Supporting Information

Synthesis of Iminoisoindolinones via a Cascade of Three-Component Ugi Reaction, Palladium Catalyzed Isocyanide Insertion, Hydroxylation and an Unexpected Rearrangement Reaction

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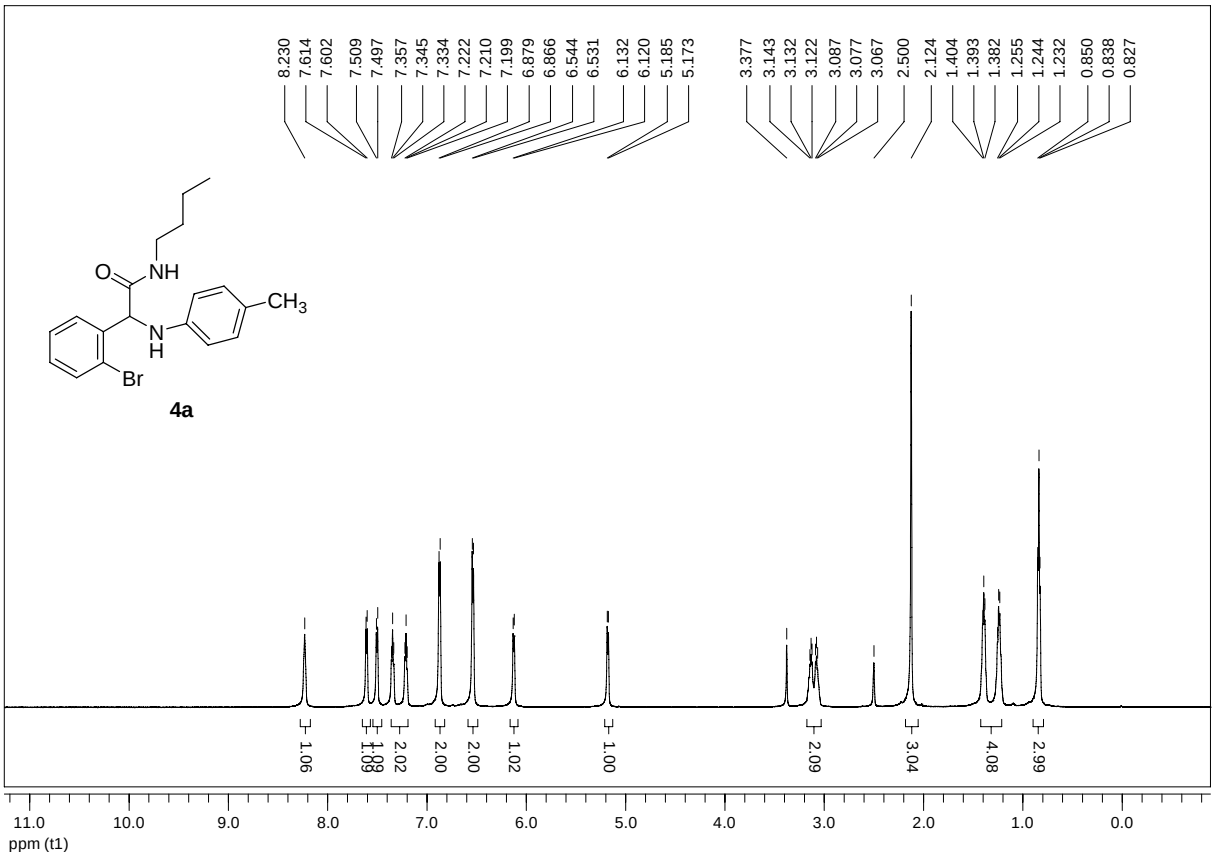
Content

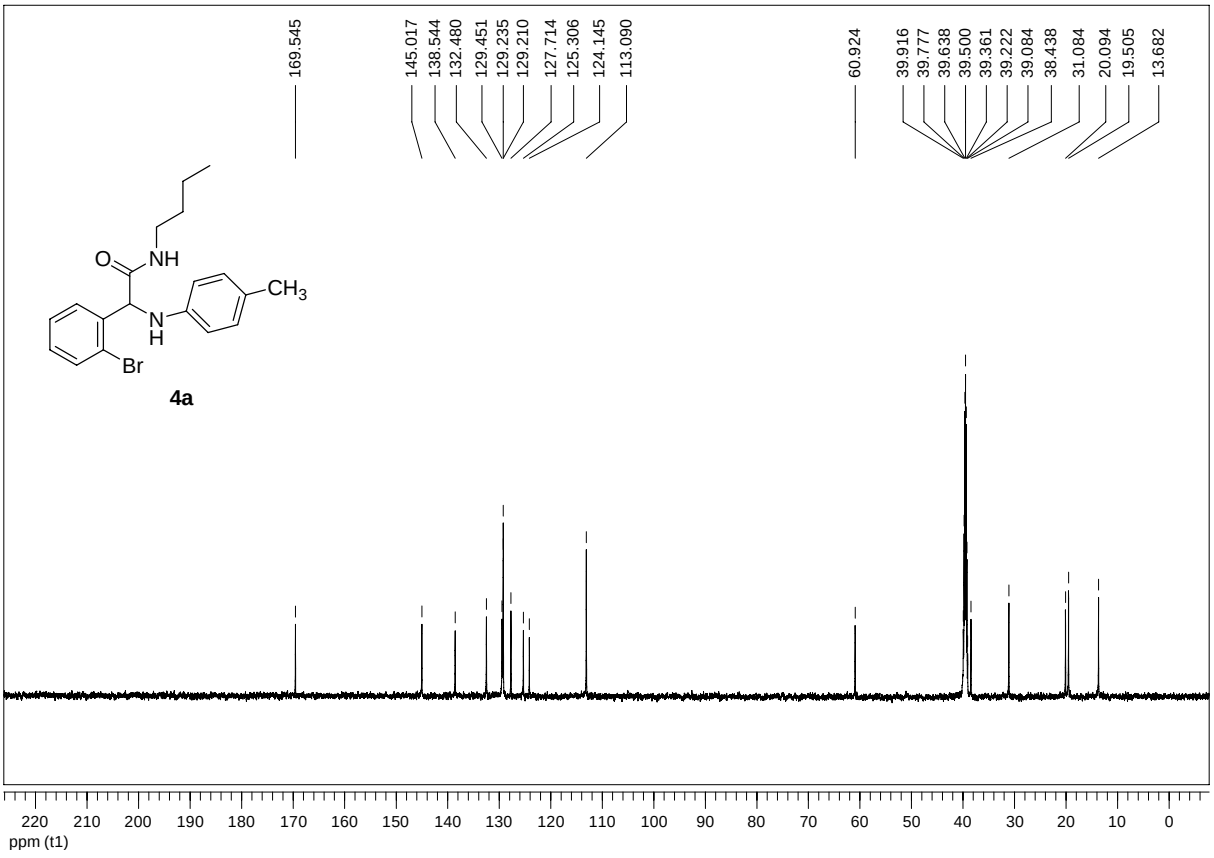
1. Crystal data and structure refinement for 6q

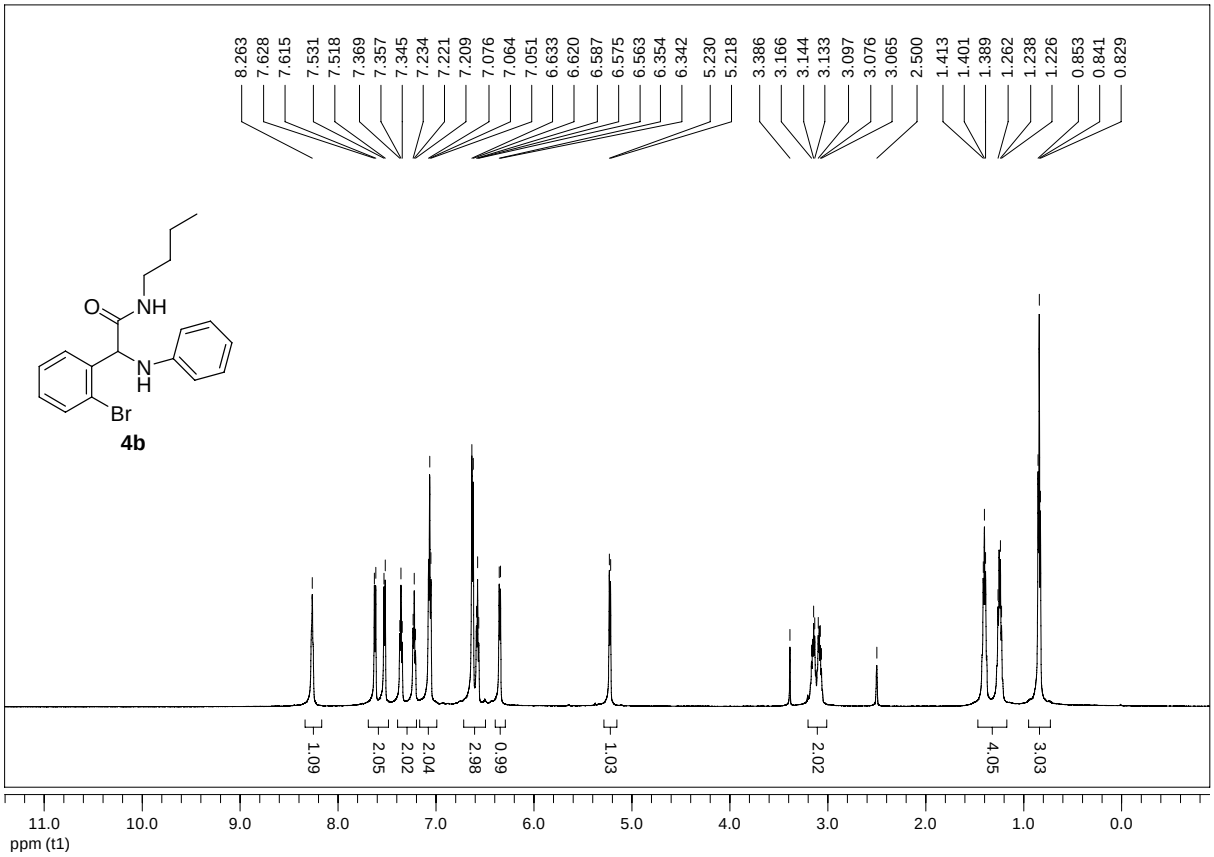
Crystal data and structure refinement for **6q**.

Identification code	6q	
Empirical formula	$C_{23}H_{28}ClN_3O_2$	
Formula weight	413.93	
Temperature	297(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 27.492(6) Å	α= 90°.
	b = 10.710(2) Å	β= 131.125(6)°.
	c = 20.869(5) Å	γ = 90°.
Volume	4628.8(18) $Å^3$	
Z	8	
Density (calculated)	1.188 Mg/m^3	
Absorption coefficient	0.187 mm^{-1}	
F(000)	1760	
Crystal size	0.200 x 0.200 x 0.100 mm^3	
Theta range for data collection	1.967 to 26.288°.	
Index ranges	-34<=h<=34, -13<=k<=13, -25<=l<=25	
Reflections collected	17217	
Independent reflections	8235 [R(int) = 0.0490]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8235 / 2 / 537	
Goodness-of-fit on F^2	0.979	
Final R indices [I>2sigma(I)]	R1 = 0.0445, wR2 = 0.1150	
R indices (all data)	R1 = 0.0605, wR2 = 0.1269	
Absolute structure parameter	0.05(4)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.512 and -0.196 $e.Å^{-3}$	

