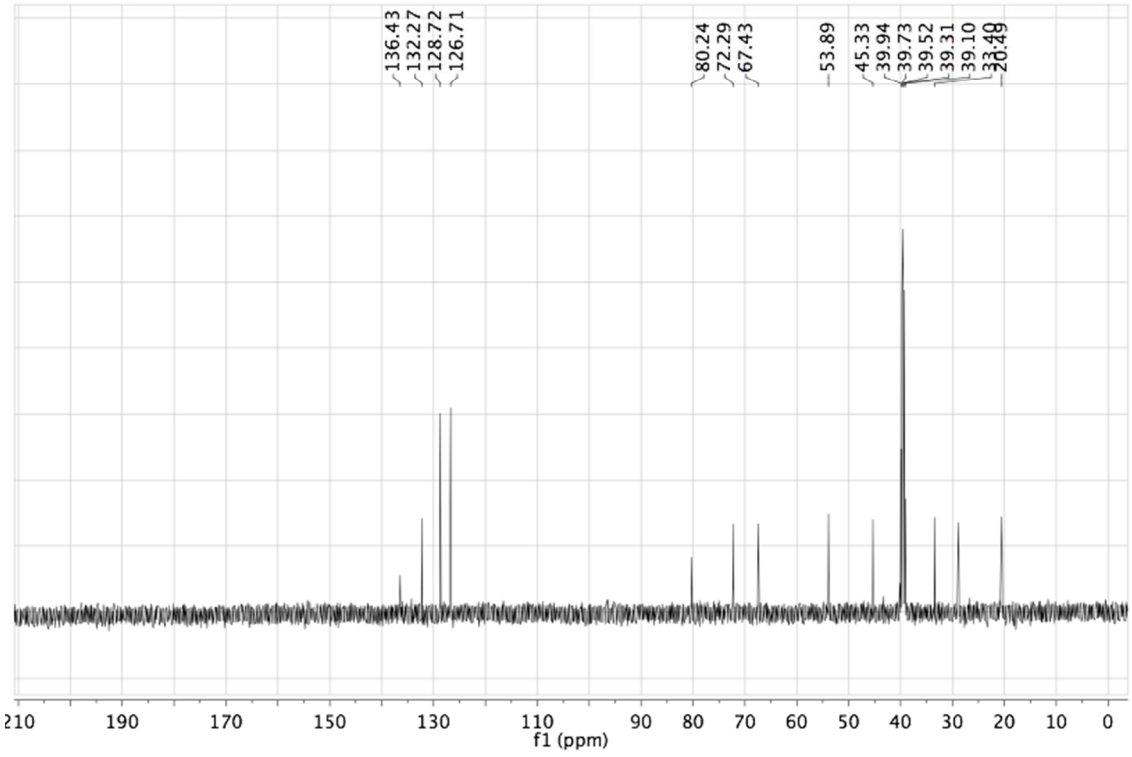

HO
TMS
N
Boc
20
4.28
3.71
3.68
3.68
3.67
3.12
3.09
3.09
2.51
2.38
2.36
1.63
1.62
1.60
1.59
1.48
1.46
1.45
1.42
0.14
0.98
2.36
2.02
2.29
2.14
11.17
9.00
f1 (ppm)

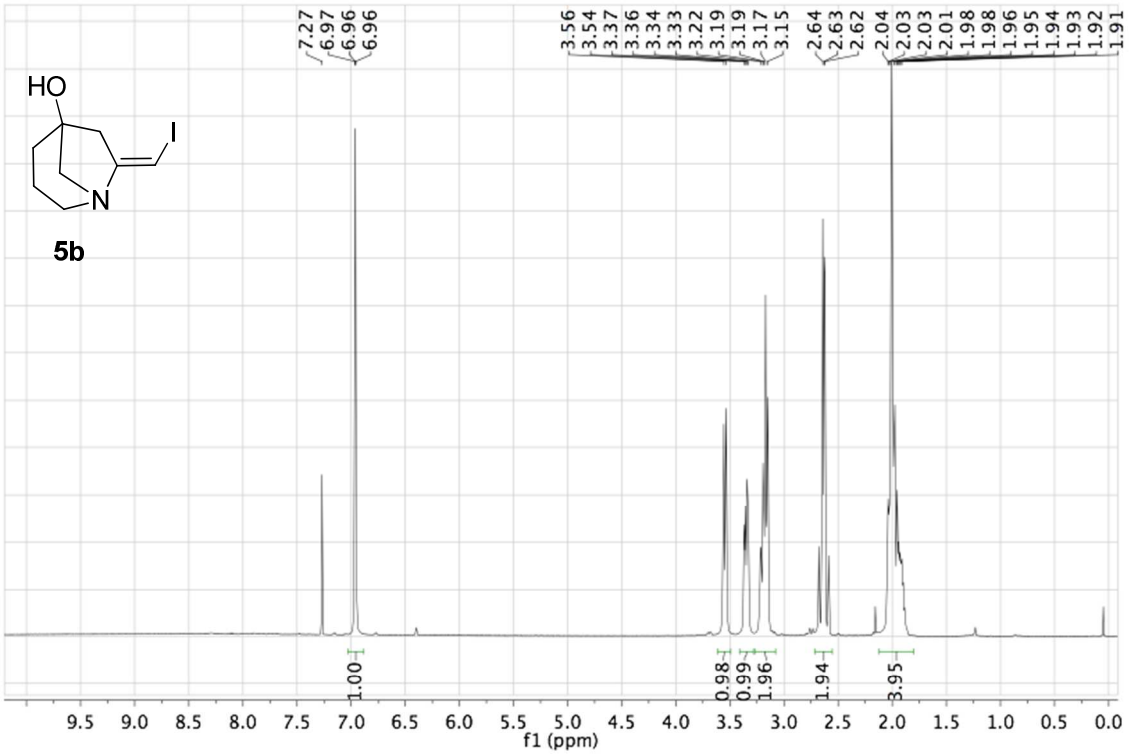

153.62
104.29
86.00
77.86
67.58
34.87
33.70
27.70
27.64
0.42
f1 (ppm)

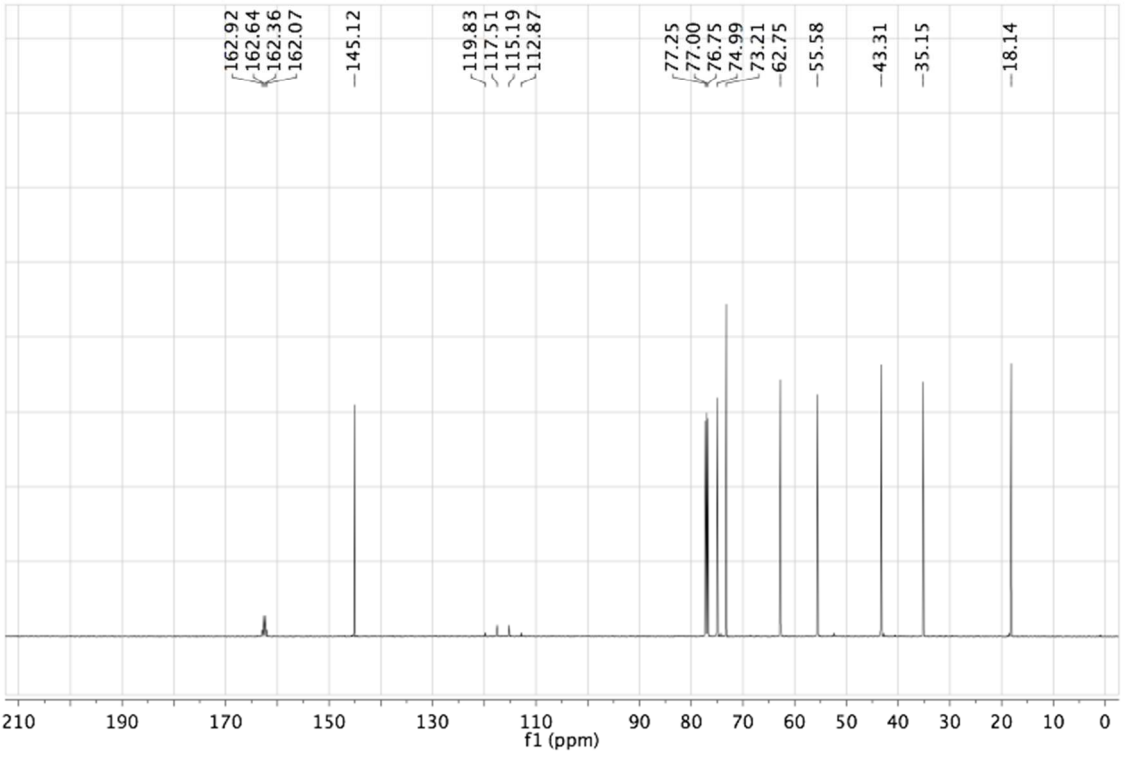

HO
N
Boc
6
4.29
3.69
3.67
3.66
3.65
3.10
3.04
2.62
2.62
2.32
2.31
1.62
1.61
1.59
1.58
1.56
1.55
1.51
1.48
1.42
0.96
2.00
2.06
0.86
2.10
2.12
2.07
9.00
f1 (ppm)

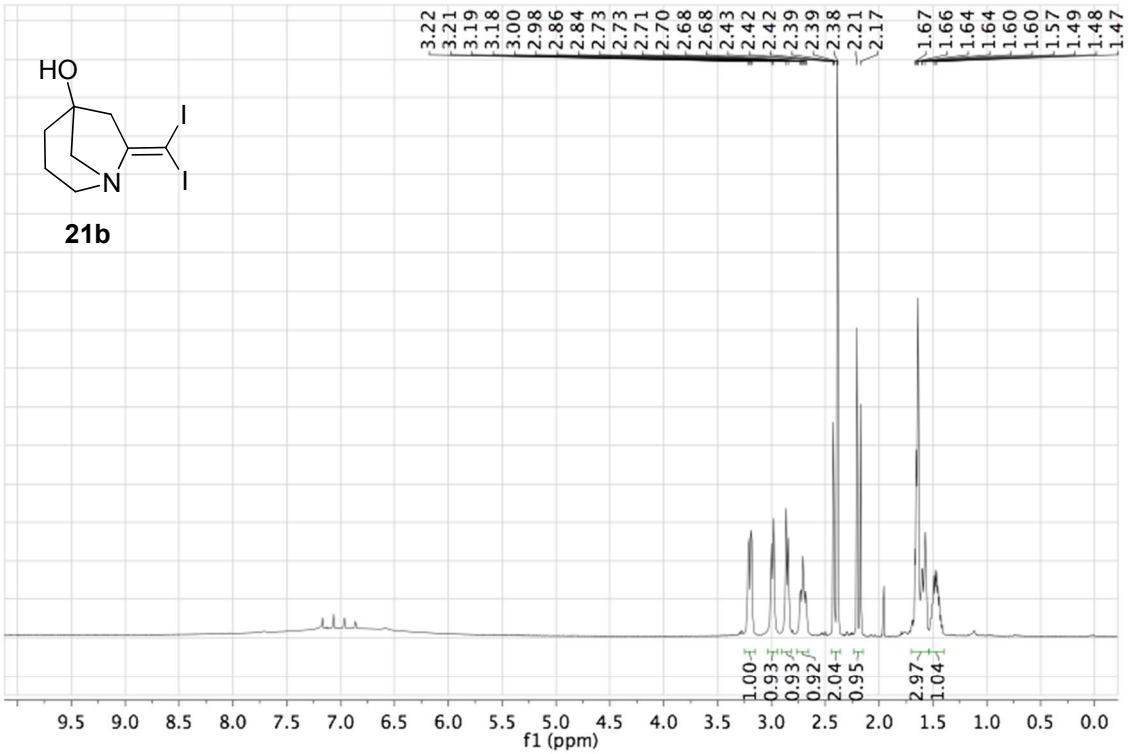

153.70
80.87
77.98
71.99
67.36
40.14
39.94
39.73
39.52
39.31
39.10
38.89
34.98
32.21
27.74
f1 (ppm)

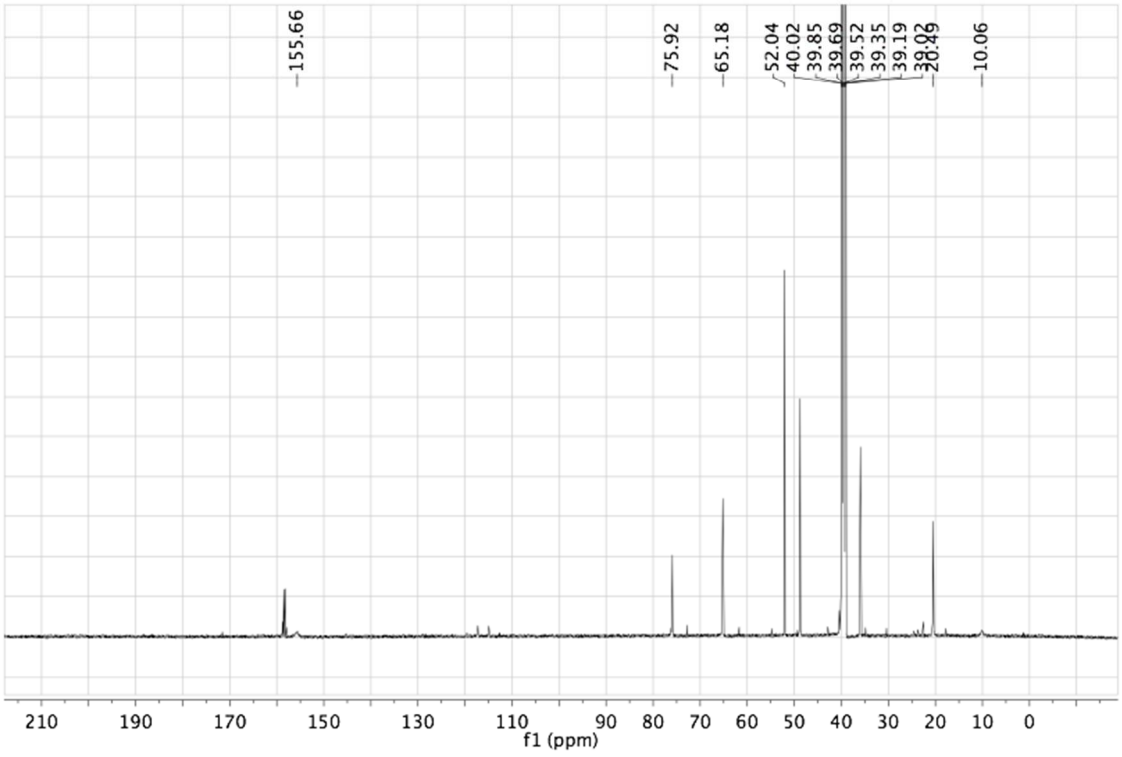

HO
N
S
O
O
8
f1 (ppm)

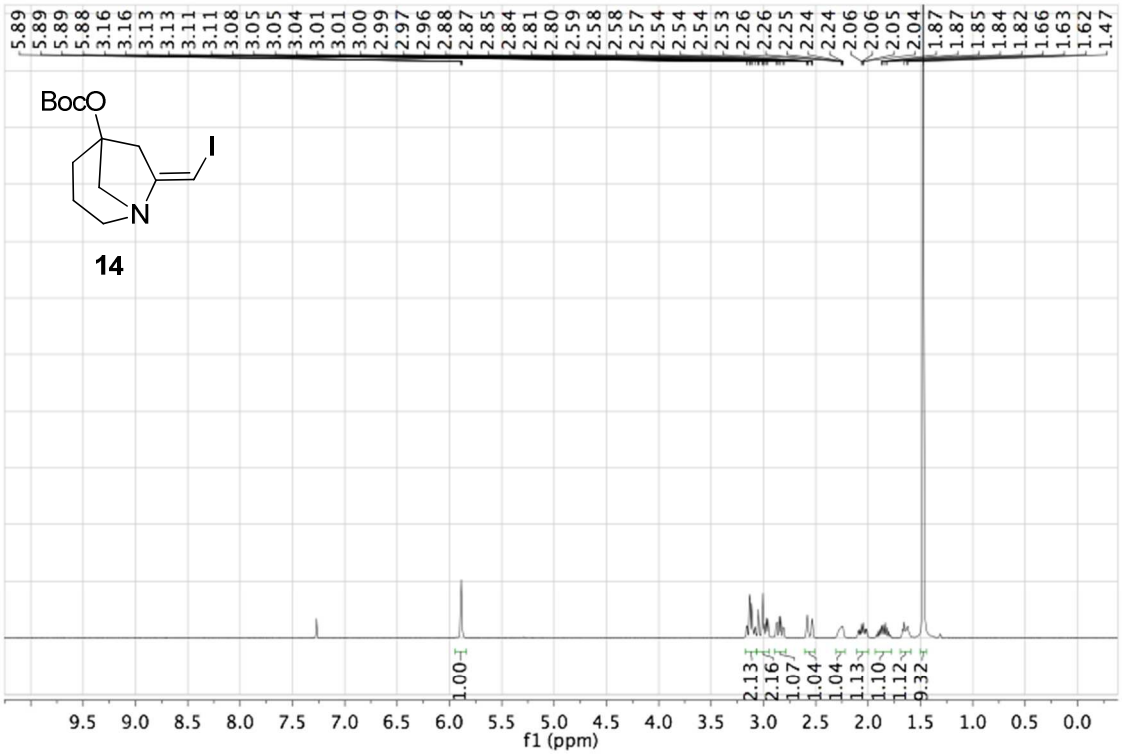

136.43
132.27
128.72
126.71
80.24
72.29
67.43
53.89
45.33
39.94
39.73
39.52
39.31
39.10
f1 (ppm)

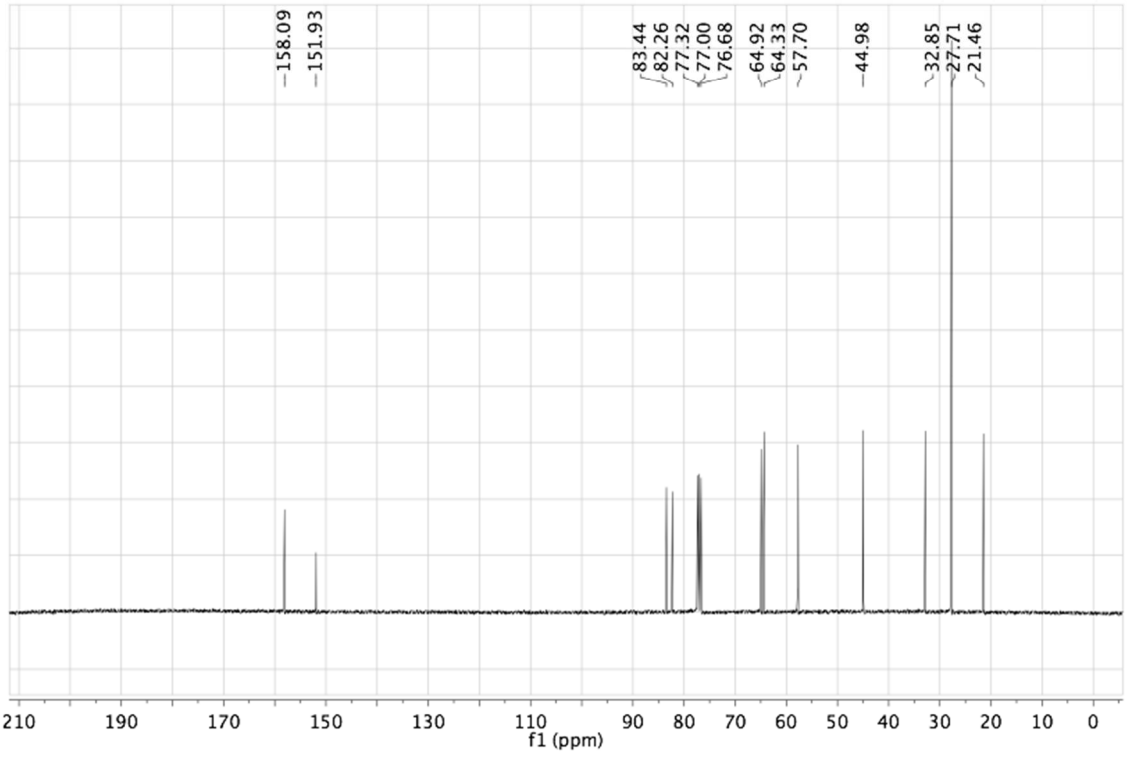

HO
I
N
5b
7.27
6.97
6.96
6.96
3.56
3.54
3.37
3.36
3.34
3.33
3.22
3.19
3.19
3.17
3.15
2.64
2.63
2.62
2.04
2.03
2.03
2.01
1.98
1.98
1.96
1.95
1.94
1.93
1.92
1.91
1.00
0.98
0.99
1.96
1.94
3.95
f1 (ppm)

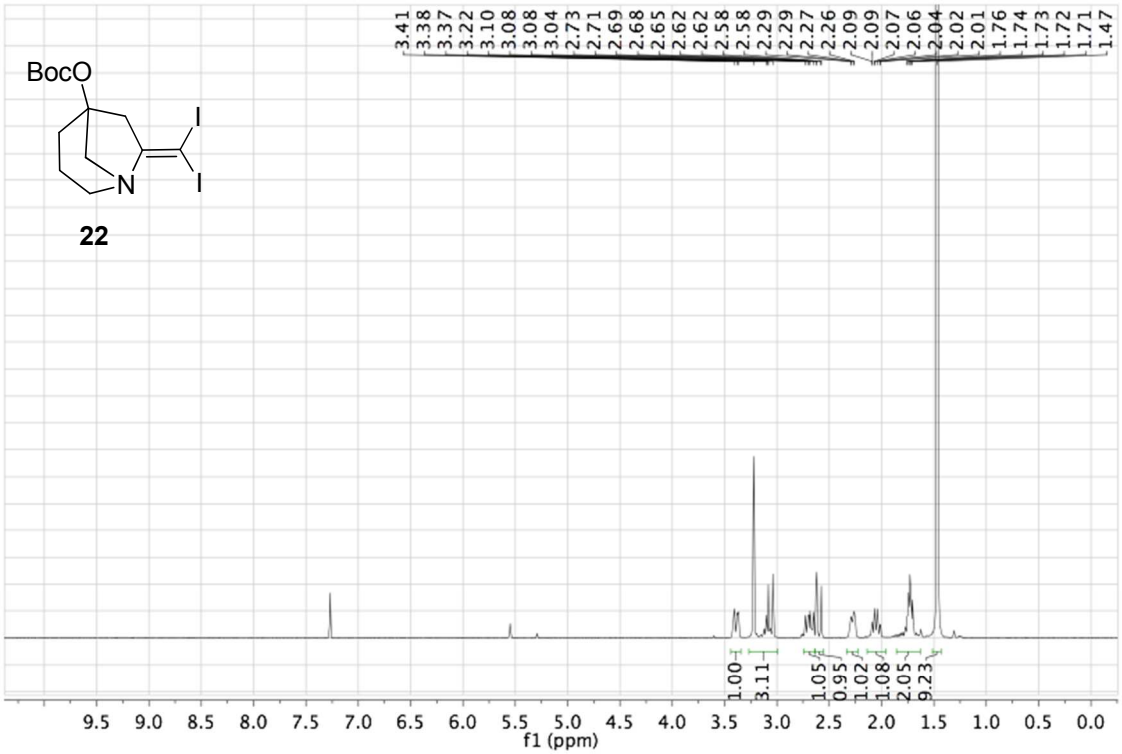

162.92
162.64
162.36
162.07
145.12
119.83
117.51
115.19
112.87
77.25
77.00
76.75
74.99
73.21
62.75
55.58
43.31
35.15
18.14
f1 (ppm)

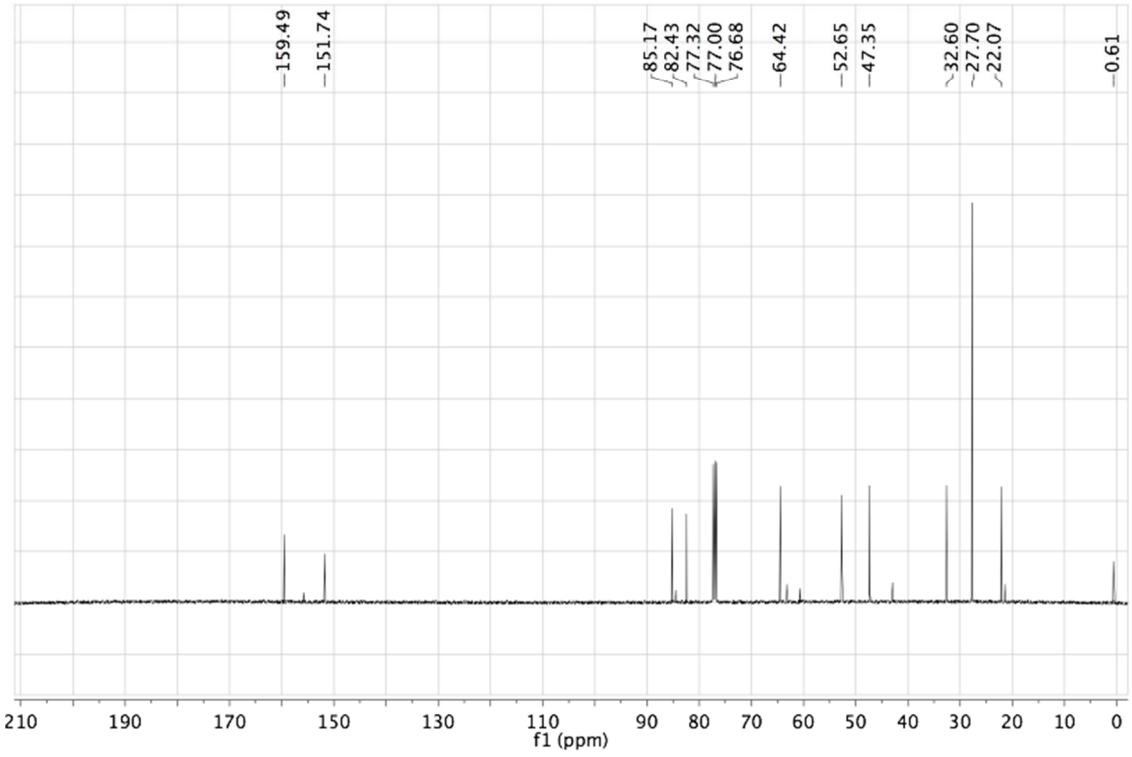

HO
I
I
N
21b
3.22
3.21
3.19
3.18
3.00
2.98
2.86
2.84
2.73
2.73
2.71
2.70
2.68
2.68
2.43
2.42
2.42
2.39
2.39
2.38
2.21
2.17
1.67
1.66
1.64
1.64
1.60
1.60
1.57
1.49
1.48
1.47
1.00
0.93
0.93
0.92
2.04
0.95
2.97
1.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

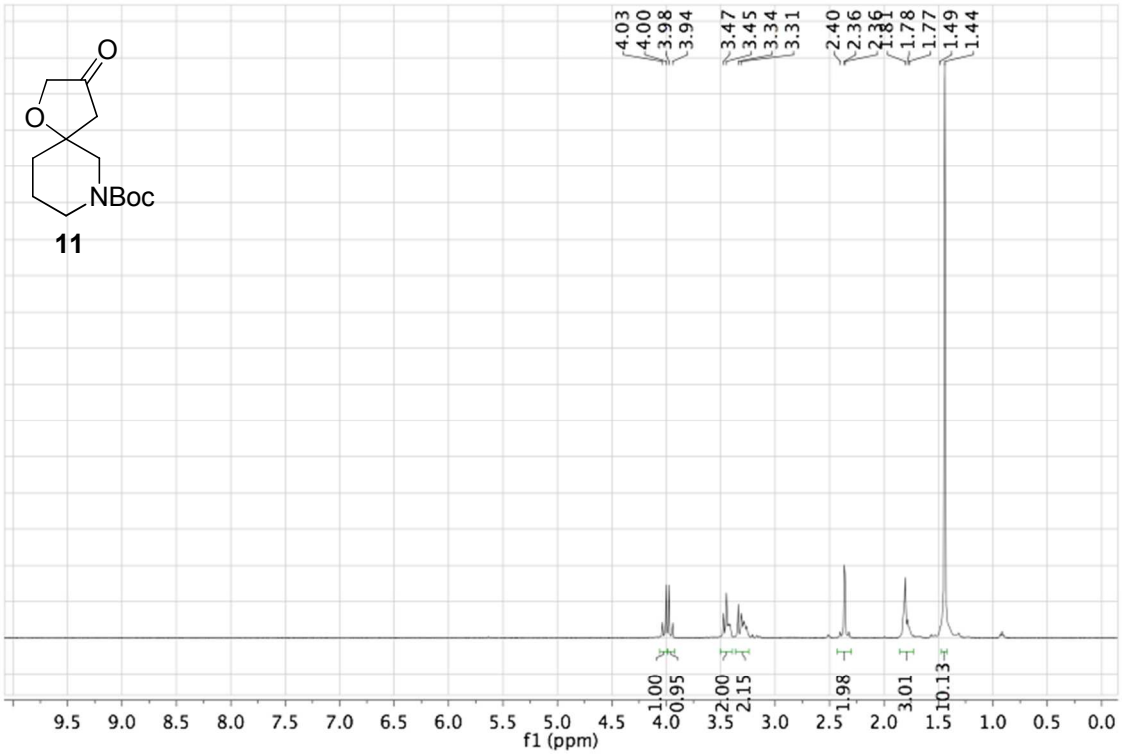

155.66
75.92
65.18
52.04
40.02
39.85
39.69
39.52
39.35
39.19
38.02
20.49
10.06
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

