Supporting Information

Formal α–Allylation of Primary Amines by a Dearomative, Palladium-Catalyzed Umpolung Allylation of N-(Aryloxy)imines

Luis M. Mori-Quiroz, Shrikant S. Londhe, and Michael D. Clift*

Department of Chemistry, The University of Kansas, Lawrence, KS, 66045

*email: michael.clift@abbvie.com

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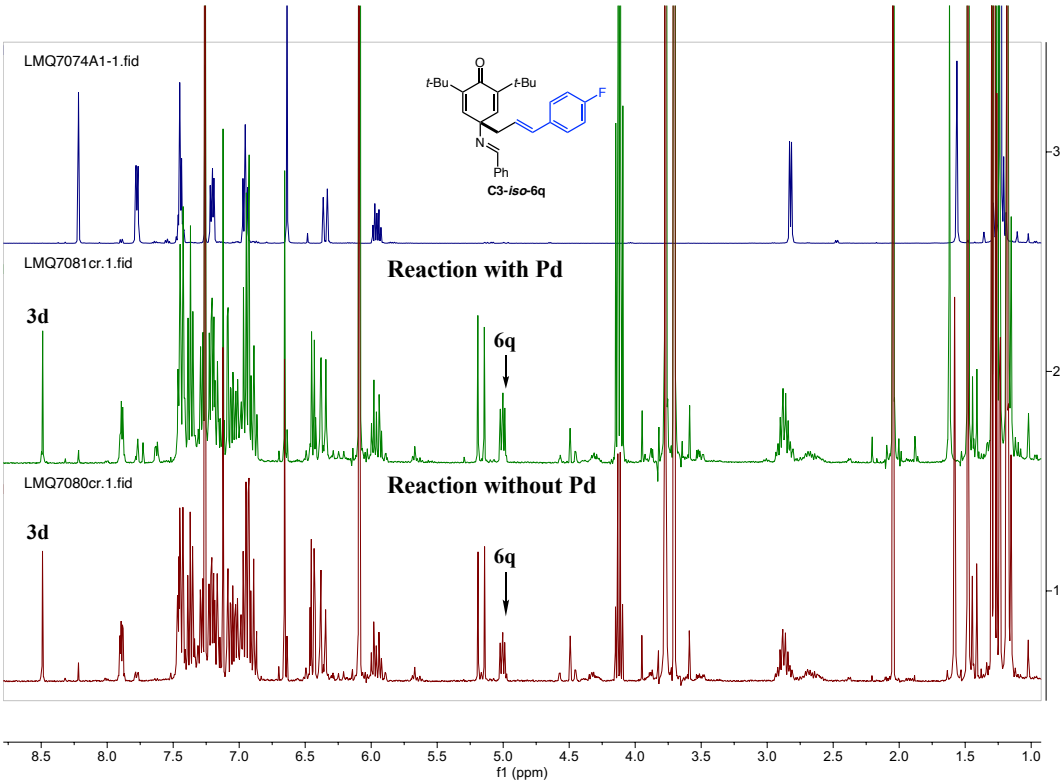
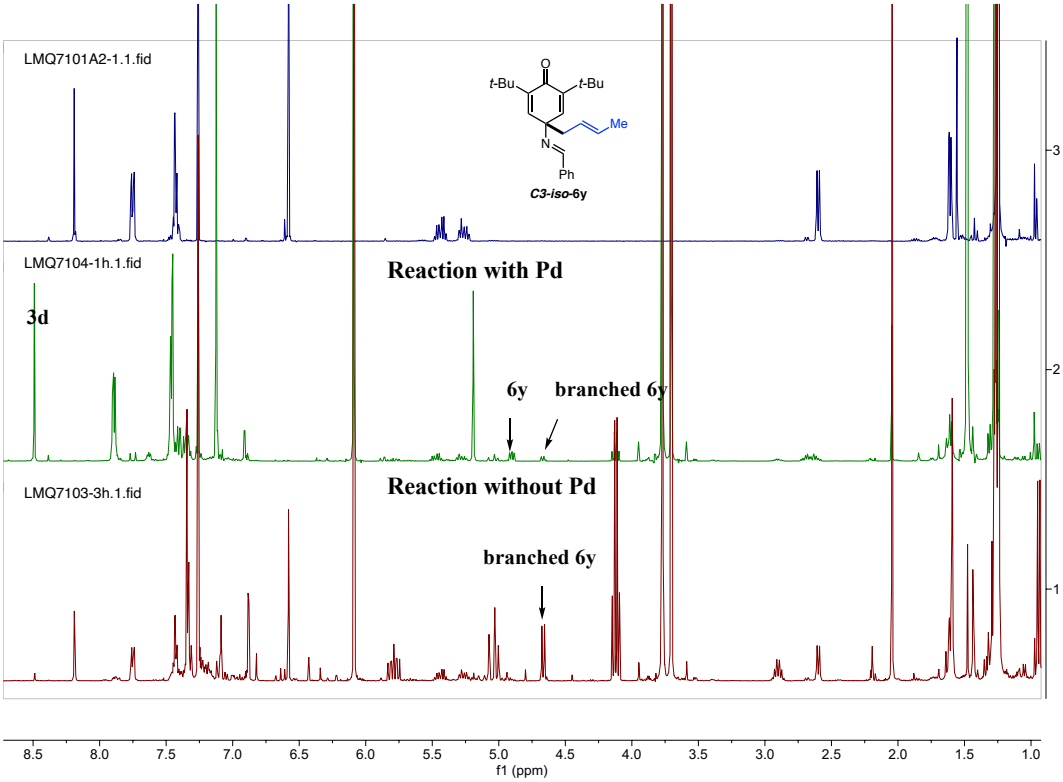
1. NMR Data for Mechanistic Experiments

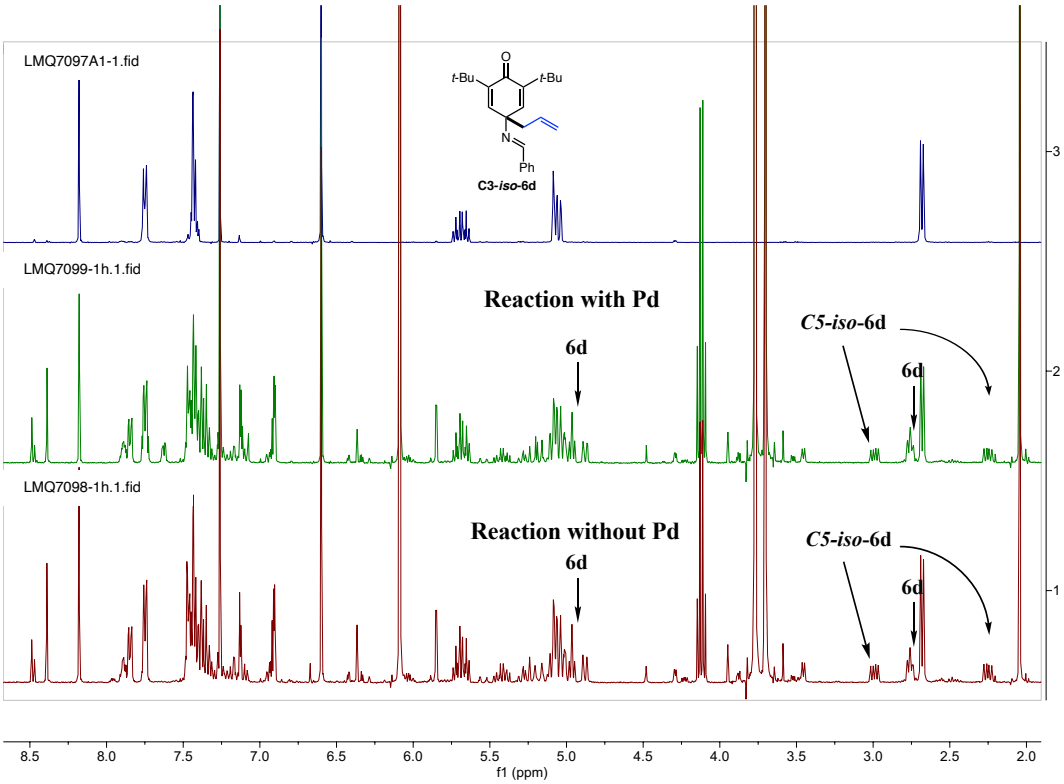
Isomerization of *C3-iso*-6q in the presence and absence of Pd



Isomerization of *C3-iso*-6y in the presence and absence of Pd



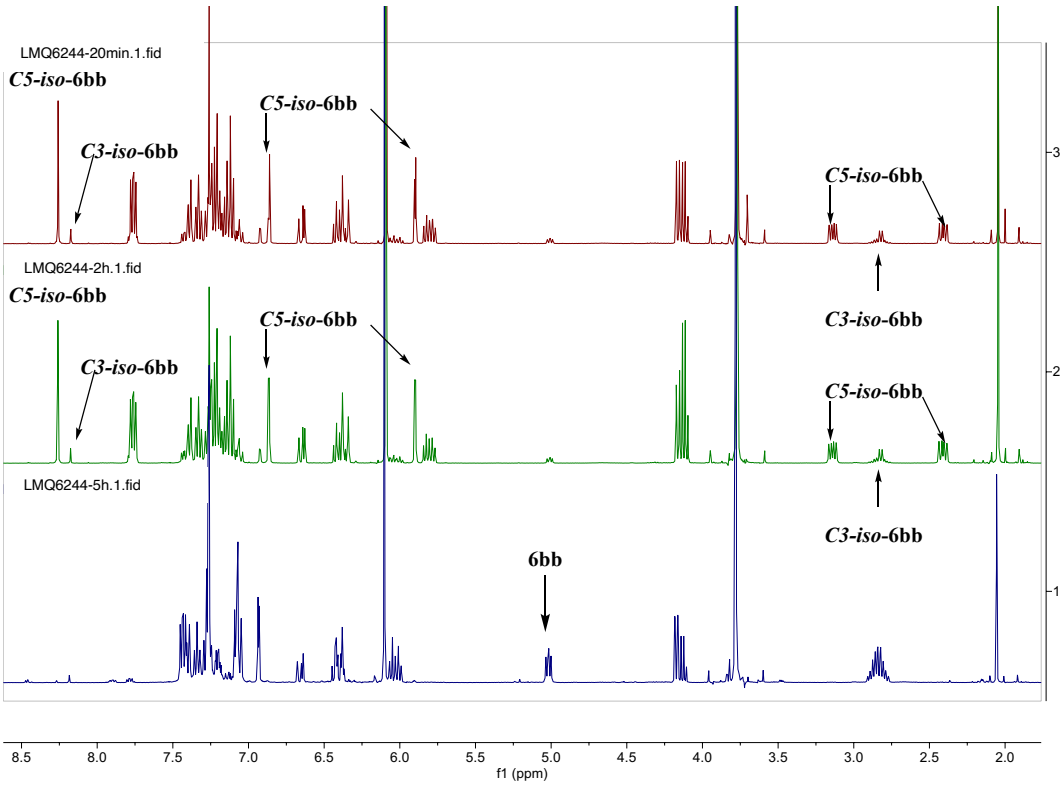
Isomerization of *C3-iso*-6d in the presence and absence of Pd



2. Thermal Isomerization of *C5-iso*-6bb

Table S1. NMR yields for the isomerization of *C5-iso*-6bb over time.

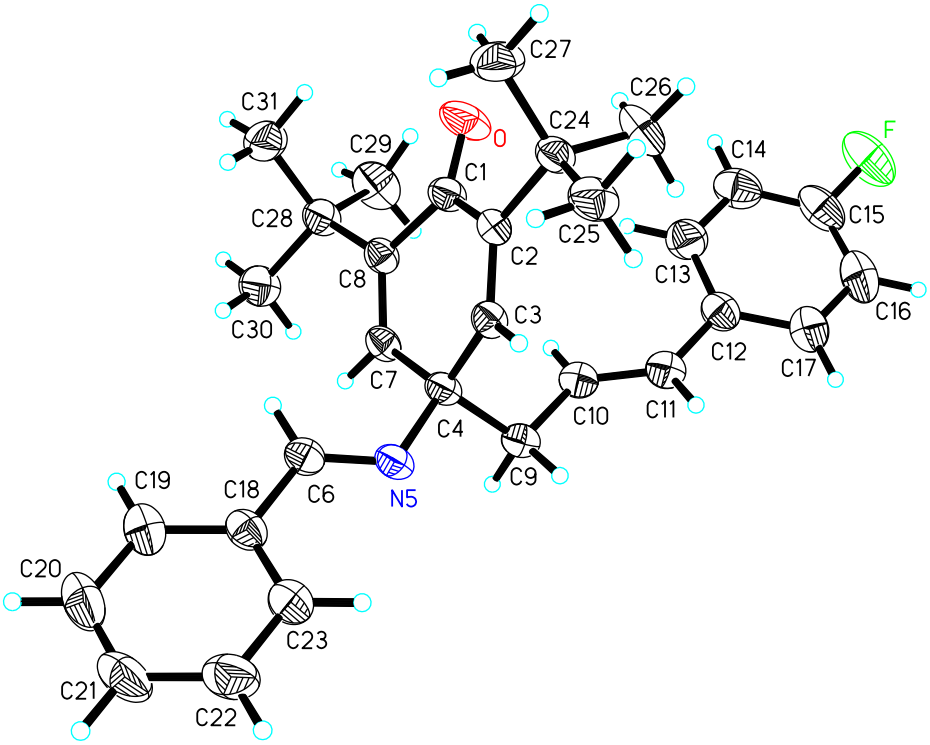
time	Temperature	conversion 3a	6bb	*C3-iso*-6bb	*C5-iso*-6bb
20 min	0 ºC	100	13	8	79
+2 h	0 ºC to rt	100	14	8	78
+2 h	rt to 65 ºC	100	92	4	2



3. Crystallographic Data for *C3-iso*-6q

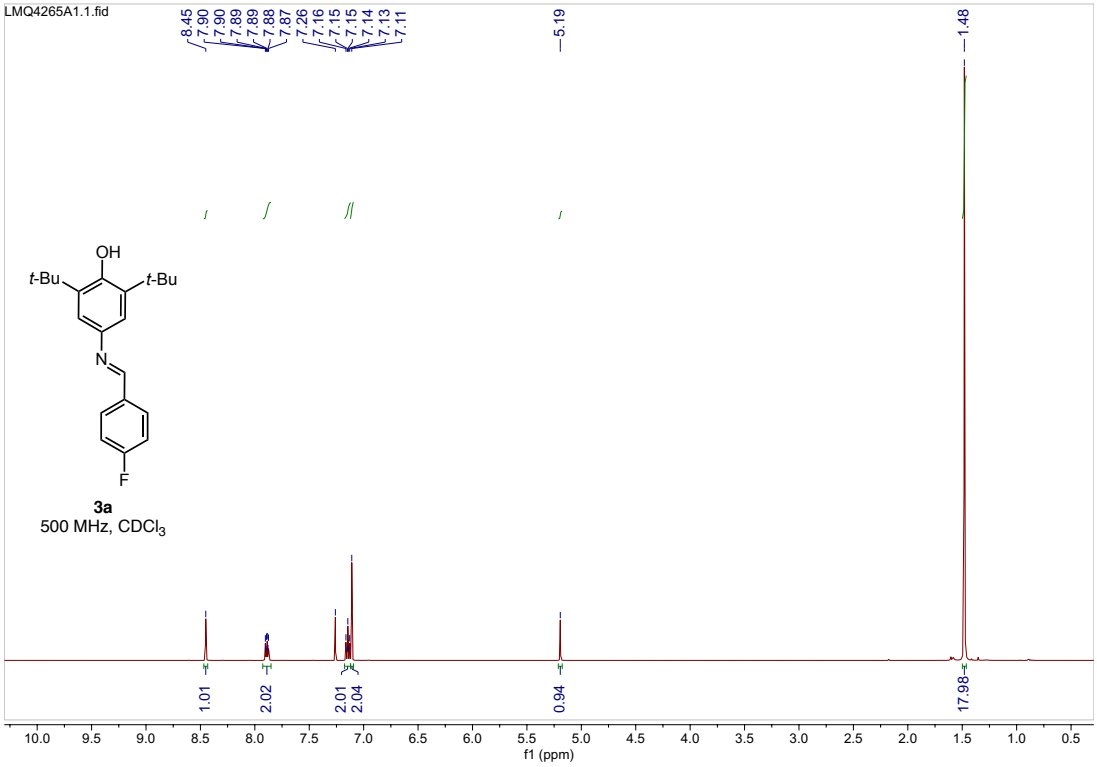
Table S2. Crystal data and structure refinement for *C3-iso*-6q.

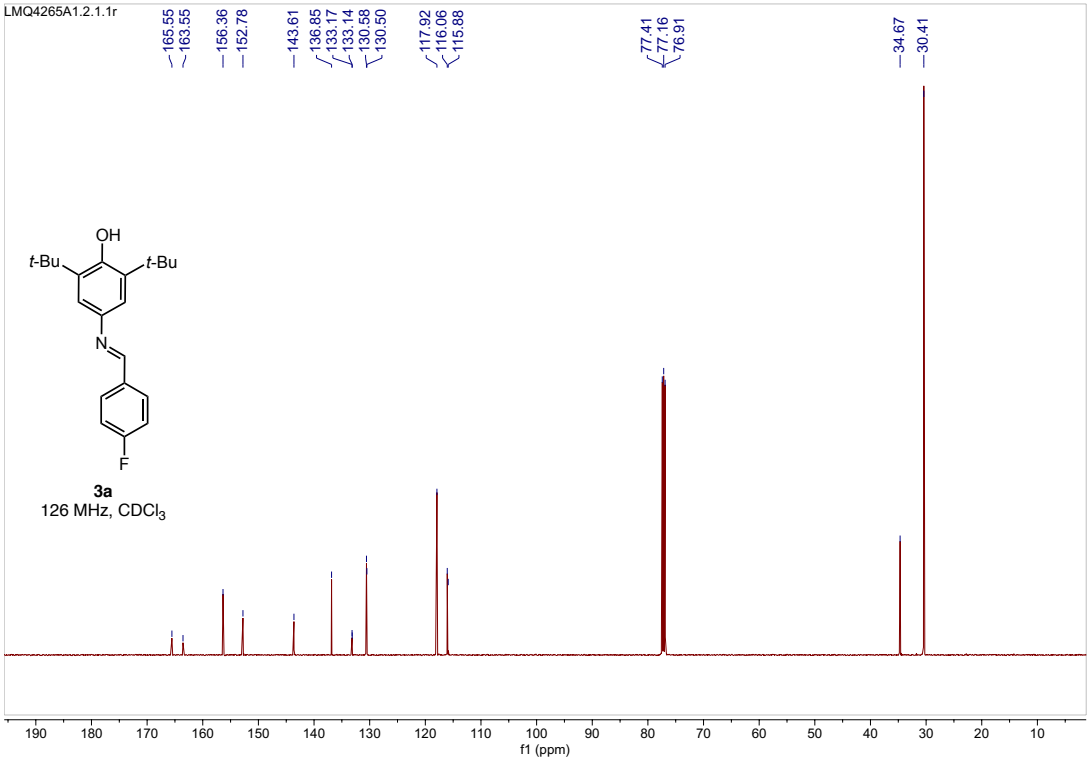
Identification code	q83h	
Empirical formula	C30 H34 F N O	
Formula weight	443.58	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.3148(3) Å	α= 90°.
	b = 20.1899(6) Å	β= 104.4280(10)°.
	c = 12.5935(4) Å	γ = 90°.
Volume	2539.94(13) $Å^3$	
Z	4	
Density (calculated)	1.160 Mg/m^3	
Absorption coefficient	0.582 mm^{-1}	
F(000)	952	
Crystal size	0.220 x 0.160 x 0.130 mm^3	
Theta range for data collection	4.380 to 70.325°.	
Index ranges	-12<=h<=10, -24<=k<=23, -15<=l<=12	
Reflections collected	12481	
Independent reflections	4677 [R(int) = 0.0276]	
Completeness to theta = 66.000°	99.1 %	
Absorption correction	Multi-scan	
Max. and min. transmission	1.000 and 0.777	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4677 / 0 / 304	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0462, wR2 = 0.1255	
R indices (all data)	R1 = 0.0495, wR2 = 0.1318	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.267 and -0.283 $e.Å^{-3}$	

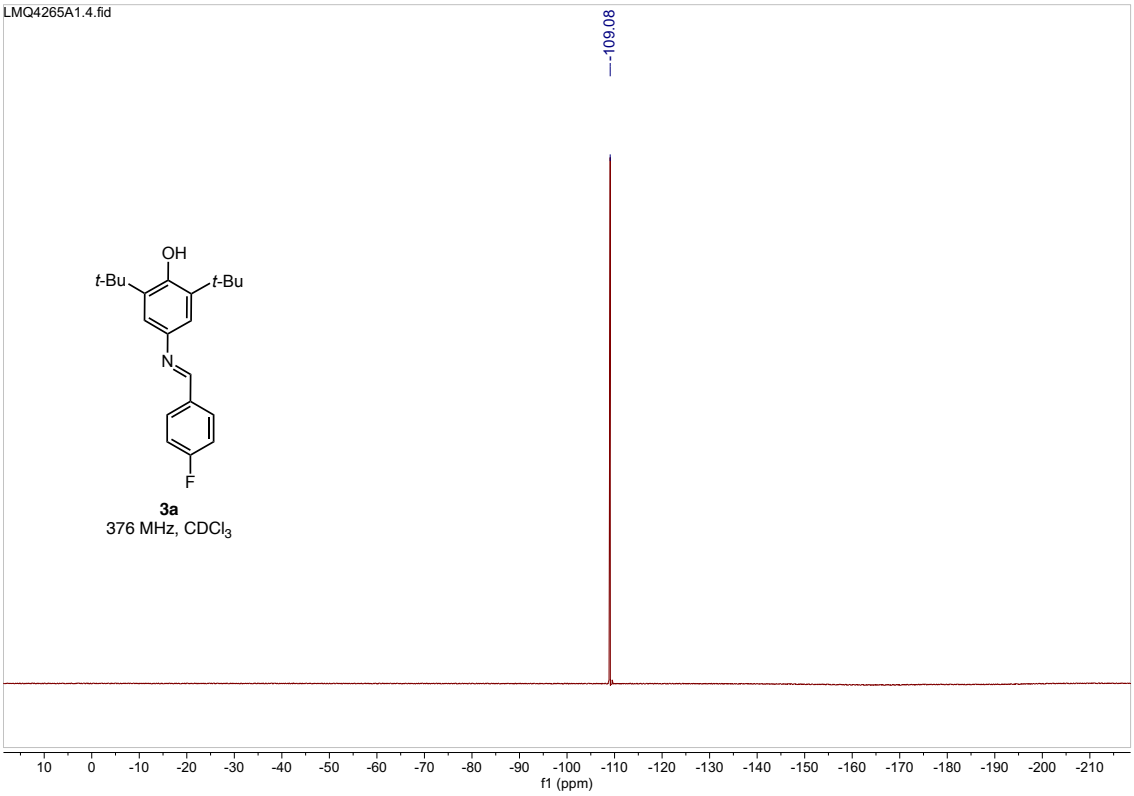


Thermal ellipsoids of *C3-iso*-6q. Ellipsoids are displayed at the 50% probability level.

