Study of Allene-Based Ligands for Transition Metal Complexes – Synthesis and Applications in Catalysis and as Metallodrugs

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Appendices

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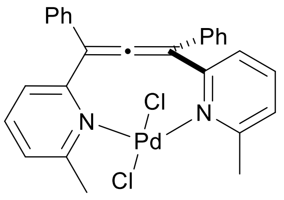
Appendix A – Structures of new complexes



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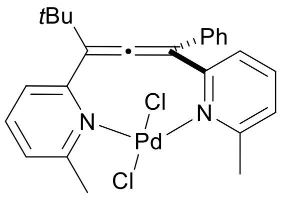

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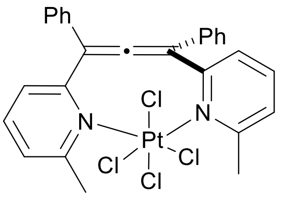

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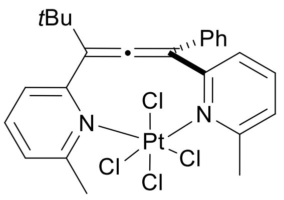

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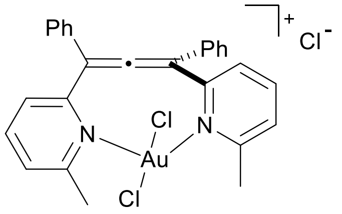

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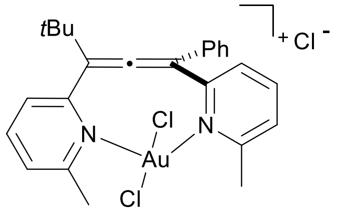

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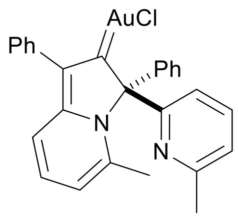

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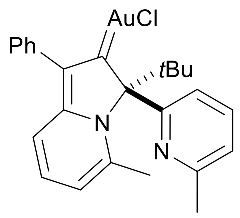

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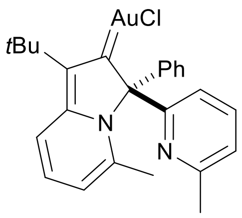

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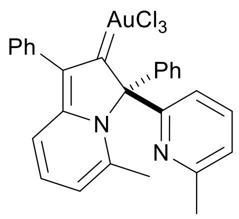

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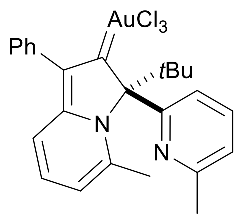

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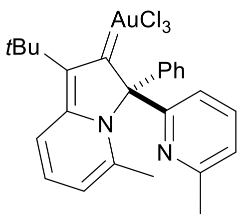

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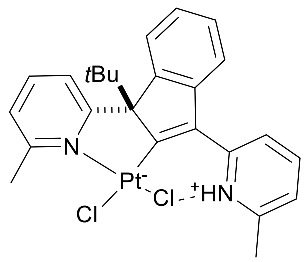

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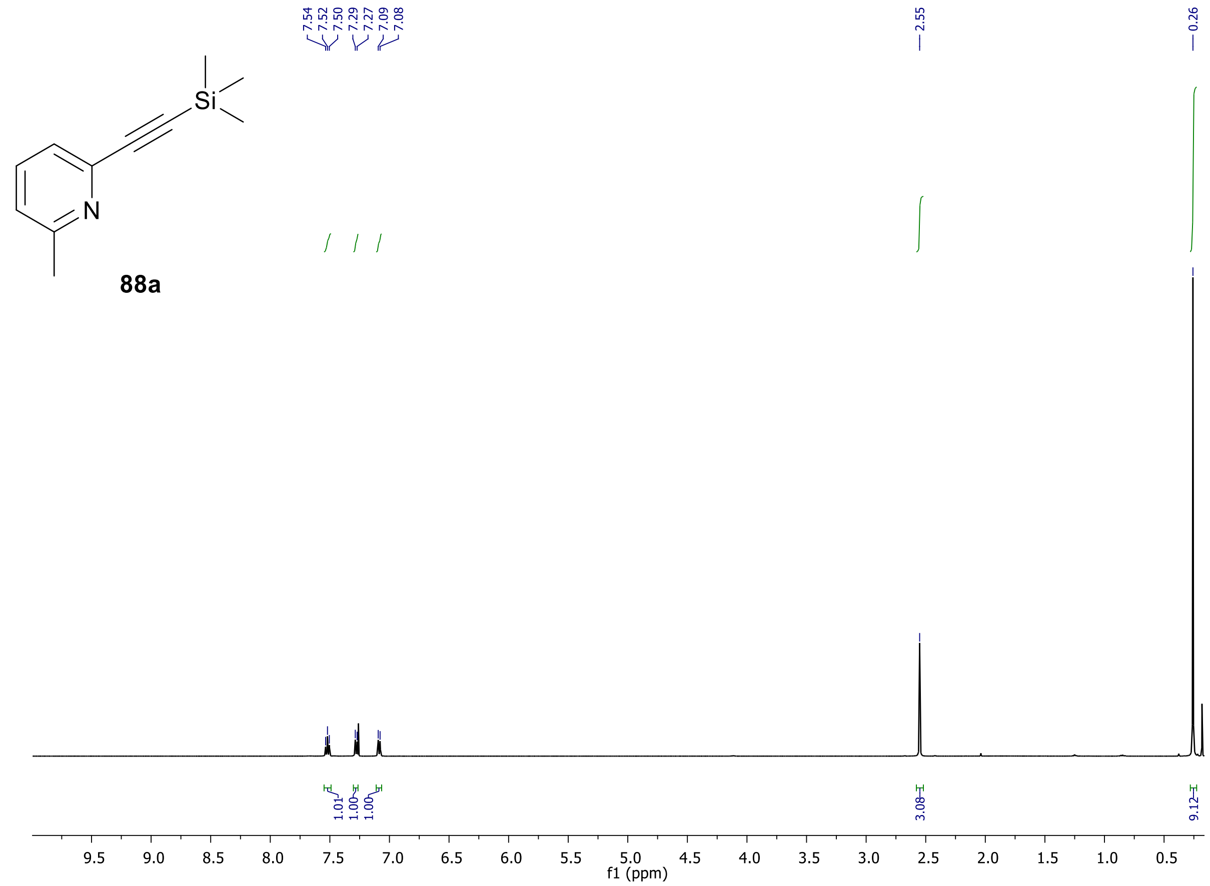
Appendix B – NMR Spectra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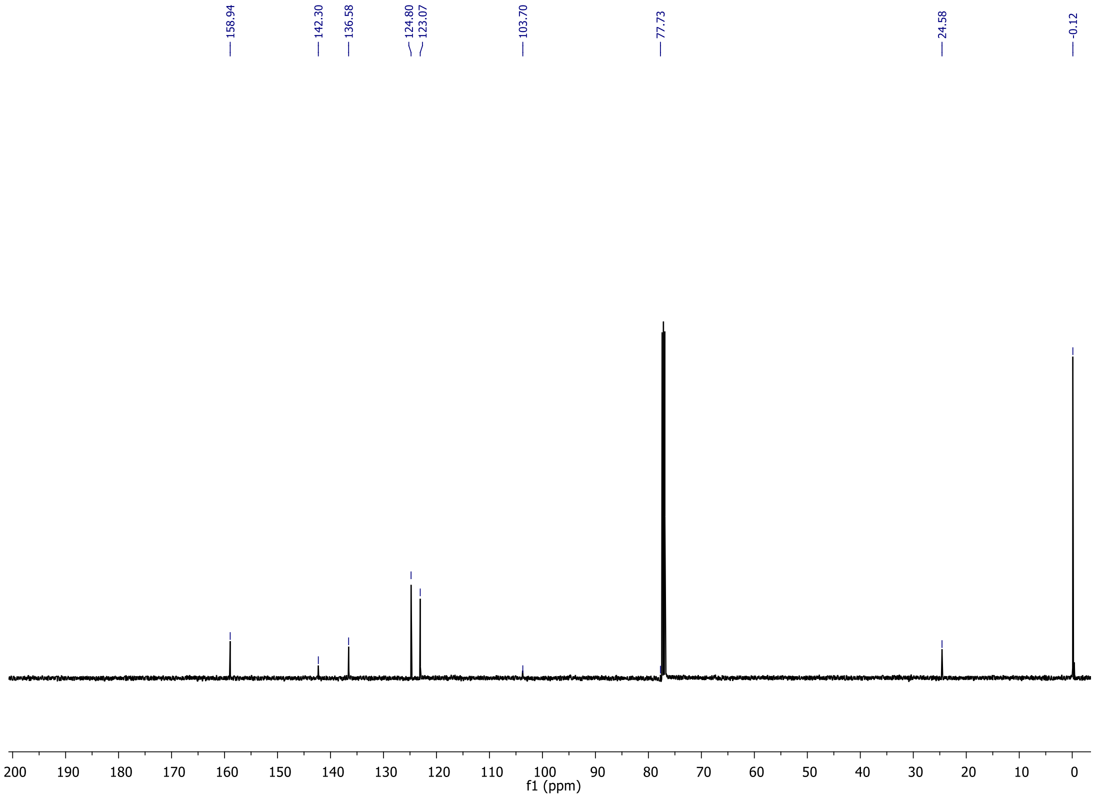

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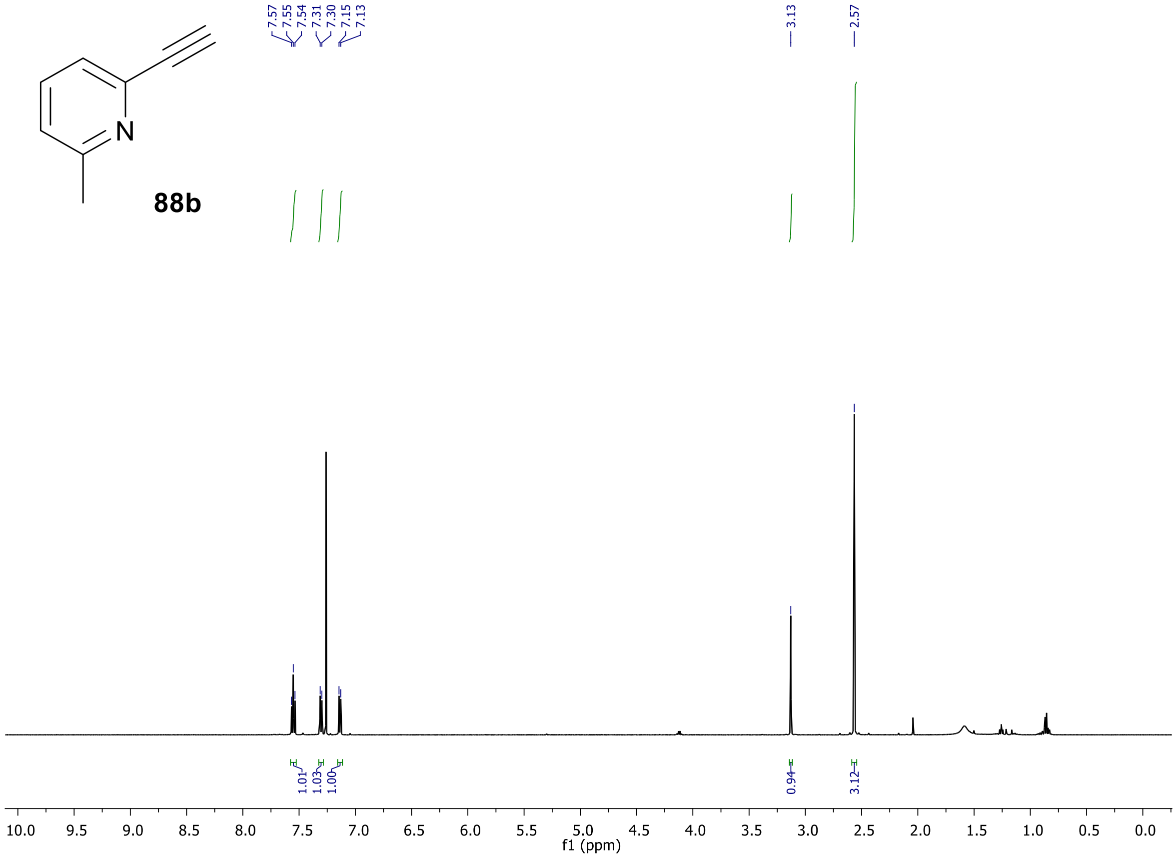
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3.12
10.0
9.5
9.0
8.5
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7.5
7.0
6.5
6.0
5.5
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2.5
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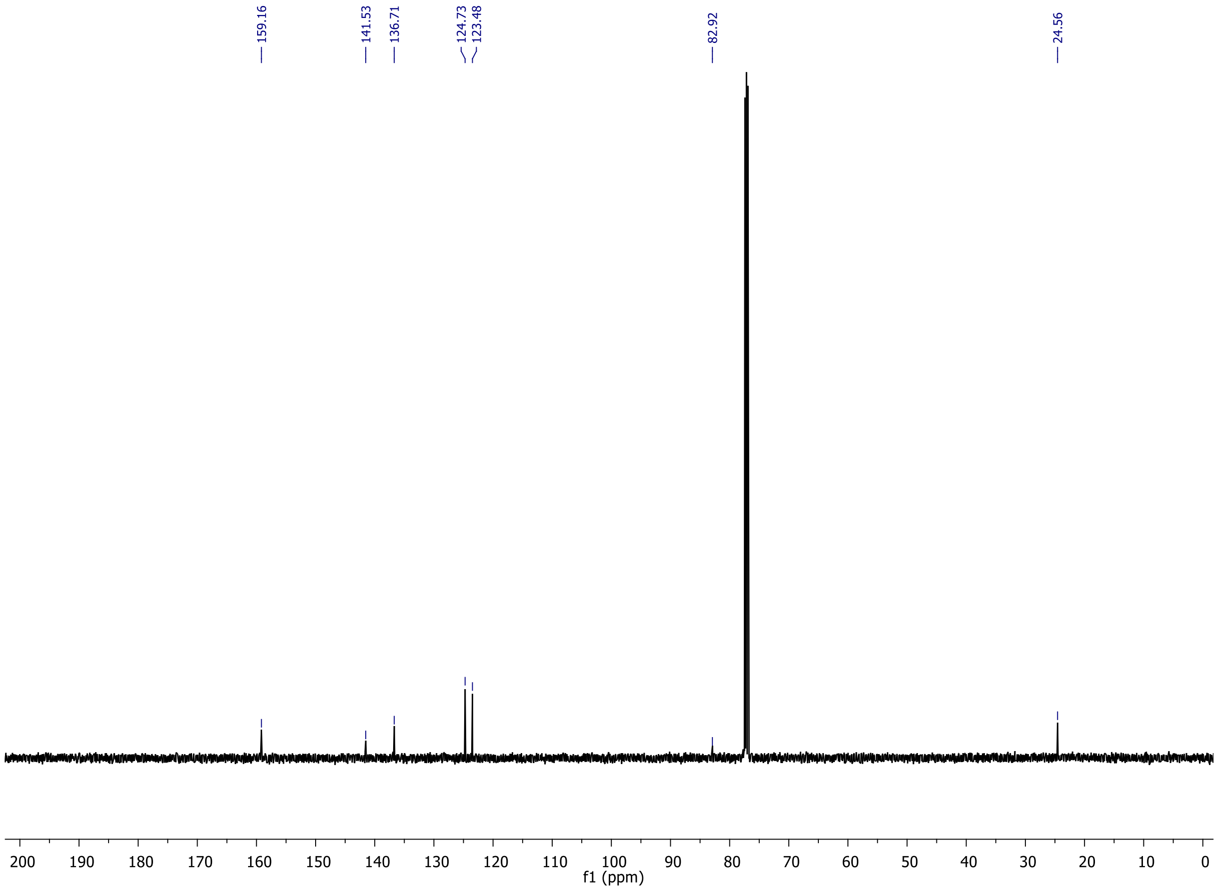
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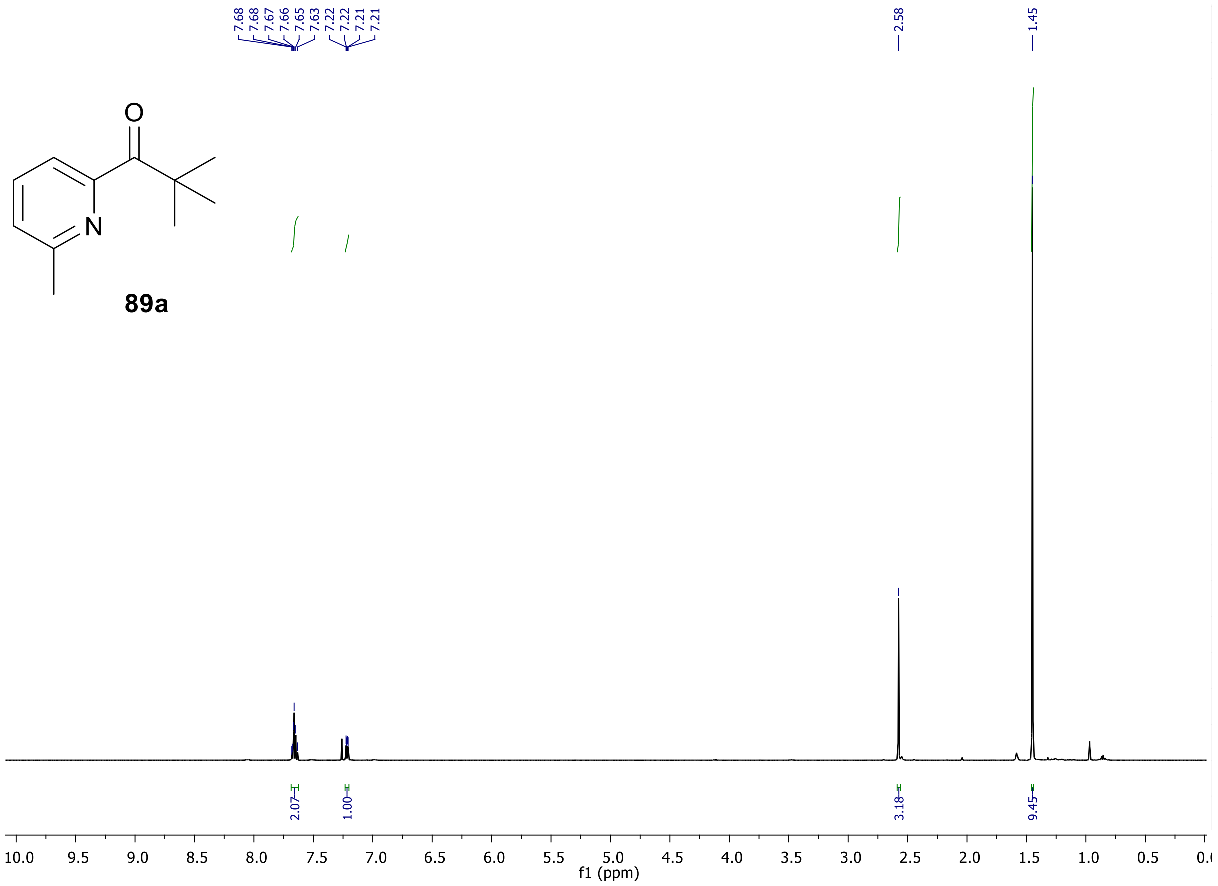
f1 (ppm)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7.21
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2.58
1.45
2.07
1.00
3.18
9.45
10.0
9.5
9.0
8.5
8.0
7.5
7.0
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6.0
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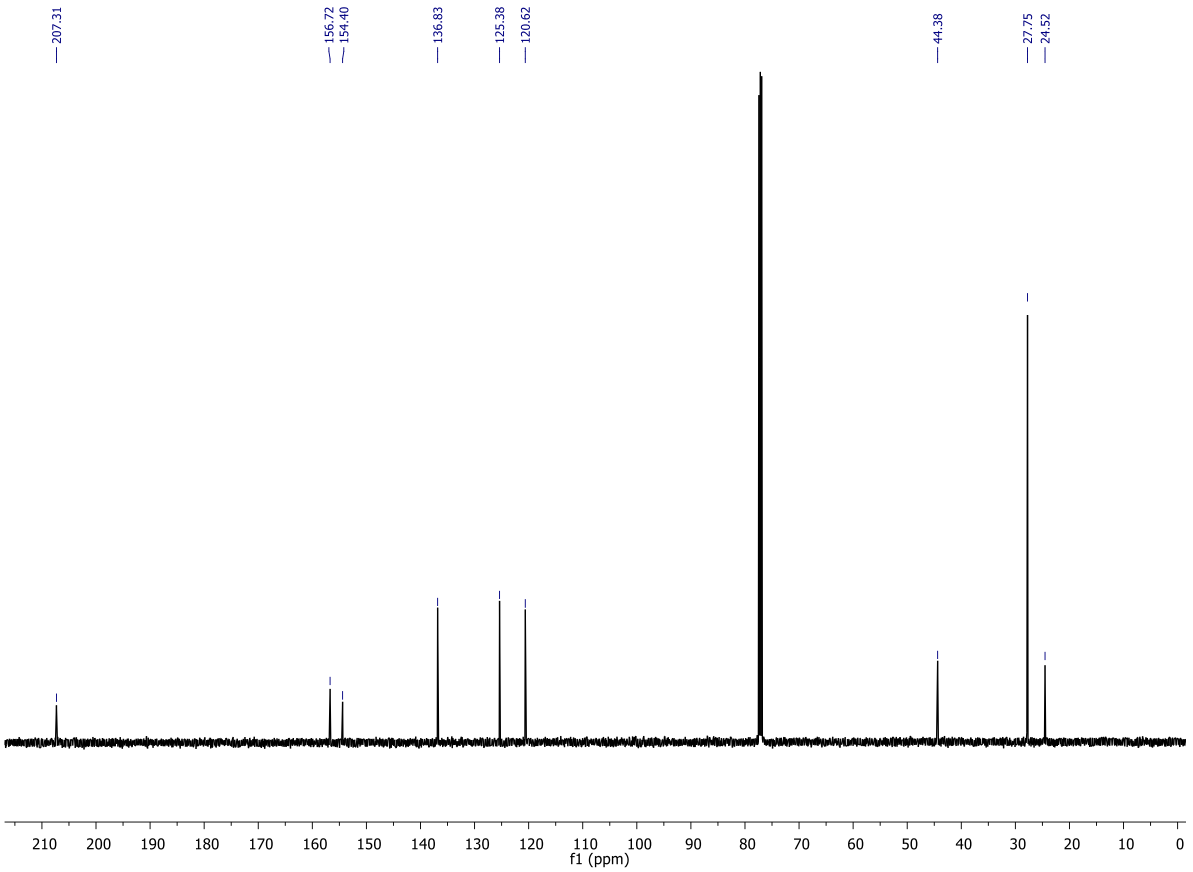
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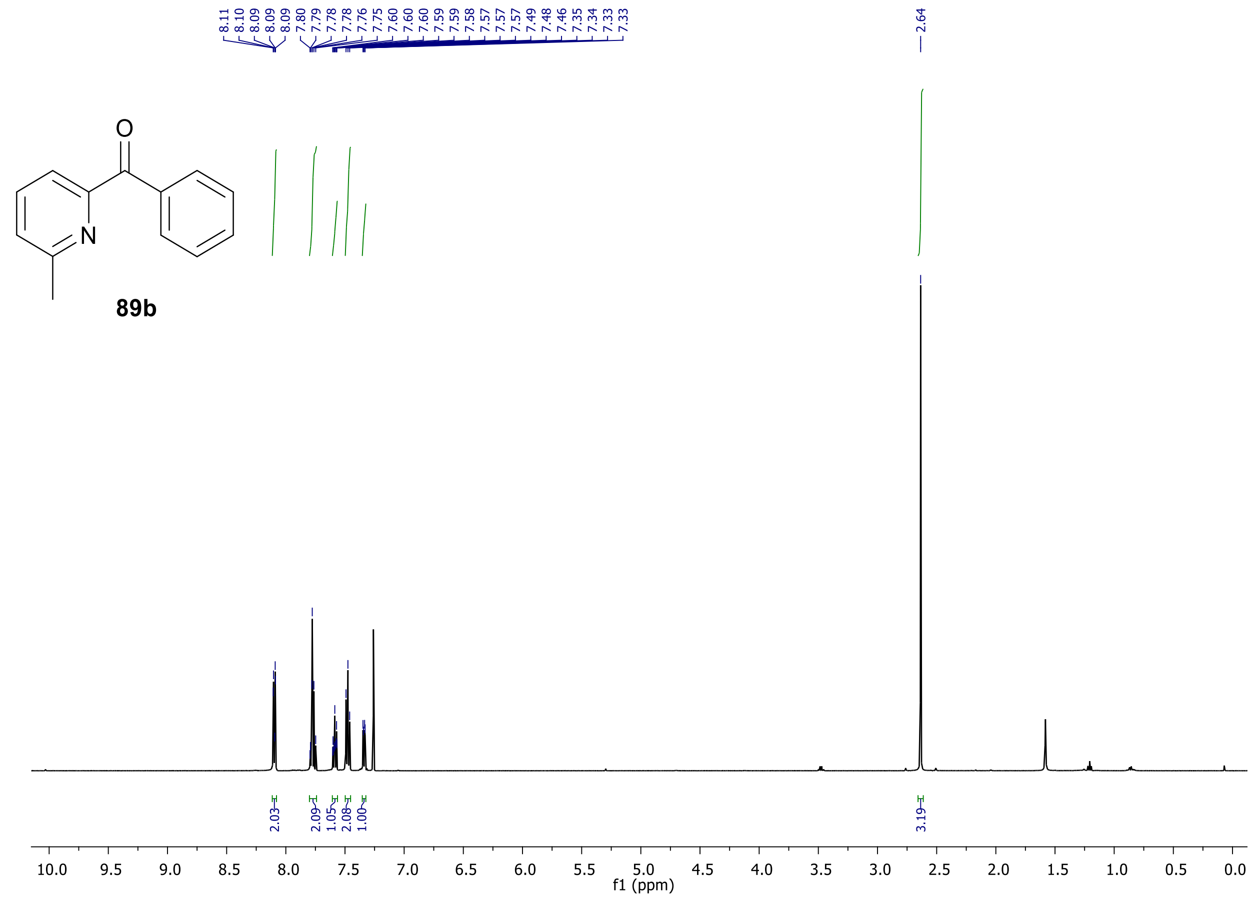
f1 (ppm)



89b

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8.10
8.09
8.09
8.09
7.80
7.79
7.78
7.78
7.76
7.75
7.60
7.60
7.59
7.59
7.58
7.57
7.57
7.57
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7.48
7.46
7.35
7.34
7.33
7.33
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2.09
1.05
2.08
1.00
3.19
10.0
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8.5
8.0
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6.0
5.5
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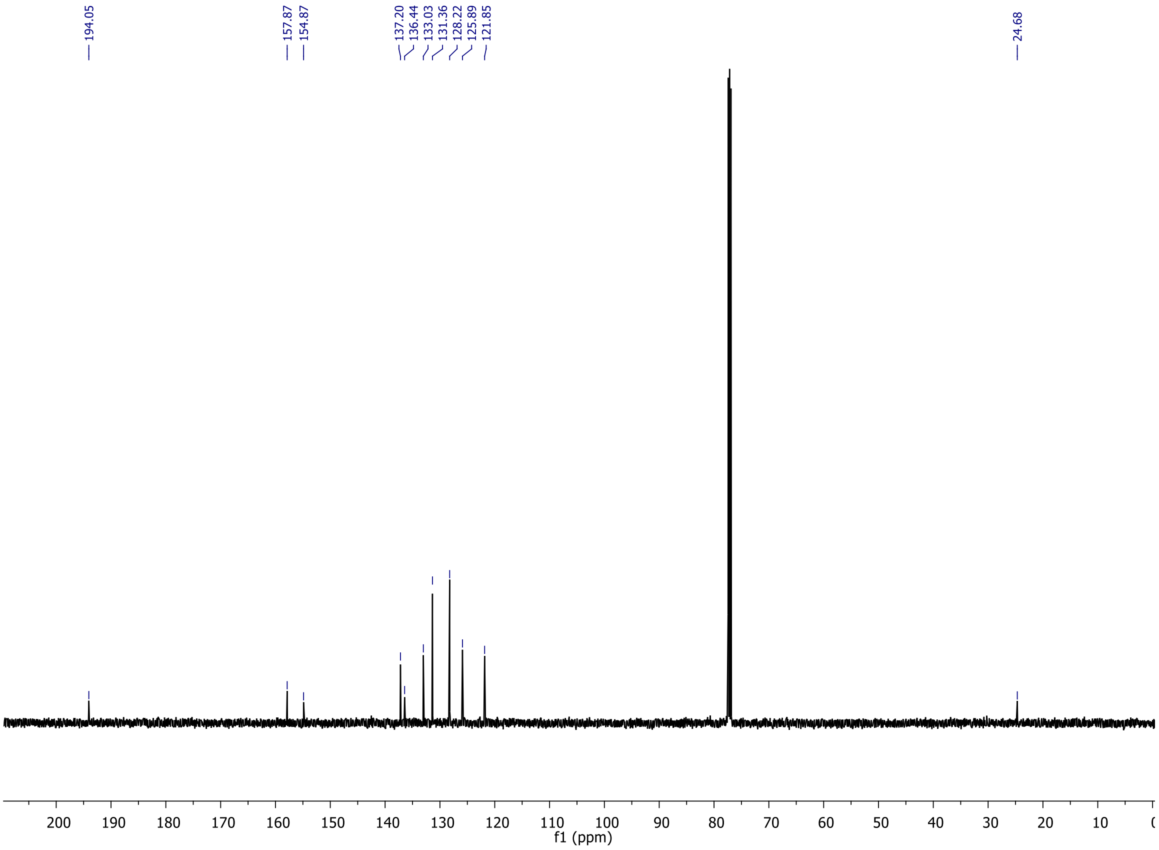

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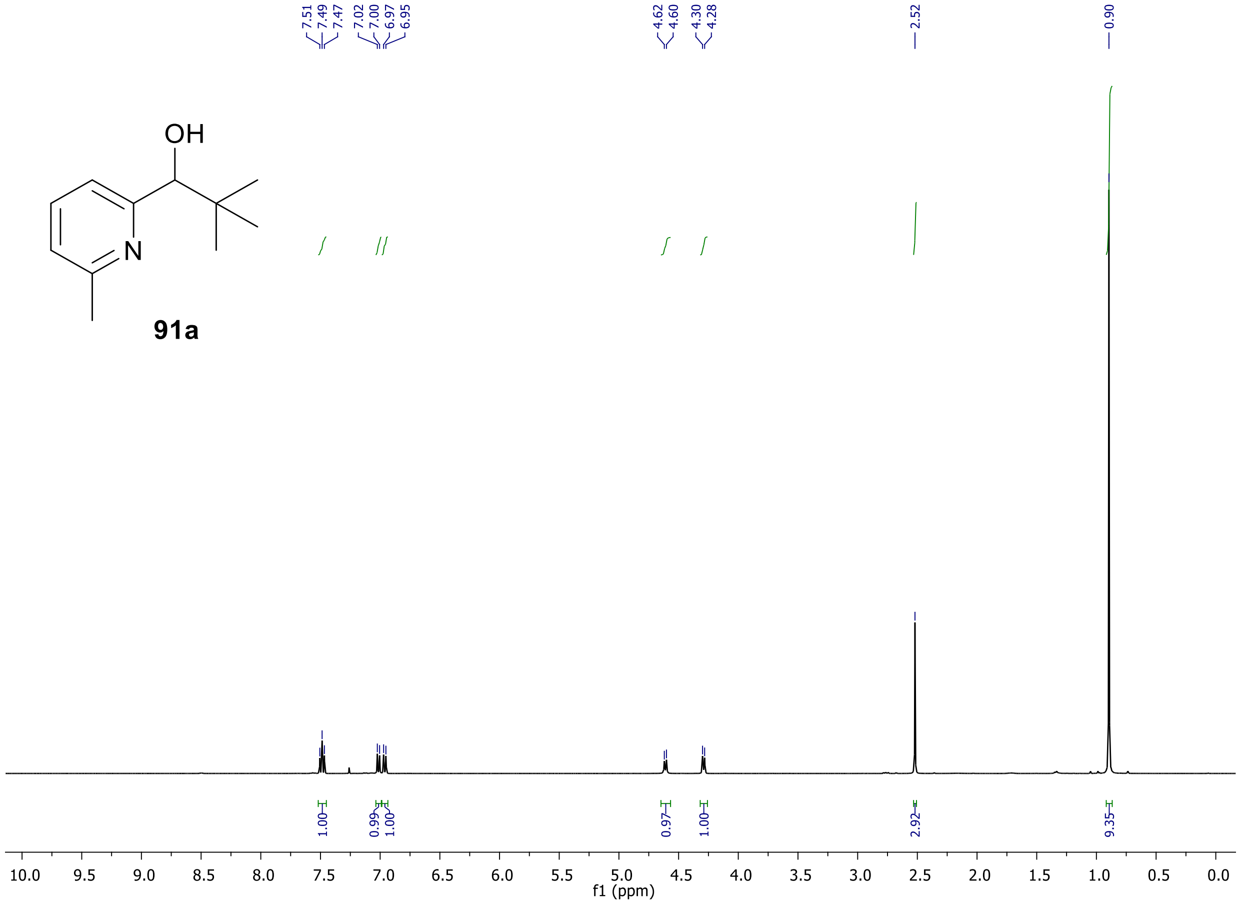
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1.00
0.97
1.00
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10.0
9.5
9.0
8.5
8.0
7.5
7.0
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5.0
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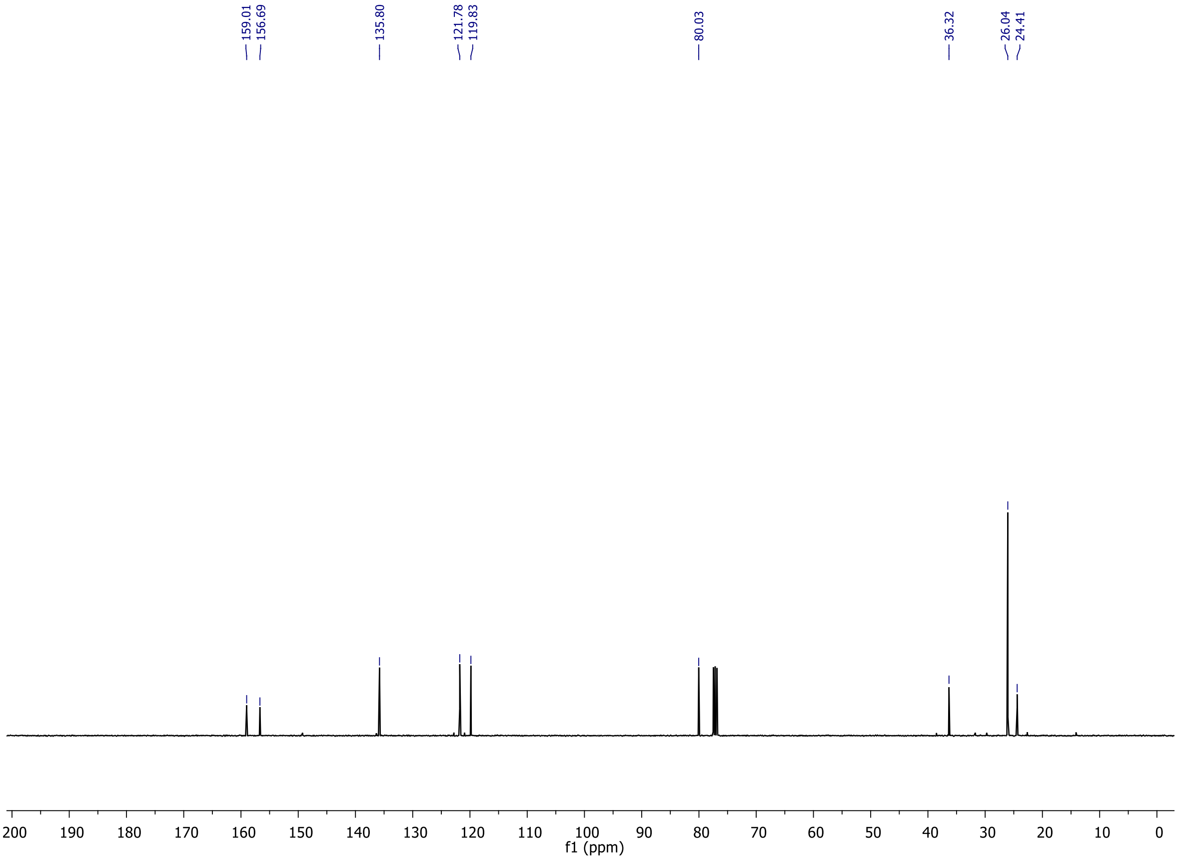
91a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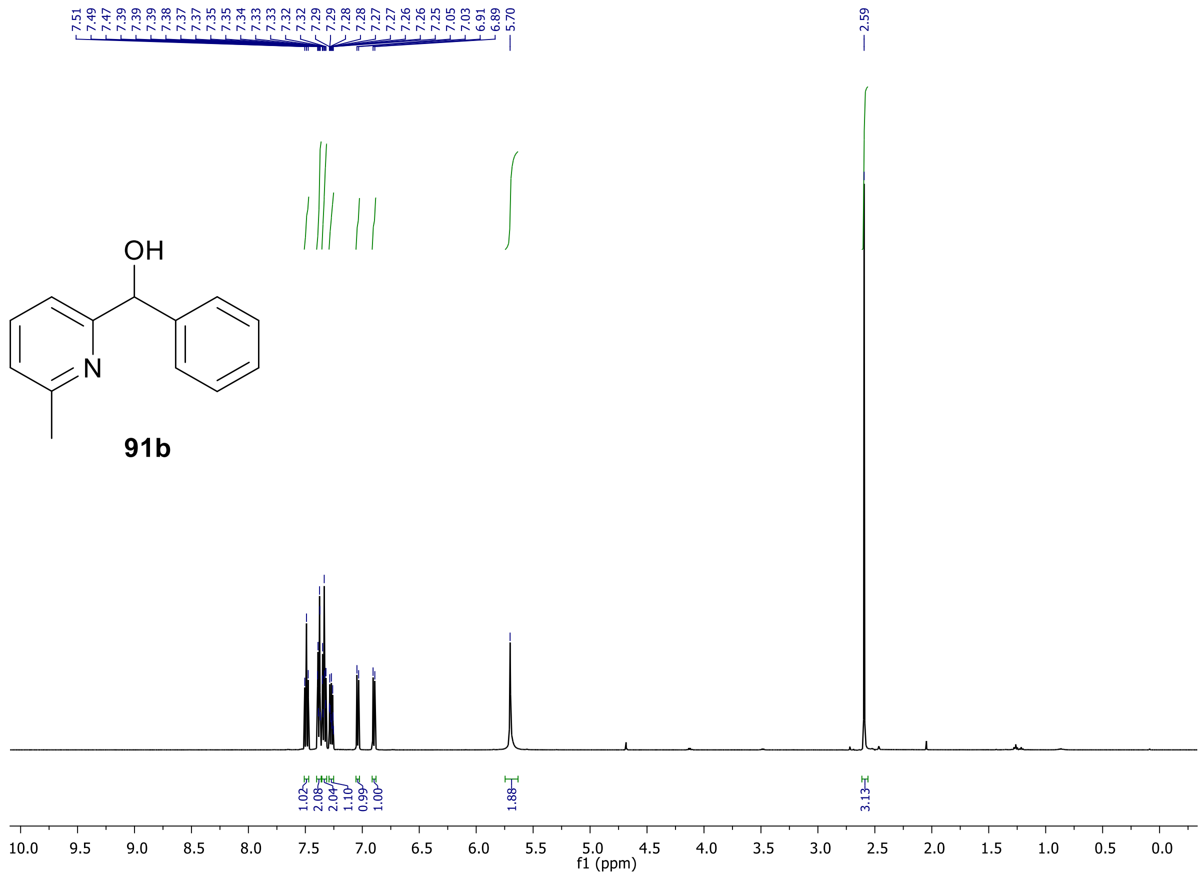
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7.25
7.05
7.03
6.91
6.89
5.70
2.59
OH
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2.08
2.04
1.10
0.99
1.00
1.88
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7.5
7.0
6.5
6.0
5.5
5.0
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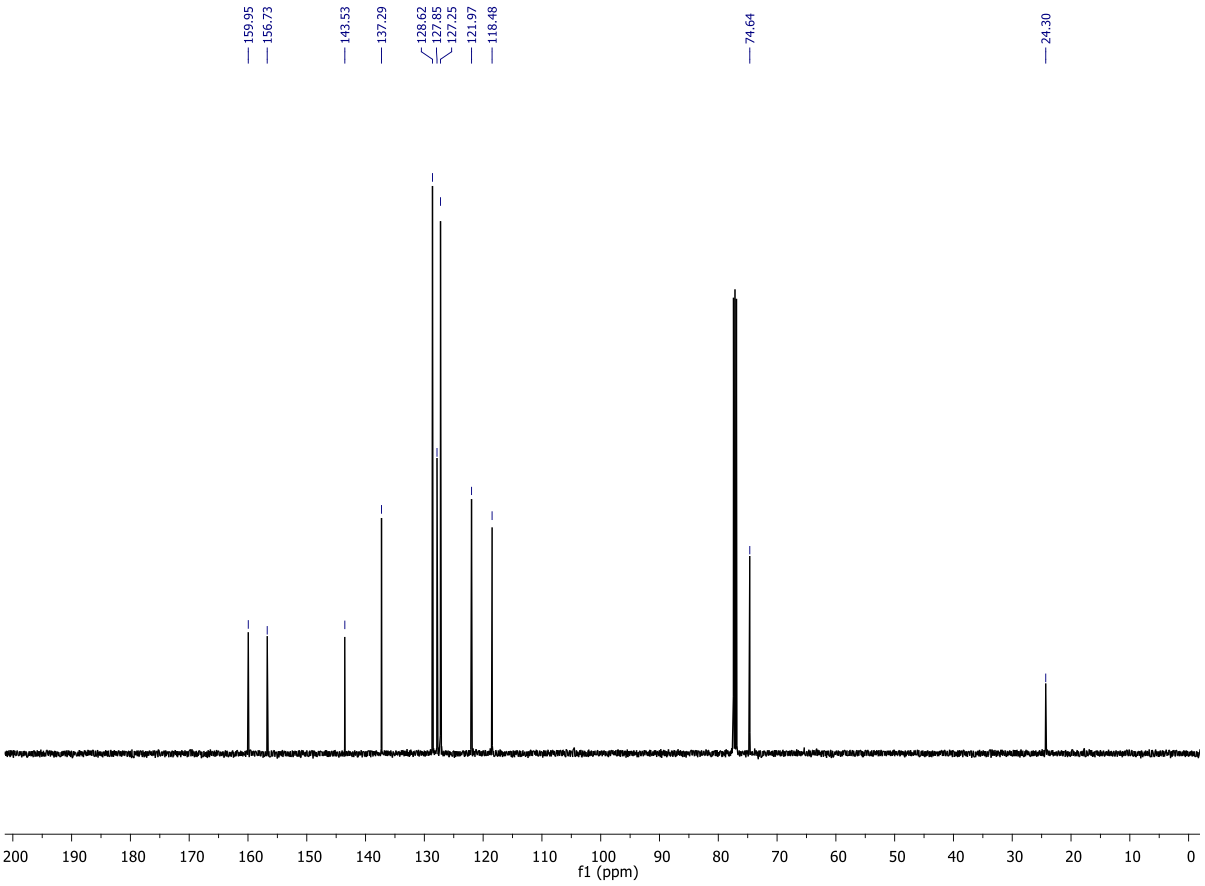
f1 (ppm)

91b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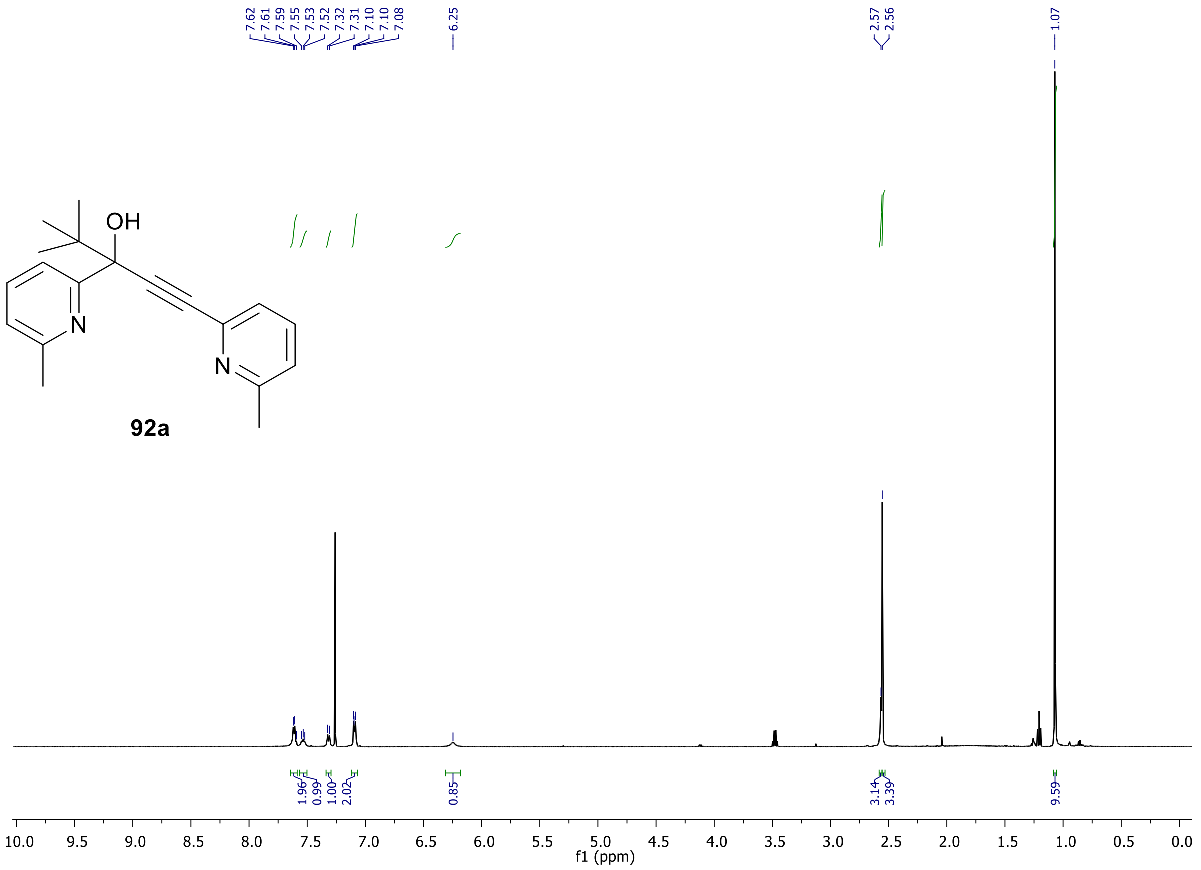
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0.85
3.14
3.39
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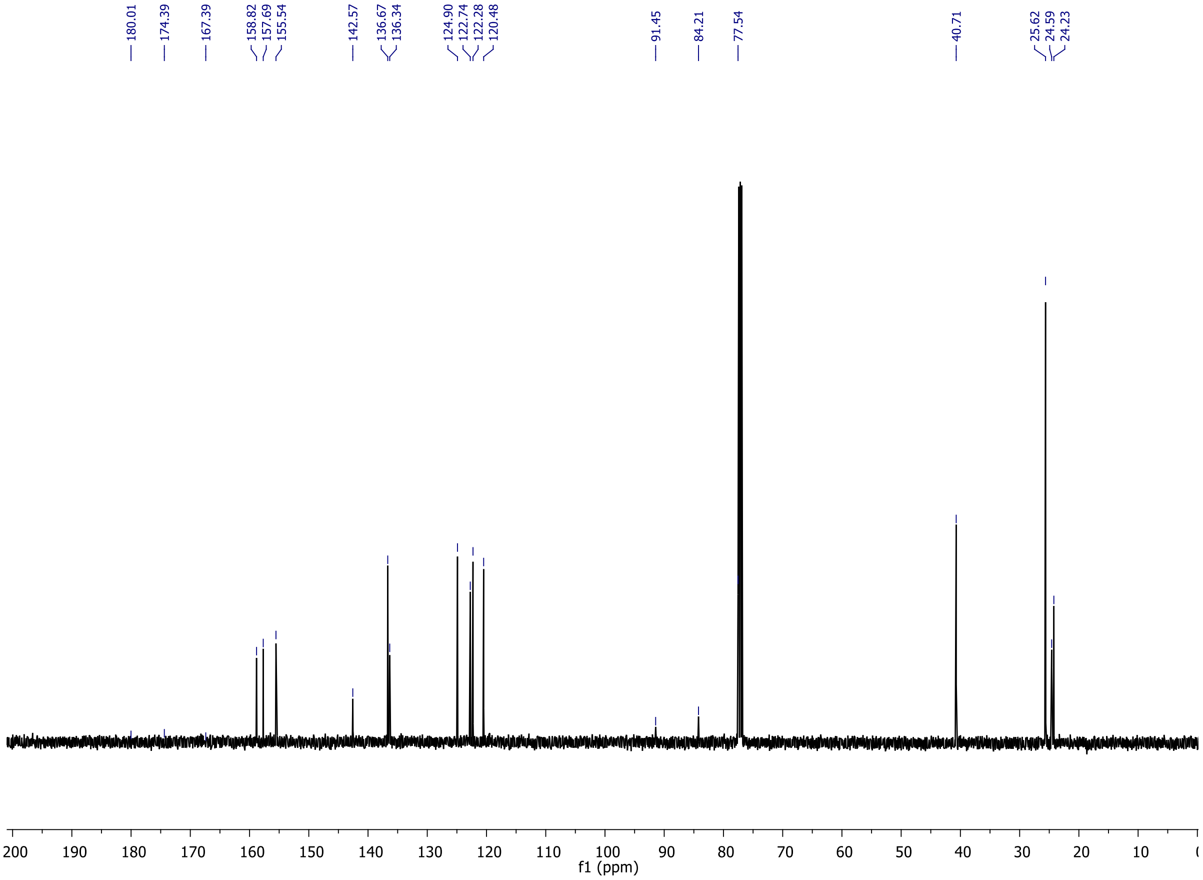
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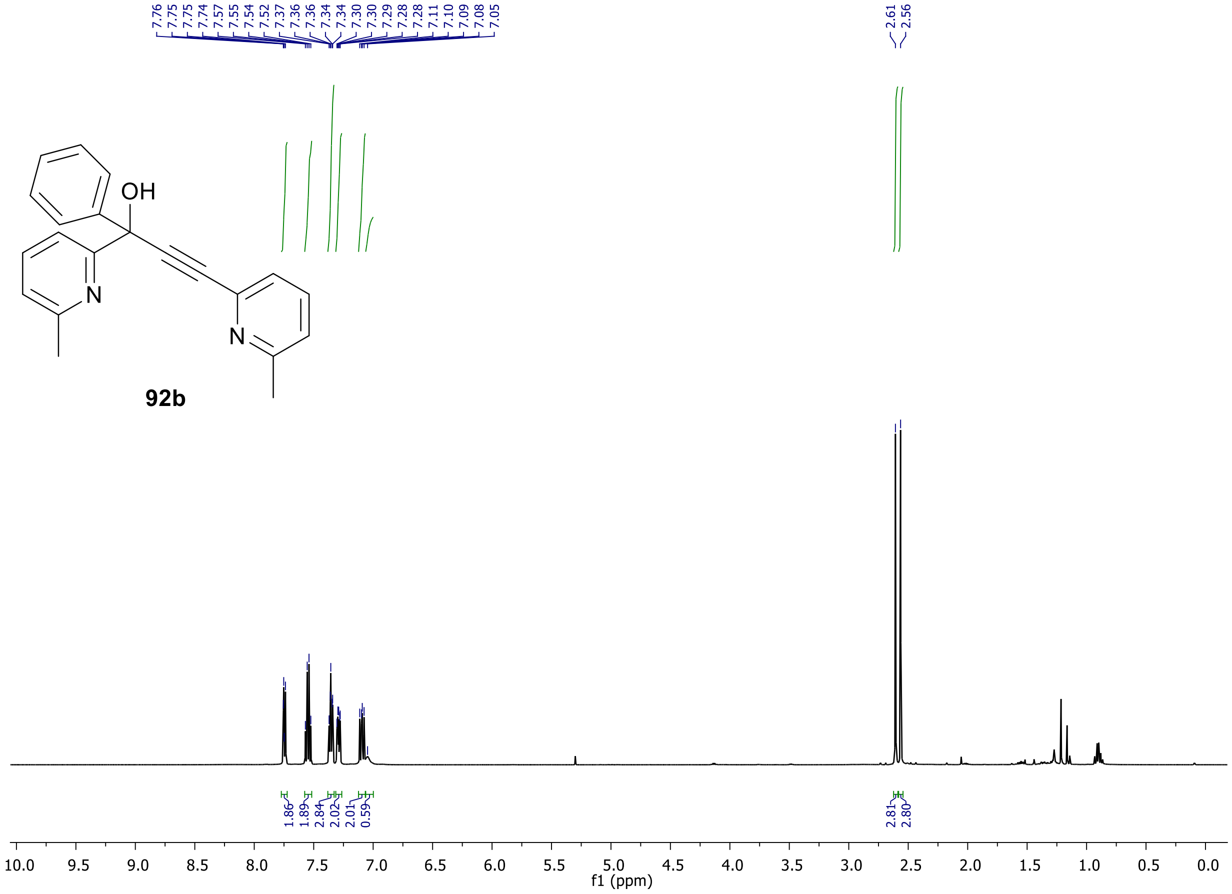
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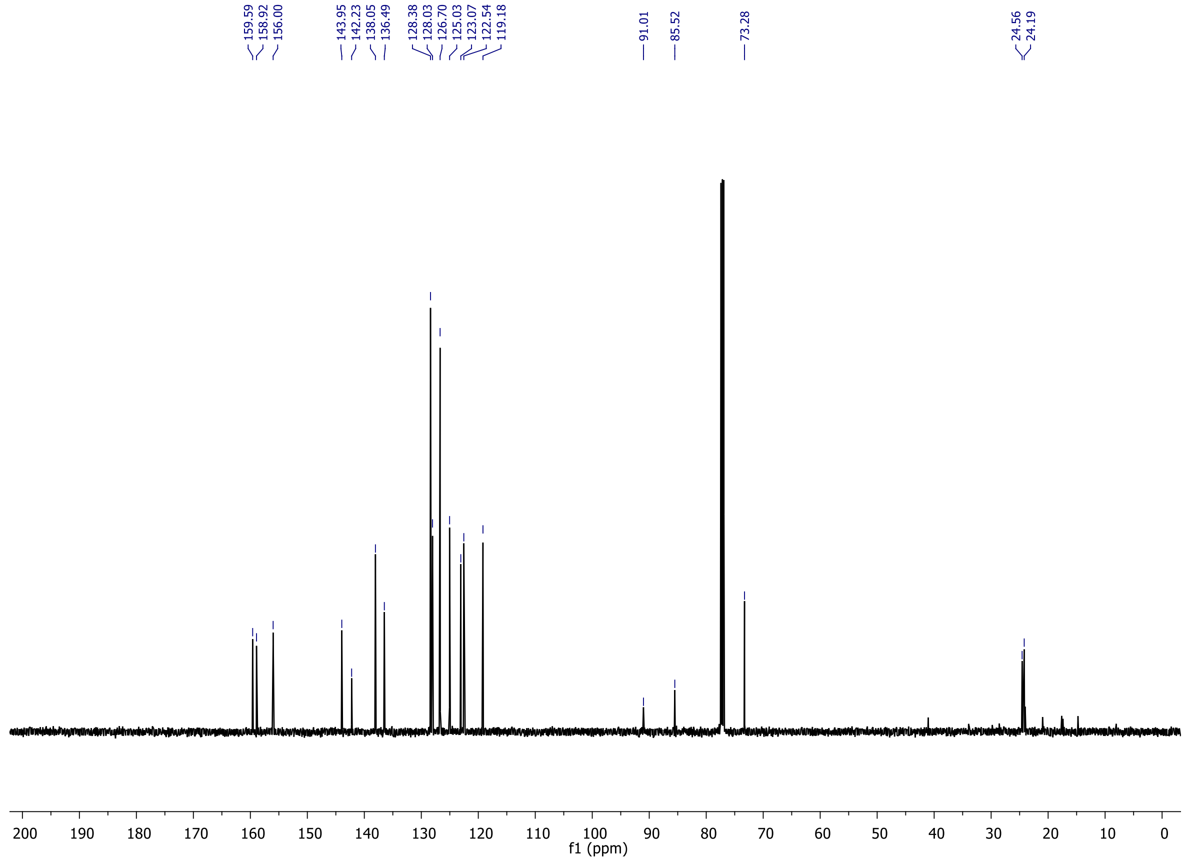
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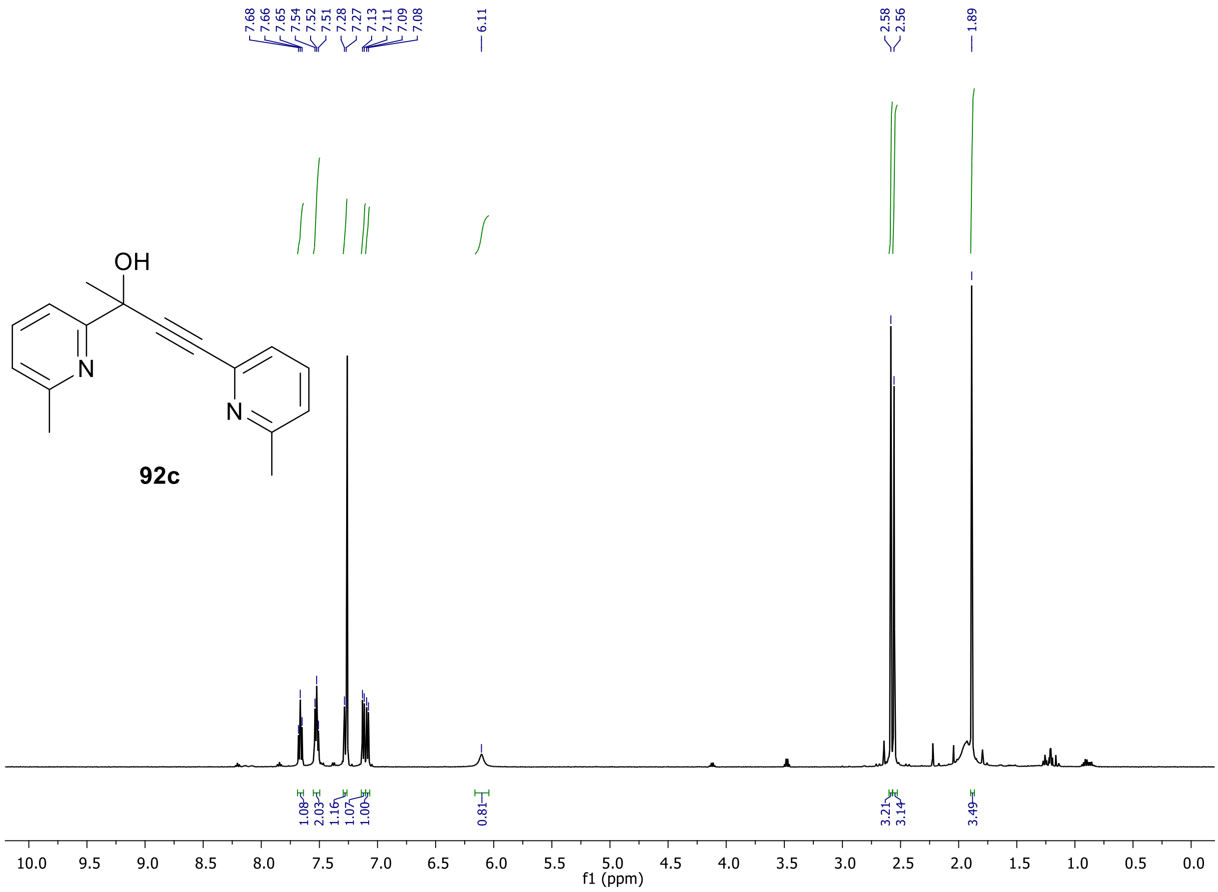
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2.56
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1.07
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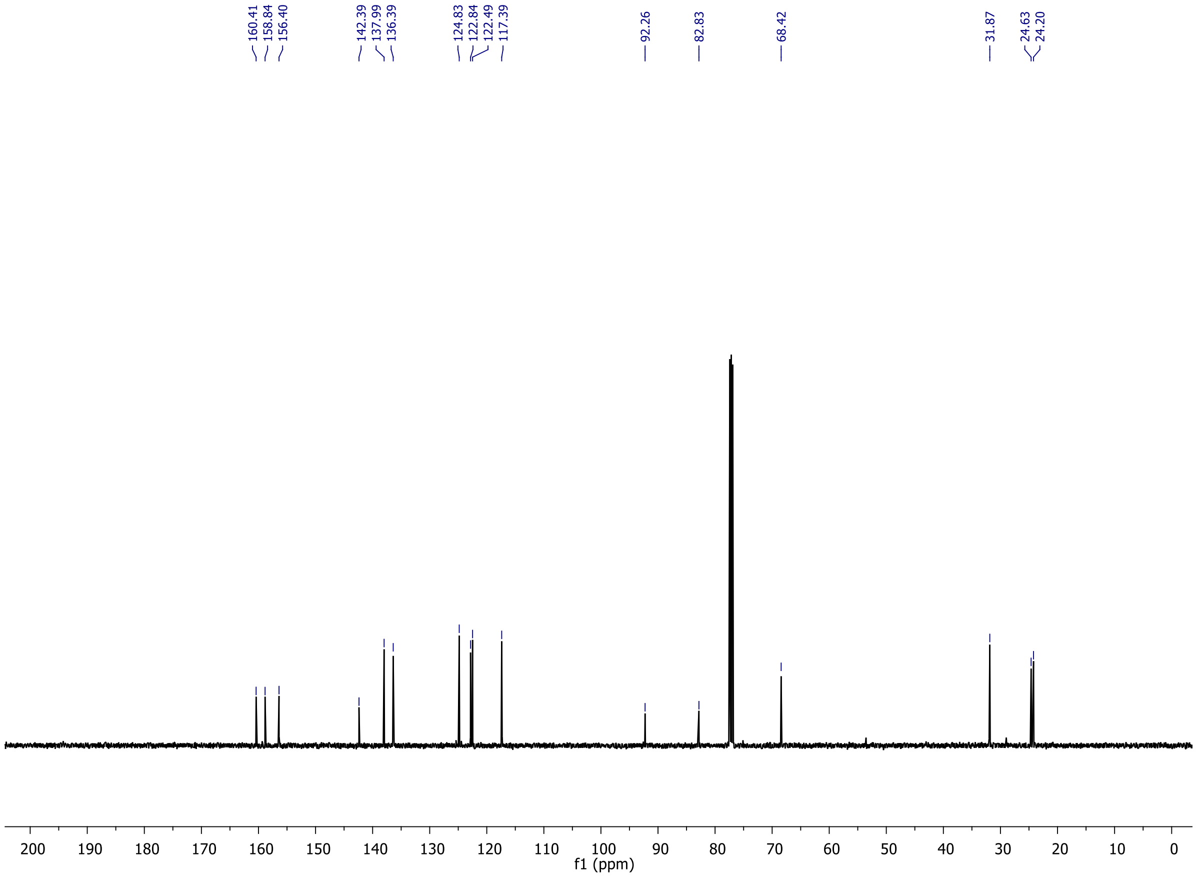
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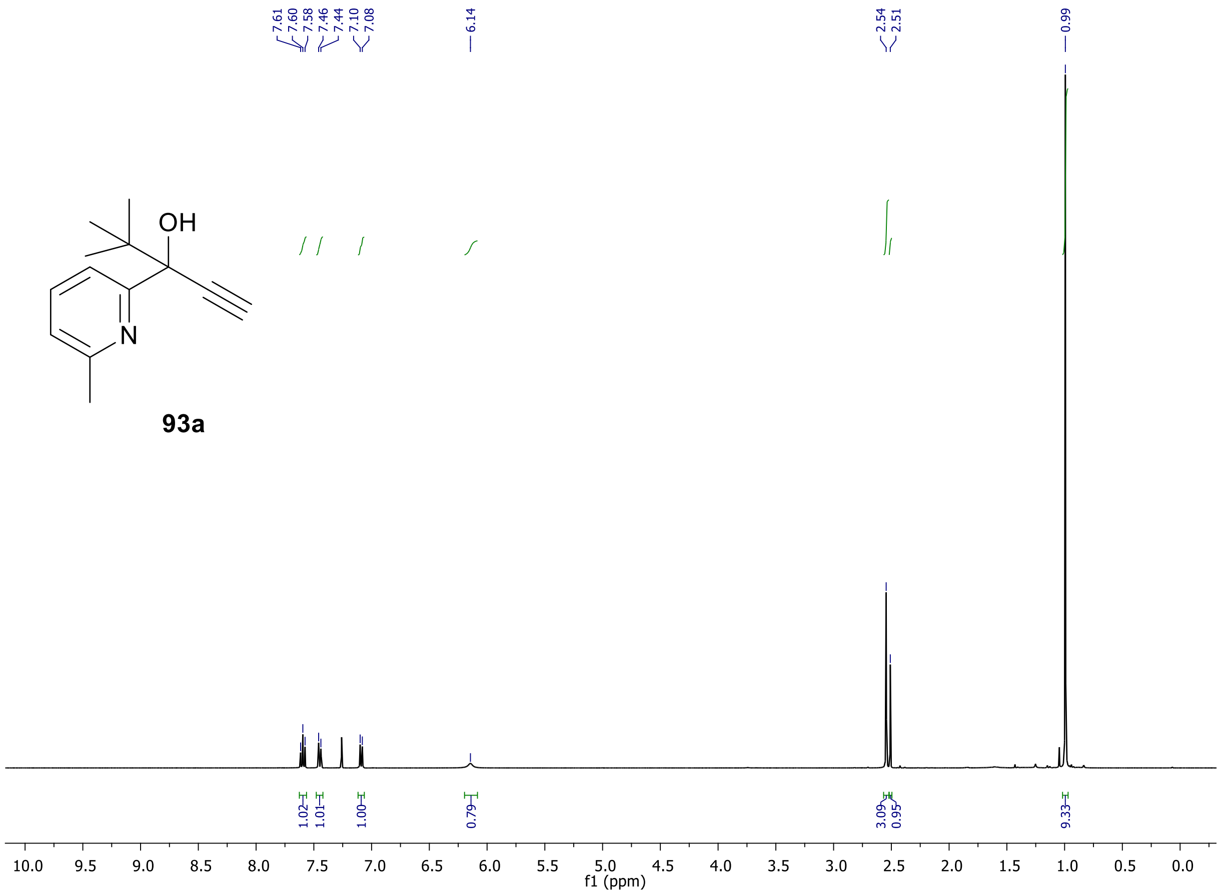
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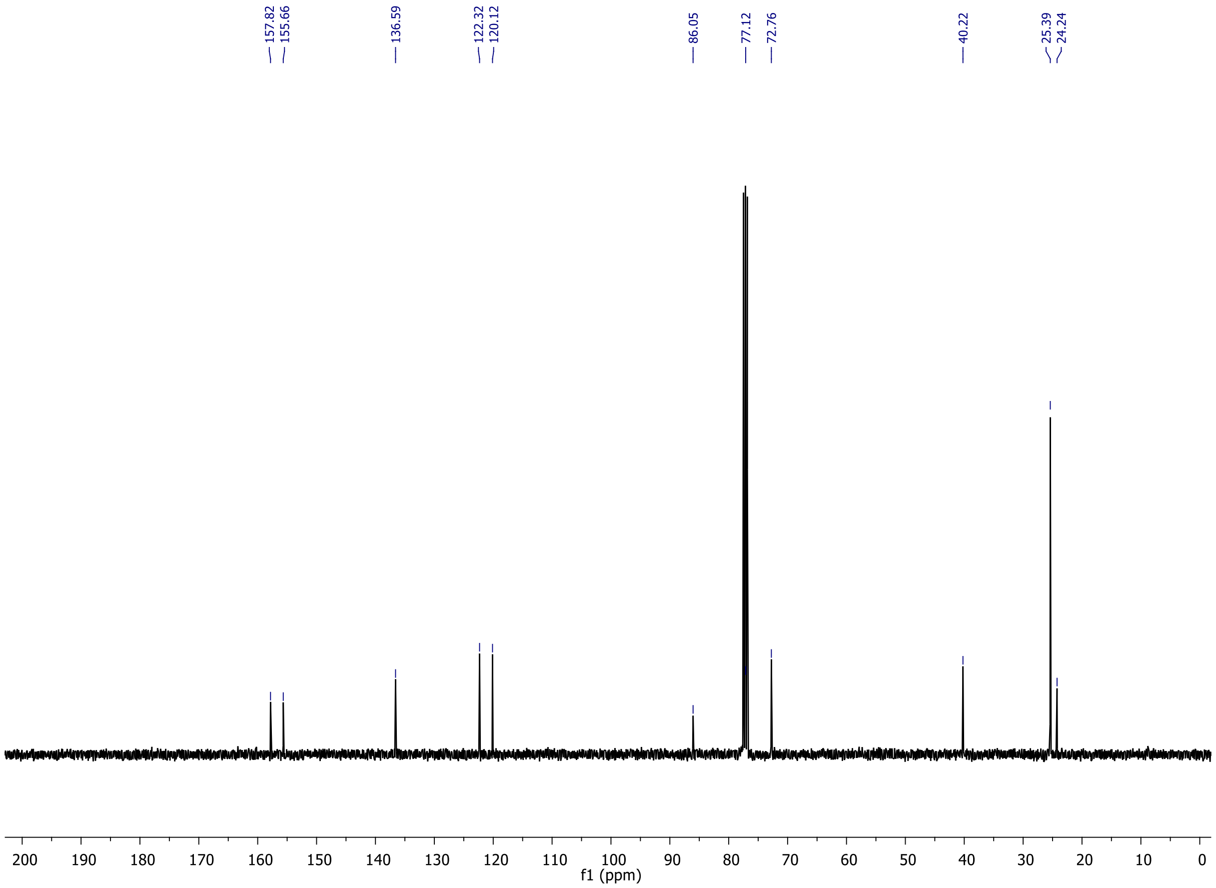
93a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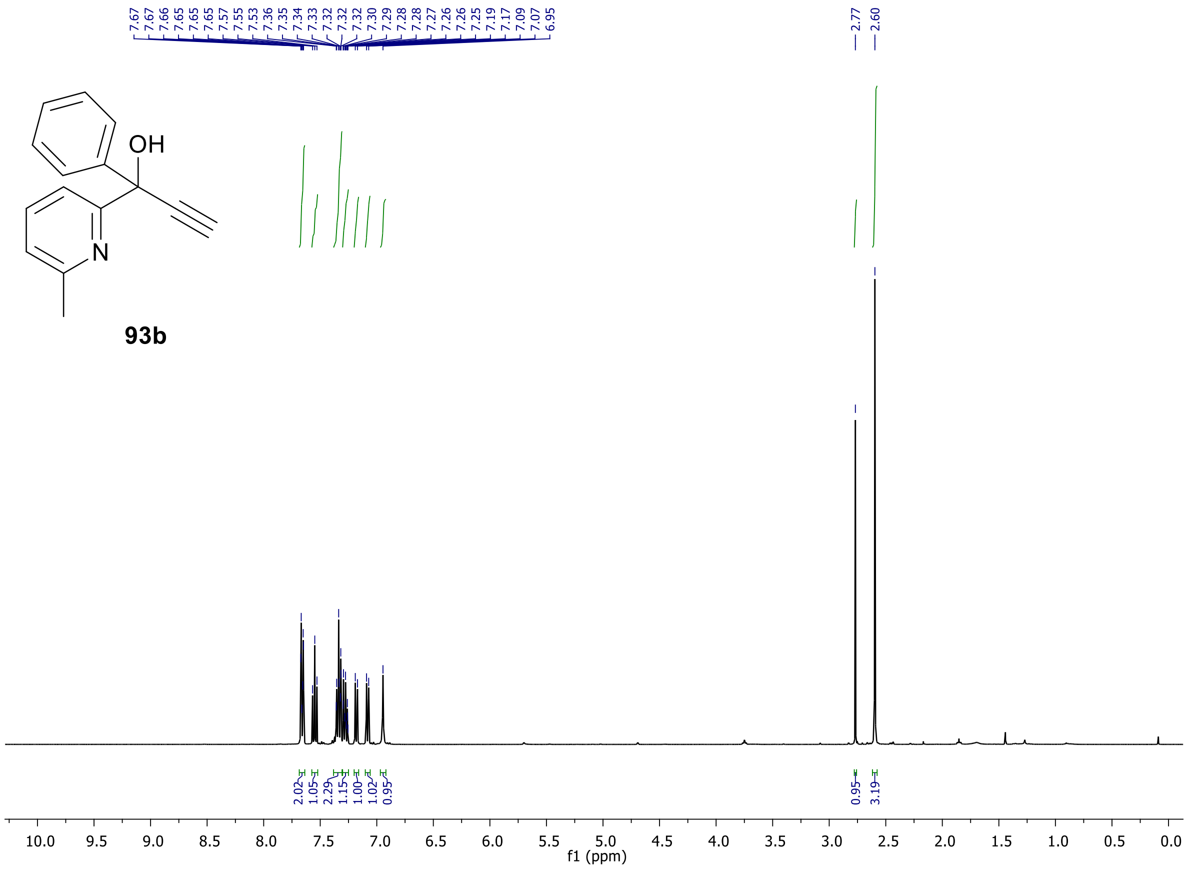
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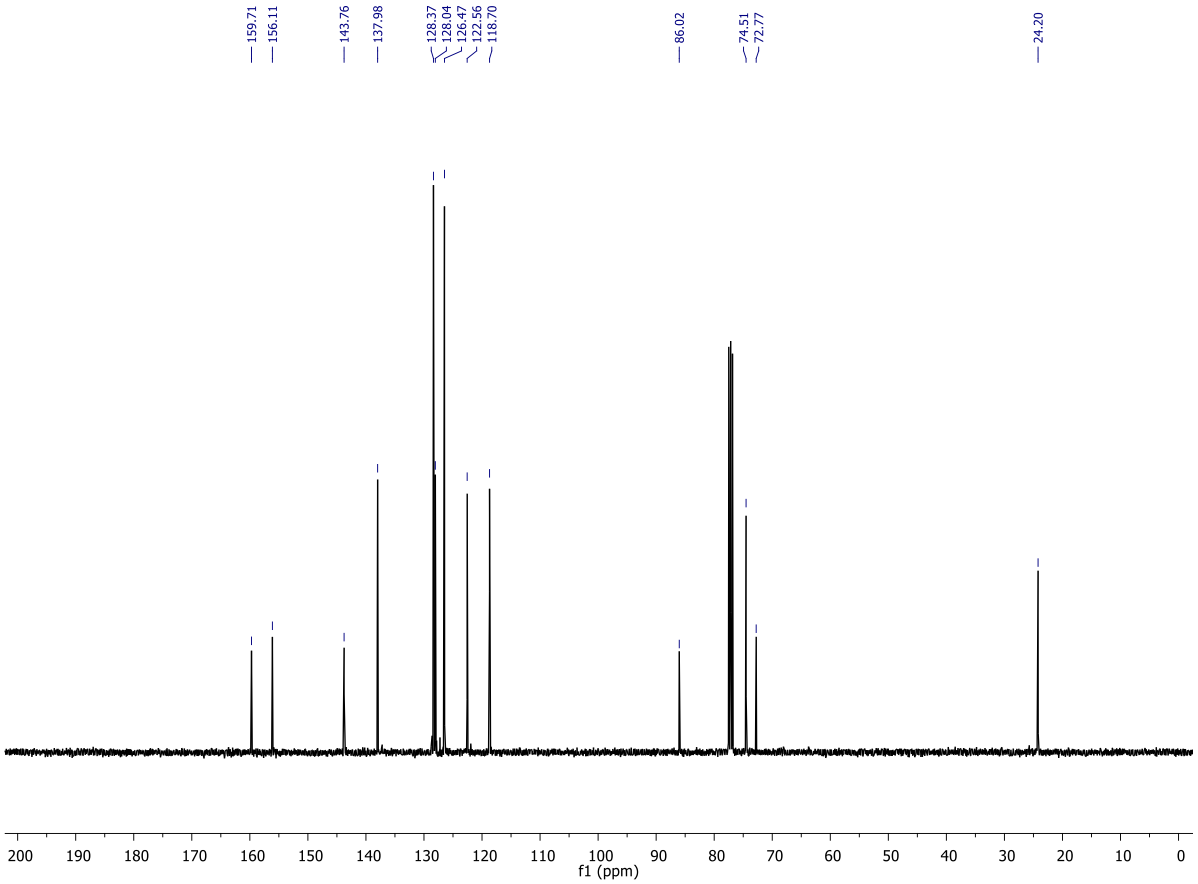
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180
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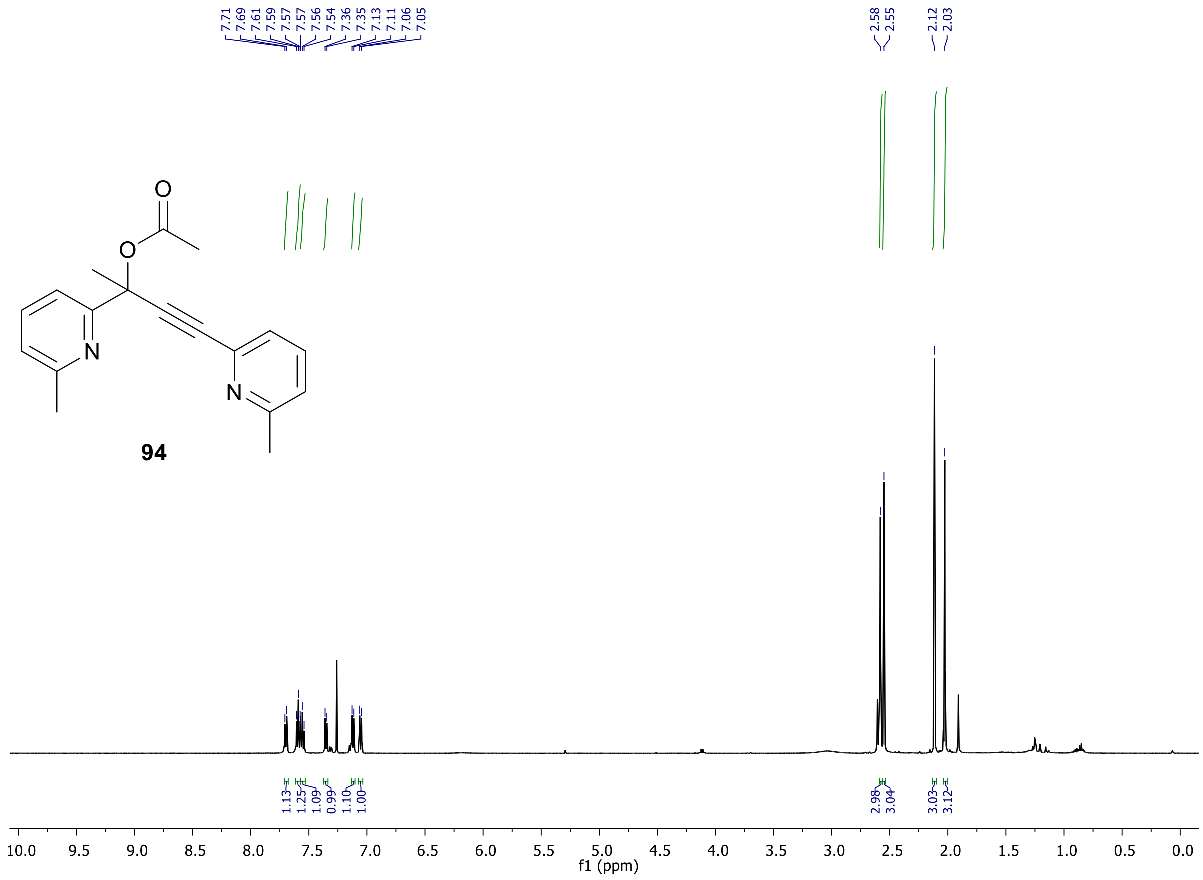
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2.03
O
O
N
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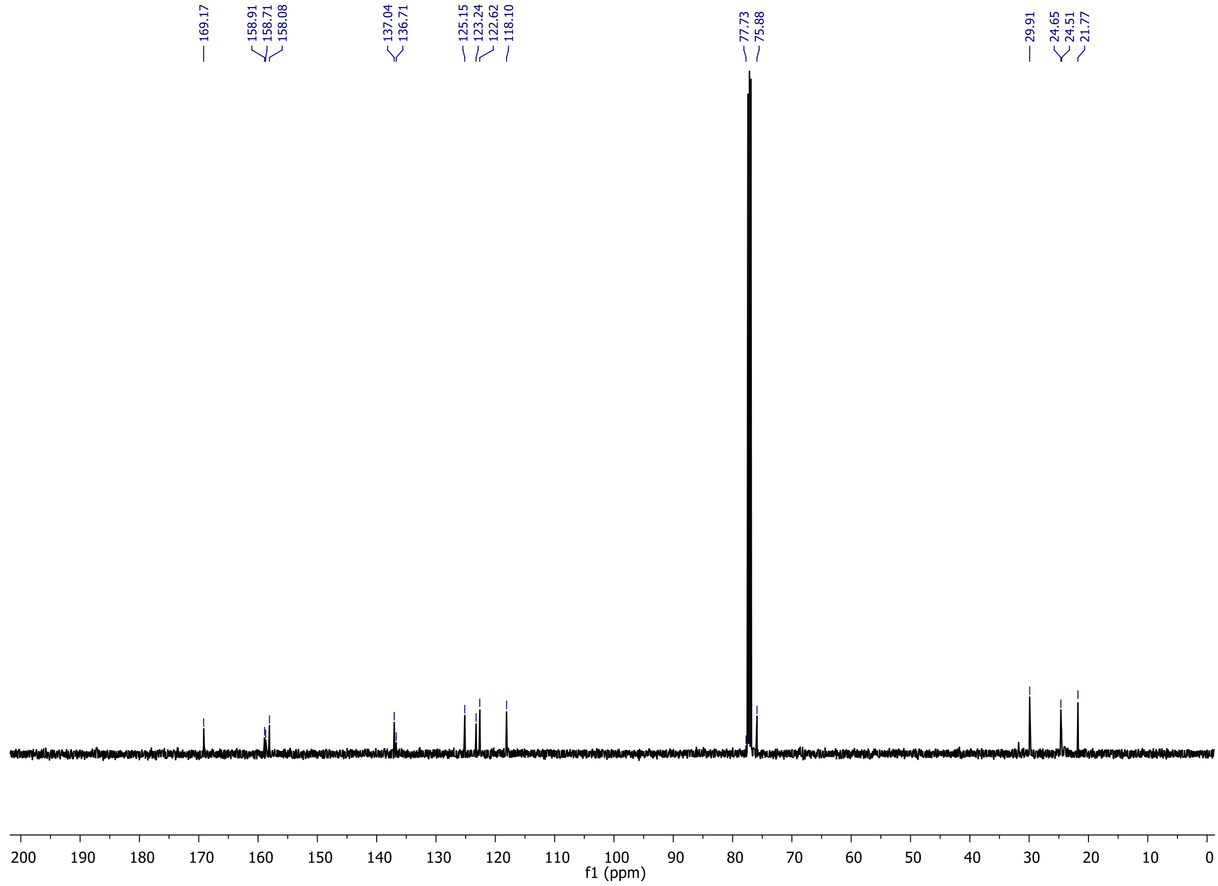
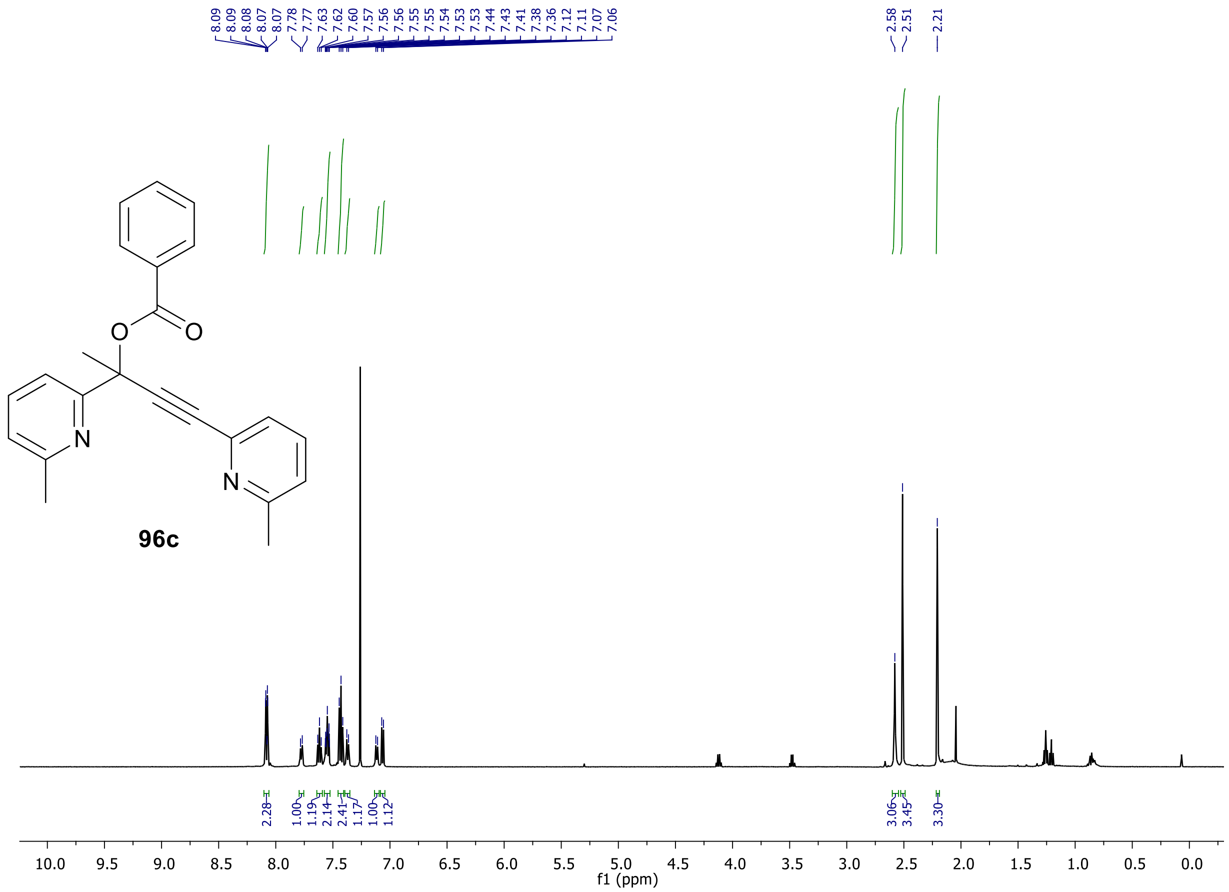
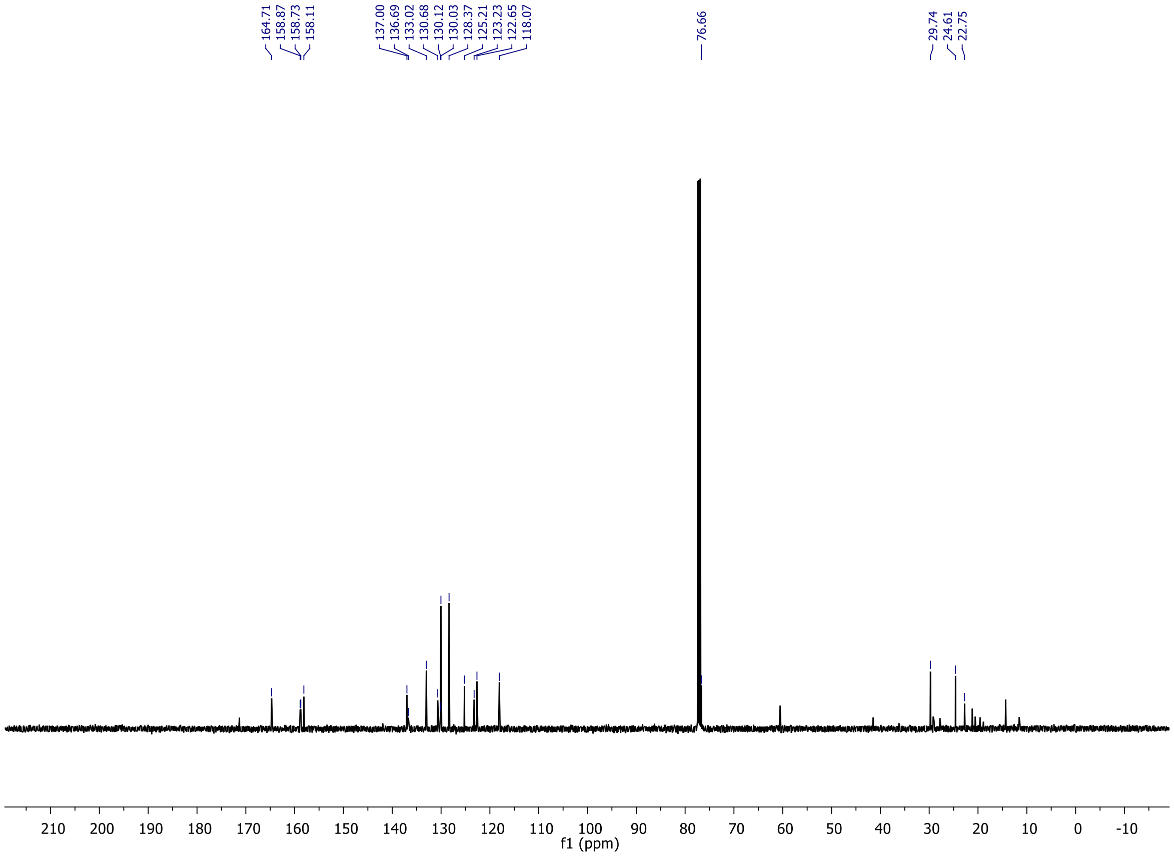
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

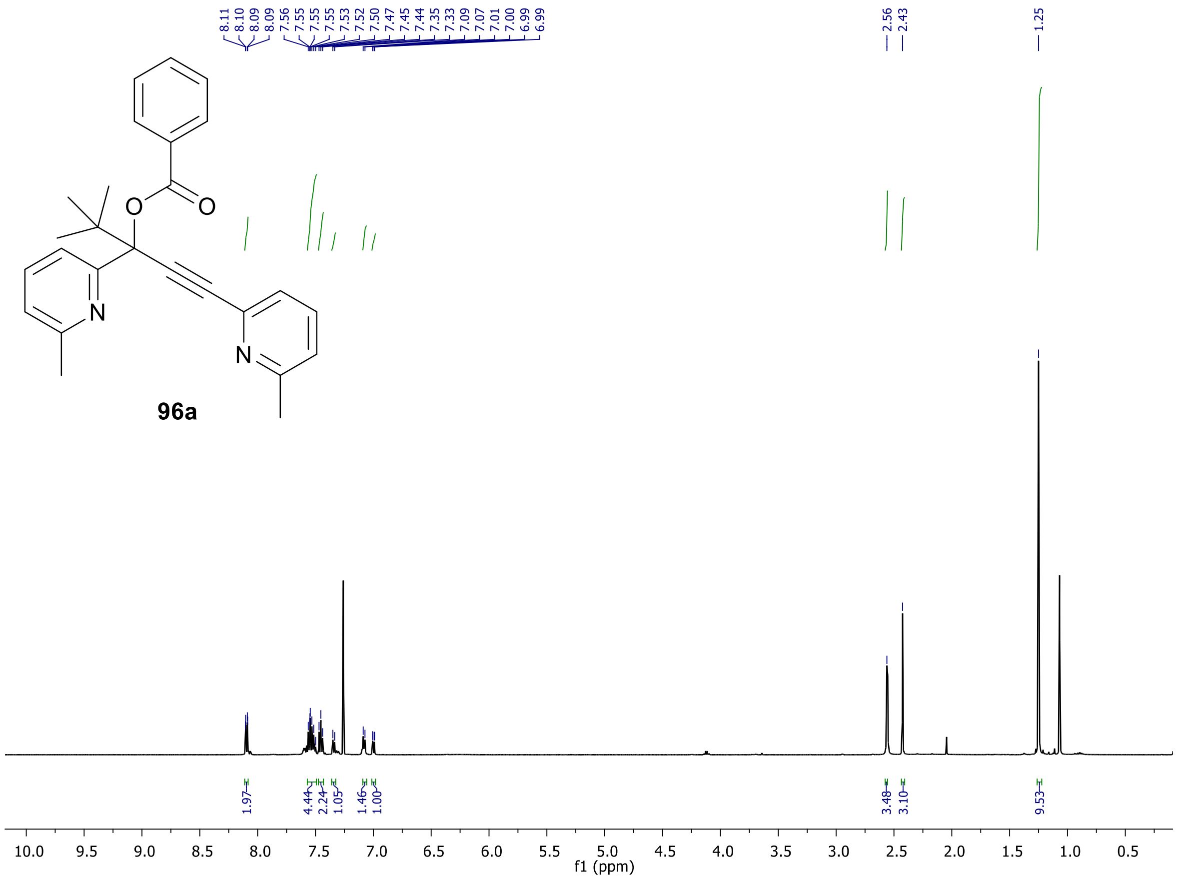
94

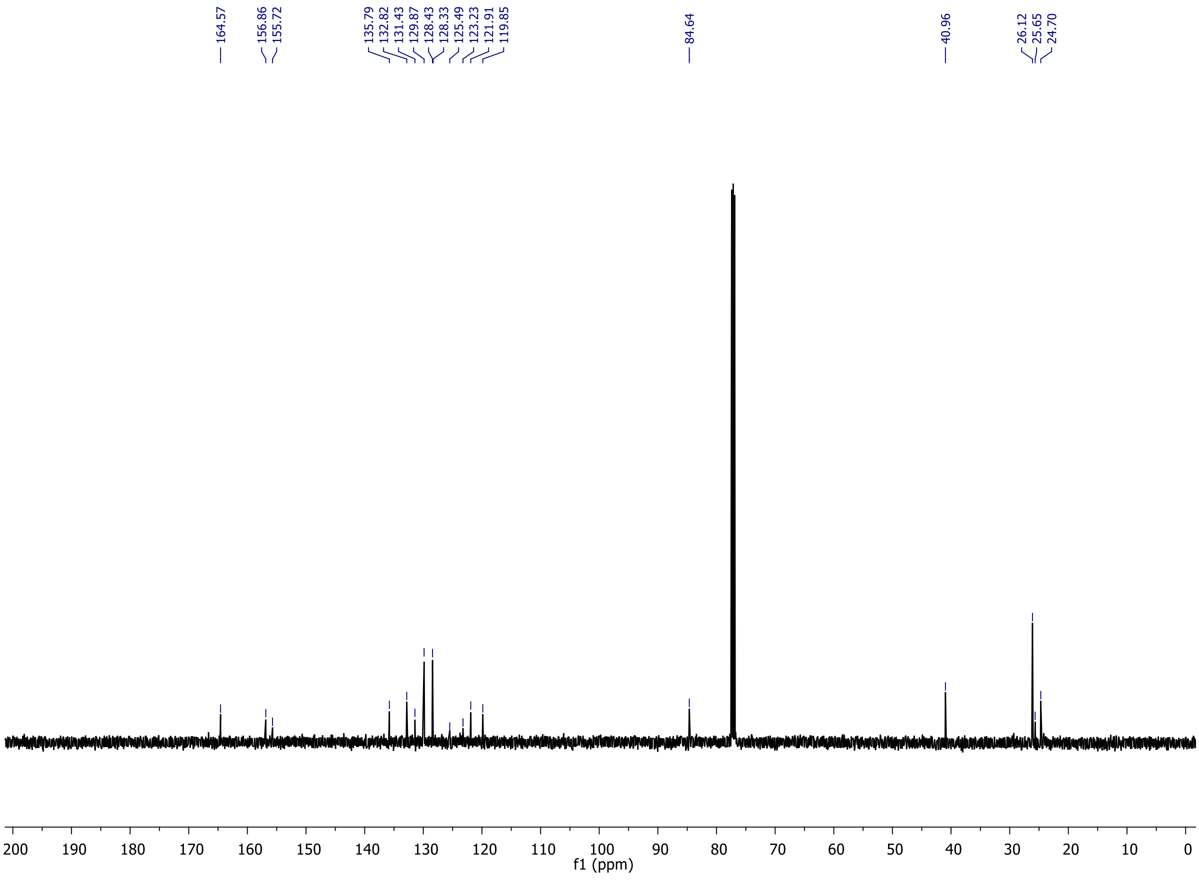

169.17
158.91
158.71
158.08
137.04
136.71
125.15
123.24
122.62
118.10
77.73
75.88
29.91
24.65
24.51
21.77
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