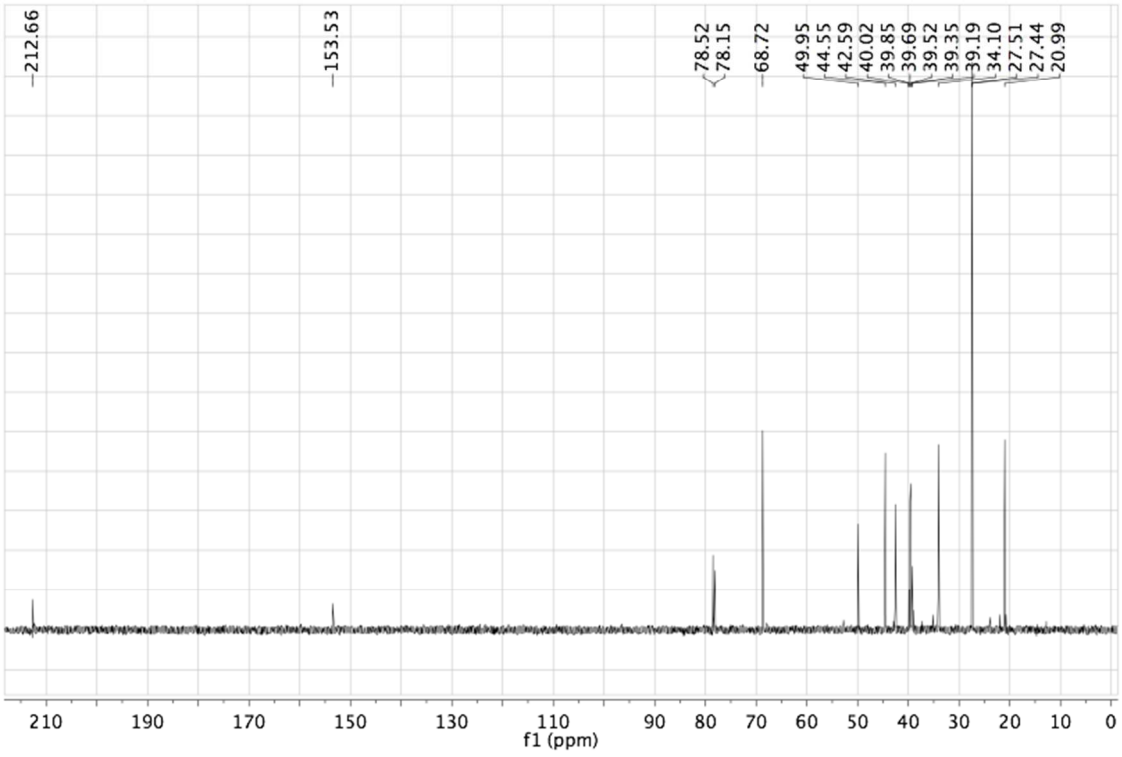

BocO
I
N
14
f1 (ppm)

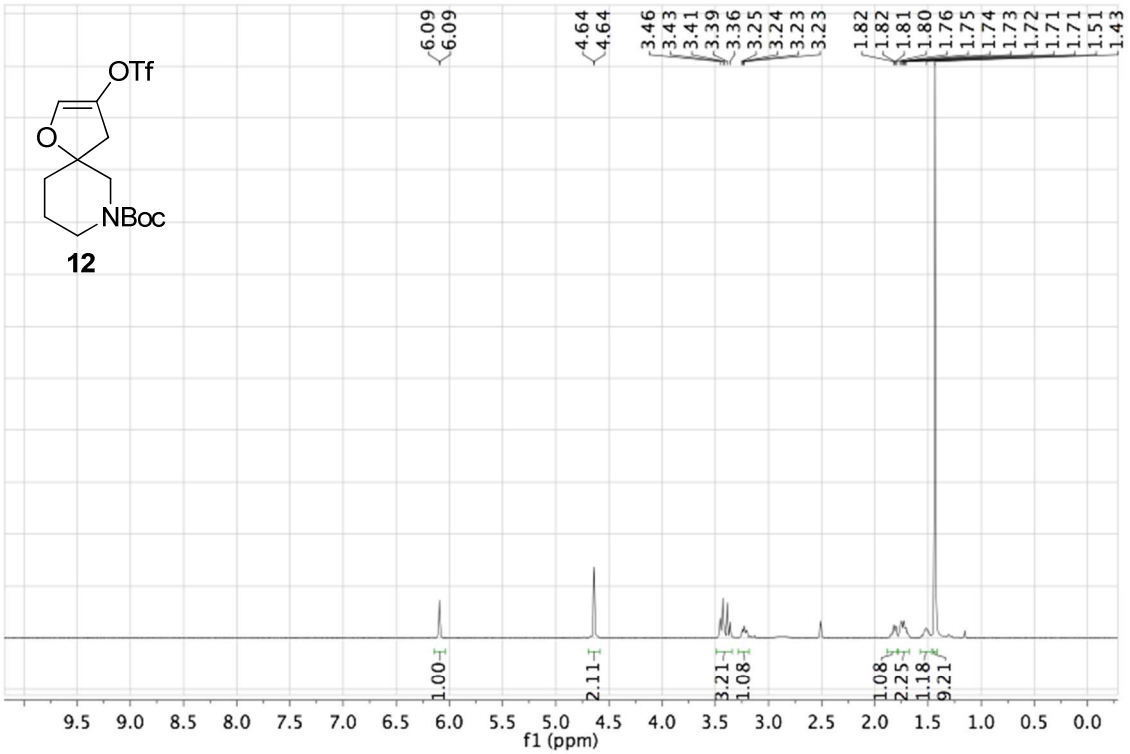

f1 (ppm)

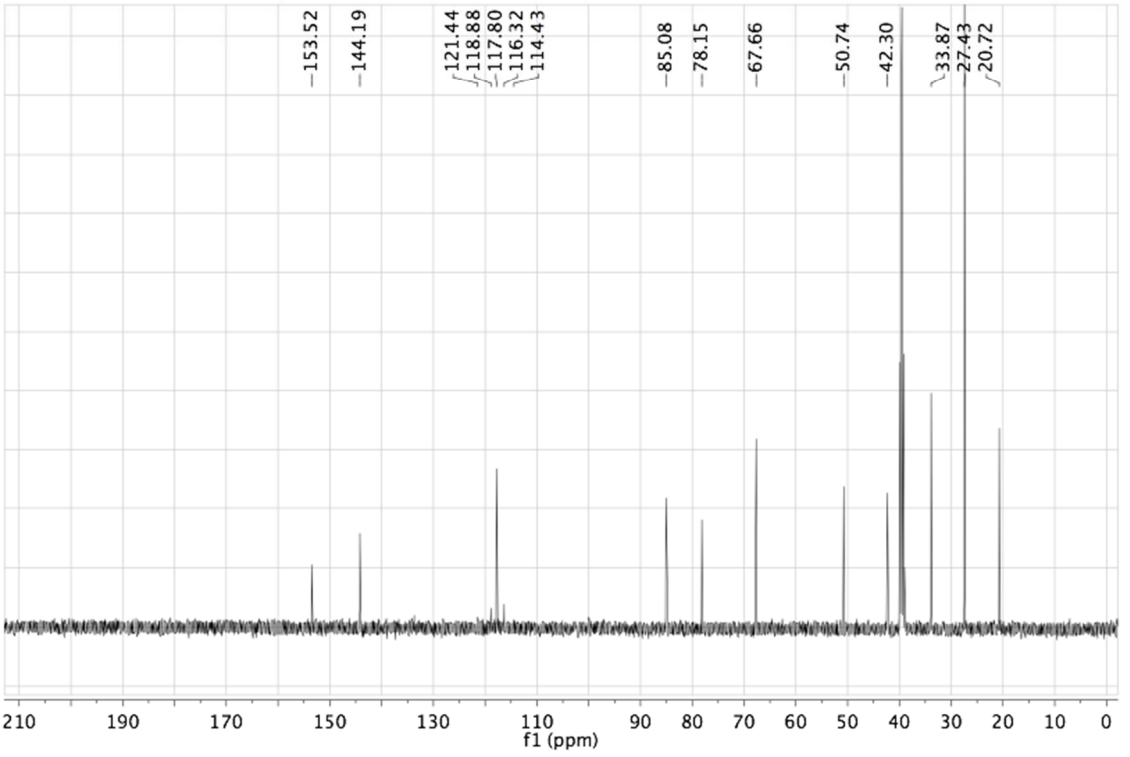

BocO
I
I
N
22
3.41
3.38
3.37
3.22
3.10
3.08
3.08
3.04
2.73
2.71
2.69
2.68
2.65
2.62
2.62
2.58
2.58
2.29
2.29
2.27
2.26
2.09
2.09
2.07
2.06
2.04
2.02
2.01
1.76
1.74
1.73
1.72
1.71
1.47
1.00
3.11
1.05
0.95
1.02
1.08
2.05
9.23
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

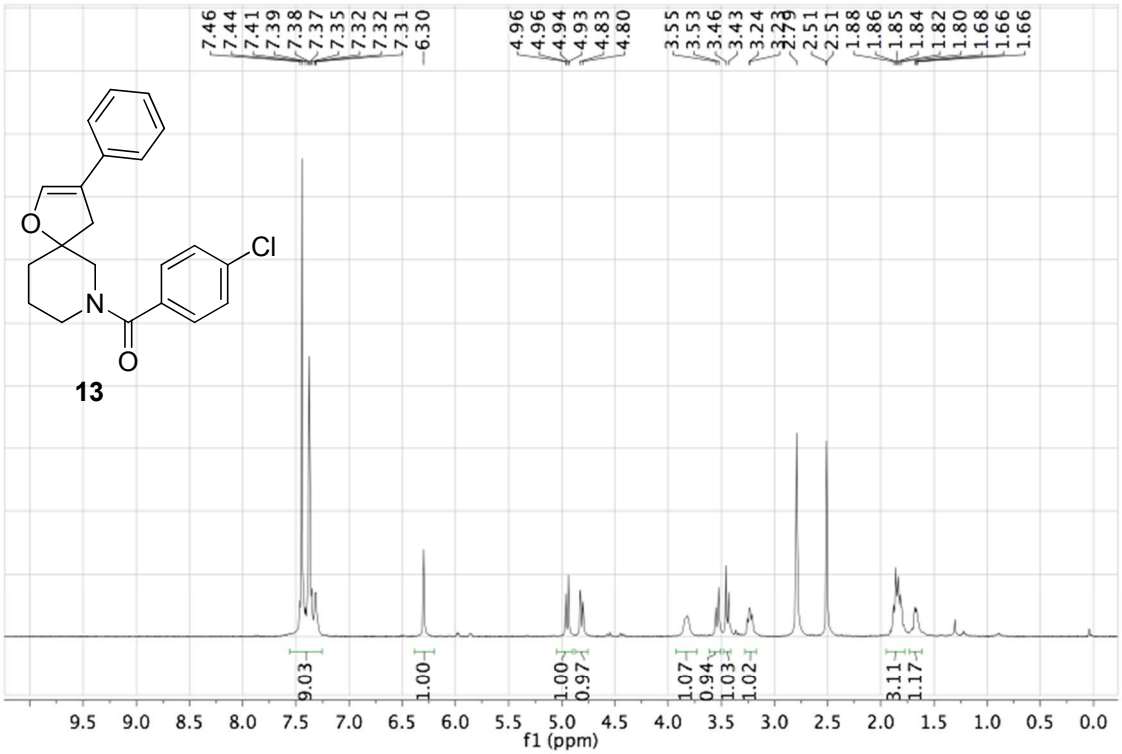

159.49
151.74
85.17
82.43
77.32
77.00
76.68
64.42
52.65
47.35
32.60
27.70
22.07
0.61
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

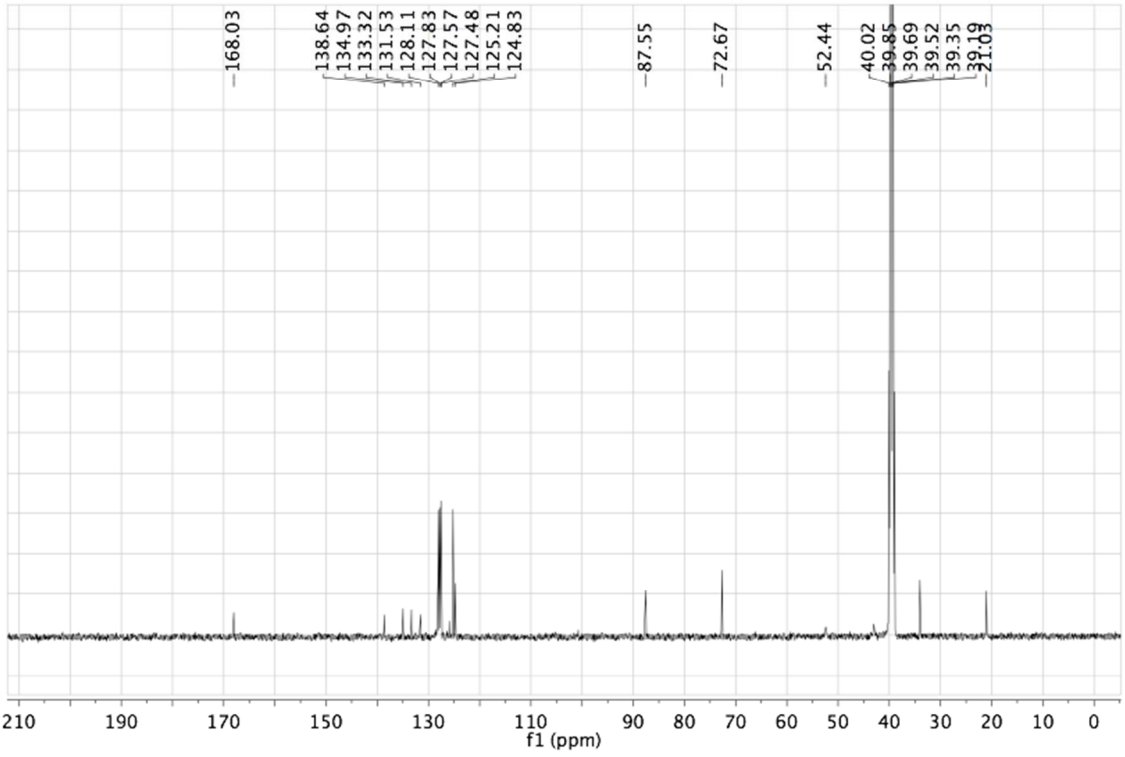

O
O
NBoc
11
4.03
4.00
3.98
3.94
3.47
3.45
3.34
3.31
2.40
2.36
2.36
1.81
1.78
1.77
1.49
1.44
1.00
0.95
2.00
2.15
1.98
3.01
10.13
f1 (ppm)

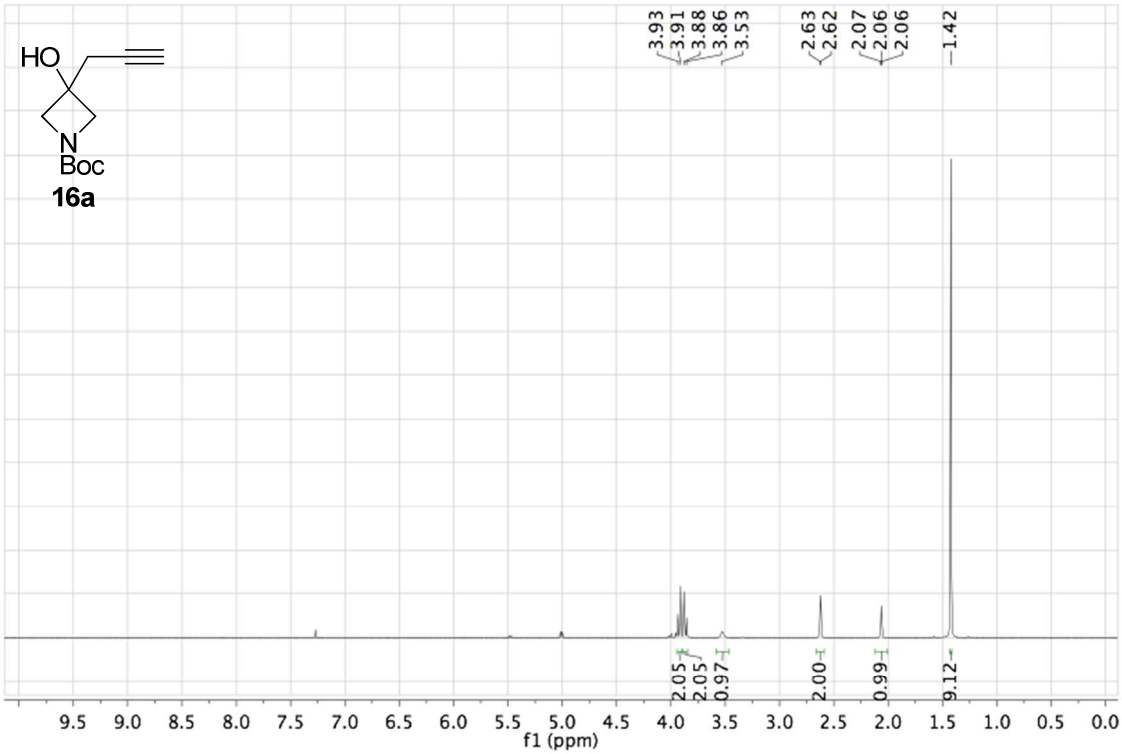

212.66
153.53
78.52
78.15
68.72
49.95
44.55
42.59
40.02
39.85
39.69
39.52
39.35
39.19
34.10
27.51
27.44
20.99
f1 (ppm)

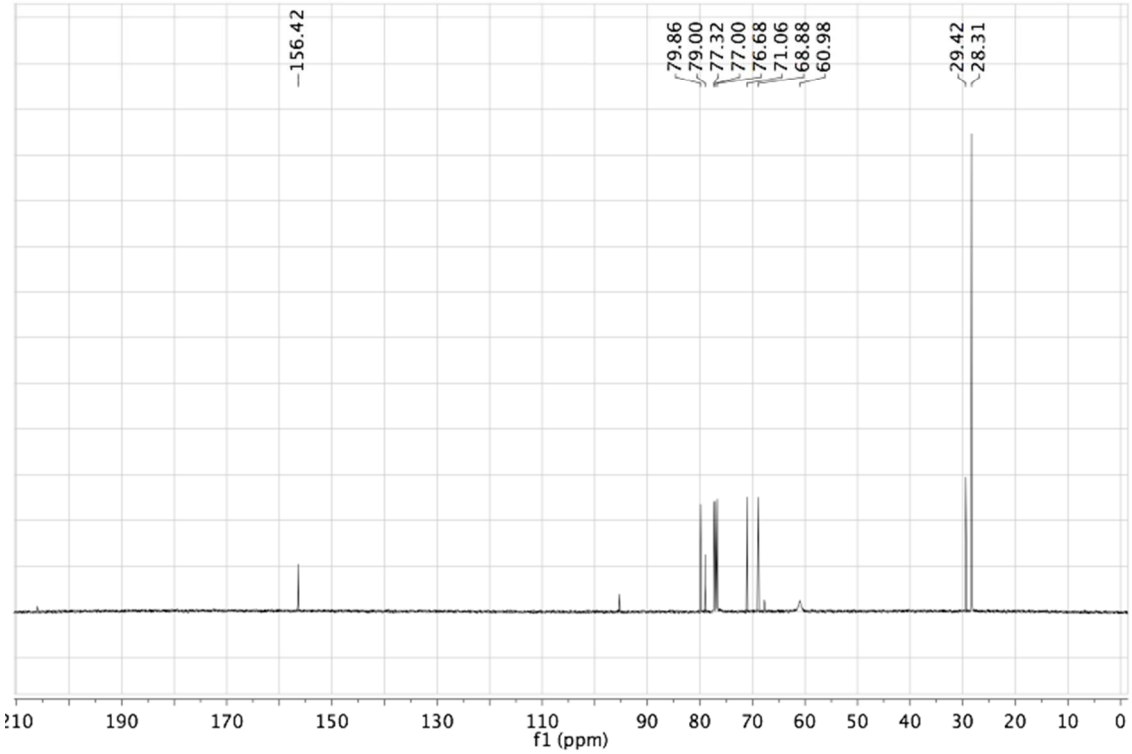

OTf
O
NBoc
12
6.09
6.09
4.64
4.64
3.46
3.43
3.41
3.39
3.36
3.25
3.24
3.23
3.23
1.82
1.82
1.81
1.80
1.76
1.75
1.74
1.73
1.72
1.71
1.71
1.51
1.43
1.00
2.11
3.21
1.08
1.08
2.25
1.18
9.21
f1 (ppm)

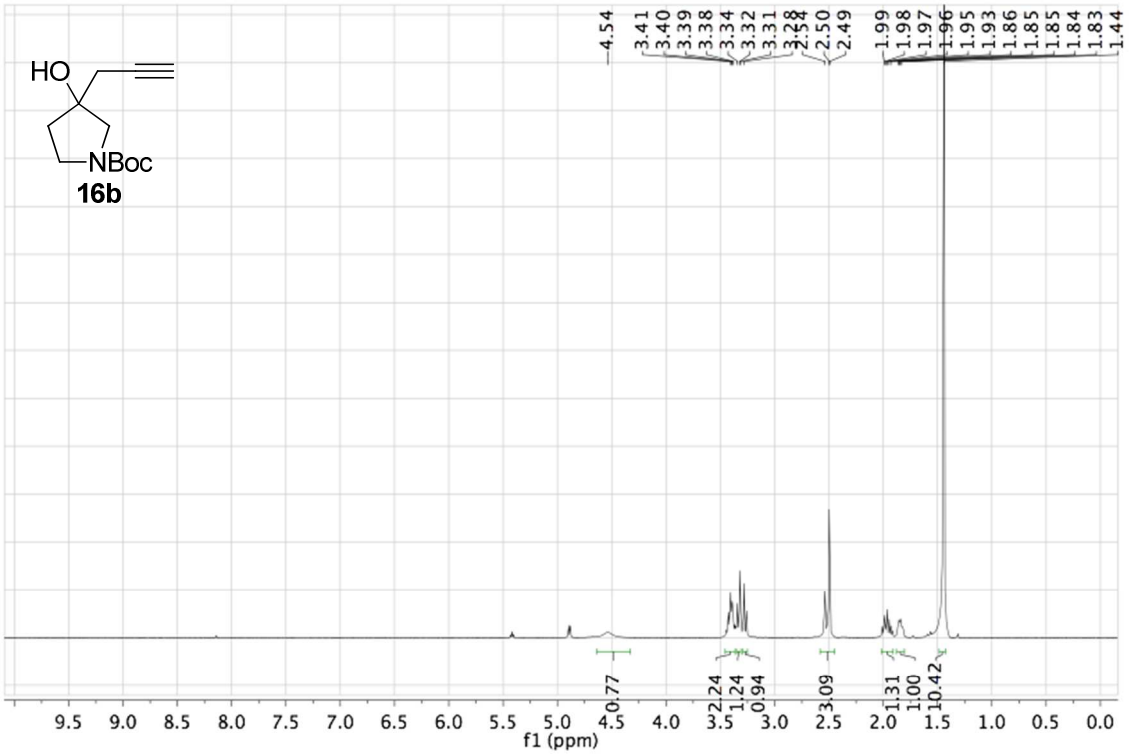

153.52
144.19
121.44
118.88
117.80
116.32
114.43
85.08
78.15
67.66
50.74
42.30
33.87
27.43
20.72
f1 (ppm)

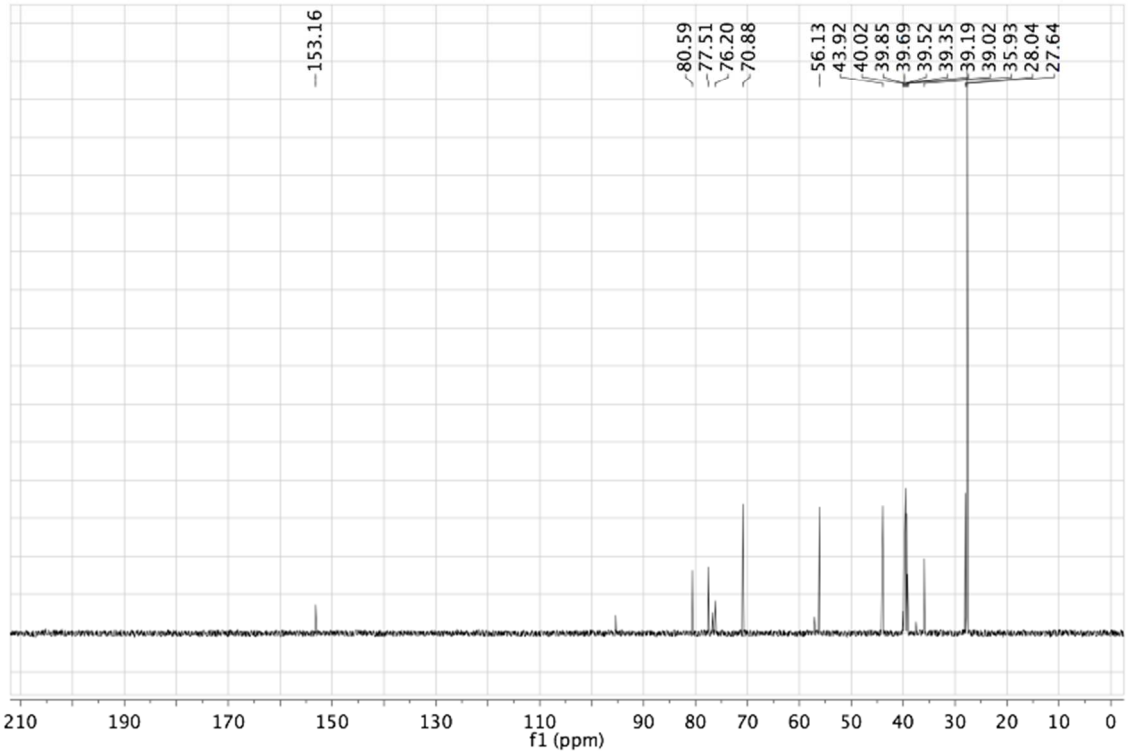

7.46
7.44
7.41
7.39
7.38
7.37
7.35
7.32
7.32
7.31
6.30
4.96
4.96
4.94
4.93
4.83
4.80
3.55
3.53
3.46
3.43
3.24
3.23
2.79
2.51
2.51
1.88
1.86
1.85
1.84
1.82
1.80
1.68
1.66
1.66
O
Cl
N
O
13
9.03
1.00
1.00
0.97
1.07
0.94
1.03
1.02
3.11
1.17
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

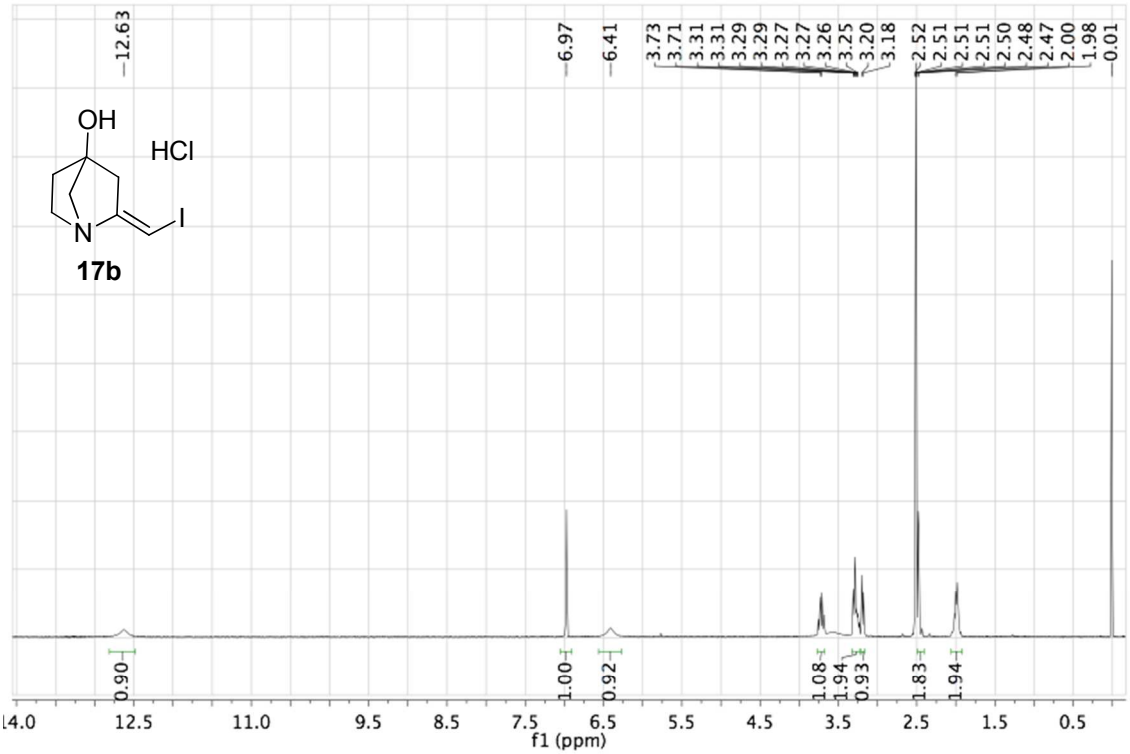

168.03
138.64
134.97
133.32
131.53
128.11
127.83
127.57
127.48
125.21
124.83
87.55
72.67
52.44
40.02
39.85
39.69
39.52
39.35
39.19
21.03
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