4. Copies of ^{1}H, ^{13}C, and ^{19}F NMR Spectra



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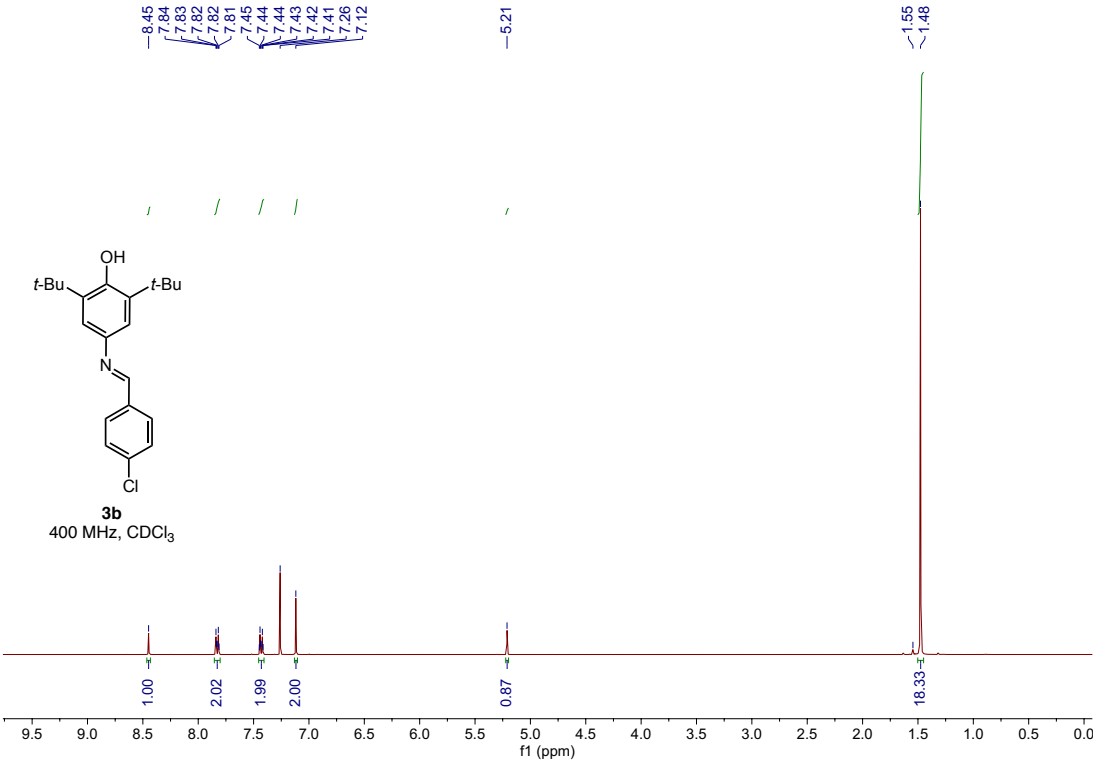
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t-Bu
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Cl
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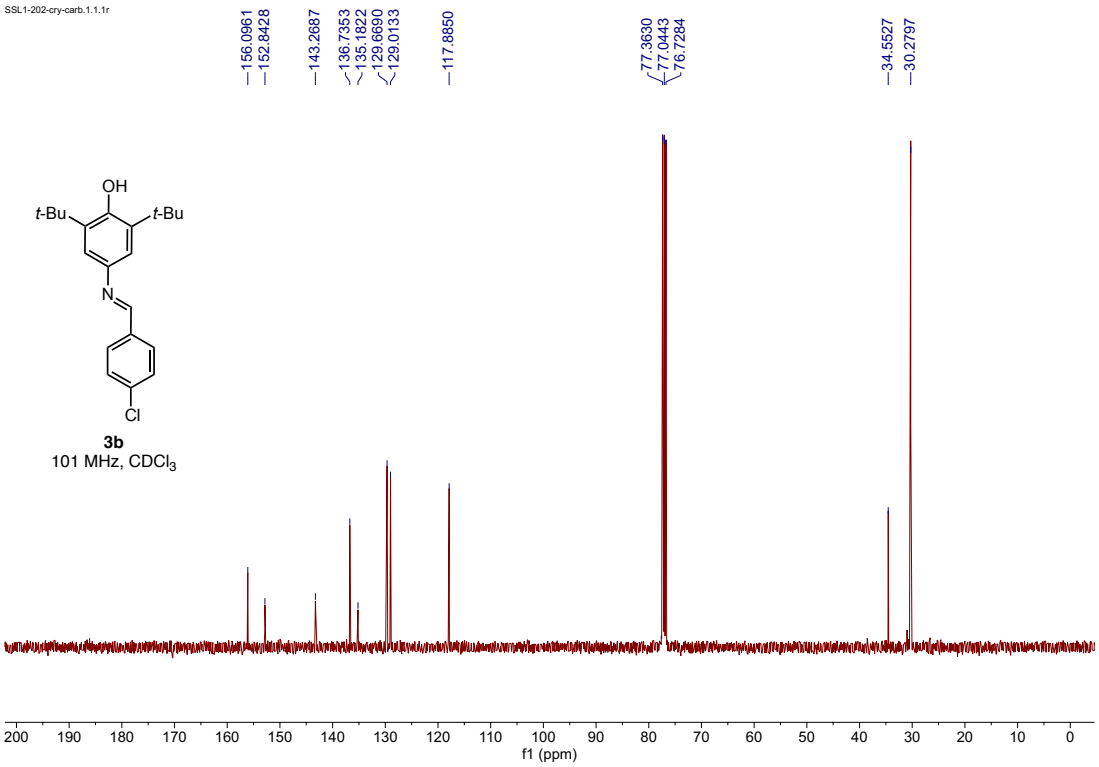
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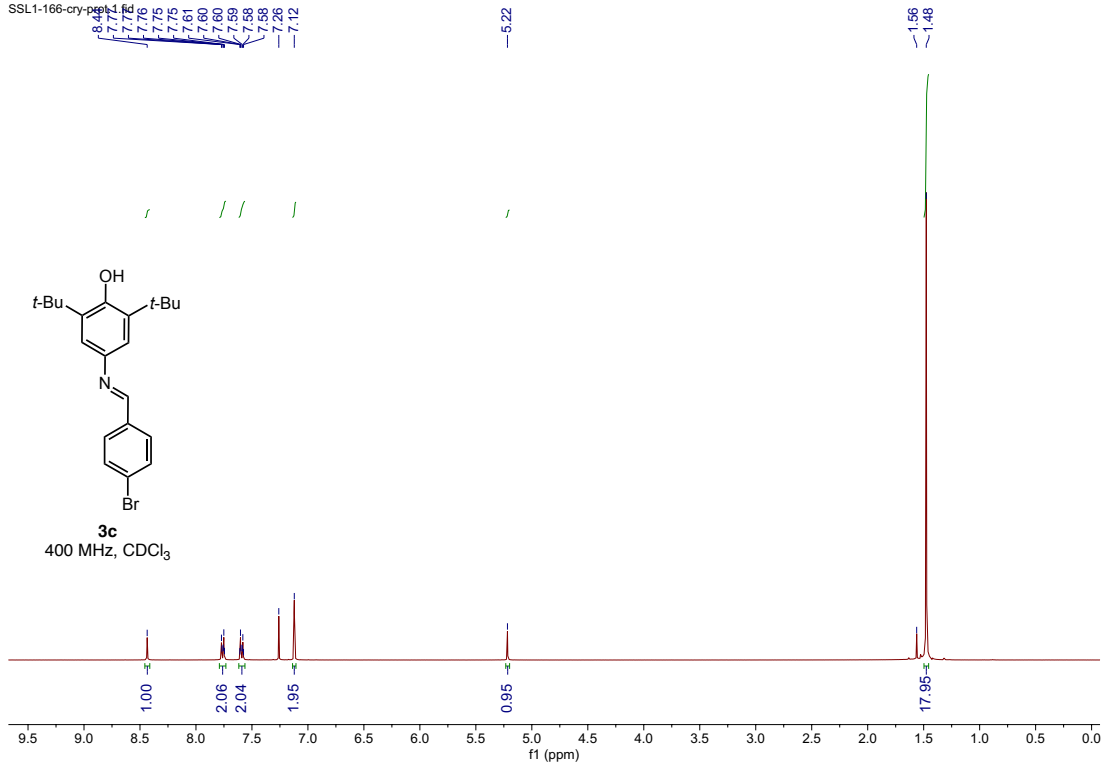
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Br
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400 MHz, CDCl3
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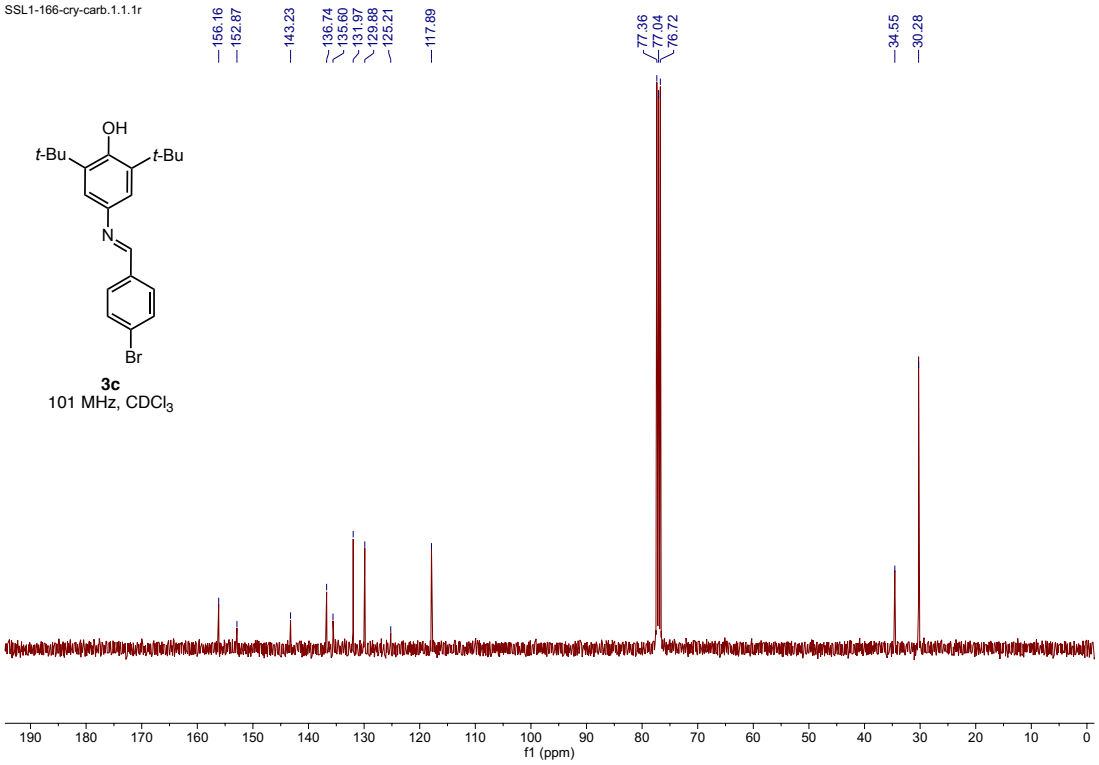
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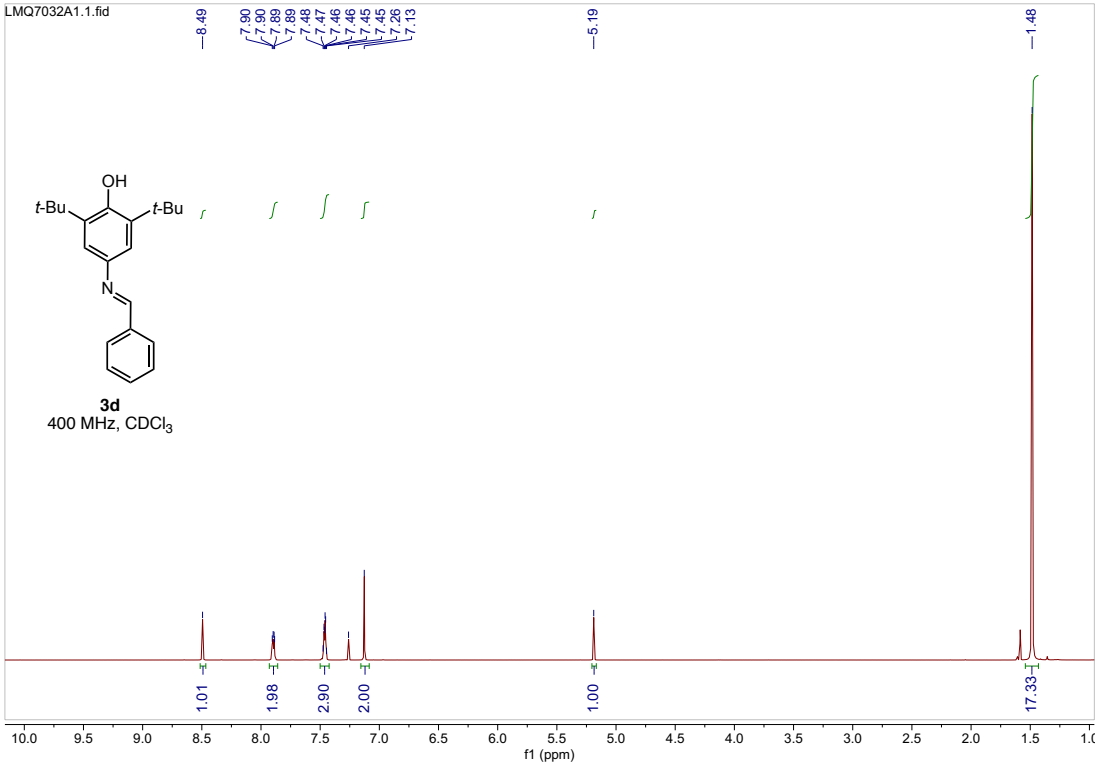
N
Br
3c
101 MHz, CDCl3
f1 (ppm)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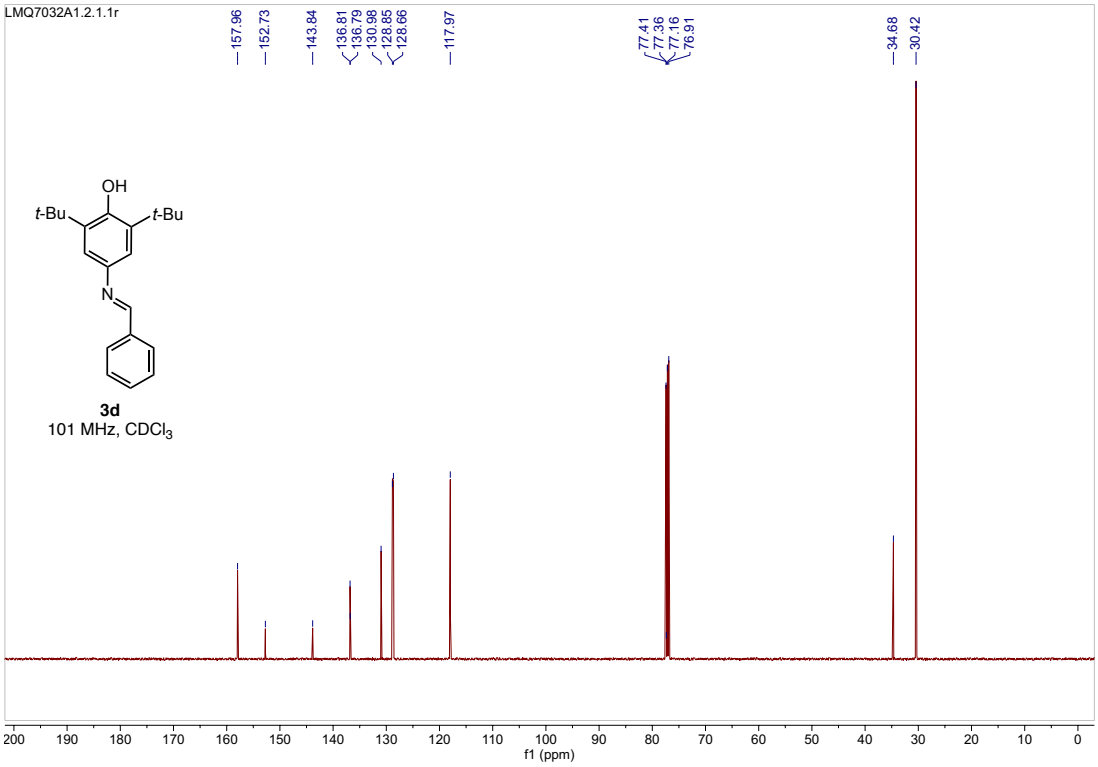
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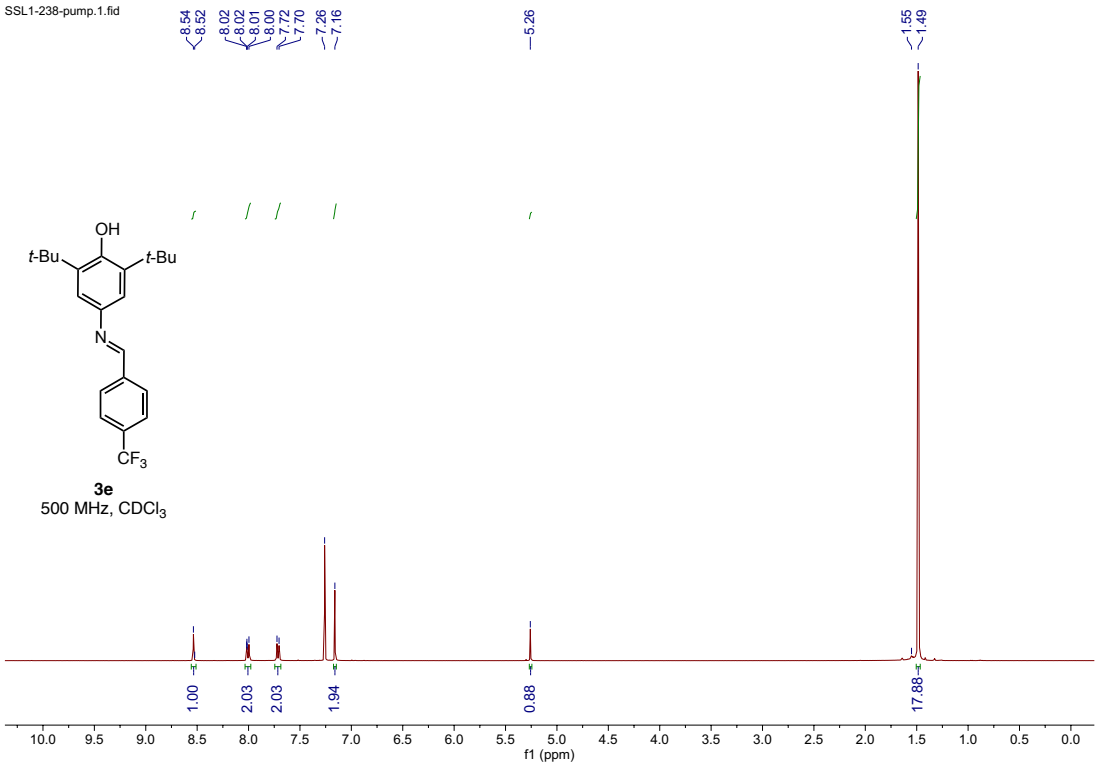
f1 (ppm)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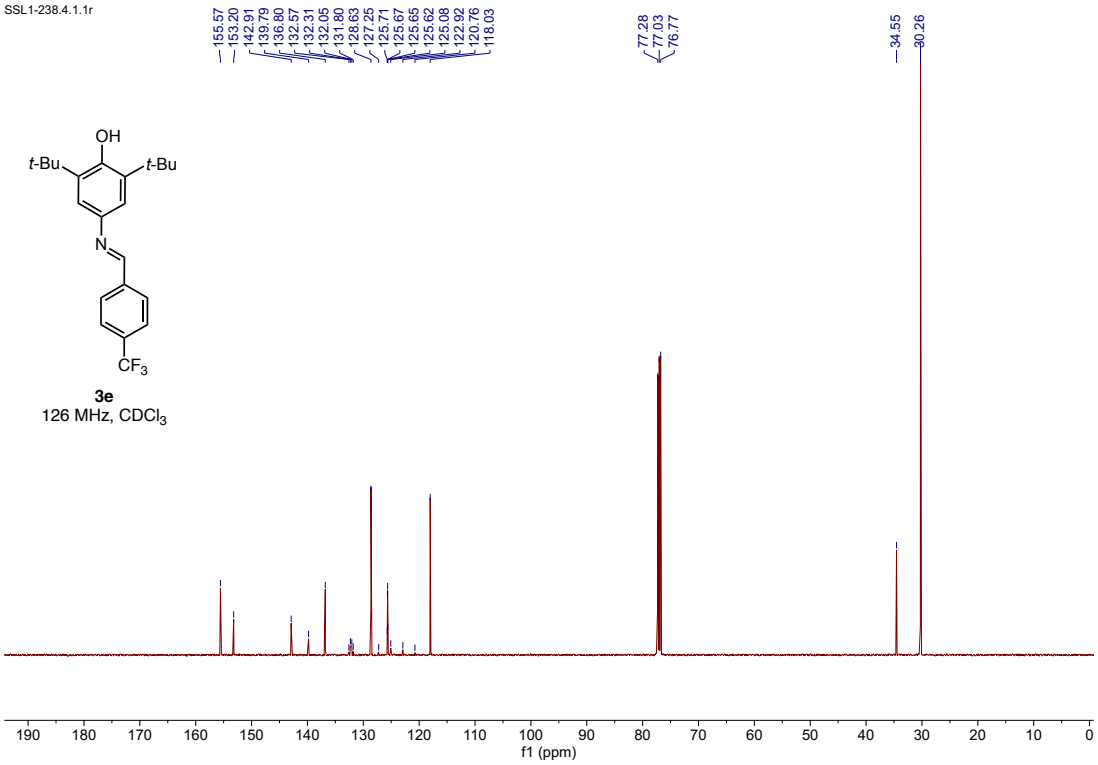
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125.67
125.65
125.62
125.08
122.92
120.76
118.03
77.28
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76.77
34.55
30.26
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t-Bu
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CF3
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126 MHz, CDCl3
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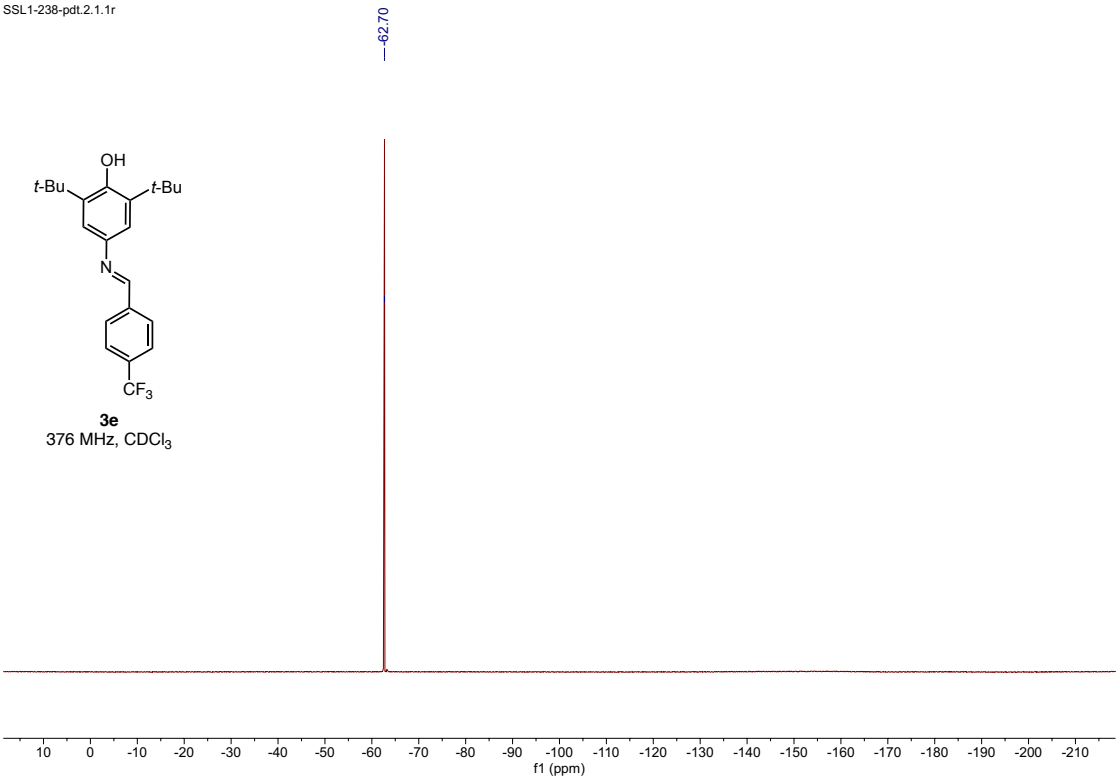
f1 (ppm)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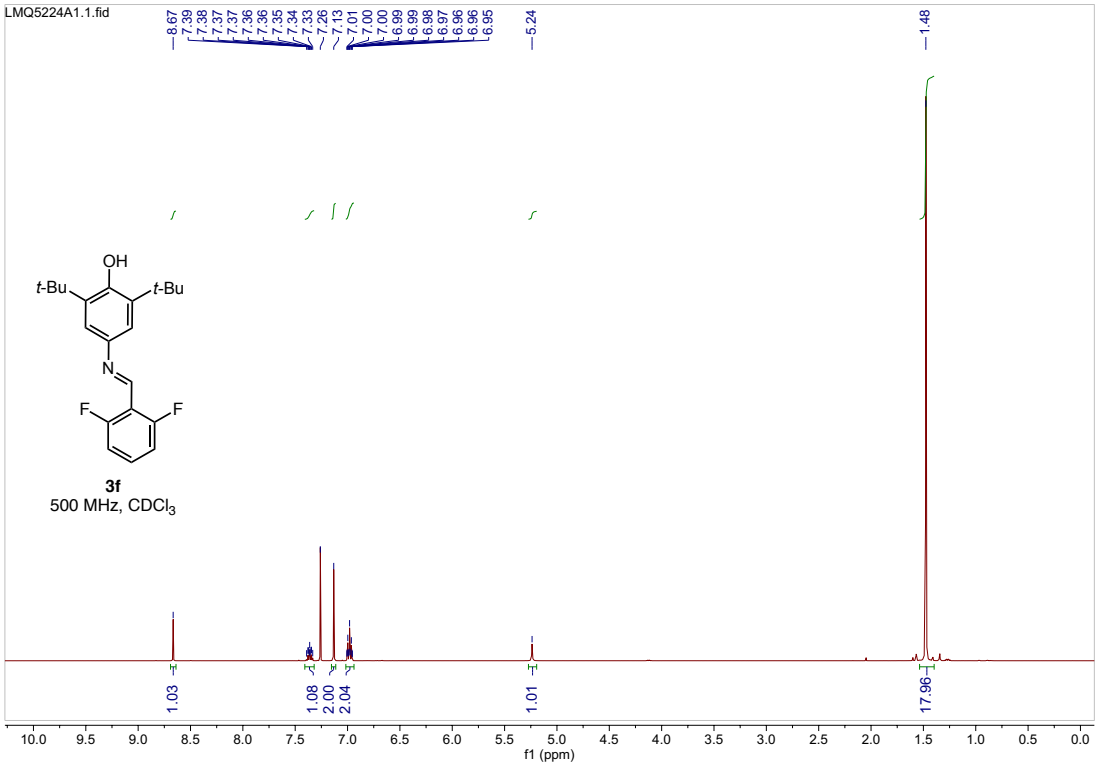
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t-Bu
N
F
F
3f
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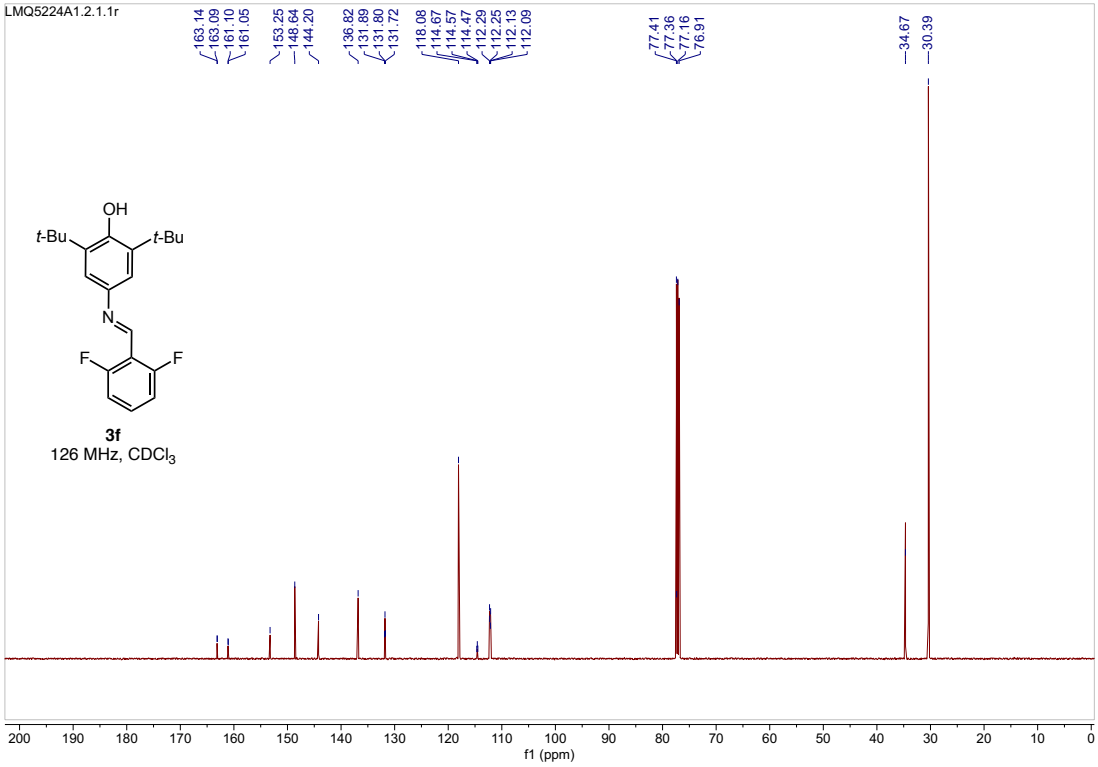
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77.16
76.91
34.67
30.39
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t-Bu
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F
F
3f
126 MHz, CDCl3
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180
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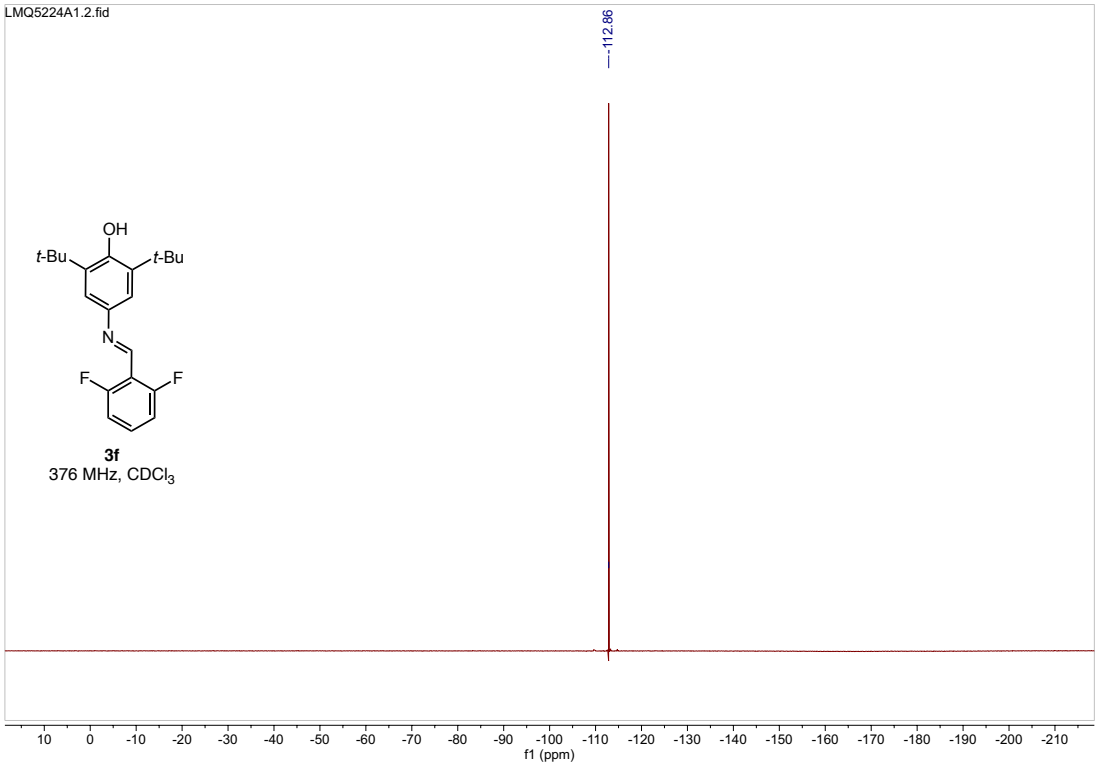
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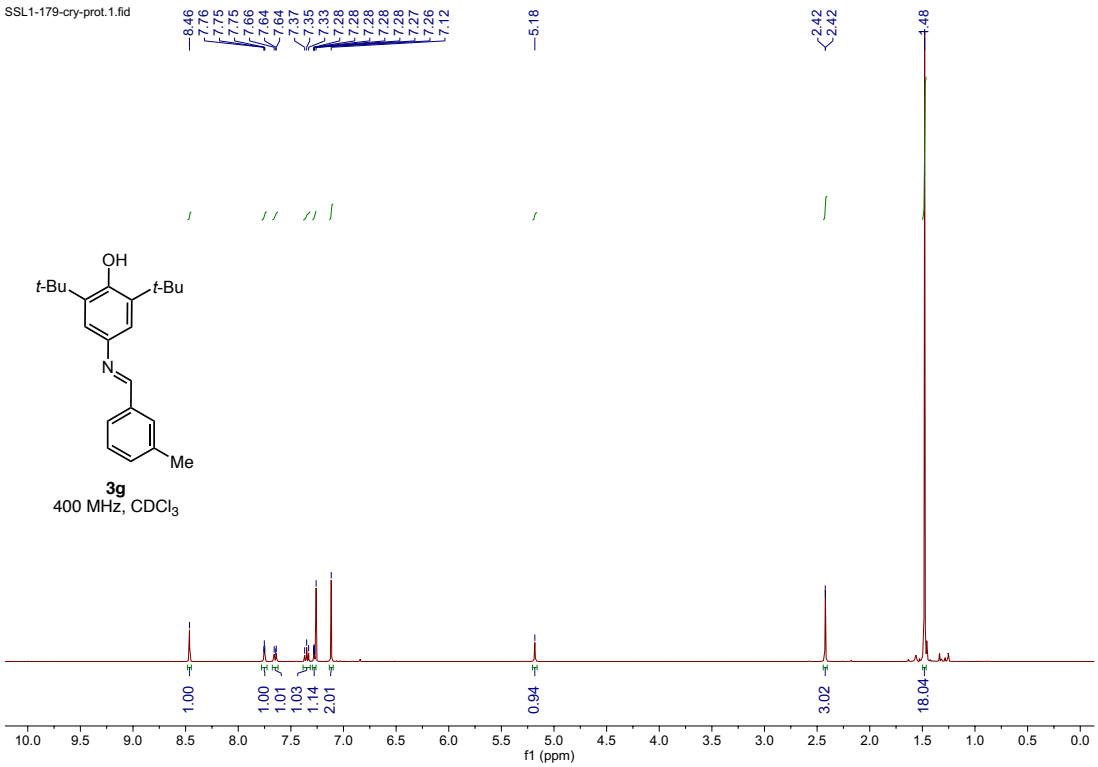
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t-Bu
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10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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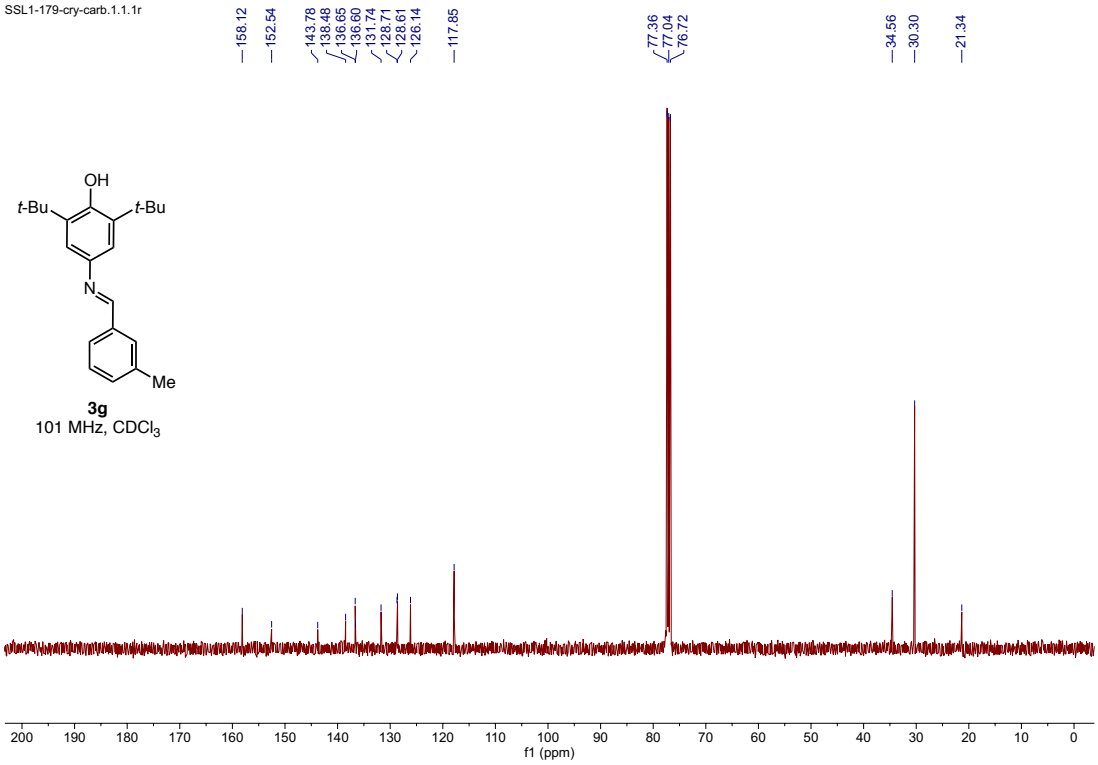
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34.56
30.30
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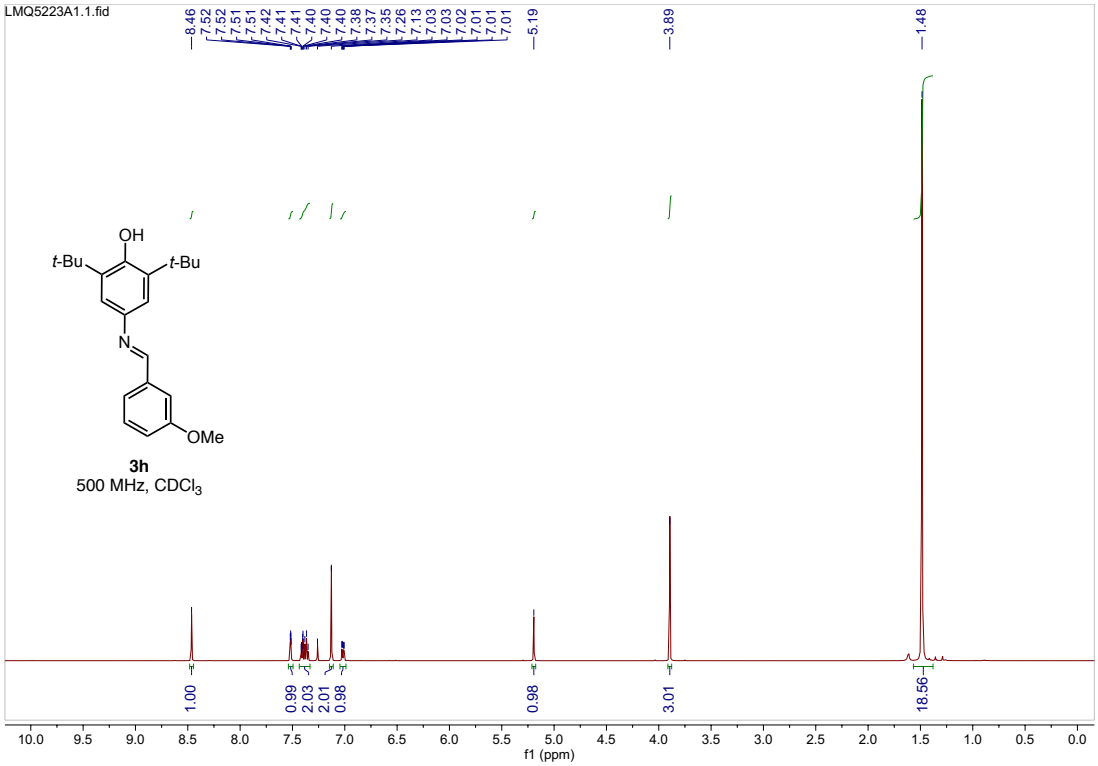
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7.01
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t-Bu
t-Bu
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OMe
3h
500 MHz, CDCl3
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3.01
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10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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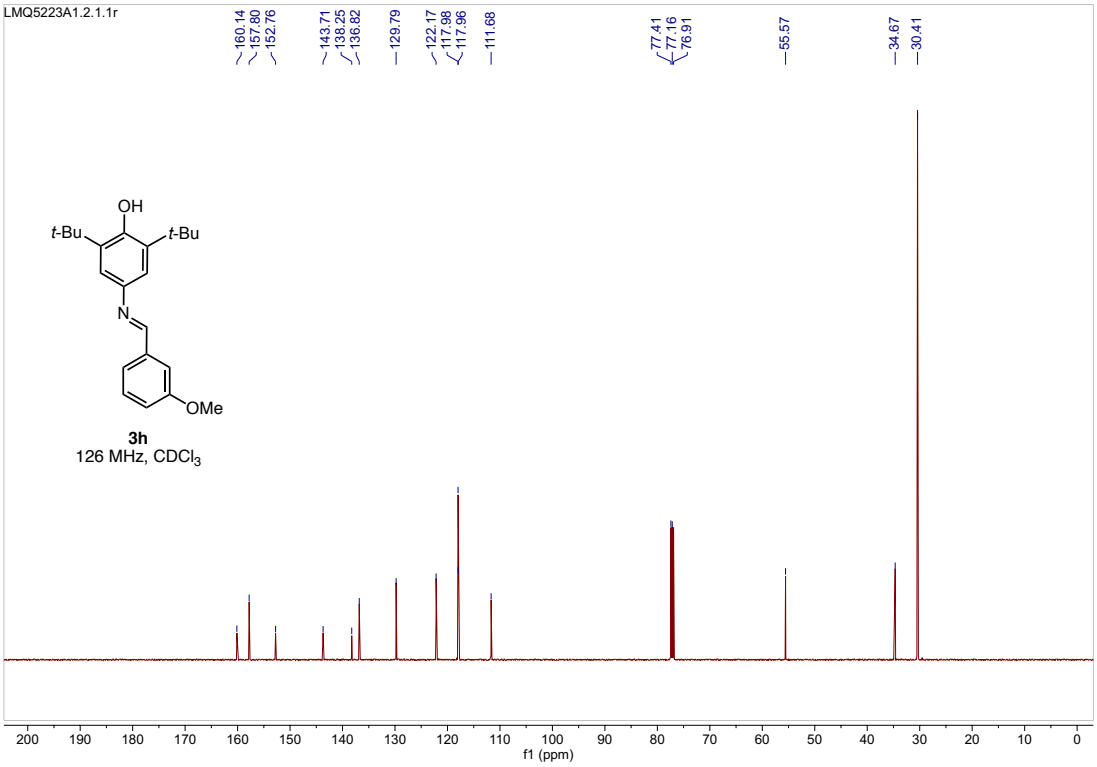
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77.16
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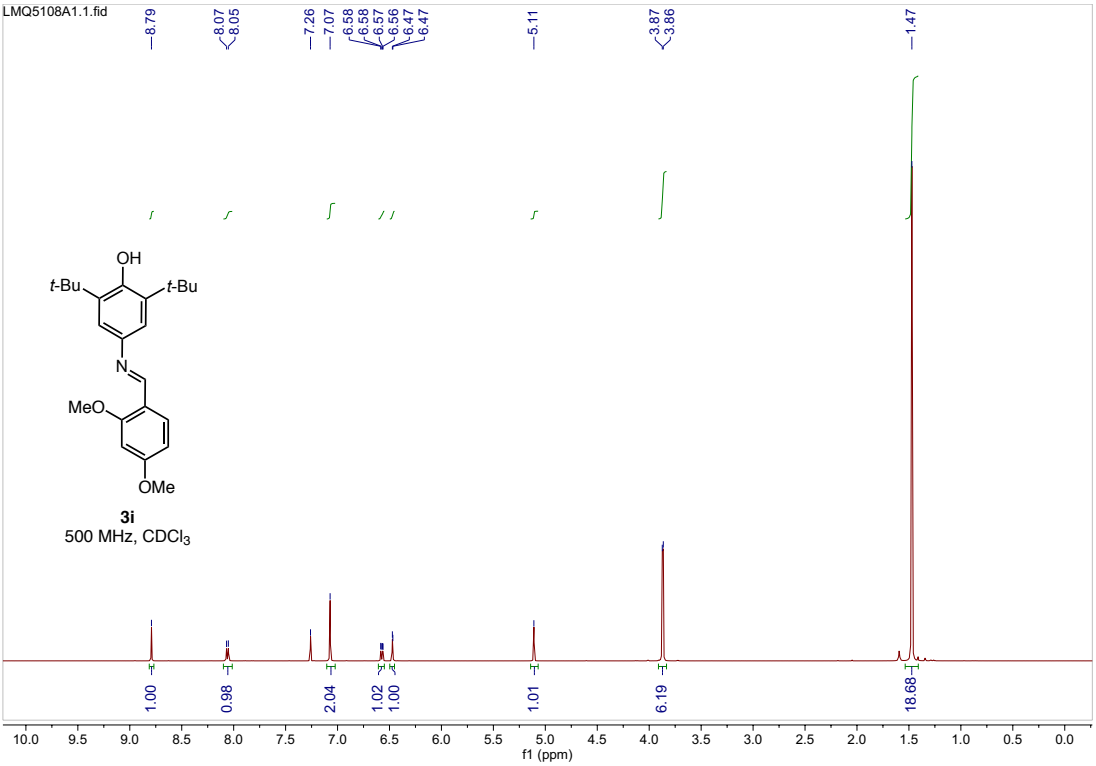
t-Bu
N
OMe
3h
126 MHz, CDCl3
f1 (ppm)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3.86
1.47
OH
t-Bu
t-Bu
N
MeO
OMe
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500 MHz, CDCl3
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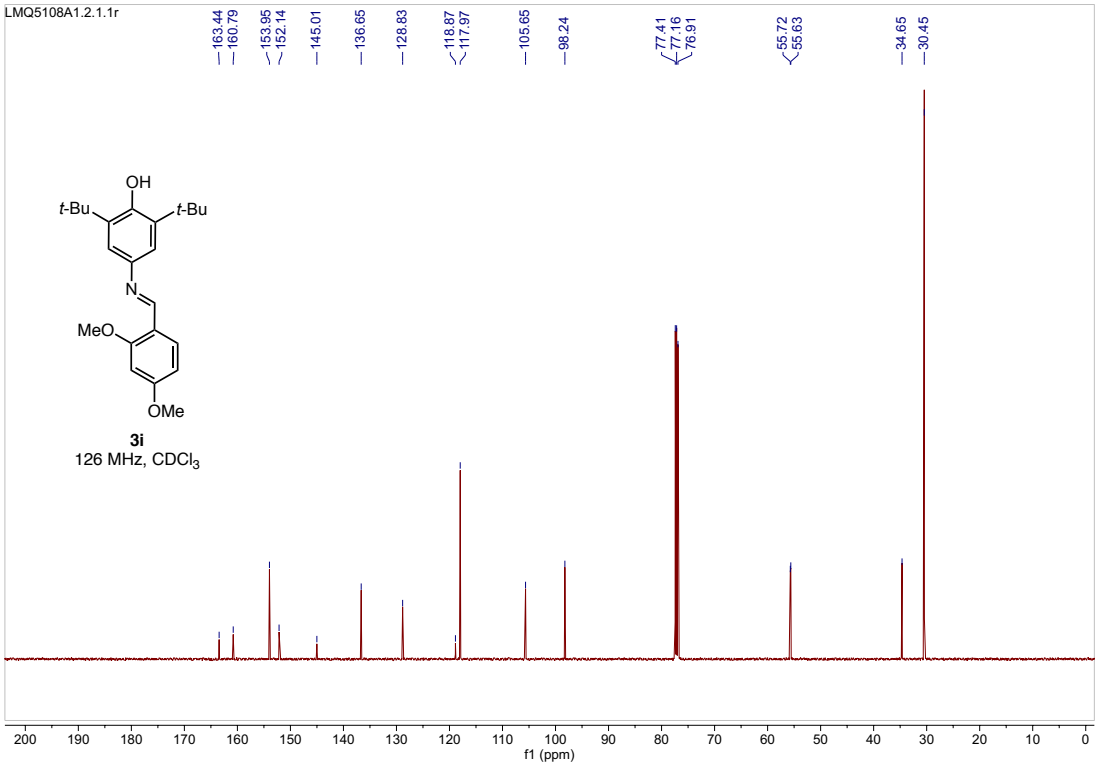
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160.79
153.95
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145.01
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118.87
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77.16
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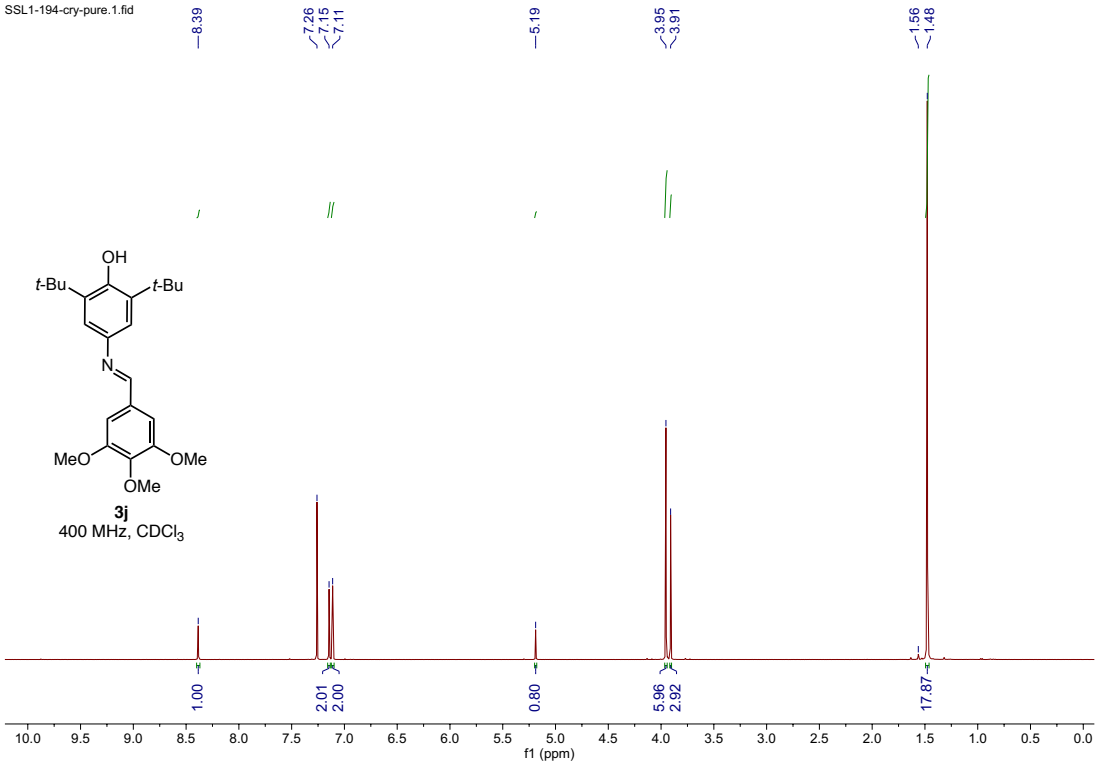
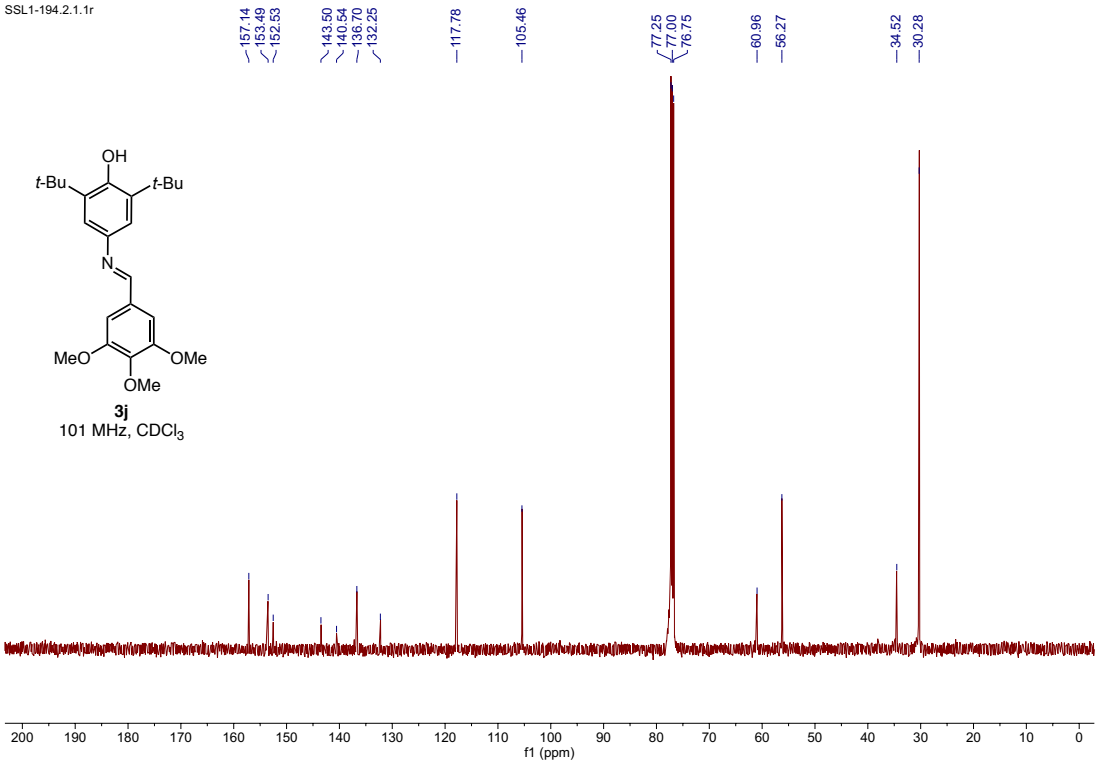
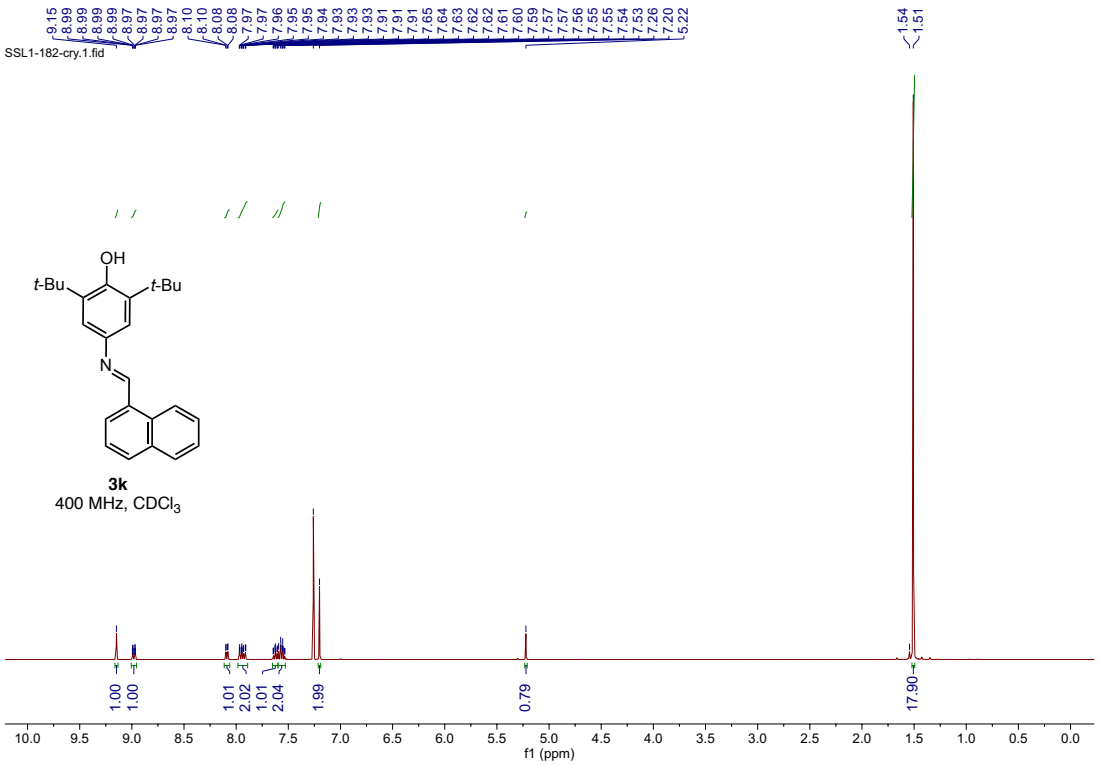
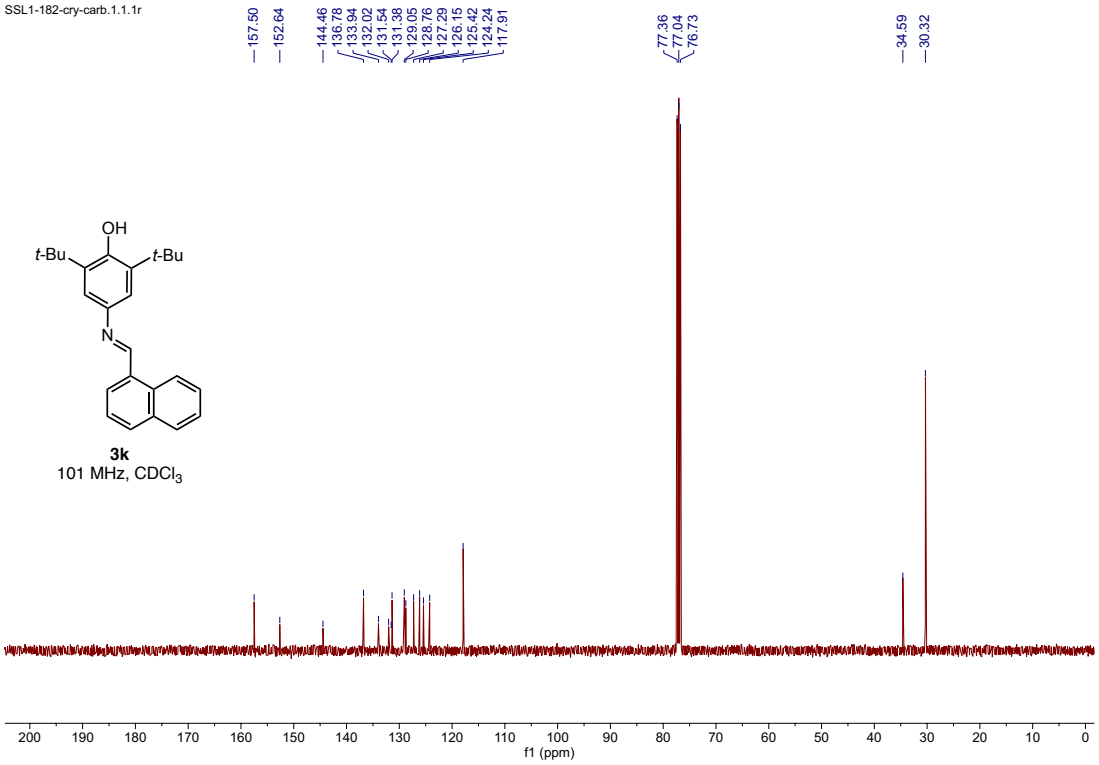
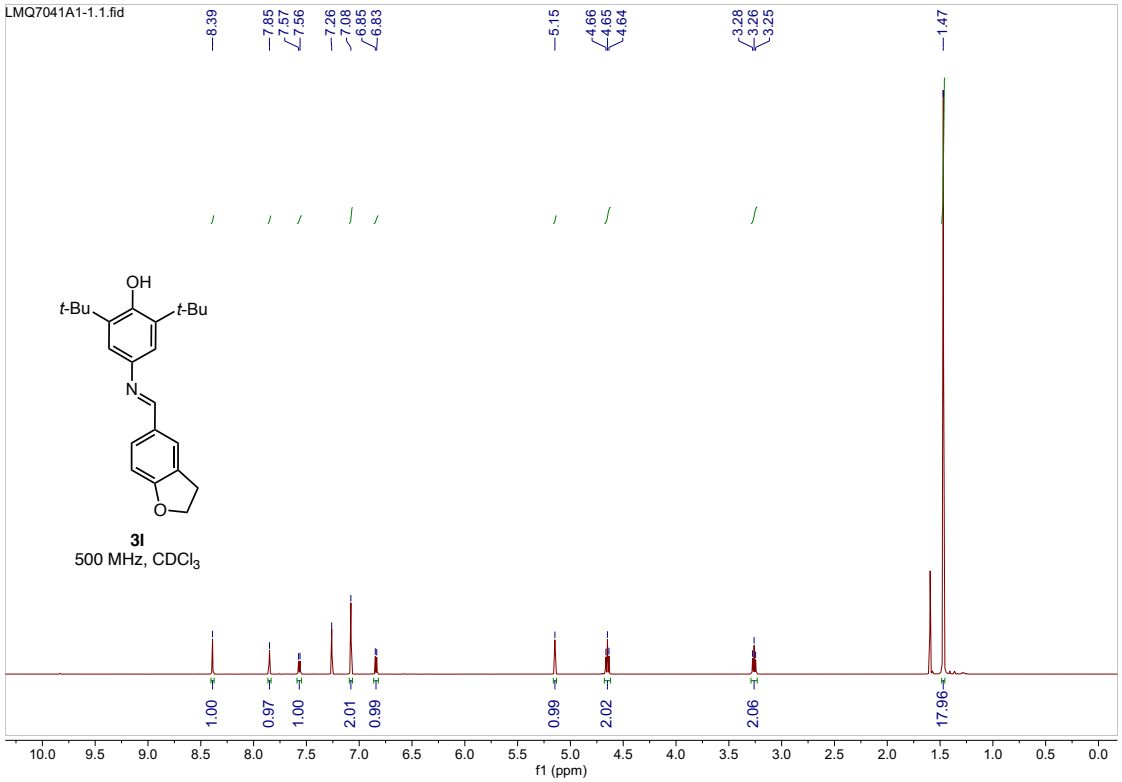
55.72
55.63
34.65
30.45
OH
t-Bu
t-Bu
N
MeO
OMe
3i
126 MHz, CDCl3
f1 (ppm)

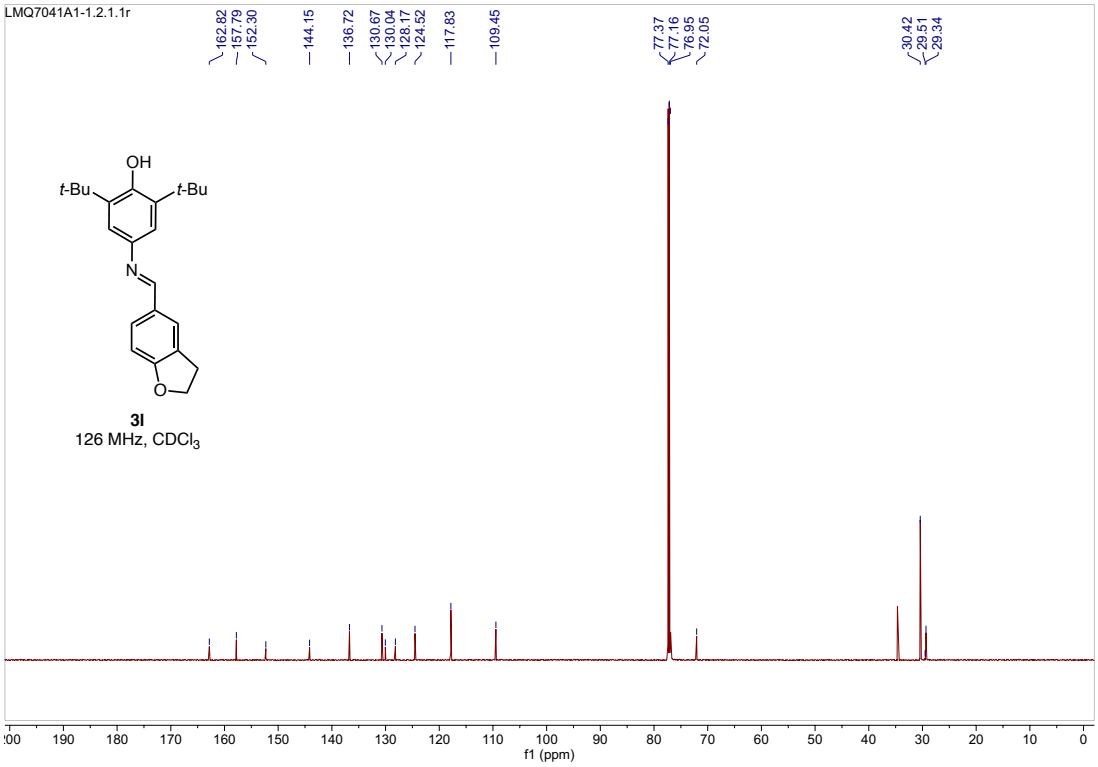

SSL1-194-cry-pure.1.fid
8.39
7.26
7.15
7.11
5.19
3.95
3.91
1.56
1.48
OH
t-Bu
t-Bu
N
MeO
OMe
OMe
3j
400 MHz, CDCl3
1.00
2.01
2.00
0.80
5.96
2.92
17.87
f1 (ppm)

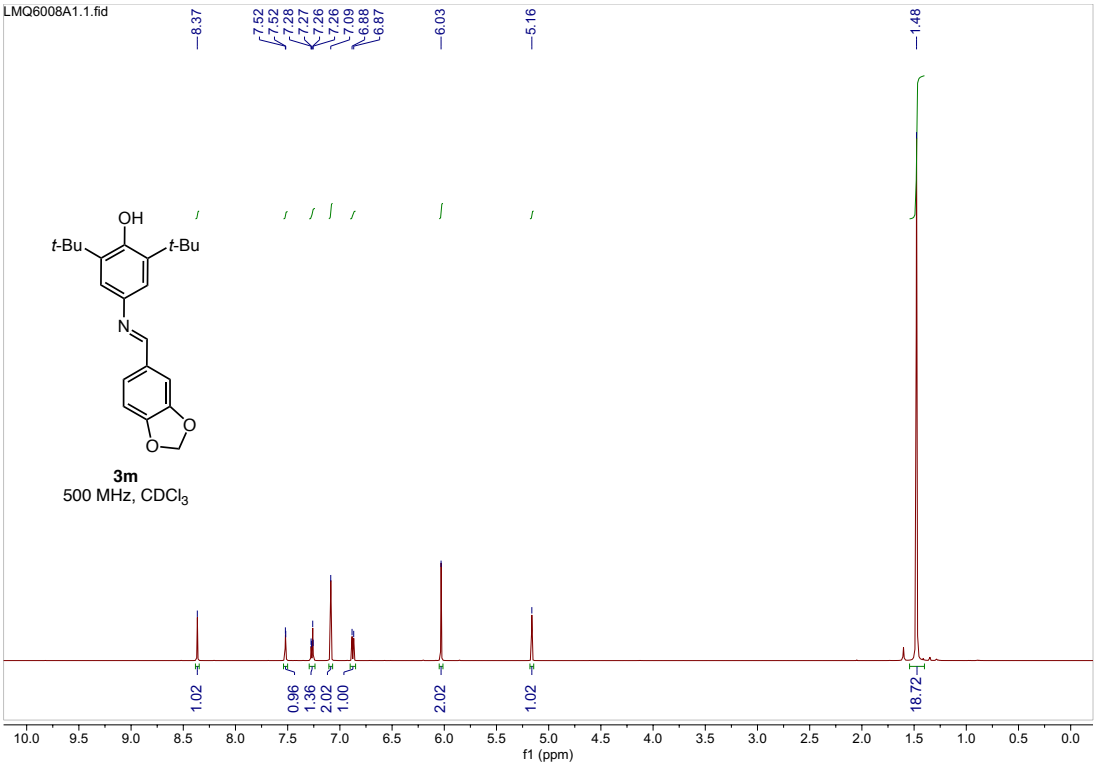

SSL1-194.2.1.1r
157.14
153.49
152.53
143.50
140.54
136.70
132.25
117.78
105.46
77.25
77.00
76.75
60.96
56.27
34.52
30.28
OH
t-Bu
t-Bu
N
MeO
OMe
OMe
3j
101 MHz, CDCl3
f1 (ppm)

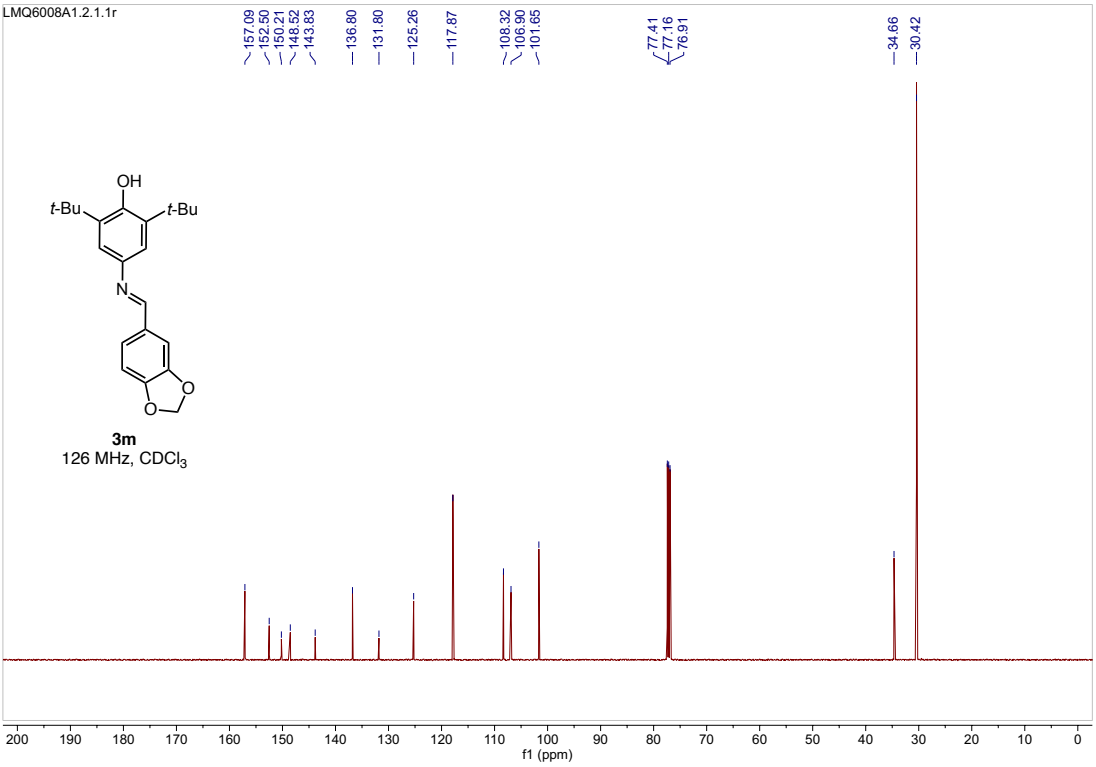

SSL1-182-cry.1.fid
9.15
8.99
8.97
8.10
8.08
7.97
7.96
7.95
7.94
7.93
7.91
7.65
7.64
7.63
7.62
7.61
7.60
7.59
7.57
7.56
7.55
7.54
7.53
7.26
7.20
5.22
1.54
1.51
OH
t-Bu
t-Bu
N
3k
400 MHz, CDCl3
1.00
1.00
1.01
2.02
1.01
2.04
1.99
0.79
17.90
f1 (ppm)