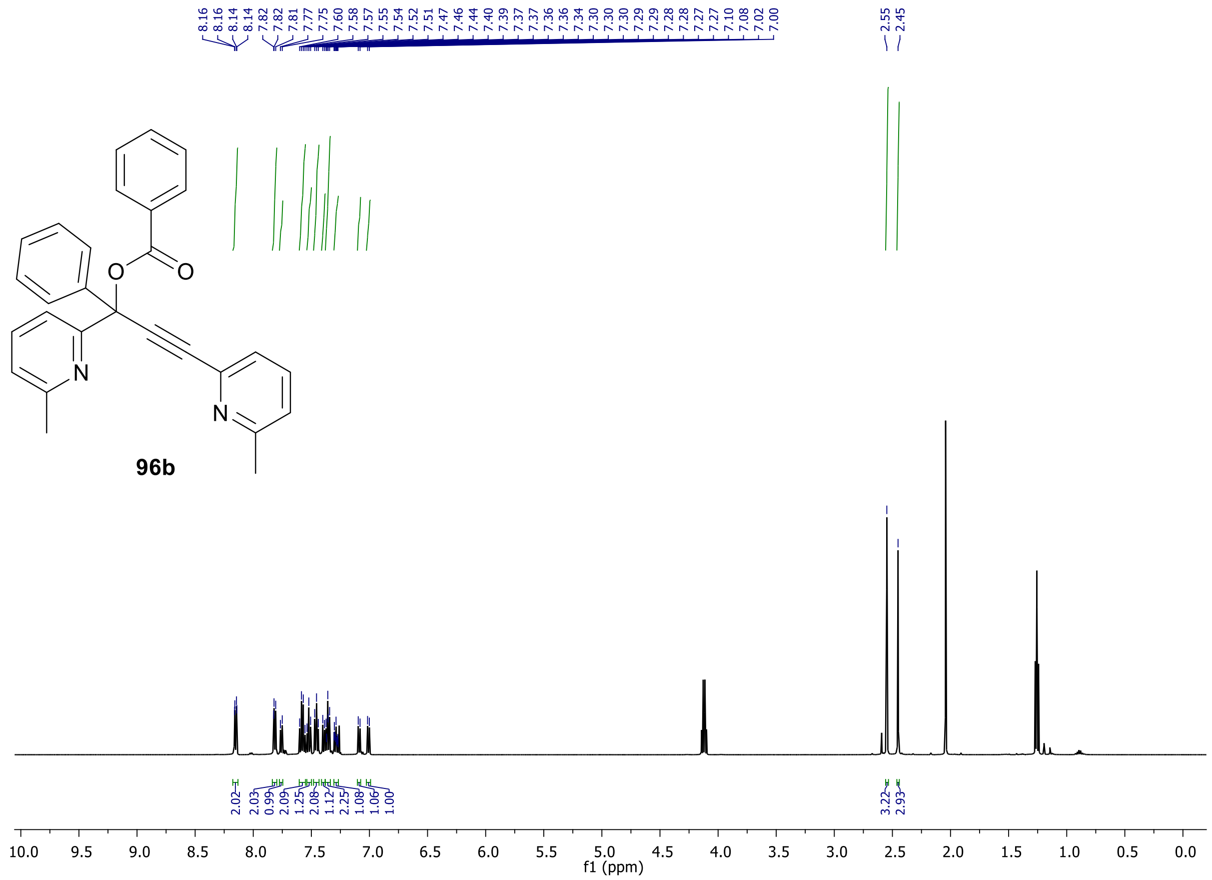

8.09
8.09
8.08
8.07
8.07
7.78
7.77
7.63
7.62
7.60
7.57
7.56
7.55
7.55
7.54
7.53
7.53
7.44
7.43
7.41
7.38
7.36
7.12
7.11
7.07
7.06
2.58
2.51
2.21
O
O
N
N
2.28
1.00
1.19
2.14
2.41
1.17
1.00
1.12
3.06
3.45
3.30
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

96c


164.71
158.87
158.73
158.11
137.00
136.69
133.02
130.68
130.12
130.03
128.37
125.21
123.23
122.65
118.07
76.66
29.74
24.61
22.75
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)

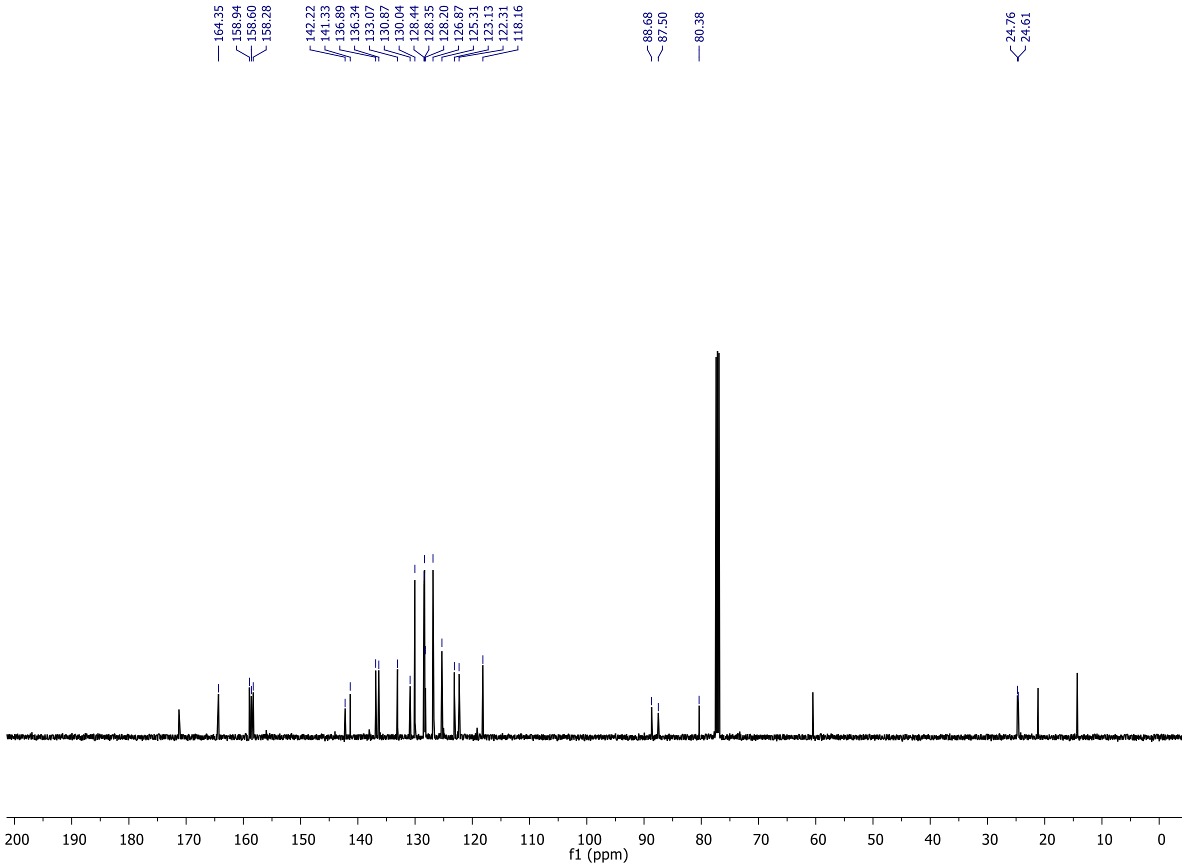

96a
N
N
O
O
8.11
8.10
8.09
8.09
7.56
7.55
7.55
7.55
7.53
7.52
7.50
7.47
7.45
7.44
7.35
7.33
7.09
7.07
7.01
7.00
6.99
6.99
2.56
2.43
1.25
1.97
4.44
2.24
1.05
1.46
1.00
3.48
3.10
9.53
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


164.57
156.86
155.72
135.79
132.82
131.43
129.87
128.43
128.33
125.49
123.23
121.91
119.85
84.64
40.96
26.12
25.65
24.70
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

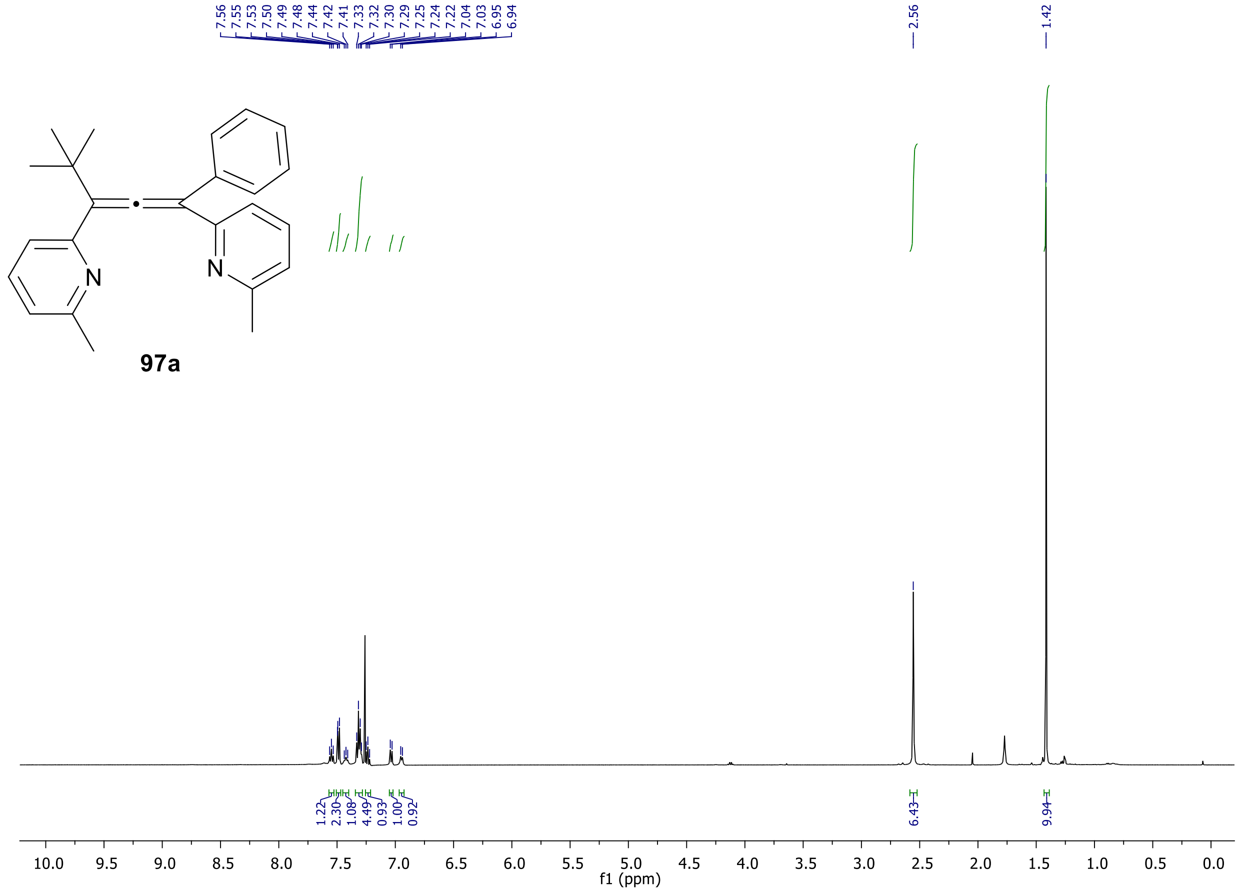


96b

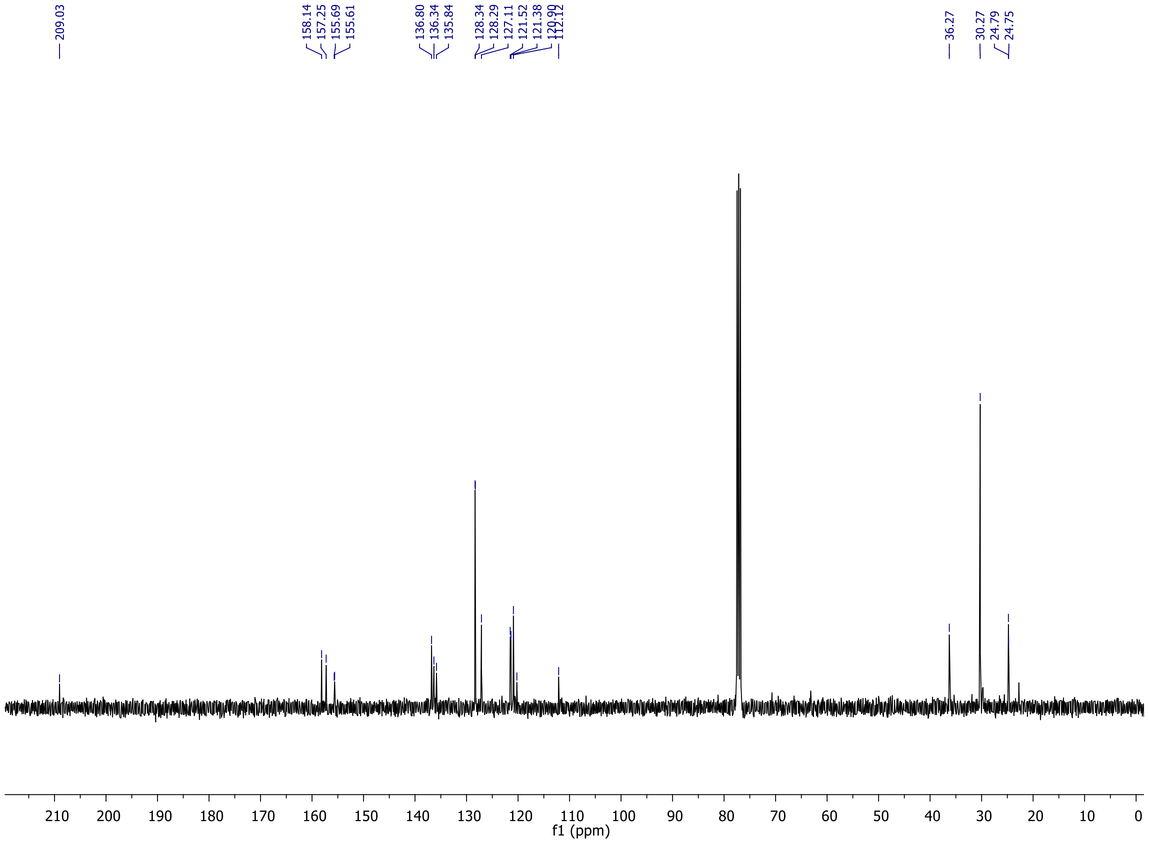
8.16
8.16
8.14
8.14
7.82
7.82
7.81
7.77
7.75
7.60
7.58
7.57
7.55
7.54
7.52
7.51
7.47
7.46
7.44
7.40
7.39
7.37
7.37
7.36
7.34
7.30
7.30
7.30
7.29
7.29
7.28
7.28
7.27
7.27
7.10
7.08
7.02
7.00
2.55
2.45
O
O
N
N
2.02
2.03
0.99
2.09
1.25
2.08
1.12
2.25
1.08
1.06
1.00
3.22
2.93
10.0
9.5
9.0
8.5
8.0
7.5
7.0
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)

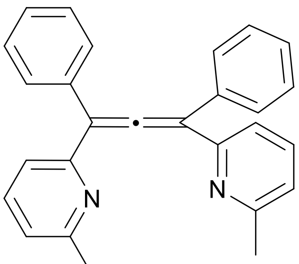


164.35
158.94
158.60
158.28
142.22
141.33
136.89
136.34
133.07
130.87
130.04
128.44
128.35
128.20
126.87
125.31
123.13
122.31
118.16
88.68
87.50
80.38
24.76
24.61
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

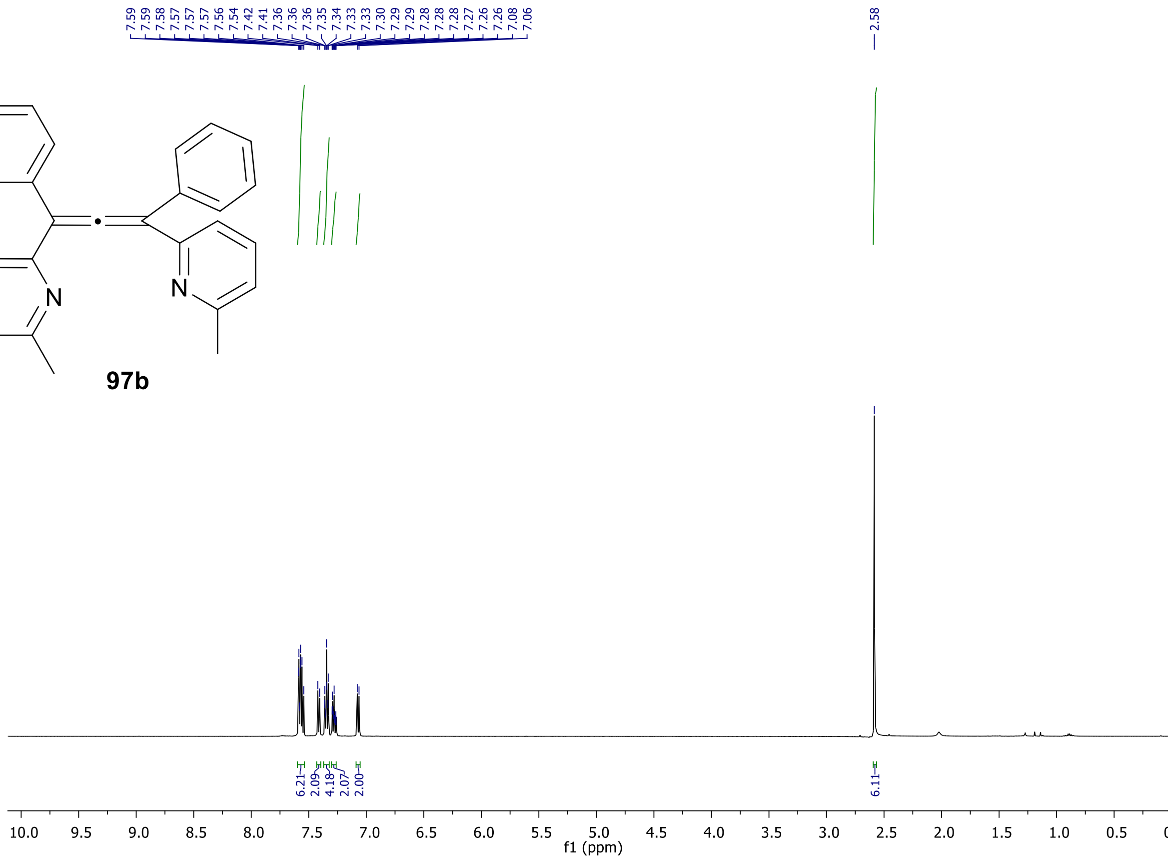

7.56
7.55
7.53
7.50
7.49
7.48
7.44
7.42
7.41
7.33
7.32
7.30
7.29
7.25
7.24
7.22
7.04
7.03
6.95
6.94
2.56
1.42
N
N
1.22
2.30
1.08
4.49
0.93
1.00
0.92
6.43
9.94
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

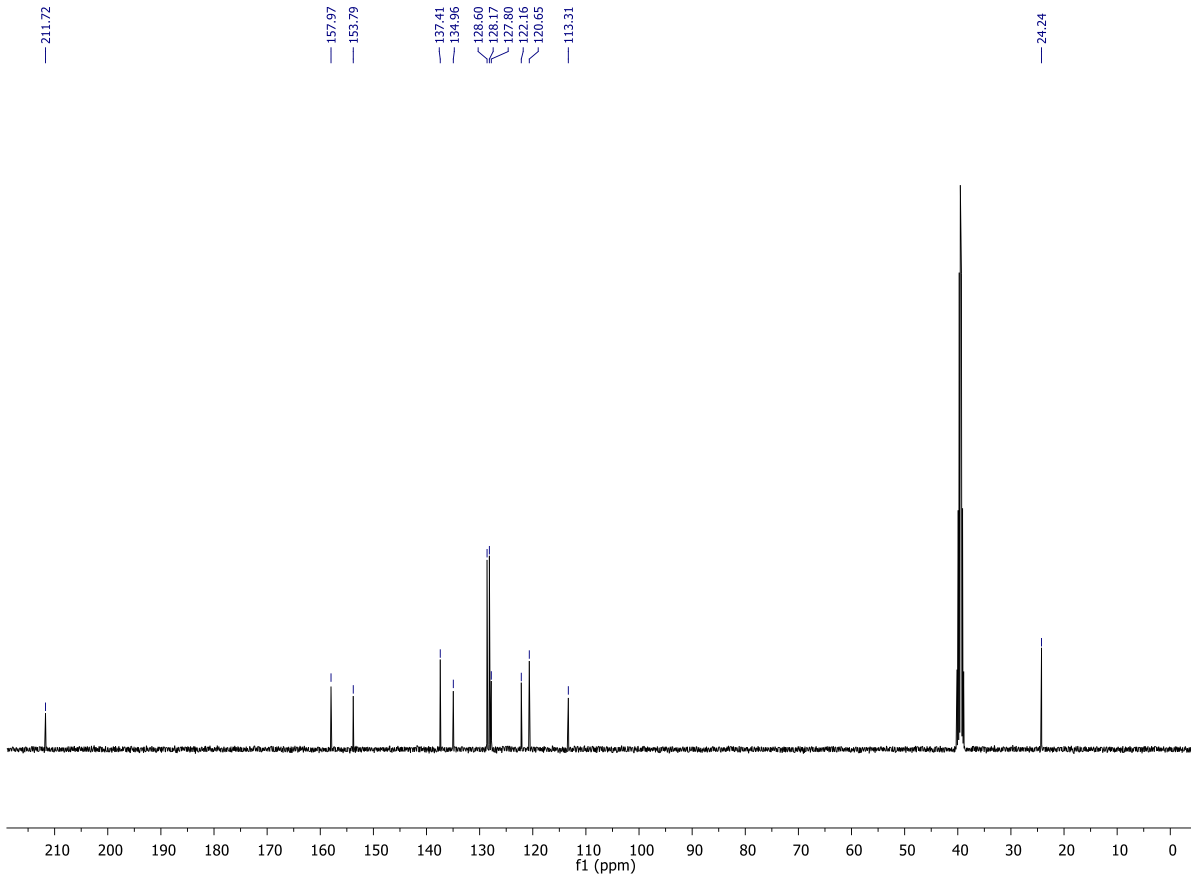
97a

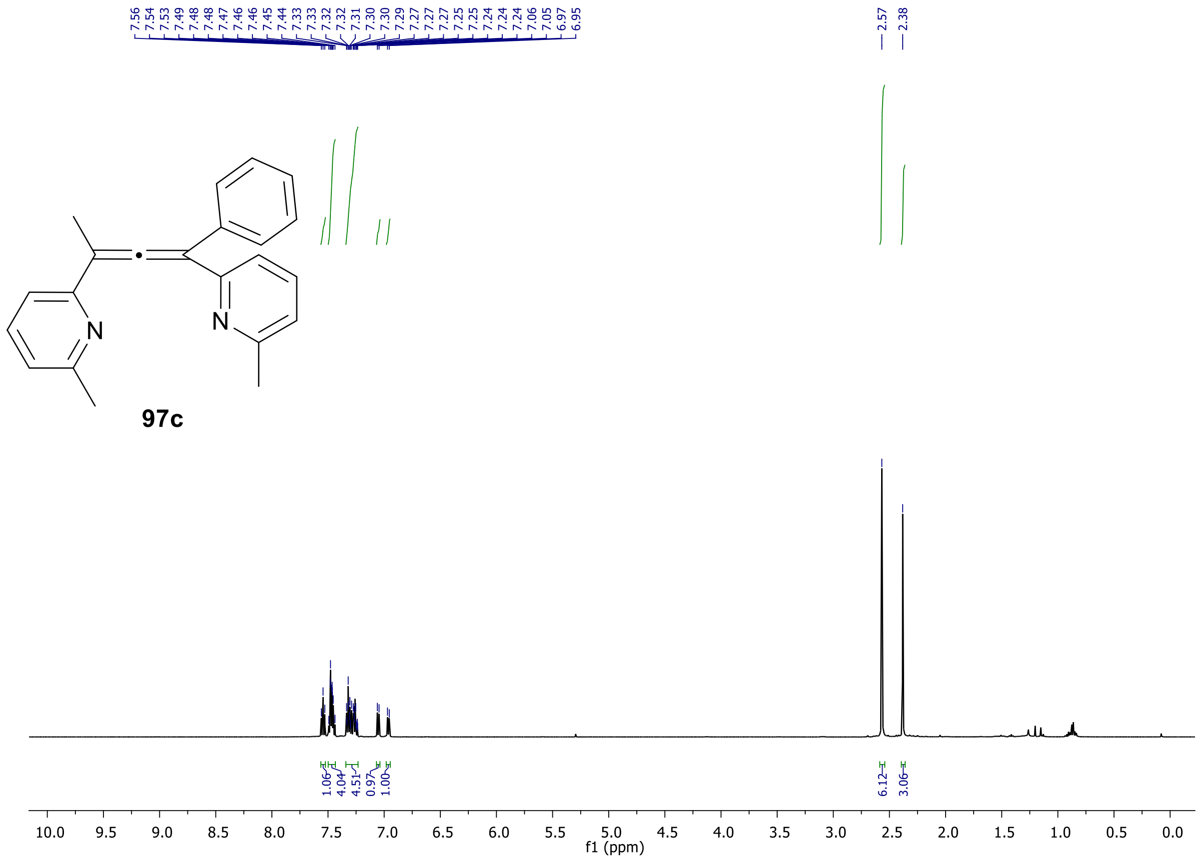

209.03
158.14
157.25
155.69
155.61
136.80
136.34
135.84
128.34
128.29
127.11
121.52
121.38
120.90
112.12
36.27
30.27
24.79
24.75
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

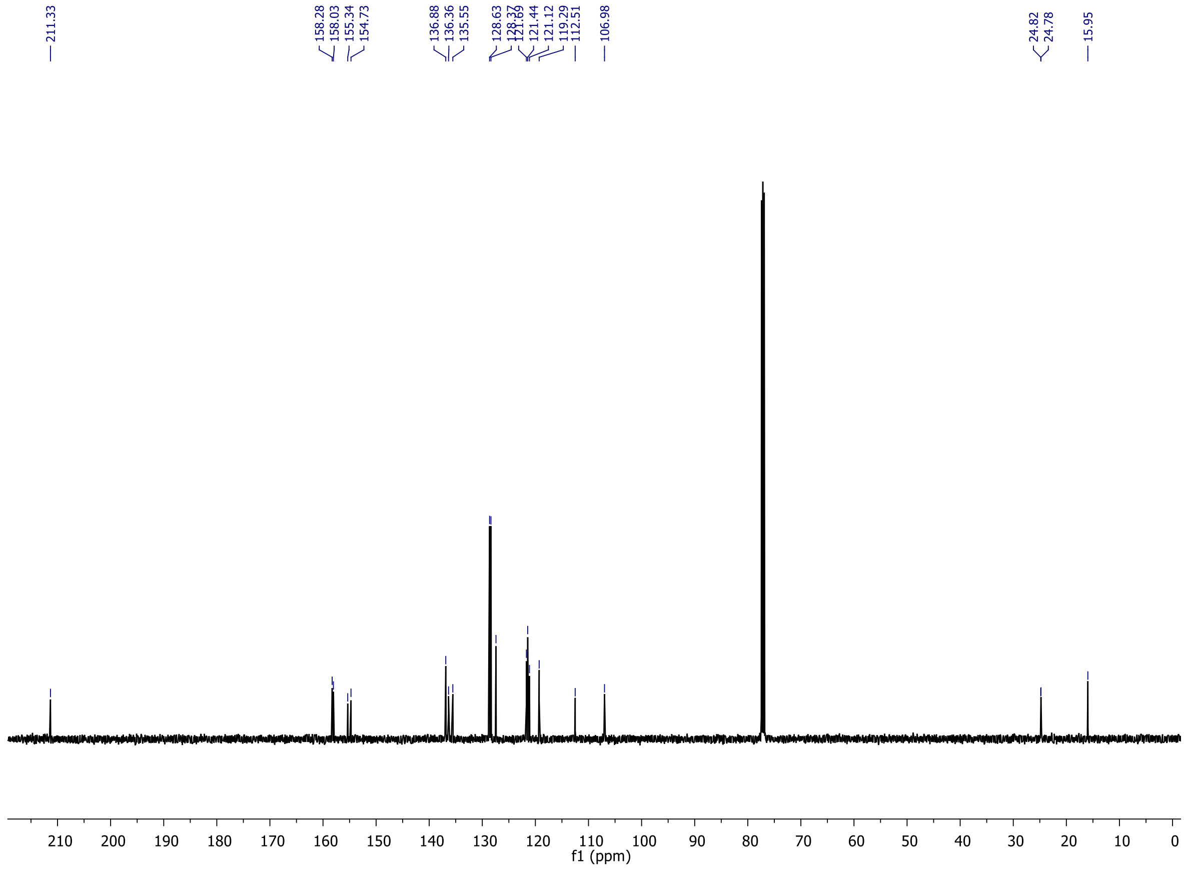

N
N

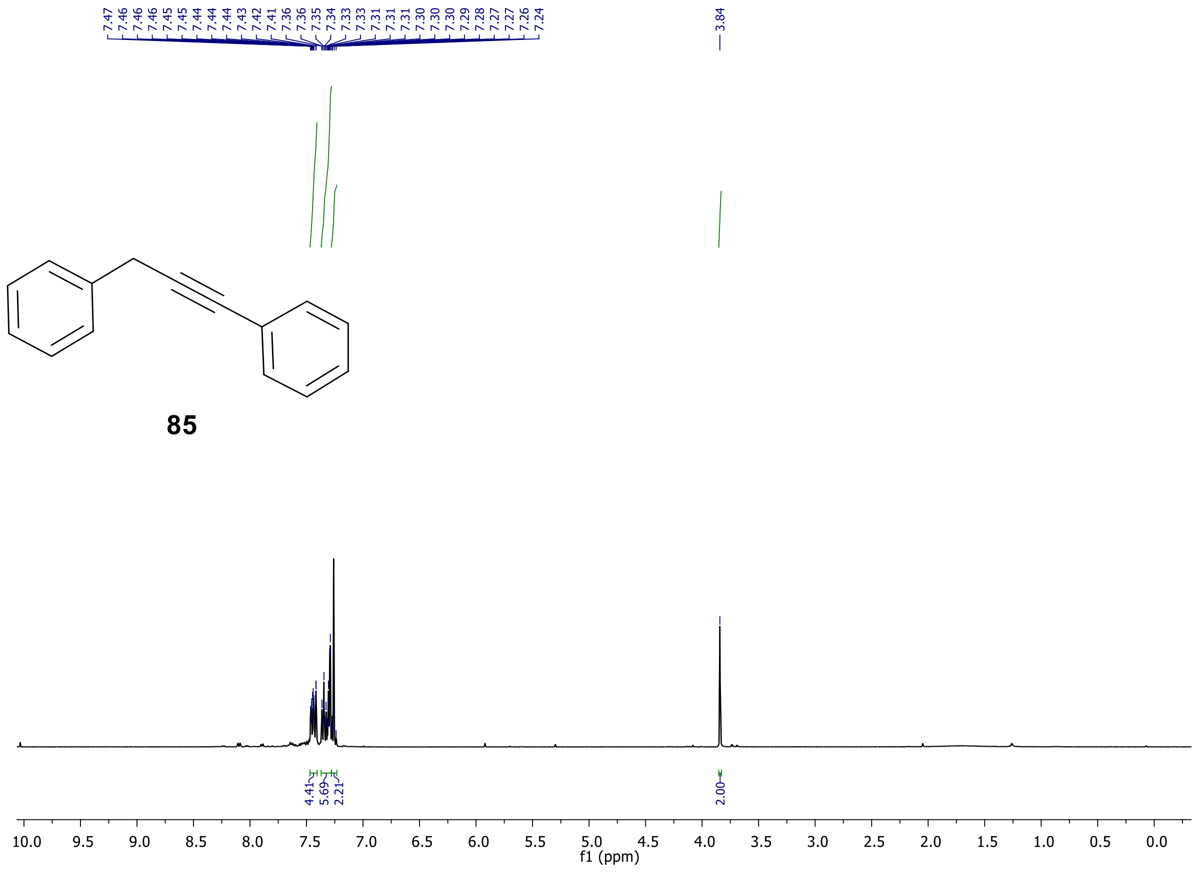
97b


7.59
7.59
7.58
7.57
7.57
7.57
7.56
7.54
7.42
7.41
7.36
7.36
7.36
7.35
7.34
7.33
7.33
7.30
7.29
7.29
7.28
7.28
7.28
7.27
7.26
7.26
7.08
7.06
2.58
6.21
2.09
4.18
2.07
2.00
6.11
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)

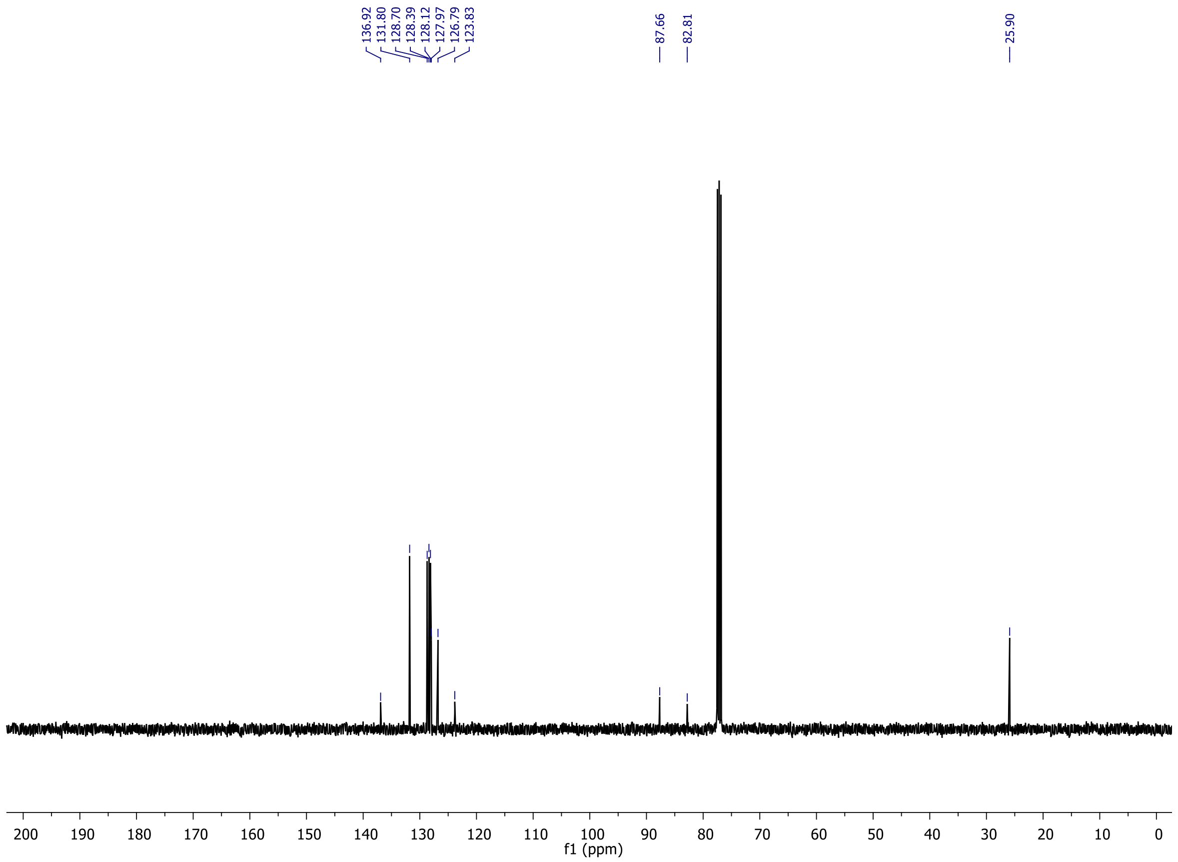

211.72
157.97
153.79
137.41
134.96
128.60
128.17
127.80
122.16
120.65
113.31
24.24
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

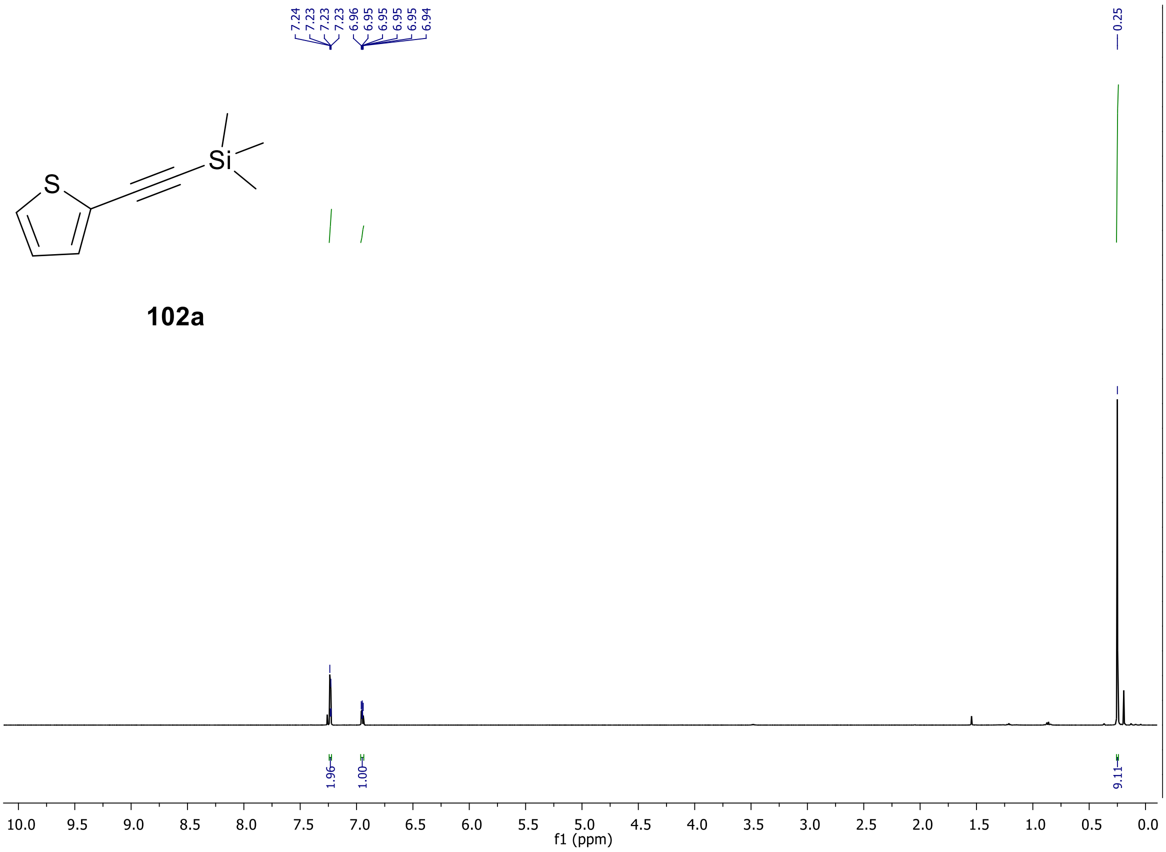

97c
7.56
7.54
7.53
7.49
7.48
7.48
7.47
7.46
7.46
7.45
7.44
7.33
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.27
7.27
7.27
7.25
7.25
7.24
7.24
7.24
7.06
7.05
6.97
6.95
2.57
2.38
N
N
1.06
4.04
4.51
0.97
1.00
6.12
3.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


211.33
158.28
158.03
155.34
154.73
136.88
136.36
135.55
128.63
128.37
127.69
121.44
121.12
119.29
112.51
106.98
24.82
24.78
15.95
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

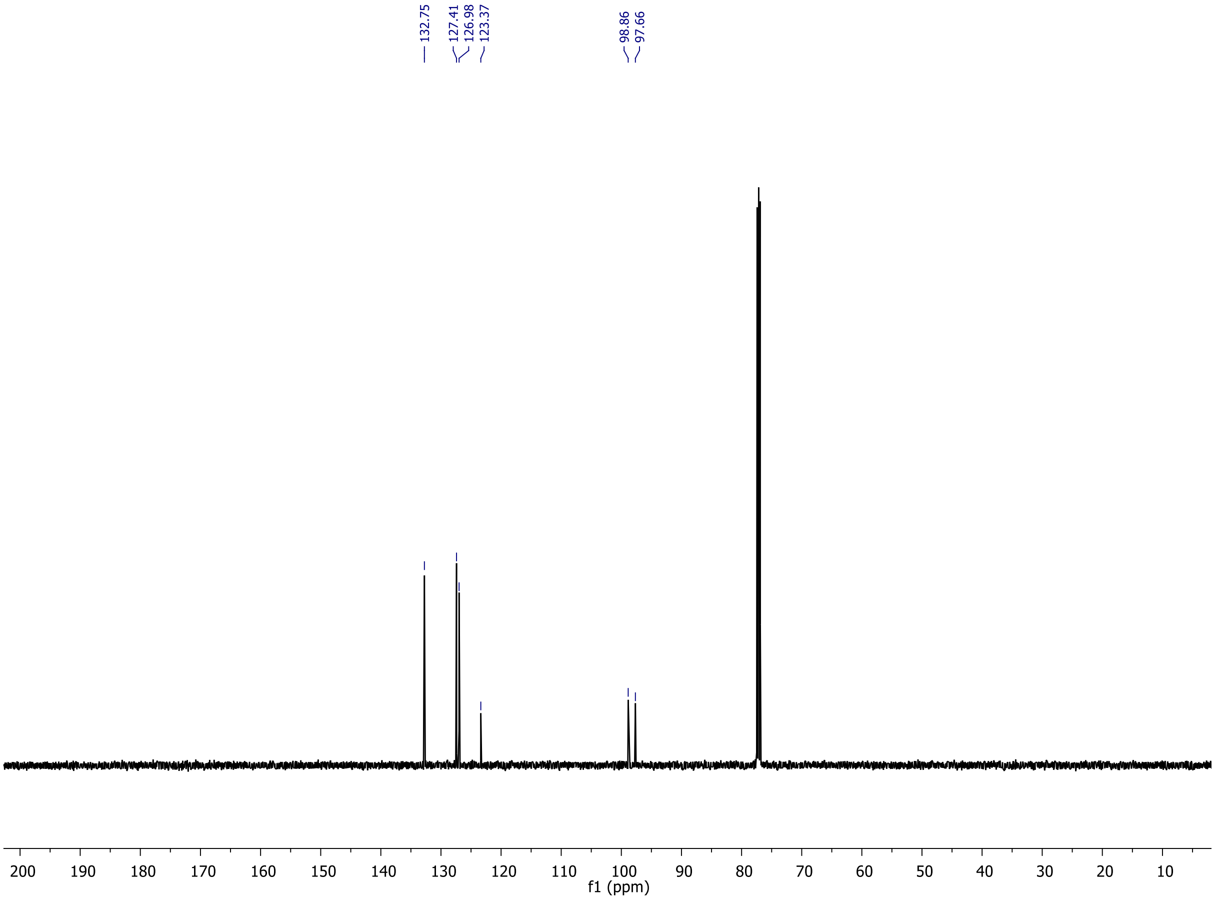

7.47
7.46
7.46
7.45
7.45
7.44
7.44
7.44
7.43
7.42
7.41
7.36
7.36
7.35
7.34
7.33
7.33
7.31
7.31
7.30
7.30
7.30
7.29
7.28
7.27
7.27
7.26
7.24
3.84
4.41
5.69
2.21
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

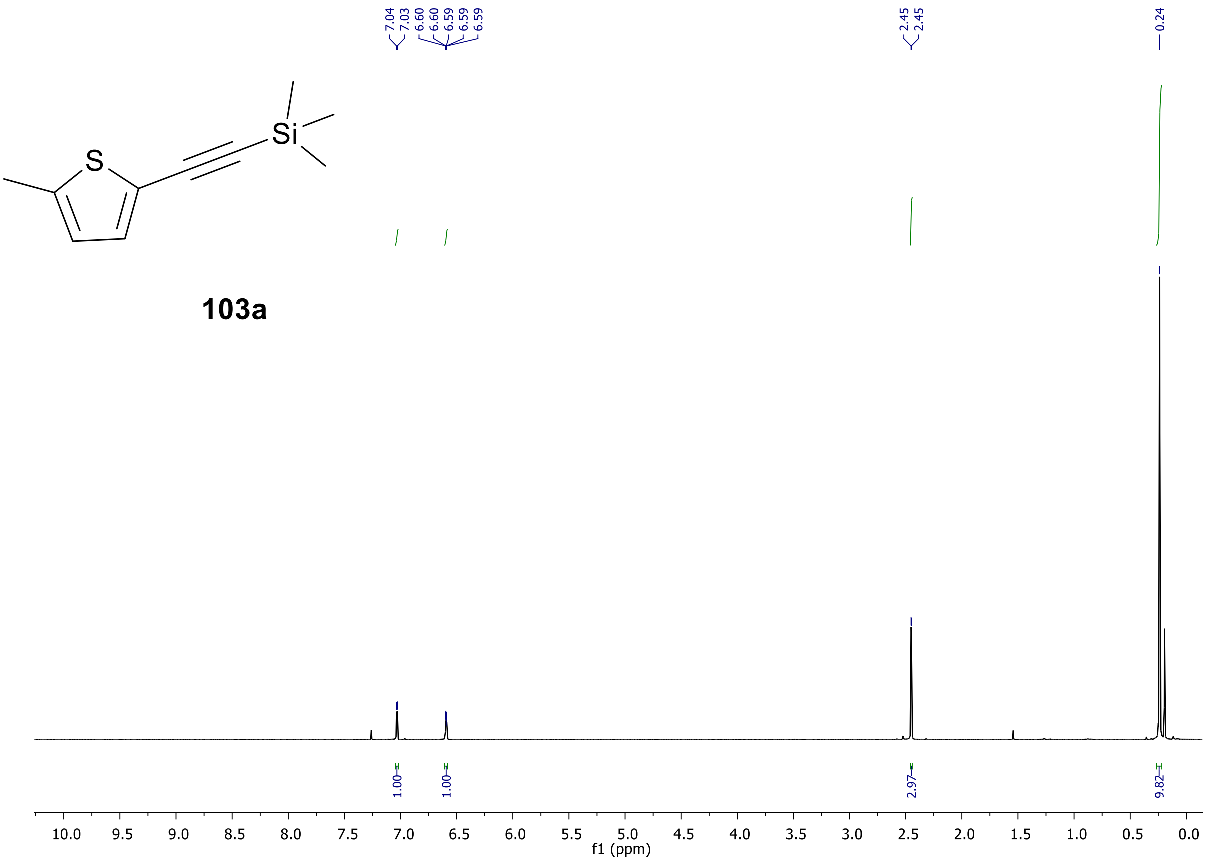
85


136.92
131.80
128.70
128.39
128.12
127.97
126.79
123.83
87.66
82.81
25.90
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

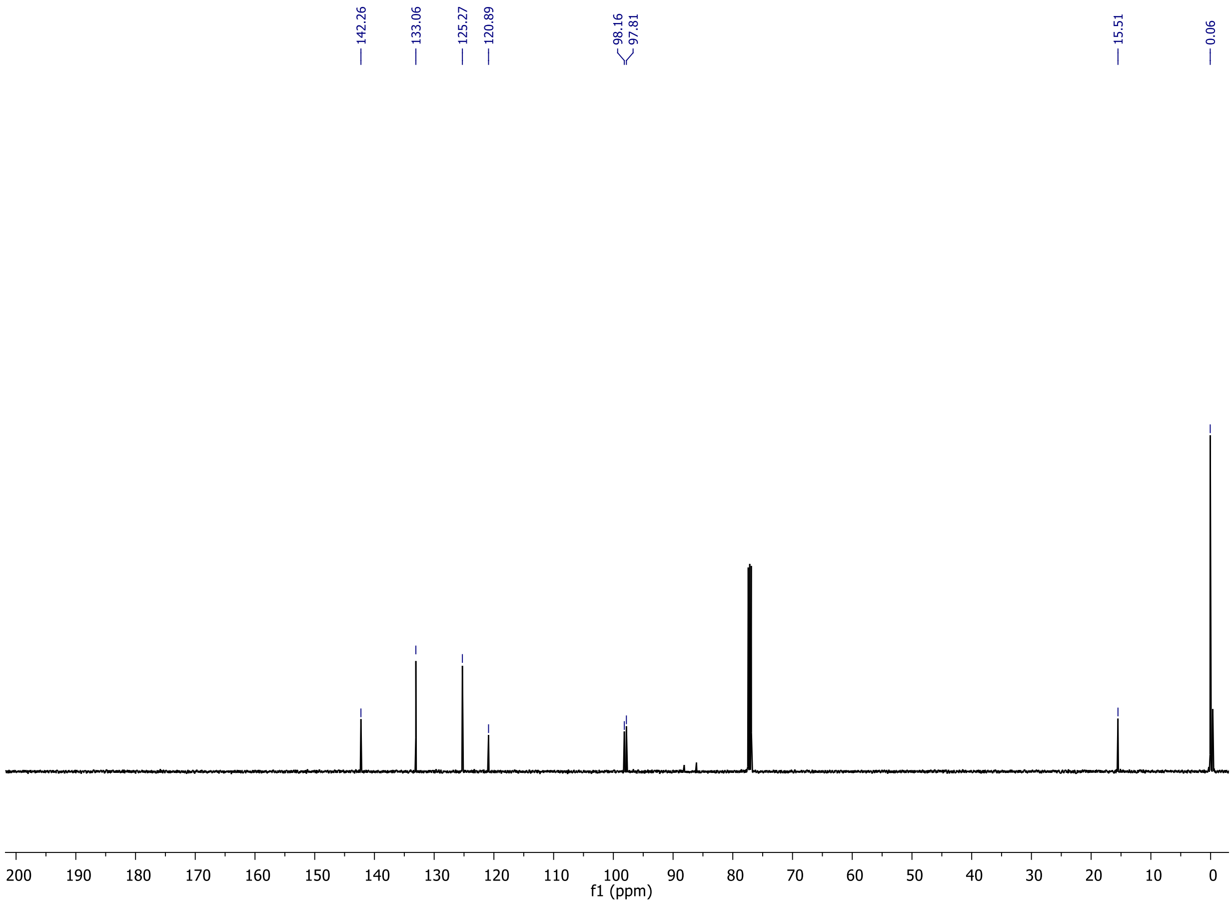

S
Si
7.24
7.23
7.23
7.23
6.96
6.95
6.95
6.95
6.95
6.94
0.25
1.96
1.00
9.11
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

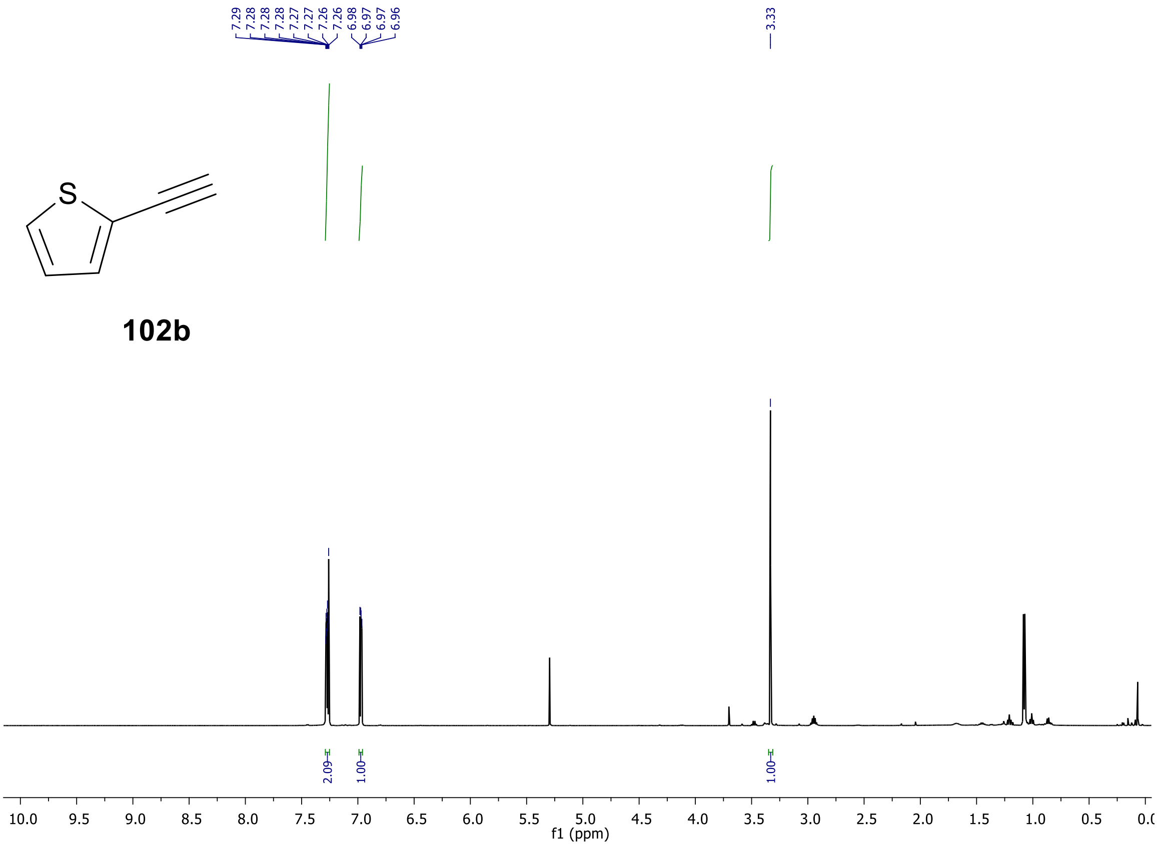
102a


132.75
127.41
126.98
123.37
98.86
97.66
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


S
Si
7.04
7.03
6.60
6.60
6.59
6.59
6.59
2.45
2.45
0.24
1.00
1.00
2.97
9.82
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)

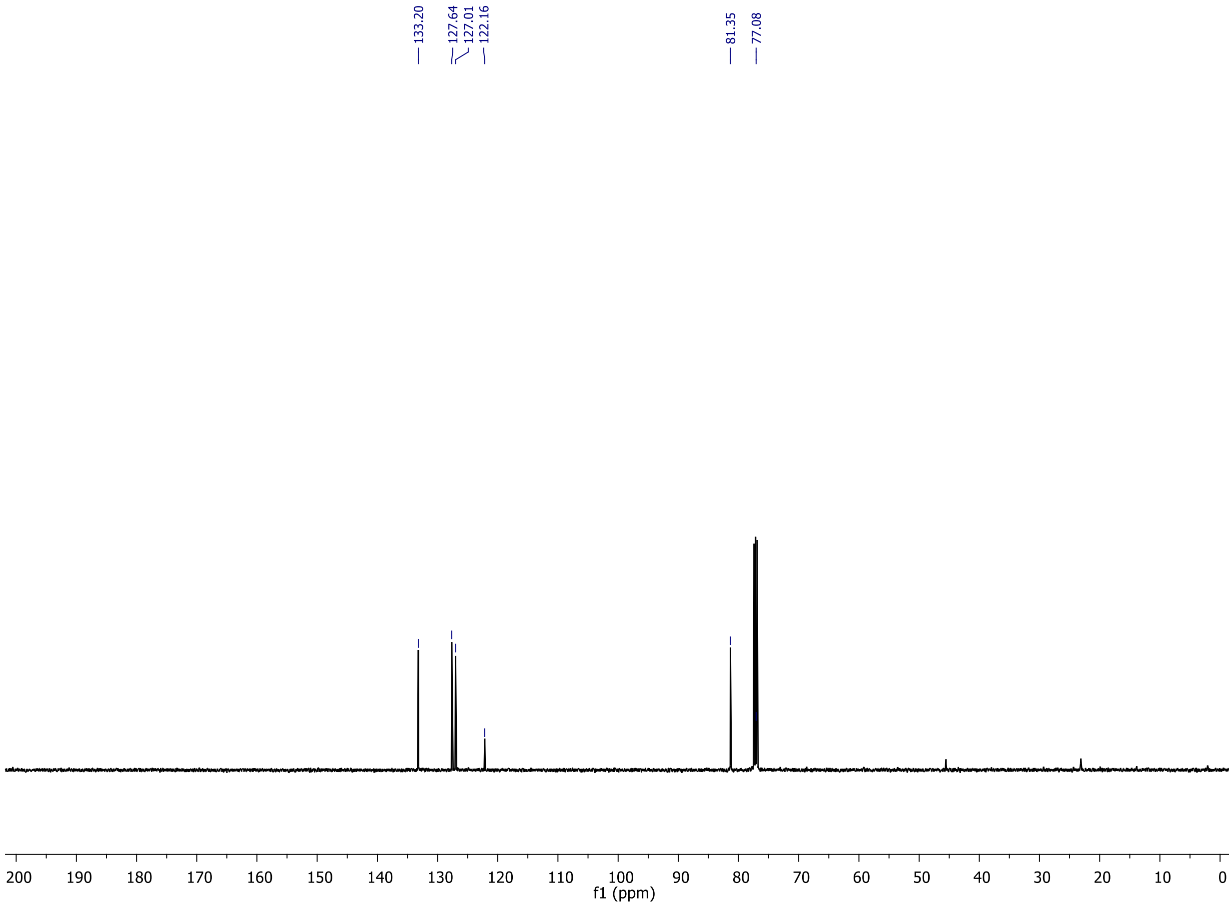
103a


142.26
133.06
125.27
120.89
98.16
97.81
15.51
0.06
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

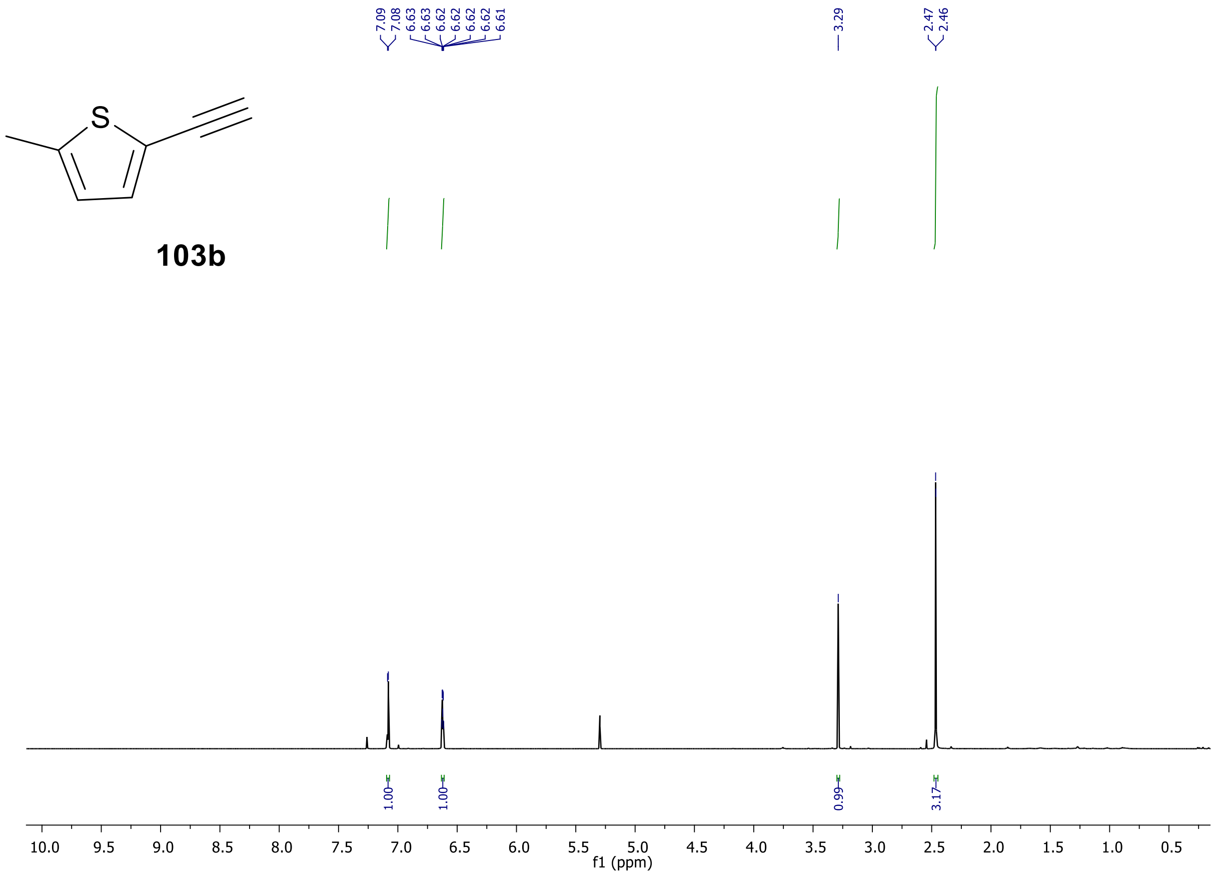


102b

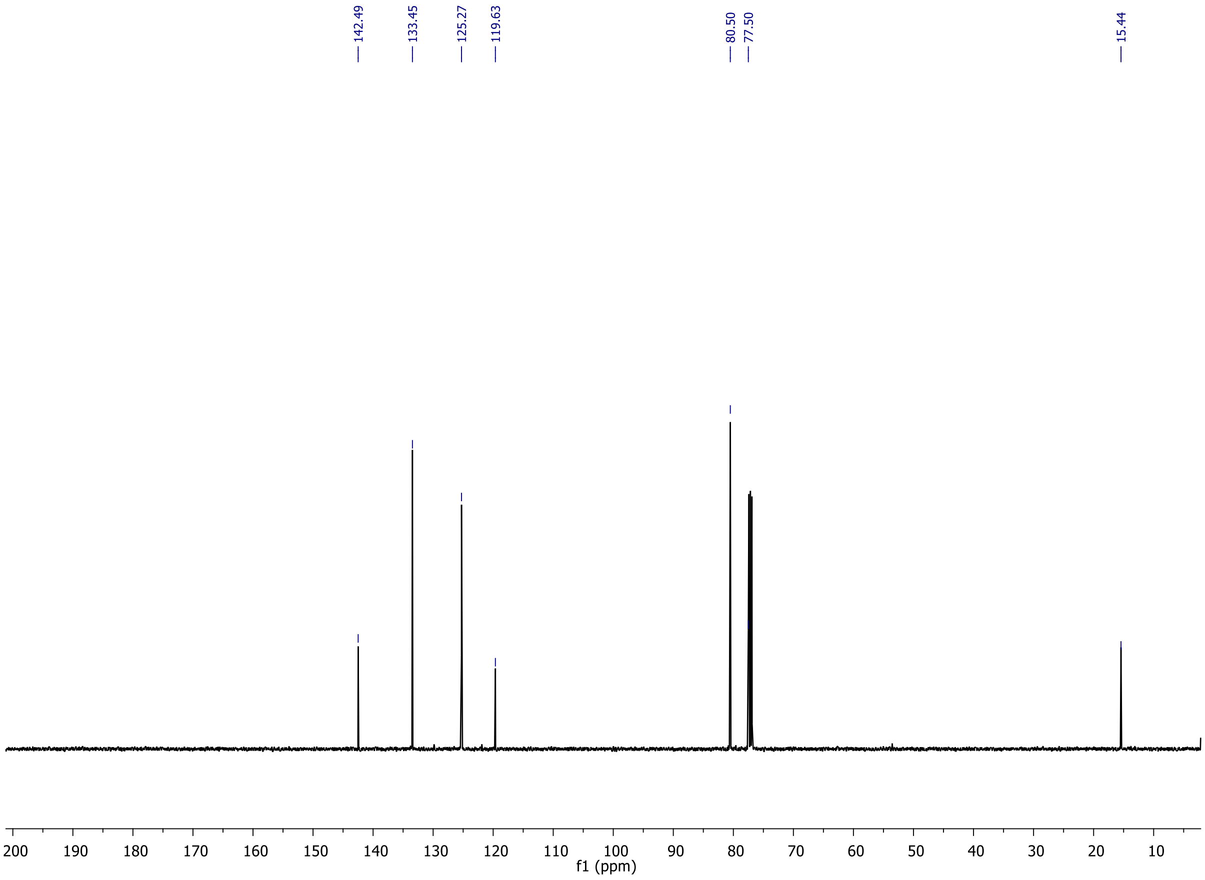
7.29
7.28
7.28
7.28
7.27
7.27
7.26
7.26
6.98
6.97
6.97
6.96
3.33
S
2.09
1.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.(
f1 (ppm)

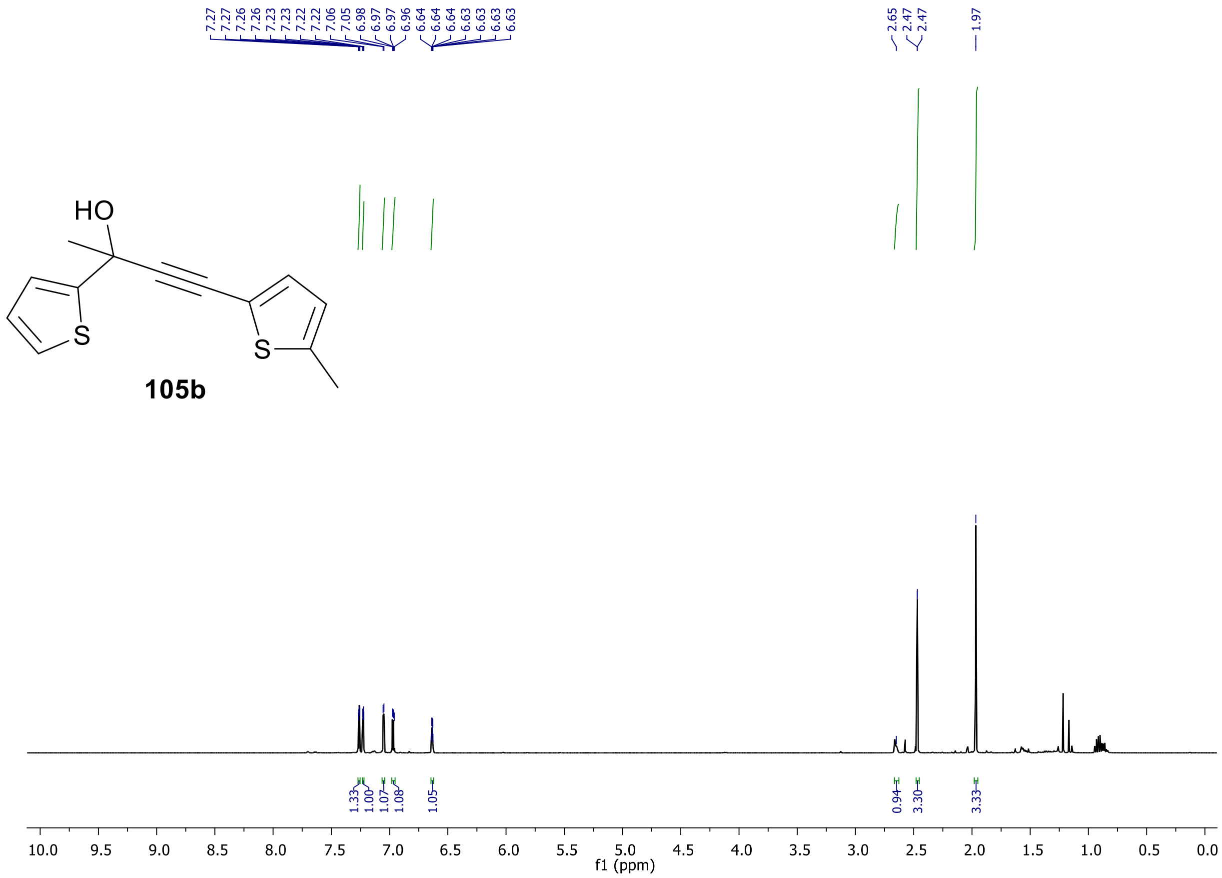


133.20
127.64
127.01
122.16
81.35
77.08
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

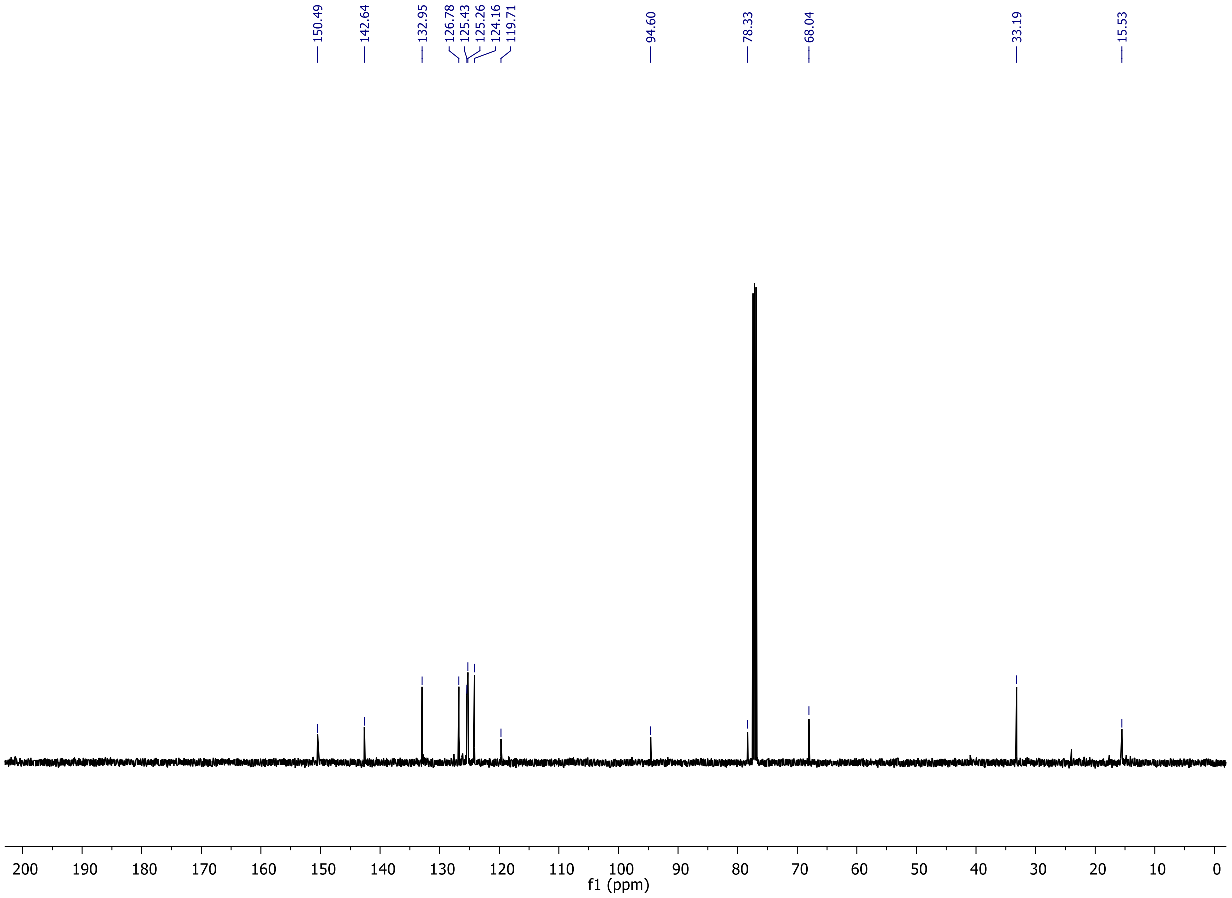

S
7.09
7.08
6.63
6.63
6.62
6.62
6.62
6.62
6.61
3.29
2.47
2.46
1.00
1.00
0.99
3.17
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

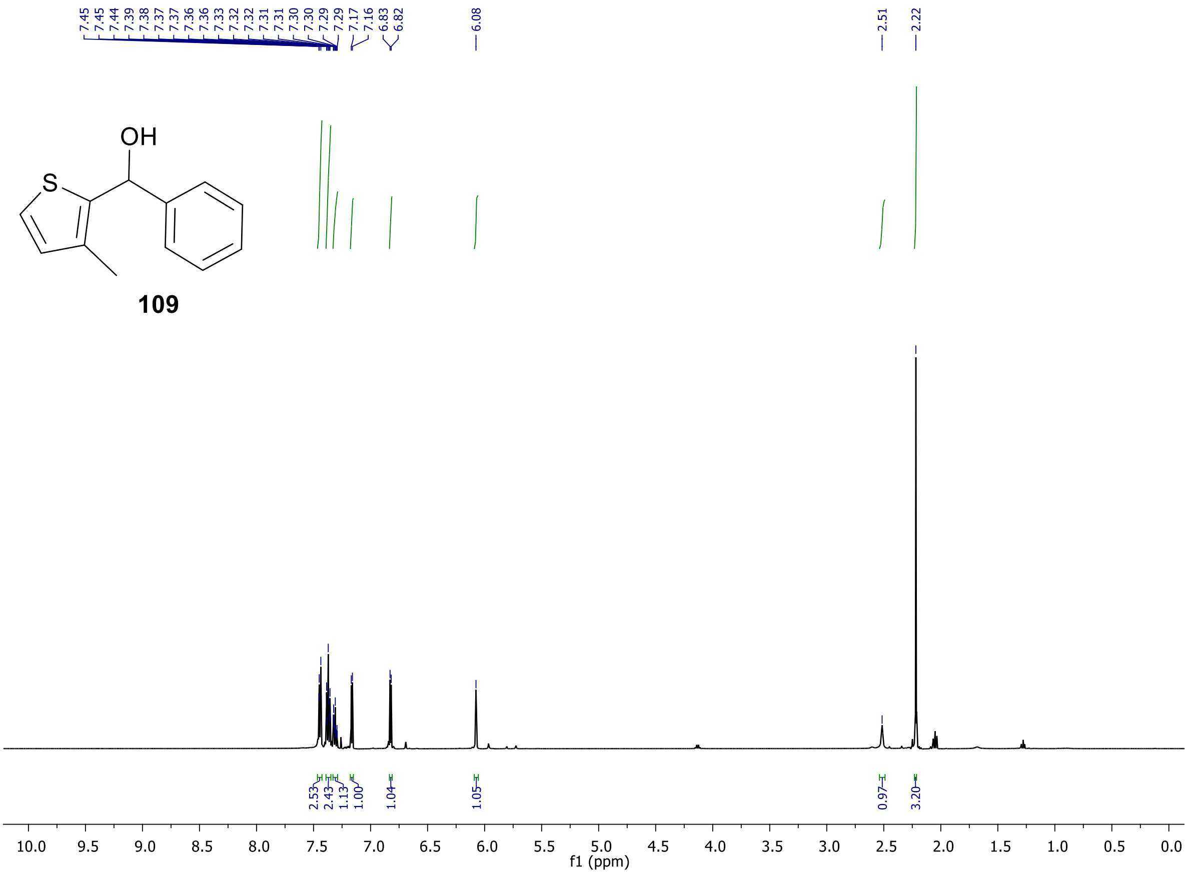
103b


142.49
133.45
125.27
119.63
80.50
77.50
15.44
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

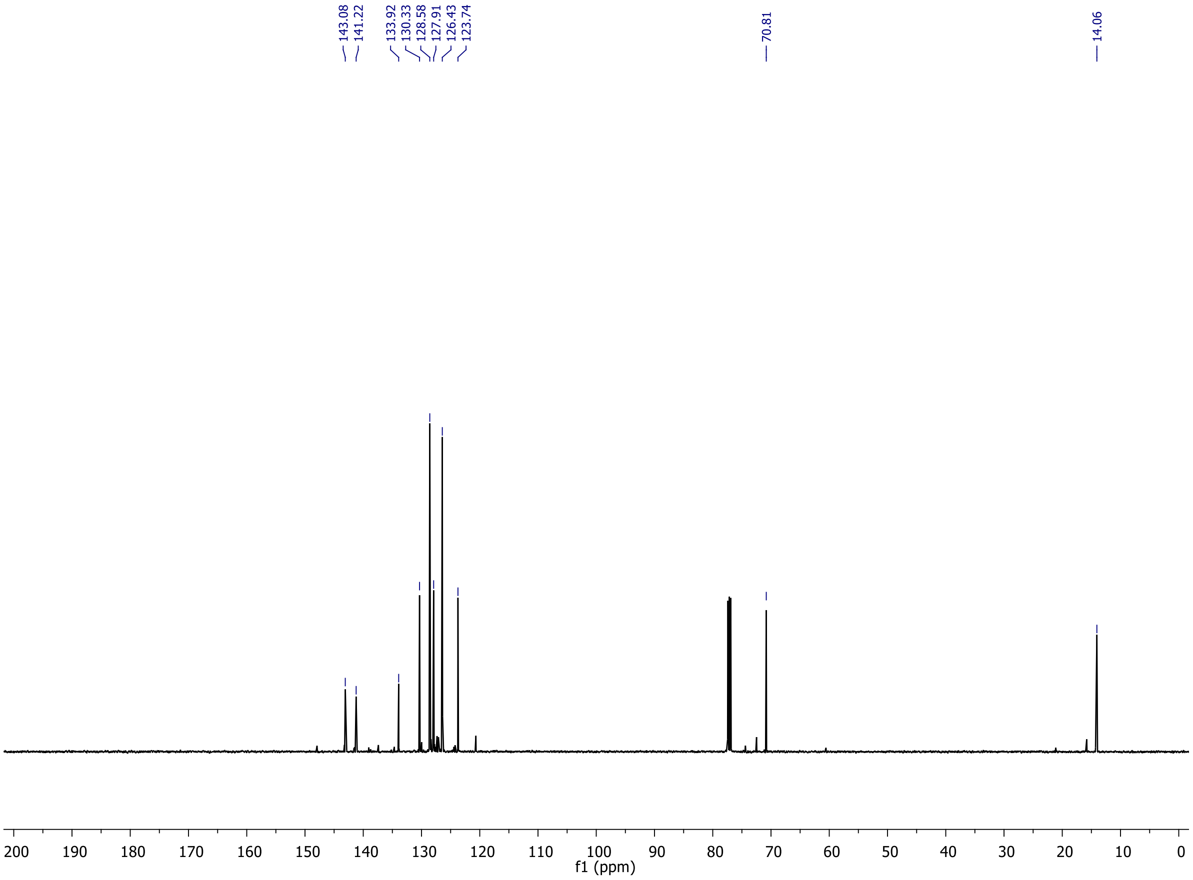

7.27
7.27
7.26
7.26
7.23
7.23
7.22
7.22
7.06
7.05
6.98
6.97
6.97
6.96
6.64
6.64
6.64
6.63
6.63
6.63
6.63
2.65
2.47
2.47
1.97
HO
S
S
1.33
1.00
1.07
1.08
1.05
0.94
3.30
3.33
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

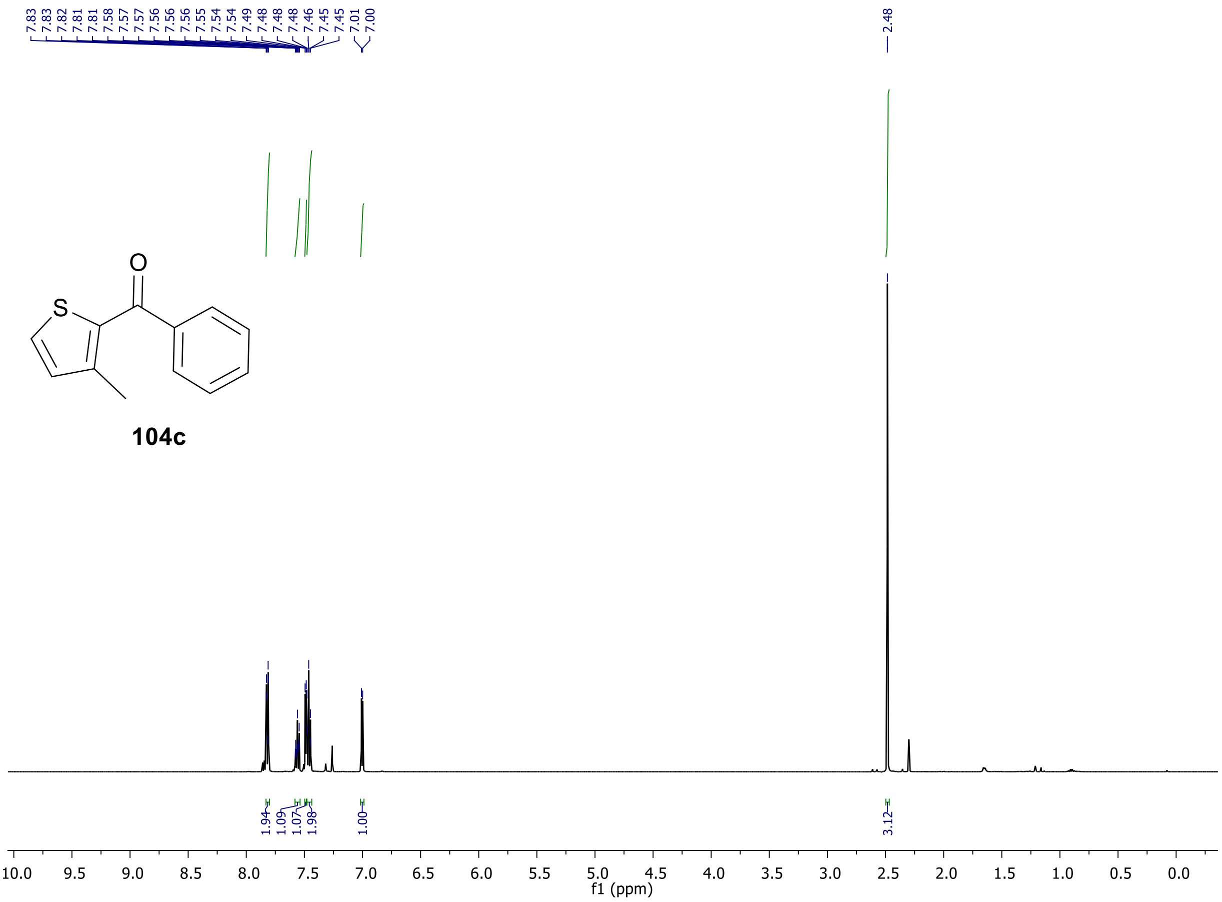
105b

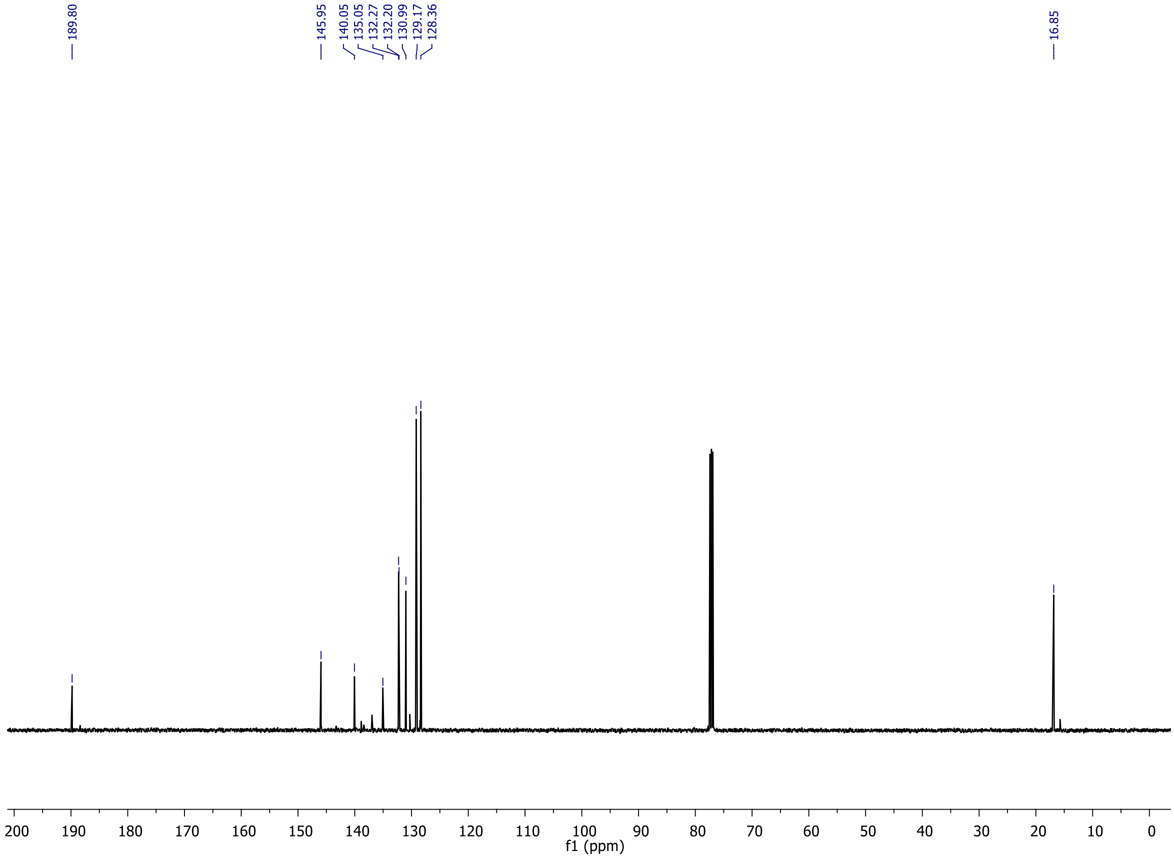

150.49
142.64
132.95
126.78
125.43
125.26
124.16
119.71
94.60
78.33
68.04
33.19
15.53
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

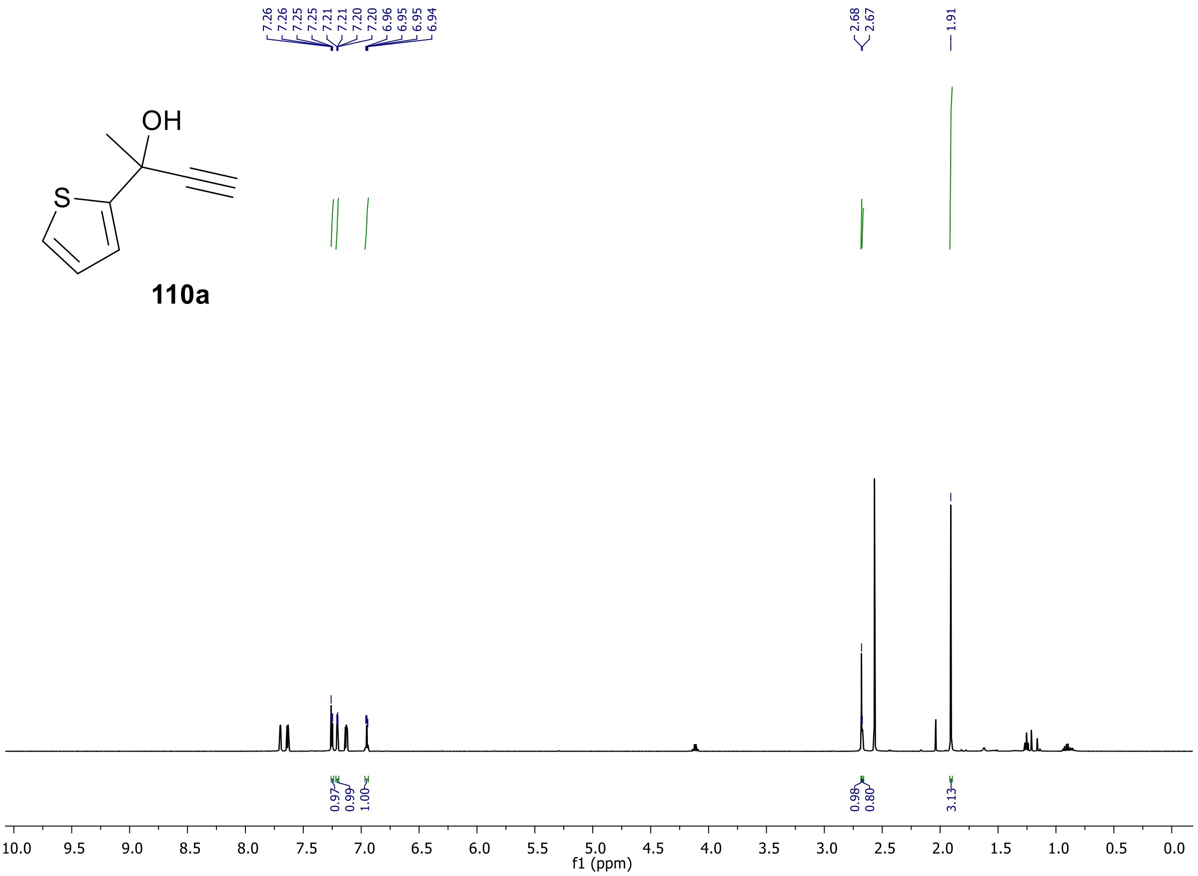

7.45
7.45
7.44
7.39
7.38
7.37
7.37
7.36
7.36
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.29
7.17
7.16
6.83
6.82
6.08
2.51
2.22
OH
S
2.53
2.43
1.13
1.00
1.04
1.05
0.97
3.20
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

109

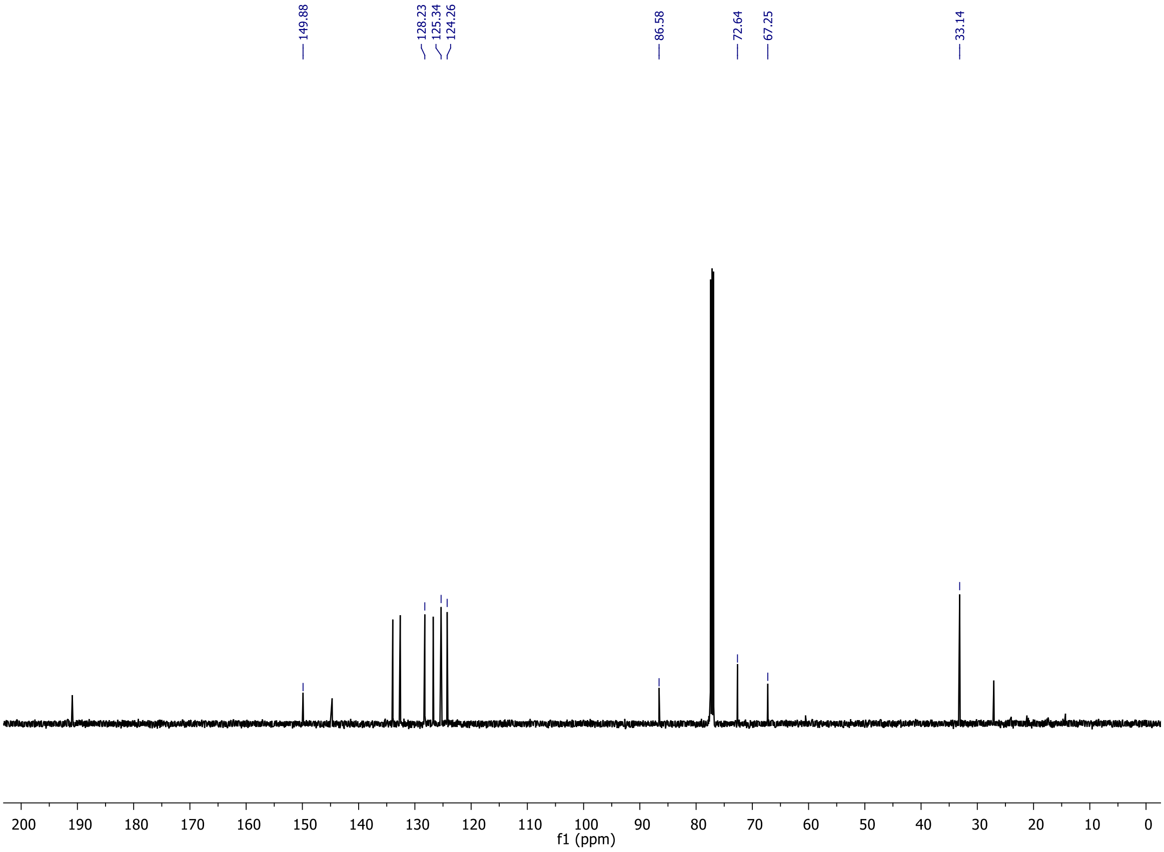

143.08
141.22
133.92
130.33
128.58
127.91
126.43
123.74
70.81
14.06
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

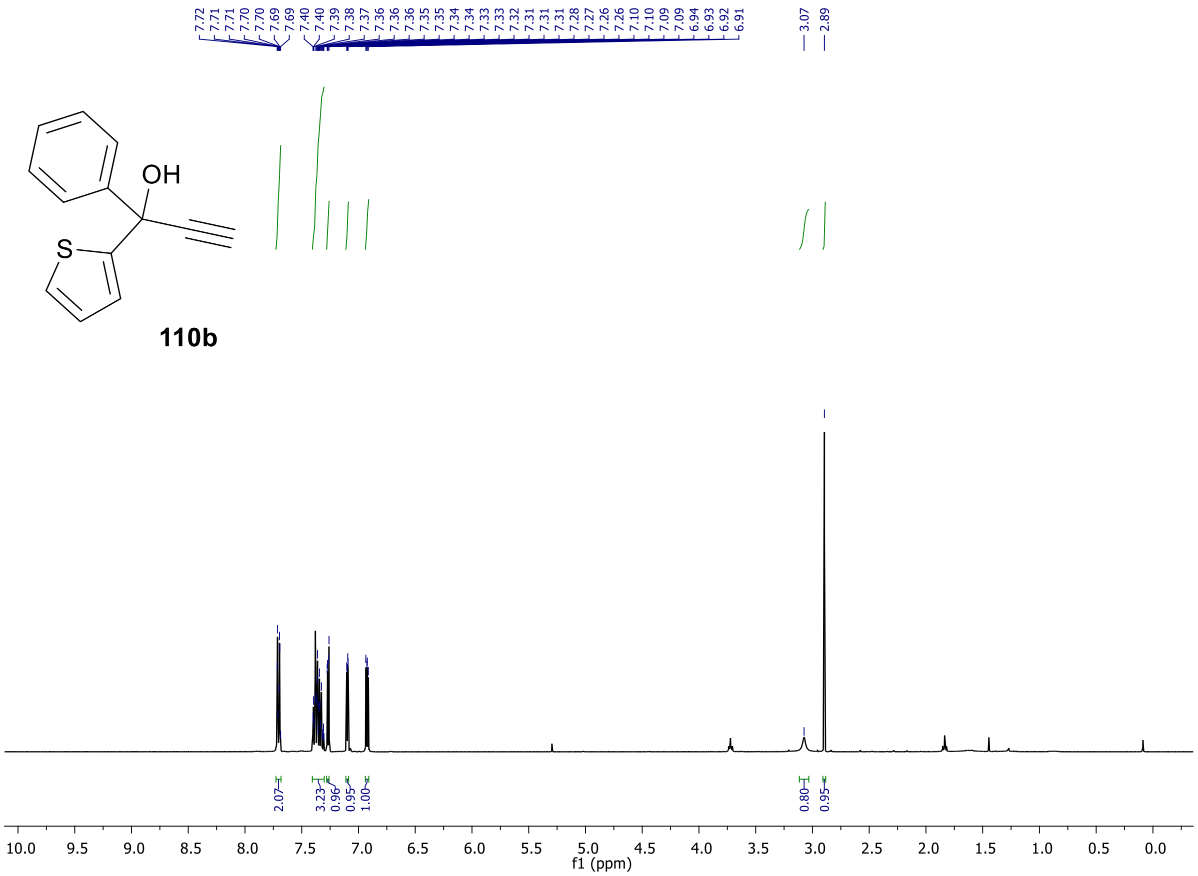

104c
7.83
7.83
7.82
7.81
7.81
7.58
7.57
7.57
7.56
7.56
7.55
7.54
7.54
7.49
7.48
7.48
7.46
7.45
7.45
7.01
7.00
2.48
S
O
1.94
1.09
1.07
1.98
1.00
3.12
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


189.80
145.95
140.05
135.05
132.27
132.20
130.99
129.17
128.36
16.85
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

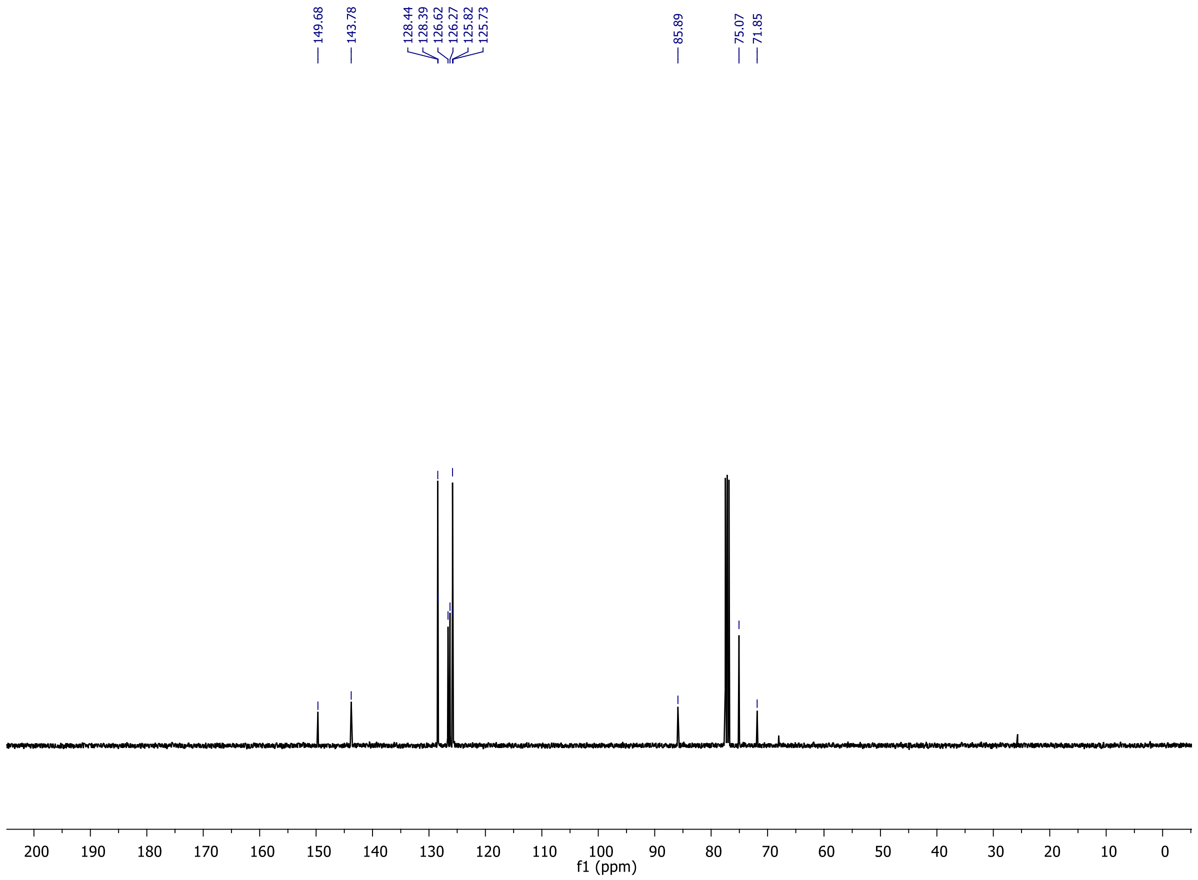

7.26
7.26
7.25
7.25
7.21
7.21
7.20
7.20
6.96
6.95
6.95
6.94
2.68
2.67
1.91
OH
S
0.97
0.99
1.00
0.98
0.80
3.13
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

