Supporting Information for

Oxidative Aromatic C-N Bond Formation: Convenient Synthesis of *N*-Aminoindole-3-carbonitriles via $FeBr_3$-Mediated Intramolecular Cyclization

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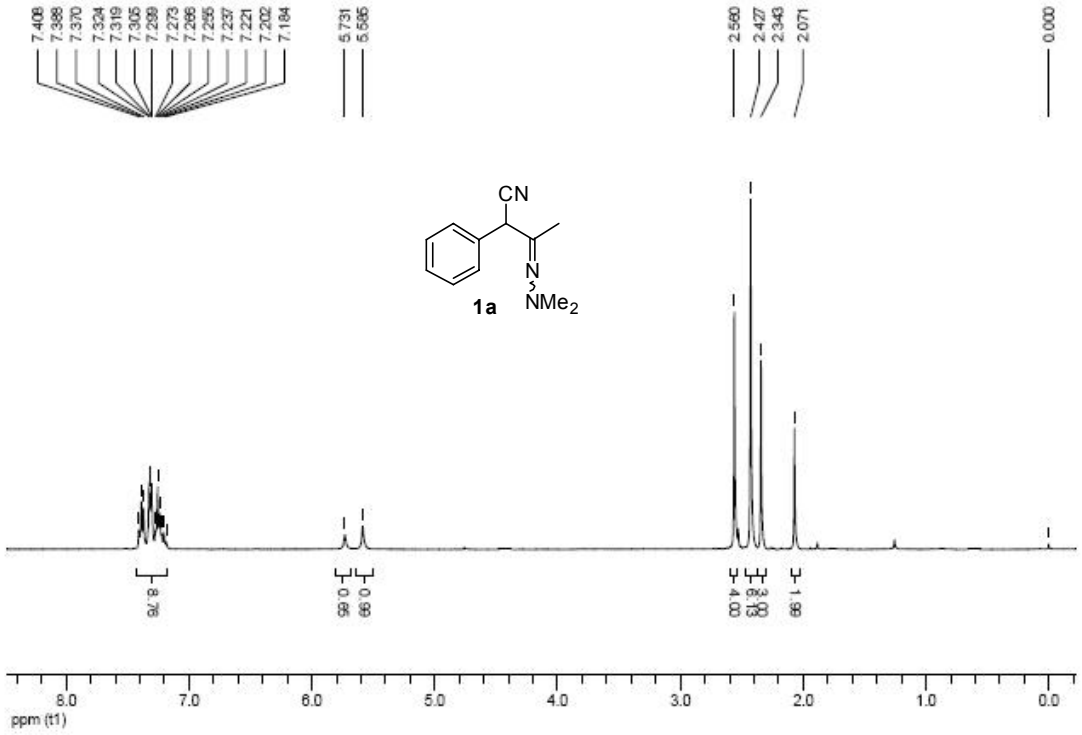
Fax: +86-22-27404031 Tel: +86-22-27404031

Supplementary Material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NMe2
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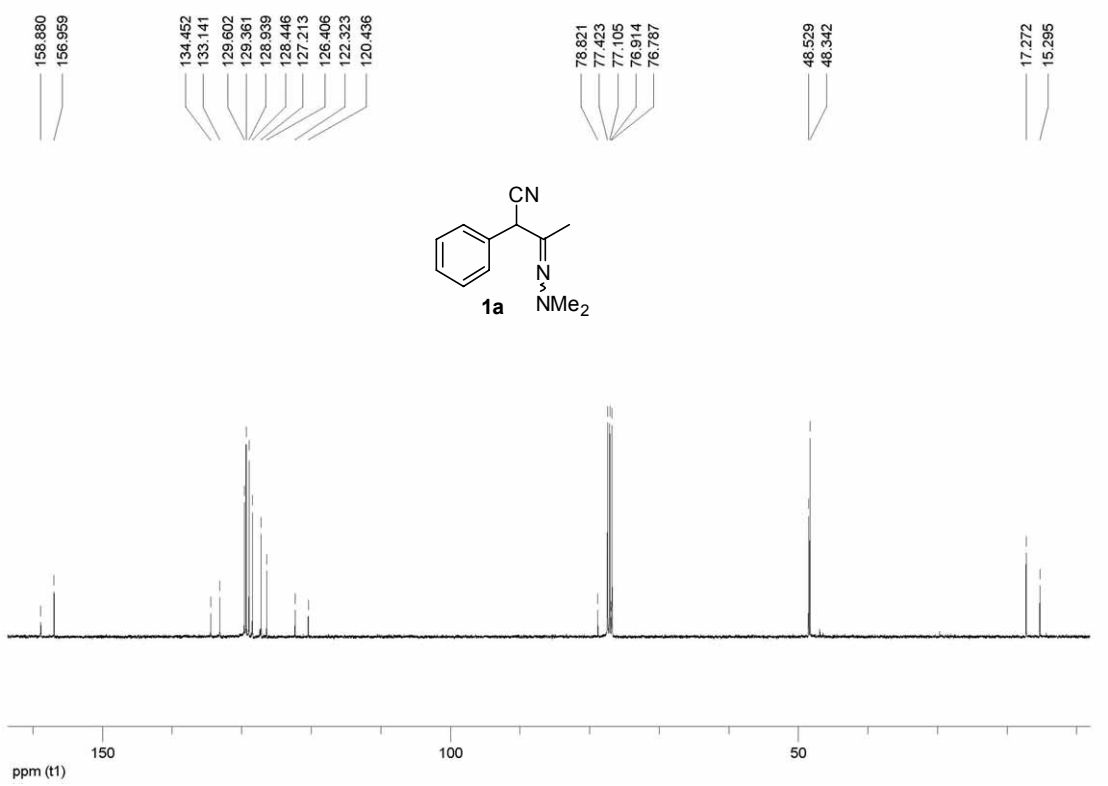
ppm (t1)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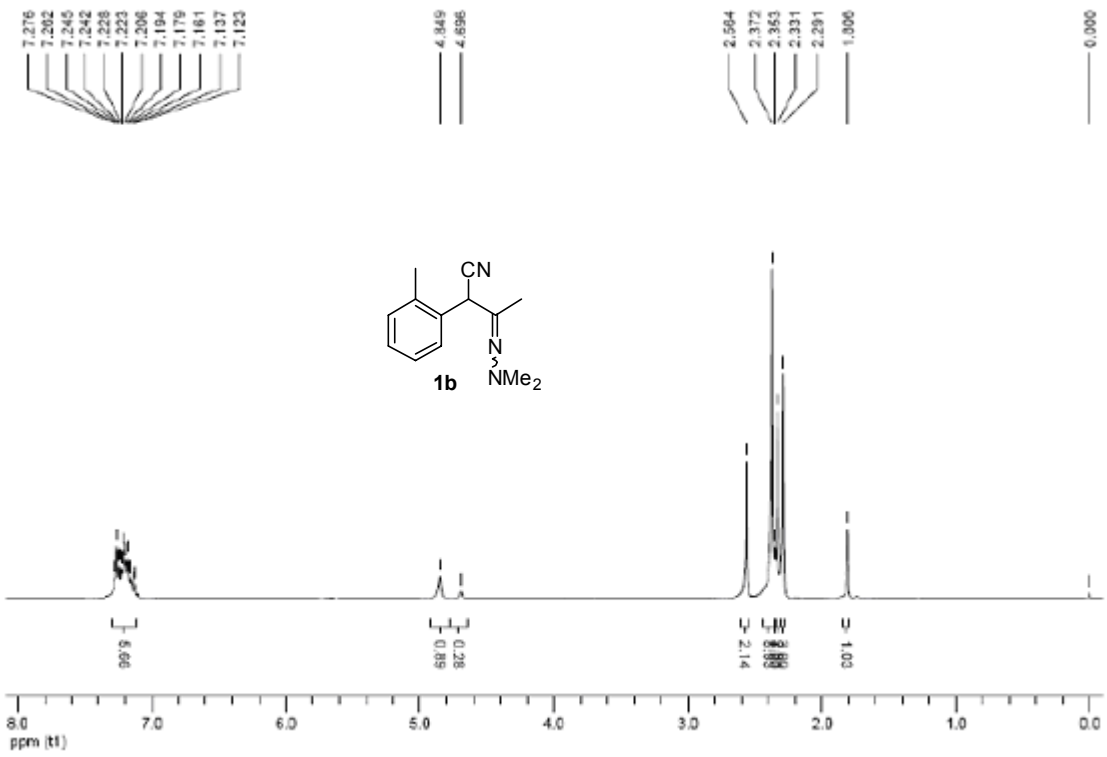
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4.696
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2.372
2.353
2.331
2.291
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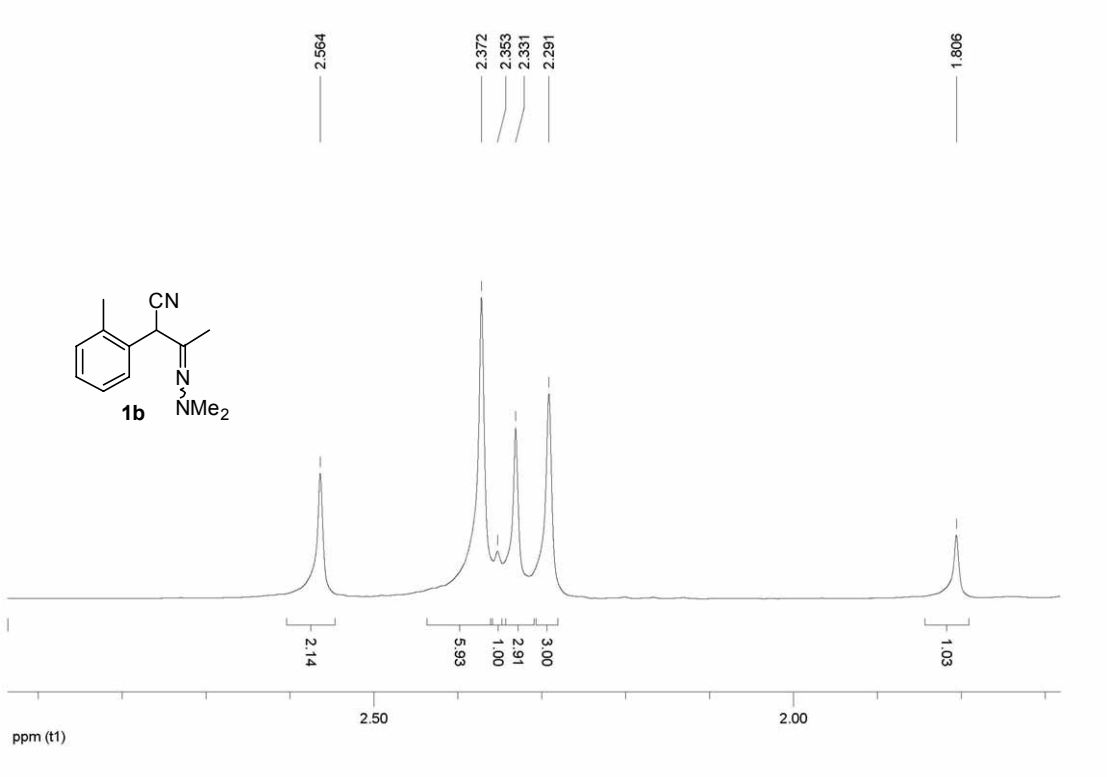
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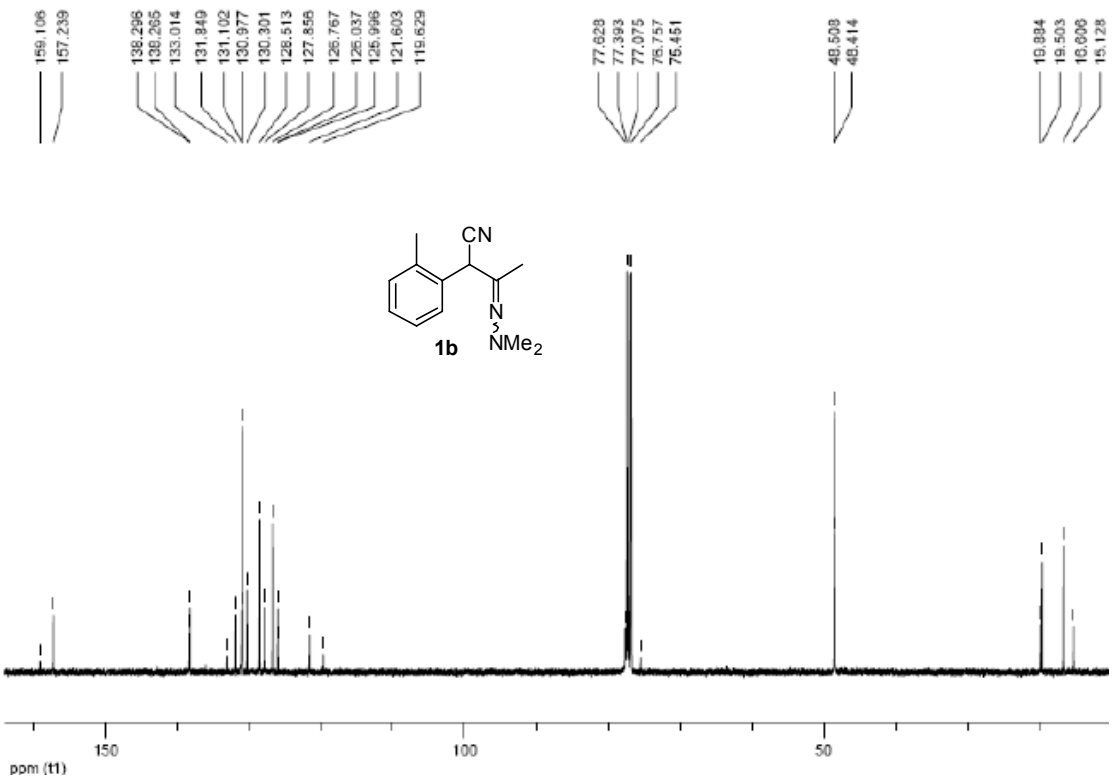
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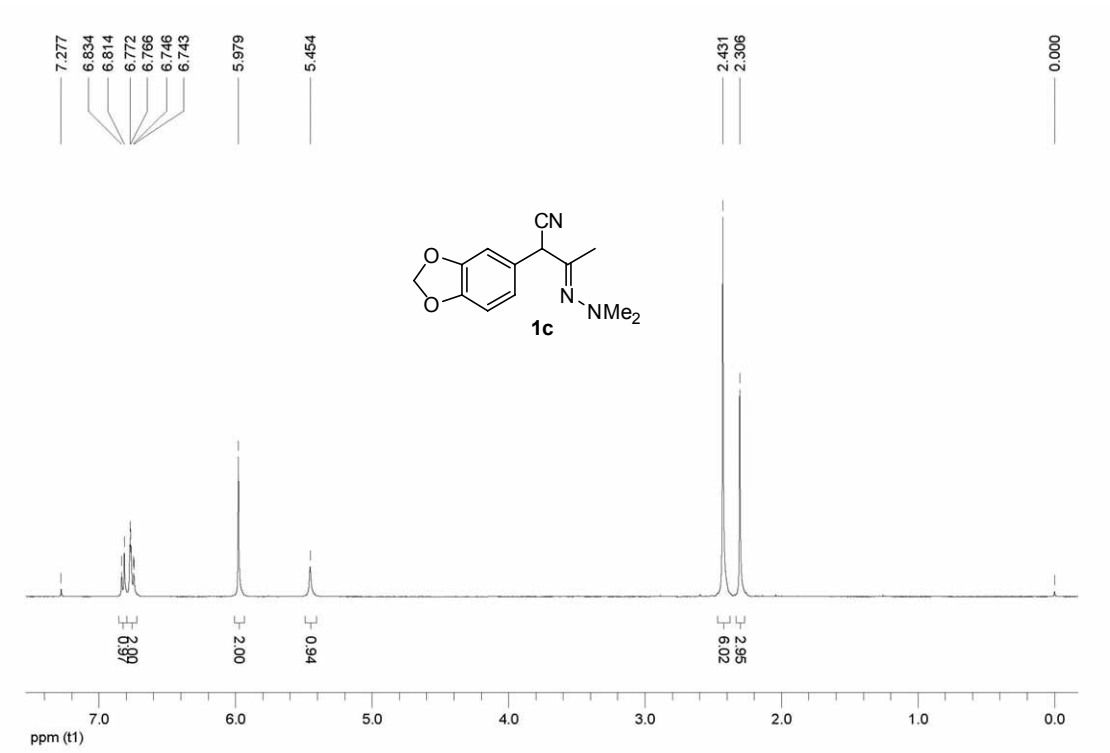
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O
N
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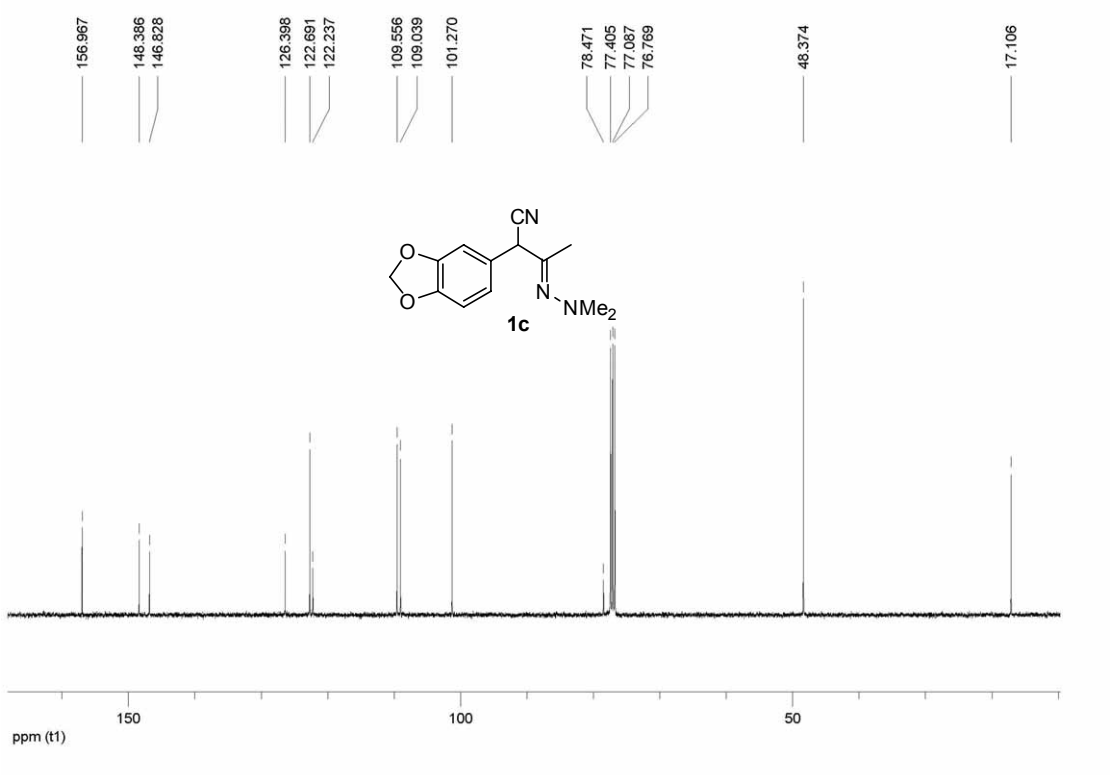