2. Copies of ^{1}H and ^{13}C NMR spectrum of compounds 4 and 6



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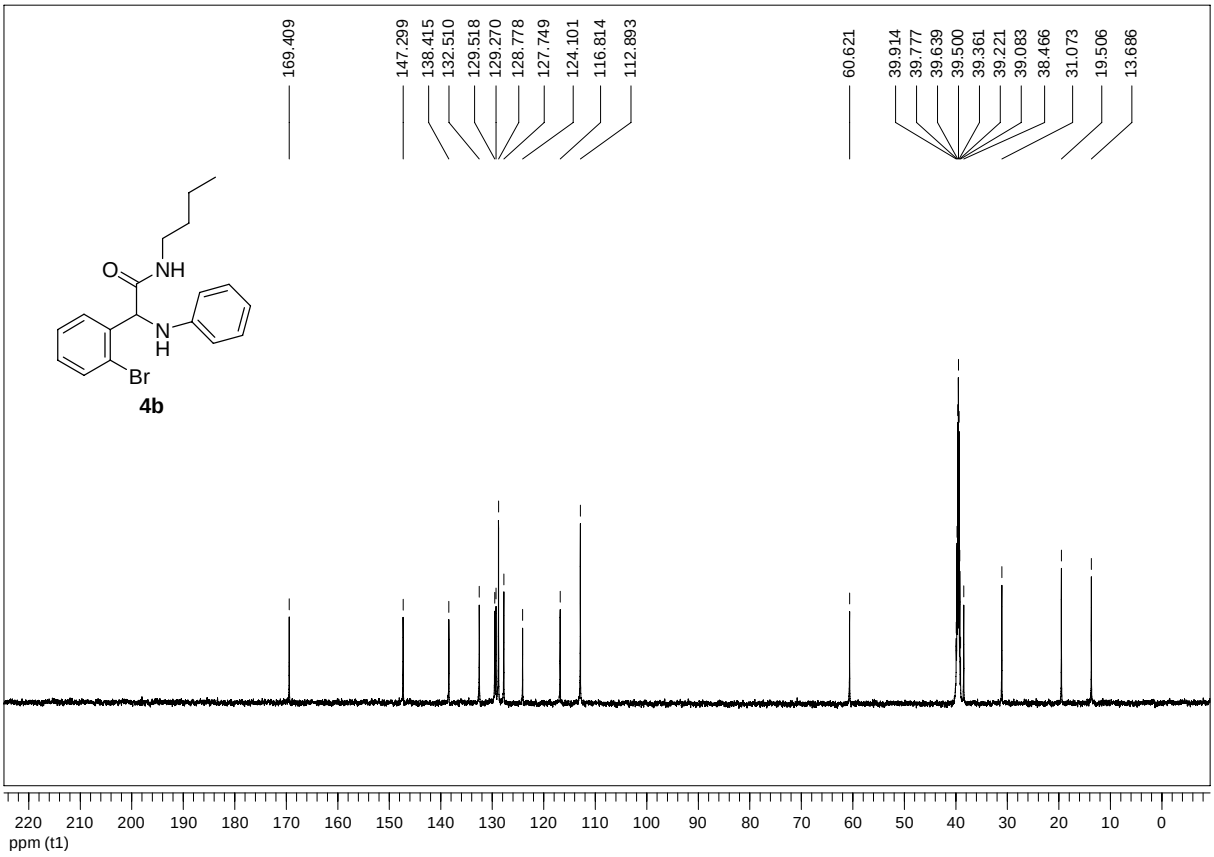
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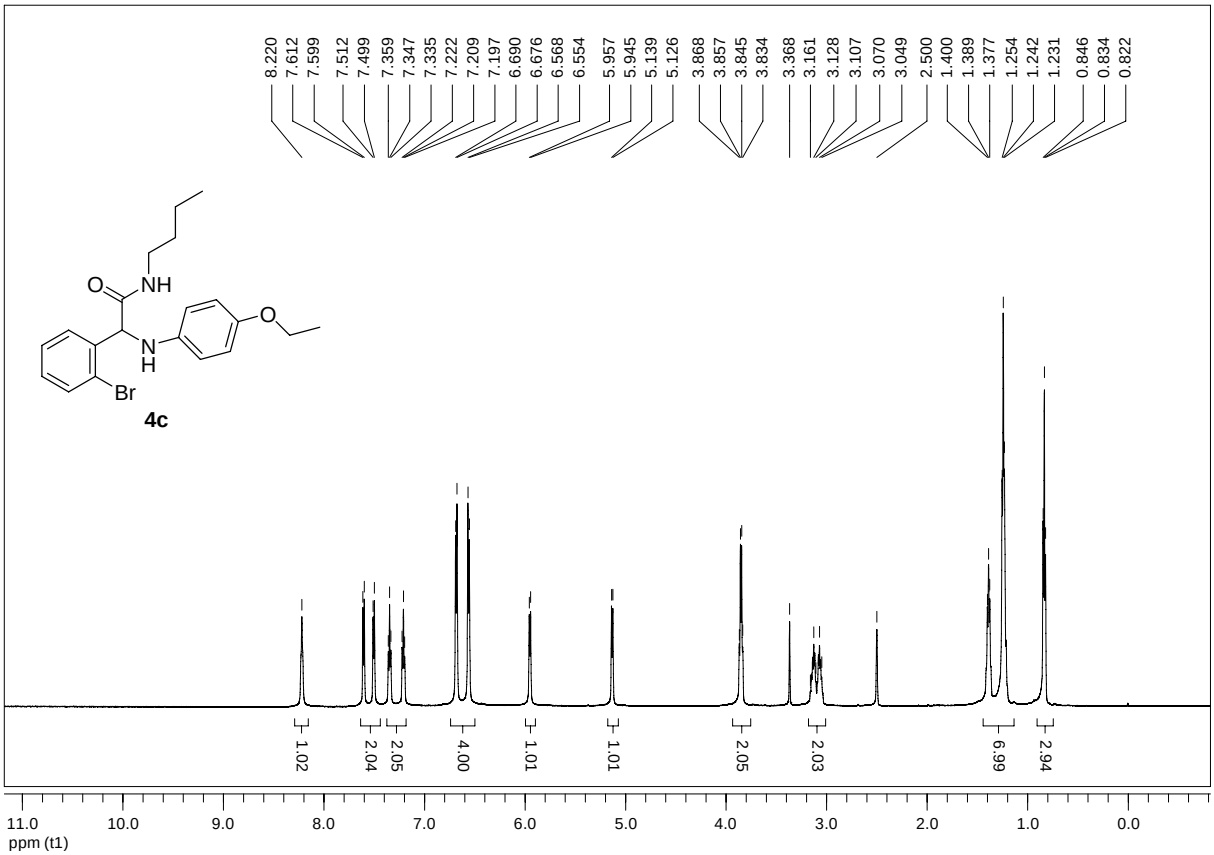
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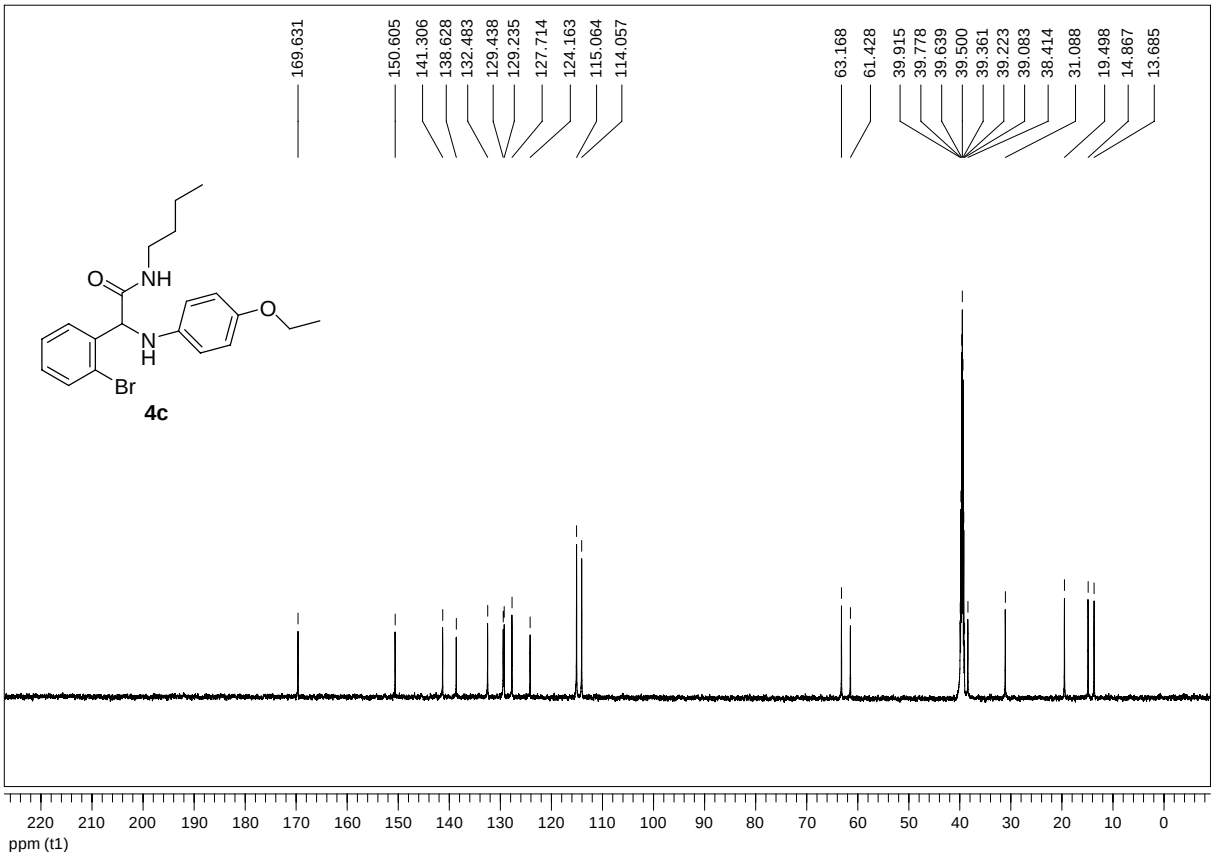
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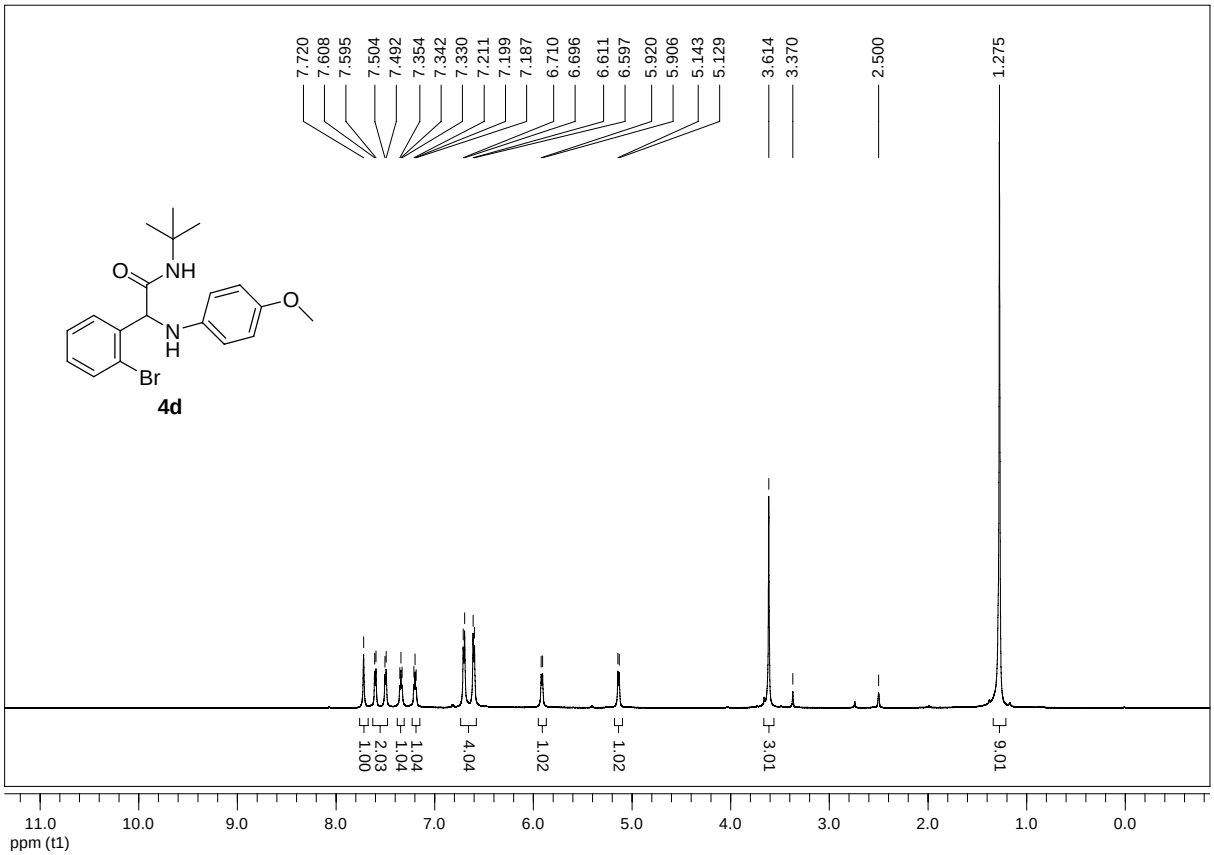
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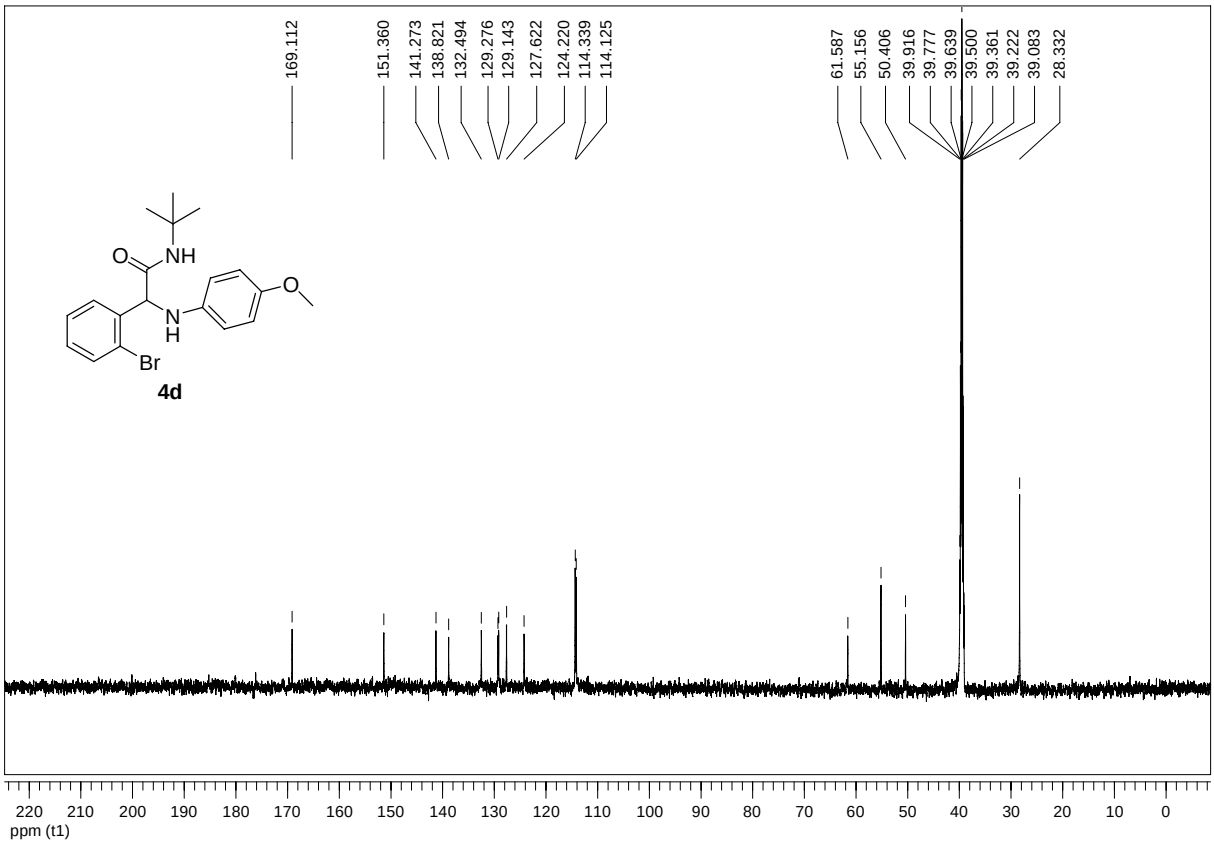
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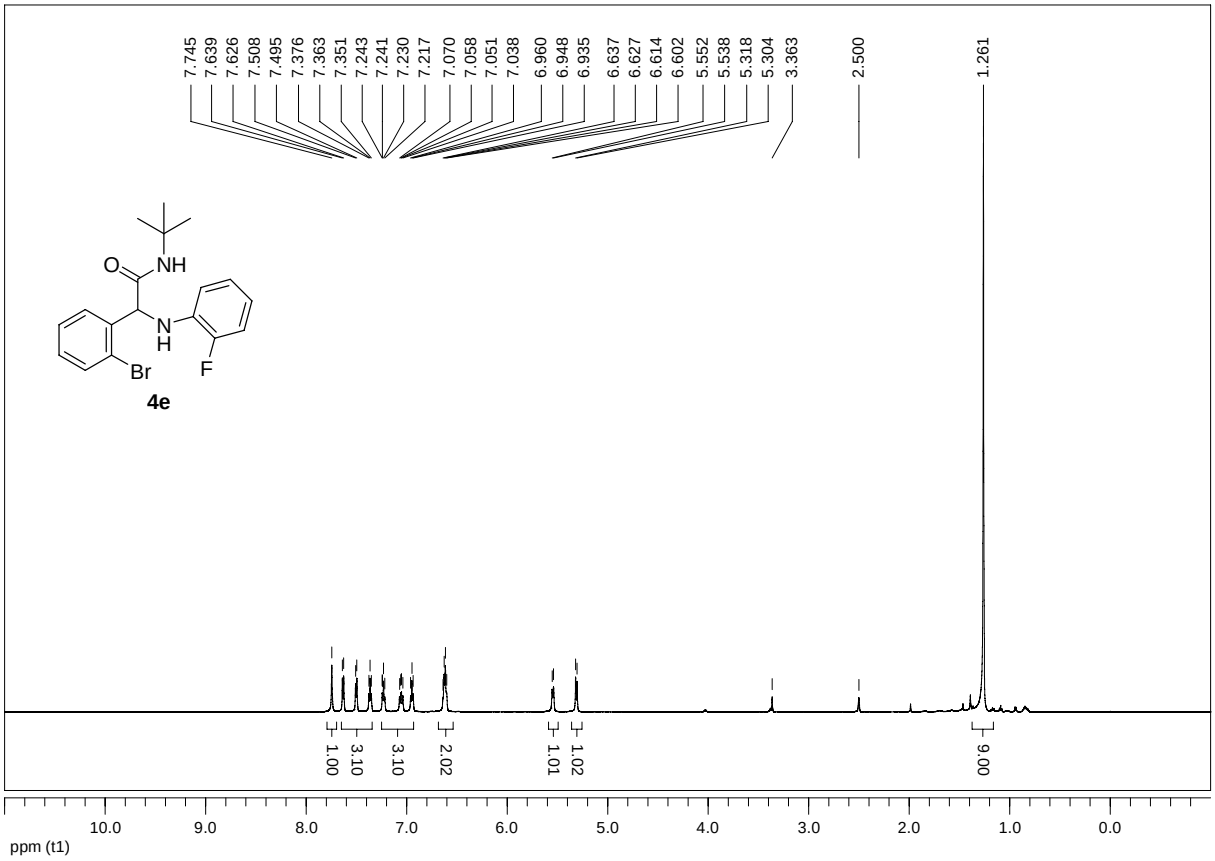
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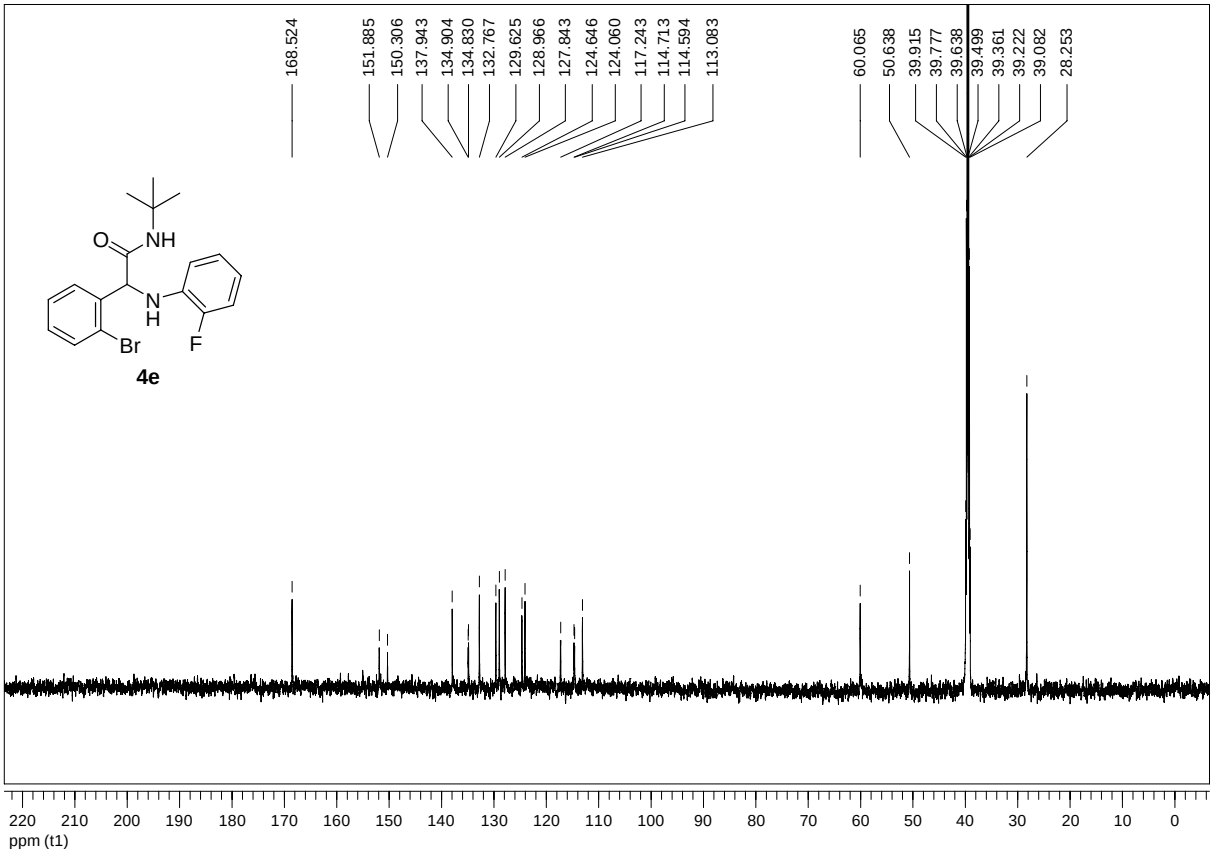
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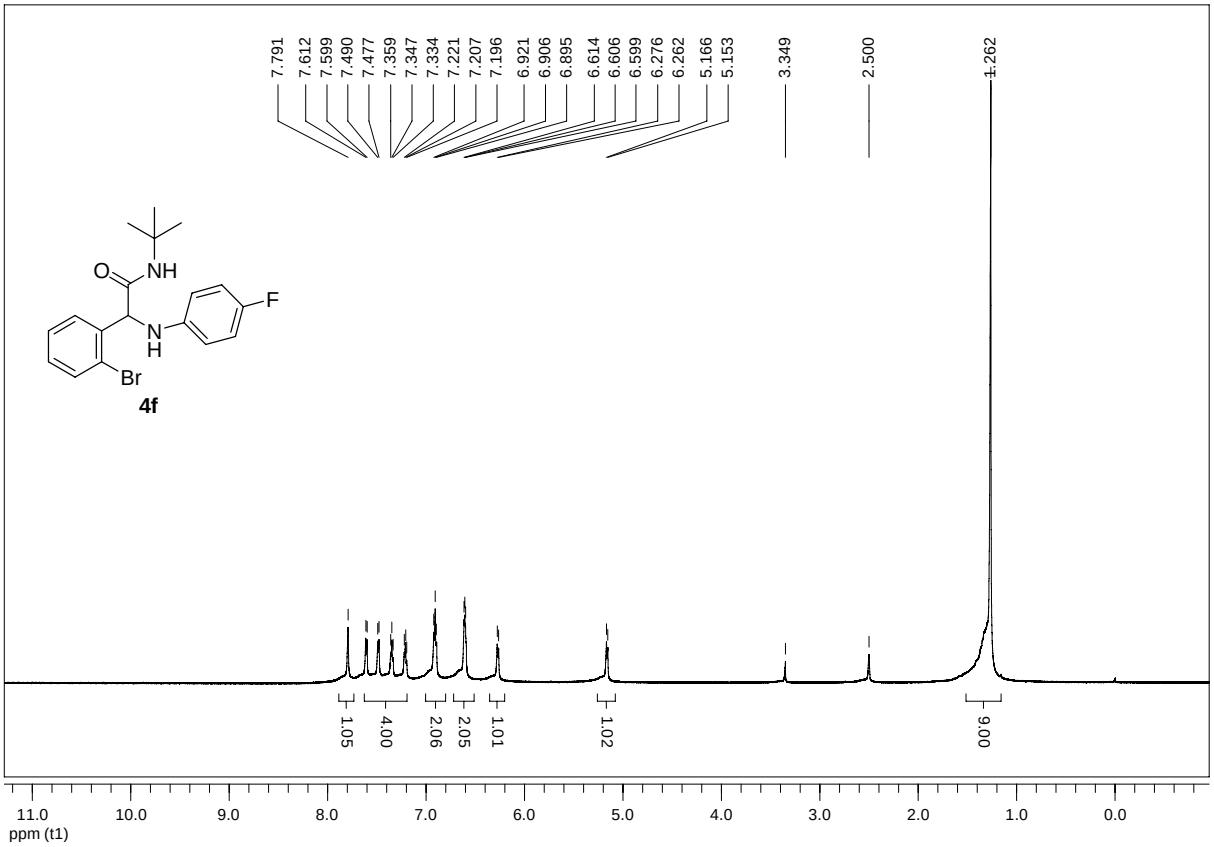
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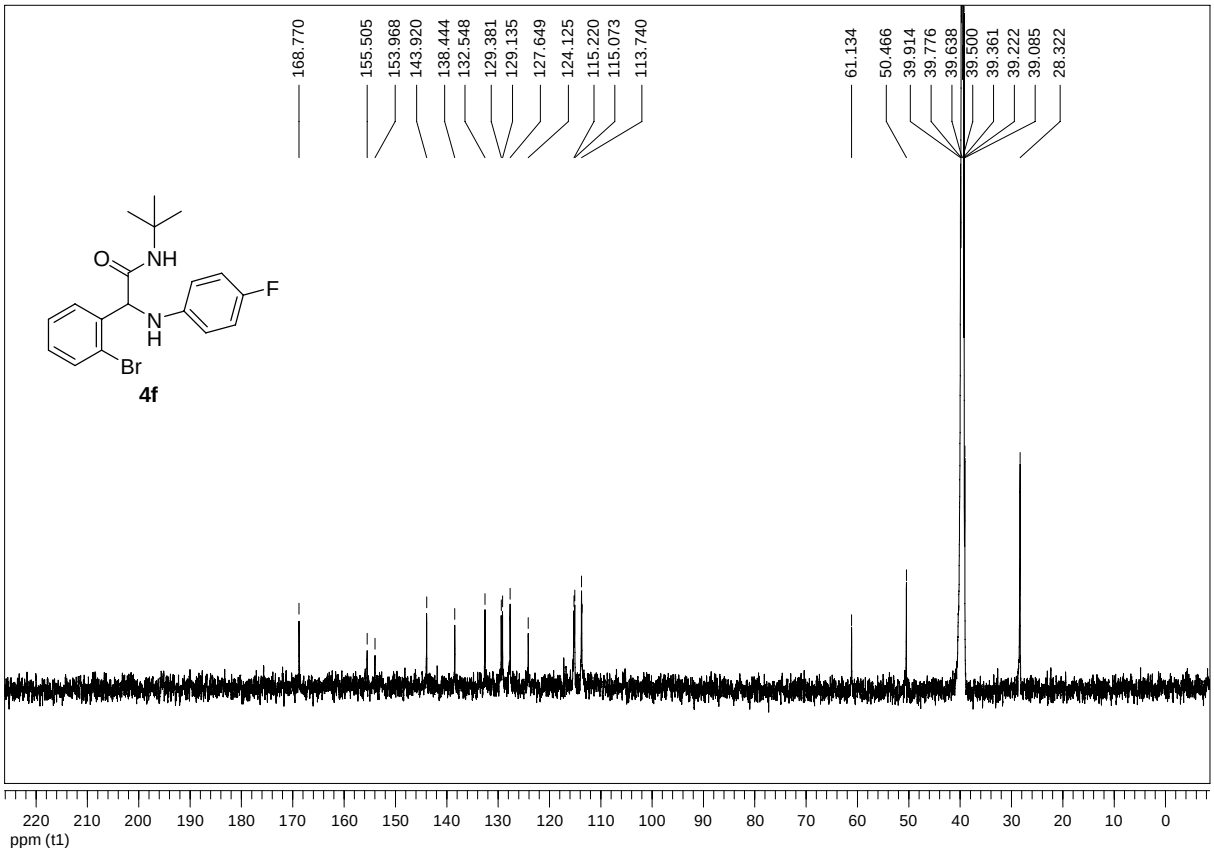
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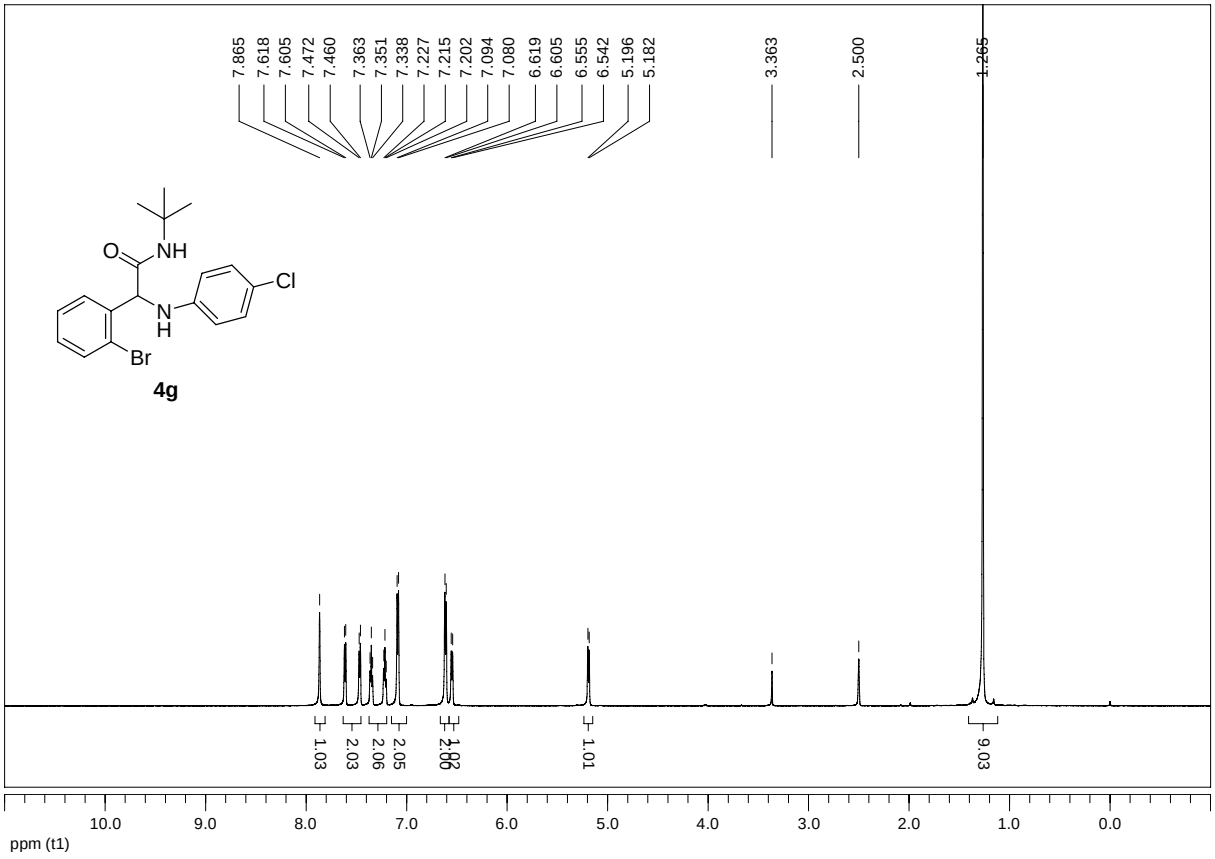
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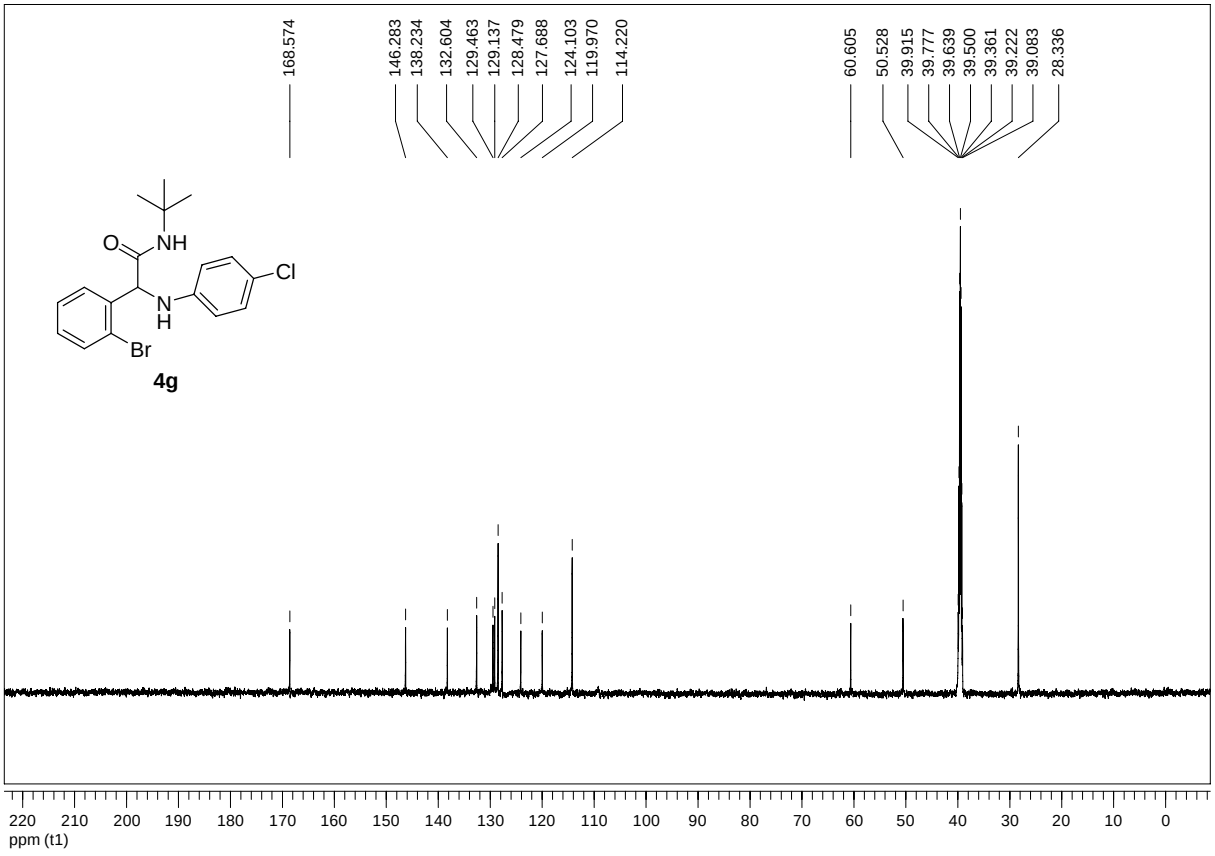
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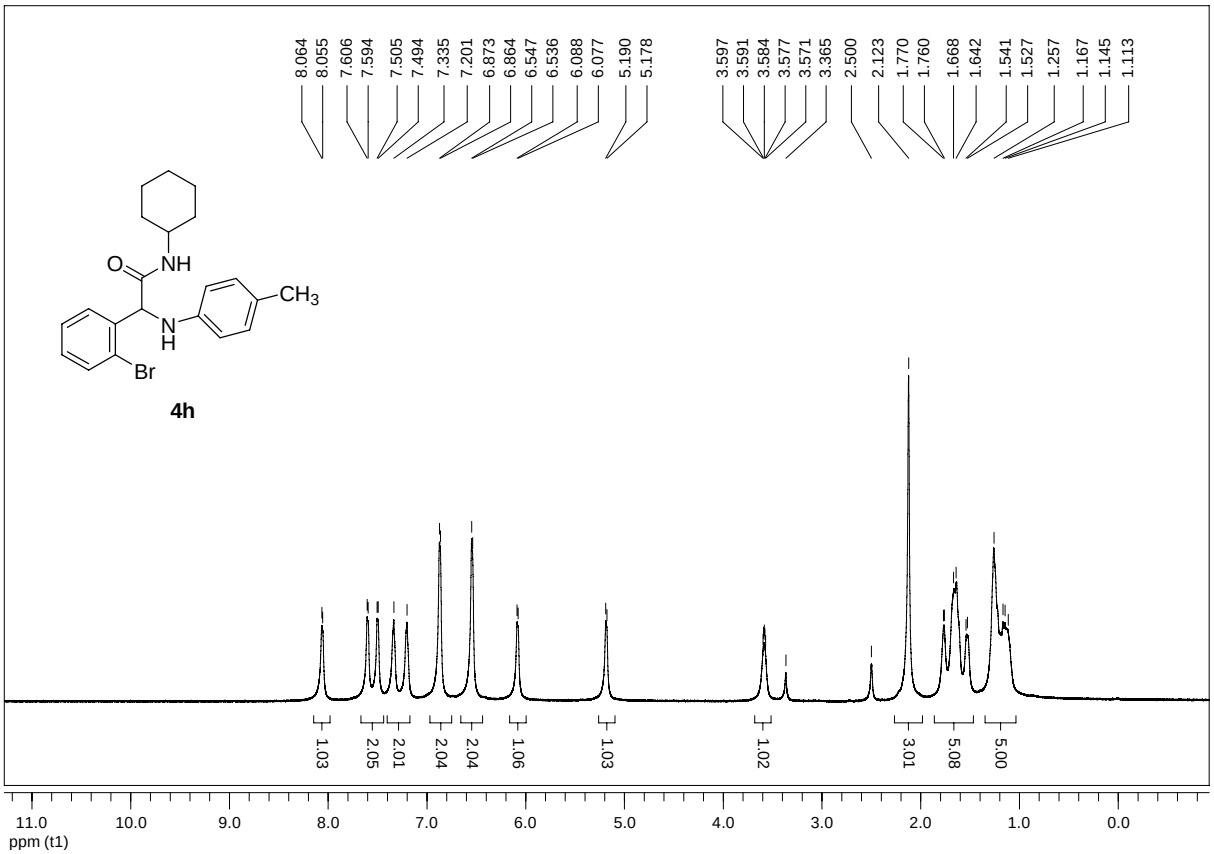
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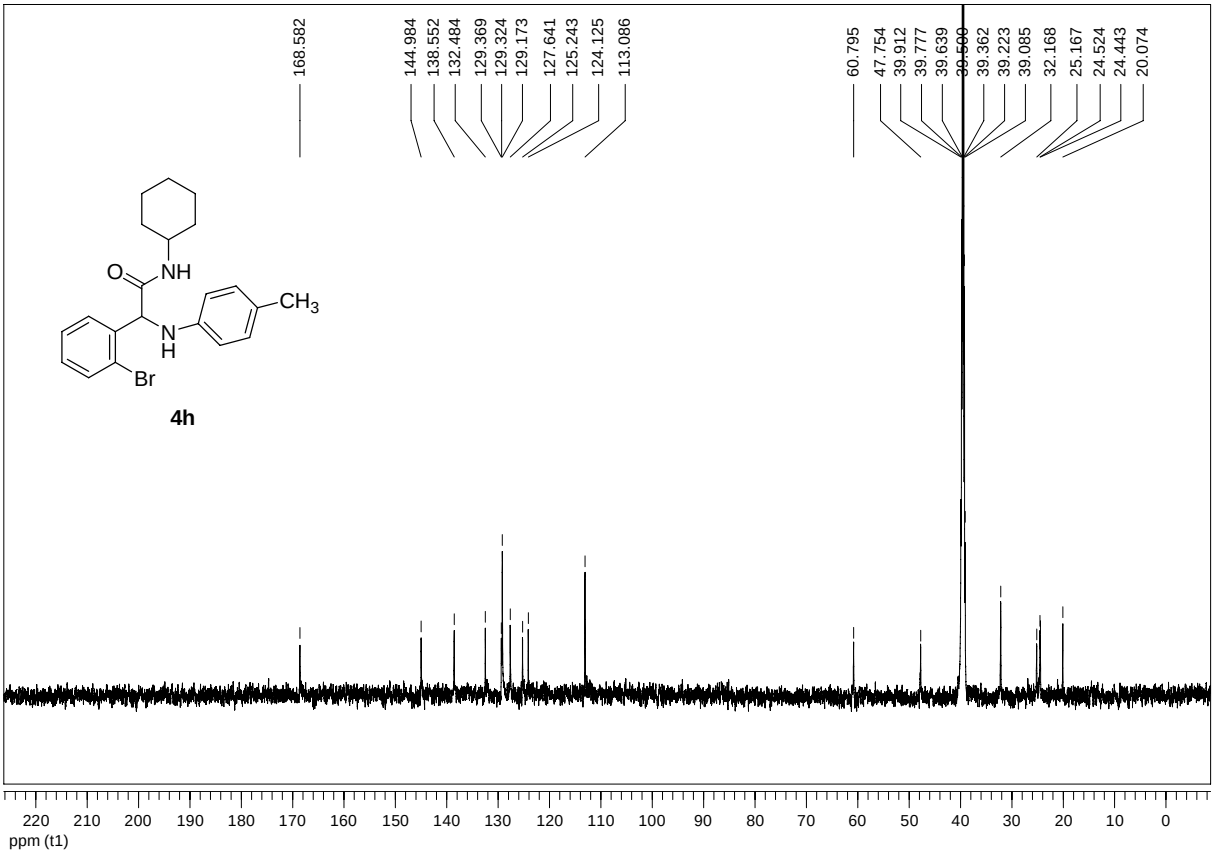
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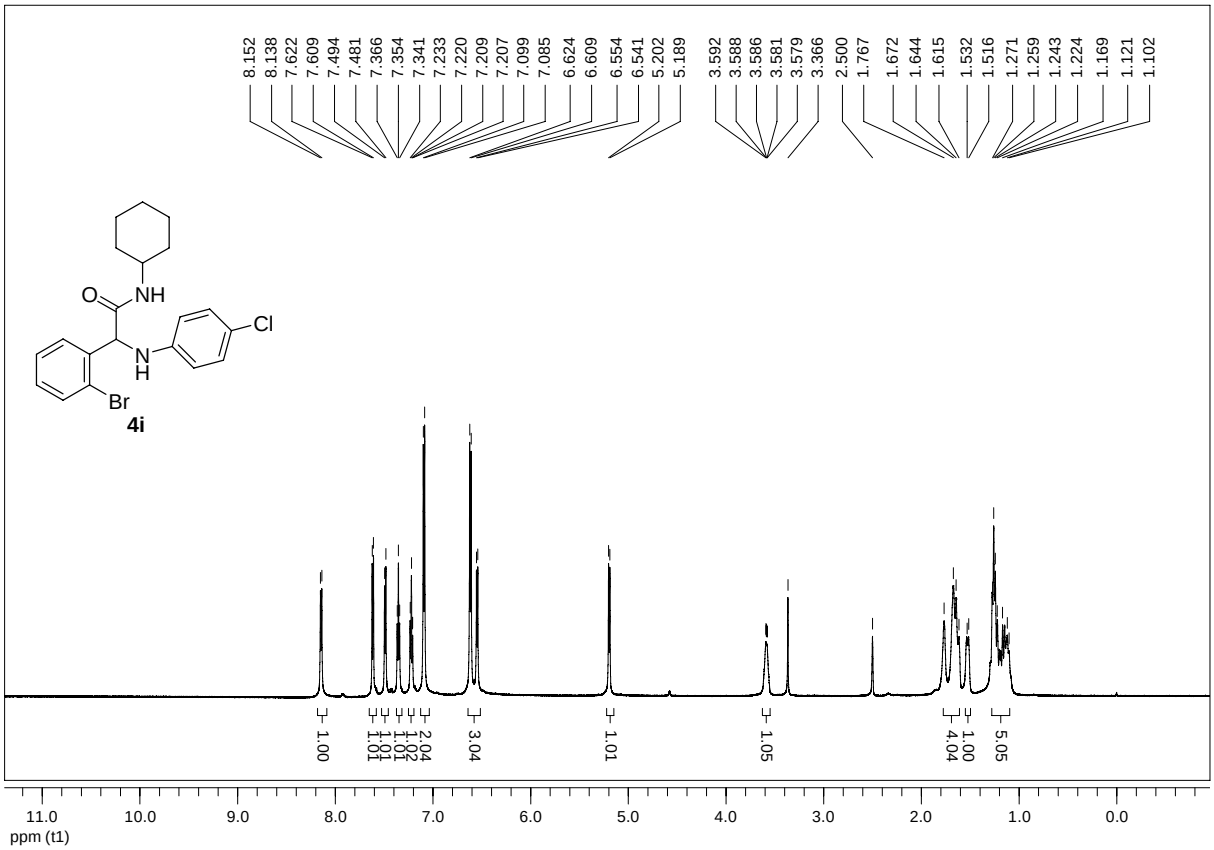
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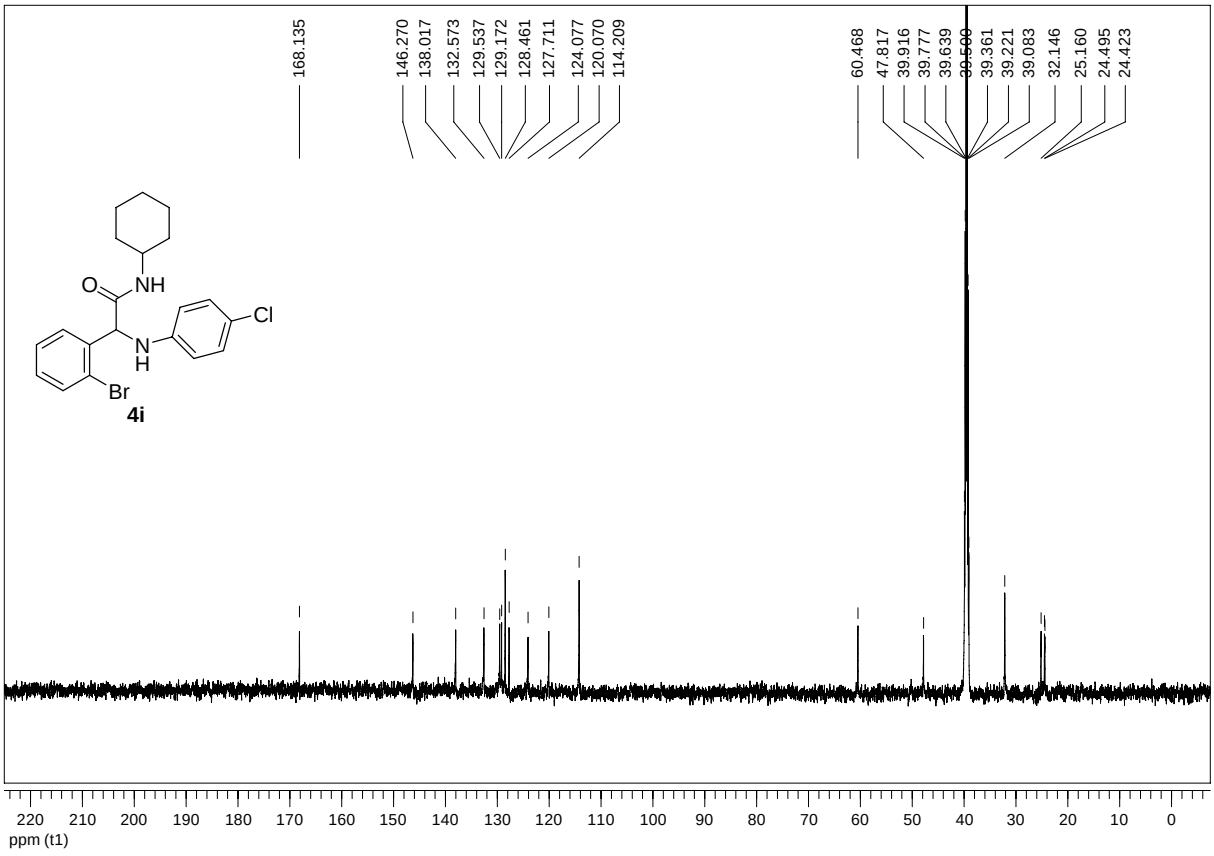
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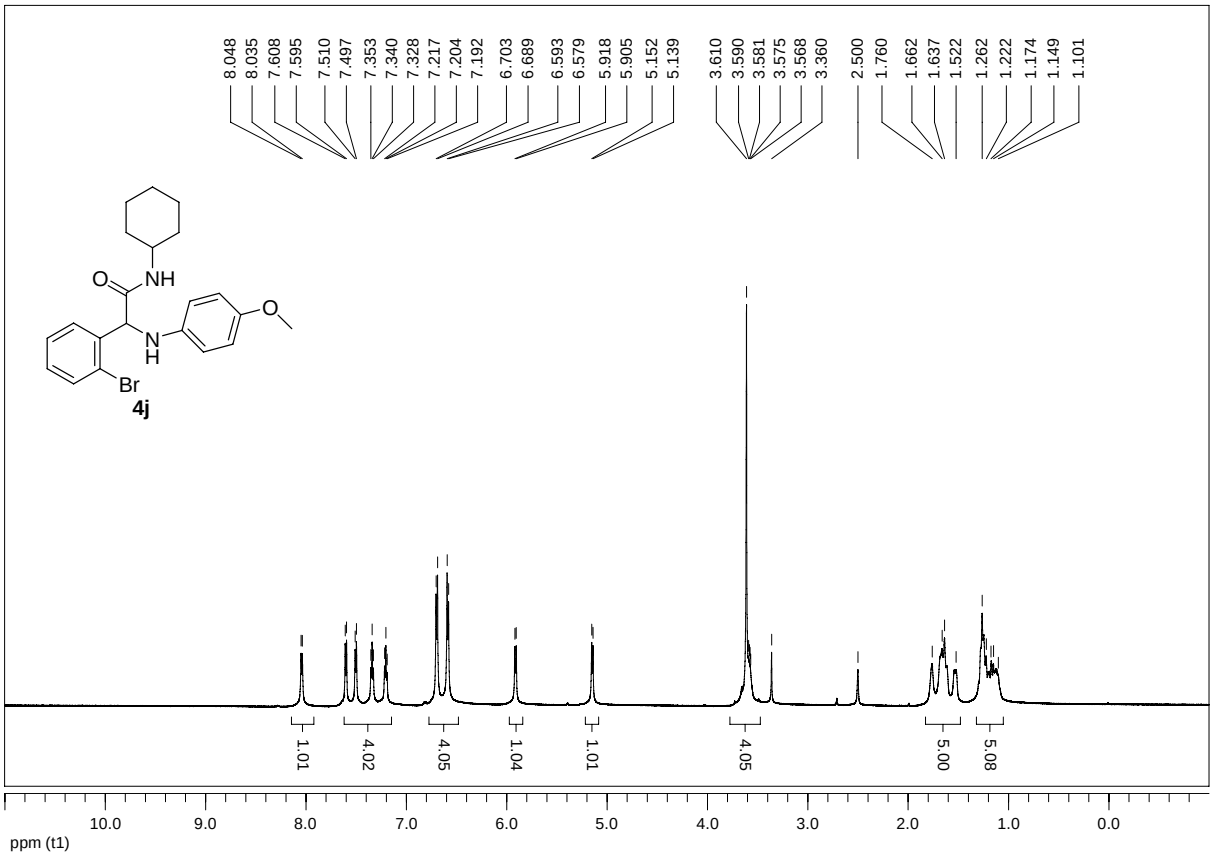
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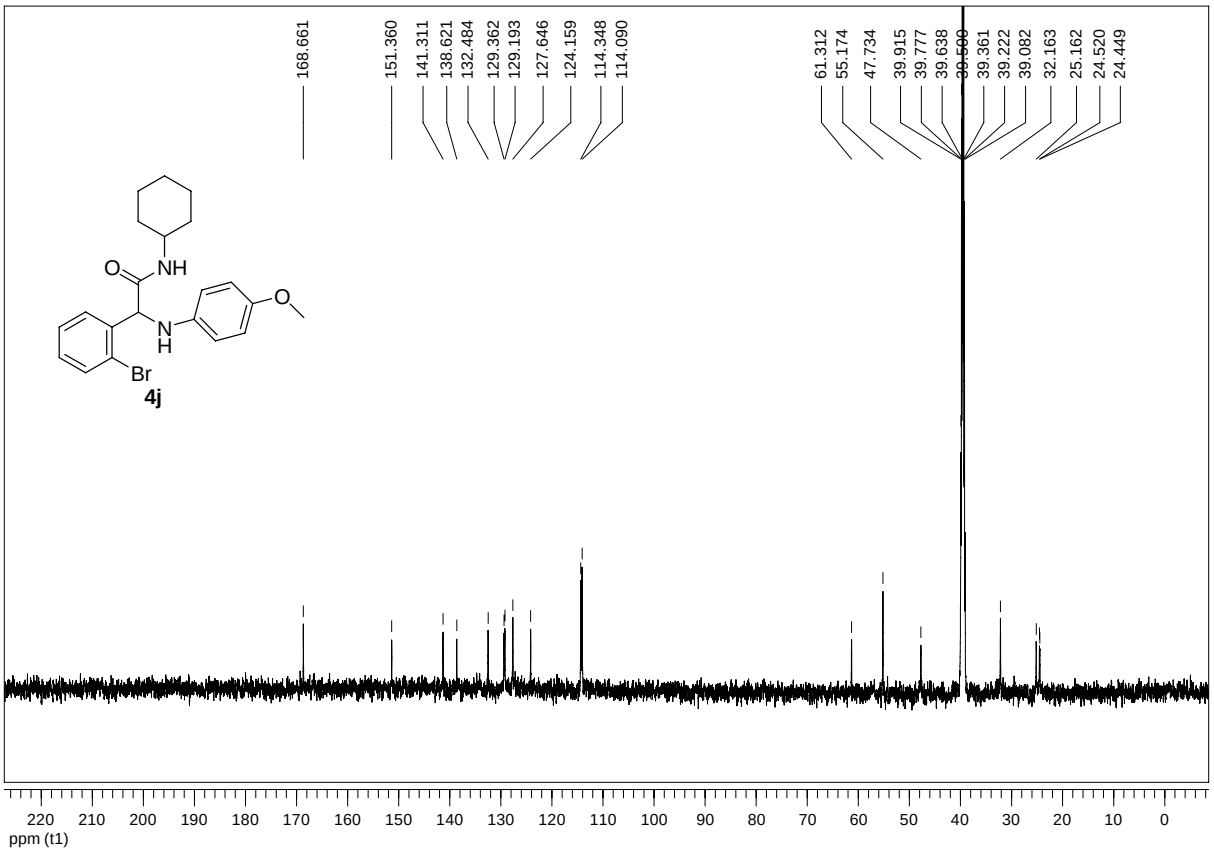
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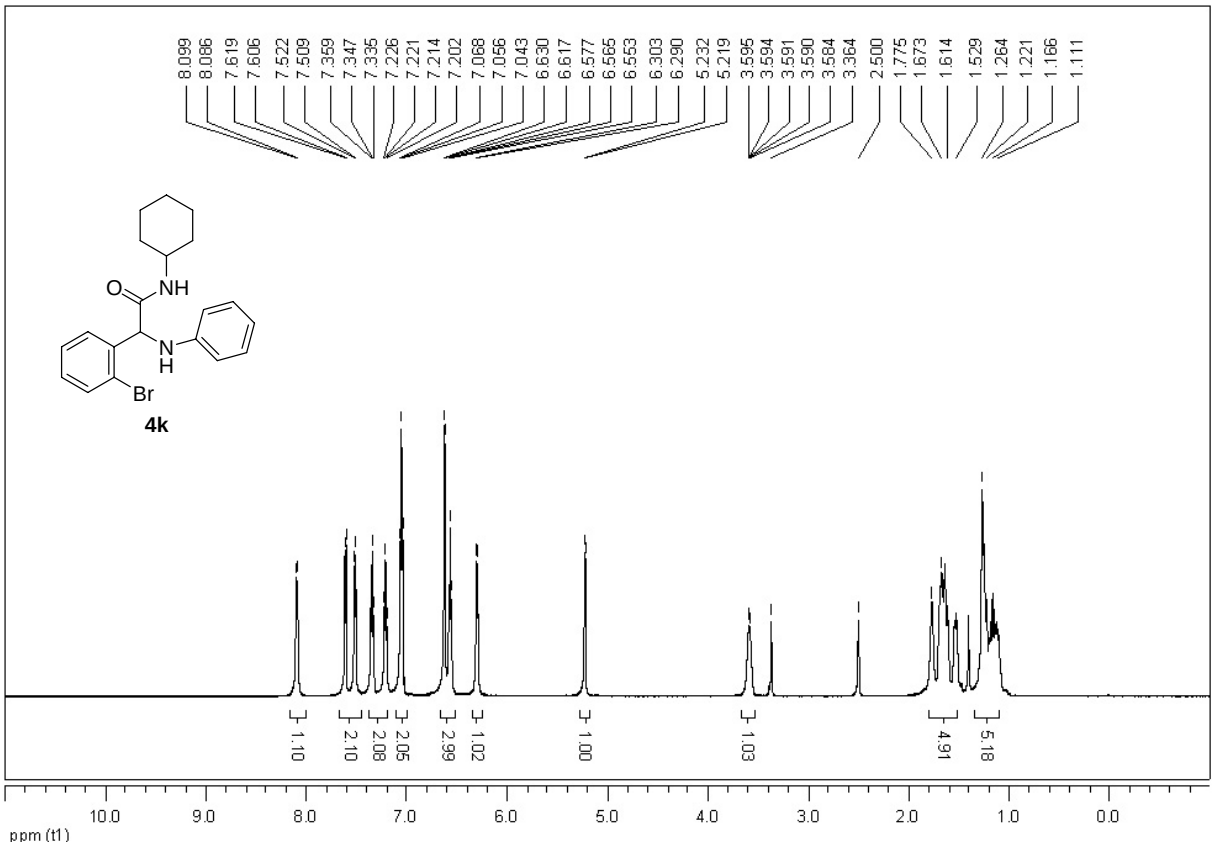
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6.553
6.303
6.290
5.232
5.219
3.595
3.594
3.591
3.590
3.584
3.364
2.500
1.775
1.673
1.614
1.529
1.264
1.221
1.166
1.111
O
NH
N
H
Br
4k
1.10
2.10
2.08
2.05
2.99
2.02
3.00
1.03
4.91
5.18
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5.0
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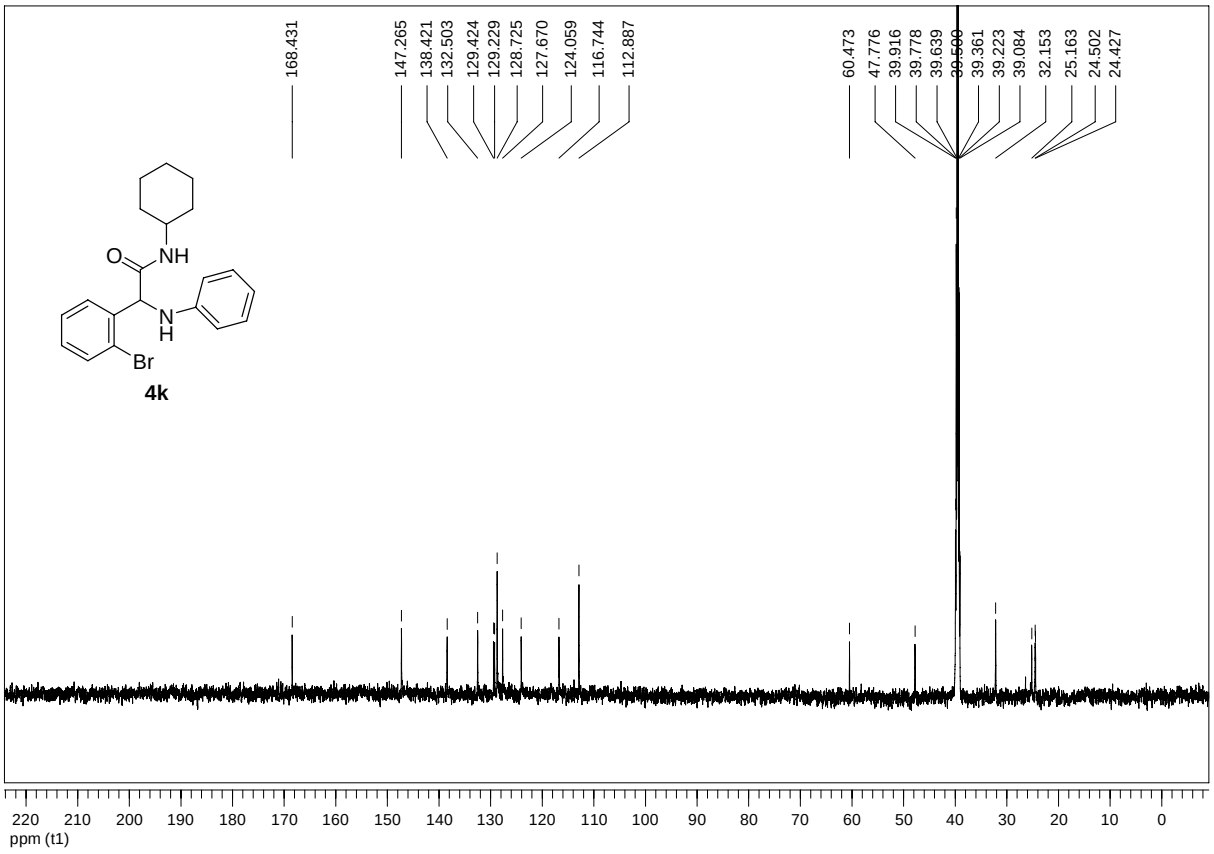
1.0
0.0
ppm (t1)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129.229
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127.670
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112.887
60.473
47.776
39.916
39.778
39.639
39.500
39.361
39.223
39.084
32.153
25.163
24.502
24.427
O
NH
N
H
Br
4k
220
210
200
190
180
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90
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50
40
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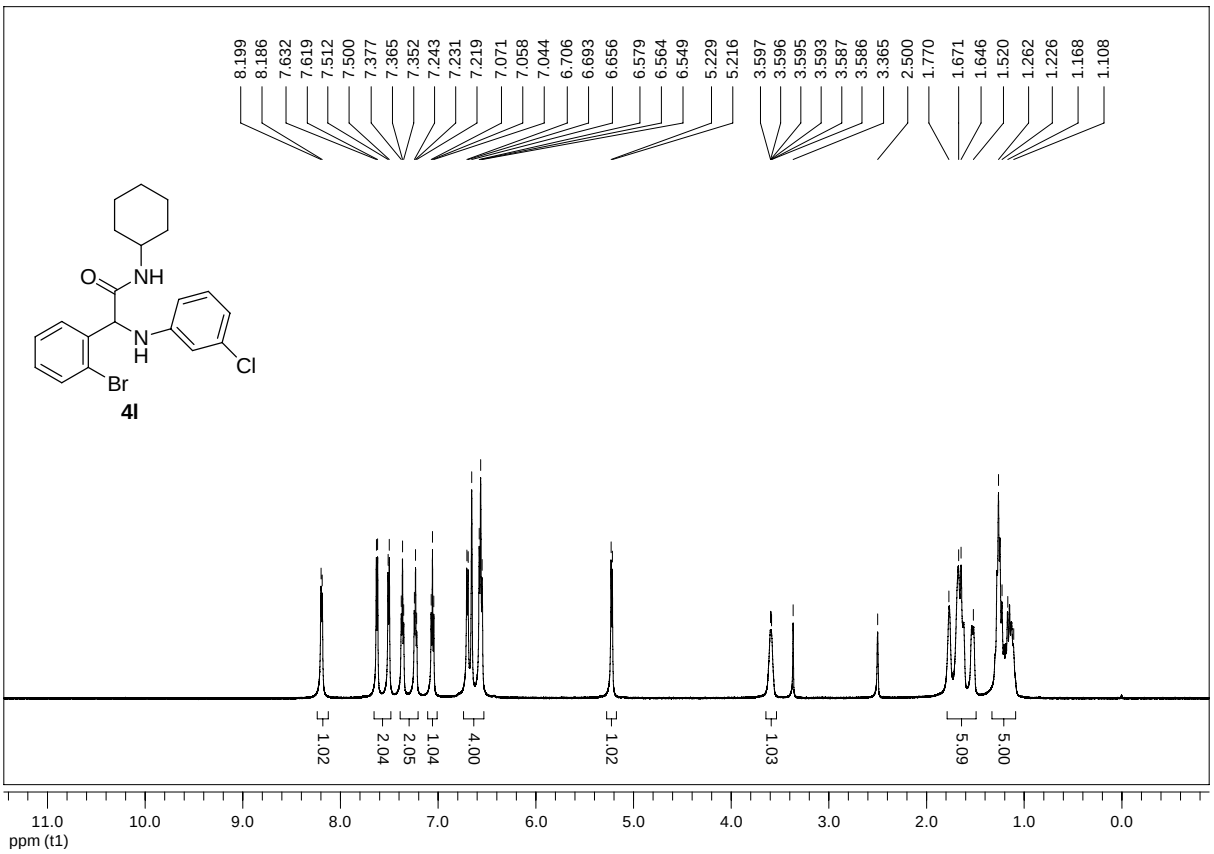
ppm (t1)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7.377
7.365
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7.243
7.231
7.219
7.071
7.058
7.044
6.706
6.693
6.656
6.579
6.564
6.549
5.229
5.216
3.597
3.596
3.595
3.593
3.587
3.586
3.365
2.500
1.770
1.671
1.646
1.520
1.262
1.226
1.168
1.108
O
NH
N
H
Br
Cl
4l
1.02
2.04
2.05
1.04
4.00
1.02
1.03
5.09
5.00
11.0
10.0
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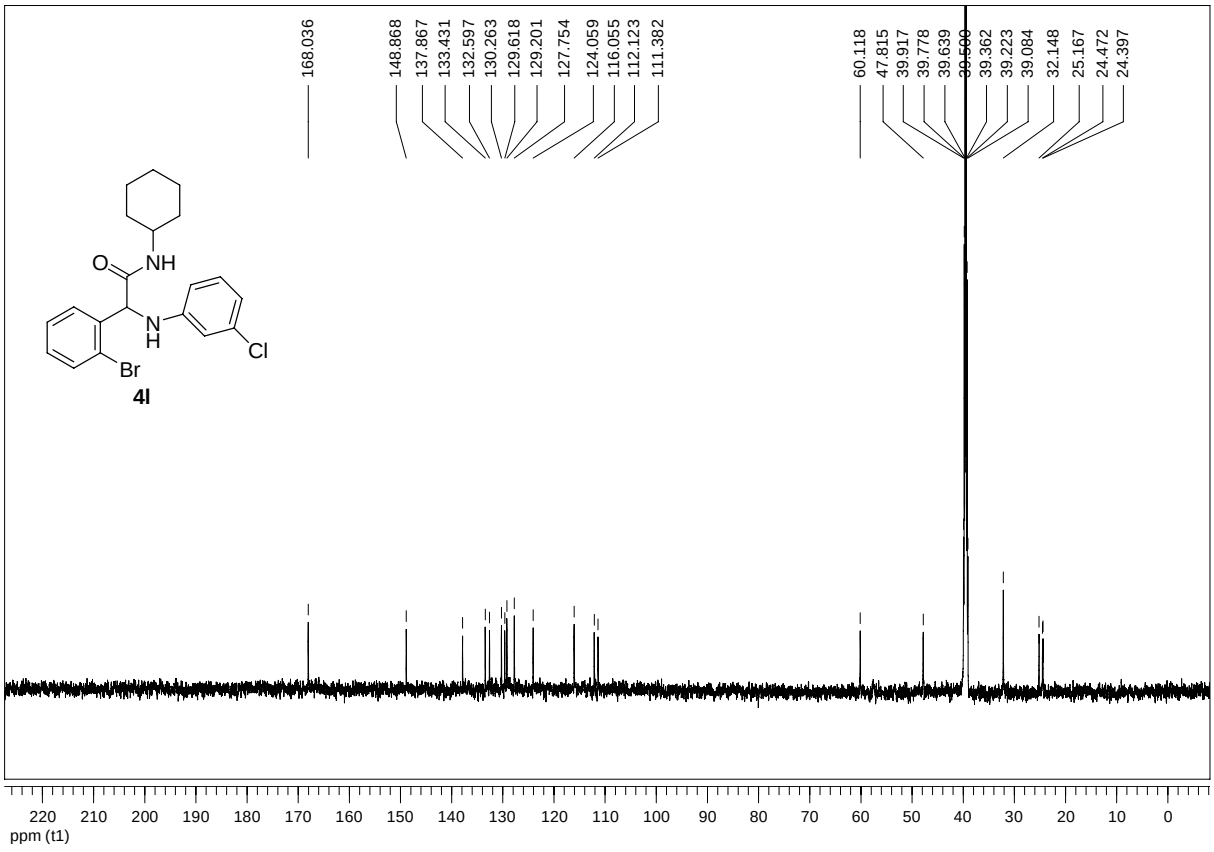
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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111.382
60.118
47.815
39.917
39.778
39.639
39.500
39.362
39.223
39.084
32.148
25.167
24.472
24.397
O
NH
N
H
Br
Cl
4l
220
210
200
190
180
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150
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130
120
110
100
90
80
70
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50
40
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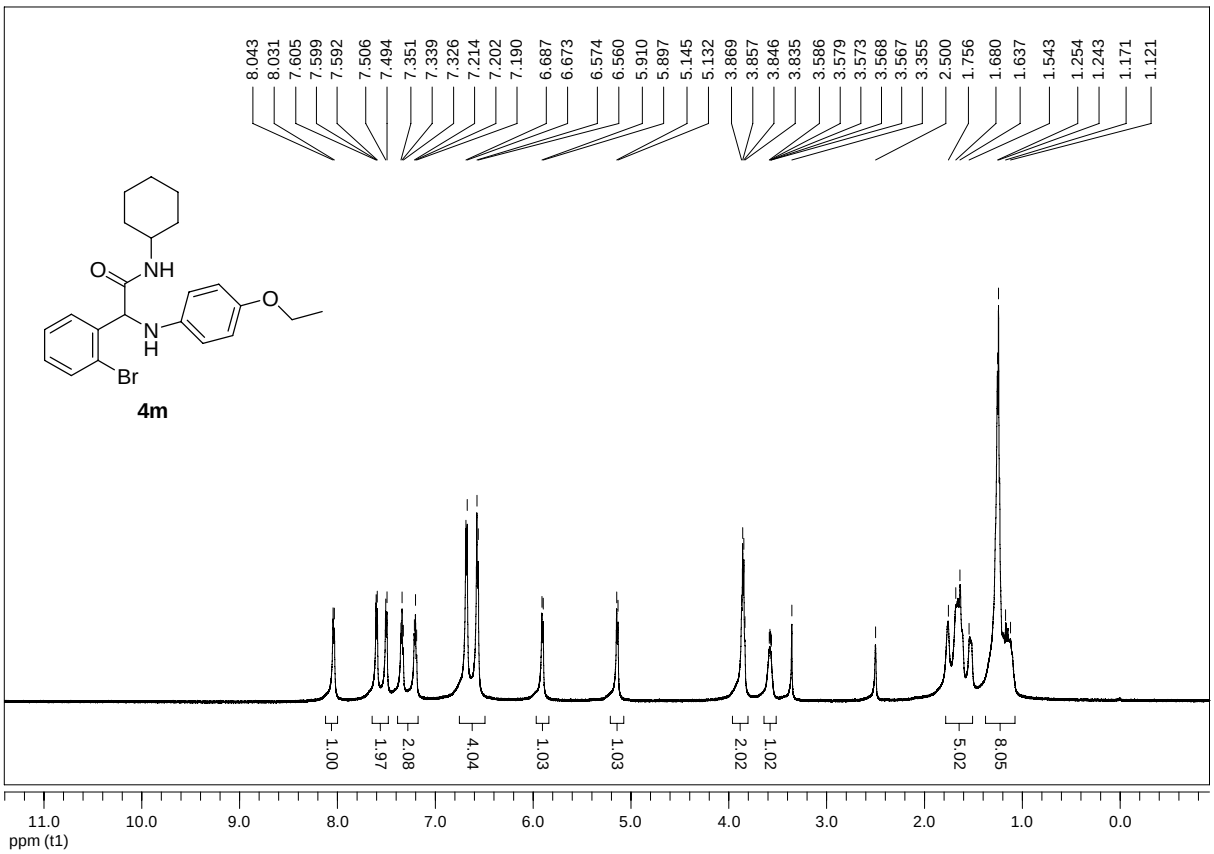
ppm (t1)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7.599
7.592
7.506
7.494
7.351
7.339
7.326
7.214
7.202
7.190
6.687
6.673
6.574
6.560
5.910
5.897
5.145
5.132
3.869
3.857
3.846
3.835
3.586
3.579
3.573
3.568
3.567
3.355
2.500
1.756
1.680
1.637
1.543
1.254
1.243
1.171
1.121
NH
O
N
H
O
Br
4m
1.00
1.97
2.08
4.04
1.03
1.03
2.02
1.02
5.02
8.05
11.0
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6.0
5.0
4.0
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2.0
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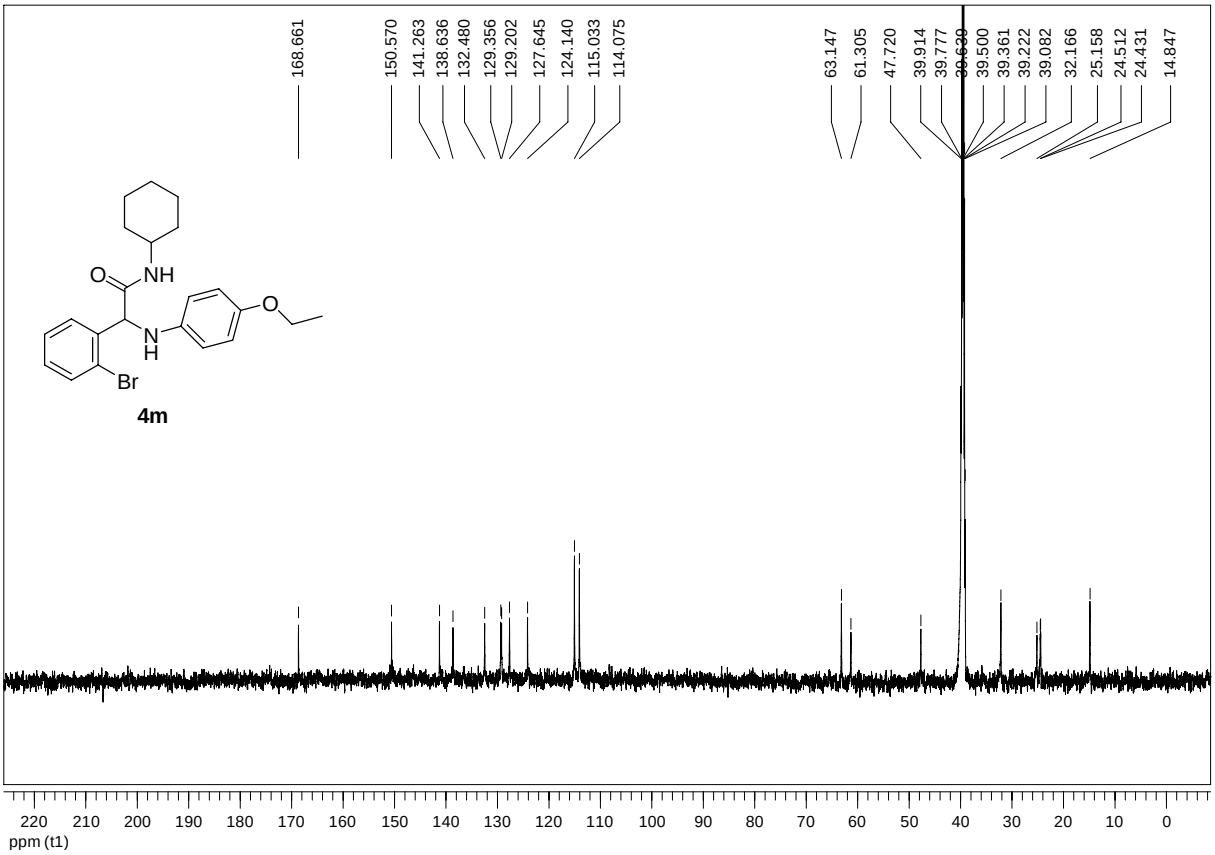
ppm (t1)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114.075
63.147
61.305
47.720
39.914
39.777
39.639
39.500
39.361
39.222
39.082
32.166
25.158
24.512
24.431
14.847
NH
O
N
H
O
Br
4m
220
210
200
190
180
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150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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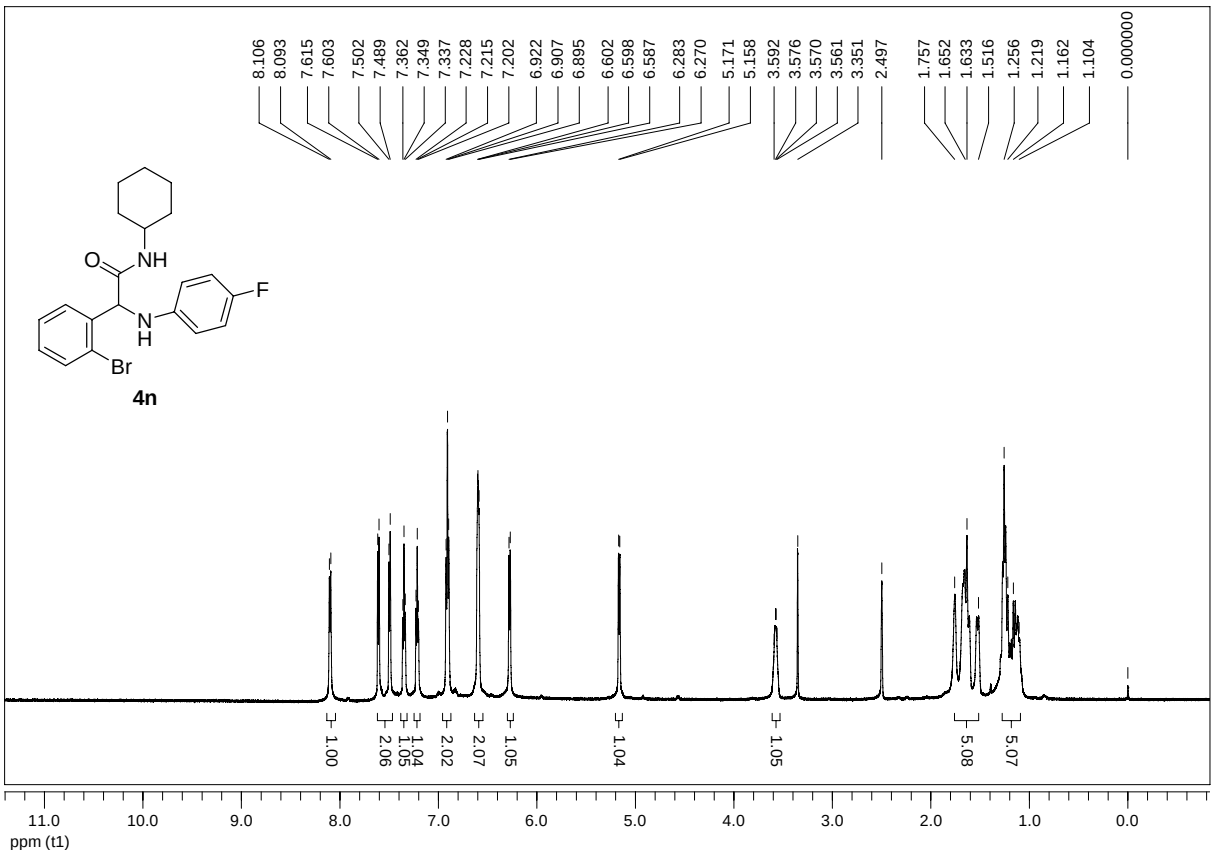
ppm (t1)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7.603
7.502
7.489
7.362
7.349
7.337
7.228
7.215
7.202
6.922
6.907
6.895
6.602
6.598
6.587
6.283
6.270
5.171
5.158
3.592
3.576
3.570
3.561
3.351
2.497
1.757
1.652
1.633
1.516
1.256
1.219
1.162
1.104
0.000000
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NH
F
N
H
Br
4n
1.00
2.06
1.05
1.04
2.02
2.07
1.05
1.04
1.05
5.08
5.07
11.0