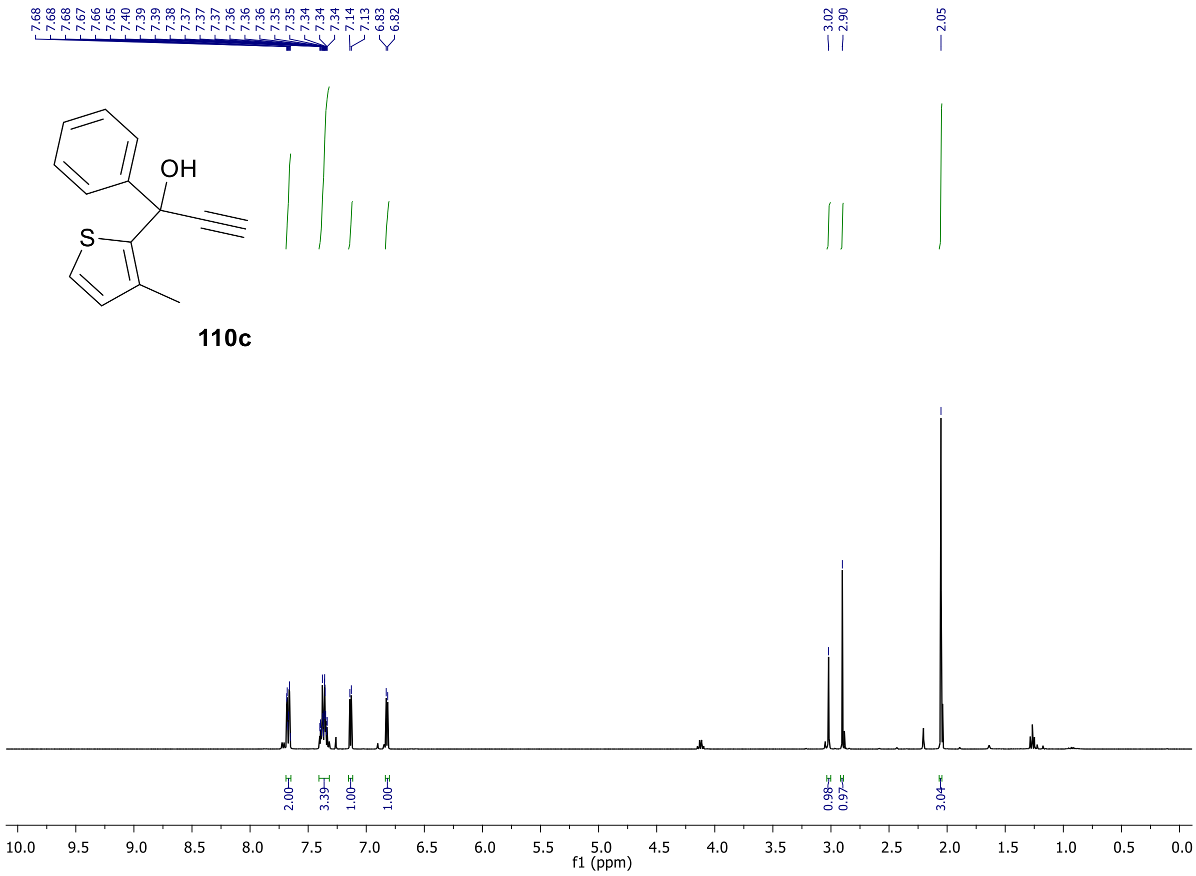
110a


149.88
128.23
125.34
124.26
86.58
72.64
67.25
33.14
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

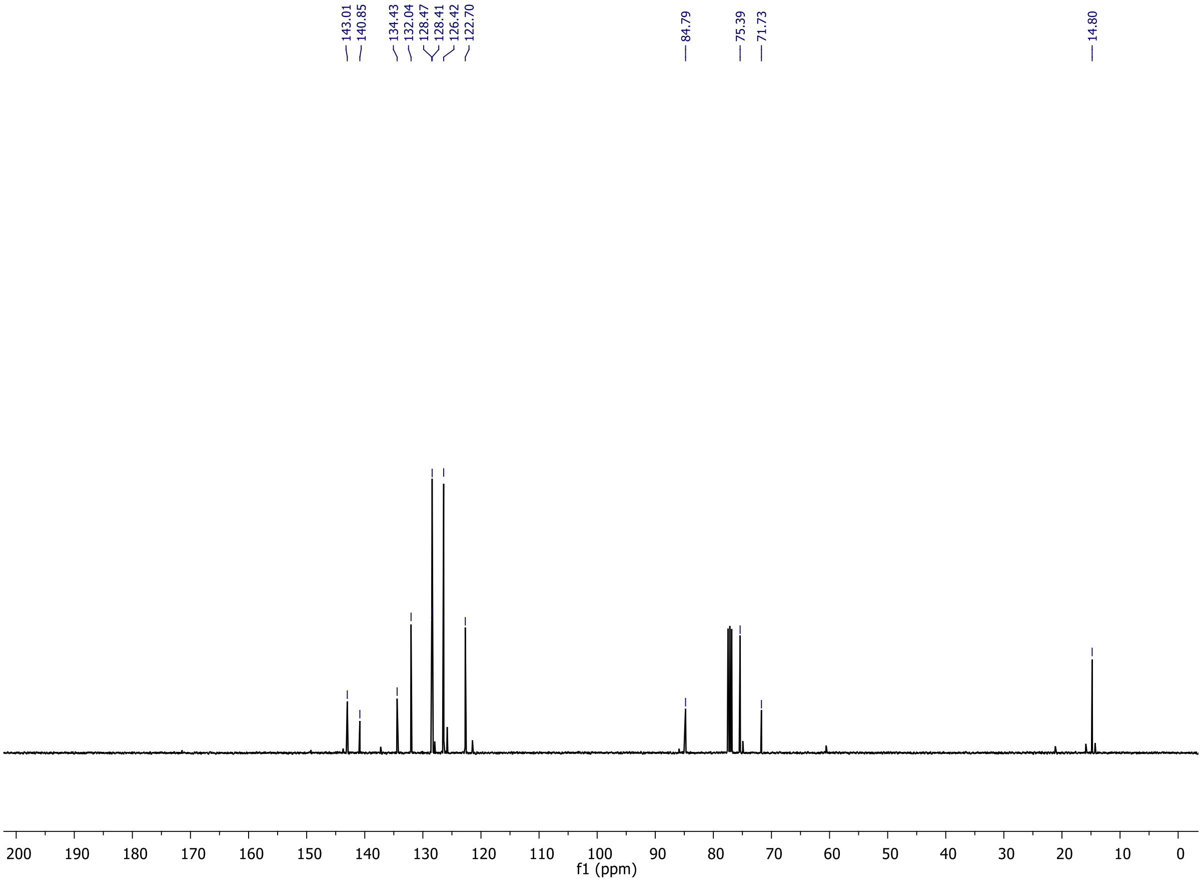

OH
S
7.72
7.71
7.71
7.70
7.70
7.69
7.69
7.40
7.40
7.39
7.38
7.37
7.36
7.36
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.31
7.31
7.28
7.27
7.26
7.26
7.10
7.10
7.09
7.09
6.94
6.93
6.92
6.91
3.07
2.89
2.07
3.23
0.96
0.95
1.00
0.80
0.95
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

110b


149.68
143.78
128.44
128.39
126.62
126.27
125.82
125.73
85.89
75.07
71.85
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.68
7.68
7.68
7.67
7.66
7.65
7.40
7.39
7.39
7.38
7.37
7.37
7.37
7.36
7.36
7.35
7.35
7.34
7.34
7.34
7.14
7.13
6.83
6.82
3.02
2.90
2.05
OH
S
2.00
3.39
1.00
1.00
0.98
0.97
3.04
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)

110c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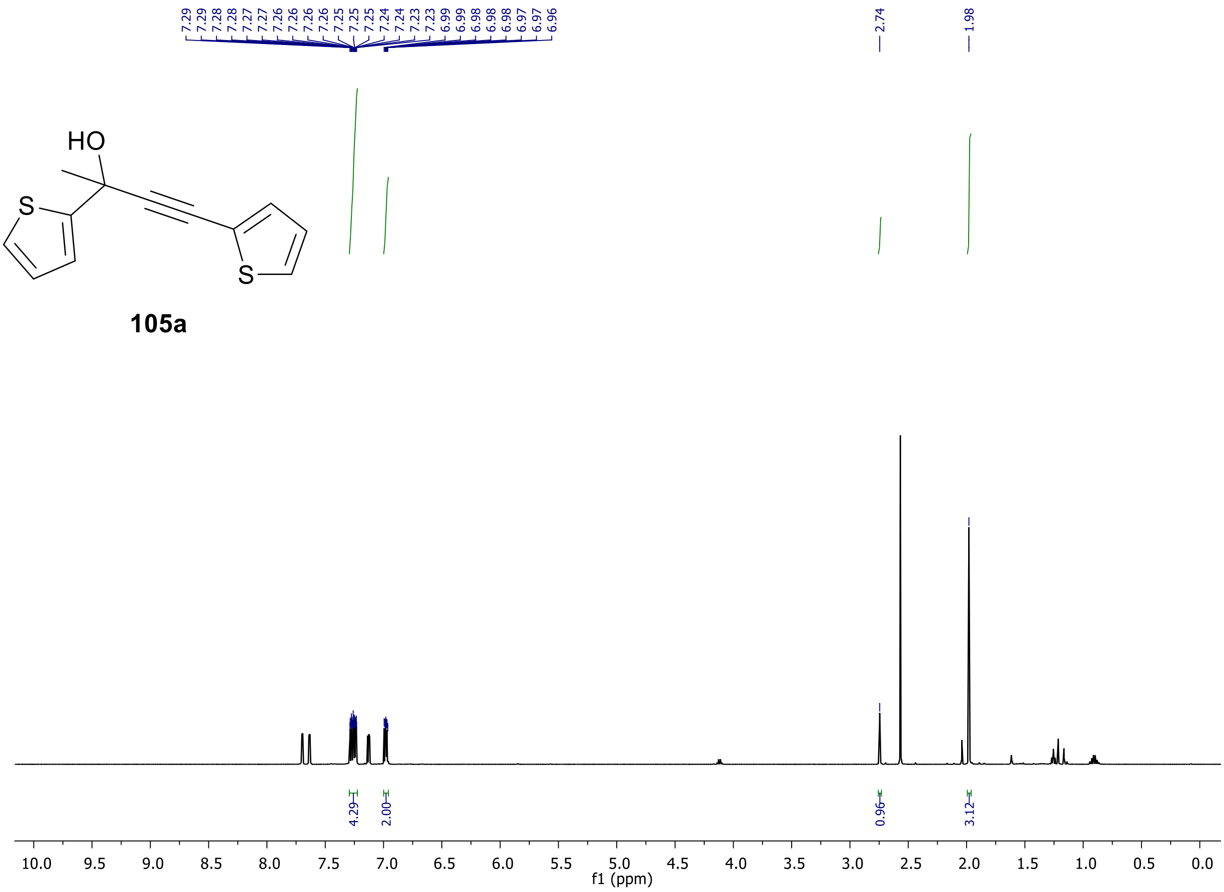
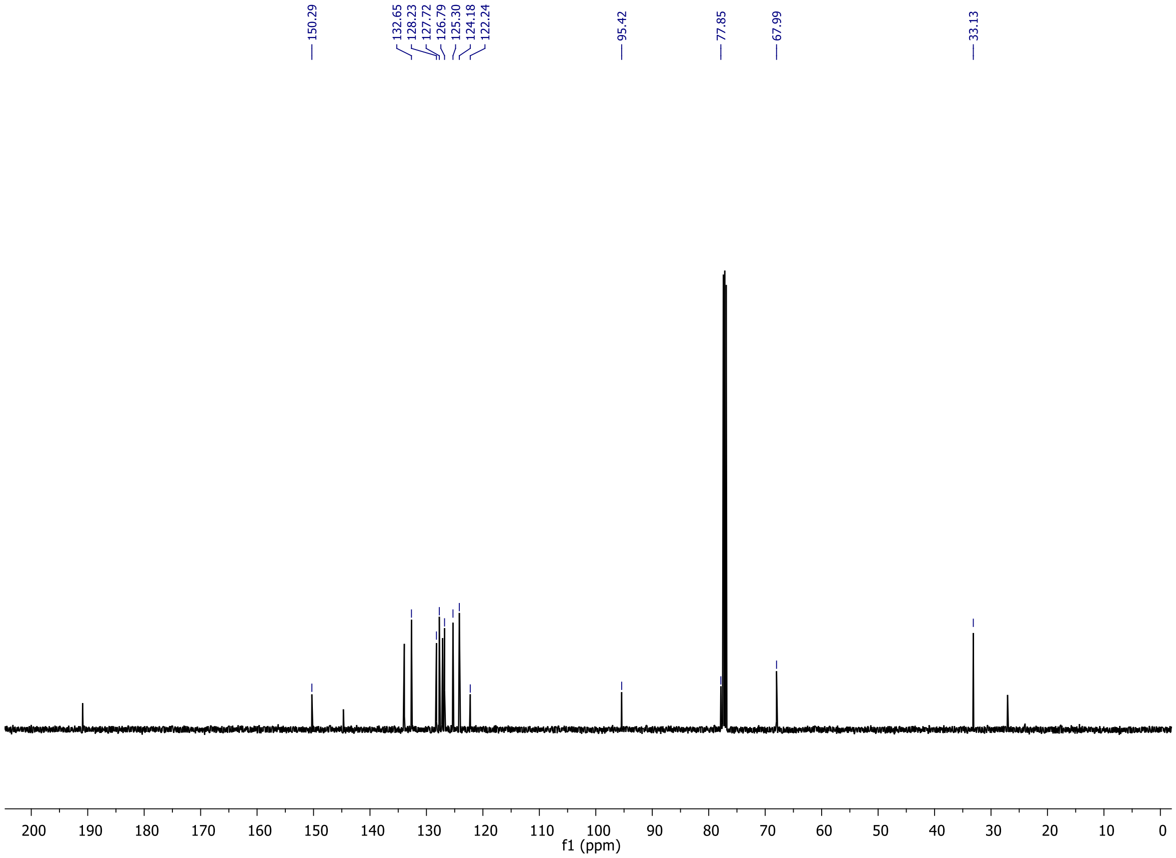
140.85
134.43
132.04
128.47
128.41
126.42
122.70
84.79
75.39
71.73
14.80
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

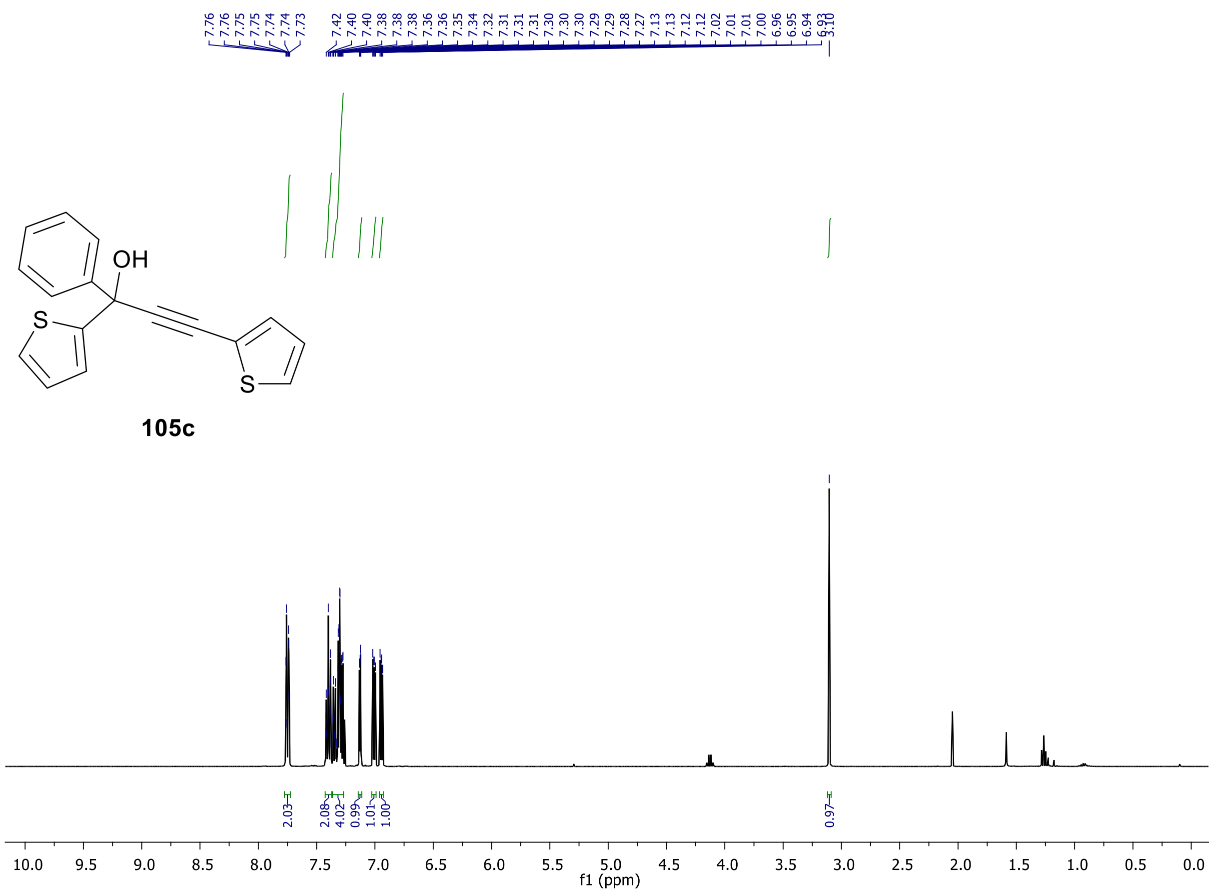


HO
S
S

105a

7.29
7.29
7.28
7.28
7.27
7.27
7.26
7.26
7.26
7.26
7.25
7.25
7.25
7.24
7.24
7.23
7.23
6.99
6.99
6.98
6.98
6.98
6.97
6.97
6.96
2.74
1.98
4.29
2.00
0.96
3.12
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)


150.29
132.65
128.23
127.72
126.79
125.30
124.18
122.24
95.42
77.85
67.99
33.13
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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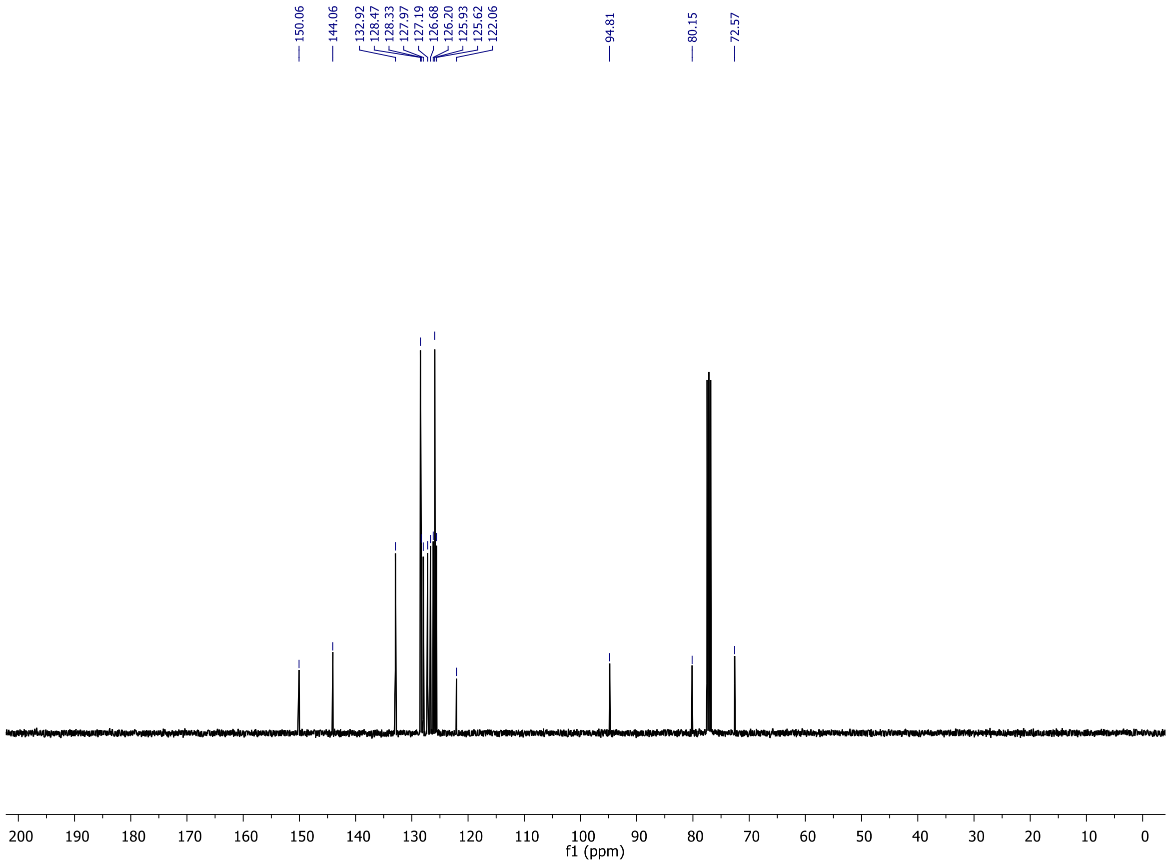
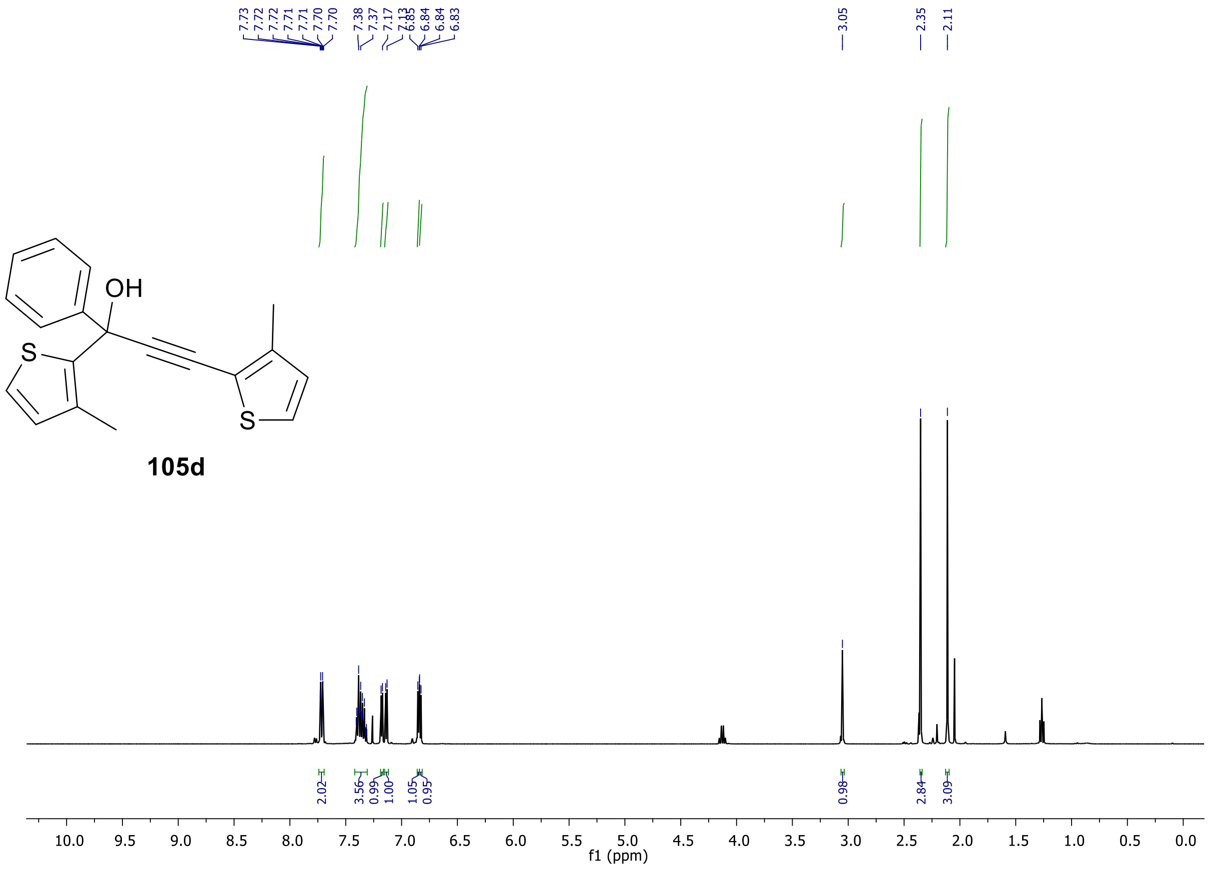
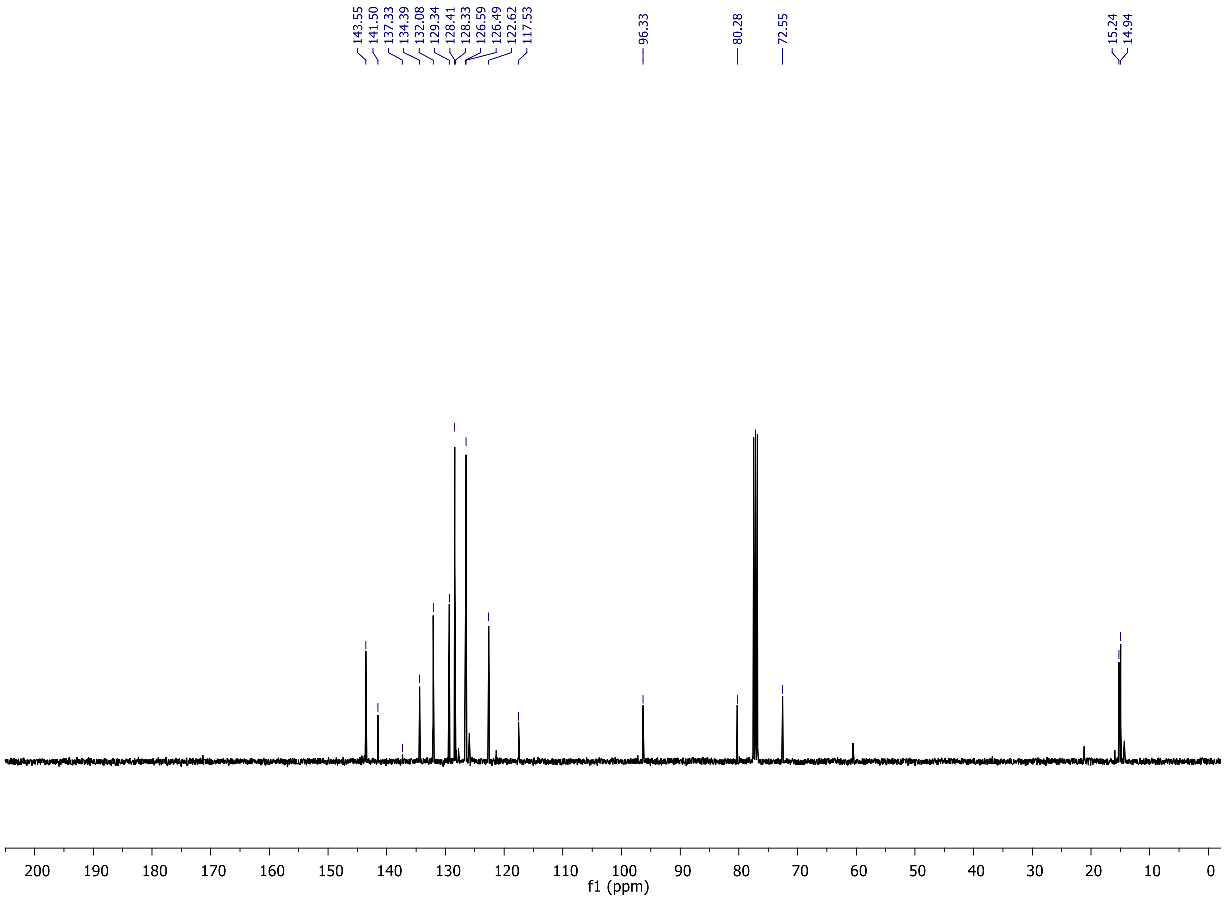
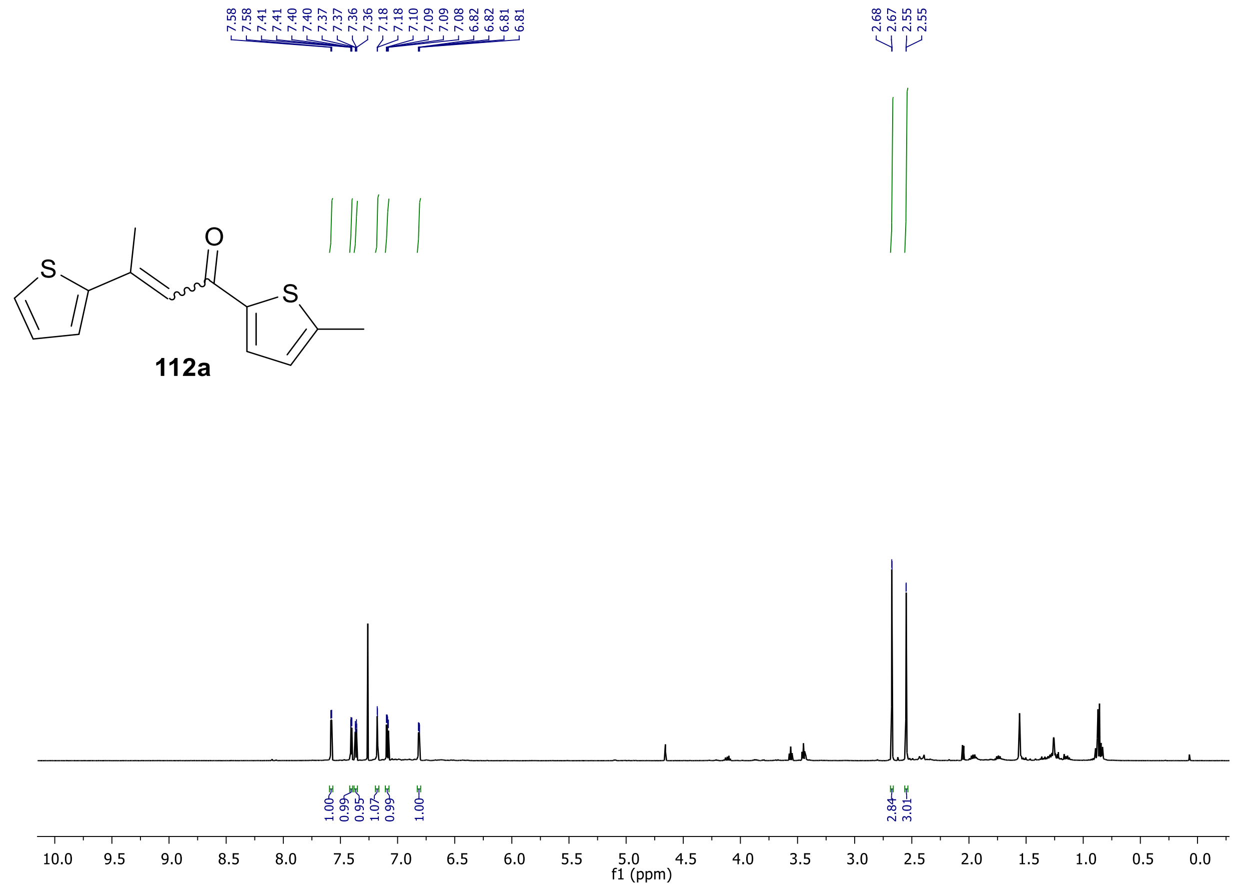
7.76
7.75
7.75
7.74
7.74
7.73
7.42
7.40
7.40
7.38
7.38
7.38
7.36
7.36
7.35
7.34
7.32
7.31
7.31
7.31
7.30
7.30
7.30
7.29
7.29
7.28
7.27
7.13
7.13
7.12
7.12
7.02
7.01
7.01
7.00
6.96
6.95
6.94
6.93
3.10
OH
S
S
105c
2.03
2.08
4.02
0.99
1.01
1.00
0.97
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


150.06
144.06
132.92
128.47
128.33
127.97
127.19
126.68
126.20
125.93
125.62
122.06
94.81
80.15
72.57
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.73
7.72
7.72
7.71
7.71
7.70
7.70
7.38
7.37
7.17
7.13
6.85
6.84
6.84
6.83
3.05
2.35
2.11
OH
S
S
2.02
3.56
0.99
1.00
1.05
0.95
0.98
2.84
3.09
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)

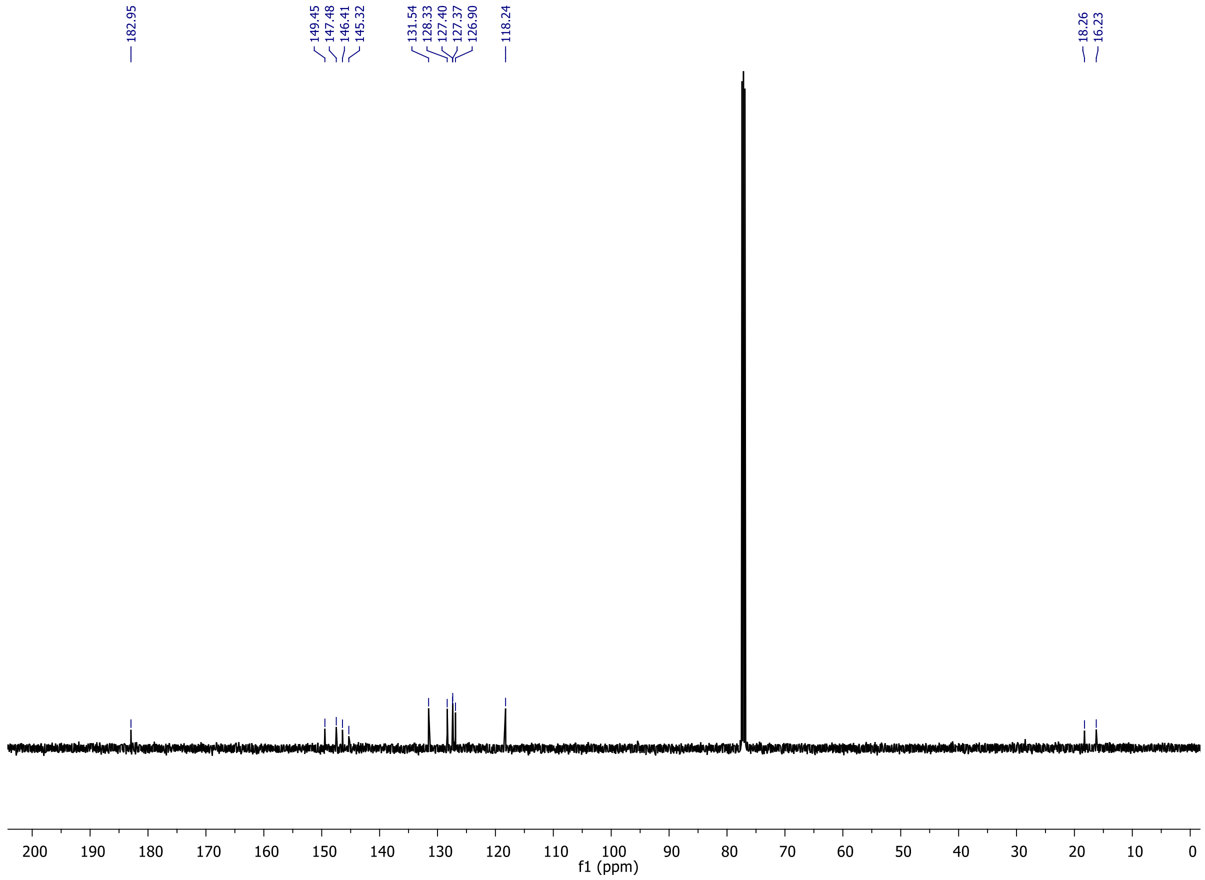
105d


143.55
141.50
137.33
134.39
132.08
129.34
128.41
128.33
126.59
126.49
122.62
117.53
96.33
80.28
72.55
15.24
14.94
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



112a

7.58
7.58
7.41
7.41
7.40
7.40
7.37
7.37
7.36
7.36
7.18
7.18
7.10
7.09
7.09
7.08
6.82
6.82
6.81
6.81
2.68
2.67
2.55
2.55
S
O
S
1.00
0.99
0.95
1.07
0.99
1.00
2.84
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)



182.95
149.45
147.48
146.41
145.32
131.54
128.33
127.40
127.37
126.90
118.24
18.26
16.23
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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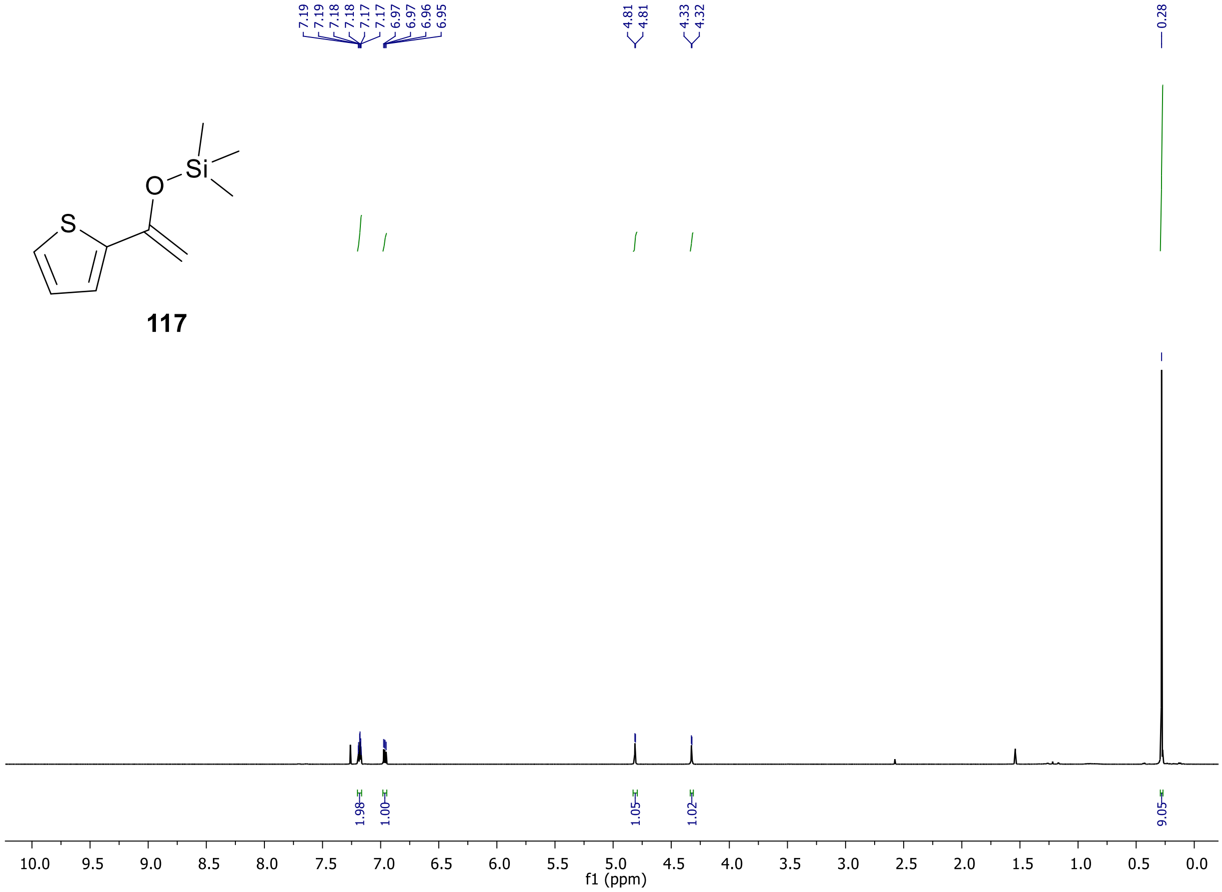
50
40
30
20
10
0
f1 (ppm)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7.18
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7.17
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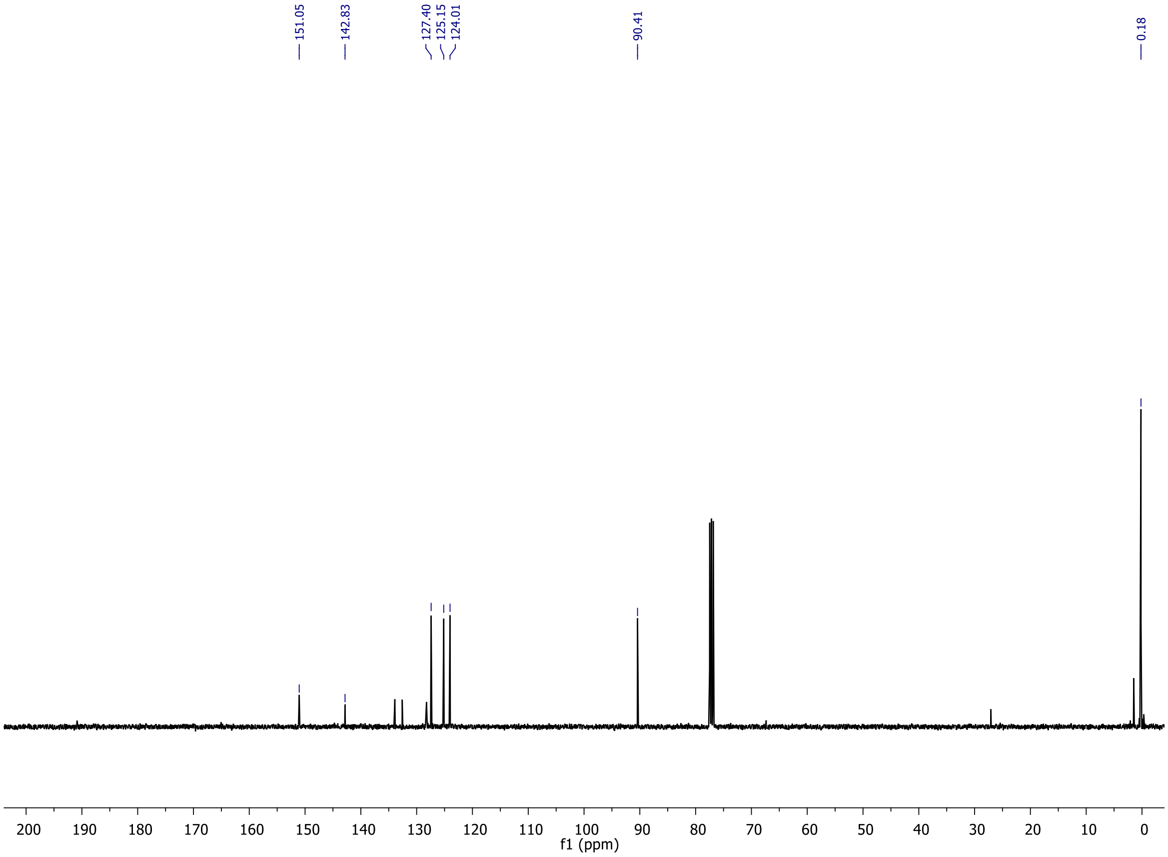
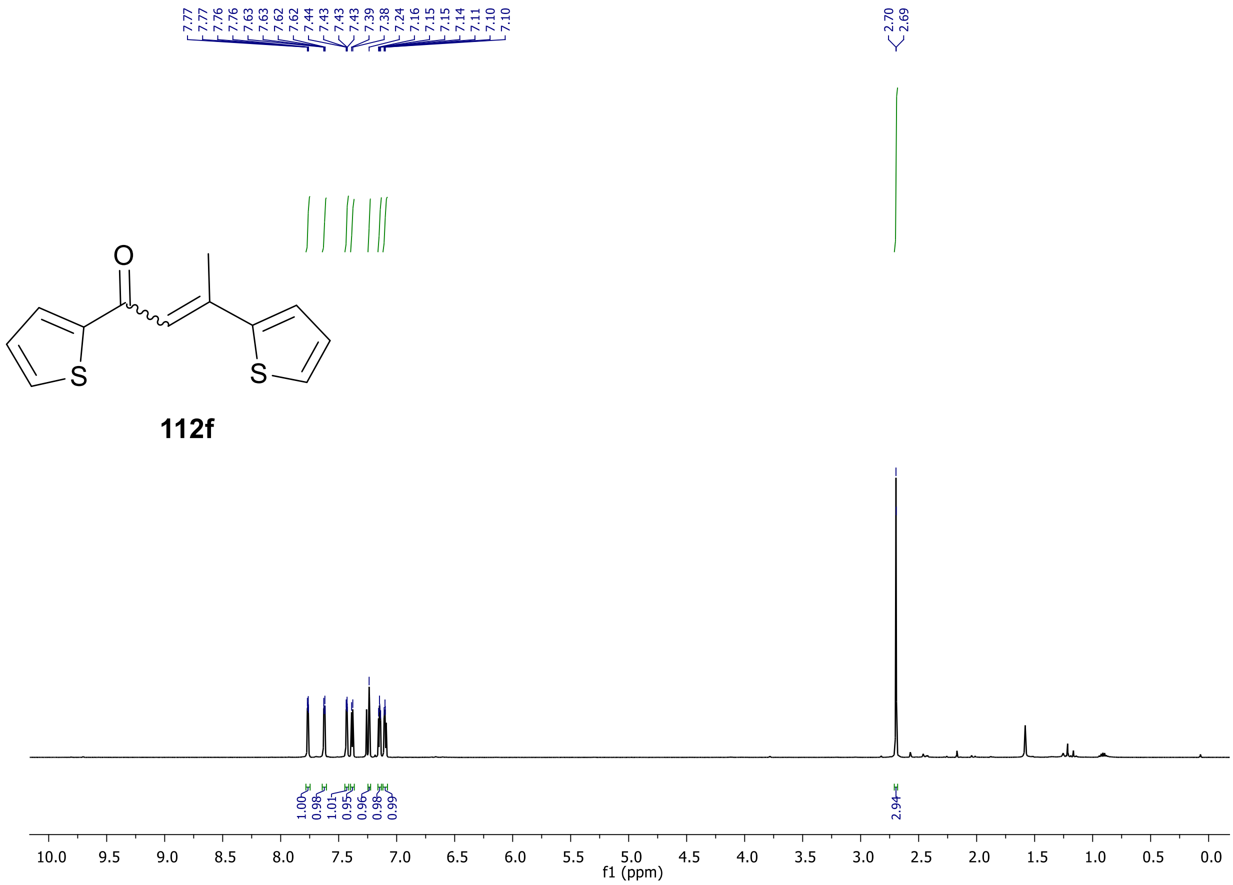
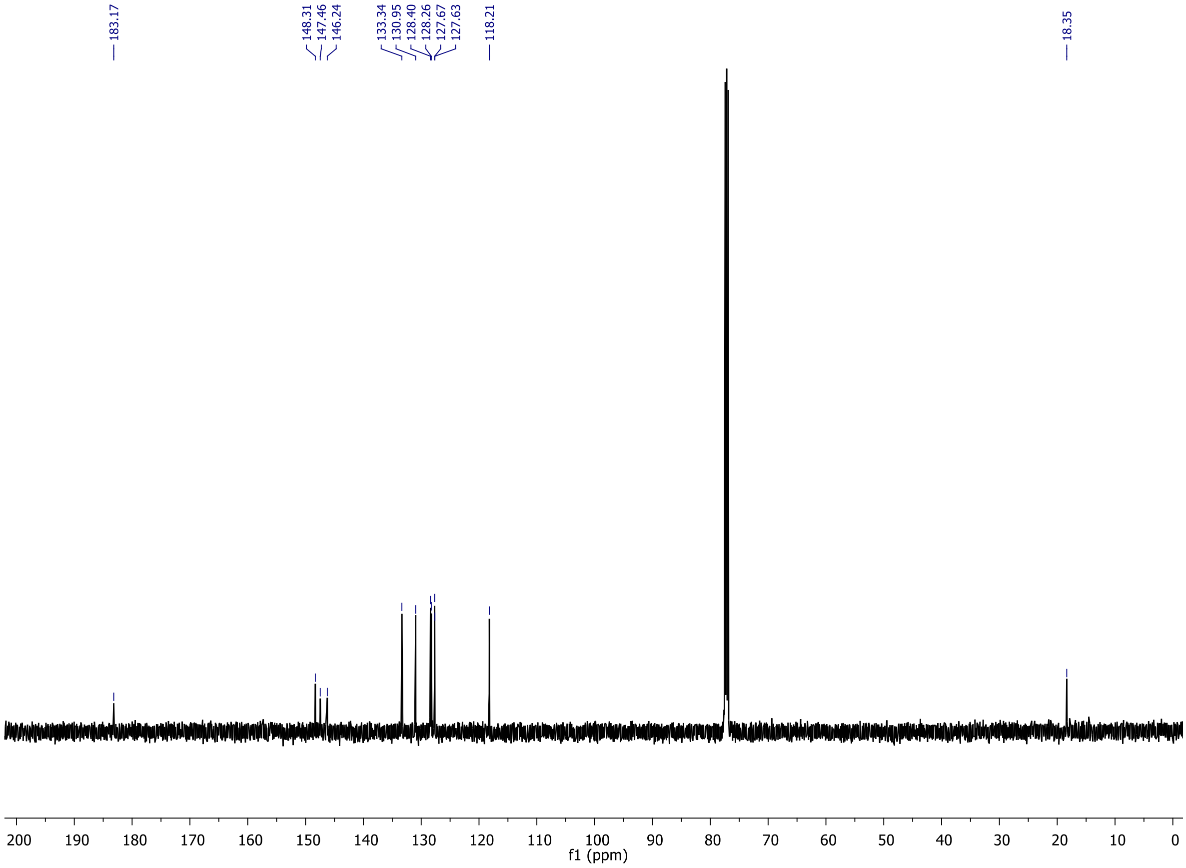
6.97
6.96
6.95
4.81
4.81
4.33
4.32
0.28
S
O
Si
1.98
1.00
1.05
1.02
9.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

117


151.05
142.83
127.40
125.15
124.01
90.41
0.18
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.77
7.77
7.76
7.63
7.63
7.62
7.62
7.44
7.43
7.43
7.43
7.39
7.38
7.24
7.16
7.15
7.15
7.14
7.11
7.10
7.10
2.70
2.69
O
S
S
1.00
0.98
1.01
0.95
0.96
0.98
0.99
2.94
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)

112f


183.17
148.31
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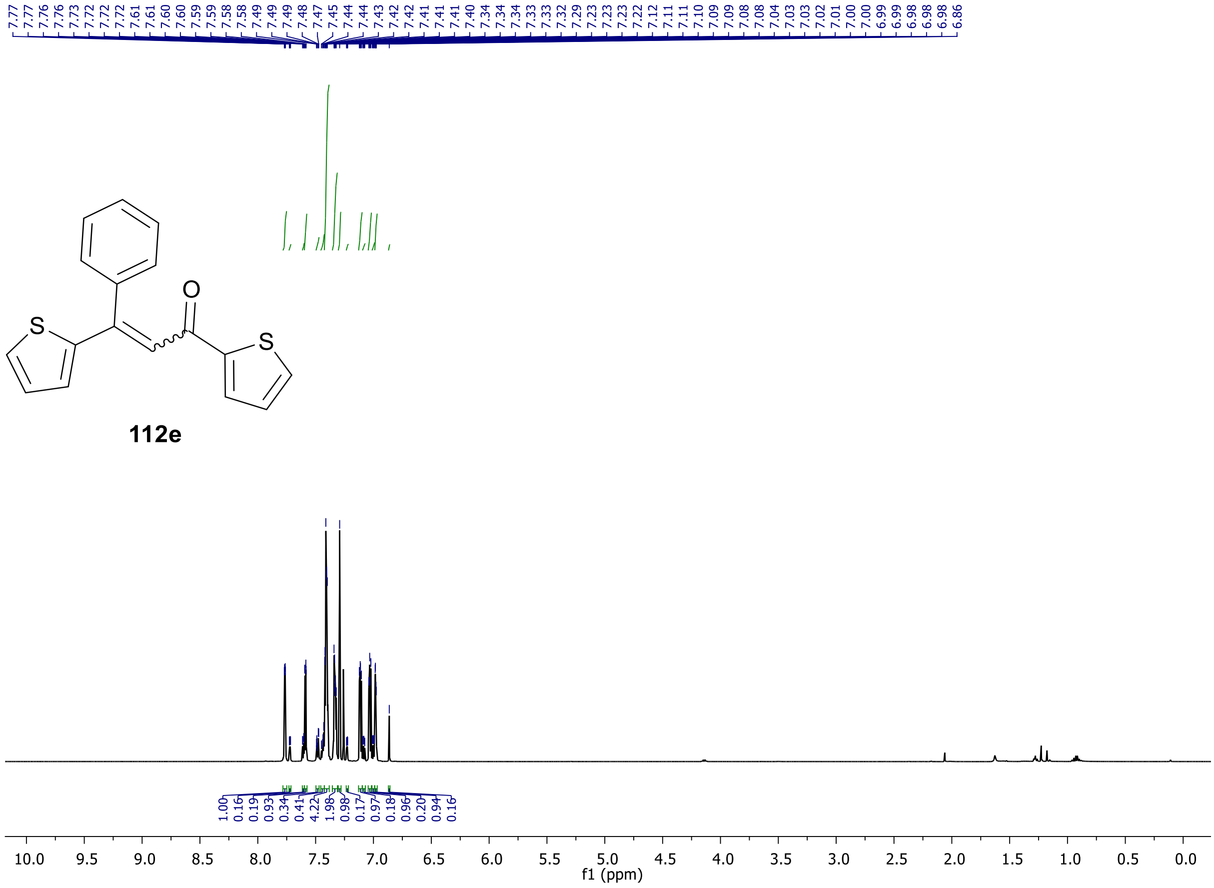
146.24
133.34
130.95
128.40
128.26
127.67
127.63
118.21
18.35
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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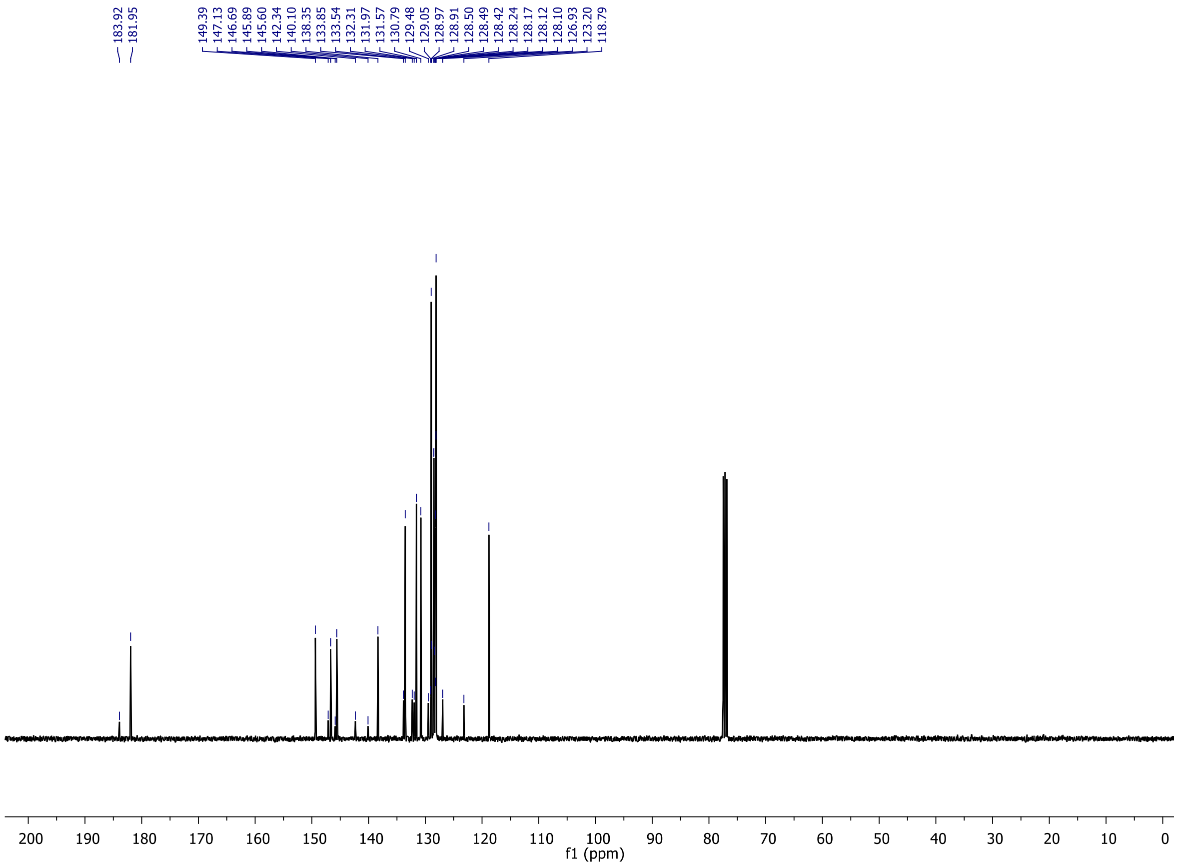
7.60
7.59
7.59
7.58
7.49
7.49
7.48
7.47
7.45
7.44
7.44
7.43
7.42
7.42
7.41
7.41
7.41
7.40
7.34
7.34
7.34
7.33
7.32
7.29
7.23
7.23
7.23
7.22
7.12
7.11
7.10
7.09
7.09
7.08
7.04
7.03
7.03
7.02
7.01
7.00
6.99
6.99
6.98
6.98
6.98
6.86
O
S
S
1.00
0.16
0.19
0.93
0.34
0.41
4.22
1.98
0.98
0.17
0.97
0.18
0.96
0.20
0.94
0.16
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
f1 (ppm)

112e


183.92
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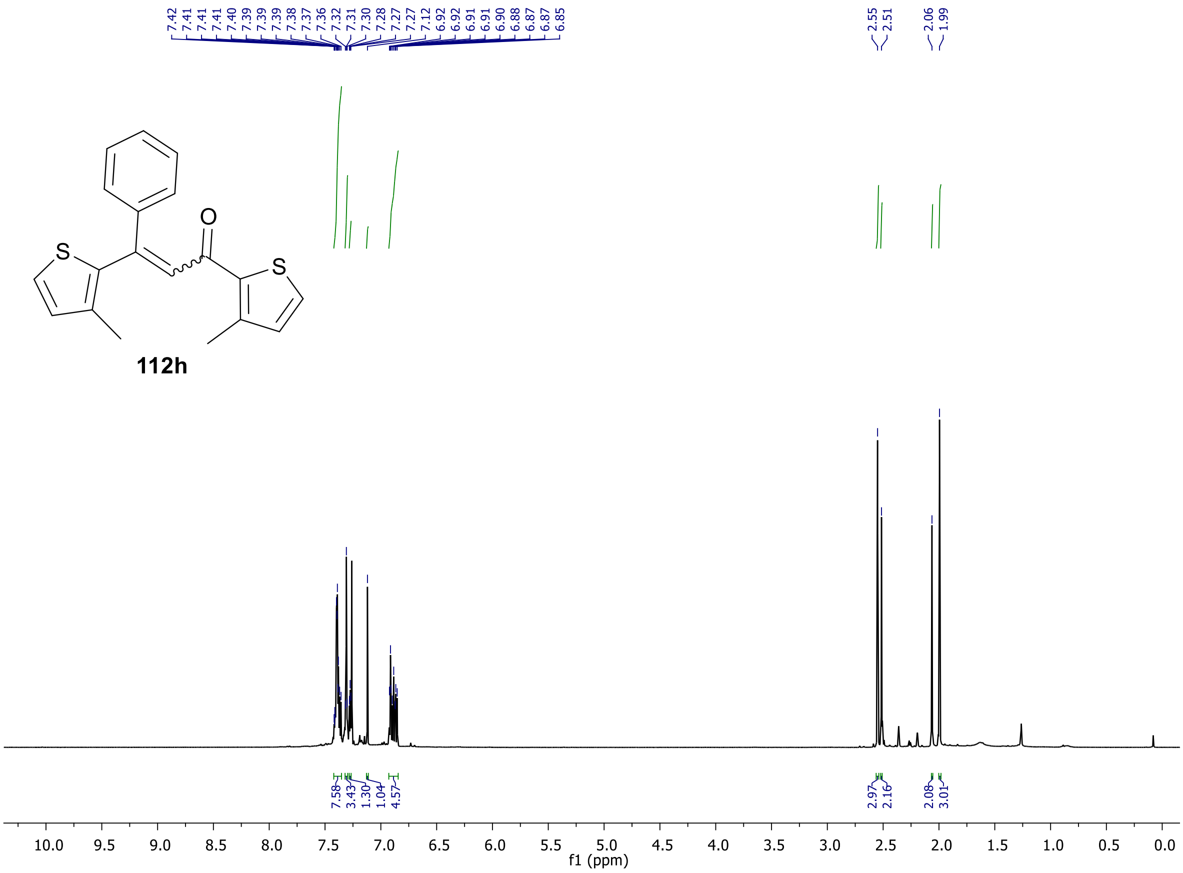
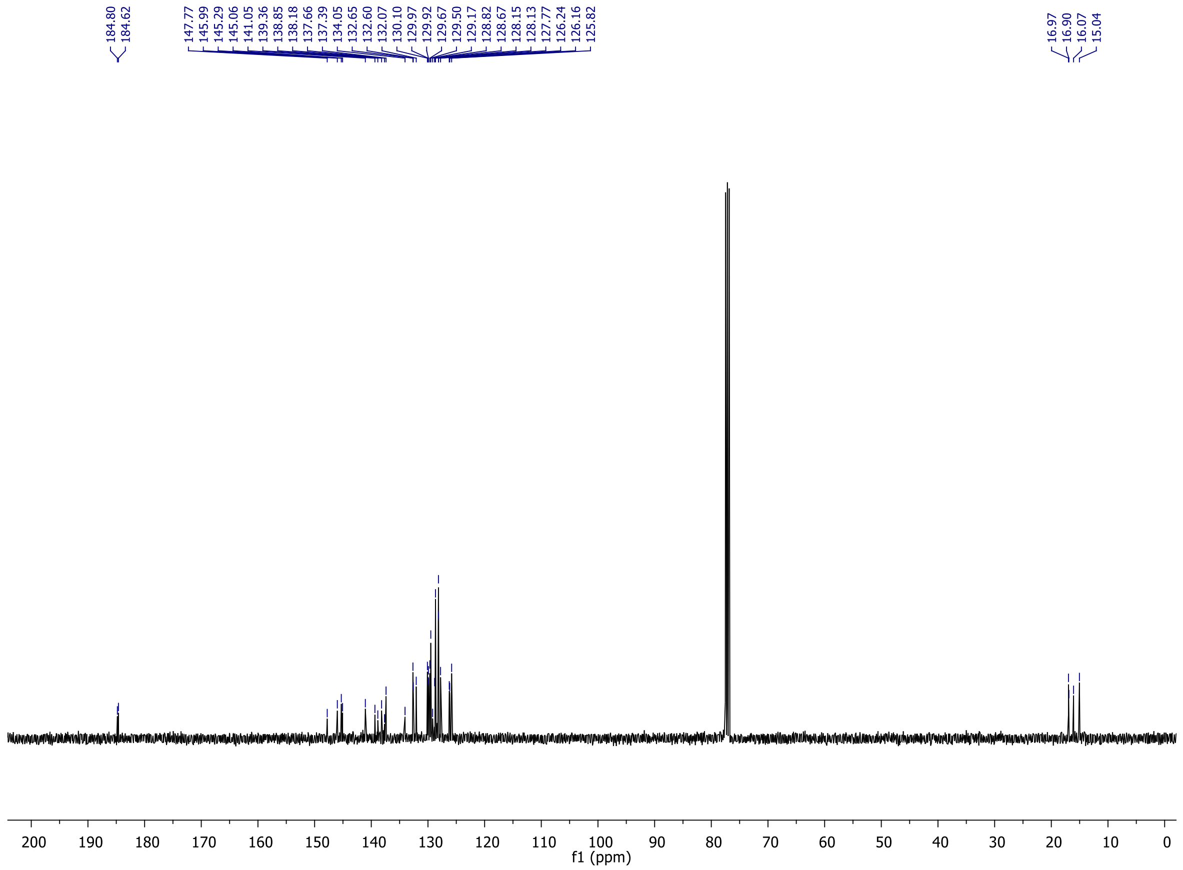
149.39
147.13
146.69
145.89
145.60
142.34
140.10
138.35
133.85
133.54
132.31
131.97
131.57
130.79
129.48
129.05
128.97
128.91
128.50
128.49
128.42
128.24
128.17
128.12
128.10
126.93
123.20
118.79
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



112h

7.42
7.41
7.41
7.41
7.40
7.39
7.39
7.39
7.38
7.37
7.36
7.32
7.31
7.30
7.28
7.27
7.27
7.12
6.92
6.92
6.91
6.91
6.90
6.88
6.87
6.87
6.85
2.55
2.51
2.06
1.99
S
O
S
7.58
3.43
1.30
1.04
4.57
2.97
2.16
2.08
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)



184.80
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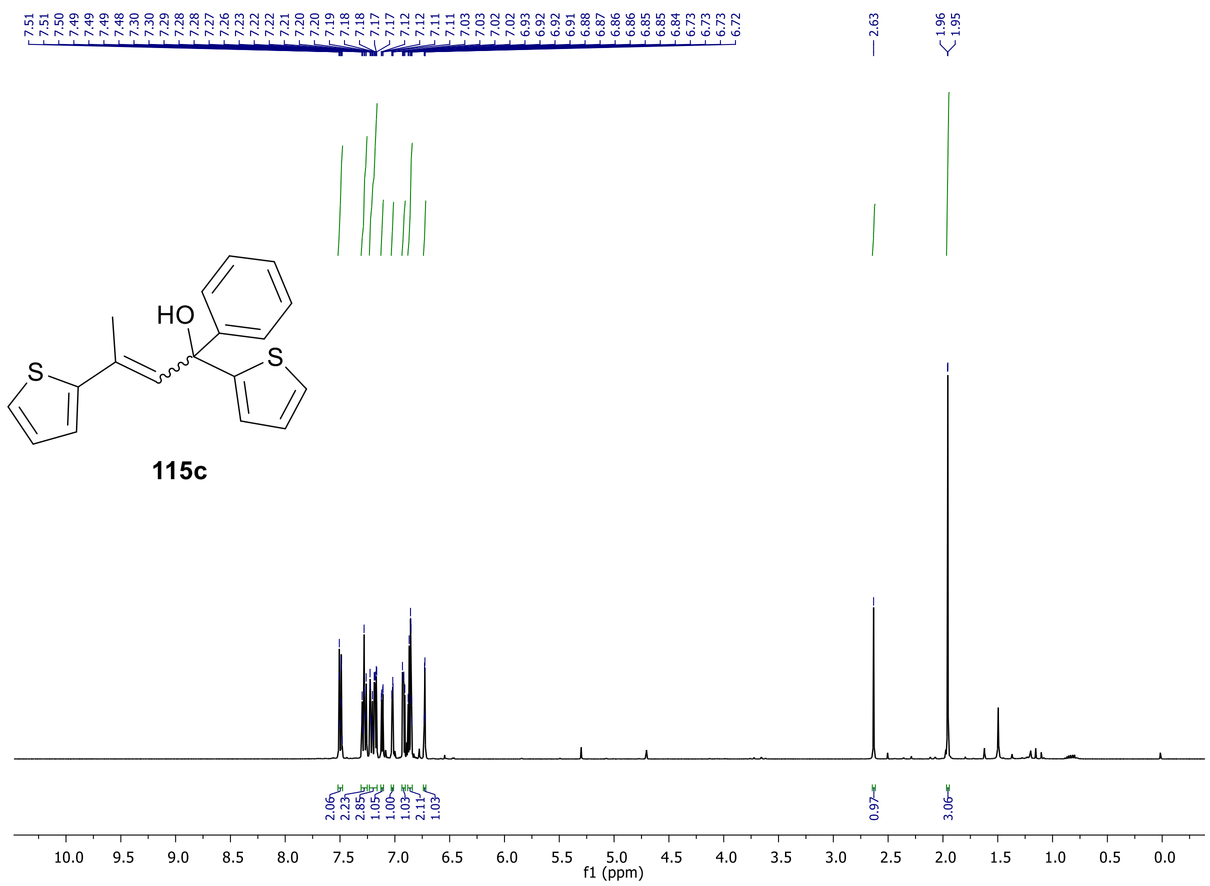
137.39
134.05
132.65
132.60
132.07
130.10
129.97
129.92
129.67
129.50
129.17
128.82
128.67
128.15
128.13
127.77
126.24
126.16
125.82
16.97
16.90
16.07
15.04
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.51
7.51
7.50
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7.49
7.48
7.30
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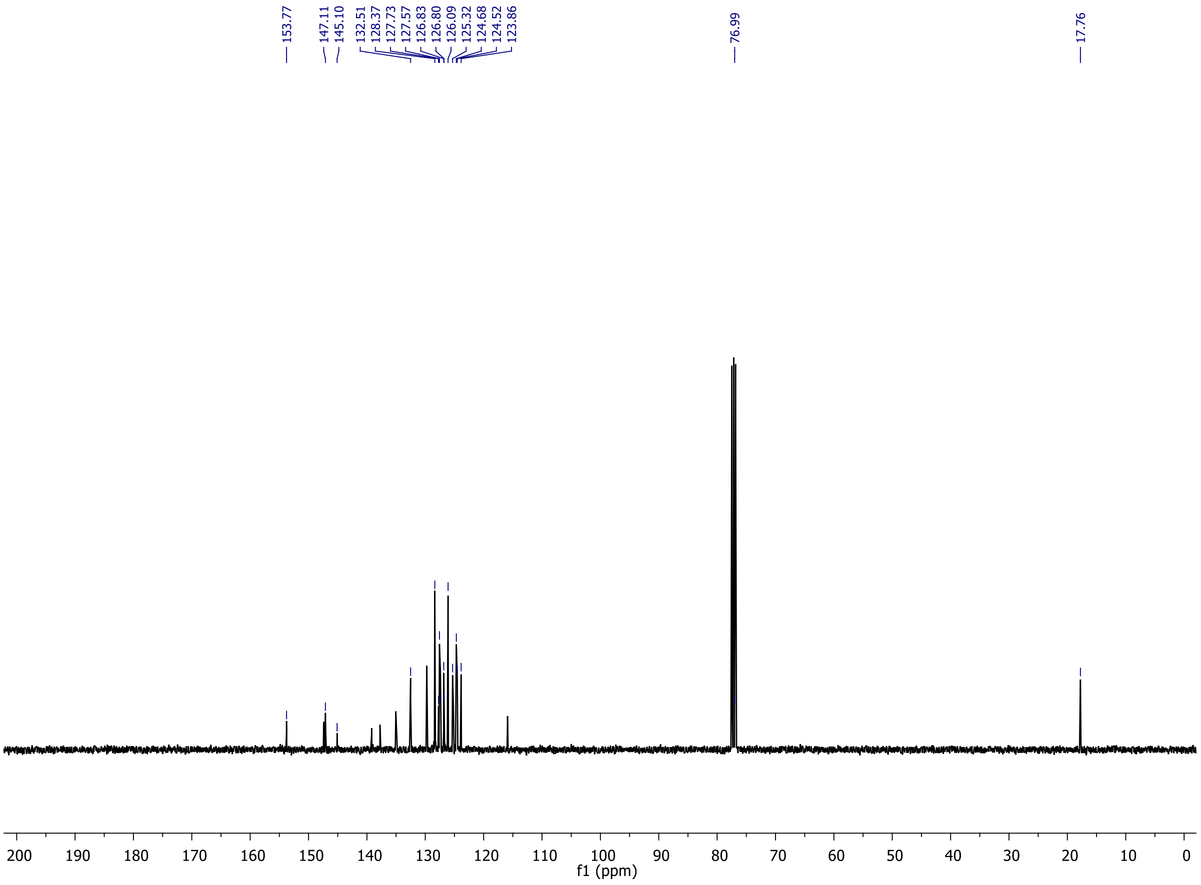
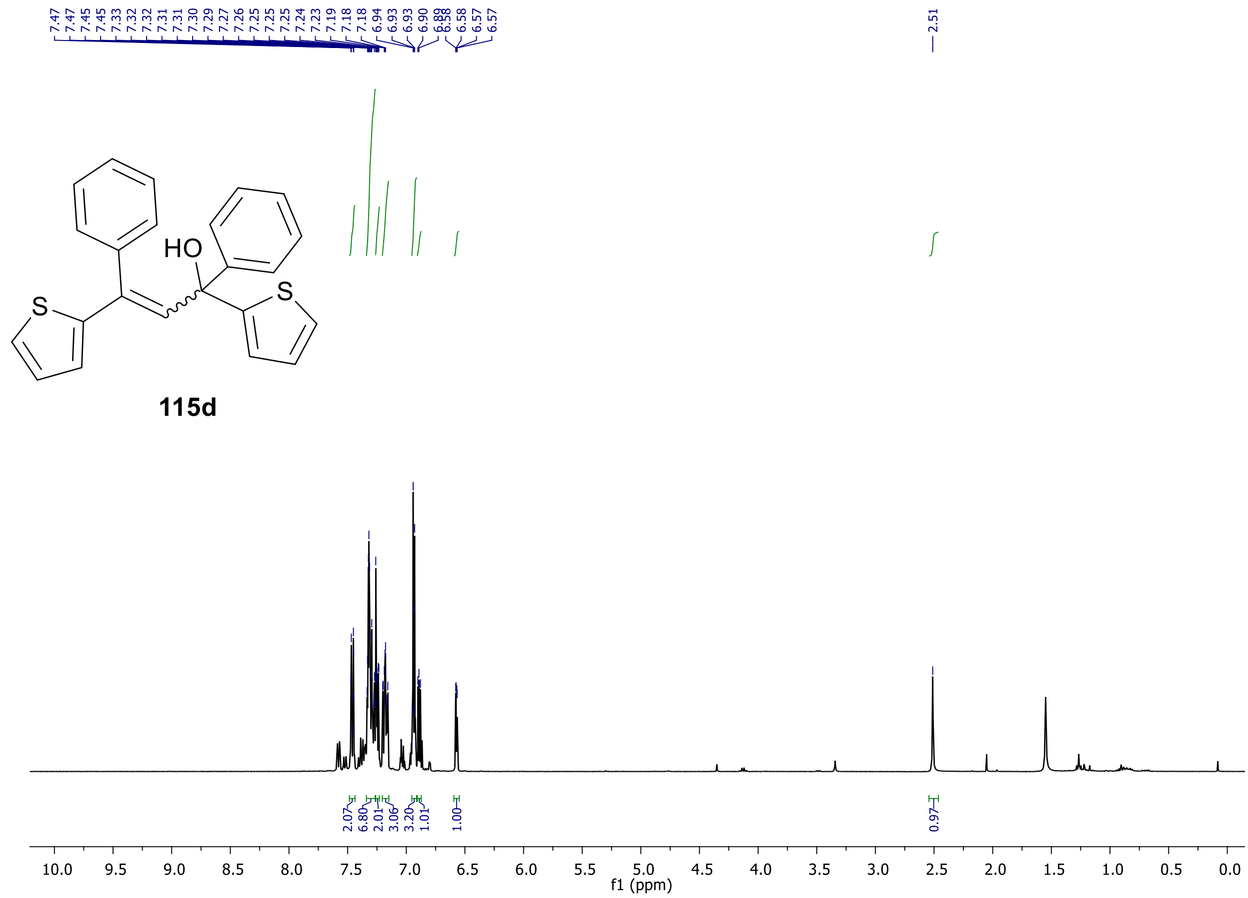
7.29
7.28
7.28
7.27
7.26
7.23
7.22
7.22
7.21
7.20
7.20
7.19
7.18
7.18
7.17
7.17
7.12
7.12
7.11
7.11
7.03
7.03
7.02
7.02
6.93
6.92
6.92
6.91
6.88
6.87
6.86
6.86
6.85
6.85
6.84
6.73
6.73
6.73
6.72
2.63
1.96
1.95
HO
S
S
2.06
2.23
2.85
1.05
1.00
1.03
2.11
1.03
0.97
3.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

115c


153.77
147.11
145.10
132.51
128.37
127.73
127.57
126.83
126.80
126.09
125.32
124.68
124.52
123.86
76.99
17.76
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.47
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7.45
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7.32
7.31
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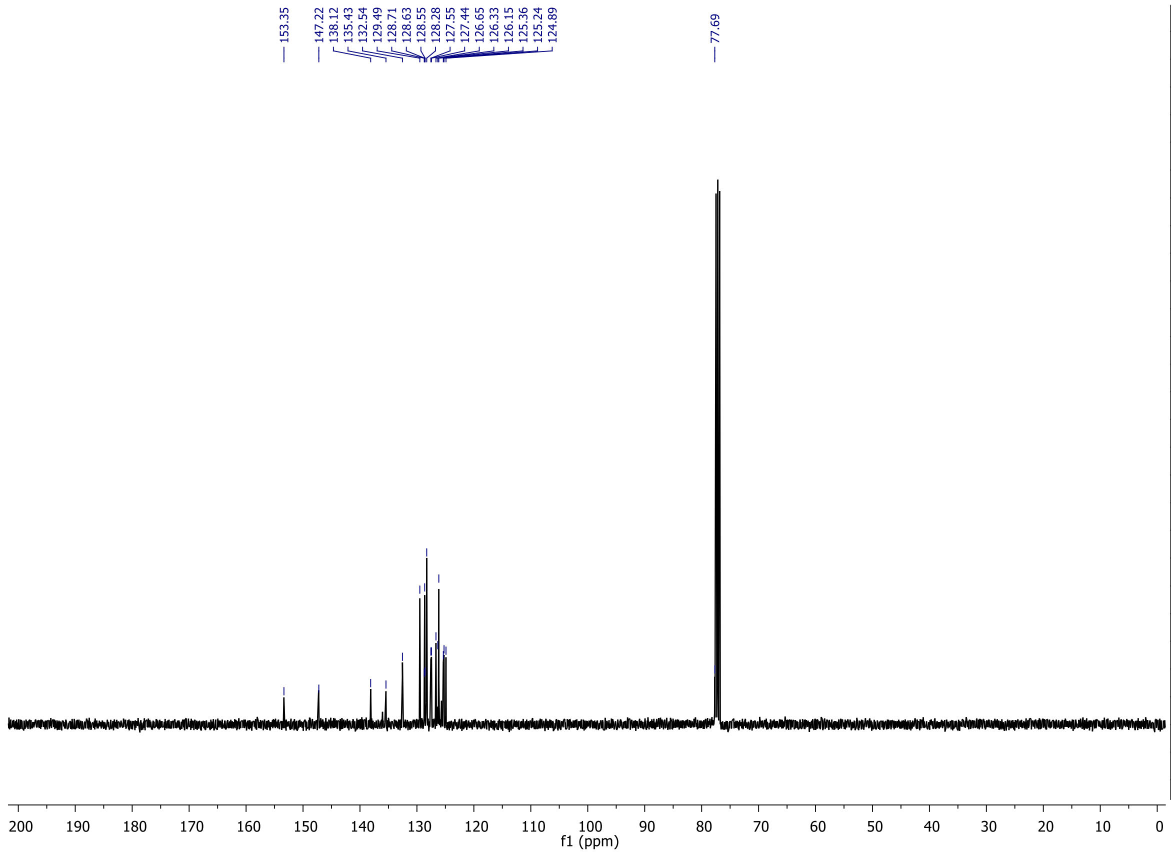
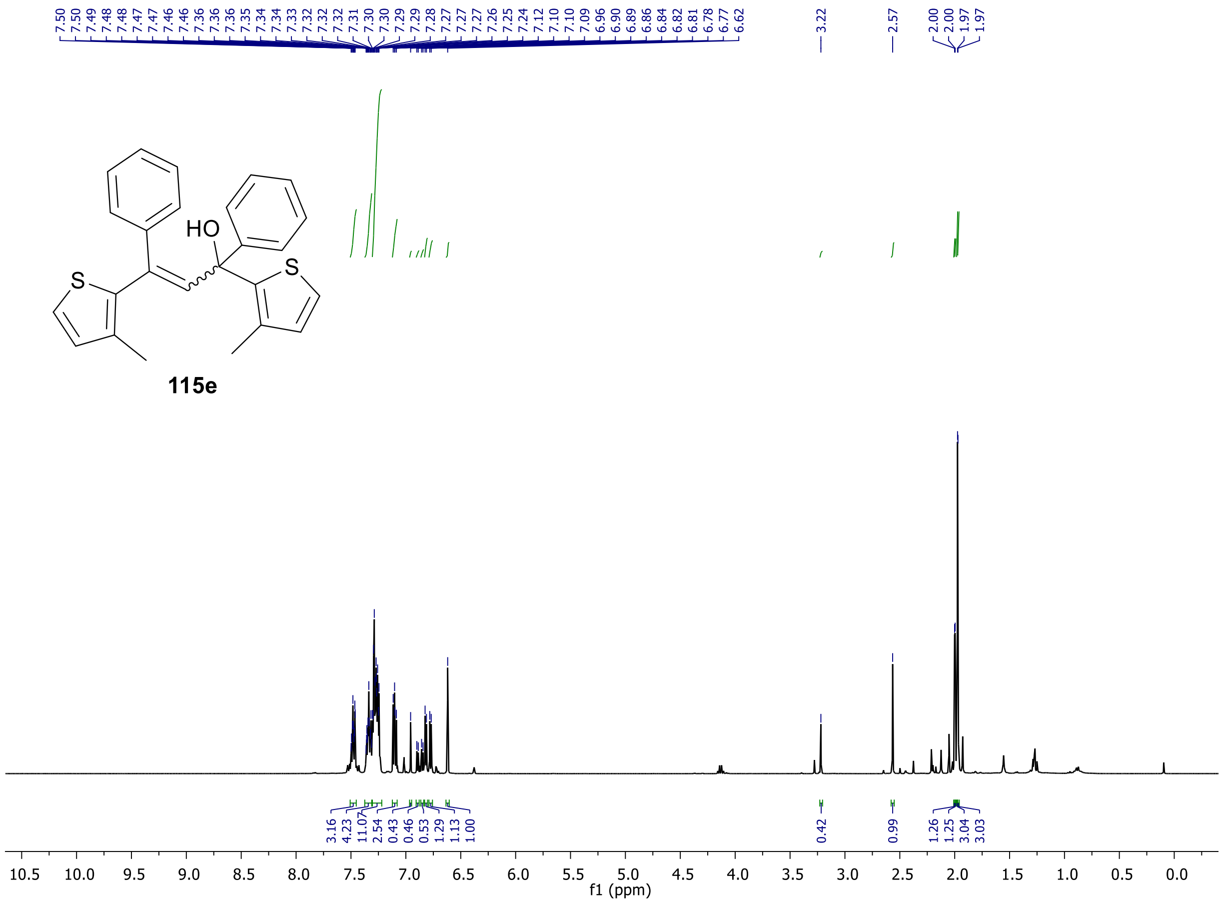
7.30
7.29
7.27
7.26
7.25
7.25
7.25
7.24
7.23
7.19
7.18
7.18
6.94
6.93
6.93
6.90
6.89
6.88
6.58
6.57
6.57
2.51
HO
S
S
2.07
6.80
2.01
3.06
3.20
1.01
1.00
0.97
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

115d


153.35
147.22
138.12
135.43
132.54
129.49
128.71
128.63
128.55
128.28
127.55
127.44
126.65
126.33
126.15
125.36
125.24
124.89
77.69
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.50
7.50
7.49
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7.47
7.47
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7.46
7.36
7.36
7.36
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7.34
7.34
7.33
7.32
7.32
7.32
7.31
7.30
7.30
7.29
7.29
7.28
7.27
7.27
7.27
7.26
7.25
7.24
7.12
7.10
7.10
7.09
6.96
6.90
6.89
6.86
6.84
6.82
6.81
6.78
6.77
6.62
3.22
2.57
2.00
2.00
1.97
1.97
HO
S
S
115e
3.16
4.23
11.07
2.54
0.43
0.46
0.53
1.29
1.13
1.00
0.42
0.99
1.26
1.25
3.04
3.03
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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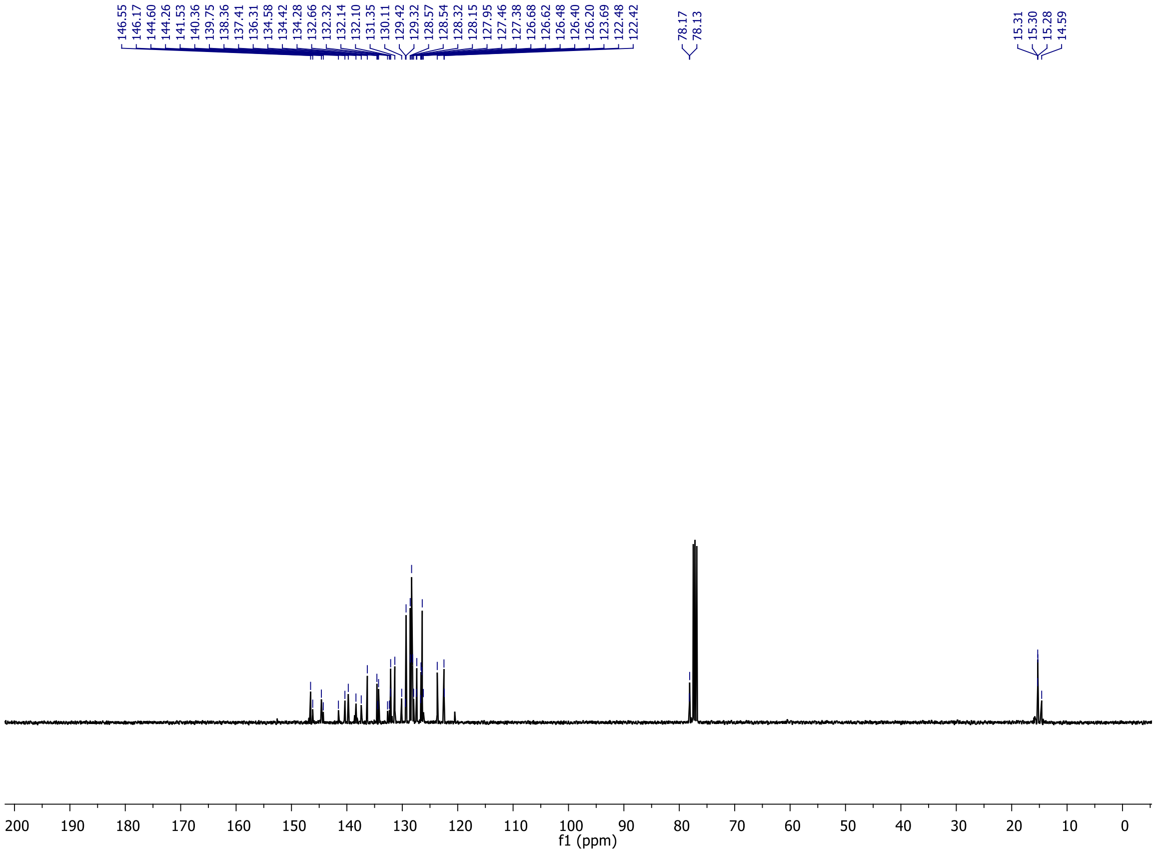
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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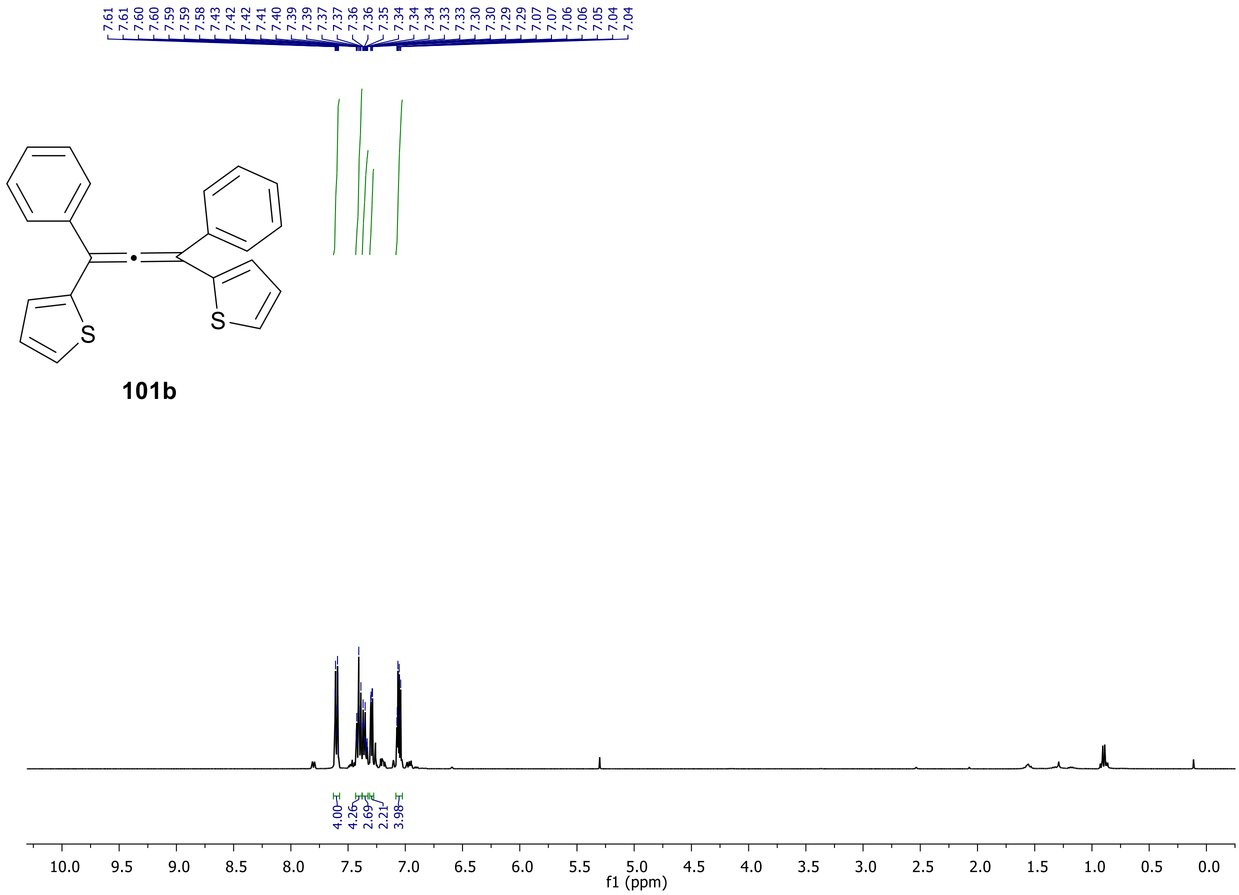
140.36
139.75
138.36
137.41
136.31
134.58
134.42
134.28
132.66
132.32
132.14
132.10
131.35
130.11
129.42
129.32
128.57
128.54
128.32
128.15
127.95
127.46
127.38
126.68
126.62
126.48
126.40
126.20
123.69
122.48
122.42
78.17
78.13
15.31
15.30
15.28
14.59
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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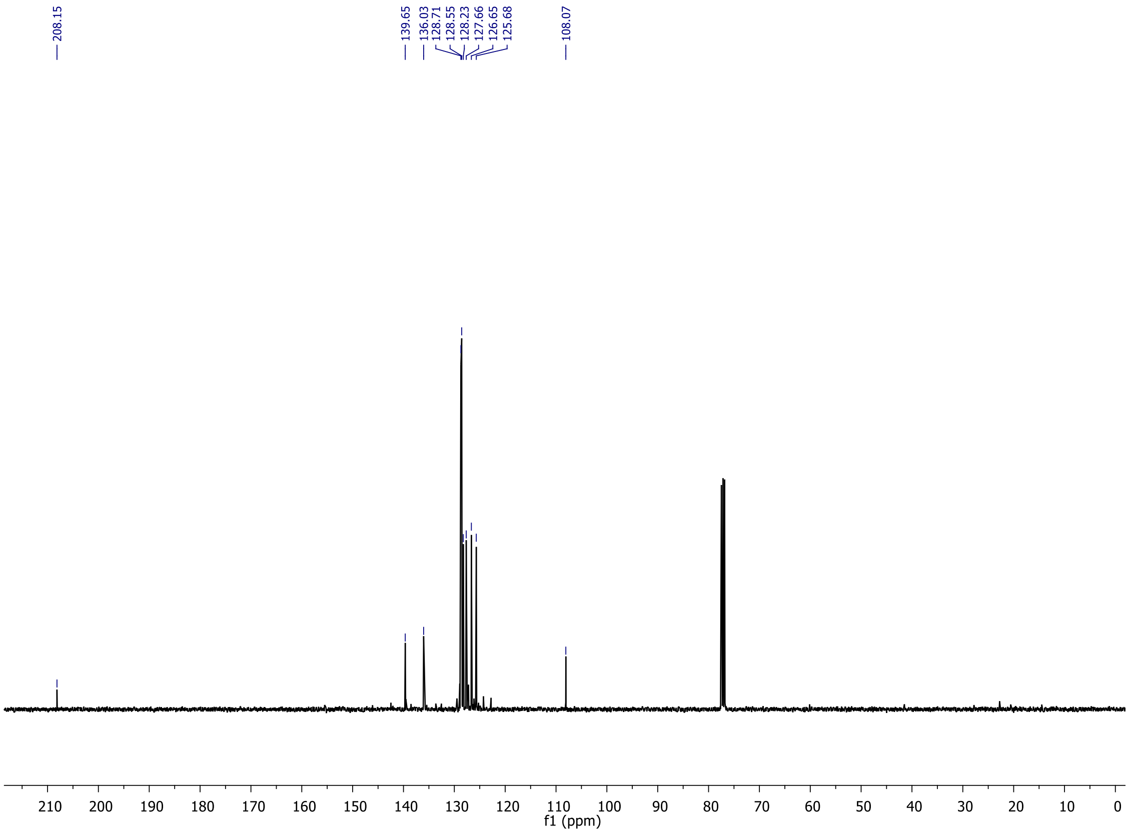
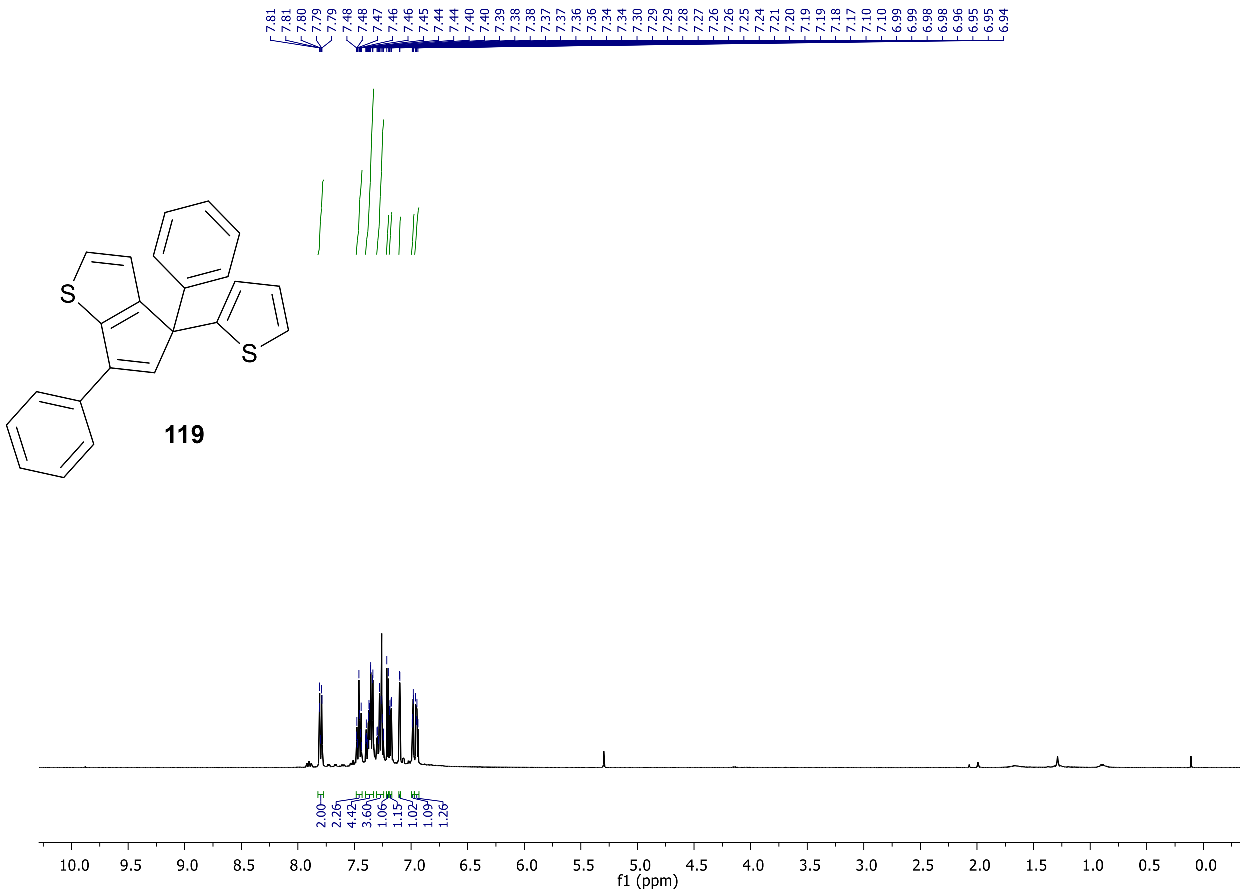
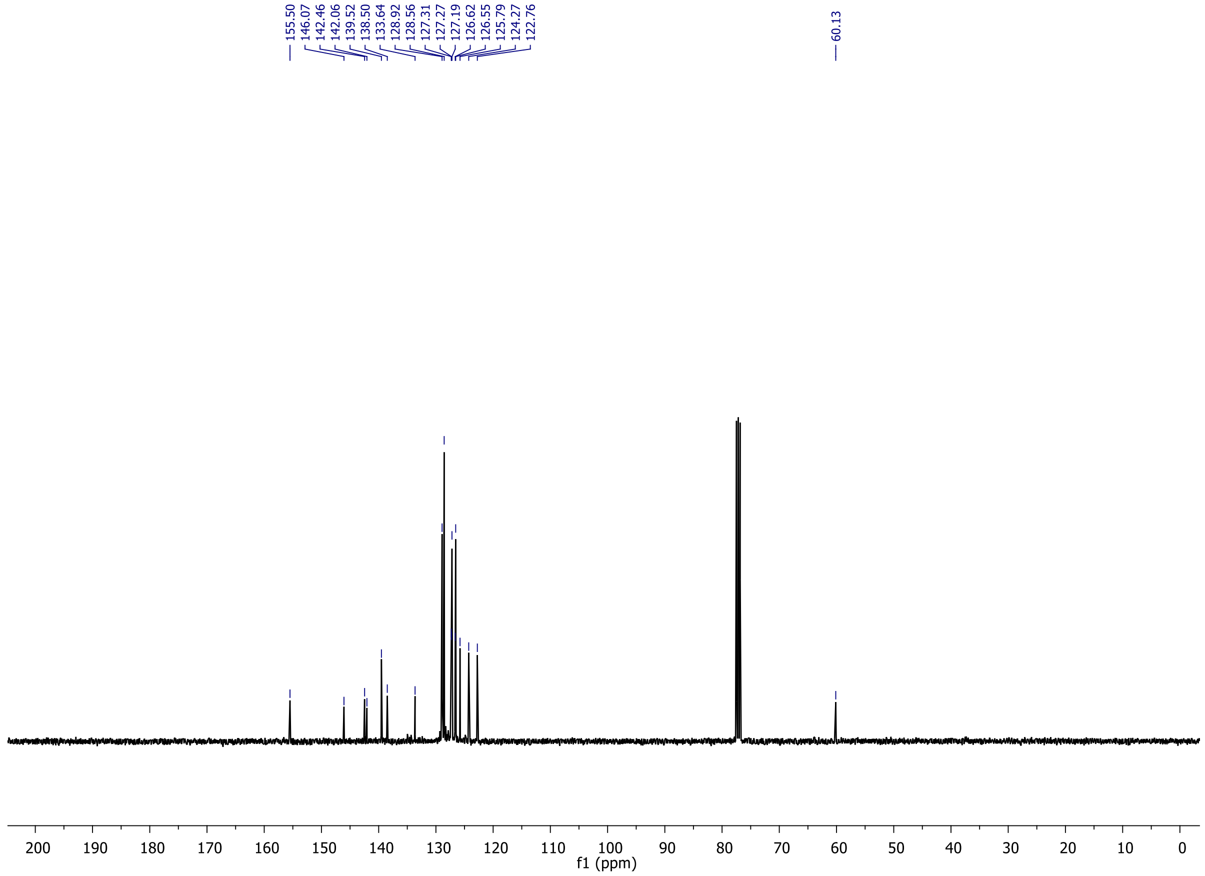
7.61
7.60
7.60
7.59
7.59
7.58
7.43
7.42
7.42
7.41
7.40
7.39
7.39
7.37
7.37
7.36
7.36
7.35
7.34
7.34
7.34
7.33
7.33
7.30
7.30
7.29
7.29
7.07
7.07
7.06
7.06
7.05
7.04
7.04
S
S
4.00
4.26
2.69
2.21
3.98
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