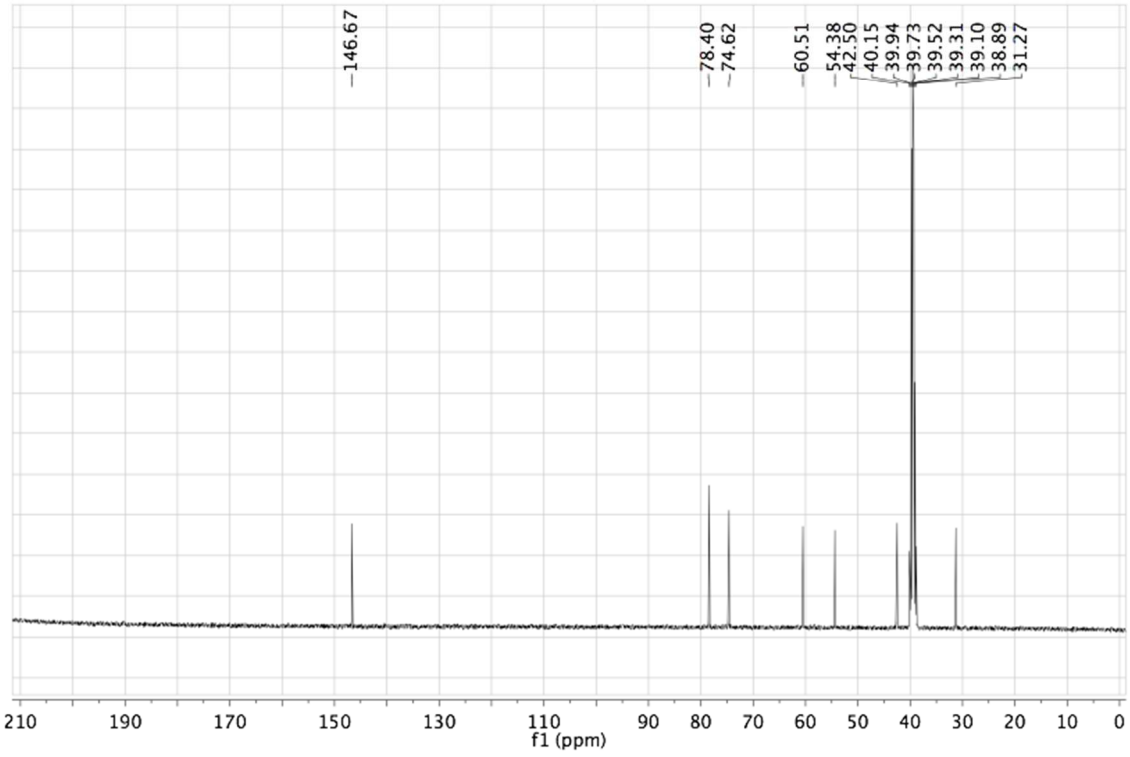

HO
N
Boc
16a
3.93
3.91
3.88
3.86
3.53
2.63
2.62
2.07
2.06
2.06
1.42
2.05
2.05
0.97
2.00
0.99
9.12
f1 (ppm)

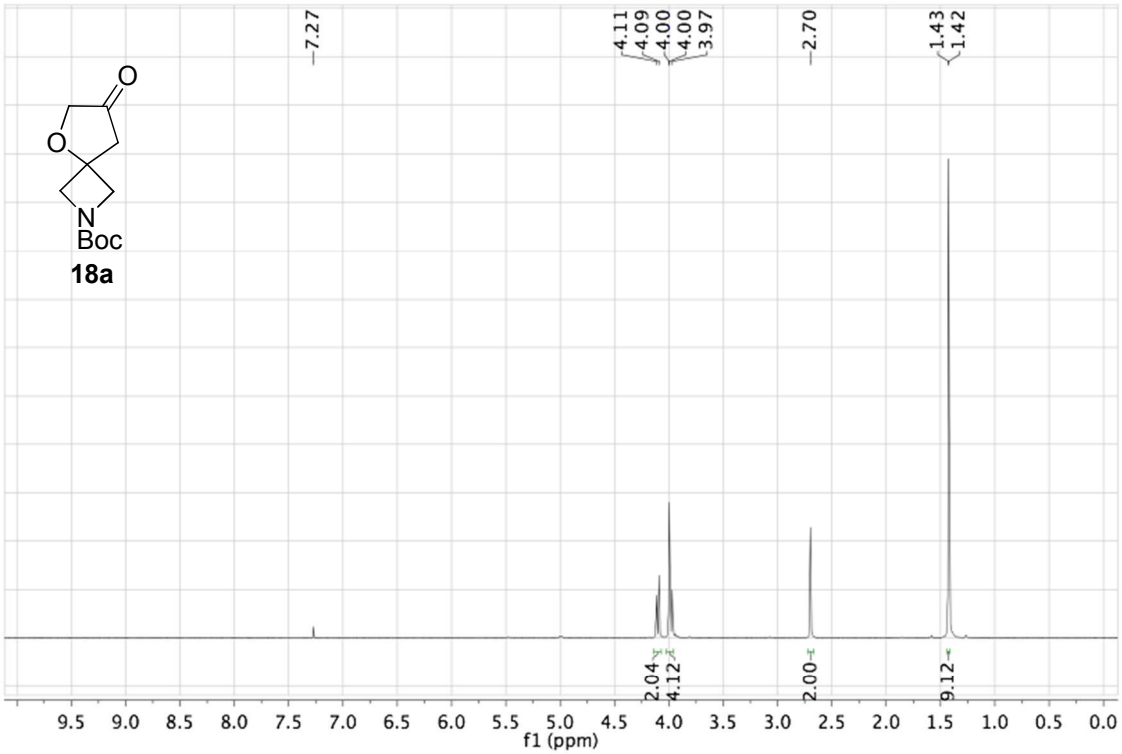

156.42
79.86
79.00
77.32
77.00
76.68
71.06
68.88
60.98
29.42
28.31
f1 (ppm)

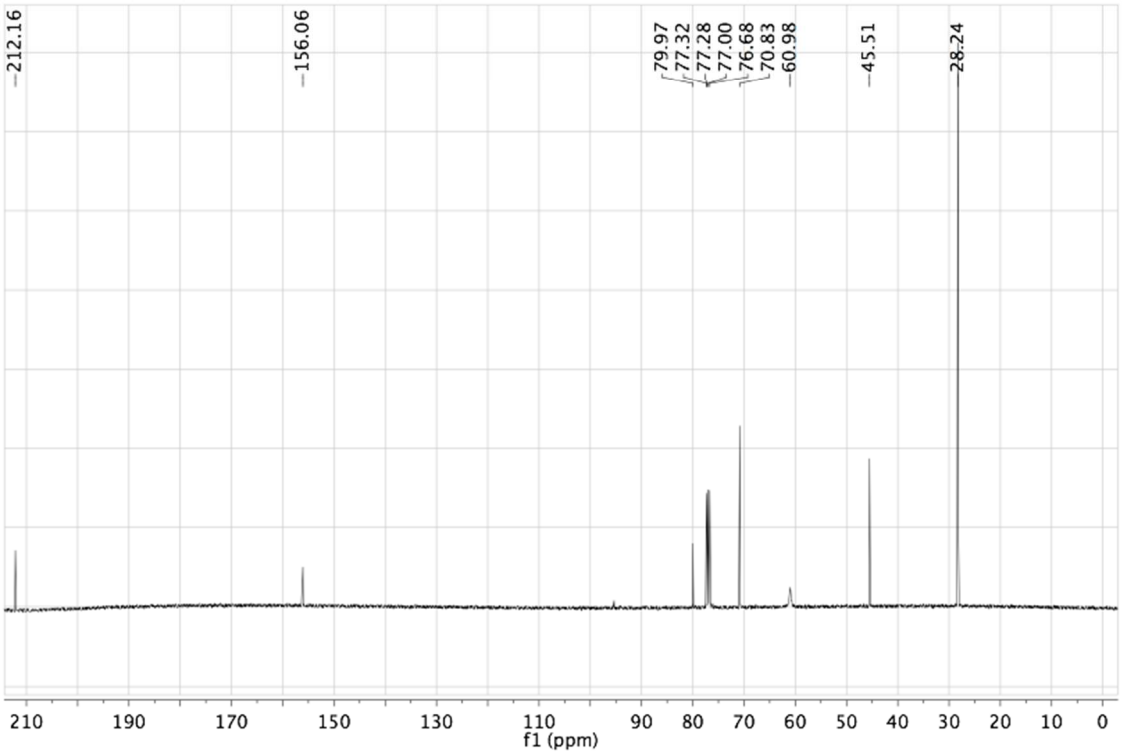

HO
NBoc
16b
4.54
3.41
3.40
3.39
3.38
3.34
3.32
3.31
3.28
2.54
2.50
2.49
1.99
1.98
1.97
1.96
1.95
1.93
1.86
1.85
1.85
1.84
1.83
1.44
0.77
2.24
1.24
0.94
3.09
1.31
1.00
10.42
f1 (ppm)

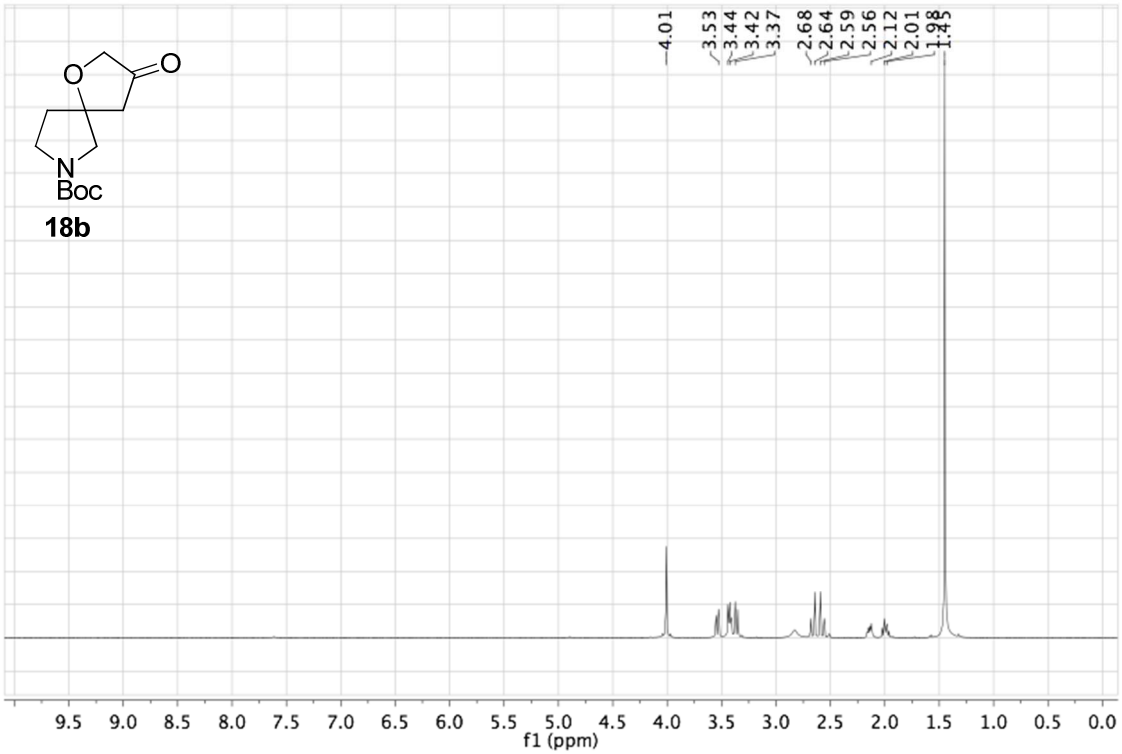

153.16
80.59
77.51
76.20
70.88
56.13
43.92
40.02
39.85
39.69
39.52
39.35
39.19
39.02
35.93
28.04
27.64
f1 (ppm)

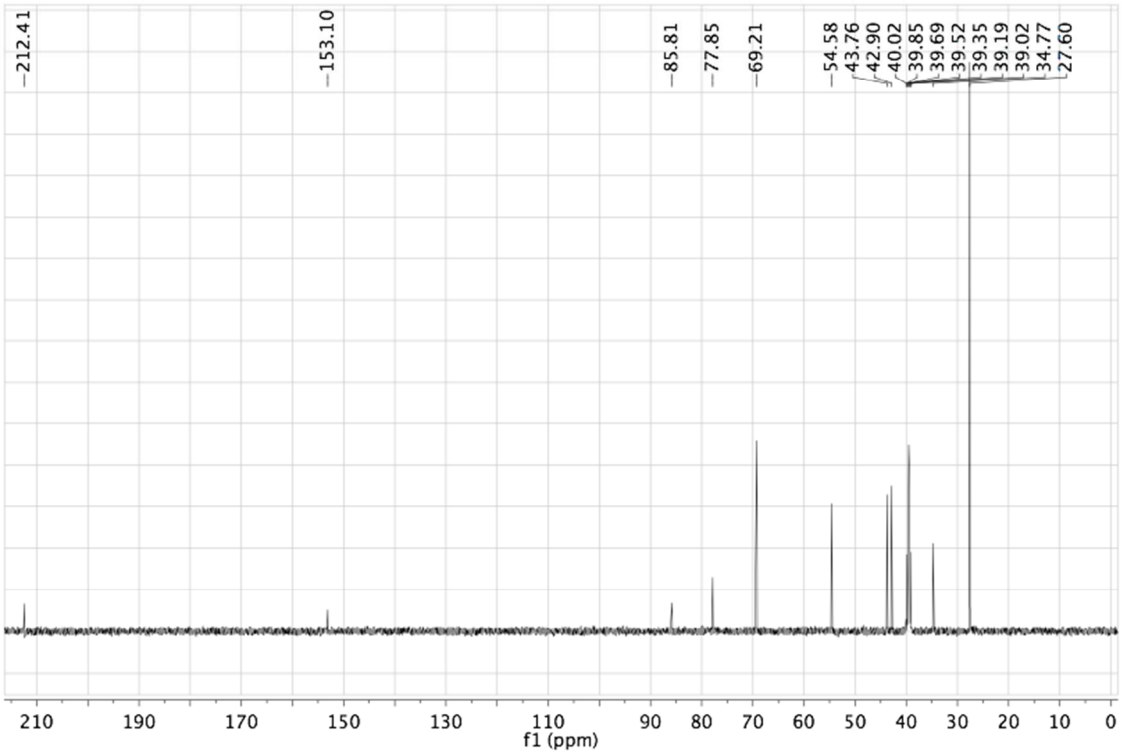

12.63
6.97
6.41
3.73
3.71
3.31
3.31
3.29
3.29
3.27
3.27
3.26
3.25
3.20
3.18
2.52
2.51
2.51
2.51
2.50
2.48
2.47
2.00
1.98
0.01
OH
HCl
I
N
17b
0.90
1.00
0.92
1.08
1.94
0.93
1.83
1.94
f1 (ppm)

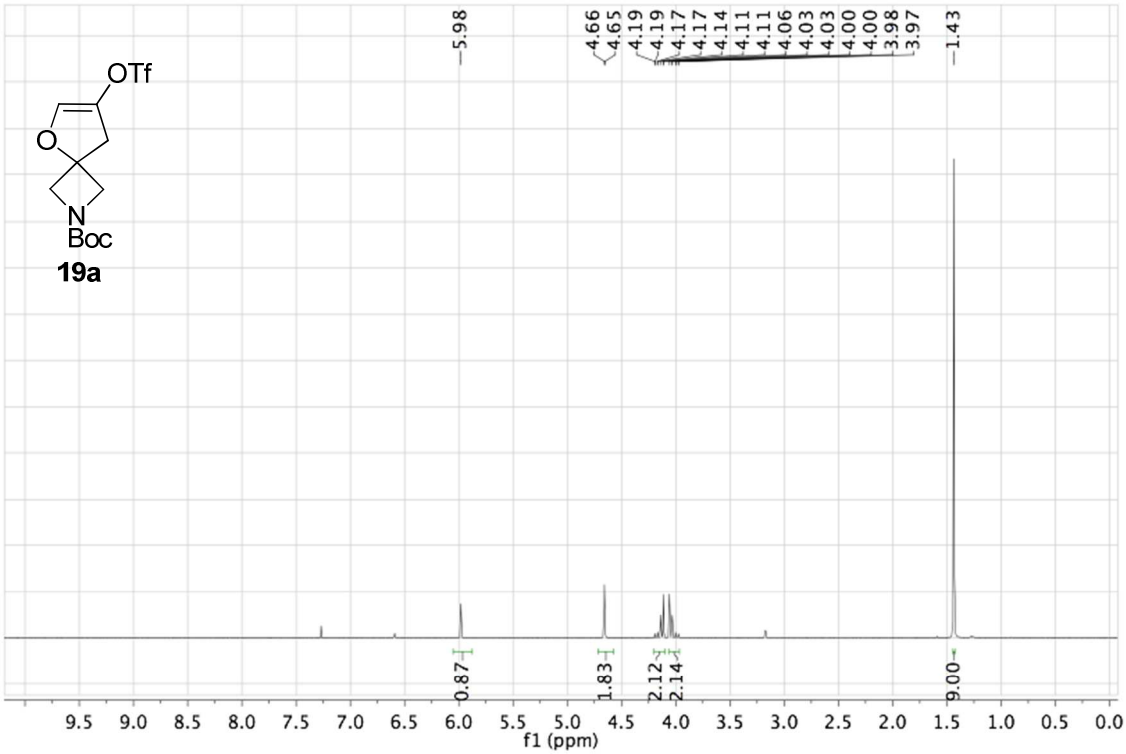

146.67
78.40
74.62
60.51
54.38
42.50
40.15
39.94
39.73
39.52
39.31
39.10
38.89
31.27
f1 (ppm)

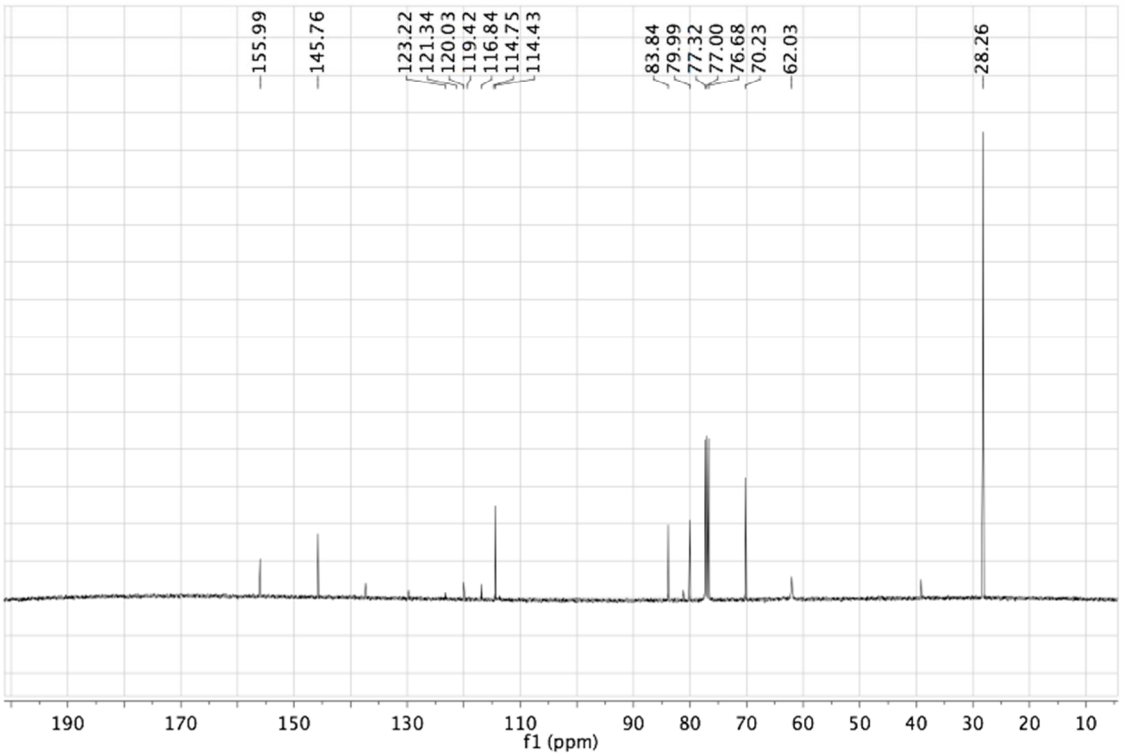

O
O
N
Boc
18a
7.27
4.11
4.09
4.00
4.00
3.97
2.70
1.43
1.42
2.04
4.12
2.00
9.12
f1 (ppm)

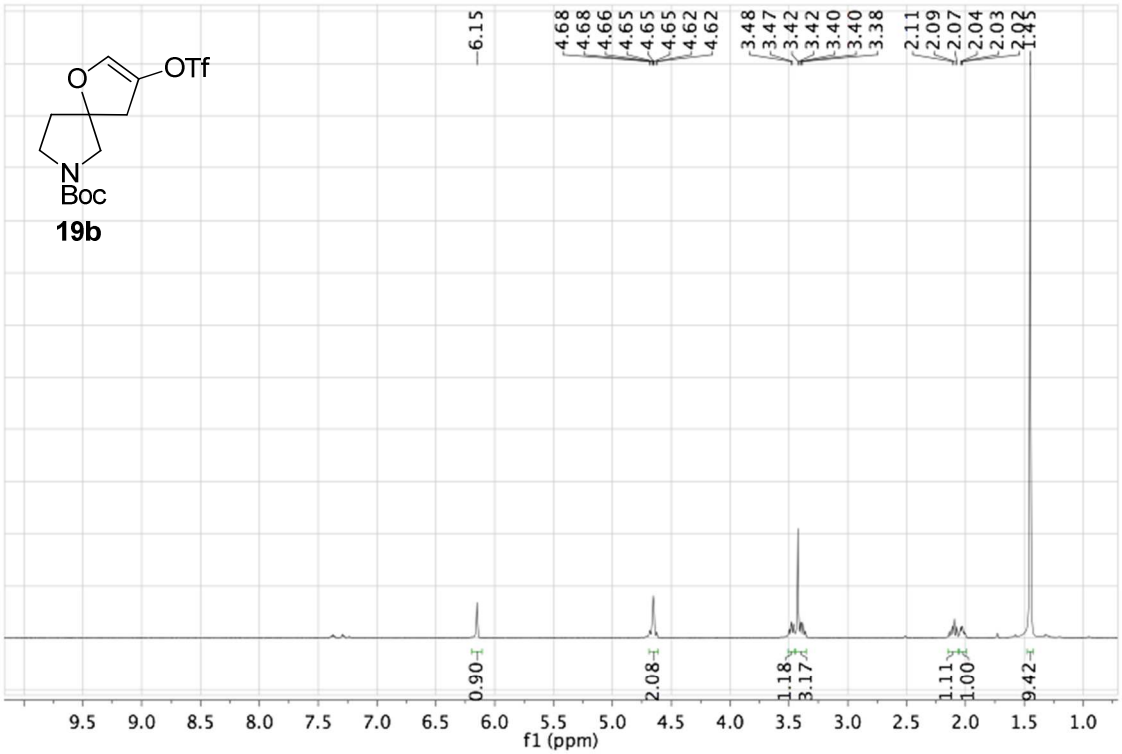

212.16
156.06
79.97
77.32
77.28
77.00
76.68
70.83
60.98
45.51
28.24
f1 (ppm)

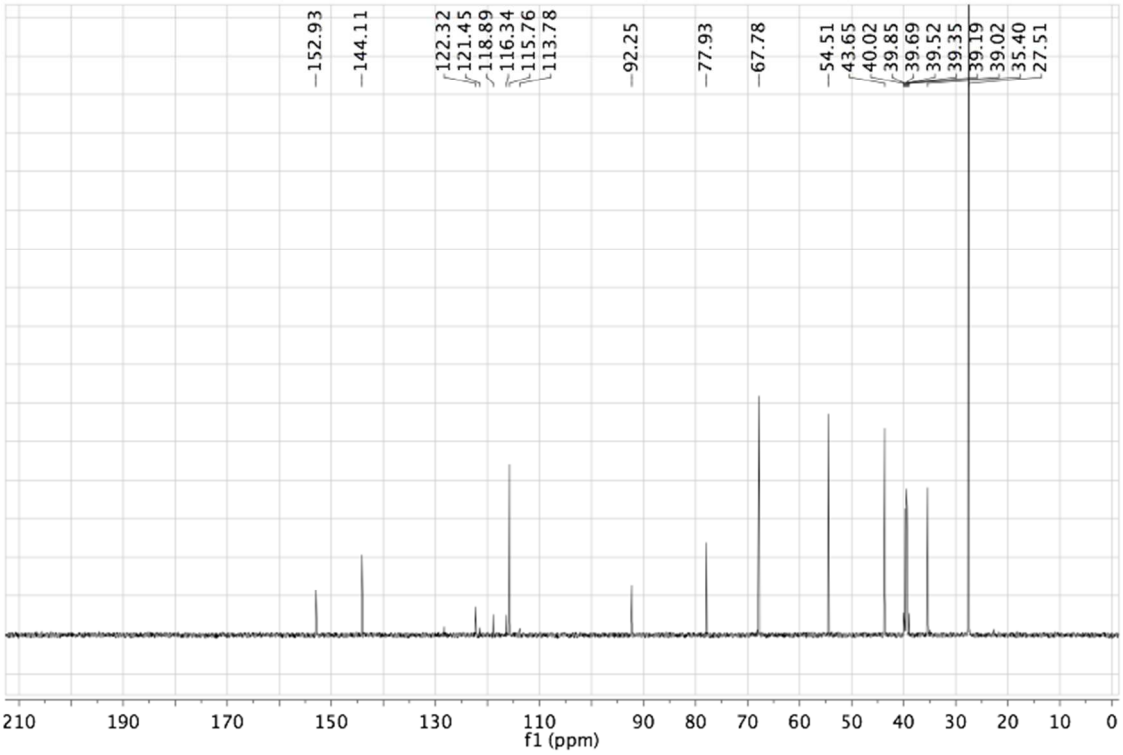

4.01
3.53
3.44
3.42
3.37
2.68
2.64
2.59
2.56
2.12
2.01
1.98
1.45
O
O
N
Boc
18b
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


212.41
153.10
85.81
77.85
69.21
54.58
43.76
42.90
40.02
39.85
39.69
39.52
39.35
39.19
39.02
34.77
27.60
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

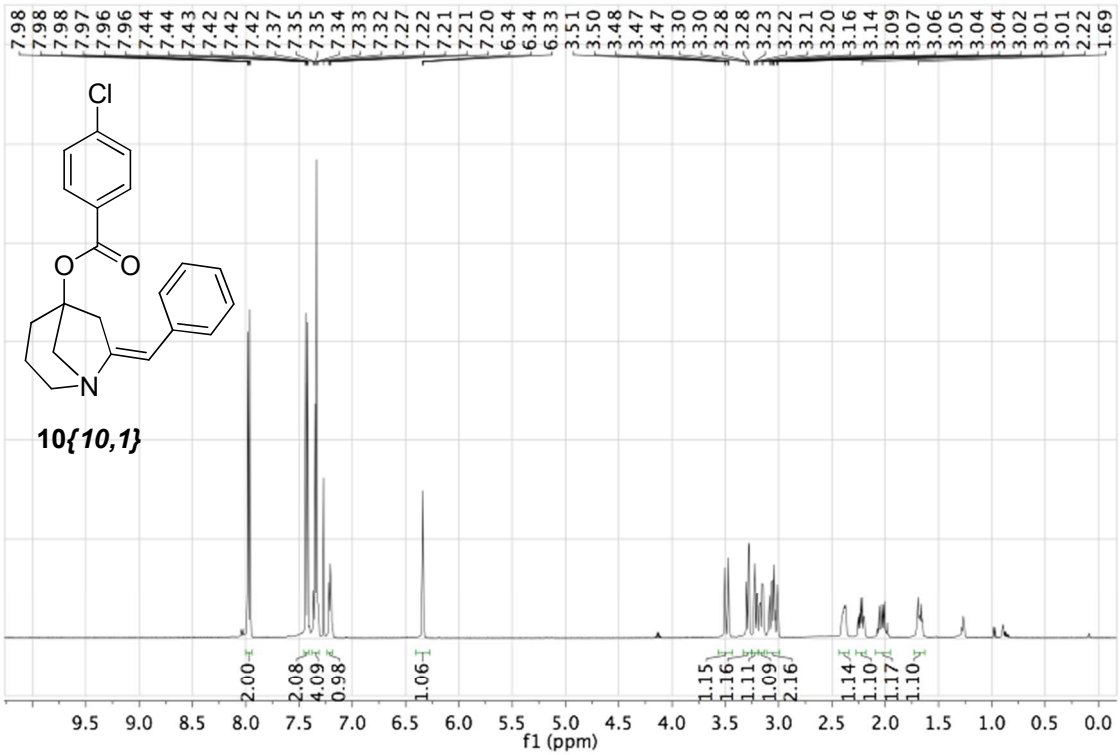

OTf
O
N
Boc
19a
5.98
4.66
4.65
4.19
4.19
4.17
4.17
4.14
4.11
4.11
4.06
4.03
4.03
4.00
4.00
3.98
3.97
1.43
0.87
1.83
2.12
2.14
9.00
f1 (ppm)

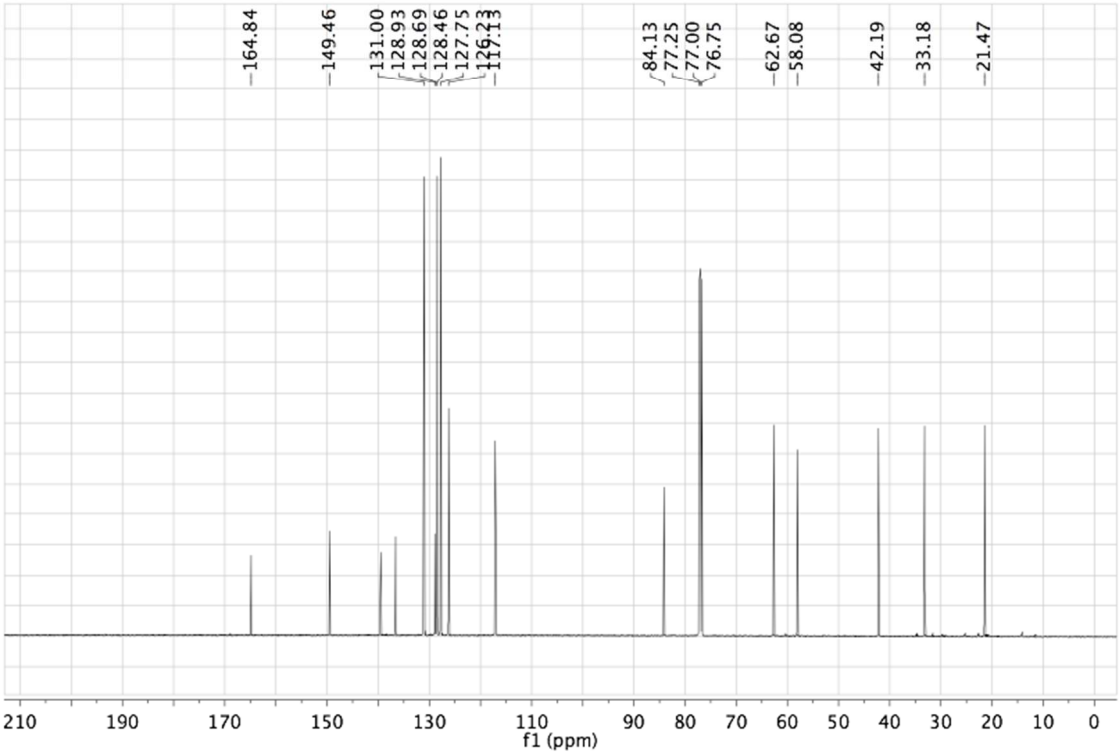

155.99
145.76
123.22
121.34
120.03
119.42
116.84
114.75
114.43
83.84
79.99
77.32
77.00
76.68
70.23
62.03
28.26
f1 (ppm)