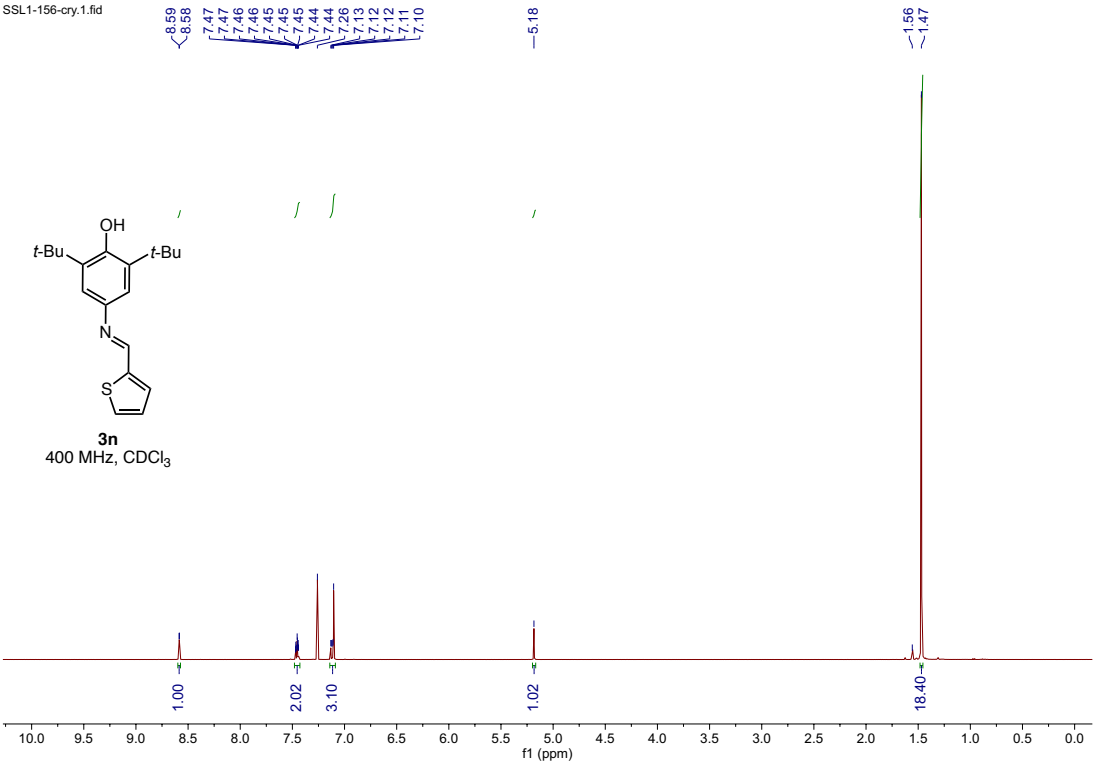

SSL1-182-cry-carb.1.1.1r
157.50
152.64
144.46
136.78
133.94
132.02
131.54
131.38
129.05
128.76
127.29
126.15
125.42
124.24
117.91
77.36
77.04
76.73
34.59
30.32
OH
t-Bu
t-Bu
N
3k
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

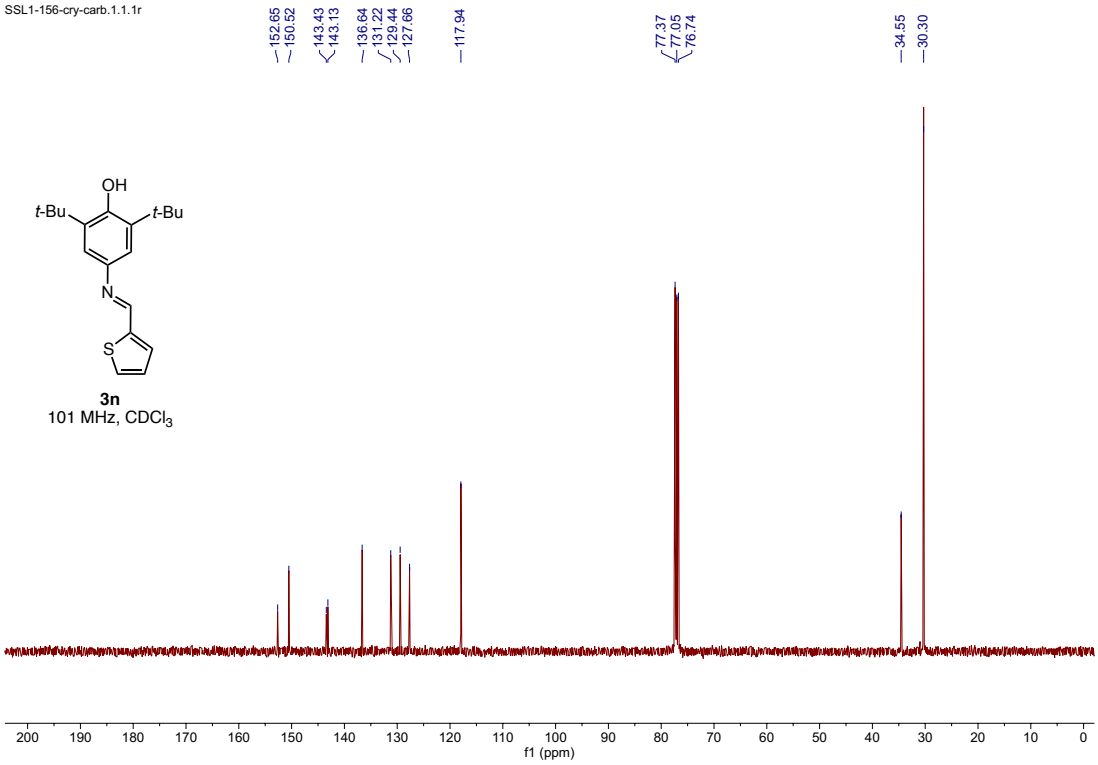

LMQ7041A1-1.1.fid
8.39
7.85
7.57
7.56
7.26
7.08
6.85
6.83
5.15
4.66
4.65
4.64
3.28
3.26
3.25
1.47
OH
t-Bu
t-Bu
N
O
3l
500 MHz, CDCl3
1.00
0.97
1.00
2.01
0.99
0.99
2.02
2.06
17.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

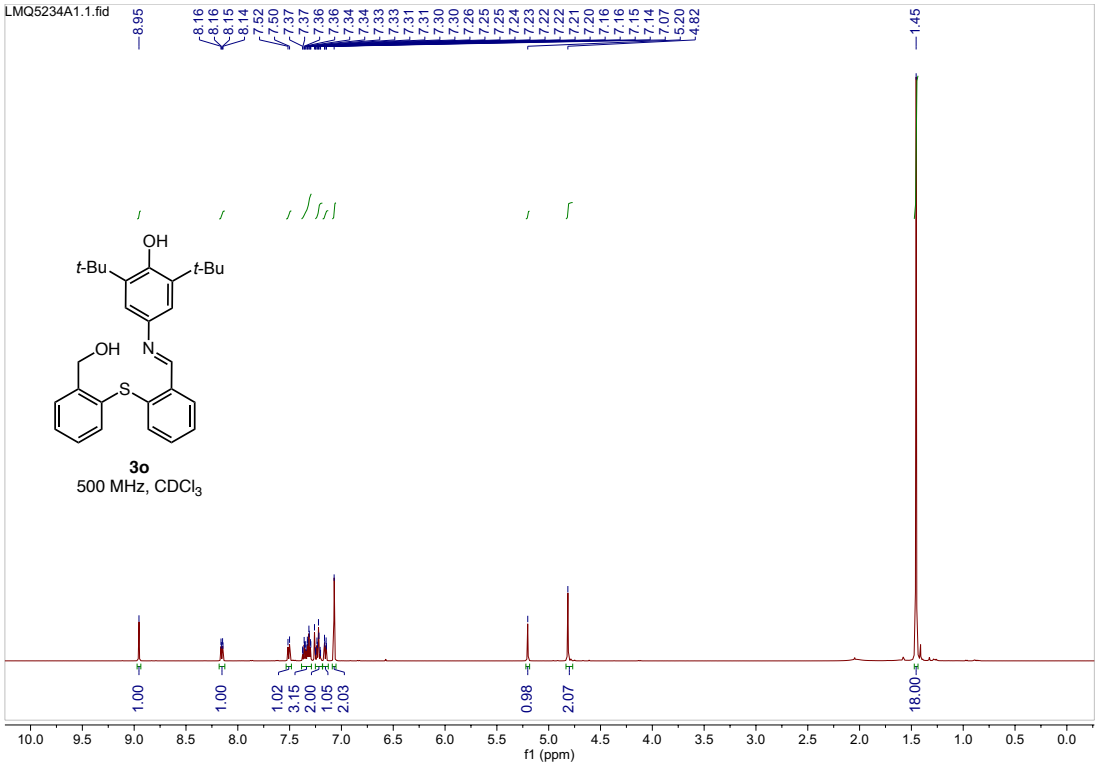

LMQ7041A1-1.2.1.1r
162.82
157.79
152.30
144.15
136.72
130.67
130.04
128.17
124.52
117.83
109.45
77.37
77.16
76.95
72.05
30.42
29.51
29.34
OH
t-Bu
t-Bu
N
O
3l
126 MHz, CDCl3
f1 (ppm)

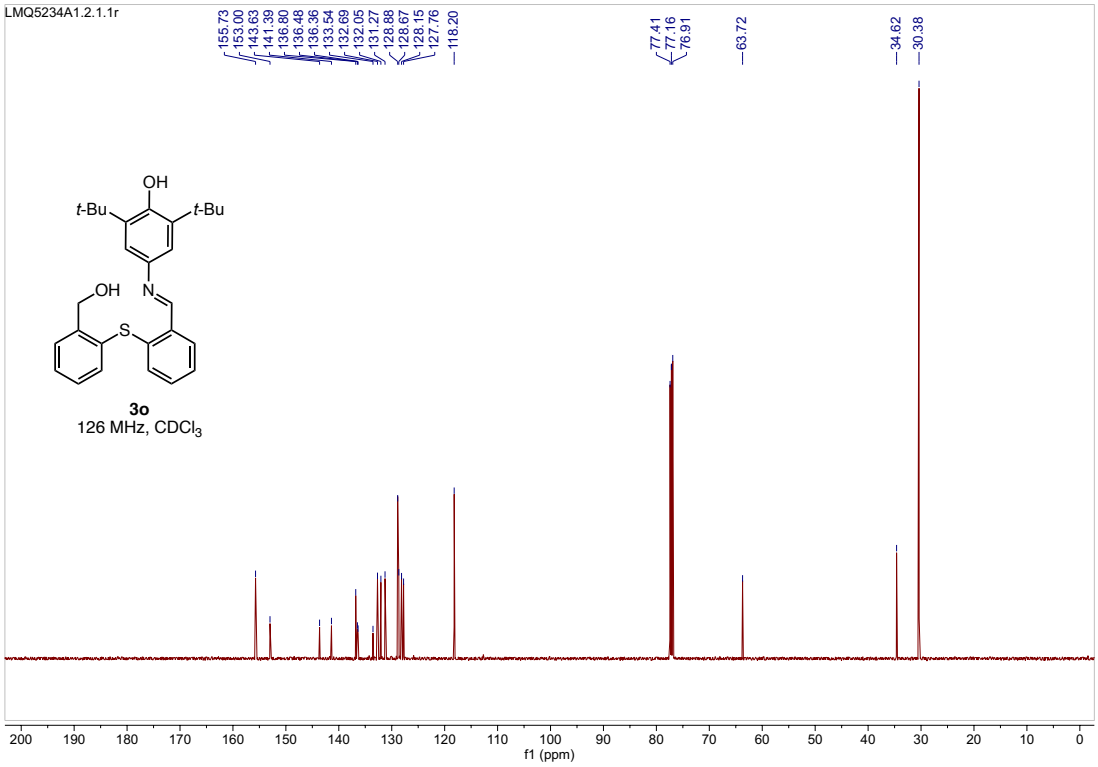

LMQ6008A1.1.fid
8.37
7.52
7.52
7.28
7.27
7.26
7.26
7.09
6.88
6.87
6.03
5.16
1.48
OH
t-Bu
t-Bu
N
O
O
3m
500 MHz, CDCl3
1.02
0.96
1.36
2.02
1.00
2.02
1.02
18.72
f1 (ppm)

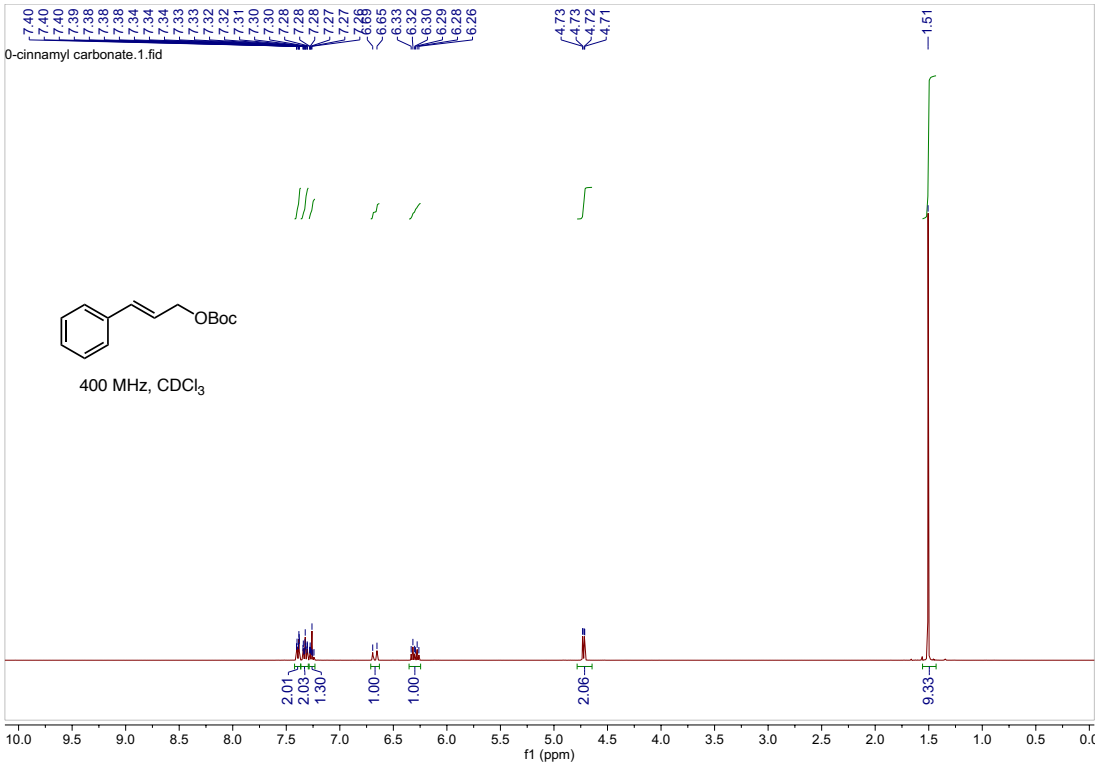

LMQ6008A1.2.1.1r
157.09
152.50
150.21
148.52
143.83
136.80
131.80
125.26
117.87
108.32
106.90
101.65
77.41
77.16
76.91
34.66
30.42
OH
t-Bu
t-Bu
N
O
O
3m
126 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

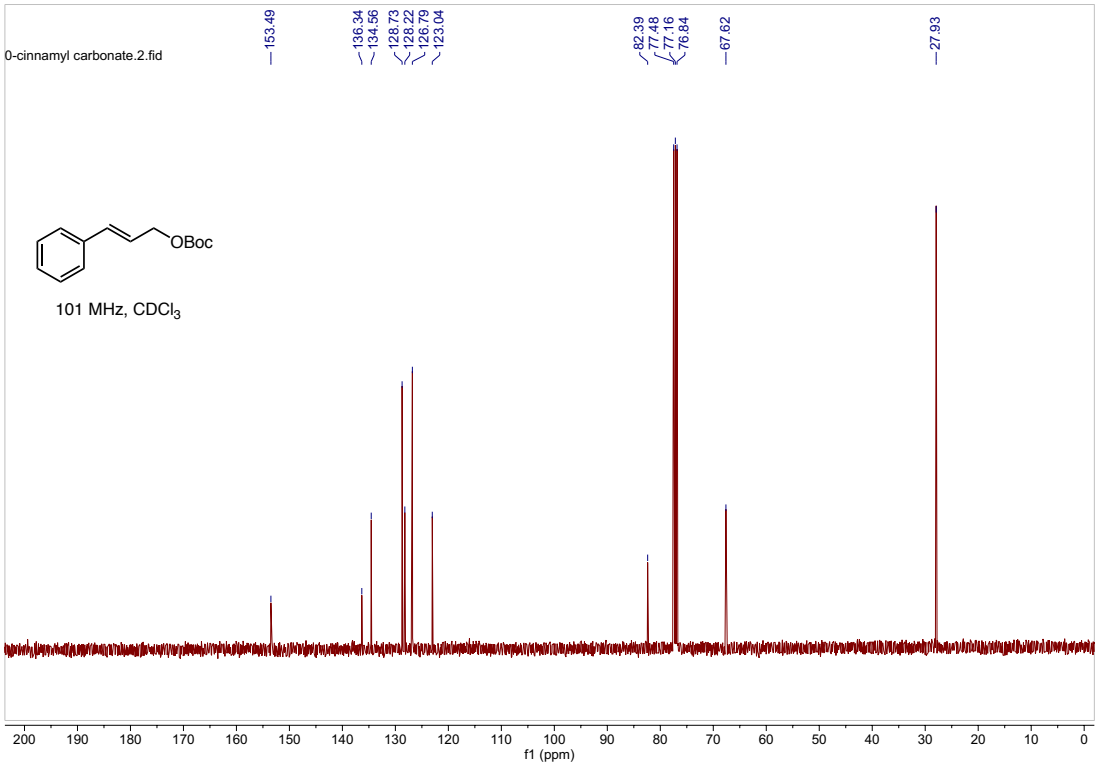

SSL1-156-cry.1.fid
8.59
8.58
7.47
7.47
7.46
7.46
7.45
7.45
7.45
7.44
7.44
7.26
7.13
7.12
7.12
7.11
7.10
5.18
1.56
1.47
OH
t-Bu
t-Bu
N
S
3n
400 MHz, CDCl3
1.00
2.02
3.10
1.02
18.40
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

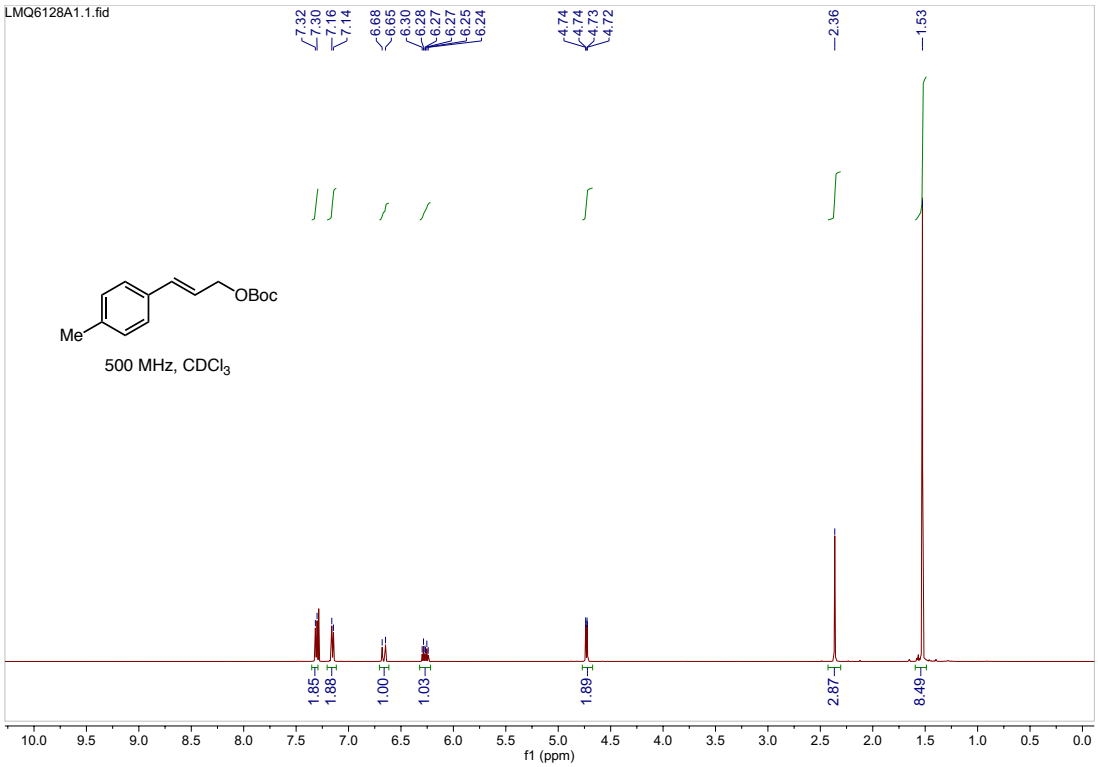

SSL1-156-cry-carb.1.1.1r
152.65
150.52
143.43
143.13
136.64
131.22
129.44
127.66
117.94
77.37
77.05
76.74
34.55
30.30
OH
t-Bu
t-Bu
N
S
3n
101 MHz, CDCl3
f1 (ppm)

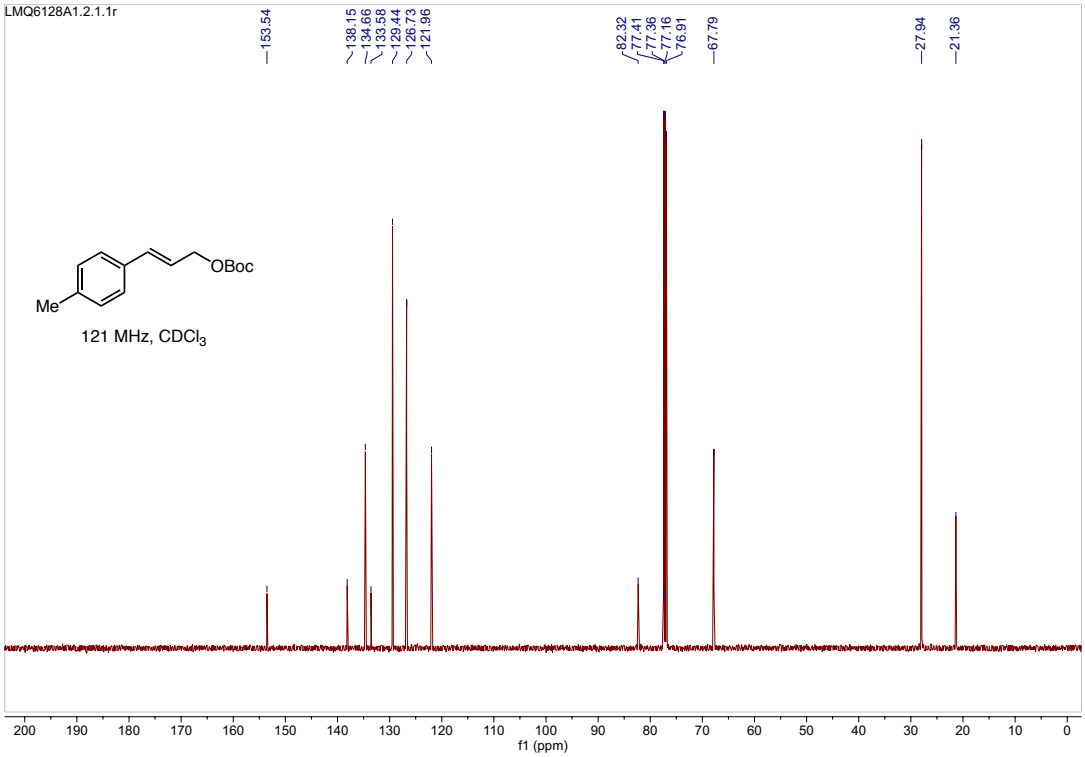

LMQ5234A1.1.fid
8.95
8.16
8.16
8.15
8.14
7.52
7.50
7.37
7.37
7.36
7.36
7.34
7.34
7.33
7.33
7.31
7.31
7.30
7.30
7.26
7.25
7.25
7.24
7.23
7.22
7.22
7.21
7.20
7.16
7.16
7.15
7.14
7.07
5.20
4.82
1.45
OH
t-Bu
t-Bu
OH
N
S
3o
500 MHz, CDCl3
1.00
1.00
1.02
3.15
2.00
1.05
2.03
0.98
2.07
18.00
f1 (ppm)

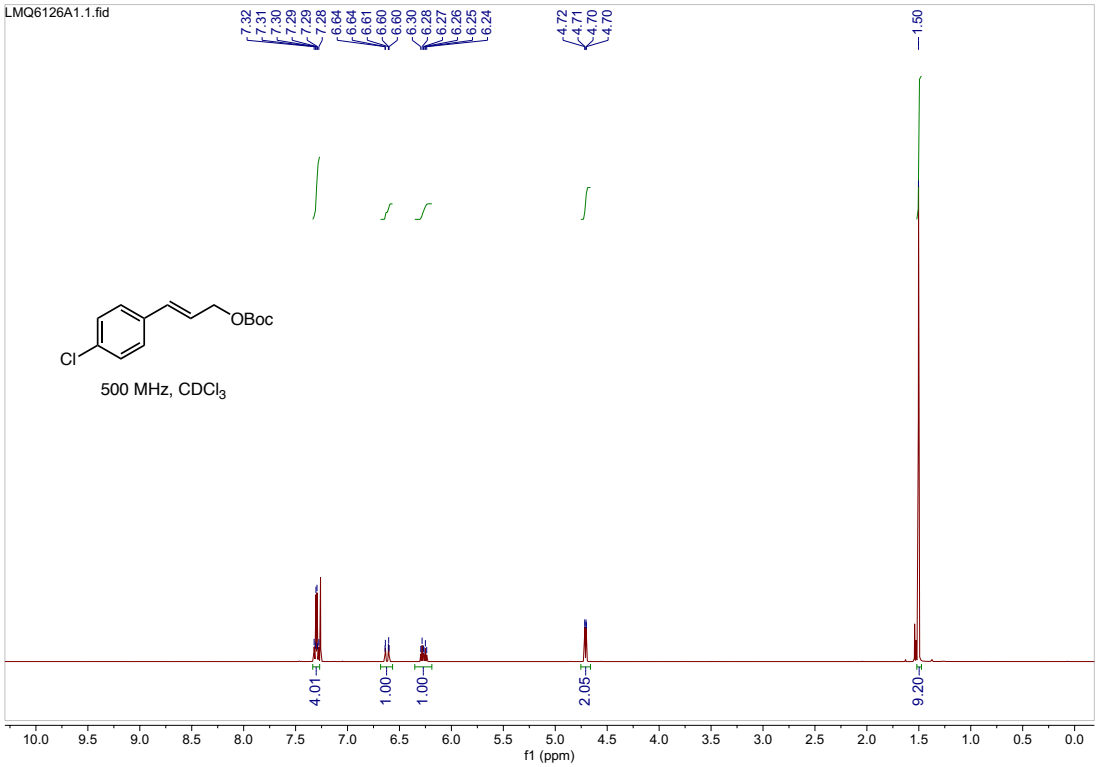

LMQ5234A1.2.1.1r
155.73
153.00
143.63
141.39
136.80
136.48
136.36
133.54
132.69
132.05
131.27
128.88
128.67
128.15
127.76
118.20
77.41
77.16
76.91
63.72
34.62
30.38
OH
t-Bu
t-Bu
OH
N
S
3o
126 MHz, CDCl3
f1 (ppm)

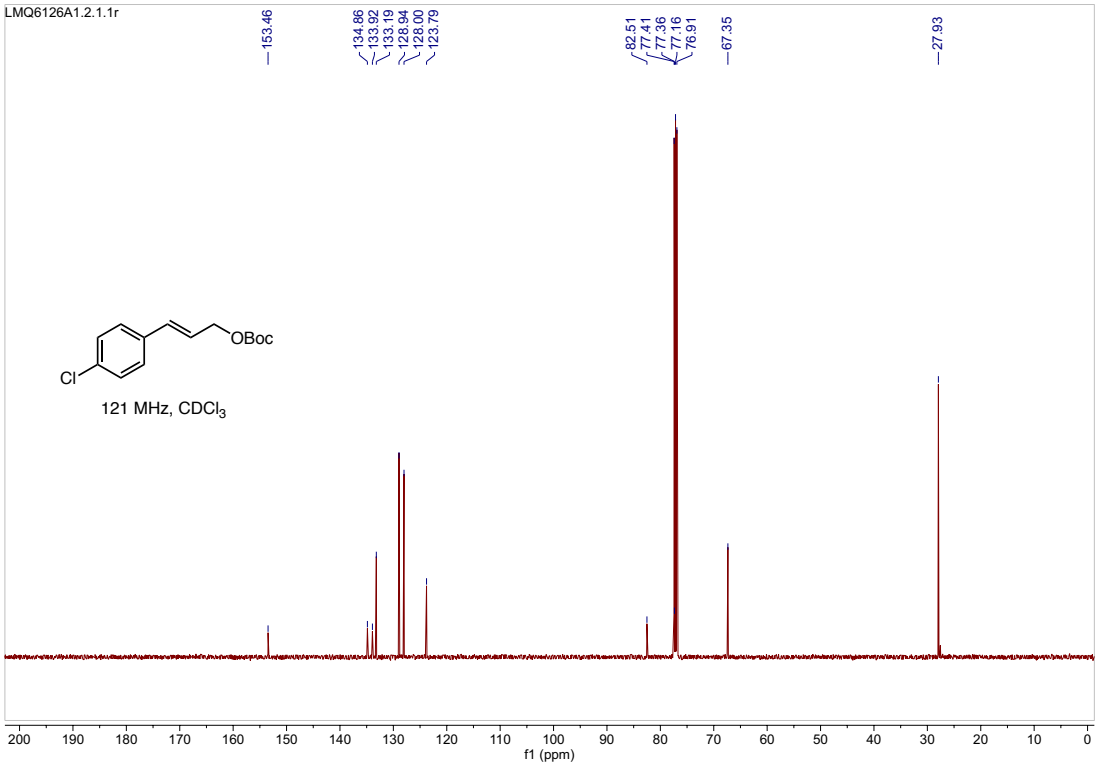

0-cinnamyl carbonate.1.fid
7.40
7.40
7.40
7.39
7.38
7.38
7.38
7.34
7.34
7.34
7.33
7.33
7.32
7.32
7.31
7.30
7.30
7.28
7.28
7.28
7.27
7.27
6.69
6.65
6.33
6.32
6.30
6.29
6.28
6.26
4.73
4.73
4.72
4.71
1.51
OBoc
400 MHz, CDCl3
2.01
2.03
1.30
1.00
1.00
2.06
9.33
f1 (ppm)

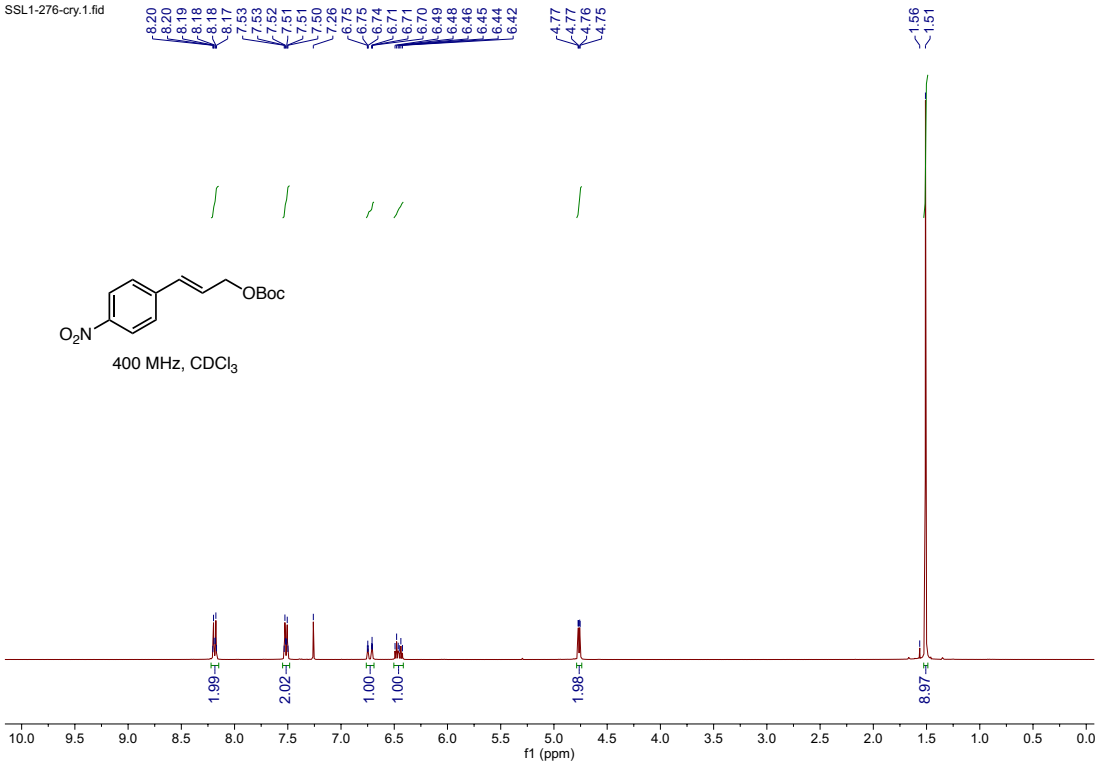

0-cinnamyl carbonate.2.fid
153.49
136.34
134.56
128.73
128.22
126.79
123.04
82.39
77.48
77.16
76.84
67.62
27.93
OBoc
101 MHz, CDCl3
f1 (ppm)

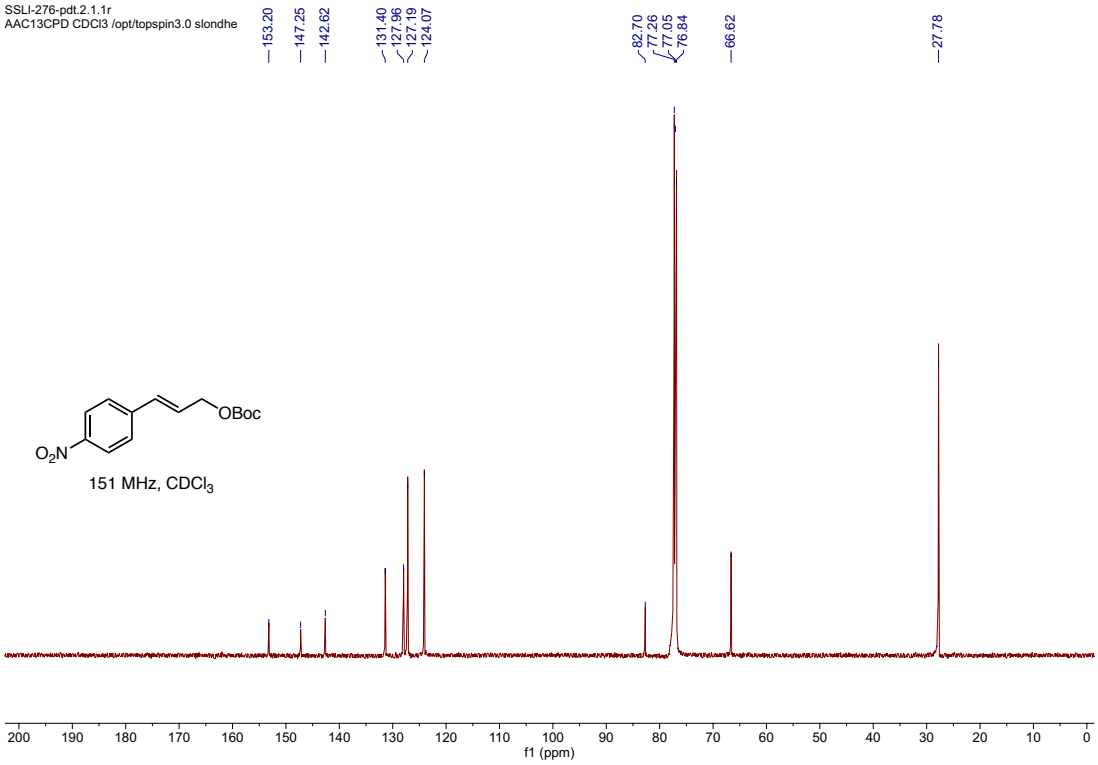

LMQ6128A1.1.fid
7.32
7.30
7.16
7.14
6.68
6.65
6.30
6.28
6.27
6.27
6.25
6.24
4.74
4.74
4.73
4.72
2.36
1.53
OBoc
Me
500 MHz, CDCl3
1.85
1.88
1.00
1.03
1.89
2.87
8.49
f1 (ppm)

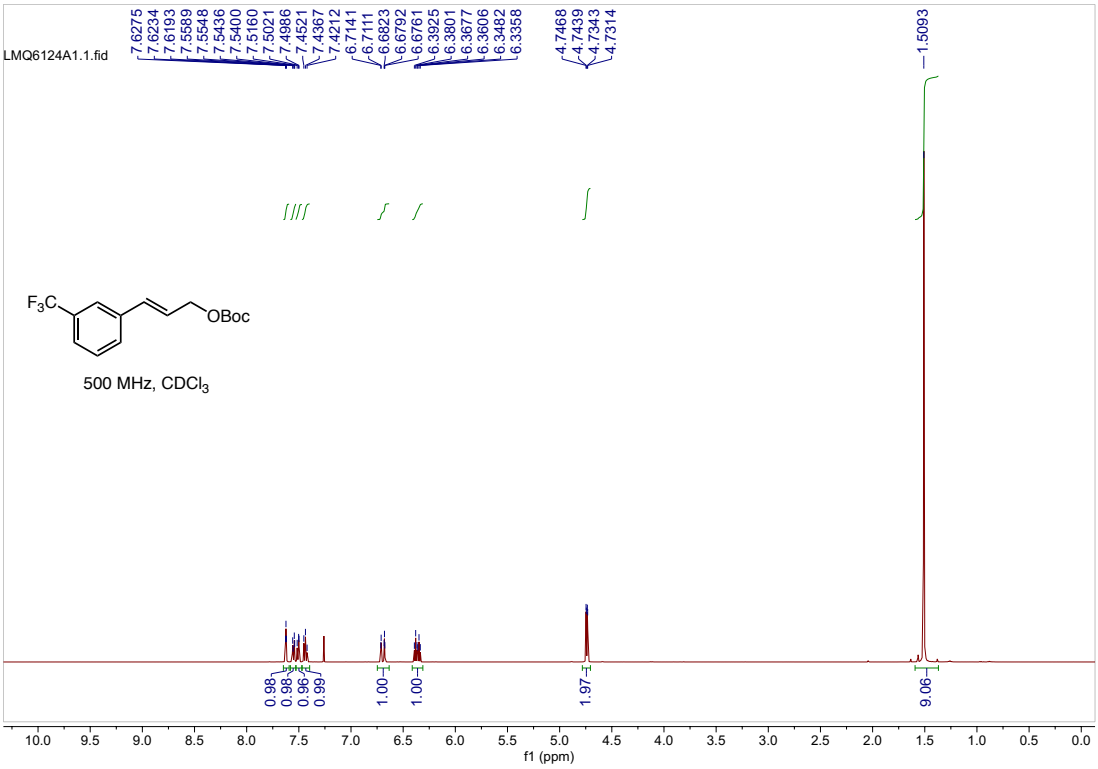

LMQ6128A1.2.1.1r
153.54
138.15
134.66
133.58
129.44
126.73
121.96
82.32
77.41
77.36
77.16
76.91
67.79
27.94
21.36
OBoc
Me
121 MHz, CDCl3
f1 (ppm)

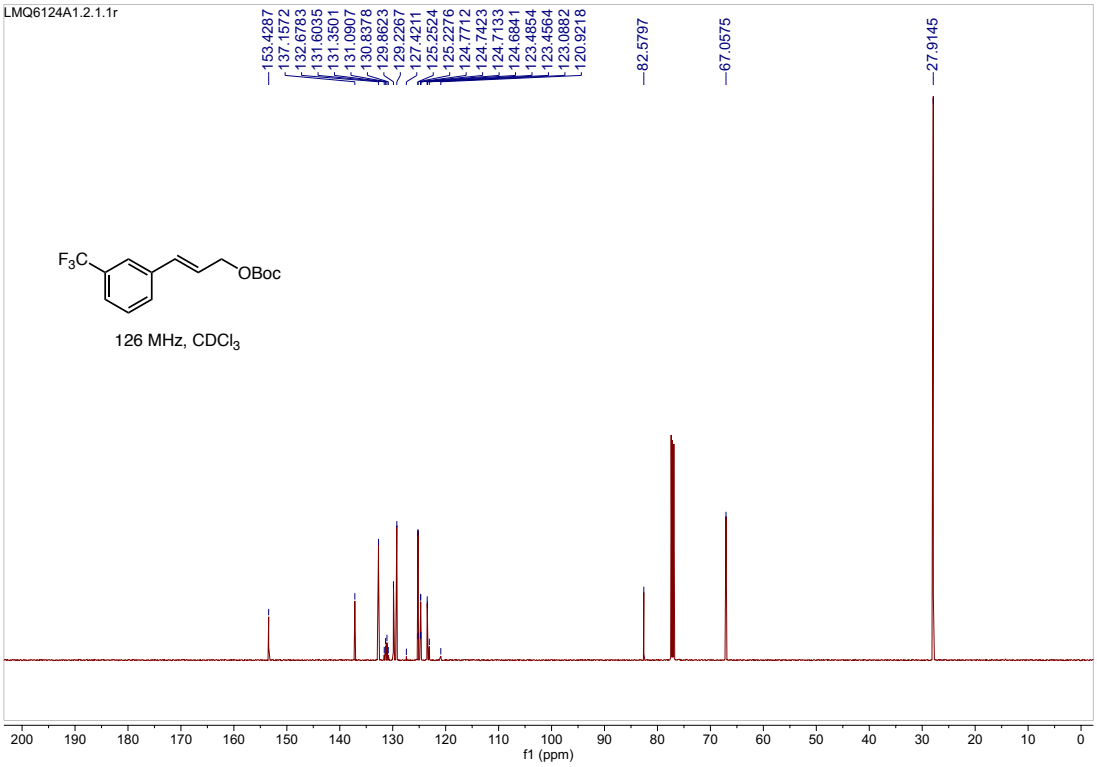

LMQ6126A1.1.fid
7.32
7.31
7.30
7.29
7.29
7.28
6.64
6.64
6.61
6.60
6.60
6.30
6.28
6.27
6.26
6.25
6.24
4.72
4.71
4.70
4.70
1.50
OBoc
Cl
500 MHz, CDCl3
4.01
1.00
1.00
2.05
9.20
f1 (ppm)

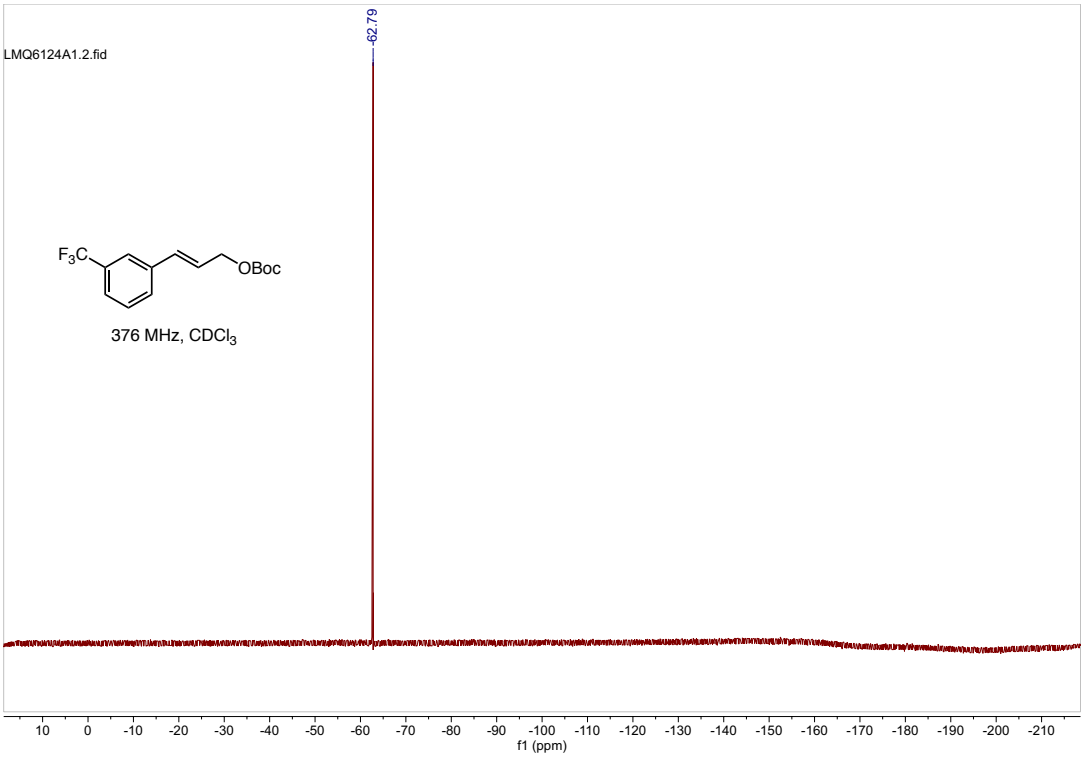

LMQ6126A1.2.1.1r
153.46
134.86
133.92
133.19
128.94
128.00
123.79
82.51
77.41
77.36
77.16
76.91
67.35
27.93
OBoc
Cl
121 MHz, CDCl3
f1 (ppm)