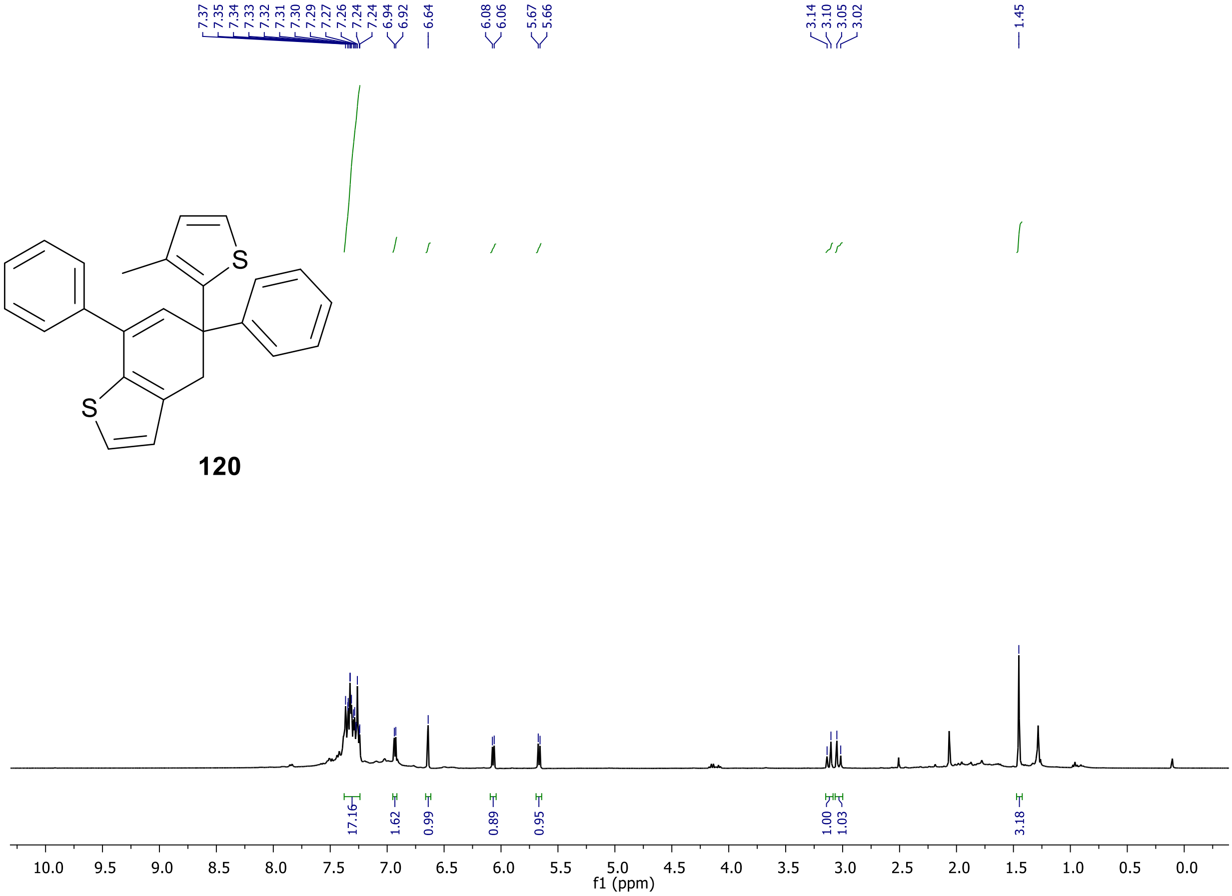
101b


208.15
139.65
136.03
128.71
128.55
128.23
127.66
126.65
125.68
108.07
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

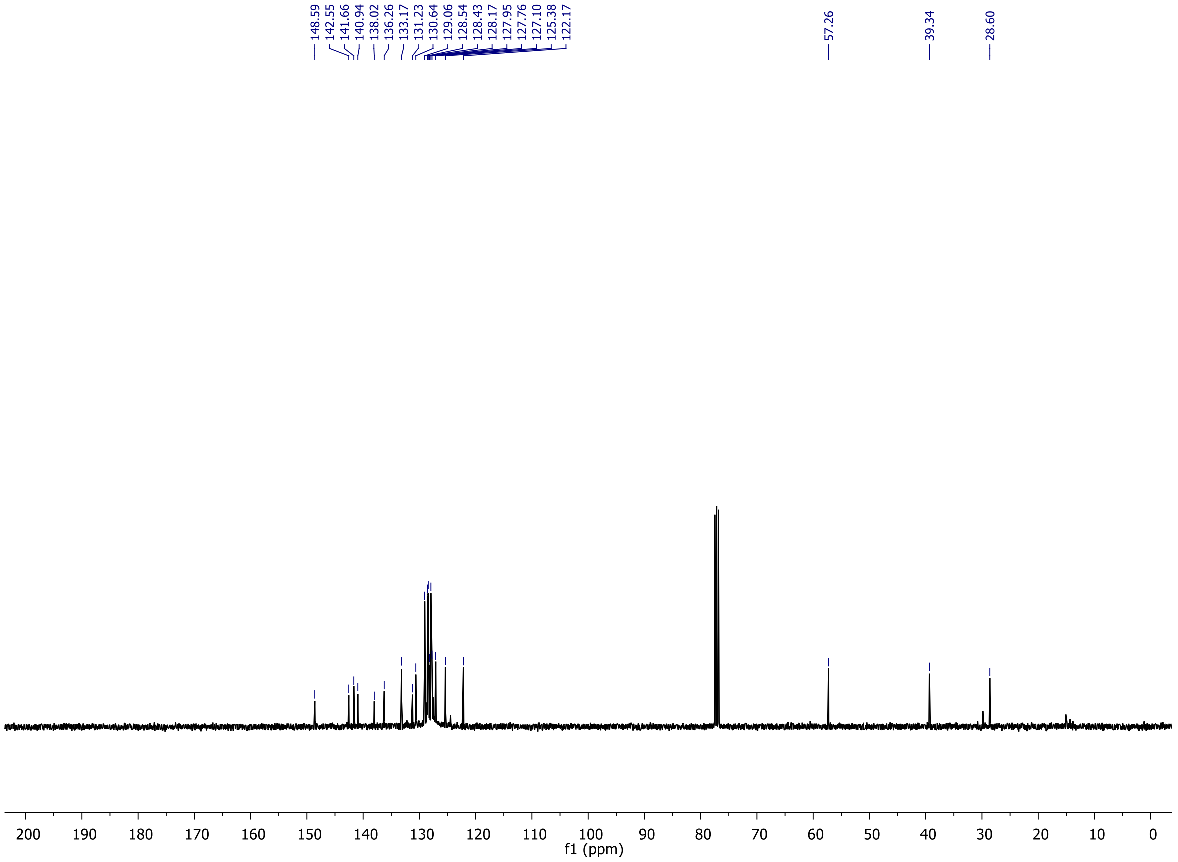

7.81
7.81
7.80
7.79
7.79
7.48
7.48
7.47
7.46
7.46
7.45
7.44
7.44
7.40
7.40
7.39
7.38
7.38
7.37
7.37
7.36
7.36
7.34
7.34
7.30
7.29
7.29
7.28
7.27
7.26
7.26
7.25
7.24
7.21
7.20
7.19
7.19
7.18
7.17
7.10
6.99
6.99
6.98
6.98
6.96
6.95
6.95
6.94
S
S
2.00
2.26
4.42
3.60
1.06
1.15
1.02
1.09
1.26
10.0
9.5
9.0
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)

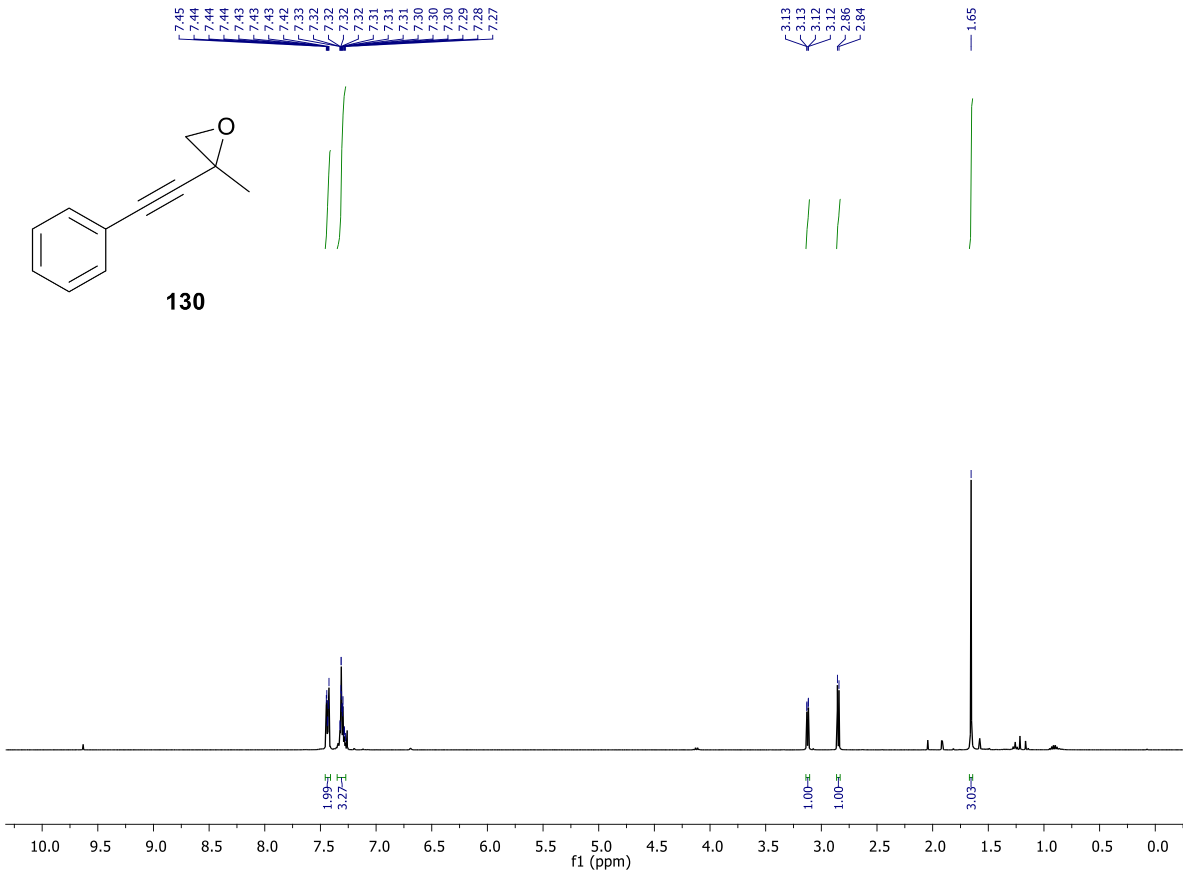
119

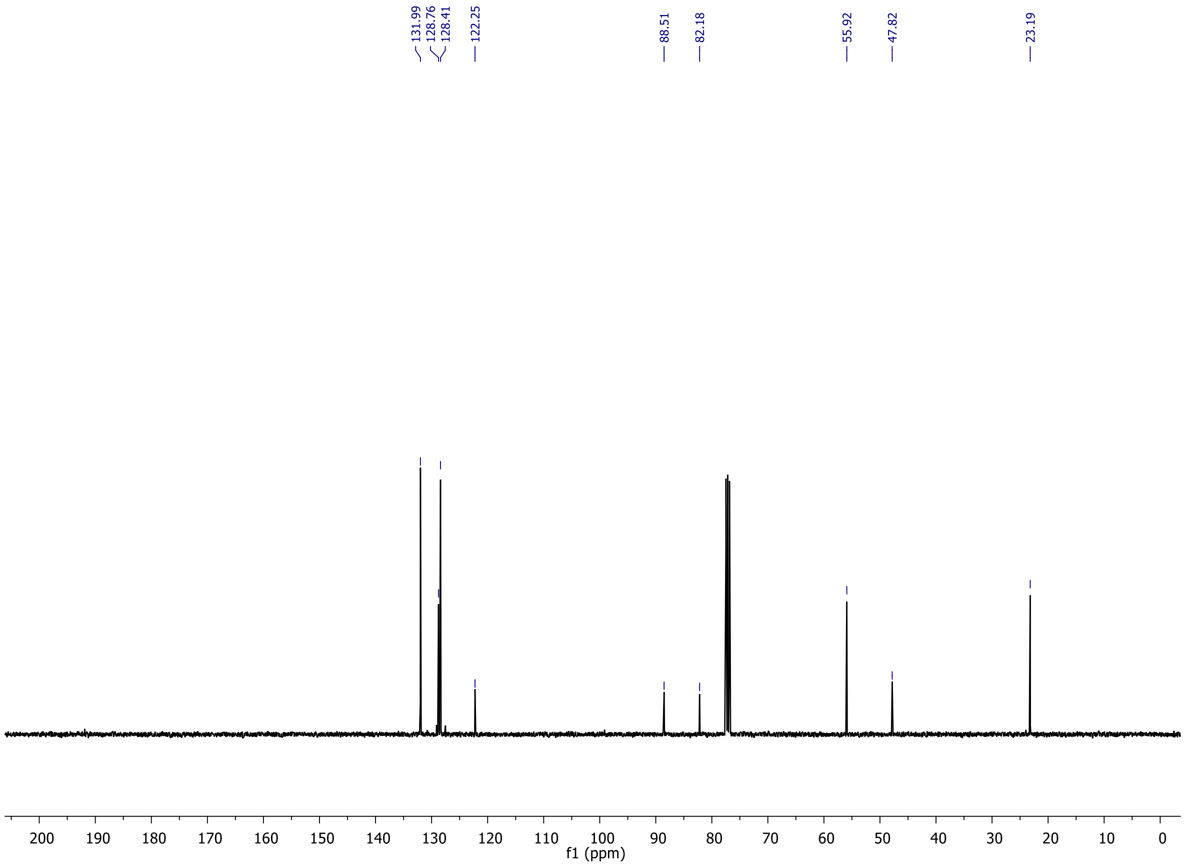

155.50
146.07
142.46
142.06
139.52
138.50
133.64
128.92
128.56
127.31
127.27
127.19
126.62
126.55
125.79
124.27
122.76
60.13
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

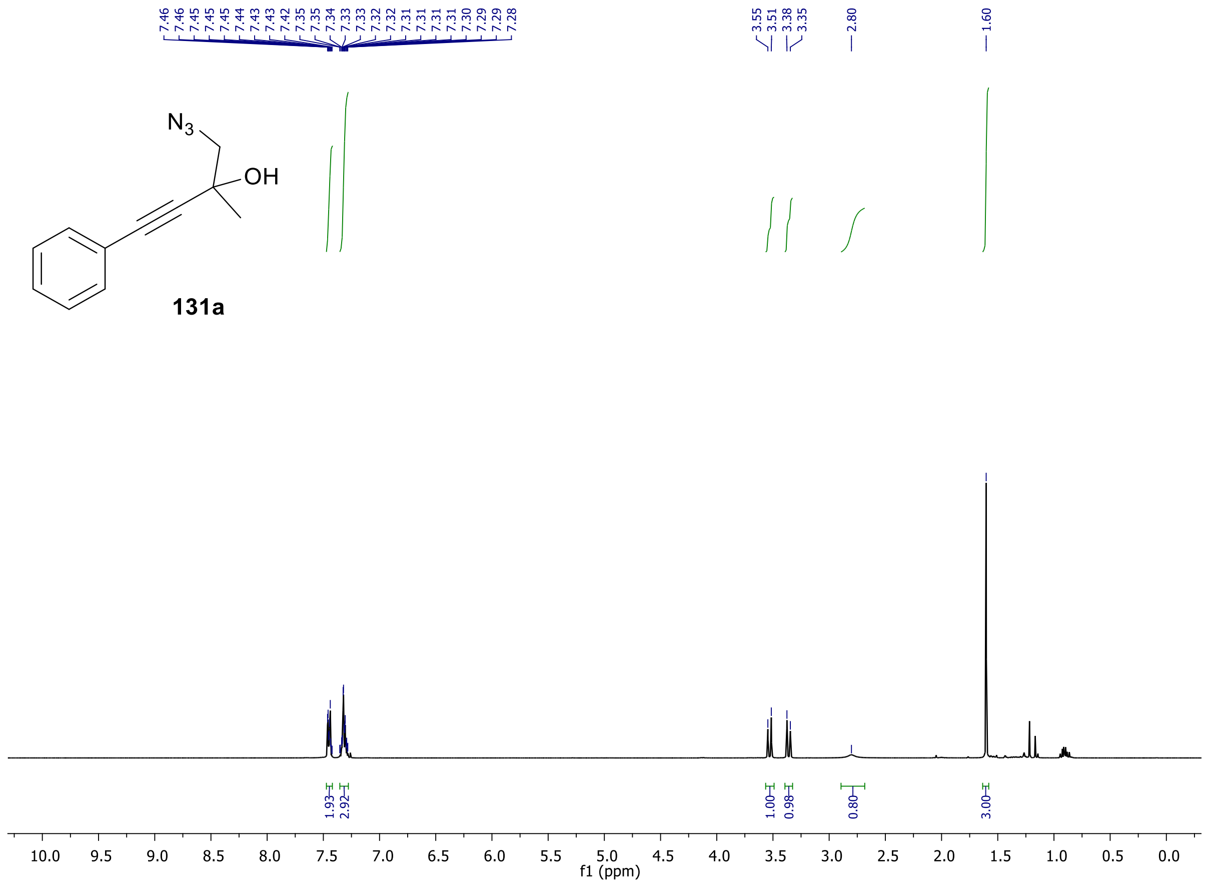

7.37
7.35
7.34
7.33
7.32
7.31
7.30
7.29
7.27
7.26
7.24
7.24
6.94
6.92
6.64
6.08
6.06
5.67
5.66
3.14
3.10
3.05
3.02
1.45
S
S
17.16
1.62
0.99
0.89
0.95
1.00
1.03
3.18
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

120

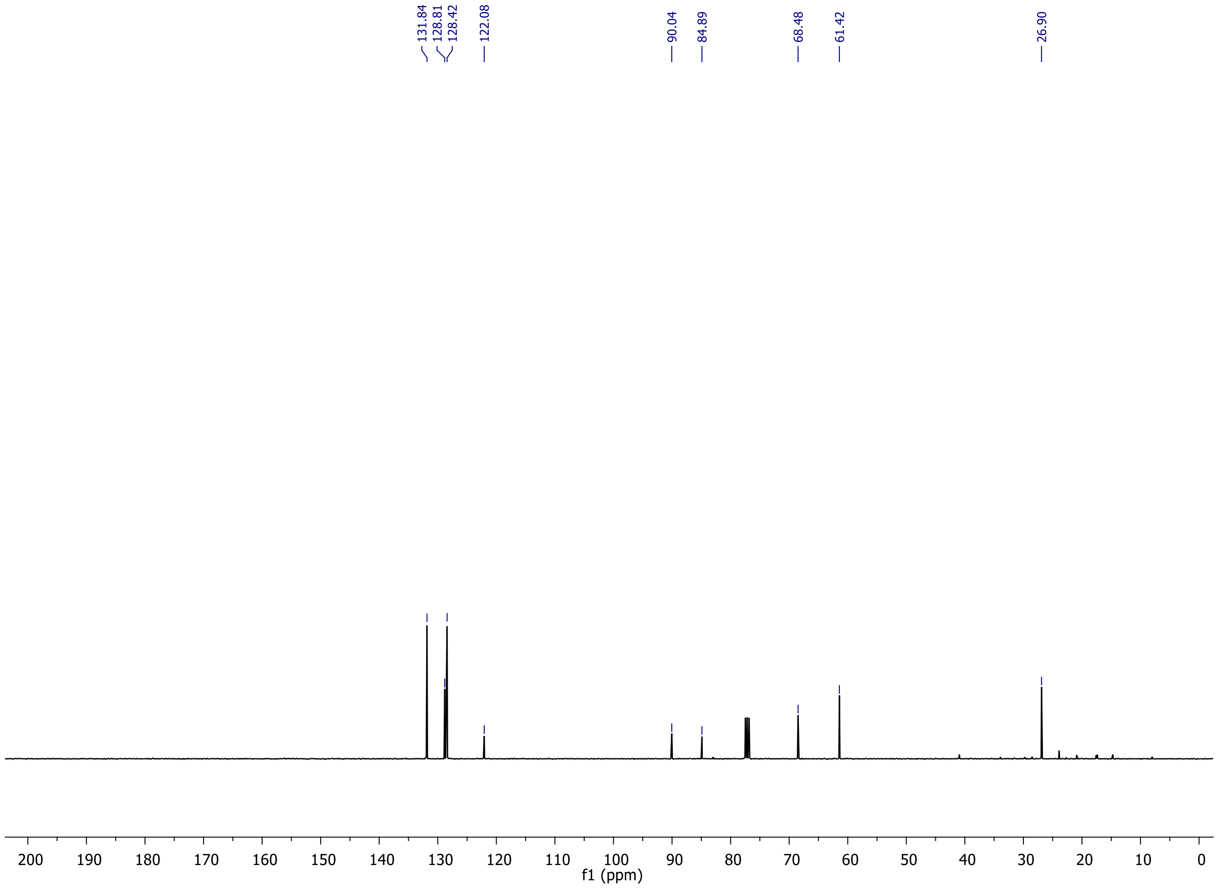

148.59
142.55
141.66
140.94
138.02
136.26
133.17
131.23
130.64
129.06
128.54
128.43
128.17
127.95
127.76
127.10
125.38
122.17
57.26
39.34
28.60
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

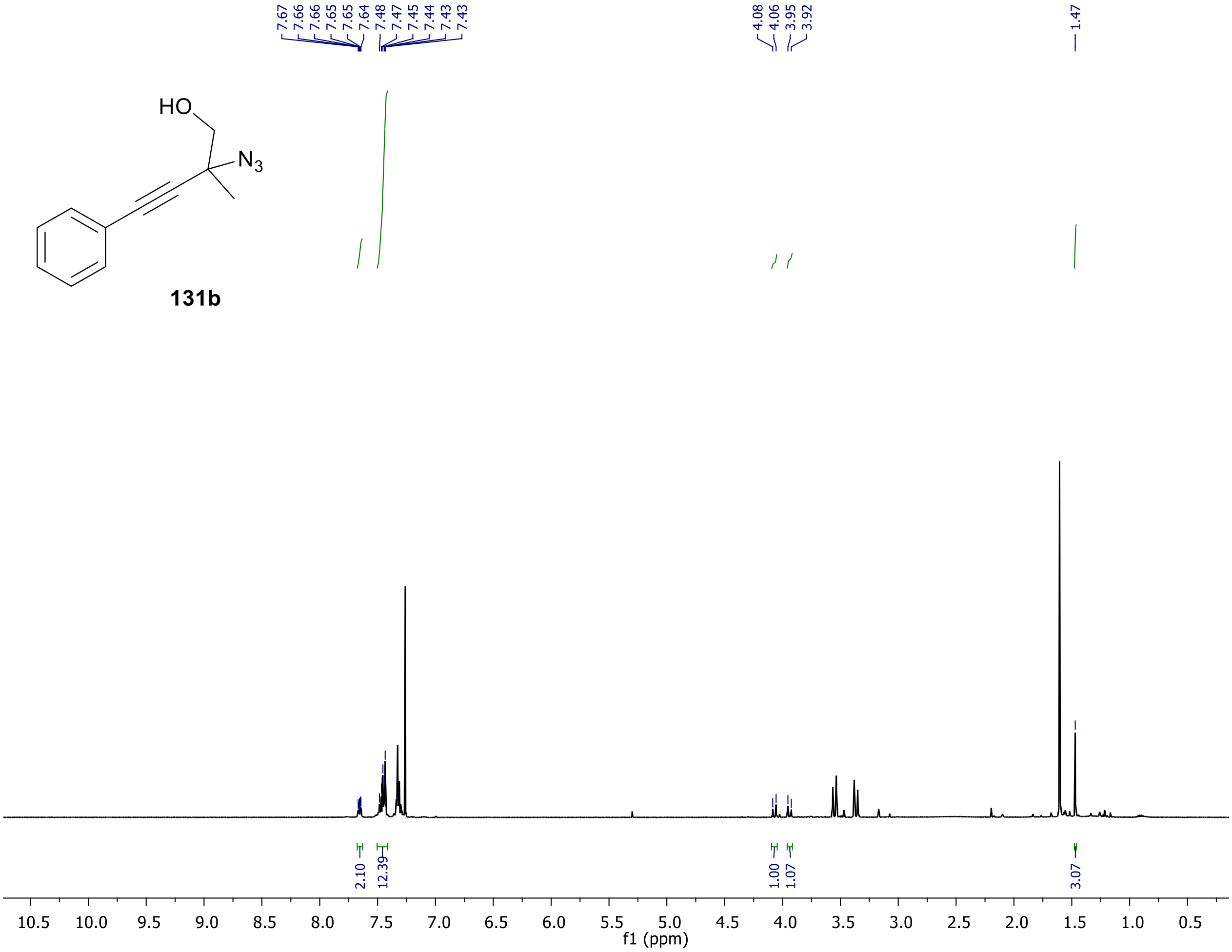

130
7.45
7.44
7.44
7.44
7.43
7.43
7.43
7.42
7.33
7.32
7.32
7.32
7.32
7.31
7.31
7.31
7.30
7.30
7.30
7.29
7.28
7.27
3.13
3.13
3.12
3.12
2.86
2.84
1.65
1.99
3.27
1.00
1.00
3.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


131.99
128.76
128.41
122.25
88.51
82.18
55.92
47.82
23.19
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.46
7.46
7.45
7.45
7.45
7.44
7.43
7.43
7.42
7.35
7.35
7.34
7.33
7.33
7.32
7.32
7.31
7.31
7.31
7.31
7.30
7.29
7.29
7.28
3.55
3.51
3.38
3.35
2.80
1.60
N3
OH
1.93
2.92
1.00
0.98
0.80
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

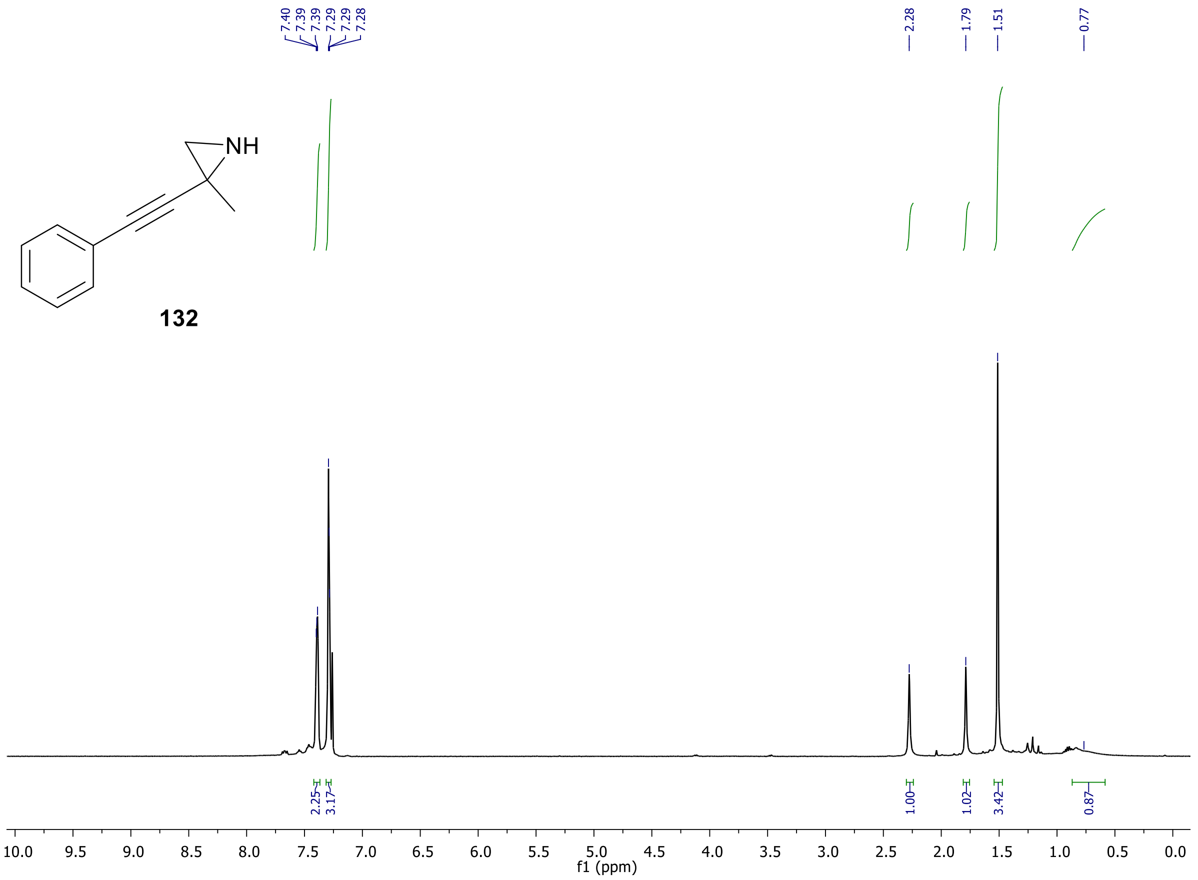
131a

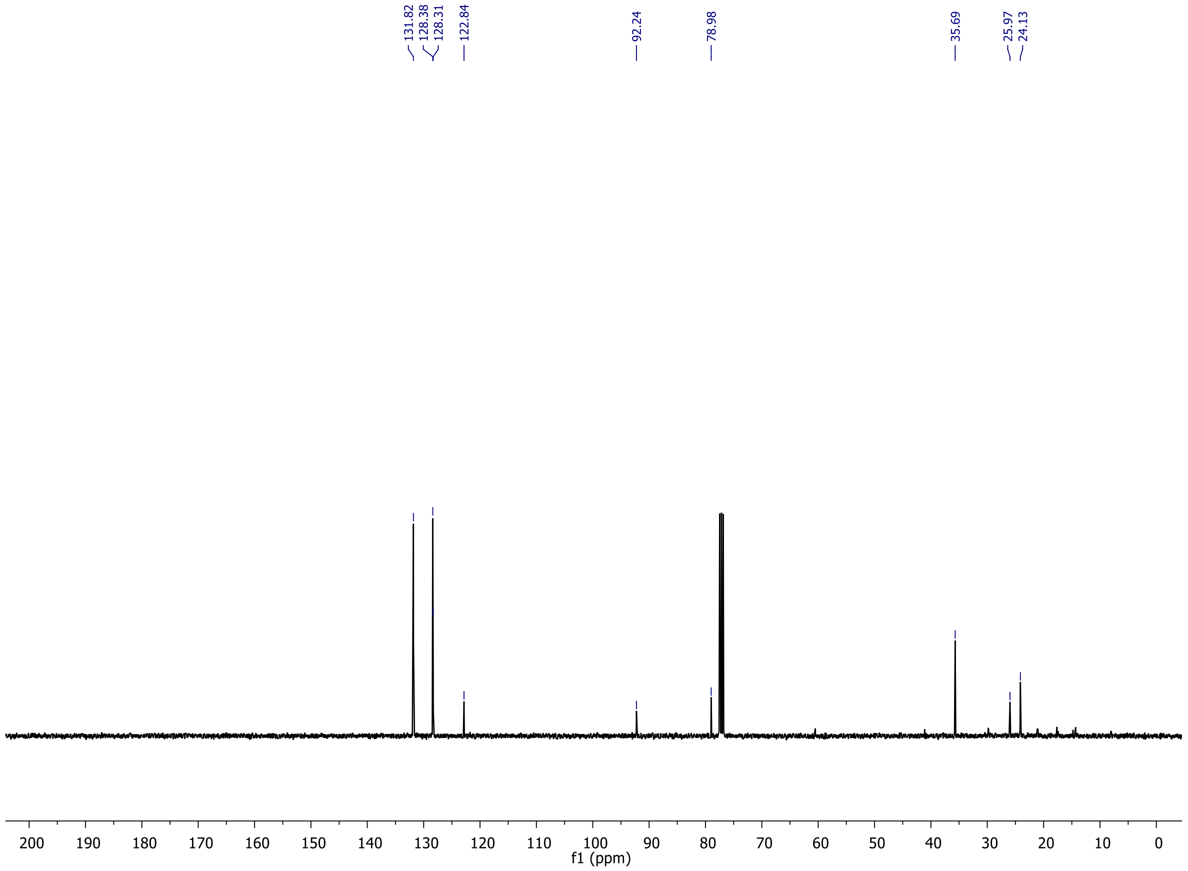

131.84
128.81
128.42
122.08
90.04
84.89
68.48
61.42
26.90
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

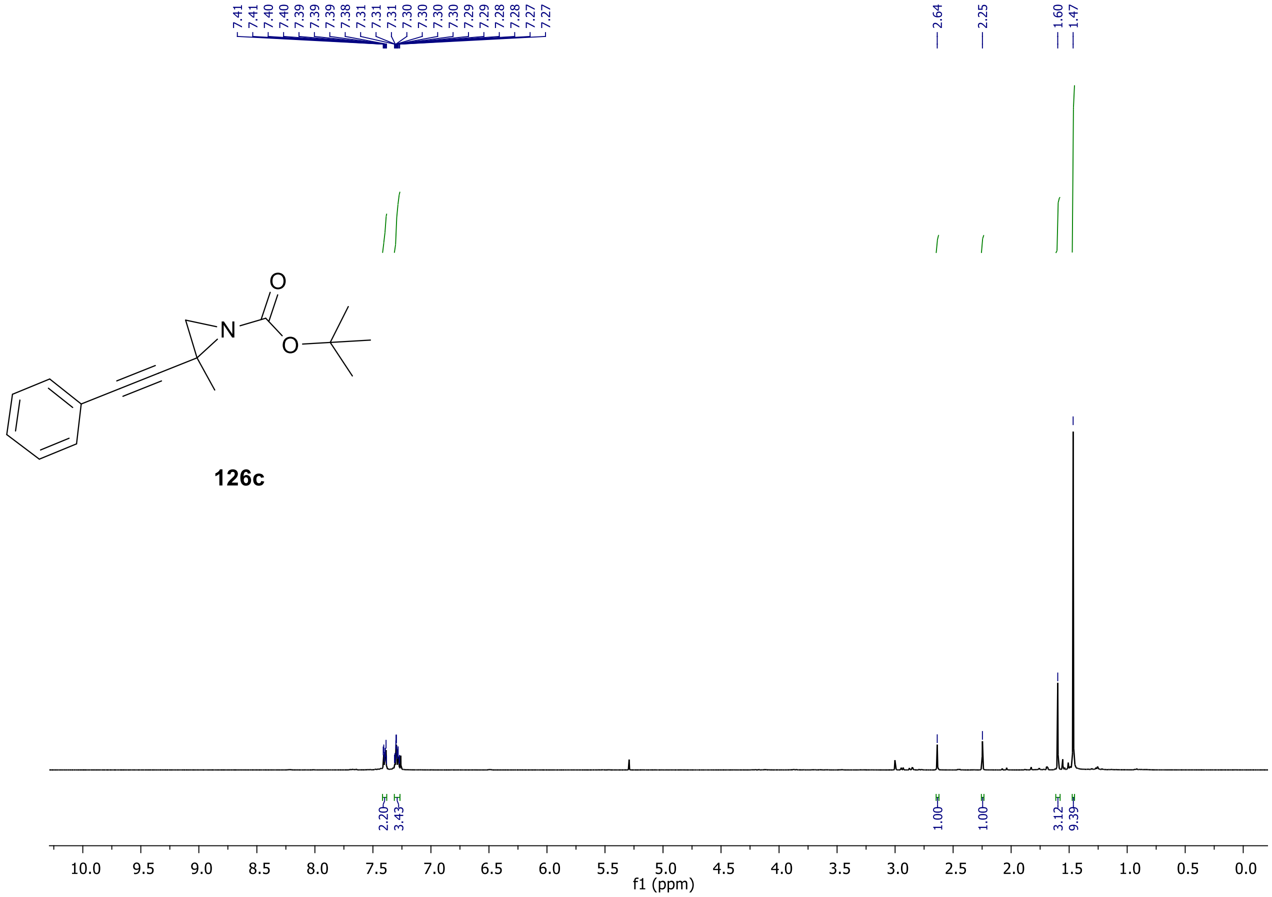


131b

HO
N3
7.67
7.66
7.66
7.65
7.65
7.64
7.48
7.47
7.45
7.44
7.43
7.43
4.08
4.06
3.95
3.92
1.47
2.10
12.39
1.00
1.07
3.07
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)

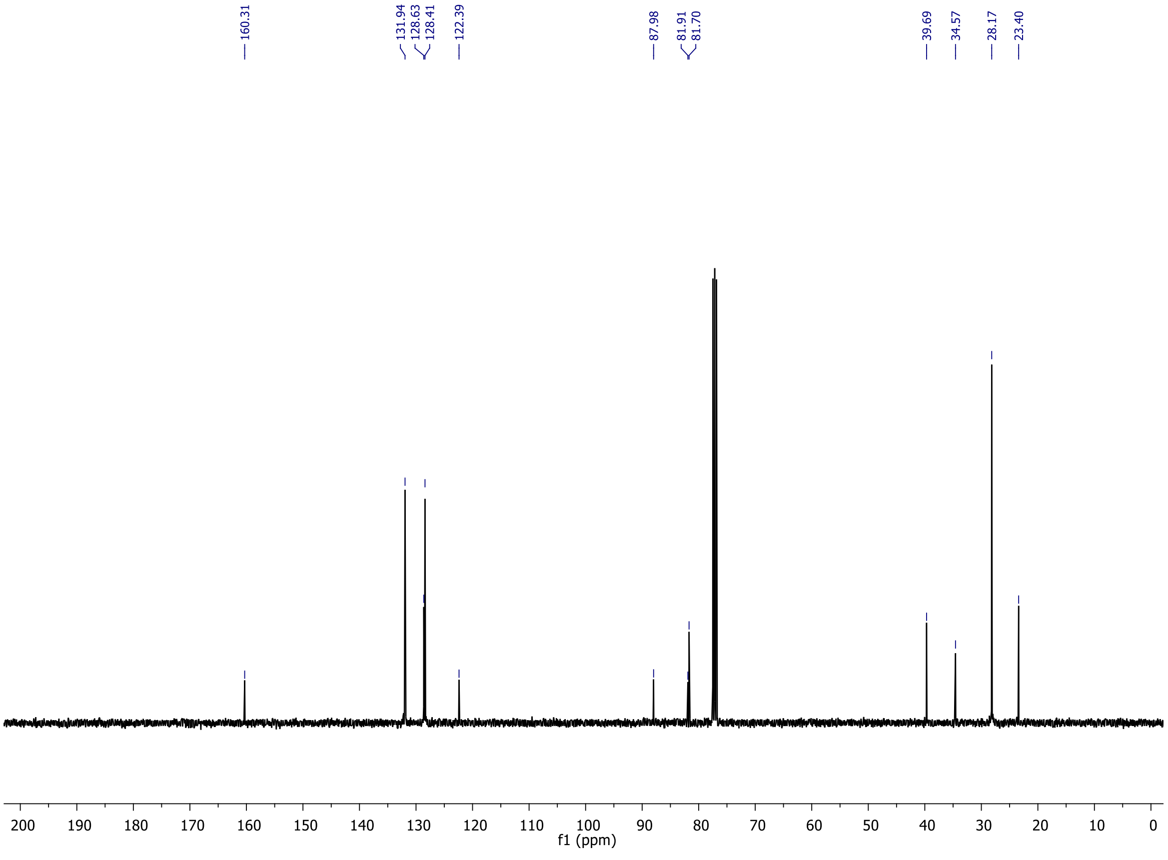

132
NH
7.40
7.39
7.39
7.29
7.29
7.28
2.28
1.79
1.51
0.77
2.25
3.17
1.00
1.02
3.42
0.87
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


131.82
128.38
128.31
122.84
92.24
78.98
35.69
25.97
24.13
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

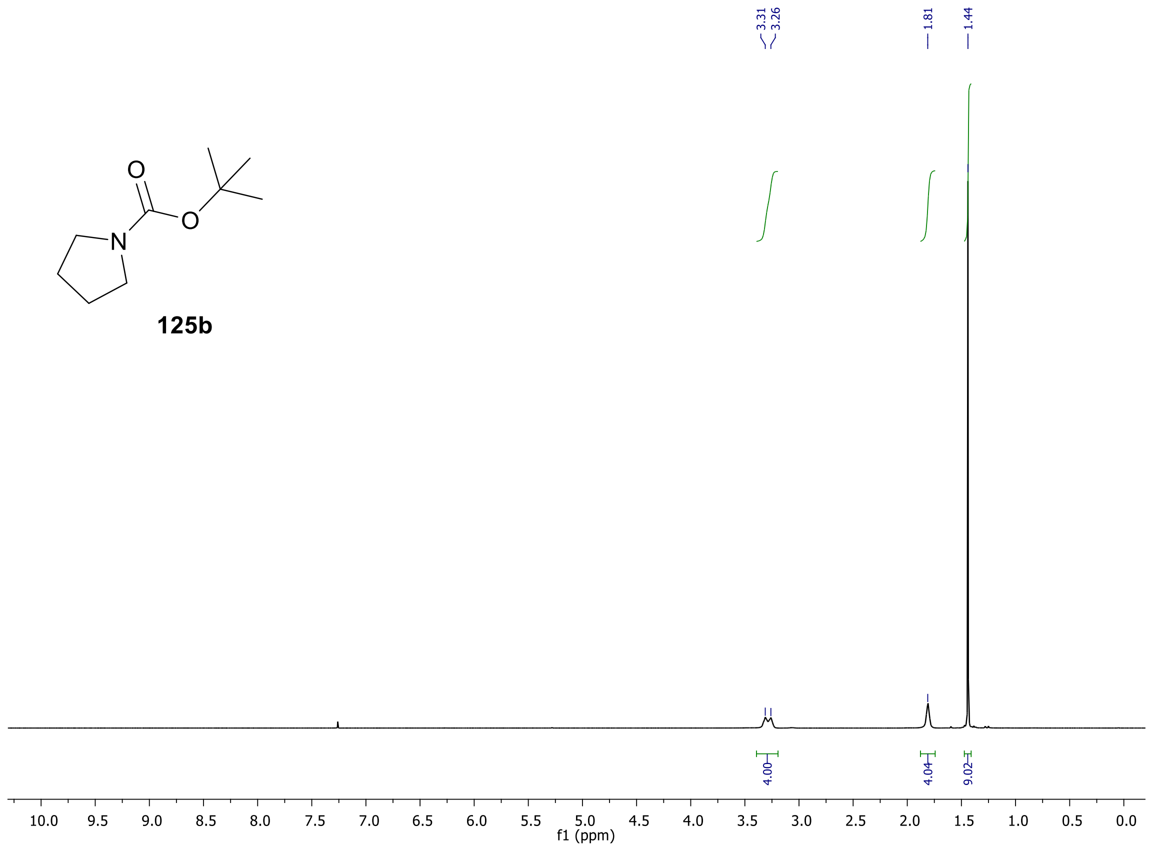


126c

7.41
7.41
7.40
7.39
7.39
7.39
7.38
7.31
7.31
7.30
7.30
7.30
7.29
7.29
7.28
7.28
7.27
7.27
2.64
2.25
1.60
1.47
2.20
3.43
1.00
1.00
3.12
9.39
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)
O
N
O

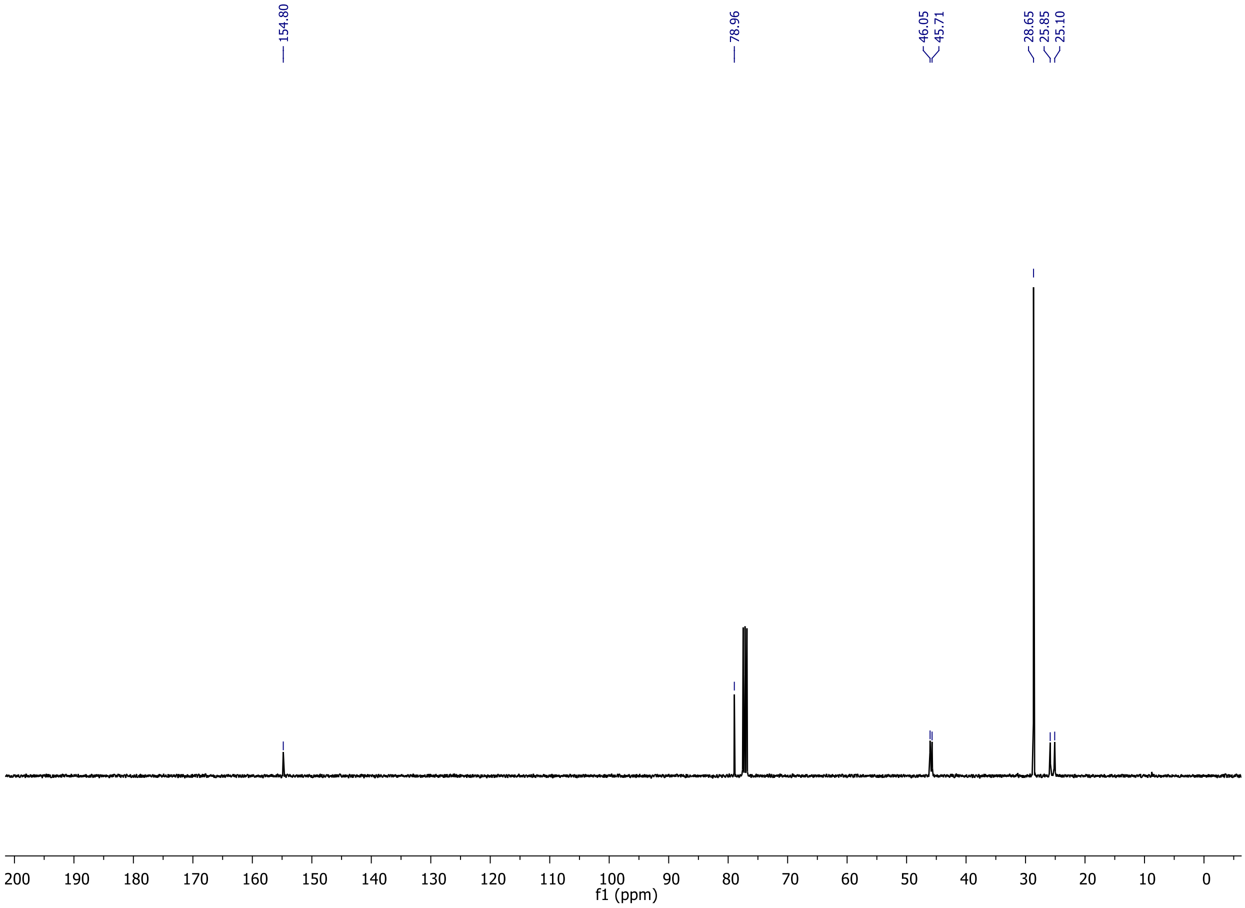


160.31
131.94
128.63
128.41
122.39
87.98
81.91
81.70
39.69
34.57
28.17
23.40
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

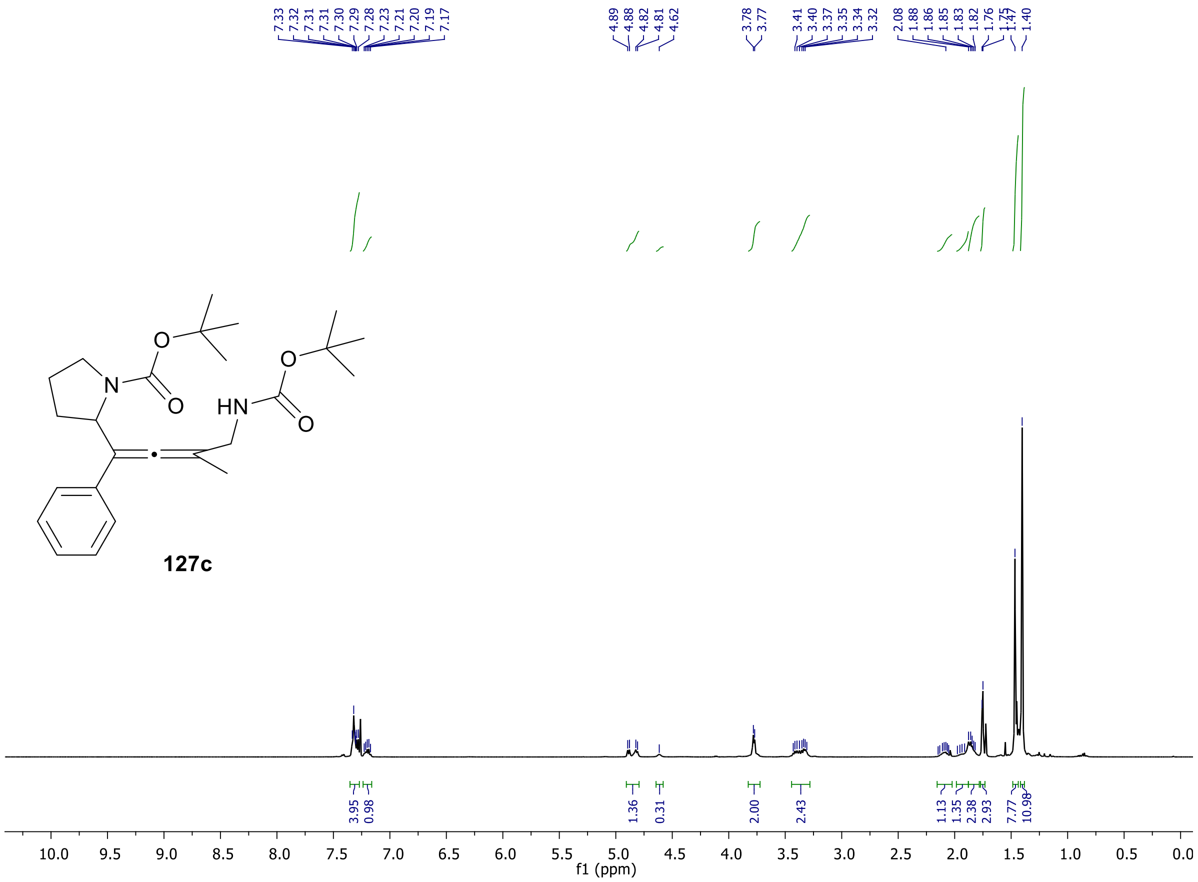


125b

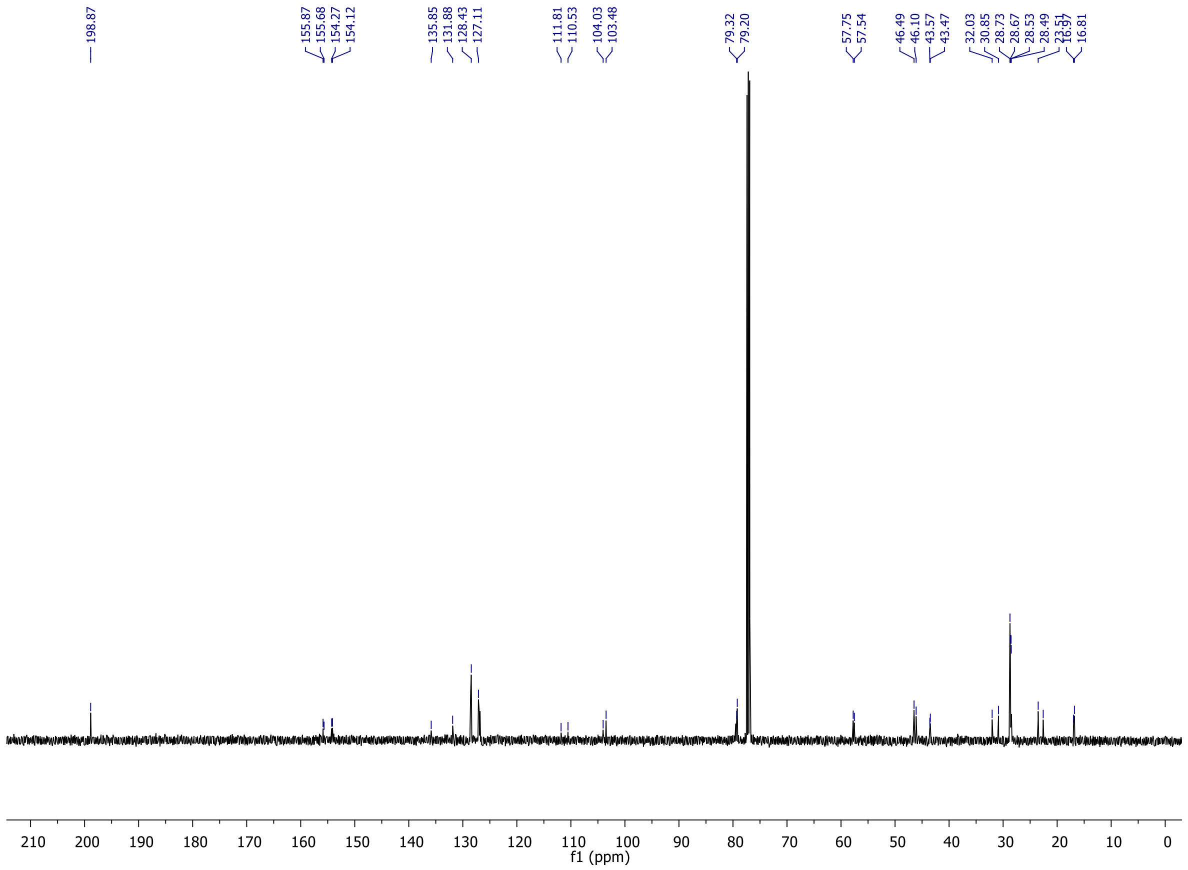
3.31
3.26
1.81
1.44
4.00
4.04
9.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
O
N
O

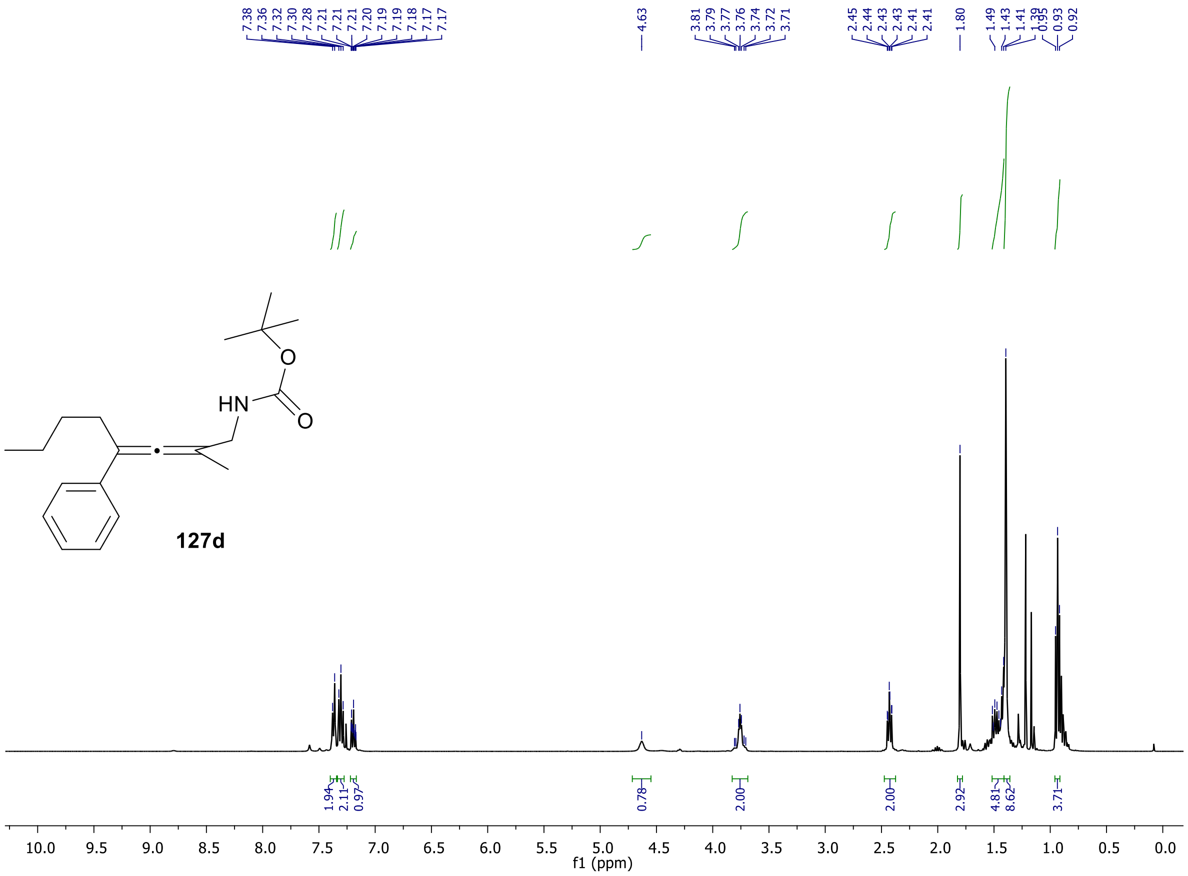


154.80
78.96
46.05
45.71
28.65
25.85
25.10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.33
7.32
7.31
7.31
7.30
7.29
7.28
7.23
7.21
7.20
7.19
7.17
4.89
4.88
4.82
4.81
4.62
3.78
3.77
3.41
3.40
3.37
3.35
3.34
3.32
2.08
1.88
1.86
1.85
1.83
1.82
1.76
1.75
1.47
1.40
HN
N
O
3.95
0.98
1.36
0.31
2.00
2.43
1.13
1.35
2.38
2.93
7.77
10.98
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)

127c


198.87
155.87
155.68
154.27
154.12
135.85
131.88
128.43
127.11
111.81
110.53
104.03
103.48
79.32
79.20
57.75
57.54
46.49
46.10
43.57
43.47
32.03
30.85
28.73
28.67
28.53
28.49
23.51
16.97
16.81
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.38
7.36
7.32
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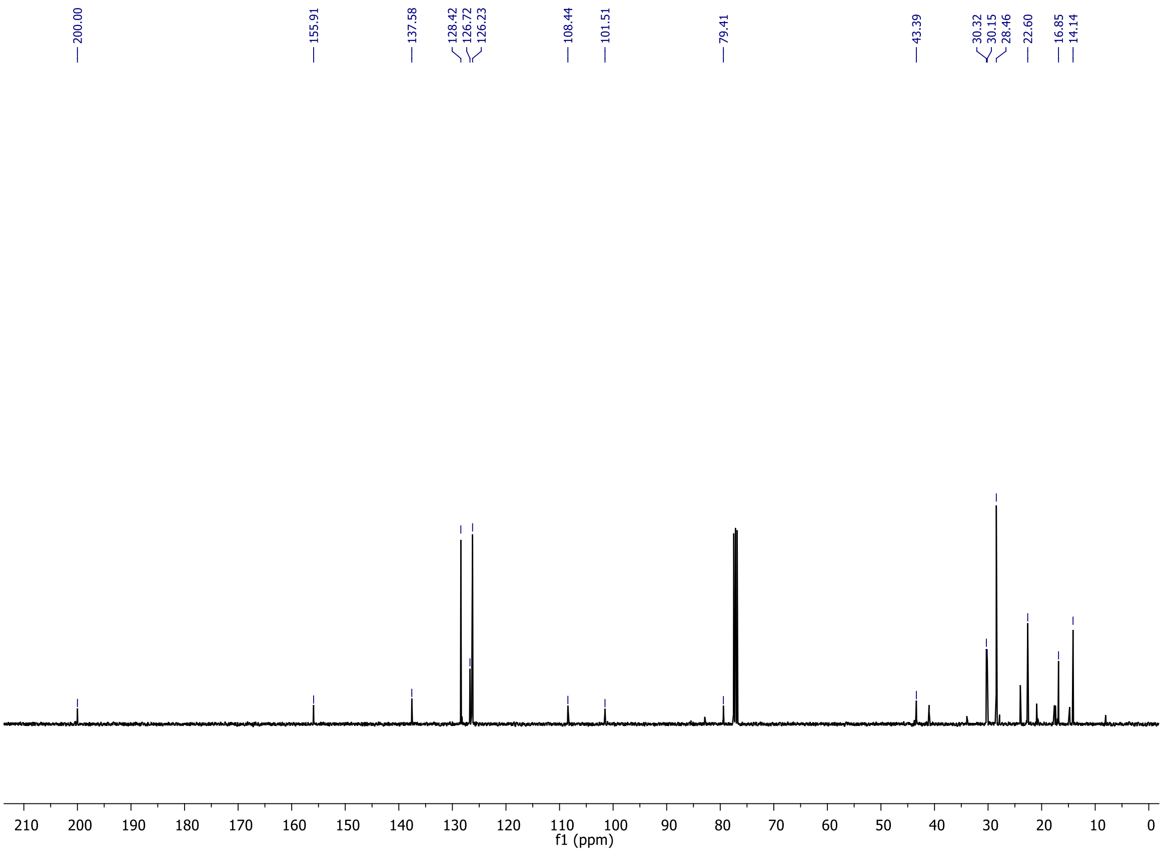
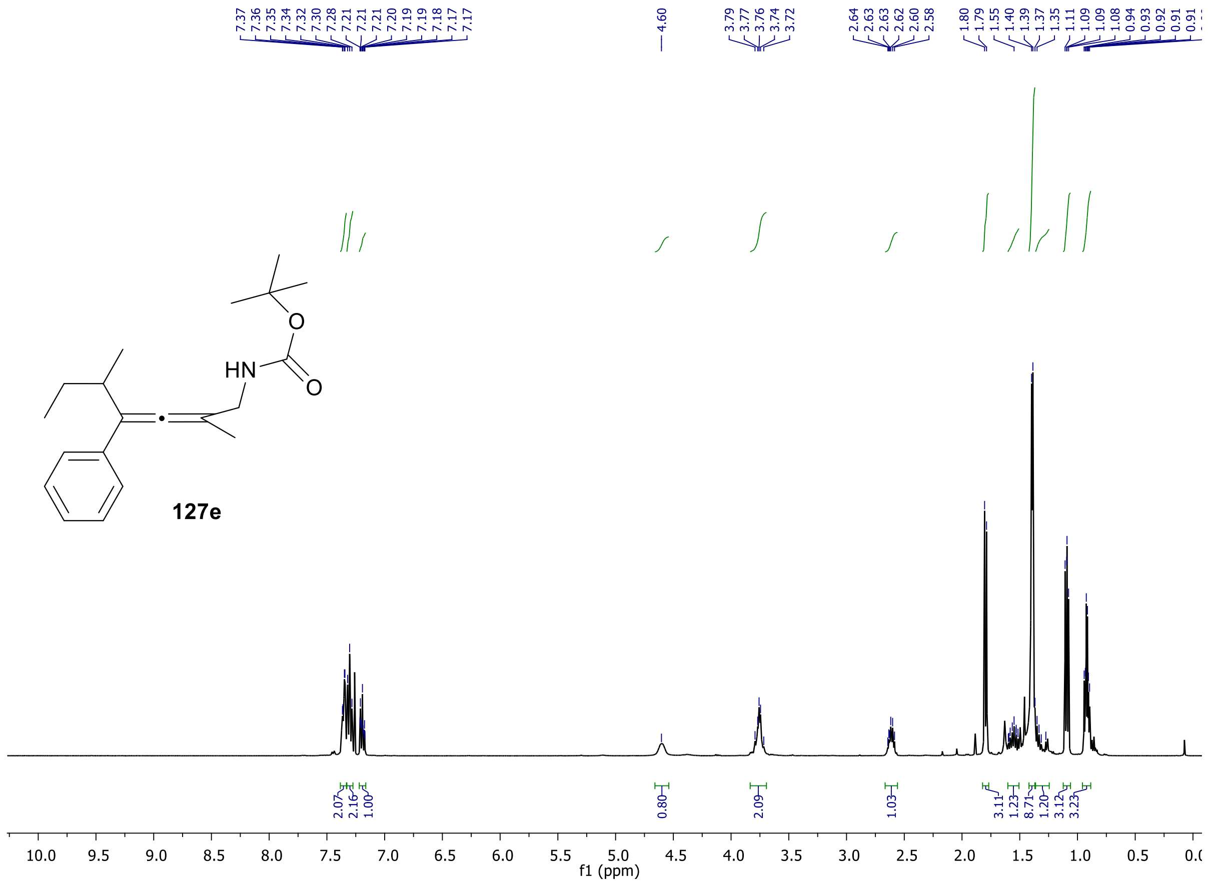
7.28
7.21
7.21
7.21
7.20
7.19
7.19
7.18
7.17
7.17
4.63
3.81
3.79
3.77
3.76
3.74
3.72
3.71
2.45
2.44
2.43
2.43
2.41
2.41
1.80
1.49
1.43
1.41
1.39
0.95
0.93
0.92
HN
O
O
1.94
2.11
0.97
0.78
2.00
2.00
2.92
4.81
8.62
3.71
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

127d


200.00
155.91
137.58
128.42
126.72
126.23
108.44
101.51
79.41
43.39
30.32
30.15
28.46
22.60
16.85
14.14
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.37
7.36
7.35
7.34
7.32
7.30
7.28
7.21
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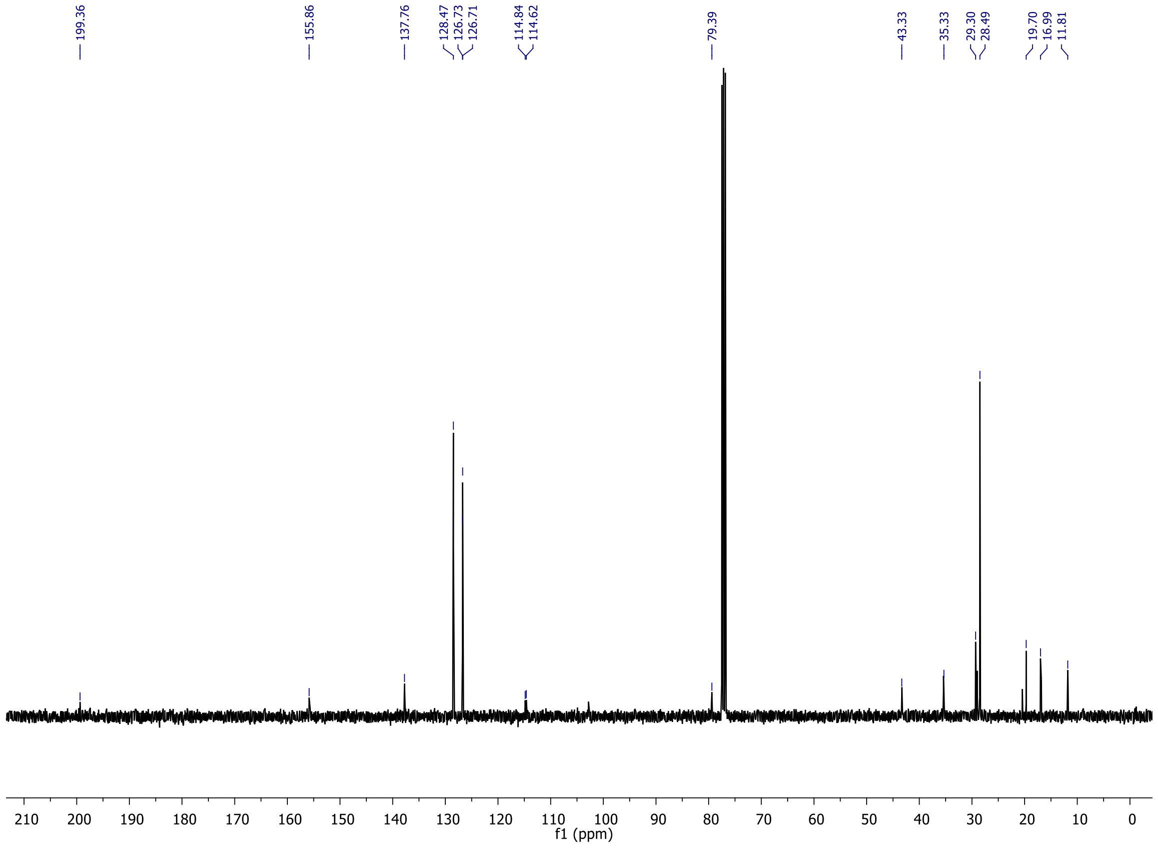
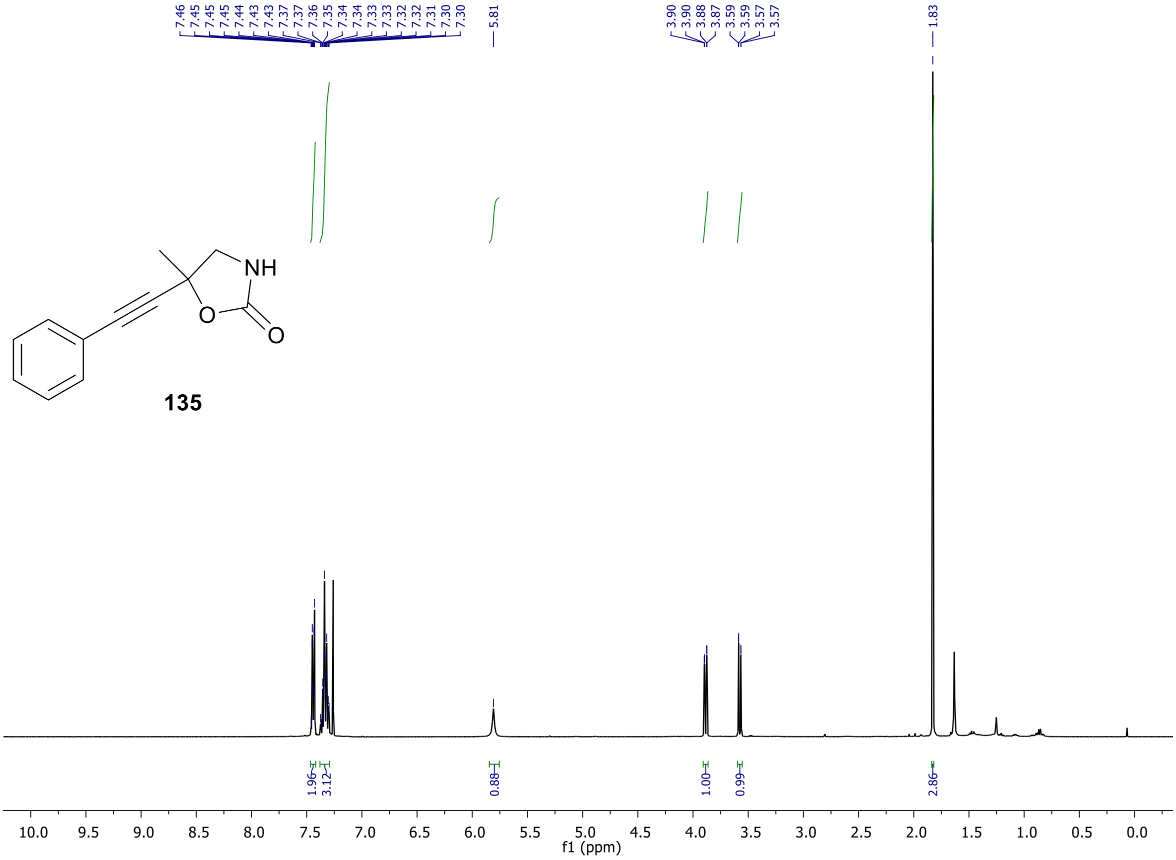
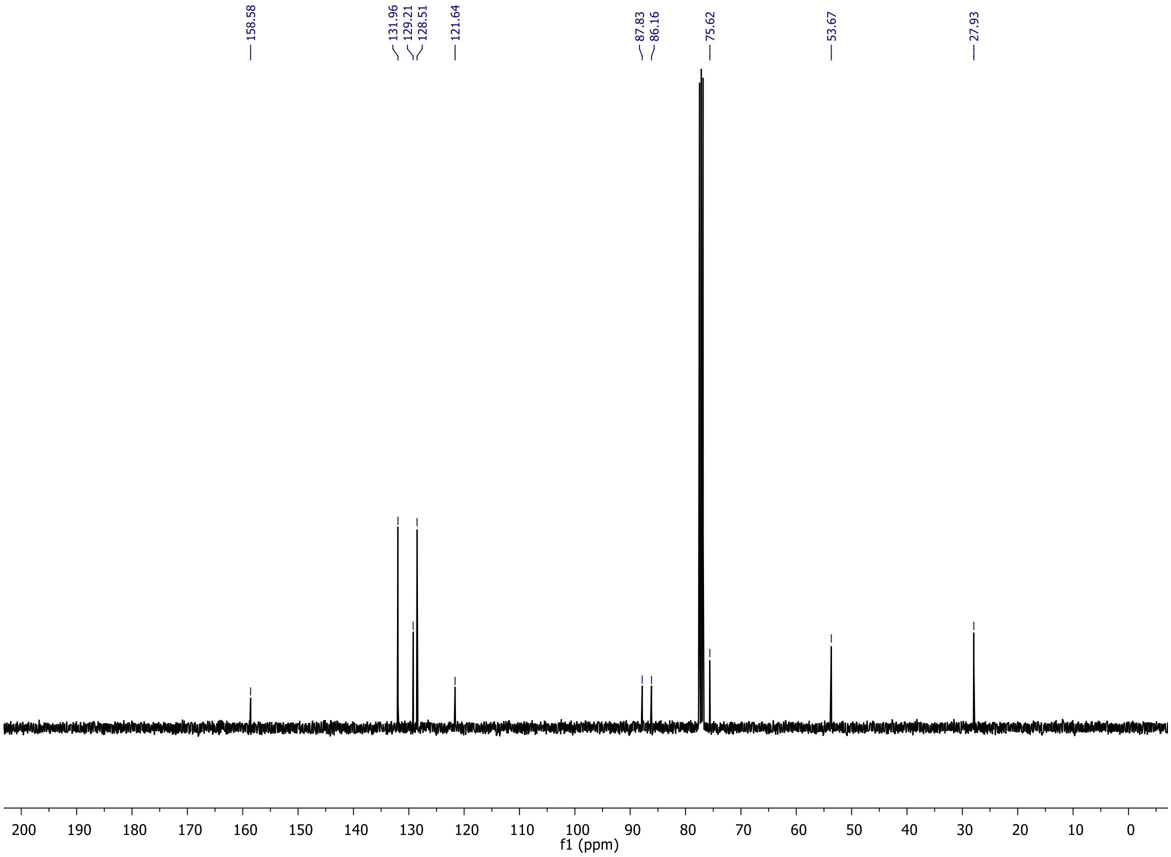
7.20
7.19
7.19
7.18
7.17
7.17
4.60
3.79
3.77
3.76
3.74
3.72
2.64
2.63
2.63
2.62
2.60
2.58
1.80
1.79
1.55
1.40
1.39
1.37
1.35
1.11
1.09
1.08
0.94
0.93
0.92
0.91
0.91
HN
O
O
2.07
2.16
1.00
0.80
2.09
1.03
3.11
1.23
8.71
1.20
3.12
3.23
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

127e


199.36
155.86
137.76
128.47
126.73
126.71
114.84
114.62
79.39
43.33
35.33
29.30
28.49
19.70
16.99
11.81
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

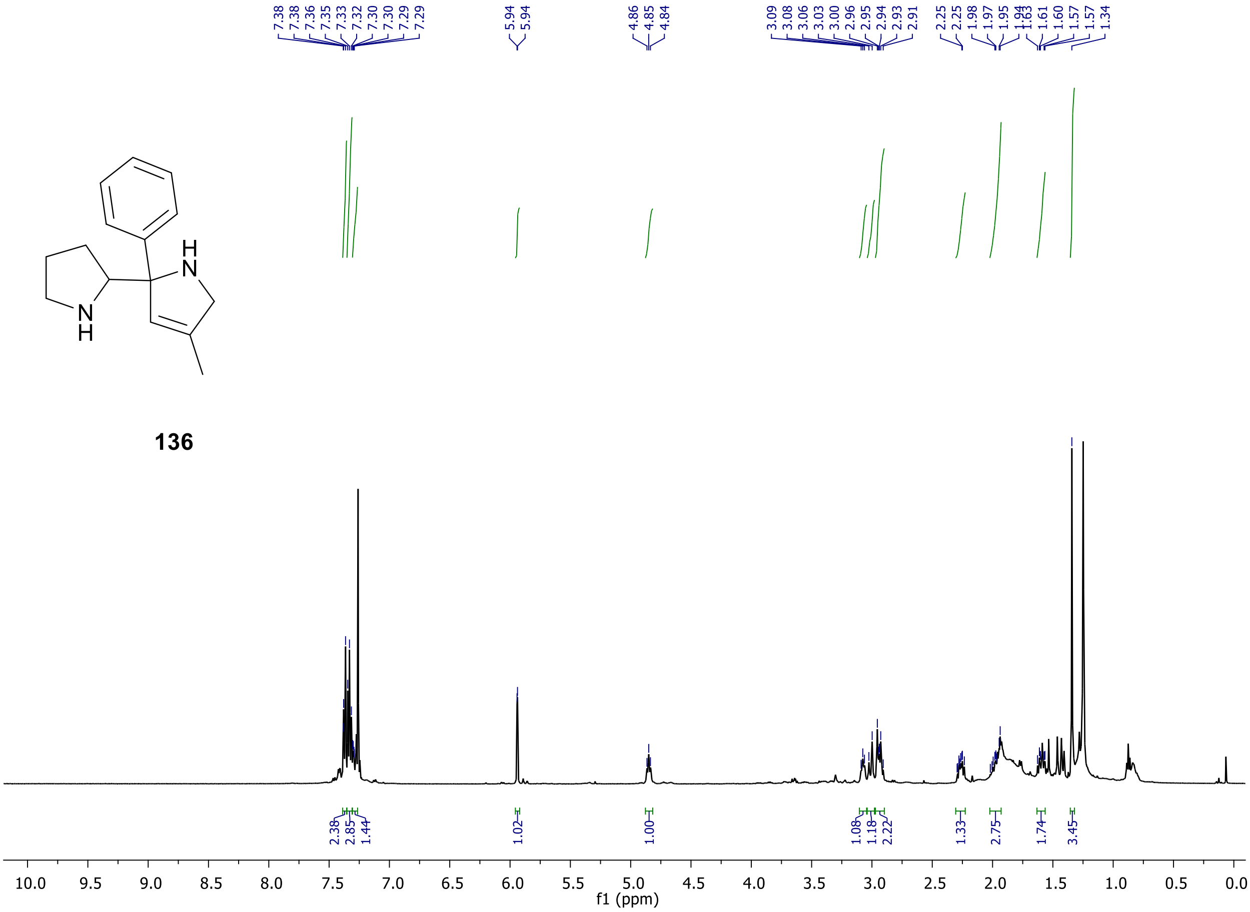

7.46
7.45
7.45
7.45
7.44
7.43
7.43
7.37
7.37
7.36
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.31
7.30
7.30
5.81
3.90
3.90
3.88
3.87
3.59
3.59
3.57
3.57
1.83
NH
O
O
1.96
3.12
0.88
1.00
0.99
2.86
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

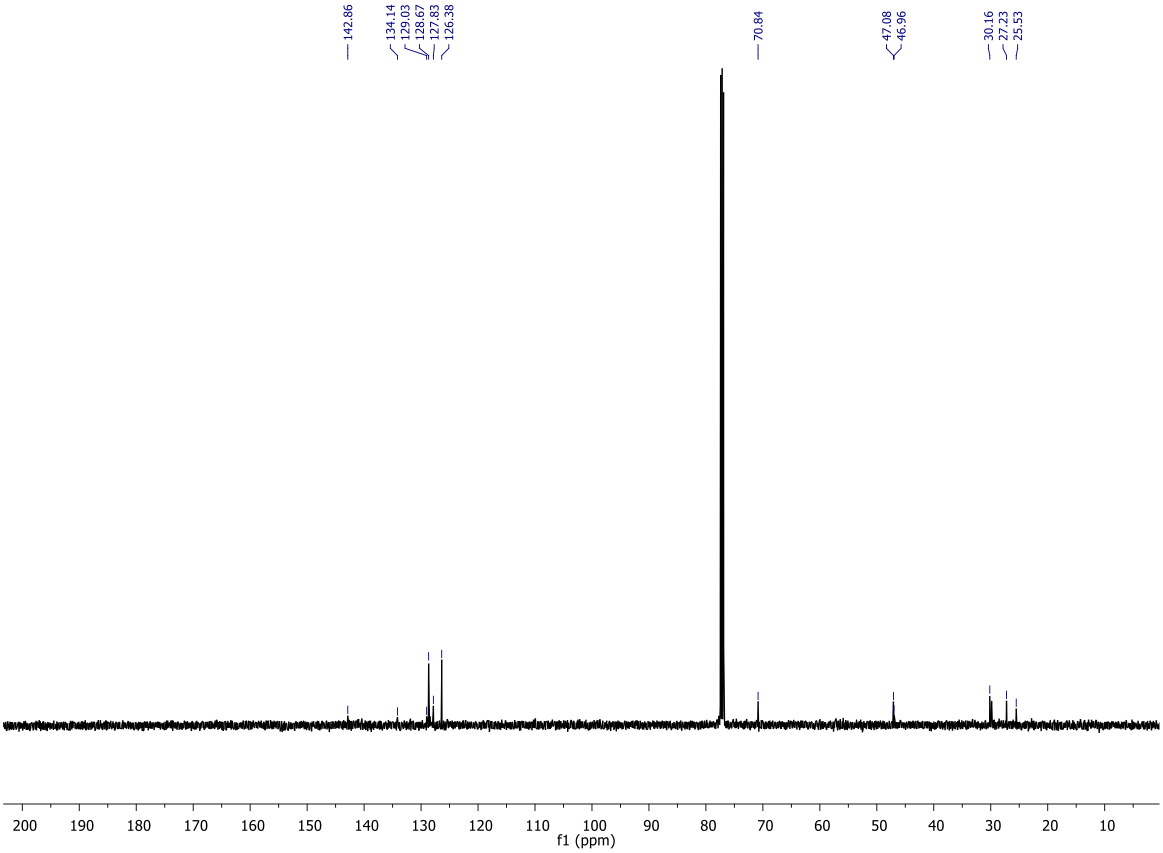
135

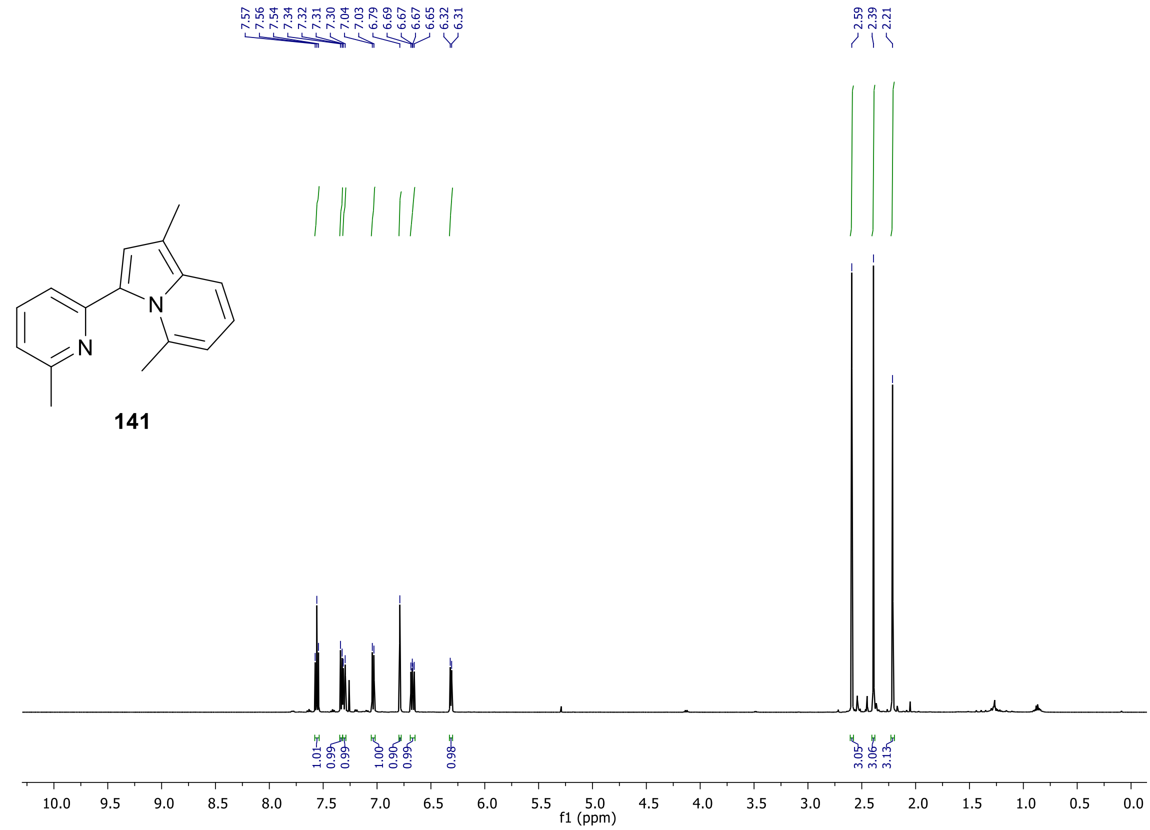

158.58
131.96
129.21
128.51
121.64
87.83
86.16
75.62
53.67
27.93
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

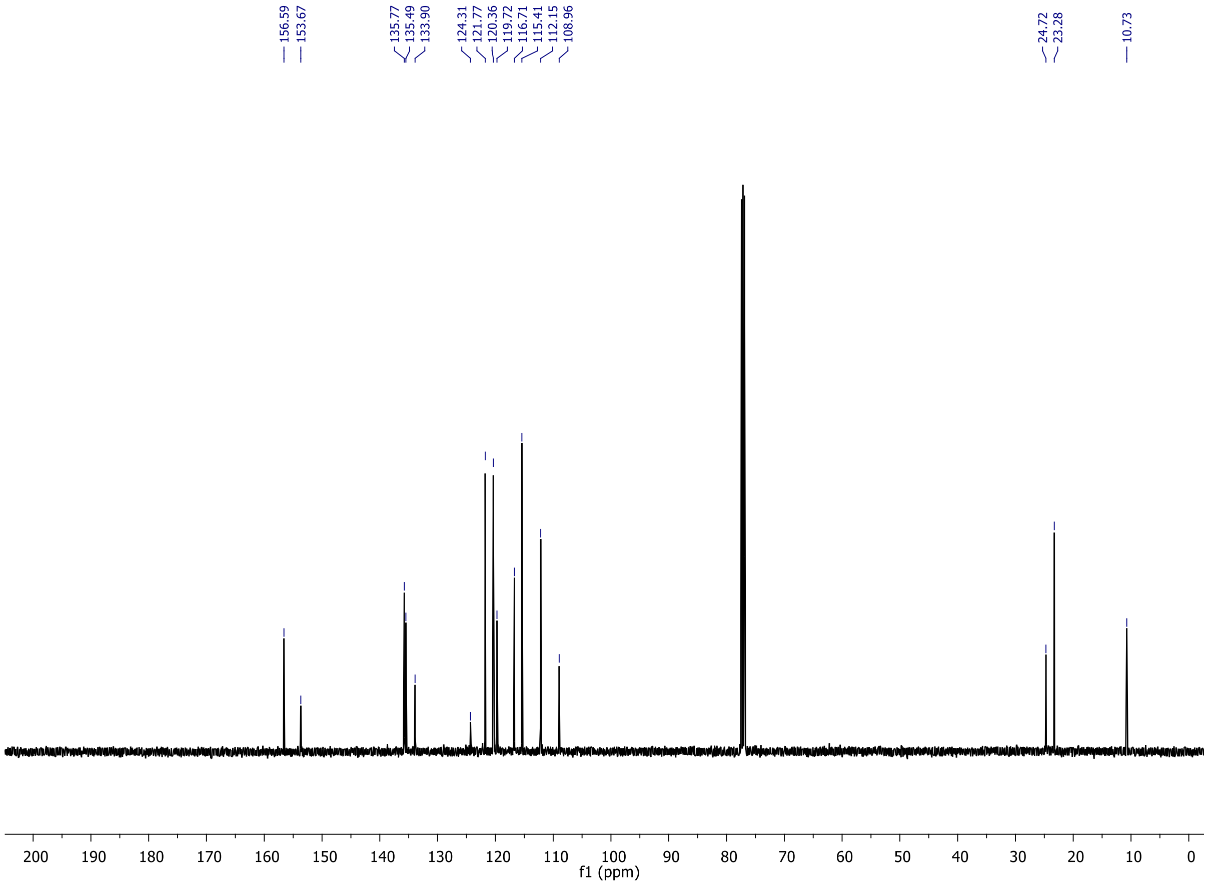
H
N
N
H

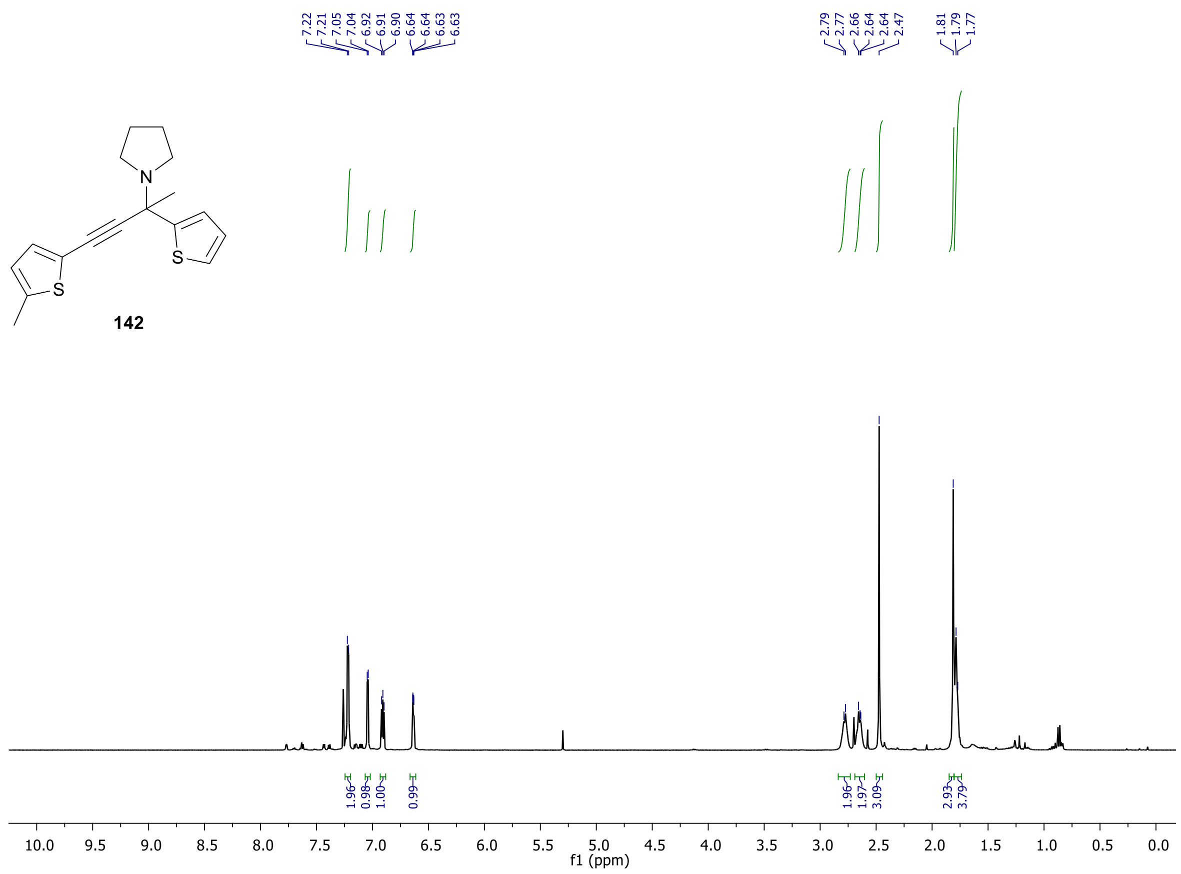
136


7.38
7.38
7.36
7.35
7.33
7.32
7.30
7.30
7.29
7.29
5.94
5.94
4.86
4.85
4.84
3.09
3.08
3.06
3.03
3.00
2.96
2.95
2.94
2.93
2.91
2.25
2.25
1.98
1.97
1.95
1.94
1.63
1.61
1.60
1.57
1.57
1.34
2.38
2.85
1.44
1.02
1.00
1.08
1.18
2.22
1.33
2.75
1.74
3.45
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)


142.86
134.14
129.03
128.67
127.83
126.38
70.84
47.08
46.96
30.16
27.23
25.53
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