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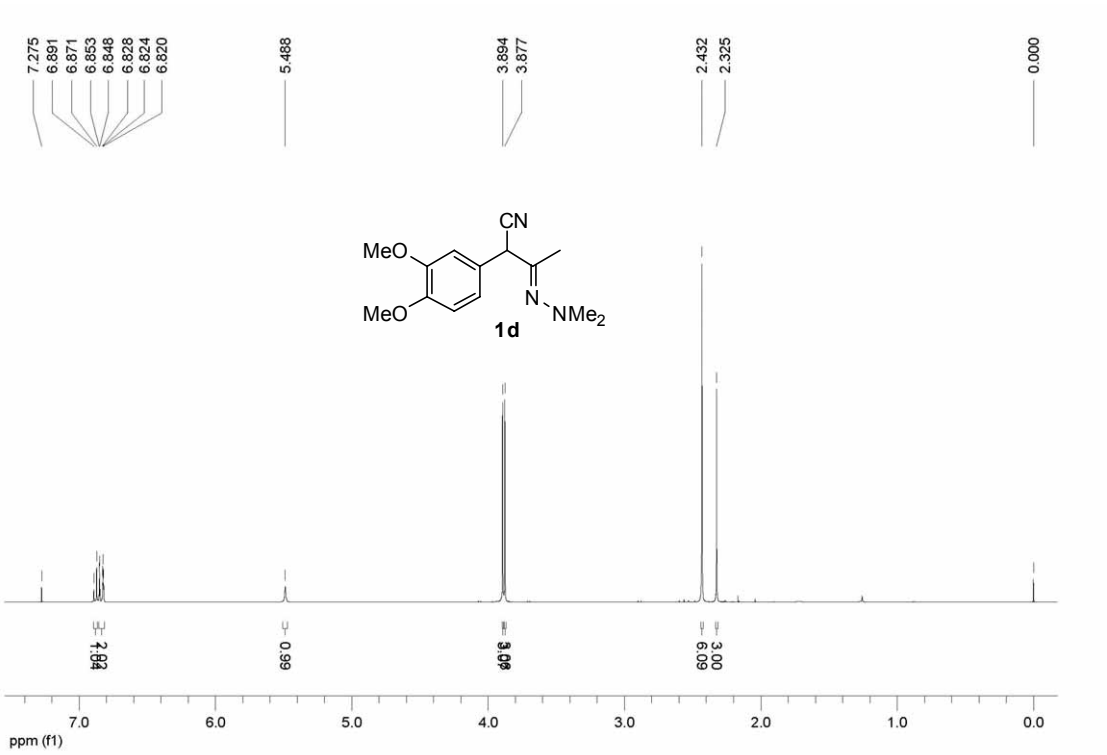
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MeO
N
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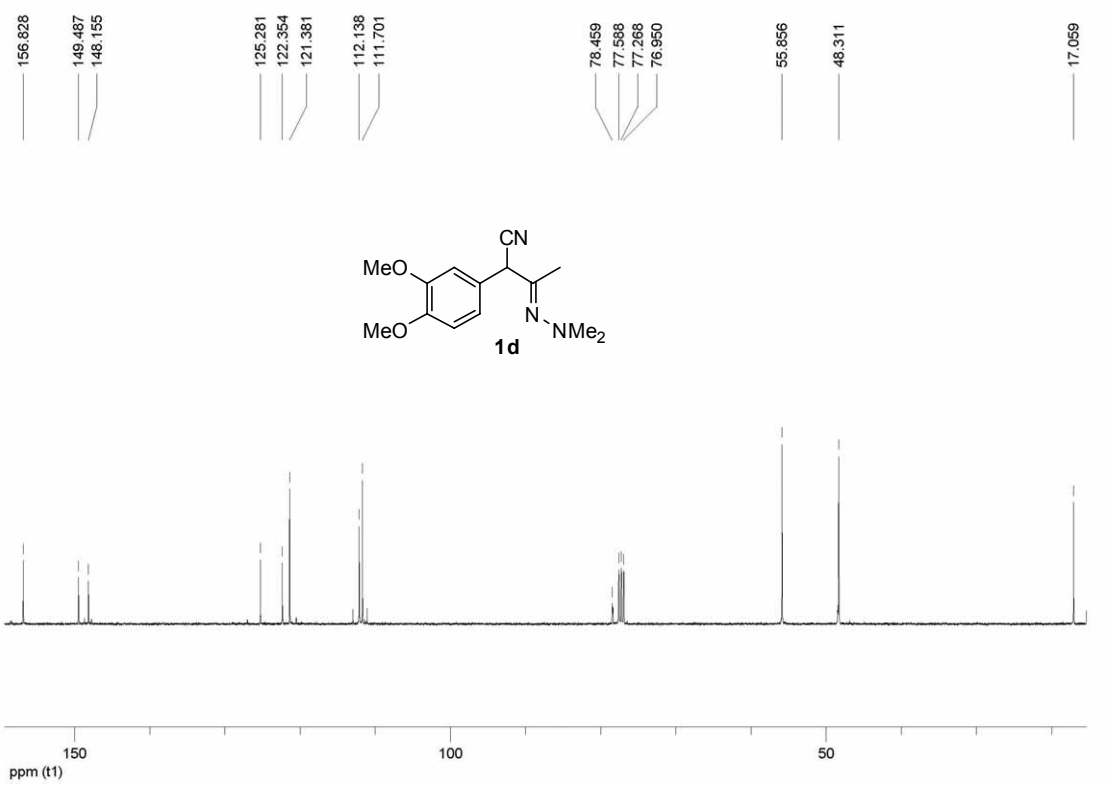
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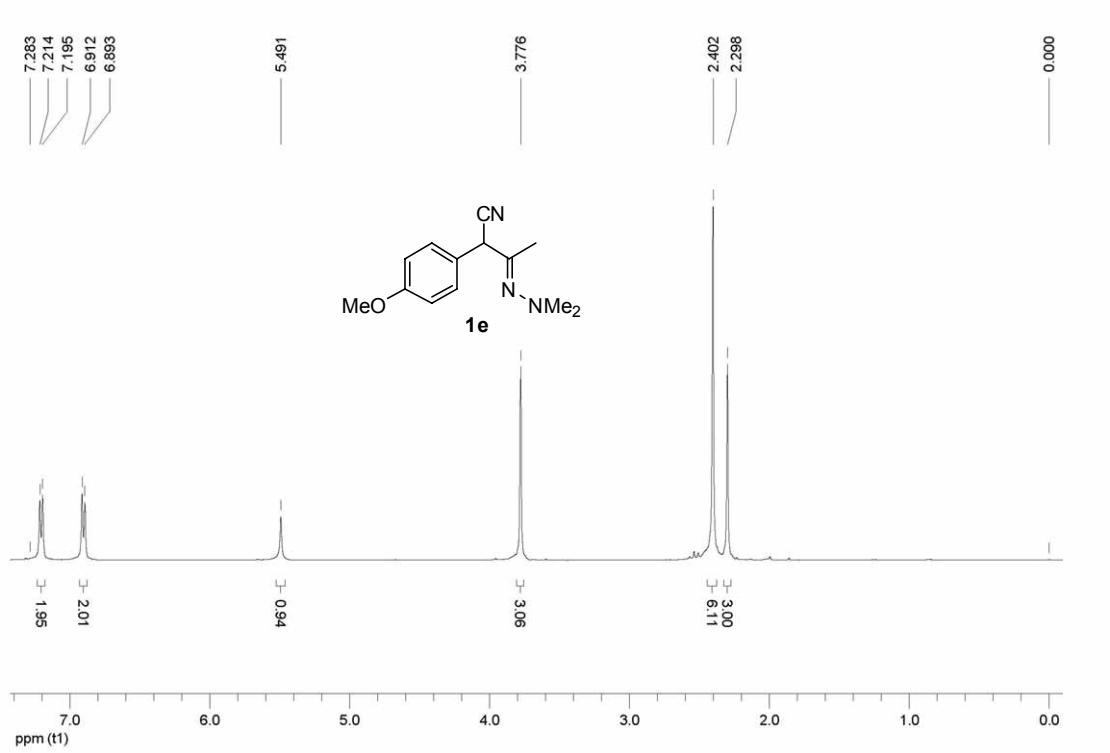
50
ppm (t1)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2.01
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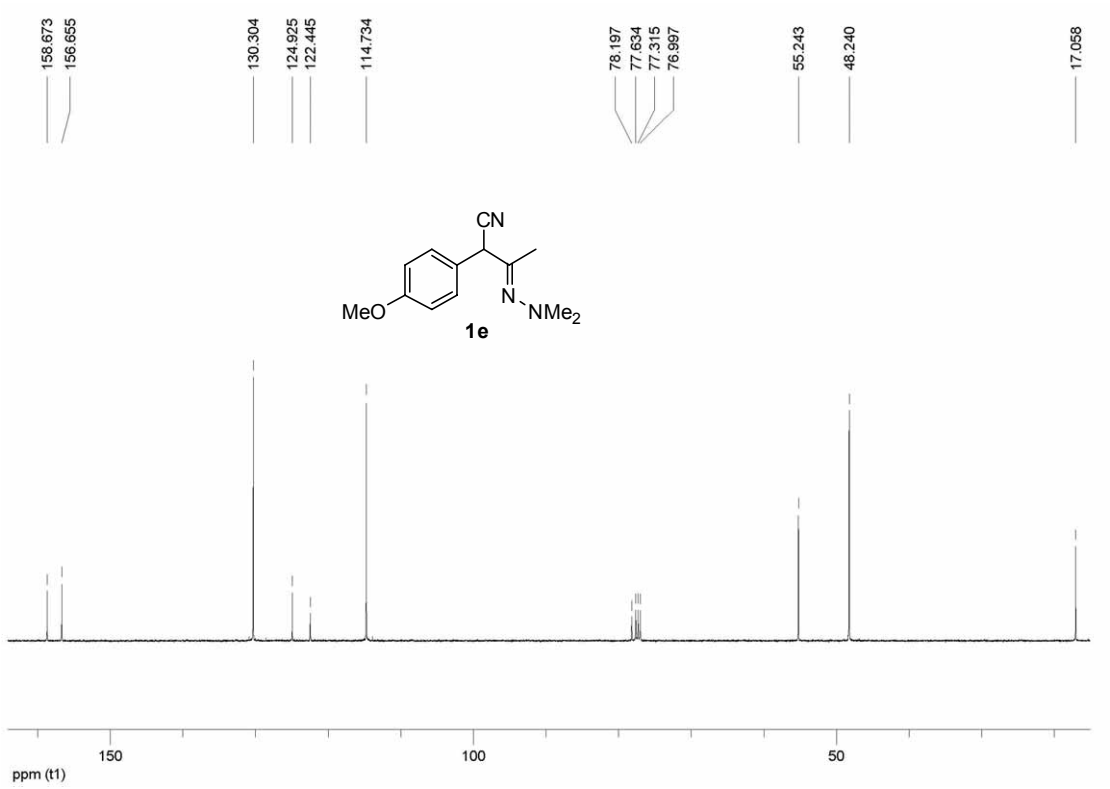
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MeO
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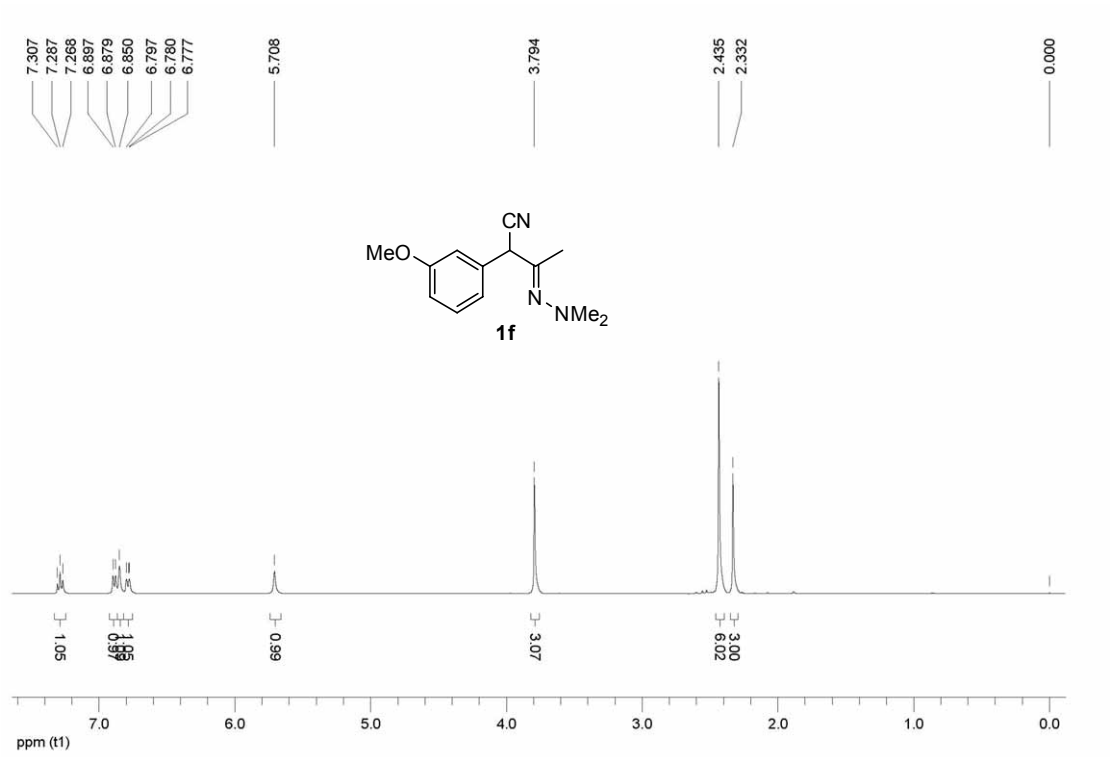
ppm (t1)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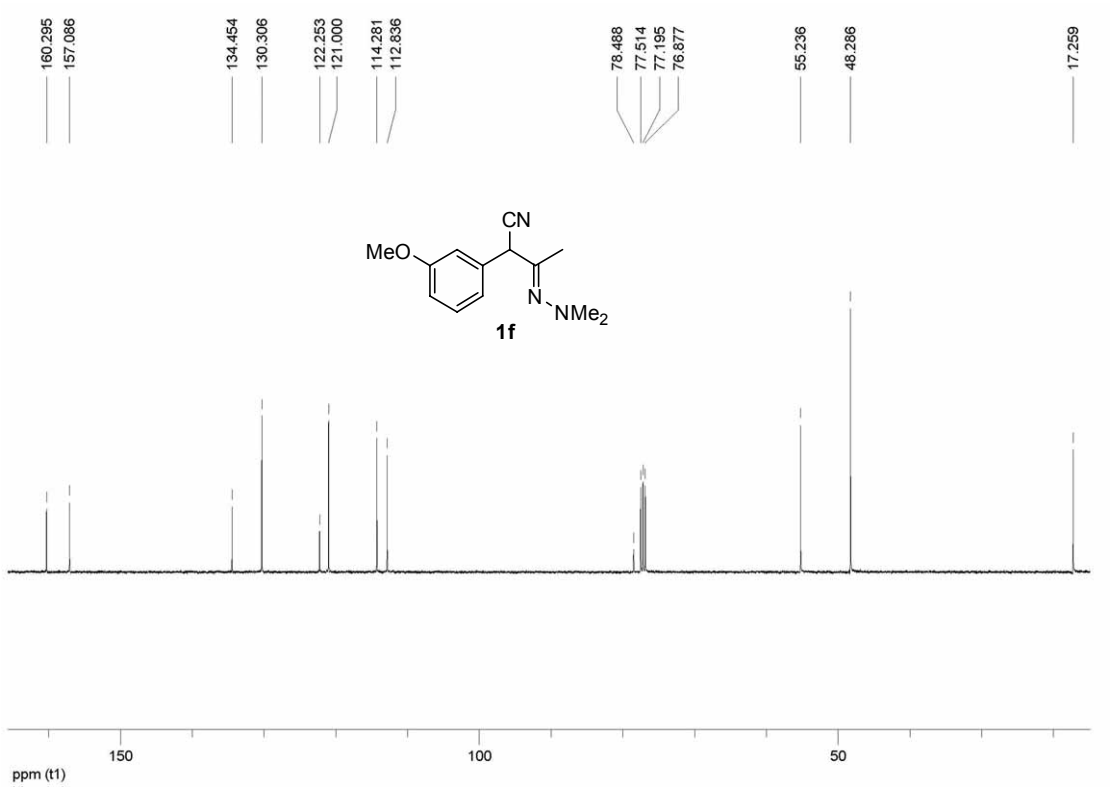
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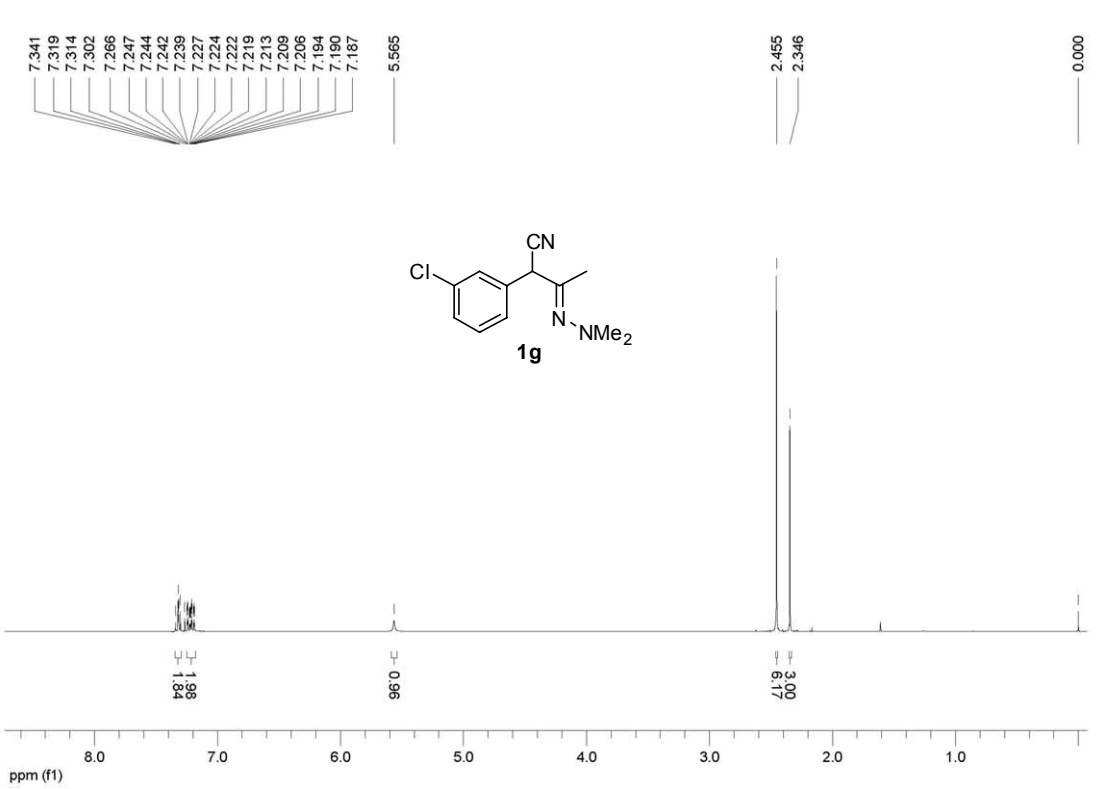
ppm (t1)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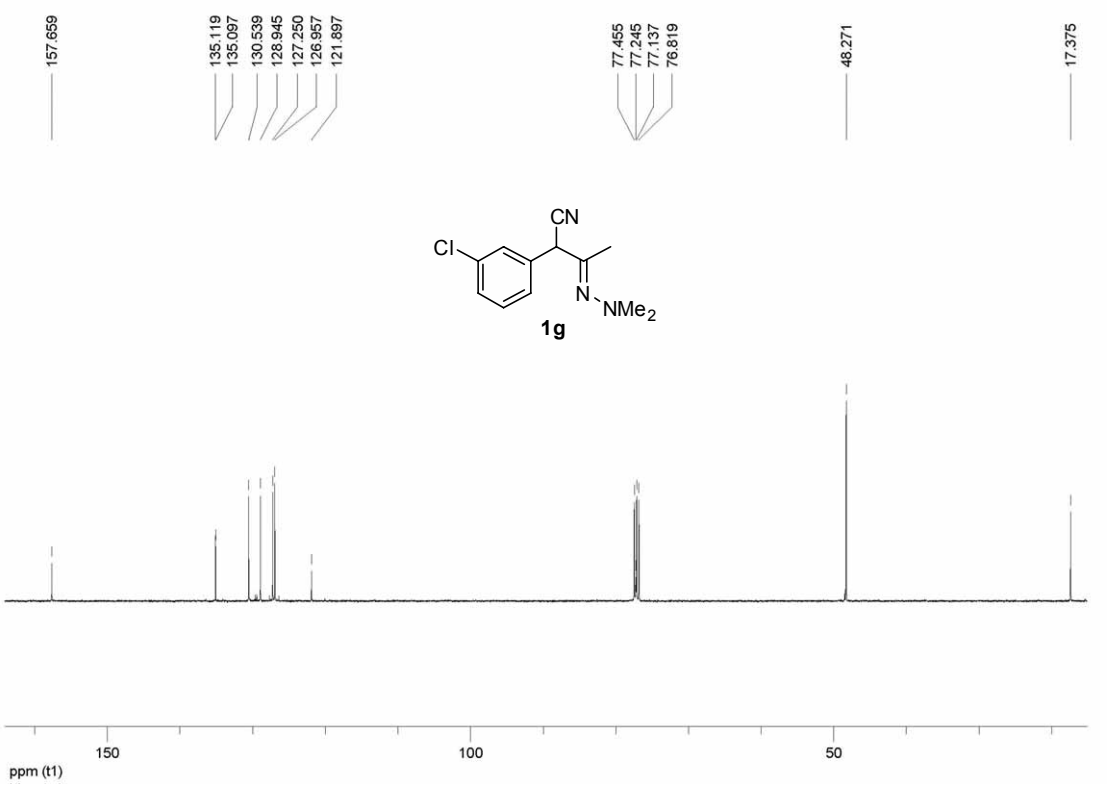
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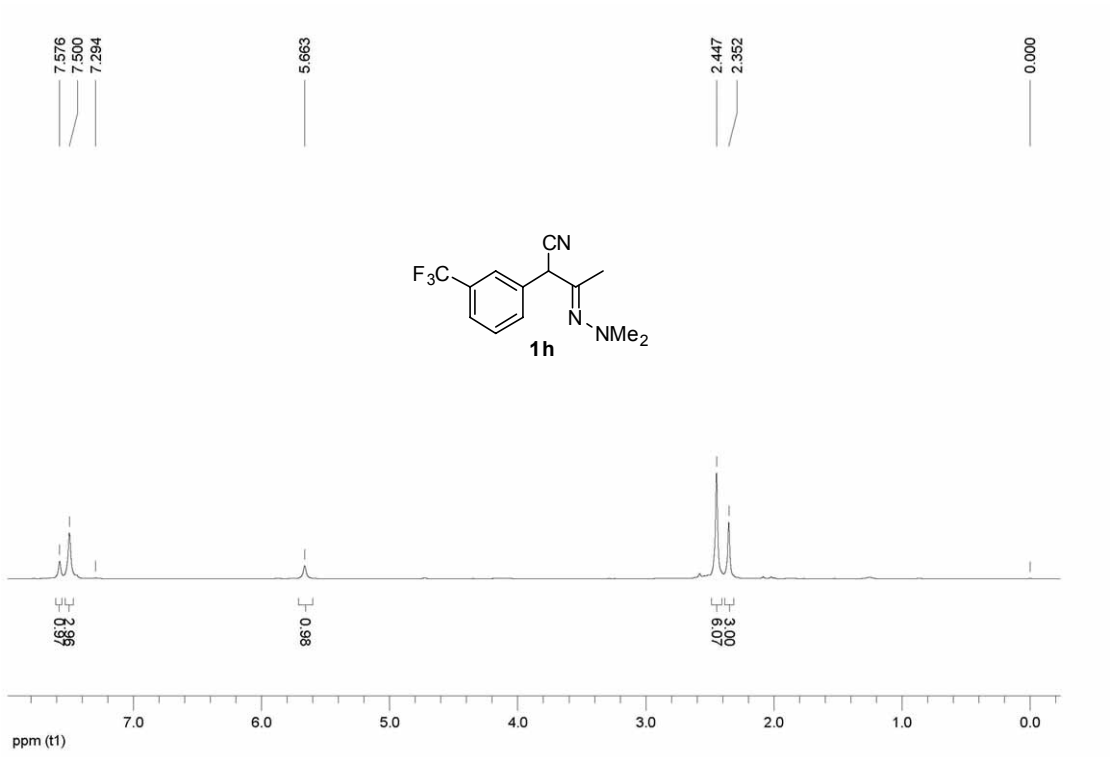
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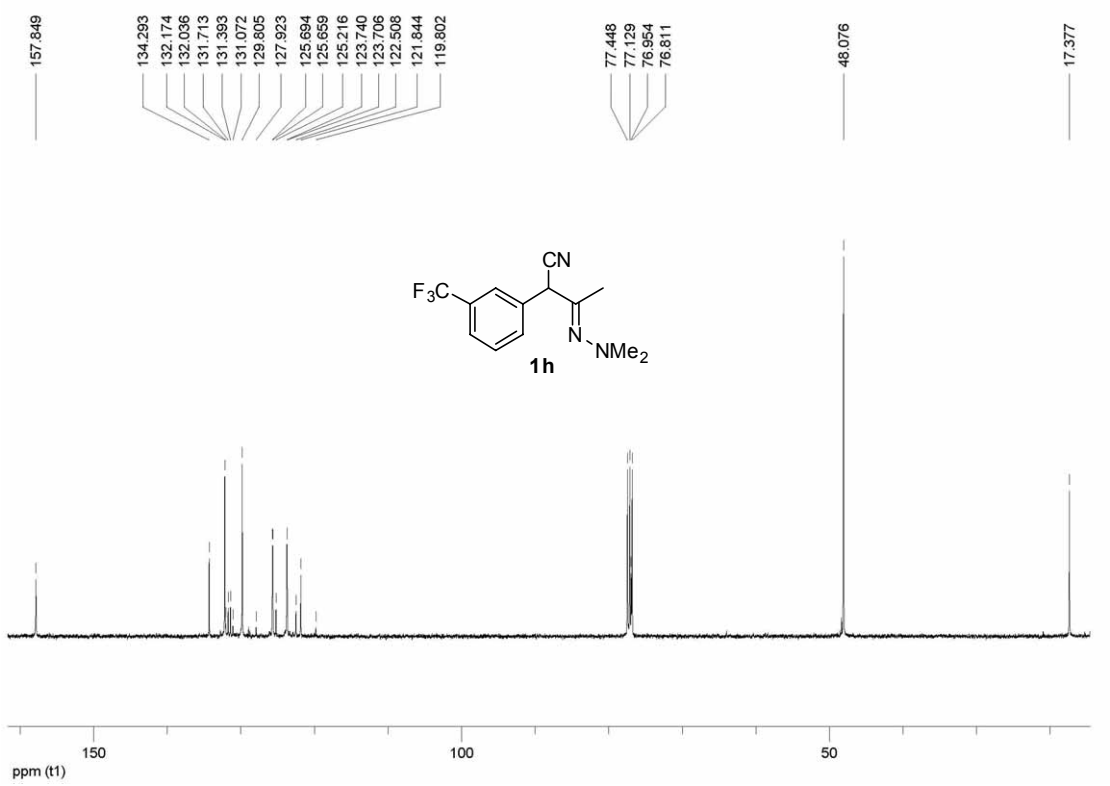