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7.0
6.0
5.0
4.0
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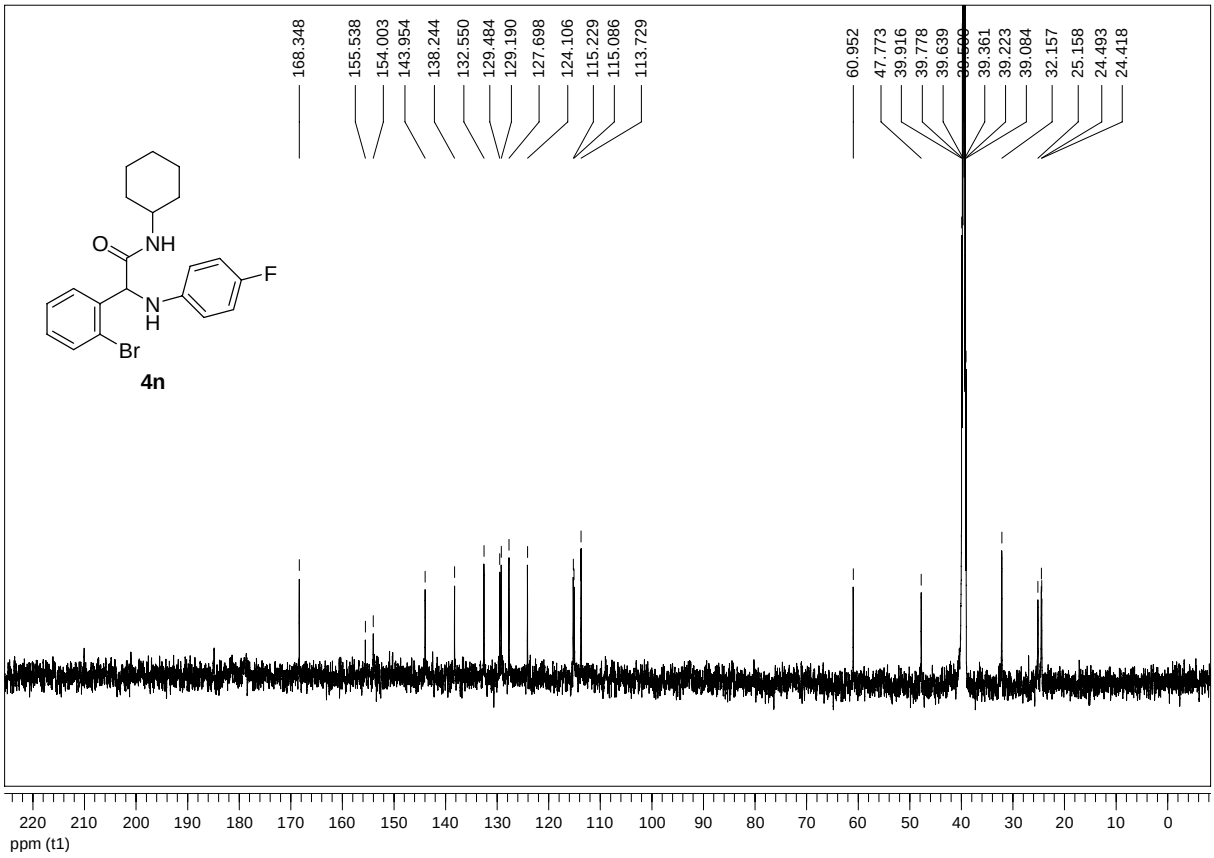
2.0
1.0
0.0
ppm (t1)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154.003
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132.550
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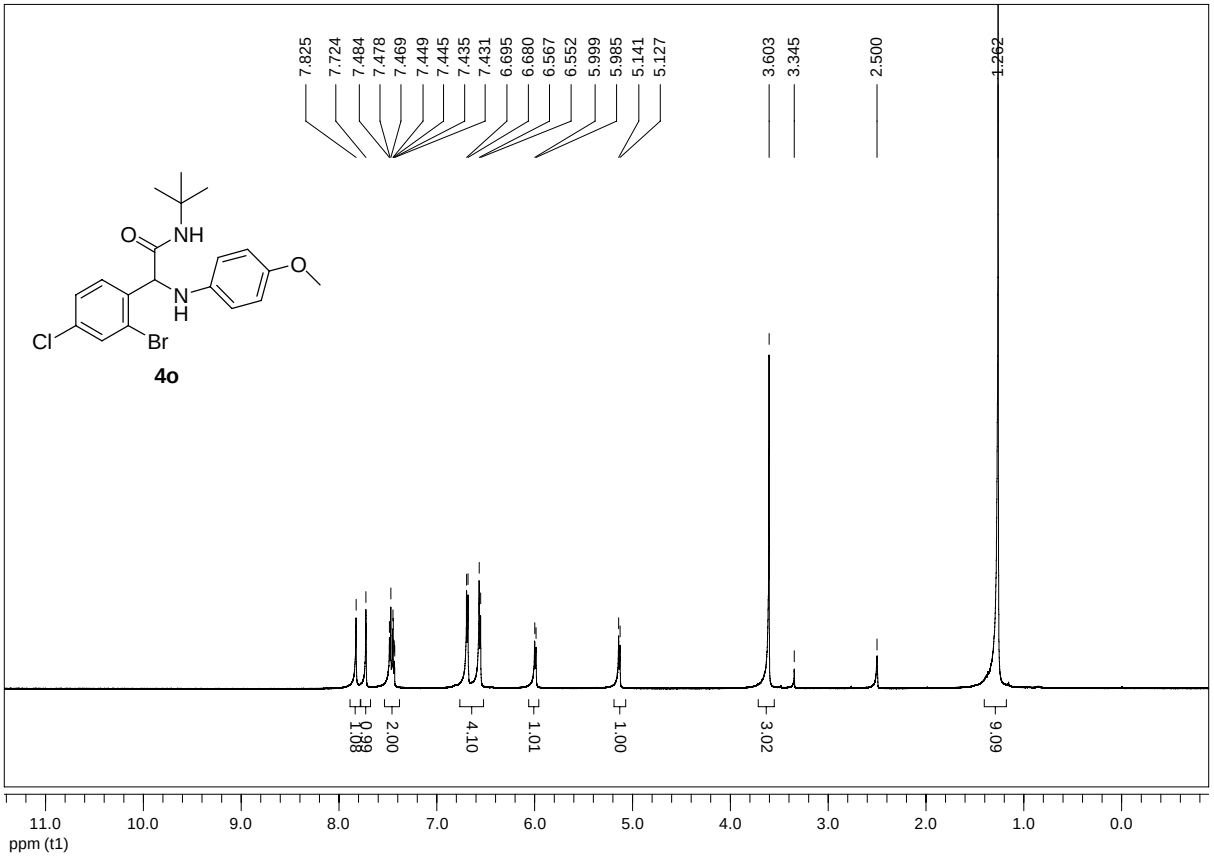
129.190
127.698
124.106
115.229
115.086
113.729
60.952
47.773
39.916
39.778
39.639
39.361
39.223
39.084
32.157
25.158
24.493
24.418
O
NH
F
N
H
Br
4n
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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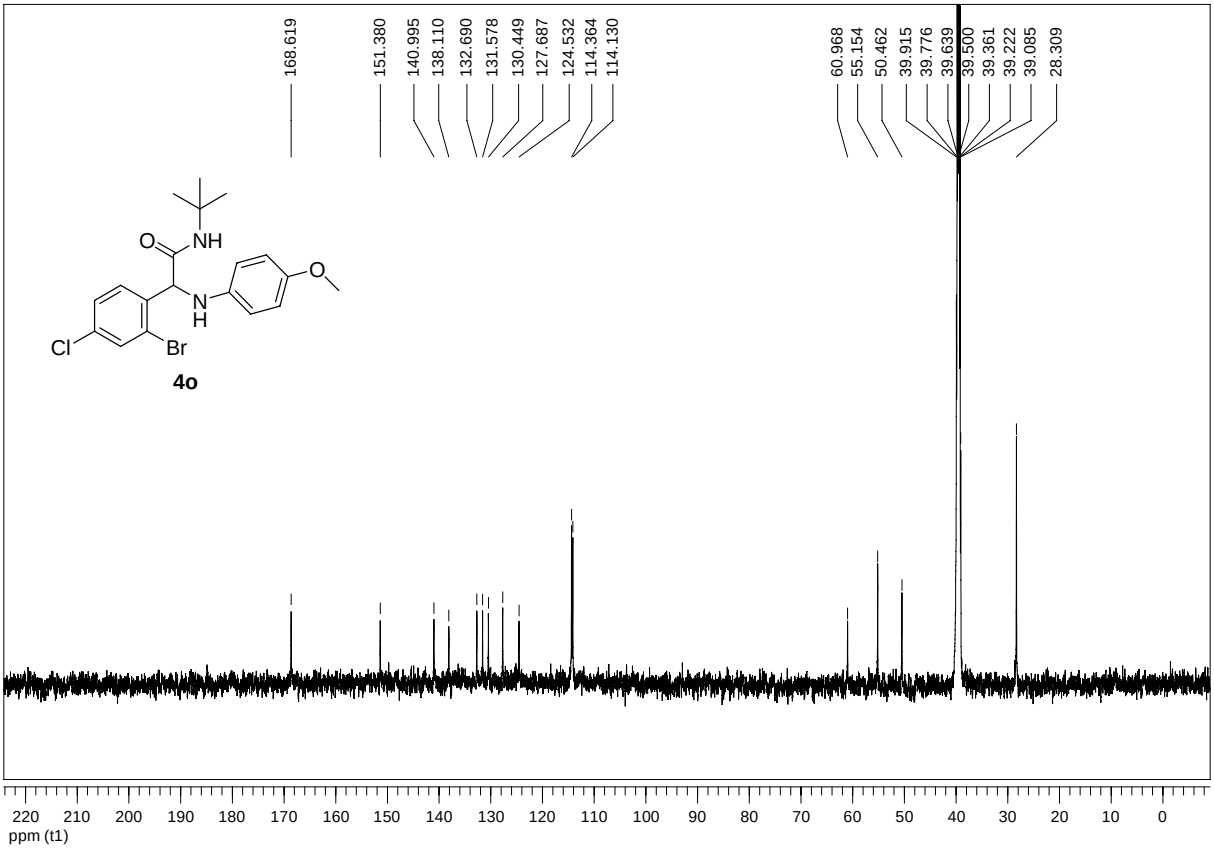
7.484
7.478
7.469
7.449
7.445
7.435
7.431
6.695
6.680
6.567
6.552
5.999
5.985
5.141
5.127
3.603
3.345
2.500
1.262
1.08
0.88
2.00
4.10
1.01
1.00
3.02
9.09
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
O
NH
N
H
O
Cl
Br
4o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130.449
127.687
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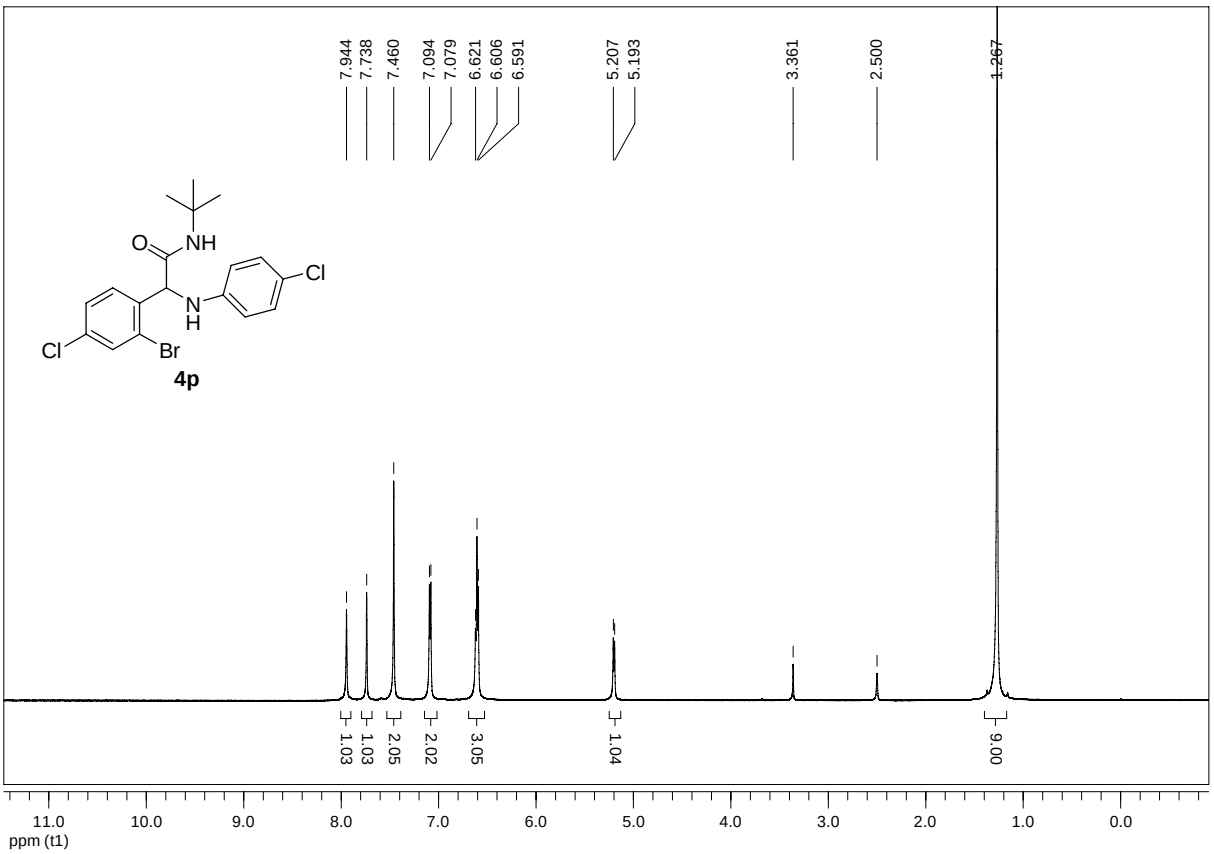
114.130
60.968
55.154
50.462
39.915
39.776
39.639
39.500
39.361
39.222
39.085
28.309
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)
O
NH
N
H
O
Cl
Br
4o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7.738
7.460
7.094
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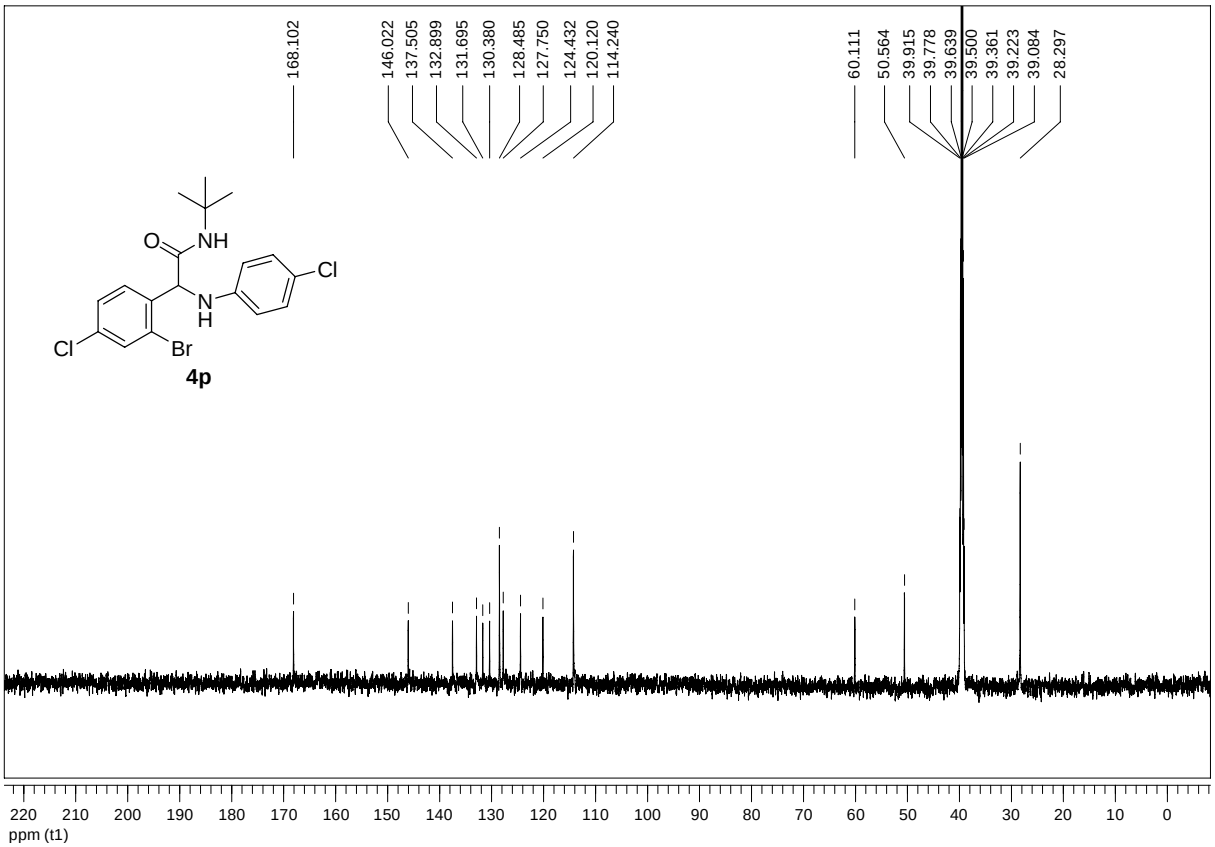
6.621
6.606
6.591
5.207
5.193
3.361
2.500
1.267
O
NH
N
H
Cl
Cl
Br
4p
1.03
1.03
2.05
2.02
3.05
1.04
9.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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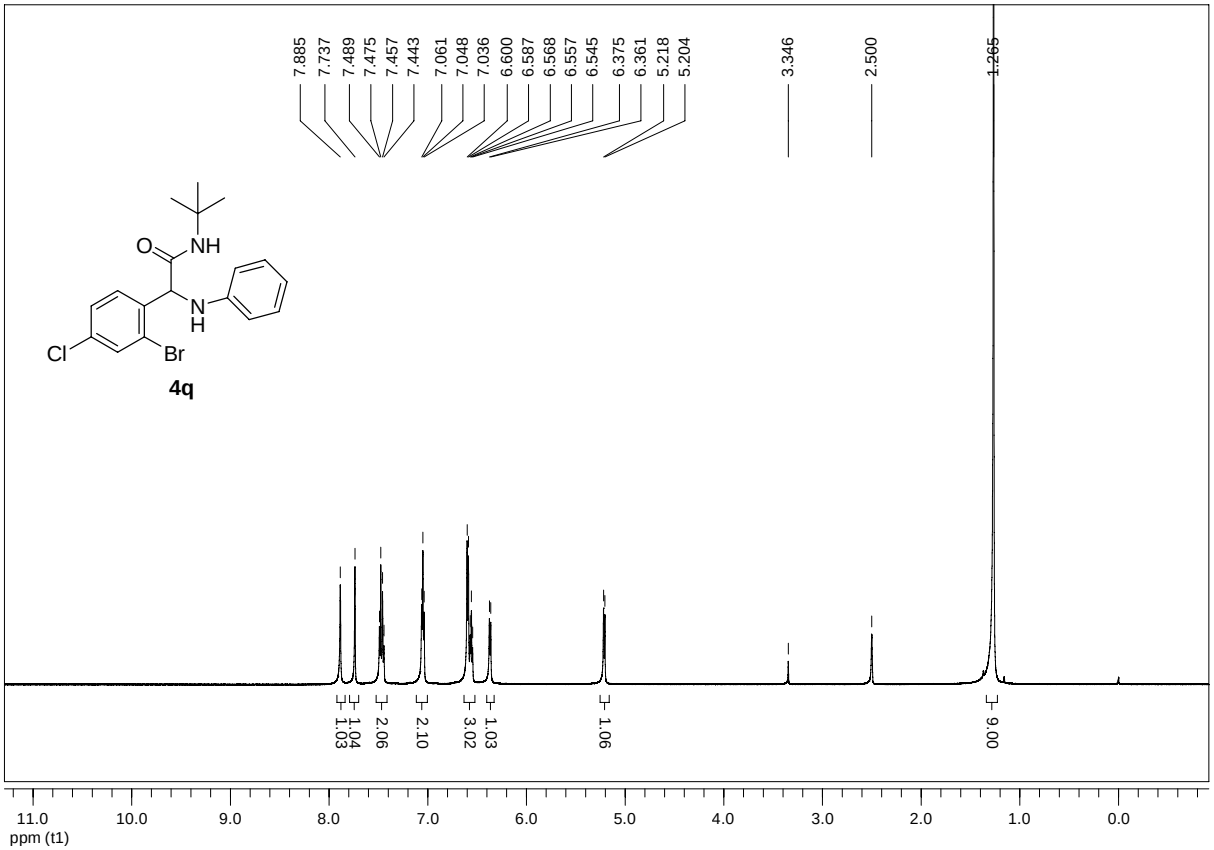
131.695
130.380
128.485
127.750
124.432
120.120
114.240
60.111
50.564
39.915
39.778
39.639
39.500
39.361
39.223
39.084
28.297
O
NH
N
H
Cl
Cl
Br
4p
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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7.443
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7.048
7.036
6.600
6.587
6.568
6.557
6.545
6.375
6.361
5.218
5.204
3.346
2.500
1.265
1.03
1.04
2.06
2.10
3.02
1.03
1.06
9.00
O
NH
N
H
Cl
Br
4q
11.0
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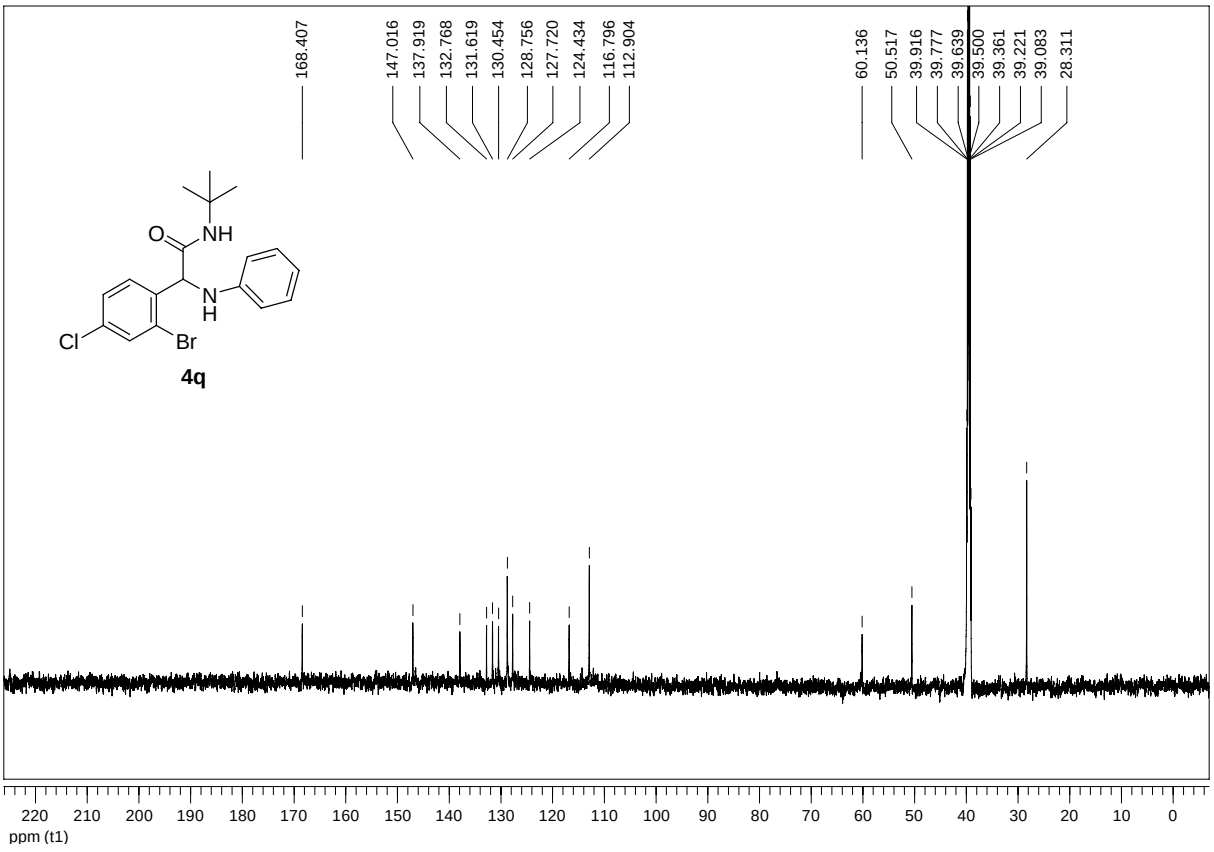
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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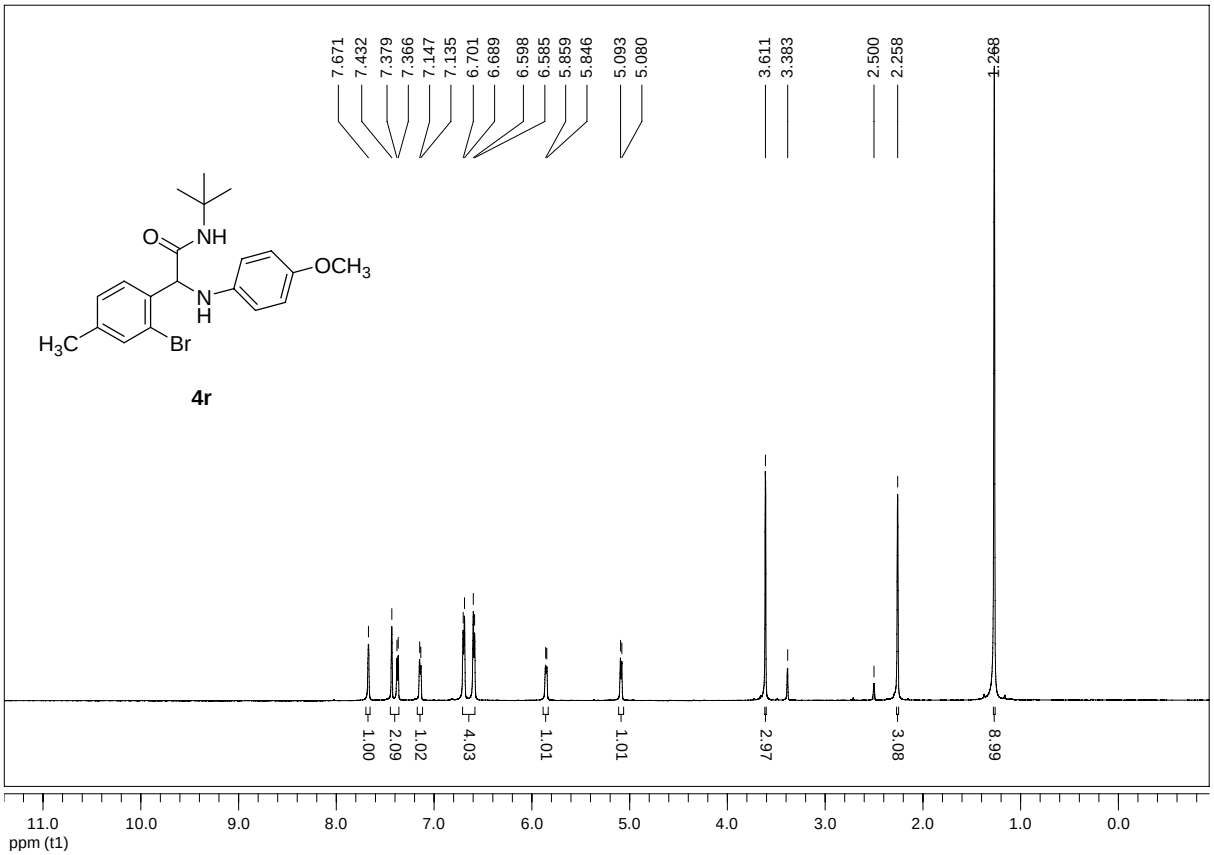
127.720
124.434
116.796
112.904
60.136
50.517
39.916
39.777
39.639
39.500
39.361
39.221
39.083
28.311
O
NH
N
H
Cl
Br
4q
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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7.147
7.135
6.701
6.689
6.598
6.585
5.859
5.846
5.093
5.080
3.611
3.383
2.500
2.258
1.268
O
NH
OCH3
N
H
H3C
Br
4r
1.00
2.09
1.02
4.03
1.01
1.01
2.97
3.08
8.99
11.0
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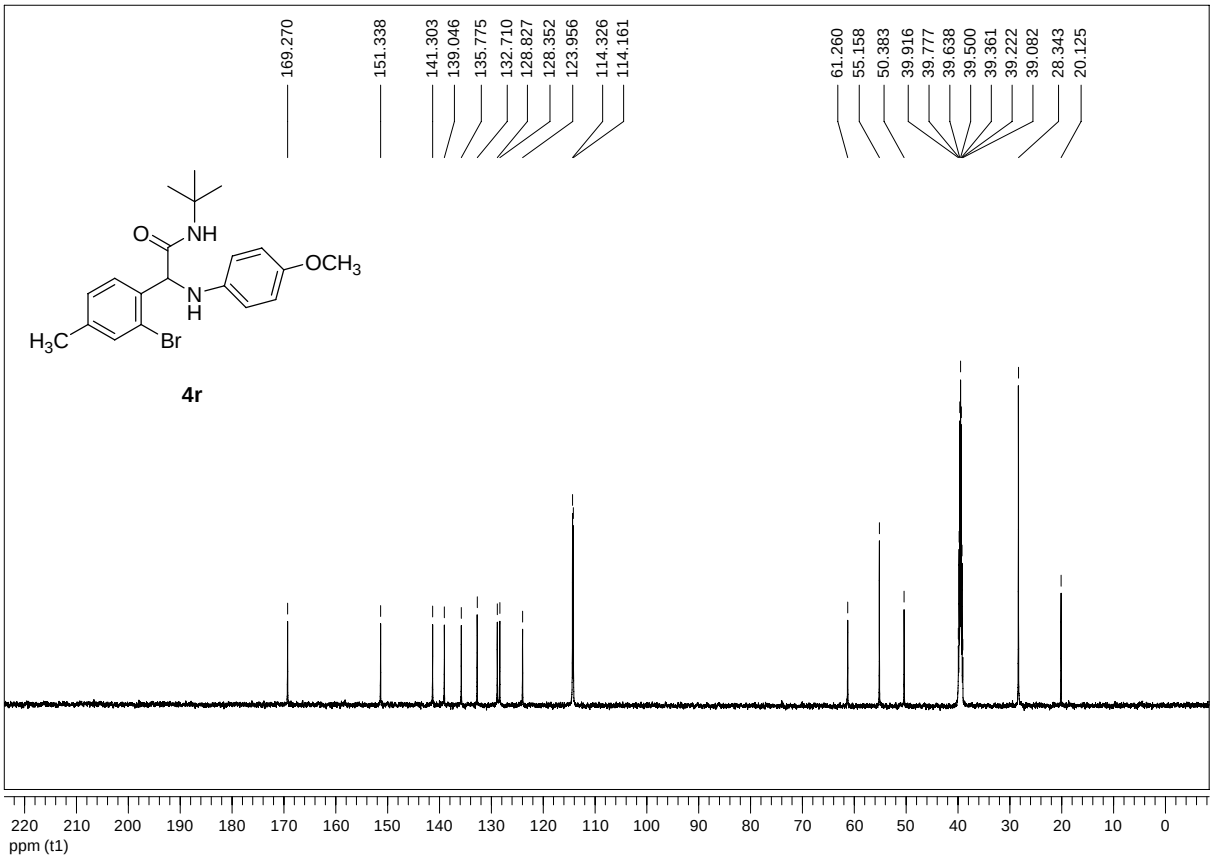
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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128.352
123.956
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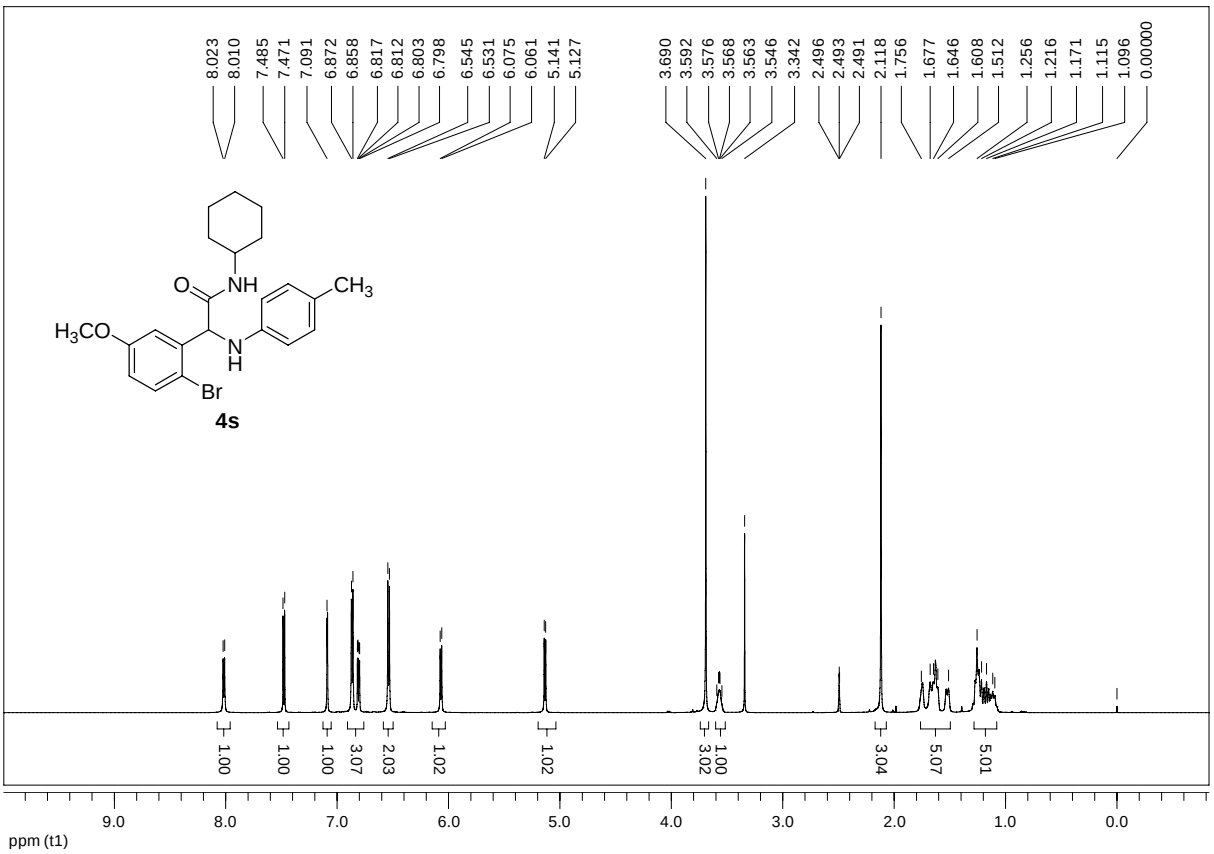
114.161
61.260
55.158
50.383
39.916
39.777
39.638
39.500
39.361
39.222
39.082
28.343
20.125
O
NH
OCH3
N
H
H3C
Br
4r
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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6.817
6.812
6.803
6.798
6.545
6.531
6.075
6.061
5.141
5.127
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3.592
3.576
3.568
3.563
3.546
3.342
2.496
2.493
2.491
2.118
1.756
1.677
1.646
1.608
1.512
1.256
1.216
1.171
1.115
1.096
0.00000
O
NH
CH3
H3CO
N
H
Br
4s
1.00
1.00
1.00
3.07
2.03
1.02
1.02
3.02
1.00
3.04
5.07
5.01
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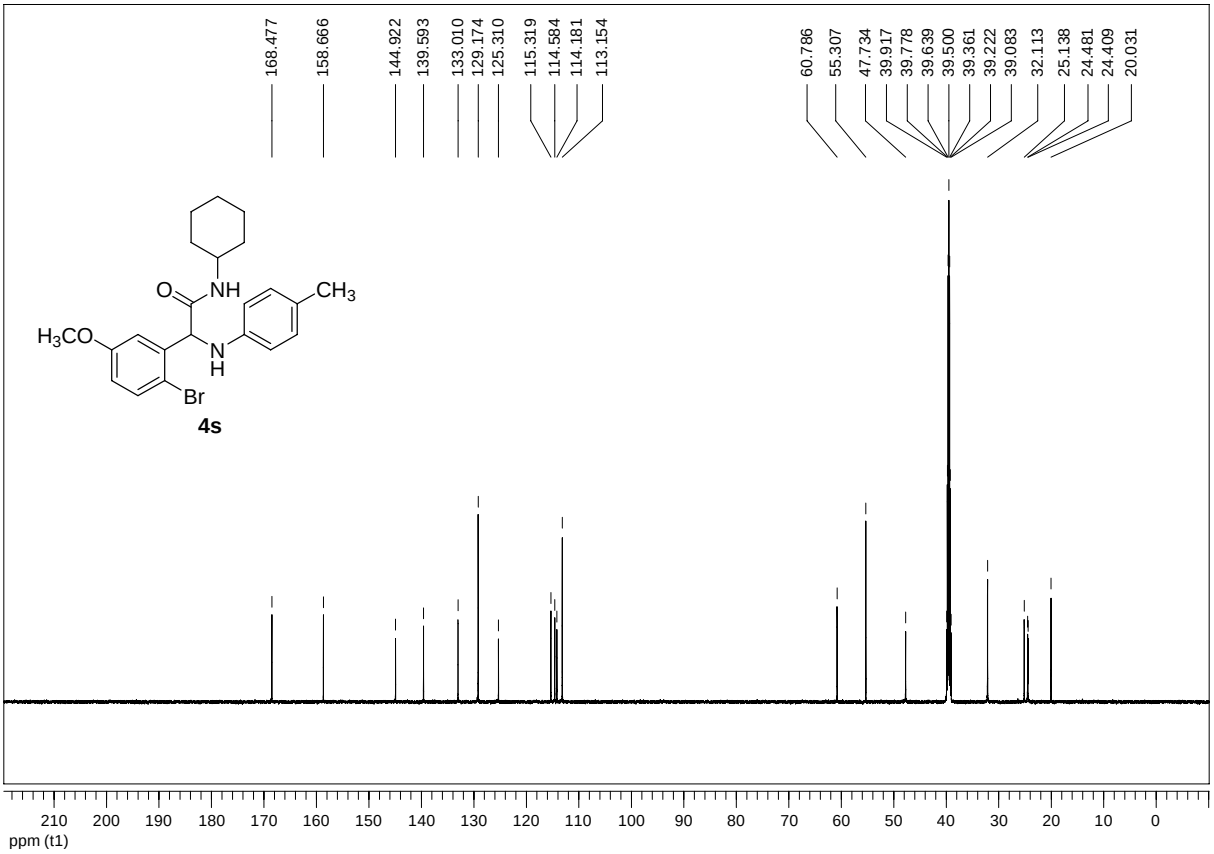
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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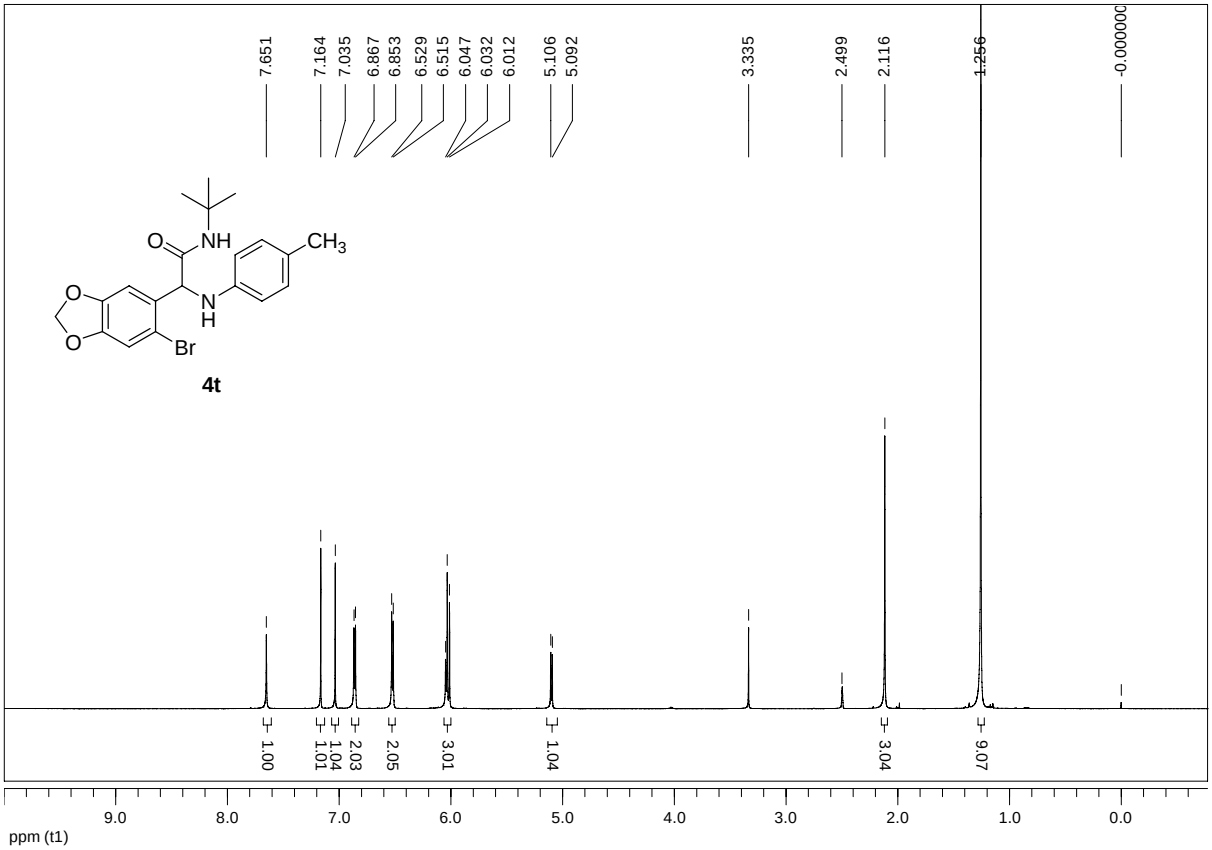
115.319
114.584
114.181
113.154
60.786
55.307
47.734
39.917
39.778
39.639
39.500
39.361
39.222
39.083
32.113
25.138
24.481
24.409
20.031
O
NH
CH3
H3CO
N
H
Br
4s
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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6.529
6.515
6.047
6.032
6.012
5.106
5.092
3.335
2.499
2.116
1.256
-0.000000
1.00
1.01
1.04
2.03
2.05
3.01
1.04
3.04
9.07
O
NH
CH3
O
N
H
O
Br
4t
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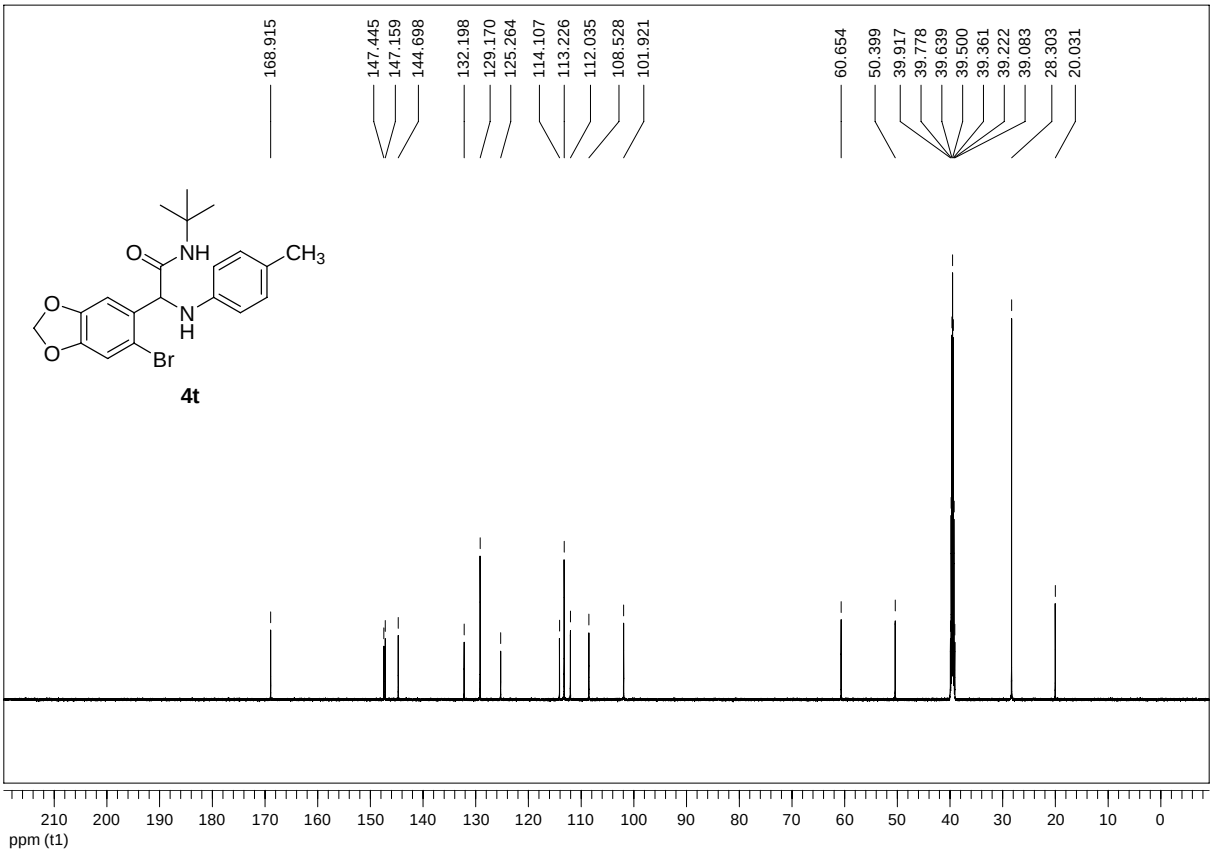
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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108.528
101.921
60.654
50.399
39.917
39.778
39.639
39.500
39.361
39.222
39.083
28.303
20.031
O
NH
CH3
O
N
H
O
Br
4t
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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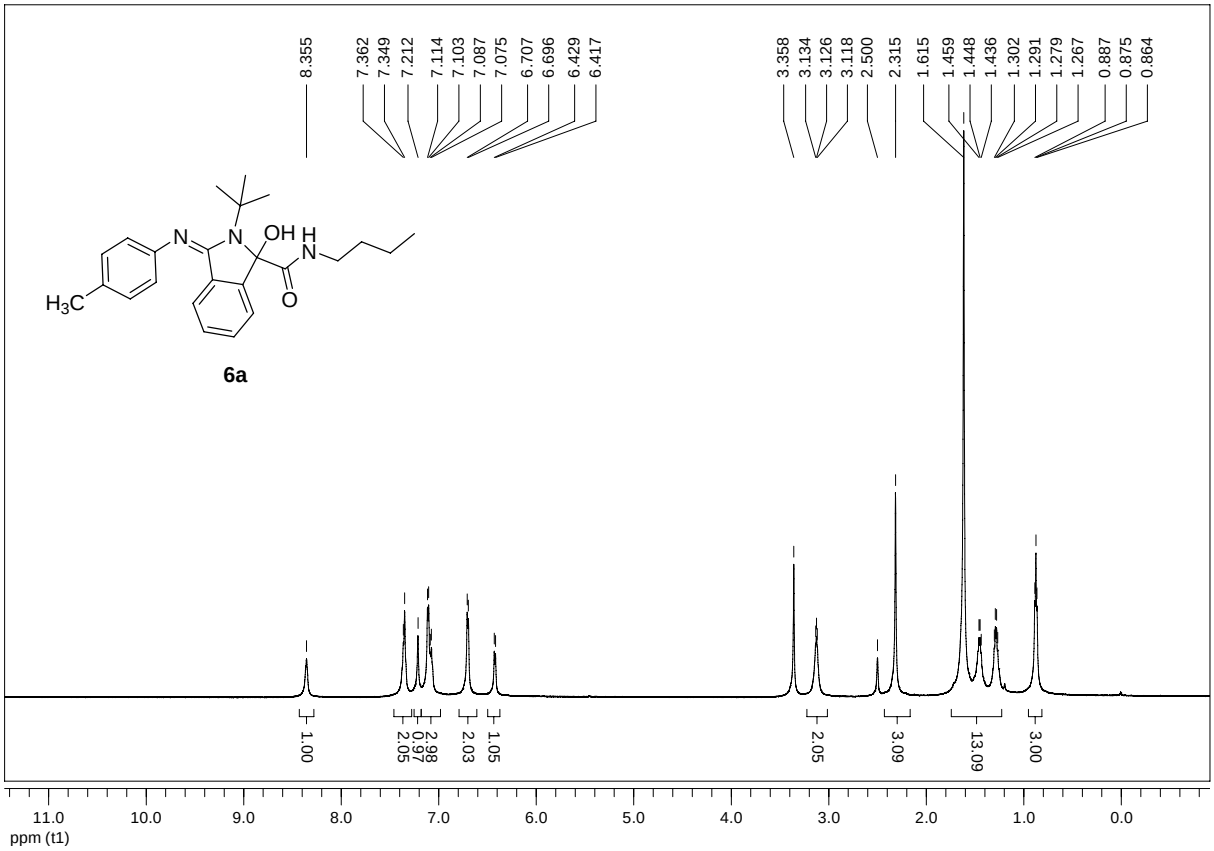
ppm (t1)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6.429
6.417
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3.134
3.126
3.118
2.500
2.315
1.615
1.459
1.448
1.436
1.302
1.291
1.279
1.267
0.887
0.875
0.864
1.00
2.05
0.97
2.98
2.03
1.05
2.05
3.09
13.09
3.00
11.0
10.0
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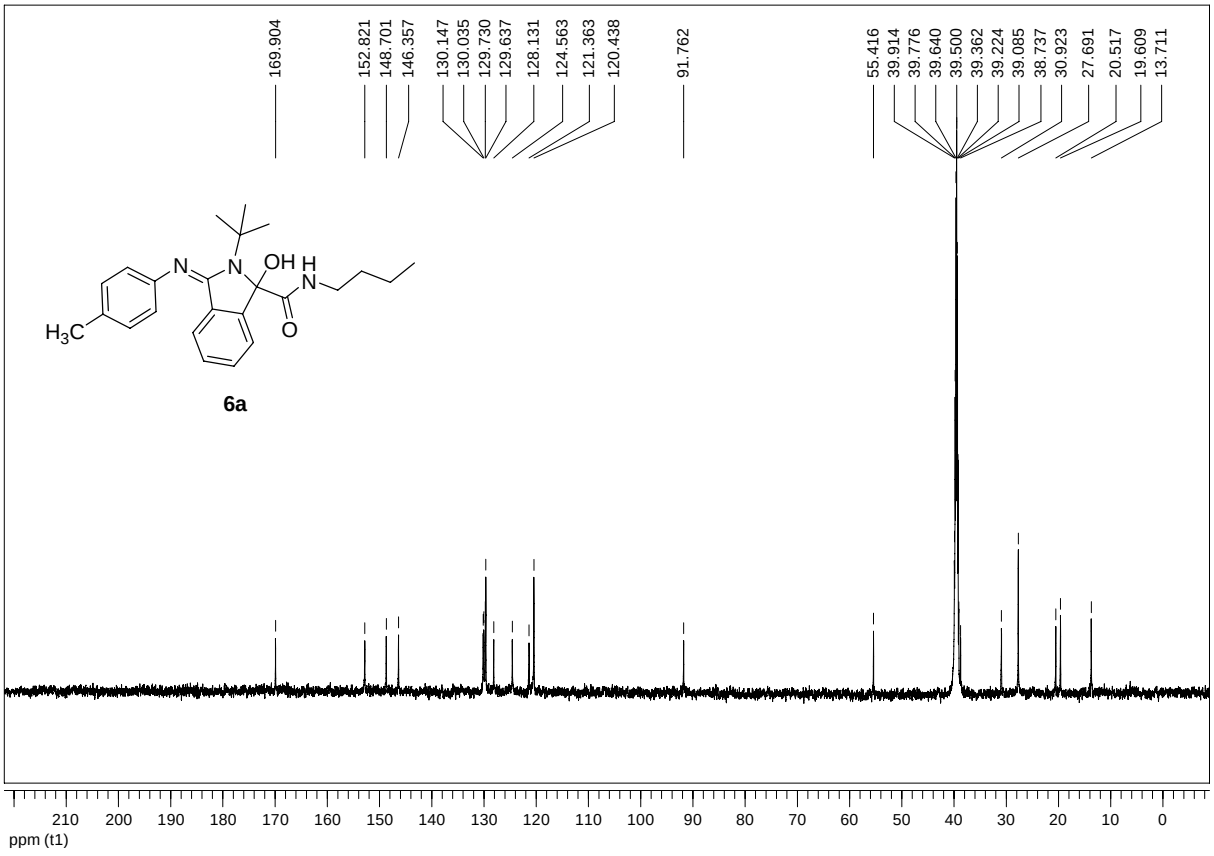
ppm (t1)