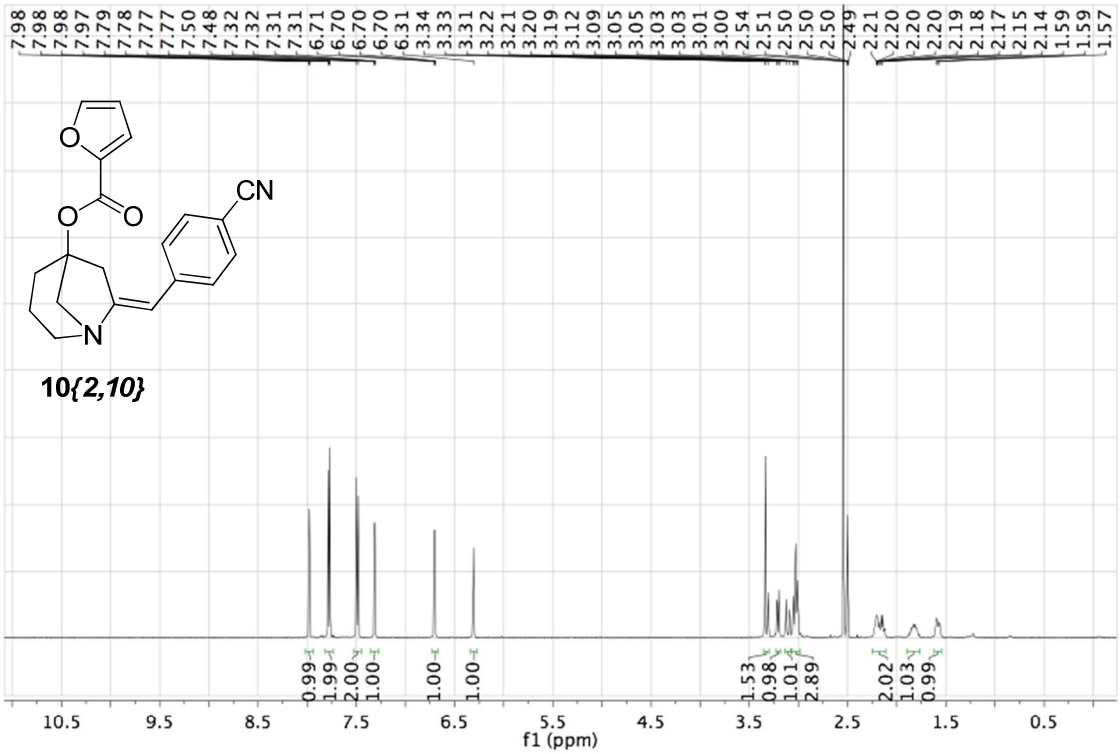

OTf
O
N
Boc
19b
6.15
4.68
4.68
4.66
4.65
4.65
4.62
4.62
3.48
3.47
3.42
3.42
3.40
3.40
3.38
2.11
2.09
2.07
2.04
2.03
2.02
1.45
0.90
2.08
1.18
3.17
1.11
1.00
9.42
f1 (ppm)

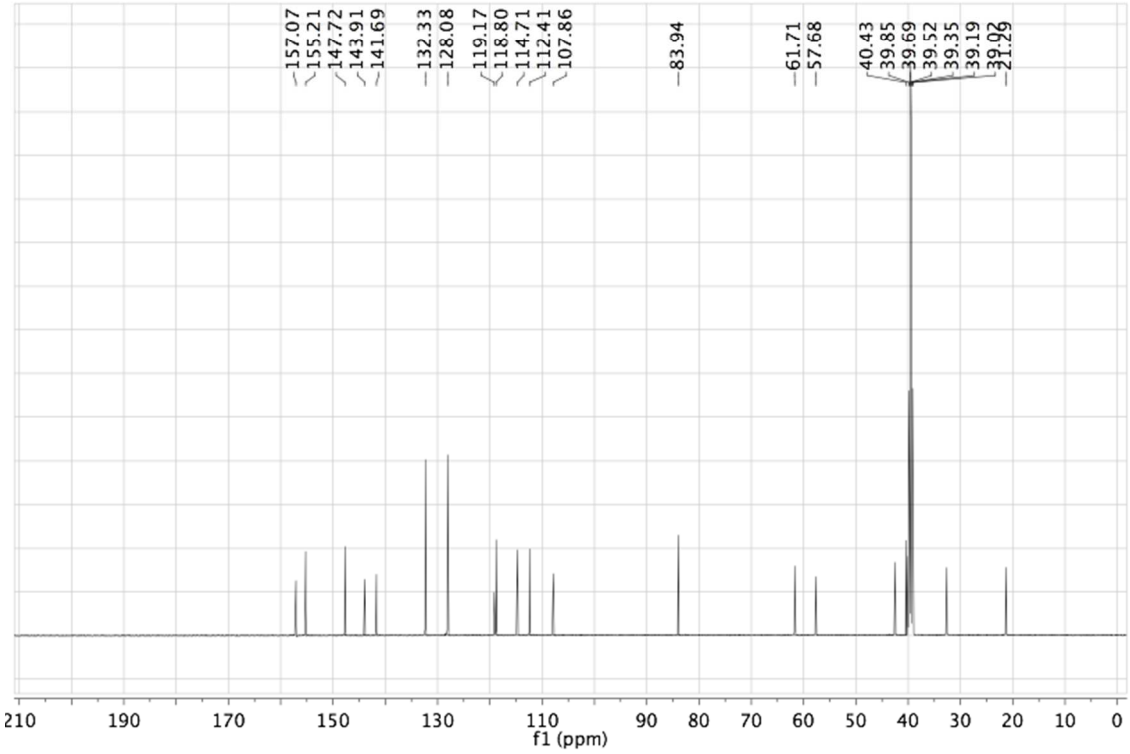

152.93
144.11
122.32
121.45
118.89
116.34
115.76
113.78
92.25
77.93
67.78
54.51
43.65
40.02
39.85
39.69
39.52
39.35
39.19
39.02
35.40
27.51
f1 (ppm)

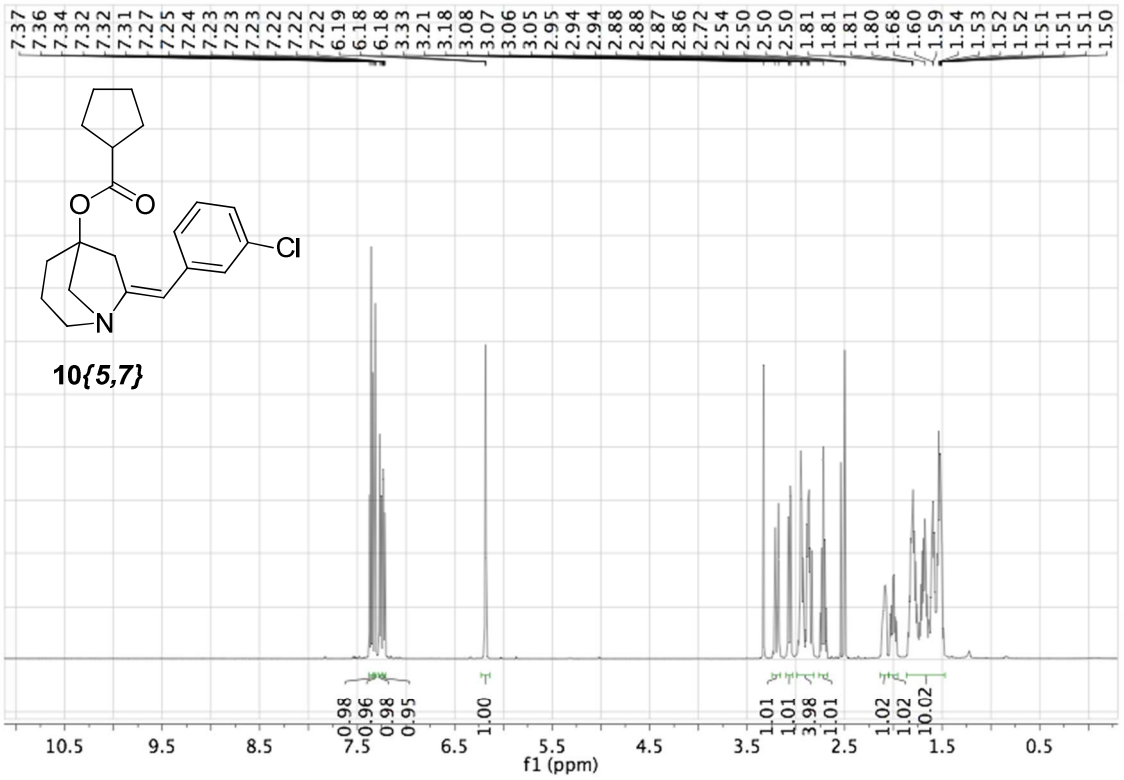
Library Compounds

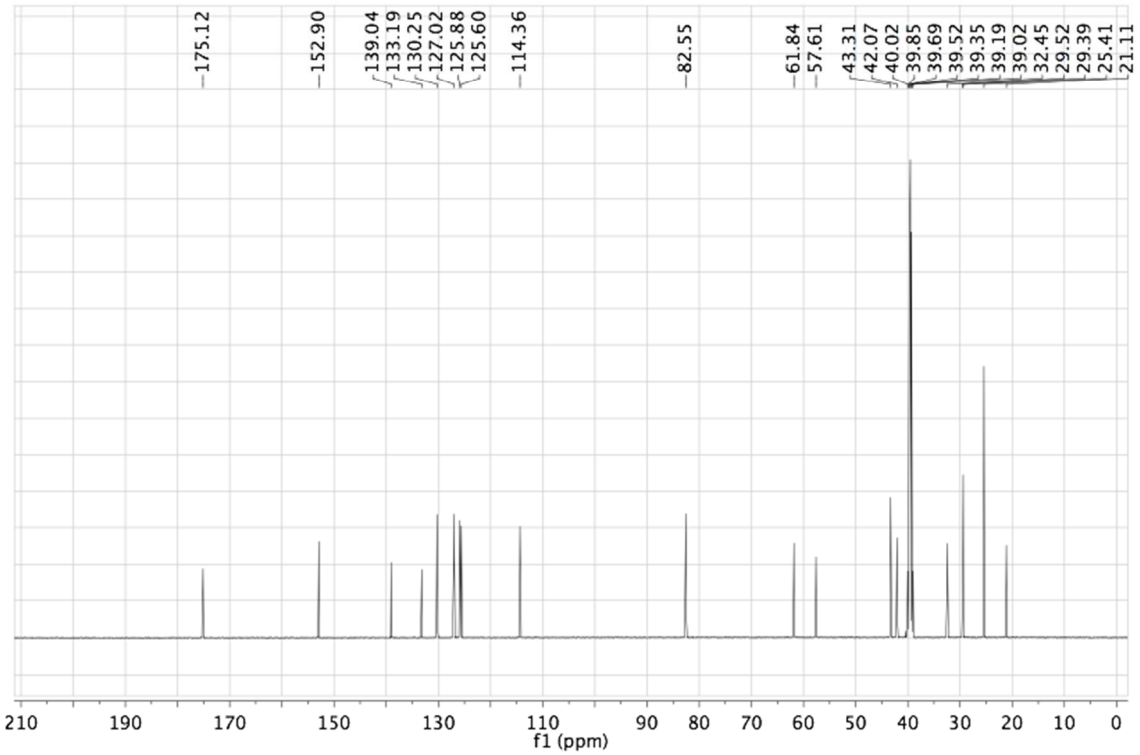


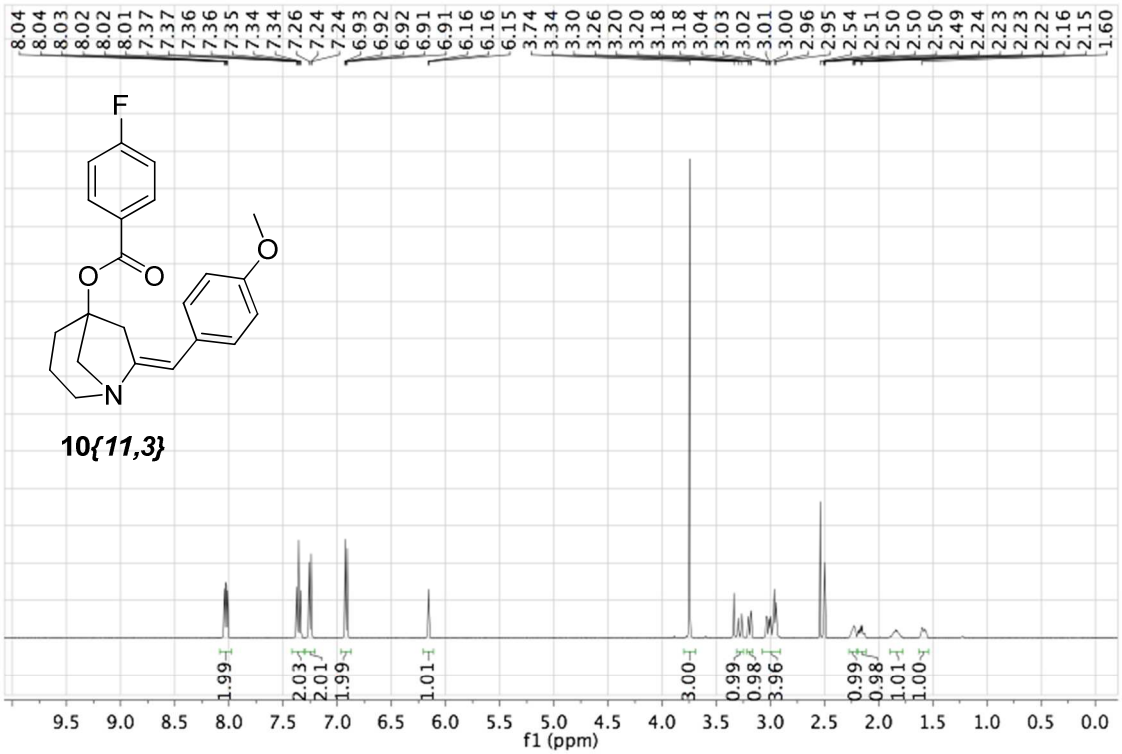


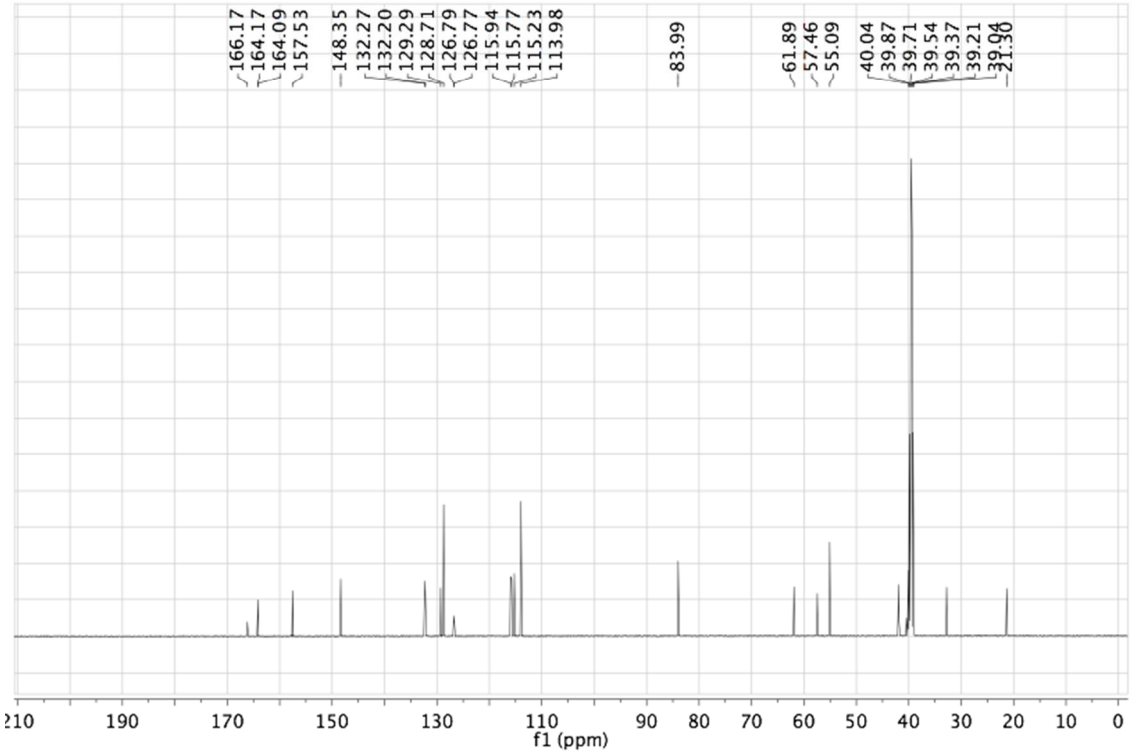

7.98 7.98 7.98 7.97 7.79 7.78 7.77 7.77 7.50 7.48 7.32 7.31 7.31 6.71 6.70 6.70 6.31 3.34 3.33 3.31 3.22 3.21 3.20 3.19 3.12 3.09 3.05 3.05 3.03 3.03 3.01 3.00 2.54 2.51 2.50 2.50 2.50 2.49 2.21 2.20 2.20 2.20 2.19 2.18 2.17 2.15 2.14 1.59 1.59 1.57
O
O
O
CN
N
10{2,10}
0.99 1.99 2.00 1.00 1.00 1.00 1.53 0.98 1.01 2.89 2.02 1.03 0.99
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)

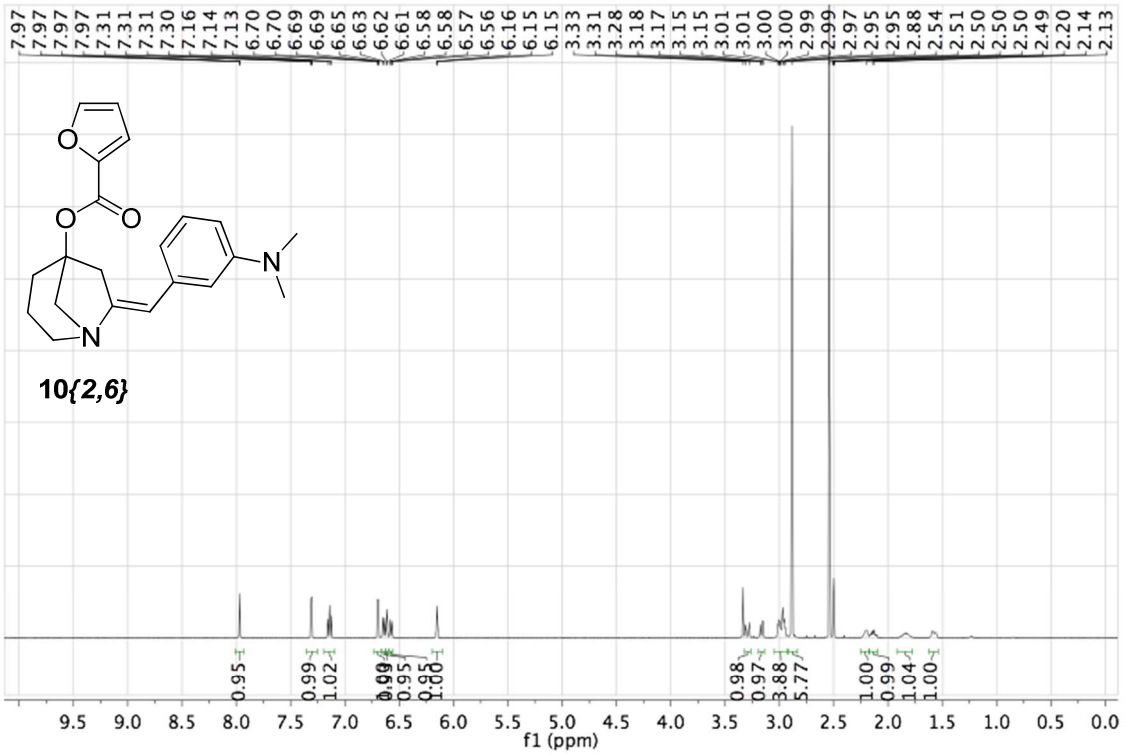

157.07 155.21 147.72 143.91 141.69 132.33 128.08 119.17 118.80 114.71 112.41 107.86 83.94 61.71 57.68 40.43 39.85 39.69 39.52 39.35 39.19 39.02 21.29
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

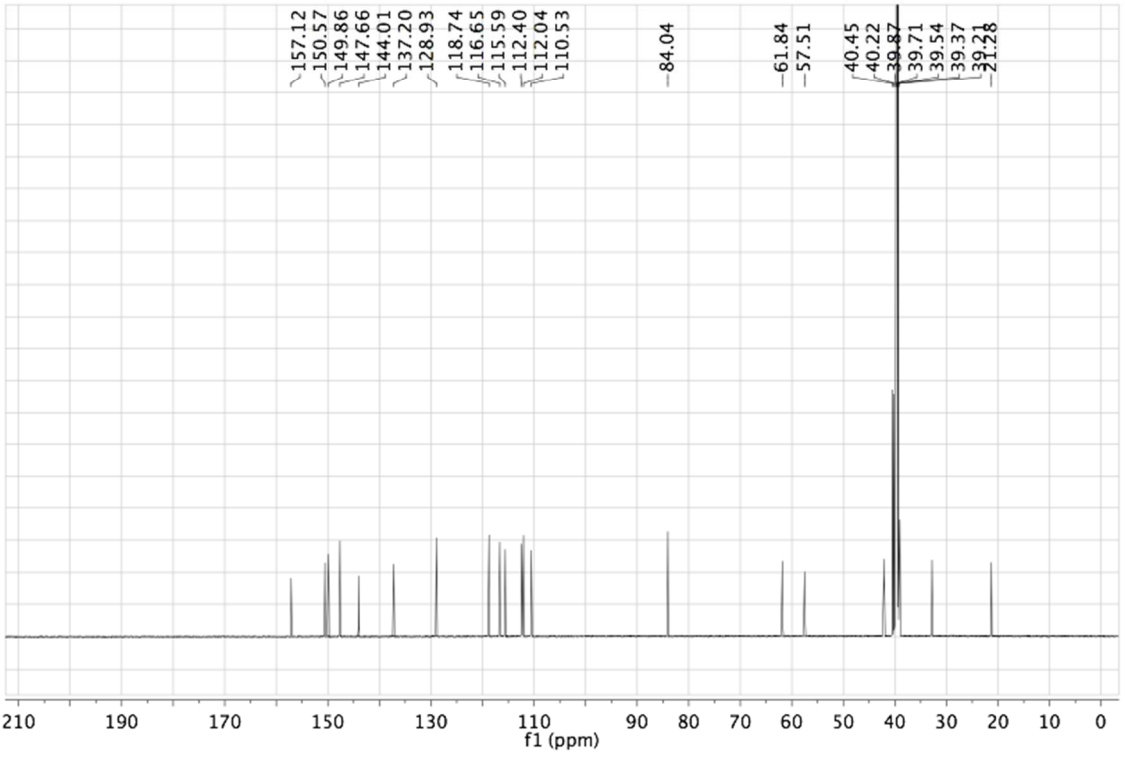

7.37 7.36 7.34 7.32 7.32 7.31 7.27 7.25 7.24 7.23 7.23 7.23 7.22 7.22 7.22 6.19 6.18 6.18 3.33 3.21 3.18 3.08 3.07 3.06 3.05 2.95 2.94 2.94 2.88 2.88 2.87 2.86 2.72 2.54 2.50 2.50 2.50 1.81 1.81 1.81 1.80 1.68 1.60 1.59 1.54 1.53 1.52 1.52 1.51 1.51 1.51 1.50
O
O
Cl
N
10{5,7}
0.98 0.96 0.98 0.95 1.00 1.01 1.01 3.98 1.01 1.02 1.02 10.02
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)

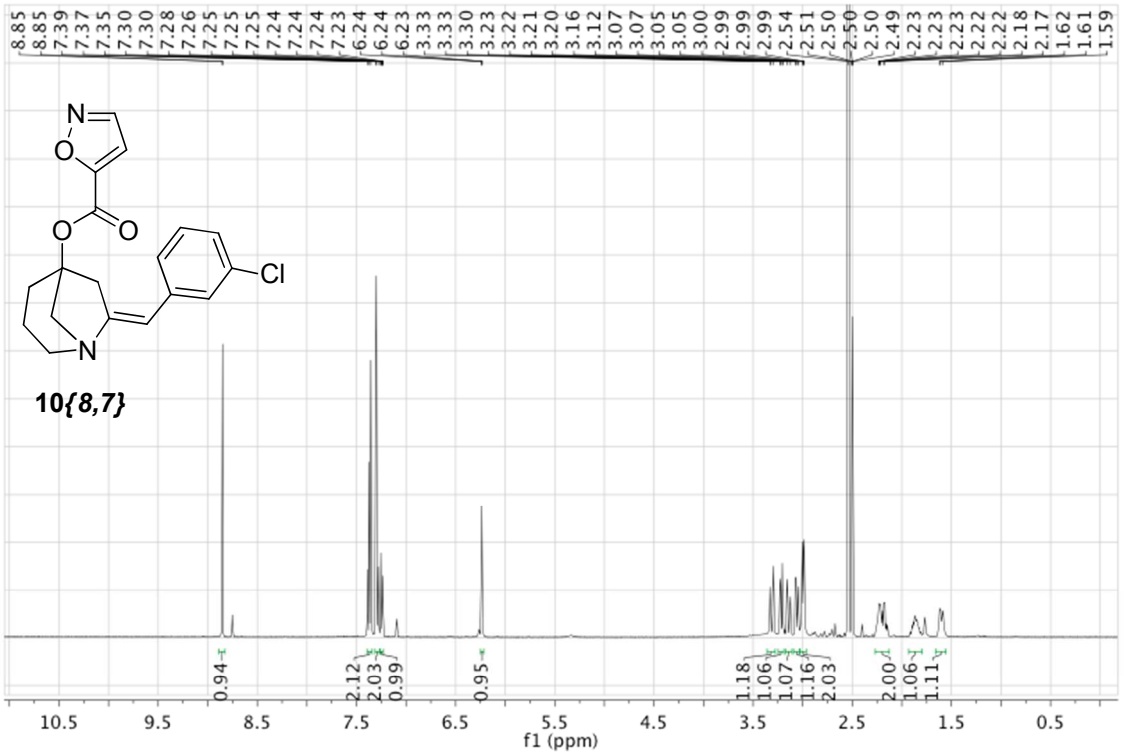

175.12 152.90 139.04 133.19 130.25 127.02 125.88 125.60 114.36 82.55 61.84 57.61 43.31 42.07 40.02 39.85 39.69 39.52 39.35 39.19 39.02 32.45 29.52 29.39 25.41 21.11
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

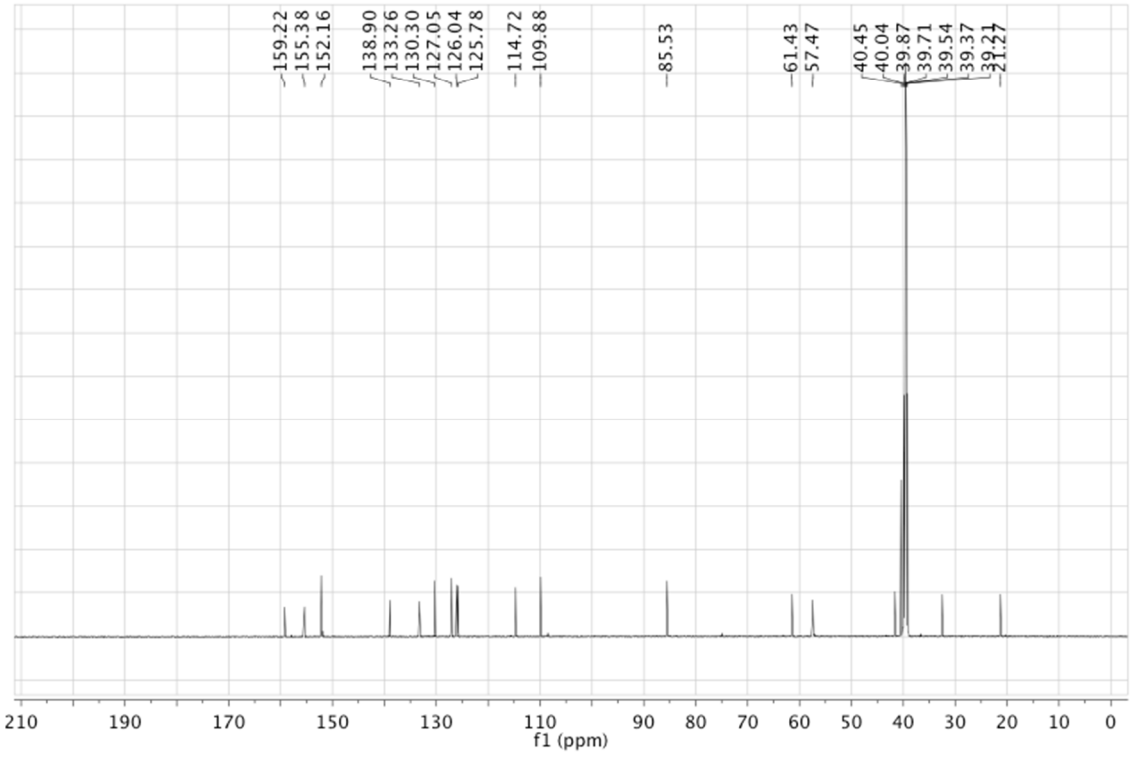

F
O
O
O
N
10{11,3}
f1 (ppm)