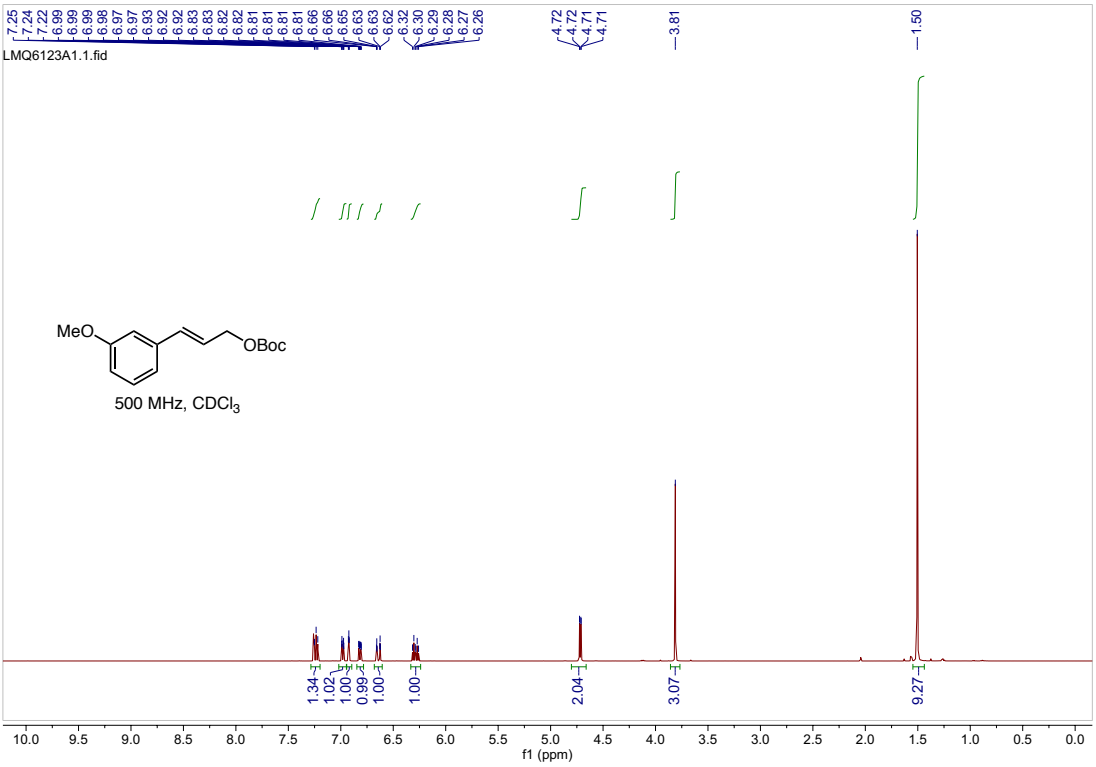

SSL1-276-cry.1.fid
8.20
8.20
8.19
8.18
8.18
8.17
7.53
7.53
7.52
7.51
7.51
7.50
7.26
6.75
6.75
6.74
6.71
6.71
6.70
6.49
6.48
6.46
6.45
6.44
6.42
4.77
4.77
4.76
4.75
1.56
1.51
OBoc
O2N
400 MHz, CDCl3
1.99
2.02
1.00
1.00
1.98
8.97
f1 (ppm)

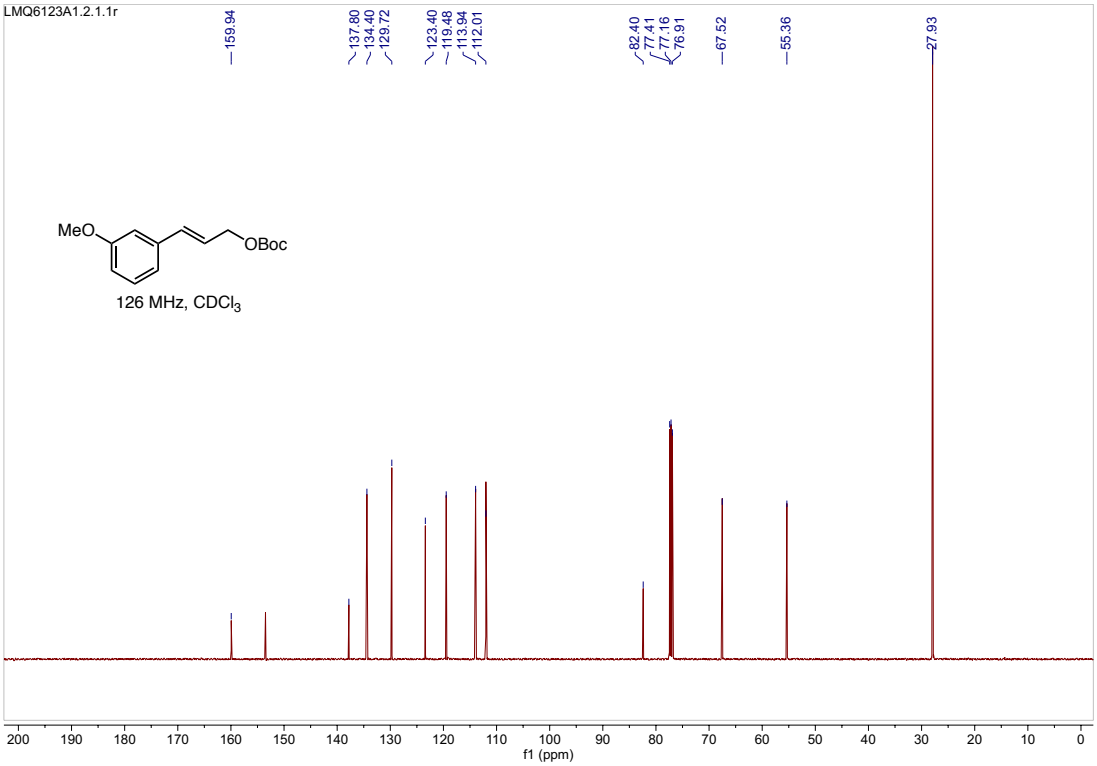

SSLI-276-pdt.2.1.1r
AAC13CPD CDCl3 /opt/topspin3.0 slondhe
153.20
147.25
142.62
131.40
127.96
127.19
124.07
82.70
77.26
77.05
76.84
66.62
27.78
OBoc
O2N
151 MHz, CDCl3
f1 (ppm)

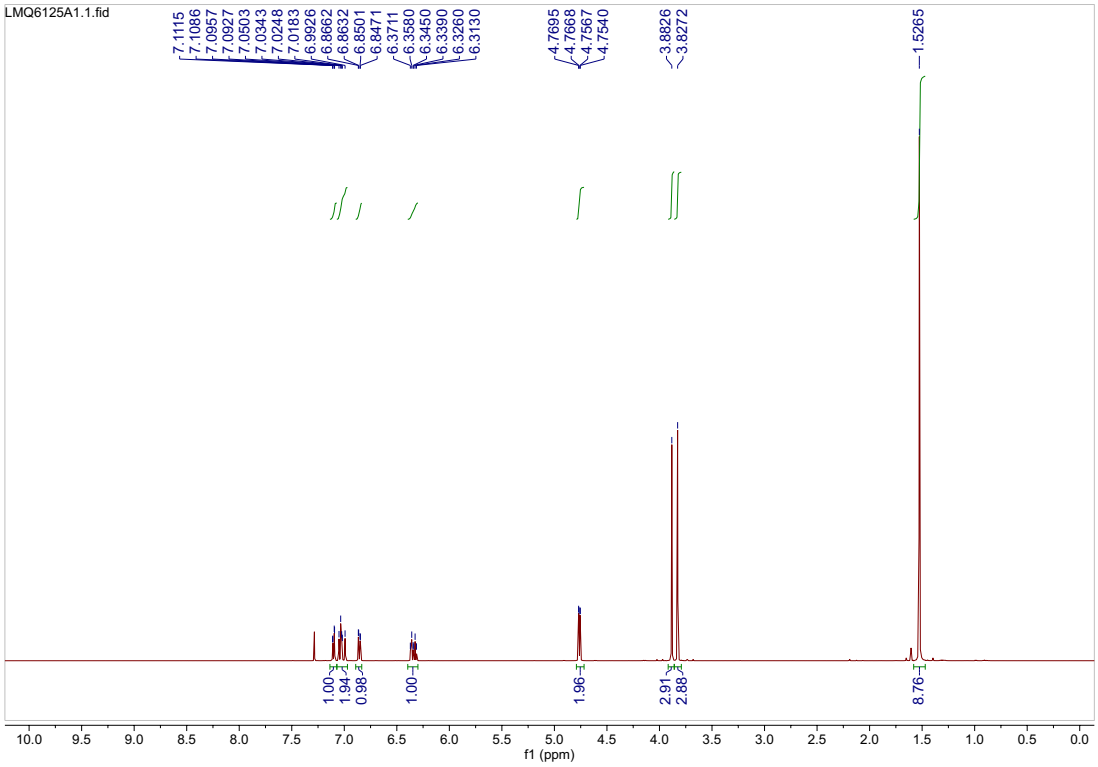

LMQ6124A1.1.fid
7.6275
7.6234
7.6193
7.5589
7.5548
7.5436
7.5400
7.5160
7.5021
7.4986
7.4521
7.4367
7.4212
6.7141
6.7111
6.6823
6.6792
6.6761
6.3925
6.3801
6.3677
6.3606
6.3482
6.3358
4.7468
4.7439
4.7343
4.7314
1.5093
F3C
OBoc
500 MHz, CDCl3
0.98
0.98
0.96
0.99
1.00
1.00
1.97
9.06
f1 (ppm)

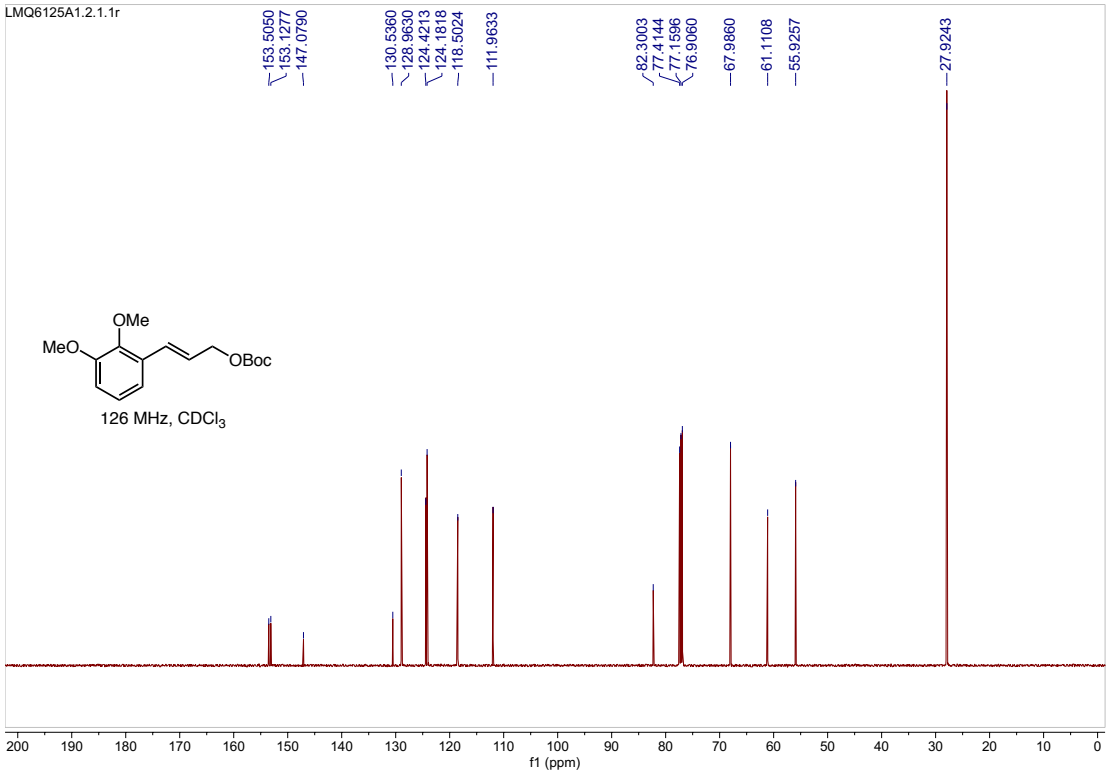

LMQ6124A1.2.1.1r
153.4287
137.1572
132.6783
131.6035
131.3501
131.0907
130.8378
129.8623
129.2267
127.4211
125.2524
125.2276
124.7712
124.7423
124.7133
124.6841
123.4854
123.4564
123.0882
120.9218
82.5797
67.0575
27.9145
F3C
OBoc
126 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

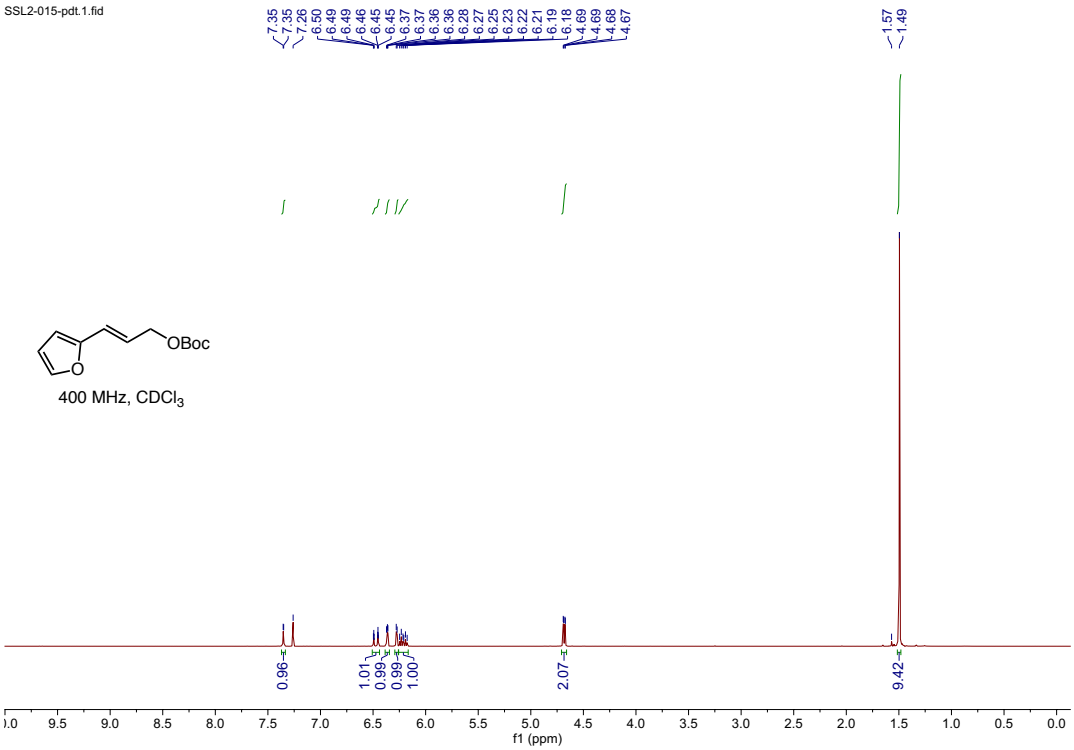

LMQ6124A1.2.fid
-62.79
F3C
OBoc
376 MHz, CDCl3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

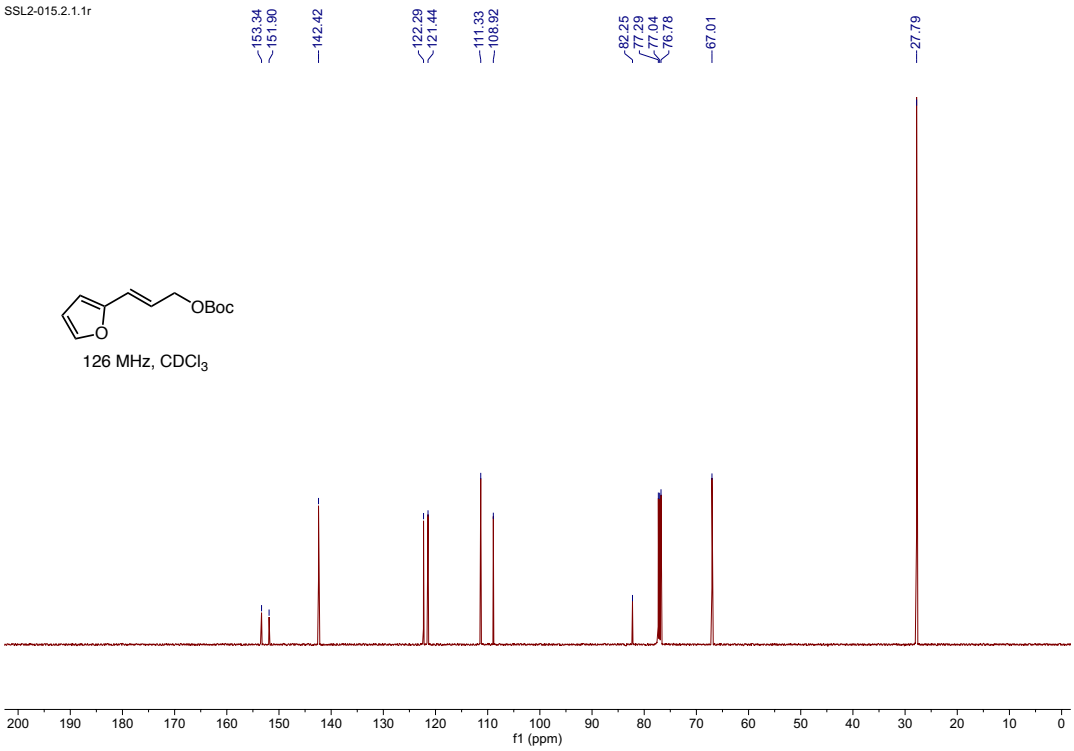

LMQ6123A1.1.fid
7.25
7.24
7.22
6.99
6.99
6.99
6.98
6.97
6.97
6.93
6.92
6.83
6.83
6.82
6.82
6.81
6.81
6.81
6.81
6.66
6.66
6.65
6.63
6.63
6.62
6.32
6.30
6.29
6.28
6.27
6.26
4.72
4.72
4.71
4.71
3.81
1.50
MeO
OBoc
500 MHz, CDCl3
1.34
1.02
1.00
0.99
1.00
1.00
2.04
3.07
9.27
f1 (ppm)

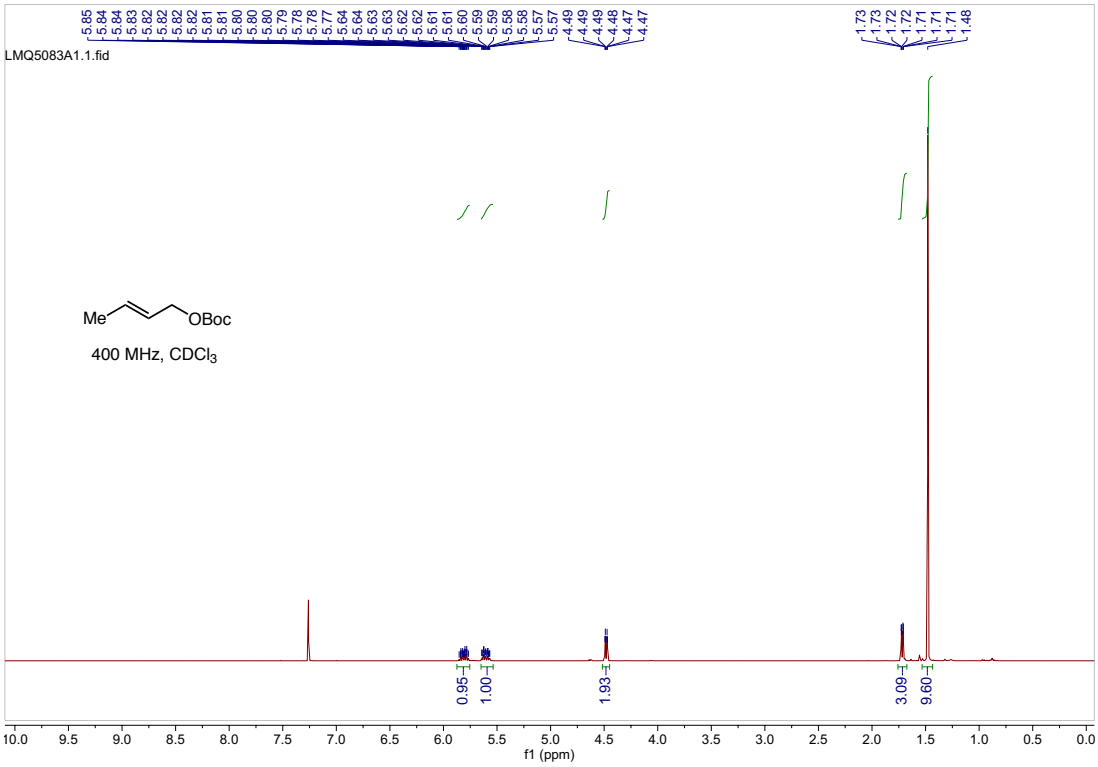

LMQ6123A1.2.1.1r
159.94
137.80
134.40
129.72
123.40
119.48
113.94
112.01
82.40
77.41
77.16
76.91
67.52
55.36
27.93
MeO
OBoc
126 MHz, CDCl3
f1 (ppm)

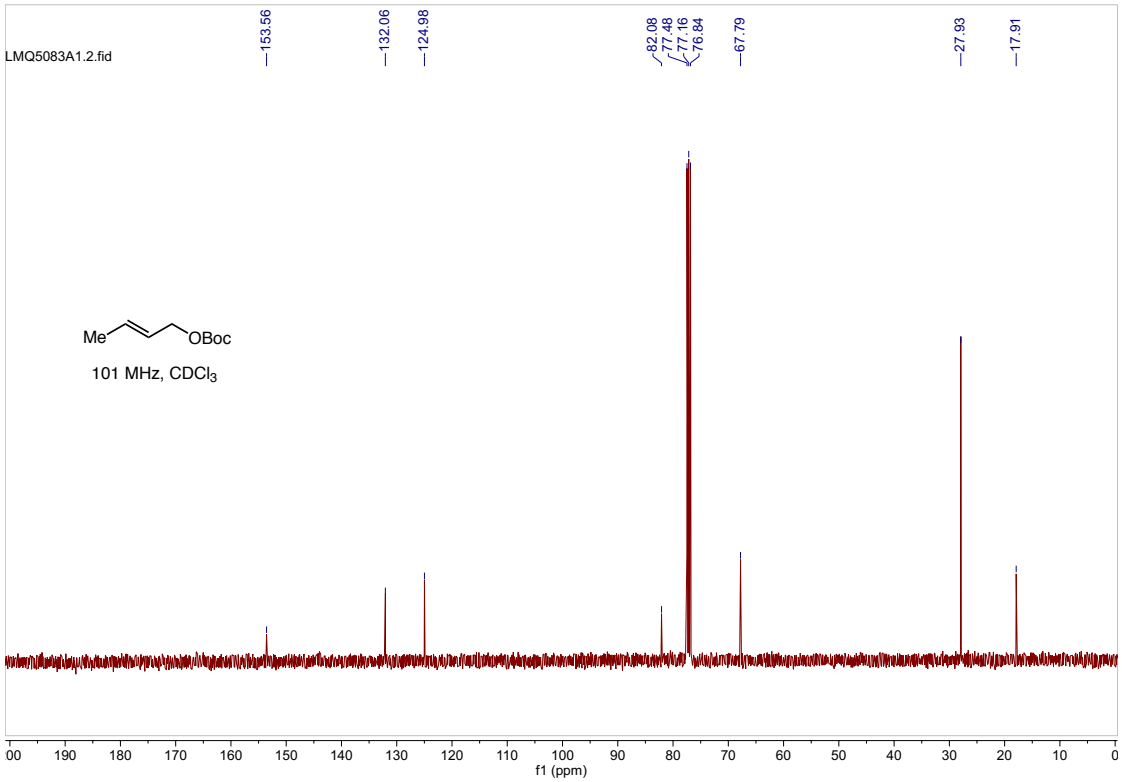

LMQ6125A1.1.fid
7.1115
7.1086
7.0957
7.0927
7.0503
7.0343
7.0248
7.0183
6.9926
6.8662
6.8632
6.8501
6.8471
6.3711
6.3580
6.3450
6.3390
6.3260
6.3130
4.7695
4.7668
4.7567
4.7540
3.8826
3.8272
1.5265
1.00
1.94
0.98
1.00
1.96
2.91
2.88
8.76
f1 (ppm)

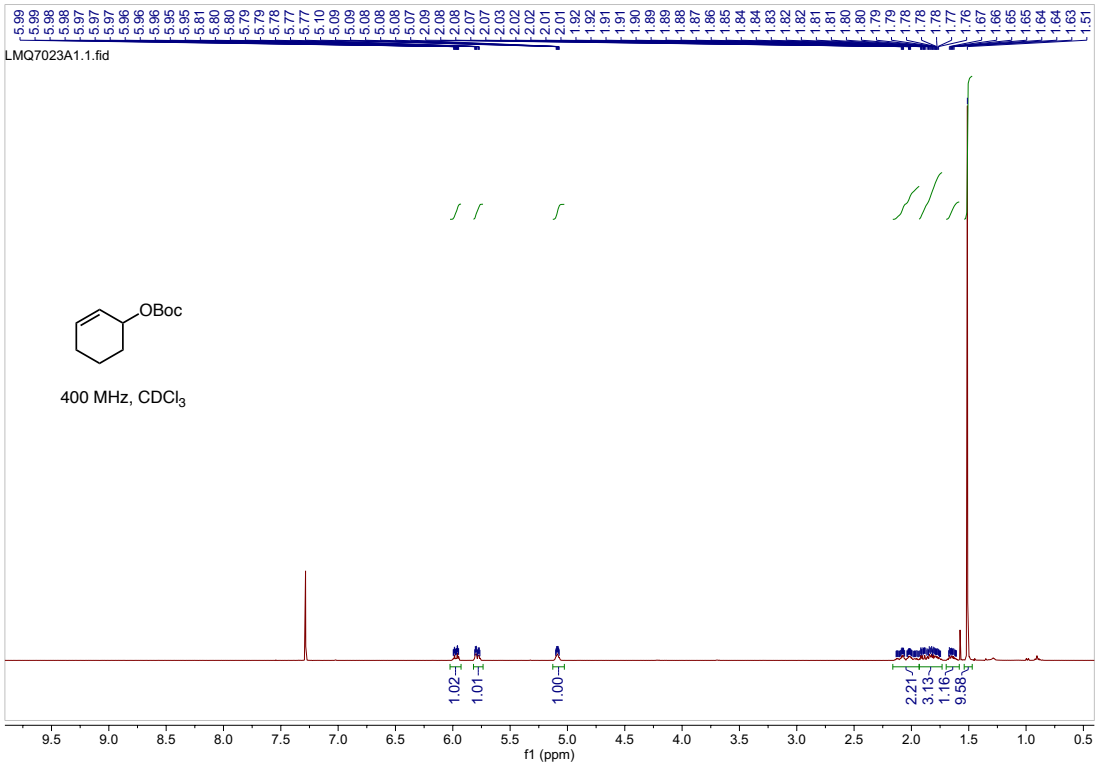

LMQ6125A1.2.1.1r
153.5050
153.1277
147.0790
130.5360
128.9630
124.4213
124.1818
118.5024
111.9633
82.3003
77.4144
77.1596
76.9060
67.9860
61.1108
55.9257
27.9243
OMe
MeO
OBoc
126 MHz, CDCl3
f1 (ppm)

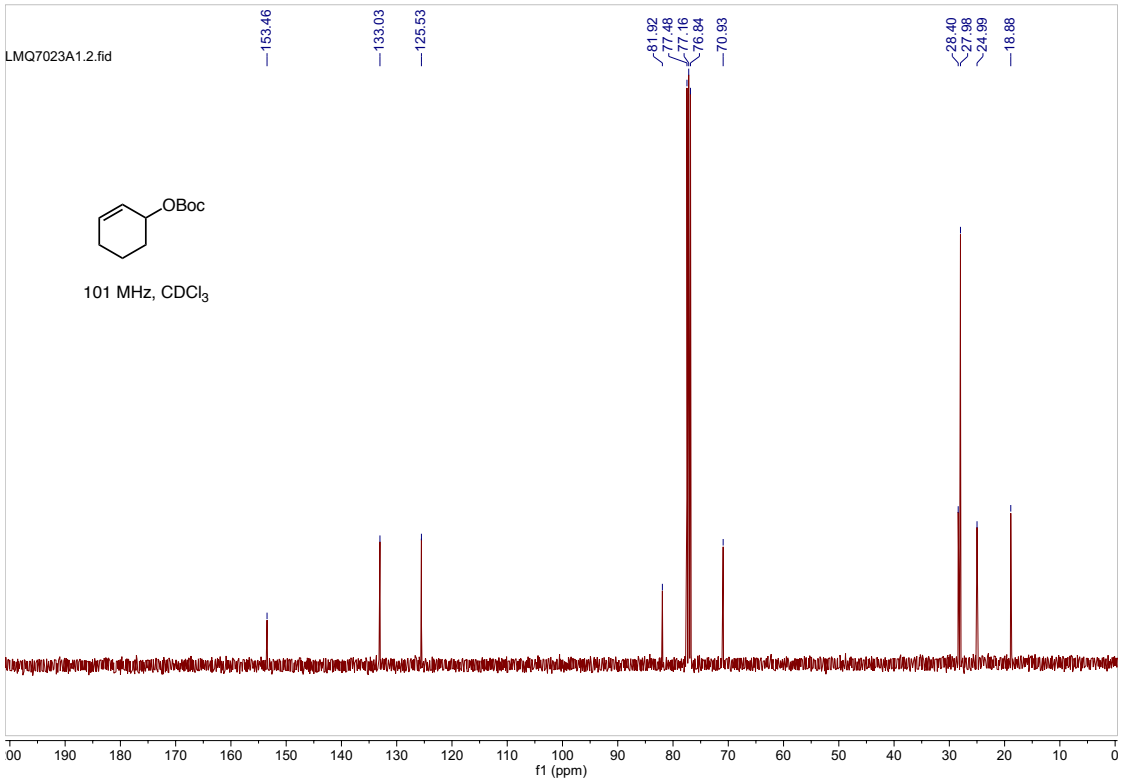

SSL2-015-pdt.1.fid
7.35
7.35
7.26
6.50
6.49
6.49
6.46
6.45
6.45
6.37
6.37
6.36
6.36
6.28
6.27
6.25
6.23
6.22
6.21
6.19
6.18
4.69
4.69
4.68
4.67
1.57
1.49
OBoc
O
400 MHz, CDCl3
0.96
1.01
0.99
0.99
1.00
2.07
9.42
f1 (ppm)

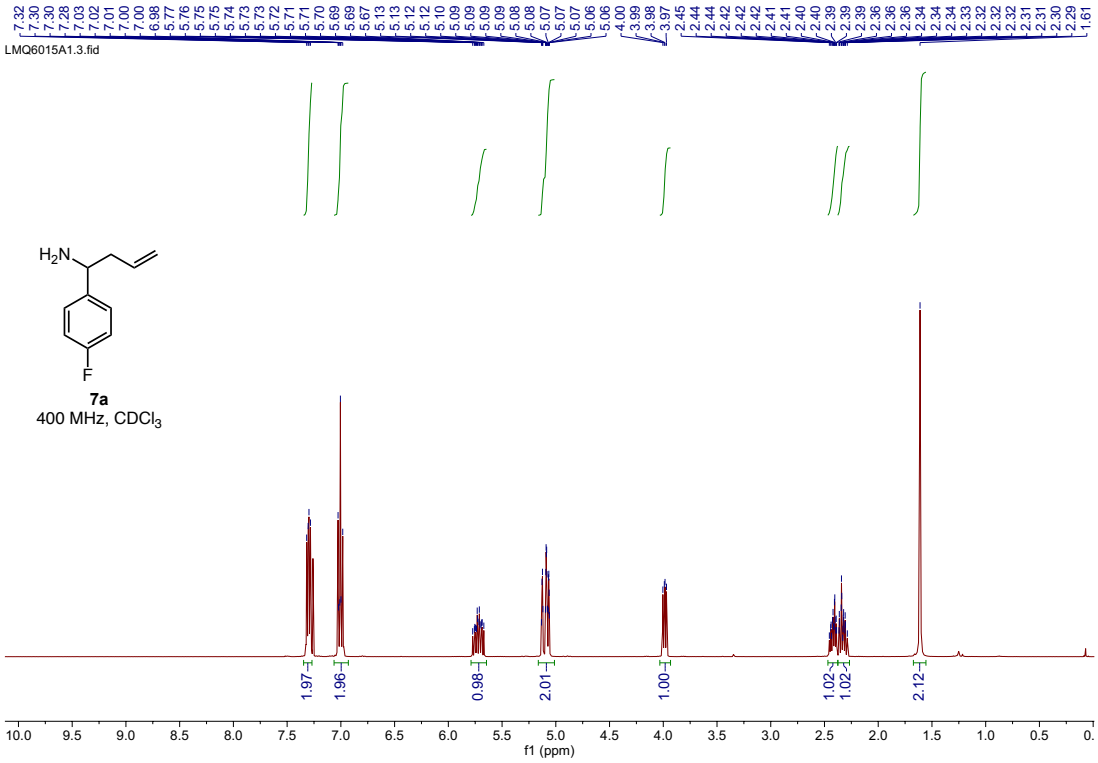

SSL2-015.2.1.1r
153.34
151.90
142.42
122.29
121.44
111.33
108.92
82.25
77.29
77.04
76.78
67.01
27.79
OBoc
O
126 MHz, CDCl3
f1 (ppm)

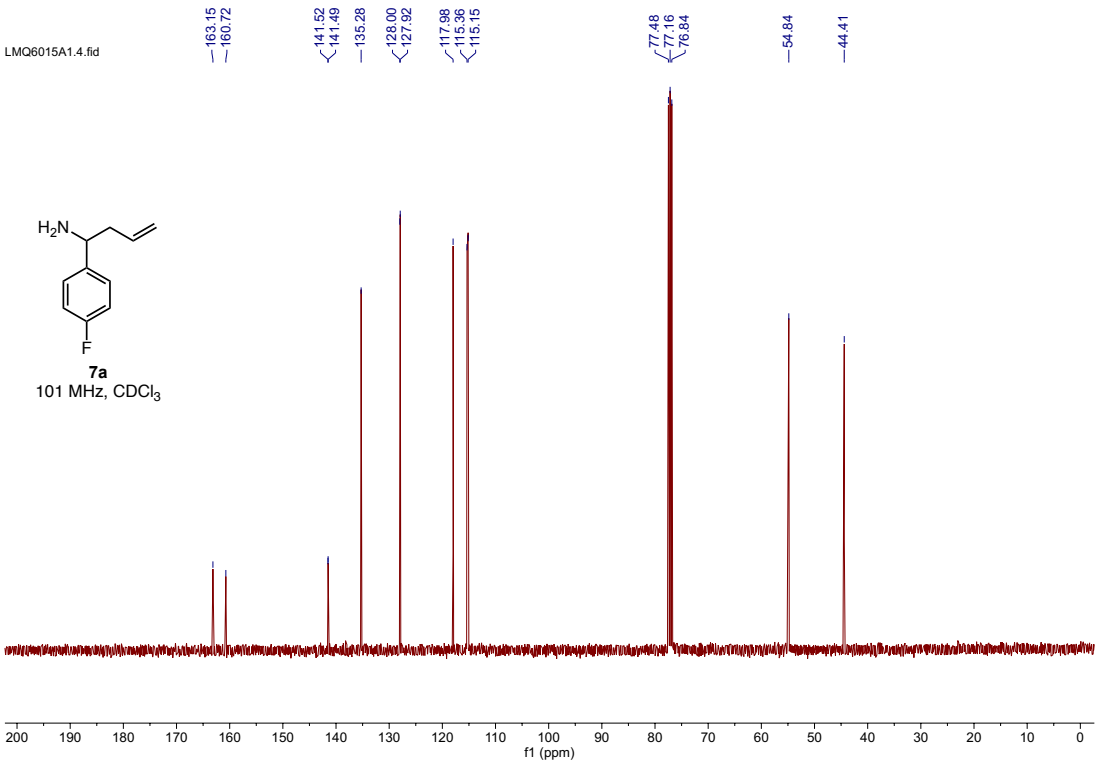

LMQ5083A1.1.fid
Me
OBoc
400 MHz, CDCl3
0.95
1.00
1.93
3.09
9.60
f1 (ppm)

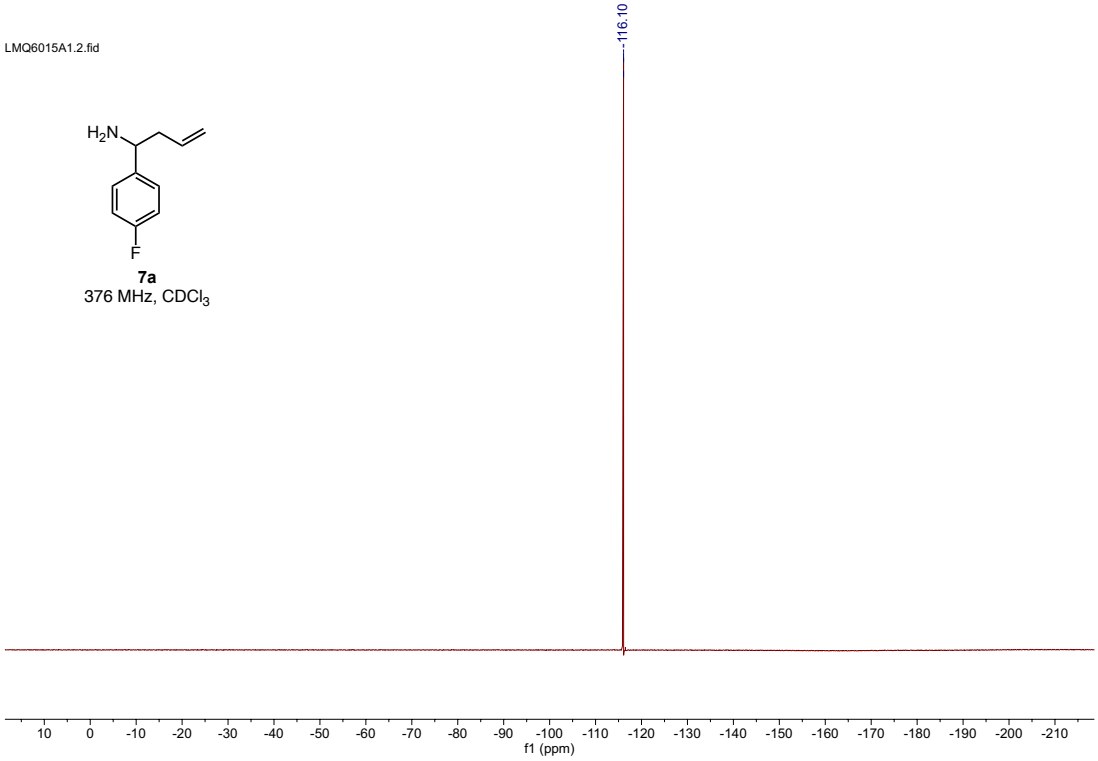

LMQ5083A1.2.fid
153.56
132.06
124.98
82.08
77.48
77.16
76.84
67.79
27.93
17.91
Me
OBoc
101 MHz, CDCl3
f1 (ppm)

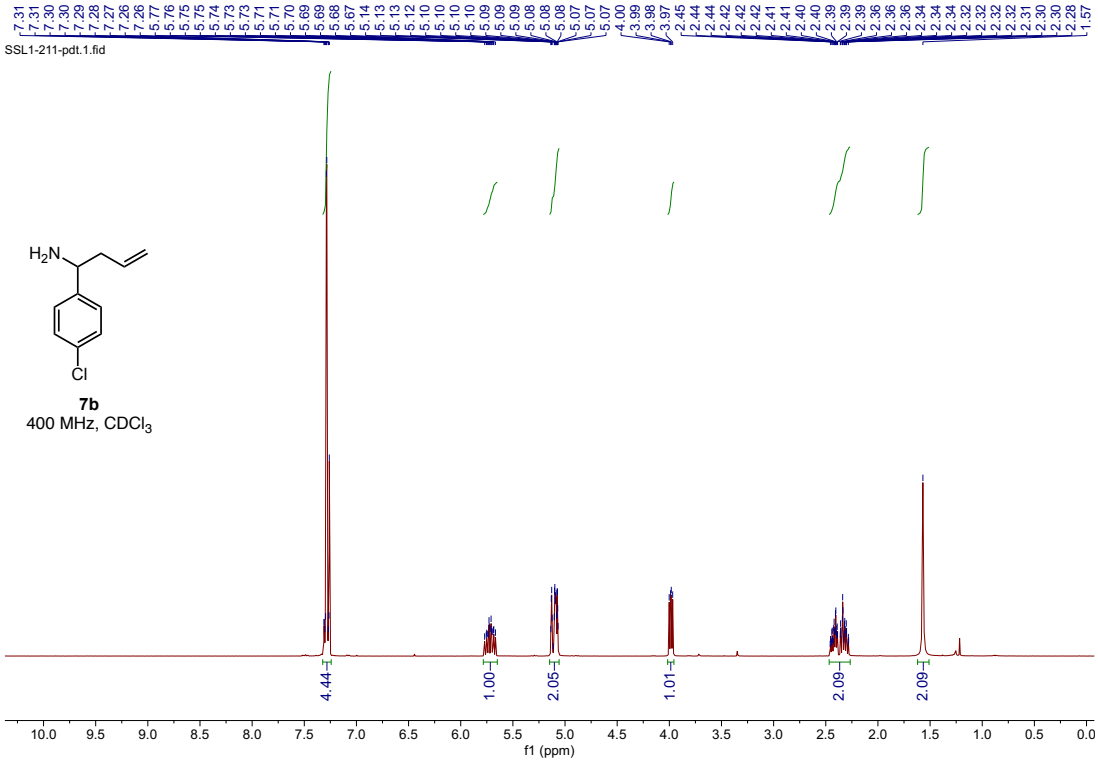

LMQ7023A1.1.fid
OBoc
400 MHz, CDCl3
1.02
1.01
1.00
2.21
3.13
1.16
9.58
f1 (ppm)

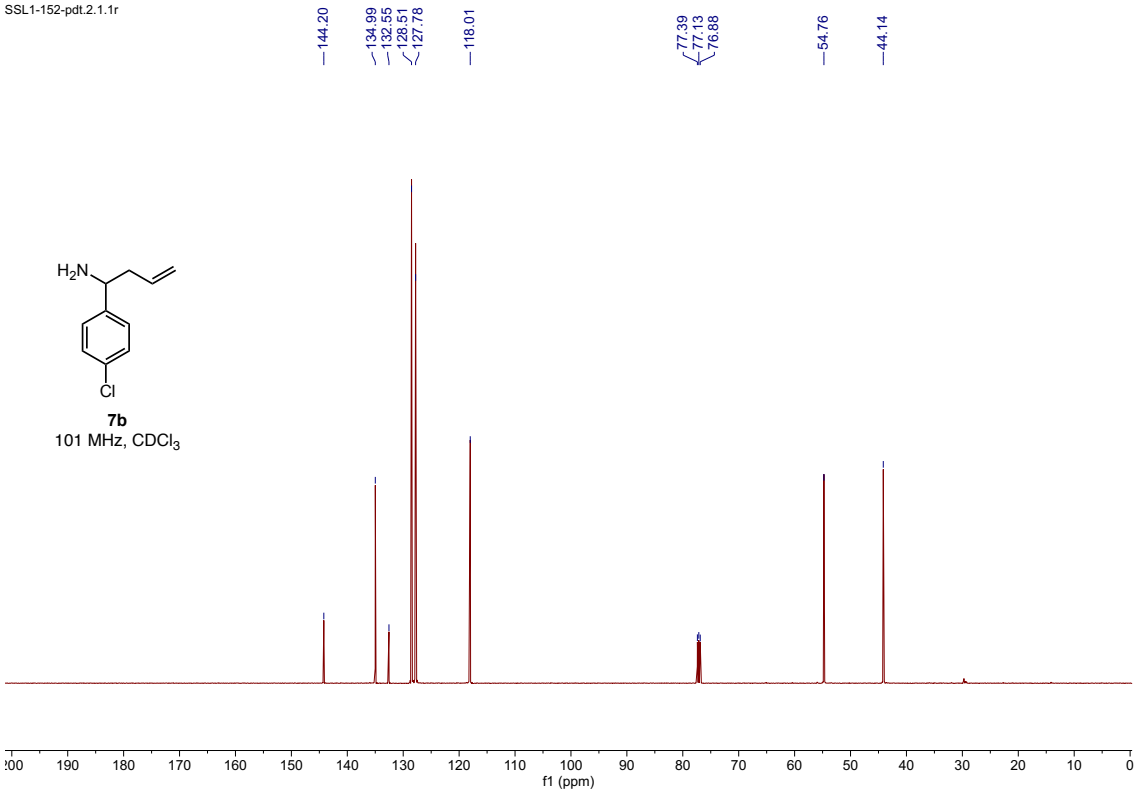

LMQ7023A1.2.fid
153.46
133.03
125.53
81.92
77.48
77.16
76.84
70.93
28.40
27.98
24.99
18.88
OBoc
101 MHz, CDCl3
f1 (ppm)

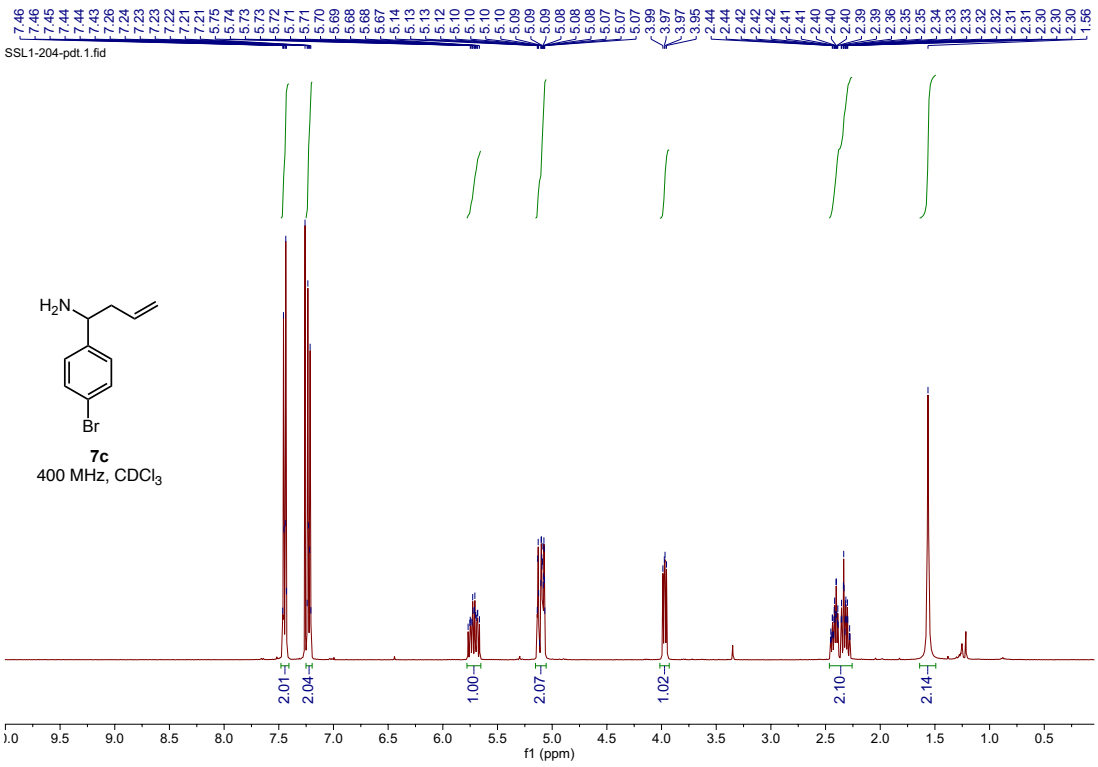

LMQ6015A1.3.fid
7.32 7.30 7.30 7.28 7.03 7.02 7.01 7.00 7.00 6.98 5.77 5.76 5.75 5.75 5.74 5.73 5.73 5.72 5.71 5.71 5.70 5.69 5.69 5.67 5.13 5.12 5.12 5.10 5.09 5.09 5.09 5.08 5.08 5.07 5.07 5.07 5.06 5.06 4.00 3.99 3.98 3.97 2.45 2.44 2.44 2.42 2.42 2.42 2.41 2.41 2.40 2.40 2.39 2.39 2.39 2.36 2.36 2.36 2.34 2.34 2.34 2.33 2.32 2.32 2.32 2.31 2.31 2.30 2.29 1.61
H2N
F
7a
400 MHz, CDCl3
1.97
1.96
0.98
2.01
1.00
1.02
1.02
2.12
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.
f1 (ppm)