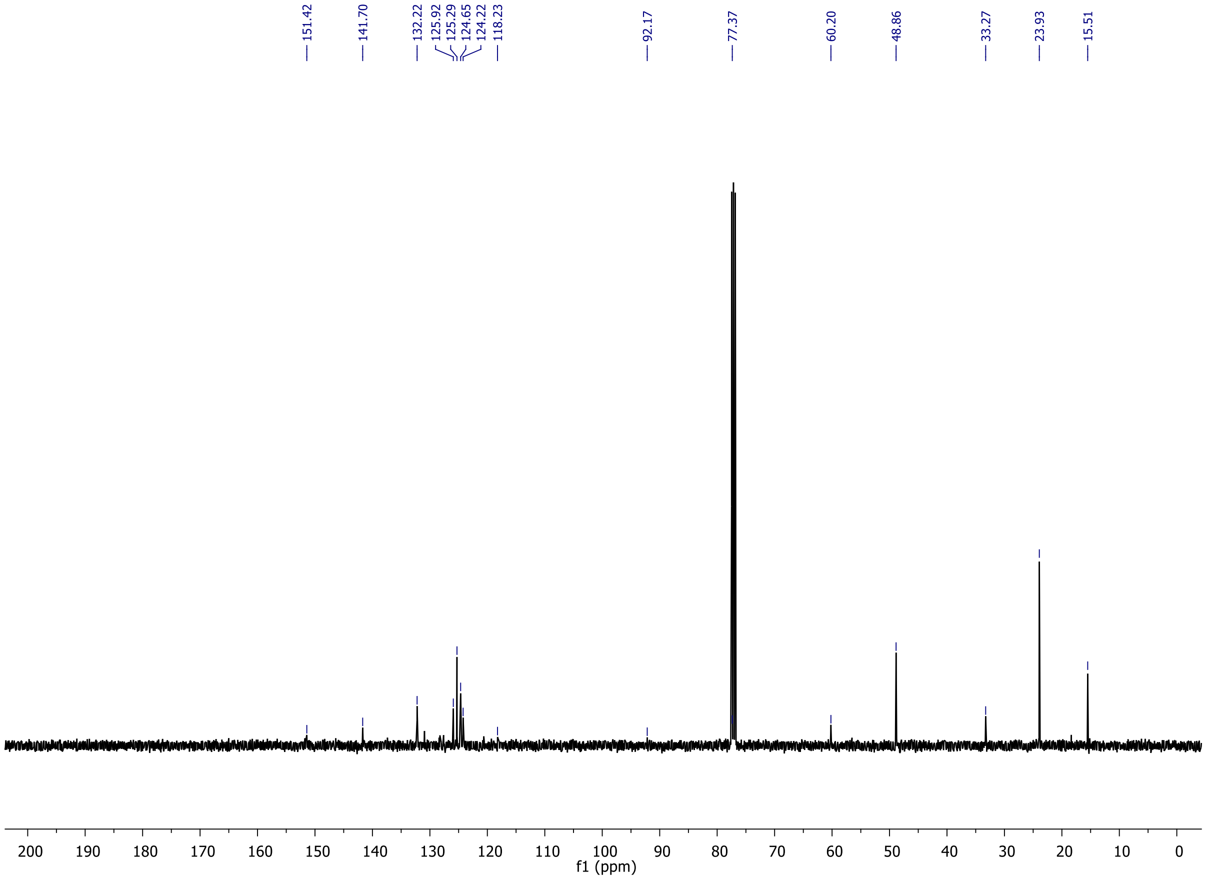

7.57
7.56
7.54
7.34
7.32
7.31
7.30
7.04
7.03
6.79
6.69
6.67
6.67
6.65
6.32
6.31
2.59
2.39
2.21
N
N
141
1.01
0.99
0.99
1.00
0.90
0.99
0.98
3.05
3.06
3.13
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


156.59
153.67
135.77
135.49
133.90
124.31
121.77
120.36
119.72
116.71
115.41
112.15
108.96
24.72
23.28
10.73
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

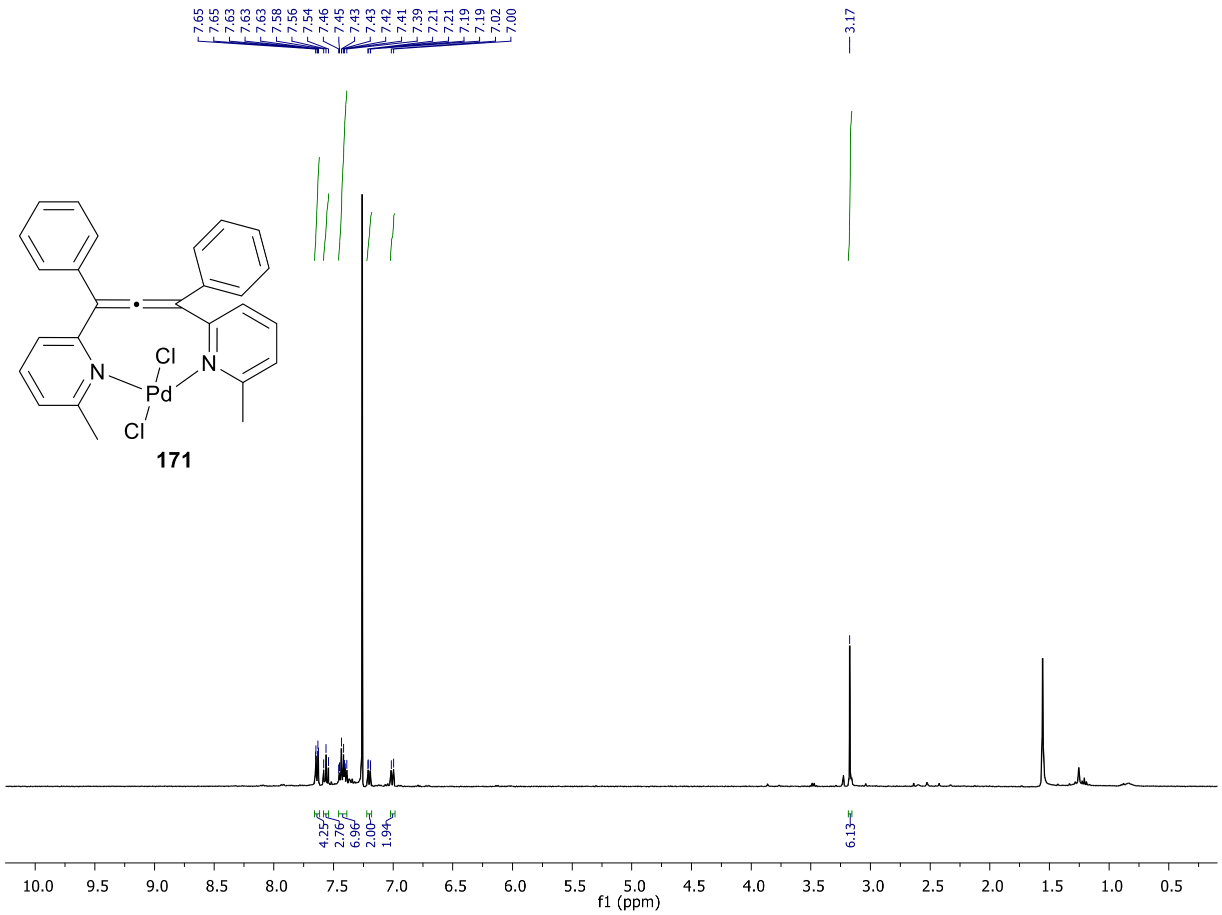


142

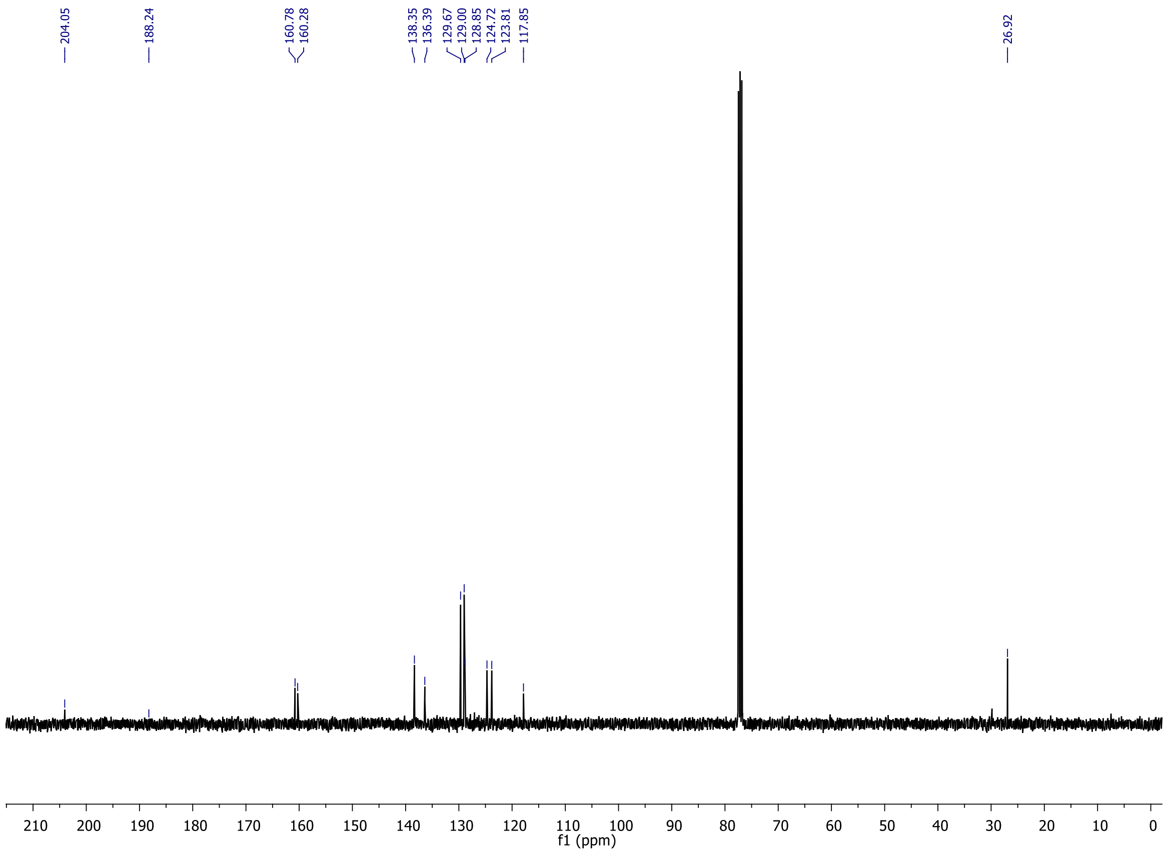
N
S
S
7.22
7.21
7.05
7.04
6.92
6.91
6.90
6.64
6.64
6.63
6.63
2.79
2.77
2.66
2.64
2.64
2.47
1.81
1.79
1.77
1.96
0.98
1.00
0.99
1.96
1.97
3.09
2.93
3.79
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

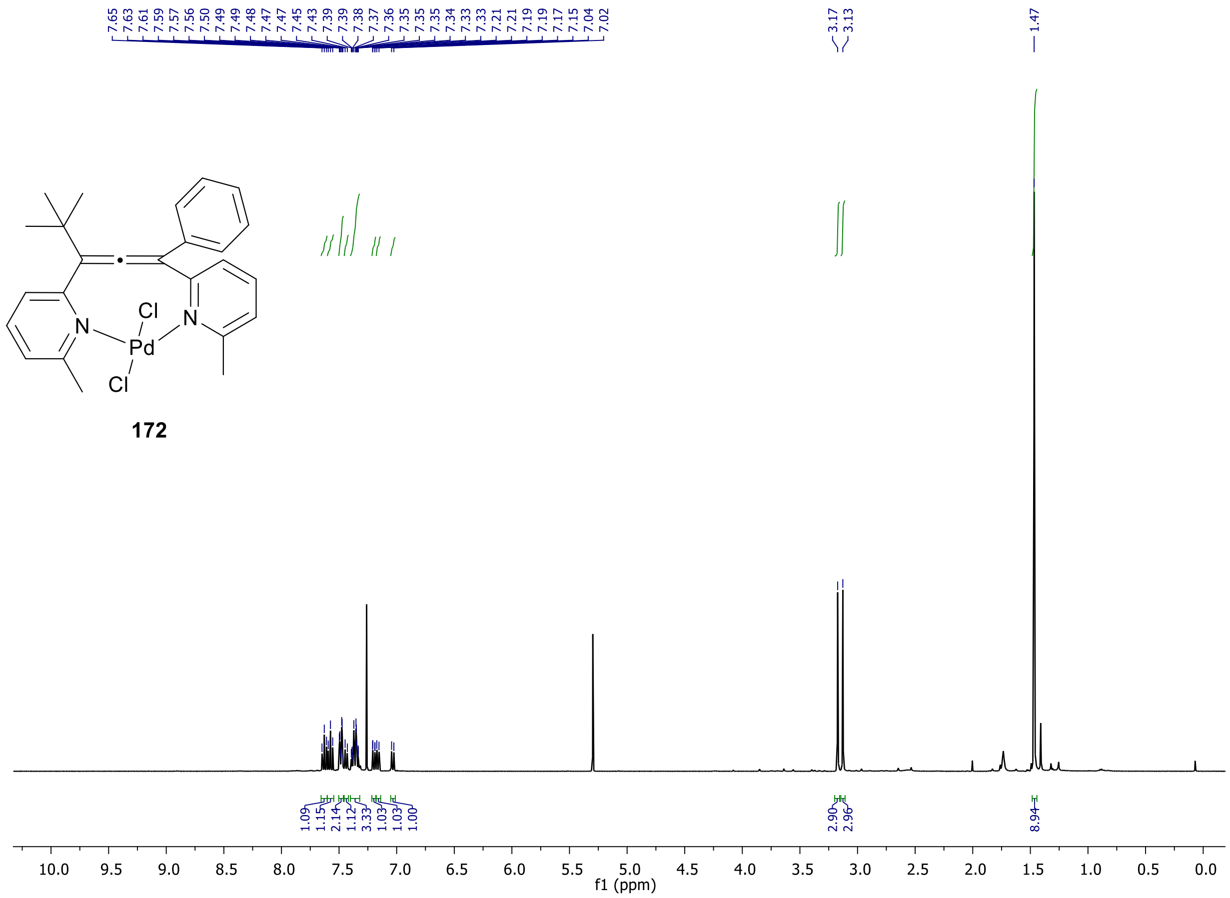


151.42
141.70
132.22
125.92
125.29
124.65
124.22
118.23
92.17
77.37
60.20
48.86
33.27
23.93
15.51
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

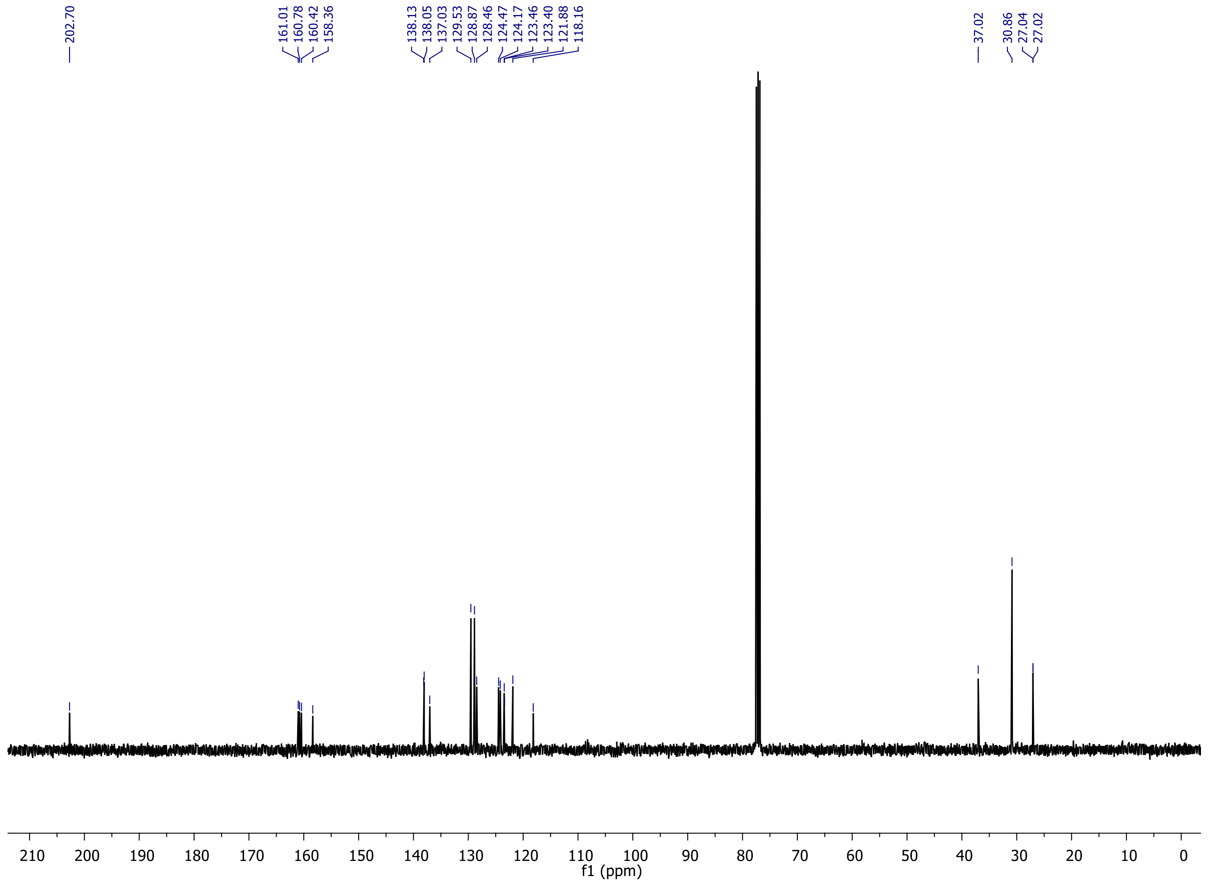

7.65
7.65
7.63
7.63
7.63
7.58
7.56
7.54
7.46
7.45
7.43
7.43
7.42
7.41
7.39
7.21
7.21
7.19
7.02
7.00
3.17
Cl
Pd
Cl
N
N
4.25
2.76
6.96
2.00
1.94
6.13
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

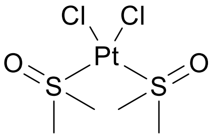
171


204.05
188.24
160.78
160.28
138.35
136.39
129.67
129.00
128.85
124.72
123.81
117.85
26.92
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

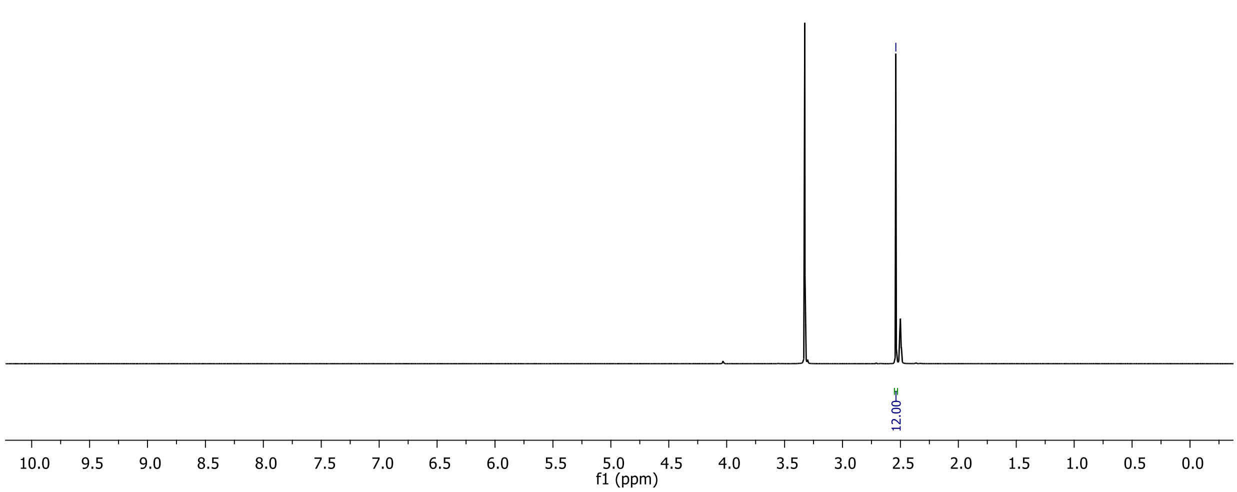

7.65
7.63
7.61
7.59
7.57
7.56
7.50
7.49
7.49
7.48
7.47
7.47
7.45
7.43
7.39
7.39
7.38
7.37
7.36
7.35
7.35
7.34
7.33
7.33
7.21
7.21
7.19
7.19
7.17
7.15
7.04
7.02
3.17
3.13
1.47
Cl
N
N
Pd
Cl
1.09
1.15
2.14
1.12
3.33
1.03
1.03
1.00
2.90
2.96
8.94
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

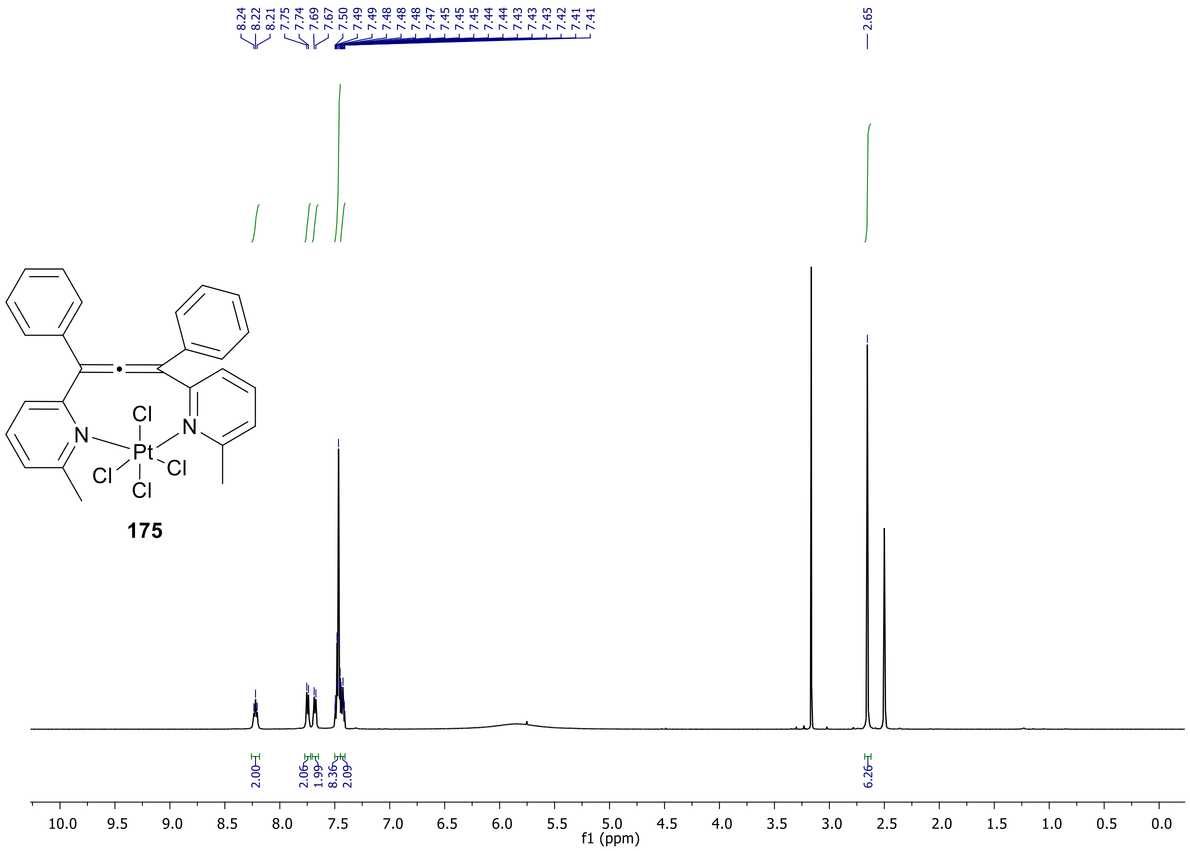
172


202.70
161.01
160.78
160.42
158.36
138.13
138.05
137.03
129.53
128.87
128.46
124.47
124.17
123.46
123.40
121.88
118.16
37.02
30.86
27.04
27.02
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

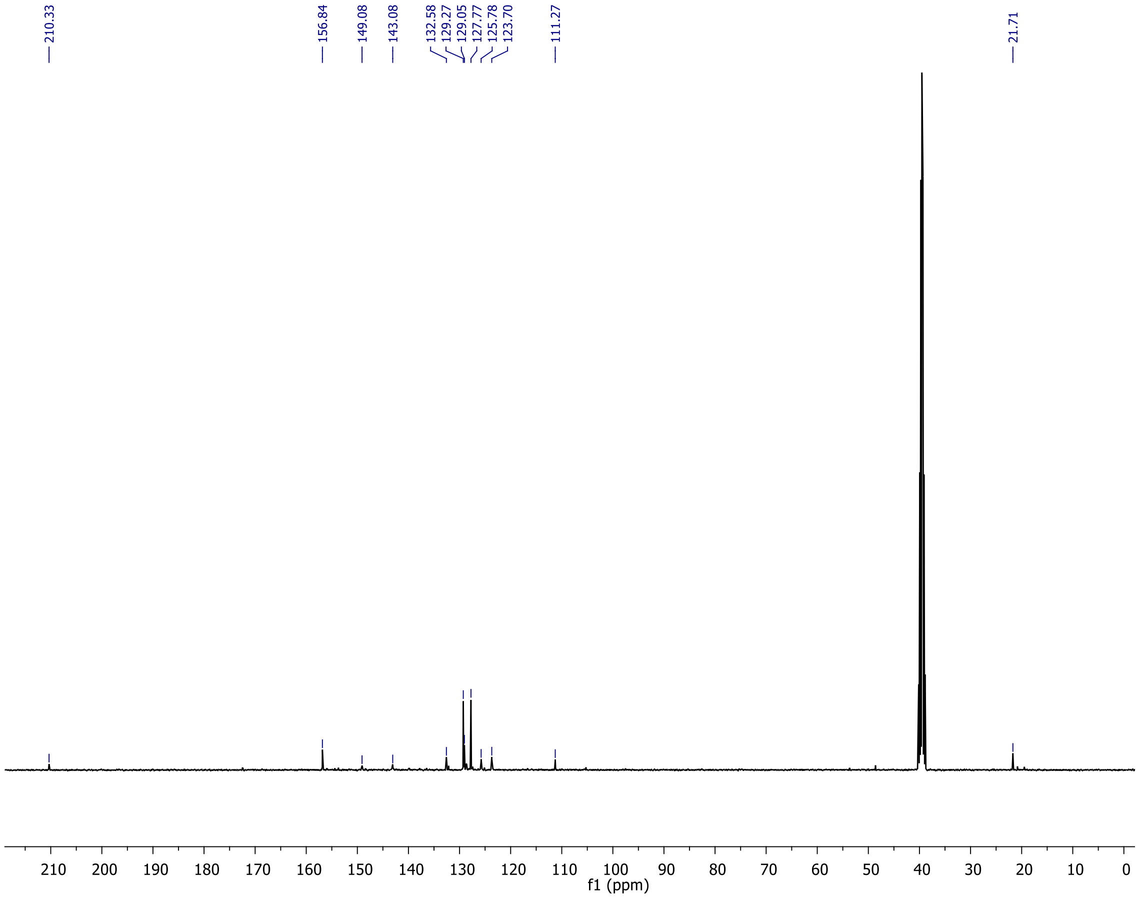


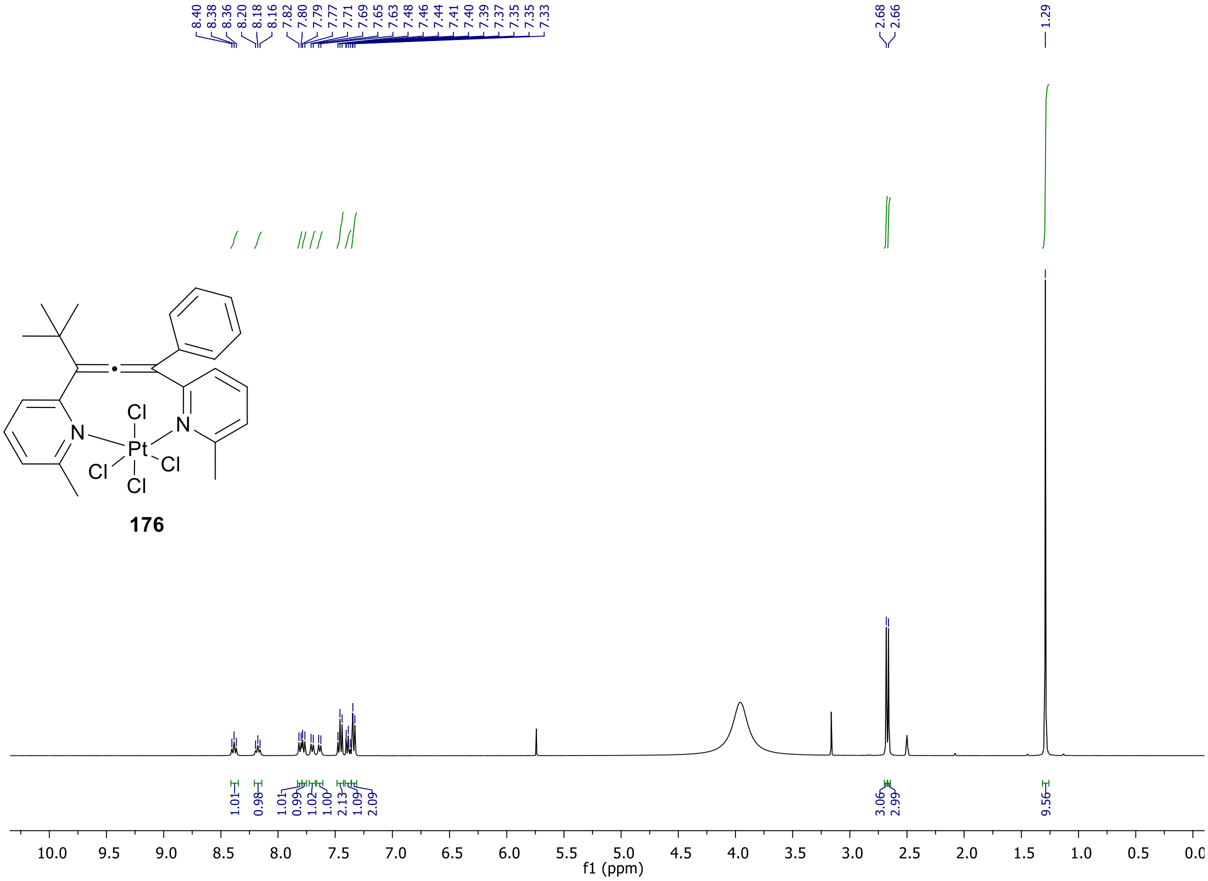
173


2.54
12.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

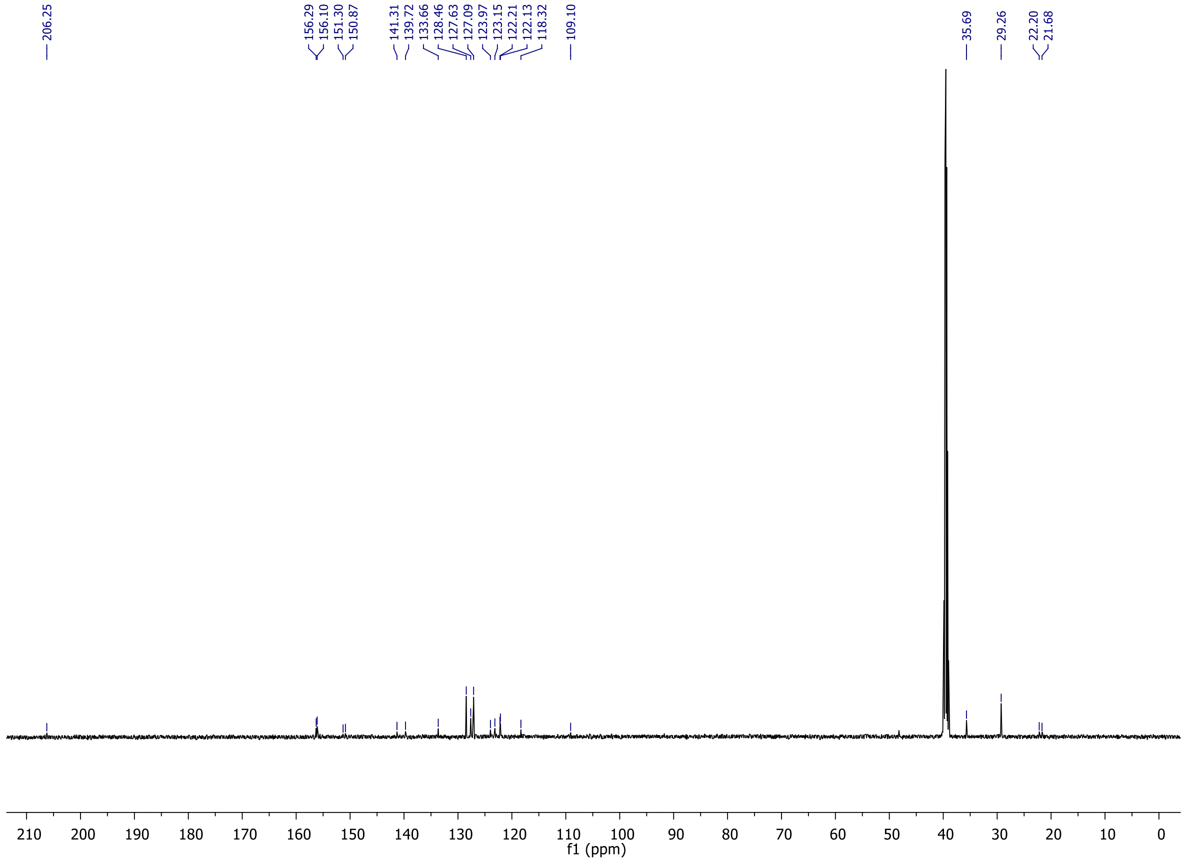

8.24
8.22
8.21
7.75
7.74
7.69
7.67
7.50
7.49
7.49
7.48
7.48
7.48
7.47
7.45
7.45
7.45
7.44
7.44
7.43
7.43
7.43
7.42
7.41
7.41
2.65
Cl
N
Pt
N
Cl
Cl
Cl
2.00
2.06
1.99
8.36
2.09
6.26
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

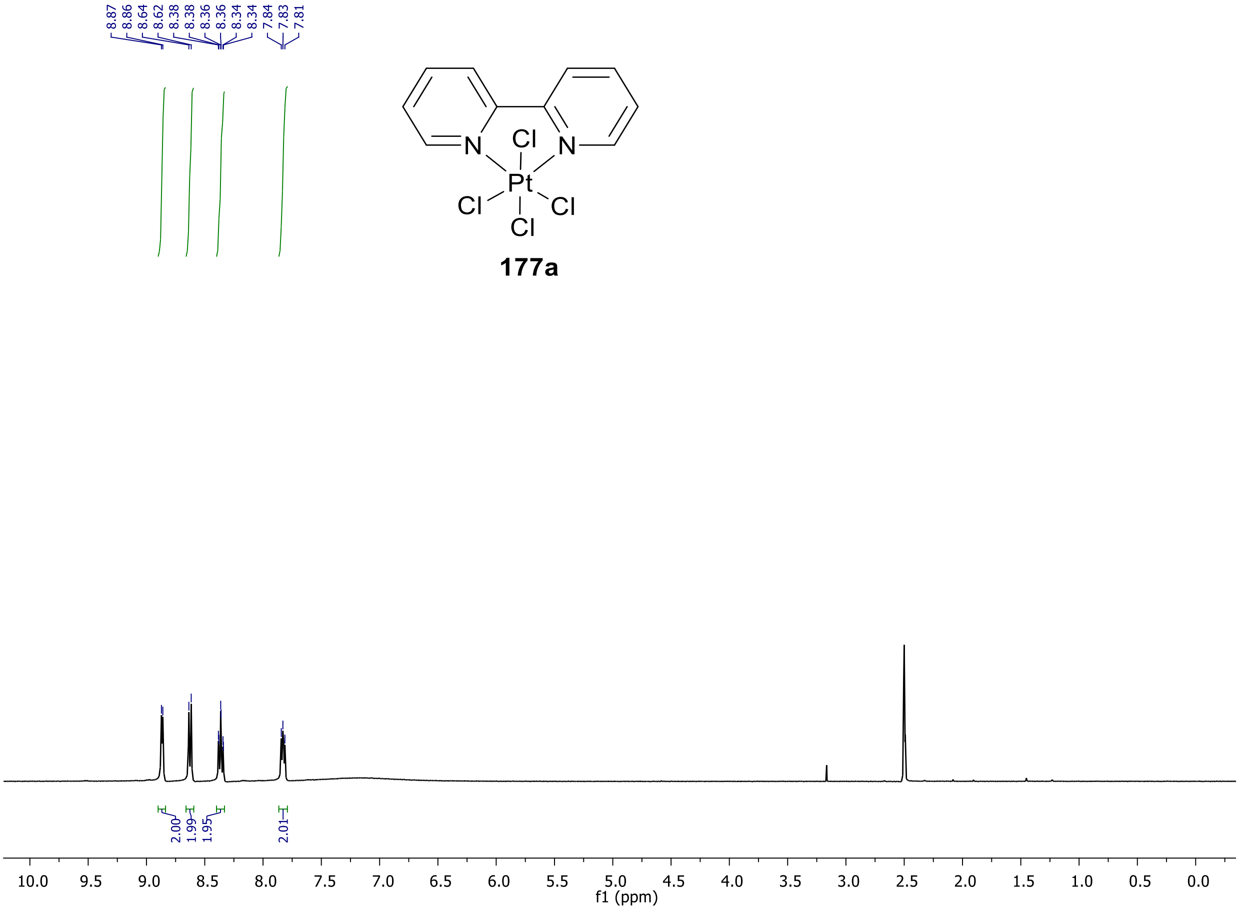
175


210.33
156.84
149.08
143.08
132.58
129.27
129.05
127.77
125.78
123.70
111.27
21.71
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

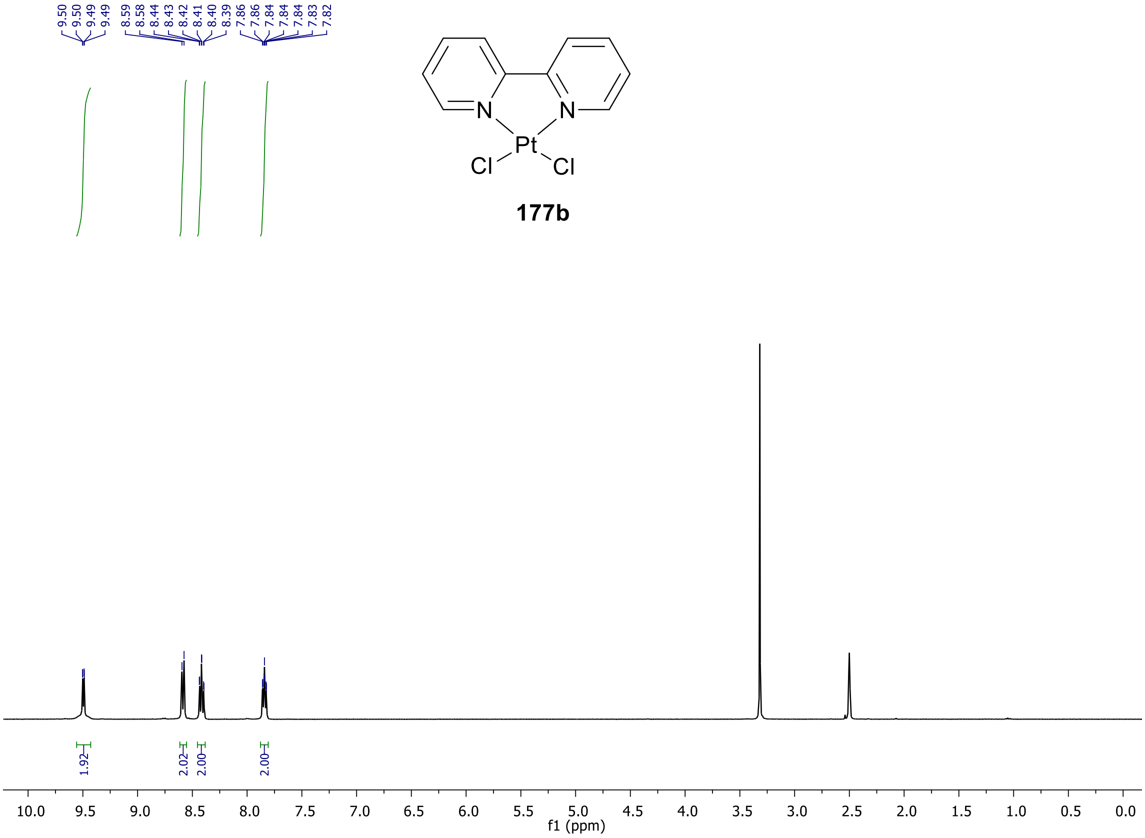

8.40
8.38
8.36
8.20
8.18
8.16
7.82
7.80
7.79
7.77
7.71
7.69
7.65
7.63
7.48
7.46
7.44
7.41
7.40
7.39
7.37
7.35
7.35
7.33
2.68
2.66
1.29
Cl
N
Pt
N
Cl
Cl
Cl
1.01
0.98
1.01
0.99
1.02
1.00
2.13
1.09
2.09
3.06
2.99
9.56
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

176

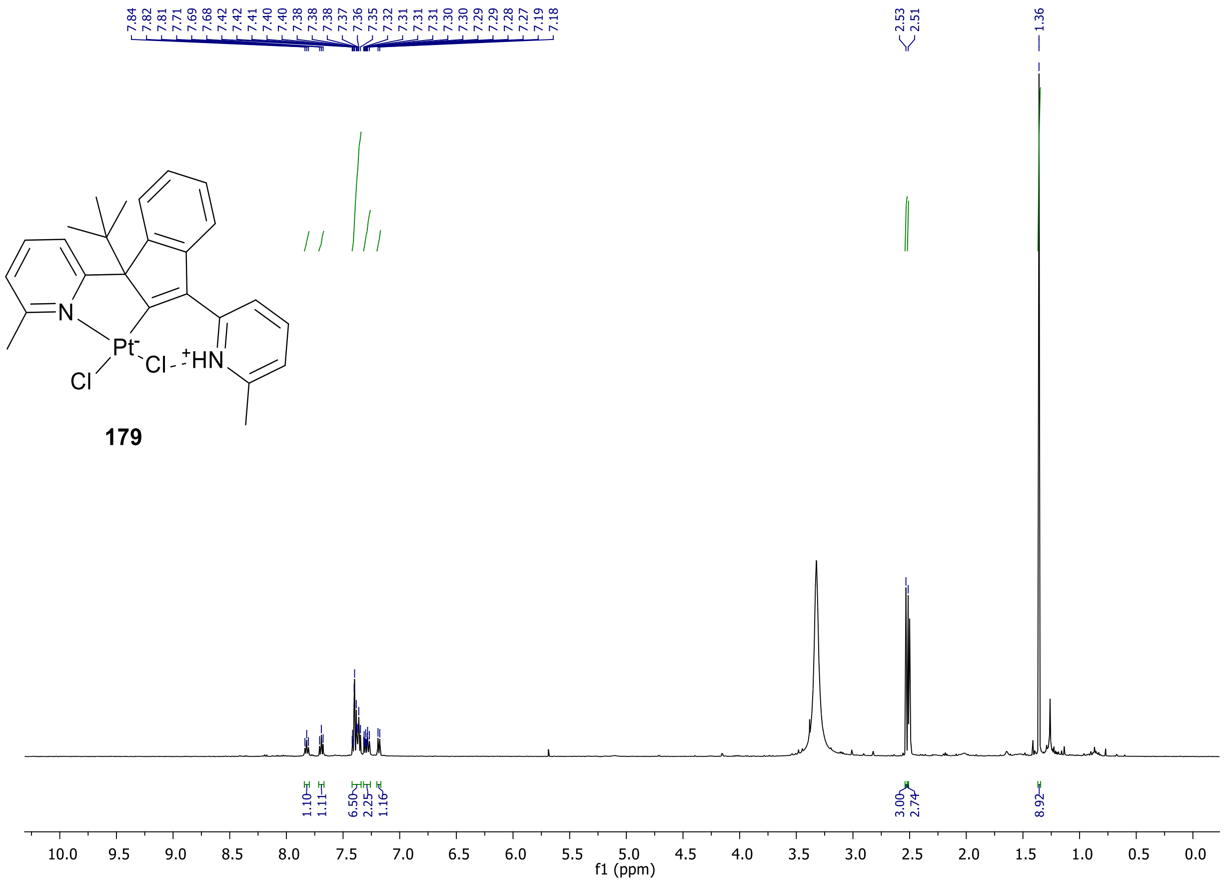

206.25
156.29
156.10
151.30
150.87
141.31
139.72
133.66
128.46
127.63
127.09
123.97
123.15
122.21
122.13
118.32
109.10
35.69
29.26
22.20
21.68
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.87
8.86
8.64
8.62
8.38
8.38
8.36
8.36
8.34
8.34
7.84
7.83
7.81
Cl
N
N
Pt
Cl
Cl
Cl
2.00
1.99
1.95
2.01
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)

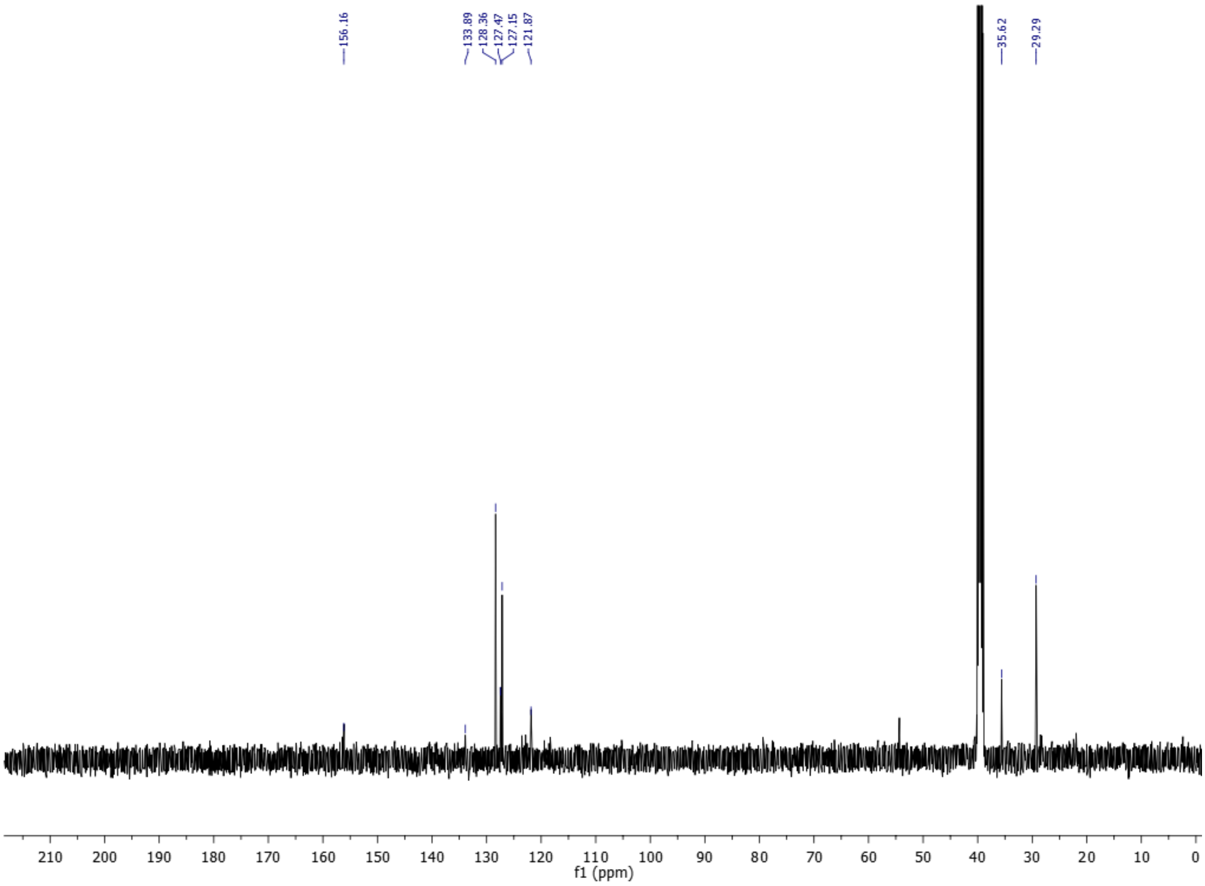
177a

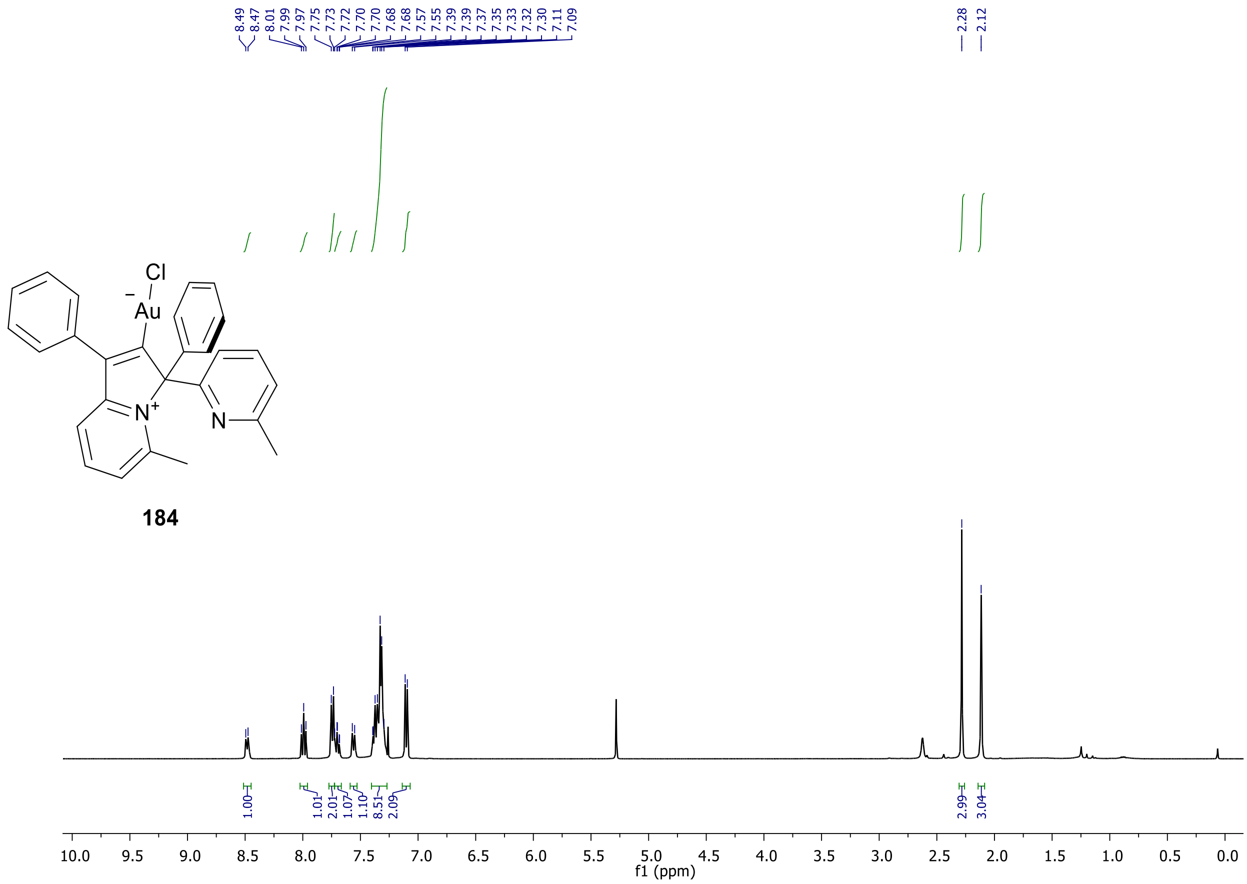

9.50
9.50
9.49
9.49
8.59
8.58
8.44
8.43
8.42
8.41
8.40
8.39
7.86
7.86
7.84
7.84
7.84
7.83
7.82
N
N
Pt
Cl
Cl
1.92
2.02
2.00
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

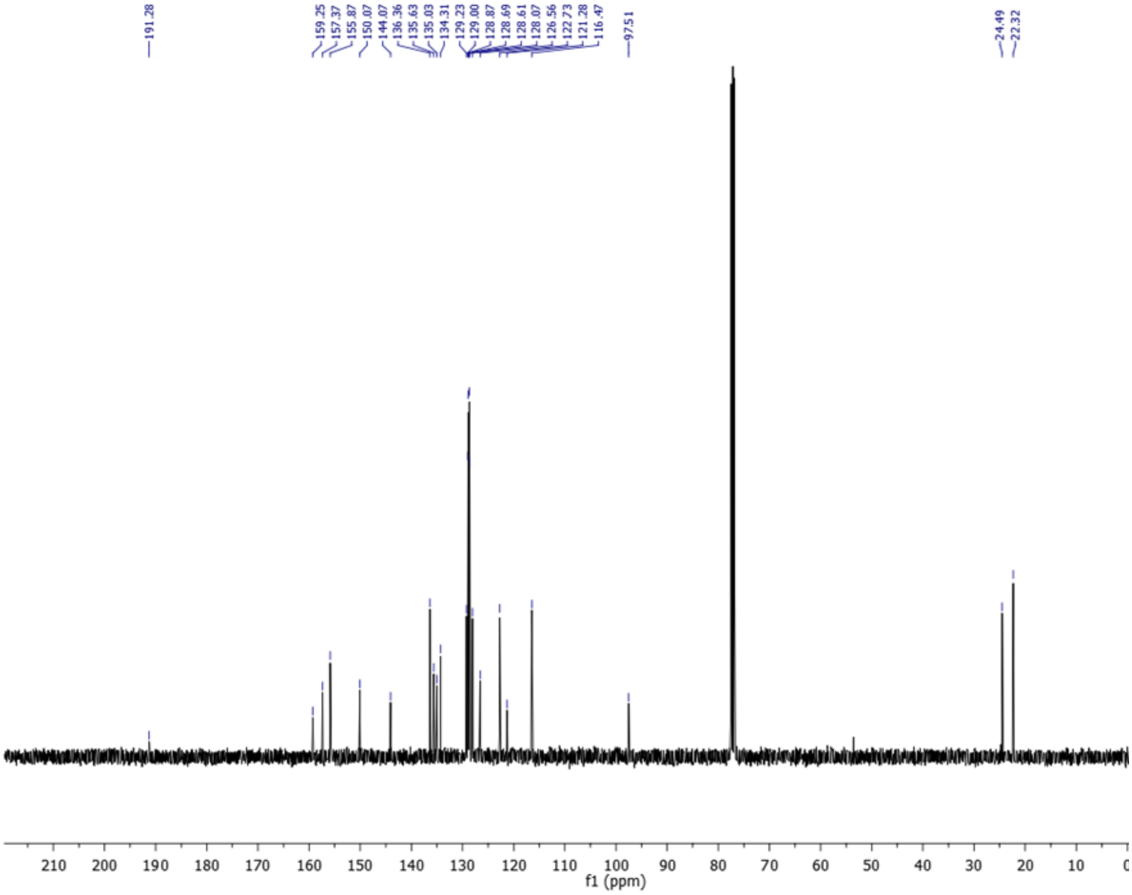
177b


7.84
7.82
7.81
7.71
7.69
7.68
7.42
7.42
7.41
7.40
7.38
7.38
7.38
7.37
7.36
7.35
7.32
7.31
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.27
7.19
7.18
2.53
2.51
1.36
N
Pt-
Cl
Cl
+HN
1.10
1.11
6.50
2.25
1.16
3.00
2.74
8.92
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)

179

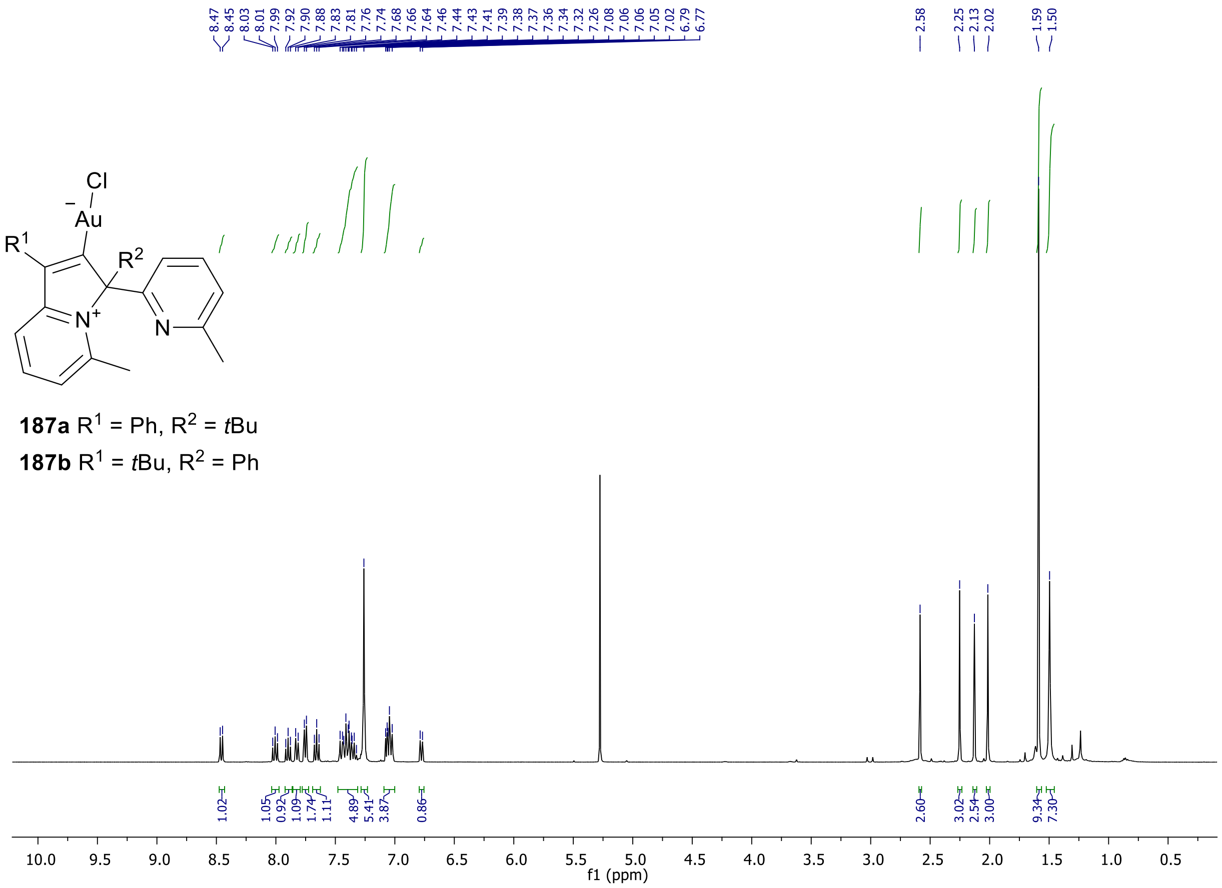

156.16
133.89
128.36
127.47
127.15
121.87
35.62
29.29
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

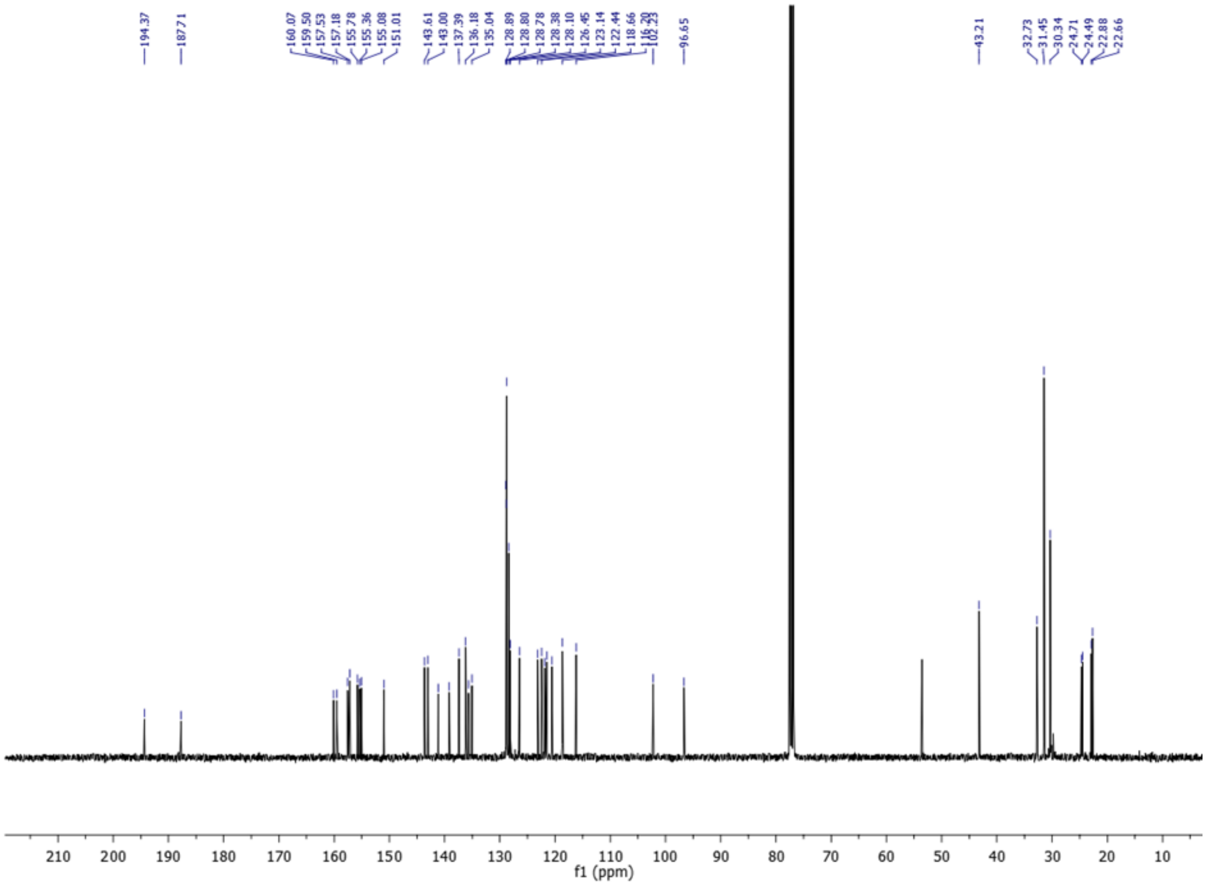

8.49
8.47
8.01
7.99
7.97
7.75
7.73
7.72
7.70
7.70
7.68
7.68
7.57
7.55
7.39
7.39
7.37
7.35
7.33
7.32
7.30
7.11
7.09
2.28
2.12
Cl
Au
N+
N
184
1.00
1.01
2.01
1.07
1.10
8.51
2.09
2.99
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

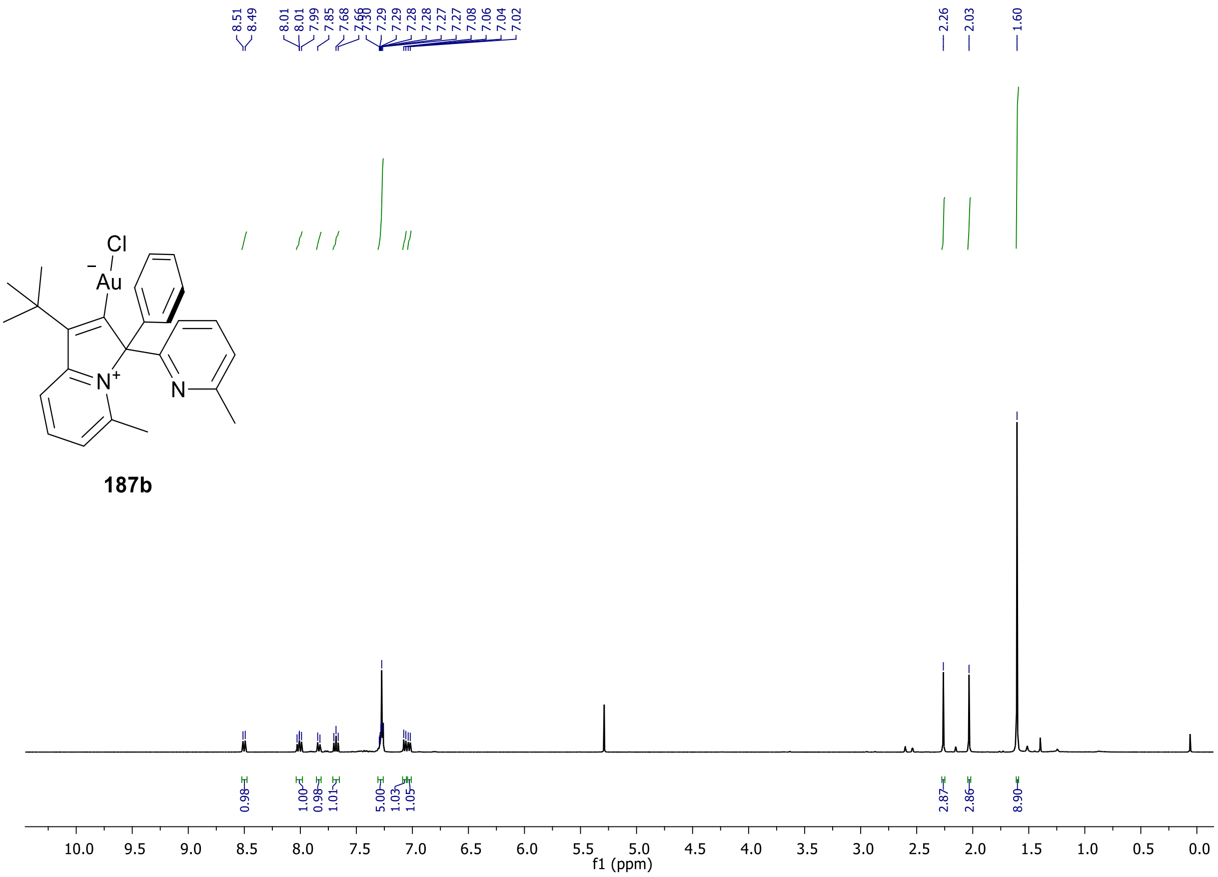

191.28
159.25
157.37
155.87
150.07
144.07
136.36
135.63
135.03
134.31
129.23
129.00
128.87
128.69
128.61
128.07
126.56
122.73
121.28
116.47
97.51
24.49
22.32
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

187a R^1 = Ph, R^2 = *t*Bu

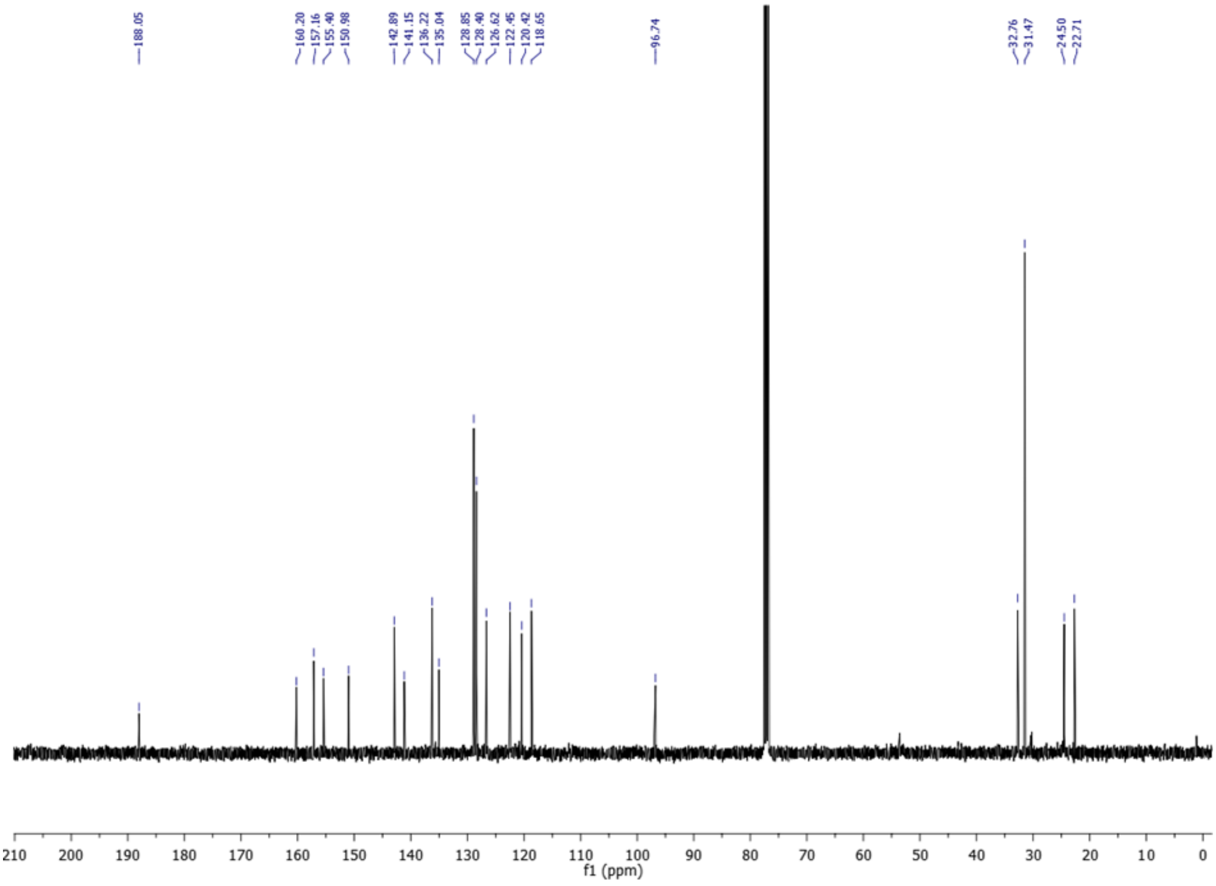
187b R^1 = *t*Bu, R^2 = Ph





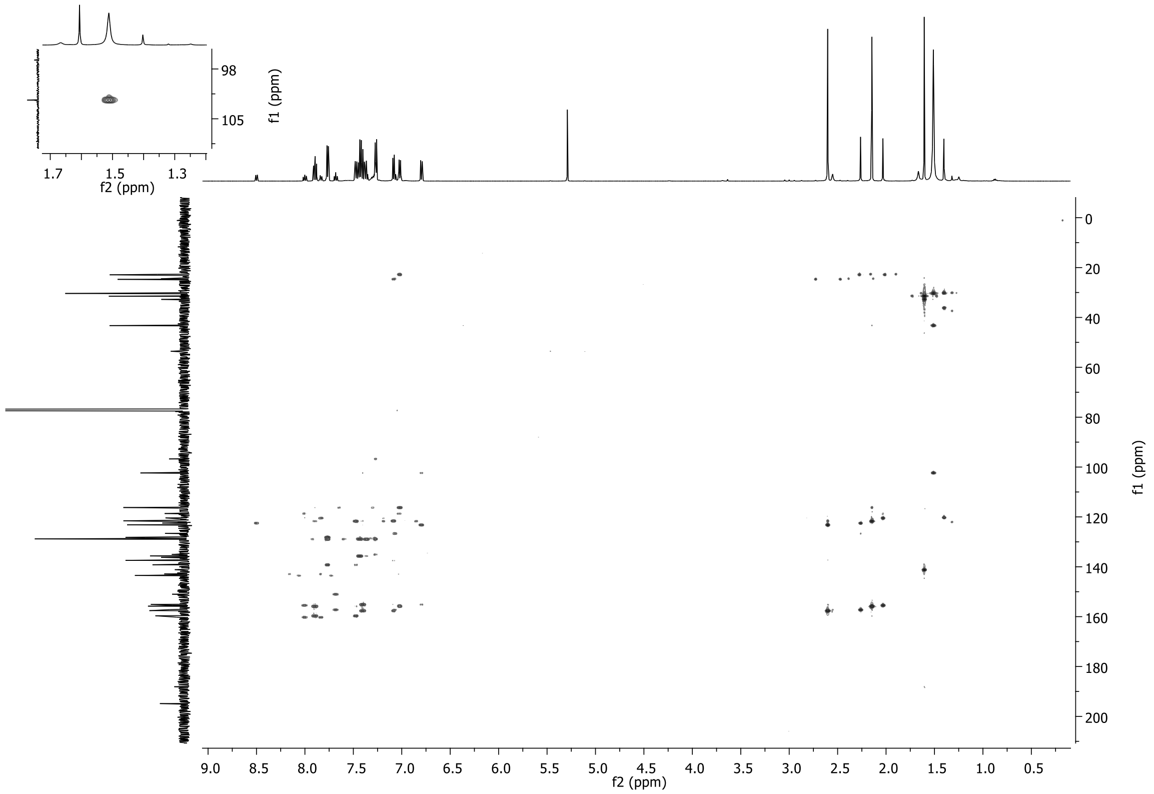

Cl
Au
N+
N
8.51
8.49
8.01
8.01
7.99
7.85
7.68
7.66
7.30
7.29
7.29
7.28
7.28
7.27
7.27
7.08
7.06
7.04
7.02
2.26
2.03
1.60
0.98
1.00
0.98
1.01
5.00
1.03
1.05
2.87
2.86
8.90
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

187b

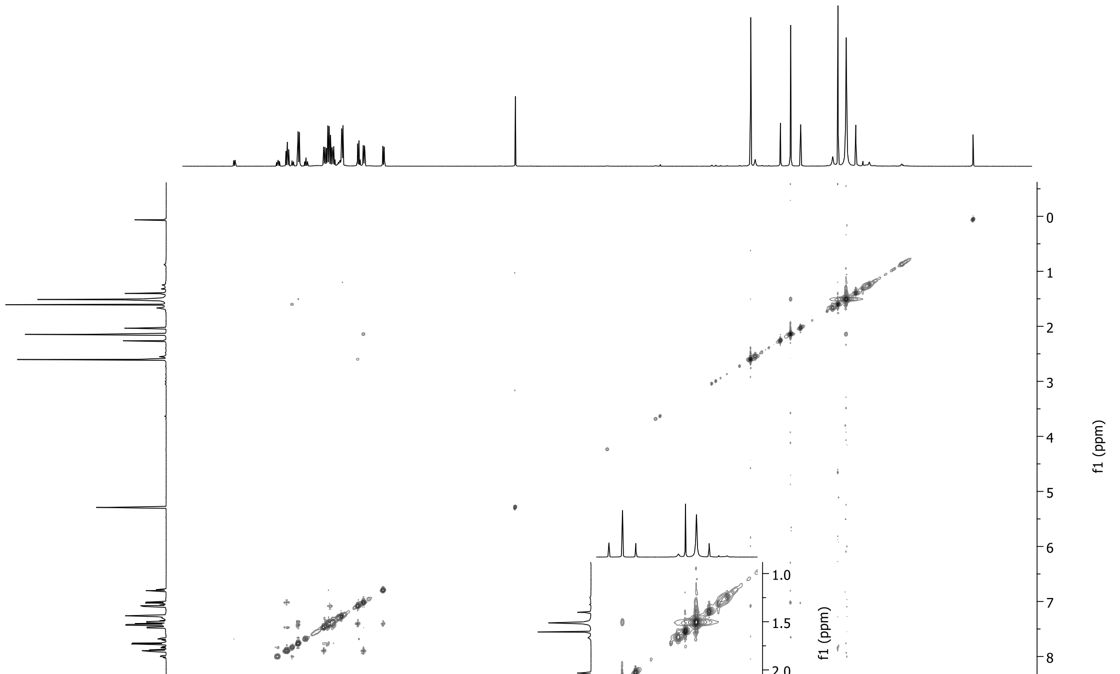

188.05
160.20
157.16
155.40
150.98
142.89
141.15
136.22
135.04
128.85
128.40
126.62
122.45
120.42
118.65
96.74
32.76
31.47
24.50
22.71
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

2D NMRs of 187 at 1:0.3 187a:187b

HMBC

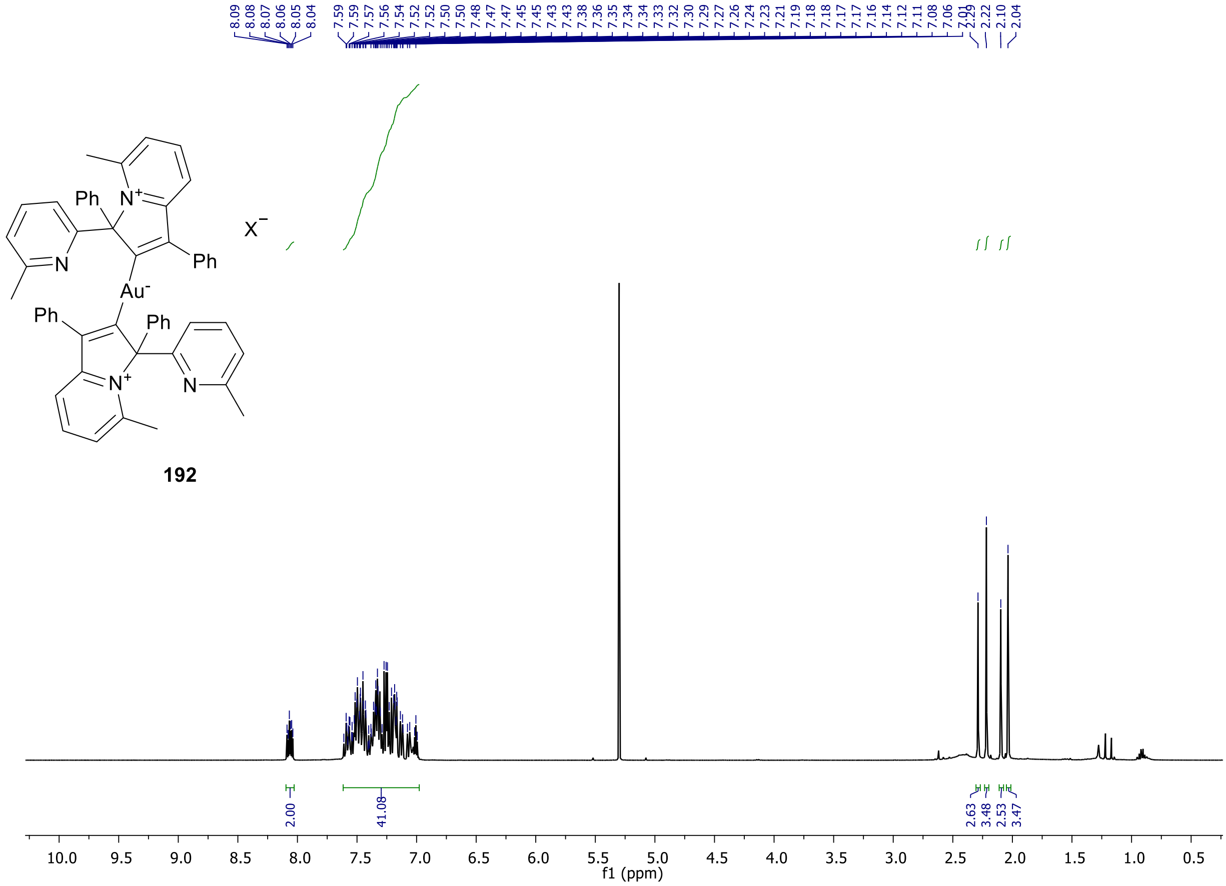


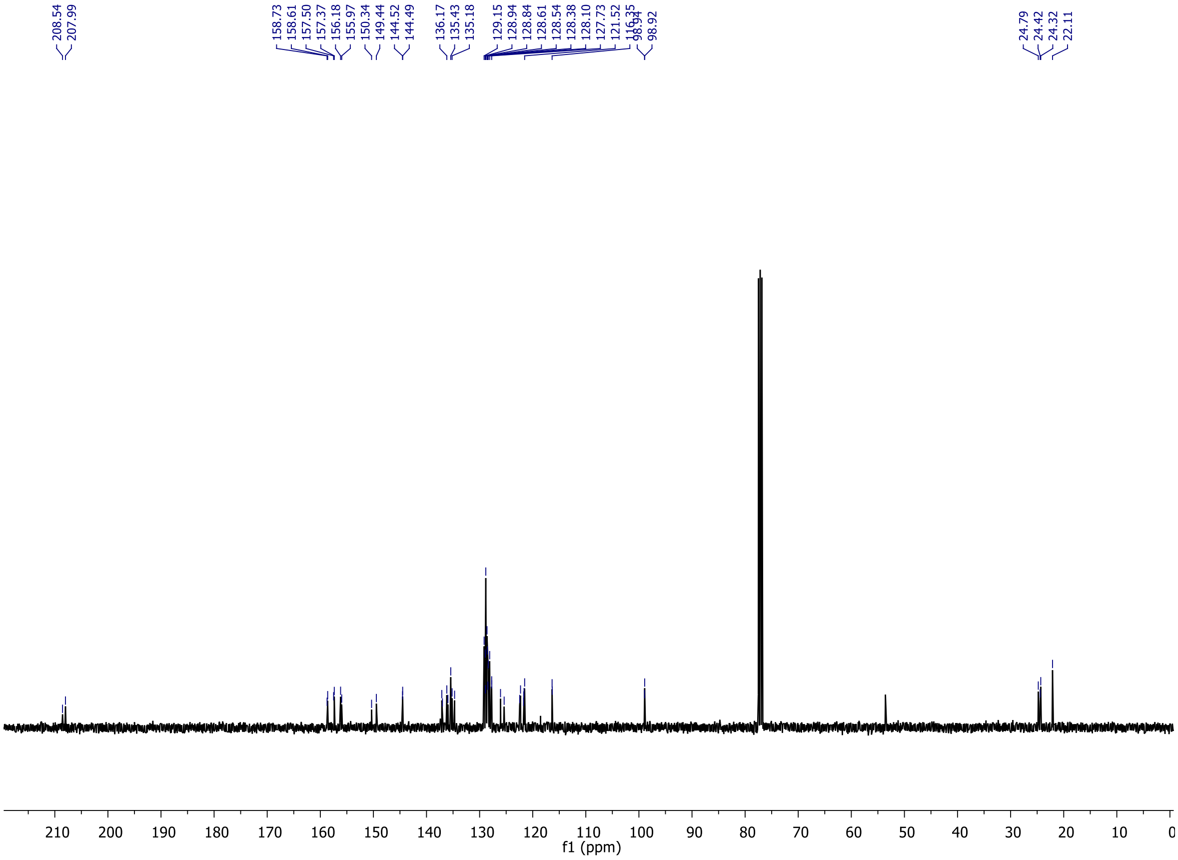
NOESY

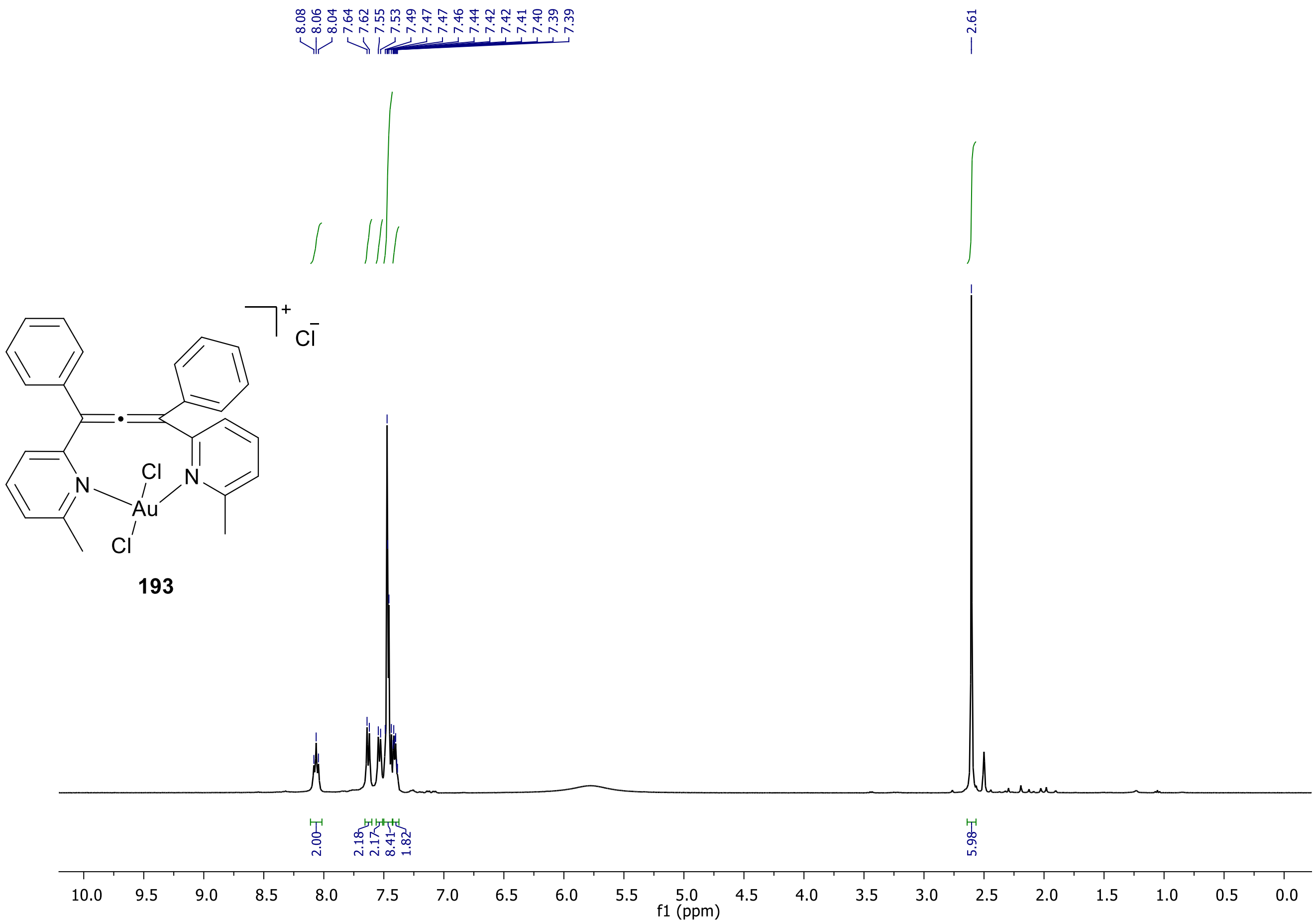


Ph
N+
X−
N
Ph
Au−
Ph
Ph
N+
N

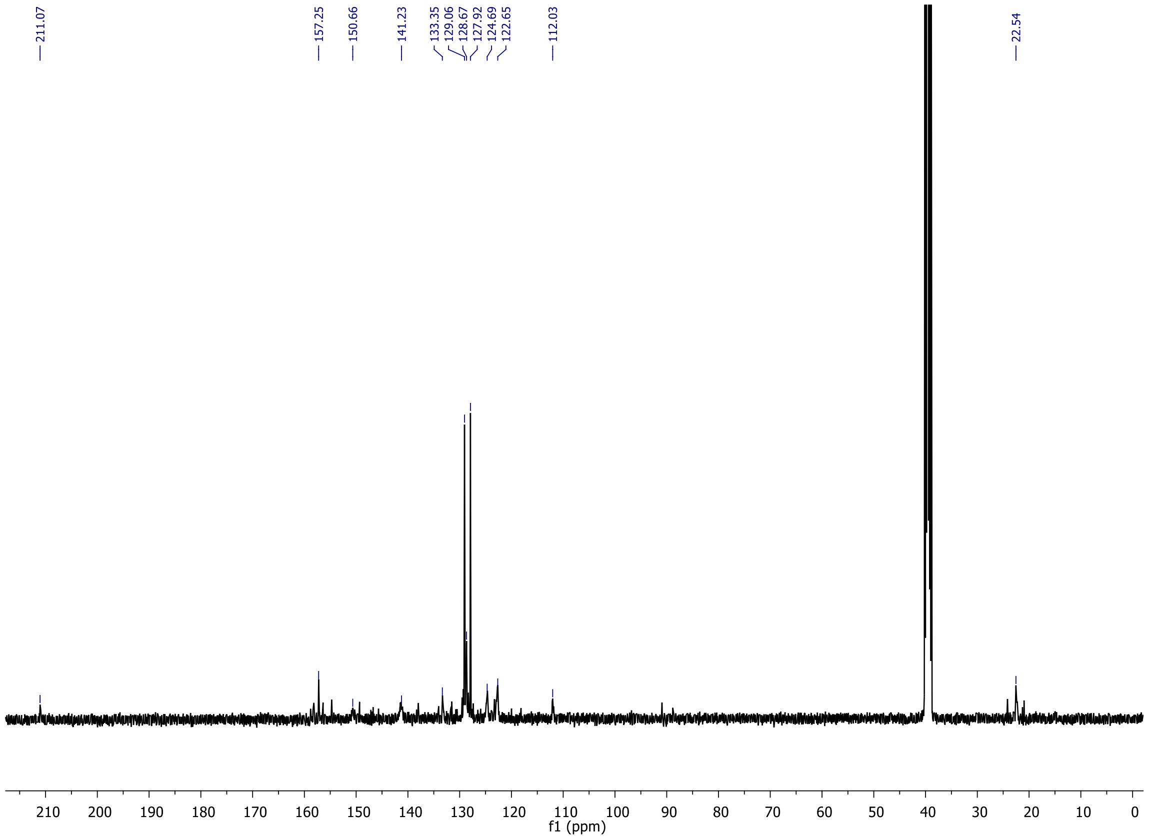
192

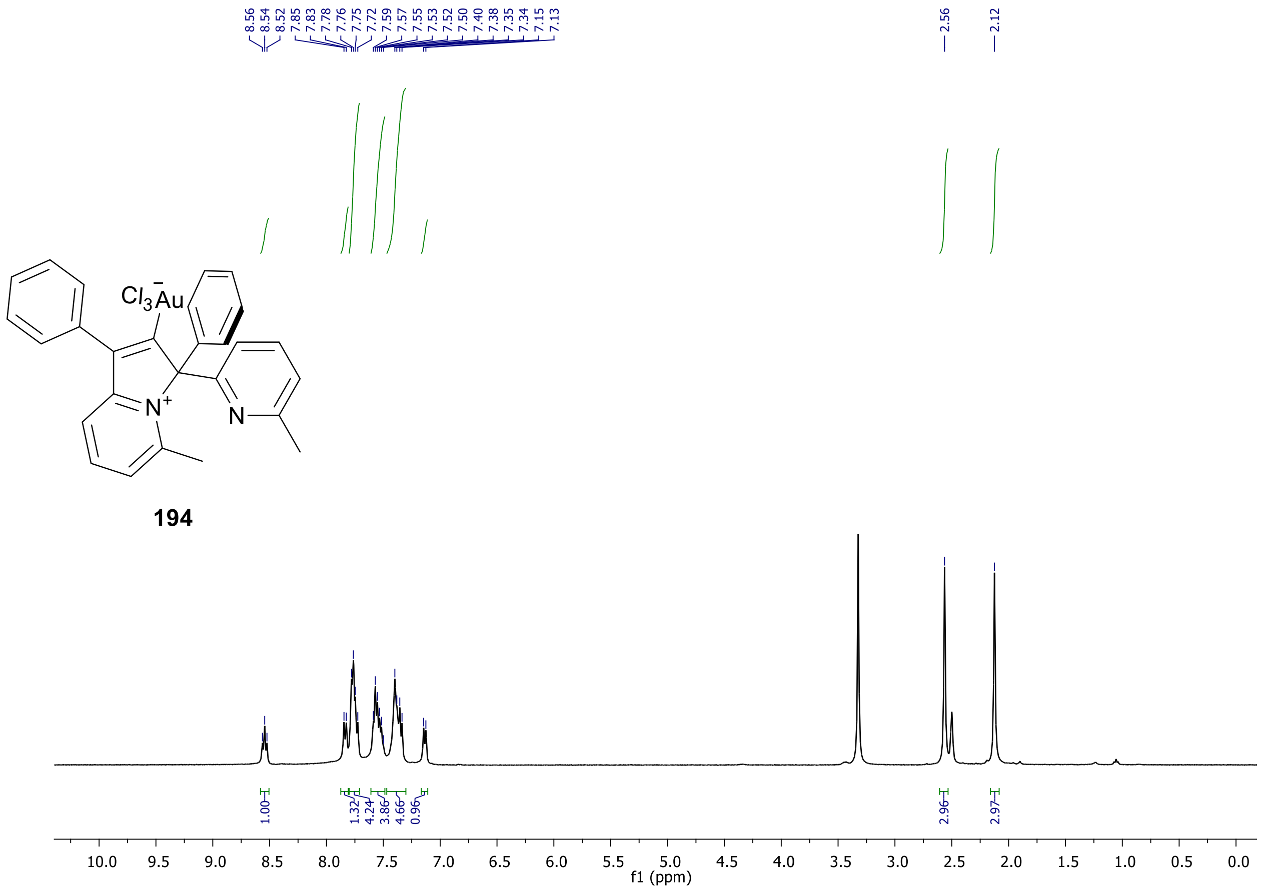

8.09
8.08
8.07
8.06
8.05
8.04
7.59
7.59
7.57
7.56
7.54
7.52
7.52
7.50
7.50
7.48
7.47
7.45
7.45
7.43
7.43
7.38
7.36
7.35
7.34
7.34
7.33
7.32
7.30
7.29
7.27
7.26
7.24
7.23
7.21
7.19
7.18
7.18
7.17
7.17
7.16
7.14
7.12
7.11
7.08
7.06
7.01
2.29
2.22
2.10
2.04
2.00
41.08
2.63
3.48
2.53
3.47
10.0
9.5
9.0
8.5
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)


208.54
207.99
158.73
158.61
157.50
157.37
156.18
155.97
150.34
149.44
144.52
144.49
136.17
135.43
135.18
129.15
128.94
128.84
128.61
128.54
128.38
128.10
127.73
121.52
116.35
98.94
98.92
24.79
24.42
24.32
22.11
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

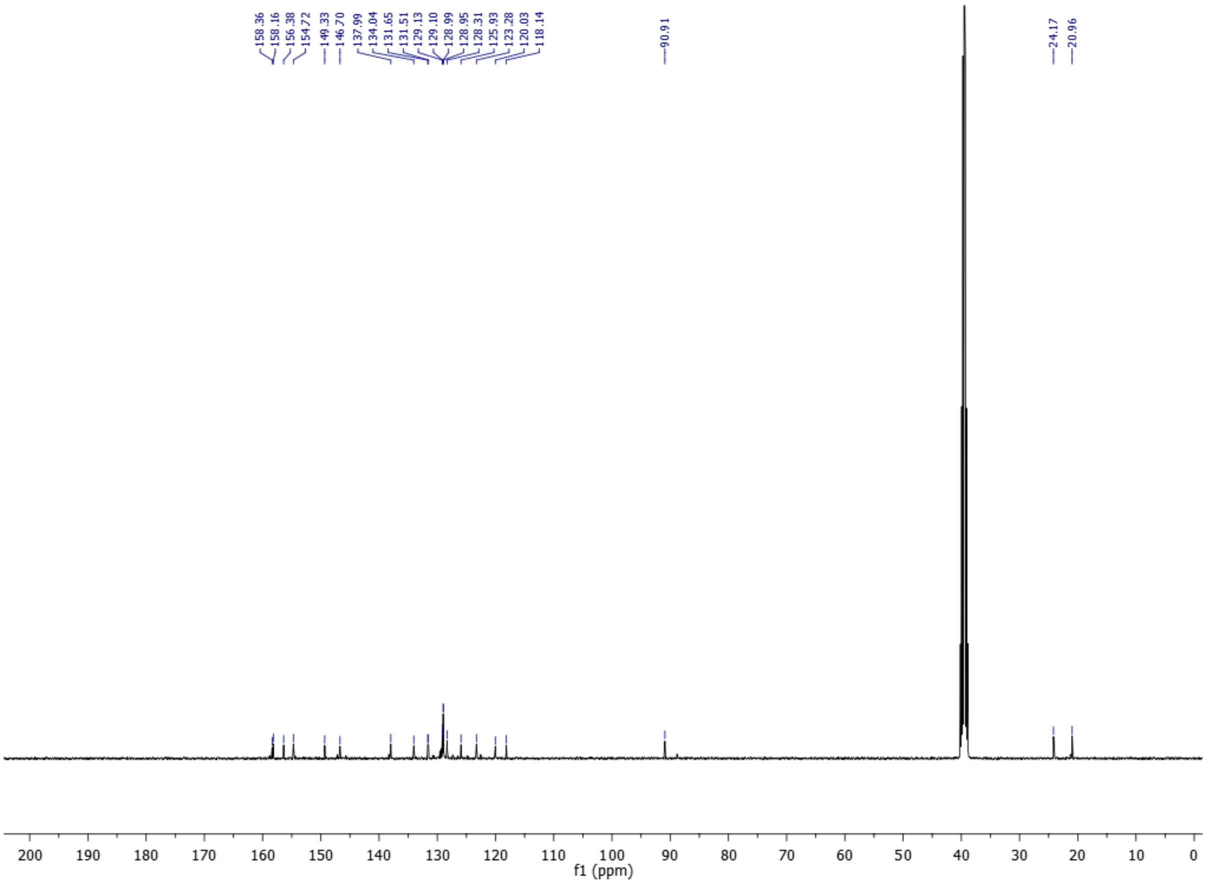

8.08
8.06
8.04
7.64
7.62
7.55
7.53
7.49
7.47
7.47
7.46
7.44
7.42
7.42
7.41
7.40
7.39
7.39
2.61
Cl
N
Au
N
Cl
+
Cl−
2.00
2.18
2.17
8.41
1.82
5.98
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