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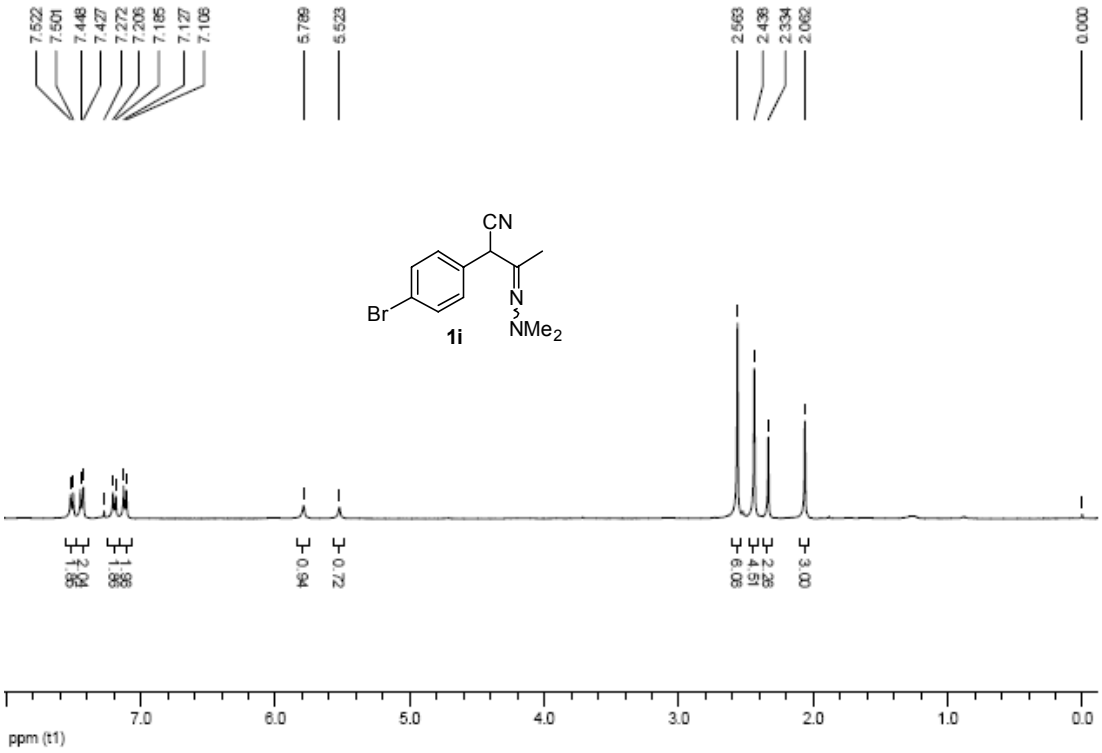
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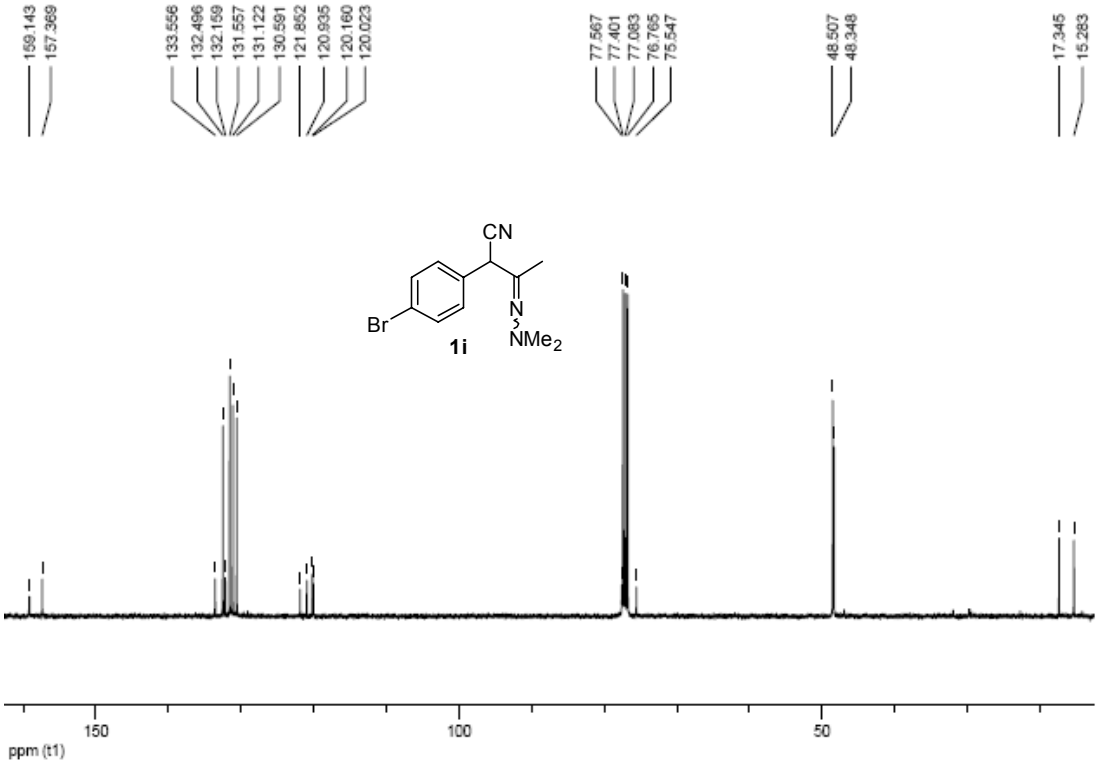
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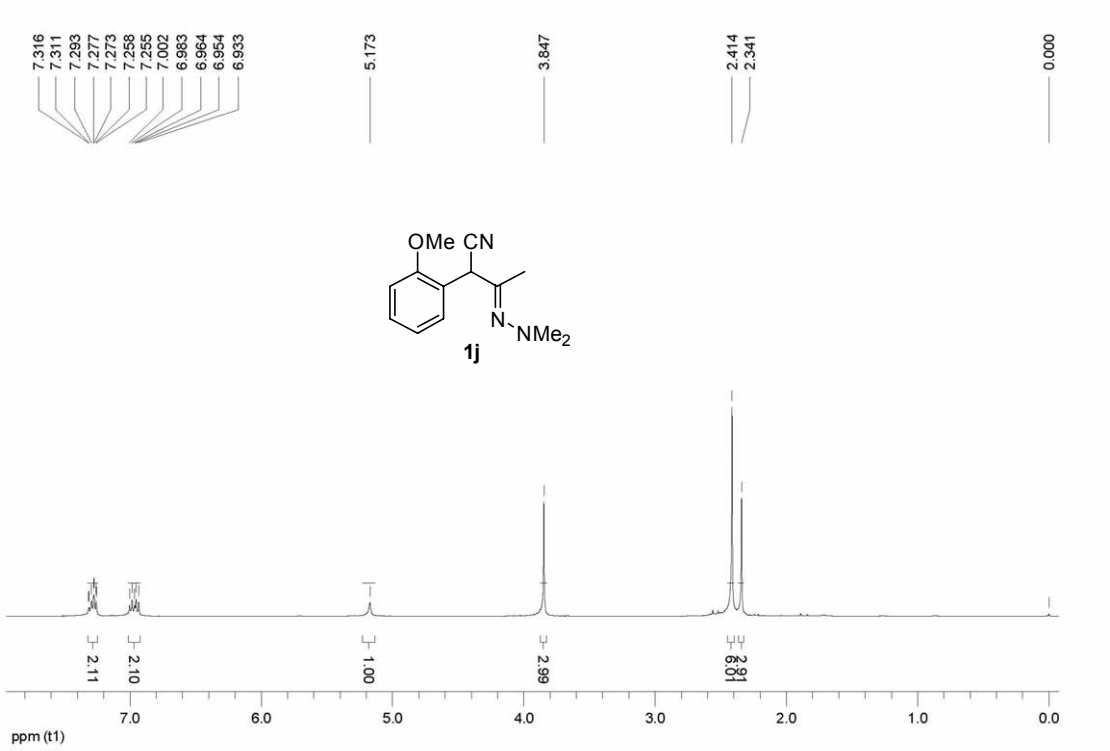
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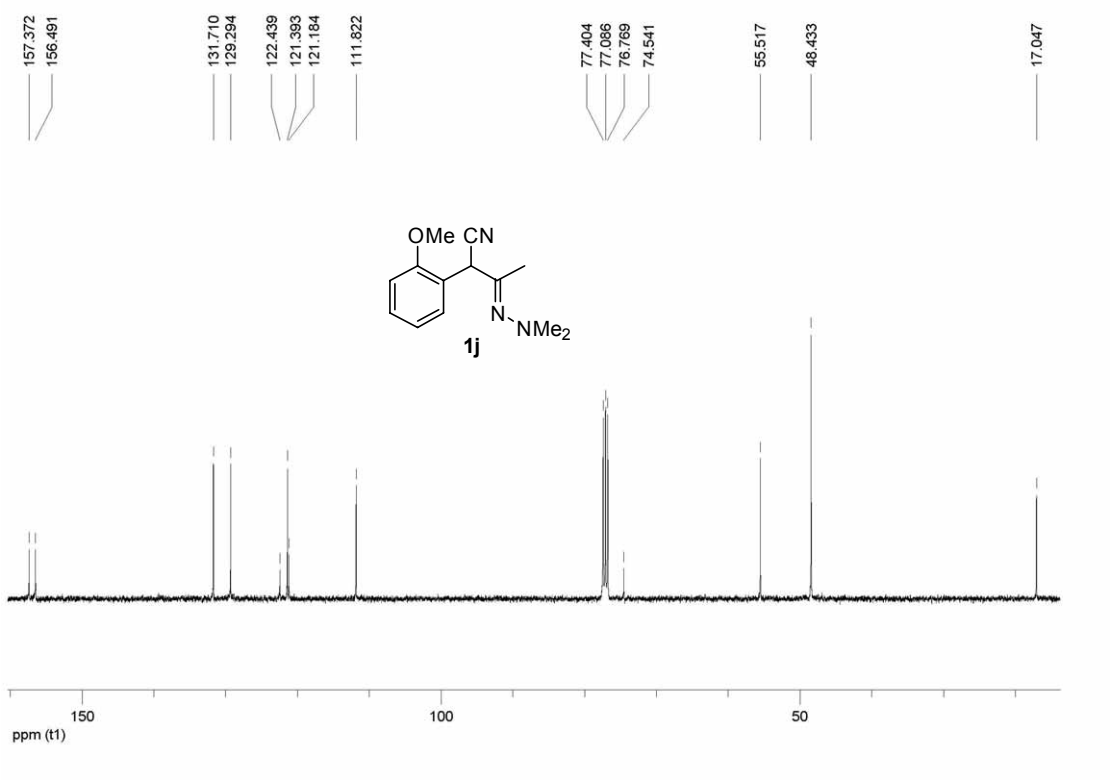
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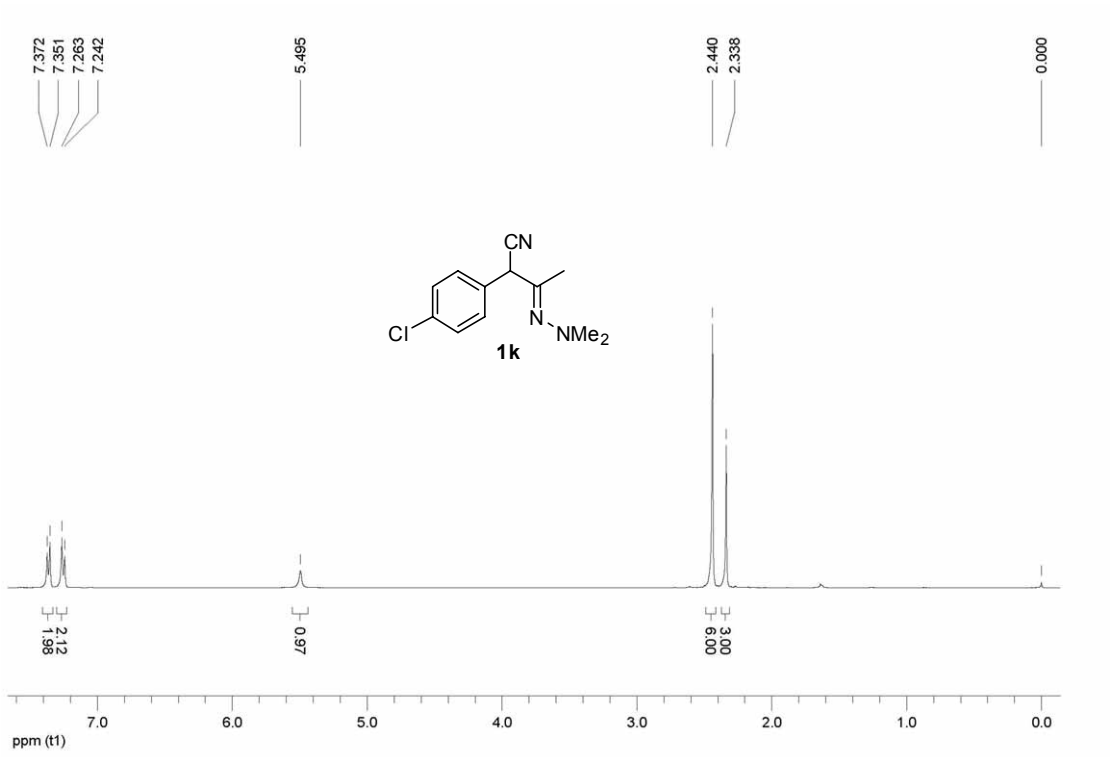
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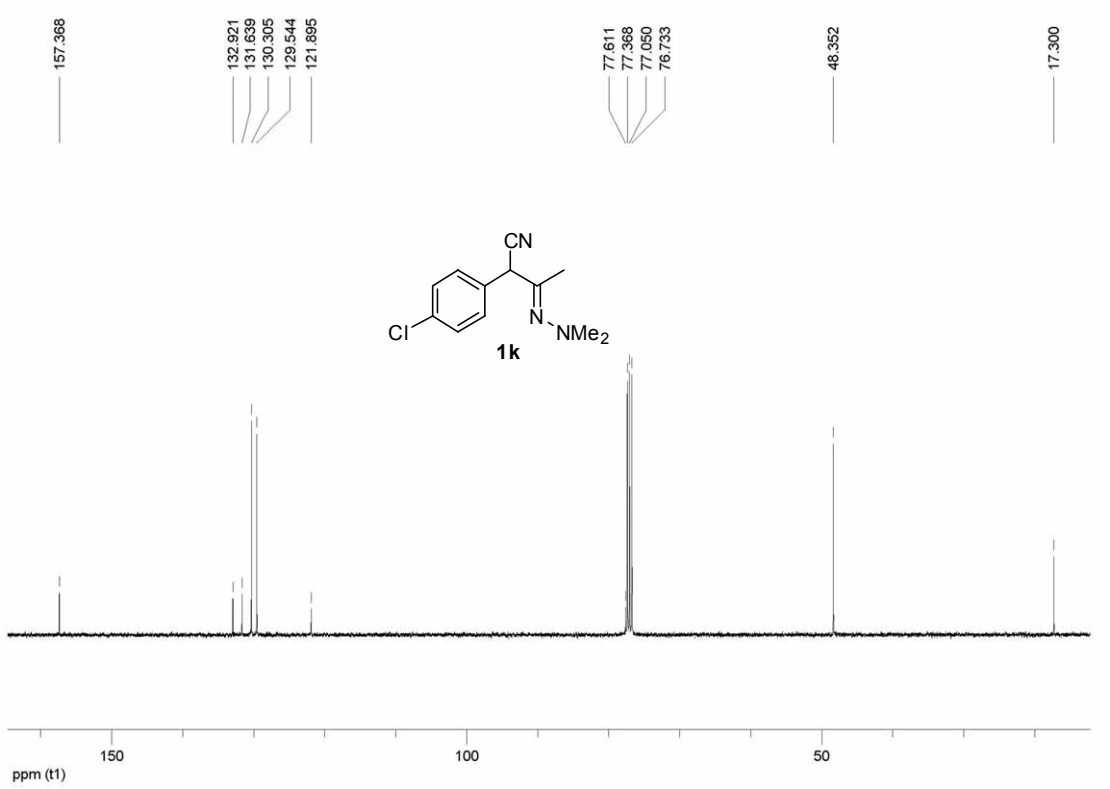
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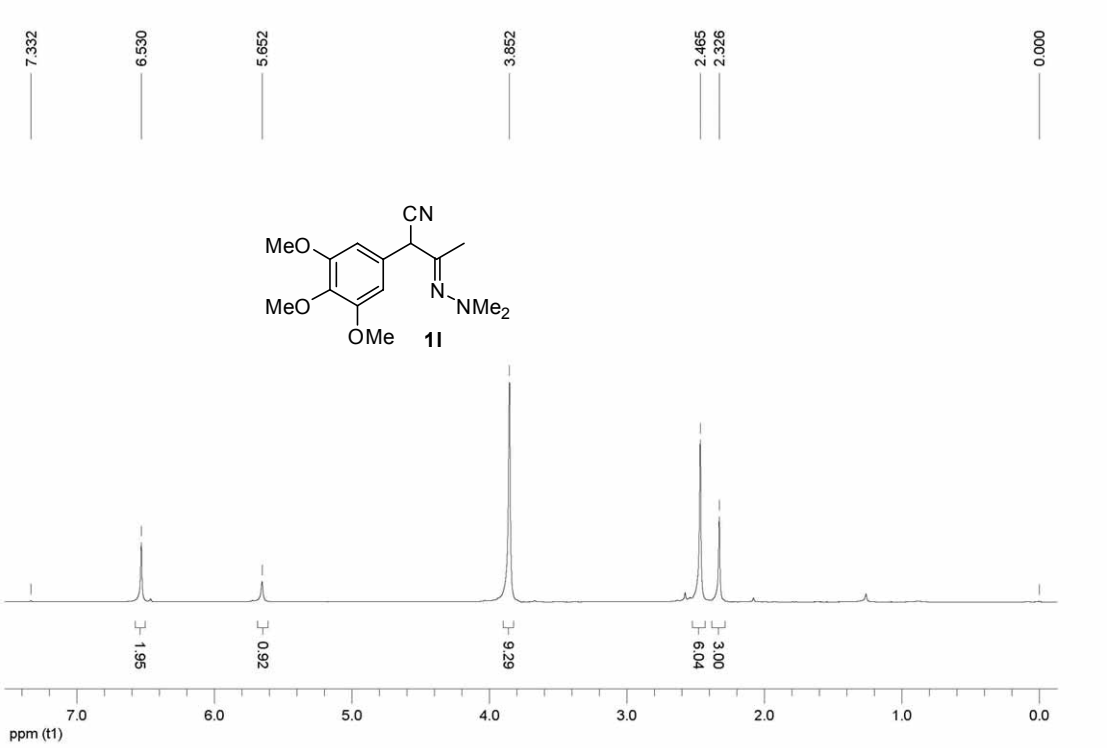
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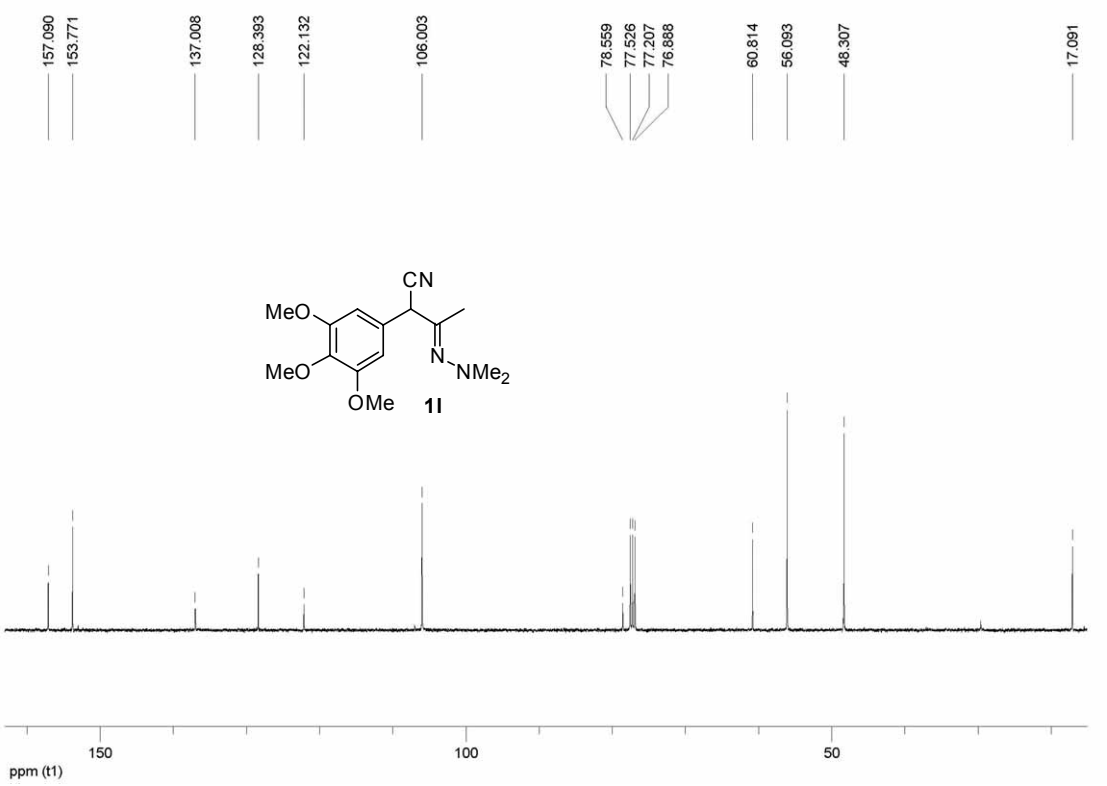
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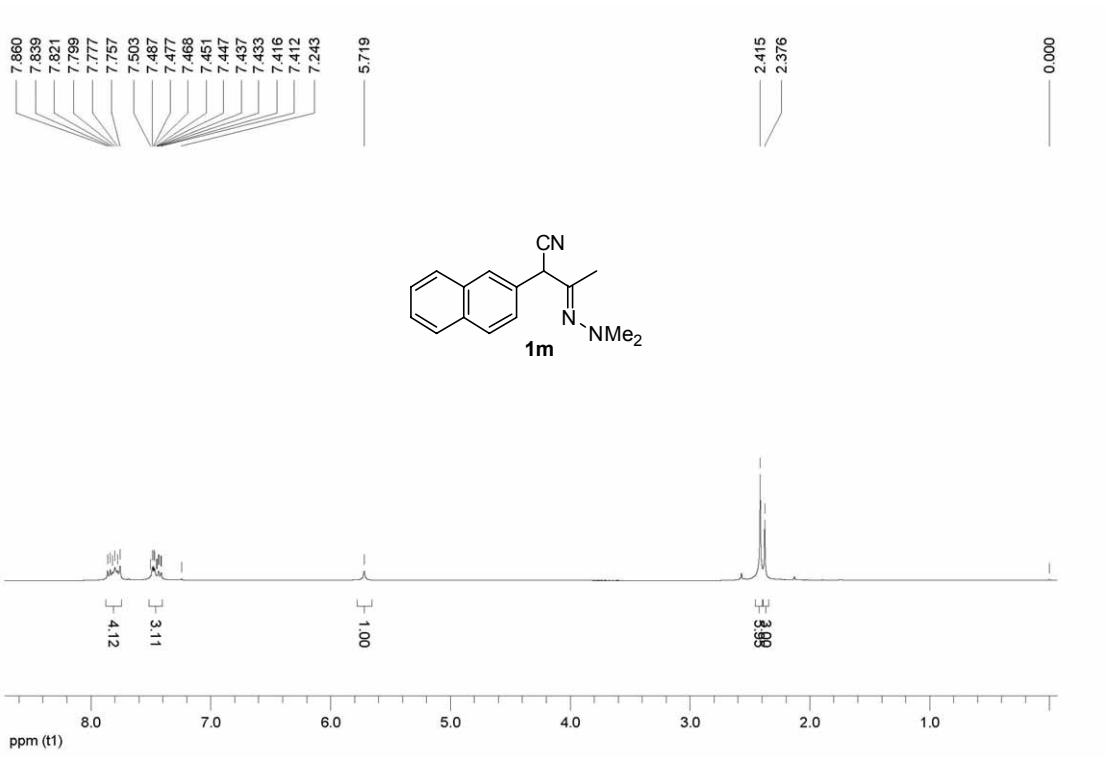
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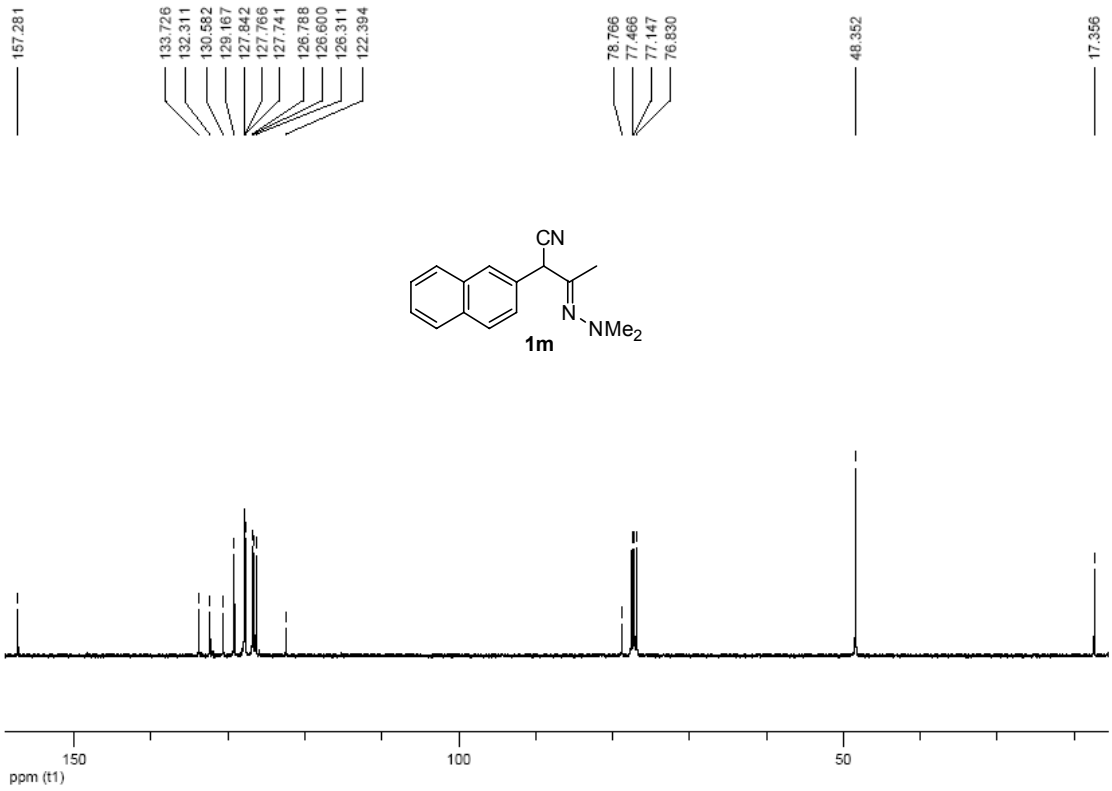
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100
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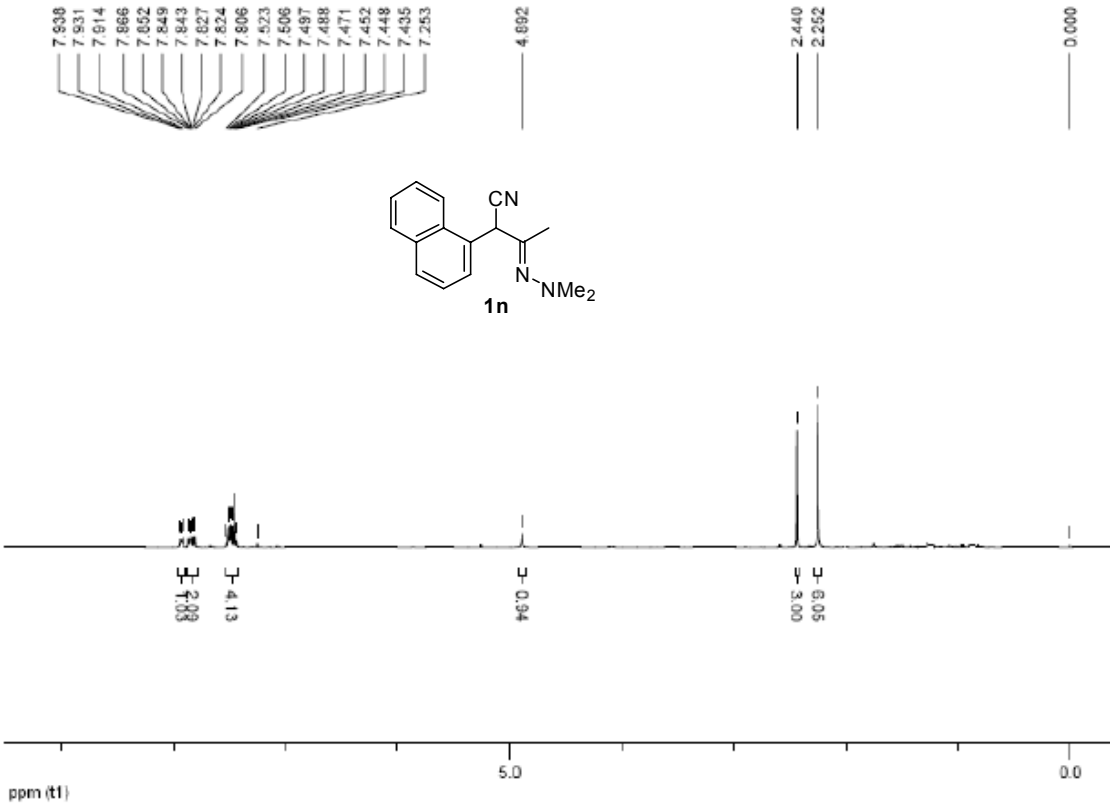
ppm (t1)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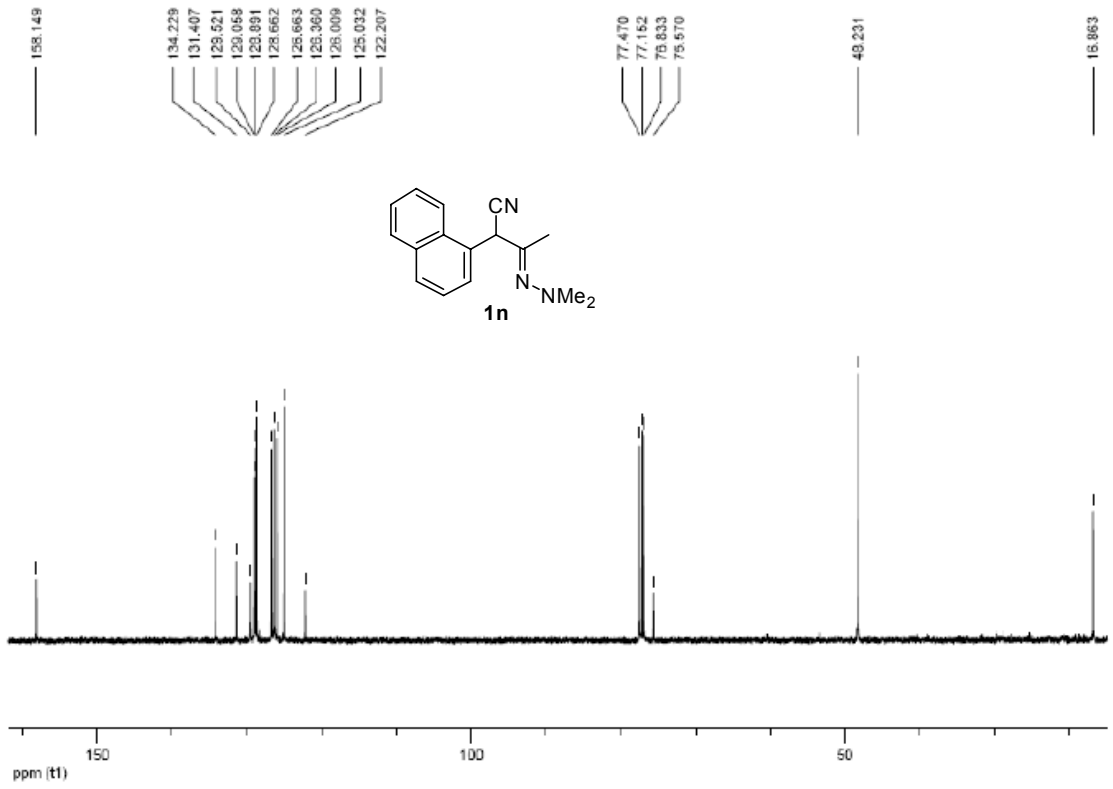