6a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129.637
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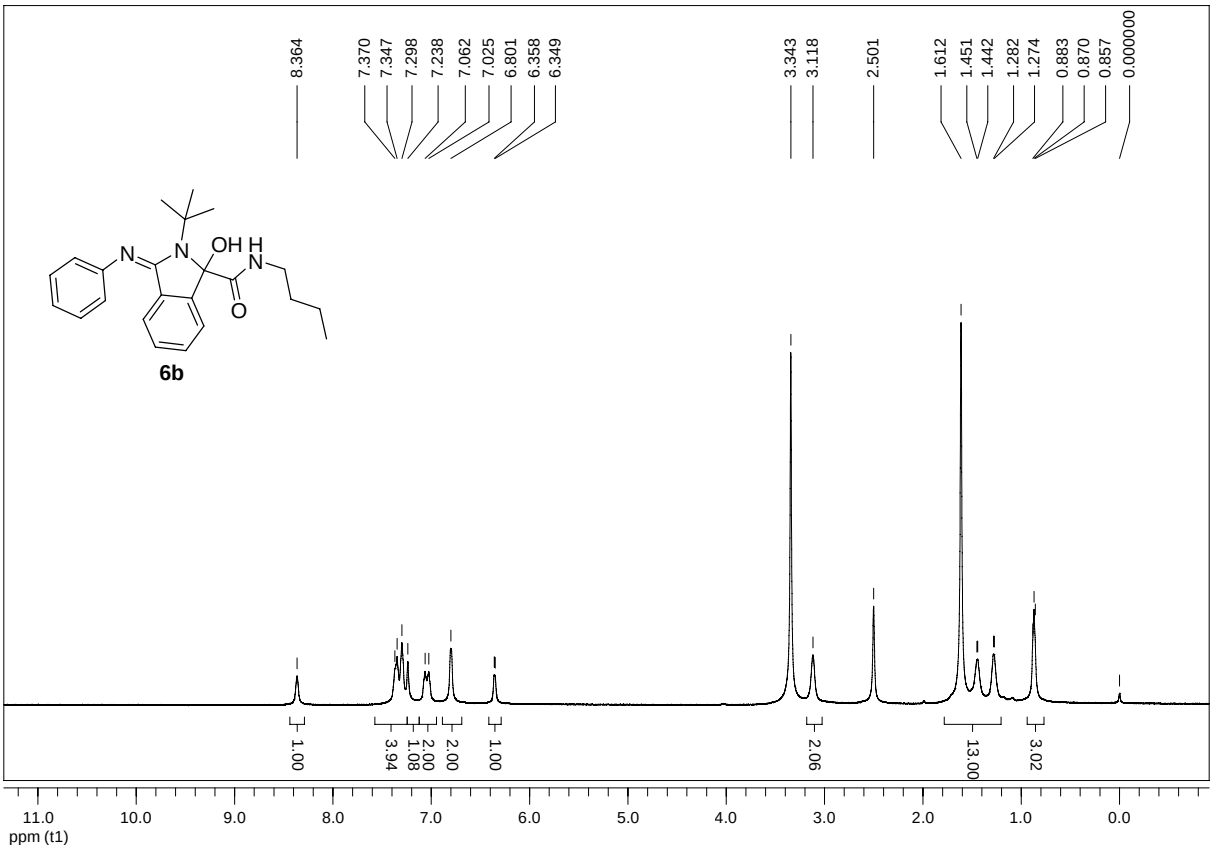
124.563
121.363
120.438
91.762
55.416
39.914
39.776
39.640
39.500
39.362
39.224
39.085
38.737
30.923
27.691
20.517
19.609
13.711
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