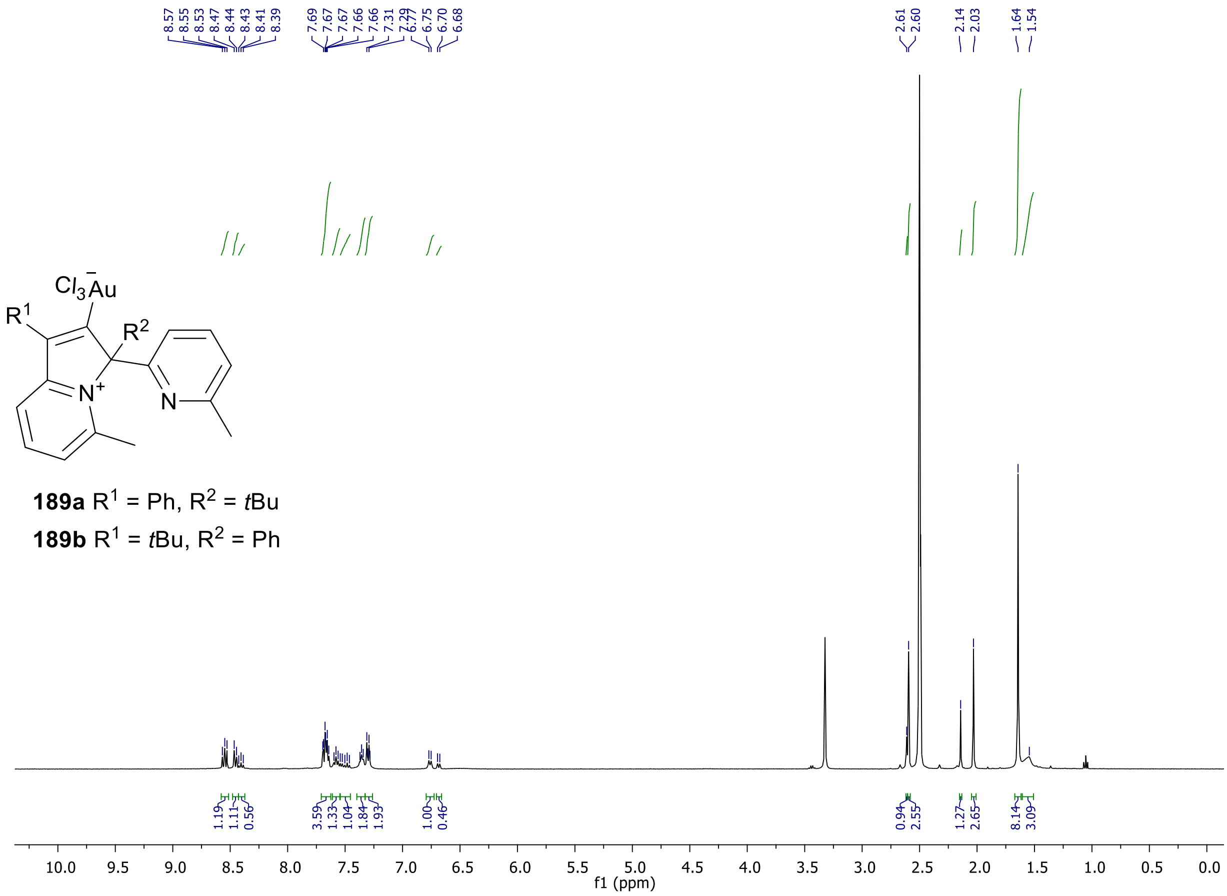
193


211.07
157.25
150.66
141.23
133.35
129.06
128.67
127.92
124.69
122.65
112.03
22.54
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Cl3Au
−
N+
N
8.56
8.54
8.52
7.85
7.83
7.78
7.76
7.75
7.72
7.59
7.57
7.55
7.53
7.52
7.50
7.40
7.38
7.35
7.34
7.15
7.13
2.56
2.12
1.00
1.32
4.24
3.86
4.66
0.96
2.96
2.97
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)

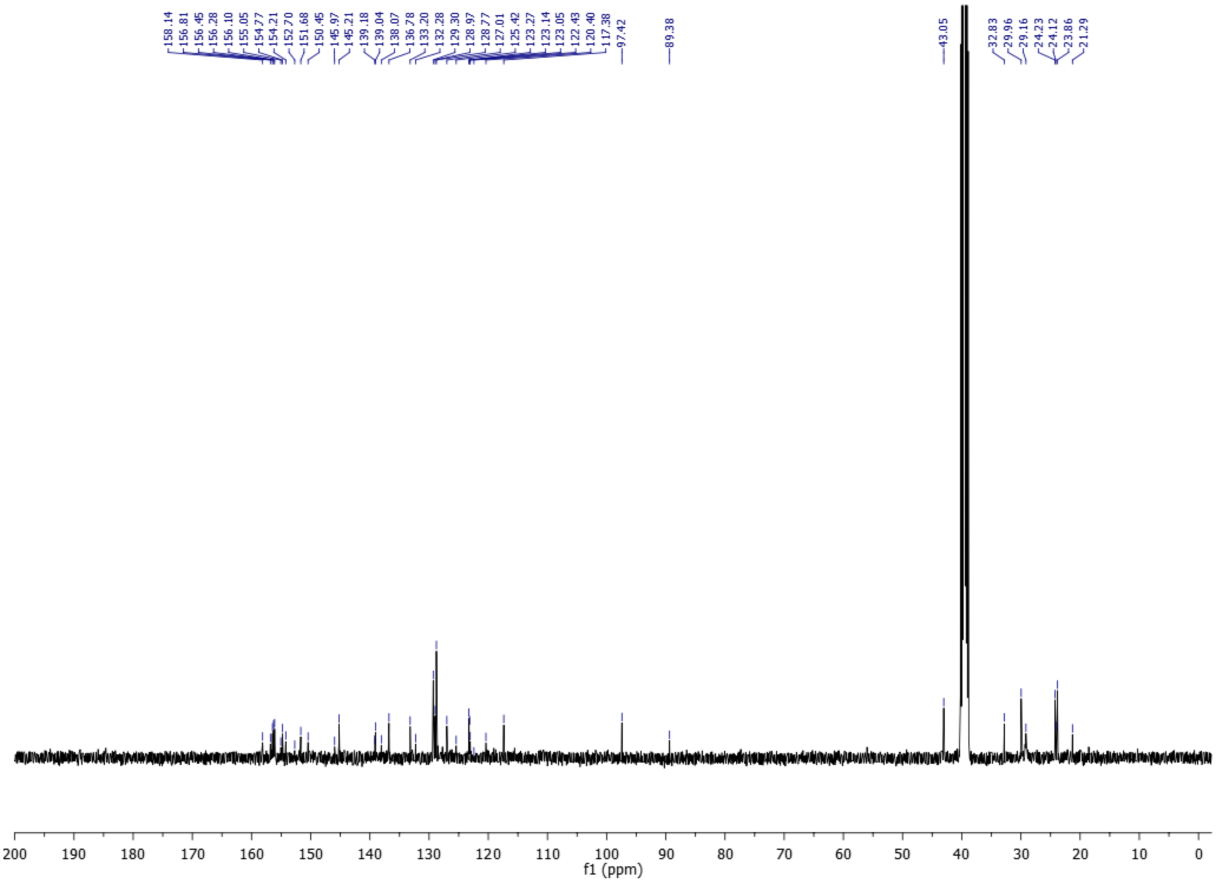
194


158.36
158.16
156.38
154.72
149.33
146.70
137.99
134.04
131.65
131.51
129.13
129.10
128.99
128.95
128.31
125.93
123.28
120.03
118.14
90.91
24.17
20.96
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



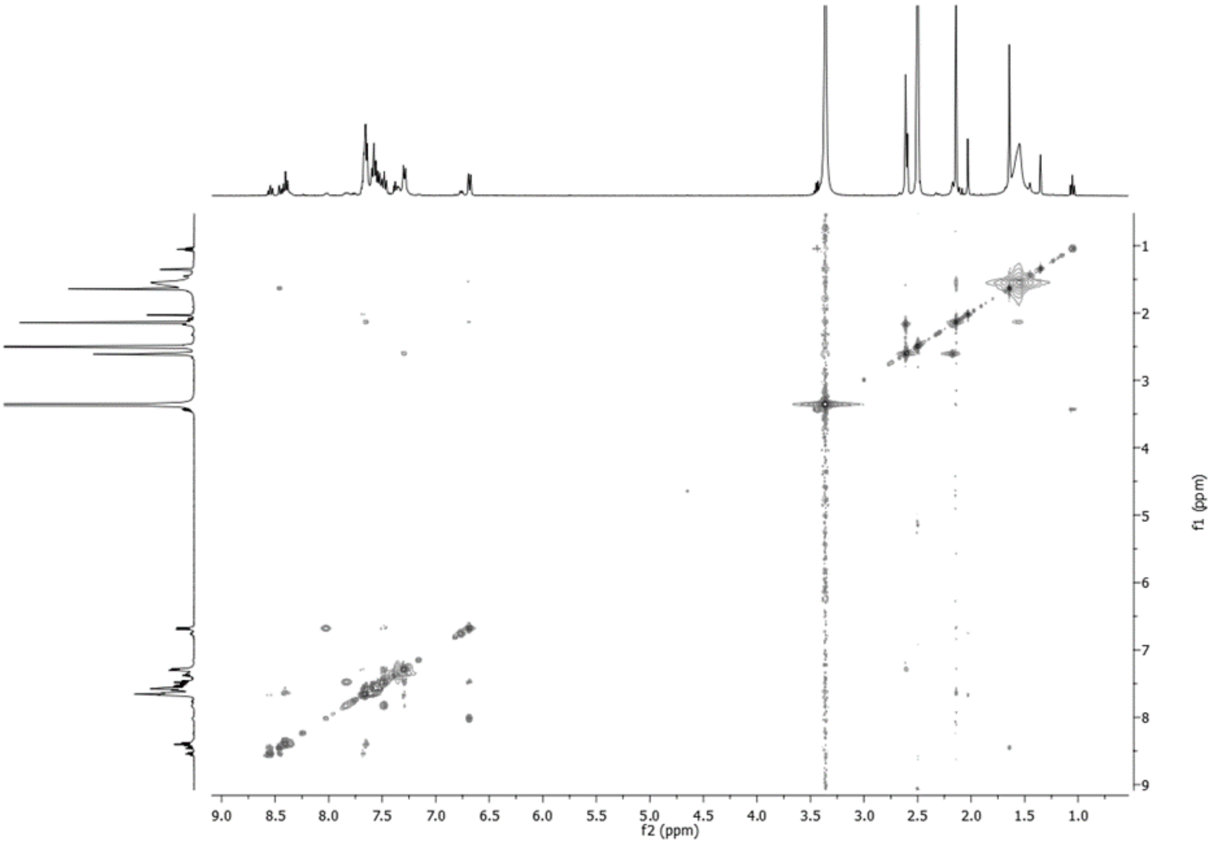
189a R^1 = Ph, R^2 = *t*Bu

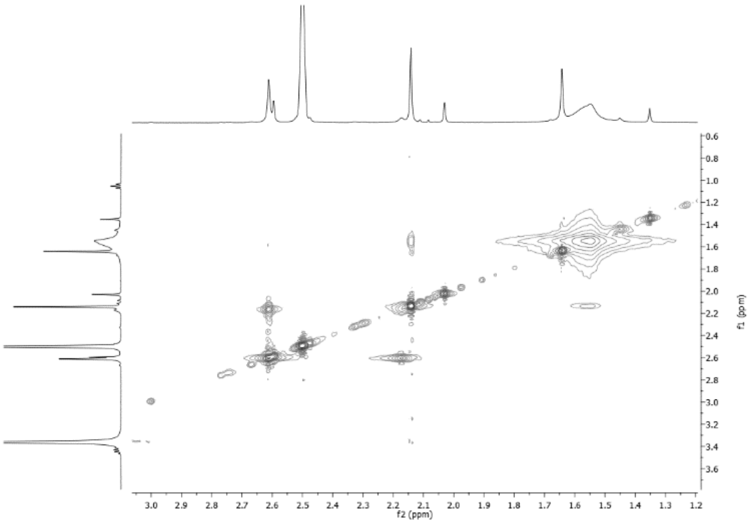
189b R^1 = *t*Bu, R^2 = Ph

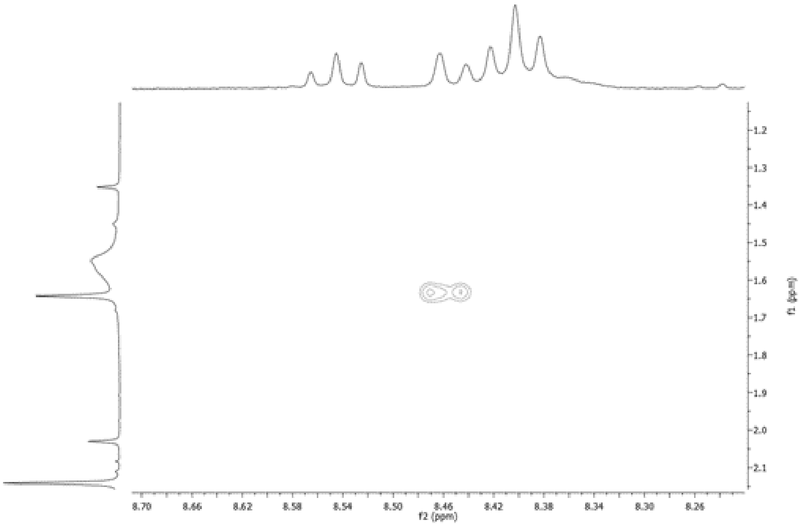


2D NMRs of 189 at 1:0.4 ratio of 189a:189b

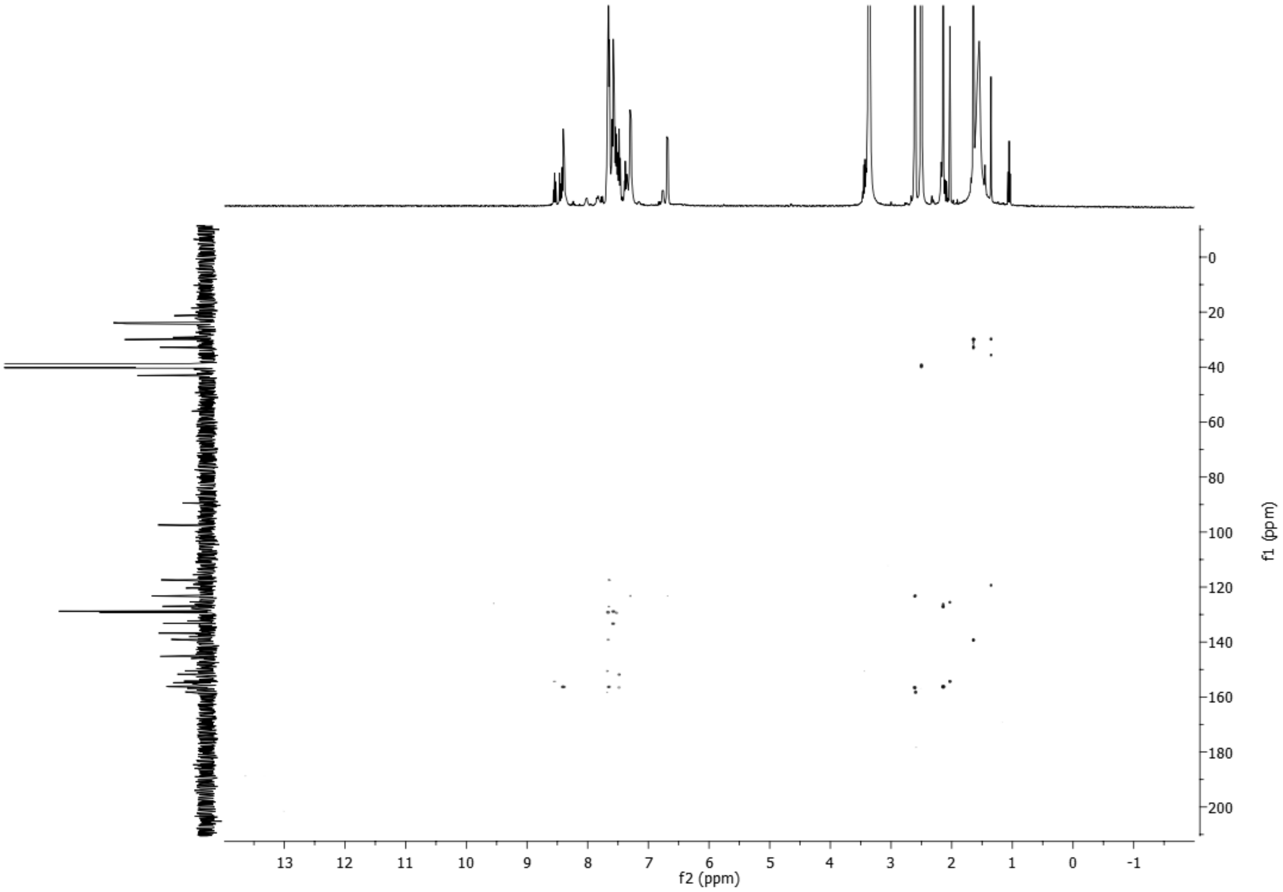
NOESY

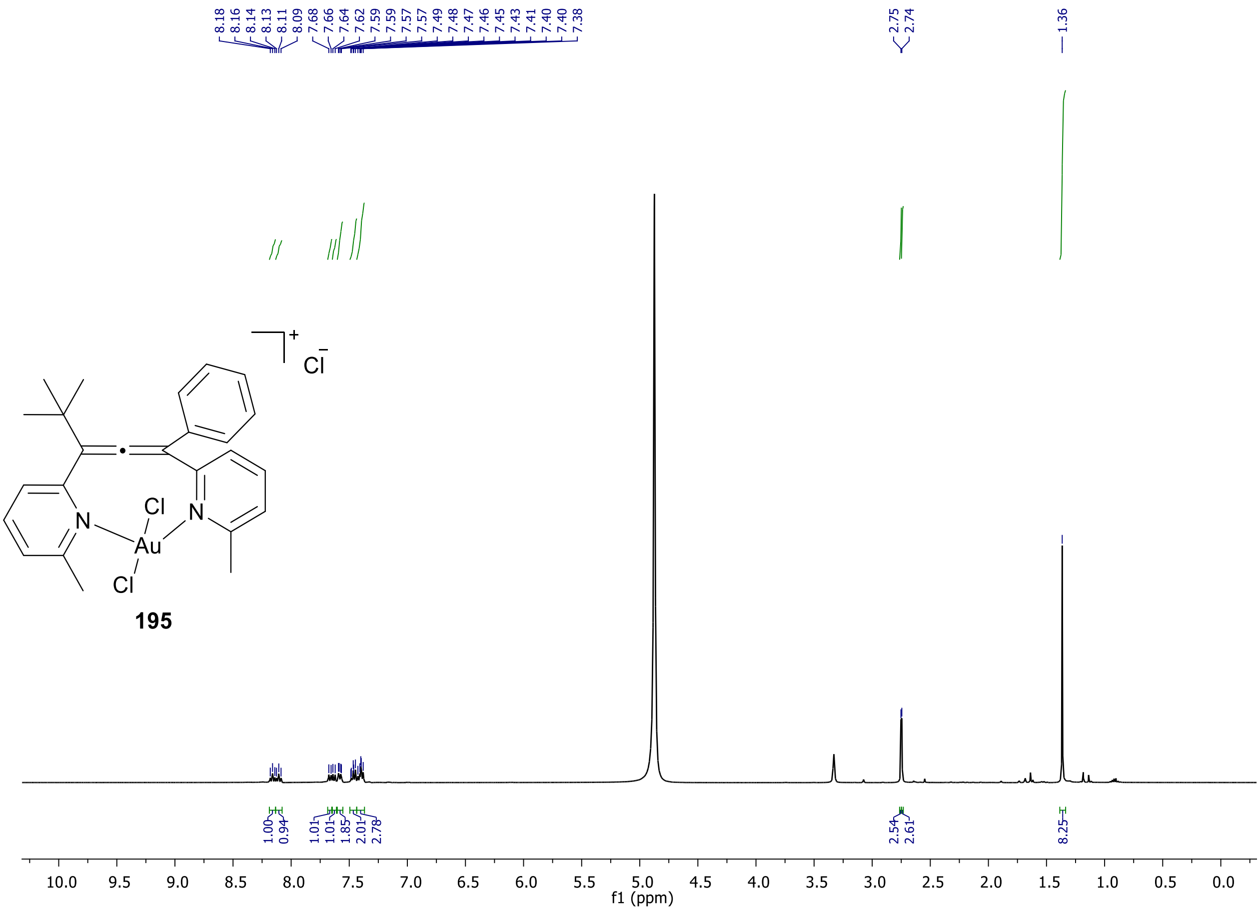




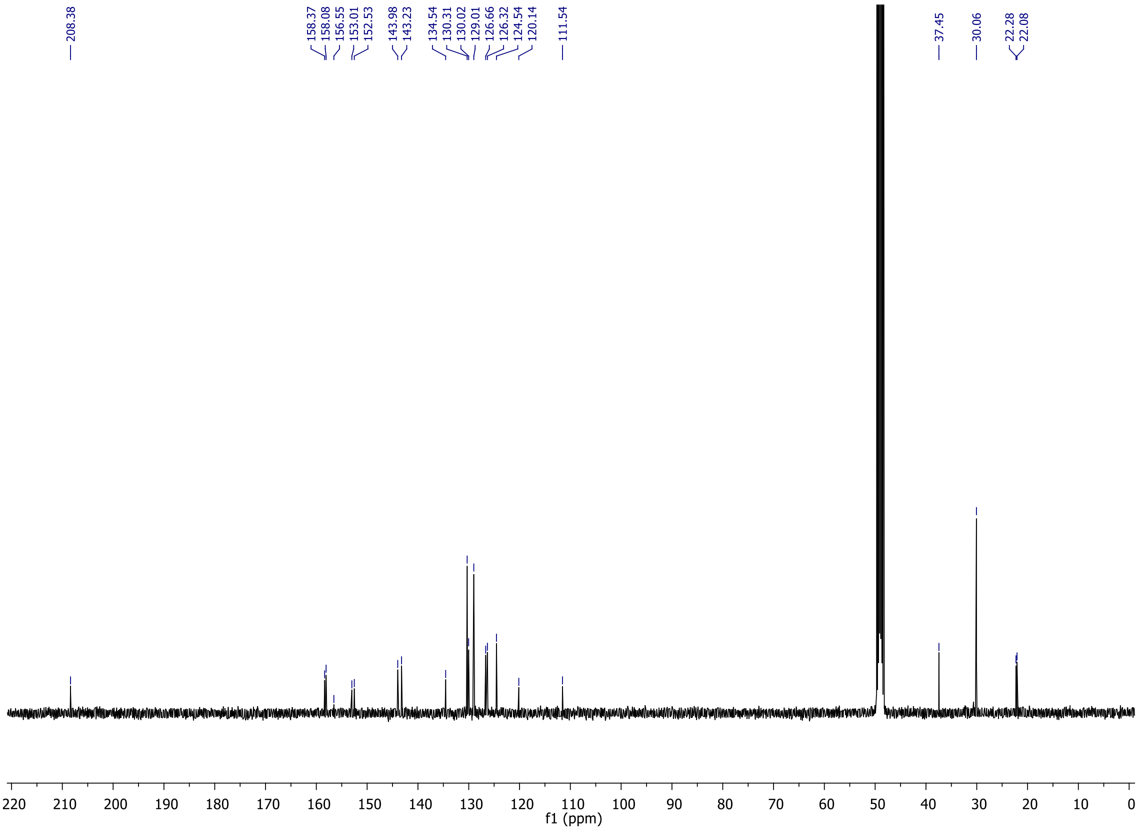

1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
2.0
2.1
f1 (ppm)
8.70
8.66
8.62
8.58
8.54
8.50
8.46
8.42
8.38
8.34
8.30
8.26
f2 (ppm)

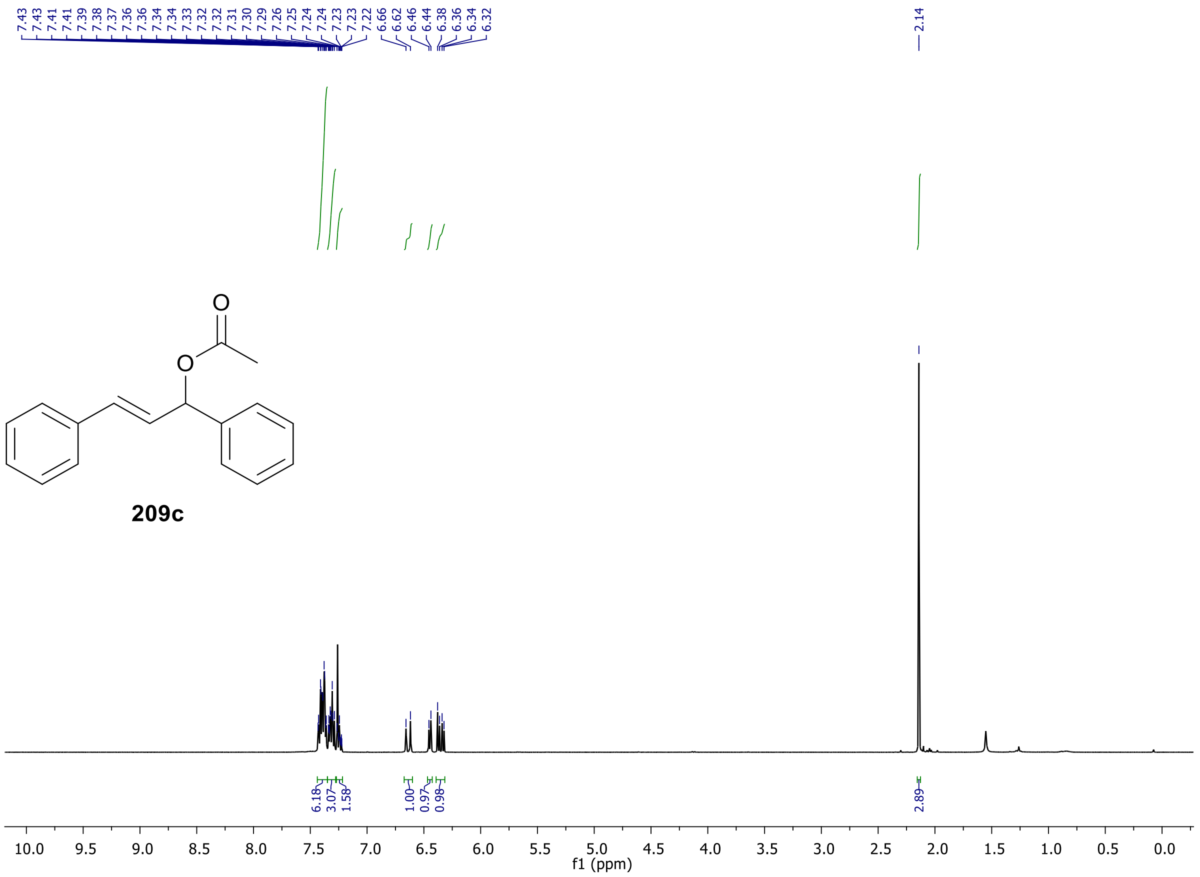
HMBC


0
20
40
60
80
100
120
140
160
180
200
f1 (ppm)
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f2 (ppm)

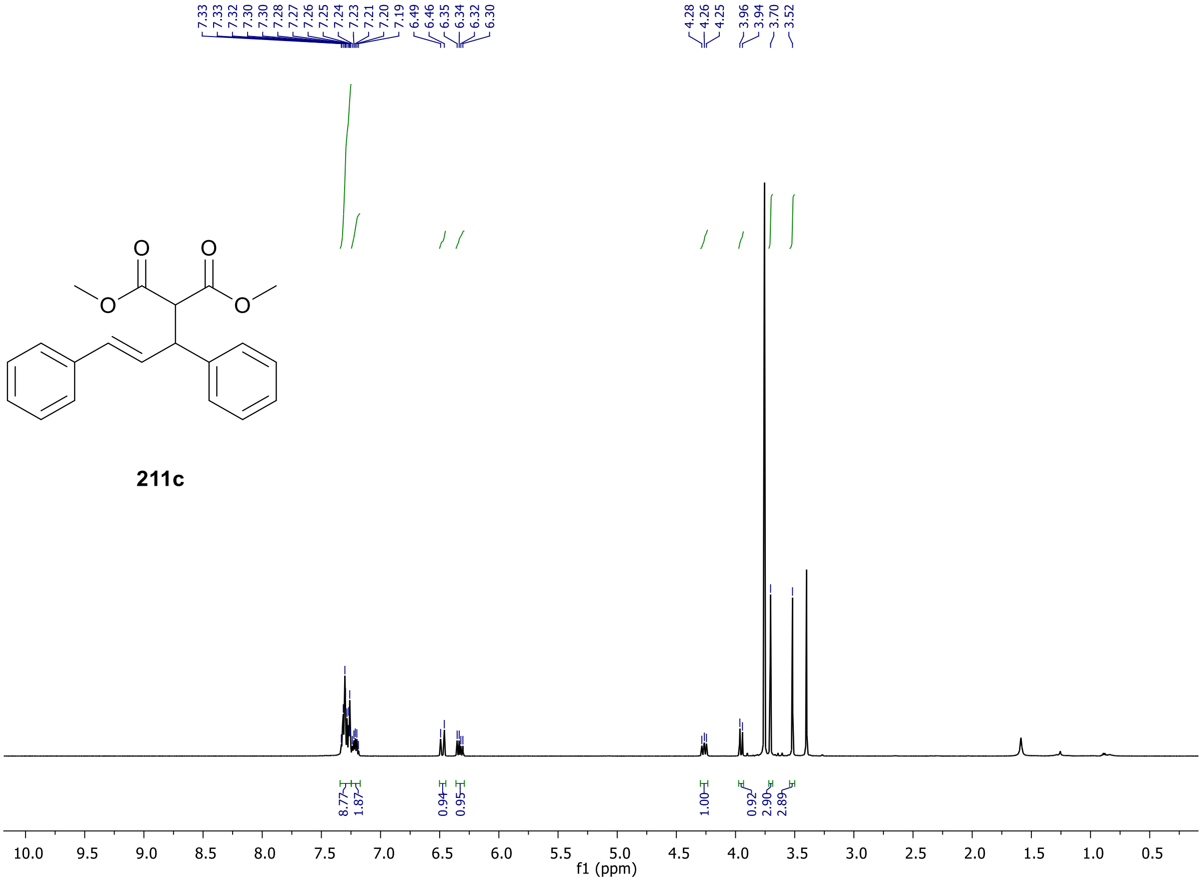

8.18
8.16
8.14
8.13
8.11
8.09
7.68
7.66
7.64
7.62
7.59
7.59
7.57
7.57
7.49
7.48
7.47
7.46
7.45
7.43
7.41
7.40
7.40
7.38
2.75
2.74
1.36
Cl
Cl
N
Au
N
Cl
+
–
1.00
0.94
1.01
1.01
1.85
2.01
2.78
2.54
2.61
8.25
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

195

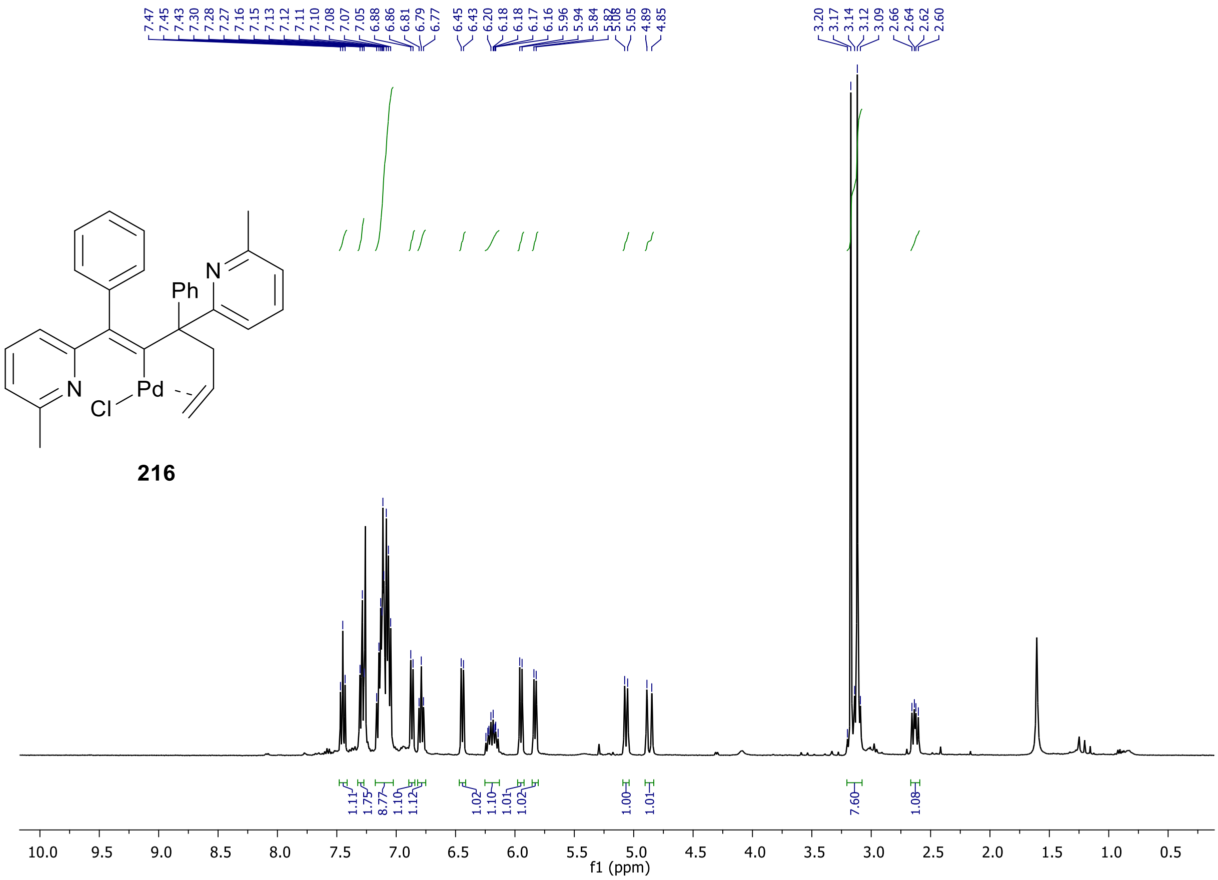

208.38
158.37
158.08
156.55
153.01
152.53
143.98
143.23
134.54
130.31
130.02
129.01
126.66
126.32
124.54
120.14
111.54
37.45
30.06
22.28
22.08
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.43
7.43
7.41
7.41
7.39
7.38
7.37
7.36
7.36
7.34
7.34
7.33
7.32
7.32
7.31
7.30
7.29
7.26
7.25
7.24
7.24
7.23
7.23
7.22
6.66
6.62
6.46
6.44
6.38
6.36
6.34
6.32
2.14
O
O
6.18
3.07
1.58
1.00
0.97
0.98
2.89
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)

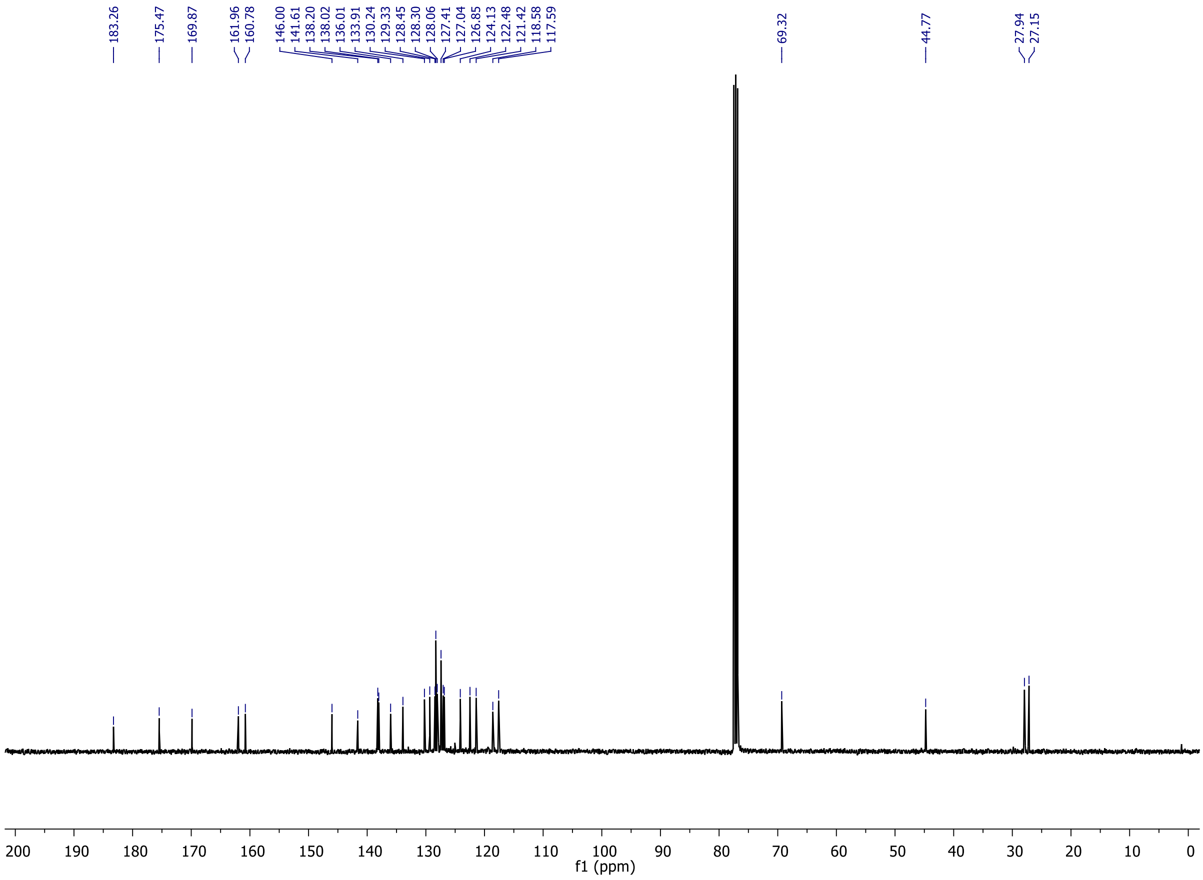
209c


7.33
7.33
7.32
7.30
7.30
7.28
7.27
7.26
7.25
7.24
7.23
7.21
7.20
7.19
6.49
6.46
6.35
6.34
6.32
6.30
4.28
4.26
4.25
3.96
3.94
3.70
3.52
O
O
O
O
8.77
1.87
0.94
0.95
1.00
0.92
2.90
2.89
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)

211c

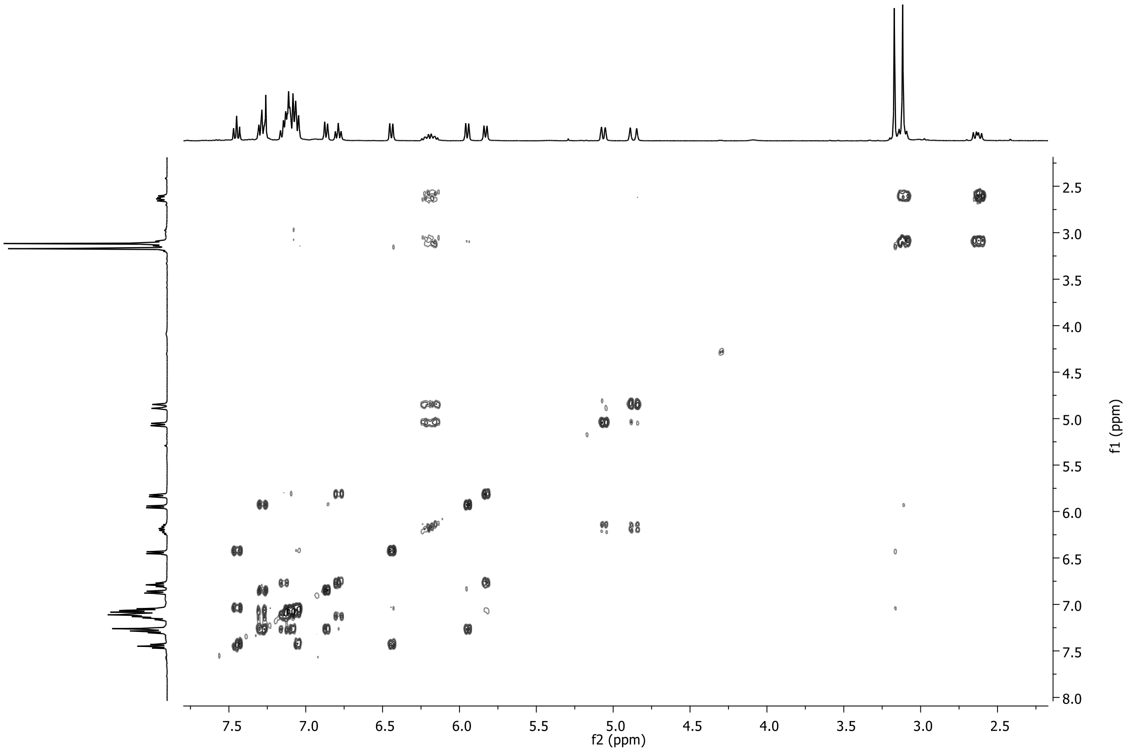

7.47
7.45
7.43
7.30
7.28
7.27
7.16
7.15
7.13
7.12
7.11
7.10
7.08
7.07
7.05
6.88
6.86
6.81
6.79
6.77
6.45
6.43
6.20
6.18
6.18
6.17
6.16
5.96
5.94
5.84
5.82
5.08
5.05
4.89
4.85
3.20
3.17
3.14
3.12
3.09
2.66
2.64
2.62
2.60
Ph
N
N
Pd
Cl
1.11
1.75
8.77
1.10
1.12
1.02
1.10
1.01
1.02
1.00
1.01
7.60
1.08
10.0
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)

216

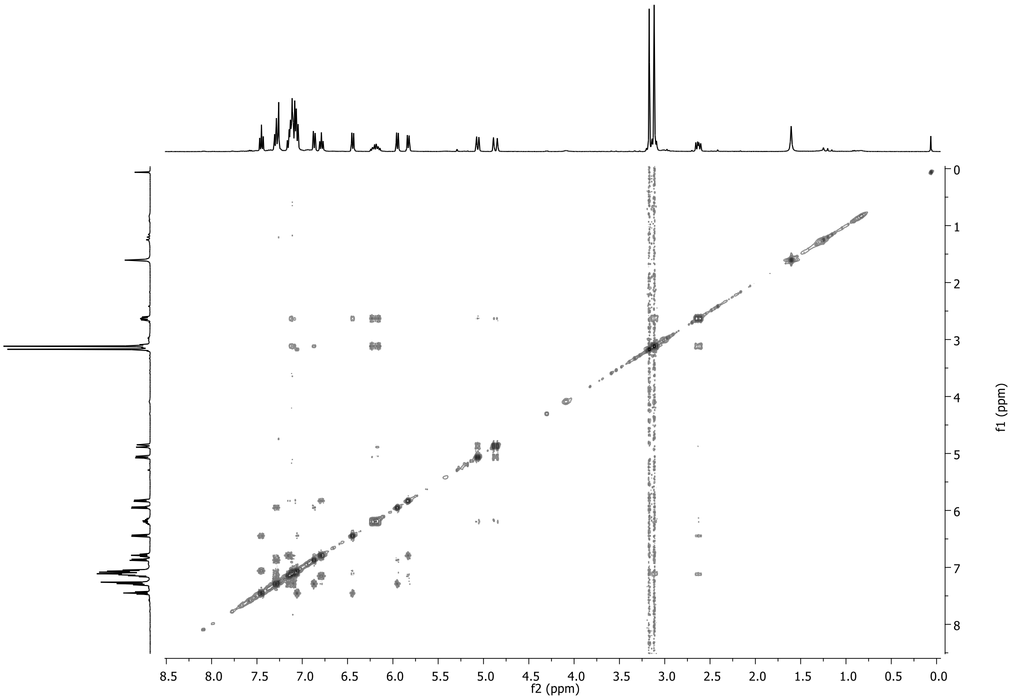

183.26
175.47
169.87
161.96
160.78
146.00
141.61
138.20
138.02
136.01
133.91
130.24
129.33
128.45
128.30
128.06
127.41
127.04
126.85
124.13
122.48
121.42
118.58
117.59
69.32
44.77
27.94
27.15
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2D NMR of 216

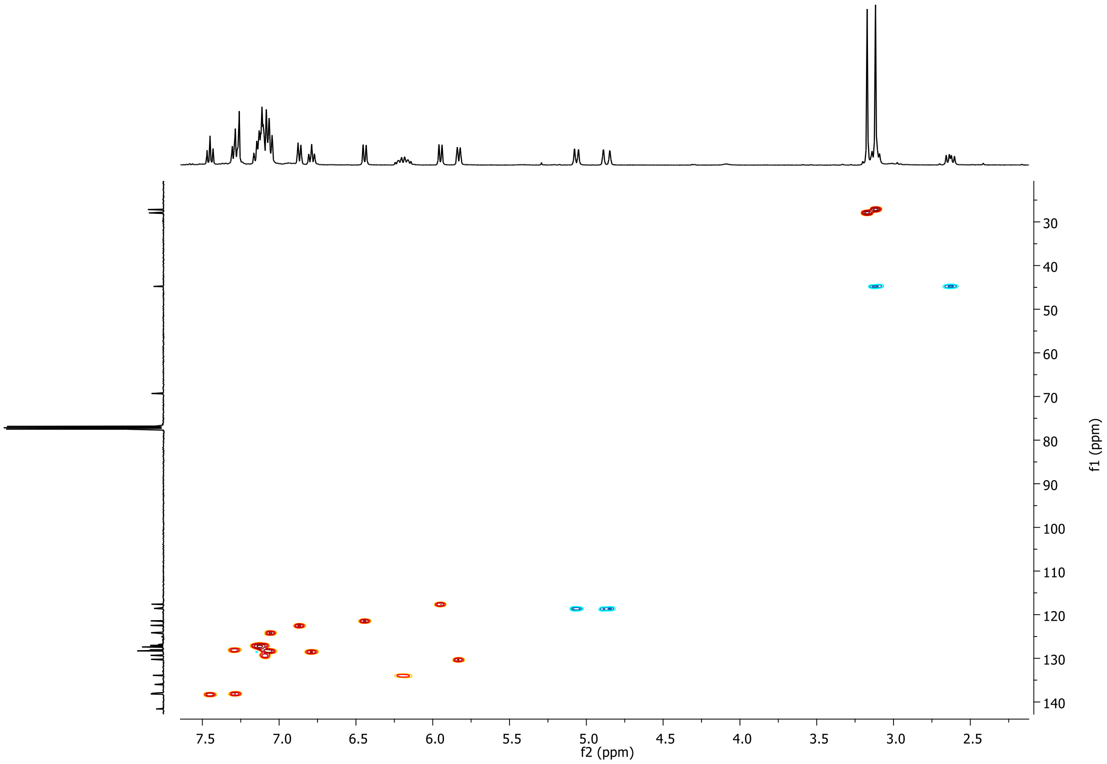
COSY



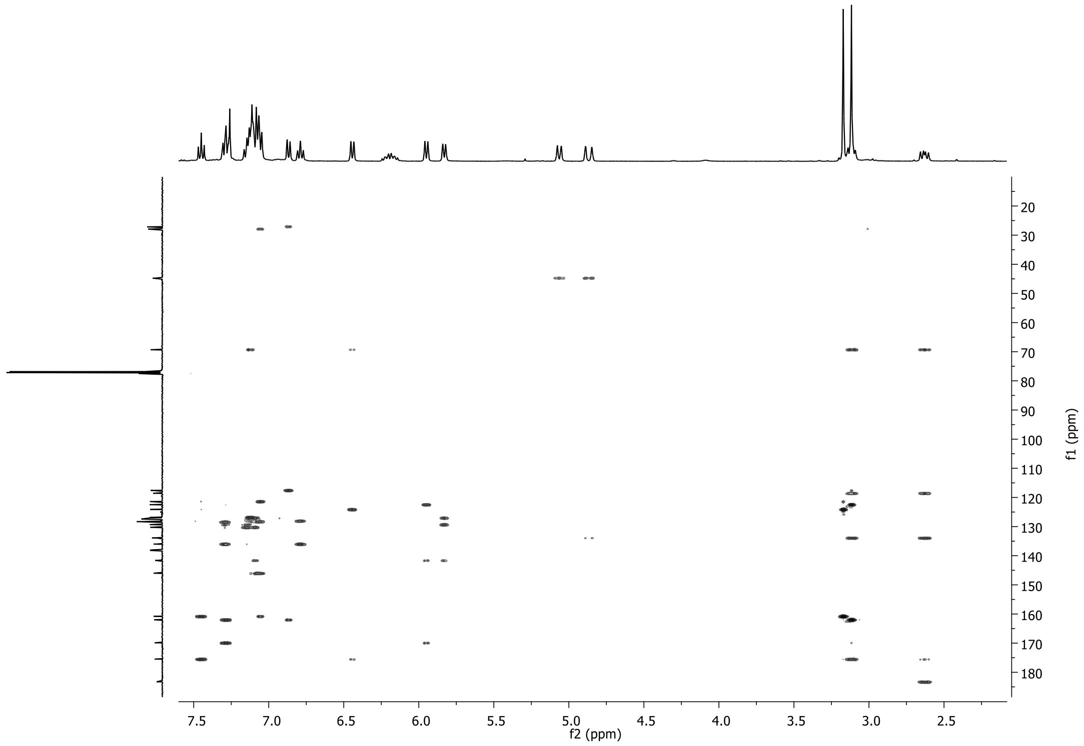
NOESY

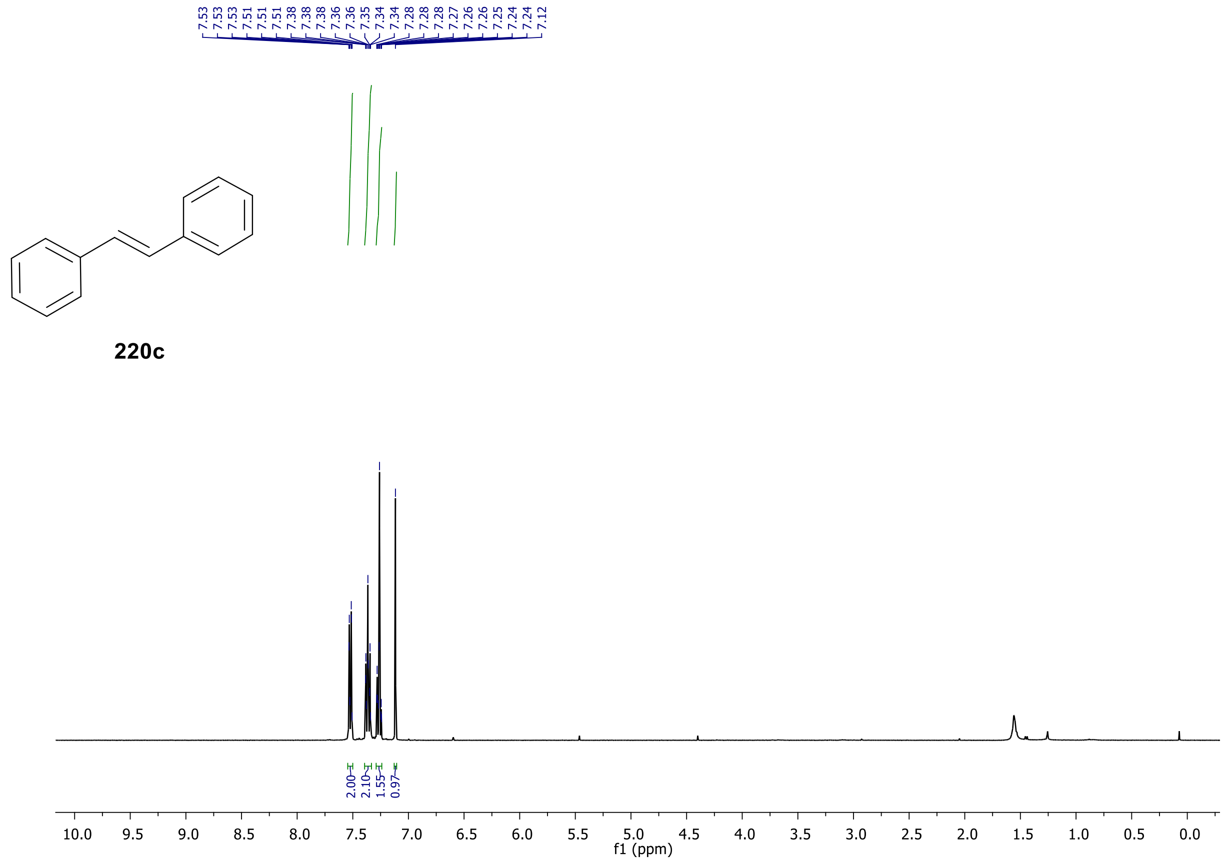


HSQC

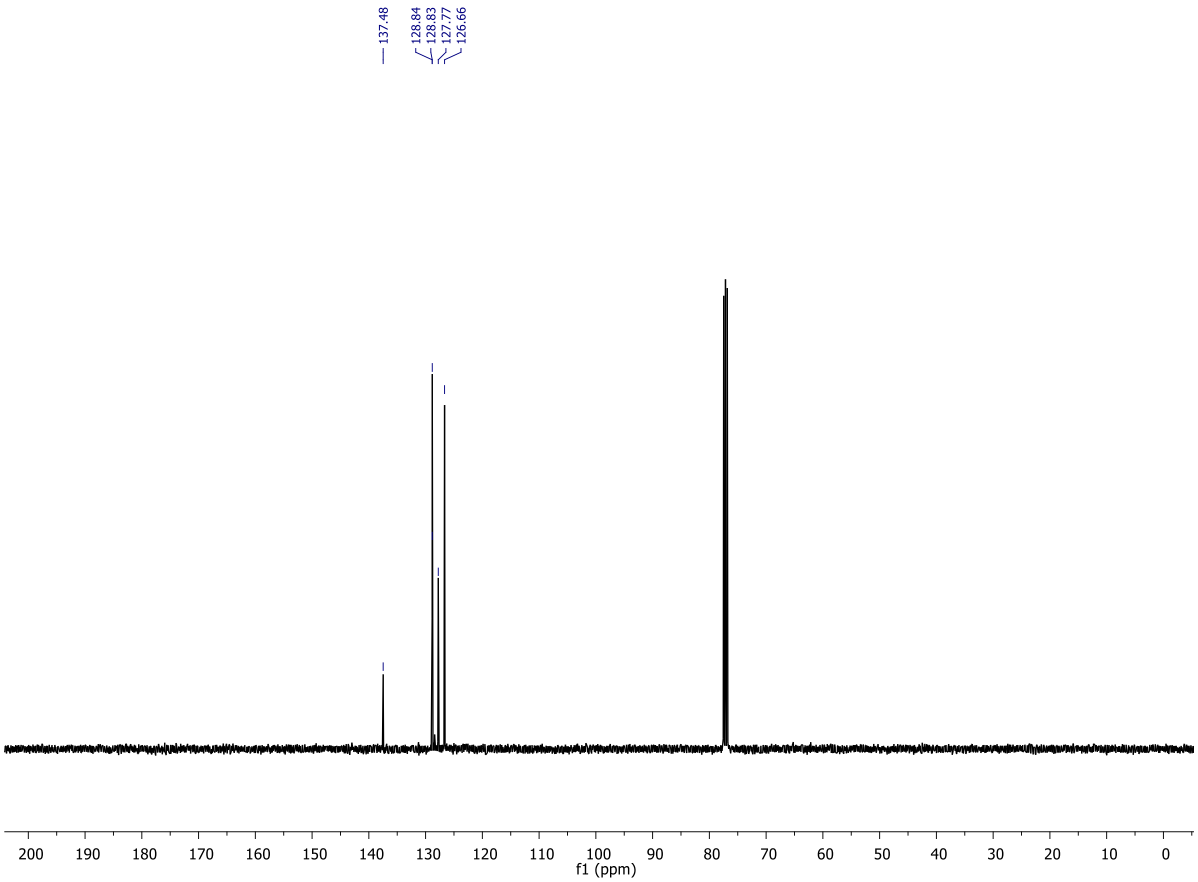

7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
f2 (ppm)
30
40
50
60
70
80
90
100
110
120
130
140
f1 (ppm)

HMBC


7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
f2 (ppm)
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
f1 (ppm)

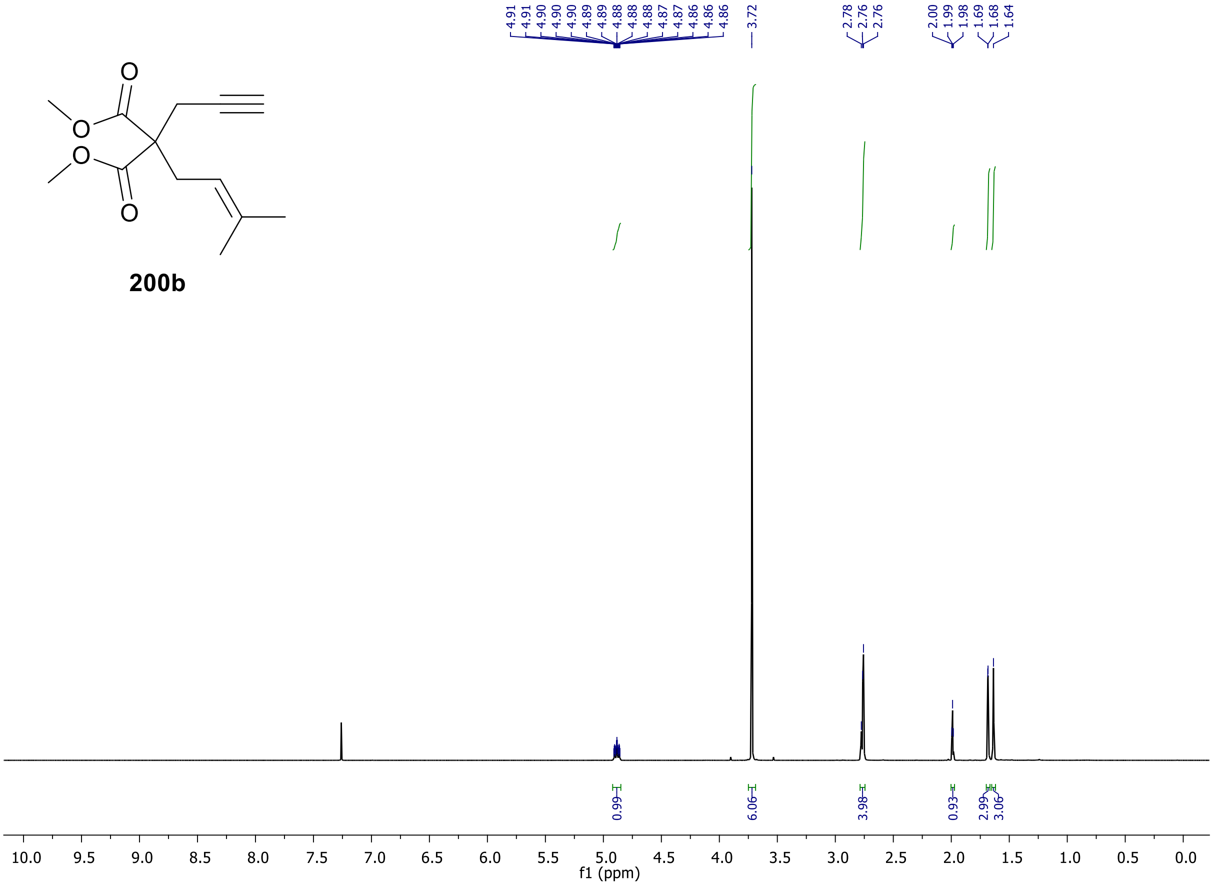

7.53
7.53
7.53
7.51
7.51
7.51
7.38
7.38
7.38
7.36
7.35
7.34
7.34
7.28
7.28
7.28
7.27
7.26
7.26
7.25
7.24
7.24
7.12
2.00
2.10
1.55
0.97
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

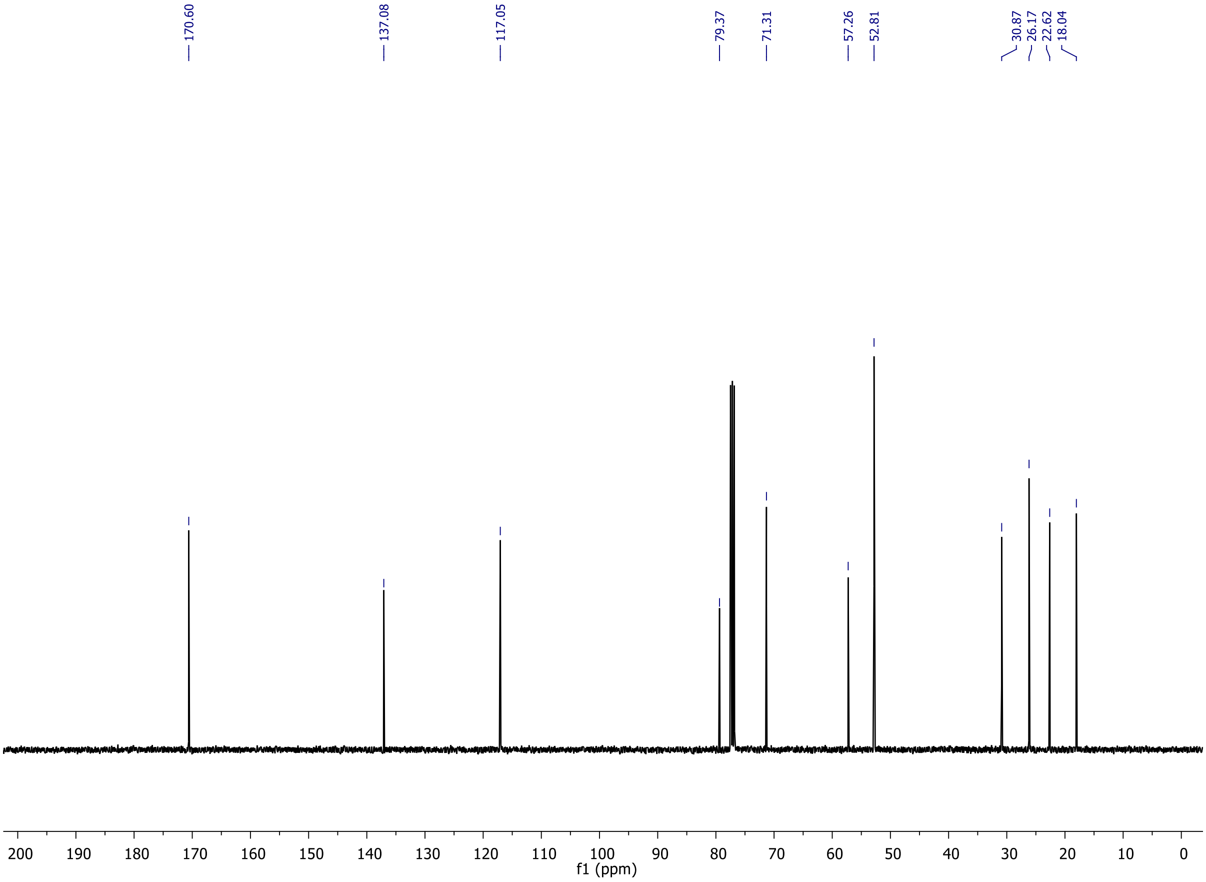
220c

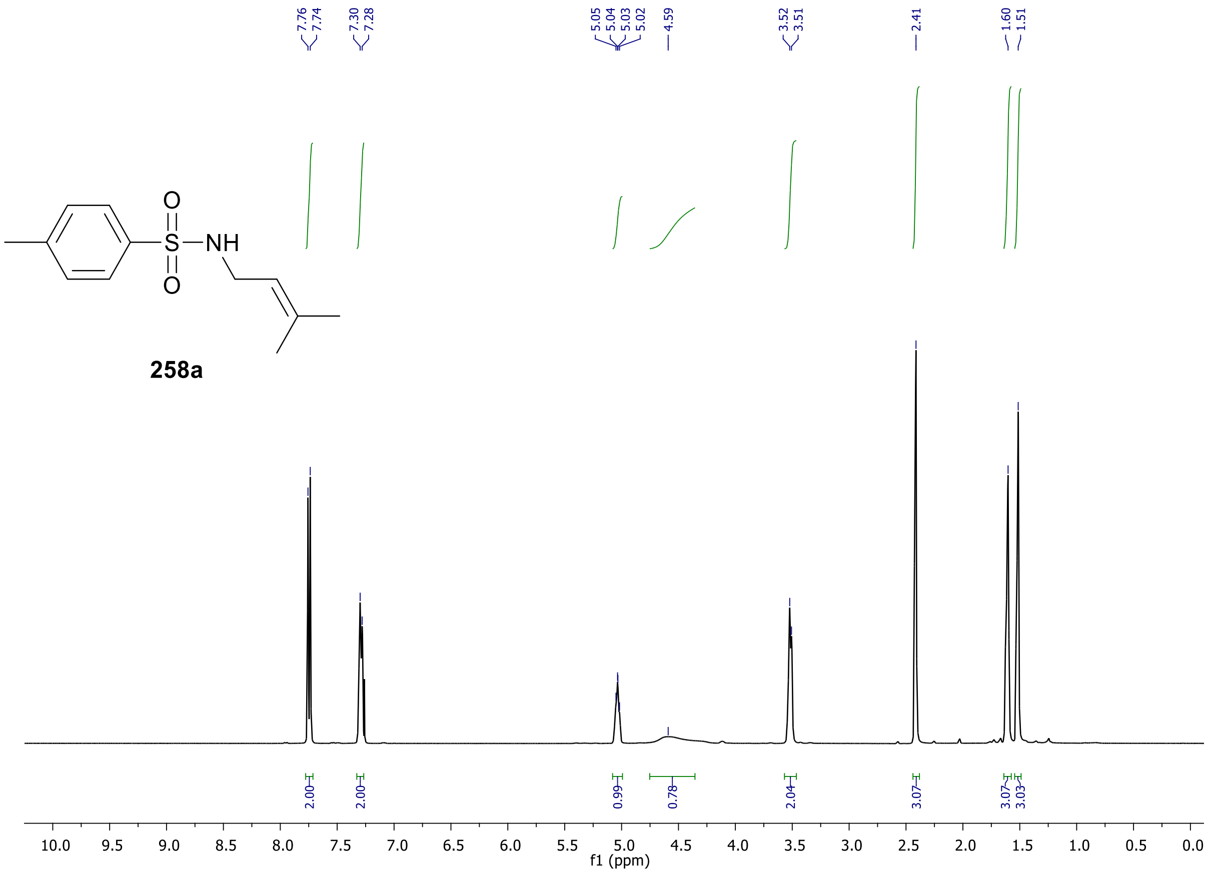

137.48
128.84
128.83
127.77
126.66
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

O
O
O
O

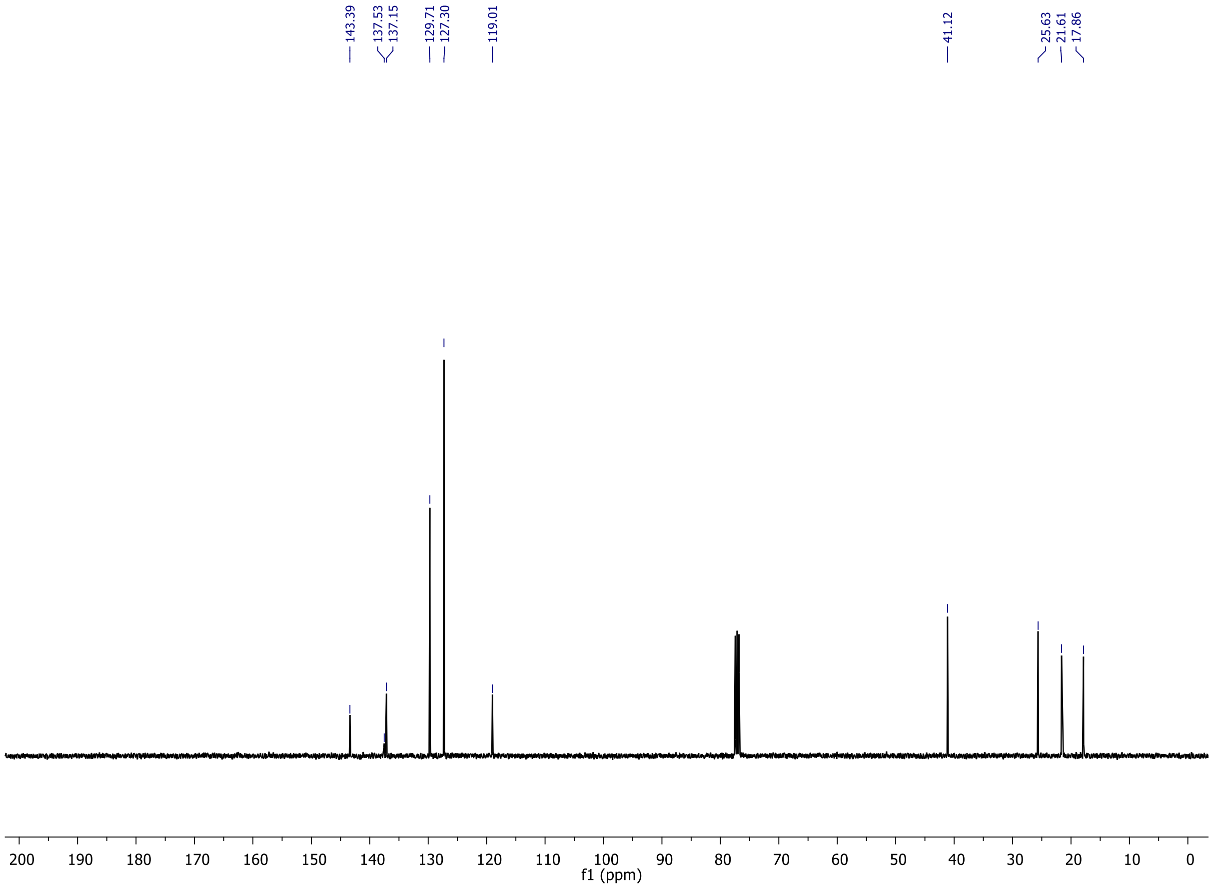
200b

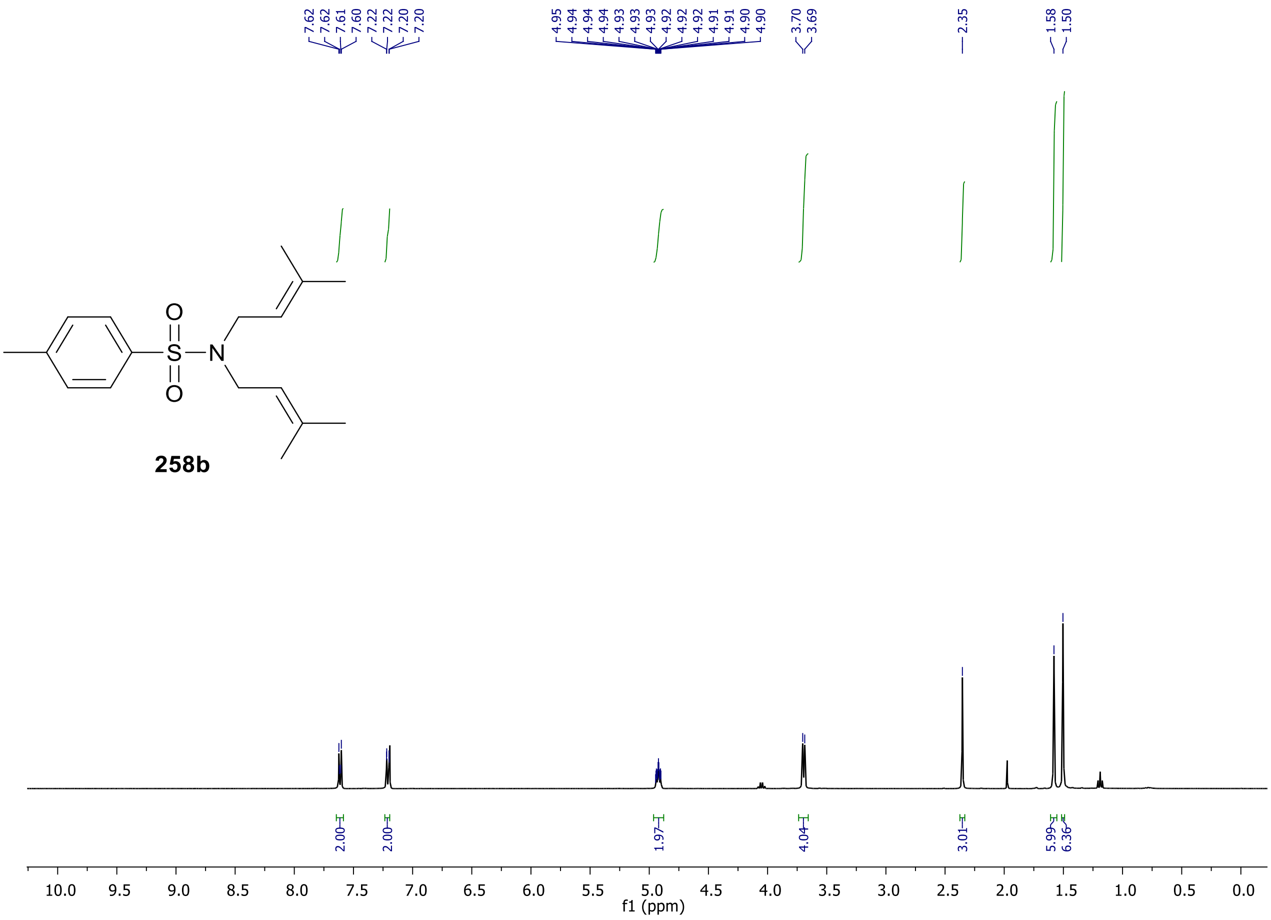

4.91
4.91
4.90
4.90
4.90
4.89
4.89
4.88
4.88
4.88
4.87
4.87
4.86
4.86
4.86
3.72
2.78
2.76
2.76
2.00
1.99
1.98
1.69
1.68
1.64
0.99
6.06
3.98
0.93
2.99
3.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


170.60
137.08
117.05
79.37
71.31
57.26
52.81
30.87
26.17
22.62
18.04
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

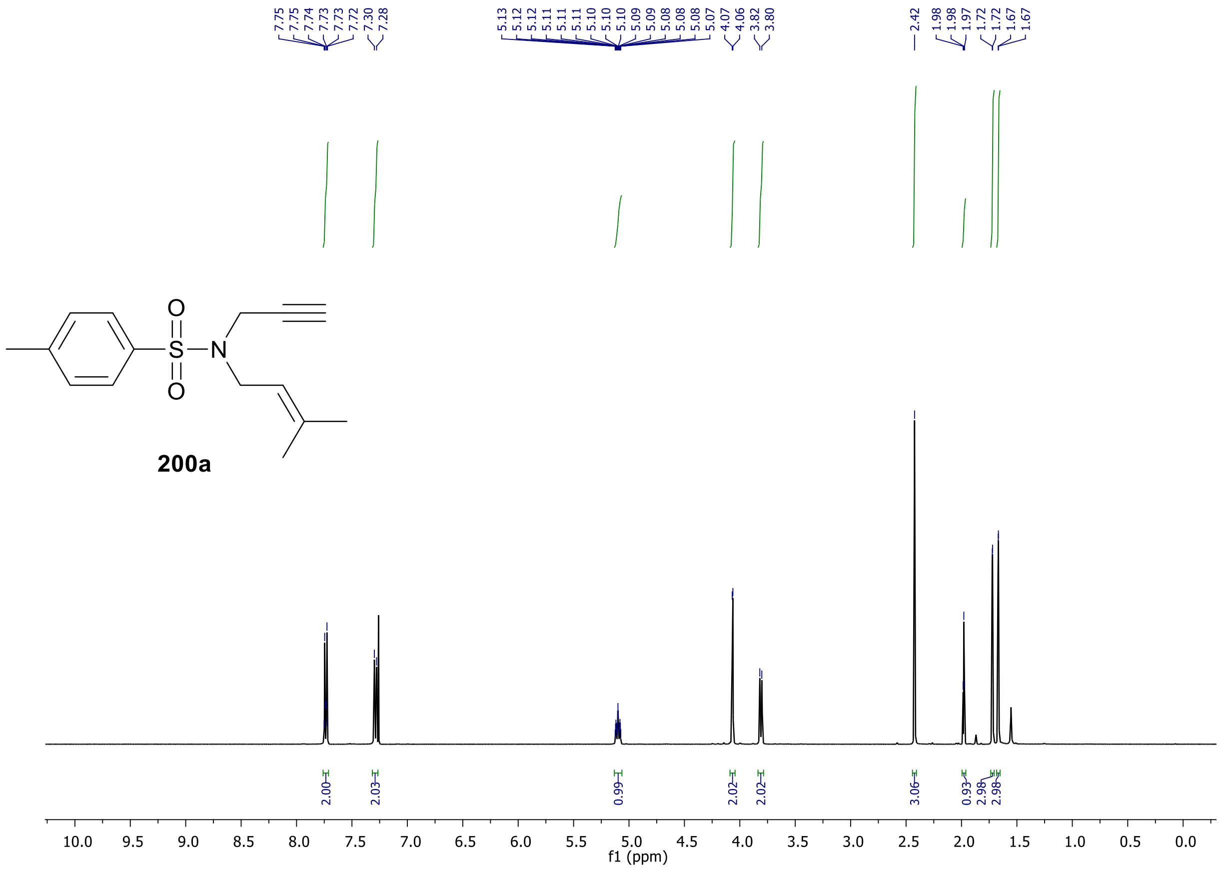

258a

7.76
7.74
7.30
7.28
5.05
5.04
5.03
5.02
4.59
3.52
3.51
2.41
1.60
1.51
2.00
2.00
0.99
0.78
2.04
3.07
3.07
3.03
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)
O
S
NH
O

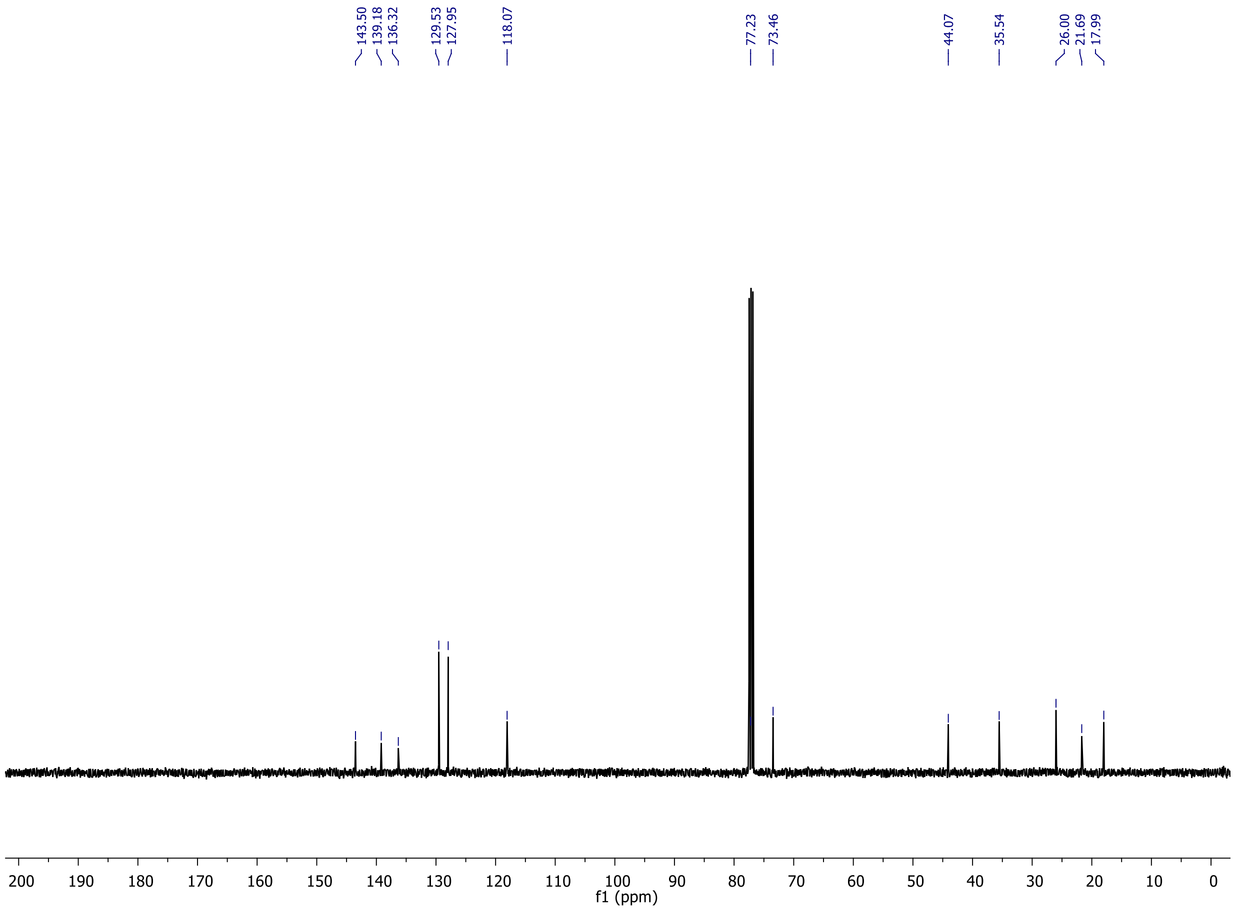

143.39
137.53
137.15
129.71
127.30
119.01
41.12
25.63
21.61
17.86
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

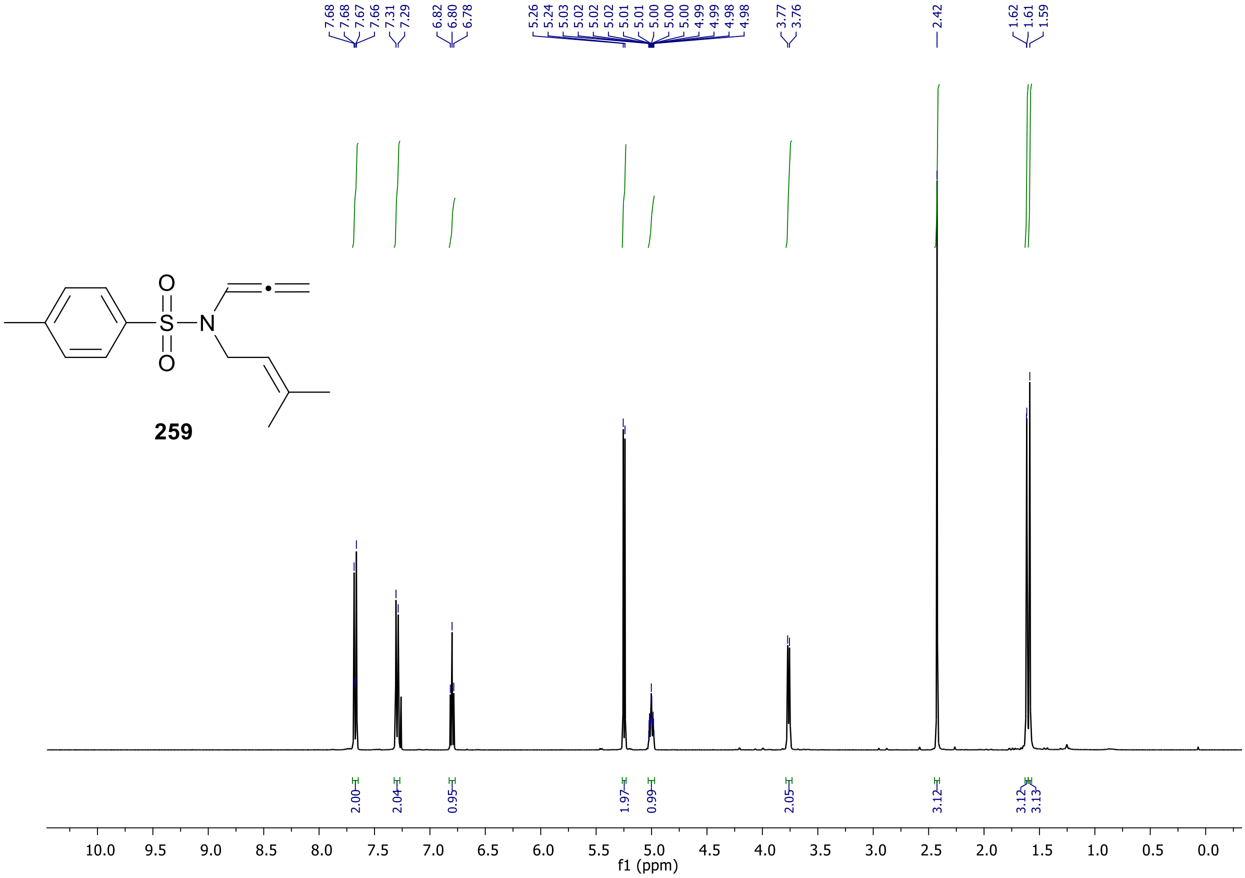

7.62
7.62
7.61
7.60
7.22
7.22
7.20
7.20
4.95
4.94
4.94
4.94
4.93
4.93
4.93
4.92
4.92
4.92
4.91
4.91
4.90
4.90
3.70
3.69
2.35
1.58
1.50
O
S
N
O
2.00
2.00
1.97
4.04
3.01
5.99
6.36
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

258b


7.75
7.75
7.74
7.73
7.73
7.72
7.30
7.28
5.13
5.12
5.12
5.11
5.11
5.11
5.10
5.10
5.09
5.09
5.08
5.08
5.08
5.07
4.07
4.06
3.82
3.80
2.42
1.98
1.98
1.97
1.72
1.72
1.67
1.67
O
S
N
O
2.00
2.03
0.99
2.02
2.02
3.06
0.93
2.98
2.98
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)

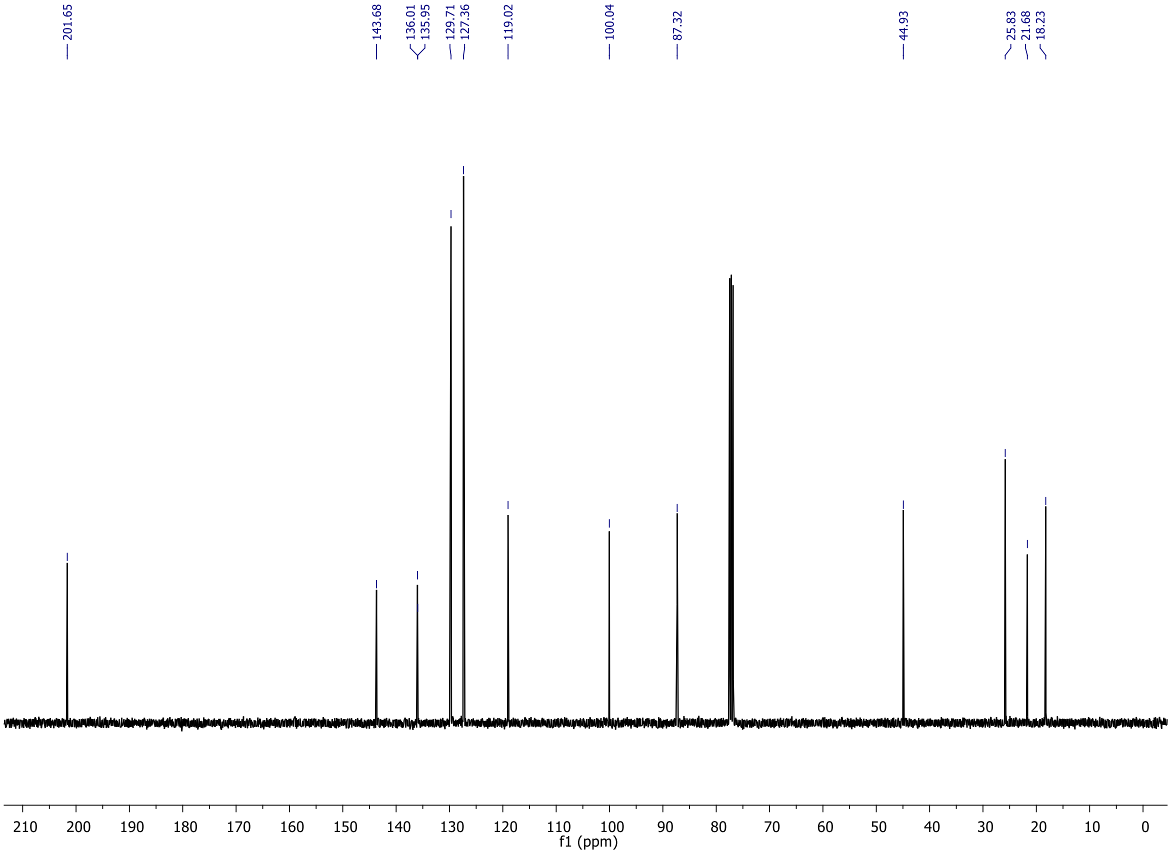
200a


143.50
139.18
136.32
129.53
127.95
118.07
77.23
73.46
44.07
35.54
26.00
21.69
17.99
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

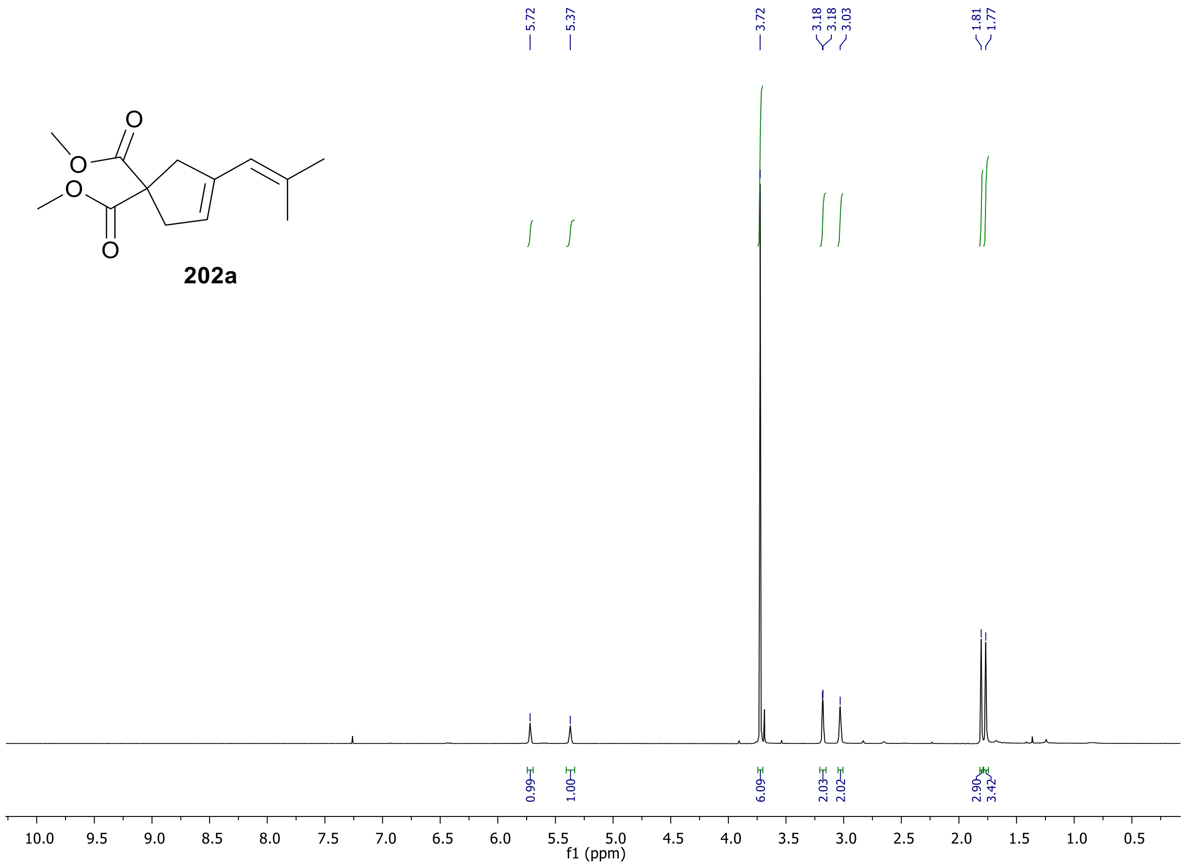


259

7.68
7.68
7.67
7.66
7.31
7.29
6.82
6.80
6.78
5.26
5.24
5.03
5.02
5.02
5.02
5.01
5.01
5.00
5.00
5.00
4.99
4.99
4.98
4.98
3.77
3.76
2.42
1.62
1.61
1.59
2.00
2.04
0.95
1.97
0.99
2.05
3.12
3.12
3.13
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)

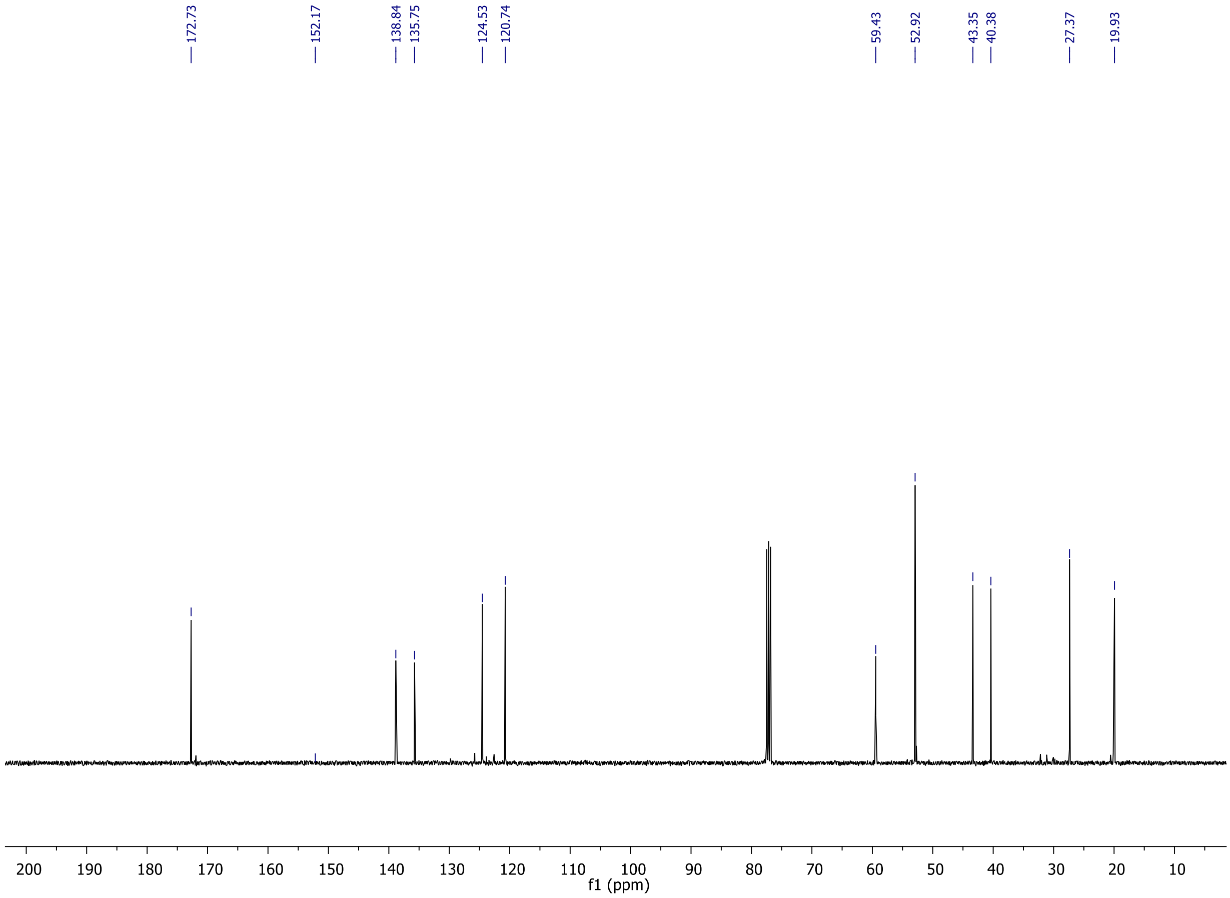


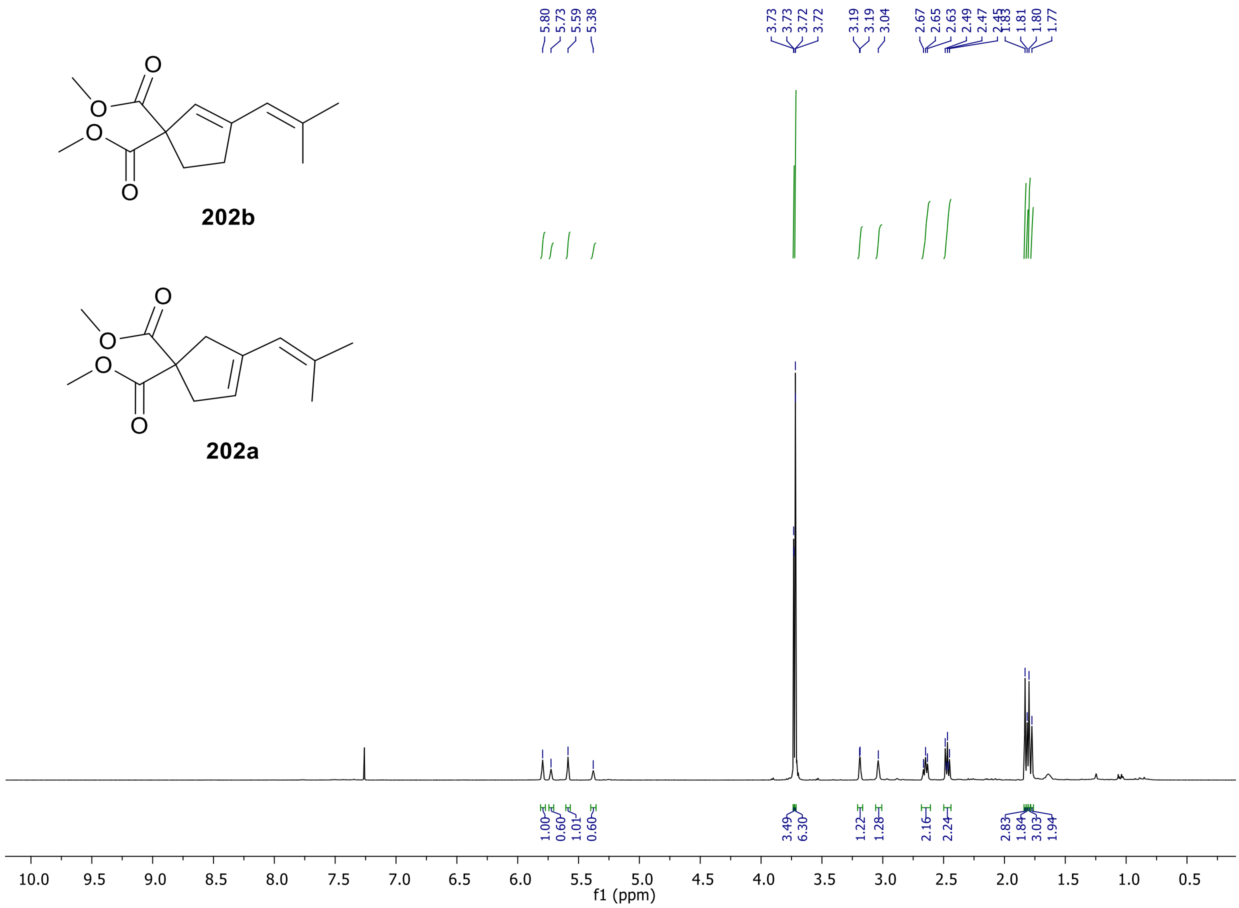
201.65
143.68
136.01
135.95
129.71
127.36
119.02
100.04
87.32
44.93
25.83
21.68
18.23
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