0.0
ppm (t1)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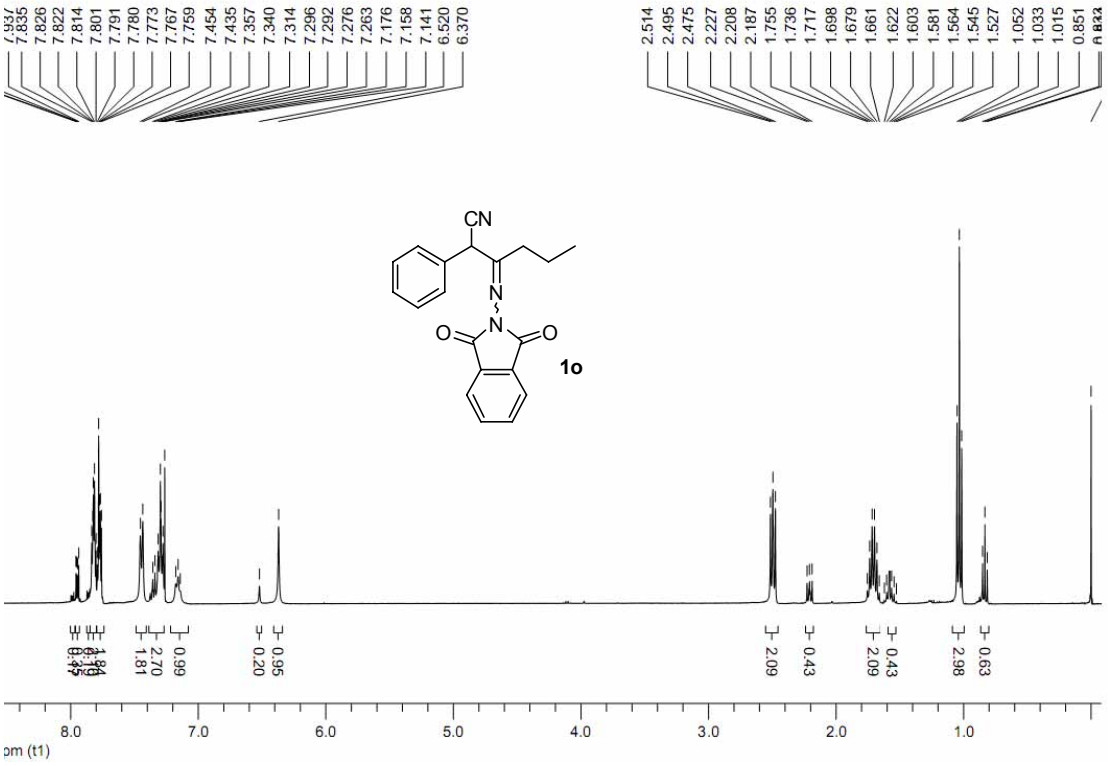
134.229
131.407
129.521
129.058
128.891
128.662
126.663
126.360
126.009
125.032
122.207
77.470
77.152
76.833
75.570
48.231
16.863
CN
N
NMe2
1n
150
100
50
ppm (t1)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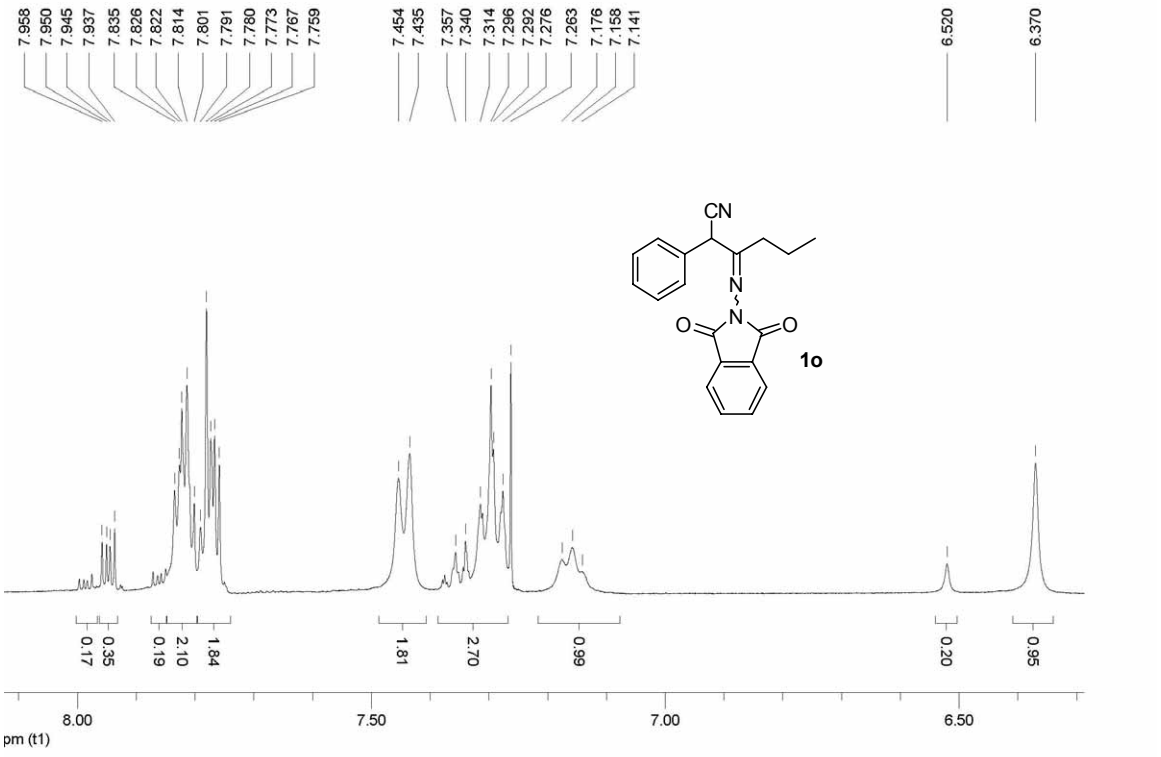
7.826
7.822
7.814
7.801
7.791
7.780
7.773
7.767
7.759
7.454
7.435
7.357
7.340
7.314
7.296
7.292
7.276
7.263
7.176
7.158
7.141
6.520
6.370
2.514
2.495
2.475
2.227
2.208
2.187
1.755
1.736
1.717
1.698
1.679
1.661
1.622
1.603
1.581
1.564
1.545
1.527
1.052
1.033
1.015
0.851
CN
N
O
O
N
O
1o
1.81
0.99
0.20
0.95
2.09
0.43
2.09
0.43
2.98
0.63
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
pm (t1)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7.950
7.945
7.937
7.835
7.826
7.822
7.814
7.801
7.791
7.780
7.773
7.767
7.759
7.454
7.435
7.357
7.340
7.314
7.296
7.292
7.276
7.263
7.176
7.158
7.141
6.520
6.370
CN
N
O
O
N
O
1o
0.17
0.35
0.19
2.10
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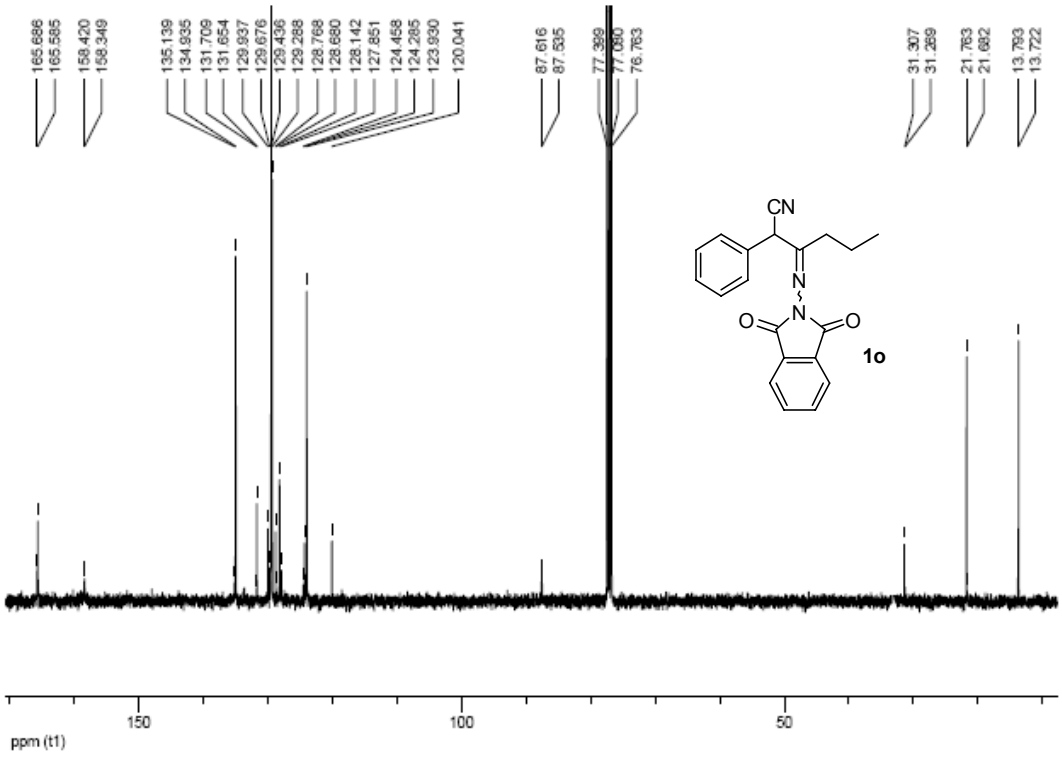