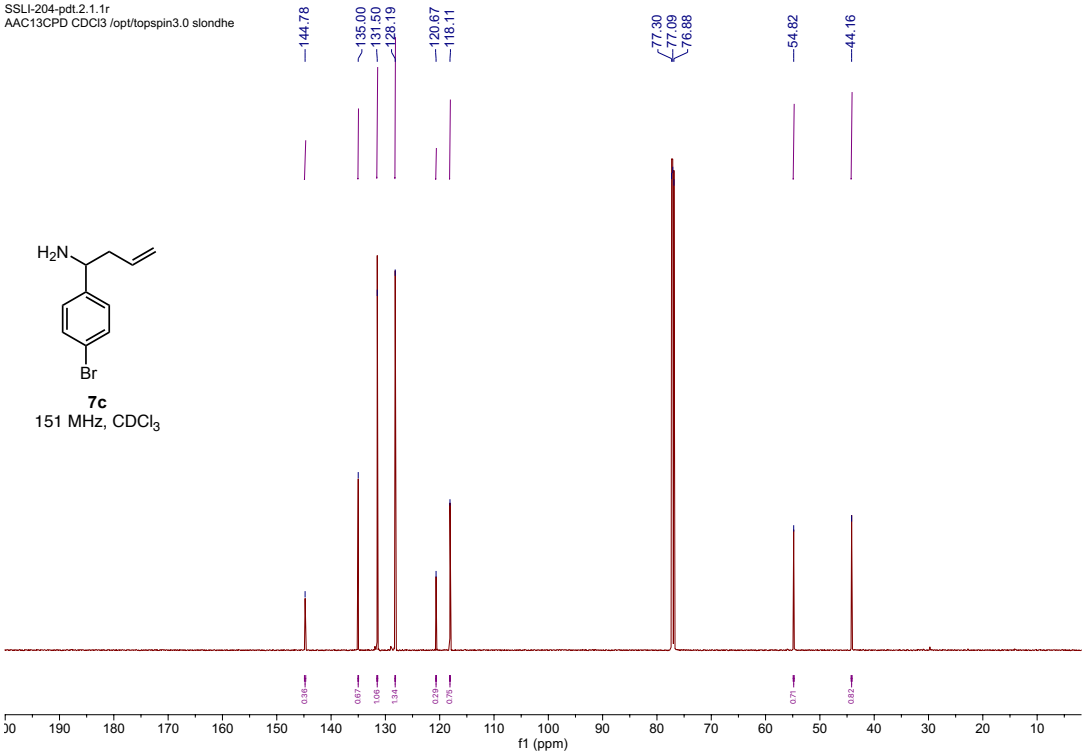

LMQ6015A1.4.fid
163.15
160.72
141.52
141.49
135.28
128.00
127.92
117.98
115.36
115.15
77.48
77.16
76.84
54.84
44.41
H2N
F
7a
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

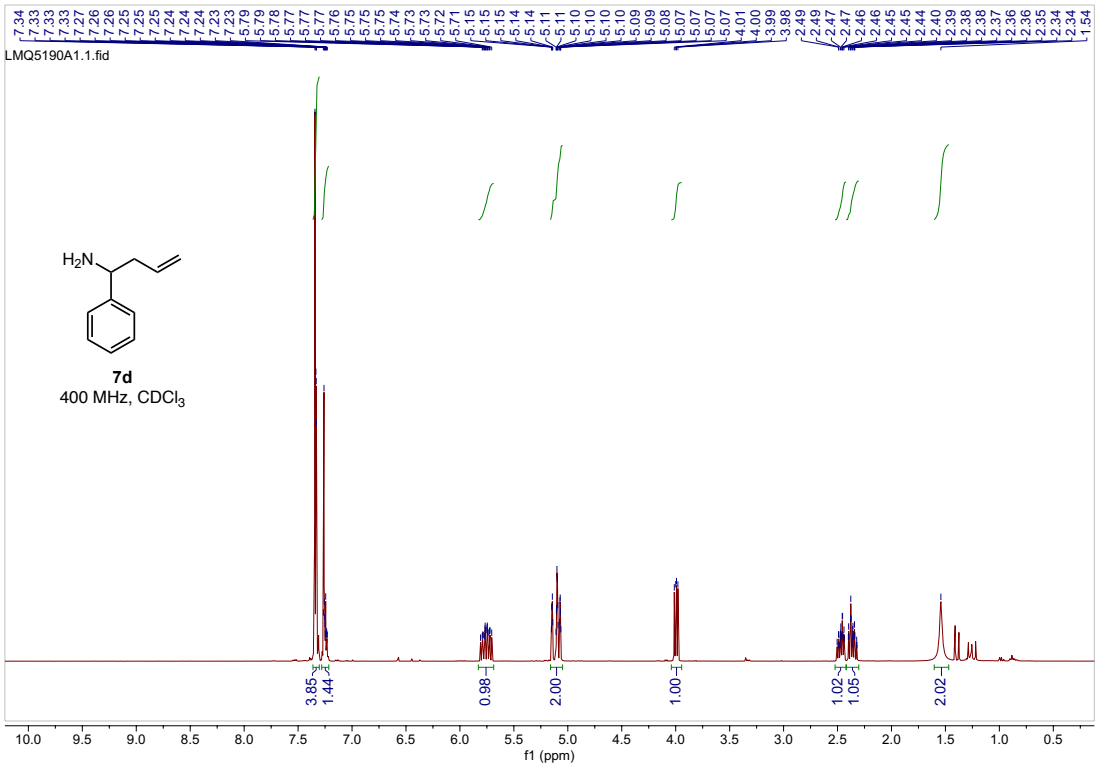

LMQ6015A1.2.fid
116.10
H2N
F
7a
376 MHz, CDCl3
f1 (ppm)

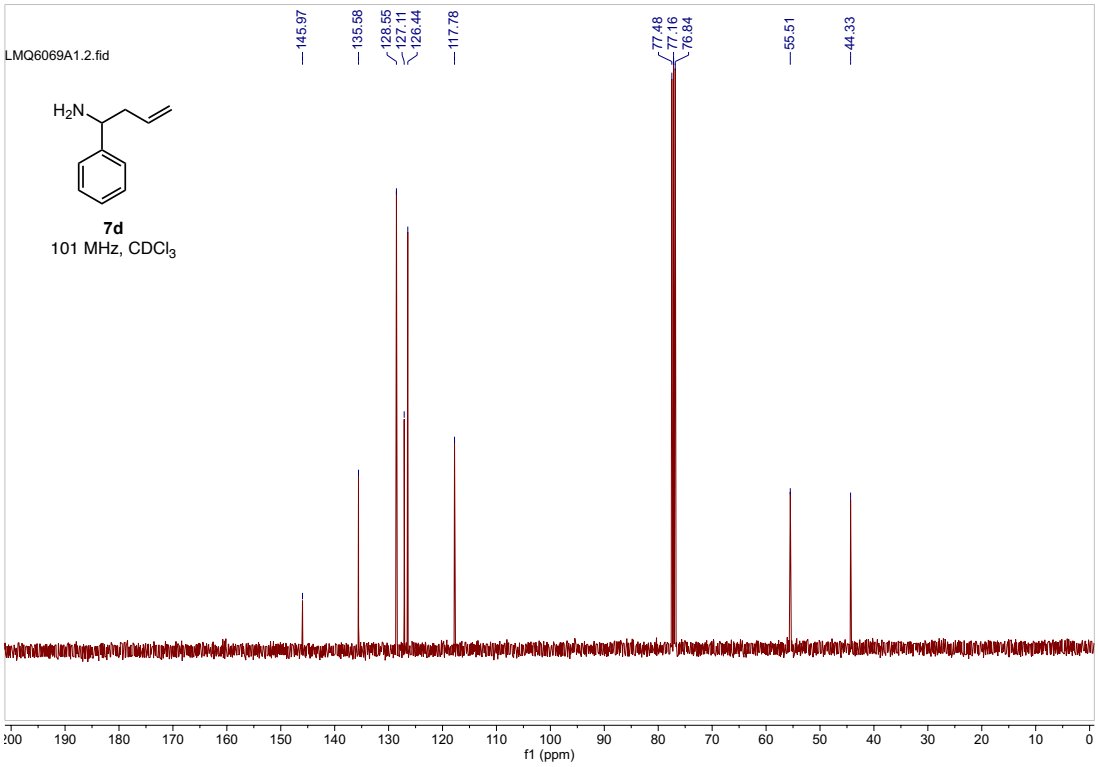

SSL1-211-pdt.1.fid
H2N
Cl
7b
400 MHz, CDCl3
4.44
1.00
2.05
1.01
2.09
2.09
f1 (ppm)

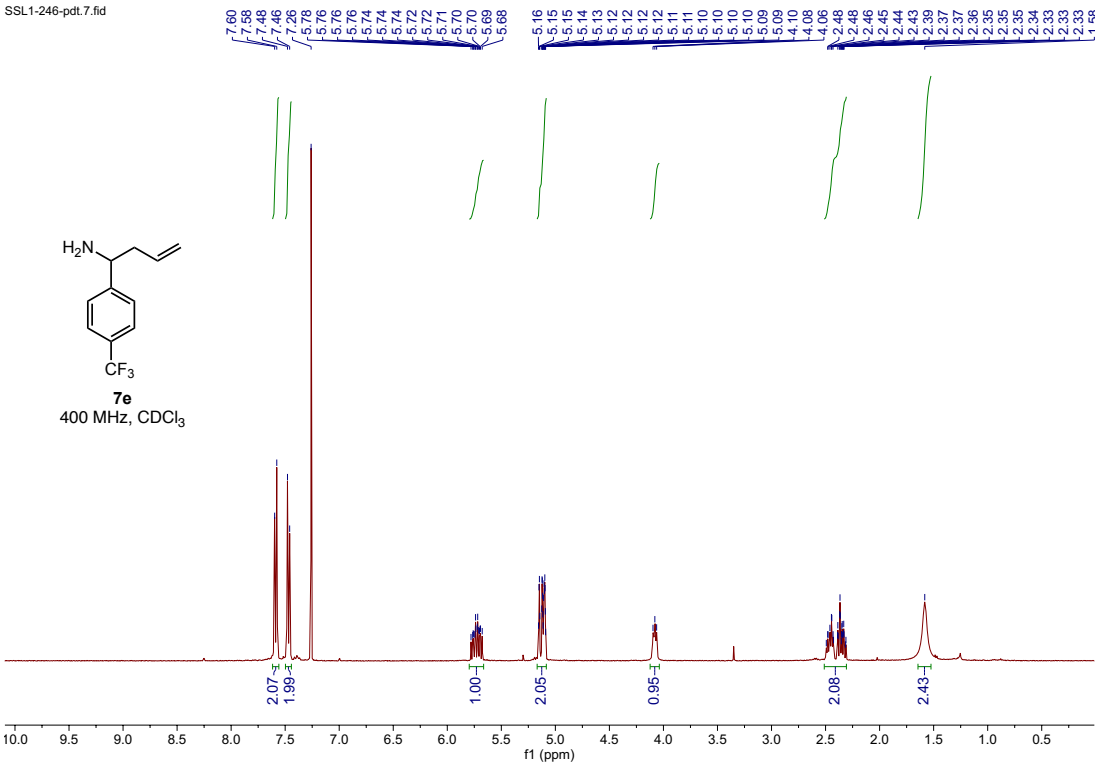

SSL1-152-pdt.2.1.1r
144.20
134.99
132.55
128.51
127.78
118.01
77.39
77.13
76.88
54.76
44.14
H2N
Cl
7b
101 MHz, CDCl3
f1 (ppm)

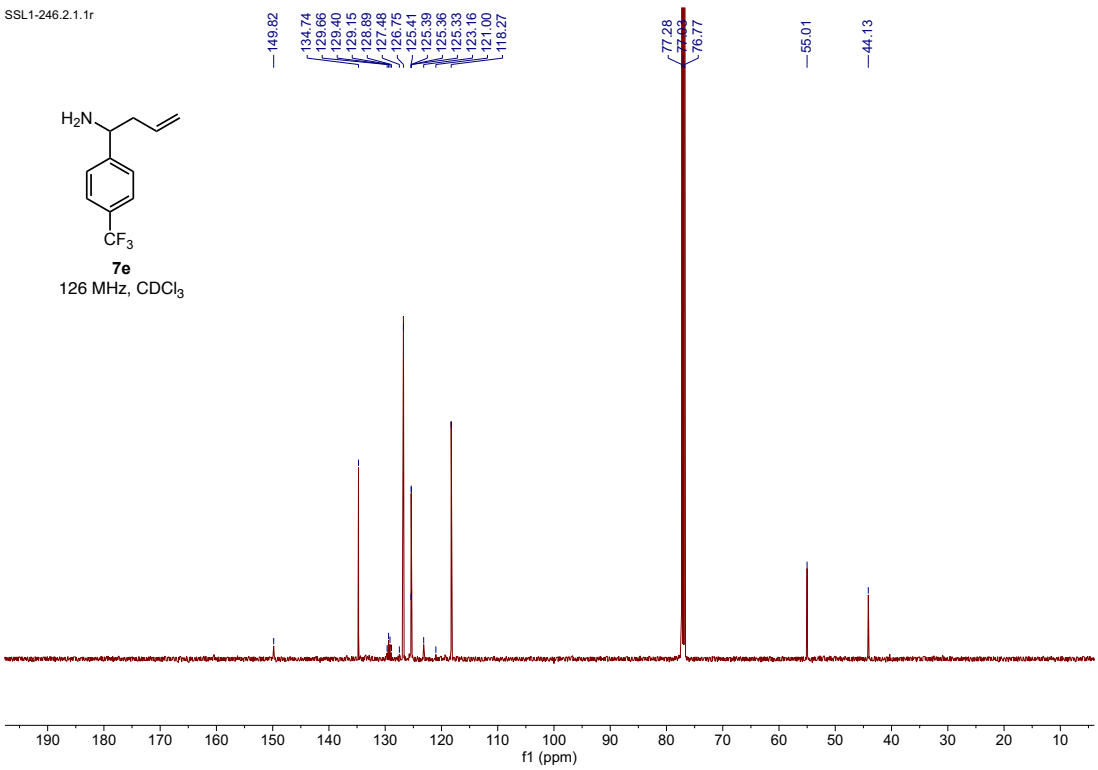

SSL1-204-pdt.1.fid
H2N
Br
7c
400 MHz, CDCl3
2.01
2.04
1.00
2.07
1.02
2.10
2.14
f1 (ppm)

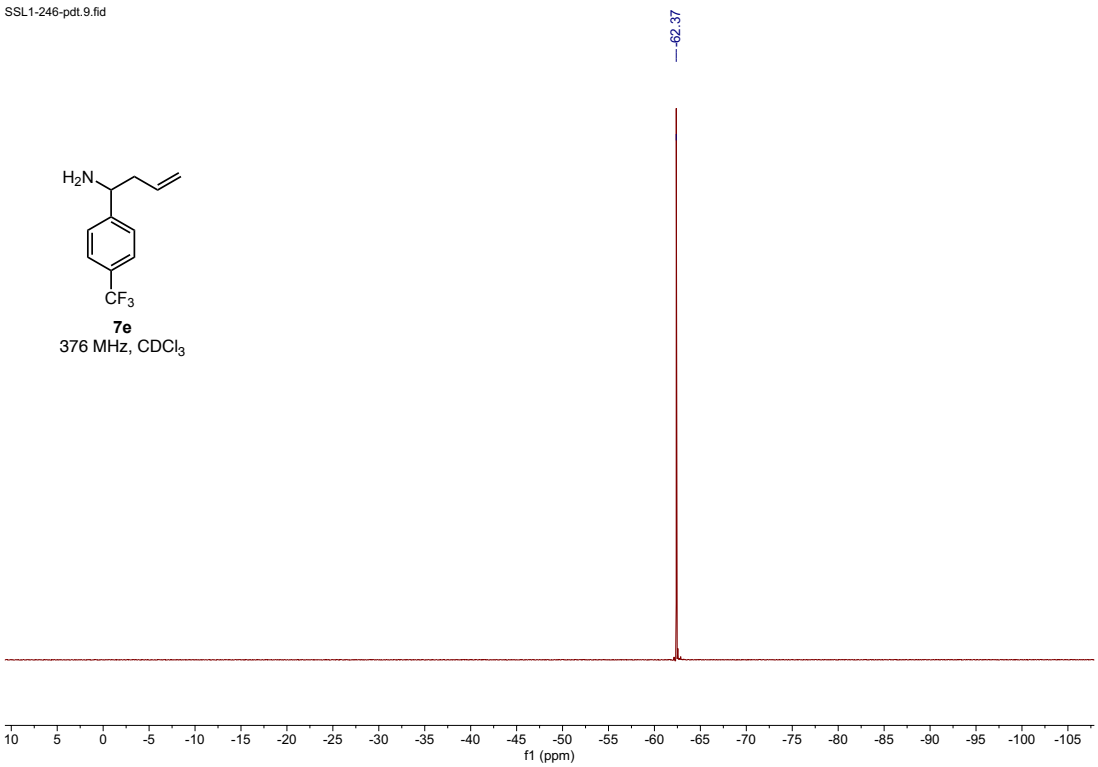

SSLI-204-pdt.2.1.1r
AAC13CPD CDCl3 /opt/topspin3.0 slondhe
144.78
135.00
131.50
129.19
120.67
118.11
77.30
77.09
76.88
54.82
44.16
H2N
Br
7c
151 MHz, CDCl3
f1 (ppm)

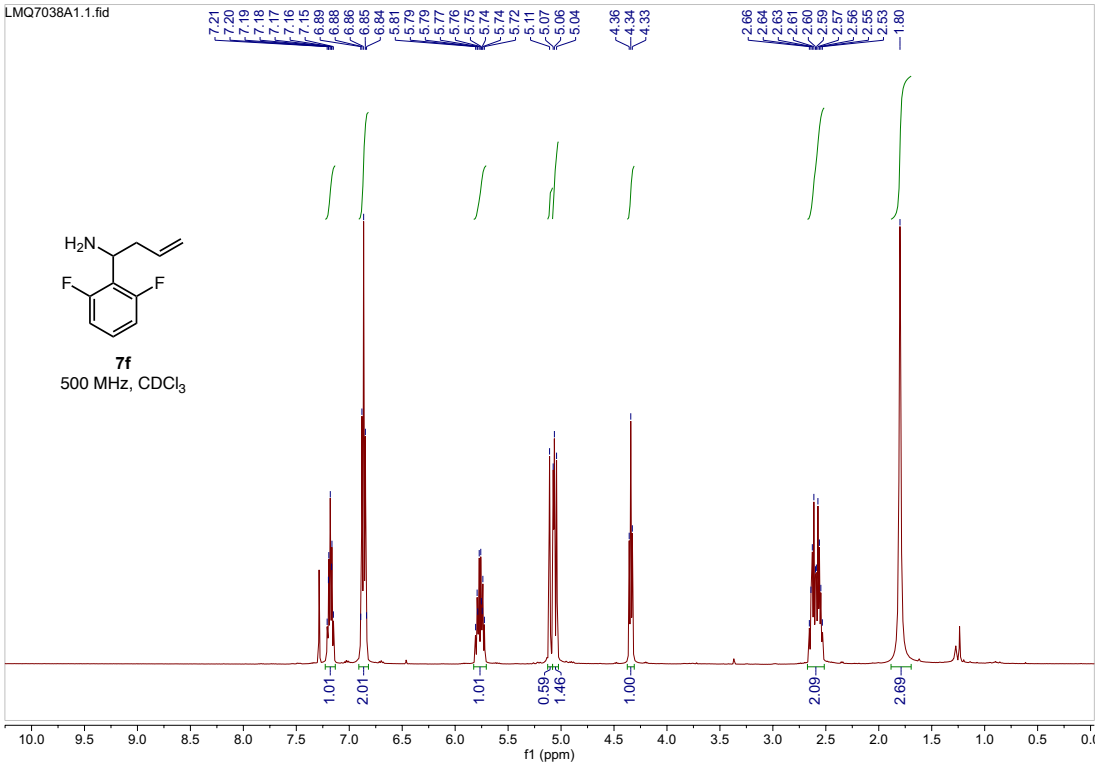

LMQ5190A1.1.fid
H2N
7d
400 MHz, CDCl3
3.85
1.44
0.98
2.00
1.00
1.02
1.05
2.02
f1 (ppm)

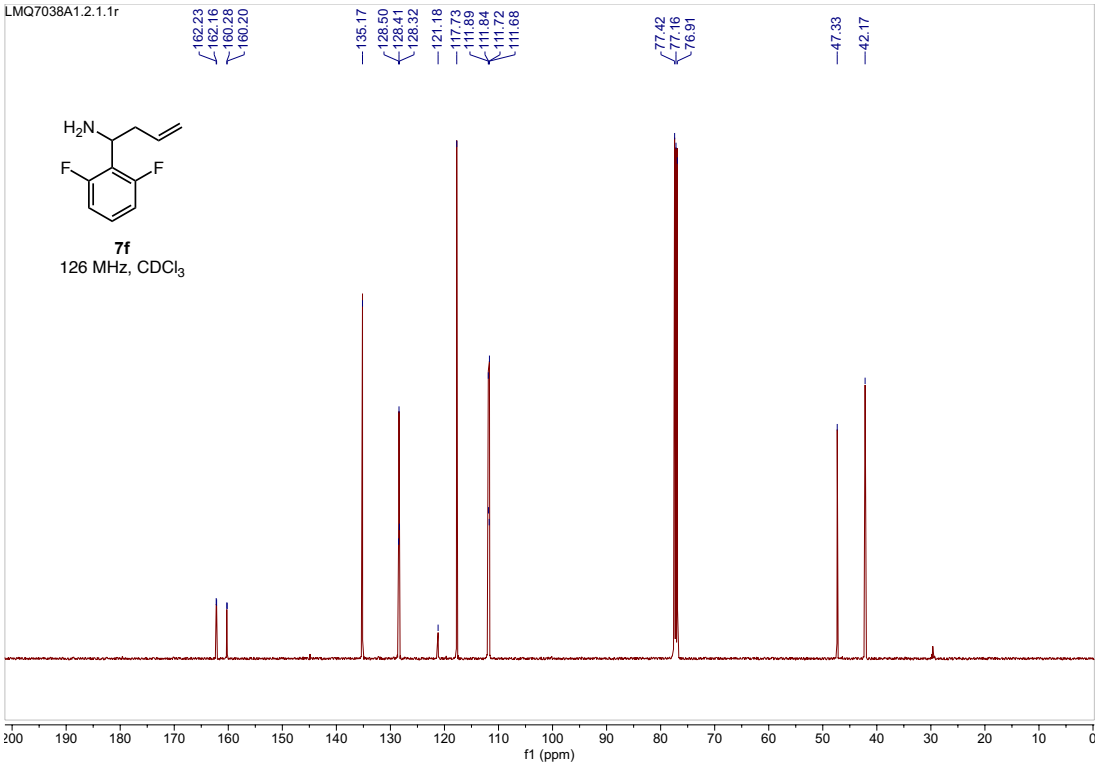

LMQ6069A1.2.fid
145.97
135.58
128.55
127.11
126.44
117.78
77.48
77.16
76.84
55.51
44.33
H_2N
7d
101 MHz, $CDCl_3$
f1 (ppm)

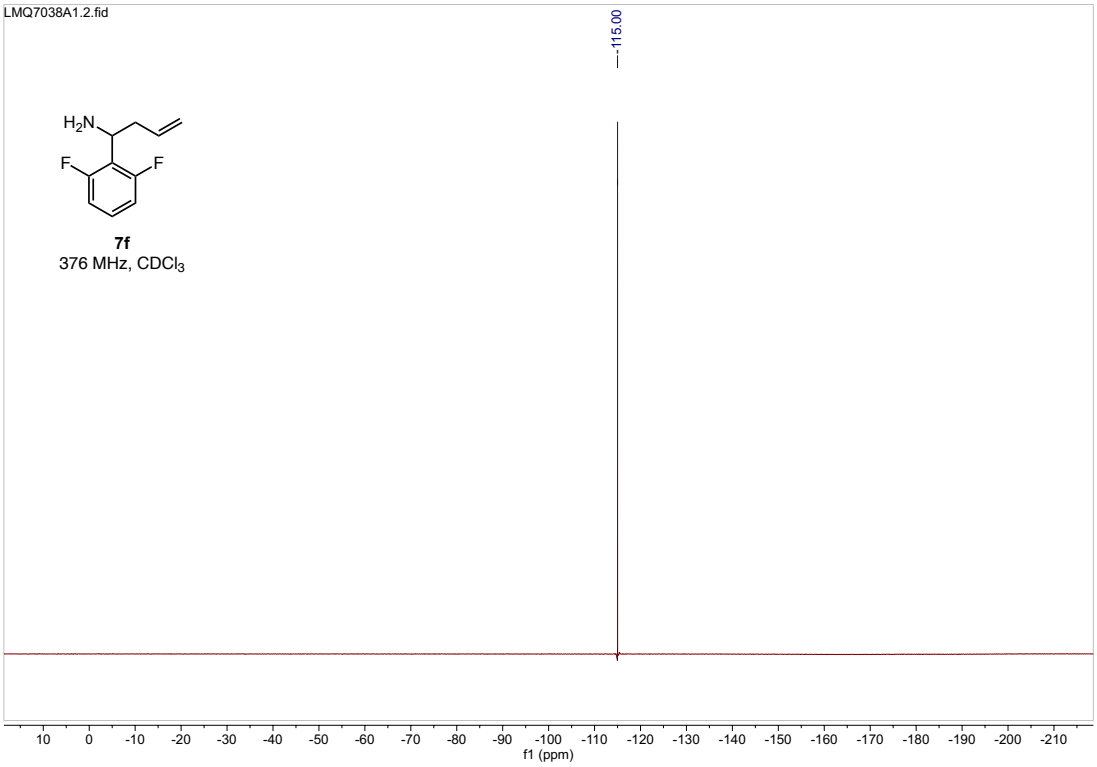

SSL1-246-pdt.7.fid
H_2N
CF_3
7e
400 MHz, $CDCl_3$
2.07
1.99
1.00
2.05
0.95
2.08
2.43
f1 (ppm)

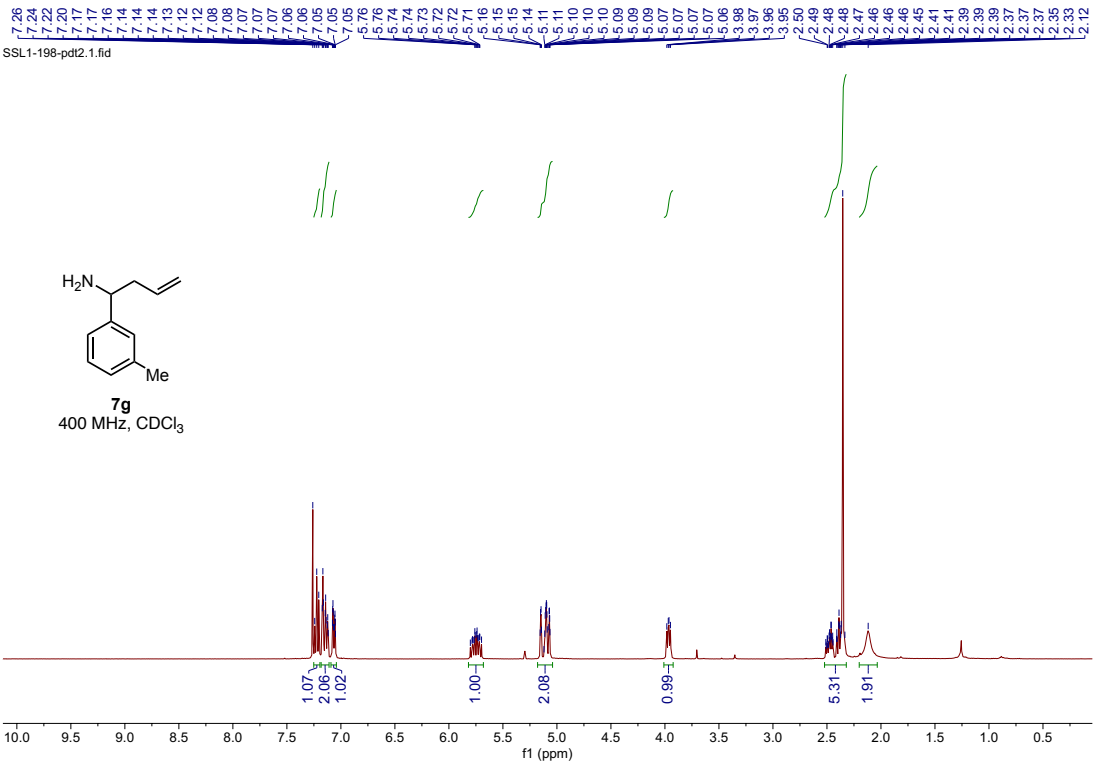

SSL1-246.2.1.1r
149.82
134.74
129.66
129.40
129.15
128.89
127.48
126.75
125.41
125.39
125.36
125.33
123.16
121.00
118.27
77.28
77.03
76.77
55.01
44.13
H2N
CF3
7e
126 MHz, CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

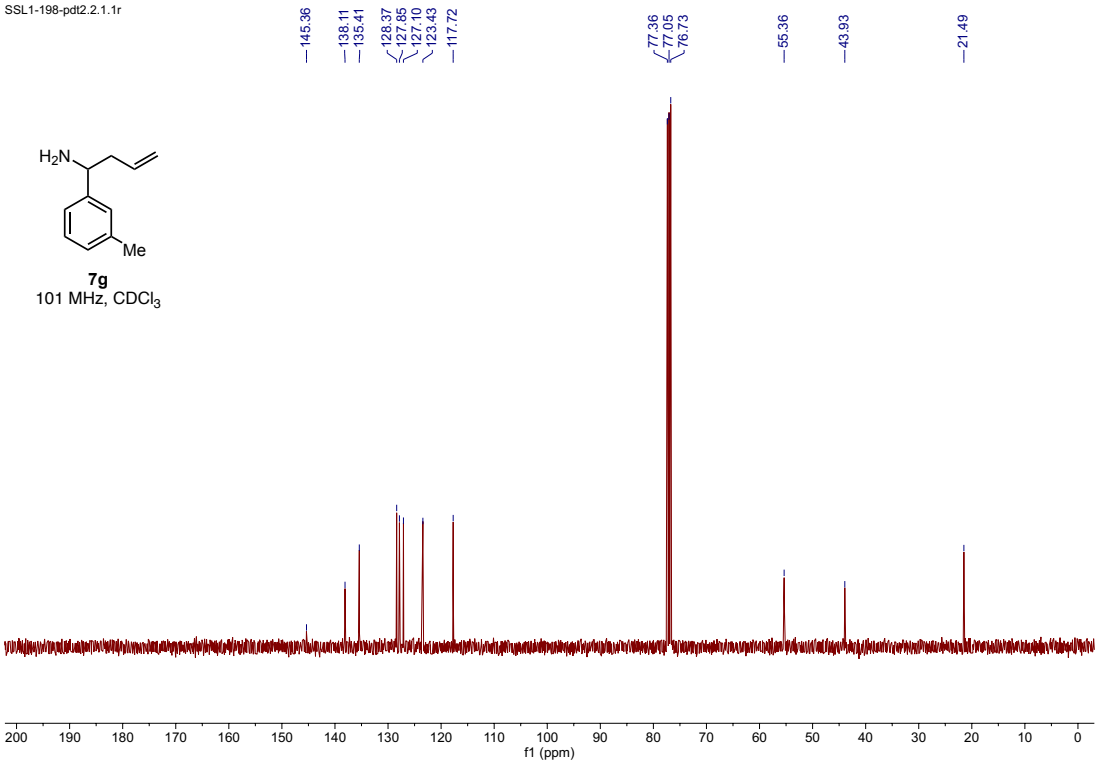

SSL1-246-pdt.9.fid
-62.37
H2N
CF3
7e
376 MHz, CDCl3
10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105
f1 (ppm)

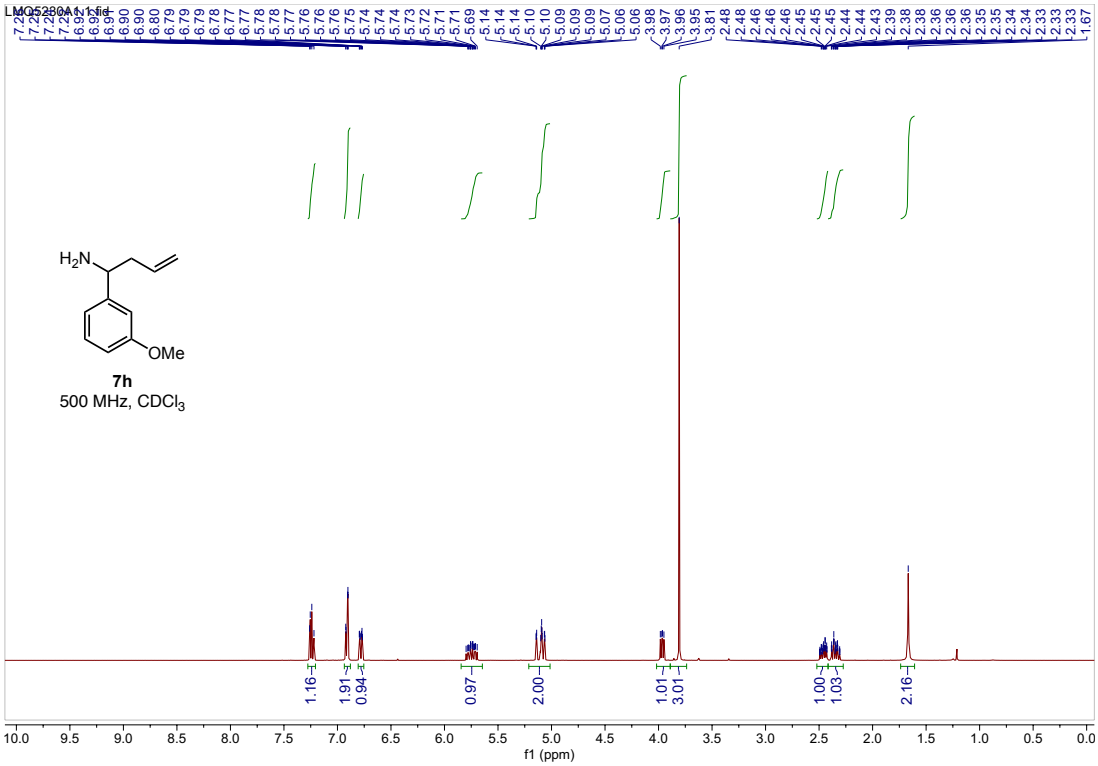

LMQ7038A1.1.fid
7.21
7.20
7.19
7.18
7.17
7.16
7.15
6.89
6.88
6.86
6.85
6.84
5.81
5.79
5.79
5.77
5.76
5.75
5.74
5.74
5.72
5.11
5.07
5.06
5.04
4.36
4.34
4.33
2.66
2.64
2.63
2.61
2.60
2.59
2.57
2.56
2.55
2.53
1.80
H2N
F
F
7f
500 MHz, CDCl3
1.01
2.01
1.01
0.59
1.46
1.00
2.09
2.69
10.0
9.5
9.0
8.5
8.0
7.5
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)

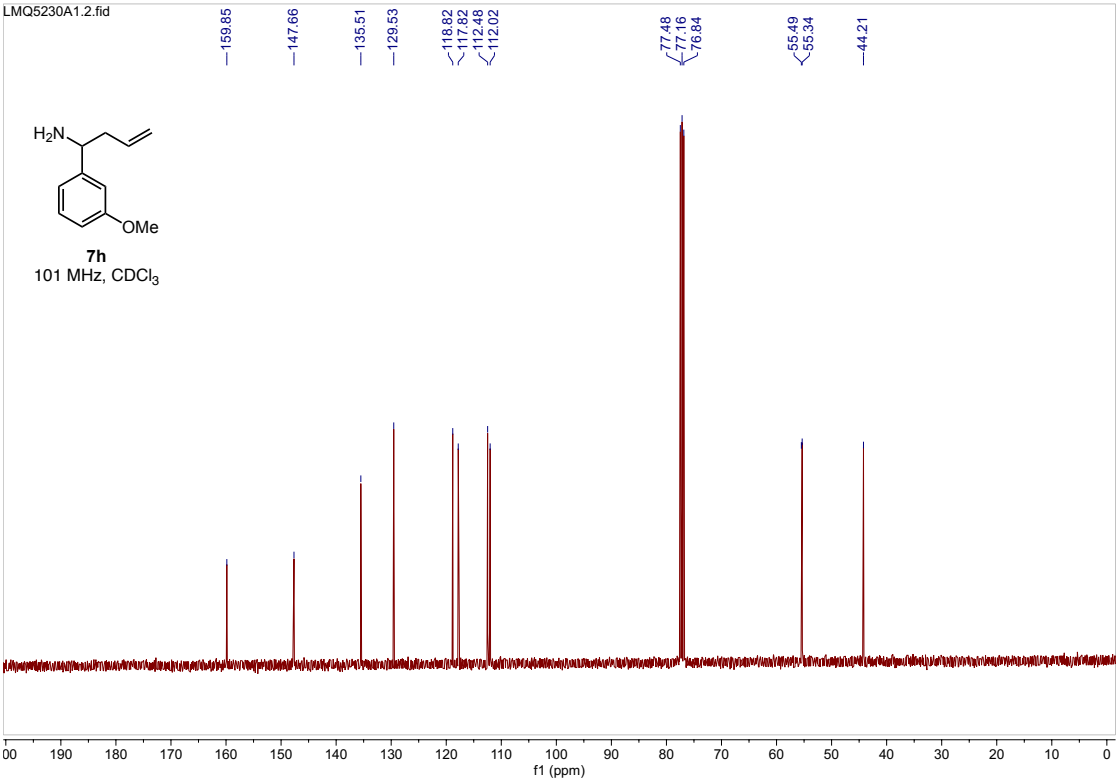

LMQ7038A1.2.1.1r
162.23
162.16
160.28
160.20
135.17
128.50
128.41
128.32
121.18
117.73
111.89
111.84
111.72
111.68
77.42
77.16
76.91
47.33
42.17
H2N
F
F
7f
126 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

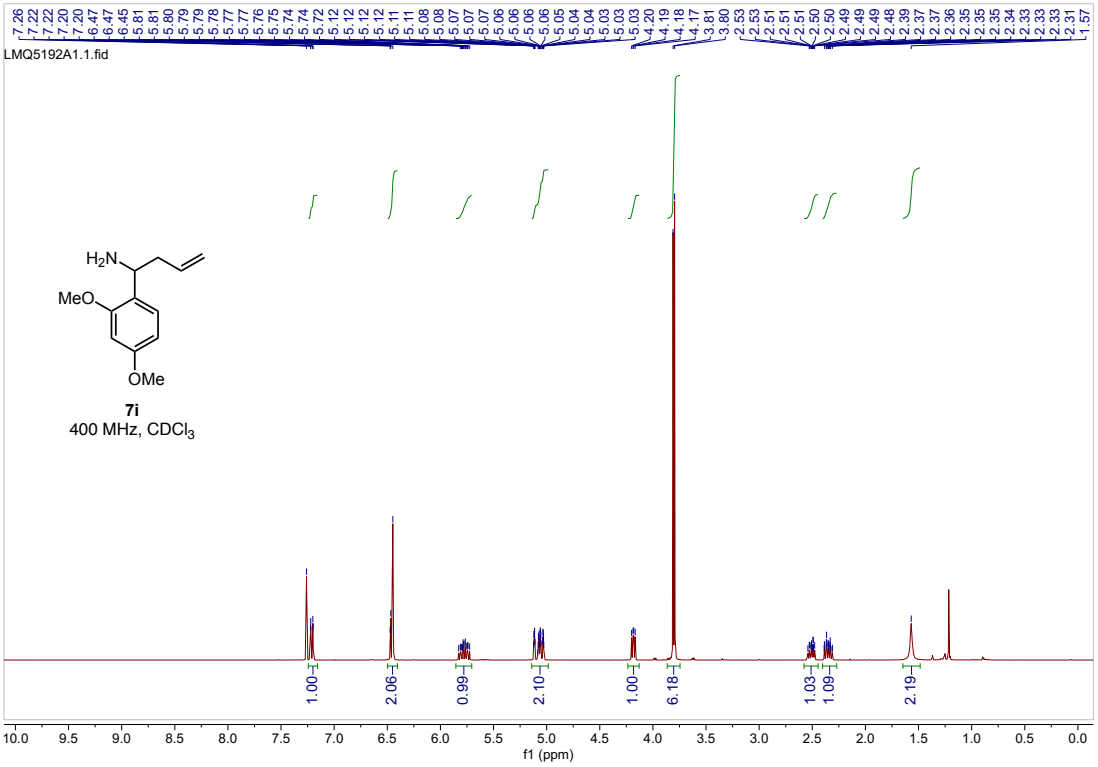

LMQ7038A1.2.fid
-115.00
H2N
F
F
7f
376 MHz, CDCl3
f1 (ppm)

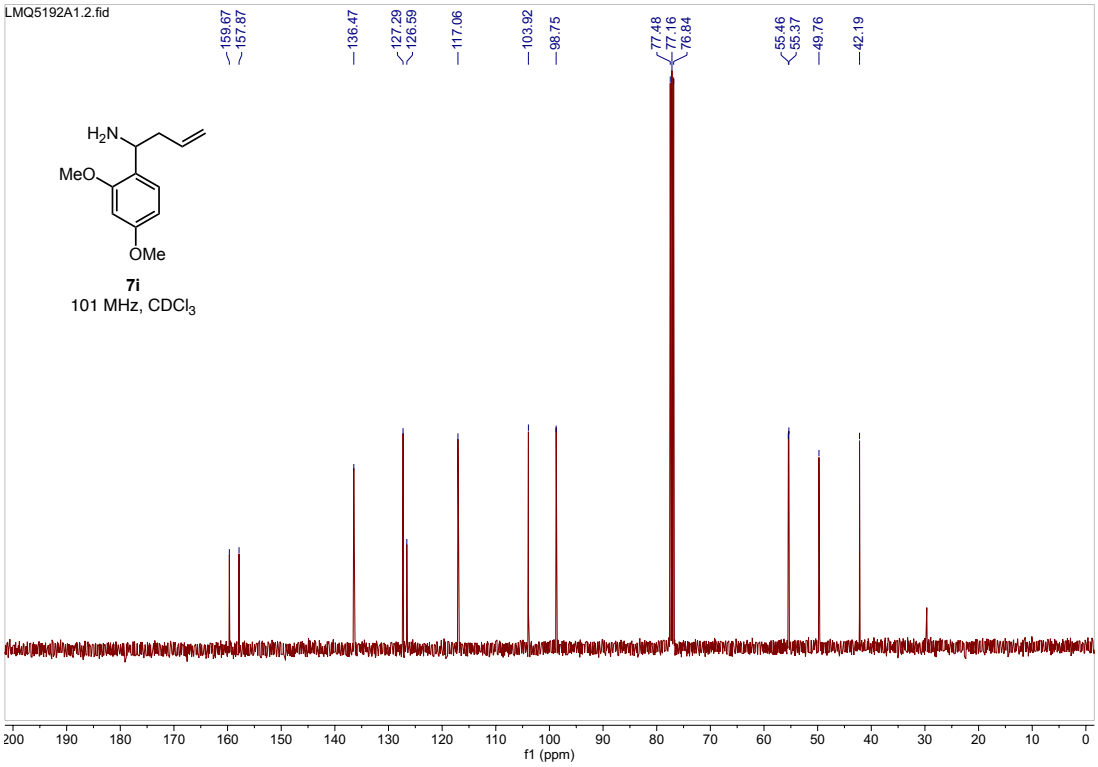

SSL1-198-pdt2.1.fid
H2N
Me
7g
400 MHz, CDCl3
1.07
2.06
1.02
1.00
2.08
0.99
5.31
1.91
f1 (ppm)

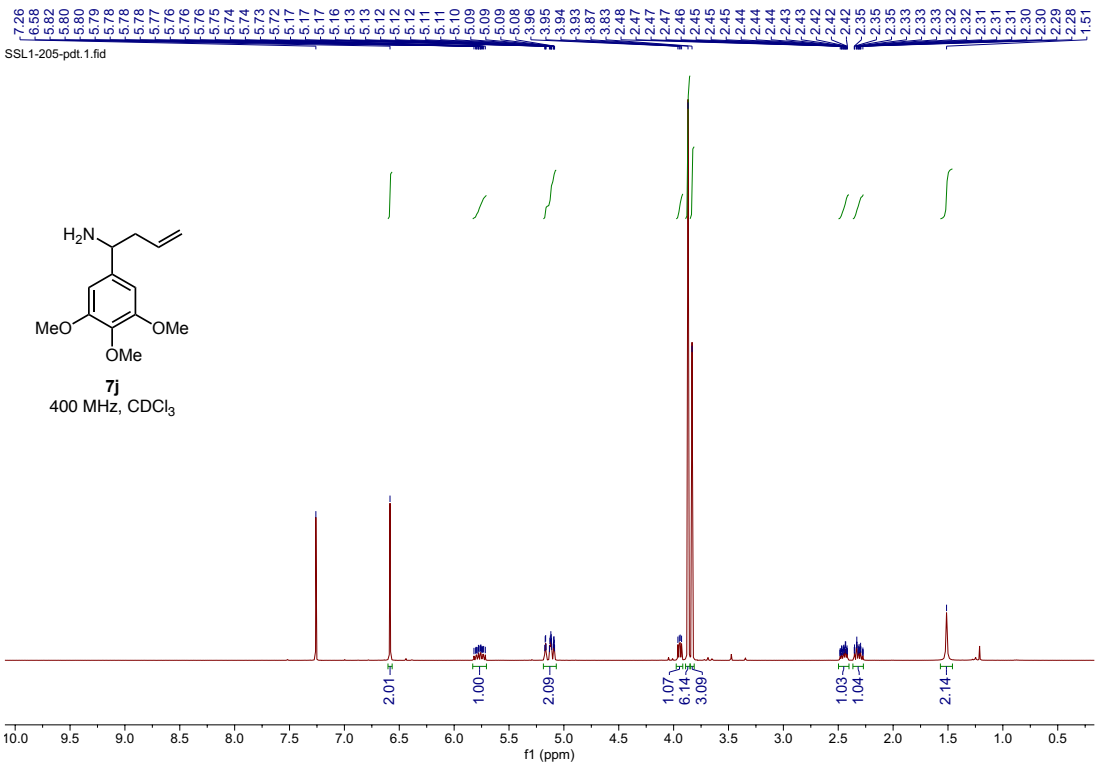

SSL1-198-pdt2.2.1.1r
145.36
138.11
135.41
128.37
127.85
127.10
123.43
117.72
77.36
77.05
76.73
55.36
43.93
21.49
H2N
Me
7g
101 MHz, CDCl3
f1 (ppm)