6a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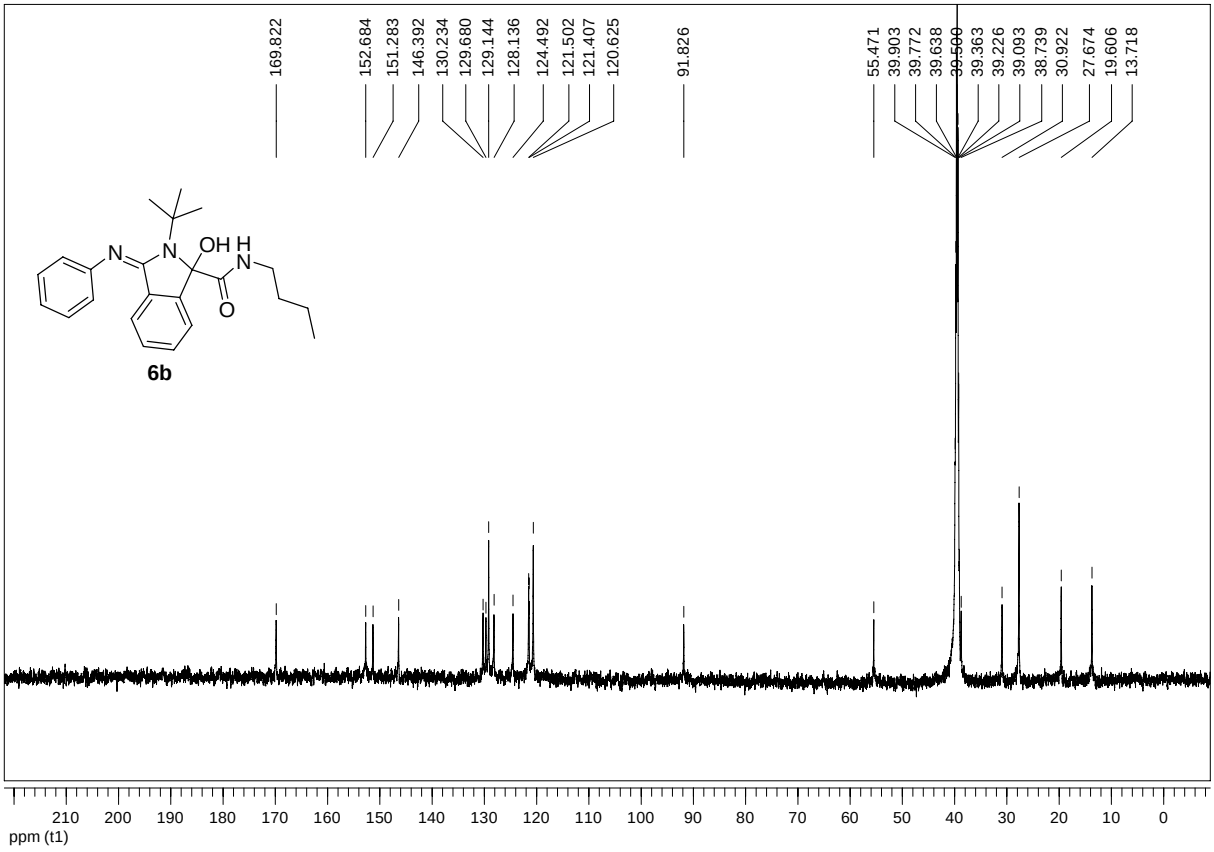
7.370
7.347
7.298
7.238
7.062
7.025
6.801
6.358
6.349
3.343
3.118
2.501
1.612
1.451
1.442
1.282
1.274
0.883
0.870
0.857
0.000000
1.00
3.94
1.08
2.00
2.00
1.00
2.06
13.00
3.02
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
OH
H
N
N
N
O
6b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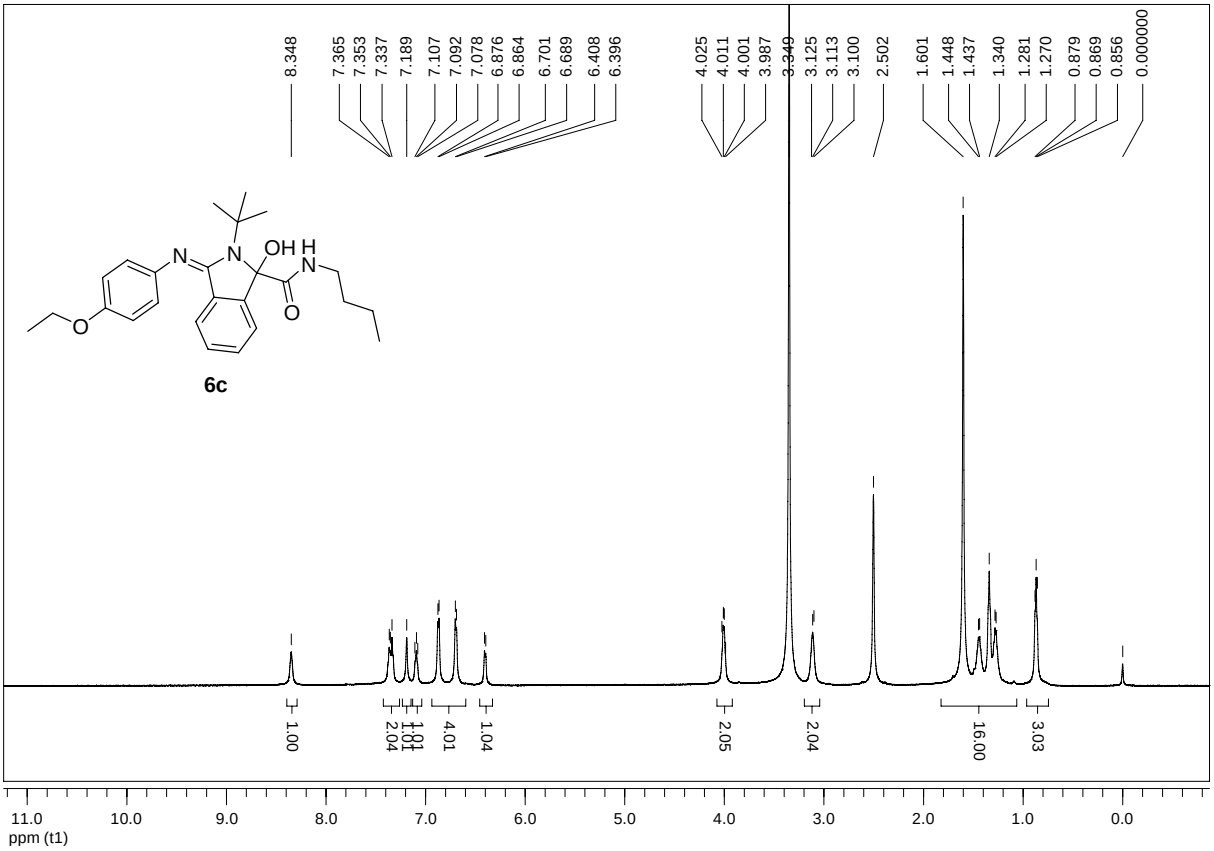
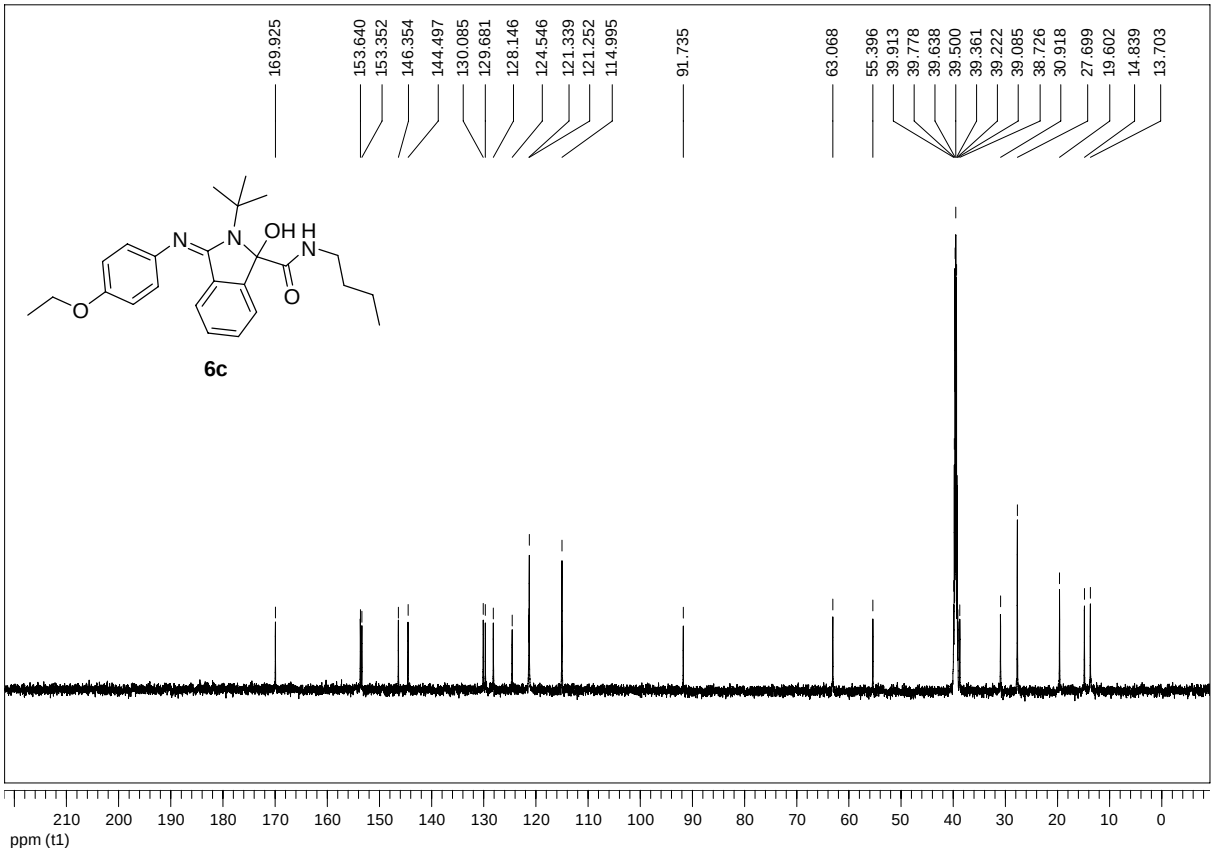
152.684
151.283
146.392
130.234
129.680
129.144
128.136
124.492
121.502
121.407
120.625
91.826
55.471
39.903
39.772
39.638
39.500
39.363
39.226
39.093
38.739
30.922
27.674
19.606
13.718
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)
OH
H
N
N
N
O
6b


8.348
7.365
7.353
7.337
7.189
7.107
7.092
7.078
6.876
6.864
6.701
6.689
6.408
6.396
4.025
4.011
4.001
3.987
3.349
3.125
3.113
3.100
2.502
1.601
1.448
1.437
1.340
1.281
1.270
0.879
0.869
0.856
0.000000
1.00
2.04
1.01
1.01
4.01
1.04
2.05
2.04
16.00
3.03
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
OH
H
N
N
N
O
O

6c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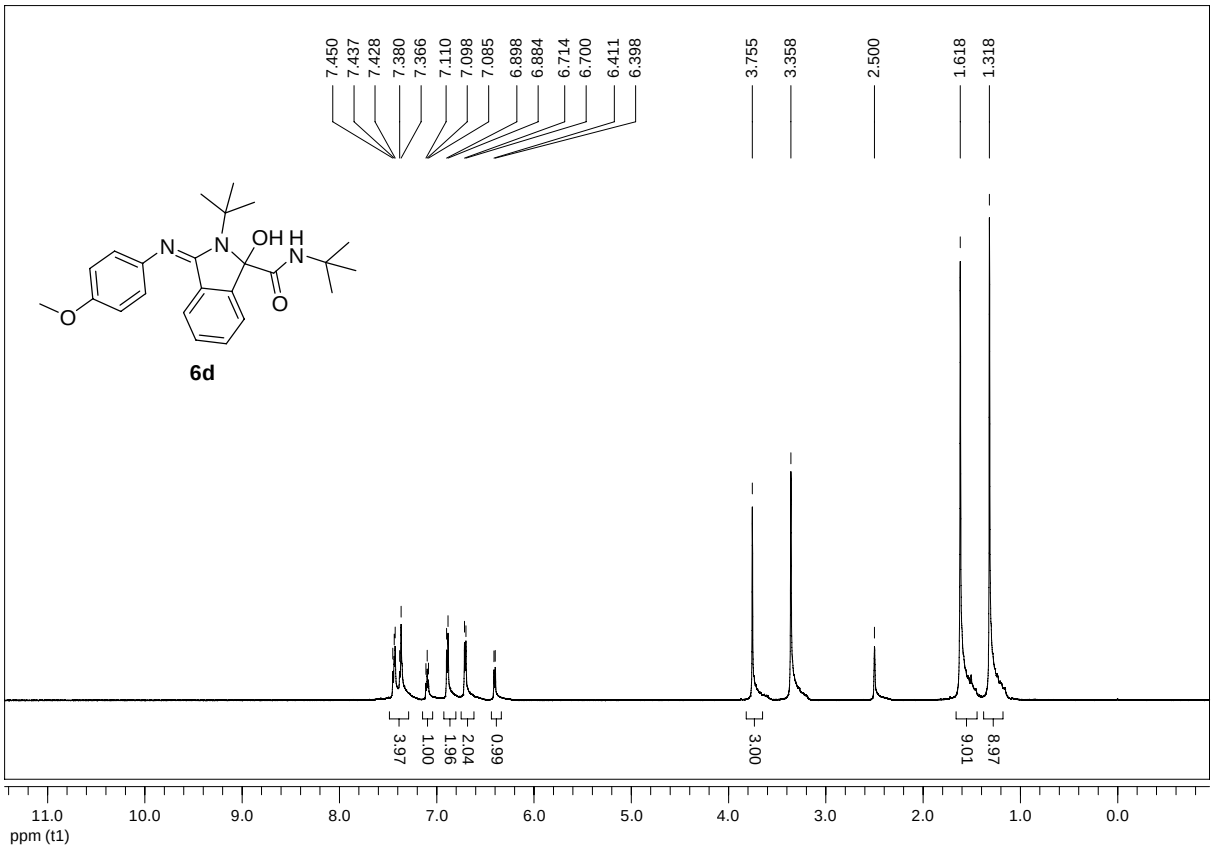
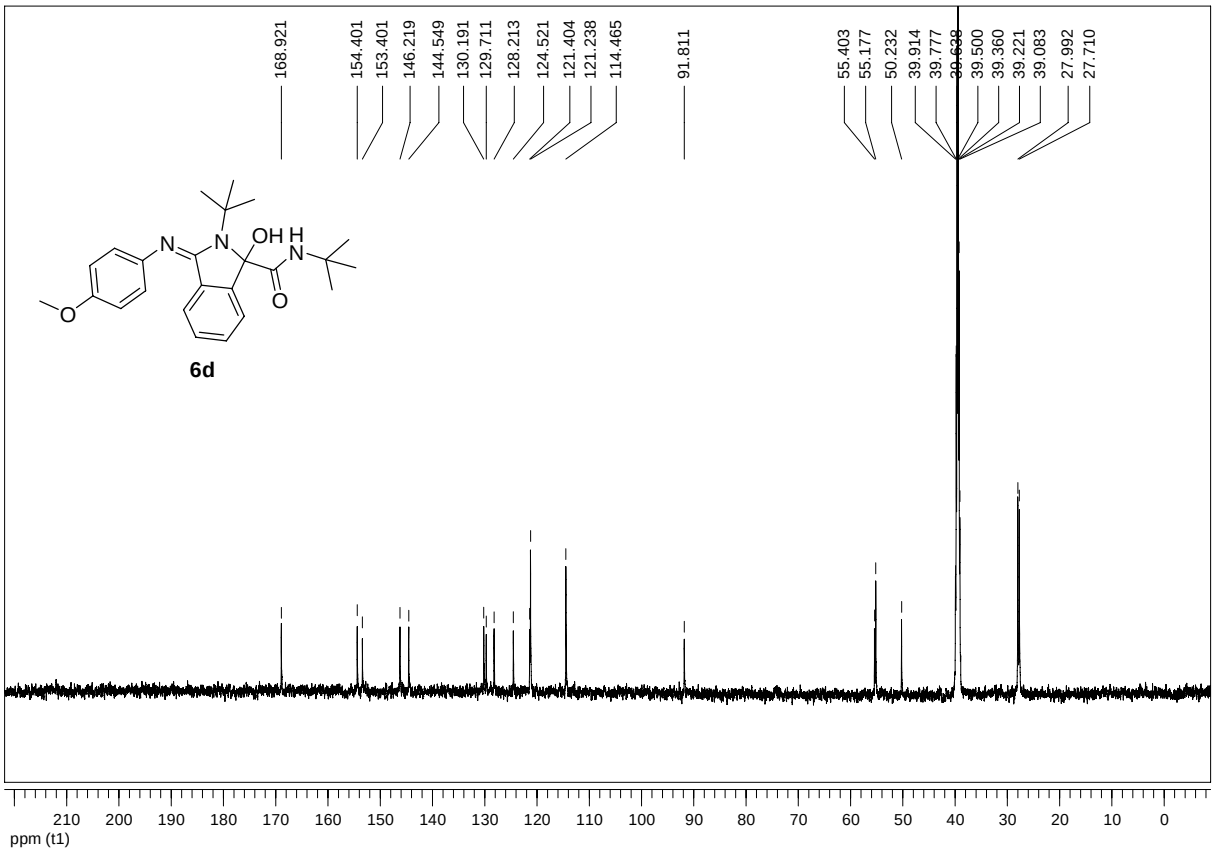
153.640
153.352
146.354
144.497
130.085
129.681
128.146
124.546
121.339
121.252
114.995
91.735
63.068
55.396
39.913
39.778
39.638
39.500
39.361
39.222
39.085
38.726
30.918
27.699
19.602
14.839
13.703
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)
OH
H
N
N
N
O
O

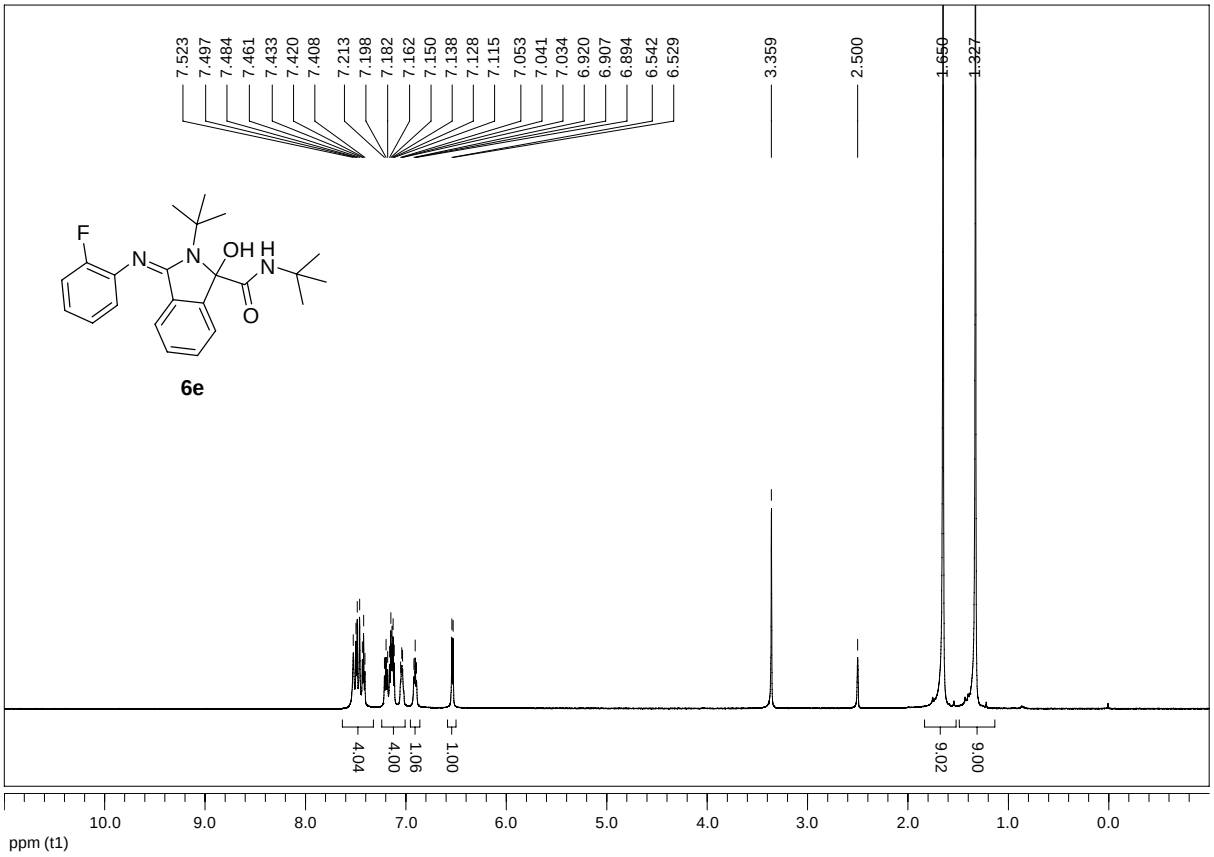
6c


7.450
7.437
7.428
7.380
7.366
7.110
7.098
7.085
6.898
6.884
6.714
6.700
6.411
6.398
3.755
3.358
2.500
1.618
1.318
3.97
1.00
1.96
2.04
0.99
3.00
9.01
8.97
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

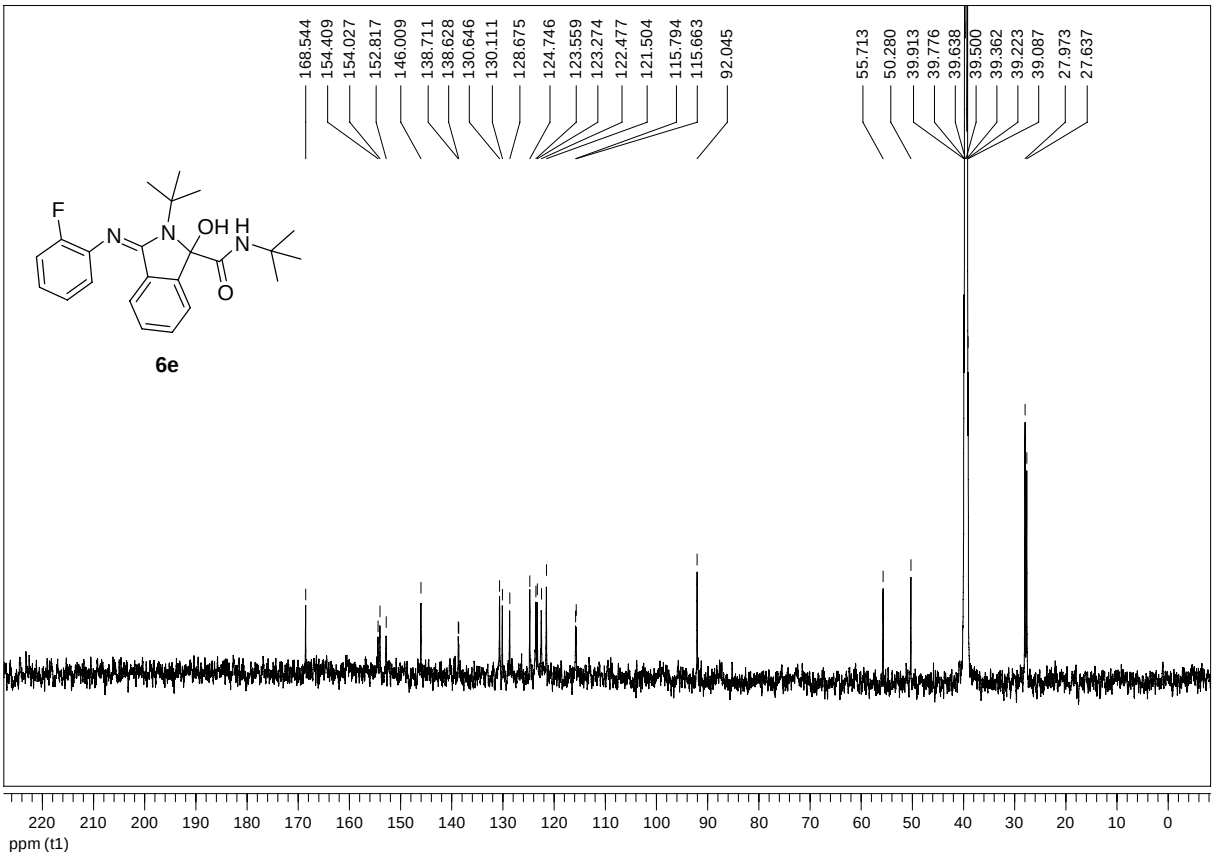
6d


168.921
154.401
153.401
146.219
144.549
130.191
129.711
128.213
124.521
121.404
121.238
114.465
91.811
55.403
55.177
50.232
39.914
39.777
39.638
39.500
39.360
39.221
39.083
27.992
27.710
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

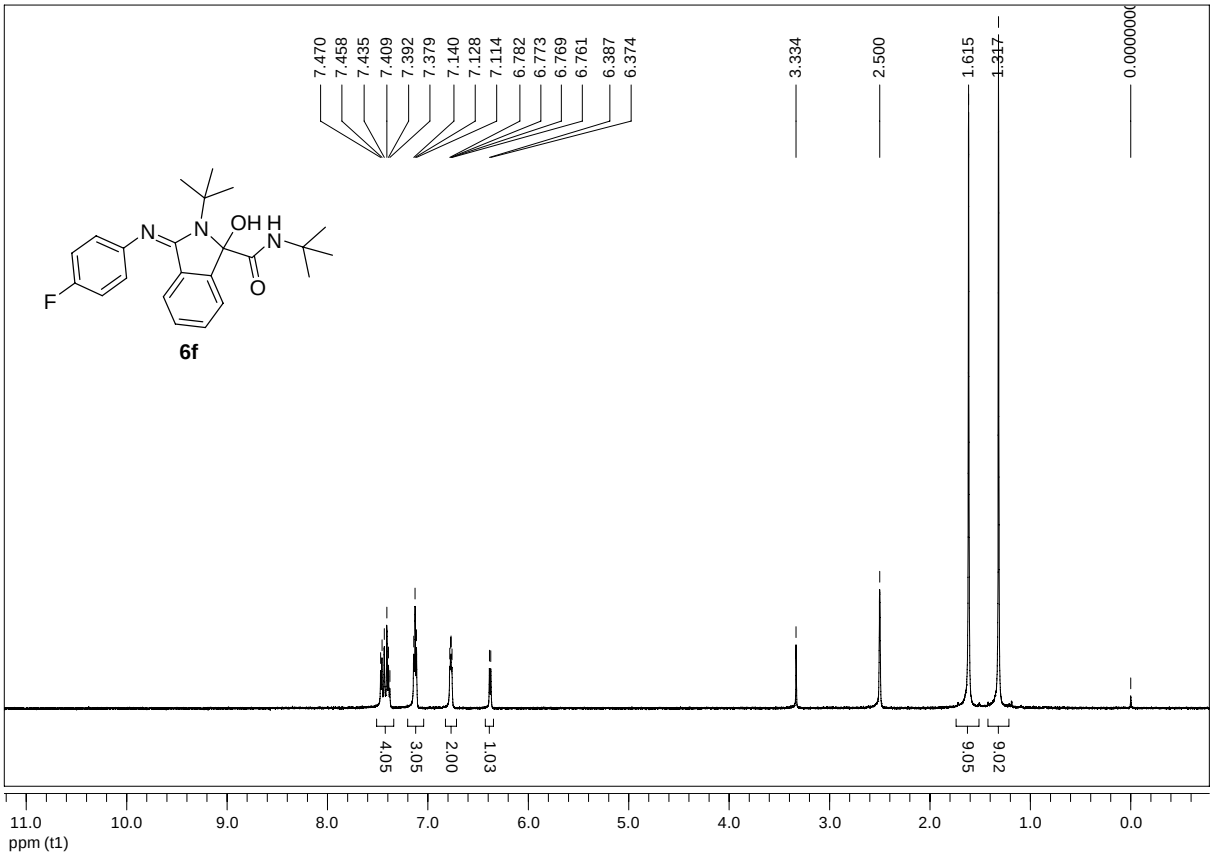
6d


7.523
7.497
7.484
7.461
7.433
7.420
7.408
7.213
7.198
7.182
7.162
7.150
7.138
7.128
7.115
7.053
7.041
7.034
6.920
6.907
6.894
6.542
6.529
3.359
2.500
1.650
1.327
F
N
N
OH H
N
O
4.04
4.00
1.06
1.00
9.02
9.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

6e


168.544
154.409
154.027
152.817
146.009
138.711
138.628
130.646
130.111
128.675
124.746
123.559
123.274
122.477
121.504
115.794
115.663
92.045
55.713
50.280
39.913
39.776
39.638
39.500
39.362
39.223
39.087
27.973
27.637
F
N
N
OH H
N
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

6e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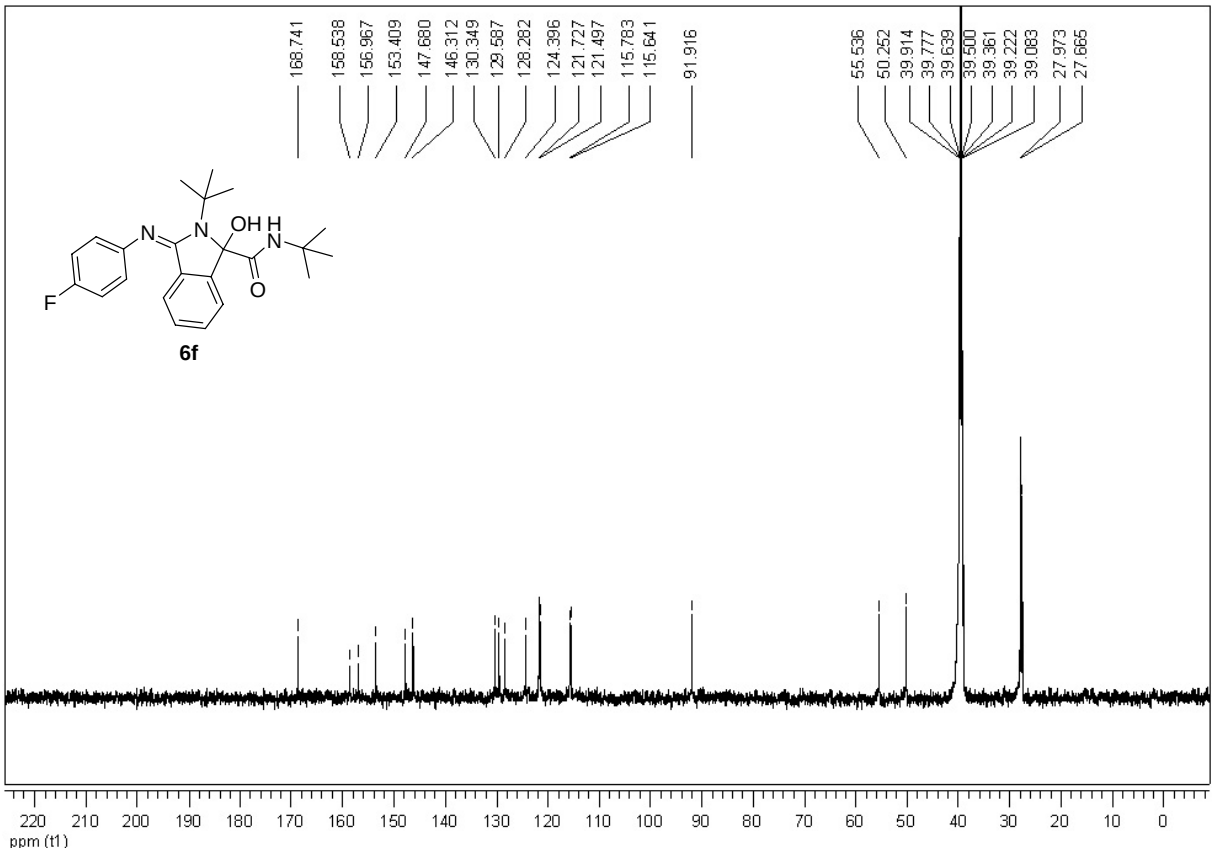
7.458
7.435
7.409
7.392
7.379
7.140
7.128
7.114
6.782
6.773
6.769
6.761
6.387
6.374
3.334
2.500
1.615
1.317
0.000000
4.05
3.05
2.00
1.03
9.05
9.02
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
OH
H
N
N
N
O
F

6f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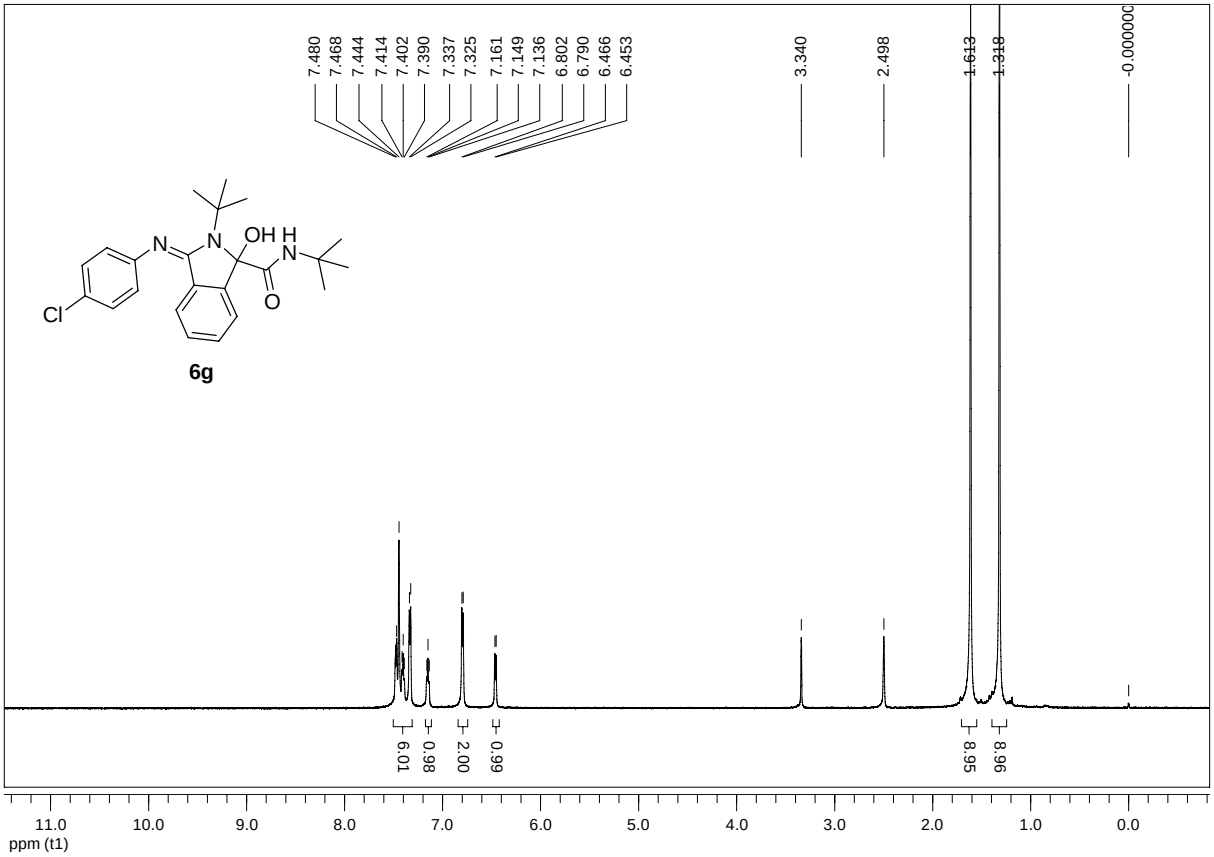
158.538
156.967
153.409
147.680
146.312
130.349
129.587
128.282
124.396
121.727
121.497
115.783
115.641
91.916
55.536
50.252
39.914
39.777
39.639
39.500
39.361
39.222
39.083
27.973
27.665
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)
OH
H
N
N
N
O
F

6f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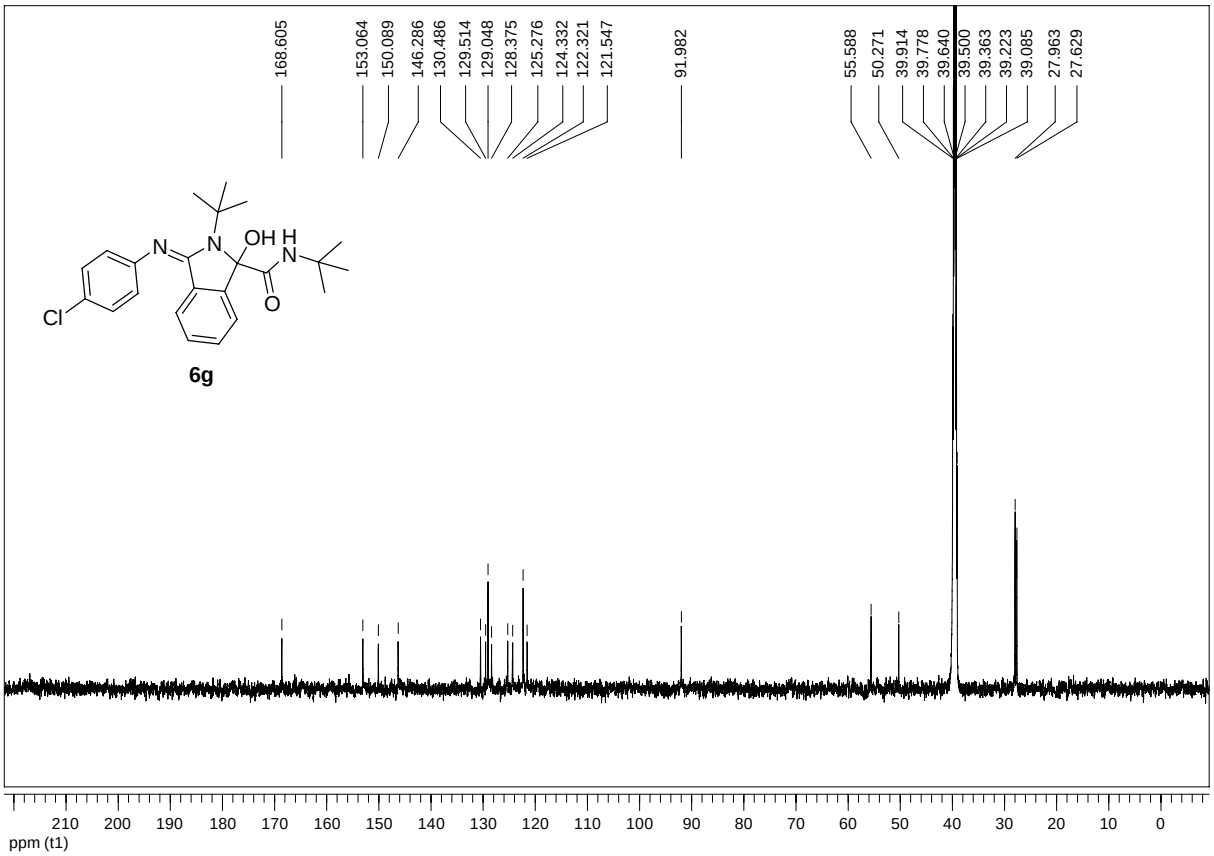
7.444
7.414
7.402
7.390
7.337
7.325
7.161
7.149
7.136
6.802
6.790
6.466
6.453
3.340
2.498
1.613
1.318
-0.000000
6.01
0.98
2.00
0.99
8.95
8.96
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
N
N
OH
H
N
O
Cl

6g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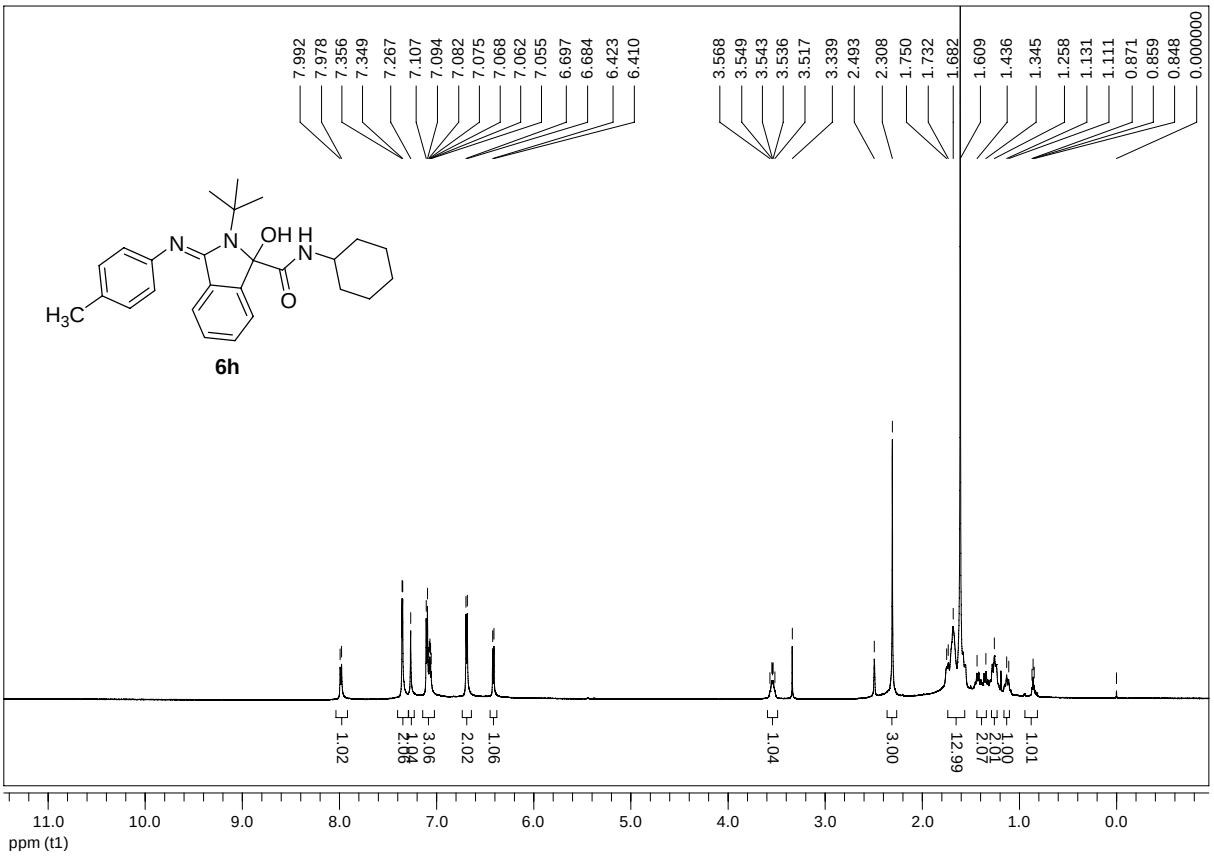
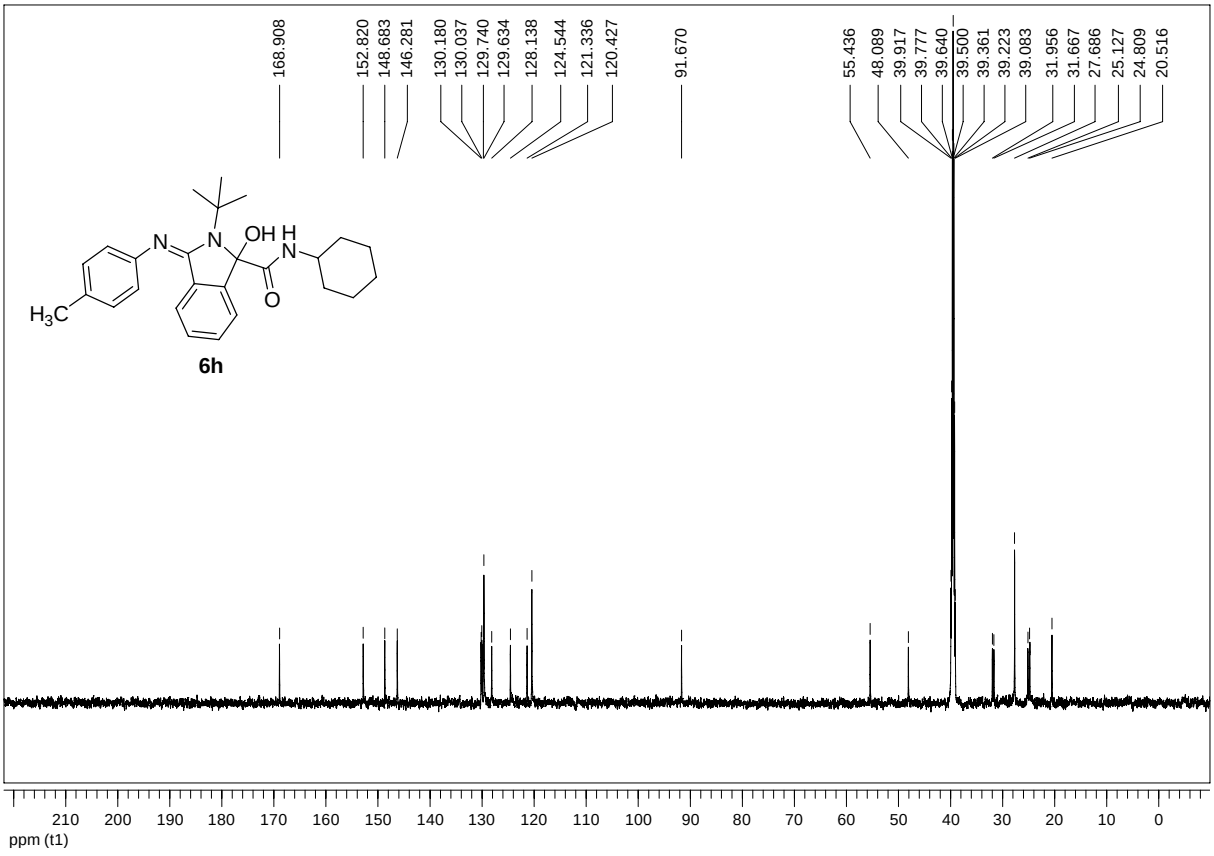
153.064
150.089
146.286
130.486
129.514
129.048
128.375
125.276
124.332
122.321
121.547
91.982
55.588
50.271
39.914
39.778
39.640
39.500
39.363
39.223
39.085
27.963
27.629
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)
N
N
OH
H
N
O
Cl