1.81
2.70
0.99
0.20
0.95
8.00
7.50
7.00
6.50
pm (t1)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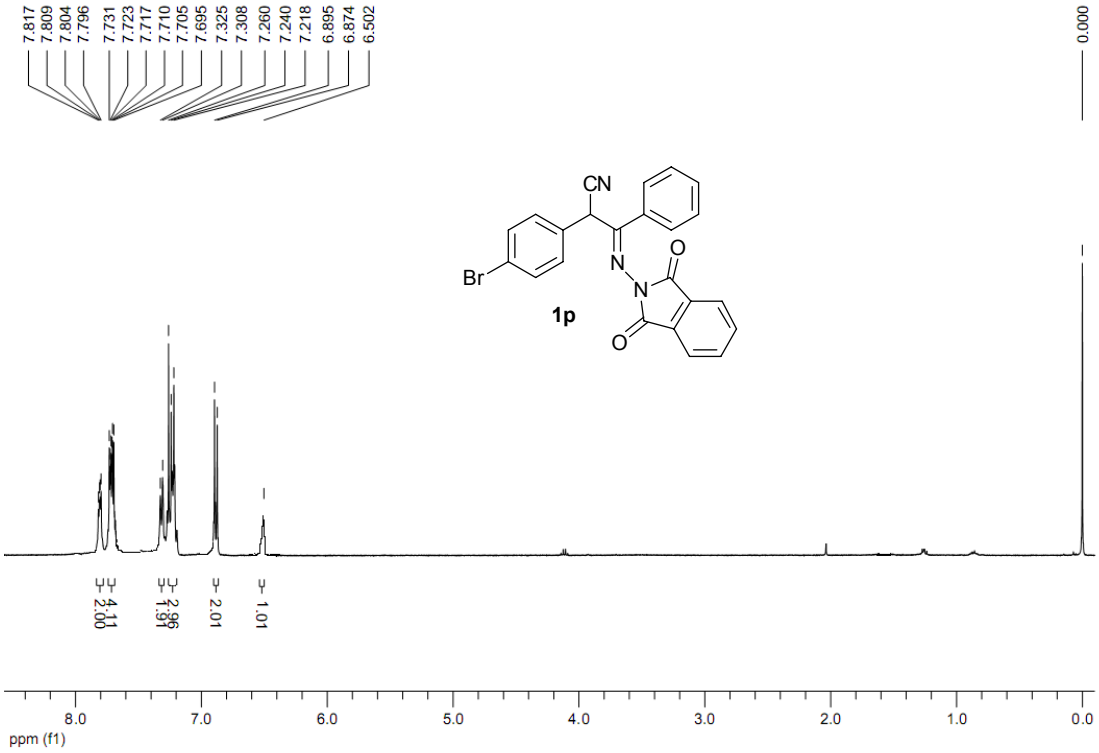
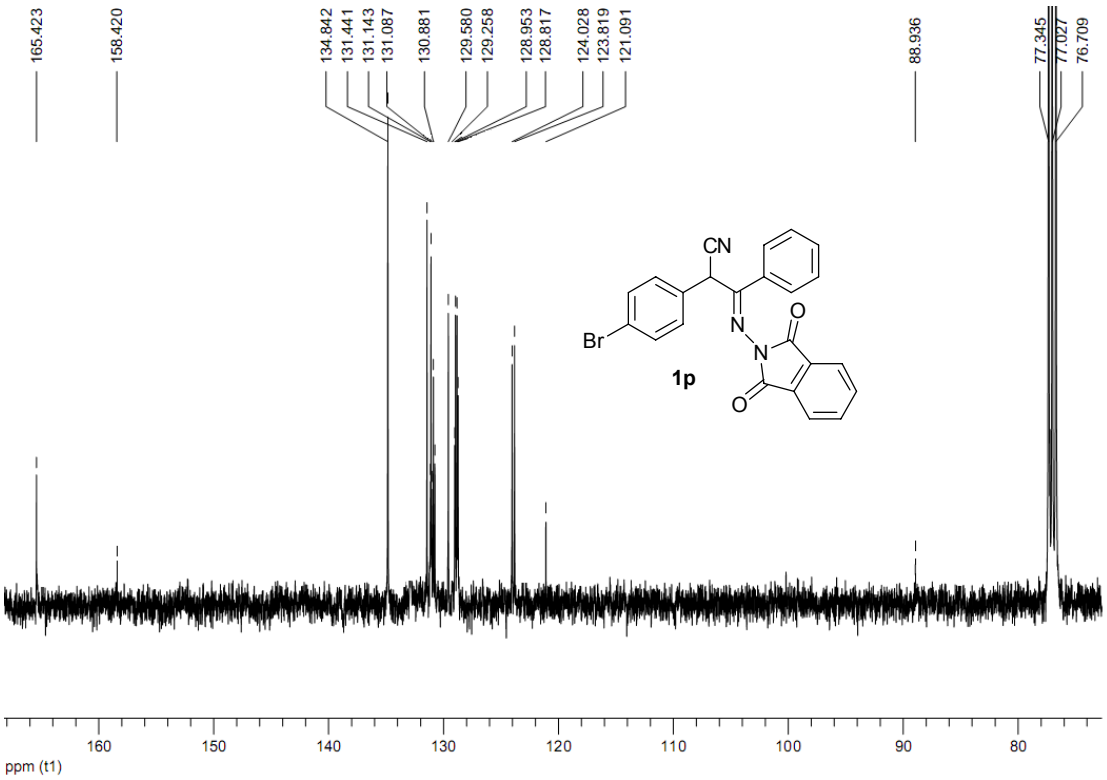
165.585
158.420
158.349
135.139
134.935
131.709
131.654
129.937
129.676
129.436
129.288
128.768
128.680
128.142
127.851
124.458
124.285
123.930
120.041
87.616
87.535
77.399
77.080
76.763
31.307
31.269
21.763
21.682
13.793
13.722
CN
N
N
O
O
1o
150
100
50
ppm (t1)


7.817
7.809
7.804
7.796
7.731
7.723
7.717
7.710
7.705
7.695
7.325
7.308
7.260
7.240
7.218
6.895
6.874
6.502
0.000
CN
Br
N
O
N
O
1p
4.11
2.96
2.01
1.01
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)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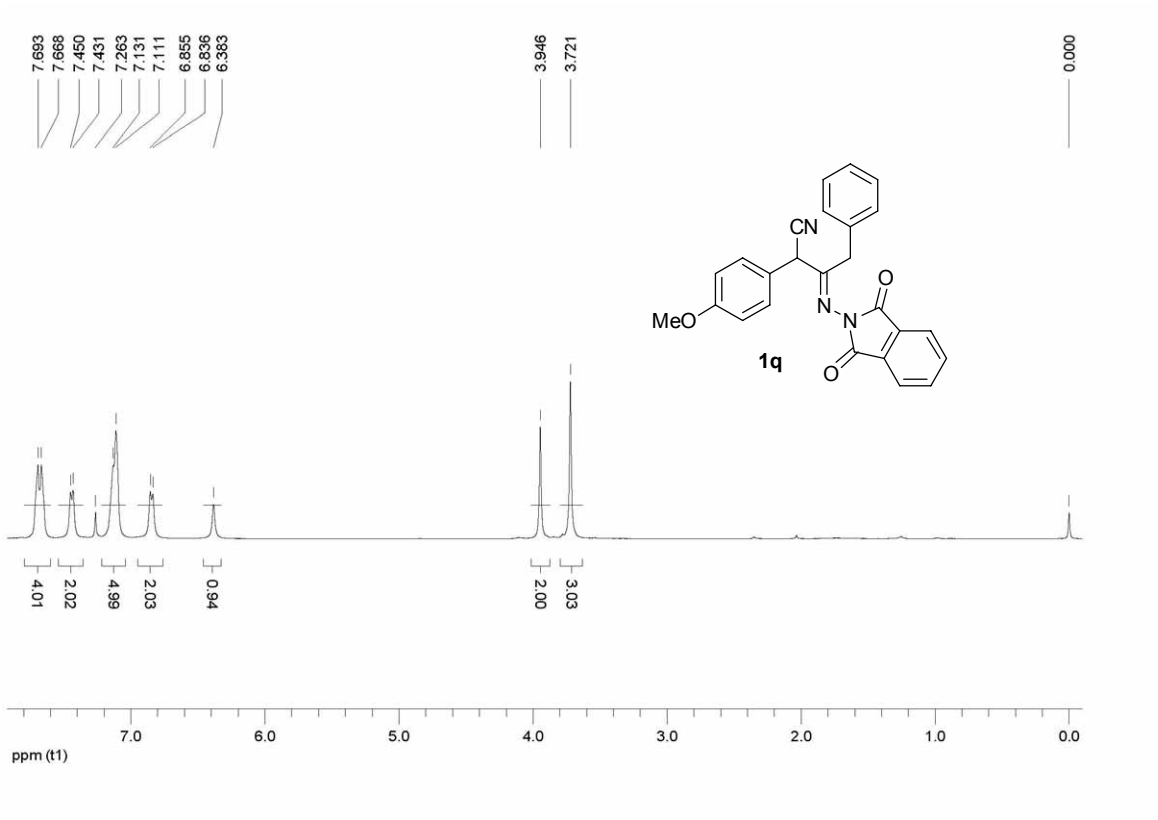
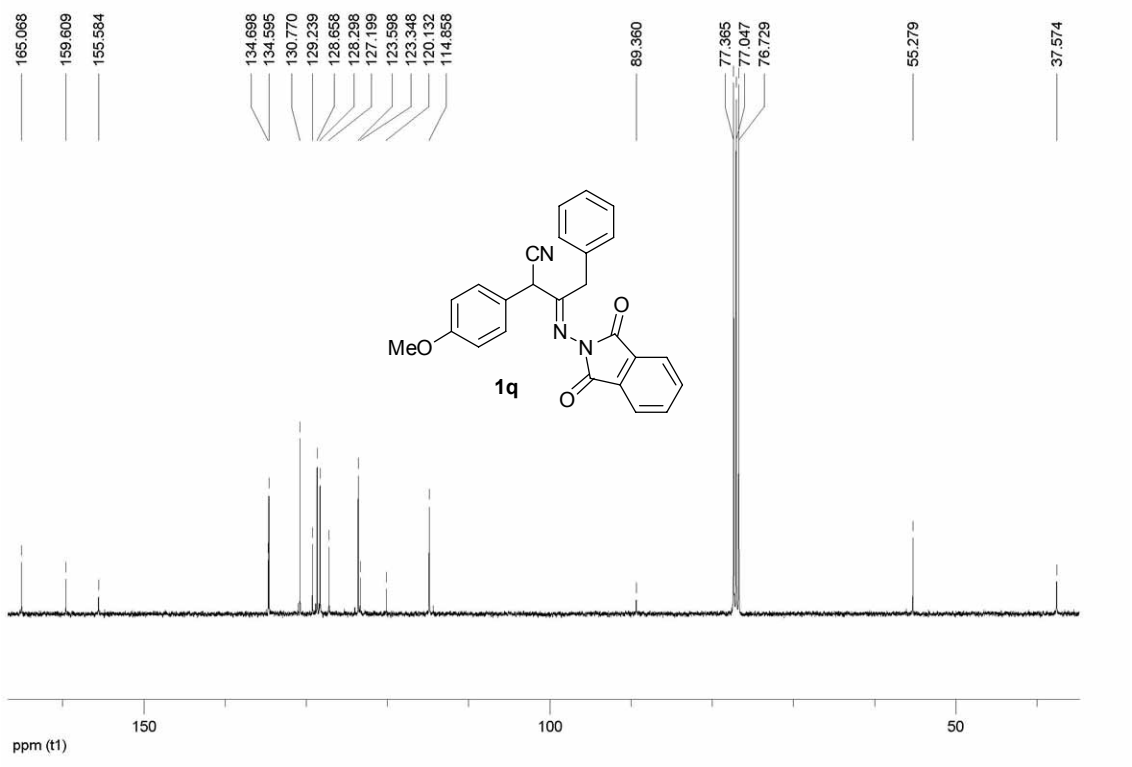
134.842
131.441
131.143
131.087
130.881
129.580
129.258
128.953
128.817
124.028
123.819
121.091
88.936
77.345
77.027
76.709
CN
Br
N
O
N
O
1p
160
150
140
130
120
110
100
90
80
ppm (t1)


7.693
7.668
7.450
7.431
7.263
7.131
7.111
6.855
6.836
6.383
3.946
3.721
0.000
CN
MeO
N
N
O
O
1q
4.01
2.02
4.99
2.03
0.64
2.00
3.03