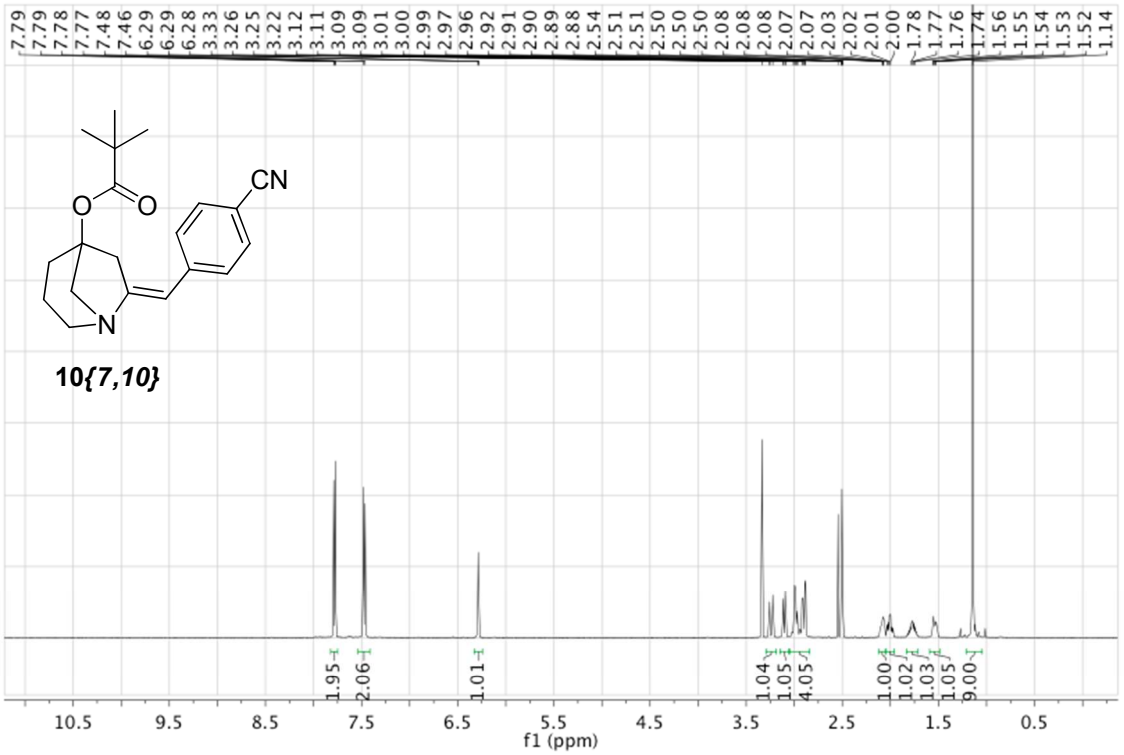

f1 (ppm)

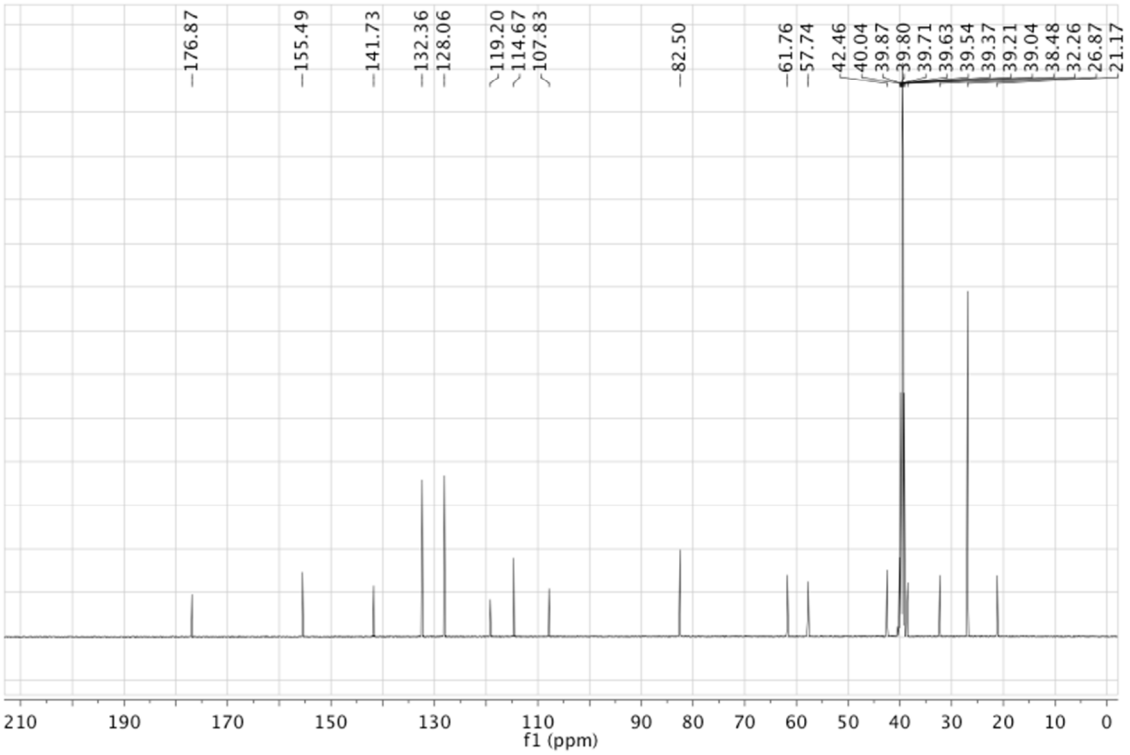

10{2,6}
f1 (ppm)

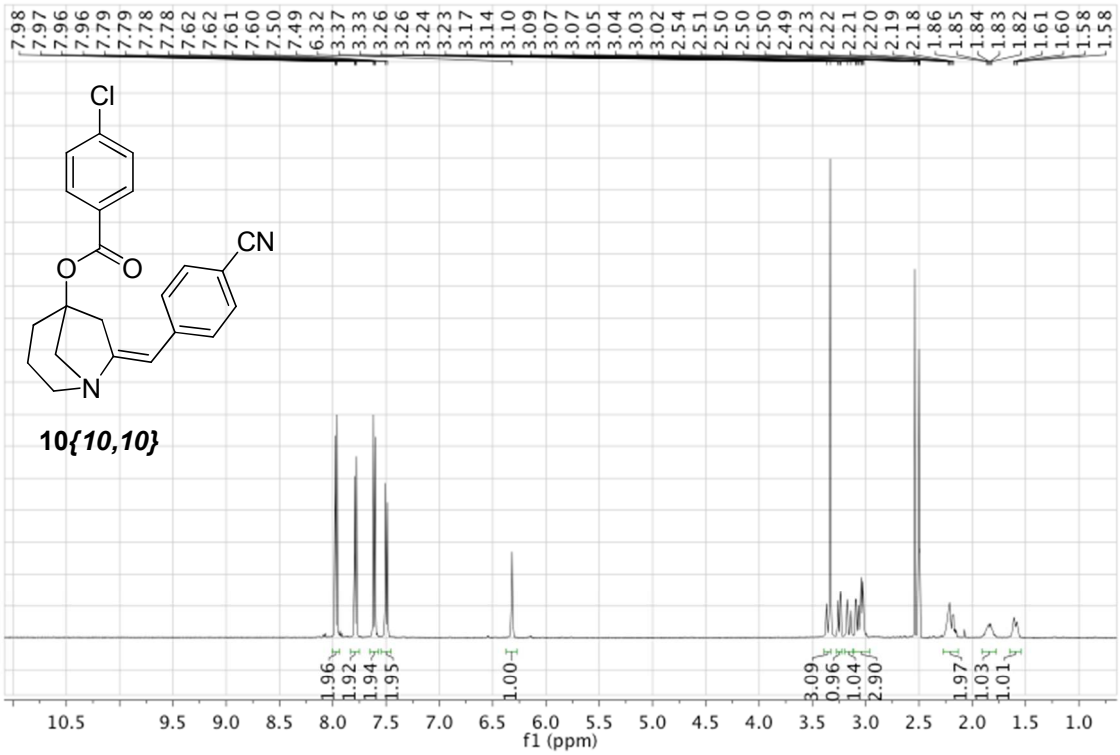

f1 (ppm)

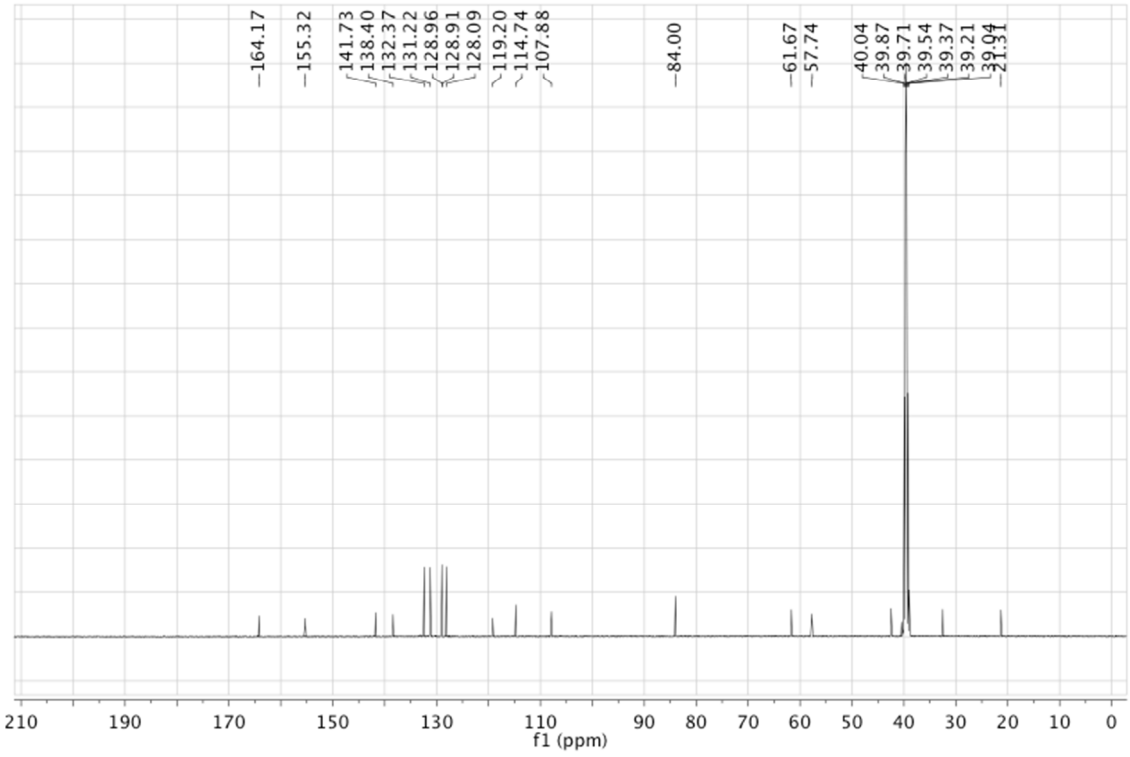

10{8,7}
f1 (ppm)

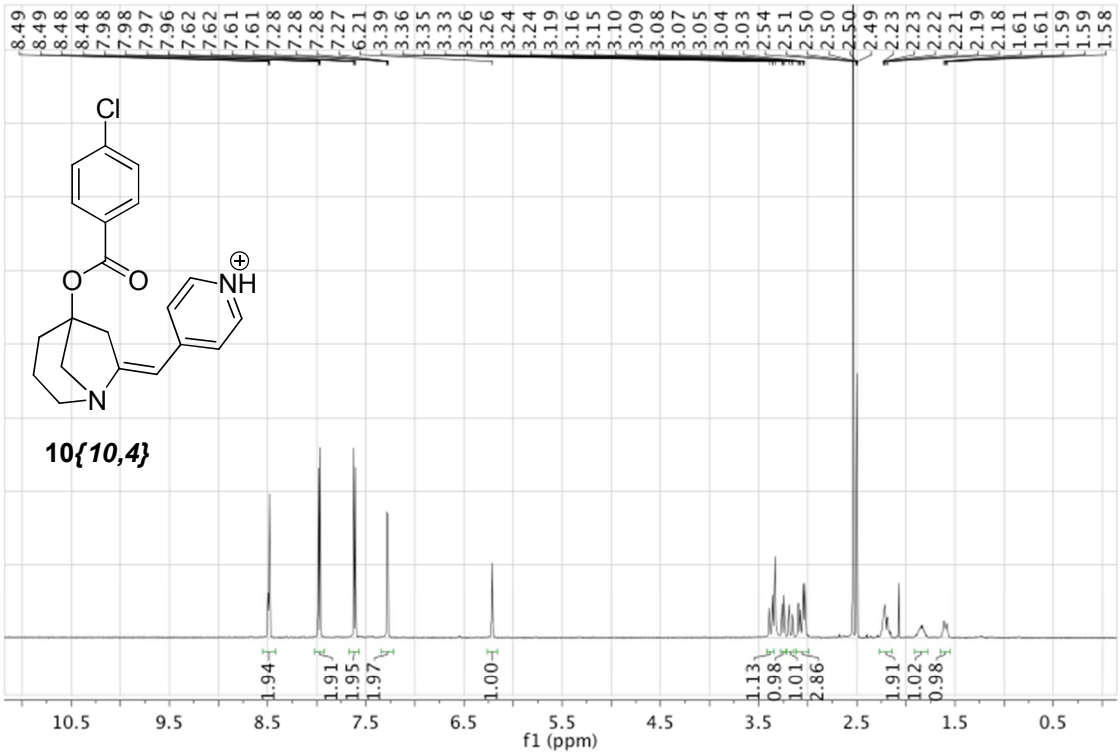

f1 (ppm)

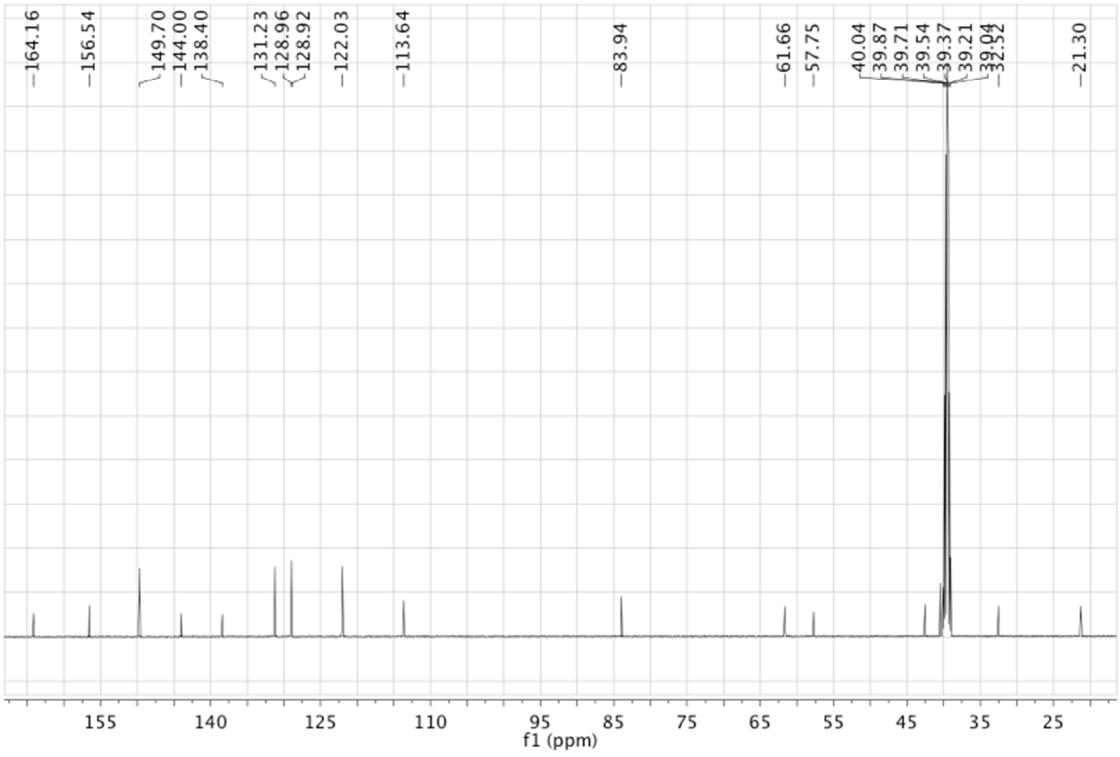

7.79 7.79 7.78 7.77 7.48 7.46 6.29 6.28 3.33 3.26 3.25 3.22 3.12 3.11 3.09 3.09 3.01 3.00 2.99 2.97 2.96 2.92 2.91 2.90 2.89 2.88 2.54 2.51 2.51 2.50 2.50 2.50 2.08 2.08 2.08 2.07 2.07 2.03 2.02 2.01 2.00 1.78 1.77 1.76 1.74 1.56 1.55 1.54 1.53 1.52 1.14
O
O
CN
N
10{7,10}
1.95 2.06 1.01 1.04 1.05 4.05 1.00 1.02 1.03 1.05 9.00
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)

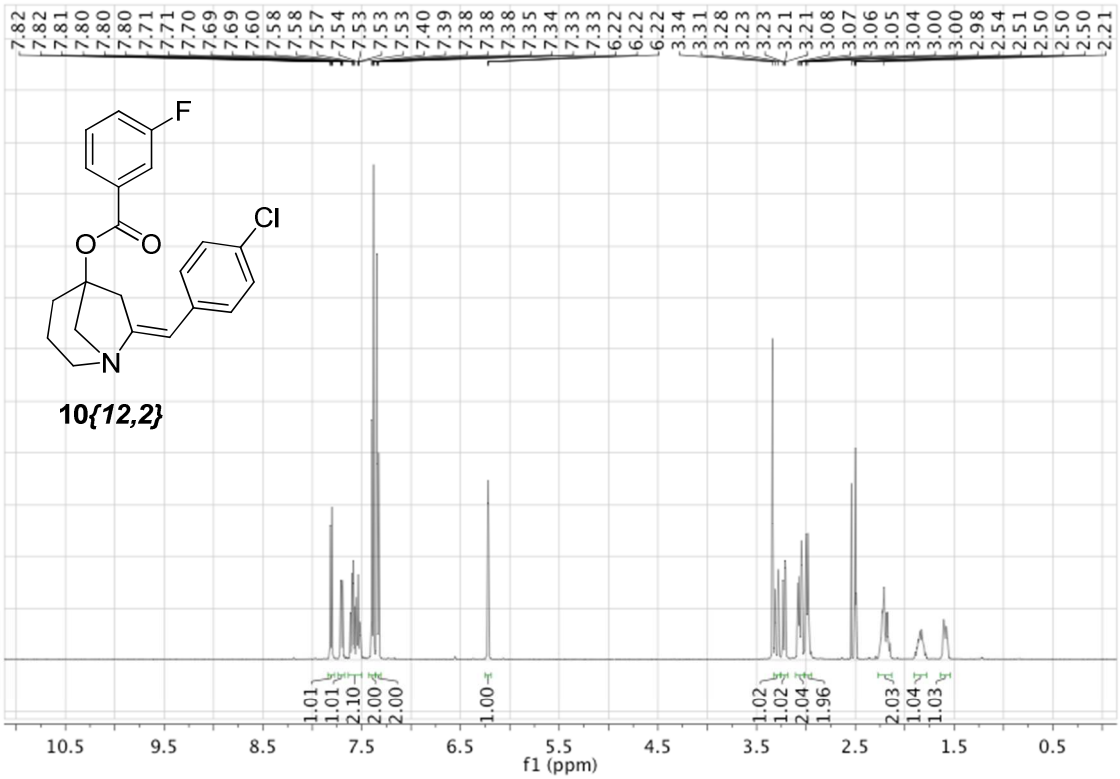

176.87 155.49 141.73 132.36 128.06 119.20 114.67 107.83 82.50 61.76 57.74 42.46 40.04 39.87 39.80 39.71 39.63 39.54 39.37 39.21 39.04 38.48 32.26 26.87 21.17
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

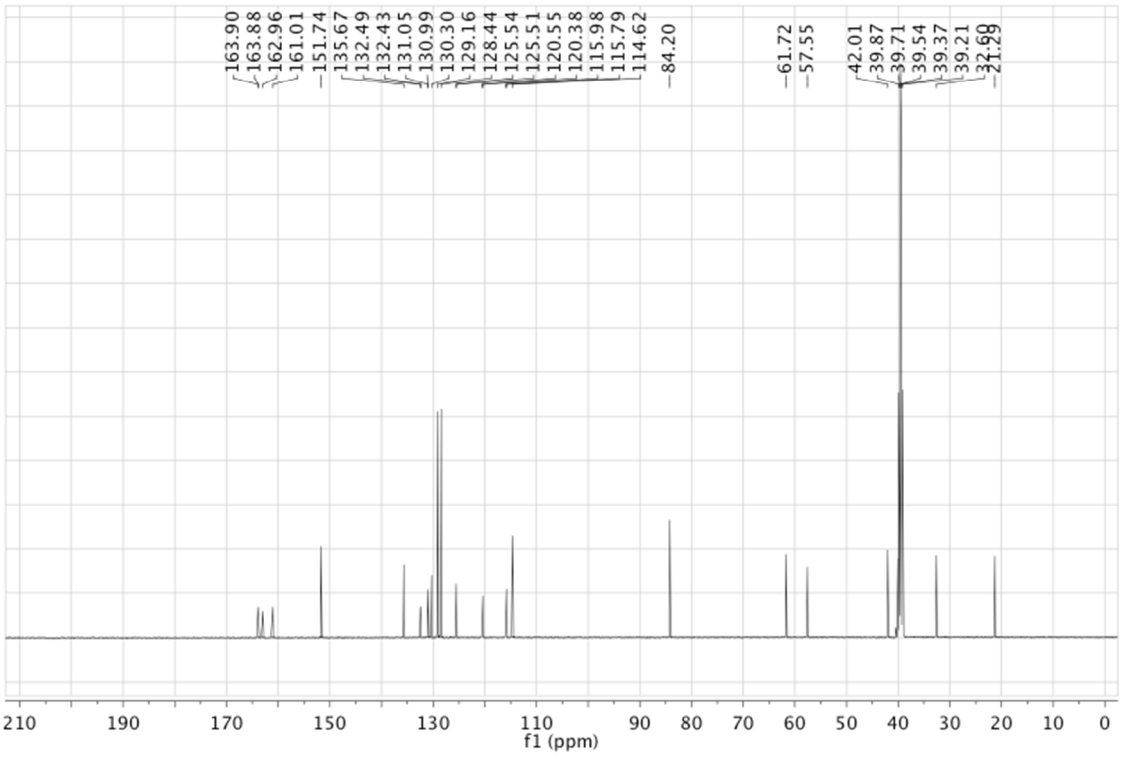

Cl
CN
O
O
N
10{10,10}
f1 (ppm)

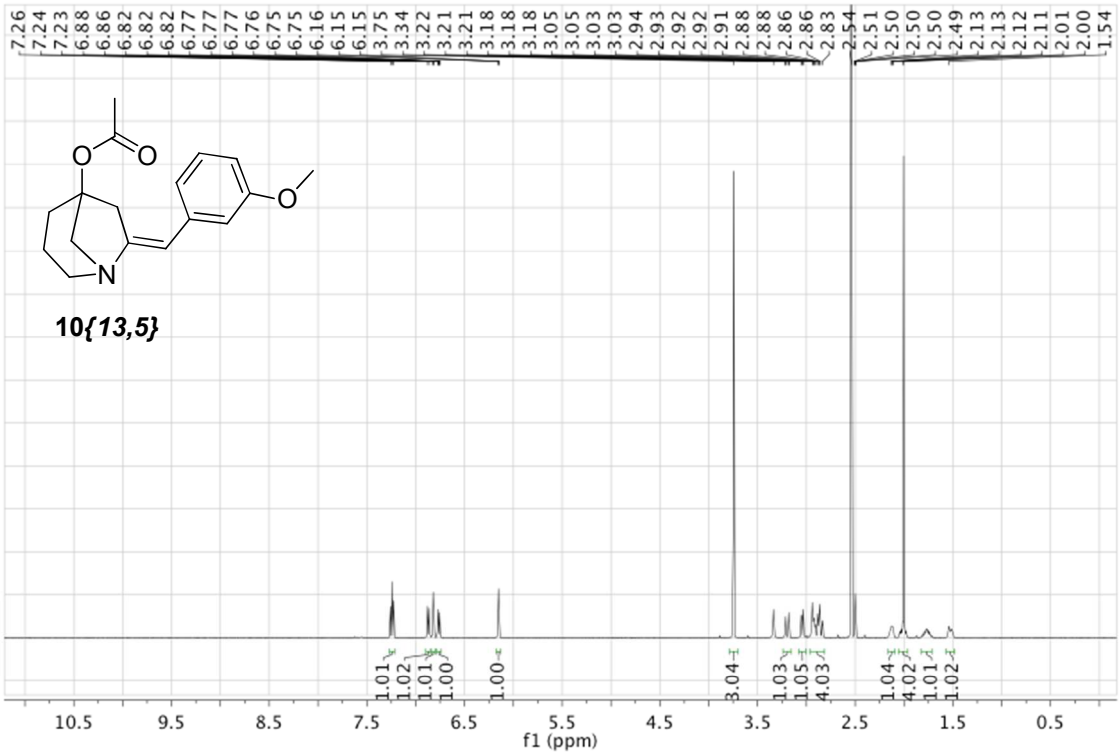

f1 (ppm)


Cl
O
O
NH
N
10{10,4}
f1 (ppm)

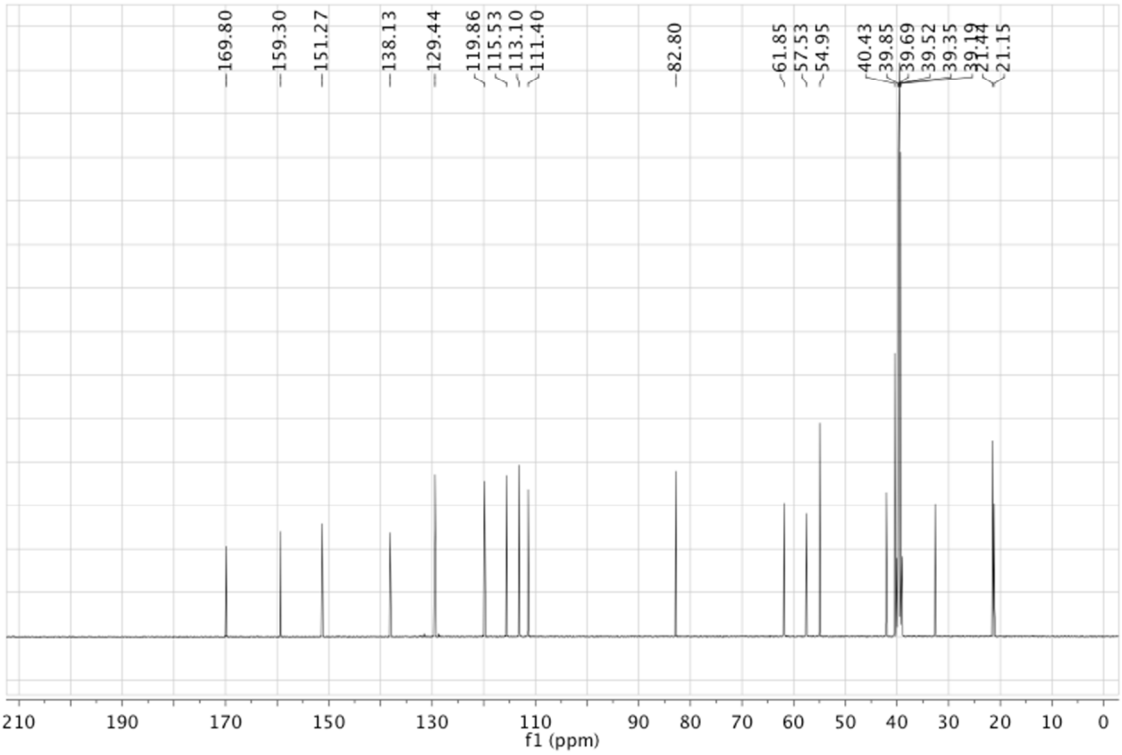

f1 (ppm)