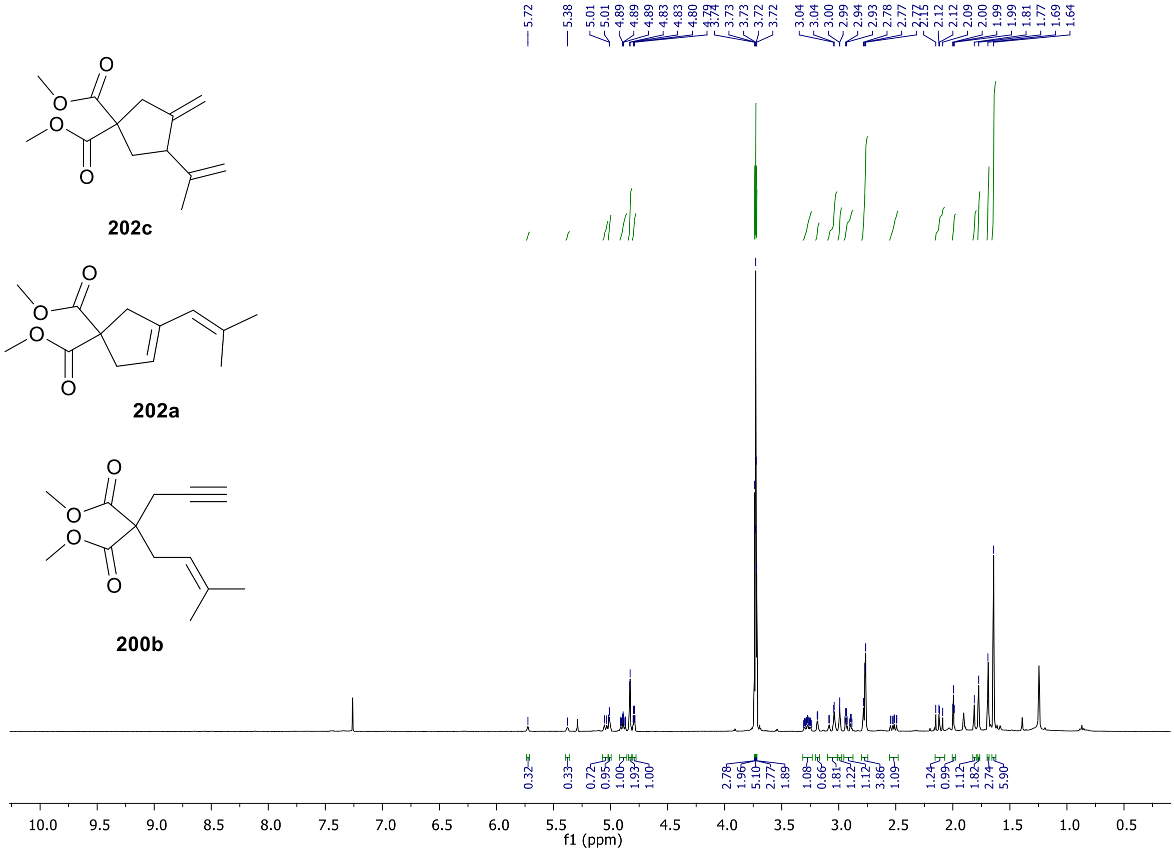
202a

5.72
5.37
3.72
3.18
3.18
3.03
1.81
1.77
0.99
1.00
6.09
2.03
2.02
2.90
3.42
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)


172.73
152.17
138.84
135.75
124.53
120.74
59.43
52.92
43.35
40.38
27.37
19.93
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

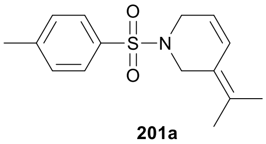

202b

202a

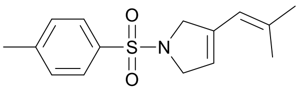

202c

202a

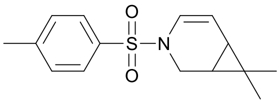
200b



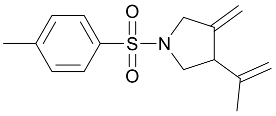
201a



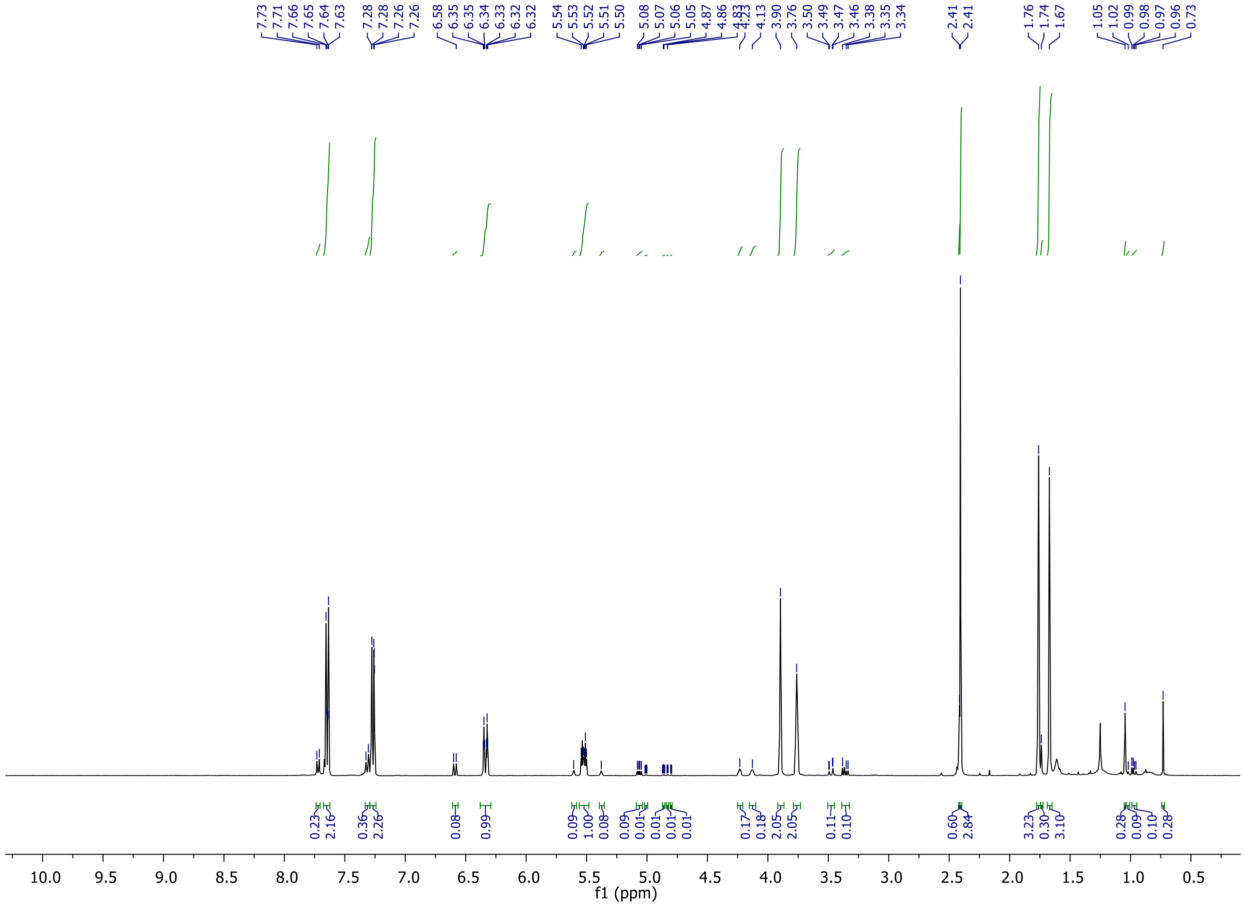
201b

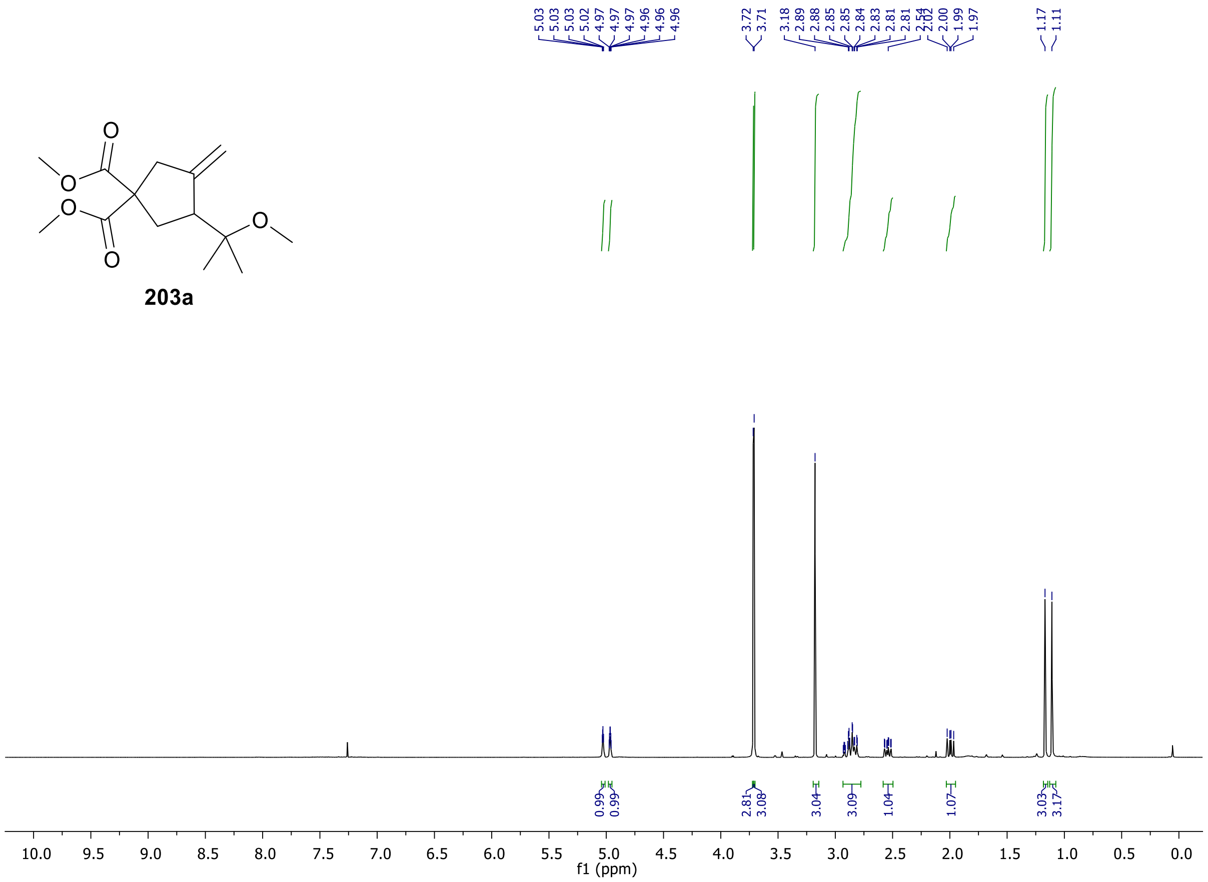


201c



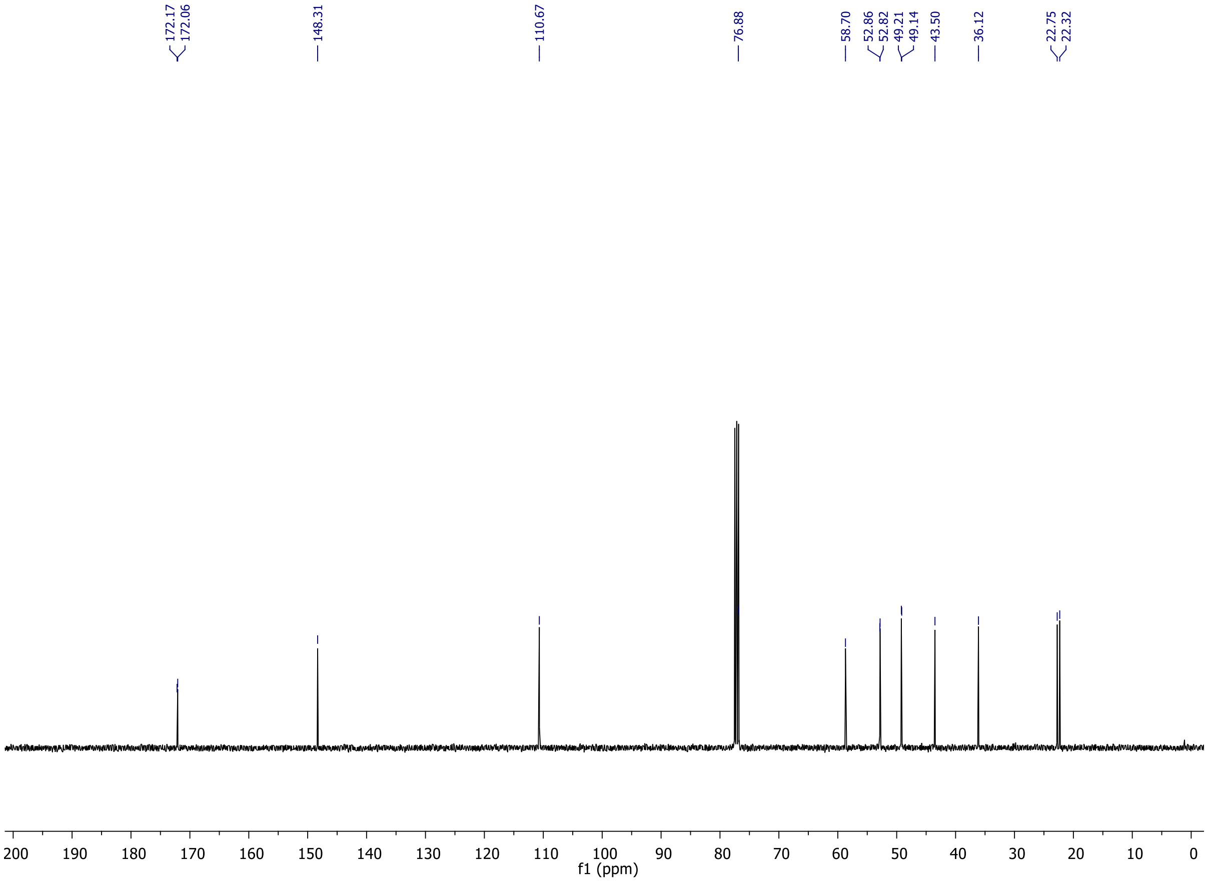
201d

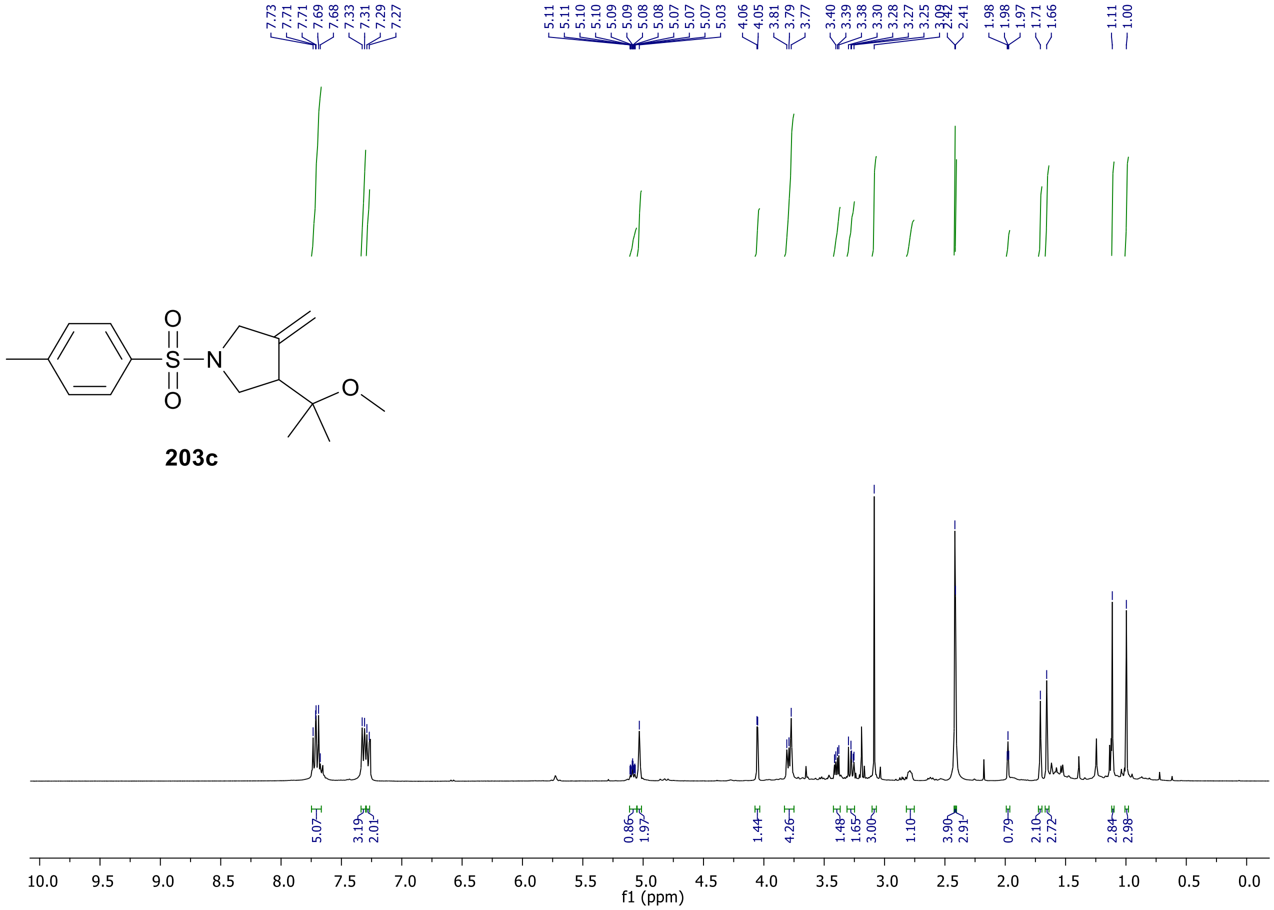



O
O
O
O
O

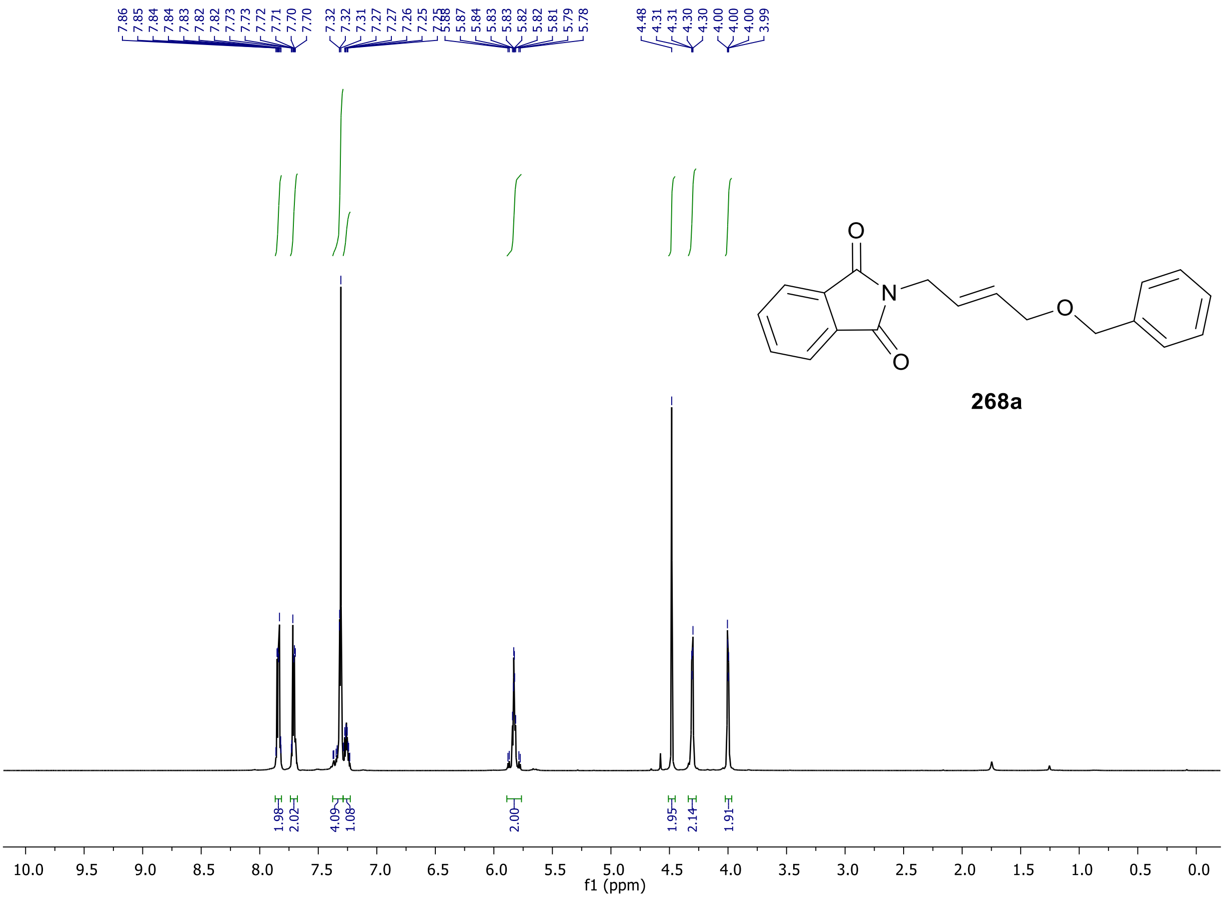
203a

5.03
5.03
5.03
5.02
4.97
4.97
4.97
4.96
4.96
4.96
3.72
3.71
3.18
2.89
2.88
2.85
2.85
2.84
2.83
2.81
2.81
2.54
2.02
2.00
1.99
1.97
1.17
1.11
0.99
0.99
2.81
3.08
3.04
3.09
1.04
1.07
3.03
3.17
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)

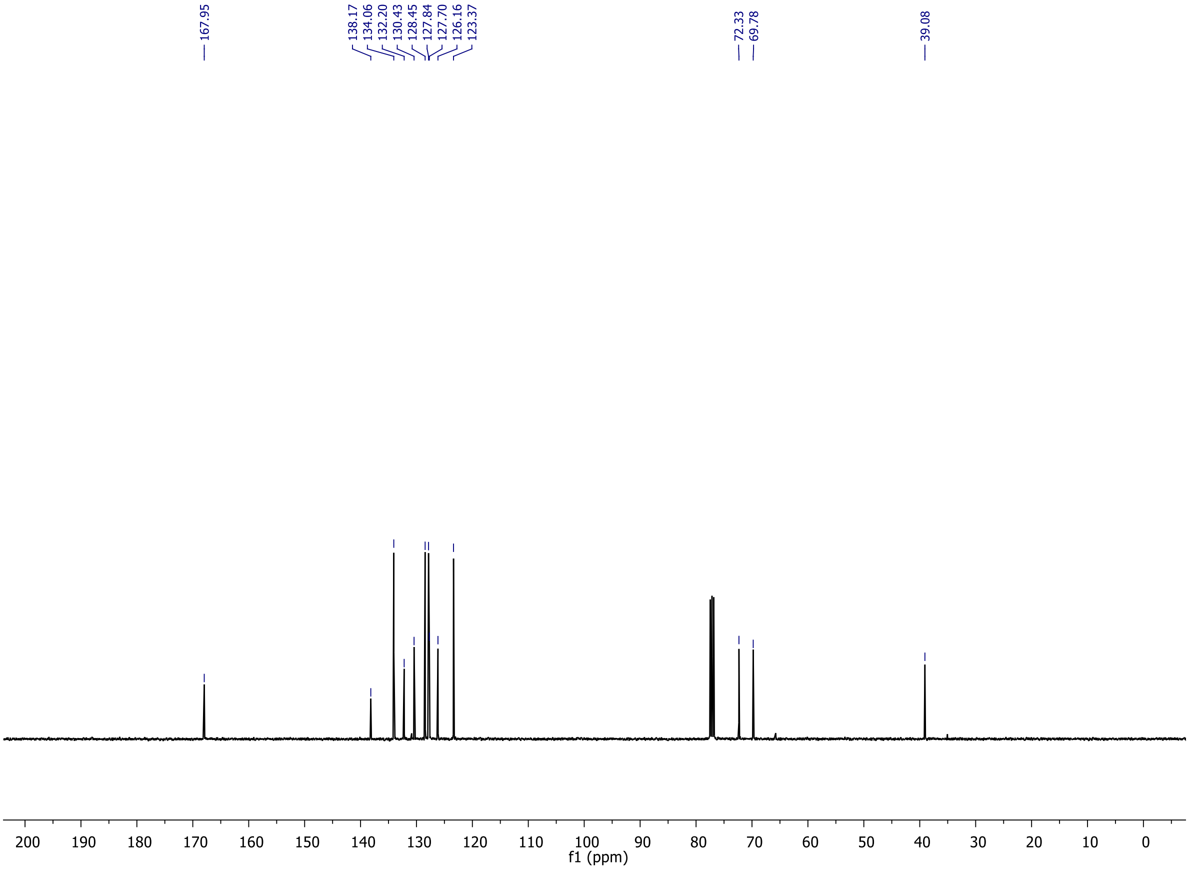

172.17
172.06
148.31
110.67
76.88
58.70
52.86
52.82
49.21
49.14
43.50
36.12
22.75
22.32
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

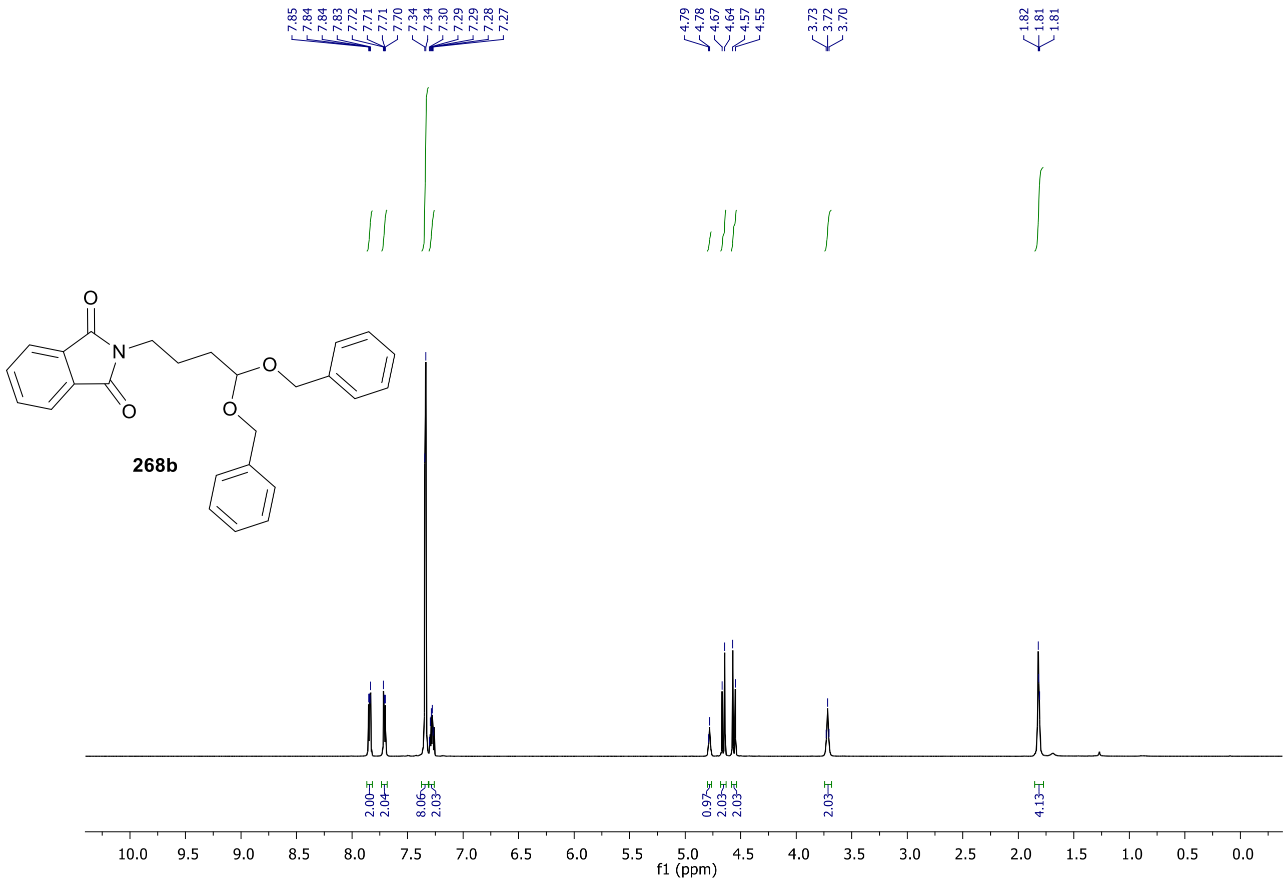

7.73
7.71
7.71
7.69
7.68
7.33
7.31
7.29
7.27
5.11
5.11
5.10
5.10
5.09
5.09
5.08
5.08
5.07
5.07
5.07
5.03
4.06
4.05
3.81
3.79
3.77
3.40
3.39
3.38
3.30
3.28
3.27
3.25
3.09
2.42
2.41
1.98
1.98
1.97
1.71
1.66
1.11
1.00
O
S
N
O
O
5.07
3.19
2.01
0.86
1.97
1.44
4.26
1.48
1.65
3.00
1.10
3.90
2.91
0.79
2.10
2.72
2.84
2.98
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)

203c


7.86
7.85
7.84
7.84
7.83
7.82
7.82
7.73
7.73
7.72
7.71
7.70
7.70
7.32
7.32
7.31
7.27
7.27
7.26
7.25
7.25
5.88
5.87
5.84
5.83
5.83
5.82
5.82
5.81
5.79
5.78
4.48
4.31
4.31
4.30
4.30
4.00
4.00
4.00
3.99
O
N
O
O
1.98
2.02
4.09
1.08
2.00
1.95
2.14
1.91
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)

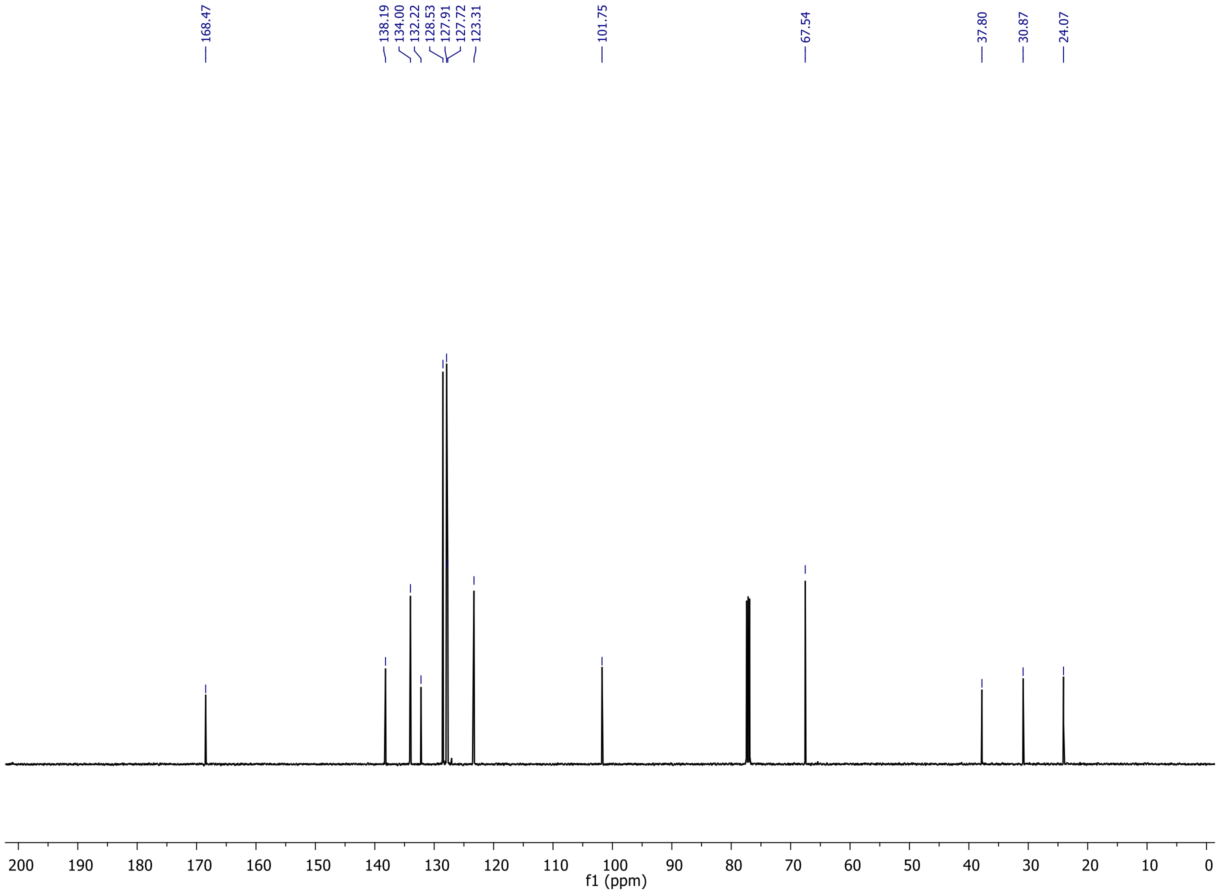
268a


167.95
138.17
134.06
132.20
130.43
128.45
127.84
127.70
126.16
123.37
72.33
69.78
39.08
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

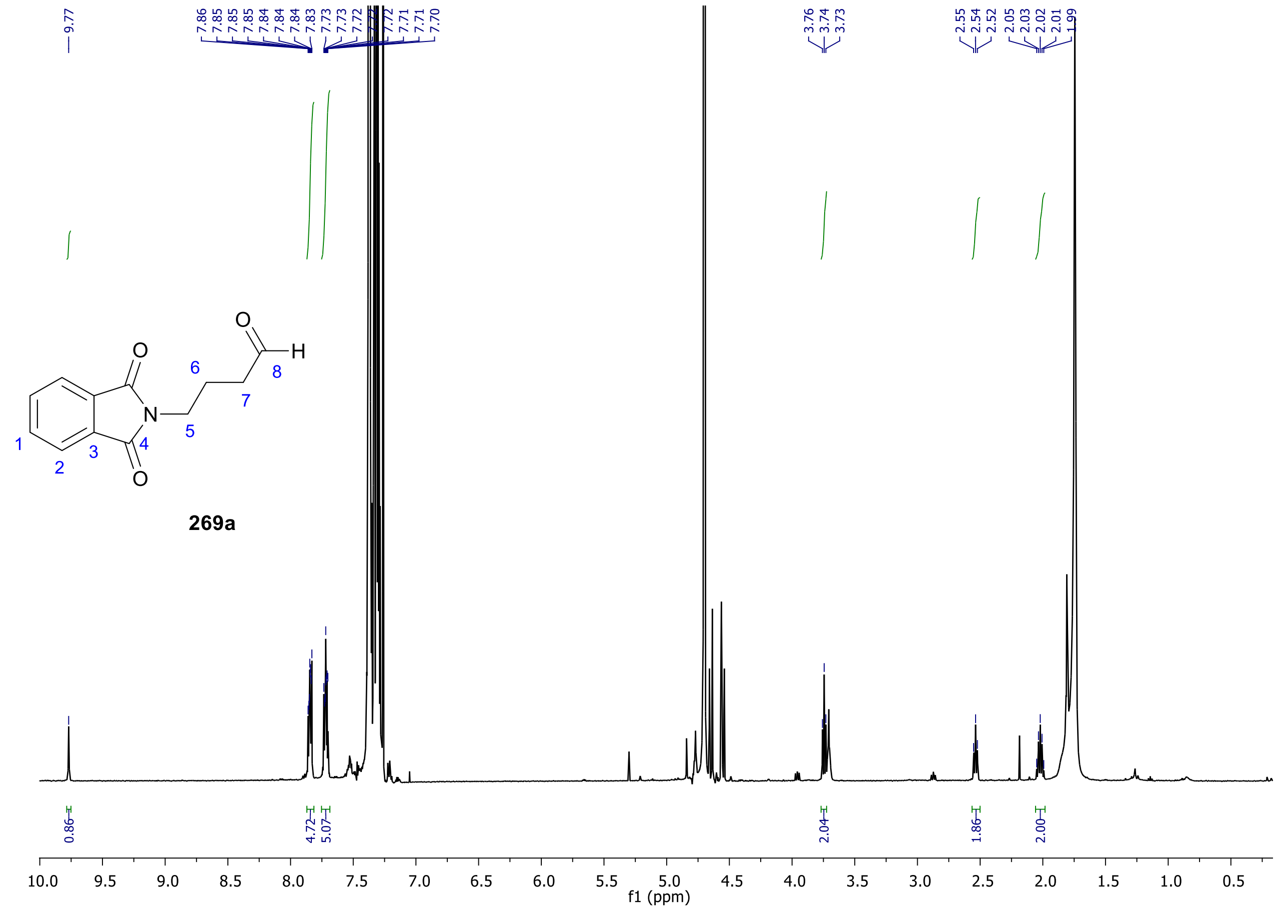


268b

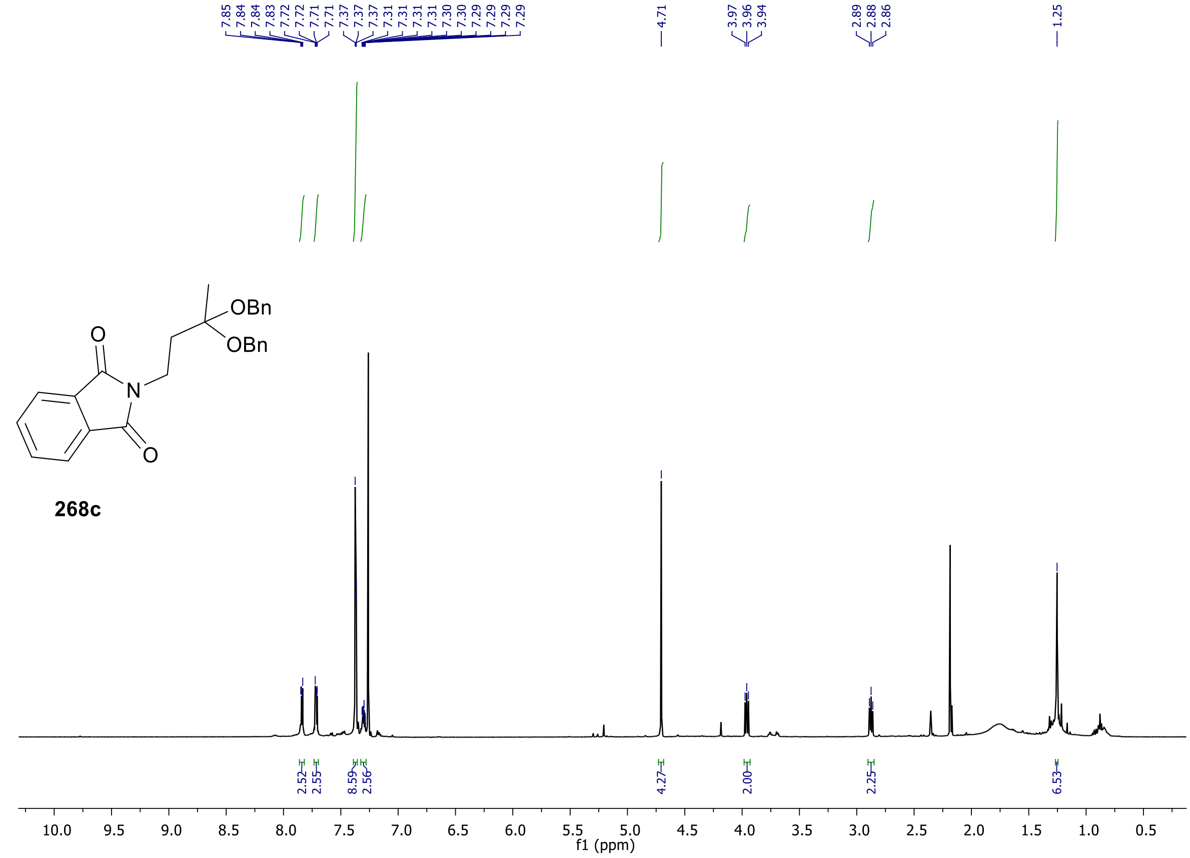
7.85
7.84
7.84
7.83
7.72
7.71
7.71
7.70
7.34
7.34
7.30
7.29
7.29
7.28
7.27
4.79
4.78
4.67
4.64
4.57
4.55
3.73
3.72
3.70
1.82
1.81
1.81
2.00
2.04
8.06
2.03
0.97
2.03
2.03
2.03
4.13
O
N
O
O
O
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



168.47
138.19
134.00
132.22
128.53
127.91
127.72
123.31
101.75
67.54
37.80
30.87
24.07
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.77
7.86
7.85
7.85
7.85
7.84
7.84
7.84
7.83
7.73
7.73
7.72
7.72
7.72
7.71
7.71
7.70
3.76
3.74
3.73
2.55
2.54
2.52
2.05
2.03
2.02
2.01
1.99
1
2
3
4
5
6
7
8
O
N
H
0.86
4.72
5.07
2.04
1.86
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

269a


7.85
7.84
7.84
7.83
7.72
7.72
7.71
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7.37
7.31
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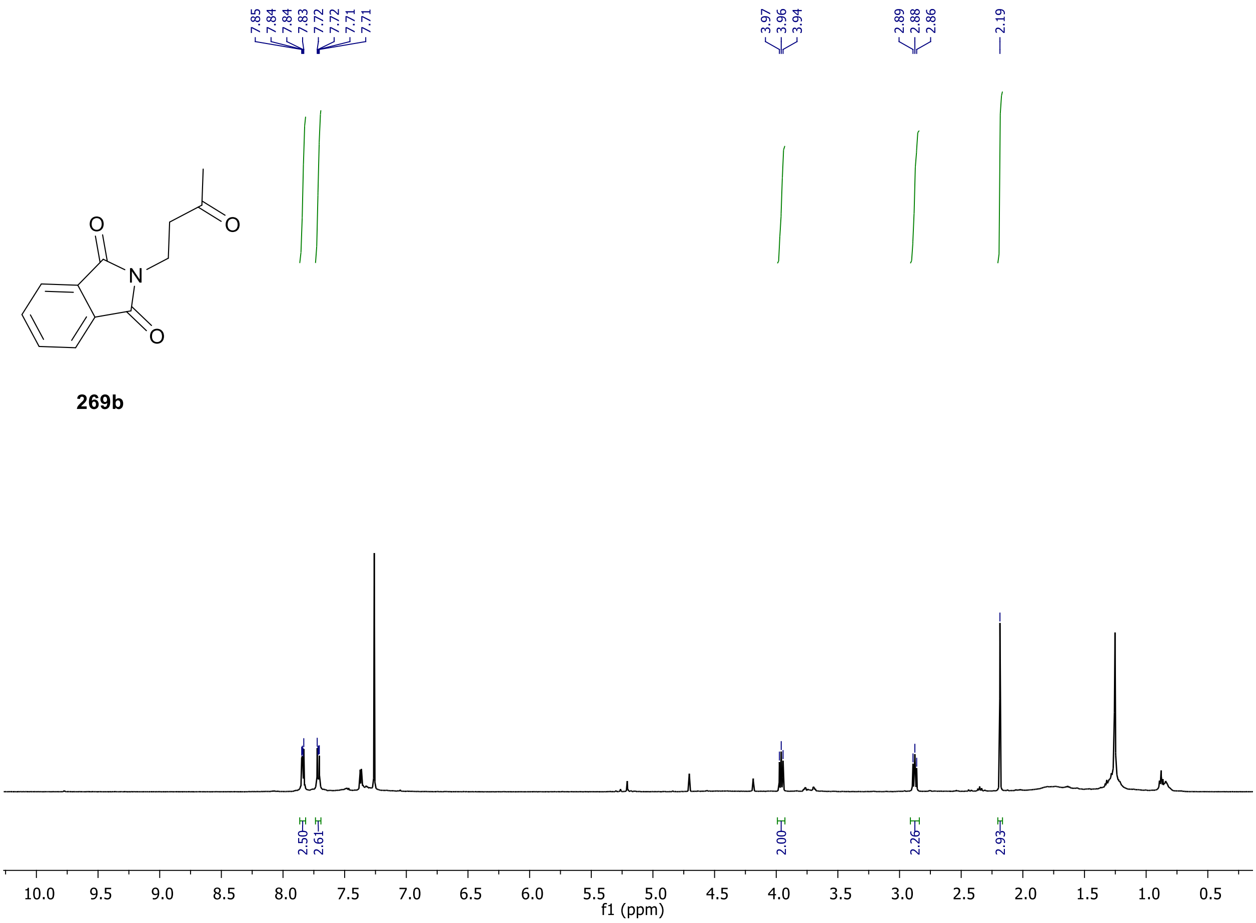
7.31
7.30
7.30
7.29
7.29
7.29
7.29
4.71
3.97
3.96
3.94
2.89
2.88
2.86
1.25
O
N
OBn
OBn
2.52
2.55
8.59
2.56
4.27
2.00
2.25
6.53
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

268c



269b

7.85
7.84
7.84
7.83
7.72
7.72
7.71
7.71
3.97
3.96
3.94
2.89
2.88
2.86
2.19
O
N
O
O
2.50
2.61
2.00
2.26
2.93
10.0
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1.5
1.0
0.5
f1 (ppm)

Appendix C – X-ray data

Data for complexes **179**, **184**, **187b**, **194** and **189b** can be found at: https://doi.org/10.1039/D0DT00665C.

Table 1 Summary of X-ray data.

	Complex 184	**Complex 194**	**Complex 179**	**Complex 189b**
Elemental formula	$C_{27}H_{22}AuClN_2$	$C_{27}H_{22}AuCl_3N_2$, Dichloromethane	$C_{25}H_{26}Cl_2N_2Pt$, $CHCl_3$	$C_{25}H_{26}AuCl_3N_2$
Formula weight	606.88	762.71	739.83	657.79
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space group	P 2_1/n (equiv. to no. 14)	P 2_1/c (no. 14)	P -1 (no. 2)	P 2_1/n (equiv. to no. 14)
Unit cell dimensions: a = (Å)	13.6080(2)	10.7752(2)	9.3270(3)	9.46335(14)
b =	12.09078(15)	14.9805(3)	11.8674(5)	19.7083(2)
c =	14.8143(2)	17.3390(3)	12.9754(4)	14.0613(2)
α = (°)	90	90	105.467(3	90
β =	110.984(2)	96.371(2)	91.480(3)	108.2848(15)
γ =	90	90	102.873(3)	90
Volume (Å^3)	2275.77(6)	2781.54(9)	1343.84(9)	2490.10(6)
Z, Calculated density (Mg/m^3)	4, 1.771	4, 1.821	2, 1.828	4, 1.755
F(000)	1176	1480	720	1280
Absorption coefficient (mm^{-1})	6.598	5.790	5.737	6.245

Temperature (K)	100.01(10) K	140(1)	140(1)	100.01(10)
Crystal colour, shape	colourless plate	pale yellow plate	pale yellow prism	yellow plate
Crystal size (mm)	0.07 x 0.10 x 0.16	0.56 x 0.32 x 0.09	0.44 x 0.115 x 0.110	0.16 x 0.11 x 0.026
On the diffractometer:				
Theta range for data collection	2.237 to 29.995	3.594 to 29.999	3.575 to 29.999	1.842 to 30.000
Limiting indices	-19<=h<=19, -17<=k<=17, -20<=l<=20	-15<=h<=15, -21<=k<=21, -24<=l<=24	-13<=h<=13, -16<=k<=16, -18<=l<=18	-13<=h<=13, -27<=k<=27, -19<=l<=19
Completeness to theta = 25.242 (%)	100.0	99.7	99.7	100.0
Absorption correction: Semi-empirical from equivalents				
Max. and min. transmission	1.00000 and 0.45490	1.000 and 0.236	1.000 and 0.1190	1.00000 and 0.39824
Reflections collected (not including absences)	82534	53936	26150	93429
No. of unique reflections, R(int) for equivalents	6634, 0.056	8091, 0.037	7821, 0.094	7264, 0.036
No. of 'observed' reflections (I > $2\sigma_I$)	6115	7083	7106	6792
Refinement:				
Data / restraints / parameters	6634 / 0 / 282	8091 / 0 / 327	7821 / 0 / 313	7264 / 0 / 282

Goodness-of-fit on F^2	1.106	1.046	1.065	1.053
Final R indices ('obsd' data)	R_1 = 0.025, wR_2 = 0.056	R_1 = 0.023, wR_2 = 0.047	R1 = 0.054, wR_2 = 0.134	R1 = 0.018, wR_2 = 0.041
Final R indices (all data)	R_1 = 0.030, wR_2 = 0.057	R_1 = 0.031, wR_2 = 0.048	R1 = 0.059, wR_2 = 0.141	R1 = 0.021, wR_2 = 0.042
Reflections weighted: 1/w = *	$\sigma^2(Fo^2)+(0.0231P)^2+4.323P$	$\sigma^2(Fo^2)+(0.0186P)^2+2.648P$	$\sigma^2(Fo^2)+(0.0835P)^2+1.455P$	$\sigma^2(Fo^2)+(0.0191P)^2+3.303P$
Largest diff. peak and hole (e.Å^{-3})	1.49 and -1.11	1.42 and -0.77	7.42 and -4.37	1.27 and -0.48
Location of largest difference peak	near the Au atom	near the Au atom	near the Pt atom	near Cl(1)

Table 2 Summary of X-Ray data continued.

	Complex 187b	**Compound 141**	**Complex 189a**	**Complex 172**
Elemental formula	$C_{25}H_{26}AuClN_2$	$C_{16}H_{16}N_2$	$C_{25}H_{26}AuCl_3N_2$	$C_{25}H_{26}Cl_2N_2Pd$
Formula weight	586.89	236.31	657.79	531.78
Crystal system	Tetragonal	Monoclinic	Monoclinic	Monoclinic
Space group	$P\ 4_1$ (no. 76)	$P\ 2_1/c$ (no. 14)	$P\ 2_1/n$ (equiv. to no. 14)	$P\ 2_1/c$ (no. 14)
Unit cell dimensions: a = (Å)	10.03923(5)	15.9846(3)	9.0844(2)	9.3560(3)
b =	10.03923(5)	6.86460(10)	15.9007(4)	14.1423(4)
c =	21.99014(18)	12.1208(2)	17.2456(4)	17.5530(5)
α = (°)	90	90	90	90

β =	90	110.310(2)	102.833(2)	103.017(3)
γ =	90	90	90	90
Volume (Å^3)	2216.28(2)	1247.30(4)	2428.87(10)	2262.85(12)
Z, Calculated density (Mg/m^3)	4, 1.759	4, 1.258	4, 1.799	4, 1.561
F(000)	1144	504	1280	1080
Absorption coefficient (mm^{-1})	6.772	0.576	6.402	1.071
Temperature (K)	100.01(10)	100(2)	100.00(10)	100.00(10)
Crystal colour, shape	yellow cuboid	colourless plate	yellow plate	red irregular
Crystal size (mm)	0.10 x 0.09 x 0.07	0.150 × 0.100 × 0.020	0.154 × 0.108 × 0.010	0.332 × 0.286 × 0.019
On the diffractometer:				
Theta range for data collection(°)	2.029 to 29.990	5.903 to 70.105	2.3290 to 30.9370	2.2200 to 31.1750
Limiting indices	-14<=h<=14, -14<=k<=14, -30<=l<=30	–18 ≤ h ≤ 17, –8 ≤ k ≤ 8, –14 ≤ l ≤ 14	-11 ≤ h ≤ 12, -19 ≤ k ≤ 22, -23 ≤ l ≤ 21	-11 ≤ h ≤ 12, -19 ≤ k ≤ 17, -22 ≤ l ≤ 21
Completeness to theta = 25.242 (%)	100.0	99.8	99.9	99.9
Absorption correction: Semi-empirical from equivalents				
Max. and min. transmission	1.00000 and 0.48497	1.000 and 0.702	1.00000 and 0.60590	1.00000 and 0.55327
Reflections collected (not including absences)	84333	33713	29087	26885

No. of unique reflections, R(int) for equivalents	6451, 0.036	2356, 0.0468	6308, 0.0447	5767, 0.0316
No. of 'observed' reflections (I > $2\sigma_I$)	6283	n/a	n/a	n/a
Refinement:				
Data / restraints / parameters	6451 / 1 / 264	2356 / 0 / 168	6308/0/285	5767/0/276
Goodness-of-fit on F^2	1.087	0.947	1.063	1.063
Final R indices ('obsd' data)	R1 = 0.013, wR_2 = 0.029	R1 = 0.0407, wR_2 = 0.0903	R_1 = 0.0256, wR_2 = 0.0496	R_1 = 0.0240, wR_2 = 0.0567
Final R indices (all data)	R1 = 0.014, wR_2 = 0.029	R1 = 0.0438, wR_2 = 0.0924	R_1 = 0.0330, wR_2 = 0.0513	R1 = 0.0262, wR2 = 0.0574
Reflections weighted: 1/w = *	$\sigma^2(Fo^2)+(0.0127P)^2+1.184P$	n/a	n/a	n/a
Largest diff. peak and hole (e.Å^{-3})	0.61 and -0.44	0.171 and –0.198	1.57 and -0.77	0.65 and -0.71
Location of largest difference peak	near the Au atom	n/a	near the Au atom	near the Pd atom

Compound 141

Table 3 Atomic coordinates [× 10^4], equivalent isotropic displacement parameters [Å^2 × 10^3] and site occupancy factors. *Ueq* is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}
N2	2034(1)	5329(2)	5883(1)	21(1)
N1	3686(1)	3425(2)	5715(1)	22(1)
C5	2765(1)	2489(2)	3756(1)	23(1)
C2	4407(1)	2826(2)	5478(1)	23(1)

C6	2878(1)	3265(2)	4863(1)	20(1)
C11	1295(1)	4980(2)	6246(1)	24(1)
C7	2095(1)	3772(2)	5181(1)	22(1)
C15	2482(1)	7114(2)	6119(1)	24(1)
C9	893(1)	3248(2)	5743(1)	25(1)
C3	4341(1)	2051(2)	4387(1)	25(1)
C8	1390(1)	2529(2)	5081(1)	24(1)
C12	1106(1)	6334(2)	7004(1)	29(1)
C16	3119(1)	7635(2)	5509(1)	27(1)
C14	2275(1)	8379(2)	6851(1)	29(1)
C4	3510(1)	1880(2)	3518(1)	25(1)
C13	1599(1)	7978(2)	7332(1)	31(1)
C1	5287(1)	2996(2)	6465(1)	29(1)
C10	112(1)	2310(2)	5952(1)	33(1)

Table 4 Bond lengths [Å] and angles [°].

N2–C7	1.3903(17)	N1–C2–C3	122.08(12)
N2–C15	1.3971(18)	N1–C2–C1	116.12(12)
N2–C11	1.4176(17)	C3–C2–C1	121.79(12)
N1–C2	1.3451(17)	N1–C6–C5	122.47(12)
N1–C6	1.3494(17)	N1–C6–C7	117.11(11)
C5–C4	1.3827(19)	C5–C6–C7	120.18(12)
C5–C6	1.3966(18)	C9–C11–C12	132.79(13)
C5–H5	0.9500	C9–C11–N2	108.50(11)
C2–C3	1.3947(19)	C12–C11–N2	118.71(13)
C2–C1	1.5017(19)	C8–C7–N2	107.45(11)
C6–C7	1.4741(18)	C8–C7–C6	124.83(12)
C11–C9	1.388(2)	N2–C7–C6	125.95(12)
C11–C12	1.4108(19)	C14–C15–N2	118.09(13)
C7–C8	1.3851(19)	C14–C15–C16	122.03(13)
C15–C14	1.361(2)	N2–C15–C16	119.75(12)
C15–C16	1.4956(19)	C11–C9–C8	106.59(12)
C9–C8	1.4002(19)	C11–C9–C10	125.31(13)
C9–C10	1.5017(19)	C8–C9–C10	127.99(13)
C3–C4	1.3848(19)	C4–C3–C2	119.34(12)
C3–H3	0.9500	C4–C3–H3	120.3
C8–H8	0.9500	C2–C3–H3	120.3
C12–C13	1.355(2)	C7–C8–C9	109.81(13)
C12–H12	0.9500	C7–C8–H8	125.1
C16–H16A	0.9800	C9–C8–H8	125.1
C16–H16B	0.9800	C13–C12–C11	120.42(13)
C16–H16C	0.9800	C13–C12–H12	119.8
C14–C13	1.422(2)	C11–C12–H12	119.8
C14–H14	0.9500	C15–C16–H16A	109.5
C4–H4	0.9500	C15–C16–H16B	109.5
C13–H13	0.9500	H16A–C16–H16B	109.5
C1–H1A	0.9800	C15–C16–H16C	109.5
C1–H1B	0.9800	H16A–C16–H16C	109.5
C1–H1C	0.9800	H16B–C16–H16C	109.5
C10–H10A	0.9800	C15–C14–C13	122.29(14)
C10–H10B	0.9800	C15–C14–H14	118.9
C10–H10C	0.9800	C13–C14–H14	118.9
		C5–C4–C3	118.96(12)
C7–N2–C15	131.32(11)	C5–C4–H4	120.5
C7–N2–C11	107.62(11)	C3–C4–H4	120.5
C15–N2–C11	120.47(11)	C12–C13–C14	119.20(13)
C2–N1–C6	118.34(11)	C12–C13–H13	120.4
C4–C5–C6	118.81(12)	C14–C13–H13	120.4
C4–C5–H5	120.6	C2–C1–H1A	109.5
C6–C5–H5	120.6	C2–C1–H1B	109.5

H1A–C1–H1B	109.5	C9–C10–H10B	109.5
C2–C1–H1C	109.5	H10A–C10–H10B	109.5
H1A–C1–H1C	109.5	C9–C10–H10C	109.5
H1B–C1–H1C	109.5	H10A–C10–H10C	109.5
C9–C10–H10A	109.5	H10B–C10–H10C	109.5

Table 5 Anisotropic displacement parameters [Å^2× 10^3]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N2	20(1)	25(1)	18(1)	1(1)	7(1)	2(1)
N1	22(1)	24(1)	20(1)	1(1)	9(1)	1(1)
C5	25(1)	24(1)	19(1)	1(1)	7(1)	0(1)
C2	24(1)	23(1)	24(1)	2(1)	11(1)	1(1)
C6	23(1)	20(1)	19(1)	2(1)	9(1)	0(1)
C11	20(1)	32(1)	21(1)	5(1)	9(1)	5(1)
C7	23(1)	24(1)	18(1)	0(1)	8(1)	1(1)
C15	22(1)	25(1)	21(1)	0(1)	3(1)	2(1)
C9	23(1)	30(1)	25(1)	5(1)	10(1)	2(1)
C3	25(1)	27(1)	26(1)	1(1)	14(1)	3(1)
C8	23(1)	26(1)	24(1)	1(1)	9(1)	−1(1)
C12	25(1)	41(1)	23(1)	2(1)	11(1)	9(1)
C16	28(1)	25(1)	27(1)	0(1)	9(1)	−3(1)
C14	26(1)	30(1)	26(1)	−4(1)	4(1)	4(1)
C4	32(1)	25(1)	21(1)	−1(1)	13(1)	1(1)
C13	29(1)	39(1)	24(1)	−5(1)	7(1)	10(1)
C1	24(1)	34(1)	27(1)	−2(1)	8(1)	2(1)
C10	28(1)	37(1)	38(1)	8(1)	18(1)	2(1)

Complex 172

Table 6 Fractional atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å2×10^3). Ueq is defined as 1/3 of the trace of the orthogonalised Uij tensor.

Atom	*x*	*y*	*z*	U(eq)
Pd01	2358.9(2)	2603.0(2)	4526.2(2)	10.33(4)
Cl02	-9.8(5)	2741.9(3)	4728.0(2)	14.91(8)
Cl03	4543.6(5)	2330.6(3)	4146.6(3)	17.11(9)
N004	2503.2(16)	1287.3(10)	4995.4(8)	12.4(3)
N005	2634.6(16)	4035.3(10)	4458.0(8)	12.1(3)
C006	2968.6(18)	4450.7(12)	5180.5(10)	12.1(3)
C007	3497.5(18)	2986.8(12)	5923.6(9)	12.2(3)
C008	3413.6(19)	1259.0(12)	5718.1(10)	12.4(3)
C009	4121.9(19)	2148.2(12)	6072.3(9)	12.4(3)
C00A	2930.1(18)	3846.3(11)	5876.9(9)	11.4(3)
C00B	3024(2)	5501.5(13)	3864.6(11)	17.2(3)
C00C	5614.3(19)	2090.6(12)	6610.4(10)	12.7(3)
C00D	8228(2)	1834.1(13)	6807.1(11)	17.8(4)
C00E	1779(2)	503.9(12)	4673.9(10)	15.3(3)
C00F	2171.1(19)	4197.5(12)	6522.4(10)	12.9(3)
C00G	6826(2)	1816.6(12)	6321.6(10)	15.6(3)
C00H	3339.1(19)	5404.0(12)	5251.0(10)	14.6(3)
C00I	3362(2)	5933.6(13)	4587.9(11)	18.2(4)
C00J	7212(2)	2335.1(13)	7882.7(11)	18.2(4)
C00K	5813(2)	2348.2(12)	7397.0(10)	15.4(3)
C00L	2671.2(19)	4542.2(12)	3810.0(10)	14.0(3)
C00M	3314(2)	4695.5(13)	7169.9(10)	16.9(3)
C00N	8415(2)	2093.6(13)	7588.7(12)	19.9(4)
C00O	1545(2)	3338.5(13)	6877.0(11)	18.4(4)
C00P	3669(2)	409.6(12)	6126.1(11)	16.3(3)
C00Q	891(2)	4866.2(13)	6186.1(11)	18.3(4)
C00R	1964(2)	-344.5(13)	5080.2(11)	17.7(3)
C00S	2329(2)	4041.2(14)	3036.2(10)	19.2(4)
C00T	2925(2)	-400.8(12)	5802.4(11)	18.8(4)
C00U	835(2)	600.6(14)	3865.5(11)	20.6(4)

Table 7 Anisotropic displacement parameters (Å^2×10^3). The anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pd01	12.37(7)	9.59(7)	8.66(7)	0.63(4)	1.57(5)	0.16(4)
Cl02	12.63(18)	15.2(2)	15.98(19)	0.16(13)	1.21(15)	-0.18(13)
Cl03	18.0(2)	19.1(2)	15.9(2)	0.99(14)	7.31(16)	2.91(15)
N004	14.9(7)	10.7(7)	11.7(7)	0.0(5)	3.5(6)	0.8(5)
N005	11.5(7)	11.5(7)	13.0(7)	1.9(5)	2.3(5)	0.1(5)
C006	9.6(7)	12.4(8)	13.9(8)	1.7(6)	1.5(6)	1.0(5)
C007	12.3(8)	16.0(8)	7.9(7)	-0.1(6)	1.7(6)	-1.3(6)
C008	12.7(8)	12.7(8)	12.6(8)	0.6(6)	4.2(6)	1.4(6)
C009	15.2(8)	12.8(8)	9.0(7)	0.5(5)	2.3(6)	0.6(6)
C00A	11.6(8)	11.1(8)	10.4(7)	-0.3(5)	0.1(6)	-0.9(5)
C00B	15.3(8)	16.9(9)	19.4(9)	7.7(6)	4.0(7)	-0.3(6)
C00C	14.7(8)	9.6(7)	13.1(8)	2.7(6)	1.3(6)	0.9(6)
C00D	13.9(8)	15.9(9)	24.2(9)	-0.3(6)	5.5(7)	0.8(6)
C00E	16.6(8)	13.4(8)	16.6(8)	-3.6(6)	5.5(7)	-0.1(6)
C00F	13.8(8)	13.0(8)	11.4(8)	-0.9(6)	1.9(6)	0.2(6)
C00G	19.4(9)	13.9(8)	13.6(8)	1.2(6)	3.9(7)	2.1(6)
C00H	14.7(8)	12.1(8)	16.3(8)	0.8(6)	1.7(7)	-0.3(6)
C00I	17.9(9)	11.2(8)	24.7(9)	5.2(6)	3.1(7)	-1.2(6)
C00J	22.3(9)	15.3(9)	14.3(8)	-1.2(6)	-1.7(7)	1.7(6)
C00K	17.7(8)	14.0(8)	14.5(8)	0.5(6)	3.5(7)	3.5(6)
C00L	12.3(8)	15.7(8)	13.6(8)	3.6(6)	2.4(6)	2.1(6)
C00M	20.0(9)	17.2(9)	12.0(8)	-3.7(6)	0.8(7)	-0.1(6)
C00N	15.7(9)	16.2(9)	24.3(9)	0.6(7)	-3.2(7)	0.1(6)
C00O	22.3(9)	19.1(9)	15.5(8)	-0.1(6)	8.1(7)	-3.2(7)
C00P	18.6(9)	13.9(8)	16.0(8)	3.5(6)	3.2(7)	3.0(6)
C00Q	16.1(8)	20.0(9)	18.7(9)	-0.2(6)	4.1(7)	5.1(6)
C00R	20.3(9)	12.3(8)	22.3(9)	-3.3(6)	8.6(7)	-1.3(6)
C00S	22.8(9)	21.7(9)	12.7(8)	3.6(6)	3.4(7)	0.6(7)
C00T	24.9(9)	9.7(8)	23.3(9)	3.2(6)	8.3(8)	1.8(6)
C00U	26.4(10)	17.9(9)	16.0(9)	-3.7(6)	1.6(7)	-3.1(7)

Table 8 Bond lengths.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd01	Cl02	2.3300(4)	C00B	C00I	1.380(3)
Pd01	Cl03	2.3203(5)	C00B	C00L	1.395(2)
Pd01	N004	2.0269(14)	C00C	C00G	1.397(3)
Pd01	N005	2.0489(14)	C00C	C00K	1.399(2)
Pd01	C007	2.5038(16)	C00D	C00G	1.394(2)
N004	C008	1.360(2)	C00D	C00N	1.393(3)
N004	C00E	1.354(2)	C00E	C00R	1.387(3)
N005	C006	1.368(2)	C00E	C00U	1.499(2)
N005	C00L	1.351(2)	C00F	C00M	1.544(2)
C006	C00A	1.499(2)	C00F	C00O	1.540(2)
C006	C00H	1.391(2)	C00F	C00Q	1.536(2)
C007	C009	1.322(2)	C00H	C00I	1.388(2)
C007	C00A	1.321(2)	C00J	C00K	1.392(3)
C008	C009	1.490(2)	C00J	C00N	1.383(3)
C008	C00P	1.391(2)	C00L	C00S	1.501(2)
C009	C00C	1.501(2)	C00P	C00T	1.394(3)
C00A	C00F	1.548(2)	C00R	C00T	1.382(3)

Table 9 Bond angles.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Cl02	Pd01	C007	92.41(4)	C007	C00A	C006	119.48(16)
Cl03	Pd01	Cl02	170.825(16)	C007	C00A	C00F	119.58(15)
Cl03	Pd01	C007	96.28(4)	C00I	C00B	C00L	119.70(17)
N004	Pd01	Cl02	89.67(4)	C00G	C00C	C009	120.17(15)
N004	Pd01	Cl03	88.97(4)	C00G	C00C	C00K	119.47(16)
N004	Pd01	N005	159.00(6)	C00K	C00C	C009	120.31(16)
N004	Pd01	C007	80.00(6)	C00N	C00D	C00G	119.95(18)
N005	Pd01	Cl02	93.56(4)	N004	C00E	C00R	120.07(16)
N005	Pd01	Cl03	90.96(4)	N004	C00E	C00U	116.92(16)
N005	Pd01	C007	79.13(6)	C00R	C00E	C00U	122.98(16)
C008	N004	Pd01	112.11(11)	C00M	C00F	C00A	109.21(14)
C00E	N004	Pd01	126.91(12)	C00O	C00F	C00A	108.78(14)
C00E	N004	C008	120.95(15)	C00O	C00F	C00M	109.02(14)
C006	N005	Pd01	112.07(11)	C00Q	C00F	C00A	111.28(14)
C00L	N005	Pd01	126.94(12)	C00Q	C00F	C00M	110.67(14)
C00L	N005	C006	120.56(15)	C00Q	C00F	C00O	107.83(15)
N005	C006	C00A	117.94(14)	C00D	C00G	C00C	120.13(17)
N005	C006	C00H	119.93(16)	C00I	C00H	C006	119.94(17)
C00H	C006	C00A	122.12(15)	C00B	C00I	C00H	119.27(16)
C009	C007	Pd01	94.04(11)	C00N	C00J	C00K	120.46(17)
C00A	C007	Pd01	93.57(11)	C00J	C00K	C00C	119.91(17)
C00A	C007	C009	172.31(17)	N005	C00L	C00B	120.59(16)
N004	C008	C009	119.37(14)	N005	C00L	C00S	118.07(15)
N004	C008	C00P	120.28(16)	C00B	C00L	C00S	121.35(16)
C00P	C008	C009	120.34(15)	C00J	C00N	C00D	120.02(17)
C007	C009	C008	122.65(15)	C008	C00P	C00T	119.22(16)
C007	C009	C00C	118.68(15)	C00T	C00R	C00E	120.12(17)
C008	C009	C00C	118.67(14)	C00R	C00T	C00P	119.25(16)
C006	C00A	C00F	120.87(14)				

Table 10 Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3).

Atom	*x*	*y*	*z*	U(eq)
H00B	3032.31	5848.6	3415.52	21
H00D	9037.56	1672.53	6609.24	21
H00G	6697.87	1622.29	5804.45	19
H00H	3571.38	5686.57	5741.83	18
H00I	3602.24	6572.46	4630.73	22
H00J	7337.62	2489.8	8408.59	22
H00K	5011.56	2527.94	7594.9	19
H00A	4083.98	4259.16	7388.06	25
H00C	2849.38	4910.6	7573.14	25
H00E	3720.83	5226.42	6951.07	25
H00N	9349.93	2104.47	7913.09	24
H00F	884.63	2999.54	6470.64	28
H00L	1026.08	3551.19	7258.79	28
H00M	2333.12	2929.31	7122.66	28
H00P	4327.58	383	6609.17	20
H00O	1259.76	5423.47	5983.72	27
H00Q	403.28	5041.04	6591.44	27
H00R	209.1	4552.2	5772.92	27
H00S	1439.4	-876.55	4866.19	21
H00T	3190.96	3719.98	2960.98	29
H00U	2018.28	4493.54	2624.42	29
H00V	1560.01	3589.59	3028.28	29
H00W	3074.64	-973.12	6069.52	23
H00X	168.86	1119.46	3852.38	31
H00Y	289.05	27.91	3724.31	31
H	1444.3	716.17	3502.17	31

Complex 189a

Table 11 Fractional atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å2×10^3). Ueq is defined as 1/3 of the trace of the orthogonalised Uij tensor.

Atom	x	y	z	U(eq)
Au01	5735.5(2)	2338.8(2)	7403.1(2)	12.93(4)
Cl02	4683.6(8)	1695.5(4)	8333.3(4)	18.17(14)
Cl03	6843.6(9)	2953.2(5)	6477.5(4)	23.91(15)
Cl04	7892.3(9)	1502.1(5)	7832.8(5)	26.96(17)
N005	1640(3)	3843.4(14)	6754.2(12)	12.8(5)
N006	3547(3)	3753.9(15)	8822.3(13)	16.1(5)
C007	3809(3)	3000.2(17)	6964.7(15)	12.6(5)
C008	2965(3)	2833.0(17)	6235.3(15)	13.2(5)
C009	3192(3)	2173.3(17)	5663.0(15)	14.0(6)
C00A	3109(3)	2353.5(17)	4861.0(15)	15.5(6)
C00B	3143(3)	3721.2(17)	7360.6(15)	13.3(5)
C00C	2768(3)	3424.1(17)	8145.0(15)	15.7(6)
C00D	1649(3)	3380.4(16)	6083.7(15)	13.0(5)
C00E	1658(3)	2811.3(18)	8115.7(17)	18.3(6)
C00F	3434(3)	1344.0(17)	5922.8(15)	15.3(6)
C00G	-705(3)	4434.7(18)	6142.7(16)	18.7(6)
C00H	487(3)	3455.4(17)	5416.3(15)	16.3(6)
C00I	3485(3)	5323.3(17)	7713.9(17)	19.1(6)
C00J	3595(3)	711.5(18)	5397.6(16)	17.9(6)
C00K	3242(3)	3476.2(19)	9510.8(16)	19.0(6)
C00L	4212(4)	4782.7(18)	6503.4(16)	20.1(6)
C00M	161(3)	4631.3(18)	7600.1(16)	18.7(6)
C00N	1339(4)	2534.8(19)	8821.8(18)	21.4(6)
C00O	3257(3)	1720.8(18)	4337.8(16)	17.7(6)
C00P	431(3)	4319.9(17)	6824.9(16)	15.1(6)
C00Q	-674(3)	4015.4(18)	5444.3(17)	20.8(6)
C00R	4127(3)	4556.5(17)	7356.6(16)	15.4(6)
C00S	3497(3)	896.9(19)	4602.1(16)	18.5(6)
C00T	5750(3)	4412.7(18)	7850.2(16)	17.6(6)
C00U	2148(4)	2877(2)	9526.9(17)	21.7(6)
C00V	4165(4)	3861(2)	10262.1(16)	25.0(7)

Table 12 Anisotropic displacement parameters (Å^2×10^3). The anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].

Atom	U11	U22	U33	U23	U13	U12
Au01	12.31(6)	11.65(6)	13.68(6)	-3.06(4)	0.41(4)	1.28(4)
Cl02	23.2(4)	15.0(3)	15.2(3)	1.9(2)	1.7(2)	1.9(3)
Cl03	23.2(4)	25.8(4)	26.4(4)	-4.3(3)	13.6(3)	-2.8(3)
Cl04	17.8(4)	21.9(4)	36.8(4)	-7.1(3)	-3.4(3)	8.1(3)
N005	13.5(13)	11.6(11)	12.5(10)	1.1(8)	1.4(9)	-1.2(9)
N006	16.0(13)	17.0(12)	14.6(11)	-0.2(9)	1.7(9)	4.4(9)
C007	12.6(14)	10.4(13)	14.6(12)	1.3(10)	2.6(10)	-1.7(10)
C008	14.4(15)	12.9(14)	13.0(12)	2.3(10)	4.3(10)	-1.9(10)
C009	12.5(15)	15.9(14)	12.5(12)	-2.4(10)	0.2(10)	-3.2(10)
C00A	15.0(16)	15.1(14)	15.7(13)	2.4(10)	1.8(11)	-0.3(11)
C00B	12.0(14)	14.5(14)	11.9(12)	0.3(10)	-0.3(10)	0.8(10)
C00C	17.7(16)	16.0(14)	13.7(12)	0.8(10)	3.9(10)	6.7(11)
C00D	15.4(15)	11.3(13)	12.9(12)	0.4(10)	4.6(10)	-2.5(10)
C00E	18.9(16)	18.7(16)	17.0(14)	1.2(10)	3.3(11)	2.1(11)
C00F	16.2(15)	17.3(14)	11.8(12)	-0.4(10)	2.1(10)	-2.8(11)
C00G	16.6(16)	14.6(14)	24.1(14)	2.1(11)	3.0(11)	1.4(11)
C00H	18.7(16)	16.3(15)	12.8(12)	1.9(10)	1.0(10)	-3.7(11)
C00I	17.4(16)	13.3(14)	24.4(15)	-2.2(11)	0.0(12)	2.4(11)
C00J	19.3(16)	13.0(14)	19.4(14)	0.0(10)	-0.1(11)	-0.3(11)
C00K	15.1(16)	23.8(16)	16.8(13)	-2.7(11)	0.8(11)	6.6(11)
C00L	23.3(17)	14.2(14)	21.5(14)	2.1(11)	2.2(12)	-3.6(11)
C00M	16.4(16)	18.0(15)	23.3(14)	-1.1(11)	7.5(12)	1.8(11)
C00N	17.9(17)	22.4(16)	24.6(15)	4.3(12)	6.1(12)	0.3(12)
C00O	16.6(16)	22.3(15)	12.6(13)	-2.1(11)	0.0(10)	-0.8(11)
C00P	12.9(15)	12.1(14)	19.9(13)	1.9(10)	2.5(11)	-1.5(10)
C00Q	16.6(16)	20.0(16)	21.8(15)	5.0(11)	-4.0(11)	-1.0(12)
C00R	12.6(15)	12.2(14)	19.4(13)	-1.0(10)	-0.5(10)	-2.2(10)
C00S	15.5(16)	21.1(16)	17.4(14)	-6.9(11)	0.9(11)	-0.7(11)
C00T	12.2(15)	16.8(14)	21.5(14)	-3.8(11)	-1.2(11)	-4.5(11)
C00U	20.7(17)	28.9(17)	16.6(14)	5.5(12)	6.4(11)	3.8(12)
C00V	26.1(19)	30.3(18)	15.9(14)	-0.6(12)	-1.1(12)	3.5(13)

Table 13 Bond lengths.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Au01	Cl02	2.2833(7)	C00B	C00R	1.602(4)
Au01	Cl03	2.2869(8)	C00C	C00E	1.395(4)
Au01	Cl04	2.3481(7)	C00D	C00H	1.384(4)
Au01	C007	2.038(3)	C00E	C00N	1.385(4)
N005	C00B	1.537(3)	C00F	C00J	1.383(4)
N005	C00D	1.373(3)	C00G	C00P	1.394(4)
N005	C00P	1.362(4)	C00G	C00Q	1.382(4)
N006	C00C	1.331(3)	C00H	C00Q	1.389(4)
N006	C00K	1.352(4)	C00I	C00R	1.538(4)
C007	C008	1.346(4)	C00J	C00S	1.387(4)
C007	C00B	1.527(4)	C00K	C00U	1.381(4)
C008	C009	1.486(4)	C00K	C00V	1.508(4)
C008	C00D	1.454(4)	C00L	C00R	1.533(4)
C009	C00A	1.398(4)	C00M	C00P	1.496(4)
C009	C00F	1.394(4)	C00N	C00U	1.385(4)
C00A	C00O	1.378(4)	C00O	C00S	1.388(4)
C00B	C00C	1.541(4)	C00R	C00T	1.547(4)

Table 14 Bond angles.

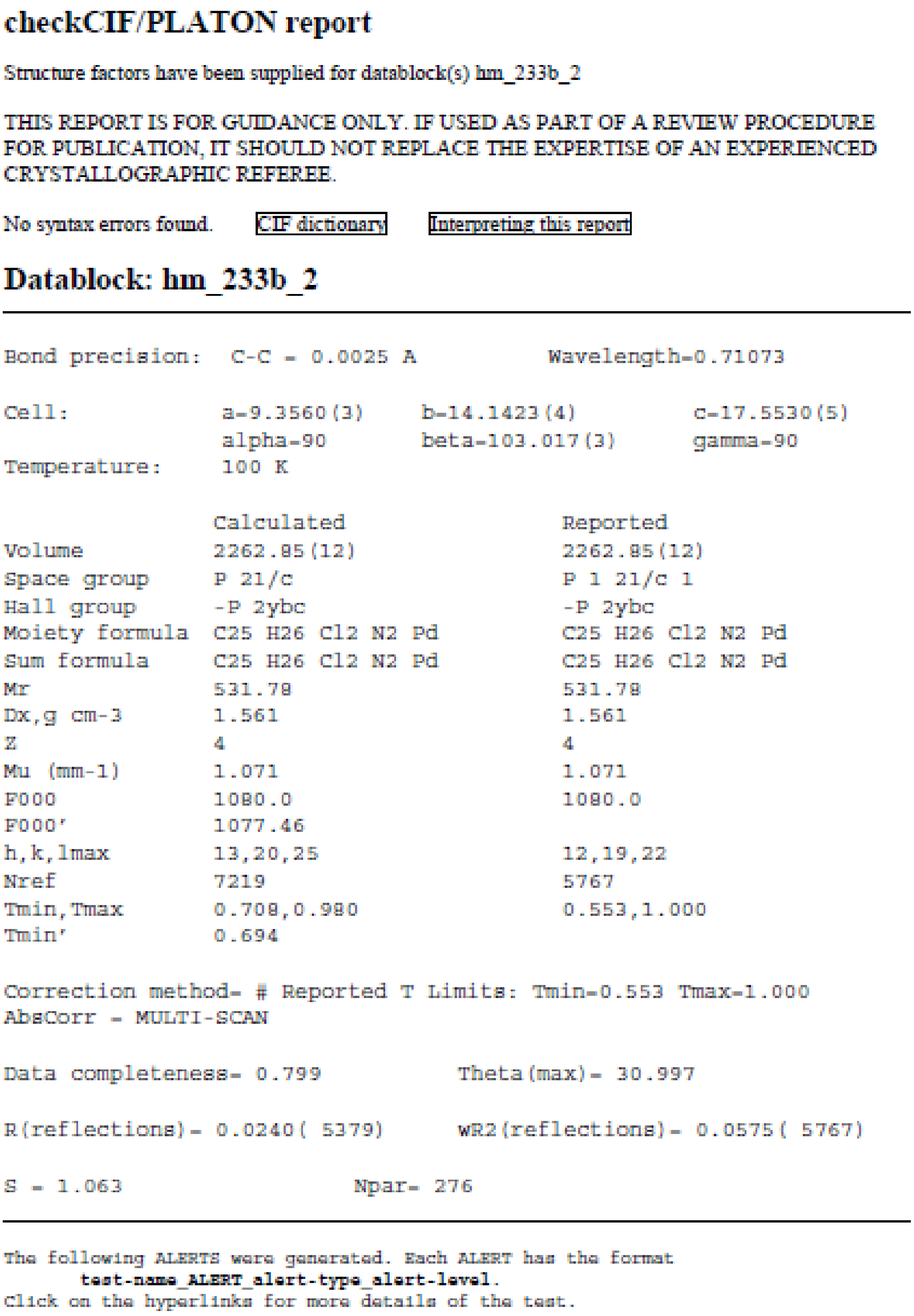
Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
Cl02	Au01	Cl03	178.30(3)	N006	C00C	C00E	123.1(3)
Cl02	Au01	Cl04	88.54(3)	C00E	C00C	C00B	118.8(2)
Cl03	Au01	Cl04	89.80(3)	N005	C00D	C008	109.2(2)
C007	Au01	Cl02	91.89(8)	N005	C00D	C00H	120.5(3)
C007	Au01	Cl03	89.74(8)	C00H	C00D	C008	130.2(2)
C007	Au01	Cl04	175.70(7)	C00N	C00E	C00C	118.7(3)
C00D	N005	C00B	109.5(2)	C00J	C00F	C009	120.6(2)
C00P	N005	C00B	128.5(2)	C00Q	C00G	C00P	121.2(3)
C00P	N005	C00D	122.0(2)	C00D	C00H	C00Q	118.1(3)
C00C	N006	C00K	118.0(3)	C00F	C00J	C00S	120.0(3)
C008	C007	Au01	120.6(2)	N006	C00K	C00U	122.1(3)
C008	C007	C00B	111.5(2)	N006	C00K	C00V	116.1(3)
C00B	C007	Au01	127.94(17)	C00U	C00K	C00V	121.8(3)
C007	C008	C009	128.7(3)	C00E	C00N	C00U	118.2(3)
C007	C008	C00D	108.9(2)	C00A	C00O	C00S	120.3(3)
C00D	C008	C009	122.2(2)	N005	C00P	C00G	117.3(2)
C00A	C009	C008	121.8(2)	N005	C00P	C00M	124.0(2)
C00F	C009	C008	119.3(2)	C00G	C00P	C00M	118.2(3)
C00F	C009	C00A	118.8(3)	C00G	C00Q	C00H	120.1(3)
C00O	C00A	C009	120.4(3)	C00I	C00R	C00B	113.2(2)
N005	C00B	C00C	107.5(2)	C00I	C00R	C00T	107.2(2)
N005	C00B	C00R	107.7(2)	C00L	C00R	C00B	110.2(2)
C007	C00B	N005	99.87(19)	C00L	C00R	C00I	107.6(2)
C007	C00B	C00C	110.4(2)	C00L	C00R	C00T	108.5(2)
C007	C00B	C00R	110.1(2)	C00T	C00R	C00B	109.9(2)
C00C	C00B	C00R	119.4(2)	C00J	C00S	C00O	119.8(3)
N006	C00C	C00B	118.1(3)	C00K	C00U	C00N	119.8(3)

Table 15 Hydrogen atom coordinates (Å×10^{4}) and isotropic displacement parameters (Å^{2}×10^{3}).