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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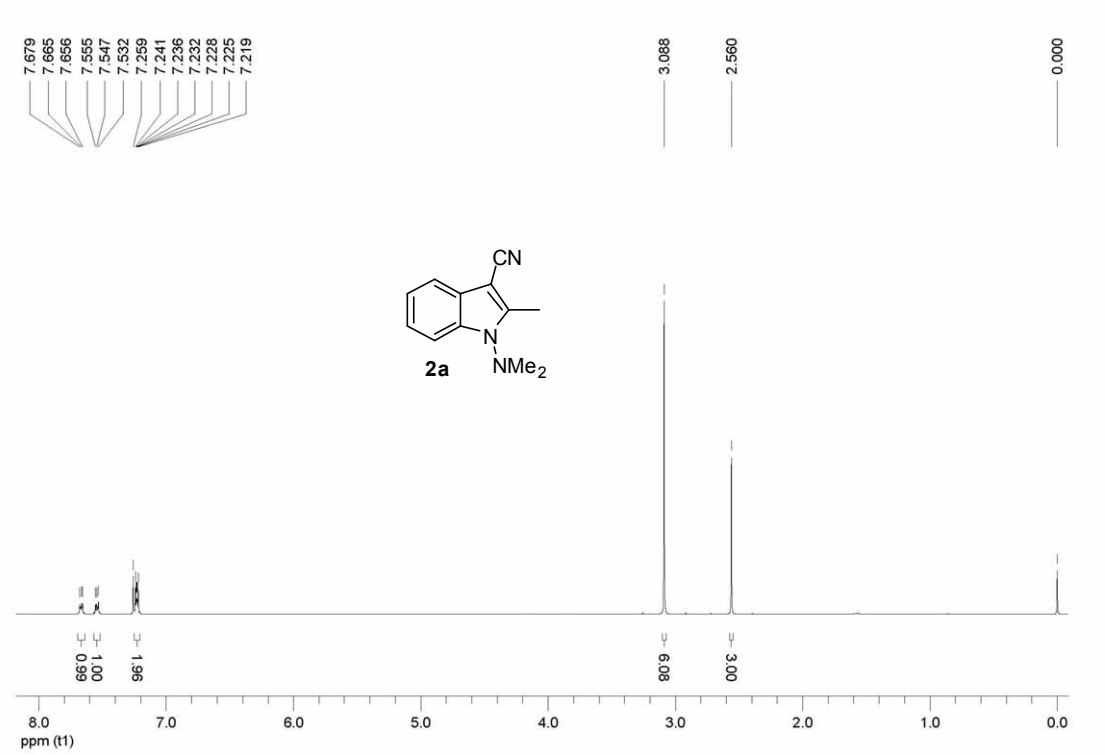
159.609
155.584
134.698
134.595
130.770
129.239
128.658
128.298
127.199
123.598
123.348
120.132
114.858
89.360
77.365
77.047
76.729
55.279
37.574
CN
MeO
N
N
O
O
1q
150
100
50
ppm (t1)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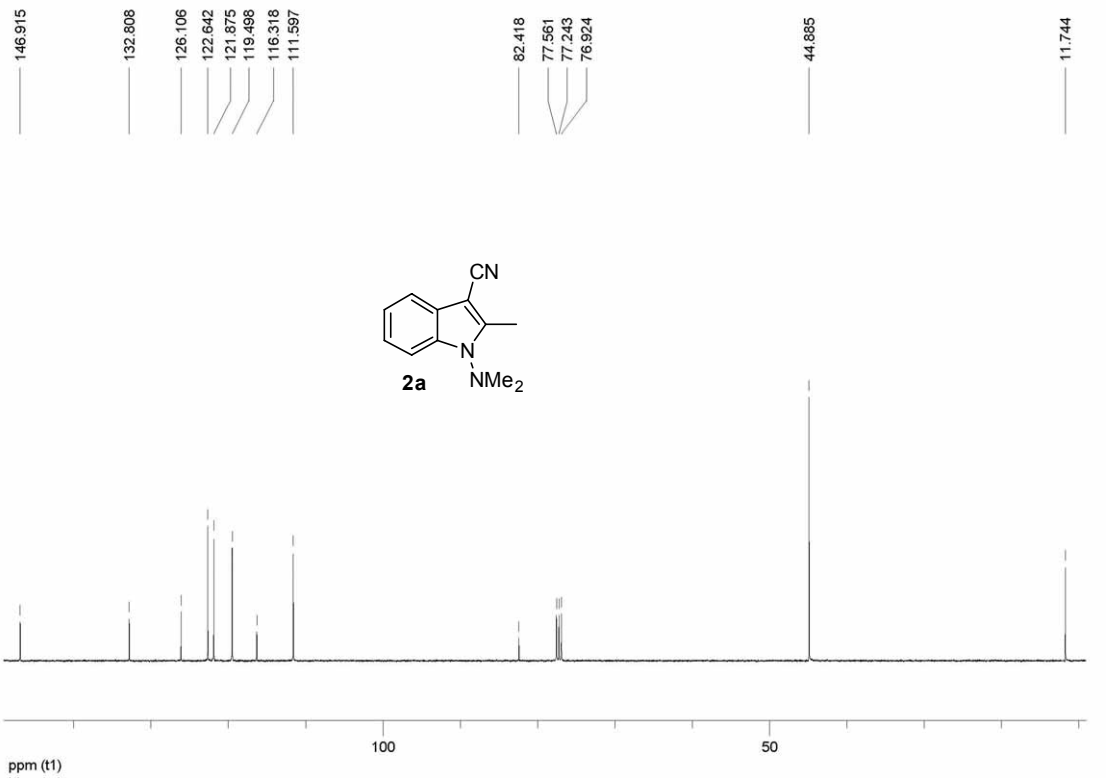
7.665
7.656
7.555
7.547
7.532
7.259
7.241
7.236
7.232
7.228
7.225
7.219
3.088
2.560
0.000
CN
N
NMe2
2a
0.99
1.00
1.96
6.08
3.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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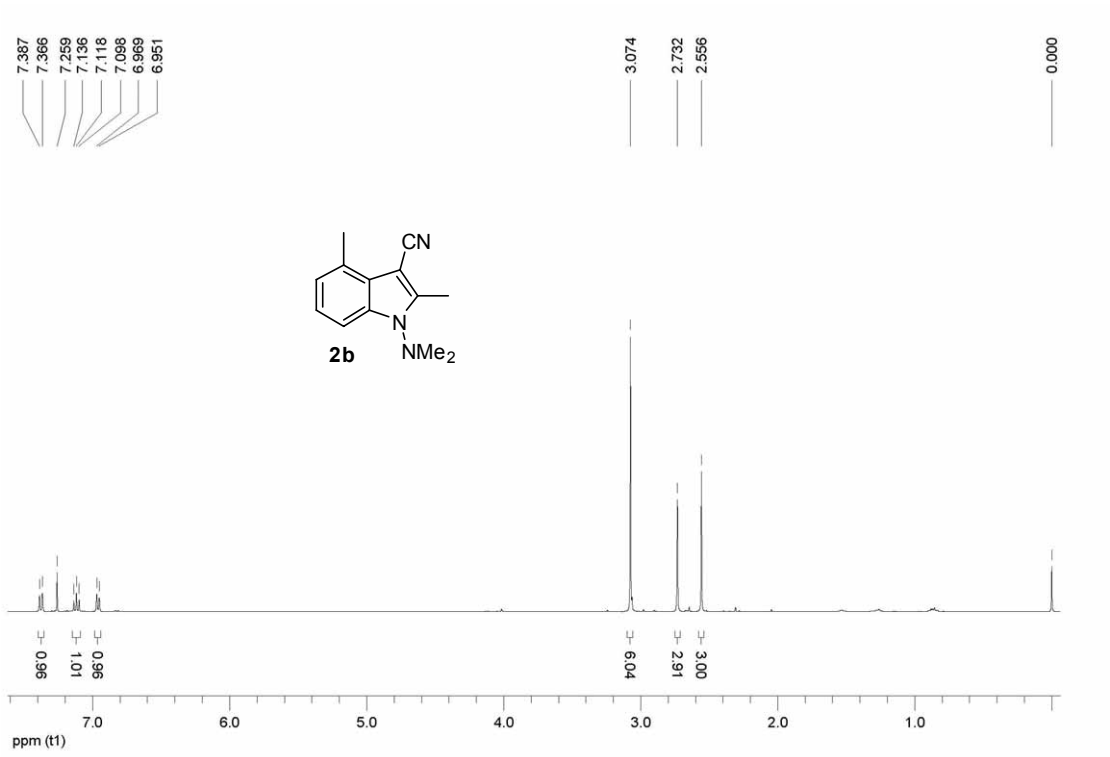
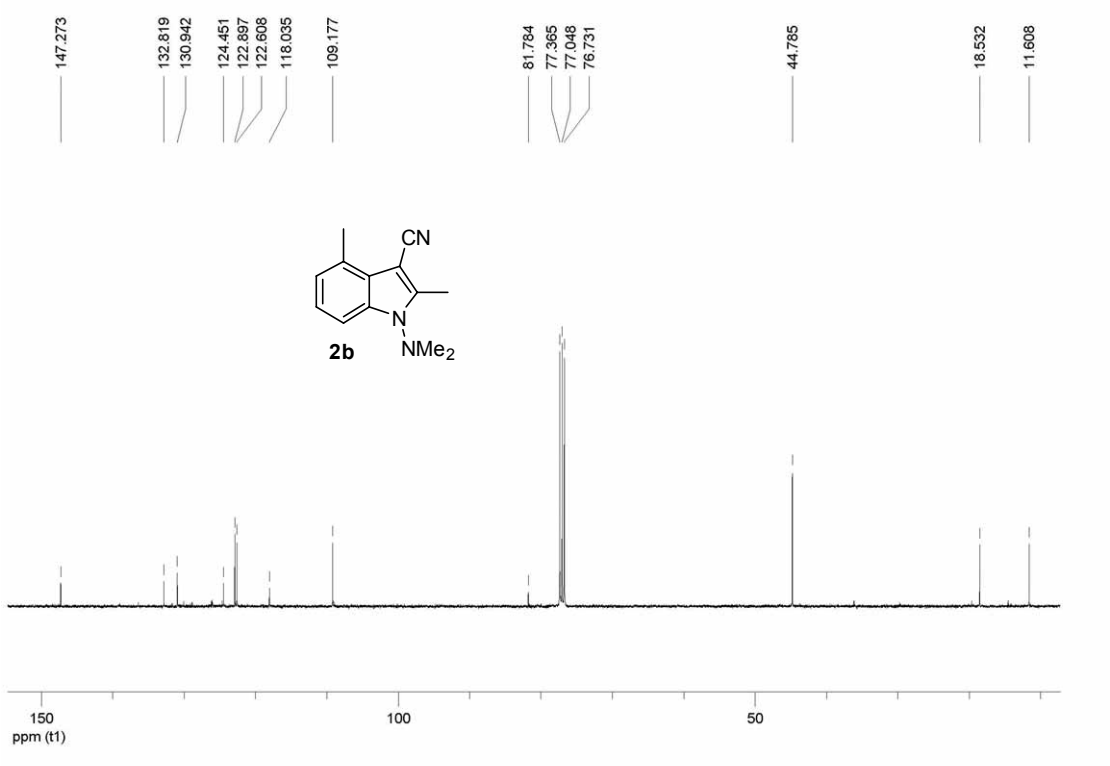
126.106
122.642
121.875
119.498
116.318
111.597
82.418
77.561
77.243
76.924
44.885
11.744
CN
N
NMe2
2a
100
50
ppm (t1)


7.387
7.366
7.259
7.136
7.118
7.098
6.969
6.951
3.074
2.732
2.556
0.000
CN
N
NMe2
2b
0.96
1.01
0.96
6.04
2.91
3.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)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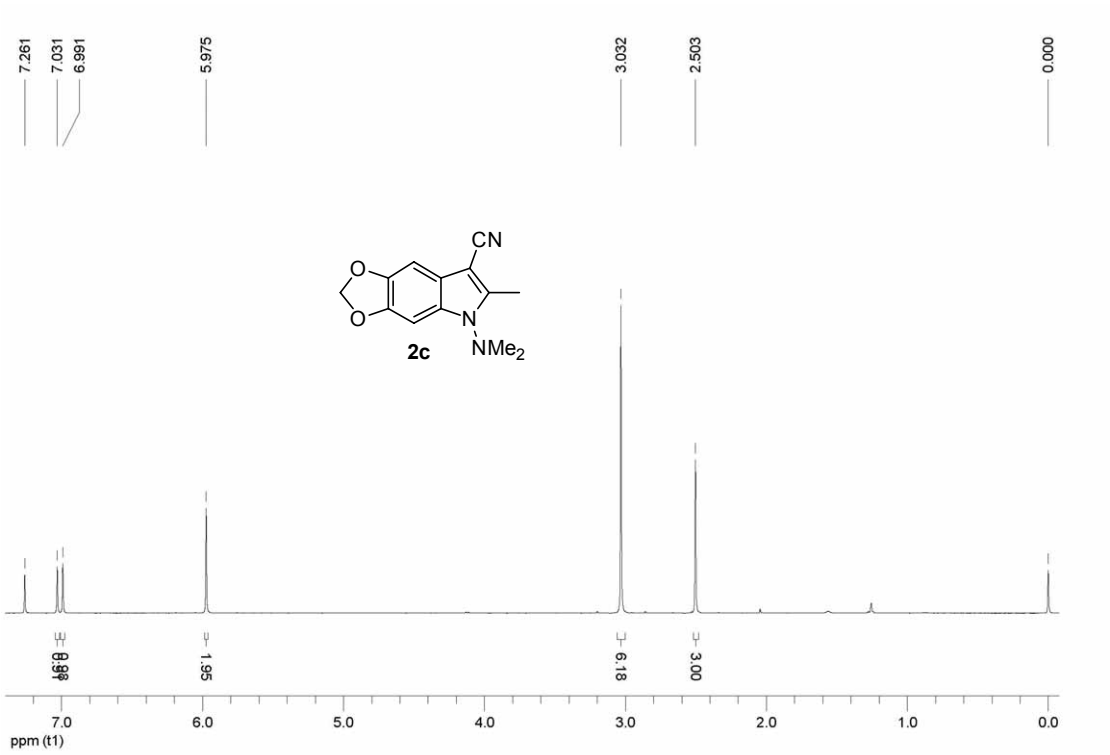
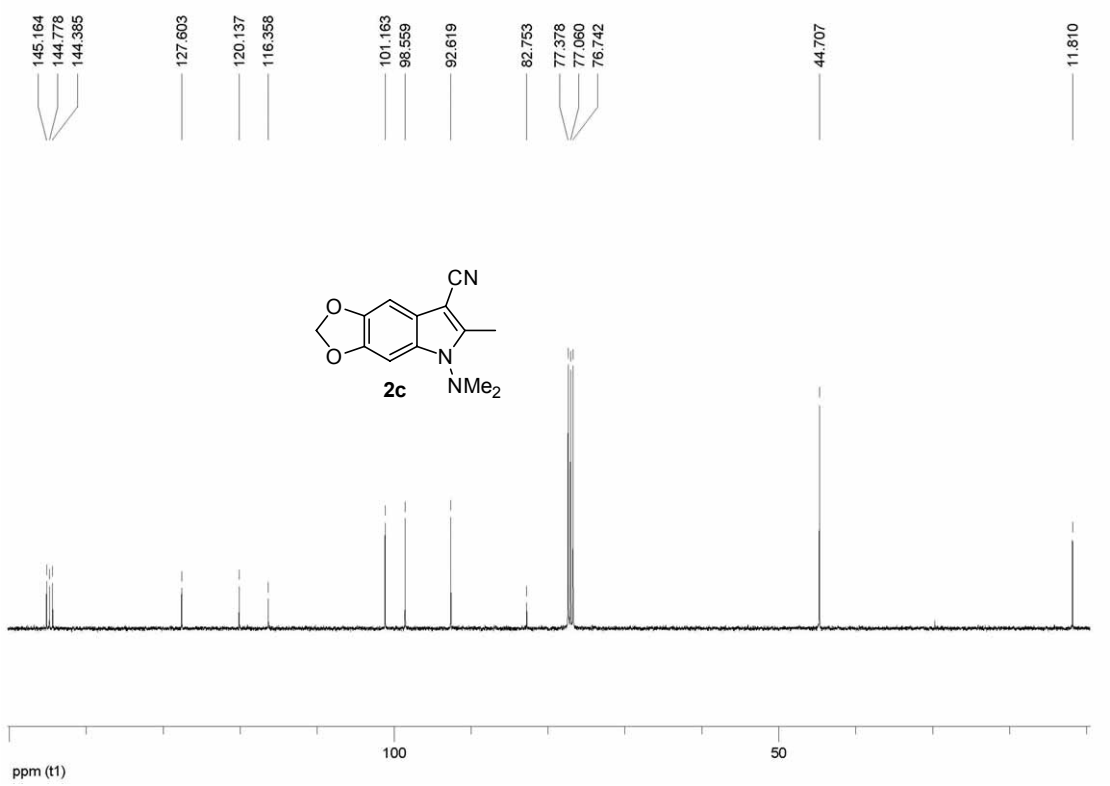
130.942
124.451
122.897
122.608