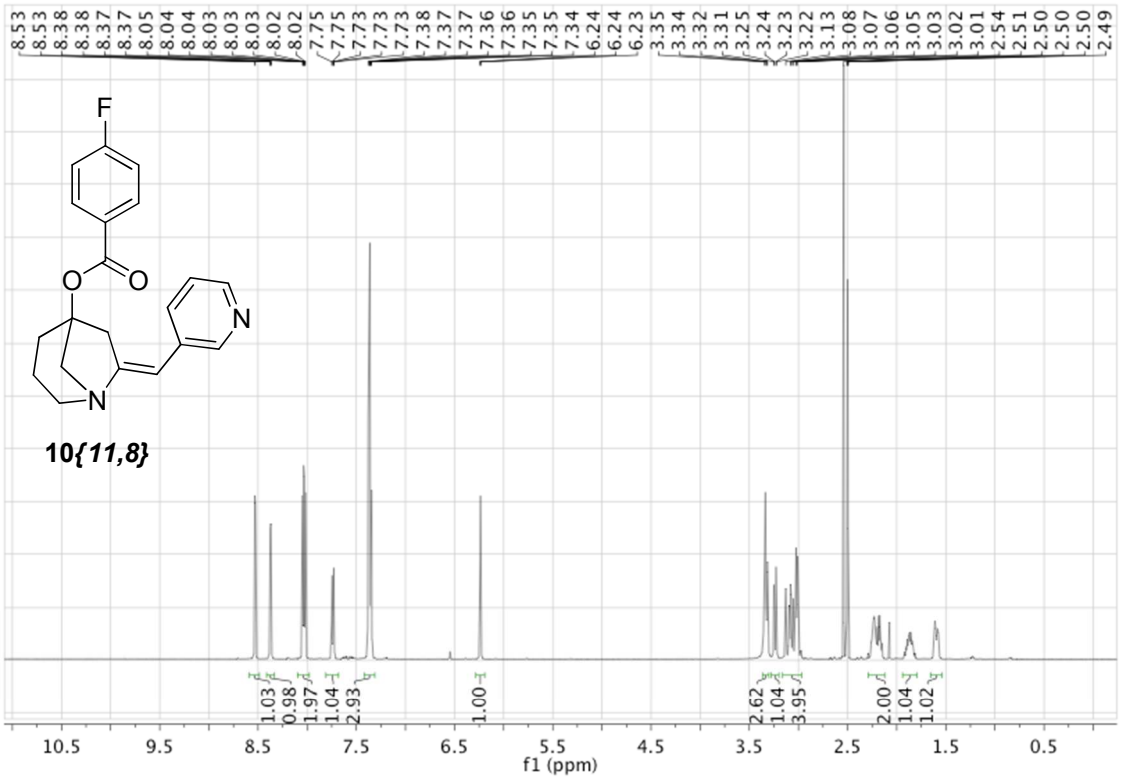

F
Cl
O
O
N
10{12,2}
f1 (ppm)

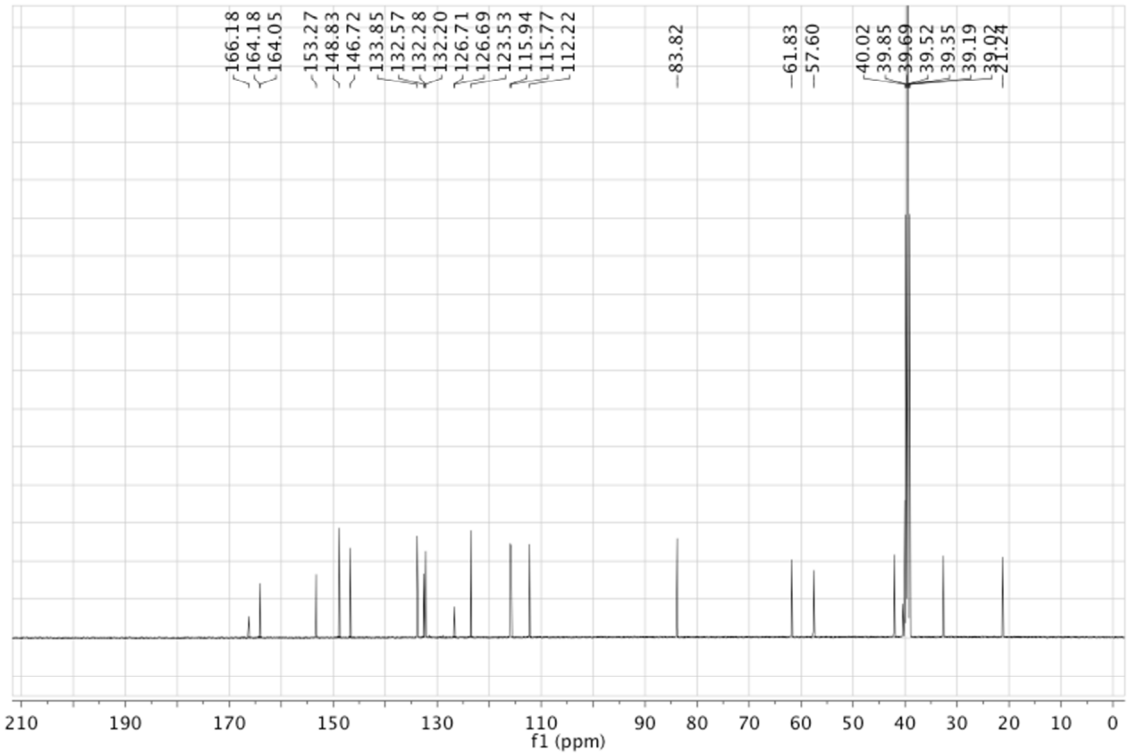

f1 (ppm)

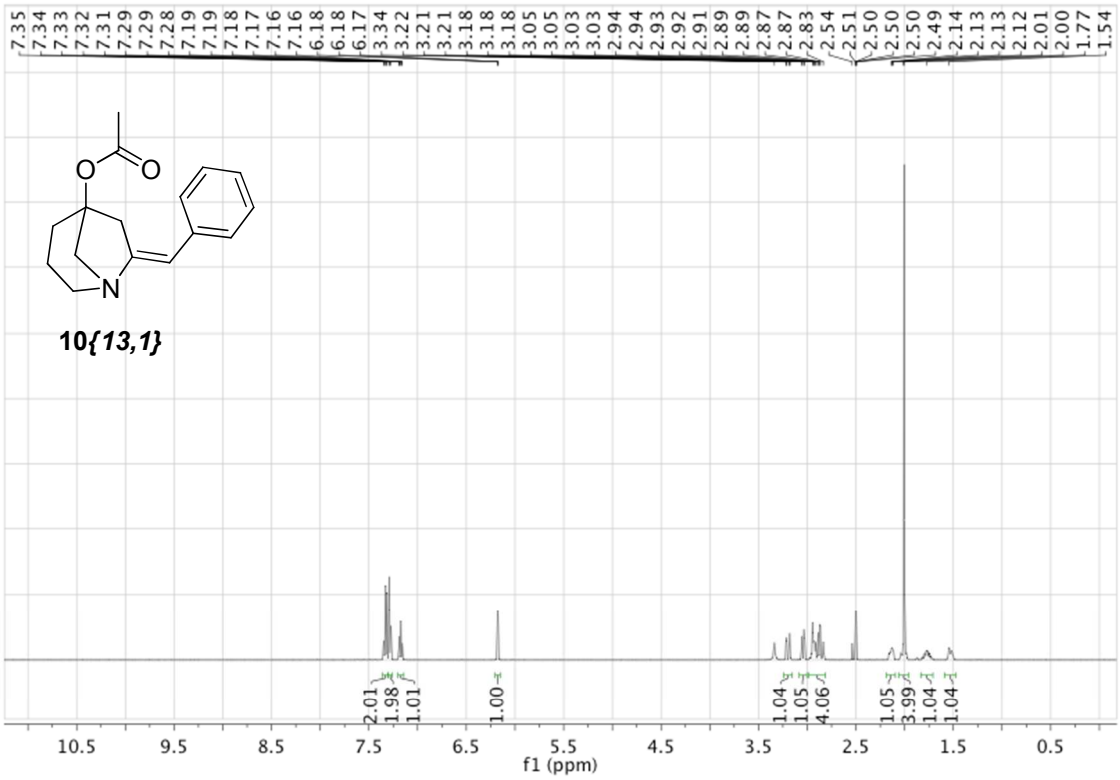

7.26 7.24 7.23 6.88 6.86 6.82 6.82 6.82 6.77 6.77 6.77 6.76 6.75 6.75 6.16 6.15 6.15 3.75 3.34 3.22 3.21 3.21 3.18 3.18 3.18 3.05 3.05 3.03 3.03 2.94 2.93 2.92 2.92 2.91 2.88 2.88 2.86 2.86 2.83 2.54 2.51 2.50 2.50 2.50 2.49 2.13 2.13 2.12 2.11 2.01 2.00 1.54
O
O
O
N
1.01 1.02 1.01 1.00 1.00 3.04 1.03 1.05 4.03 1.04 4.02 1.01 1.02
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)

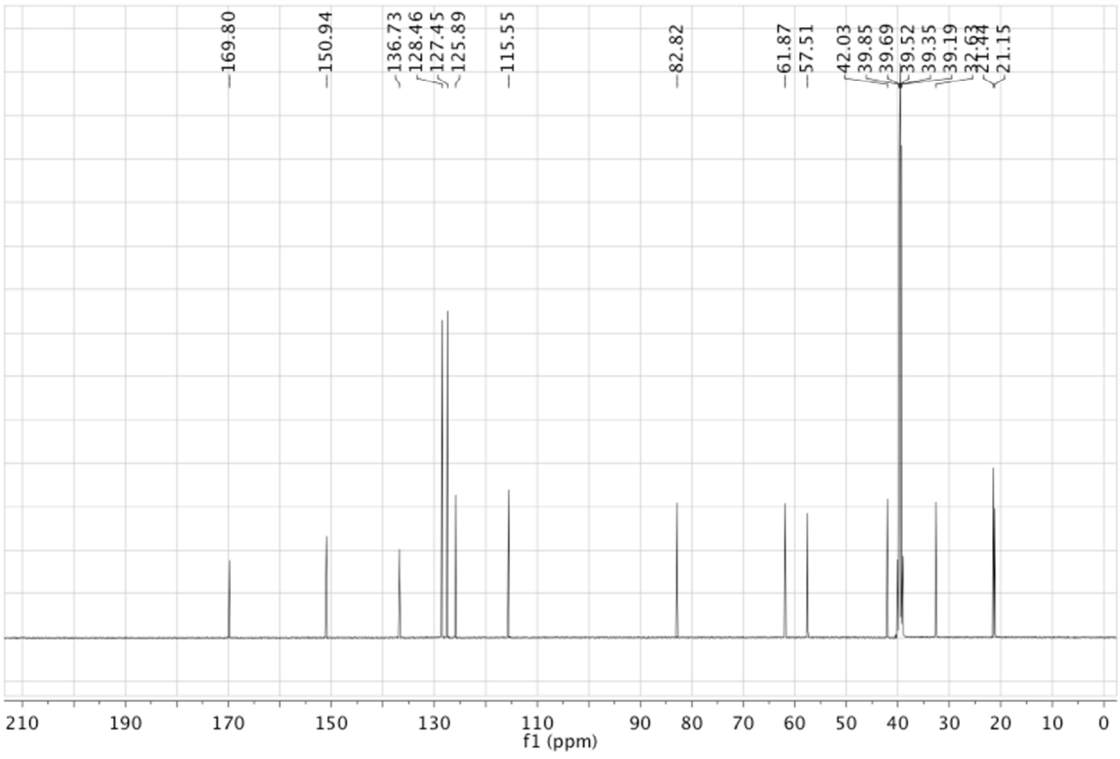
10*{13,5}*

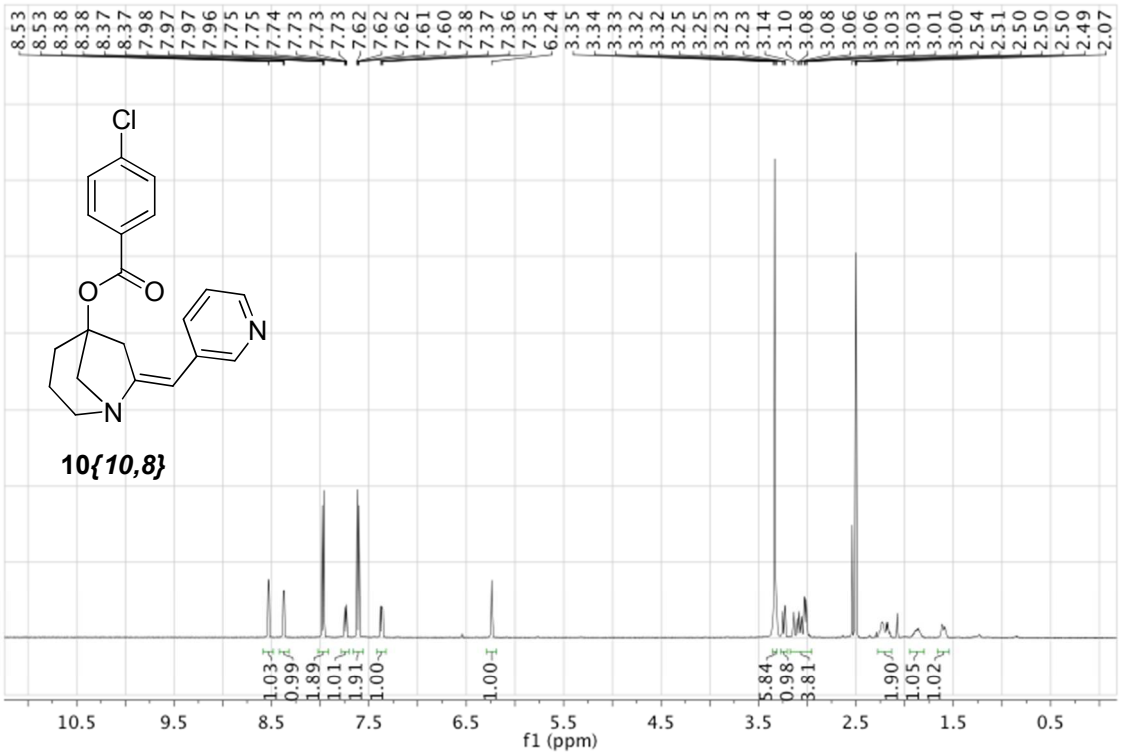

169.80 159.30 151.27 138.13 129.44 119.86 115.53 113.10 111.40 82.80 61.85 57.53 54.95 40.43 39.85 39.69 39.52 39.35 39.19 21.44 21.15
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

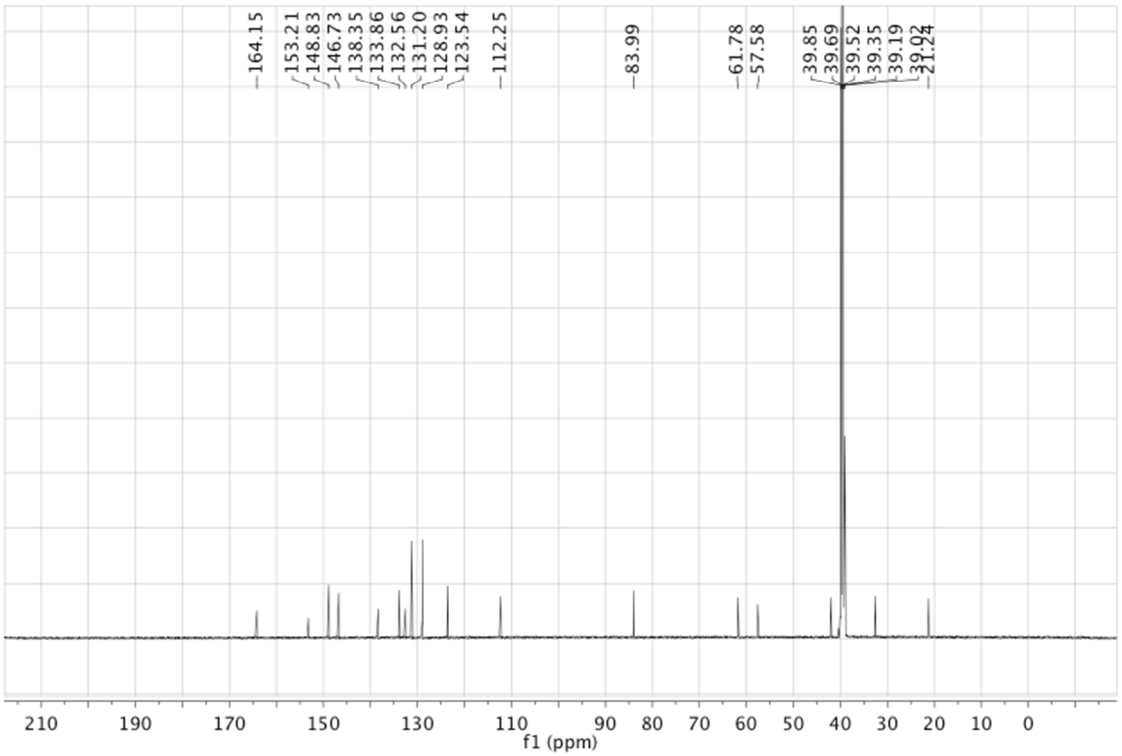

F
O
O
N
N
10{11,8}
f1 (ppm)

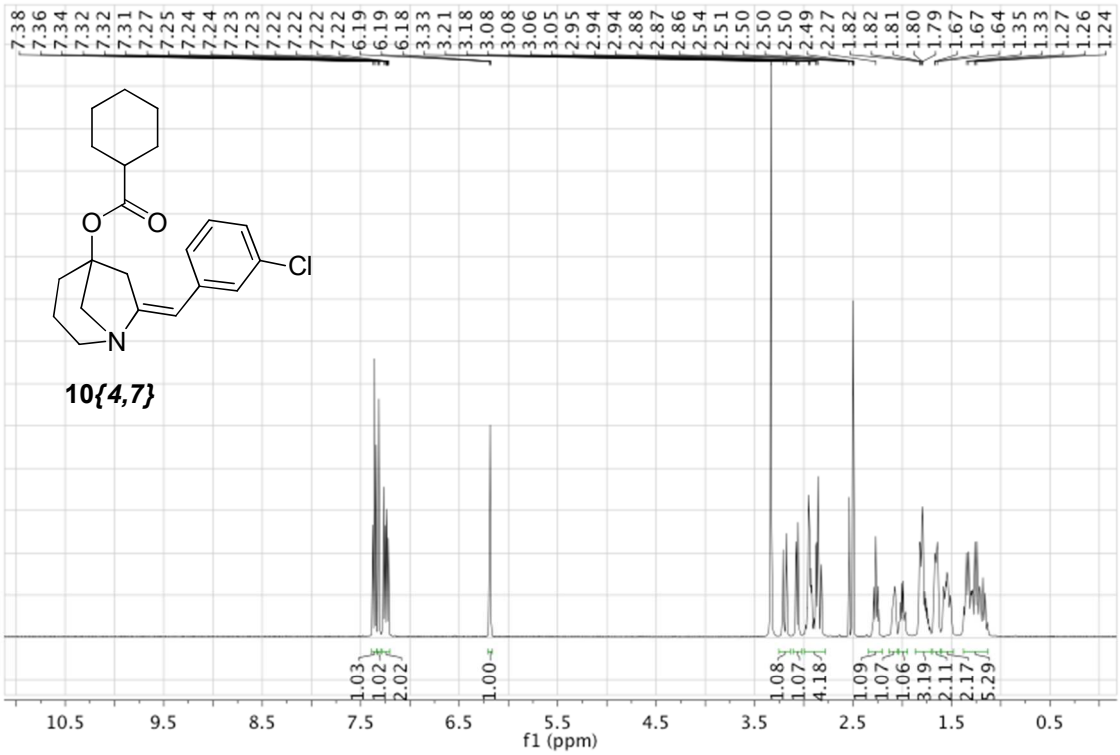

f1 (ppm)

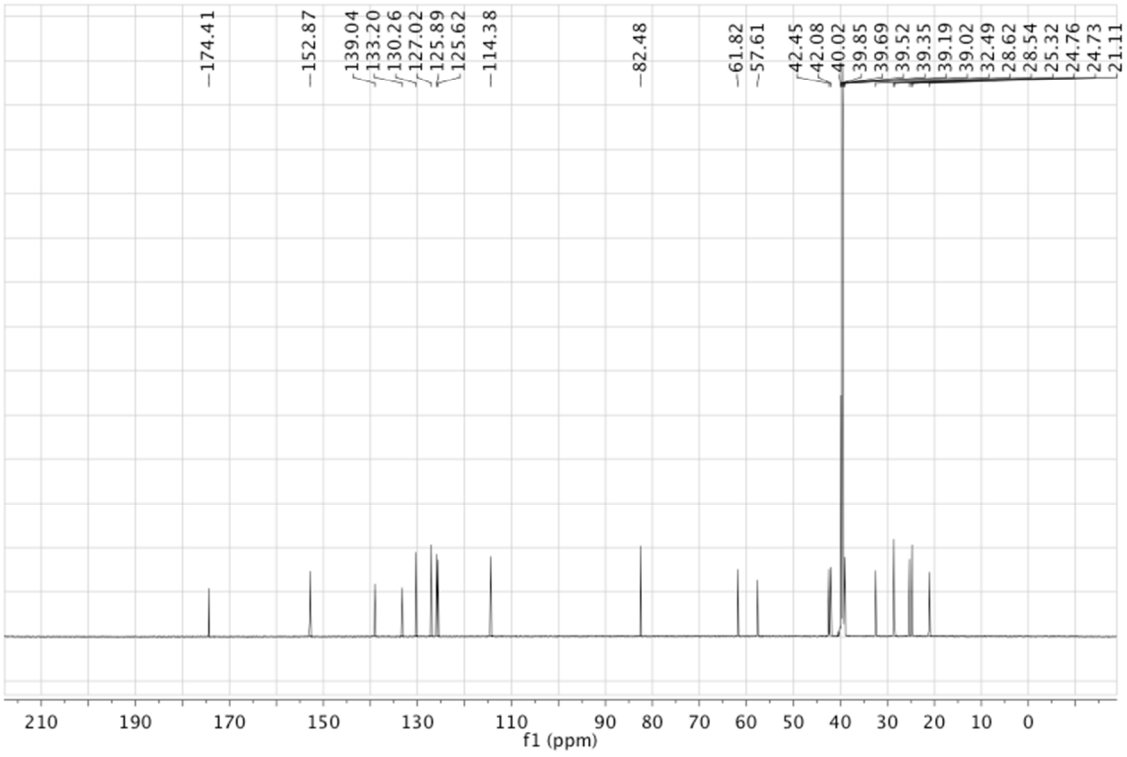

7.35 7.34 7.33 7.32 7.31 7.29 7.29 7.28 7.19 7.19 7.18 7.17 7.16 7.16 6.18 6.17 3.34 3.22 3.21 3.21 3.18 3.18 3.05 3.05 3.03 3.03 2.94 2.94 2.93 2.92 2.91 2.89 2.89 2.87 2.87 2.83 2.54 2.51 2.50 2.50 2.50 2.49 2.14 2.13 2.13 2.12 2.01 2.00 1.77 1.54
O
O
N
10{13,1}
2.01 1.98 1.01 1.00 1.04 1.05 4.06 1.05 3.99 1.04 1.04
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)

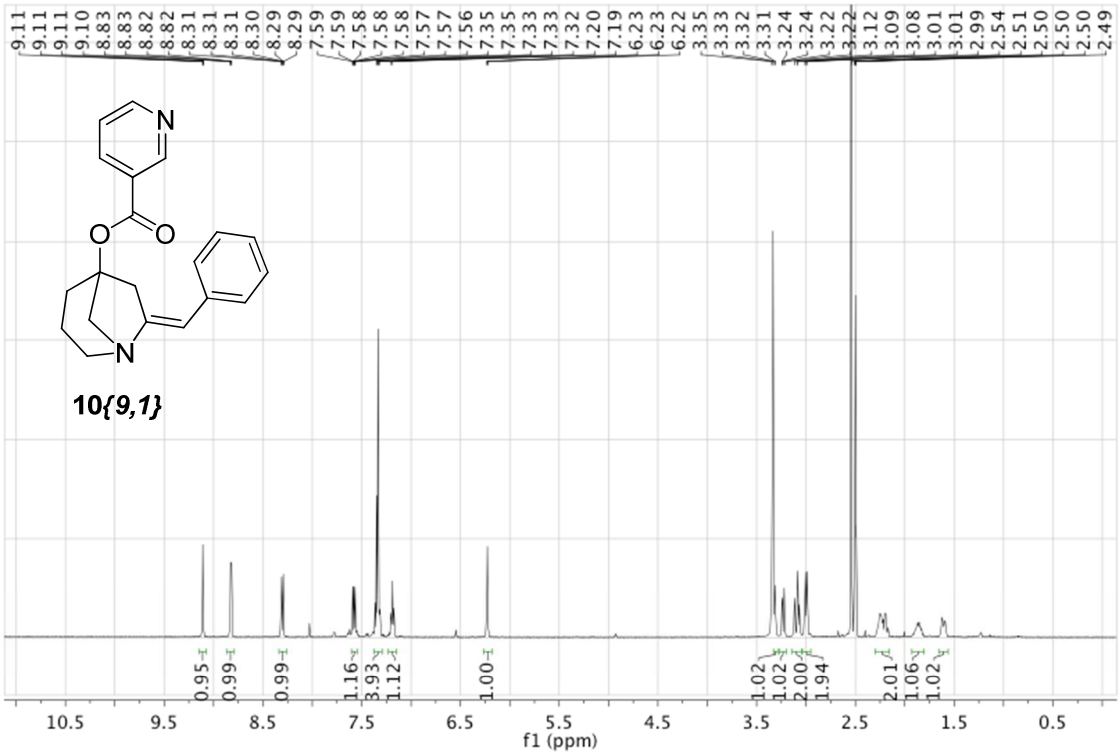

169.80 150.94 136.73 128.46 127.45 125.89 115.55 82.82 61.87 57.51 42.03 39.85 39.69 39.52 39.35 39.19 32.63 21.44 21.15
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

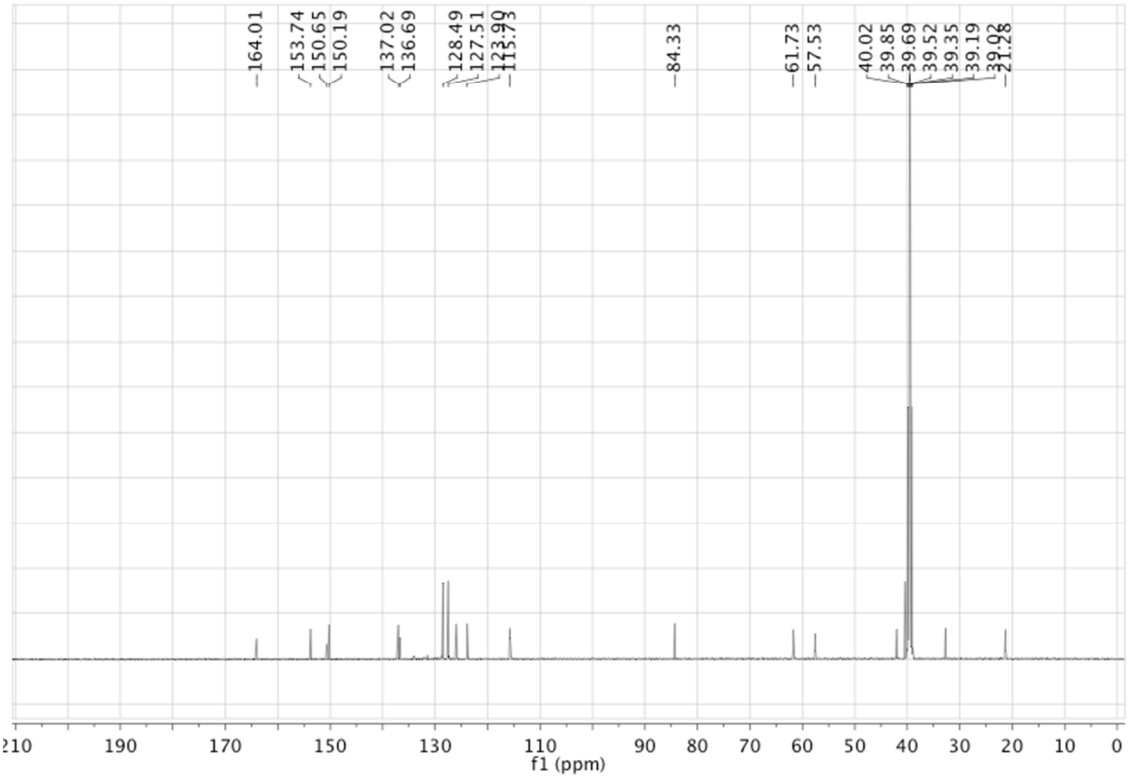

Cl
O
O
N
N
10{10,8}
f1 (ppm)

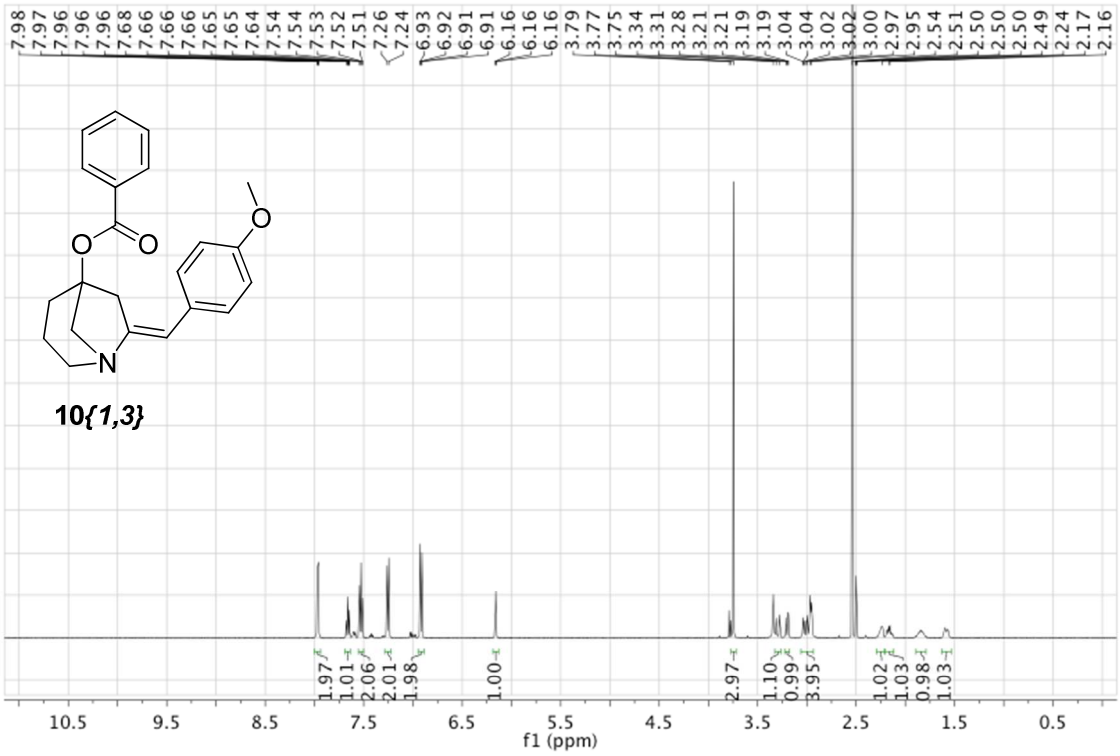

f1 (ppm)