6g


7.992
7.978
7.356
7.349
7.267
7.107
7.094
7.082
7.075
7.068
7.062
7.055
6.697
6.684
6.423
6.410
3.568
3.549
3.543
3.536
3.517
3.339
2.493
2.308
1.750
1.732
1.682
1.609
1.436
1.345
1.258
1.131
1.111
0.871
0.859
0.848
0.000000
OH H
N
N
N
O
H3C
1.02
2.04
3.06
2.02
1.06
1.04
3.00
12.99
2.07
2.01
1.00
1.01
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

6h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130.037
129.740
129.634
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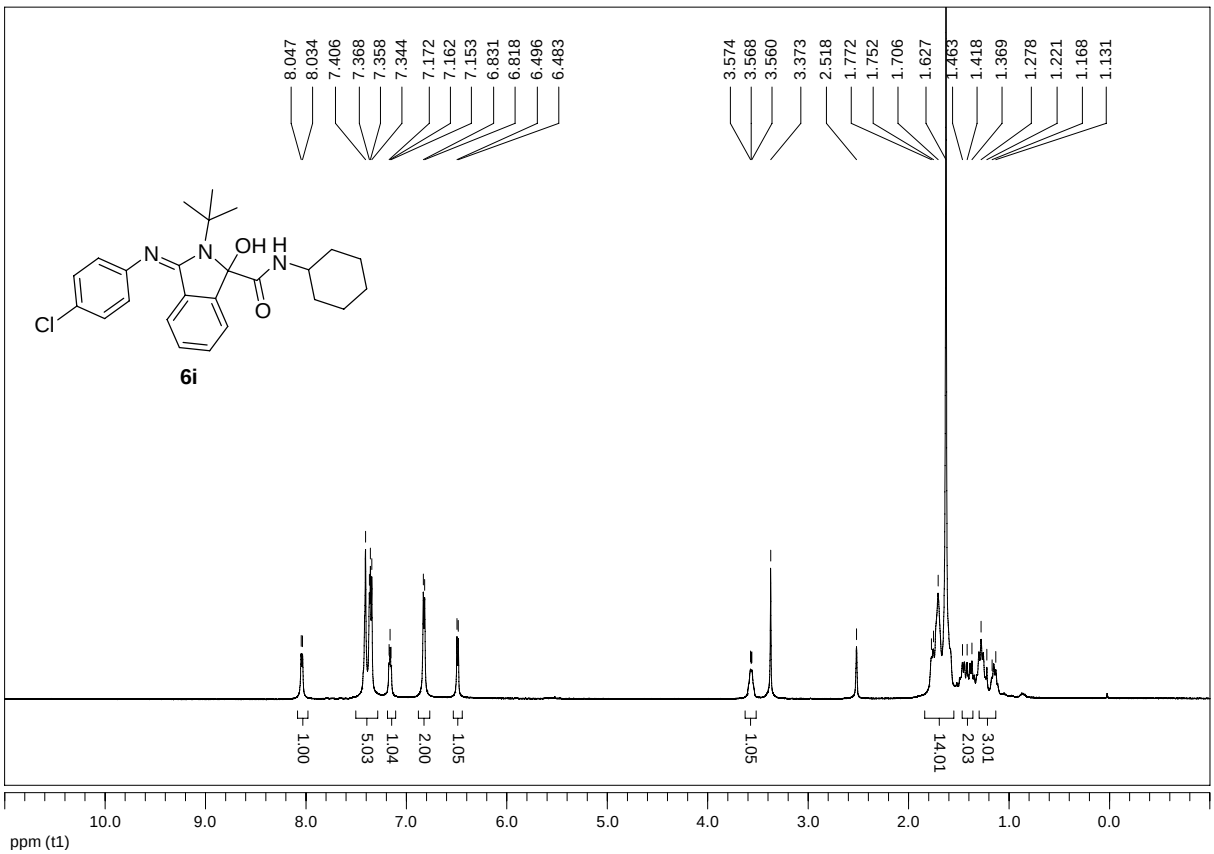
124.544
121.336
120.427
91.670
55.436
48.089
39.917
39.777
39.640
39.500
39.361
39.223
39.083
31.956
31.667
27.686
25.127
24.809
20.516
OH H
N
N
N
O
H3C
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

6h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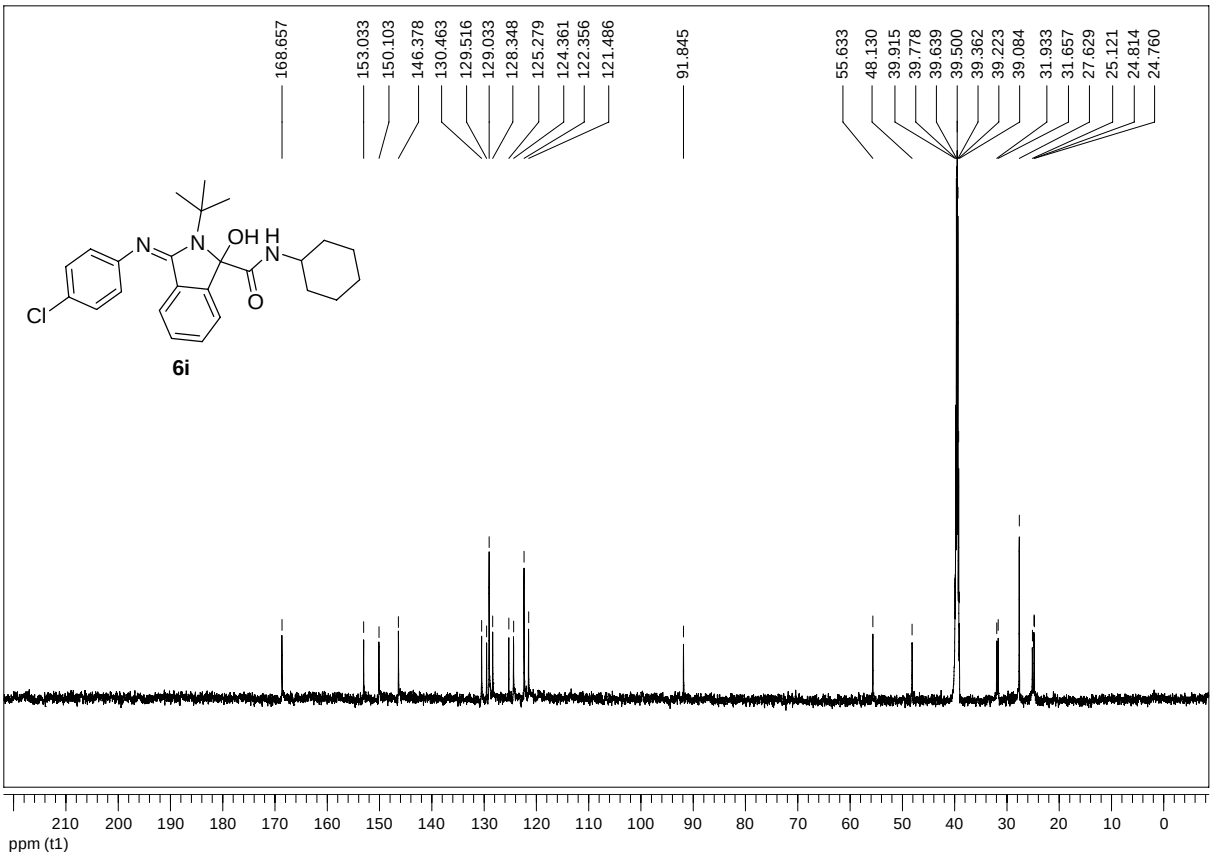
8.034
7.406
7.368
7.358
7.344
7.172
7.162
7.153
6.831
6.818
6.496
6.483
3.574
3.568
3.560
3.373
2.518
1.772
1.752
1.706
1.627
1.463
1.418
1.369
1.278
1.221
1.168
1.131
1.00
5.03
1.04
2.00
1.05
1.05
14.01
2.03
3.01
Cl
N
N
OH
H
N
O
6i
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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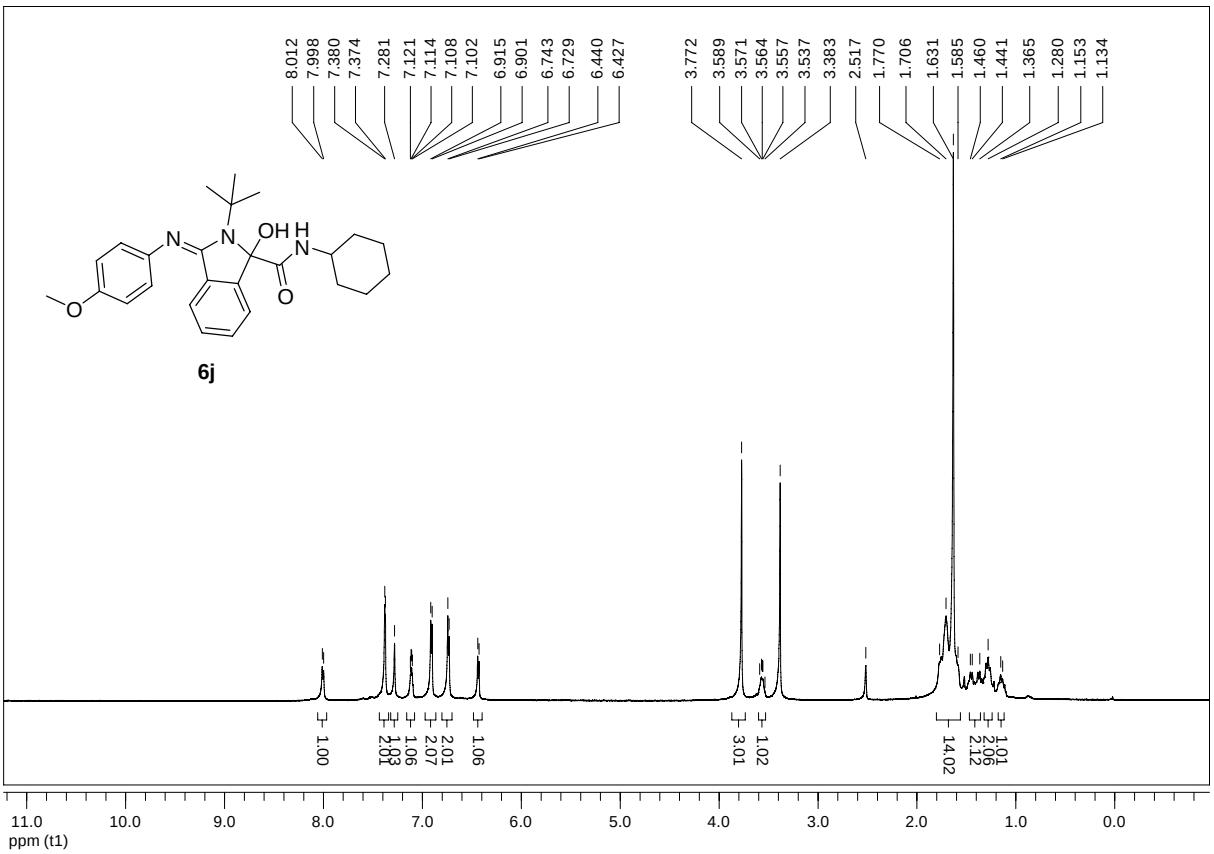
150.103
146.378
130.463
129.516
129.033
128.348
125.279
124.361
122.356
121.486
91.845
55.633
48.130
39.915
39.778
39.639
39.500
39.362
39.223
39.084
31.933
31.657
27.629
25.121
24.814
24.760
Cl
N
N
OH
H
N
O
6i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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7.114
7.108
7.102
6.915
6.901
6.743
6.729
6.440
6.427
3.772
3.589
3.571
3.564
3.557
3.537
3.383
2.517
1.770
1.706
1.631
1.585
1.460
1.441
1.365
1.280
1.153
1.134
1.00
2.01
1.03
1.06
2.07
2.01
1.06
3.01
1.02
14.02
2.12
1.08
1.01
11.0
10.0
9.0
8.0
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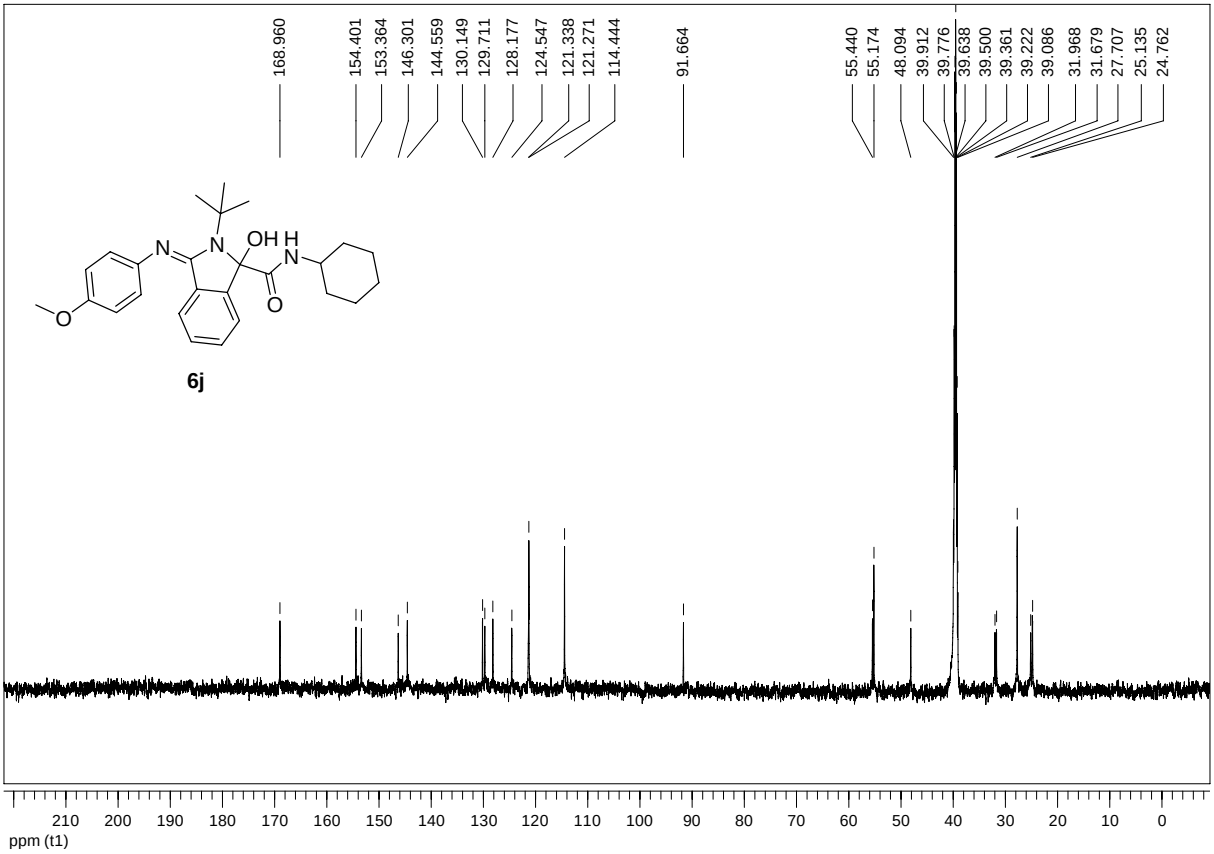
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
6j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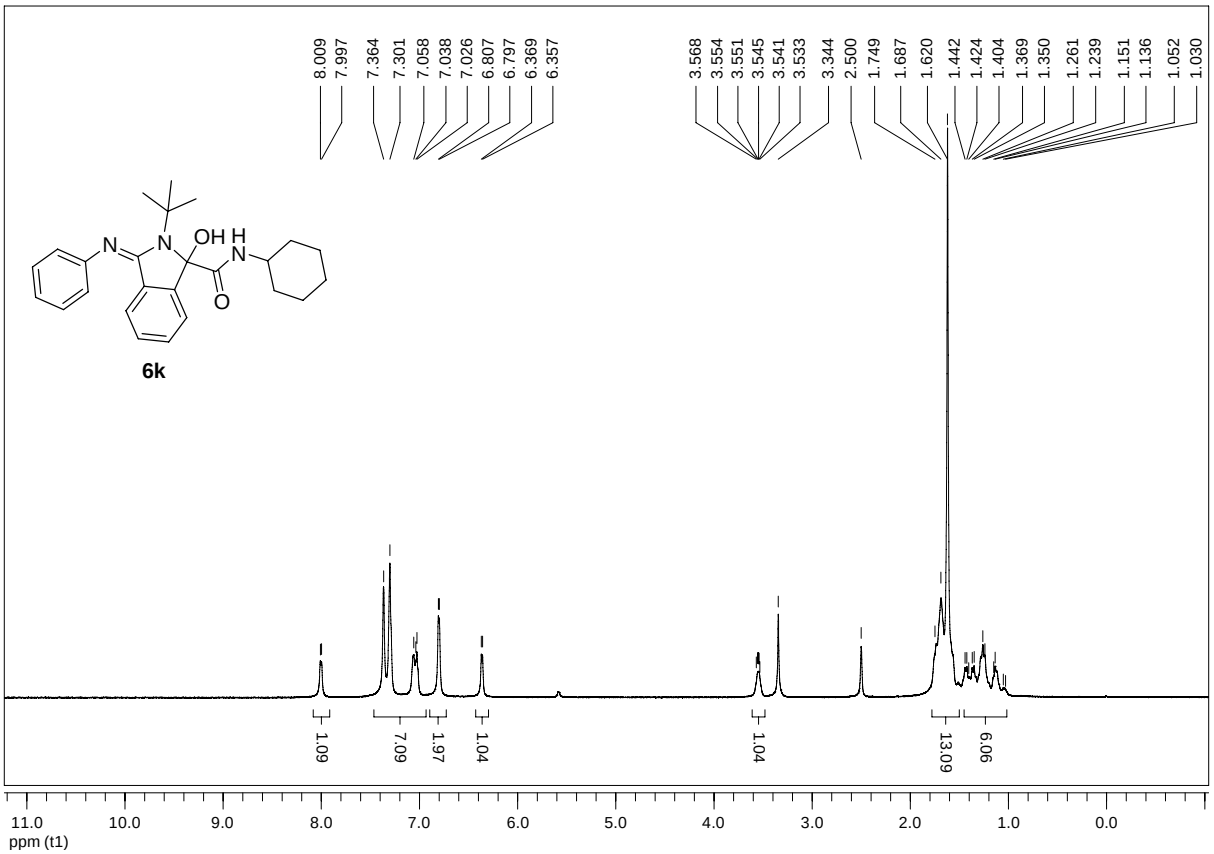
144.559
130.149
129.711
128.177
124.547
121.338
121.271
114.444
91.664
55.440
55.174
48.094
39.912
39.776
39.638
39.500
39.361
39.222
39.086
31.968
31.679
27.707
25.135
24.762
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)
6j


8.009
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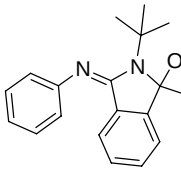
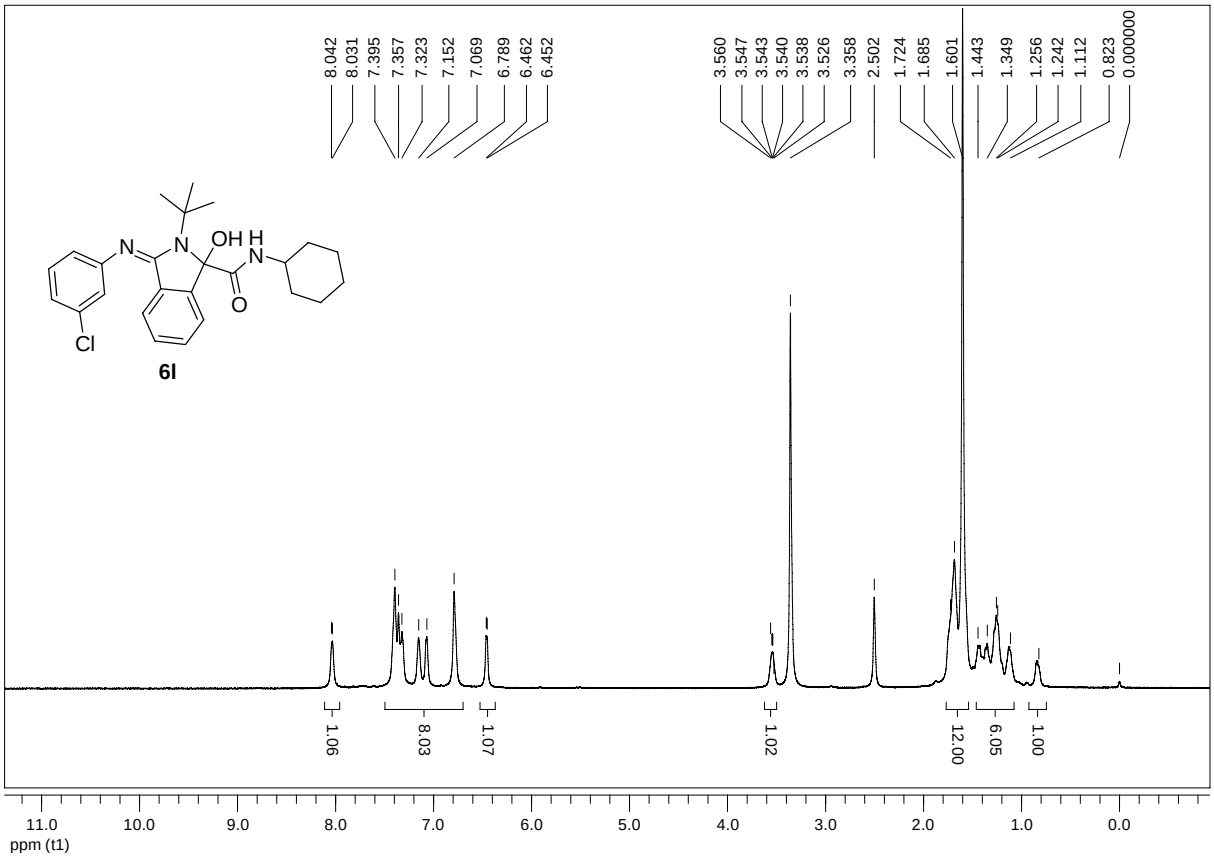
7.301
7.058
7.038
7.026
6.807
6.797
6.369
6.357
3.568
3.554
3.551
3.545
3.541
3.533
3.344
2.500
1.749
1.687
1.620
1.442
1.424
1.404
1.369
1.350
1.261
1.239
1.151
1.136
1.052
1.030
1.09
7.09
1.97
1.04
1.04
13.09
6.06
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)



6k

168.828
152.681
151.261
146.315
130.244
129.689
129.128
128.123
124.470
121.488
121.367
120.609
91.725
55.486
48.090
39.916
39.777
39.639
39.500
39.361
39.223
39.084
31.936
31.651
27.660
25.115
24.796
24.744
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

6k


8.042
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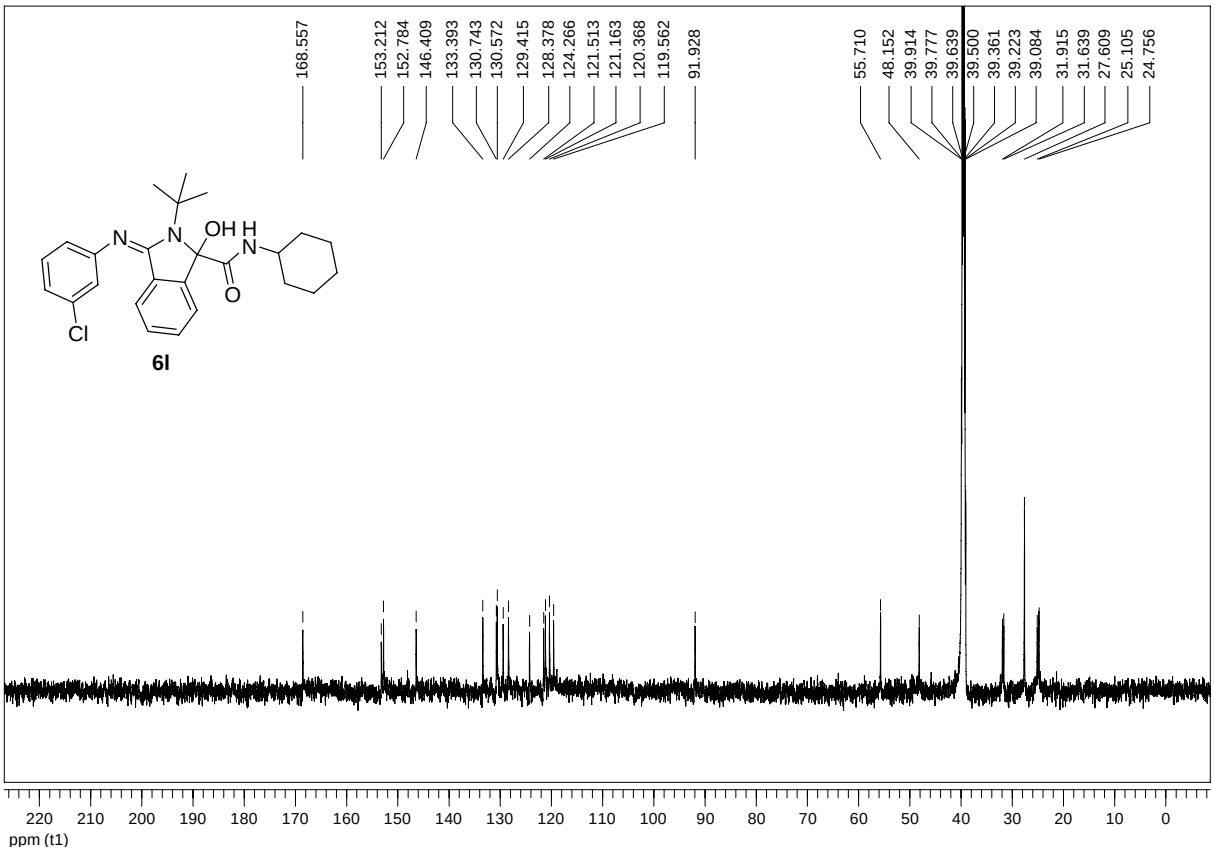
7.357
7.323
7.152
7.069
6.789
6.462
6.452
3.560
3.547
3.543
3.540
3.538
3.526
3.358
2.502
1.724
1.685
1.601
1.443
1.349
1.256
1.242
1.112
0.823
0.000000
1.06
8.03
1.07
1.02
12.00
6.05
1.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
OH H
N
N
N
O
Cl
6l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130.743
130.572
129.415
128.378
124.266
121.513
121.163
120.368
119.562
91.928
55.710
48.152
39.914
39.777
39.639
39.500
39.361
39.223
39.084
31.915
31.639
27.609
25.105
24.756
220
210
200
190
180
170
160
150
140
130
120
110
100
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50
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10
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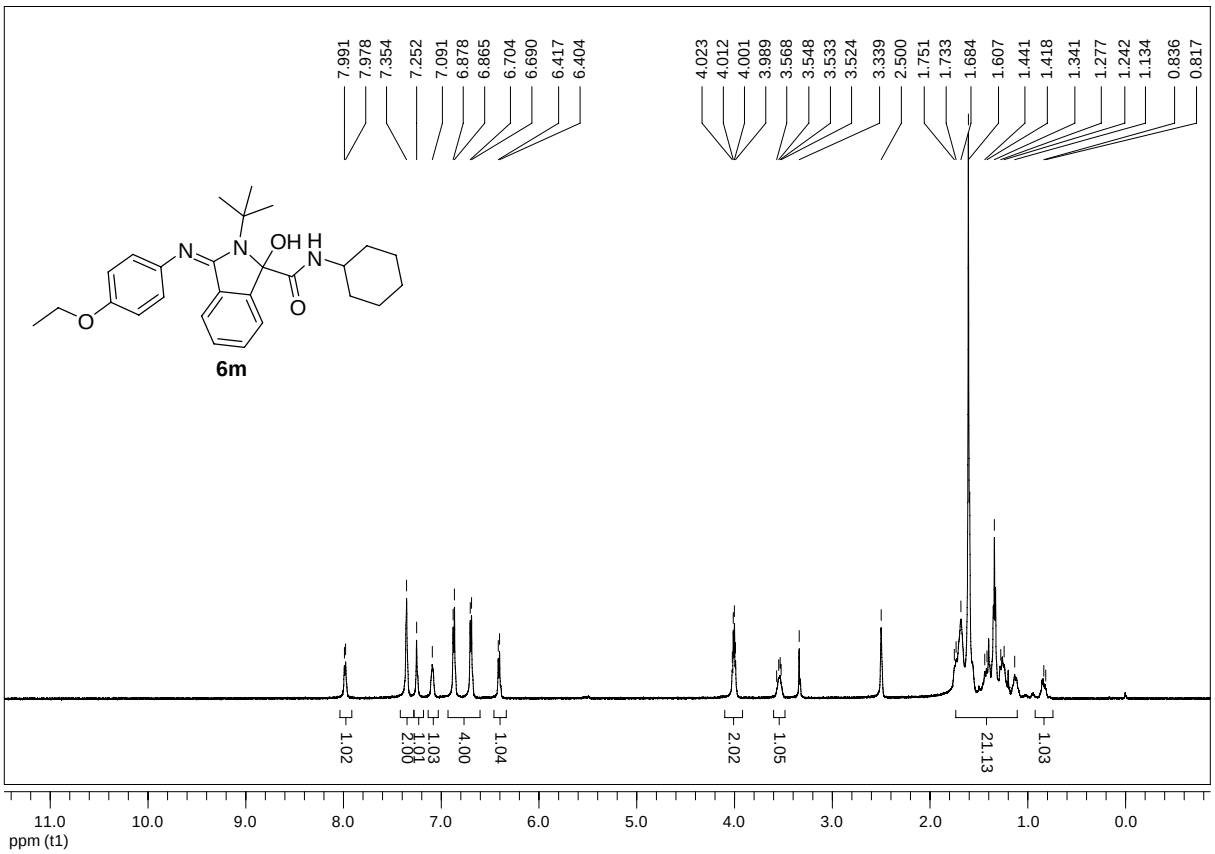
ppm (t1)
OH H
N
N
N
O
Cl
6l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6.704
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6.417
6.404
4.023
4.012
4.001
3.989
3.568
3.548
3.533
3.524
3.339
2.500
1.751
1.733
1.684
1.607
1.441
1.418
1.341
1.277
1.242
1.134
0.836
0.817
OH
H
N
N
N
O
O
6m
1.02
2.00
1.01
1.03
4.00
1.04
2.02
1.05
21.13
1.03
11.0
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2.0
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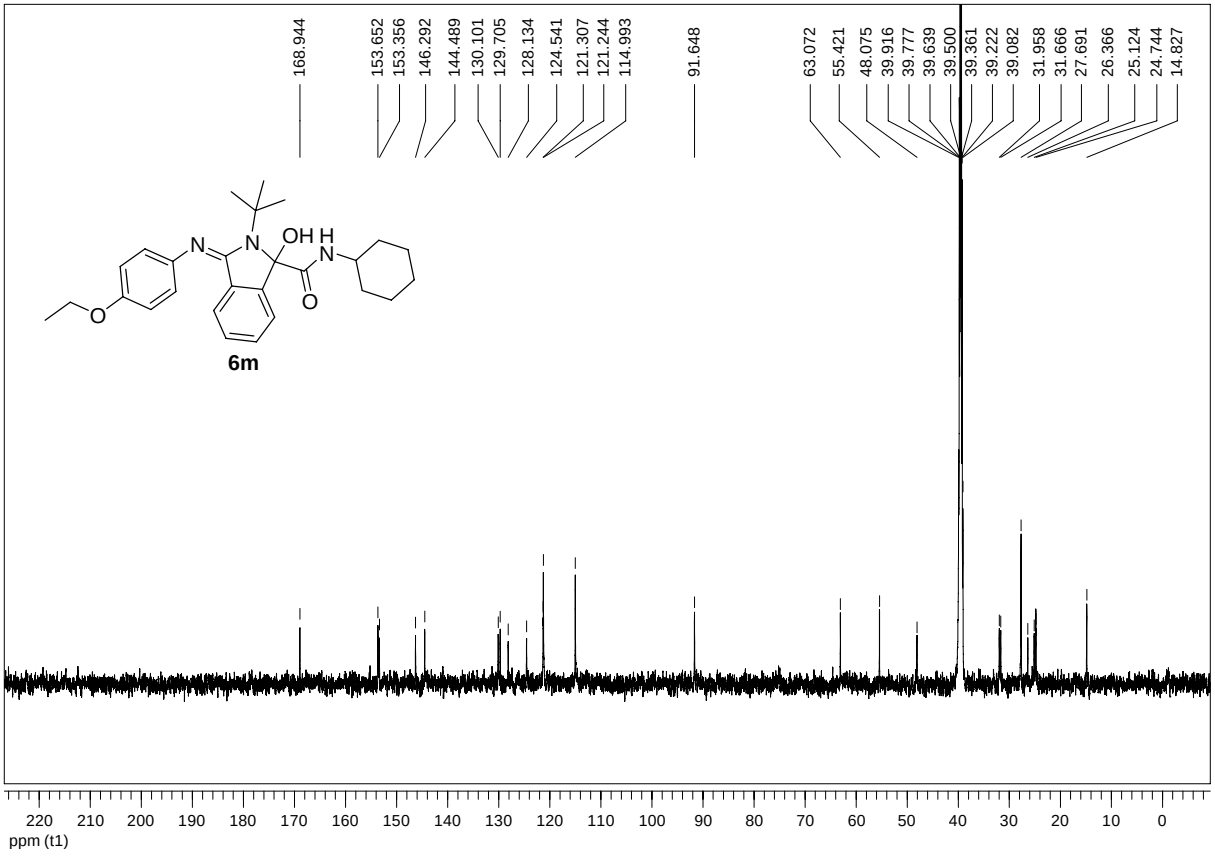
ppm (t1)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128.134
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121.244
114.993
91.648
63.072
55.421
48.075
39.916
39.777
39.639
39.500
39.361
39.222
39.082
31.958
31.666
27.691
26.366
25.124
24.744
14.827
OH
H
N
N
N
O
O
6m
220
210
200
190
180
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120
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90
80
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50
40
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10
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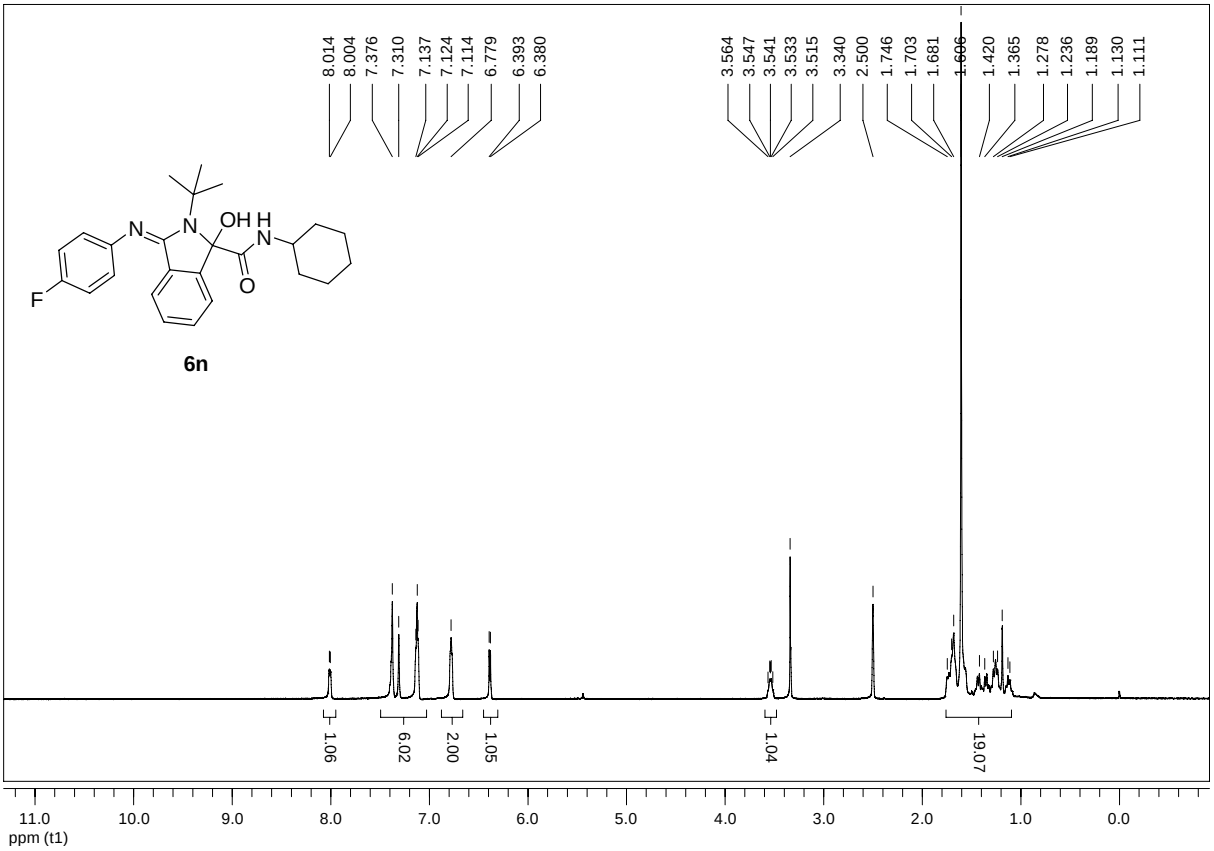
ppm (t1)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6.779
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6.380
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3.547
3.541
3.533
3.515
3.340
2.500
1.746
1.703
1.681
1.606
1.420
1.365
1.278
1.236
1.189
1.130
1.111
1.06
6.02
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1.05
1.04
19.07
11.0
10.0
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3.0
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1.0
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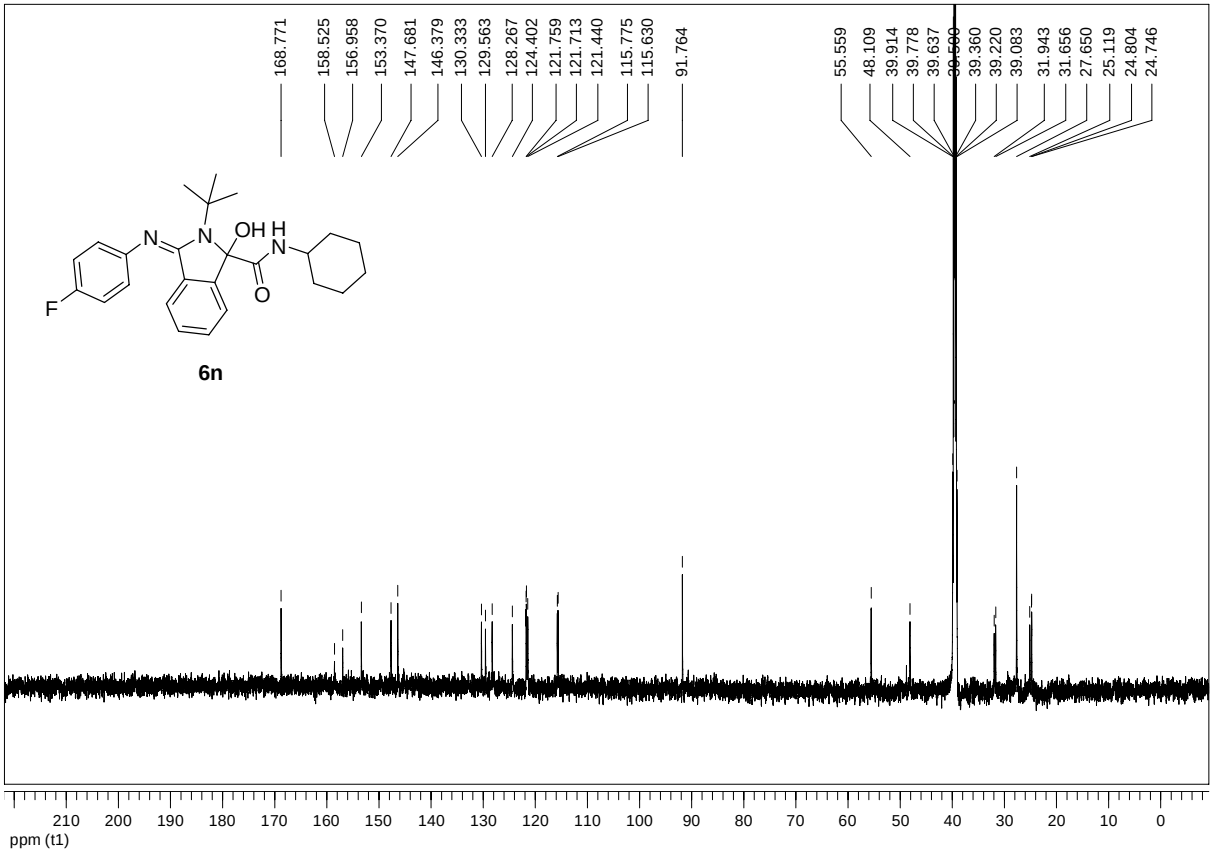
ppm (t1)