118.035
109.177
81.784
77.365
77.048
76.731
44.785
18.532
11.608
CN
N
NMe2
2b
150
100
50
ppm (t1)


7.261
7.031
6.991
5.975
3.032
2.503
0.000
CN
O
O
N
NMe2
2c
1.95
6.18
3.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


145.164
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144.385
127.603
120.137
116.358
101.163
98.559
92.619
82.753
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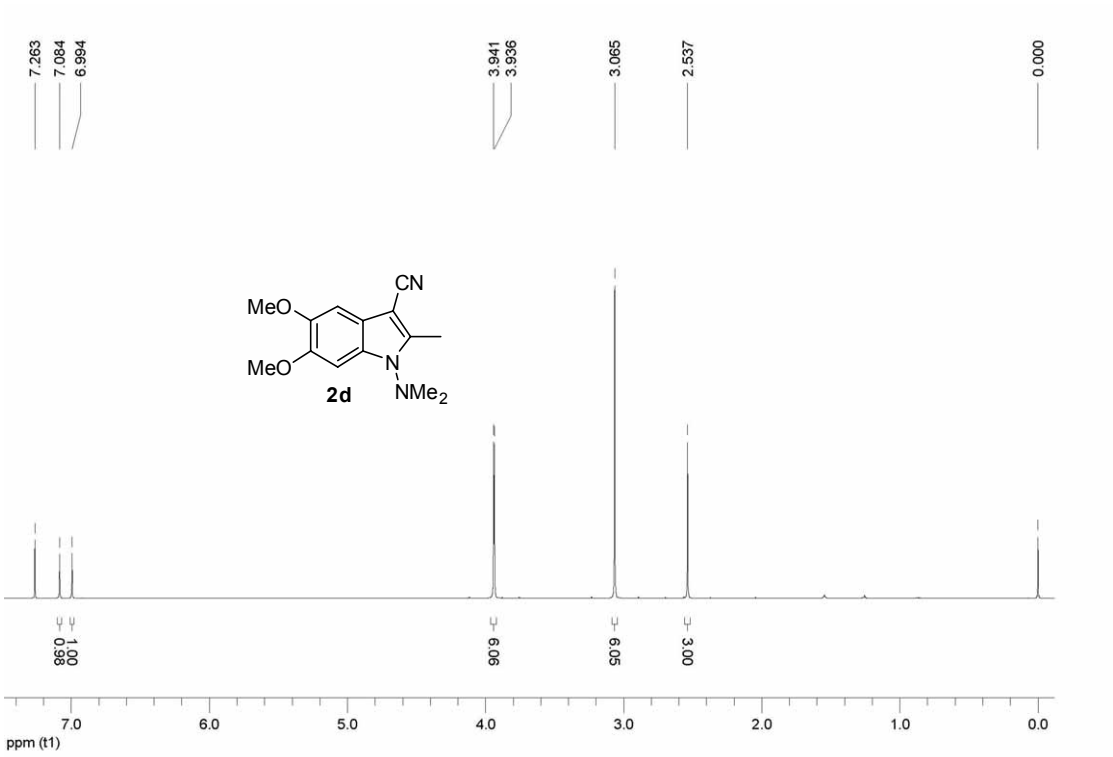
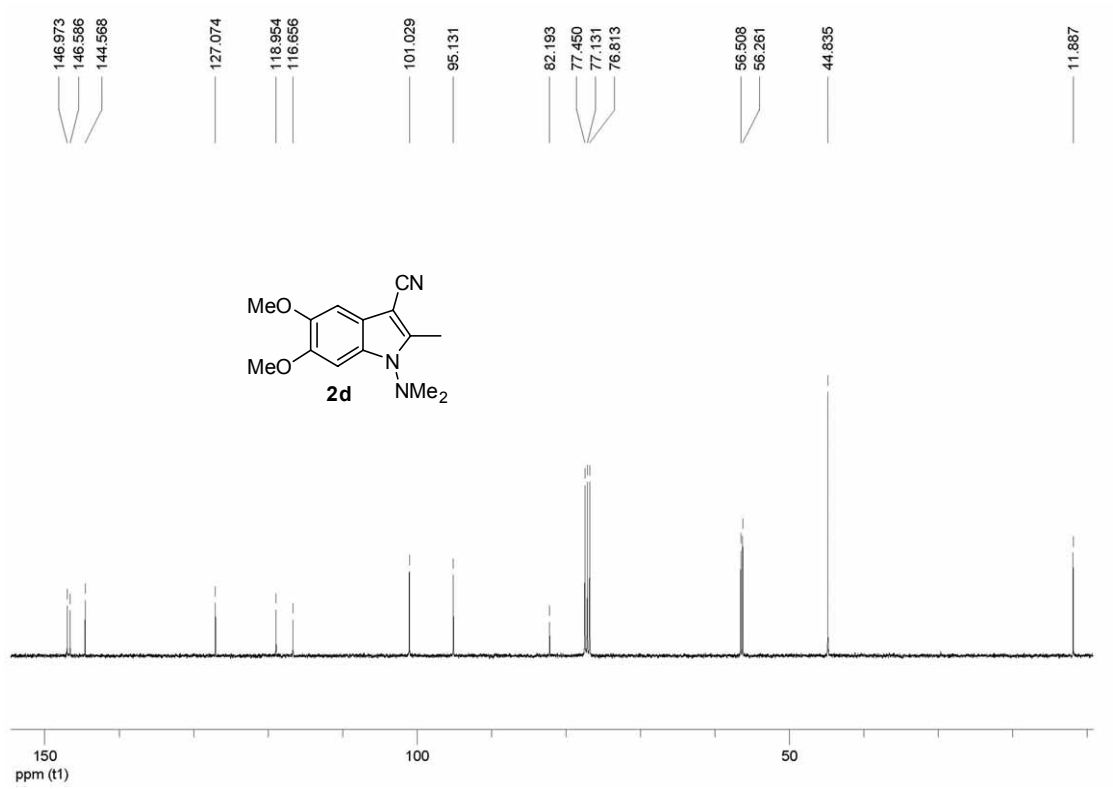
76.742
44.707
11.810
CN
O
O
N
NMe2
2c
100
50
ppm (t1)


7.263
7.084
6.994
3.941
3.936
3.065
2.537
0.000
CN
MeO
MeO
N
NMe2
2d
0.98
1.00
6.06
6.05
3.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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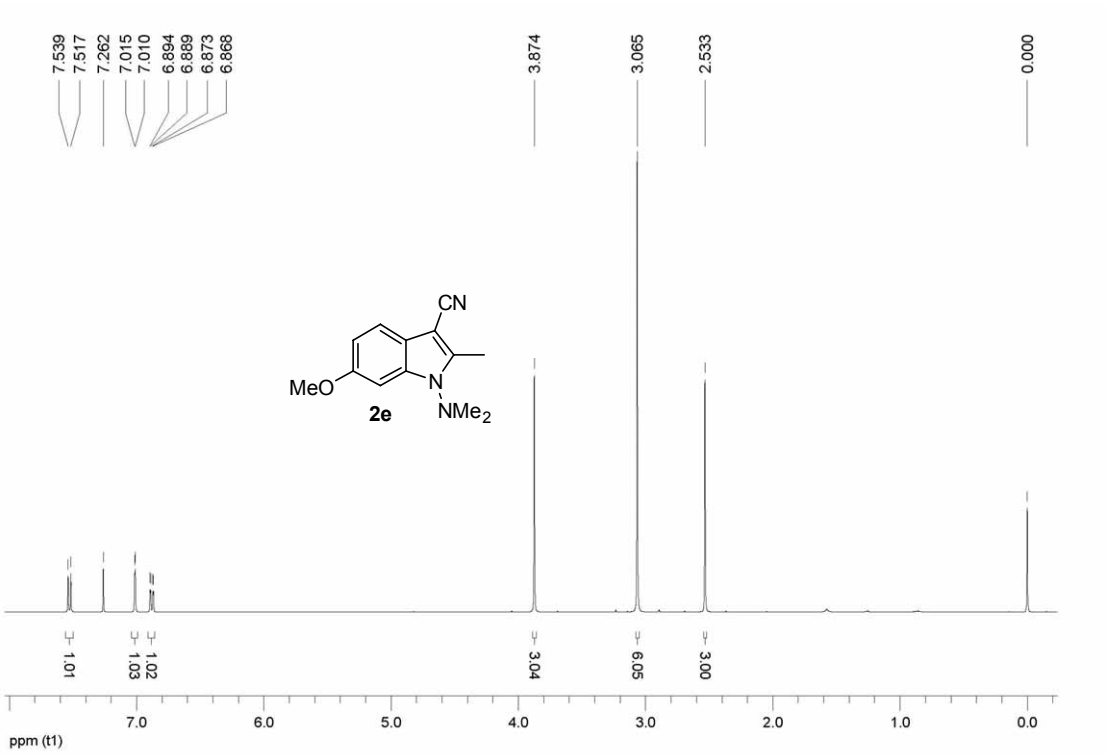
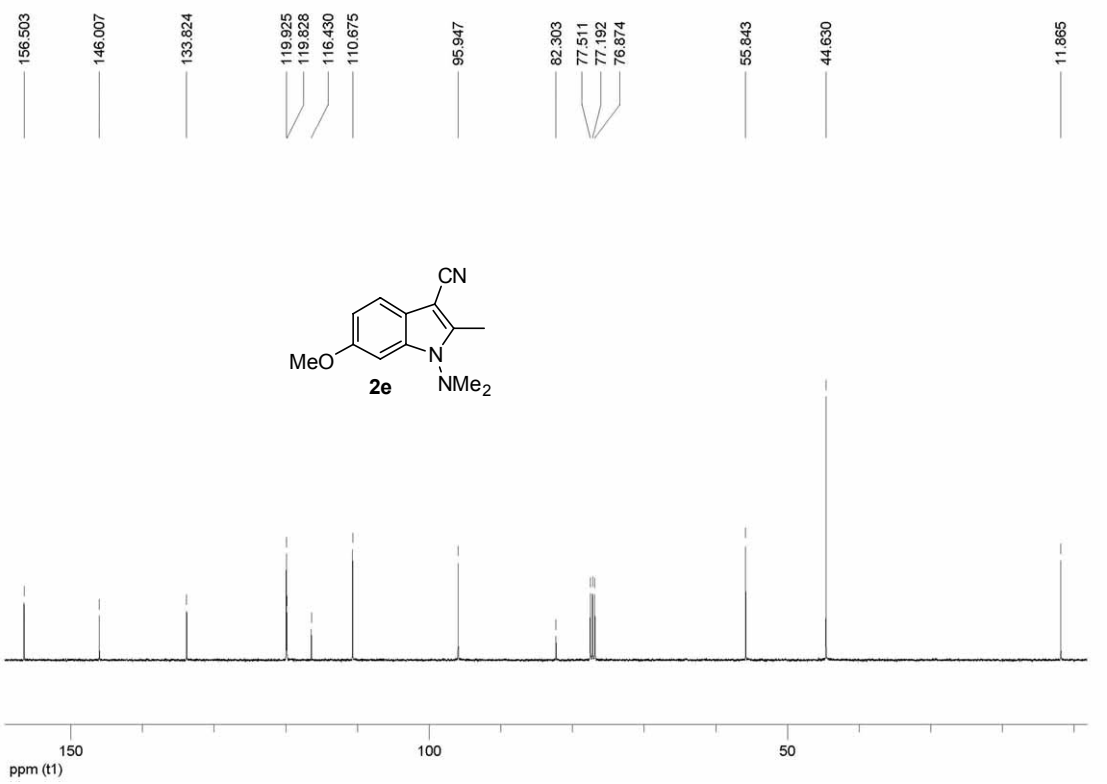
146.586
144.568
127.074
118.954
116.656
101.029
95.131
82.193
77.450
77.131
76.813
56.508
56.261
44.835
11.887
CN
MeO
MeO
N
NMe2
2d
150
100
50
ppm (t1)


7.539
7.517
7.262
7.015
7.010
6.894
6.889
6.873
6.868
3.874
3.065
2.533
0.000
CN
MeO
N
NMe2
2e
1.01
1.03
1.02
3.04
6.05