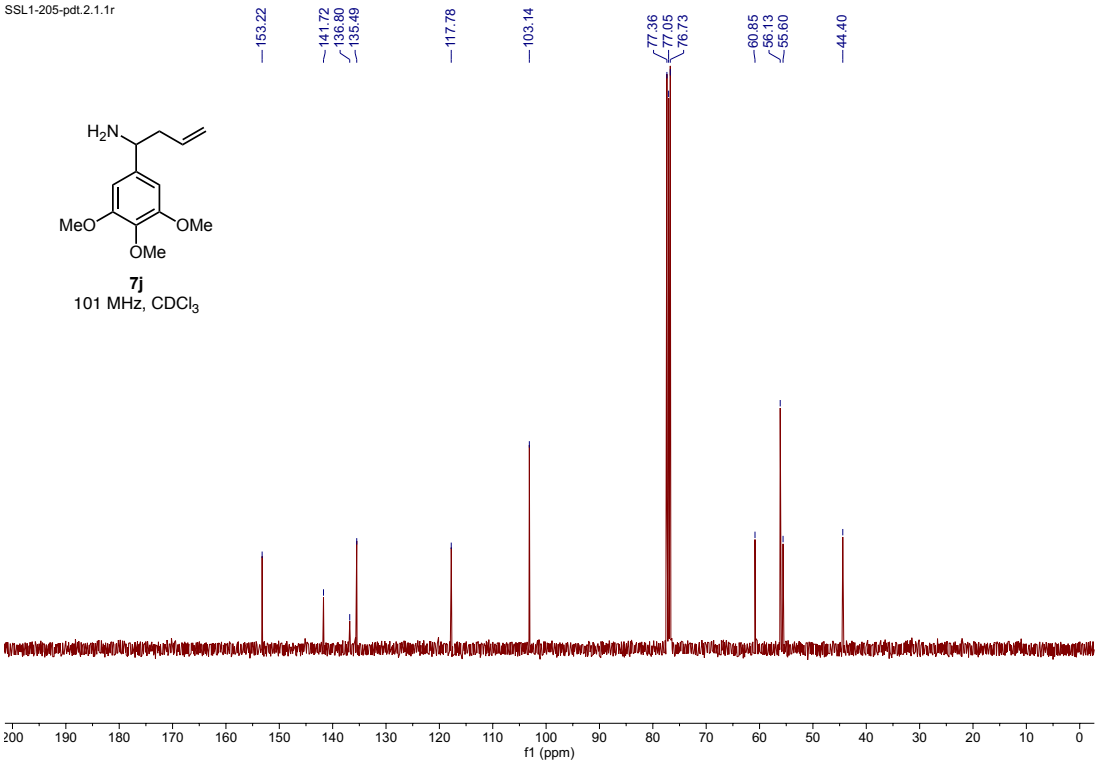

LMQ5250A11.fid
H2N
OMe
7h
500 MHz, CDCl3
1.16
1.91
0.94
0.97
2.00
1.01
3.01
1.00
1.03
2.16
f1 (ppm)

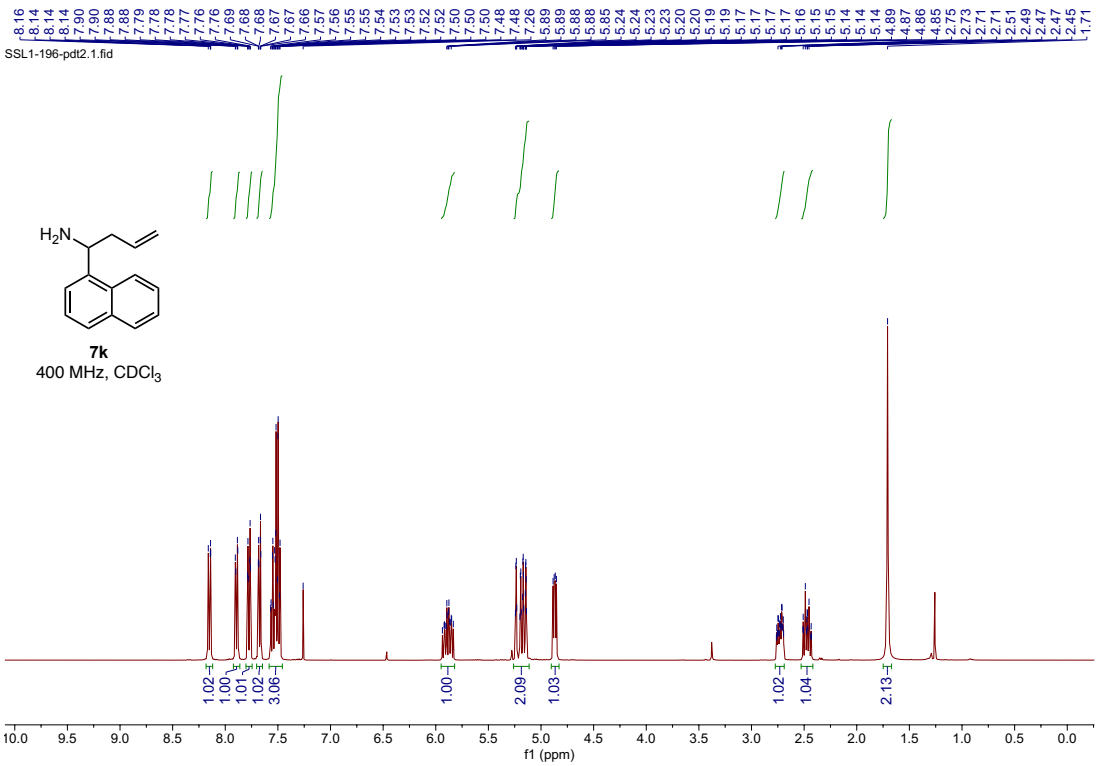

LMQ5230A1.2.fid
159.85
147.66
135.51
129.53
118.82
117.82
112.48
112.02
77.48
77.16
76.84
55.49
55.34
44.21
H2N
OMe
7h
101 MHz, CDCl3
f1 (ppm)

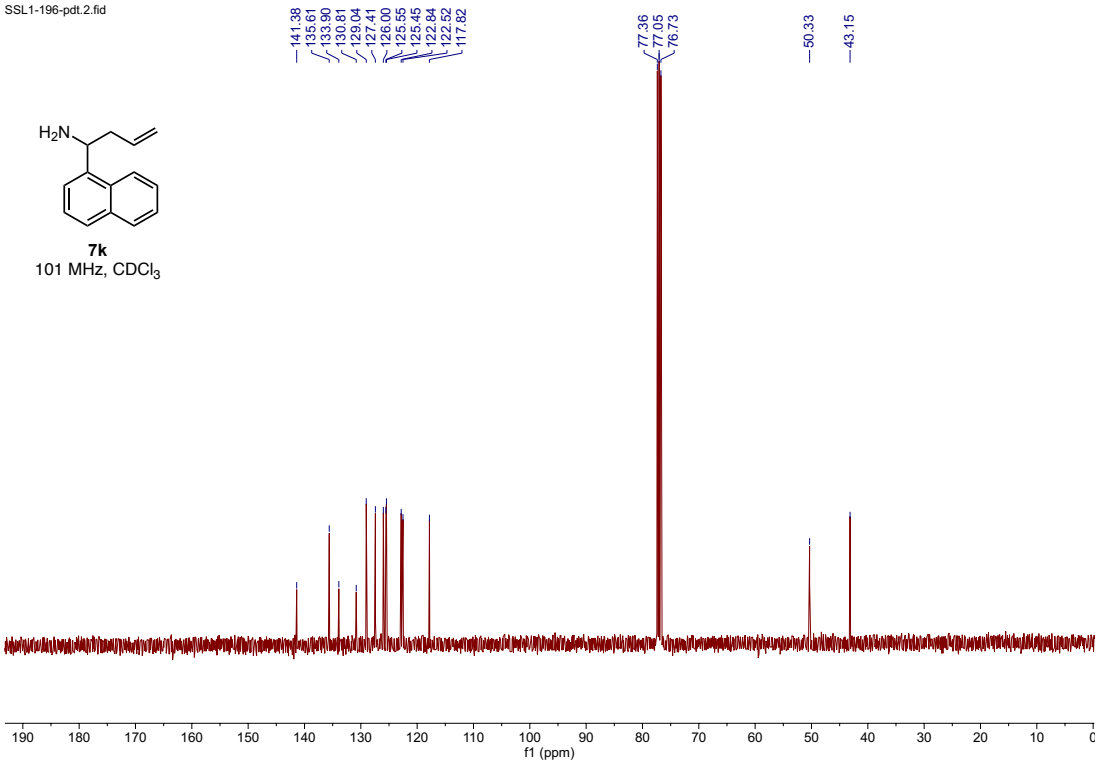

LMQ5192A1.1.fid
H2N
MeO
OMe
7i
400 MHz, CDCl3
1.00
2.06
0.99
2.10
1.00
6.18
1.03
1.09
2.19
f1 (ppm)

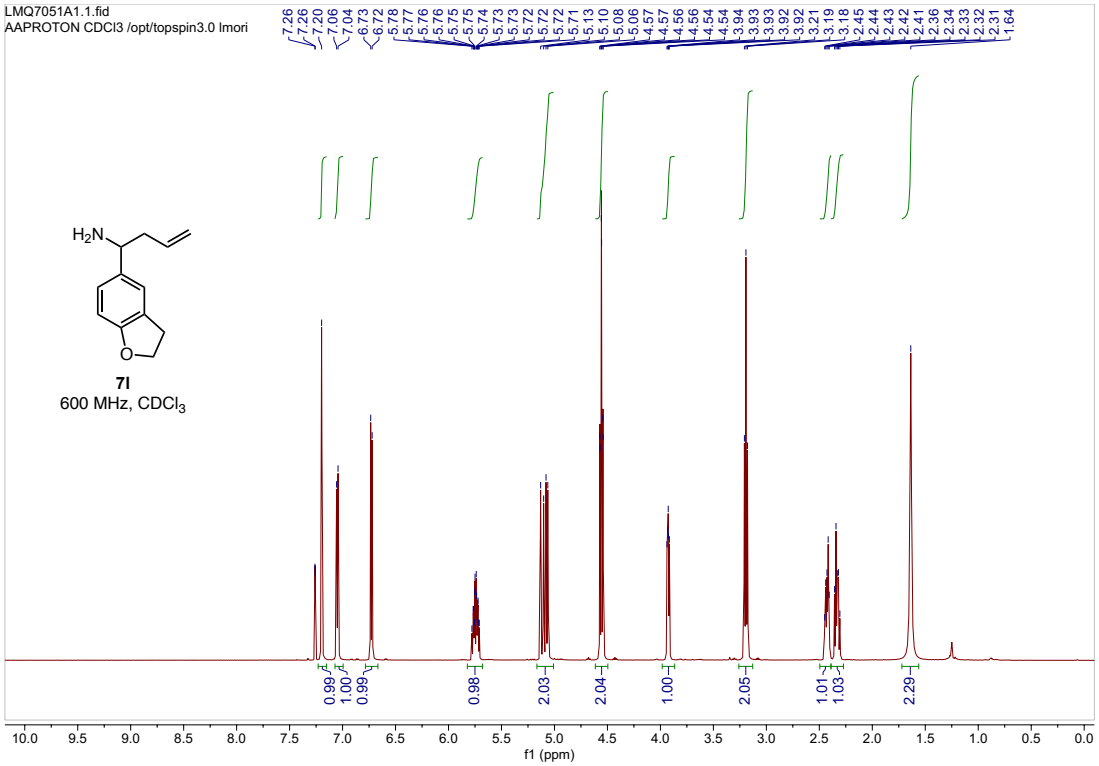

LMQ5192A1.2.fid
159.67
157.87
136.47
127.29
126.59
117.06
103.92
98.75
77.48
77.16
76.84
55.46
55.37
49.76
42.19
H2N
MeO
OMe
7i
101 MHz, CDCl3
f1 (ppm)

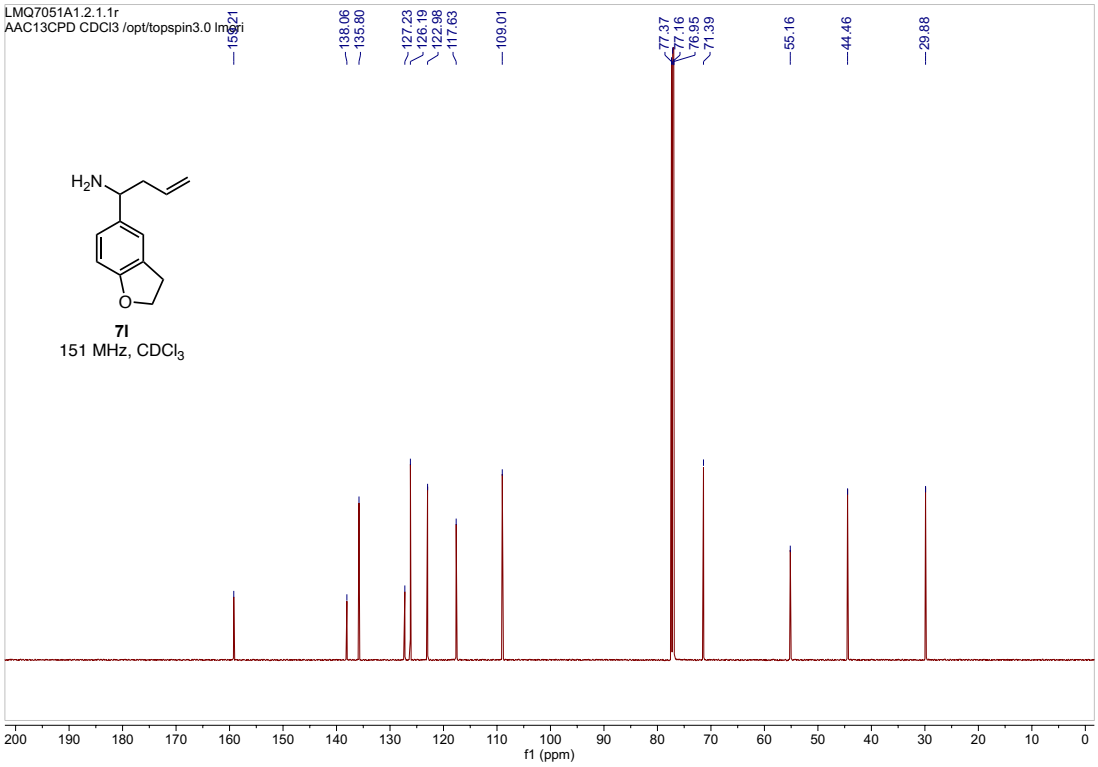

SSL1-205-pdt.1.fid
H2N
MeO
OMe
OMe
7j
400 MHz, CDCl3
2.01
1.00
2.09
1.07
6.14
3.09
1.03
1.04
2.14
f1 (ppm)

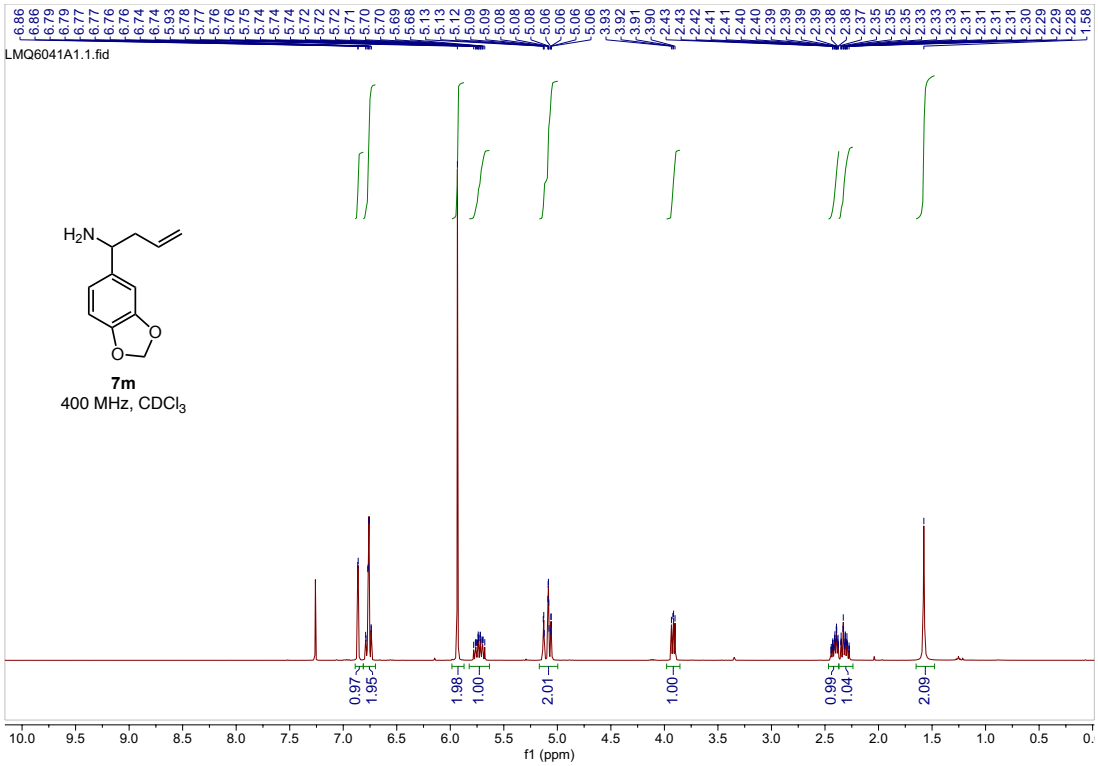

SSL1-205-pdt.2.1.1r
153.22
141.72
136.80
135.49
117.78
103.14
77.36
77.05
76.73
60.85
56.13
55.60
44.40
H2N
MeO
OMe
OMe
7j
101 MHz, CDCl3
f1 (ppm)

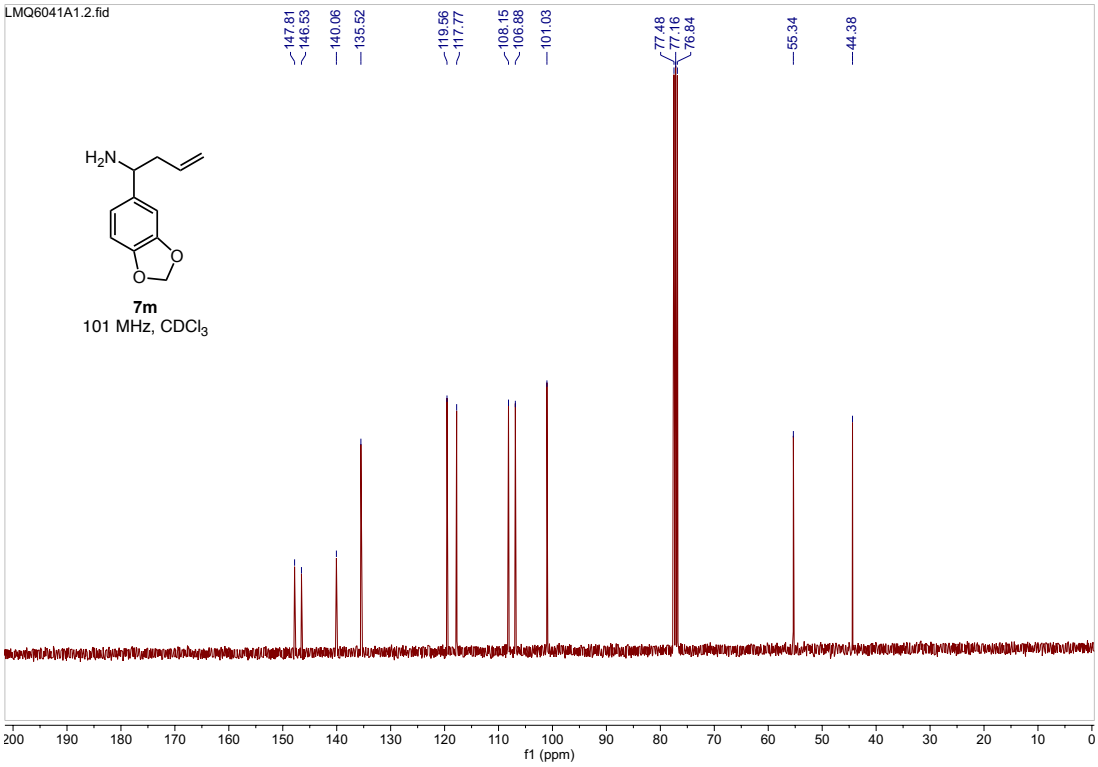

SSL1-196-pdt2.1.fid
H2N
7k
400 MHz, CDCl3
1.02
1.00
1.01
1.02
3.06
1.00
2.09
1.03
1.02
1.04
2.13
f1 (ppm)

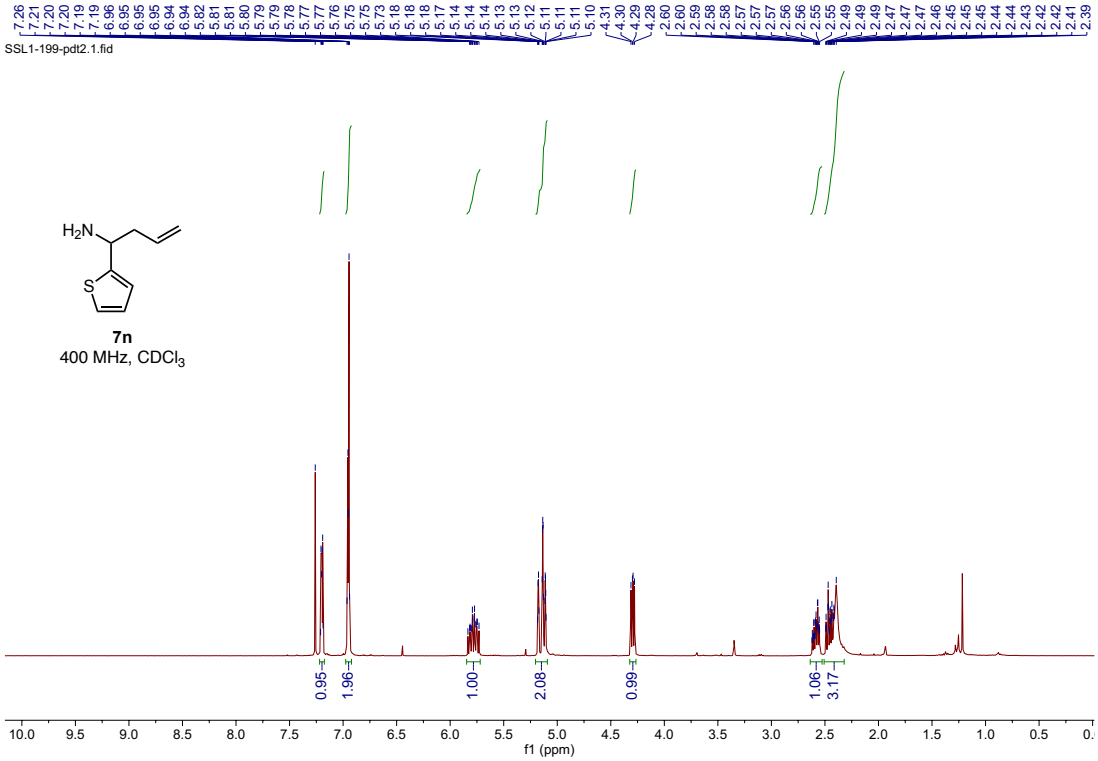

SSL1-196-pdt.2.fid
141.38
135.61
133.90
130.81
129.04
127.41
126.00
125.55
125.45
122.84
122.52
117.82
77.36
77.05
76.73
50.33
43.15
H2N
7k
101 MHz, CDCl3
f1 (ppm)

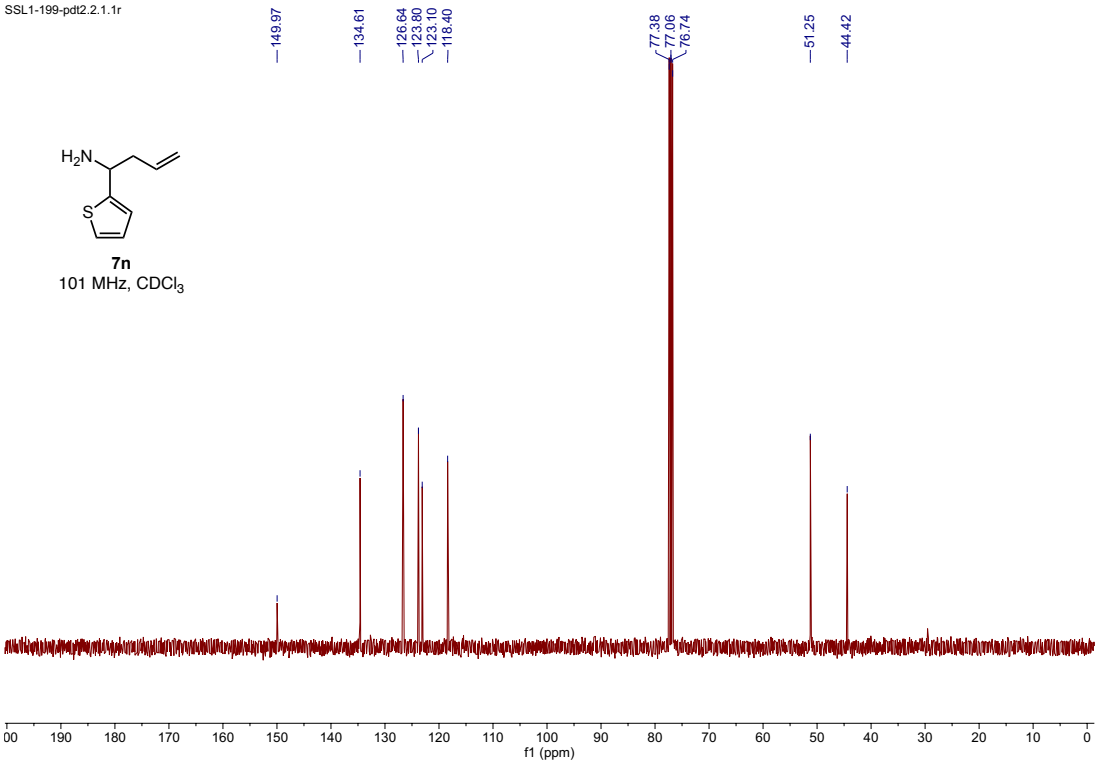

LMQ7051A1.1.fid
AAPROTON CDCl3 /opt/topspin3.0 lmori
7.26
7.26
7.20
7.06
7.04
6.73
6.72
5.78
5.77
5.76
5.76
5.75
5.75
5.74
5.73
5.73
5.72
5.72
5.72
5.71
5.13
5.10
5.08
5.06
4.57
4.57
4.56
4.56
4.54
4.54
3.94
3.93
3.93
3.92
3.92
3.21
3.19
3.18
2.45
2.44
2.43
2.42
2.41
2.36
2.34
2.33
2.32
2.31
1.64
H2N
O
7l
600 MHz, CDCl3
0.99
1.00
0.99
0.98
2.03
2.04
1.00
2.05
1.01
1.03
2.29
f1 (ppm)

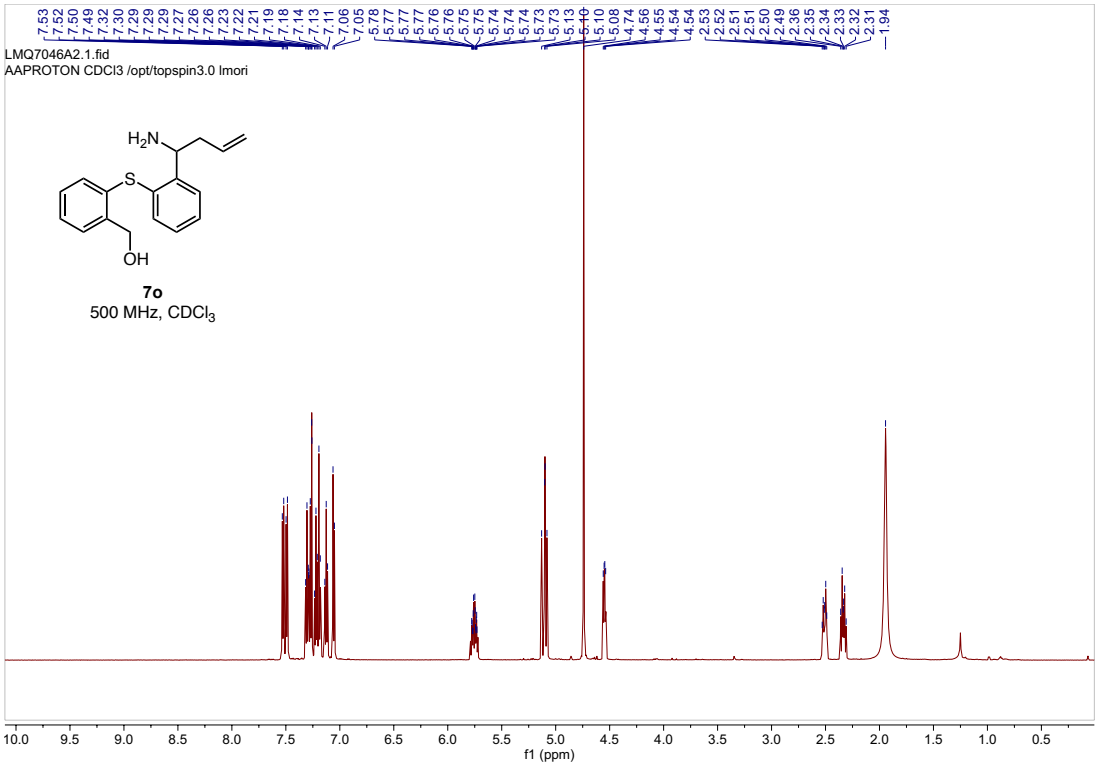

LMQ7051A1.2.1.1r
AAC13CPD CDCl3 /opt/topspin3.0 lm
159.21
138.06
135.80
127.23
126.19
122.98
117.63
109.01
77.37
77.16
76.95
71.39
55.16
44.46
29.88
H2N
O
7l
151 MHz, CDCl3
f1 (ppm)

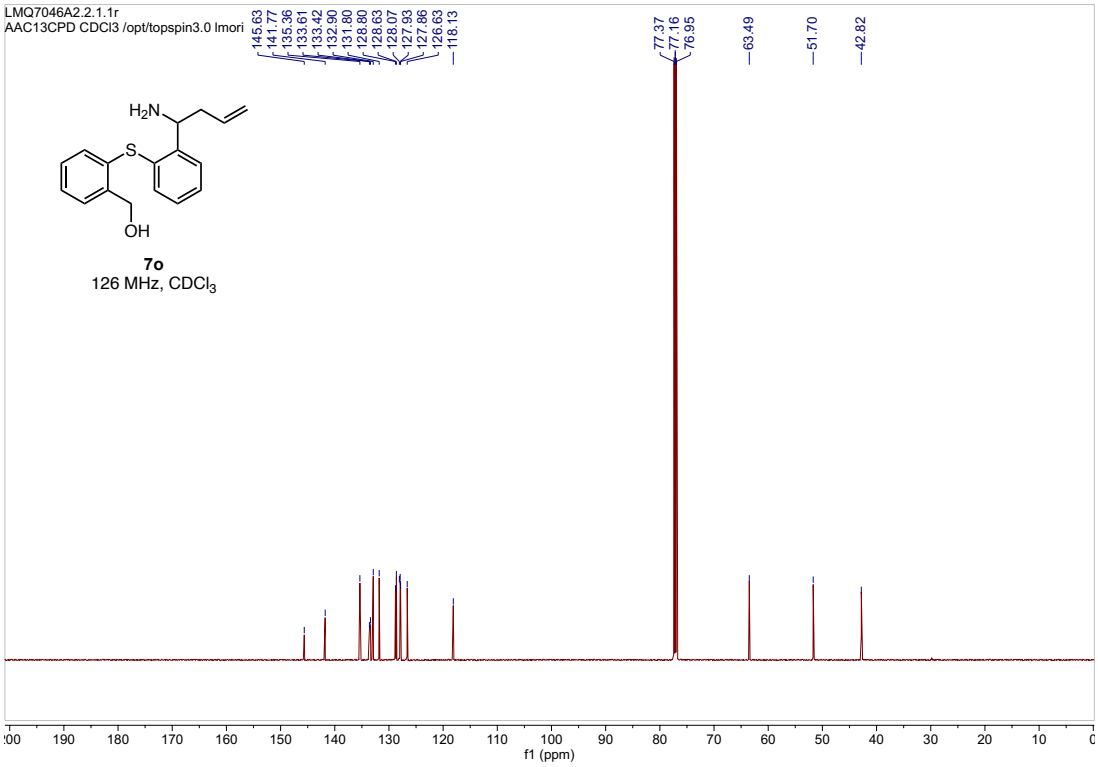

LMQ6041A1.1.fid
H2N
O
O
7m
400 MHz, CDCl3
0.97
1.95
1.98
1.00
2.01
1.00
0.99
1.04
2.09
f1 (ppm)

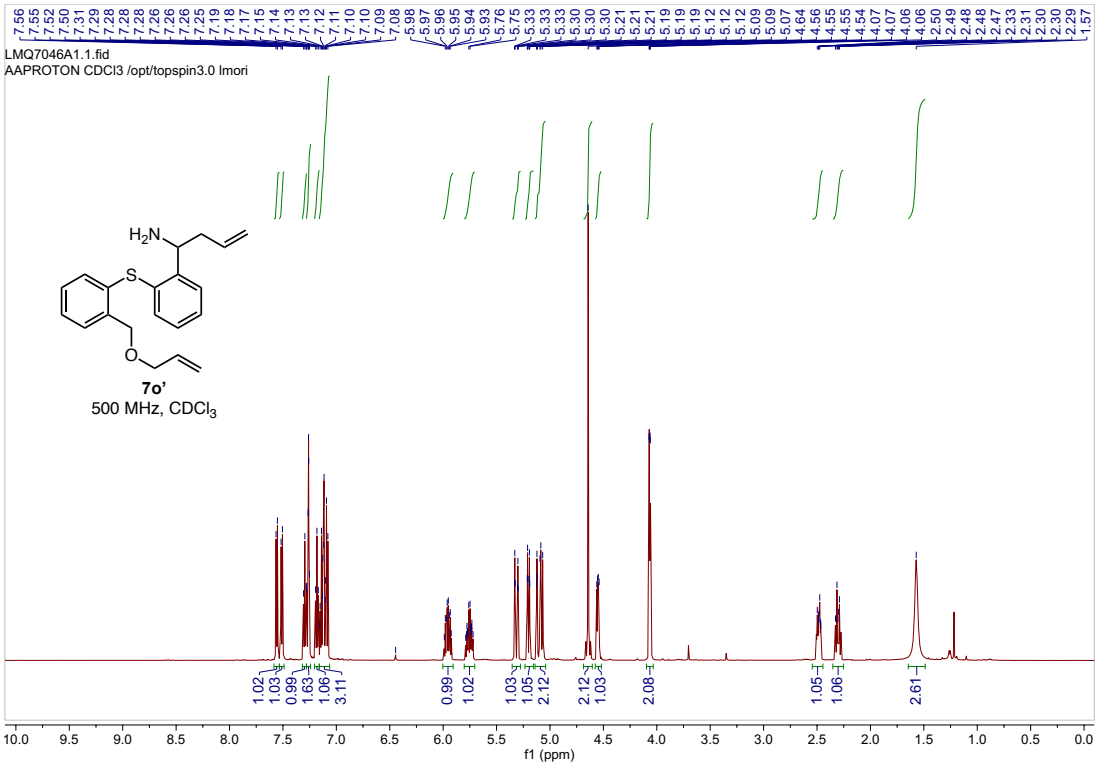

LMQ6041A1.2.fid
147.81
146.53
140.06
135.52
119.56
117.77
108.15
106.88
101.03
77.48
77.16
76.84
55.34
44.38
H2N
O
O
7m
101 MHz, CDCl3
f1 (ppm)

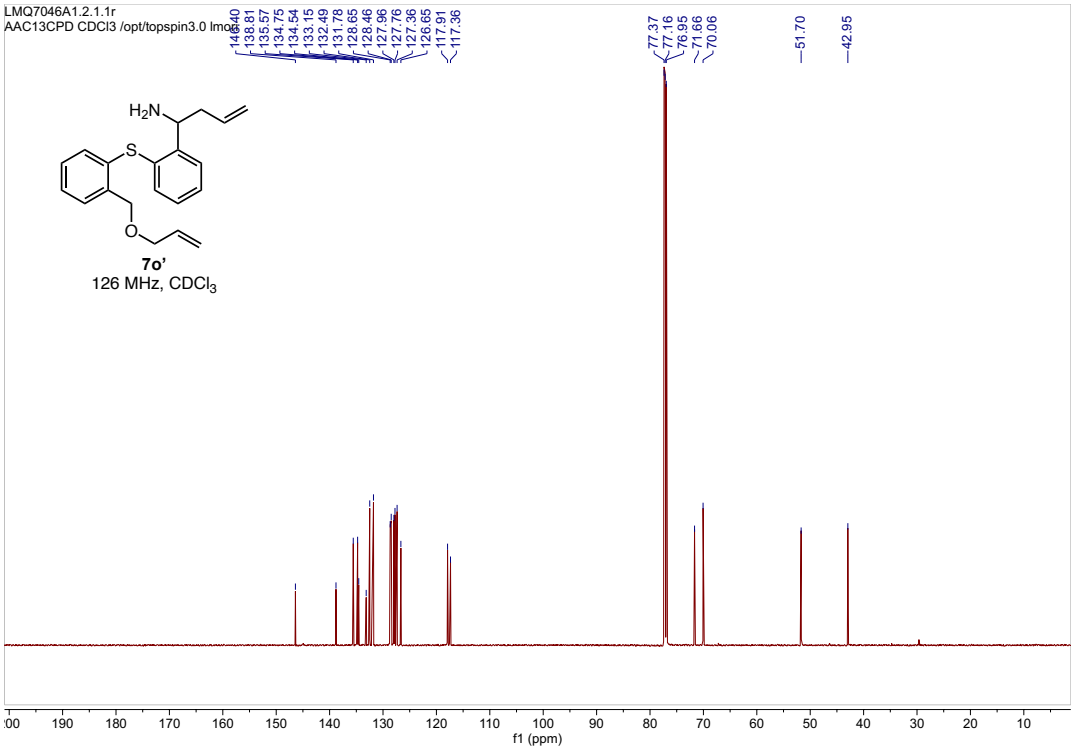

SSL1-199-pdt2.1.fid
H2N
S
7n
400 MHz, CDCl3
0.95
1.96
1.00
2.08
0.99
1.06
3.17
f1 (ppm)

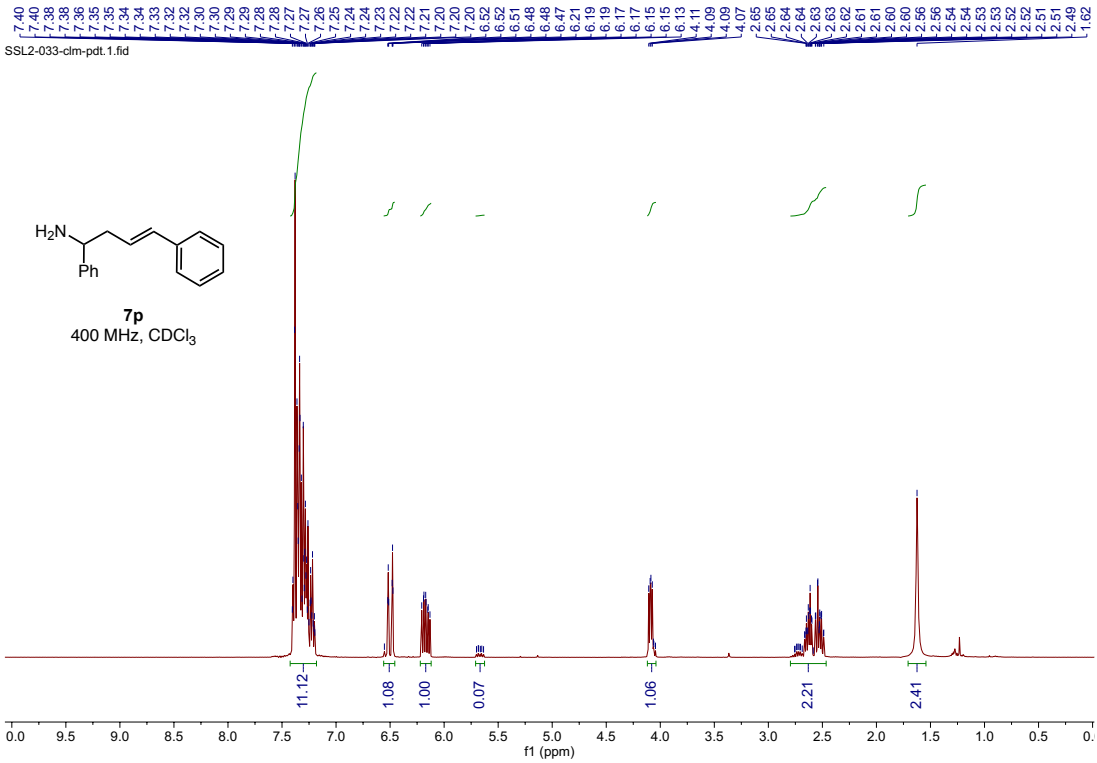

SSL1-199-pdt2.2.1.1r
149.97
134.61
126.64
123.80
123.10
118.40
77.38
77.06
76.74
51.25
44.42
H2N
S
7n
101 MHz, CDCl3
f1 (ppm)

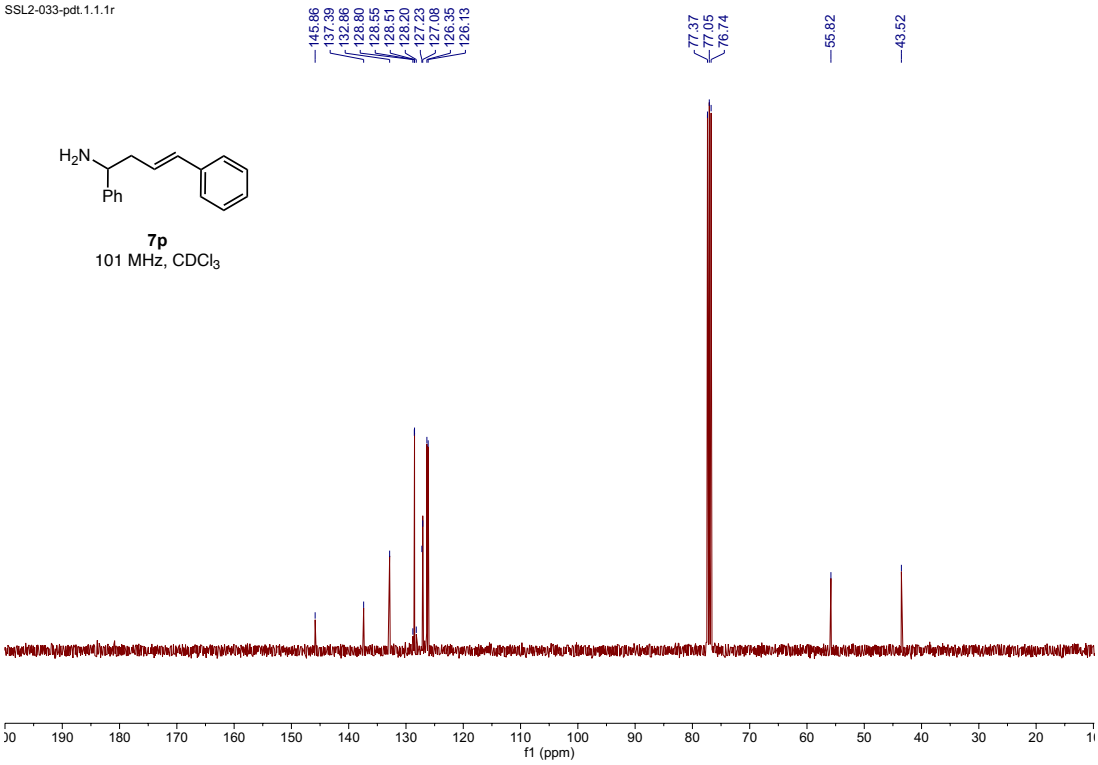

LMQ7046A2.1.fid
AAPROTON CDCl3 /opt/topspin3.0 lmori
H2N
S
OH
7o
500 MHz, CDCl3
f1 (ppm)

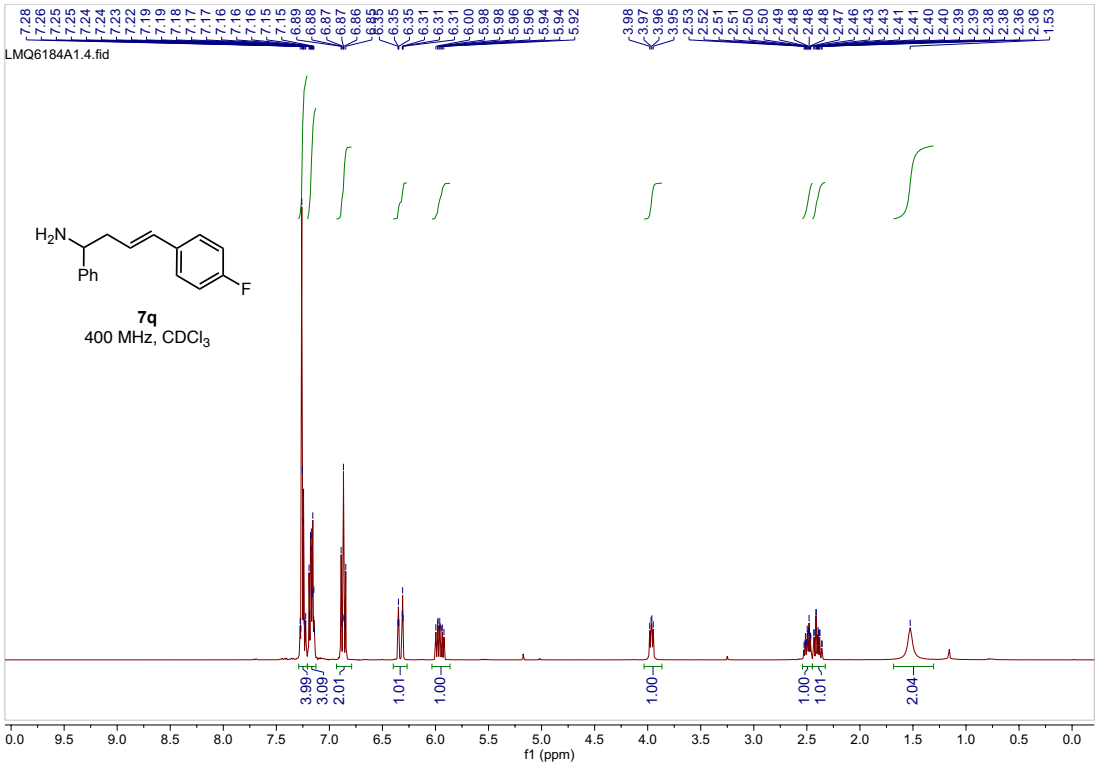

LMQ7046A2.2.1.1r
AAC13CPD CDCl3 /opt/topspin3.0 lmori
145.63
141.77
135.36
133.61
133.42
132.96
131.80
128.80
128.63
128.07
127.93
127.86
126.63
118.13
77.37
77.16
76.95
63.49
51.70
42.82
H2N
S
OH
7o
126 MHz, CDCl3
f1 (ppm)