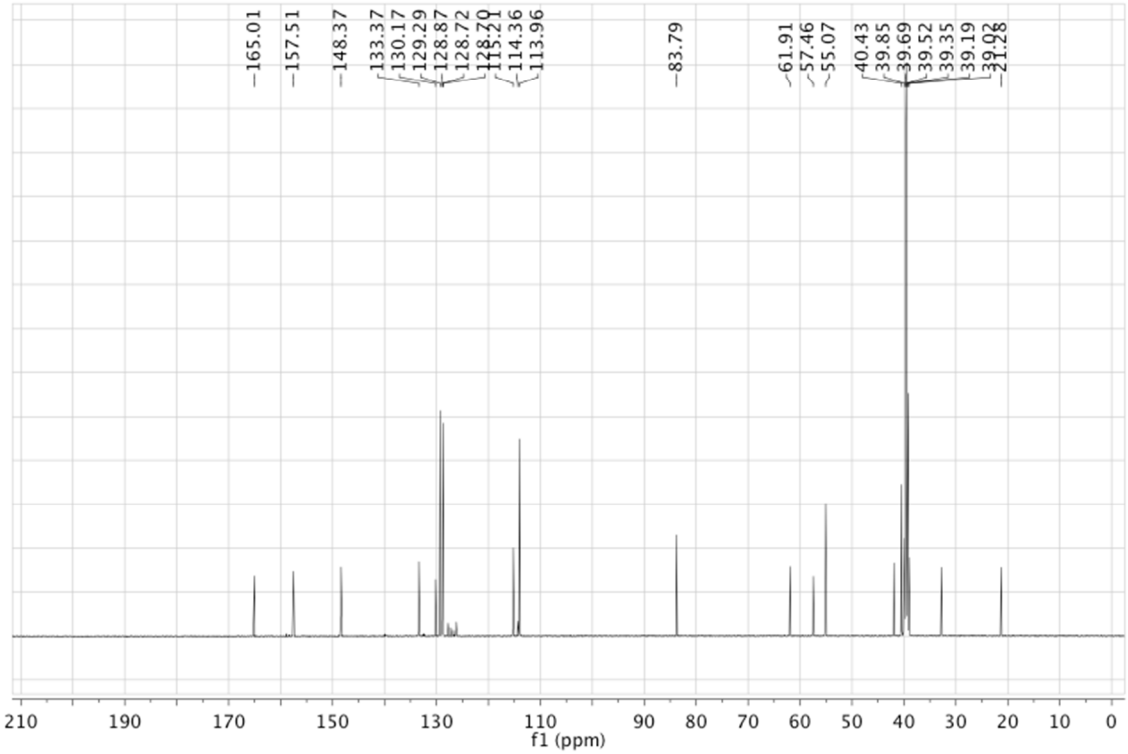

7.38
7.36
7.34
7.32
7.32
7.31
7.27
7.25
7.24
7.24
7.23
7.23
7.22
7.22
7.22
7.22
6.19
6.19
6.18
3.33
3.21
3.18
3.08
3.08
3.06
3.05
2.95
2.94
2.94
2.88
2.87
2.86
2.54
2.51
2.50
2.50
2.50
2.49
2.27
1.82
1.82
1.81
1.80
1.79
1.67
1.67
1.64
1.35
1.33
1.27
1.26
1.24
O
O
Cl
N
10{4,7}
1.03
1.02
2.02
1.00
1.08
1.07
4.18
1.09
1.07
1.06
3.19
2.11
2.17
5.29
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

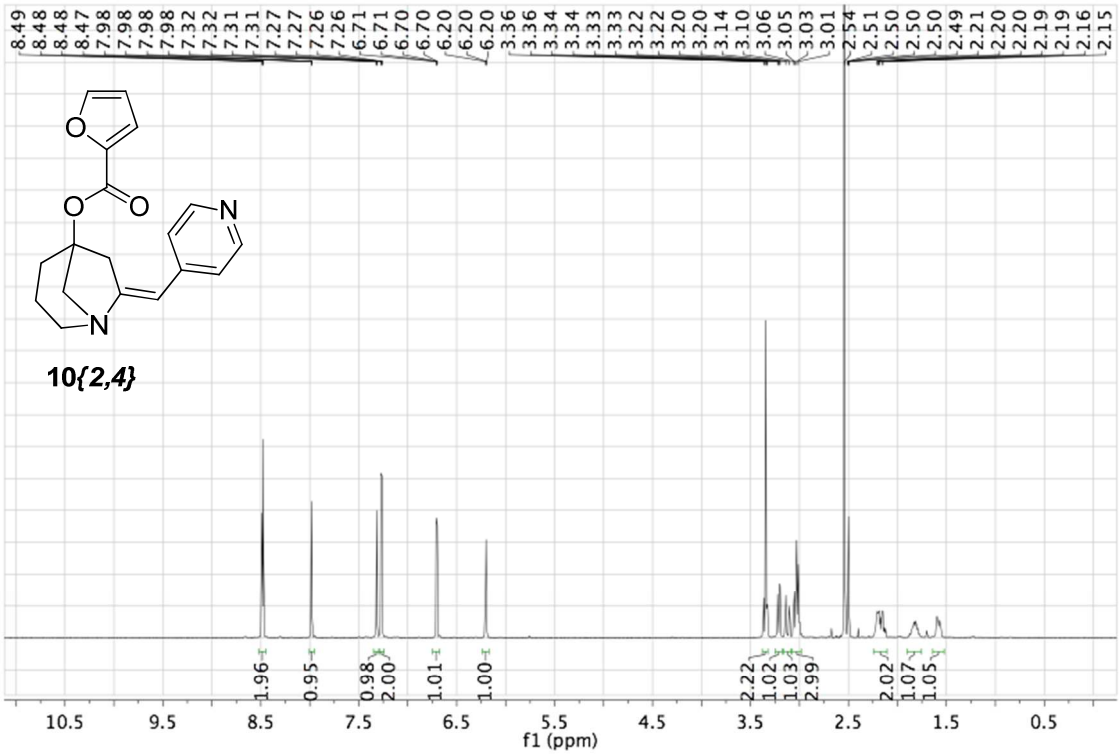

174.41
152.87
139.04
133.20
130.26
127.02
125.89
125.62
114.38
82.48
61.82
57.61
42.45
42.08
40.02
39.85
39.69
39.52
39.35
39.19
39.02
32.49
28.62
28.54
25.32
24.76
24.73
21.11
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

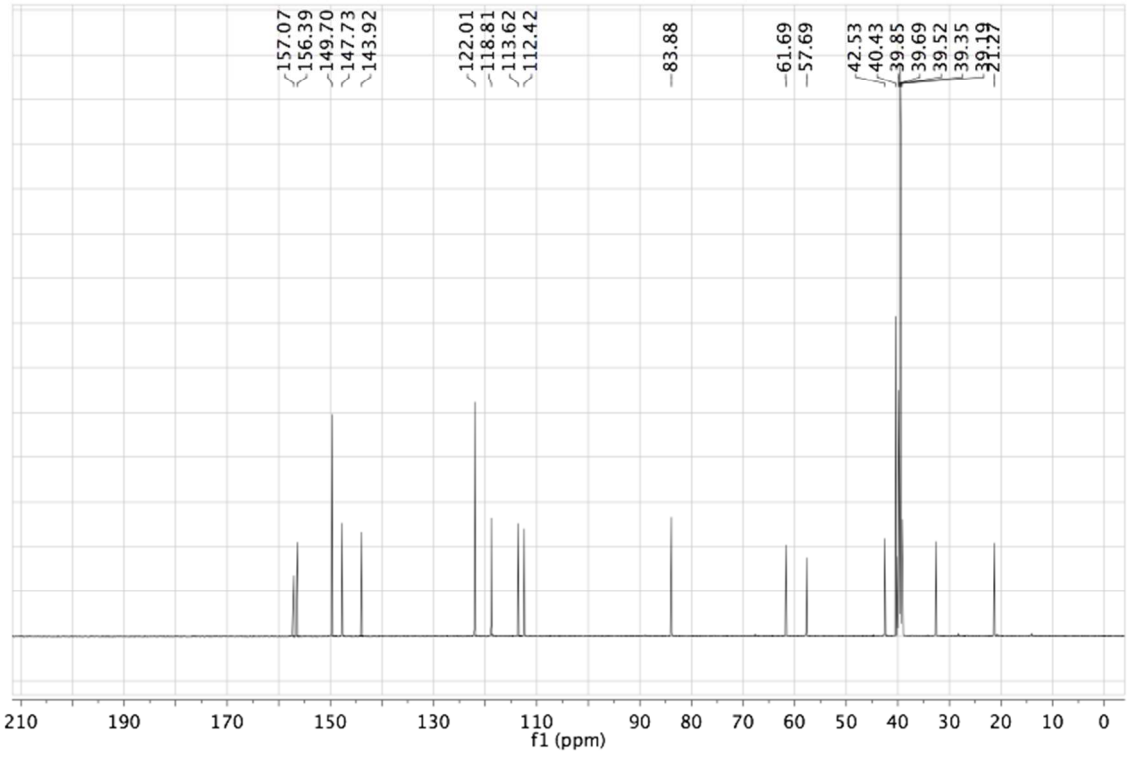

9.11
9.11
9.11
9.10
8.83
8.83
8.82
8.82
8.31
8.31
8.31
8.30
8.29
8.29
7.59
7.59
7.58
7.58
7.58
7.58
7.57
7.57
7.56
7.35
7.35
7.33
7.33
7.32
7.20
7.19
6.23
6.23
6.22
3.35
3.33
3.32
3.31
3.24
3.24
3.22
3.22
3.12
3.09
3.08
3.01
3.01
2.99
2.54
2.51
2.50
2.50
2.50
2.49
N
O
O
N
10{9,1}
0.95
0.99
0.99
1.16
3.93
1.12
1.00
1.02
1.02
2.00
1.94
2.01
1.06
1.02
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

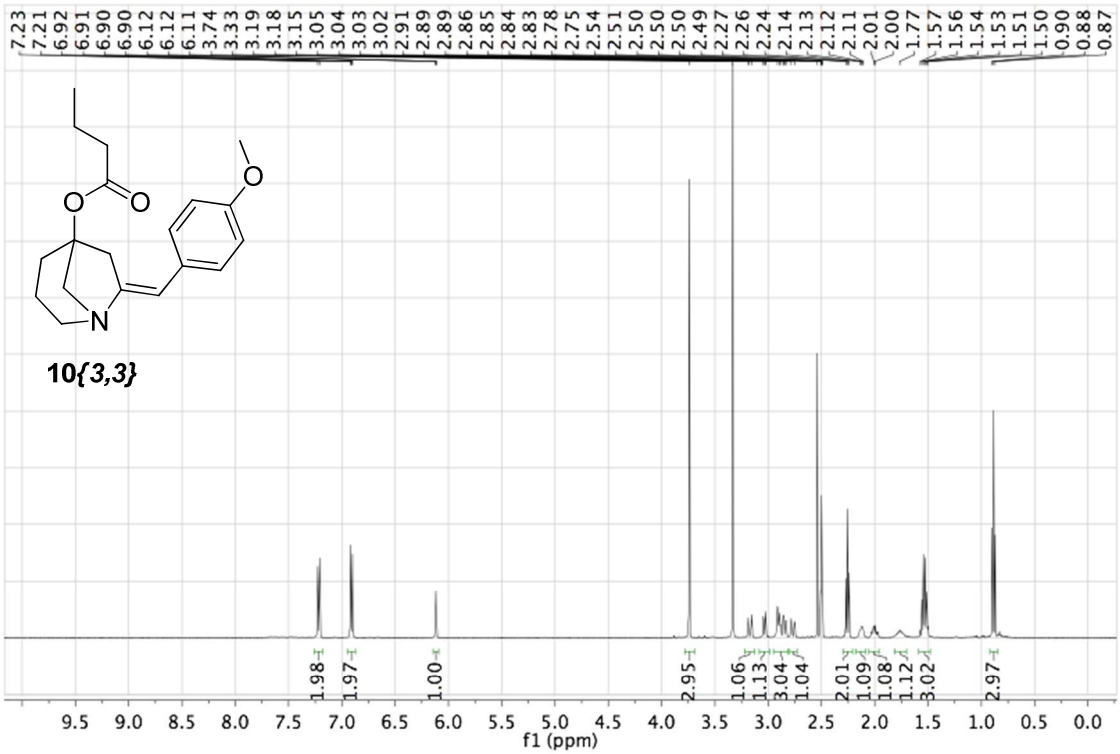

164.01
153.74
150.65
150.19
137.02
136.69
128.49
127.51
84.33
61.73
57.53
40.02
39.85
39.69
39.52
39.35
39.19
39.02
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

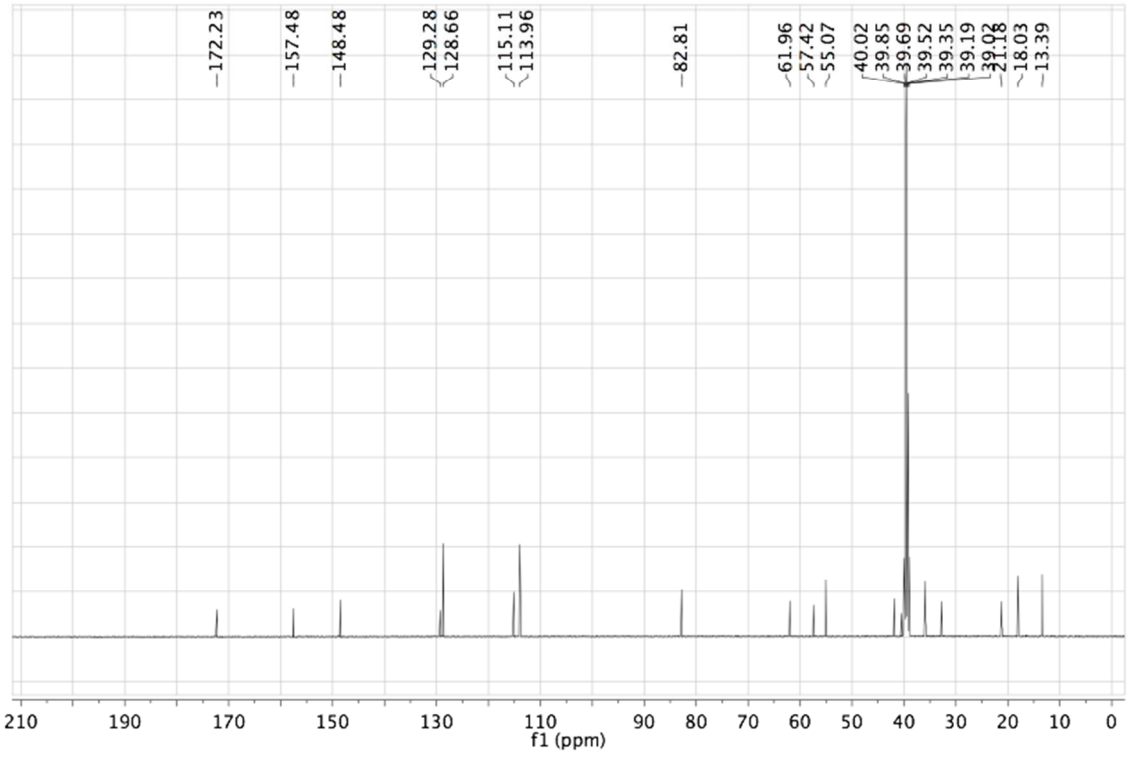

7.98 7.97 7.96 7.96 7.96 7.68 7.66 7.66 7.66 7.65 7.65 7.64 7.54 7.54 7.53 7.52 7.51 7.26 7.24 6.93 6.92 6.91 6.91 6.16 6.16 6.16 3.79 3.77 3.75 3.34 3.31 3.28 3.21 3.21 3.19 3.19 3.04 3.04 3.02 3.02 3.00 2.97 2.95 2.54 2.51 2.50 2.50 2.50 2.49 2.24 2.17 2.16
O
O
O
N
10{1,3}
1.97 1.01 2.06 2.01 1.98 1.00 2.97 1.10 0.99 3.95 1.02 1.03 0.98 1.03
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)

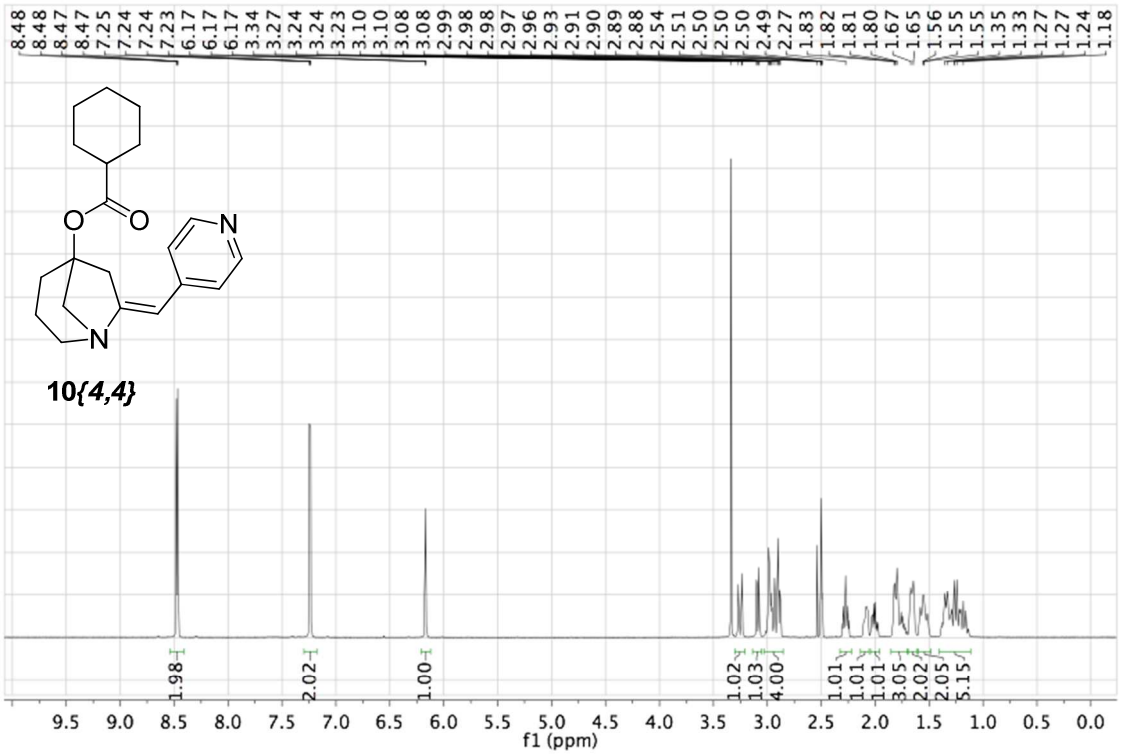

165.01 157.51 148.37 133.37 130.17 129.29 128.87 128.72 114.36 113.96 83.79 61.91 57.46 55.07 40.43 39.85 39.69 39.52 39.35 39.19 21.28
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

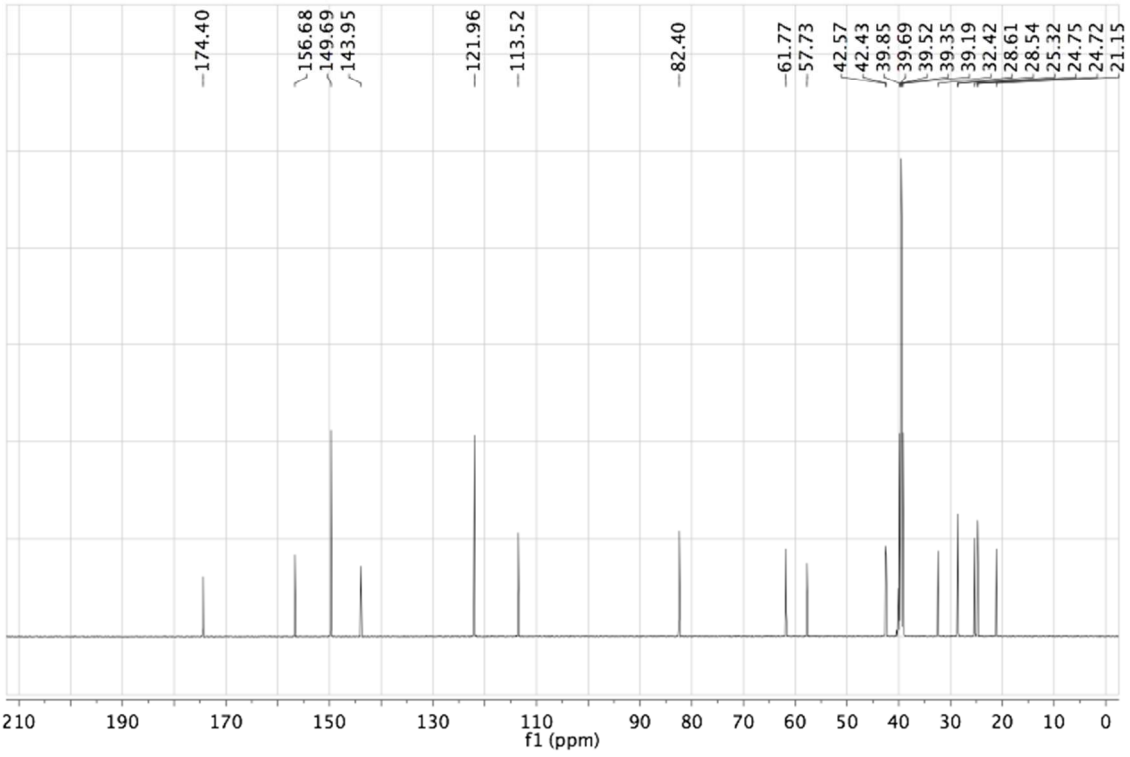

8.49 8.48 8.48 8.47 7.98 7.98 7.98 7.98 7.32 7.32 7.31 7.31 7.27 7.27 7.26 7.26 6.71 6.71 6.70 6.70 6.20 6.20 6.20 3.36 3.36 3.34 3.34 3.33 3.33 3.22 3.22 3.20 3.20 3.14 3.10 3.06 3.05 3.03 3.01 2.54 2.51 2.50 2.50 2.50 2.49 2.21 2.20 2.20 2.19 2.19 2.16 2.15
O
O
O
N
N
10{2,4}
1.96 0.95 0.98 2.00 1.01 1.00 2.22 1.02 1.03 2.99 2.02 1.07 1.05
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)

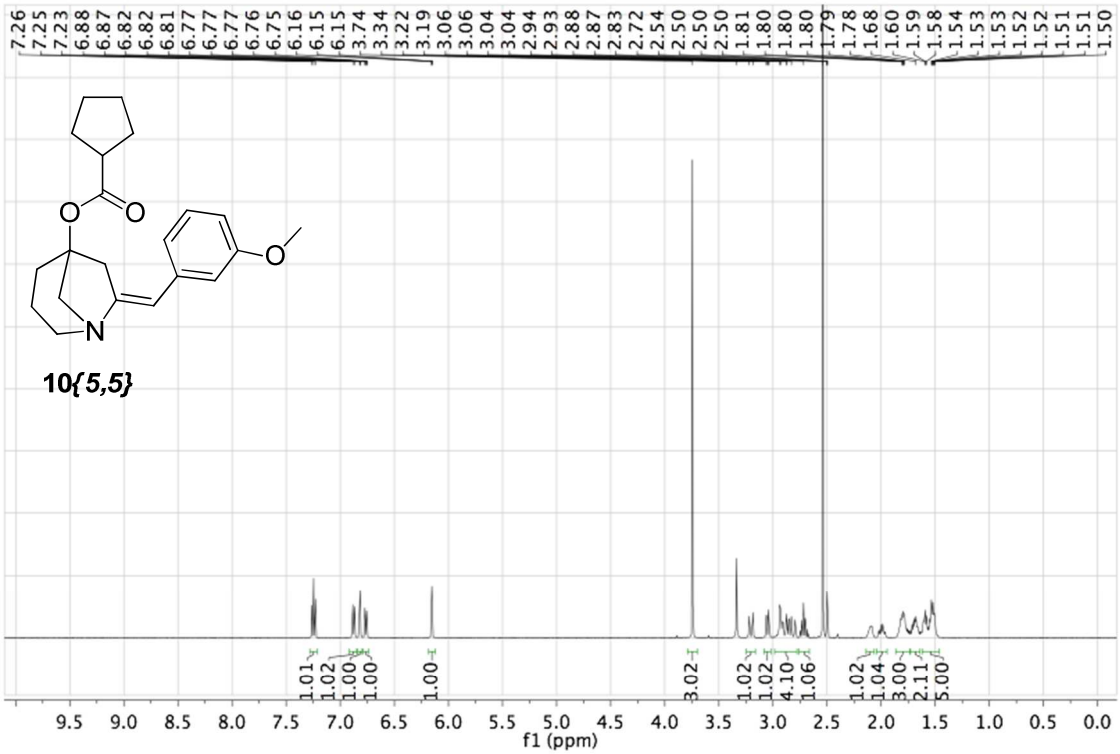

157.07 156.39 149.70 147.73 143.92 122.01 118.81 113.62 112.42 83.88 61.69 57.69 42.53 40.43 39.85 39.69 39.52 39.35 39.19 21.27
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

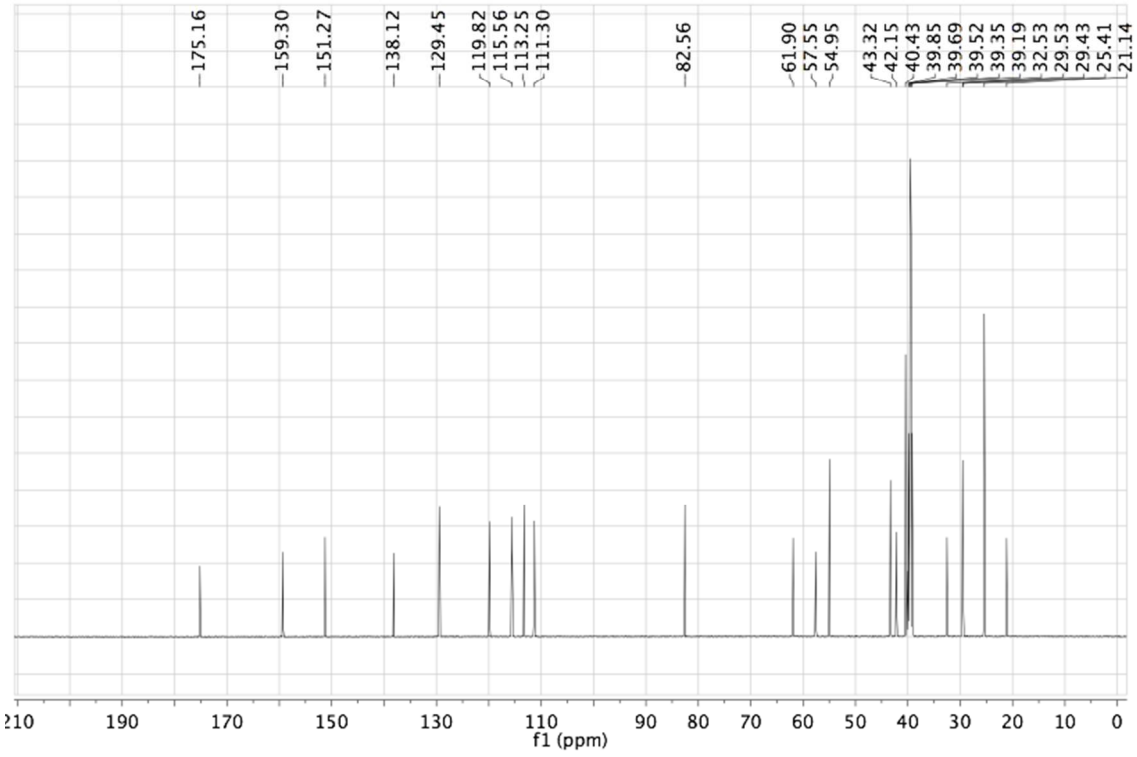

7.23 7.21 6.92 6.91 6.90 6.90 6.90 6.12 6.12 6.11 3.74 3.33 3.19 3.18 3.15 3.05 3.04 3.03 3.02 2.91 2.89 2.89 2.86 2.85 2.84 2.83 2.78 2.75 2.54 2.51 2.50 2.50 2.50 2.49 2.27 2.26 2.24 2.14 2.13 2.12 2.11 2.01 2.00 1.77 1.57 1.56 1.54 1.53 1.51 1.50 0.90 0.88 0.87
O
O
O
N
10{3,3}
1.98 1.97 1.00 2.95 1.06 1.13 3.04 1.04 2.01 1.09 1.08 1.12 3.02 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)