Atom	x	y	z	U(eq)
H00A	2949.12	2915.91	4675.53	19
H00E	1131.48	2587.98	7620.67	22
H00F	3488.24	1212.22	6465.7	18
H00G	-1515.43	4807.51	6158.03	22
H00H	482.73	3133.09	4952.02	20
H00B	2484.52	5459.79	7389.87	29
H00C	4160.92	5805.22	7721.43	29
H00D	3402.05	5193.45	8257.97	29
H00J	3773.08	149.66	5581.9	21
H00I	4610.61	4302.7	6258.28	30
H00K	4879.78	5268.31	6511.96	30
H00L	3199.87	4921.82	6194.57	30
H00M	-482.61	4231.01	7803	28
H00N	-339.64	5180.49	7520.81	28
H00O	1128.5	4686.46	7984.22	28
H00P	584.85	2121.2	8822.64	26
H00Q	3194.39	1849.01	3793.43	21
H00R	-1447.7	4110.46	4982.51	25
H00S	3593.26	461.73	4239.22	22
H00T	5708	4203.24	8379.33	26
H00U	6307.53	4944.86	7902.9	26
H00V	6262.08	3999.05	7581.2	26
H00W	1951.65	2700.65	10020.33	26
H00X	5238.2	3745.74	10297.26	37
H00Y	3859.66	3615.9	10723.74	37
H	3998.71	4469.67	10253.84	37

CheckCIF reports

Complex 172



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hm_233b_2

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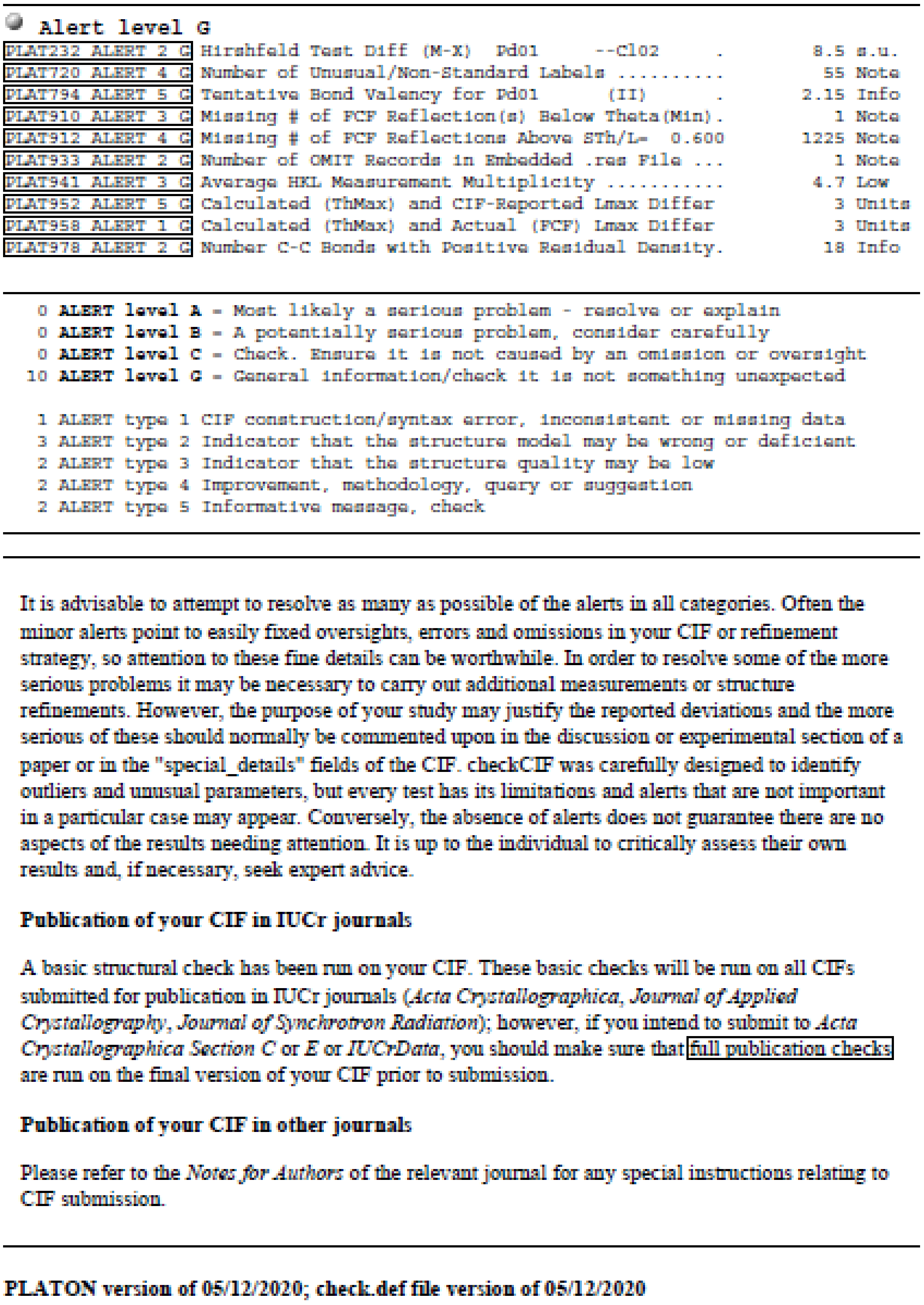
No syntax errors found. CIF dictionary Interpreting this report

Datablock: hm_233b_2

```
Bond precision:   C-C = 0.0025 A          Wavelength=0.71073

Cell:             a=9.3560(3)    b=14.1423(4)       c=17.5530(5)
                  alpha=90       beta=103.017(3)    gamma=90
Temperature:      100 K

                 Calculated                  Reported
Volume           2262.85(12)                 2262.85(12)
Space group      P 21/c                      P 1 21/c 1
Hall group       -P 2ybc                     -P 2ybc
Moiety formula   C25 H26 Cl2 N2 Pd           C25 H26 Cl2 N2 Pd
Sum formula      C25 H26 Cl2 N2 Pd           C25 H26 Cl2 N2 Pd
Mr               531.78                      531.78
Dx,g cm-3        1.561                       1.561
Z                4                           4
Mu (mm-1)        1.071                       1.071
F000             1080.0                      1080.0
F000'            1077.46
h,k,lmax         13,20,25                    12,19,22
Nref             7219                        5767
Tmin,Tmax        0.708,0.980                 0.553,1.000
Tmin'            0.694

Correction method= # Reported T Limits: Tmin=0.553 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.799          Theta(max)= 30.997

R(reflections)= 0.0240( 5379)     wR2(reflections)= 0.0575( 5767)

S = 1.063                  Npar= 276
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.



Alert level G

```
PLAT232 ALERT 2 G Hirshfeld Test Diff (M-X)  Pd01     --Cl02     .        8.5 s.u.
PLAT720 ALERT 4 G Number of Unusual/Non-Standard Labels ..........         55 Note
PLAT794 ALERT 5 G Tentative Bond Valency for Pd01      (II)      .       2.15 Info
PLAT910 ALERT 3 G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912 ALERT 4 G Missing # of FCF Reflections Above STh/L=  0.600       1225 Note
PLAT933 ALERT 2 G Number of OMIT Records in Embedded .res File ...          1 Note
PLAT941 ALERT 3 G Average HKL Measurement Multiplicity ...........        4.7 Low
PLAT952 ALERT 5 G Calculated (ThMax) and CIF-Reported Lmax Differ           3 Units
PLAT958 ALERT 1 G Calculated (ThMax) and Actual (FCF) Lmax Differ           3 Units
PLAT978 ALERT 2 G Number C-C Bonds with Positive Residual Density.         18 Info
```

```
  0 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
  0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 10 ALERT level G = General information/check it is not something unexpected

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  3 ALERT type 2 Indicator that the structure model may be wrong or deficient
  2 ALERT type 3 Indicator that the structure quality may be low
  2 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
```

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Publication of your CIF in IUCr journals

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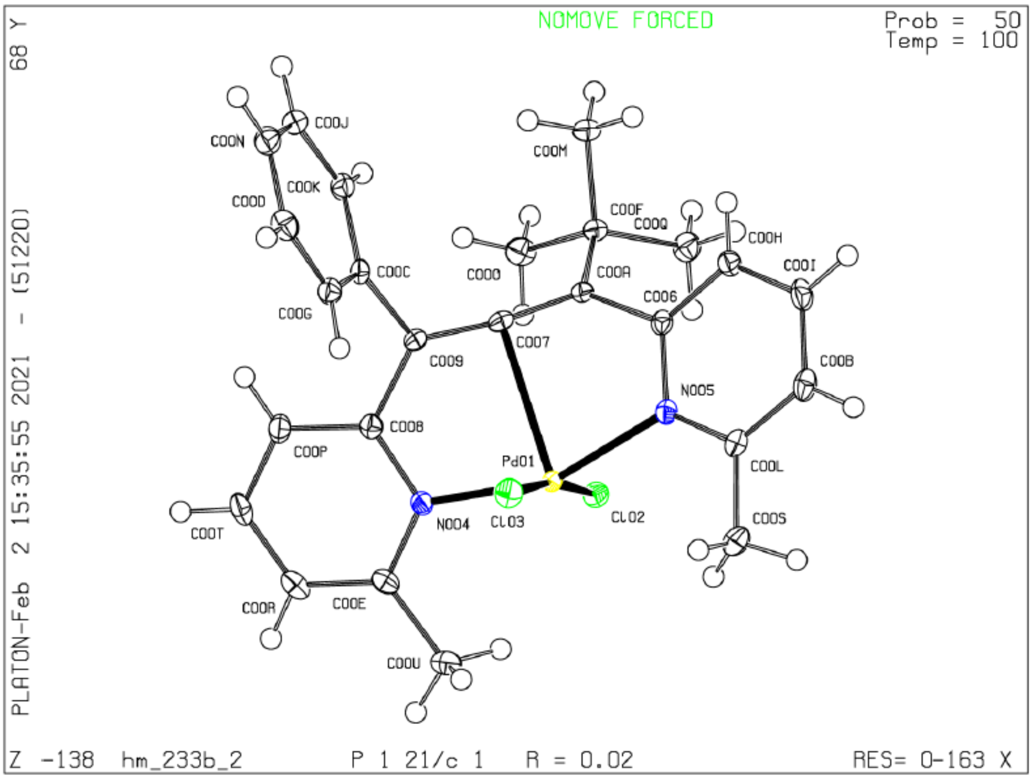
Publication of your CIF in other journals

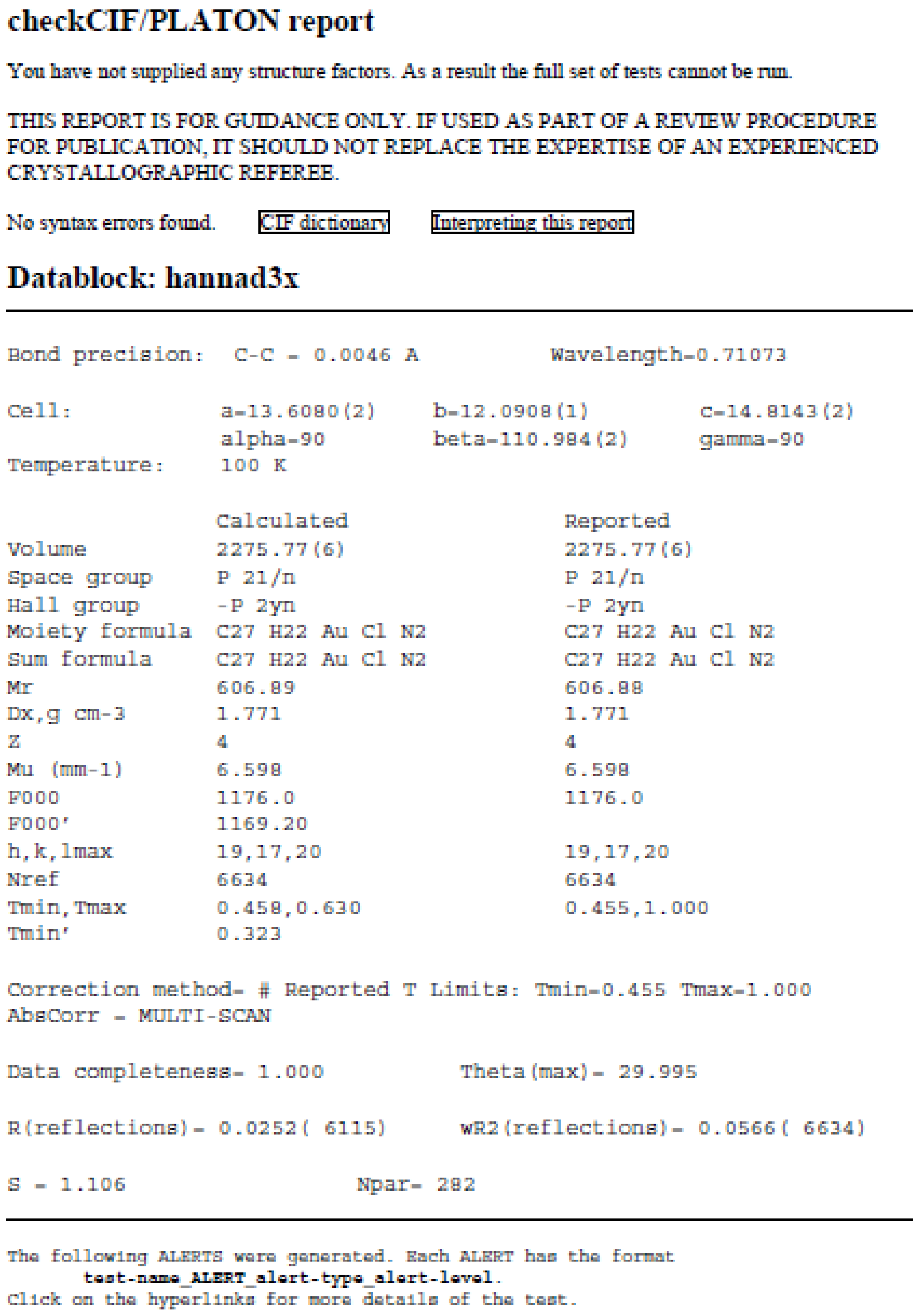
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 05/12/2020; check.def file version of 05/12/2020

Datablock hm_233b_2 - ellipsoid plot



Complex 184



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

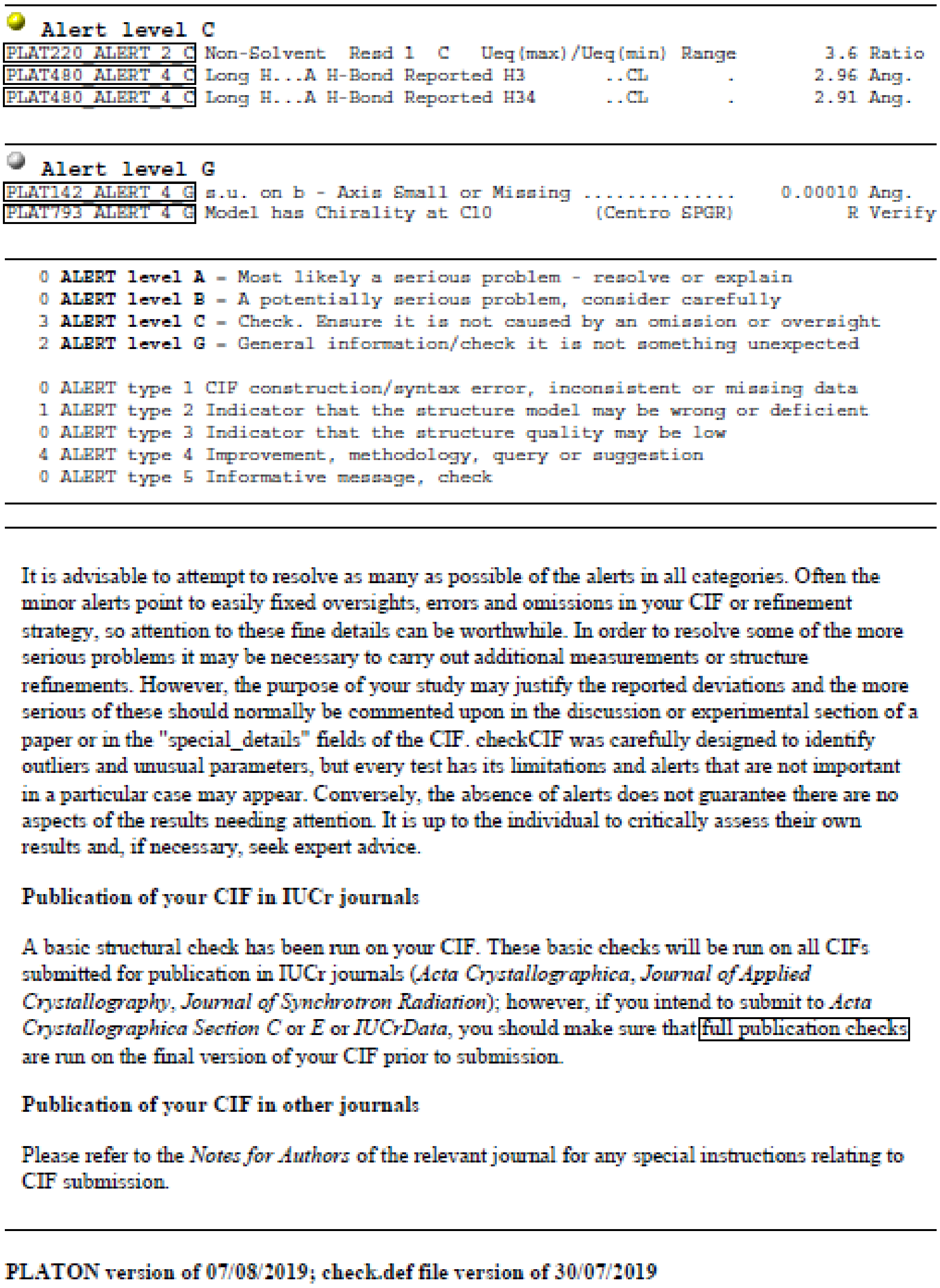
THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: hannad3x

```
Bond precision:   C-C = 0.0046 A          Wavelength=0.71073

Cell:             a=13.6080(2)     b=12.0908(1)        c=14.8143(2)
                  alpha=90         beta=110.984(2)     gamma=90
Temperature:      100 K

                 Calculated                  Reported
Volume           2275.77(6)                  2275.77(6)
Space group      P 21/n                      P 21/n
Hall group       -P 2yn                      -P 2yn
Moiety formula   C27 H22 Au Cl N2            C27 H22 Au Cl N2
Sum formula      C27 H22 Au Cl N2            C27 H22 Au Cl N2
Mr               606.89                      606.88
Dx,g cm-3        1.771                       1.771
Z                4                           4
Mu (mm-1)        6.598                       6.598
F000             1176.0                      1176.0
F000'            1169.20
h,k,lmax         19,17,20                    19,17,20
Nref             6634                        6634
Tmin,Tmax        0.458,0.630                 0.455,1.000
Tmin'            0.323

Correction method= # Reported T Limits: Tmin=0.455 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 29.995

R(reflections)= 0.0252( 6115)     wR2(reflections)= 0.0566( 6634)

S = 1.106                  Npar= 282
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.



```
Alert level C
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.6 Ratio
PLAT480_ALERT_4_C Long H...A H-Bond Reported H3        ..CL      .       2.96 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H34       ..CL      .       2.91 Ang.

Alert level G
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing .............     0.00010 Ang.
PLAT793_ALERT_4_G Model has Chirality at C10          (Centro SPGR)          R Verify

   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   2 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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Publication of your CIF in other journals

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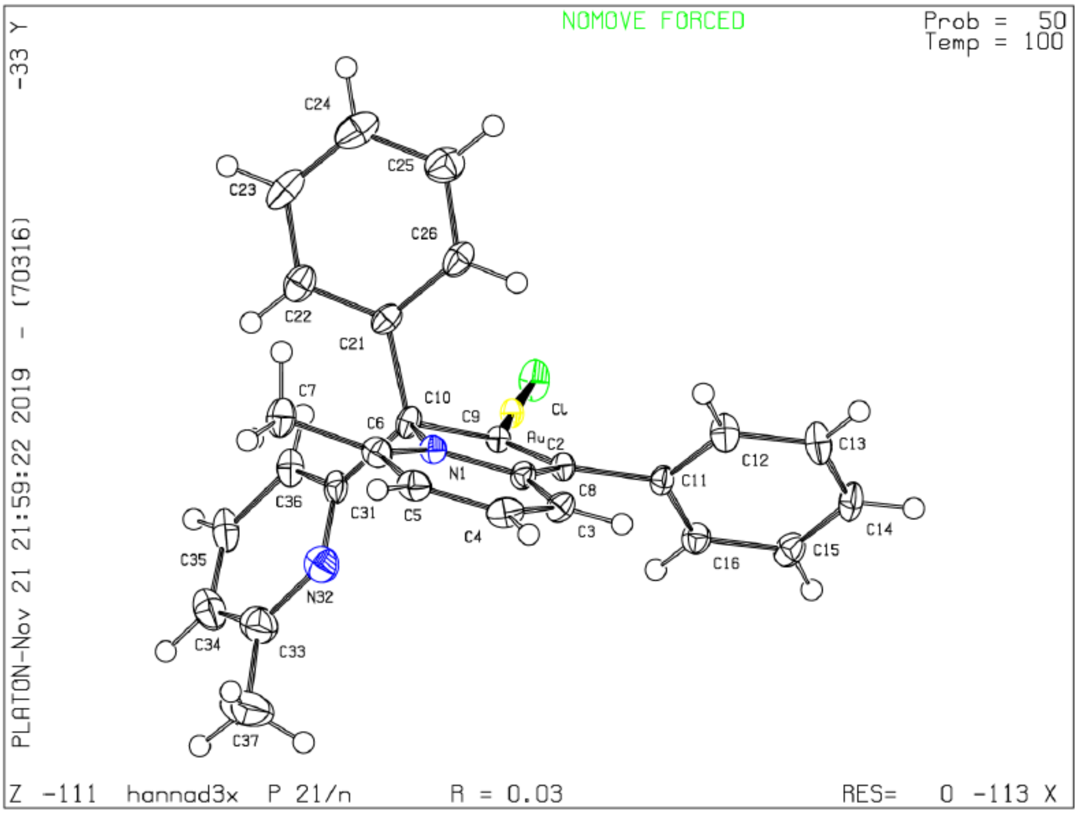
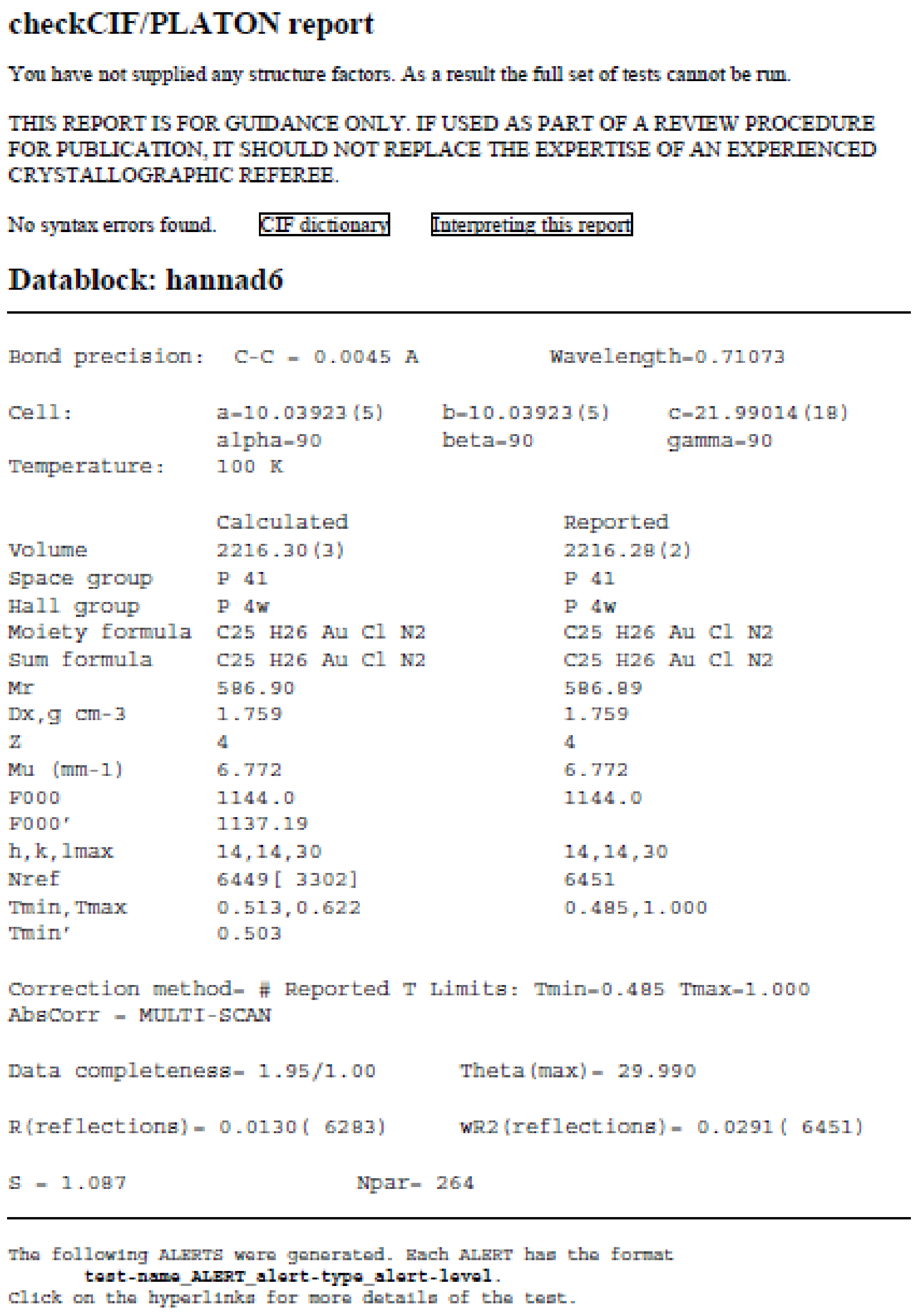
PLATON version of 07/08/2019; check.def file version of 30/07/2019

Datablock hannad3x - ellipsoid plot



Complex 187b.



checkCIF/PLATON report

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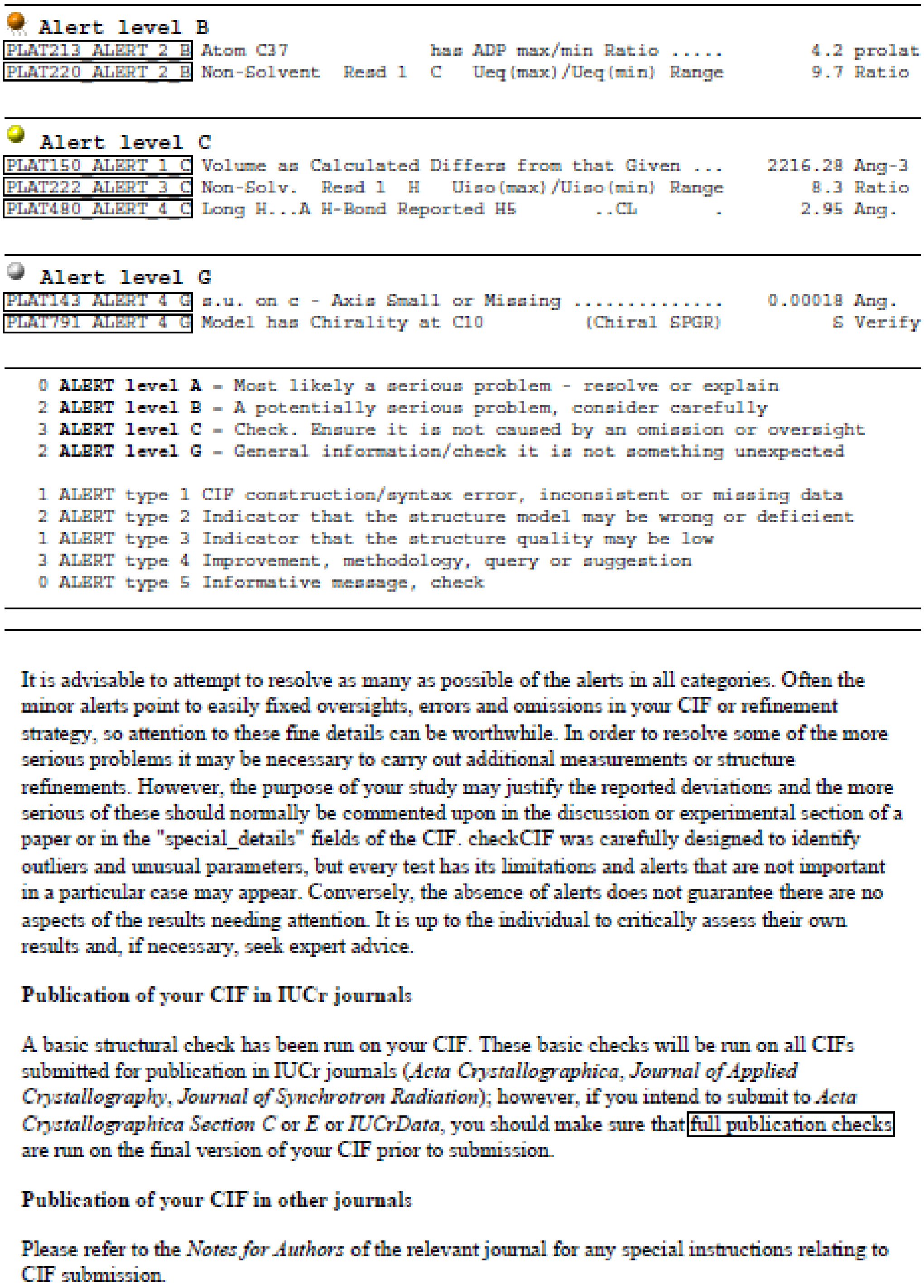
No syntax errors found. CIF dictionary Interpreting this report

Datablock: hannad6

```
Bond precision:  C-C = 0.0045 A          Wavelength=0.71073

Cell:            a=10.03923(5)     b=10.03923(5)     c=21.99014(18)
                 alpha=90          beta=90           gamma=90
Temperature:     100 K

                 Calculated                 Reported
Volume           2216.30(3)                 2216.28(2)
Space group      P 41                       P 41
Hall group       P 4w                       P 4w
Moiety formula   C25 H26 Au Cl N2           C25 H26 Au Cl N2
Sum formula      C25 H26 Au Cl N2           C25 H26 Au Cl N2
Mr               586.90                     586.89
Dx,g cm-3        1.759                      1.759
Z                4                          4
Mu (mm-1)        6.772                      6.772
F000             1144.0                     1144.0
F000'            1137.19
h,k,lmax         14,14,30                   14,14,30
Nref             6449[ 3302]                6451
Tmin,Tmax        0.513,0.622                0.485,1.000
Tmin'            0.503

Correction method= # Reported T Limits: Tmin=0.485 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.95/1.00      Theta(max)= 29.990

R(reflections)= 0.0130( 6283)     wR2(reflections)= 0.0291( 6451)

S = 1.087                 Npar= 264
```

```
The following ALERTS were generated. Each ALERT has the format
       test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.
```



```
● Alert level B
PLAT213_ALERT_2_B Atom C37             has ADP max/min Ratio .....       4.2 prolat
PLAT220_ALERT_2_B Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range       9.7 Ratio

● Alert level C
PLAT150_ALERT_1_C Volume as Calculated Differs from that Given ...   2216.28 Ang-3
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range       8.3 Ratio
PLAT480_ALERT_4_C Long H...A H-Bond Reported H5        ..CL       .     2.95 Ang.

● Alert level G
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............   0.00018 Ang.
PLAT791_ALERT_4_G Model has Chirality at C10          (Chiral SPGR)        S Verify

   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   2 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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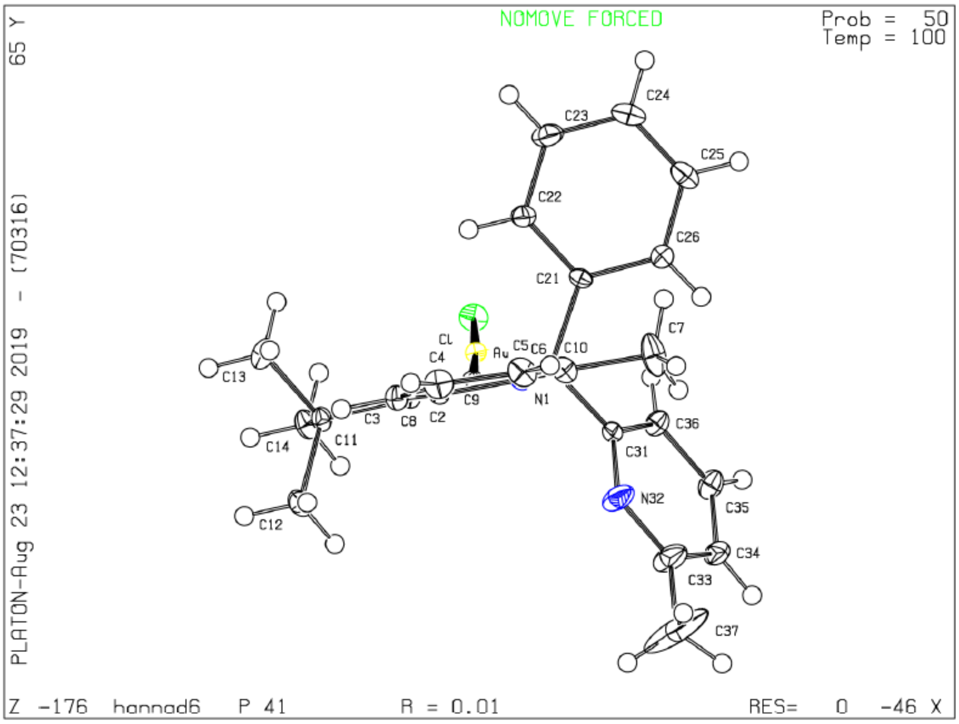
Publication of your CIF in other journals

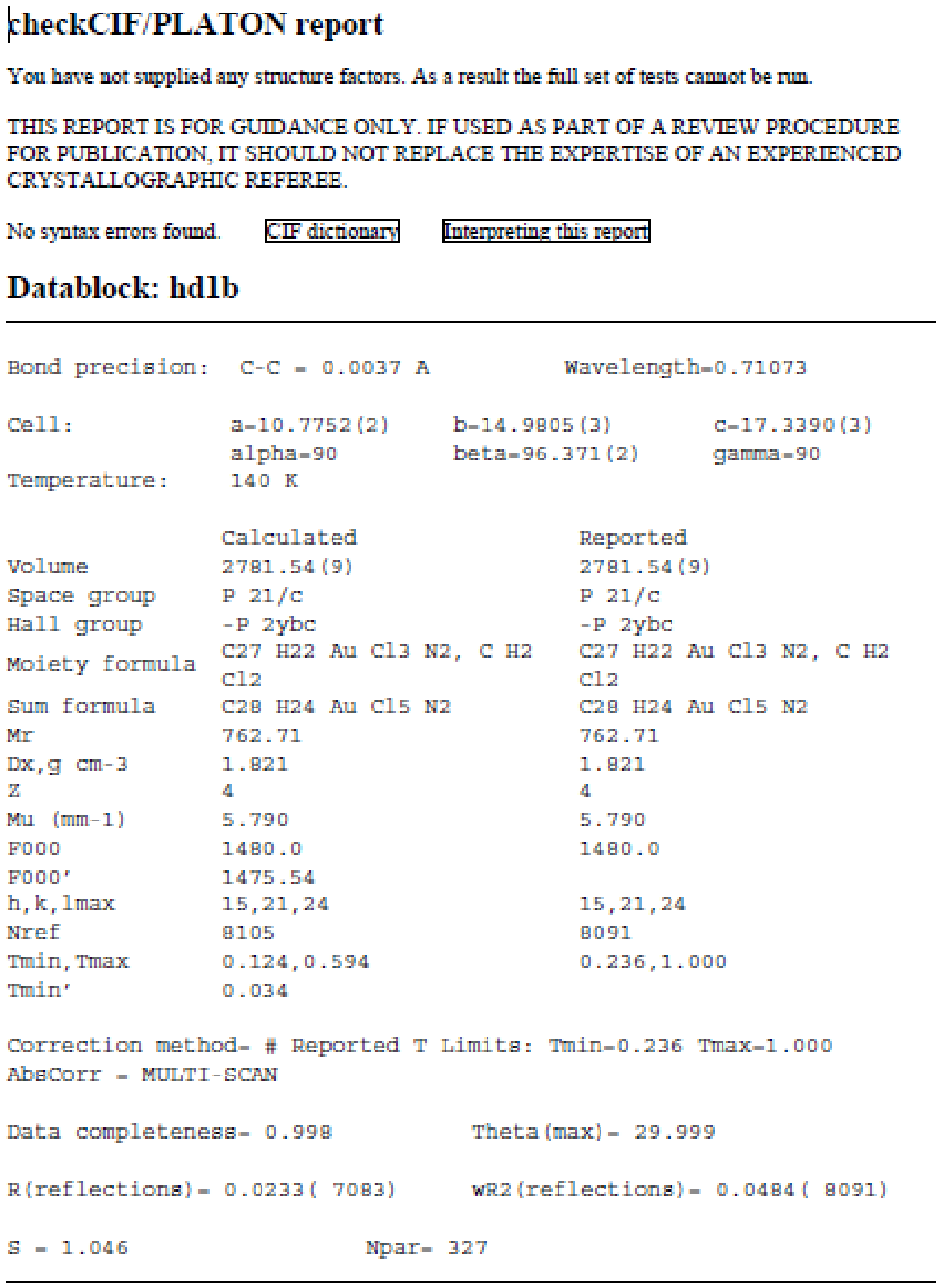
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 07/08/2019; check.def file version of 30/07/2019

Datablock hannad6 - ellipsoid plot



Complex 194



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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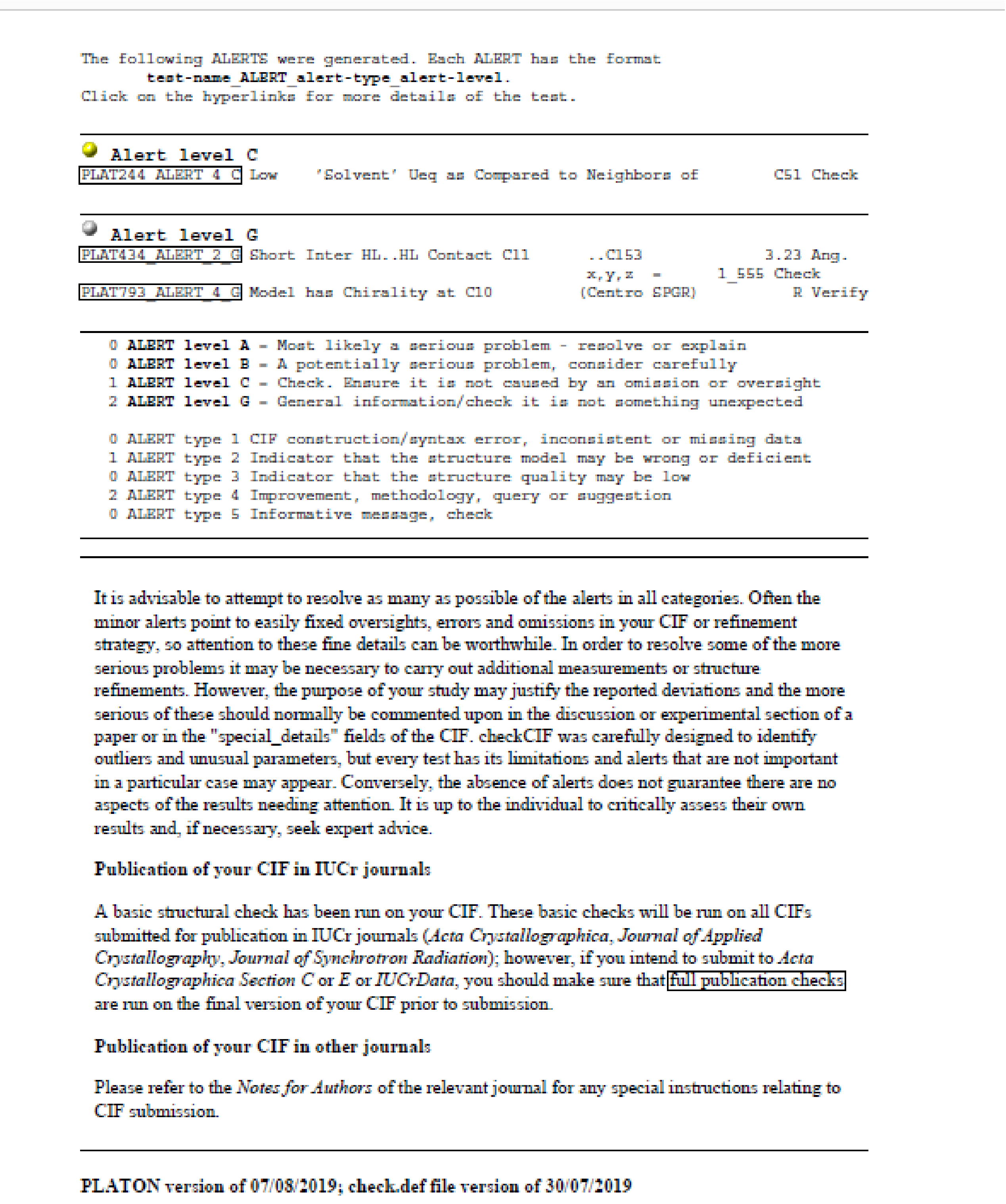
No syntax errors found. CIF dictionary Interpreting this report

Datablock: hd1b

```
Bond precision:   C-C = 0.0037 A          Wavelength=0.71073

Cell:             a=10.7752(2)     b=14.9805(3)      c=17.3390(3)
                  alpha=90         beta=96.371(2)    gamma=90
Temperature:      140 K

                 Calculated                    Reported
Volume           2781.54(9)                    2781.54(9)
Space group      P 21/c                        P 21/c
Hall group       -P 2ybc                       -P 2ybc
Moiety formula   C27 H22 Au Cl3 N2, C H2       C27 H22 Au Cl3 N2, C H2
                 Cl2                           Cl2
Sum formula      C28 H24 Au Cl5 N2             C28 H24 Au Cl5 N2
Mr               762.71                        762.71
Dx,g cm-3        1.821                         1.821
Z                4                             4
Mu (mm-1)        5.790                         5.790
F000             1480.0                        1480.0
F000'            1475.54
h,k,lmax         15,21,24                      15,21,24
Nref             8105                          8091
Tmin,Tmax        0.124,0.594                   0.236,1.000
Tmin'            0.034

Correction method= # Reported T Limits: Tmin=0.236 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 29.999

R(reflections)= 0.0233( 7083)     wR2(reflections)= 0.0484( 8091)

S = 1.046                  Npar= 327
```



```
The following ALERTS were generated. Each ALERT has the format
       test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.
```

```
● Alert level C
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C51 Check
```

```
● Alert level G
PLAT434_ALERT_2_G Short Inter HL..HL Contact C11       ..C153             3.23 Ang.
                                                       x,y,z  =       1_555 Check
PLAT793_ALERT_4_G Model has Chirality at C10          (Centro SPGR)            R Verify
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   2 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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Publication of your CIF in other journals

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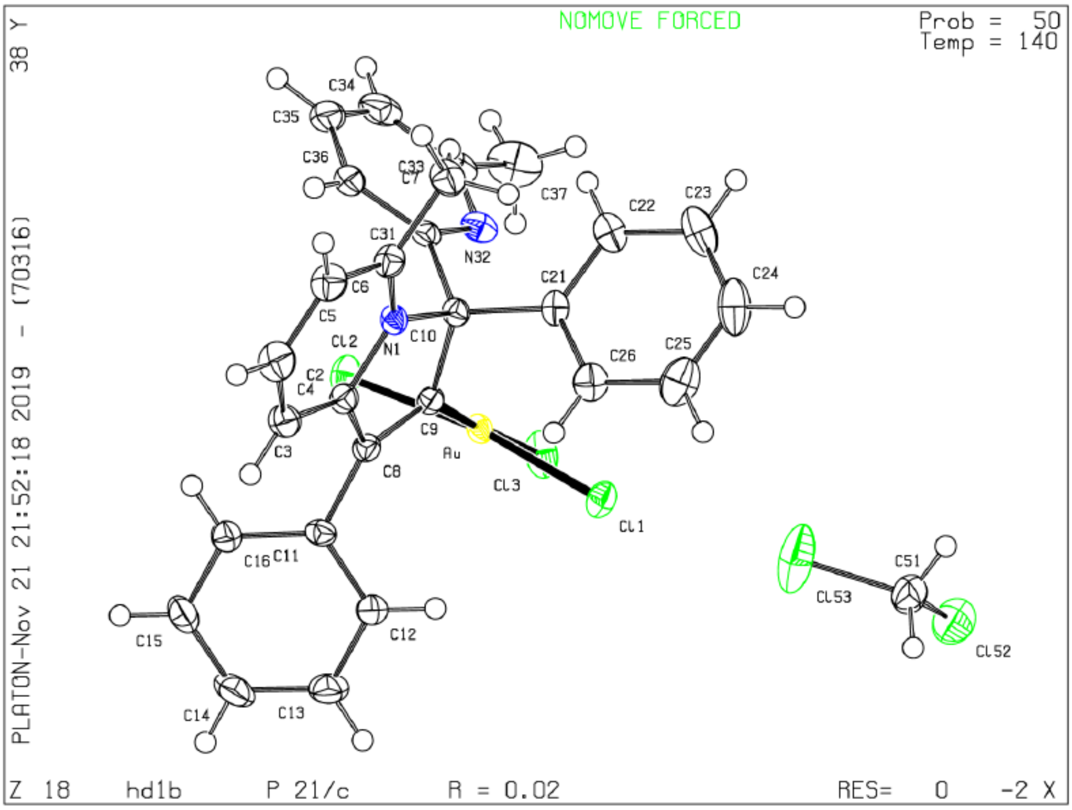
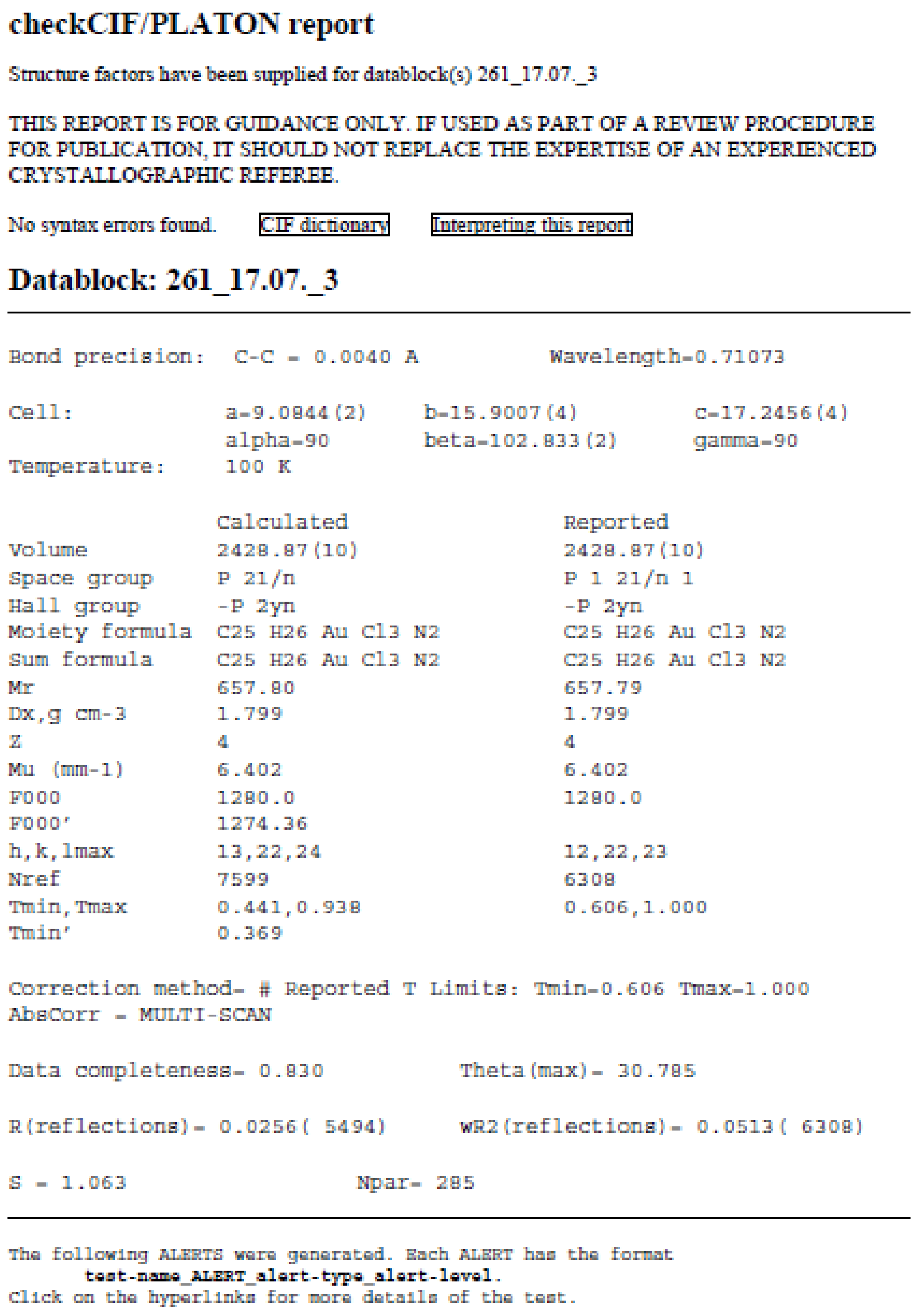
PLATON version of 07/08/2019; check.def file version of 30/07/2019

Datablock hd1b - ellipsoid plot



Complex 189a



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 261_17.07._3

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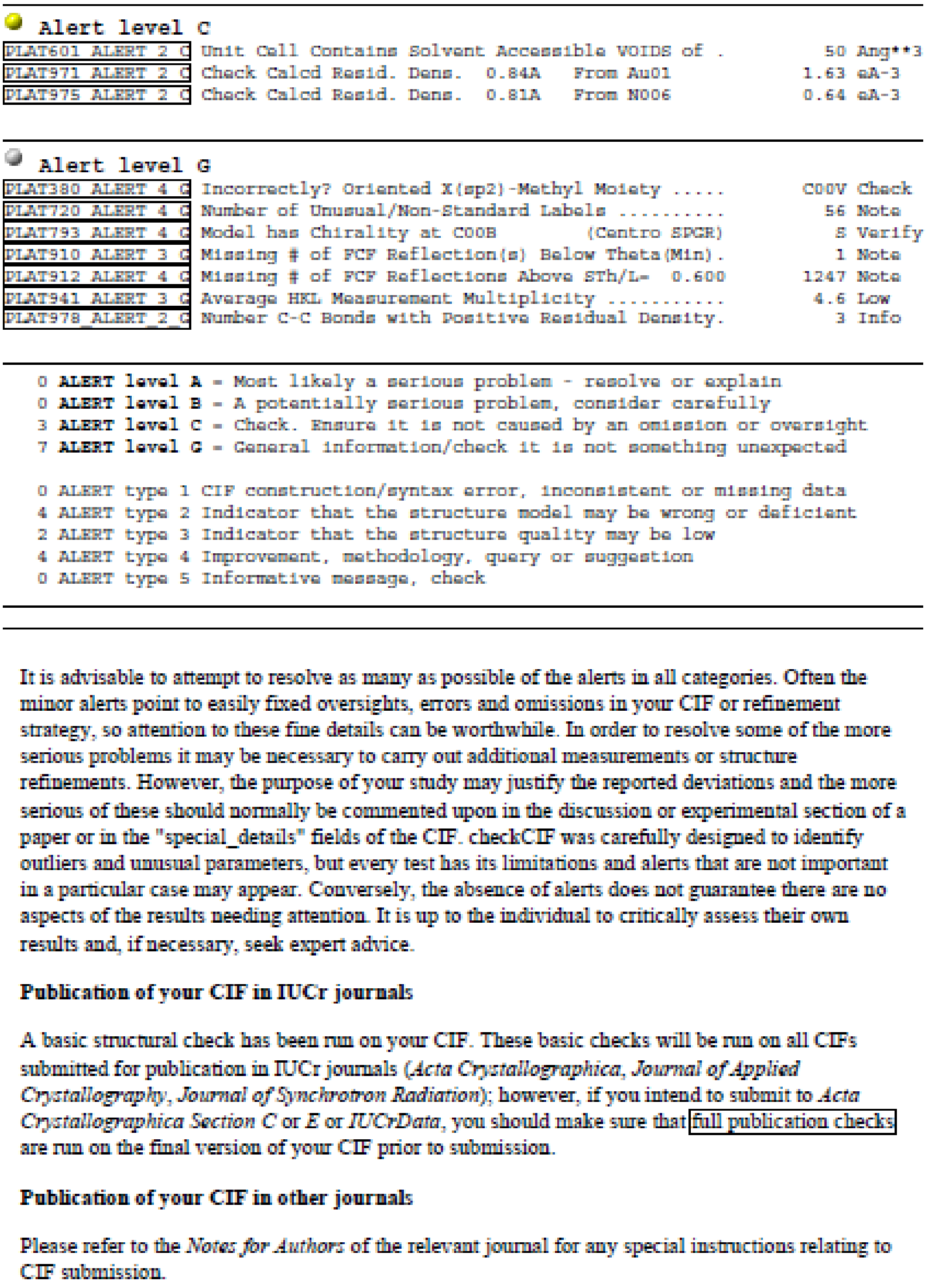
No syntax errors found. CIF dictionary Interpreting this report

Datablock: 261_17.07._3

```
Bond precision:  C-C = 0.0040 A        Wavelength=0.71073

Cell:             a=9.0844(2)    b=15.9007(4)       c=17.2456(4)
                  alpha=90       beta=102.833(2)    gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           2428.87(10)               2428.87(10)
Space group      P 21/n                    P 1 21/n 1
Hall group       -P 2yn                    -P 2yn
Moiety formula   C25 H26 Au Cl3 N2         C25 H26 Au Cl3 N2
Sum formula      C25 H26 Au Cl3 N2         C25 H26 Au Cl3 N2
Mr               657.80                    657.79
Dx,g cm-3        1.799                     1.799
Z                4                         4
Mu (mm-1)        6.402                     6.402
F000             1280.0                    1280.0
F000'            1274.36
h,k,lmax         13,22,24                  12,22,23
Nref             7599                      6308
Tmin,Tmax        0.441,0.938               0.606,1.000
Tmin'            0.369

Correction method= # Reported T Limits: Tmin=0.606 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.830          Theta(max)= 30.785

R(reflections)= 0.0256( 5494)     wR2(reflections)= 0.0513( 6308)

S = 1.063                  Npar= 285
```

```
The following ALERTS were generated. Each ALERT has the format
      test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.
```



```
   Alert level C
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .         50 Ang**3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.84A    From Au01          1.63 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.81A    From N006          0.64 eA-3

   Alert level G
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....      C00V Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        56 Note
PLAT793_ALERT_4_G Model has Chirality at C00B        (Centro SPGR)         S Verify
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      1247 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       4.6 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         3 Info

   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   7 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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Publication of your CIF in other journals

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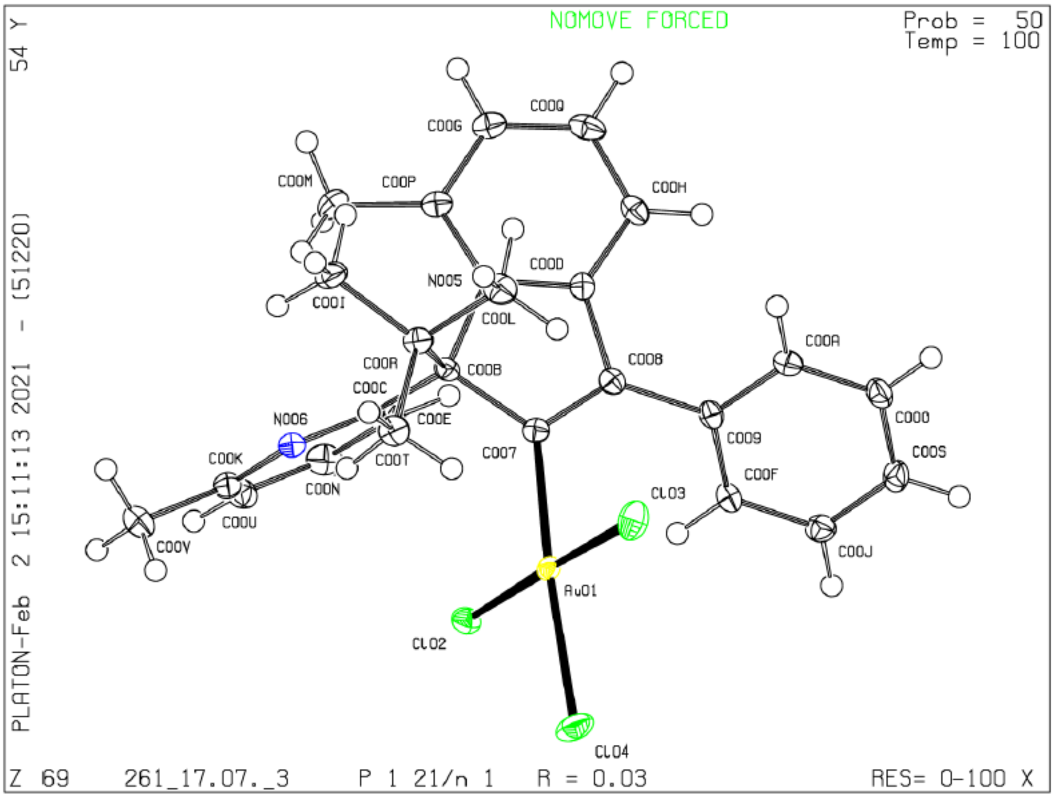
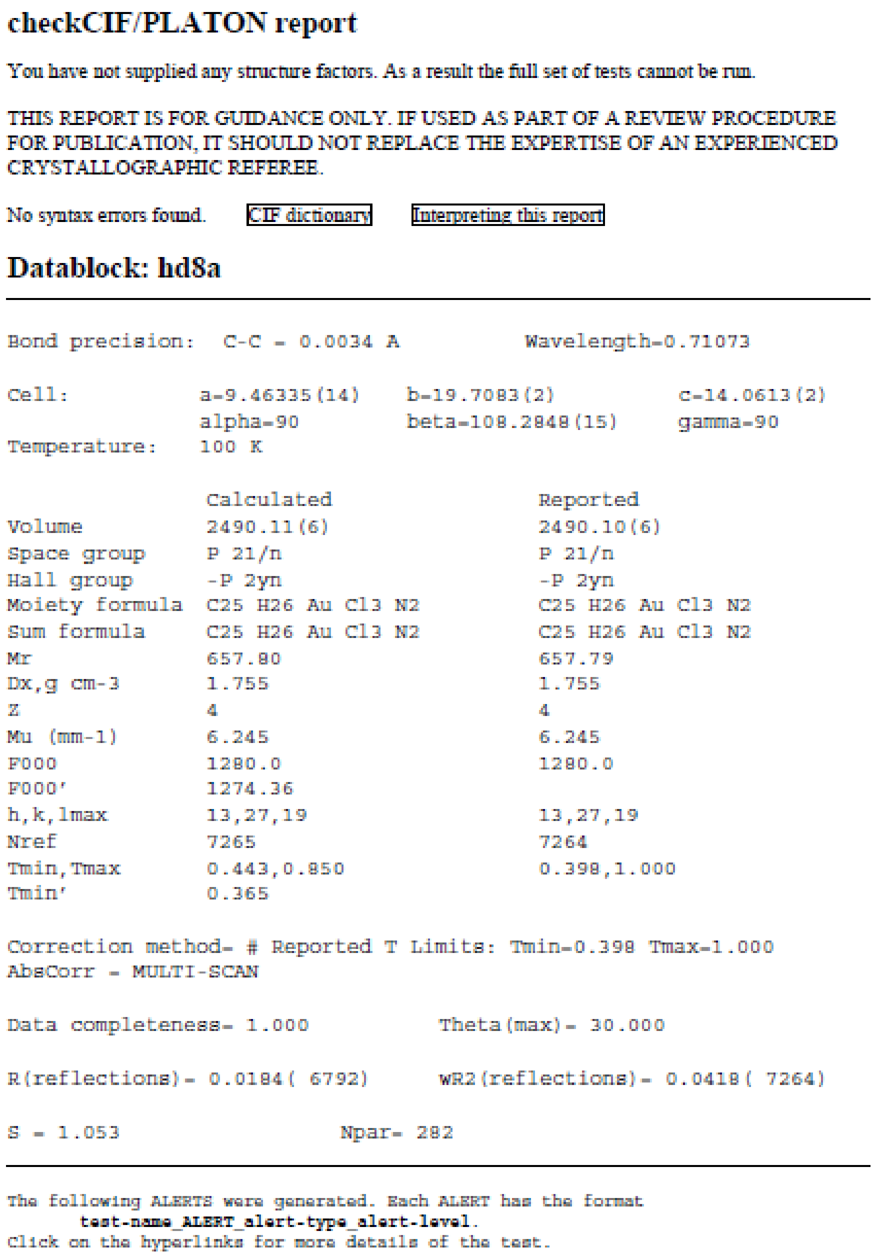
PLATON version of 05/12/2020; check.def file version of 05/12/2020

Datablock 261_17.07._3 - ellipsoid plot



Complex 189b.



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: hd8a

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Bond precision:   C-C = 0.0034 A         Wavelength=0.71073

Cell:           a=9.46335(14)    b=19.7083(2)         c=14.0613(2)
                alpha=90         beta=108.2848(15)    gamma=90
Temperature:    100 K

                Calculated                 Reported
Volume          2490.11(6)                 2490.10(6)
Space group     P 21/n                     P 21/n
Hall group      -P 2yn                     -P 2yn
Moiety formula  C25 H26 Au Cl3 N2          C25 H26 Au Cl3 N2
Sum formula     C25 H26 Au Cl3 N2          C25 H26 Au Cl3 N2
Mr              657.80                     657.79
Dx,g cm-3       1.755                      1.755
Z               4                          4
Mu (mm-1)       6.245                      6.245
F000            1280.0                     1280.0
F000'           1274.36
h,k,lmax        13,27,19                   13,27,19
Nref            7265                       7264
Tmin,Tmax       0.443,0.850                0.398,1.000
Tmin'           0.365

Correction method= # Reported T Limits: Tmin=0.398 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 30.000

R(reflections)= 0.0184( 6792)     wR2(reflections)= 0.0418( 7264)

S = 1.053                  Npar= 282
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The following ALERTS were generated. Each ALERT has the format
       test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.
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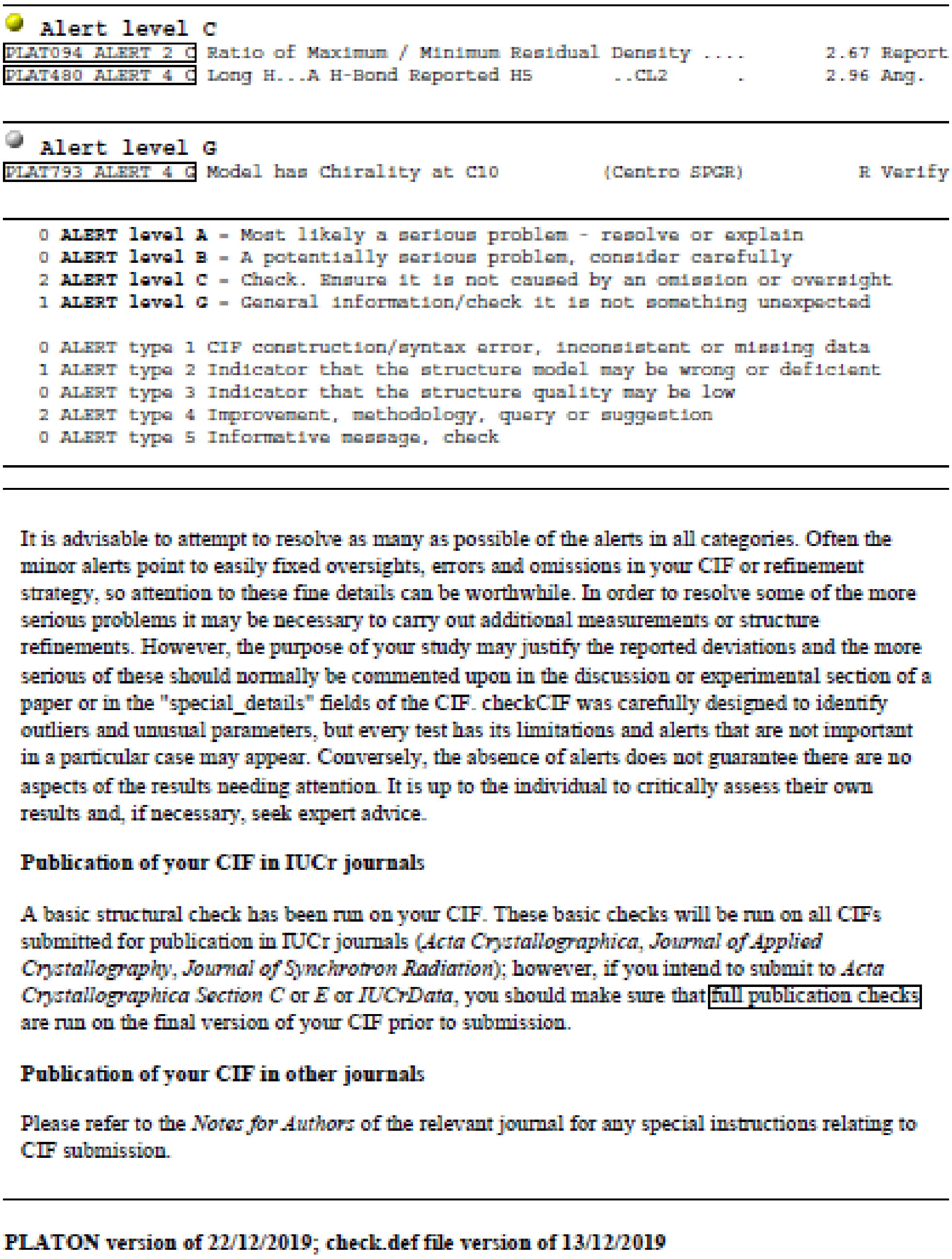

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● Alert level C
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.67 Report
PLAT480_ALERT_4_C Long H...A H-Bond Reported H5         ..CL2      .     2.96 Ang.

● Alert level G
PLAT793_ALERT_4_G Model has Chirality at C10          (Centro SPGR)          R Verify

    0 ALERT level A = Most likely a serious problem - resolve or explain
    0 ALERT level B = A potentially serious problem, consider carefully
    2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
    1 ALERT level G = General information/check it is not something unexpected

    0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
    1 ALERT type 2 Indicator that the structure model may be wrong or deficient
    0 ALERT type 3 Indicator that the structure quality may be low
    2 ALERT type 4 Improvement, methodology, query or suggestion
    0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

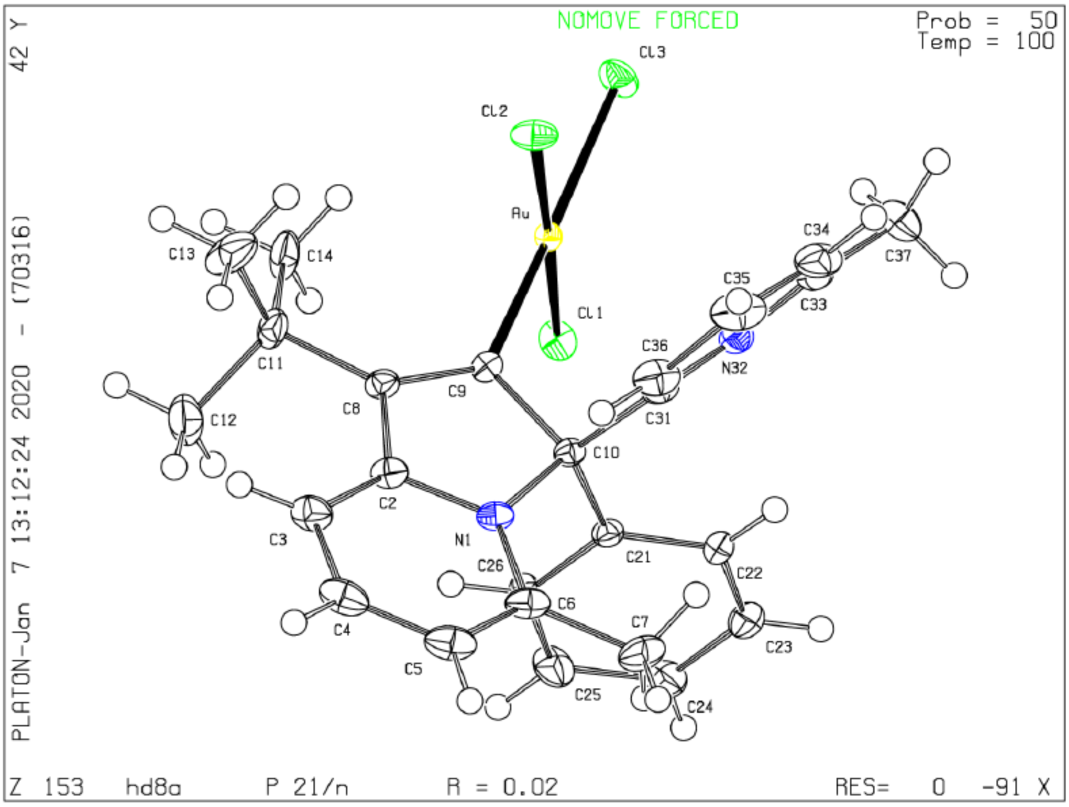
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

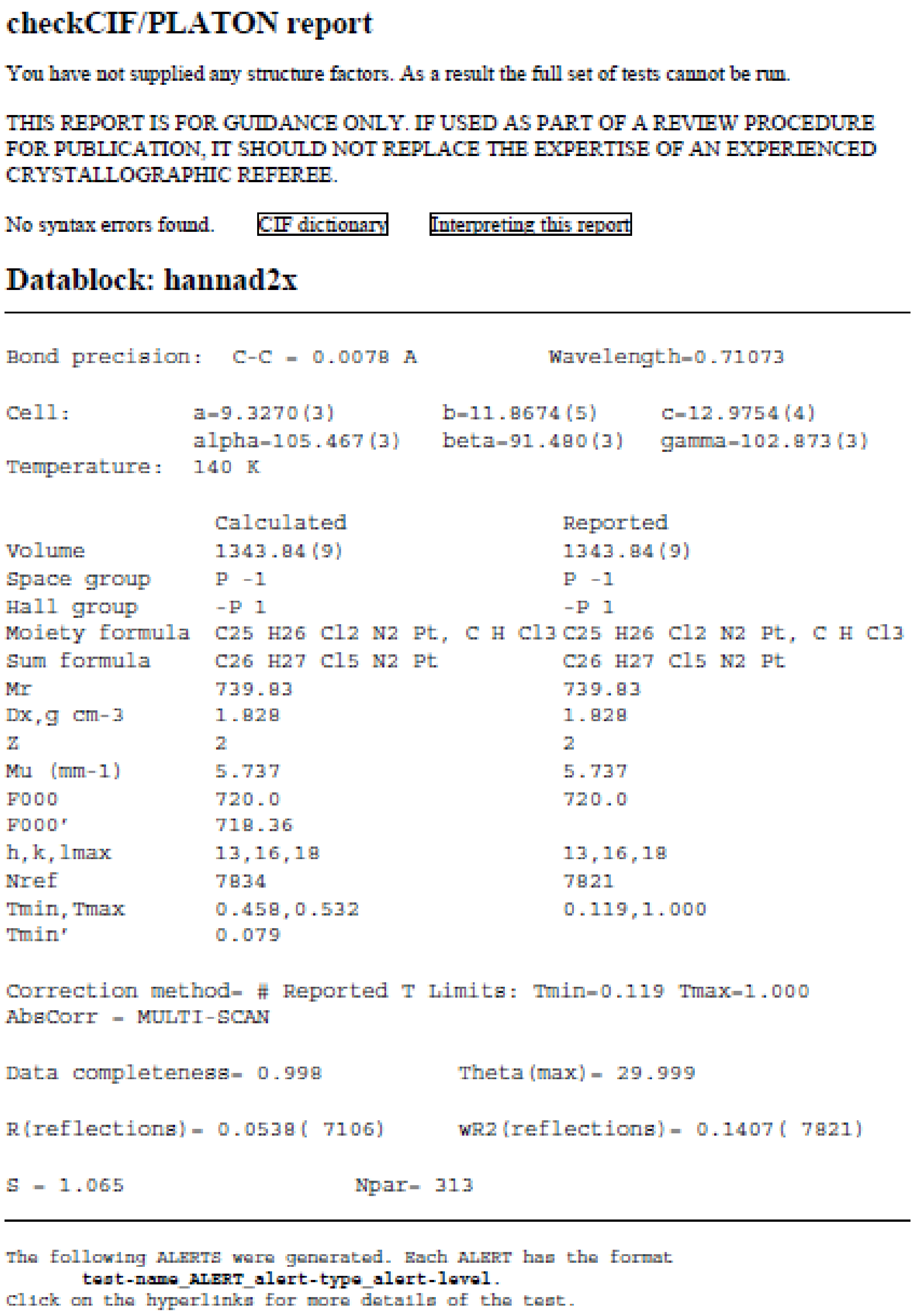
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/12/2019; check.def file version of 13/12/2019

Datablock hd8a - ellipsoid plot



Complex 179



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: hannad2x

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Bond precision:   C-C = 0.0078 A          Wavelength=0.71073

Cell:           a=9.3270(3)        b=11.8674(5)     c=12.9754(4)
                alpha=105.467(3)   beta=91.480(3)   gamma=102.873(3)
Temperature:    140 K

                  Calculated                  Reported
Volume            1343.84(9)                  1343.84(9)
Space group       P -1                        P -1
Hall group        -P 1                        -P 1
Moiety formula    C25 H26 Cl2 N2 Pt, C H Cl3 C25 H26 Cl2 N2 Pt, C H Cl3
Sum formula       C26 H27 Cl5 N2 Pt           C26 H27 Cl5 N2 Pt
Mr                739.83                      739.83
Dx,g cm-3         1.828                       1.828
Z                 2                           2
Mu (mm-1)         5.737                       5.737
F000              720.0                       720.0
F000'             718.36
h,k,lmax          13,16,18                    13,16,18
Nref              7834                        7821
Tmin,Tmax         0.458,0.532                 0.119,1.000
Tmin'             0.079

Correction method= # Reported T Limits: Tmin=0.119 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998           Theta(max)= 29.999

R(reflections)= 0.0538( 7106)      wR2(reflections)= 0.1407( 7821)

S = 1.065                 Npar= 313
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The following ALERTS were generated. Each ALERT has the format
       test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.
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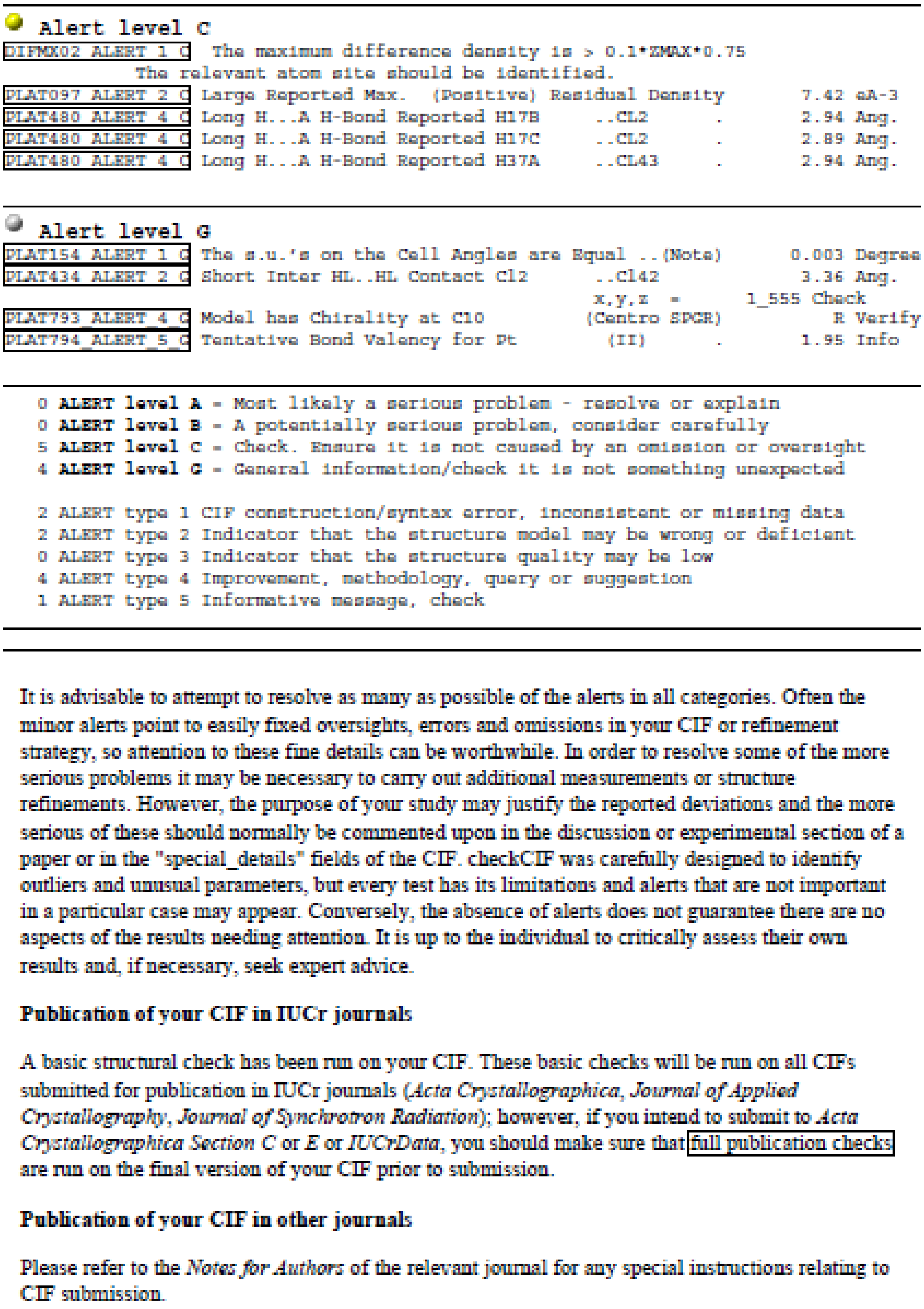

Alert level C

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            The relevant atom site should be identified.
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       7.42 eA-3
PLAT480_ALERT_4_C Long H...A H-Bond Reported H17B     ..CL2      .       2.94 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H17C     ..CL2      .       2.89 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H37A     ..CL43     .       2.94 Ang.
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Alert level G

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PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.003 Degree
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl2      ..Cl42             3.36 Ang.
                                                  x,y,z  =      1_555 Check
PLAT793_ALERT_4_G Model has Chirality at C10         (Centro SPGR)         R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Pt       (II)       .       1.95 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   4 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
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```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

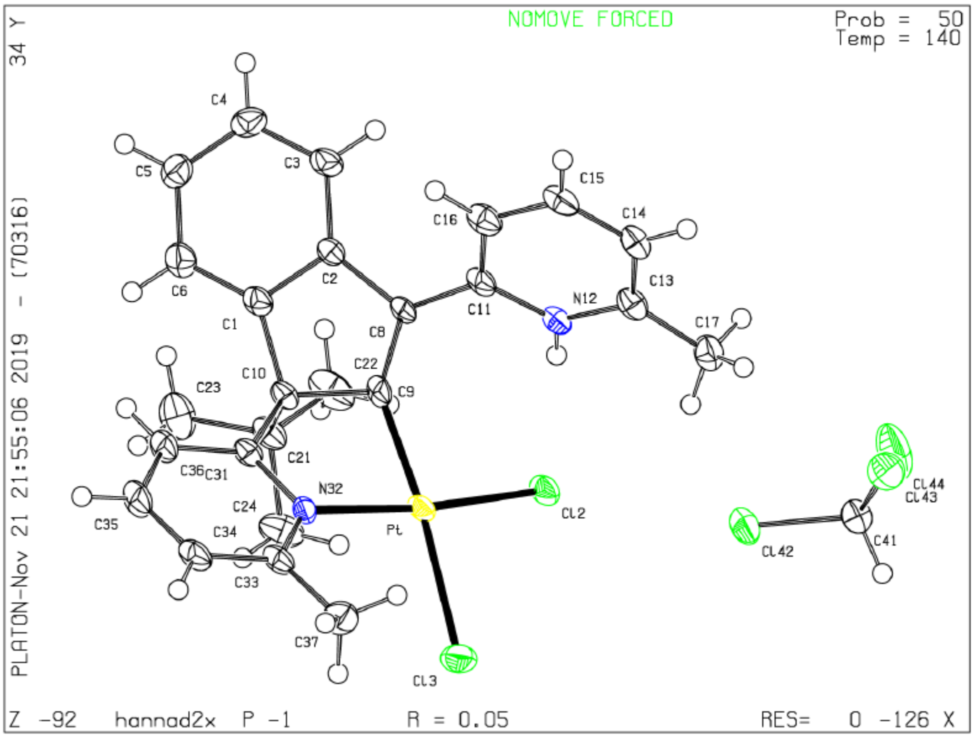
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 07/08/2019; check.def file version of 30/07/2019

Datablock hannad2x - ellipsoid plot



Appendix D – Procedures from CO-ADD

CO-ADD Community for Open Antimicrobial Drug Discovery

Primary Antimicrobial Screening

Bacterial and Fungal

Procedure and Materials

1.0 Summary

1.1 Study

Primary antimicrobial screening study by whole cell growth inhibition assays, using the provided samples at a single concentration, in duplicate (n=2). The inhibition of growth is measured against 5 bacteria: *Escherichia coli*, *Klebsiella pneumoniae, Acinetobacter baumannii, Pseudomonas aeruginosa* and *Staphylococcus aureus*, and 2 fungi: *Candida albicans* and *Cryptococcus neoformans*.

1.2 Assay Parameters

Test concentration		32 µg/mL or 20 µM ≤1% DMSO
QC		Duplicate (n=2) Control MIC: Pass
Plates		Non-Binding Surface, 384 well plate
Media	***Bacteria*** ***Fungi***	Cation-adjusted Mueller Hinton broth Yeast Nitrogen Base
Read Out	***Bacteria***	OD$_{600}$
	C. albicans	OD$_{530}$
	C. neoformans	Resazurin OD$_{600-570}$

1.3 Outcomes

Primary Screening outcomes are detailed in individual Project reports, personalised for each Project Submission for each CO-ADD user.

Please see your data sheet with file extension **P0XXX_PS_data.xlsx,** for example CO-ADD Project **P0100, P0100_PS_data.xlsx**

1.4 Comments

To confirm the inhibitory activity, the hit compound/s will be re-tested against the strains in a dose response assay to determine the minimum inhibitory concentration (MIC) of the compounds. Furthermore, to further evaluate the antimicrobial potential of the compounds they will be assayed against a mammalian cell line to determine general cell toxicity.

In order to continue with Hit Confirmation assays, CO-ADD requests (as per the standard T&C's) that chemical structures of the compound/s (both active and inactive) be supplied after receipt of the primary screening report. All structural information will be kept confidential and only used internally by CO-ADD for the purpose of evaluating novelty of the chemistry to choose compounds for further validation. No publication will result without your written consent.

If possible, please provide structures as **smiles, sdf/sd** or **cdx** files. If you do not have this means, images may also be accepted. Once we have received your structures, we will schedule the dose response assay of the active compound.

If you have not already provided structures to CO-ADD for your full compound set, please do so within a reasonable timeframe after receiving this report, so as not to delay Hit Confirmation.

1.5 Publishing CO-ADD data

If you wish to publish data provided by CO-ADD, we kindly ask that you acknowledge CO-ADD appropriately with the following reference:

> Helping Chemists Discover New Antibiotics
>
> M.A. Blaskovich, J. Zuegg, A.G. Elliott, M.A. Cooper
> *ACS Infect. Dis.*, **2015**, 1(7), 285-287.
>
> DOI: 10.1021/acsinfecdis.5b00044; PMID: 27622818

as well as an acknowledgement for the funding of CO-ADD:

> *"The antimicrobial screening performed by CO-ADD (The Community for Antimicrobial Drug Discovery) was funded by the Wellcome Trust (UK) and The University of Queensland (Australia)."*

Please advise CO-ADD at your earliest convenience that you have used provided data for publication purposes. This information is extremely helpful in keeping track of the outputs from the CO-ADD initiative and supports the program in renewed funding possibilities to continue CO-ADD as a free screening service available to the academic community.

CO-ADD also asks, that where possible you publish your data in an Open Access journals.

2.0 Methods

2.1 Sample preparation

Samples were provided by the collaborator and stored frozen at -20 □C. Samples were prepared in DMSO and water to a final testing concentration of 32 µg/mL or 20 µM (unless otherwise indicated in the data sheet), in 384-well, non-binding surface plate (NBS) for each bacterial/fungal strain, and in duplicate (n=2), and keeping the final DMSO concentration to a maximum of 1% DMSO. All the sample-preparation where done using liquid handling robots.

Compounds that showed solubility issues during stock solution preparation are detailed in the data sheet.

2.2 Antimicrobial Assay

2.2.1 Procedure

All bacteria were cultured in Cation-adjusted Mueller Hinton broth (**CAMHB**) at 37 □C overnight. A sample of each culture was then diluted 40-fold in fresh broth and incubated at 37 □C for 1.5-3 h. The resultant mid-log phase cultures were diluted (CFU/mL measured by OD_{600}), then added to each well of the compound containing plates, giving a cell density of $5\square10^{5}$ CFU/mL and a total volume of 50 µL. All the plates were covered and incubated at 37 °C for 18 h without shaking.

2.2.2 Analysis

Inhibition of bacterial growth was determined measuring absorbance at 600 nm (OD_{600}), using a Tecan M1000 Pro monochromator plate reader. The percentage of growth inhibition was calculated for each well, using the negative control (media only) and positive control (bacteria without inhibitors) on the same plate as references. The significance of the inhibition values was determined by modified Z-scores, calculated using the median and MAD of the samples (no controls) on the same plate. Samples with inhibition value above 80% and Z-Score above 2.5 for either replicate (n=2 on different plates) were classed as actives. Samples with inhibition values between 50 - 80% and Z-Score above 2.5 for either replicate (n=2 on different plates) were classed as partial actives. Samples with inhibition values between 50 - 80% and Z-Score above 2.5 for either replicate (n=2 on different plates) were classed as partial actives.

2.3 Antifungal Assay

2.3.1 Procedure

Fungi strains were cultured for 3 days on Yeast Extract-Peptone Dextrose (**YPD**) agar at 30 °C. A yeast suspension of 1 x 10^6 to 5 x 10^6 CFU/mL (as determined by OD_{530}) was prepared from five colonies. The suspension was subsequently diluted and added to each well of the compound-containing plates giving a final cell density of fungi suspension of 2.5 x 10^3 CFU/mL and a total volume of 50 µL. All plates were covered and incubated at 35 °C for 24 h without shaking.

2.3.2 Analysis

Growth inhibition of *C. albicans* was determined measuring absorbance at 530 nm (OD_{530}), while the growth inhibition of *C. neoformans* was determined measuring the difference in absorbance between 600 and 570 nm ($OD_{600-570}$), after the addition of resazurin (0.001% final concentration) and incubation at 35 °C for additional 2 h. The absorbance was measured using a Biotek Synergy HTX plate reader. The percentage of growth inhibition was calculated for each well, using the negative control (media only) and positive control (fungi without inhibitors) on the same plate. The significance of the inhibition values was determined by modified Z-scores, calculated using the median and MAD of the samples (no controls) on the same plate. Samples with inhibition value above 80% and Z-Score above 2.5 for either replicate (n=2 on different plates) were classed as actives. Samples with inhibition values between 50 - 80% and Z-Score above 2.5 for either replicate (n=2 on different plates) were classed as partial actives.

2.4 Antibiotic standards preparation and Quality control

Colistin and Vancomycin were used as positive bacterial inhibitor standards for Gramnegative and Gram-positive bacteria, respectively. Fluconazole was used as a positive fungal inhibitor standard for *C. albicans and C. neoformans.*

The antibiotics were provided in 4 concentrations, with 2 above and 2 below its MIC value, and plated into the first 8 wells of column 23 of the 384-well NBS plates.

The quality control (QC) of the assays was determined by the antimicrobial controls and the Z'-factor (using positive and negative controls). Each plate was deemed to fulfil the quality criteria (pass QC), if the Z'-factor was above 0.4, and the antimicrobial standards showed full range of activity, with full growth inhibition at their highest concentration, and no growth inhibition at their lowest concentration.

3.0 Materials

3.1 Assay materials

Material	***Code***	***Brand***	***Cat No.***
Compound preparation plate [Polypropylene]	PP	Corning	3364
Assay Plates [Non-binding surface]	NBS 384w	Corning	3640
Growth media - bacteria	CAMHB	Bacto Laboratories	212322
Culture agar - fungi	YPD	Becton Dickinson	242720
Growth media - fungi	YNB	Becton Dickinson	233520
Resazurin		Sigma-Aldrich	R7017

3.2 Standards

Sample Name	***Sample ID***	***Full MW***	***Stock Conc. (mg/mL)***	***Solvent***	***Source***
Colistin - Sulfate	MCC_000094:02	1400.63	10.0	DMSO	Sigma; C4461
Vancomycin - HCL	MCC_000095:02	1485.71	10.0	DMSO	Sigma; 861987
Fluconazole	MCC_008383:01	306.27	2.56	DMSO	Sigma; F8929

3.3 Microbial Strains

ID	**Batch**	***Organism***	***Strain***	***Description***
GN_001	02	*Escherichia coli*	ATCC 25922	FDA control strain
GN_003	02	*Klebsiella pneumoniae*	ATCC 700603	MDR
GN_034	02	*Acinetobacter baumannii*	ATCC 19606	Type strain
GN_042	02	*Pseudomonas aeruginosa*	ATCC 27853	Quality control strain
GP_020	02	*Staphylococcus aureus*	ATCC 43300	MRSA
FG_001	01	*Candida albicans*	ATCC 90028	CLSI reference
FG_002	01	*Cryptococcus neoformans*	ATCC 208821	H99 - Type strain

4.0 Controls

All antibiotic and antifungal controls displayed inhibitory values within the expected range. For further information please contact the CO-ADD team at support@co-add.org.

Strain ID	***Species***	***Antibiotic***	***Pass/Fail***
GN_001:02	*E. coli*	Colistin	Pass
GN_003:02	*K. pneumoniae* (MDR)	Colistin	Pass
GN_034:02	*A. baumannii*	Colistin	Pass
GN_042:02	*P. aeruginosa*	Colistin	Pass
GP_020:02	*S. aureus* (MRSA)	Vancomycin	Pass
FG_001:01	*C. albicans*	Fluconazole	Pass
FG_002:01	*C. neoformans* (H99)	Fluconazole	Pass

4.1 Antimicrobial susceptibility of tested strains

Values are the average of ≥ 6 independent biological replicates. All values are within the expected range as per CLSI guidelines.

4.1.1 Antibiotic standards

MIC determined by BMD method, CA-MHB, Corning 3640 384 NBS plates		**GN_001:02** ***Escherichia coli*** FDA Control ATCC 25922	**GN_003:02** ***Klebsiella pneumophila*** ESBL ATCC 700603	**GN_034:02** ***Acinetobacter baumannii*** Type strain ATCC 19606	**GN_042:02** ***Pseudomonas aeruginosa*** QC strain ATCC 27853
Compound	Compound Type	MIC (µg/mL)			
Colistin - sulfate	Antibiotic	**0.125**	**0.25**	**0.25**	**0.25**

MIC determined by BMD method, CA-MHB, Corning 3640 384 NBS plates		**GP_020:02** ***Staphylococcus aureus*** MRSA ATCC 43300
Compound	Compound Type	MIC (µg/mL)
Vancomycin - HCl	Antibiotic	**1**

4.1.2 Antifungal standard

MIC determined by BMD method, *YNB, Corning 3640 384 NBS plates*		**FG_001:02** ***Candida albicans*** CLSI reference ATCC 90028	**FG_002:02** ***Cryptococcus neoformans H99*** Type strain ATCC 208821
Compound	Compound Type	MIC (µg/mL)	
Fluconazole	Antifungal	**0.125**	**8**

CO-ADD Community for Open Antimicrobial Drug Discovery

Hit-Confirmation

Antimicrobial screening, Cytotoxicity & Haemolysis

Procedure and Materials

1.0 Summary

1.1 Study

Hit Confirmation of active compounds by whole cell growth inhibition assays was conducted as an 8-point dose response to determine the Minimum Inhibitory Concentration (MIC), in duplicate (n=2). The inhibition of growth is measured against those microorganisms that showed susceptibility to the compounds tested in the Primary Screen.

Included in the Hit Confirmation were 5 bacteria: *Escherichia coli*, *Klebsiella pneumoniae, Acinetobacter baumannii, Pseudomonas aeruginosa* and *Staphylococcus aureus*, and 2 fungi *Candida albicans* and *Cryptococcus neoformans*.

In addition to determining MIC, active compounds were counter screened for cytotoxicity against a human embryonic kidney cell line, HEK293, by determining their CC_{50} value. The compounds were also screened for haemolysis of human red blood cells.

1.2 Assay Parameters

Assay Parameters	Bacteria	Fungi	HEK293	Haemolysis
Test concentration	32 - 0.25 µg/mL or 20 – 0.15 µM ≤0.5% DMSO	32 - 0.25 µg/mL or 20 – 0.15 µM ≤0.5% DMSO	32 - 0.25 µg/mL or 20 – 0.15 µM ≤0.5% DMSO	32 - 0.25 µg/mL or 20 – 0.15 µM ≤0.5% DMSO
QC	Duplicate (n=2) Control MIC: Pass	Duplicate (n=2) Control MIC: Pass	Duplicate (n=2) Control CC_{50}: Pass	Duplicate (n=2) Control HC_{10}: Pass
Plates	Non-Binding Surface (NBS), 384-well plate	Non-Binding Surface (NBS), 384-well plate	TC, 384-well black wall/clear bottom	Polypropylene 384-well and polystyrene 384well plates
Media	Cation-adjusted Mueller Hinton broth	Yeast Nitrogen Base	DMEM supplemented with 10% FBS	0.9% NaCl
Read Out	OD_{600}	OD_{630} Resazurin $OD_{600-570}$	Resazurin $F_{560/590}$	OD_{405}

1.3 Outcomes

Hit Confirmation outcomes are detailed in individual Project reports, personalised for each Project Submission for each CO-ADD user.

Please see your data sheet with file extension **P0XXX_HC_data.xlsx,** for example CO-ADD Project **P0100, P0100_HC_data.xlsx**

1.4 Structural Novelty

As per the T&C's of CO-ADD, structures for all submitted compounds for antimicrobial screening should be disclosed to CO-ADD following Primary Screening. Without structures for all submitted compounds, Hit Confirmation assays will not be triggered.

If you have not already done so, please **provide CO-ADD with the chemical structure** of the full sample set in this study (both for compounds showing activity and those that do not), which will allow CO-ADD to filter out future samples with the same, or highly similar structure. In addition, please **notify CO-ADD** if you agree to publish the data (*i.e.* structures and activity) in the public bioactive database ChEMBL (www.ebi.ac.uk/chembl/). CO-ADD aims to increase the public knowledge of antimicrobial research, including data about non-active compounds.

All confirmed hits, without cytotoxicity or haemolytic activity, will be considered for further HitValidation, after a detailed analysis of structure-activity relationship and antimicrobial novelty, within CO-ADD samples, as well as, within public antimicrobial activity databases, like ChEMBL (www.ebi.ac.uk/chembl/).

1.5 Publishing CO-ADD Data

If you wish to publish data provided by CO-ADD, we kindly ask that you acknowledge CO-ADD appropriately with the following reference:

> Helping Chemists Discover New Antibiotics
>
> M.A. Blaskovich, J. Zuegg, A.G. Elliott, M.A. Cooper
> *ACS Infect. Dis.*, **2015**, 1(7), 285-287.
>
> DOI: 10.1021/acsinfecdis.5b00044; PMID: 27622818

as well as an acknowledgement for the funding of CO-ADD:

> *“The antimicrobial screening performed by CO-ADD (The Community for Antimicrobial Drug Discovery) was funded by the Wellcome Trust (UK) and The University of Queensland (Australia).”*

Please advise CO-ADD at your earliest convenience that you have used provided data for publication purposes. This information is extremely helpful in keeping track of the outputs from the CO-ADD initiative and supports the program in renewed funding possibilities to continue CO-ADD as a free screening service available to the academic community.

CO-ADD also asks, that where possible you publish your data in an Open Access journals.

2.0 Methods

2.1 Sample Preparation

Samples were provided by the collaborator and stored frozen at -20 °C. Samples were prepared in DMSO and water to a final testing concentration of 32 µg/mL or 20 µM (unless otherwise indicated in the data sheet) and serially diluted 1:2 fold for 8 times. Each sample concentration was prepared in 384-well plates, non-binding surface plate (**NBS;** Corning 3640) for each bacterial/fungal strain, tissue-culture treated (**TC-treated;** Corning 3712/3764) black for mammalian cell types and polypropylene 384-well (**PP**; Corning 3657) for haemolysis assays, all in duplicate (n=2), and keeping the final DMSO concentration to a maximum of 0.5%. All the sample preparation was done using liquid handling robots.

Compounds that showed notable solubility issues during stock solution preparation are detailed in the **Data sheet** for the individual Project.

2.2 Antibacterial Assay

2.2.1 Procedure

All bacteria were cultured in Cation-adjusted Mueller Hinton broth (**CAMHB**) at 37 °C overnight. A sample of each culture was then diluted 40-fold in fresh broth and incubated at 37 °C for 1.5-3 h. The resultant mid-log phase cultures were diluted (CFU/mL measured by OD_{600}), then added to each well of the compound containing plates, giving a cell density of 5 x 10^5 CFU/mL and a total volume of 50 µL. All the plates were covered and incubated at 37 °C for 18 h without shaking.

2.2.2 Analysis

Inhibition of bacterial growth was determined measuring absorbance at 600 nm (OD_{600}), using a Tecan M1000 Pro monochromator plate reader. The percentage of growth inhibition was calculated for each well, using the negative control (media only) and positive control (bacteria without inhibitors) on the same plate as references.

The percentage of growth inhibition was calculated for each well, using the negative control (media only) and positive control (bacteria without inhibitors) on the same plate. The MIC was determined as the lowest concentration at which the growth was fully inhibited, defined by an inhibition ≥ 80%. In addition, the maximal percentage of growth inhibition is reported as D_{Max}, indicating any compounds with partial activity.

Hits were classified by MIC ≤ 16 µg/mL or MIC ≤ 10 µM in either replicate (n=2 on different plates).

2.3 Antifungal Assay

2.3.1 Procedure

Fungi strains were cultured for 3 days on Yeast Extract-Peptone Dextrose (**YPD**) agar at 30 °C. A yeast suspension of 1 x 10^6 to 5 x 10^6 CFU/mL (as determined by OD_{530}) was prepared from five colonies. The suspension was subsequently diluted and added to each well of the compound-containing plates giving a final cell density of fungi suspension of 2.5 x 10^3 CFU/mL and a total volume of 50 µL. All plates were covered and incubated at 35 °C for 36 h without shaking.

2.3.2 Analysis

Growth inhibition of *C. albicans* was determined measuring absorbance at 630 nm (OD_{630}), while the growth inhibition of *C. neoformans* was determined measuring the difference in absorbance between 600 and 570 nm ($OD_{600\text{-}570}$), after the addition of resazurin (0.001% final concentration) and incubation at 35 °C for 2 h. The absorbance was measured using a Biotek Multiflo Synergy HTX plate reader.

In both cases, the percentage of growth inhibition was calculated for each well, using the negative control (media only) and positive control (fungi without inhibitors) on the same plate. The MIC was determined as the lowest concentration at which the growth was fully inhibited, defined by an inhibition ≥ 80% for *C. albicans* and an inhibition ≥ 70% for *C. neoformans.* Due to a higher variance in growth and inhibition, a lower threshold was applied to the data for *C. neoformans*. In addition, the maximal percentage of growth inhibition is reported as D_{Max}, indicating any compounds with marginal activity.

Hits were classified by MIC ≤ 16 µg/mL or MIC ≤ 10 µM in either replicate (n=2 on different plates).

2.4 Cytotoxicity Assay

2.4.1 Procedure

HEK293 cells were counted manually in a Neubauer haemocytometer and then plated in the 384-well plates containing the compounds to give a density of 5000 cells/well in a final volume of 50 µL. **DMEM** supplemented with **10% FBS** was used as growth media and the cells were incubated together with the compounds for 20 h at 37 °C in 5% CO_2.

2.4.2 Analysis

Cytotoxicity (or cell viability) was measured by fluorescence, ex: 560/10 nm, em: 590/10 nm ($F_{560/590}$), after addition of 5 µL of 25 µg/mL resazurin (2.3 µg/mL final concentration) and after incubation for further 3 h at 37 °C in 5% CO_2. The fluorescence intensity was measured using a Tecan M1000 Pro monochromator plate reader, using automatic gain calculation.

CC_{50} (concentration at 50% cytotoxicity) were calculated by curve fitting the inhibition values *vs.* log(concentration) using a sigmoidal dose-response function, with variable fitting values for bottom, top and slope. In addition, the maximal percentage of cytotoxicity is reported as D_{Max}, indicating any compounds with partial cytotoxicity.

The curve fitting was implemented using Pipeline Pilot's dose-response component, resulting in similar values to curve fitting tools such as GraphPad's Prism and IDBS's XlFit. Any value with > indicate sample with no activity (low D_{Max} value) or samples with CC_{50} values above the maximum tested concentration (higher D_{Max} value).

Cytotoxic samples were classified by $CC_{50} \leq 32$ μg/mL or $CC_{50} \leq 10$ μM in either replicate (n=2 on different plates). In addition, samples were flagged as partial cytotoxic if $D_{Max} \geq 50\%$, even with CC_{50} > the maximum tested concentration.

2.5 Haemolysis Assay

2.5.1 Procedure

Human whole blood was washed three times with 3 volumes of 0.9% NaCl and then resuspended in same to a concentration of 0.5×10^8 cells/mL, as determined by manual cell count in a Neubauer haemocytometer. The washed cells were then added to the 384-well compound-containing plates for a final volume of 50 μL. After a 10 min shake on a plate shaker the plates were then incubated for 1 h at 37 °C. After incubation, the plates were centrifuged at 1000*g* for 10 min to pellet cells and debris, 25 μL of the supernatant was then transferred to a polystyrene 384-well assay plate.

2.5.2 Analysis

Haemolysis was determined by measuring the supernatant absorbance at 405 mm (OD_{405}). The absorbance was measured using a Tecan M1000 Pro monochromator plate reader.

HC_{10} and HC_{50} (concentration at 10% and 50% haemolysis, respectively) were calculated by curve fitting the inhibition values *vs*. log(concentration) using a sigmoidal dose-response function with variable fitting values for top, bottom and slope. In addition, the maximal percentage of haemolysis is reported as D_{Max}, indicating any compounds with partial haemolysis.

The curve fitting was implemented using Pipeline Pilot's dose-response component, resulting in similar values to curve fitting tools such as GraphPad's Prism and IDBS's XlFit. Any value with > indicate sample with no activity (low D_{Max} value) or samples with HC_{10} values above the maximum tested concentration (higher D_{Max} value).

Haemolysis samples were classified by $HC_{10} \leq 32$ μg/mL or $HC_{10} \leq 10$ μM in either replicate (n=2 on different plates). In addition, samples were flagged as partial haemolytic if $D_{Max} \geq 50\%$, even with HC_{10} > the maximum tested concentration.

2.6 Antibiotic, Cytotoxic and Haemolytic Standards Preparation and Quality Control

Colistin and Vancomycin were used as positive bacterial inhibitor standards for Gramnegative and Gram-positive bacteria, respectively. Fluconazole was used as a positive fungal inhibitor standard for *C. albicans and C. neoformans.* Tamoxifen was used as a positive cytotoxicity standard. Melittin was used as a positive haemolytic standard.

Each antibiotic standard was provided in 4 concentrations, with 2 above and 2 below its MIC or CC_{50} value, and plated into the first 8 wells of column 23 of the 384-well NBS plates. Tamoxifen and melittin was used in 8 concentrations in 2 fold serial dilutions with 50 µg/mL highest concentration.

The quality control (QC) of the assays was determined by Z'-Factor, calculated from the Negative (media only) and Positive Controls (bacterial, fungal or cell culture without inhibitor), and the Standards. Plates with a Z'-Factor of ≥ 0.4 and Standards active at the highest and inactive at the lowest concentration, were accepted for further data analysis.

3.0 Materials

3.1 Assay Materials

Material	***Code***	***Brand/Supplier***	***Cat No.***
Compound preparation plate, Polypropylene	PP	Corning	3364
Assay Plates – Antimicrobial Non-binding surface	NBS 384w	Corning	3640
Assay Plates – Cytotoxicity Tissue culture treated	Black/Clear bottom 384w	Corning	3712
Assay Plates - Haemolysis	PP-Haem	Corning	3657
Reading Plates - Haemolysis	Clear 384w	Corning	3680
Growth media - bacteria	CAMHB	Bacto Laboratories	212322
Culture agar - fungi	YPD	Becton Dickinson	242720
Growth media - fungi	YNB	Becton Dickinson	233520
Resazurin		Sigma-Aldrich	R7017
Dulbecco's Modified Eagle Medium	DMEM	Life Technologies	11995-073

Foetal Bovine Serum	FBS	Bovogen	FFBS-500
0.9% NaCl	Saline	Baxter	AHF7124

3.2 Standards

Sample Name	***Sample ID***	***Full MW***	***Stock Conc. (mg/mL)***	***Solvent***	***Source***
Colistin - Sulfate	MCC_000094:02	1400.63	10.0	DMSO	Sigma; C4461
Vancomycin - HCL	MCC_000095:02	1485.71	10.0	DMSO	Sigma; 861987
Fluconazole	MCC_008383:01	306.27	2.56	DMSO	Sigma; F8929
Tamoxifen	MCC_000096:01	371.50	10	DMSO	Sigma; T5648
Melittin	MCC_008868:02	2846.46	10	Water	Sigma: M2272

3.3 Microbial strains and cell lines

ID	**Batch**	***Organism***	***Strain***	***Description***
GN_001	02	*Escherichia coli*	ATCC 25922	FDA control strain
GN_003	02	*Klebsiella pneumoniae*	ATCC 700603	MDR
GN_034	02	*Acinetobacter baumannii*	ATCC 19606	Type strain
GN_042	02	*Pseudomonas aeruginosa*	ATCC 27853	Quality control strain
GP_020	02	*Staphylococcus aureus*	ATCC 43300	MRSA
FG_001	01	*Candida albicans*	ATCC 90028	CLSI reference
FG_002	01	*Cryptococci neoformans*	ATCC 208821	H99, Type strain
MA_007	02	*Homo sapiens* embryonic kidney cells	ATCC CRL-1573	HEK 293
HA_150	-	*Homo sapiens*	ARCBS 5400 00150	Whole blood

4.0 Controls

4.1 Antimicrobial susceptibility of tested strains

Values are the average of ≥ 6 independent biological replicates. All values are within the expected range as per CLSI guidelines.

4.1.1 Antibiotic standards

MIC determined by BMD method, CA-MHB, Corning 3640 384 NBS plates		**GN_001:02** ***Escherichia coli*** FDA Control ATCC 25922	**GN_003:02** ***Klebsiella pneumophila*** ESBL ATCC 700603	**GN_034:02** ***Acinetobacter baumannii*** Type strain ATCC 19606	**GN_042:02** ***Pseudomonas aeruginosa*** QC strain ATCC 27853
Compound	Compound Type	MIC (µg/mL)			
Colistin - sulfate	Antibiotic	**0.125**	**0.25**	**0.25**	**0.25**

MIC determined by BMD method, CA-MHB, Corning 3640 384 NBS plates		**GP_020:02** ***Staphylococcus aureus*** MRSA ATCC 43300
Compound	Compound Type	MIC (µg/mL)
Vancomycin - HCl	Antibiotic	**1**

4.1.2 Antifungal standard

MIC determined by BMD method, YNB, Corning 3640 384 NBS plates		**FG_001:02** ***Candida albicans*** CLSI reference ATCC 90028	**FG_002:02** ***Cryptococcus neoformans H99*** Type strain ATCC 208821
Compound	Compound Type	MIC (µg/mL)	
Fluconazole	Antifungal	**0.125**	**8**

4.2 Susceptibility profile of cell lines

Values are the average of > 6 independent biological replicates. CC_{50} is the concentration at 50% cytotoxicity.		**MA_007** **HEK293** **ATCC CRL-1573**	
		CC_{50} (µg/mL)	
Compound	Compound Type	Average	Stdev
Tamoxifen	PKC inhibitor	**9**	**2.2**

4.3 Susceptibility profile of human washed red cells

Values are the average of > 6 independent biological replicates. HC_{10} and HC_{50} are the concentrations at 10% and 50% haemolysis, respectively.		**HA_150** **Human Whole blood** **ARCBS 00150**			
		HC_{10} (µg/mL)		HC_{50} (µg/mL)	
Compound	Compound Type	Average	Stdev	Average	Stdev
Melittin	Haemolytic peptide	**2.7**	**0.9**	**8.5**	**2.5**

4.4 Outcome

All standard compound controls displayed inhibitory values within the expected range for each assay type and each organism tested. For further information please contact the CO-ADD team at support@co-add.org.

Strain ID	***Species***	***Standard positive inhibitor control***	***Pass/Fail***
GN_001:02	*E. coli*	Colistin	Pass
GN_003:02	*K. pneumoniae* (MDR)	Colistin	Pass
GN_034:02	*A. baumannii*	Colistin	Pass
GN_042:02	*P. aeruginosa*	Colistin	Pass
GP_020:02	*S. aureus* (MRSA)	Vancomycin	Pass
FG_001:01	*C. albicans*	Fluconazole	Pass
FG_002:01	*C. neoformans* (H99)	Fluconazole	Pass
MA_007:02	*Homo sapiens* HEK293	Tamoxifen	Pass
HA_150	*Homo sapiens*	Melittin	Pass