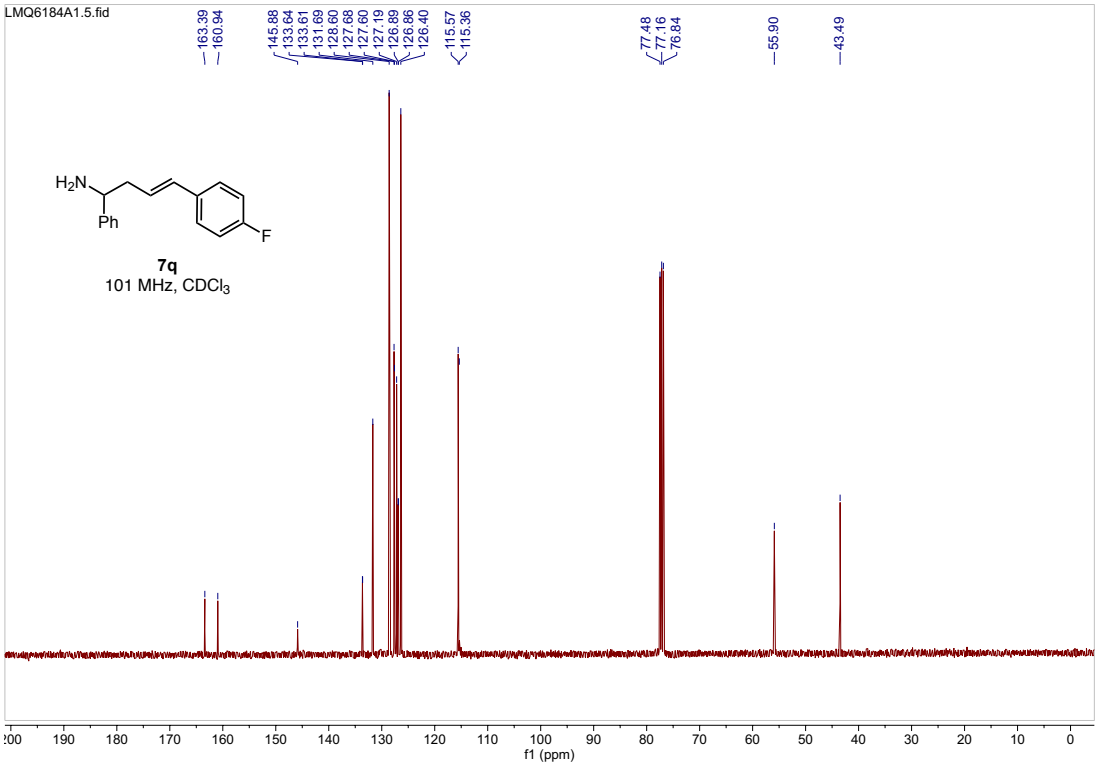

LMQ7046A1.1.fid
AAPROTON CDCl3 /opt/topspin3.0 lmori
H2N
S
O
7o'
500 MHz, CDCl3
1.02
1.03
0.99
1.63
1.06
3.11
0.99
1.02
1.03
1.05
2.12
2.12
1.03
2.08
1.05
1.06
2.61
f1 (ppm)

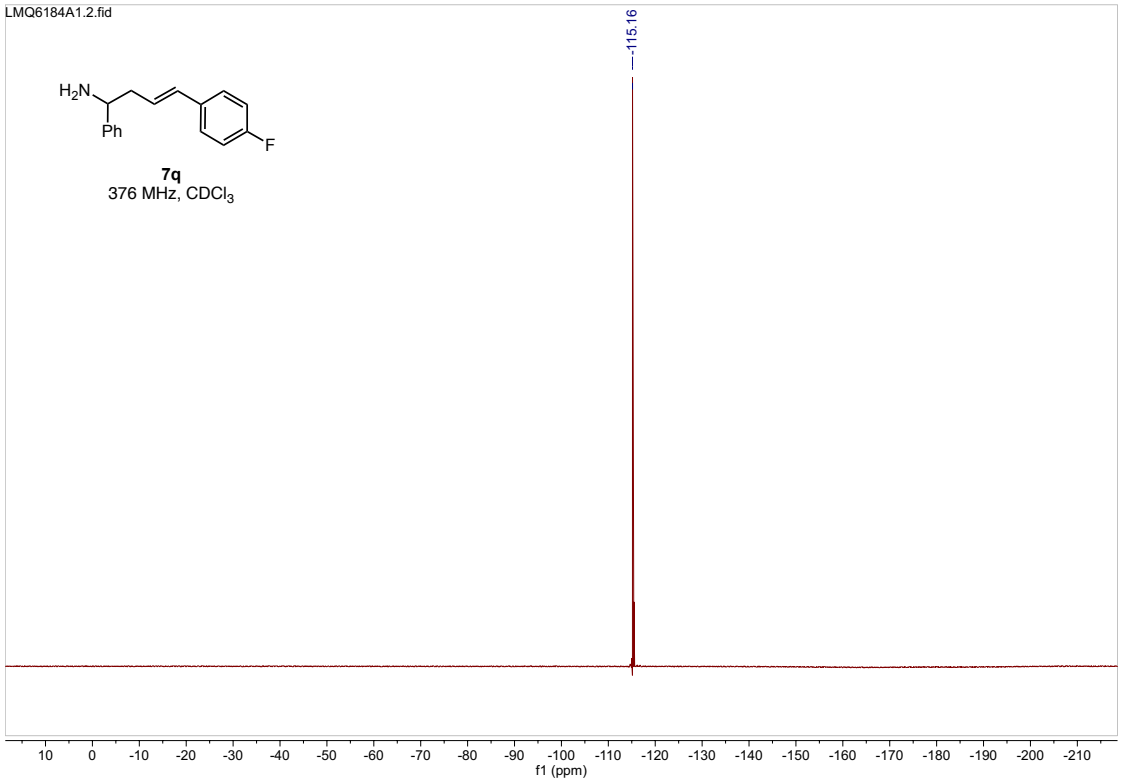

LMQ7046A1.2.1.1r
AAC13CPD CDCl3 /opt/topspin3.0 lm6
146.40
138.81
135.57
134.75
134.54
133.15
132.49
131.78
128.65
128.46
127.96
127.76
127.36
126.65
117.91
117.36
77.37
77.16
76.95
71.66
70.06
51.70
42.95
H2N
S
O
7o'
126 MHz, CDCl3
f1 (ppm)

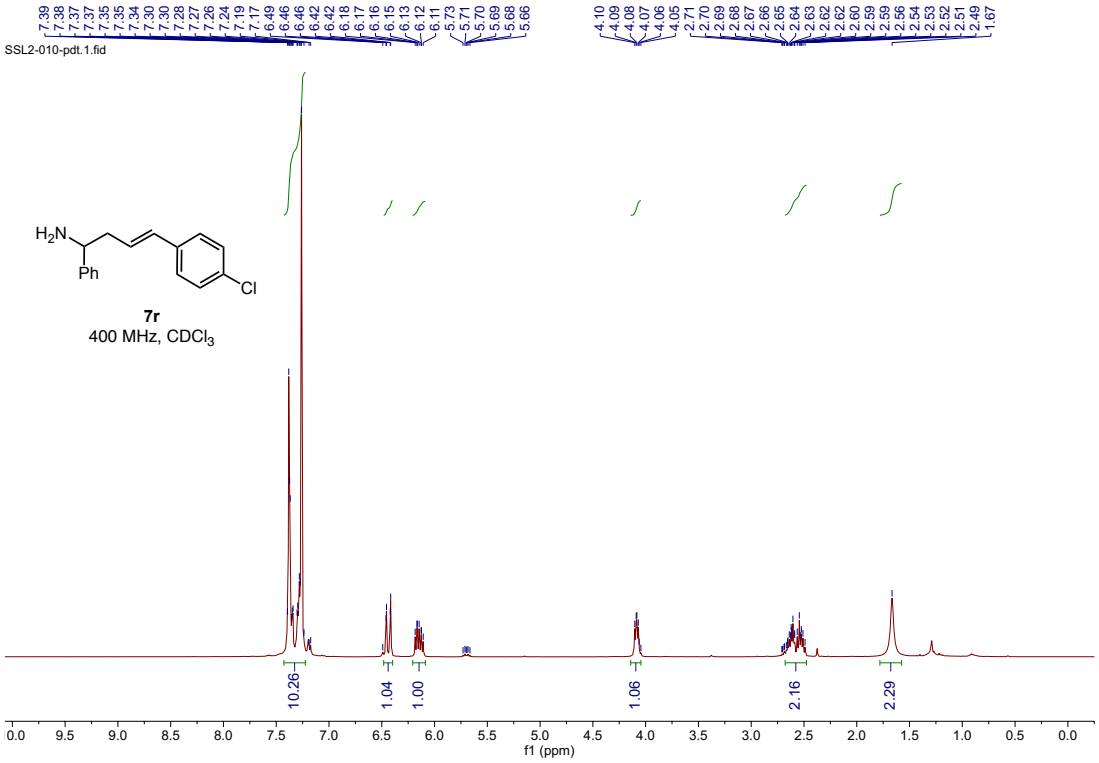

SSL2-033-clm-pdt.1.fid
H2N
Ph
7p
400 MHz, CDCl3
11.12
1.08
1.00
0.07
1.06
2.21
2.41
f1 (ppm)

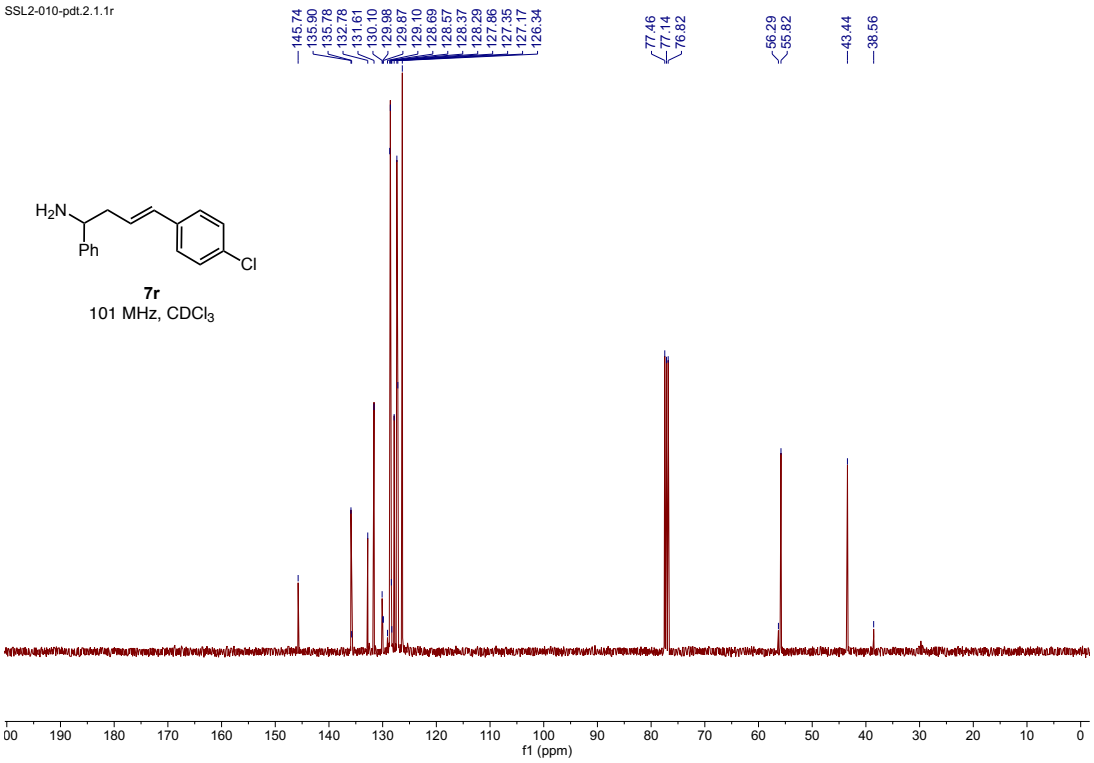

SSL2-033-pdt.1.1.1r
145.86
137.39
132.86
128.80
128.55
128.51
128.20
127.23
127.08
126.35
126.13
77.37
77.05
76.74
55.82
43.52
H2N
Ph
7p
101 MHz, CDCl3
f1 (ppm)

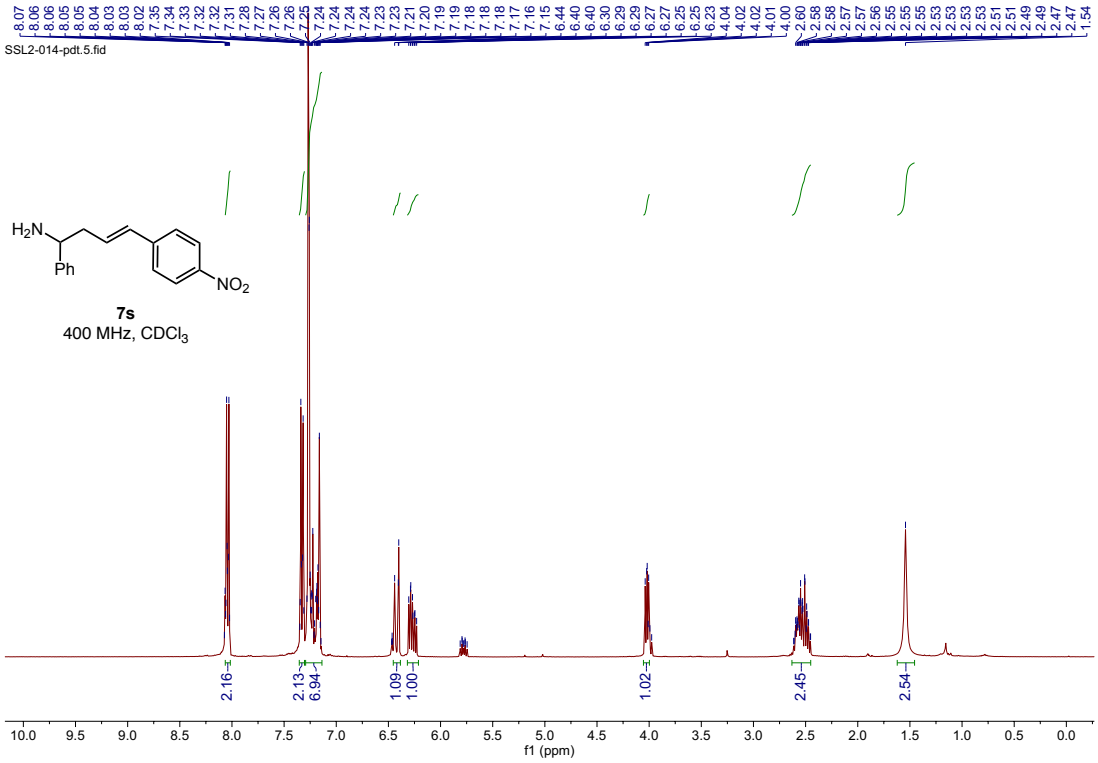

LMQ6184A1.4.fid
H2N
Ph
F
7q
400 MHz, CDCl3
3.99
3.09
2.01
1.01
1.00
1.00
1.00
1.01
2.04
f1 (ppm)

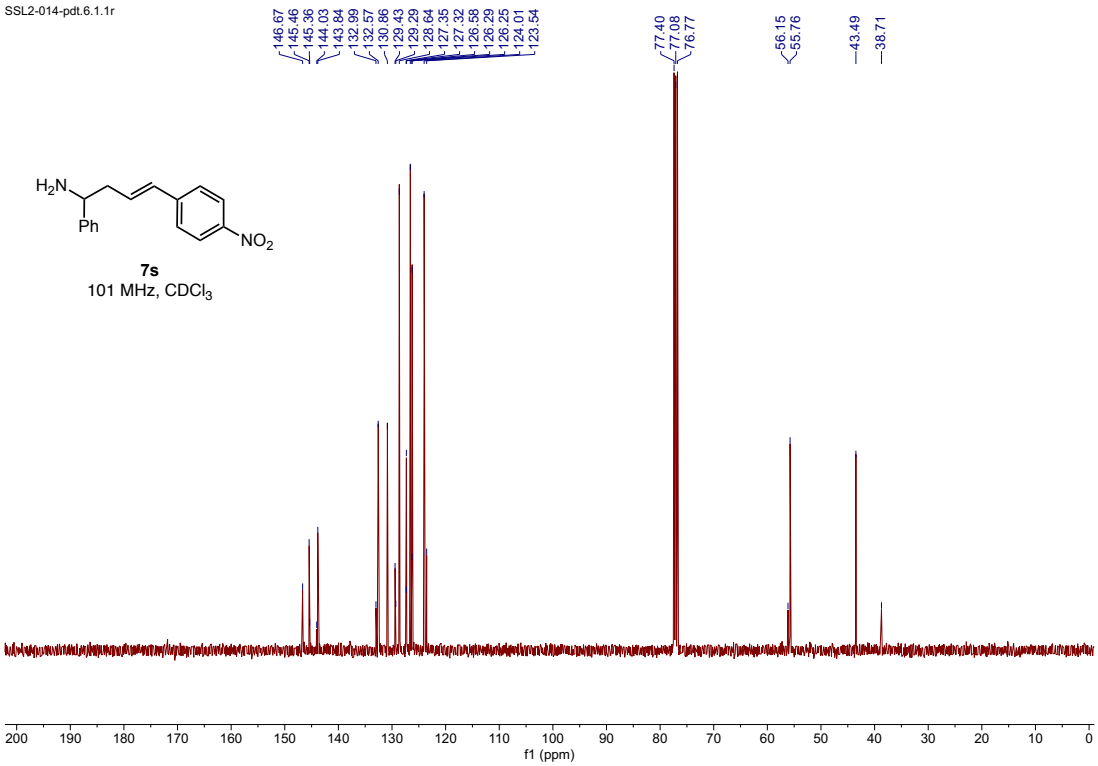

LMQ6184A1.5.fid
163.39
160.94
145.88
133.64
133.61
131.69
128.60
127.68
127.60
127.19
126.89
126.86
126.40
115.57
115.36
77.48
77.16
76.84
55.90
43.49
H2N
Ph
F
7q
101 MHz, CDCl3
f1 (ppm)

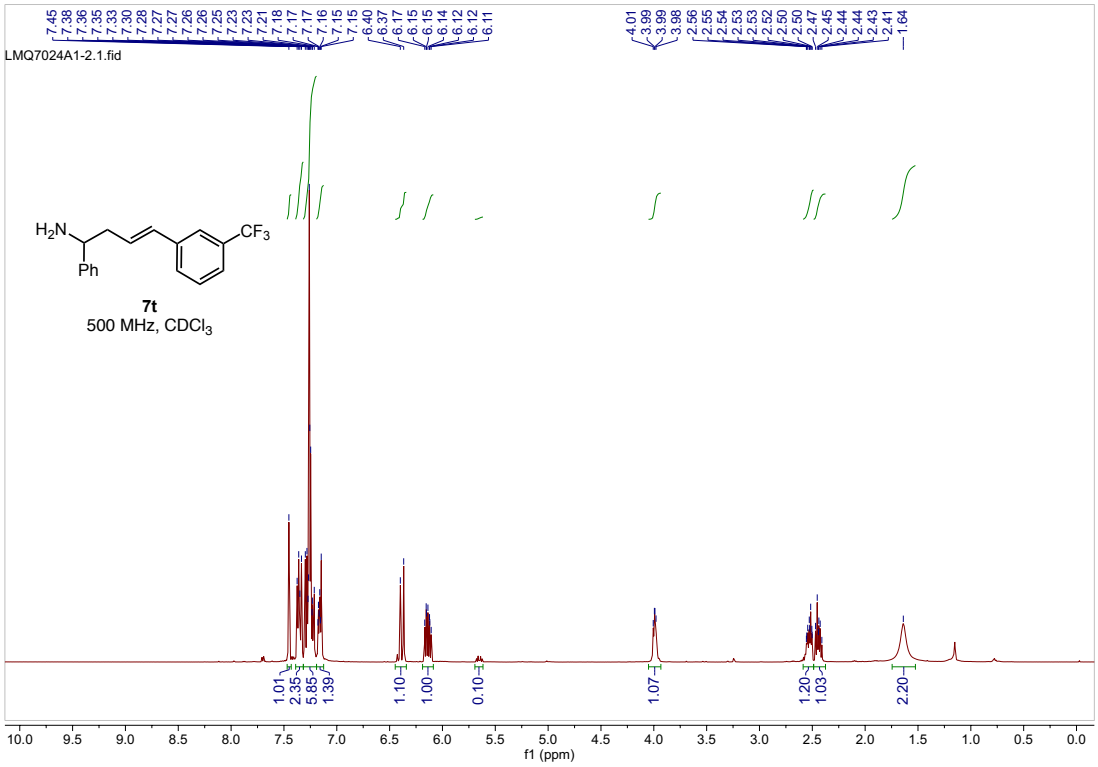

LMQ6184A1.2.fid
-115.16
H2N
Ph
F
7q
376 MHz, CDCl3
f1 (ppm)

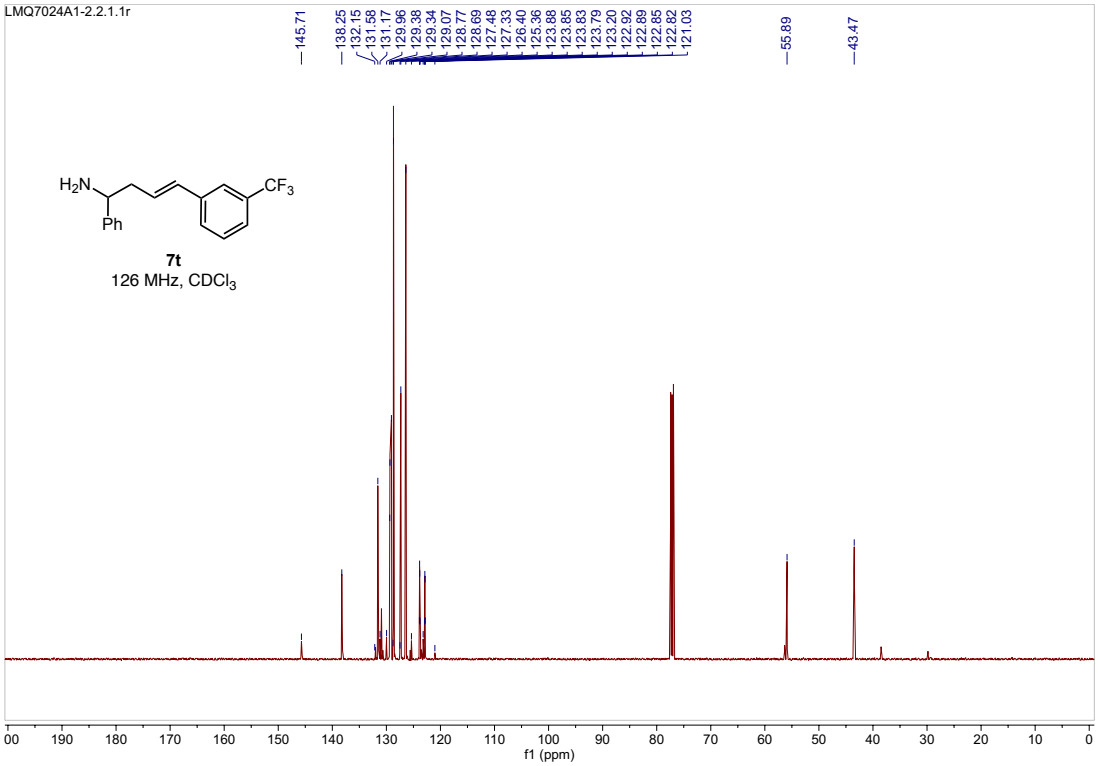

SSL2-010-pdt.1.fid
7.39 7.38 7.37 7.37 7.35 7.35 7.34 7.30 7.30 7.28 7.27 7.26 7.24 7.19 7.17 6.49 6.46 6.46 6.42 6.42 6.18 6.17 6.16 6.15 6.13 6.12 6.11 5.73 5.71 5.70 5.69 5.68 5.66
4.10 4.09 4.08 4.07 4.06 4.05 2.71 2.70 2.69 2.68 2.67 2.66 2.65 2.64 2.63 2.62 2.62 2.60 2.59 2.59 2.56 2.54 2.53 2.52 2.51 2.49 1.67
H2N
Ph
Cl
7r
400 MHz, CDCl3
10.26
1.04
1.00
1.06
2.16
2.29
f1 (ppm)

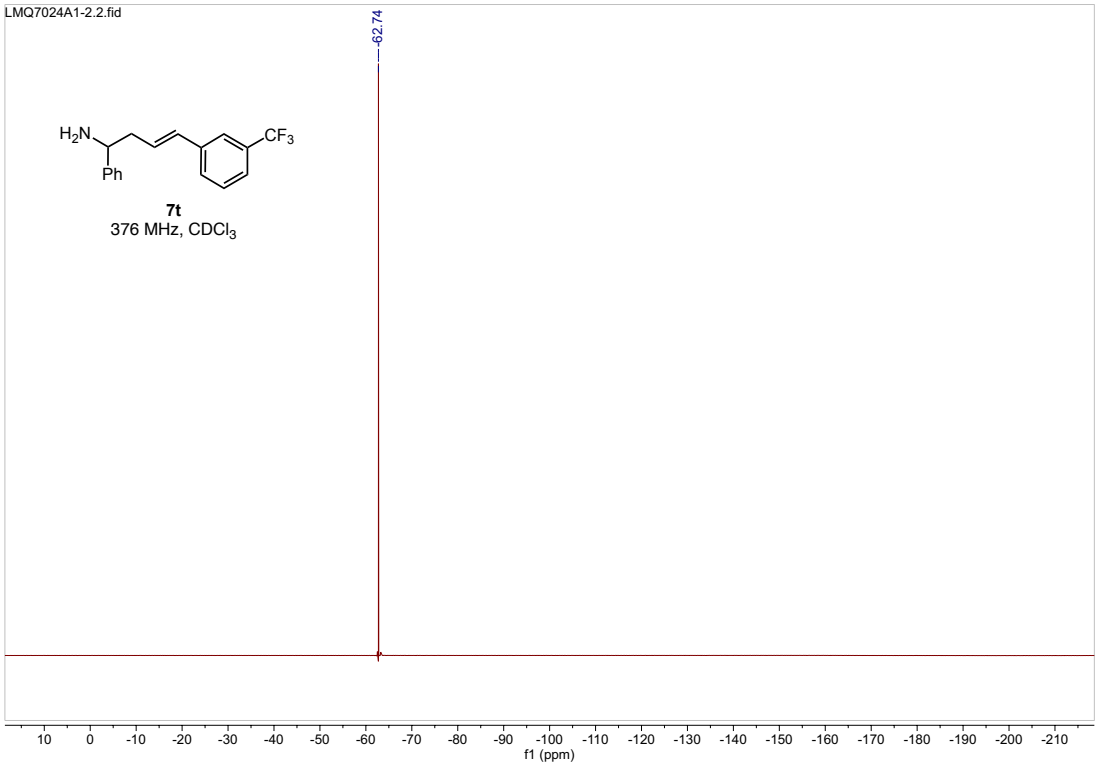

SSL2-010-pdt.2.1.1r
145.74 135.90 135.78 132.78 131.61 130.10 129.98 129.87 129.10 128.69 128.57 128.37 128.29 127.86 127.35 127.17 126.34
77.46 77.14 76.82
56.29 55.82
43.44
38.56
H2N
Ph
Cl
7r
101 MHz, CDCl3
f1 (ppm)

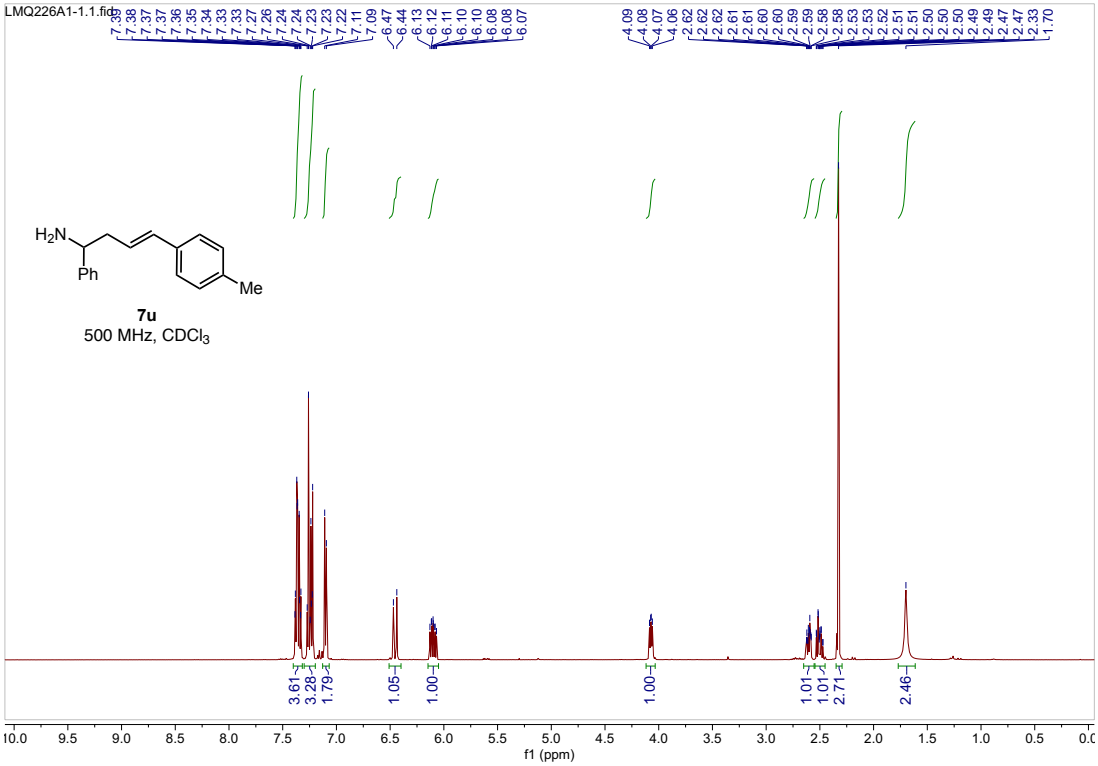

SSL2-014-pdt.5.fid
8.07 8.06 8.06 8.05 8.05 8.04 8.03 8.02 7.35 7.34 7.33 7.32 7.32 7.31 7.28 7.27 7.26 7.26 7.25 7.24 7.24 7.24 7.23 7.23 7.21 7.20 7.19 7.19 7.18 7.18 7.18 7.17 7.16 7.15 6.44 6.40 6.40 6.30 6.29 6.29 6.27 6.27 6.25 6.25 6.23 4.04 4.02 4.02 4.01 4.00 2.60 2.58 2.58 2.57 2.57 2.56 2.55 2.55 2.55 2.53 2.53 2.53 2.53 2.51 2.51 2.49 2.49 2.47 2.47 1.54
H2N
Ph
NO2
7s
400 MHz, CDCl3
2.16
2.13
6.94
1.09
1.00
1.02
2.45
2.54
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)

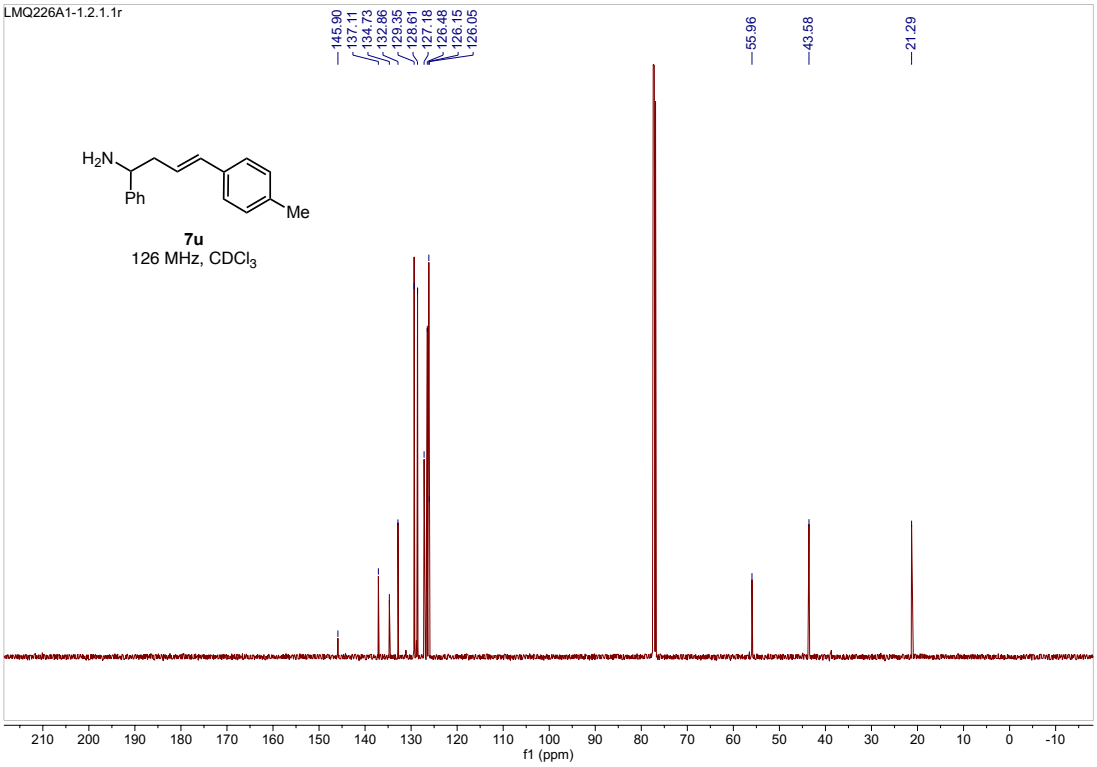

SSL2-014-pdt.6.1.1r
146.67 145.46 145.36 144.03 143.84 132.99 132.57 130.86 129.43 129.29 128.64 127.35 127.32 126.58 126.29 126.25 124.01 123.54
77.40 77.08 76.77
56.15 55.76
43.49
38.71
H2N
Ph
NO2
7s
101 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

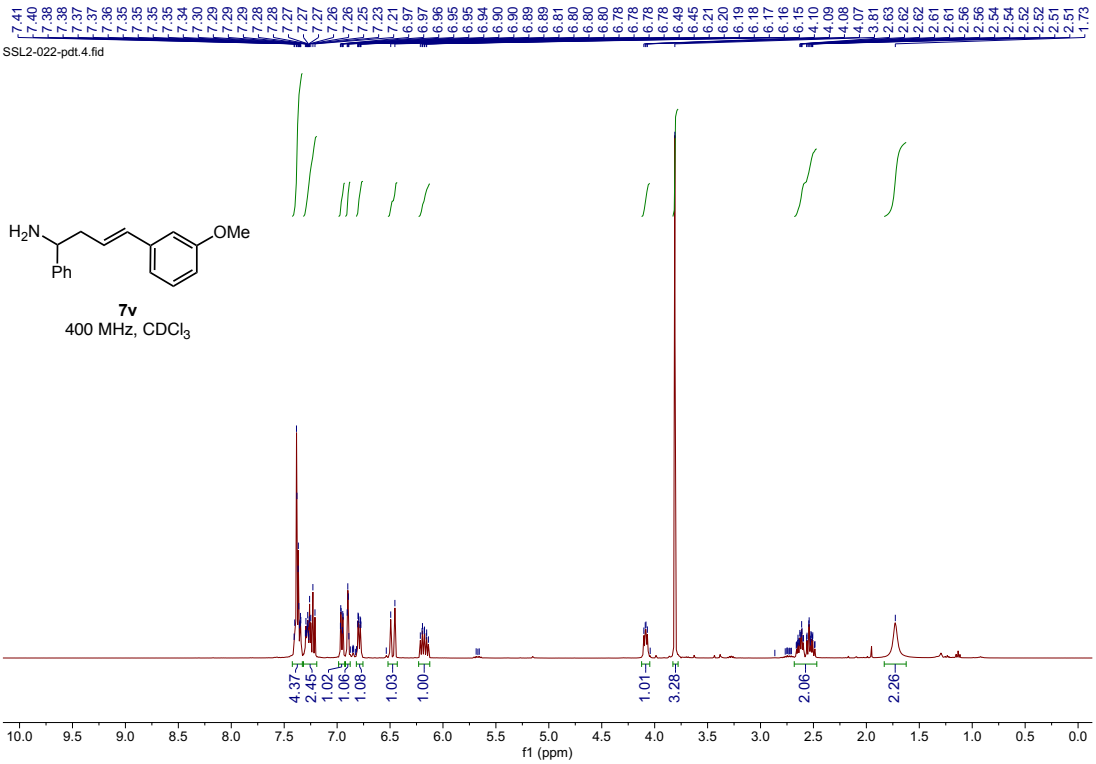

LMQ7024A1-2.1.fid
7.45 7.38 7.36 7.35 7.33 7.30 7.28 7.27 7.27 7.26 7.26 7.25 7.23 7.23 7.21 7.18 7.17 7.17 7.16 7.15 7.15 6.40 6.37 6.17 6.15 6.15 6.14 6.12 6.12 6.11
4.01 3.99 3.99 3.98 2.56 2.55 2.54 2.53 2.53 2.52 2.50 2.50 2.47 2.45 2.44 2.44 2.43 2.41 1.64
H2N
Ph
CF3
7t
500 MHz, CDCl3
1.01 2.35 5.85 1.39 1.10 1.00 0.10 1.07 1.20 1.03 2.20
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)

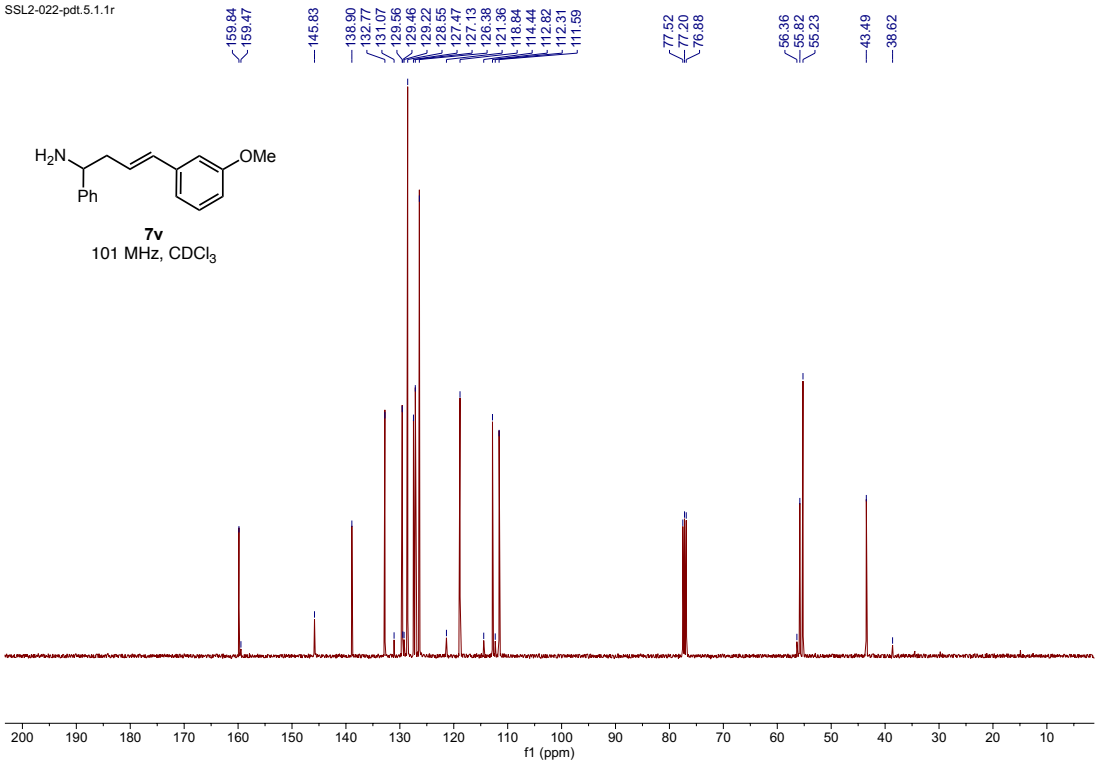

LMQ7024A1-2.2.1.1r
145.71
138.25 132.15 131.58 131.17 129.96 129.38 129.34 129.07 128.77 128.69 127.48 127.33 126.40 125.36 123.88 123.85 123.83 123.79 123.20 122.92 122.89 122.85 122.82 121.03
55.89
43.47
H2N
Ph
CF3
7t
126 MHz, CDCl3
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

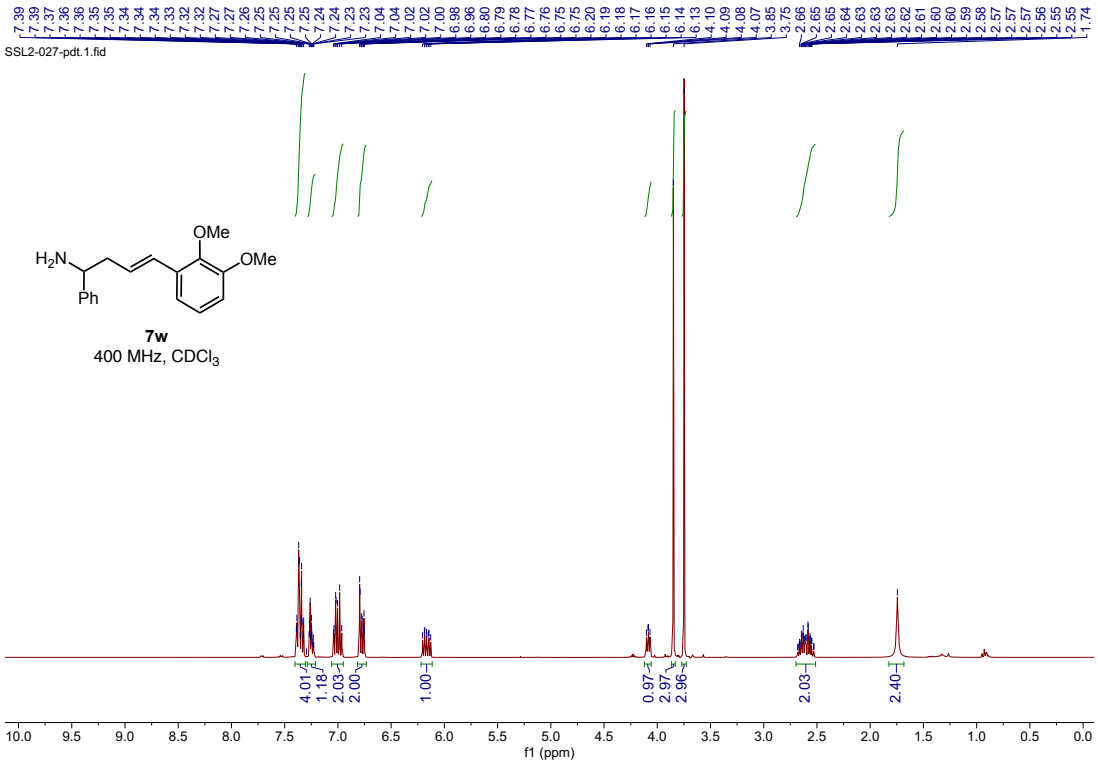

LMQ7024A1-2.2.fid
-62.74
H2N
Ph
CF3
7t
376 MHz, CDCl3
f1 (ppm)

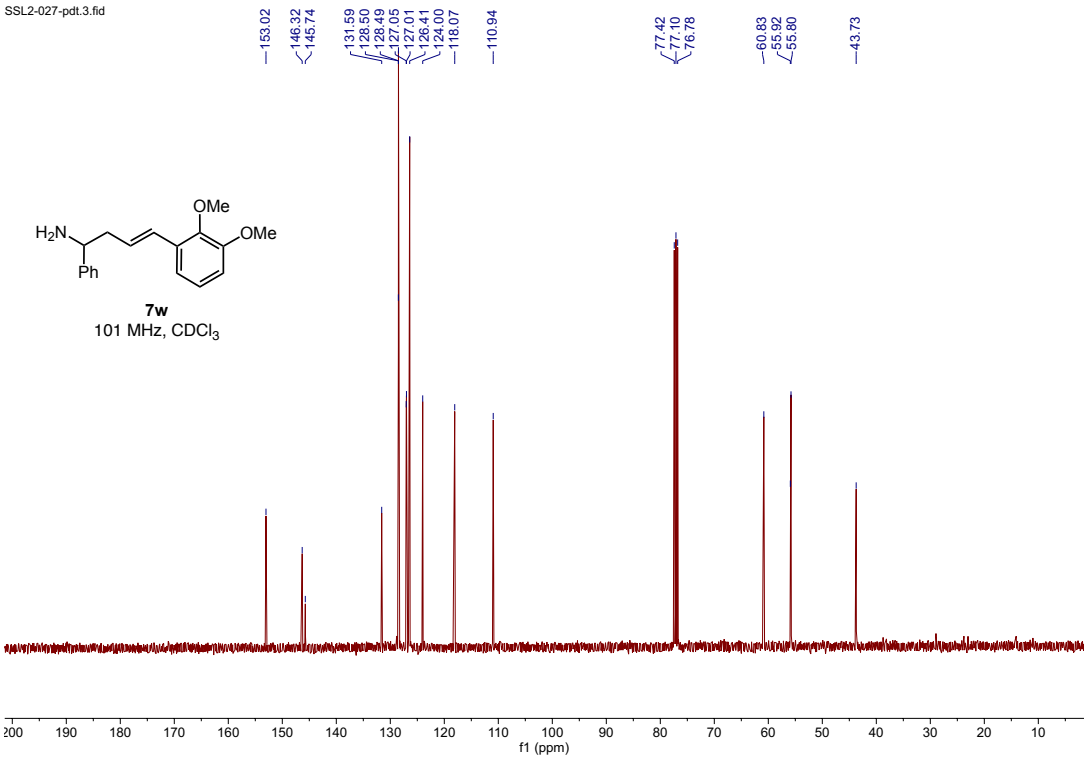

LMQ226A1-1.1.fid
H2N
Ph
Me
7u
500 MHz, CDCl3
3.61
3.28
1.79
1.05
1.00
1.00
1.01
1.01
2.71
2.46
f1 (ppm)

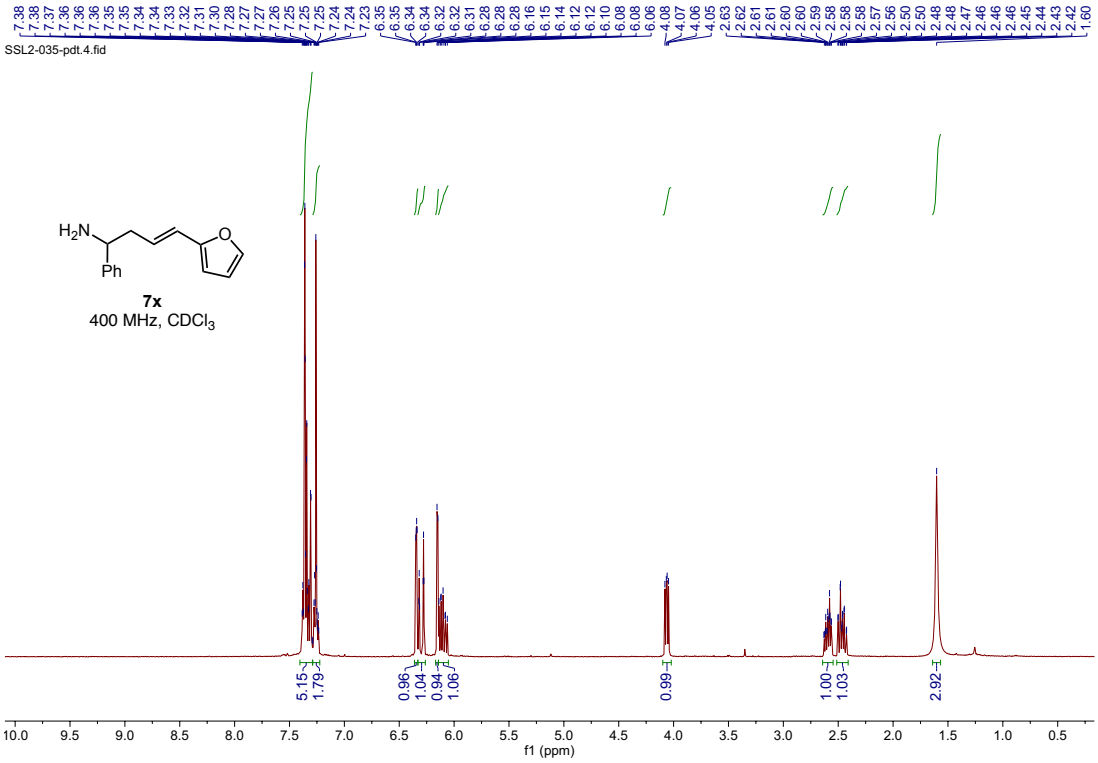

LMQ226A1-1.2.1.1r
145.90
137.11
134.73
132.86
129.35
128.61
127.18
126.48
126.15
126.05
55.96
43.58
21.29
H2N
Ph
Me
7u
126 MHz, CDCl3
f1 (ppm)