6n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115.775
115.630
91.764
55.559
48.109
39.914
39.778
39.637
39.500
39.360
39.220
39.083
31.943
31.656
27.650
25.119
24.804
24.746
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200
190
180
170
160
150
140
130
120
110
100
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80
70
60
50
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30
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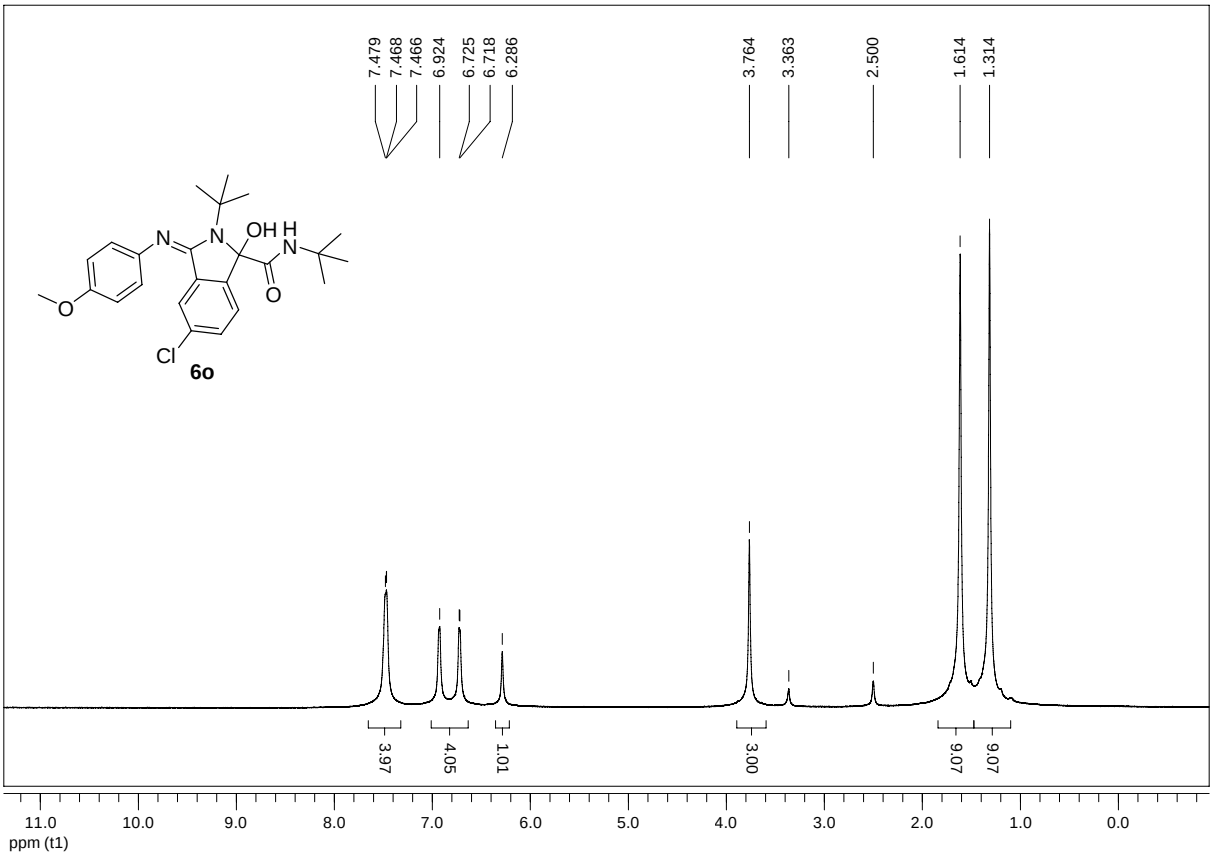
10
0
ppm (t1)

6n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6.286
3.764
3.363
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1.614
1.314
3.97
4.05
1.01
3.00
9.07
9.07
11.0
10.0
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6.0
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4.0
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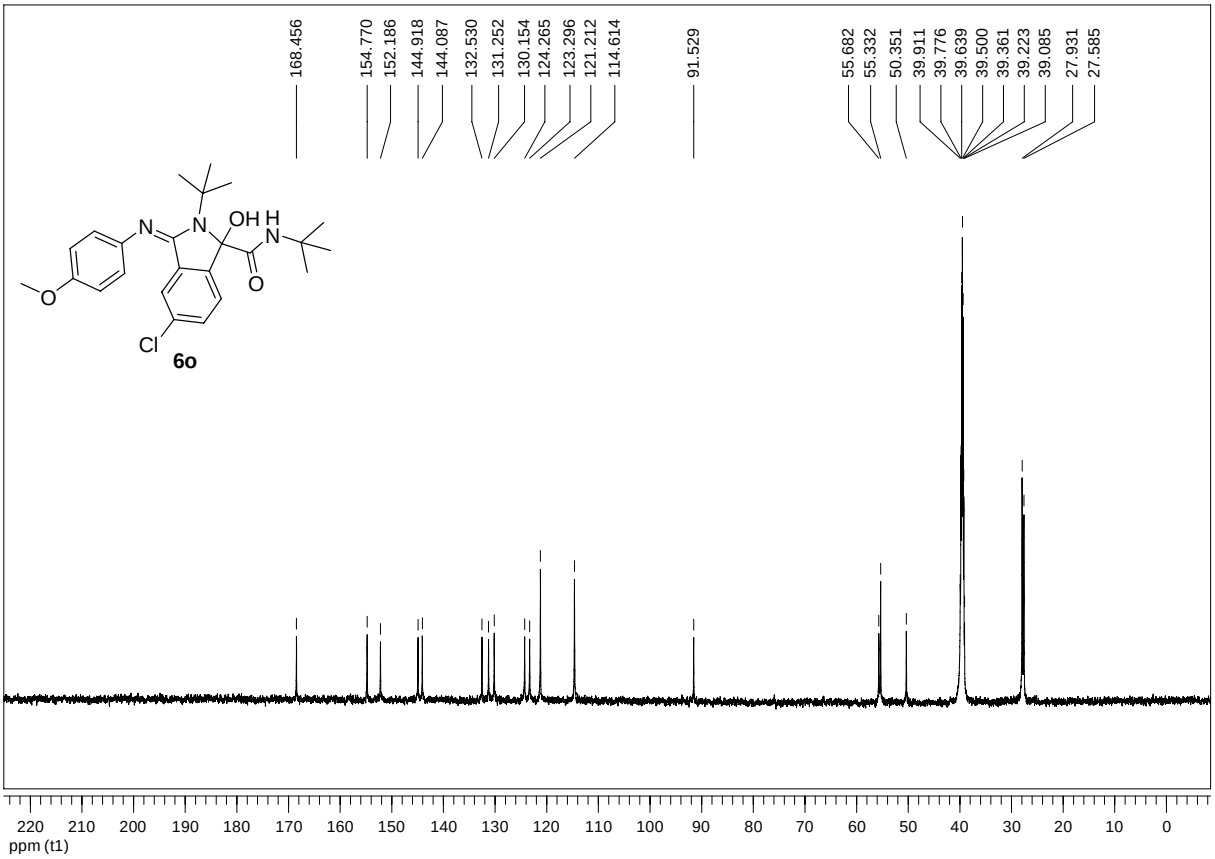
0.0
ppm (t1)
6o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130.154
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121.212
114.614
91.529
55.682
55.332
50.351
39.911
39.776
39.639
39.500
39.361
39.223
39.085
27.931
27.585
220
210
200
190
180
170
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110
100
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80
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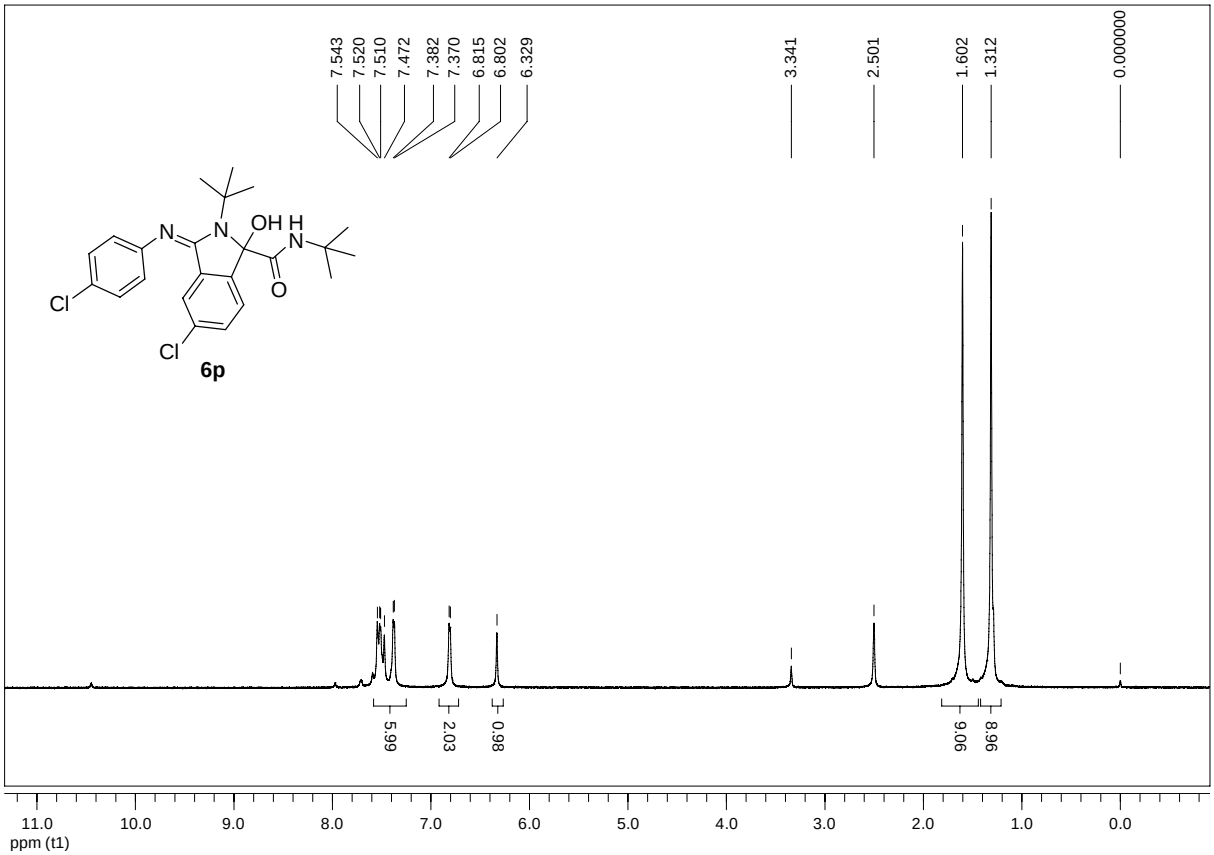
30
20
10
0
ppm (t1)
6o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6.802
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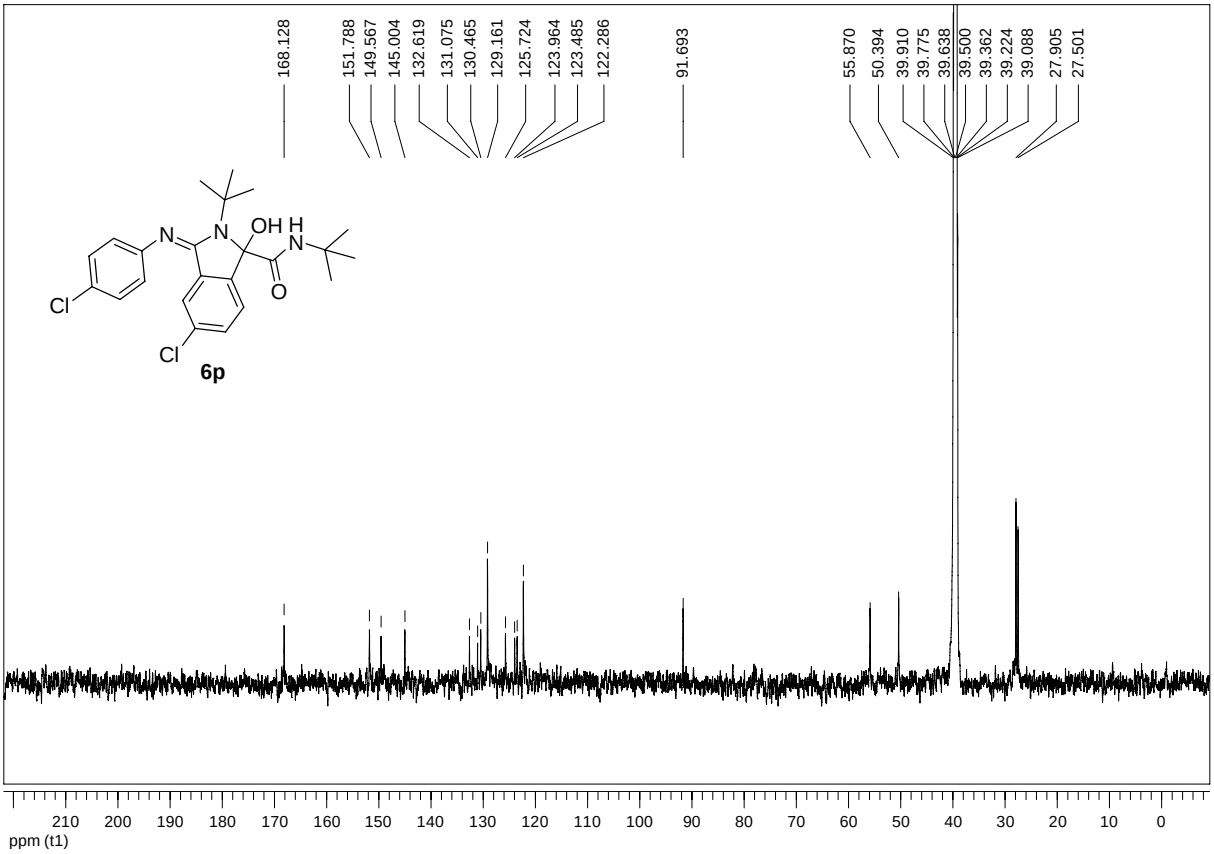
2.501
1.602
1.312
0.000000
5.99
2.03
0.98
9.06
8.96
6p
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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149.567
145.004
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129.161
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123.964
123.485
122.286
91.693
55.870
50.394
39.910
39.775
39.638
39.500
39.362
39.224
39.088
27.905
27.501
6p
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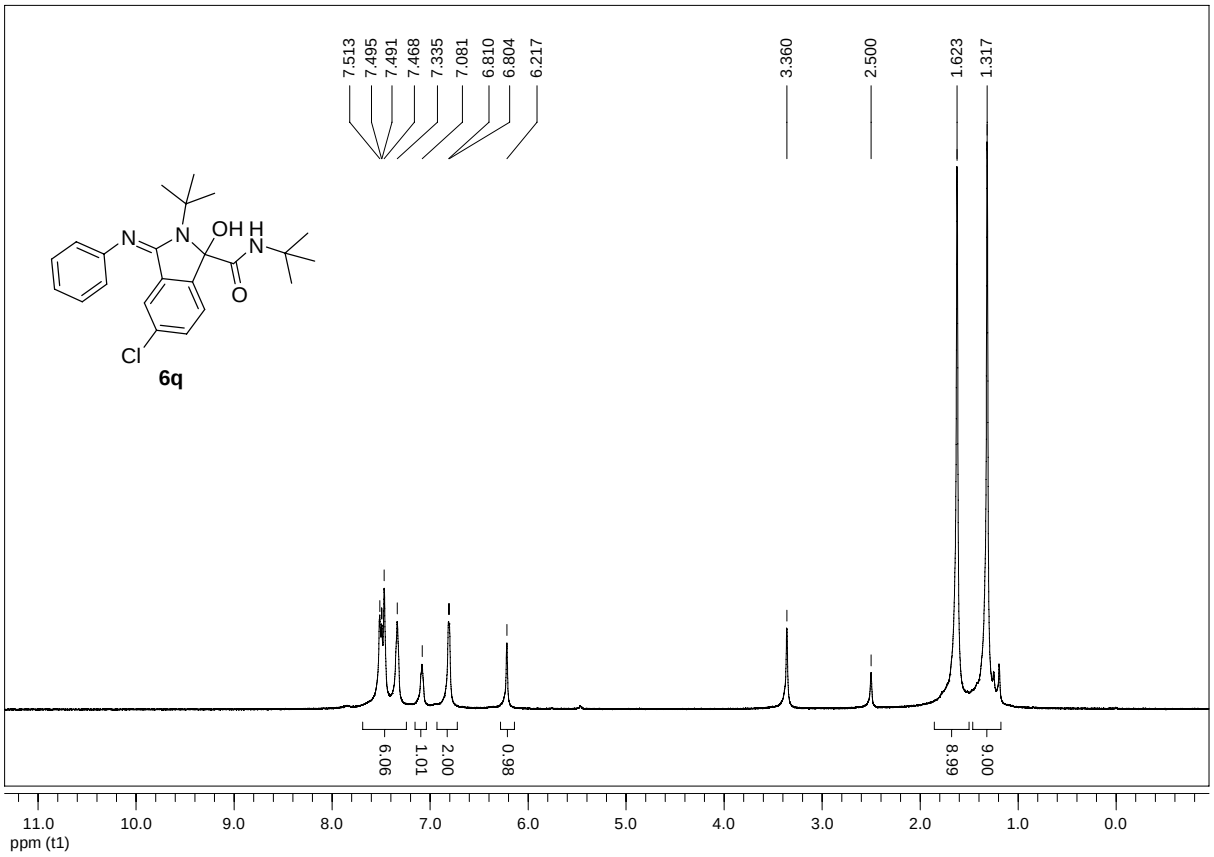
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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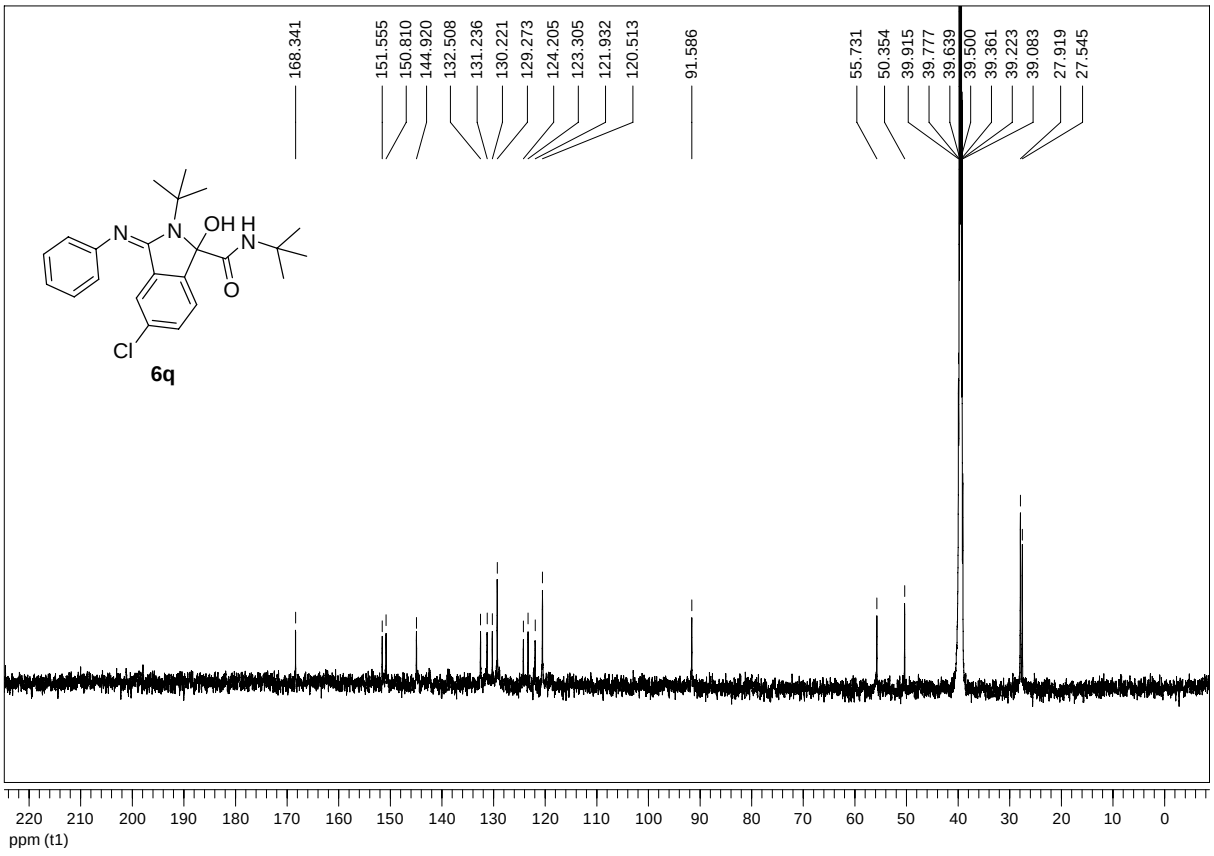
6.804
6.217
3.360
2.500
1.623
1.317
6.06
1.01
2.00
0.98
8.99
9.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
OH
H
N
N
N
O
Cl
6q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129.273
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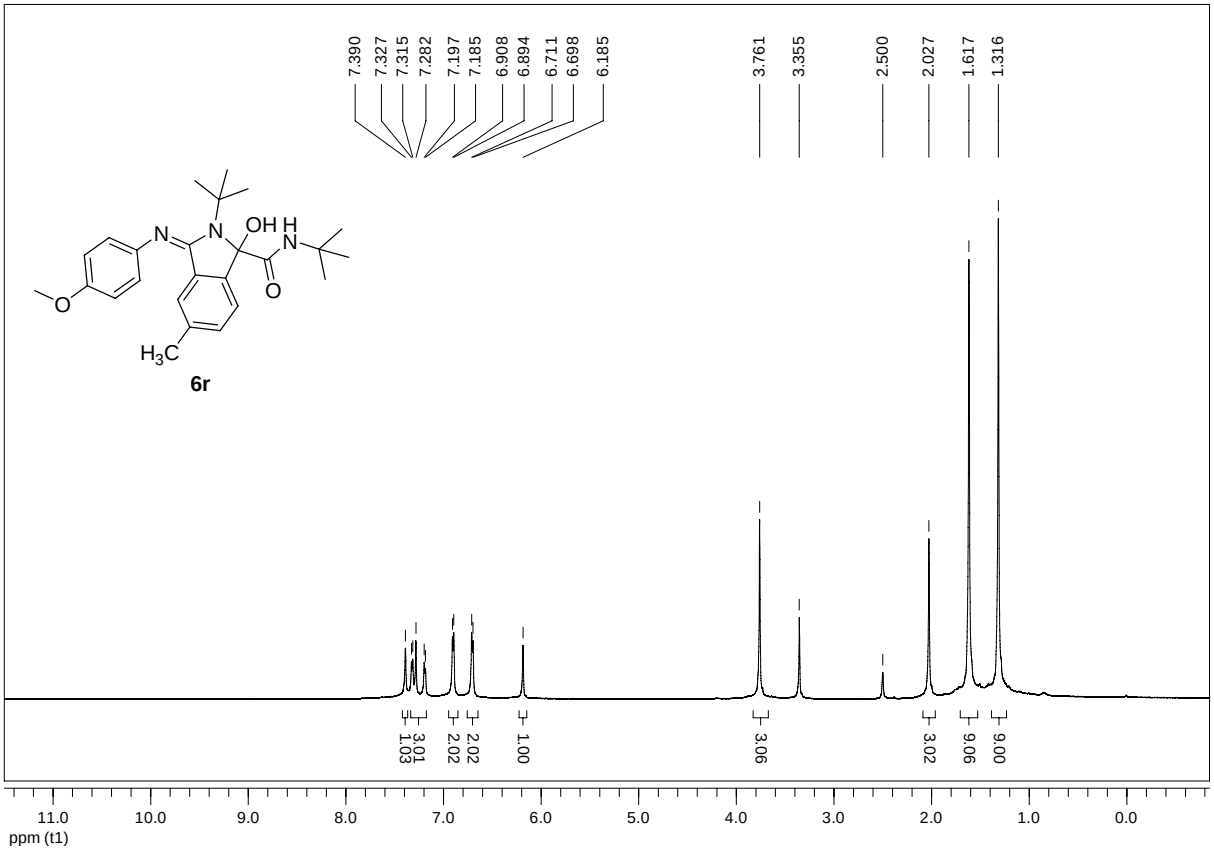
123.305
121.932
120.513
91.586
55.731
50.354
39.915
39.777
39.639
39.500
39.361
39.223
39.083
27.919
27.545
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)
OH
H
N
N
N
O
Cl
6q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6.698
6.185
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3.355
2.500
2.027
1.617
1.316
OH
H
N
N
N
O
O
H3C
6r
1.03
3.01
2.02
2.02
1.00
3.06
3.02
9.06
9.00
11.0
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9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
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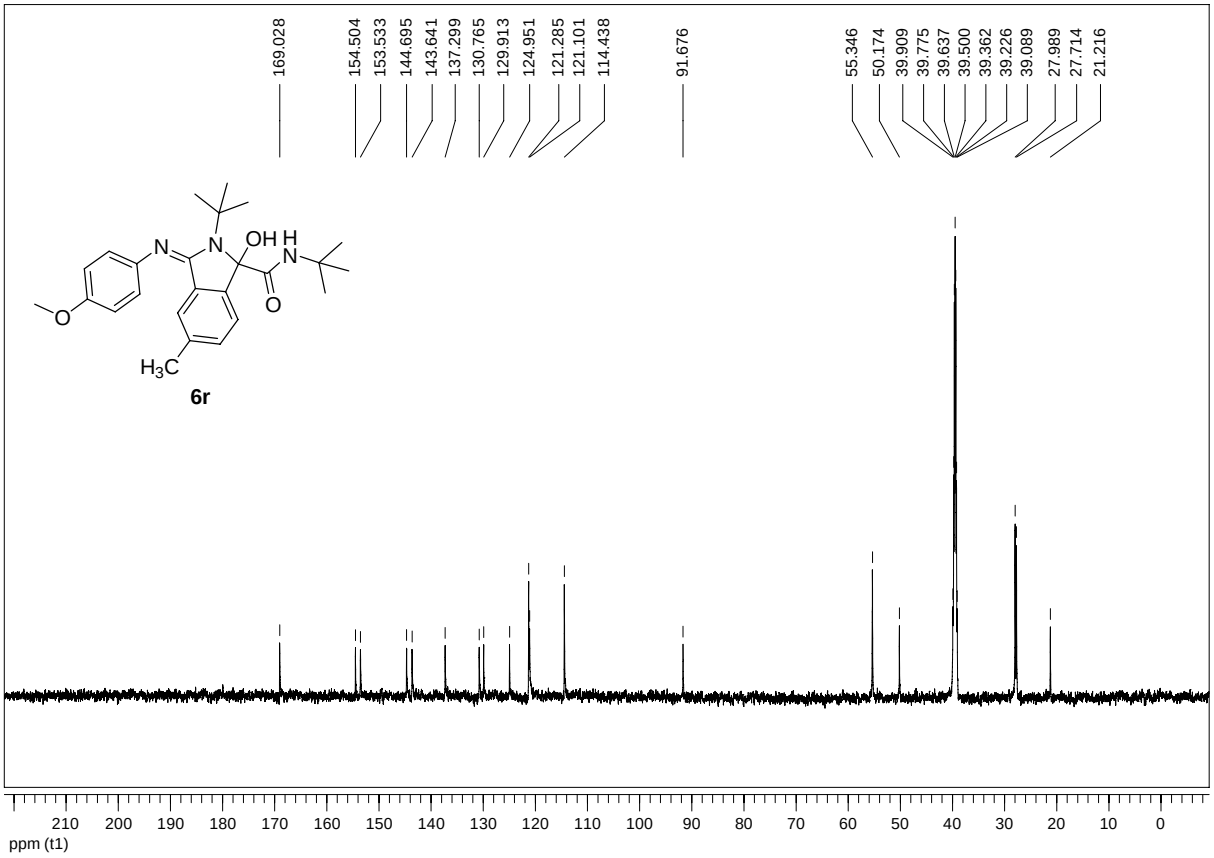
ppm (t1)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121.101
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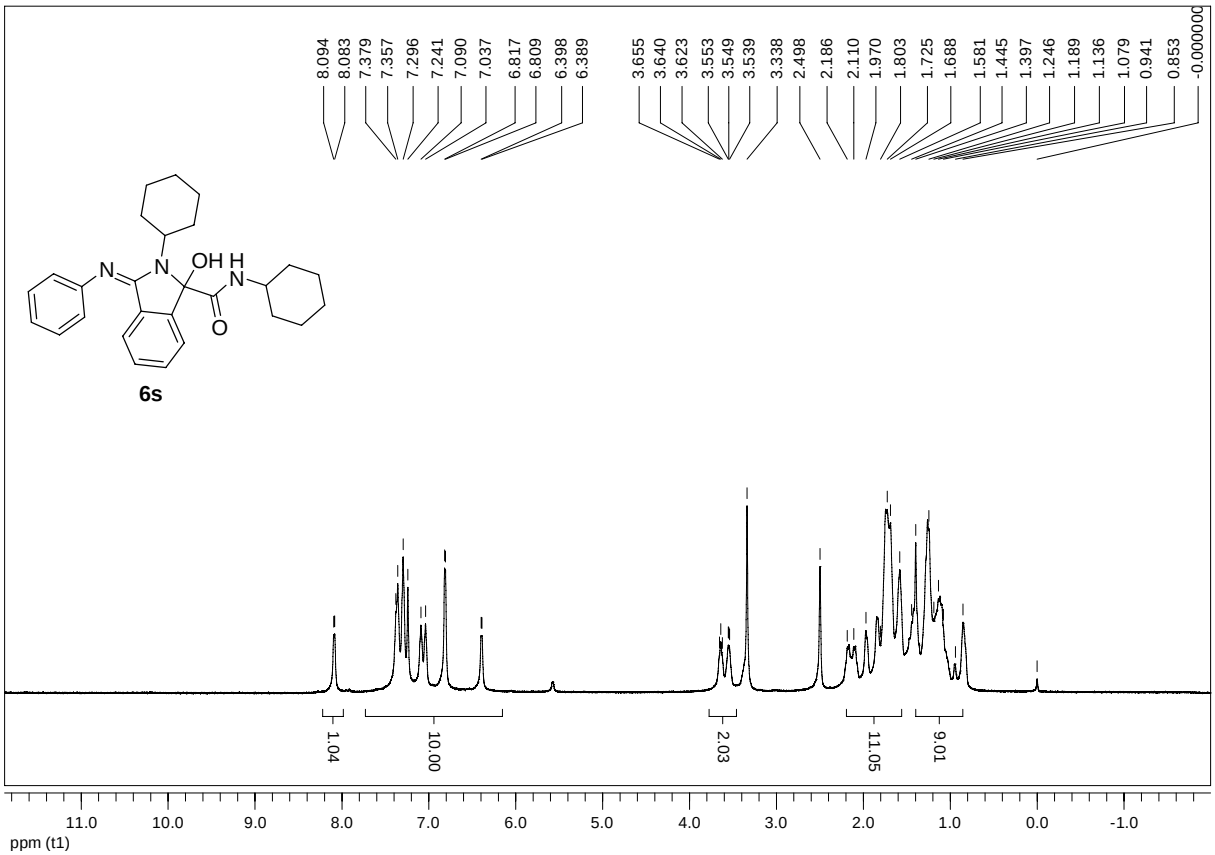
91.676
55.346
50.174
39.909
39.775
39.637
39.500
39.362
39.226
39.089
27.989
27.714
21.216
OH
H
N
N
N
O
O
H3C
6r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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7.241
7.090
7.037
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6.809
6.398
6.389
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3.640
3.623
3.553
3.549
3.539
3.338
2.498
2.186
2.110
1.970
1.803
1.725
1.688
1.581
1.445
1.397
1.246
1.189
1.136
1.079
0.941
0.853
-0.000000
OH H
N
N
N
O
6s
1.04
10.00
2.03
11.05
9.01
11.0
10.0
9.0
8.0
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5.0
4.0
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2.0
1.0
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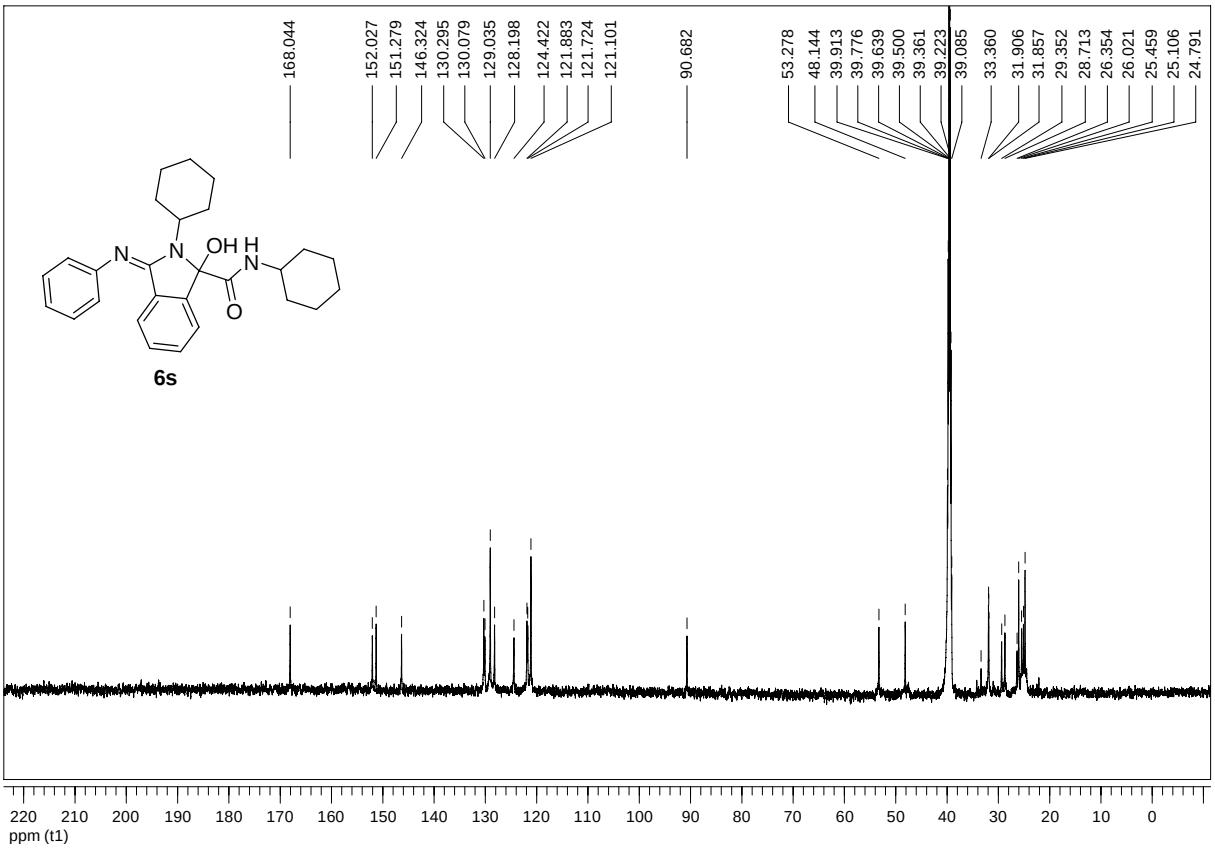
-1.0
ppm (t1)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48.144
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39.776
39.639
39.500
39.361
39.223
39.085
33.360
31.906
31.857
29.352
28.713
26.354
26.021
25.459
25.106
24.791
OH H
N
N
N
O
6s
220
210
200
190
180
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150
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120
110
100
90
80
70
60
50
40
30
20
10
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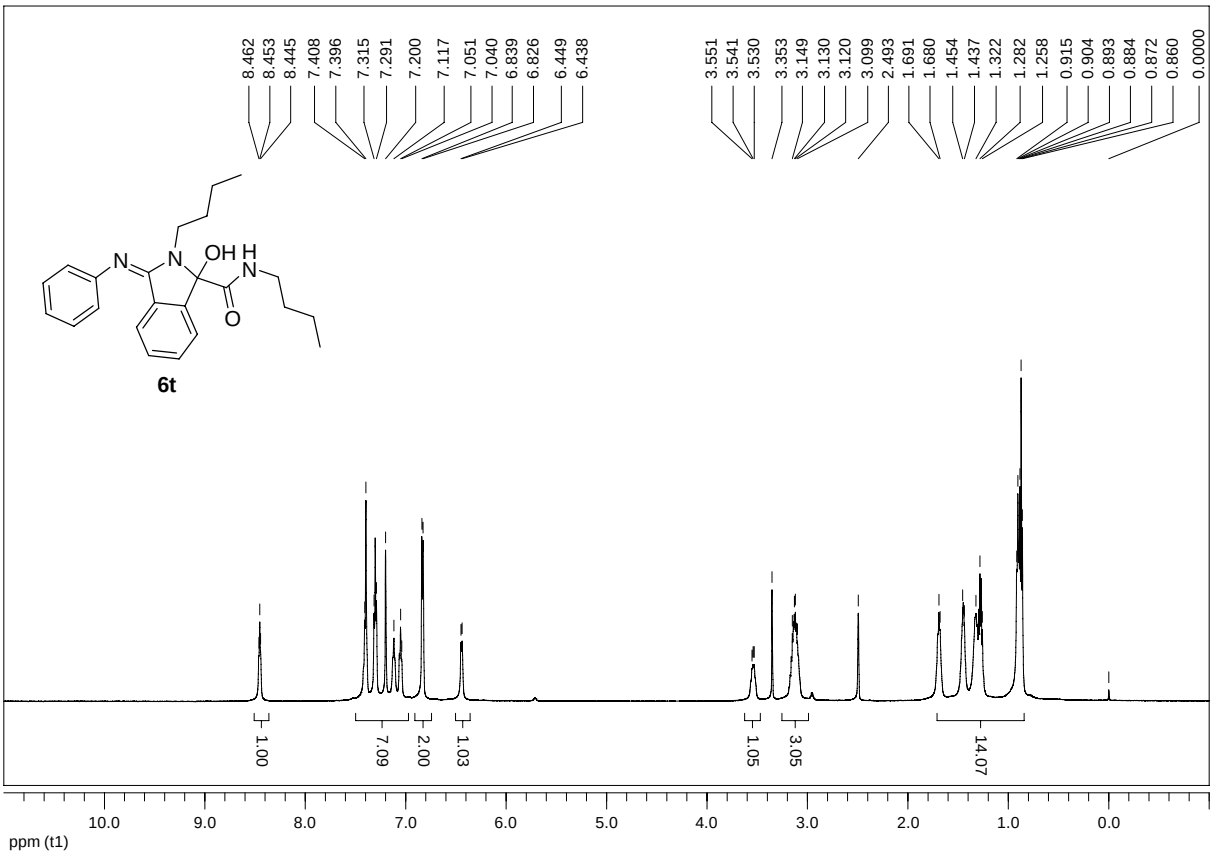
ppm (t1)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7.040
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6.826
6.449
6.438
3.551
3.541
3.530
3.353
3.149
3.130
3.120
3.099
2.493
1.691
1.680
1.454
1.437
1.322
1.282
1.258
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0.904
0.893
0.884
0.872
0.860
0.0000
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N
N
N
O
6t
1.00
7.09
2.00
1.03
1.05
3.05
14.07
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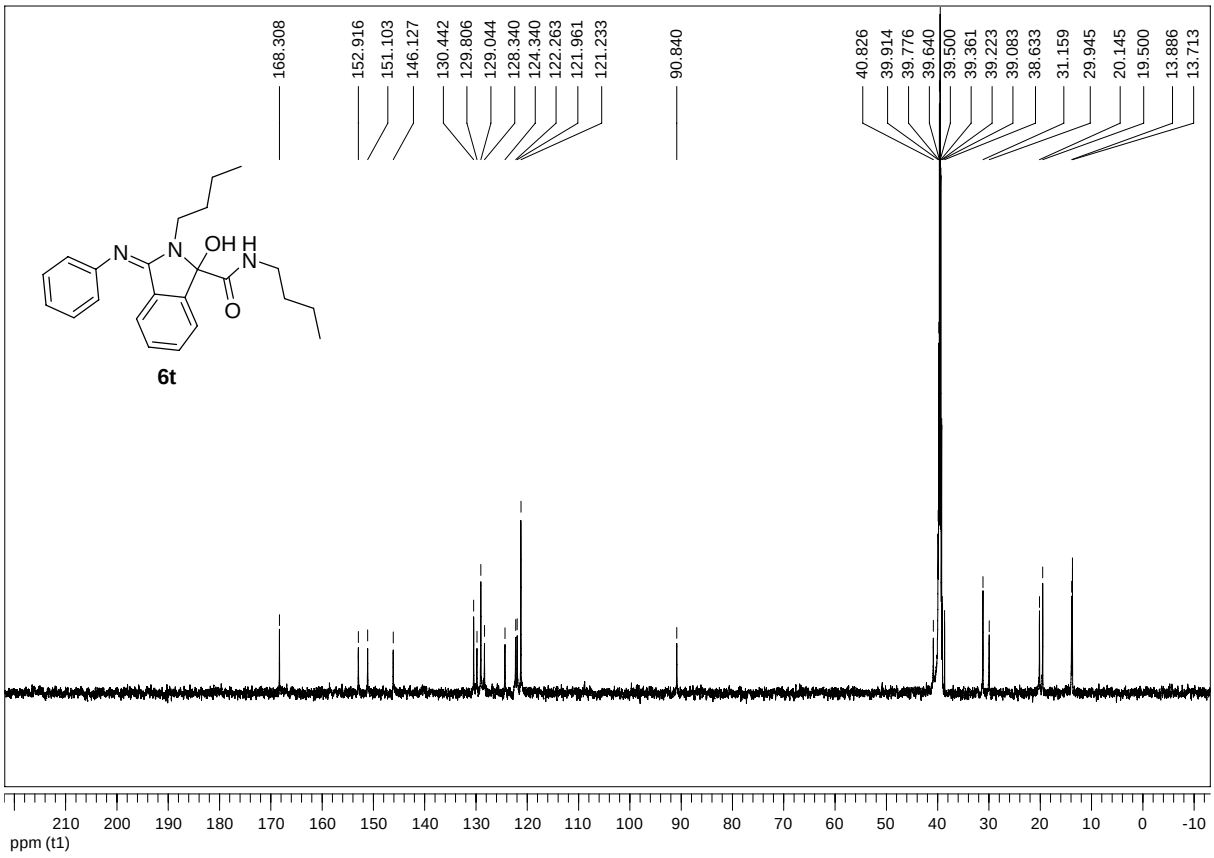
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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90.840
40.826
39.914
39.776
39.640
39.500
39.361
39.223
39.083
38.633
31.159
29.945
20.145
19.500
13.886
13.713
OH H
N
N
N
O
6t
210
200
190
180
170
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100
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80
70
60
50
40
30
20
10
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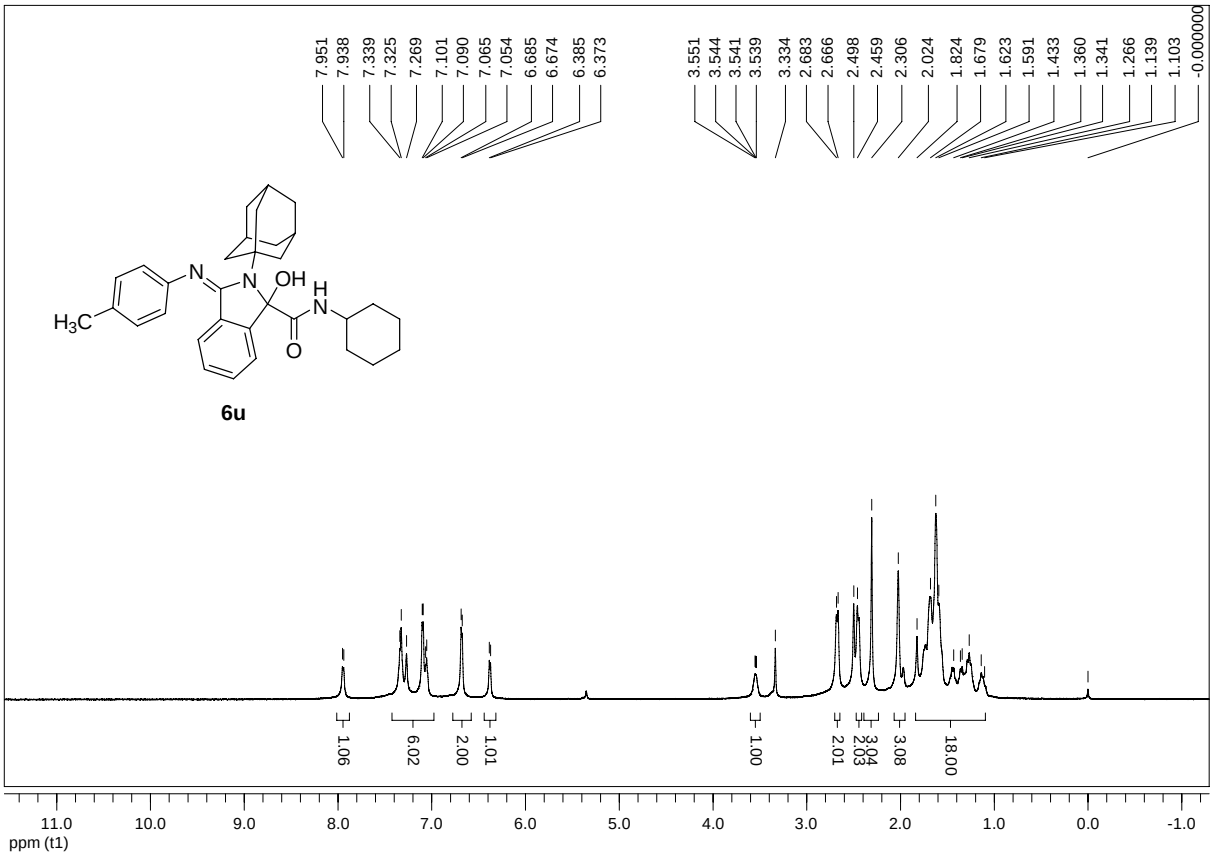
ppm (t1)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3.551
3.544
3.541
3.539
3.334
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2.666
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2.459
2.306
2.024
1.824
1.679
1.623
1.591
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1.360
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6.02
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1.01
1.00
2.01
2.03
3.04
3.08
18.00
11.0
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9.0
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3.0
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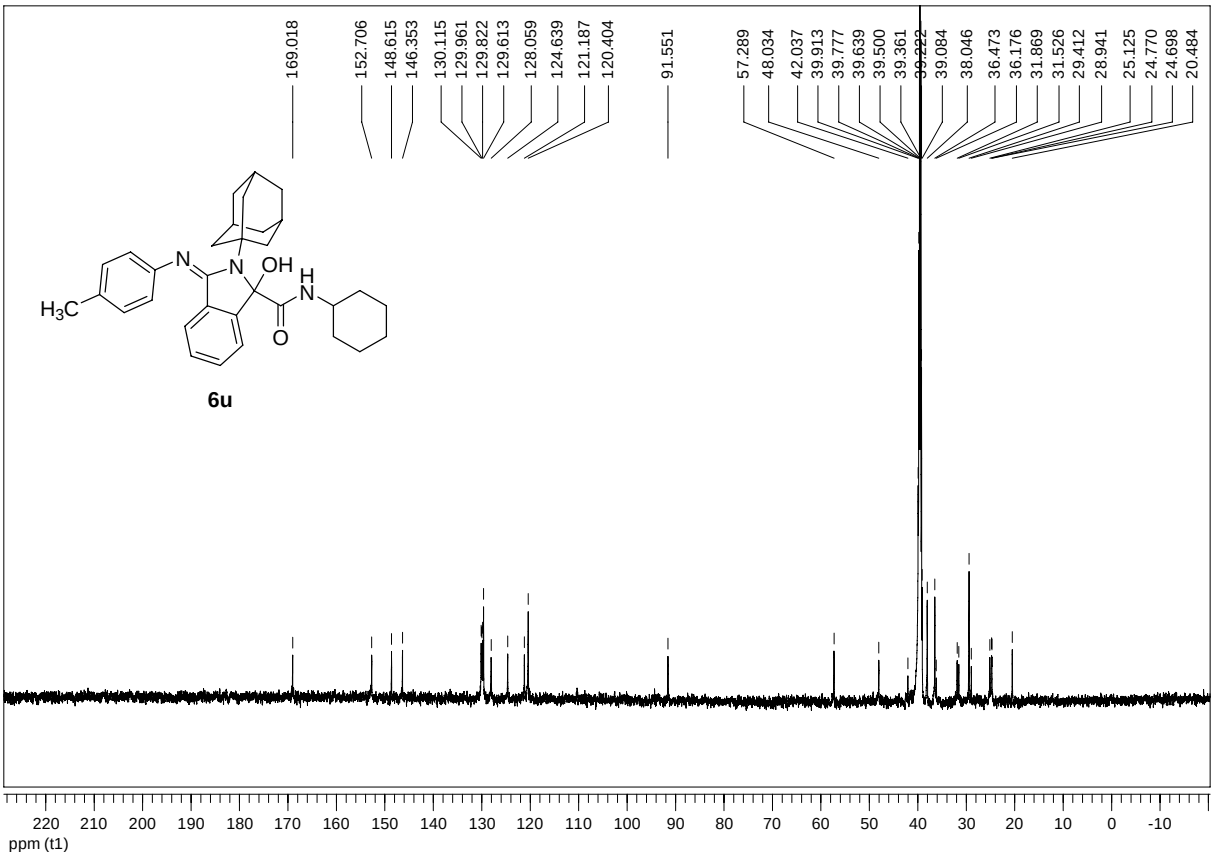
ppm (t1)