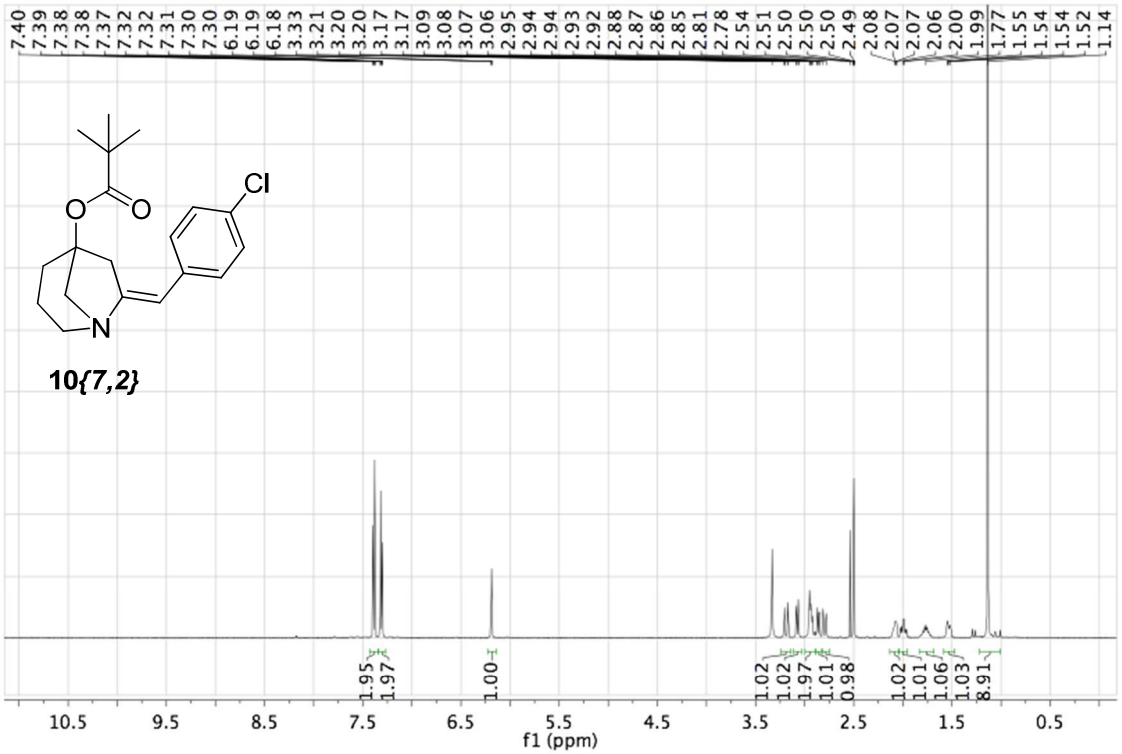

172.23 157.48 148.48 129.28 128.66 115.11 113.96 82.81 61.96 57.42 55.07 40.02 39.85 39.69 39.52 39.35 39.19 39.02 21.18 18.03 13.39
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

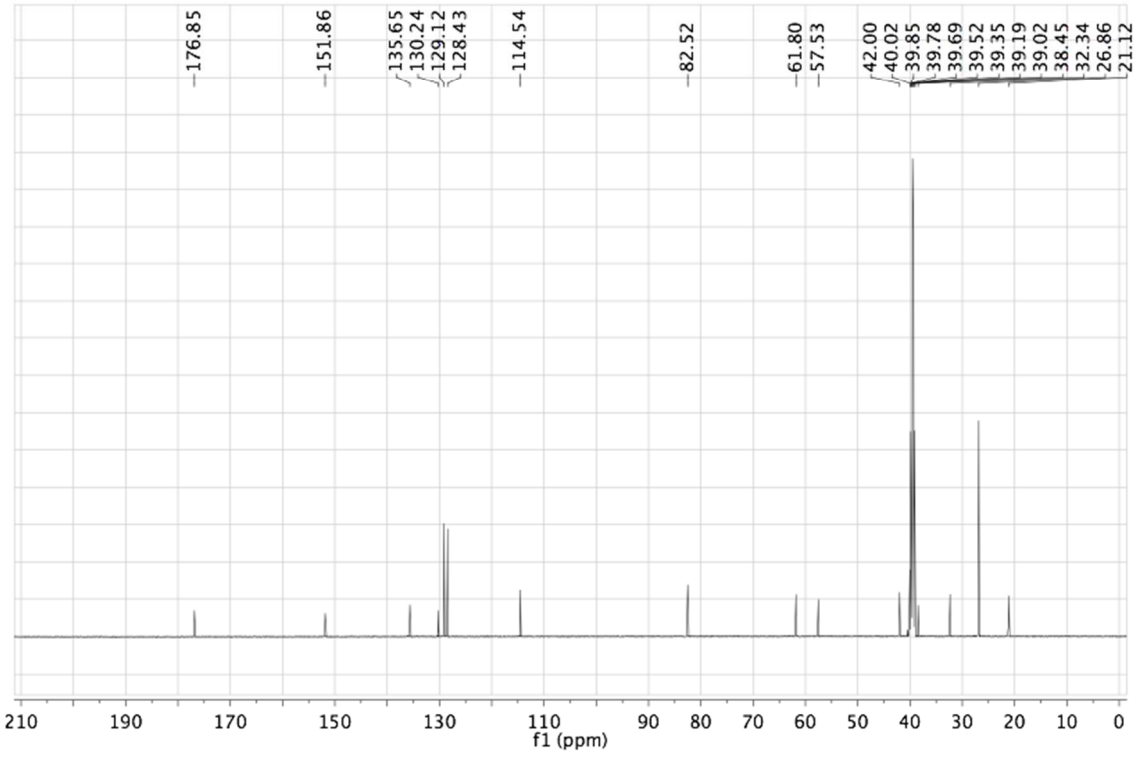

10{4,4}
f1 (ppm)

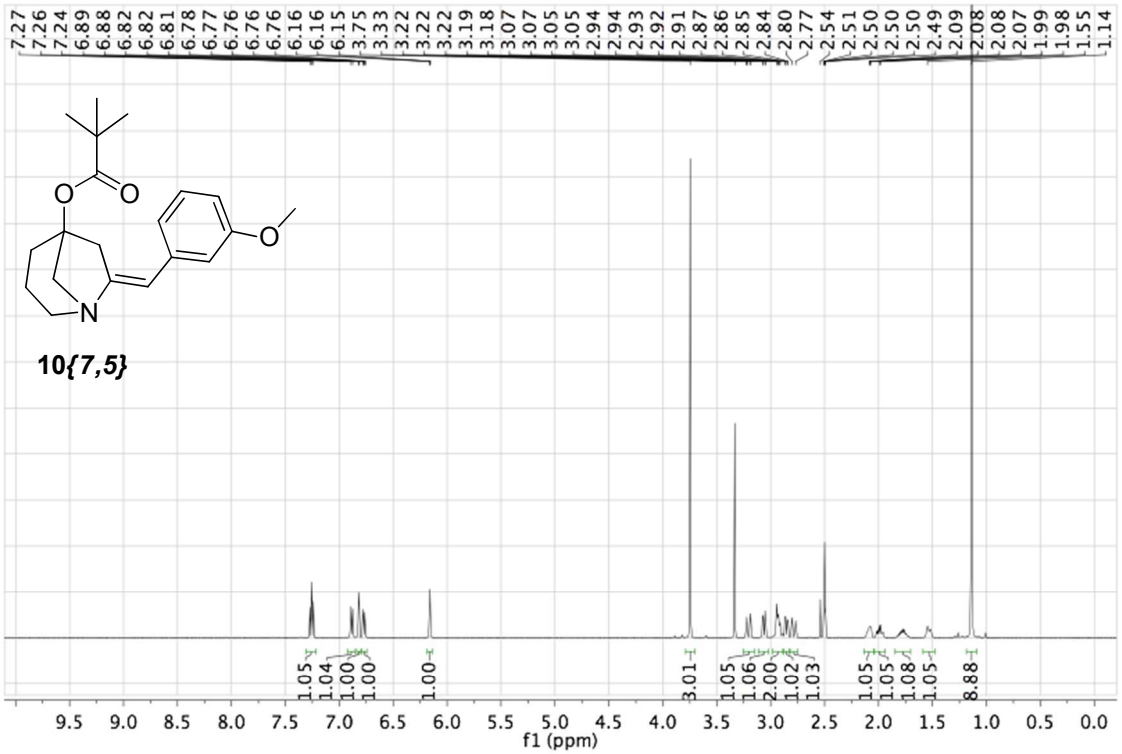

f1 (ppm)

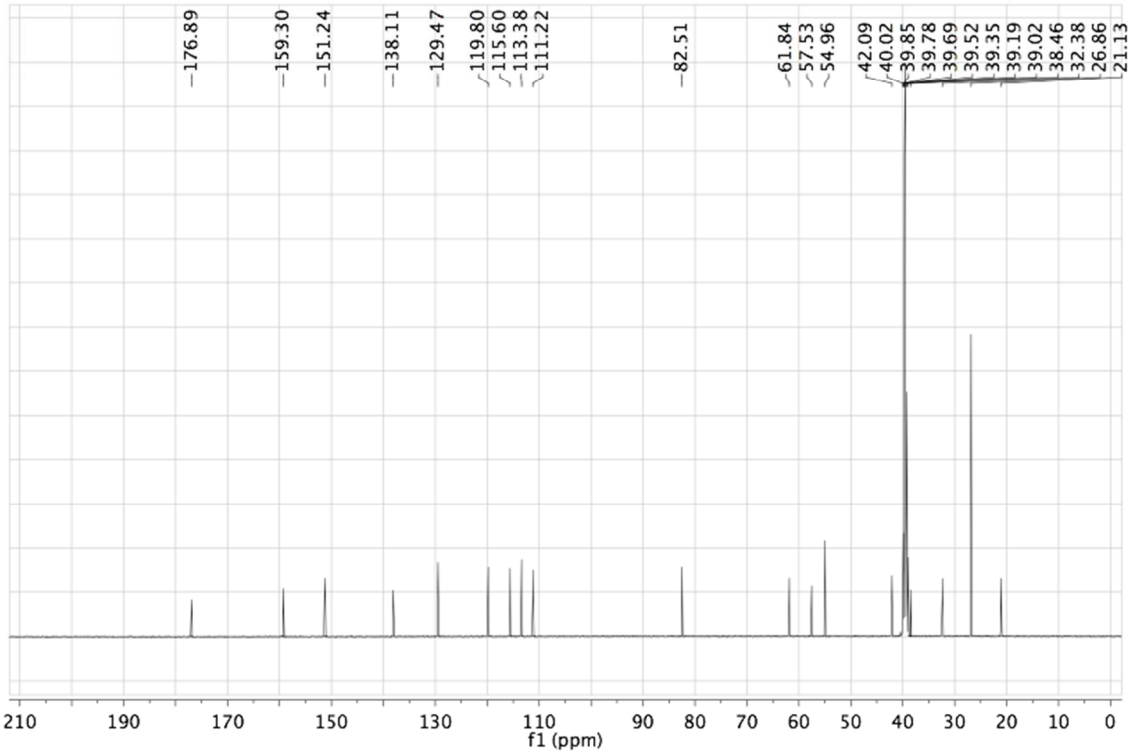

7.26 7.25 7.23 6.88 6.87 6.82 6.82 6.81 6.77 6.77 6.77 6.76 6.75 6.16 6.15 6.15 3.74 3.34 3.22 3.19 3.06 3.06 3.04 3.04 2.94 2.93 2.88 2.87 2.83 2.72 2.54 2.50 2.50 2.50 1.81 1.80 1.80 1.80 1.79 1.78 1.68 1.60 1.59 1.58 1.54 1.53 1.53 1.52 1.52 1.51 1.51 1.50
O
O
O
N
10{5,5}
1.01 1.02 1.00 1.00 1.00 3.02 1.02 1.02 4.10 1.06 1.02 1.04 3.00 2.11 5.00
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
f1 (ppm)

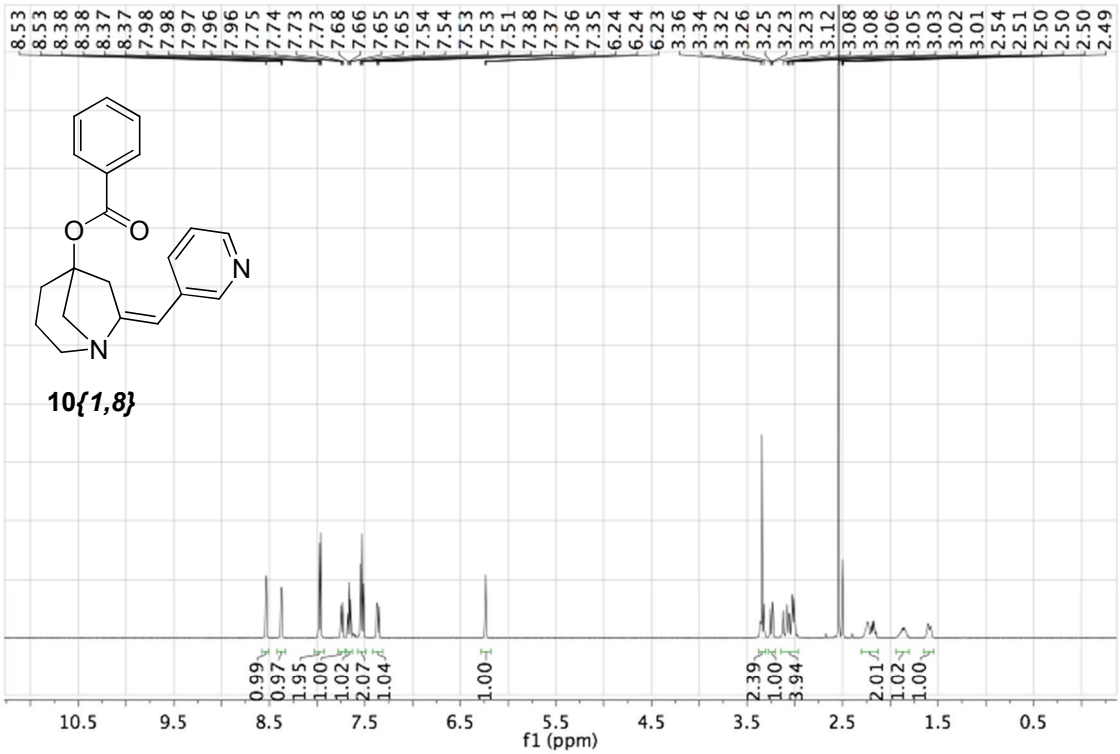

175.16 159.30 151.27 138.12 129.45 119.82 115.56 113.25 111.30 82.56 61.90 57.55 54.95 43.32 42.15 40.43 39.85 39.69 39.52 39.35 39.19 32.53 29.53 29.43 25.41 21.14
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

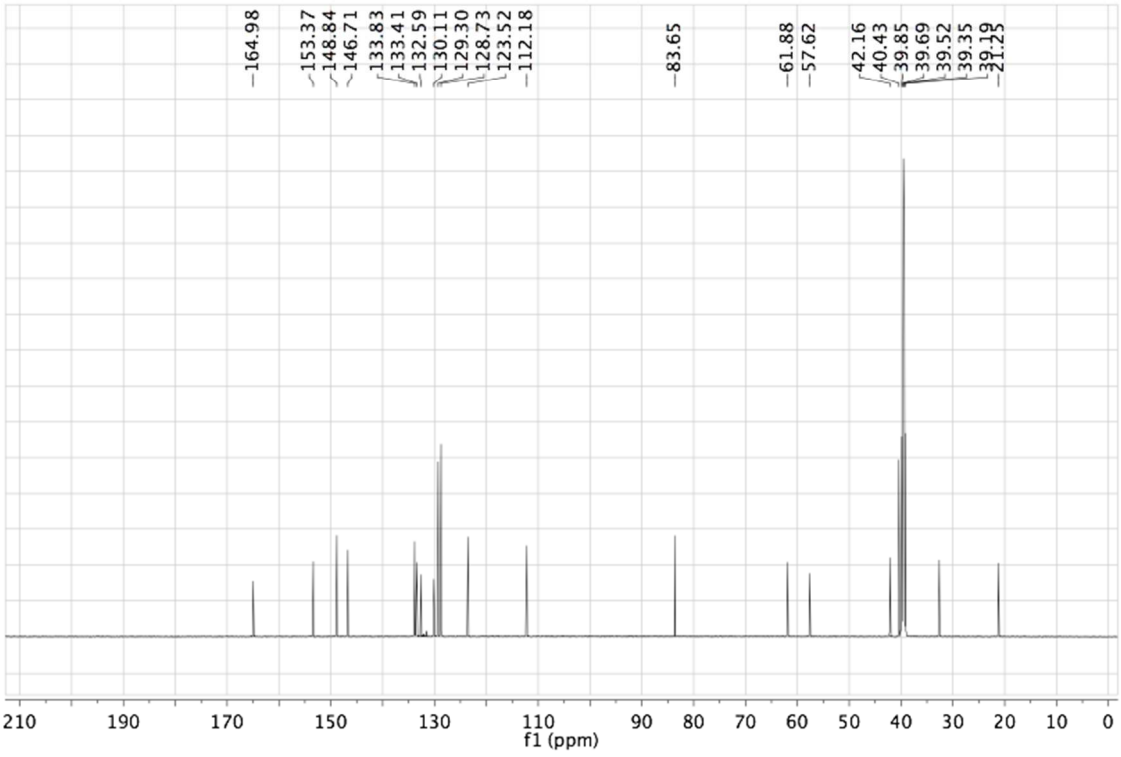

Cl
O
O
N
10{7,2}
f1 (ppm)

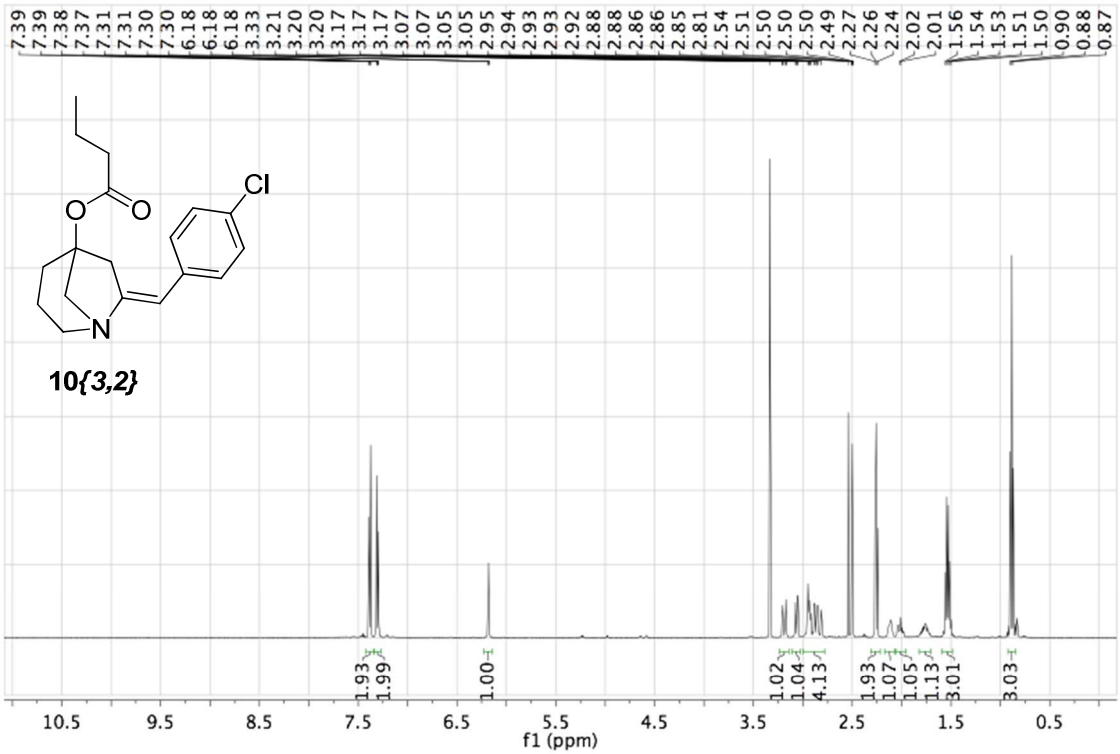

f1 (ppm)

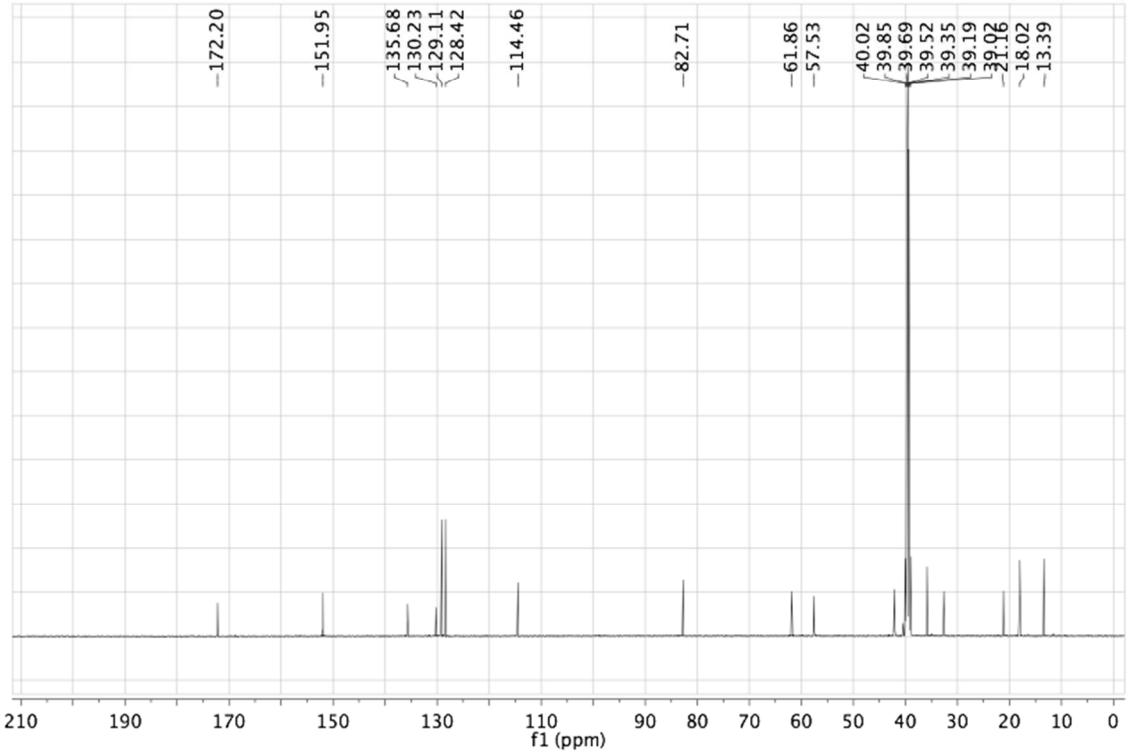

7.27 7.26 7.24 6.89 6.88 6.82 6.82 6.81 6.78 6.77 6.76 6.76 6.76 6.16 6.16 6.15 3.75 3.33 3.22 3.22 3.22 3.19 3.18 3.07 3.07 3.05 3.05 2.94 2.94 2.93 2.92 2.91 2.87 2.86 2.85 2.84 2.80 2.77 2.54 2.51 2.50 2.50 2.50 2.49 2.09 2.08 2.08 2.07 1.99 1.98 1.55 1.14
O
O
O
N
10{7,5}
1.05 1.04 1.00 1.00 1.00 3.01 1.05 1.06 2.00 1.02 1.03 1.05 1.05 1.08 1.05 8.88
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)

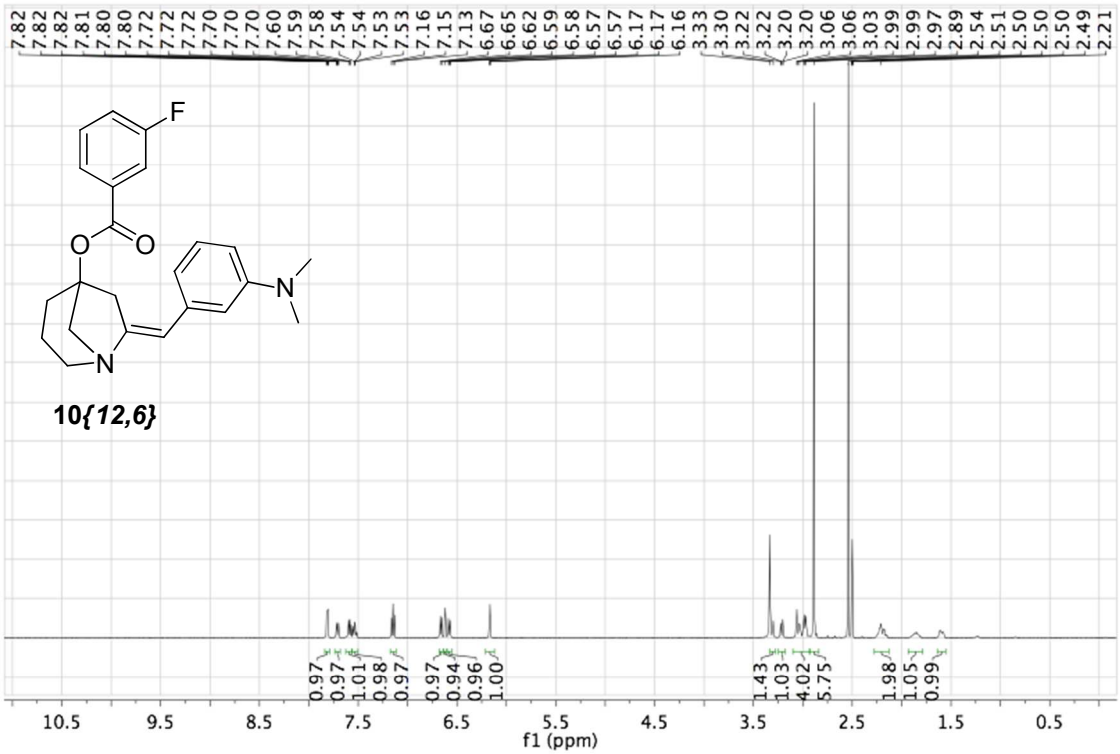

176.89 159.30 151.24 138.11 129.47 119.80 115.60 113.38 111.22 82.51 61.84 57.53 54.96 42.09 40.02 39.85 39.78 39.69 39.52 39.35 39.19 39.02 38.46 32.38 26.86 21.13
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

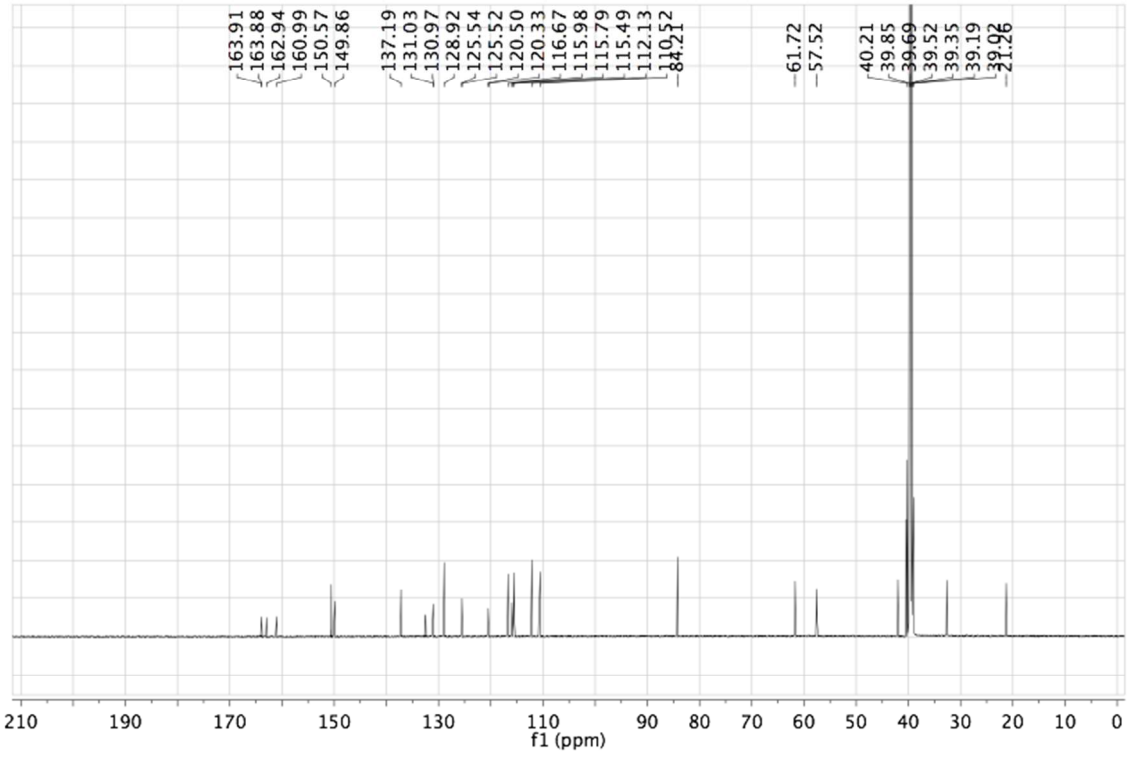

8.53 8.53 8.38 8.38 8.37 8.37 7.98 7.98 7.97 7.96 7.96 7.75 7.74 7.73 7.73 7.68 7.66 7.65 7.65 7.54 7.54 7.53 7.53 7.51 7.38 7.37 7.36 7.35 6.24 6.24 6.23 3.36 3.34 3.32 3.26 3.25 3.23 3.23 3.12 3.08 3.08 3.06 3.05 3.03 3.02 3.01 2.54 2.51 2.50 2.50 2.50 2.49
O
O
N
N
10{1,8}
0.99 0.97 1.95 1.00 1.02 2.07 1.04 1.00 2.39 1.00 3.94 2.01 1.02 1.00
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)


164.98 153.37 148.84 146.71 133.83 133.41 132.59 130.11 129.30 128.73 123.52 112.18 83.65 61.88 57.62 42.16 40.43 39.85 39.69 39.52 39.35 39.19 21.25
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.39 7.39 7.38 7.37 7.31 7.31 7.30 7.30 6.18 6.18 6.18 3.33 3.21 3.20 3.20 3.17 3.17 3.17 3.07 3.07 3.05 3.05 2.95 2.94 2.93 2.93 2.92 2.88 2.88 2.86 2.86 2.85 2.81 2.54 2.51 2.50 2.50 2.50 2.49 2.27 2.26 2.24 2.02 2.01 1.56 1.54 1.53 1.51 1.50 0.90 0.88 0.87
Cl
O
O
N
10{3,2}
1.93 1.99 1.00 1.02 1.04 4.13 1.93 1.07 1.05 1.13 3.01 3.03
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)


172.20 151.95 135.68 130.23 129.11 128.42 114.46 82.71 61.86 57.53 40.02 39.85 39.69 39.52 39.35 39.19 39.02 21.16 18.02 13.39
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


F
O
O
N
N
10{12,6}
f1 (ppm)


f1 (ppm)