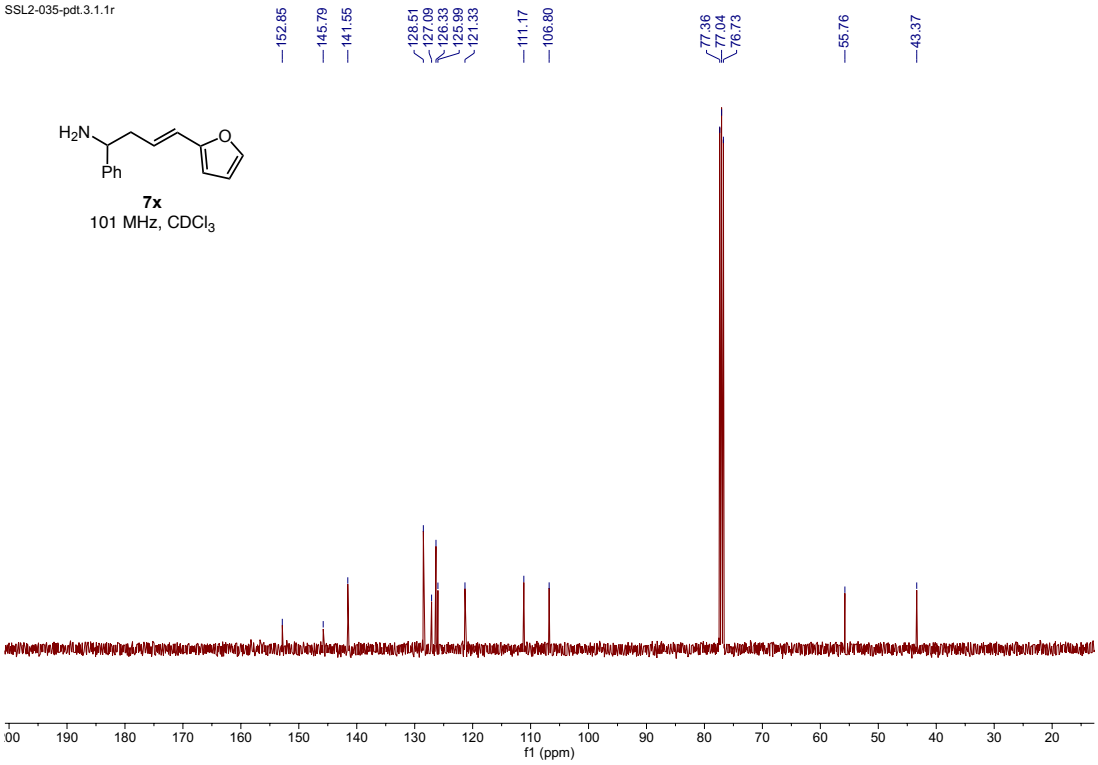

SSL2-022-pdt.4.fid
H2N
Ph
OMe
7v
400 MHz, CDCl3
4.37
2.45
1.02
1.06
1.08
1.03
1.00
1.01
3.28
2.06
2.26
f1 (ppm)

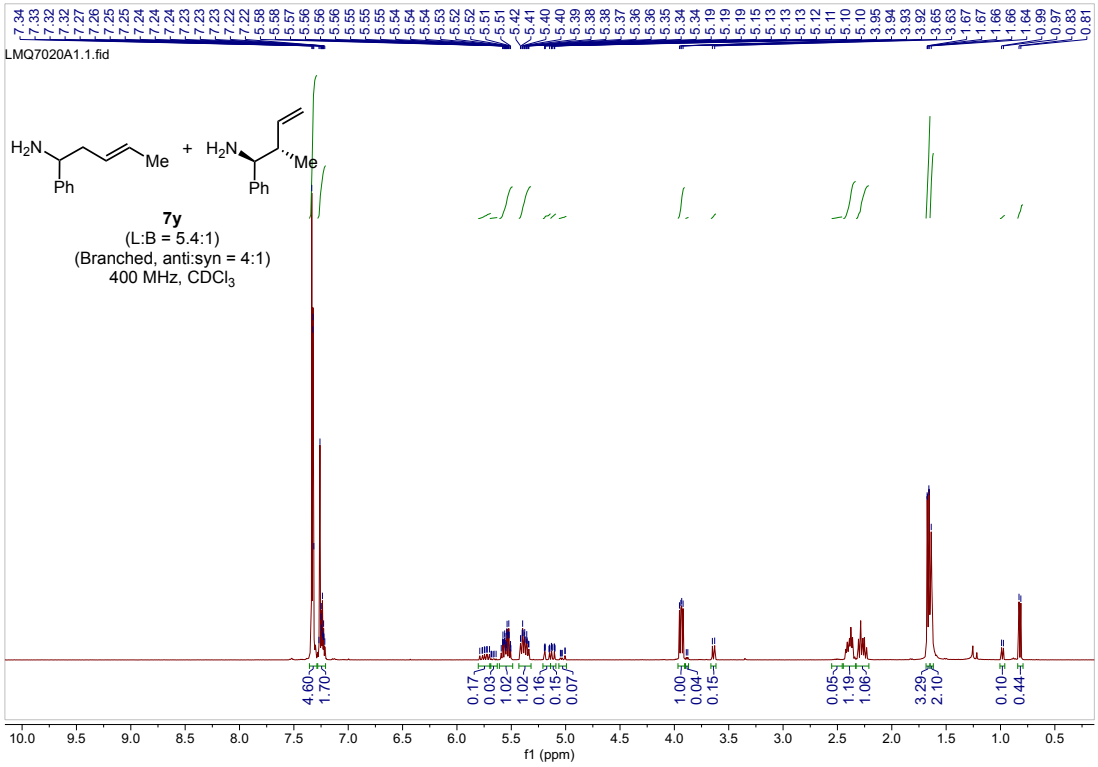

SSL2-022-pdt.5.1.1r
159.84
159.47
145.83
138.90
132.77
131.07
129.56
129.46
129.22
128.55
127.47
127.13
126.38
121.36
118.84
114.44
112.82
112.31
111.59
77.52
77.20
76.88
56.36
55.82
55.23
43.49
38.62
H2N
Ph
OMe
7v
101 MHz, CDCl3
f1 (ppm)

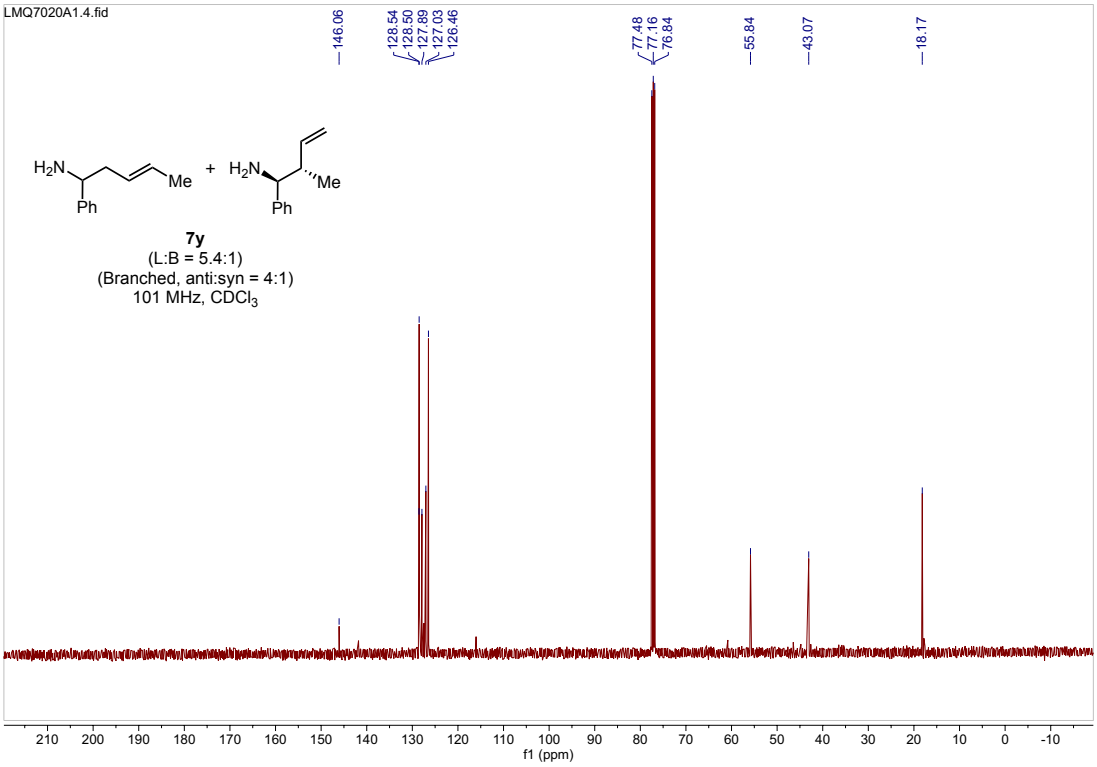

SSL2-027-pdt.1.fid
H2N
Ph
OMe
OMe
7w
400 MHz, CDCl3
4.01
1.18
2.03
2.00
1.00
0.97
2.97
2.96
2.03
2.40
f1 (ppm)

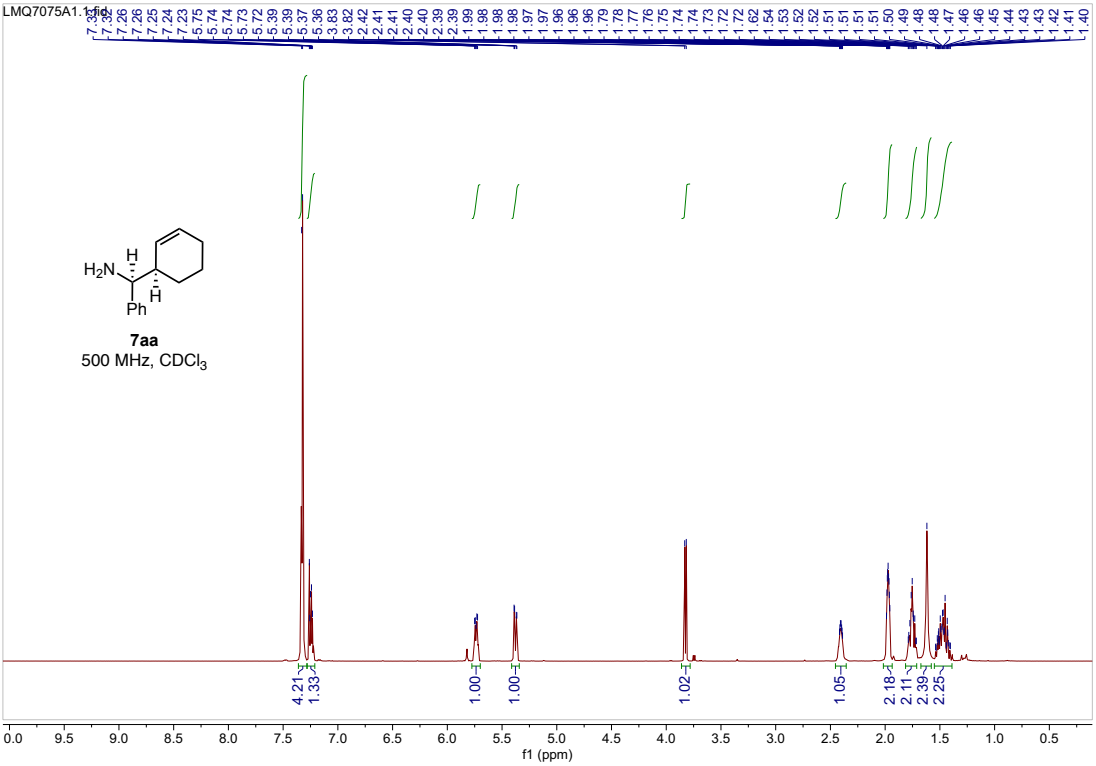

SSL2-027-pdt.3.fid
153.02
146.32
145.74
131.59
128.50
128.49
127.05
127.01
126.41
124.00
118.07
110.94
77.42
77.10
76.78
60.83
55.92
55.80
43.73
OMe
OMe
H2N
Ph
7w
101 MHz, CDCl3
f1 (ppm)

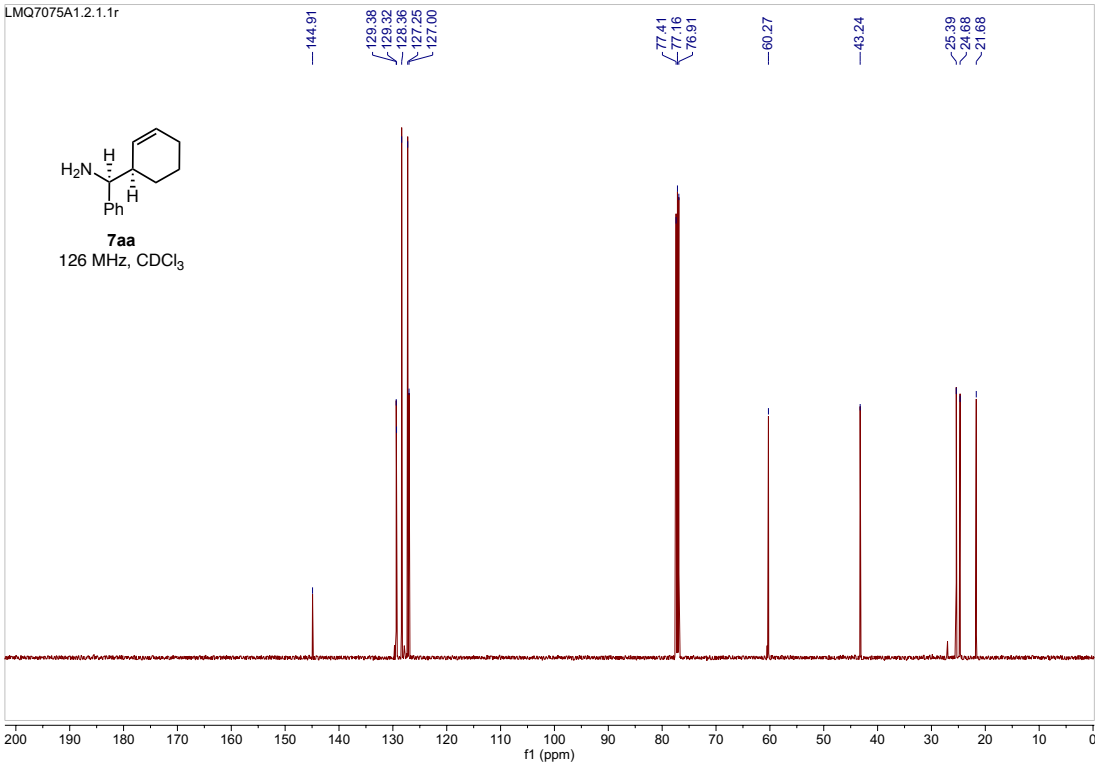

SSL2-035-pdt.4.fid
H2N
Ph
O
7x
400 MHz, CDCl3
5.15
1.79
0.96
1.04
0.94
1.06
0.99
1.00
1.03
2.92
f1 (ppm)

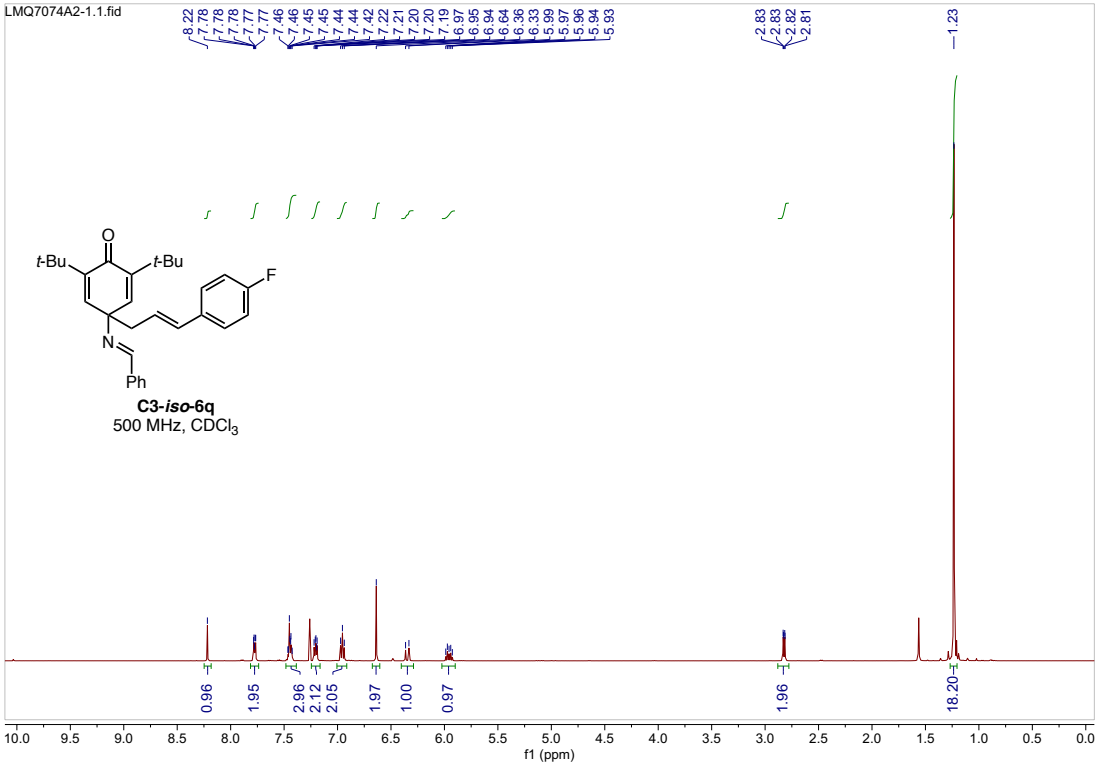

SSL2-035-pdt.3.1.1r
152.85
145.79
141.55
128.51
127.09
126.33
125.99
121.33
111.17
106.80
77.36
77.04
76.73
55.76
43.37
H2N
Ph
O
7x
101 MHz, CDCl3
f1 (ppm)

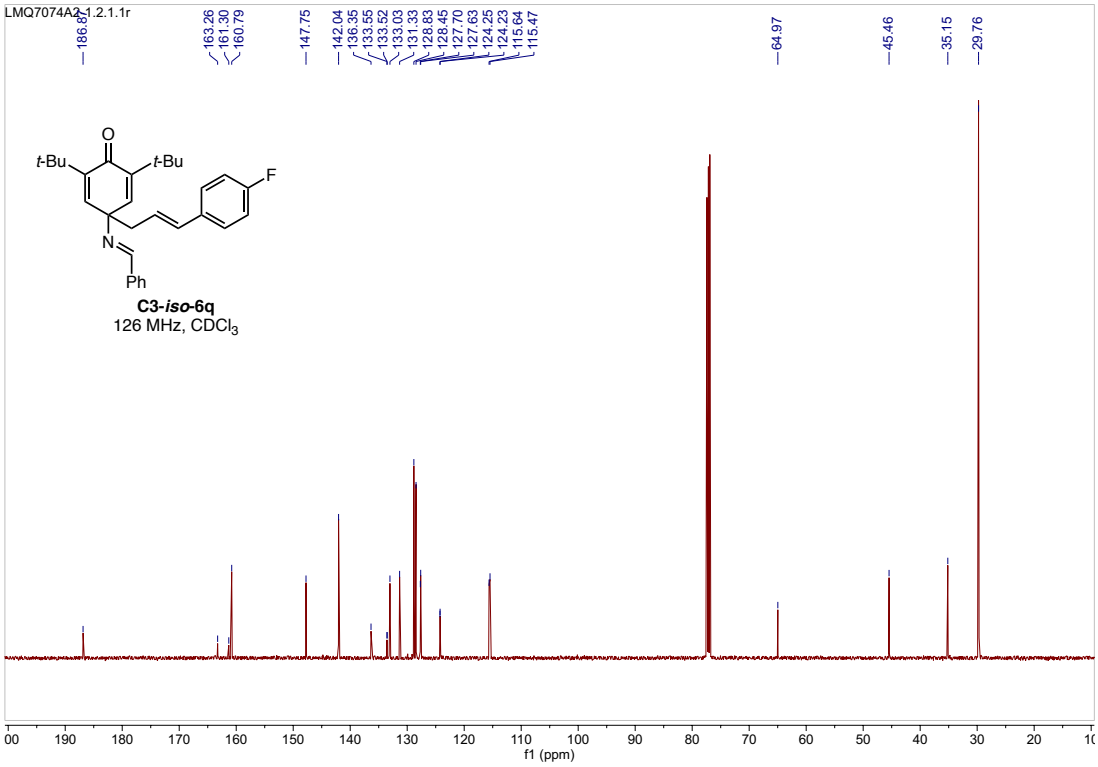

LMQ7020A1.1.fid
H2N
Ph
Me
+
H2N
Ph
Me
7y
(L:B = 5.4:1)
(Branched, anti:syn = 4:1)
400 MHz, CDCl3
4.60
1.70
0.17
0.03
1.02
1.02
0.16
0.15
0.07
1.00
0.04
0.15
0.05
1.19
1.06
3.29
2.10
0.10
0.44
f1 (ppm)

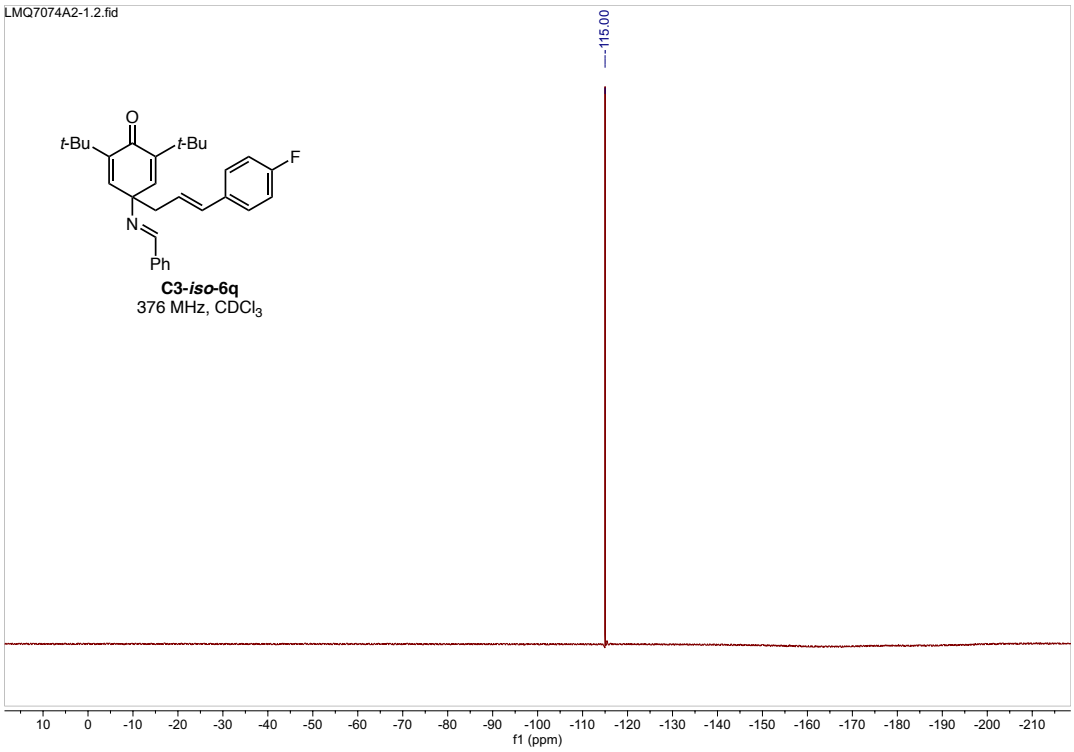

LMQ7020A1.4.fid
146.06
128.54
128.50
127.89
127.03
126.46
77.48
77.16
76.84
55.84
43.07
18.17
H2N
Me
Ph
+
H2N
Me
Ph
7y
(L:B = 5.4:1)
(Branched, anti:syn = 4:1)
101 MHz, CDCl3
f1 (ppm)

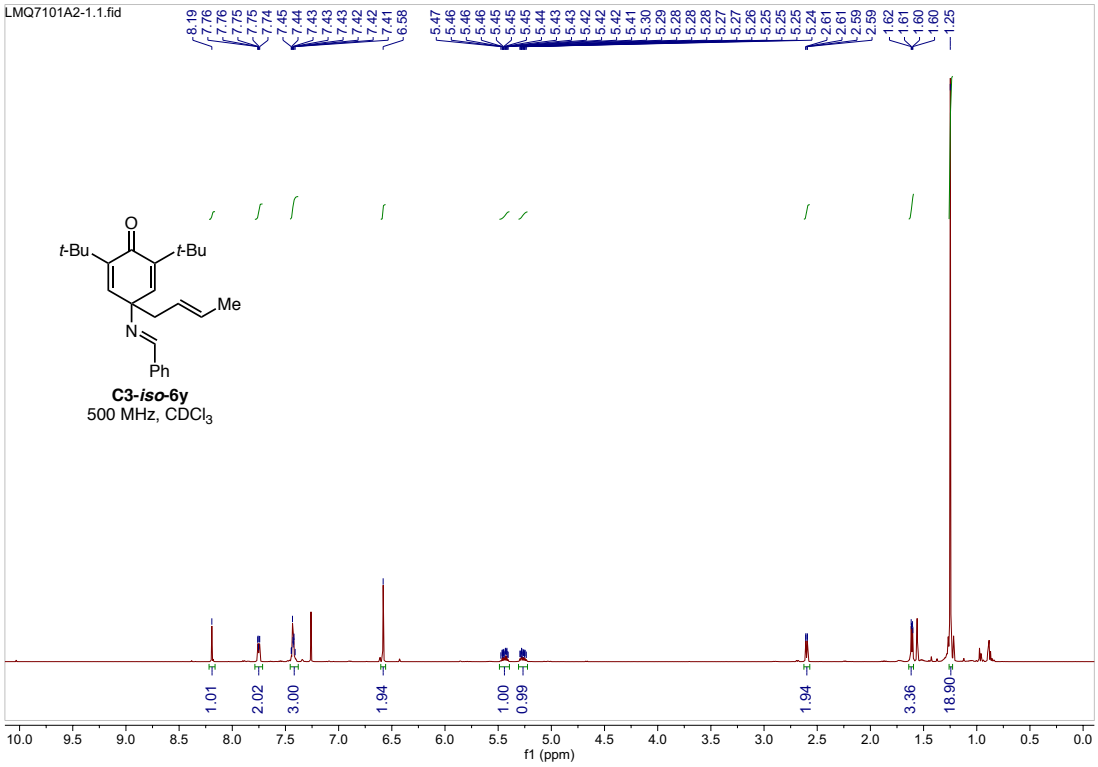

LMQ7075A1.1.fid
H2N
H
H
Ph
7aa
500 MHz, CDCl3
4.21
1.33
1.00
1.00
1.02
1.05
2.18
2.11
2.39
2.25
f1 (ppm)

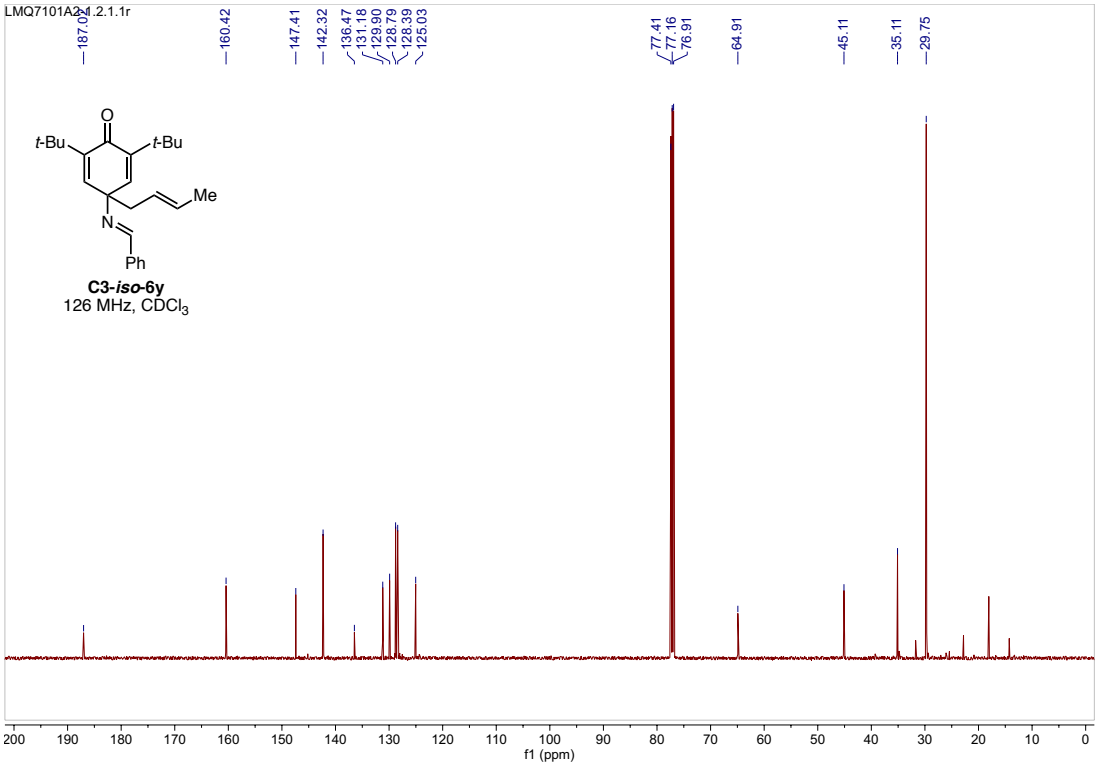

LMQ7075A1.2.1.1r
144.91
129.38
129.32
128.36
127.25
127.00
77.41
77.16
76.91
60.27
43.24
25.39
24.68
21.68
H
H_2N
H
Ph
7aa
126 MHz, $CDCl_3$
f1 (ppm)

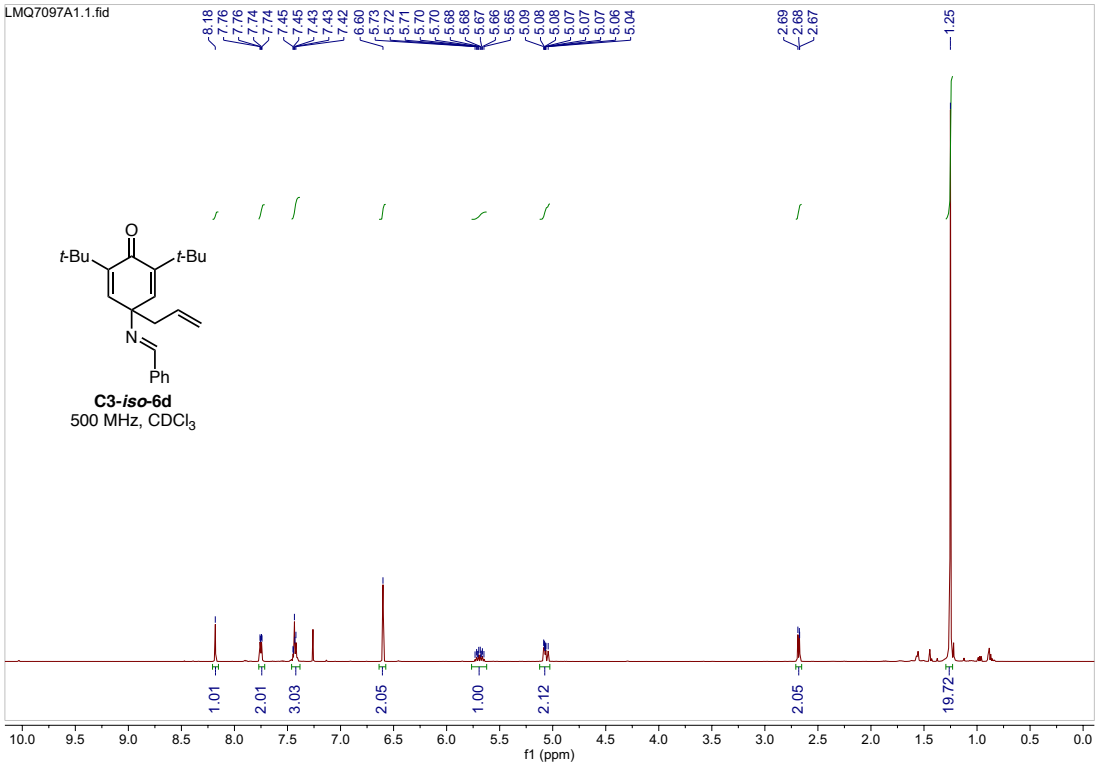

LMQ7074A2-1.1.fid
8.22
7.78
7.78
7.78
7.77
7.77
7.46
7.46
7.45
7.45
7.44
7.44
7.42
7.22
7.21
7.20
7.20
7.19
6.97
6.95
6.94
6.64
6.36
6.33
5.99
5.97
5.96
5.94
5.93
2.83
2.83
2.82
2.81
1.23
O
t-Bu
t-Bu
F
N
Ph
C3-iso-6q
500 MHz, $CDCl_3$
0.96
1.95
2.96
2.12
2.05
1.97
1.00
0.97
1.96
18.20
f1 (ppm)

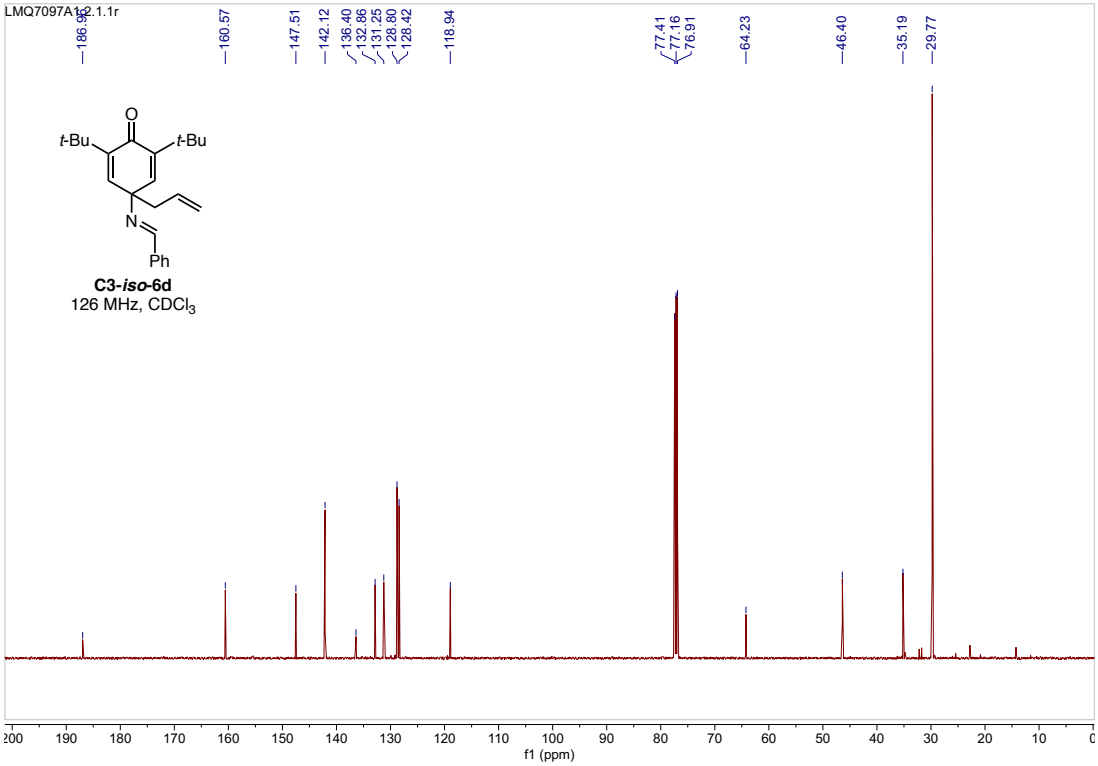

LMQ7074A2-1.2.1.1r
186.87
163.26
161.30
160.79
147.75
142.04
136.35
133.55
133.52
133.03
131.33
128.83
128.45
127.70
127.63
124.25
124.23
115.64
115.47
64.97
45.46
35.15
29.76
O
t-Bu
t-Bu
F
N
Ph
C3-iso-6q
126 MHz, CDCl3
f1 (ppm)

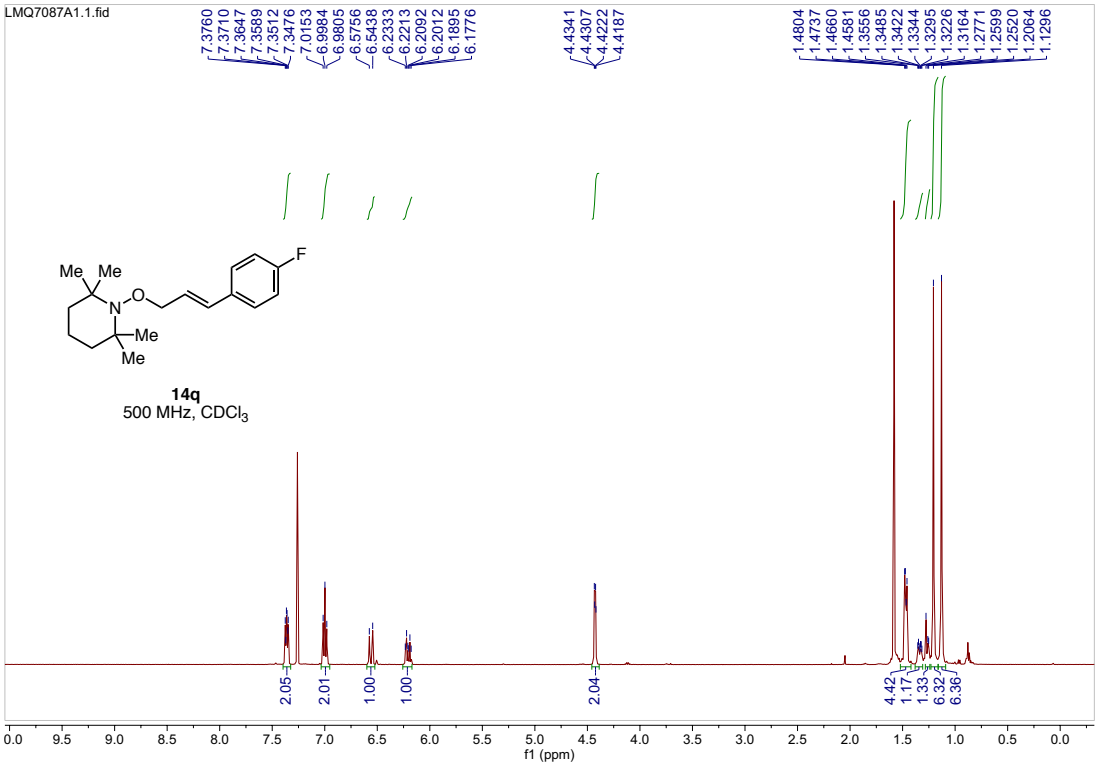

LMQ7074A2-1.2.fid
-115.00
O
t-Bu
t-Bu
F
N
Ph
C3-iso-6q
376 MHz, CDCl3
f1 (ppm)

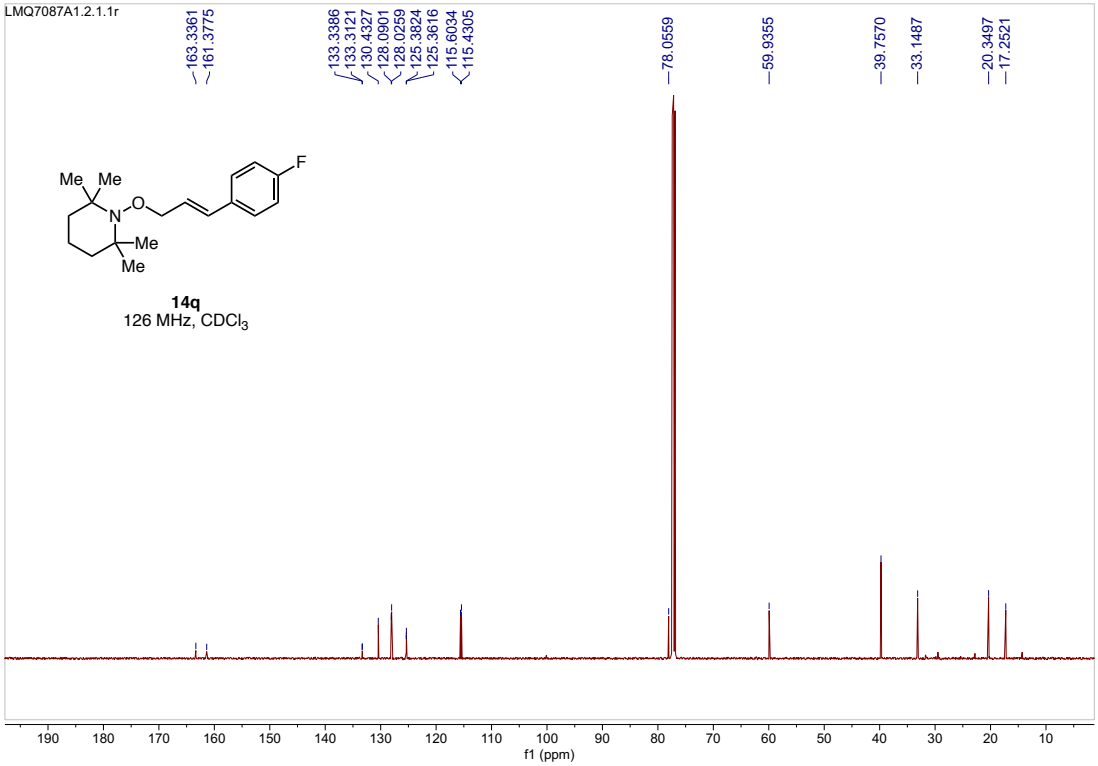

LMQ7101A2-1.1.fid
8.19 7.76 7.76 7.75 7.75 7.74 7.45 7.44 7.43 7.43 7.43 7.42 7.42 7.41 6.58
5.47 5.46 5.46 5.46 5.45 5.45 5.45 5.44 5.43 5.43 5.42 5.42 5.42 5.41 5.30 5.29 5.28 5.28 5.28 5.27 5.27 5.26 5.25 5.25 5.25 5.24
2.61 2.61 2.59 2.59
1.62 1.61 1.60 1.60 1.25
O
t-Bu
t-Bu
Me
N
Ph
C3-iso-6y
500 MHz, CDCl3
1.01 2.02 3.00 1.94 1.00 0.99 1.94 3.36 18.90
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)

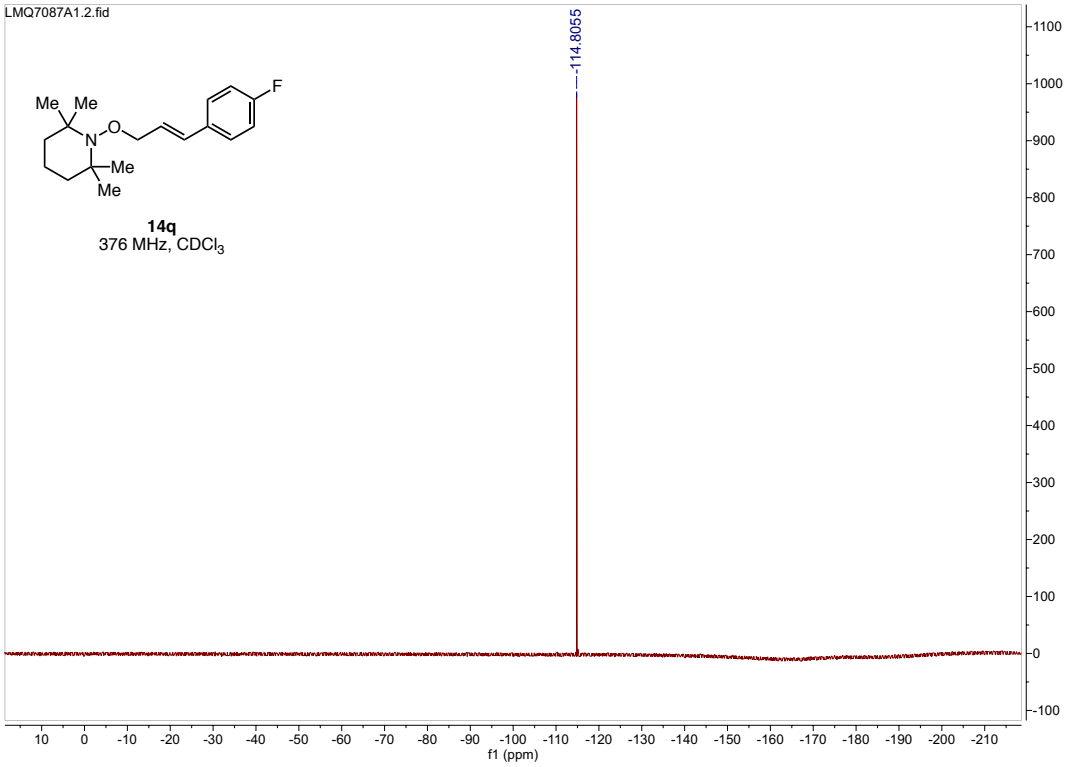

LMQ7101A2-1.2.1.1r
187.02
160.42
147.41
142.32
136.47 131.18 129.90 128.79 128.39 125.03
77.41 77.16 76.91
64.91
45.11
35.11
29.75
O
t-Bu
t-Bu
Me
N
Ph
C3-iso-6y
126 MHz, CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


LMQ7097A1.1.fid
8.18
7.76
7.76
7.74
7.74
7.45
7.45
7.43
7.43
7.42
6.60
5.73
5.72
5.71
5.70
5.70
5.68
5.68
5.67
5.66
5.65
5.09
5.08
5.08
5.07
5.07
5.07
5.06
5.04
2.69
2.68
2.67
1.25
O
t-Bu
t-Bu
N
Ph
C3-iso-6d
500 MHz, CDCl3
1.01
2.01
3.03
2.05
1.00
2.12
2.05
19.72
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)


LMQ7097A1c2.1.1r
186.91
160.57
147.51
142.12
136.40
132.86
131.25
128.80
128.42
118.94
77.41
77.16
76.91
64.23
46.40
35.19
29.77
O
t-Bu
t-Bu
N
Ph
C3-iso-6d
126 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


LMQ7087A1.1.fid
7.3760
7.3710
7.3647
7.3589
7.3512
7.3476
7.0153
6.9984
6.9805
6.5756
6.5438
6.2333
6.2213
6.2092
6.2012
6.1895
6.1776
4.4341
4.4307
4.4222
4.4187
1.4804
1.4737
1.4660
1.4581
1.3556
1.3485
1.3422
1.3344
1.3295
1.3226
1.3164
1.2771
1.2599
1.2520
1.2064
1.1296
Me
Me
N
O
Me
Me
F
14q
500 MHz, CDCl3
2.05
2.01
1.00
1.00
2.04
4.42
1.17
1.33
6.32
6.36
f1 (ppm)


LMQ7087A1.2.1.1r
163.3361
161.3775
133.3386
133.3121
130.4327
128.0901
128.0259
125.3824
125.3616
115.6034
115.4305
78.0559
59.9355
39.7570
33.1487
20.3497
17.2521
Me
Me
N
O
Me
Me
F
14q
126 MHz, CDCl3
f1 (ppm)


LMQ7087A1.2.fid
-114.8055
Me
Me
N
O
Me
Me
F
14q
376 MHz, CDCl3
f1 (ppm)