6u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91.551
57.289
48.034
42.037
39.913
39.777
39.639
39.500
39.361
39.222
39.084
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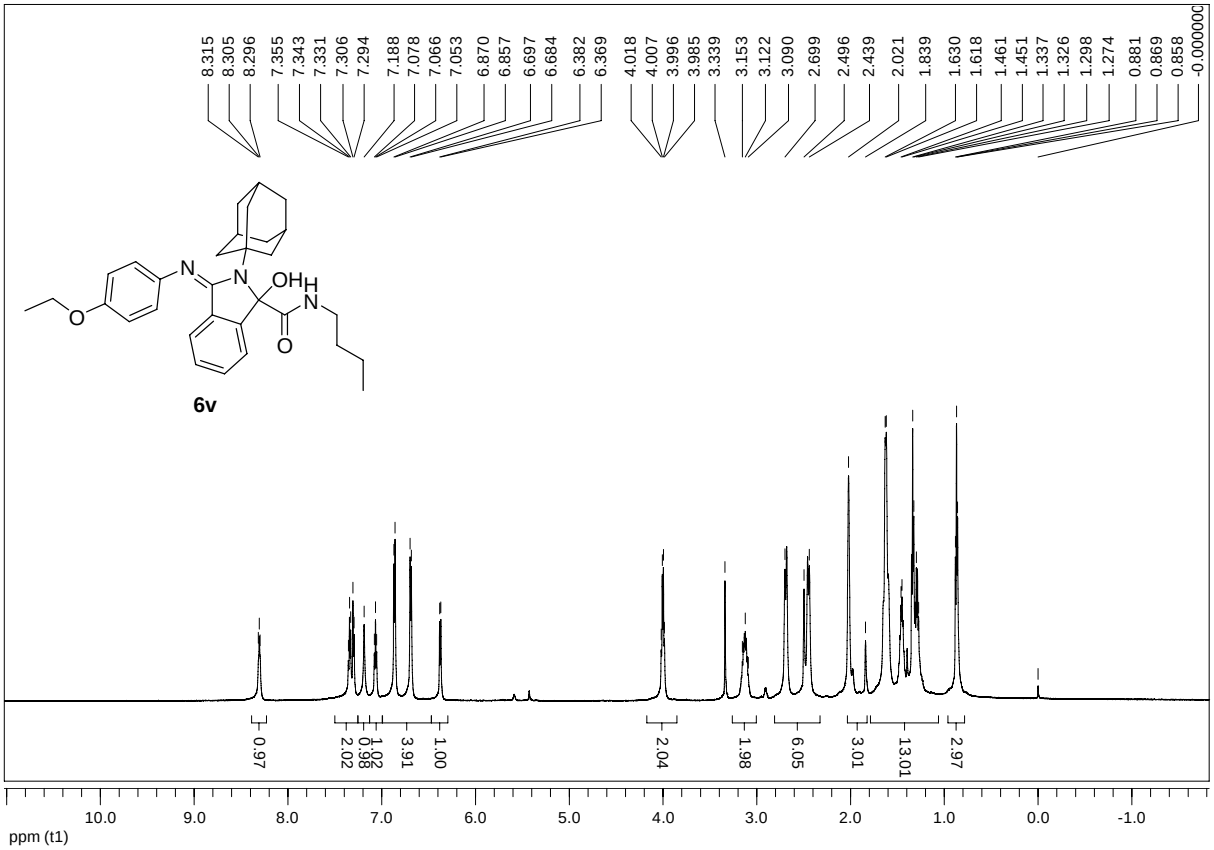
ppm (t1)

6u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7.066
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6.870
6.857
6.697
6.684
6.382
6.369
4.018
4.007
3.996
3.985
3.339
3.153
3.122
3.090
2.699
2.496
2.439
2.021
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1.630
1.618
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1.337
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O
O
6v
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1.02
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1.00
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6.05
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13.01
2.97
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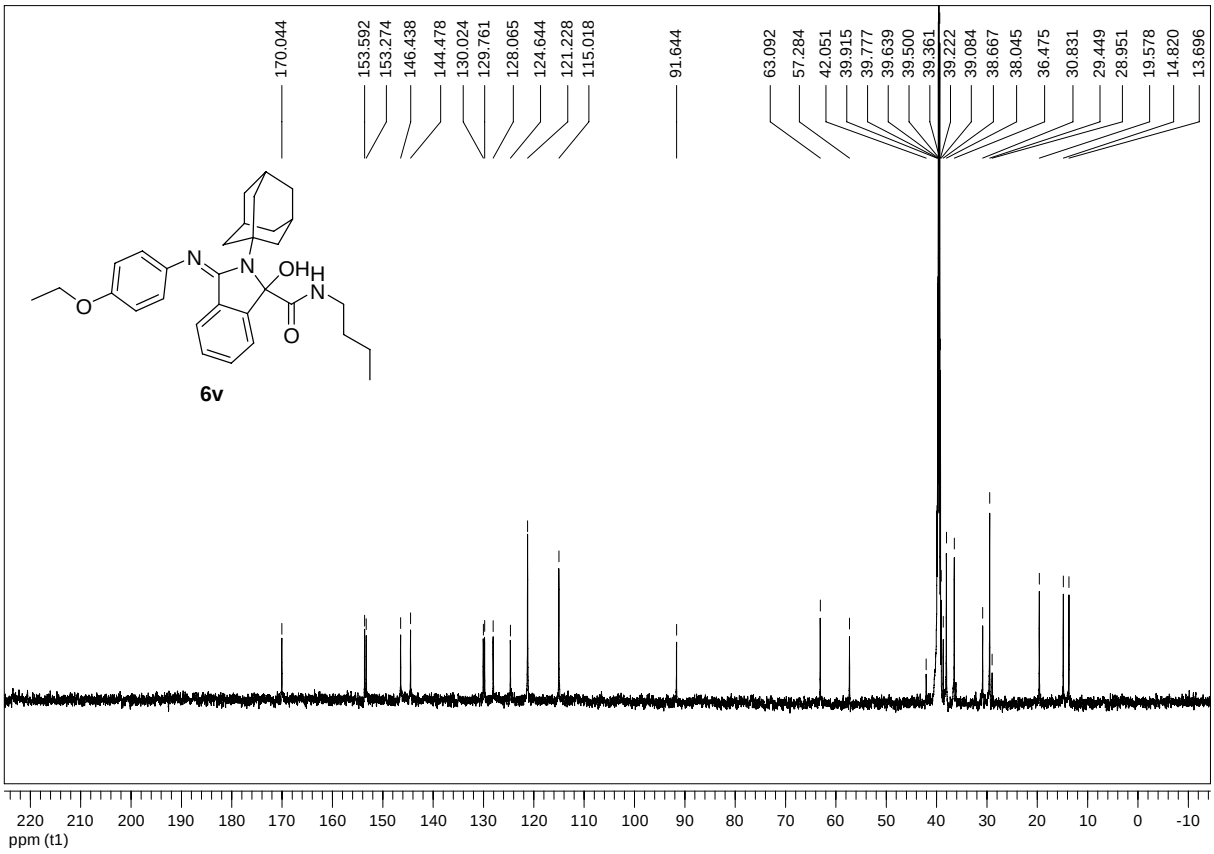
1.0
0.0
-1.0
ppm (t1)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115.018
91.644
63.092
57.284
42.051
39.915
39.777
39.639
39.500
39.361
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39.084
38.667
38.045
36.475
30.831
29.449
28.951
19.578
14.820
13.696
N
N
OH
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N
O
O
6v
220
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200
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180
170
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30
20
10
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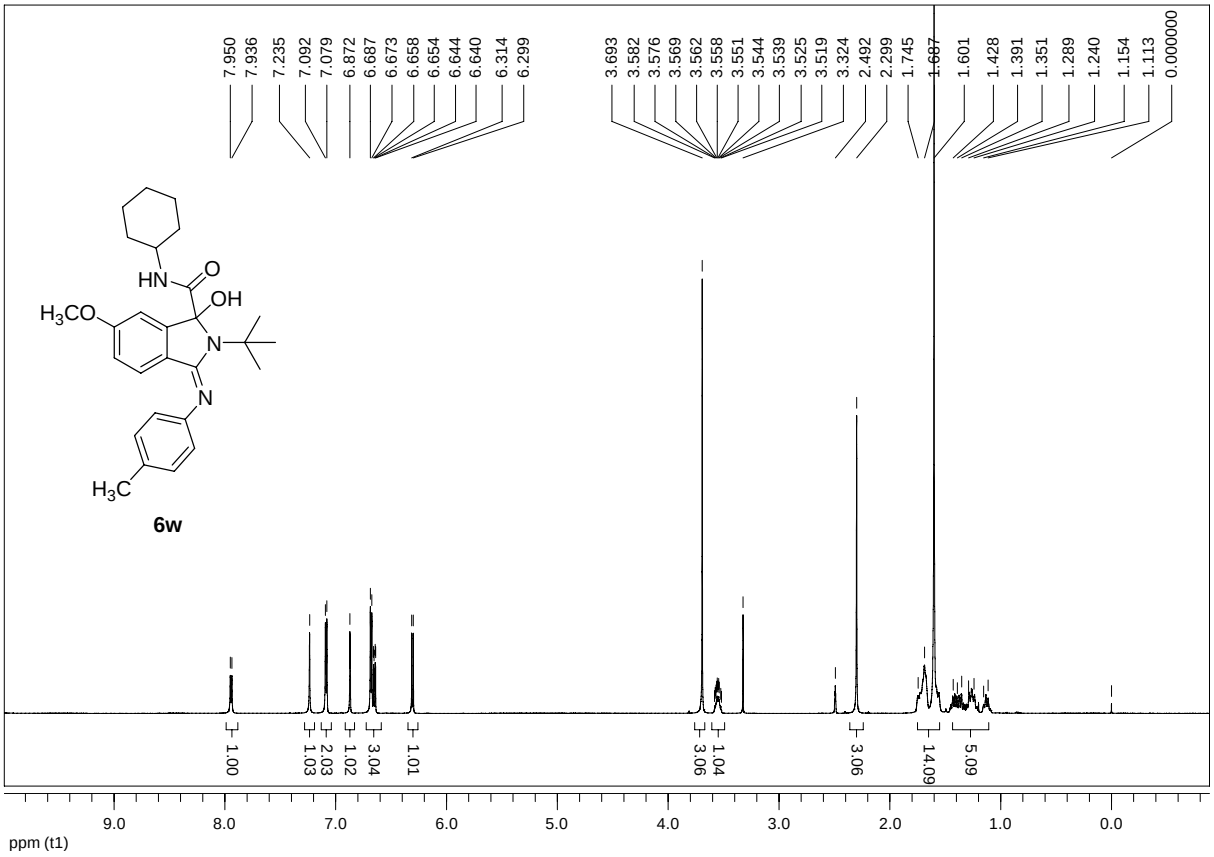
-10
ppm (t1)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6.314
6.299
3.693
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3.576
3.569
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3.558
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3.525
3.519
3.324
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1.745
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1.240
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N
N
H3C
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2.03
1.02
3.04
1.01
3.06
1.04
3.06
14.09
5.09
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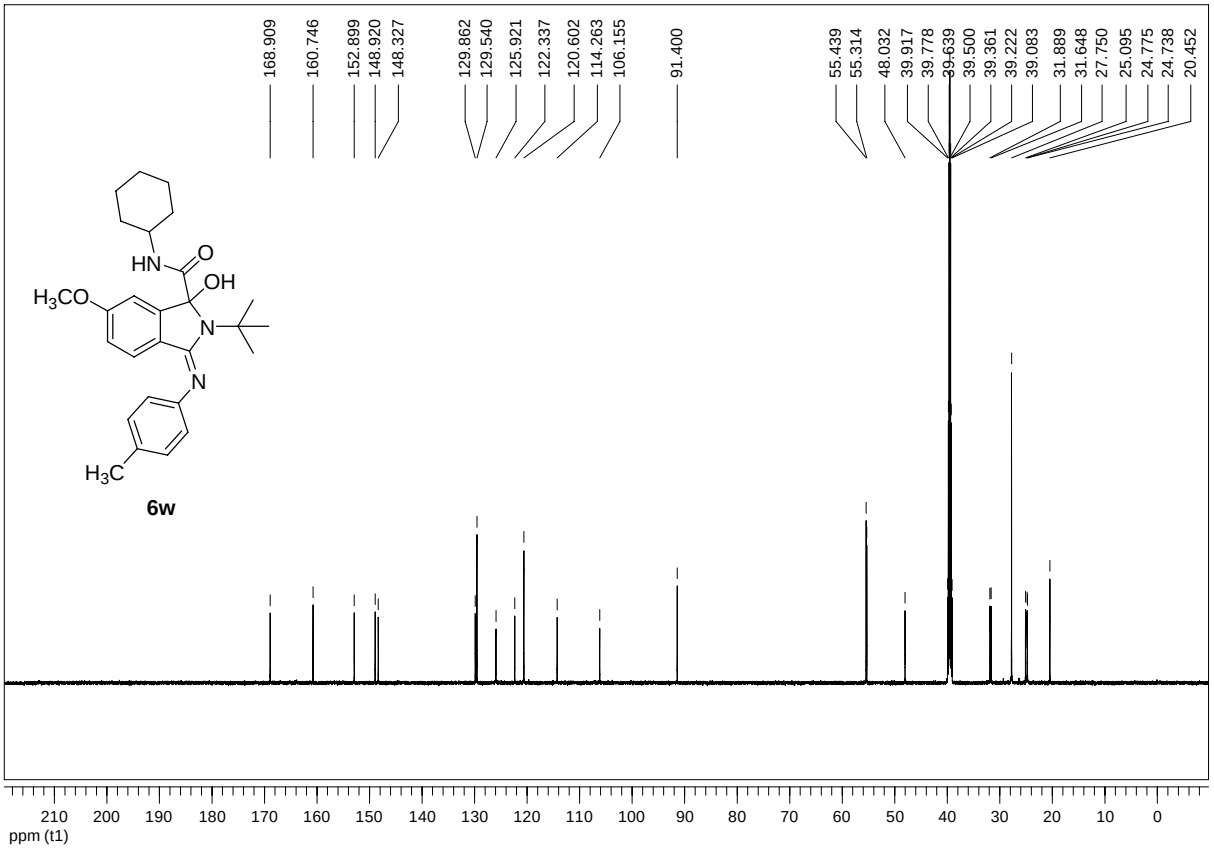
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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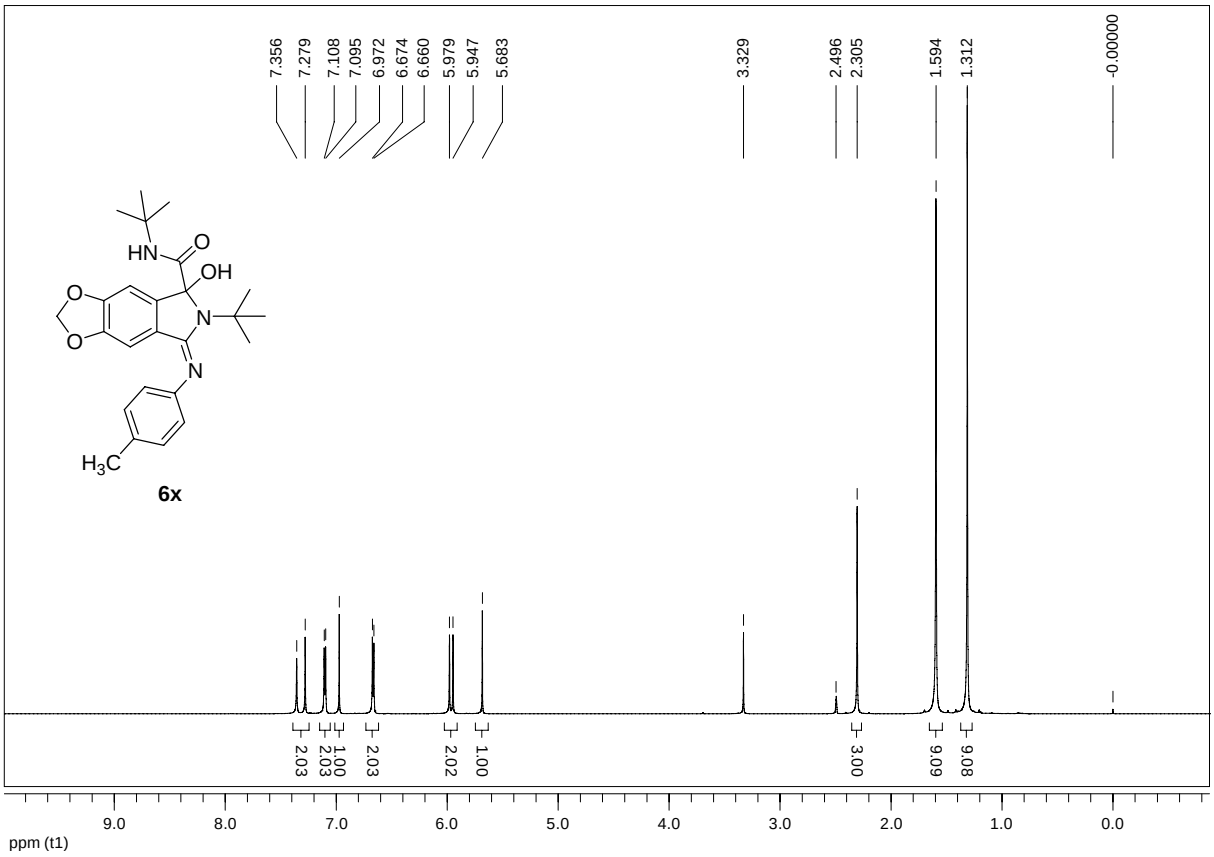
160.746
152.899
148.920
148.327
129.862
129.540
125.921
122.337
120.602
114.263
106.155
91.400
55.439
55.314
48.032
39.917
39.778
39.639
39.500
39.361
39.222
39.083
31.889
31.648
27.750
25.095
24.775
24.738
20.452
HN
O
OH
H3CO
N
N
H3C
6w
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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7.279
7.108
7.095
6.972
6.674
6.660
5.979
5.947
5.683
3.329
2.496
2.305
1.594
1.312
-0.00000
2.03
2.03
1.00
2.03
2.02
1.00
3.00
9.09
9.08
HN
O
OH
O
O
N
N
H3C
6x
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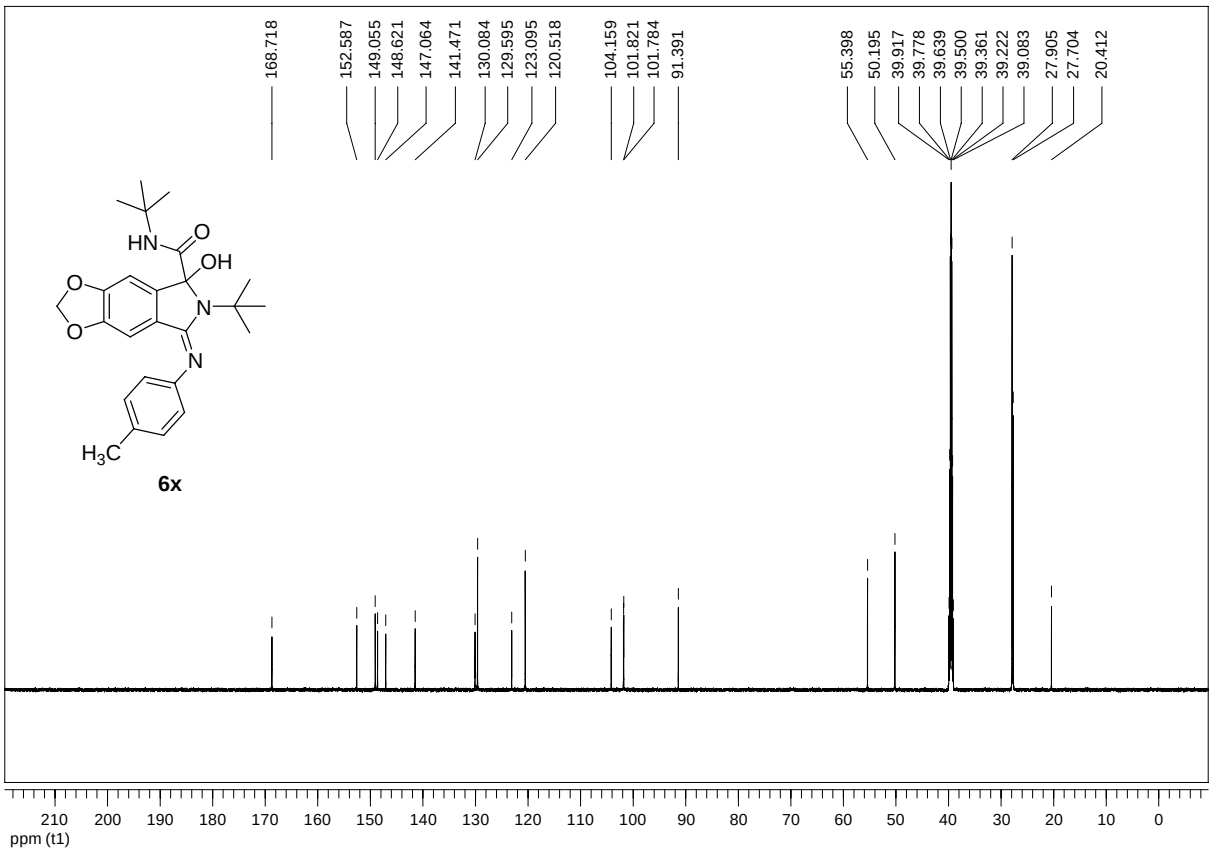
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


168.718
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149.055
148.621
147.064
141.471
130.084
129.595
123.095
120.518
104.159
101.821
101.784
91.391
55.398
50.195
39.917
39.778
39.639
39.500
39.361
39.222
39.083
27.905
27.704
20.412
HN
O
OH
O
O
N
N
H3C
6x
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)