3.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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119.925
119.828
116.430
110.675
95.947
82.303
77.511
77.192
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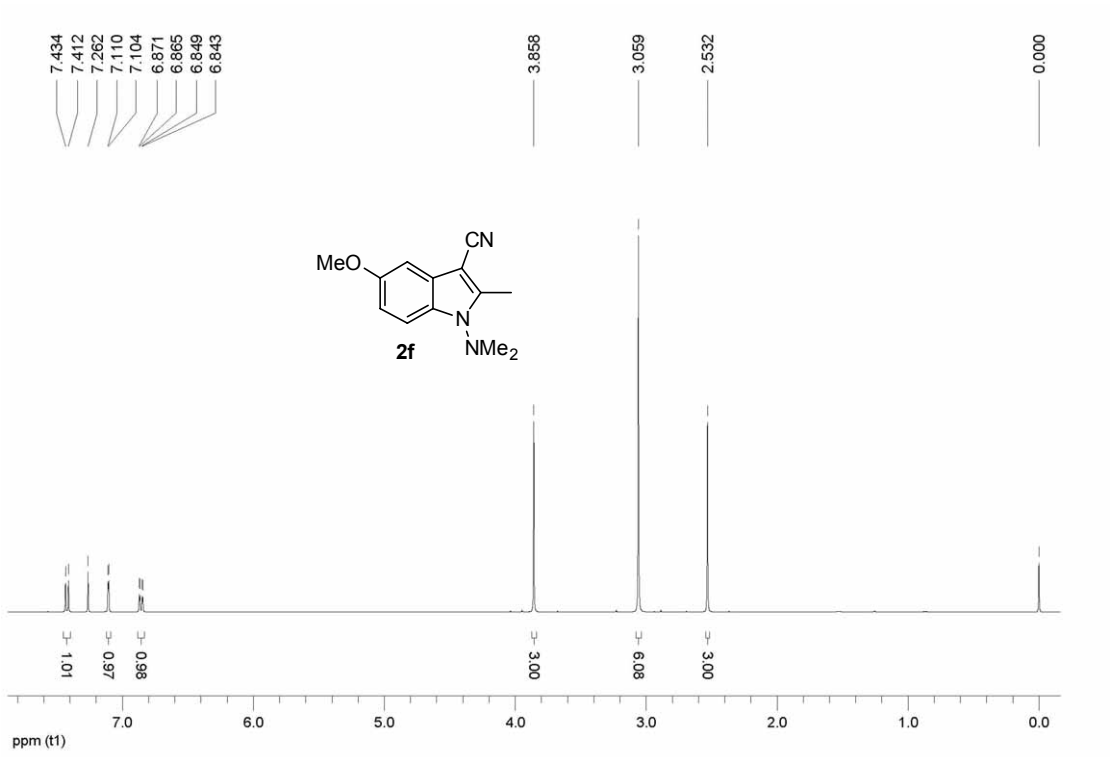
N
NMe2
2e
150
100
50
ppm (t1)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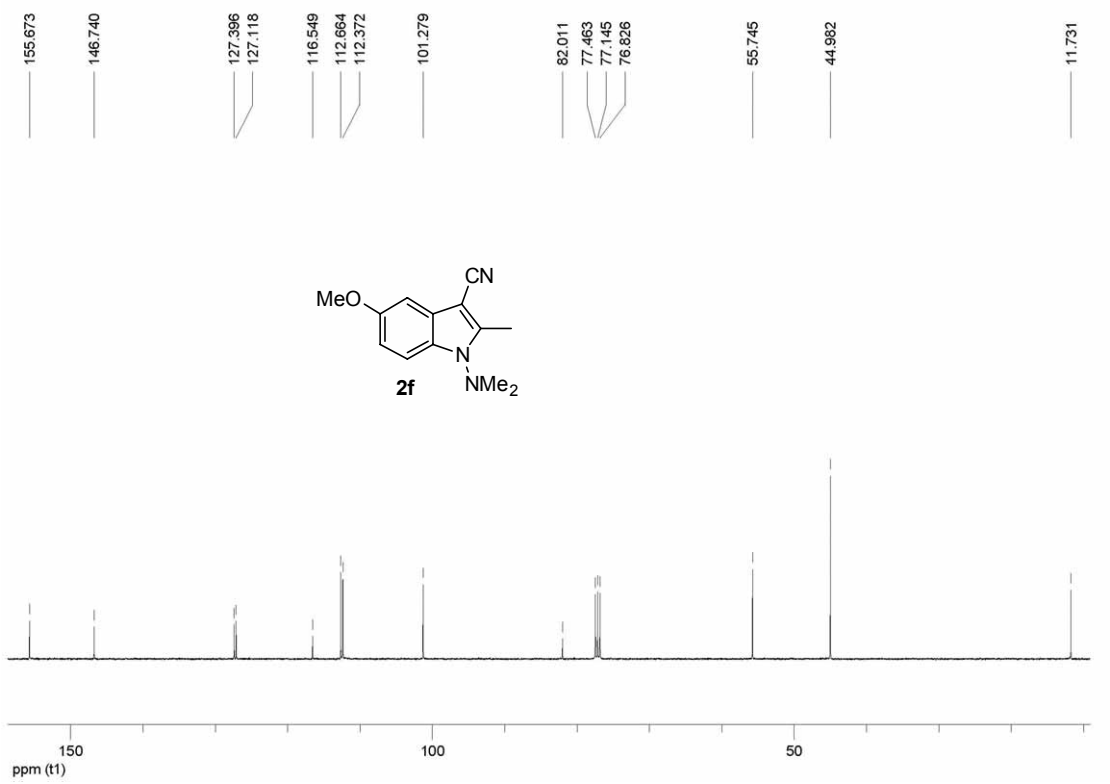
7.412
7.262
7.110
7.104
6.871
6.865
6.849
6.843
3.858
3.059
2.532
0.000
MeO
CN
N
NMe2
2f
1.01
0.97
0.98
3.00
6.08
3.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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127.118
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112.664
112.372
101.279
82.011
77.463
77.145
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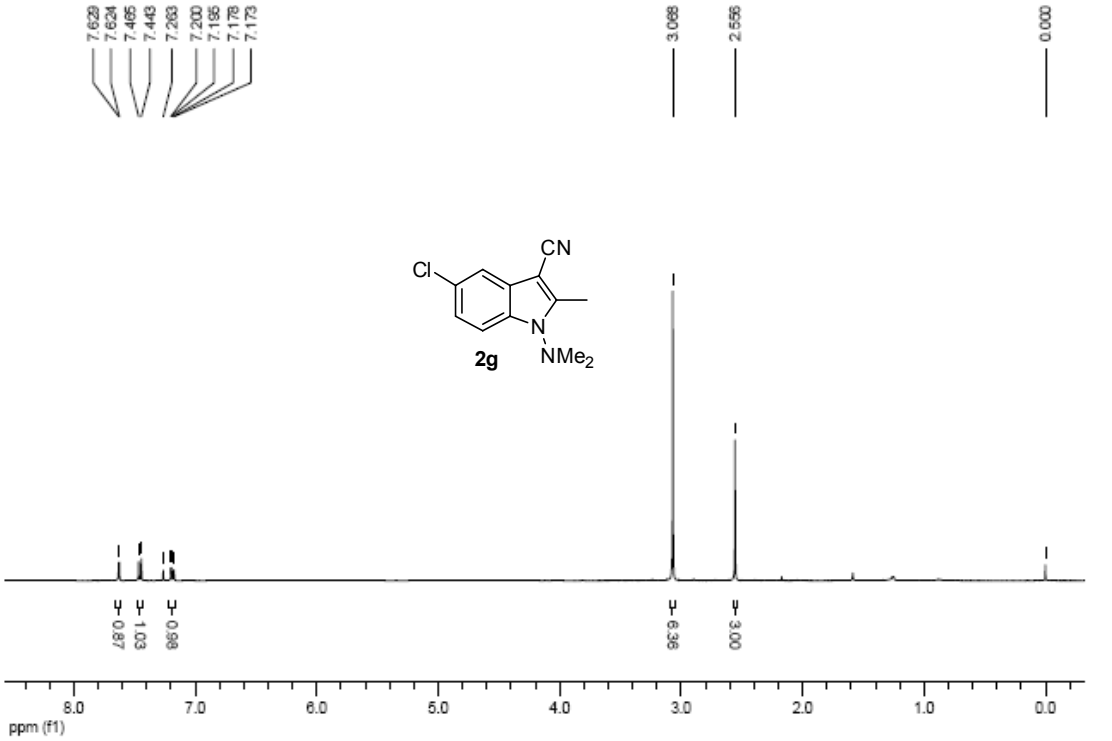
N
NMe2
2f
150
100
50
ppm (t1)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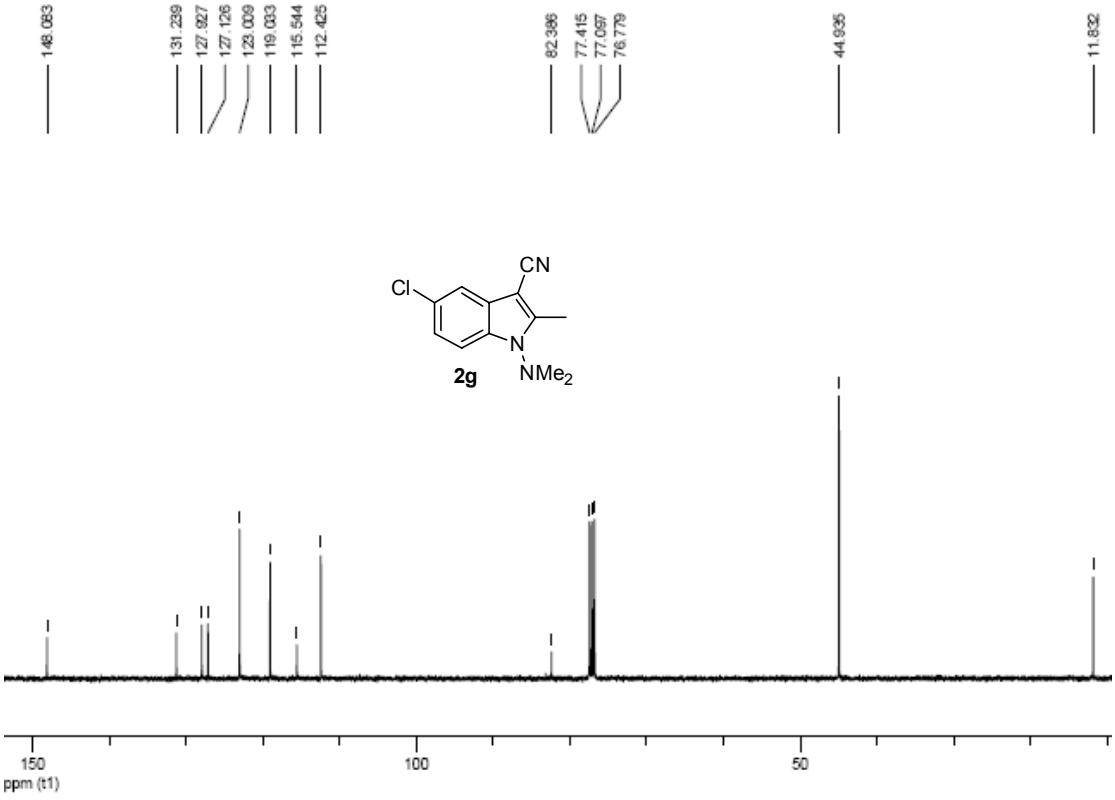
7.624
7.465
7.443
7.263
7.200
7.195
7.178
7.173
3.088
2.556
0.000
Cl
CN
N
NMe2
2g
0.87
1.03
0.98
6.36
3.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)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131.239
127.927
127.126
123.009
119.033
115.544
112.425
82.386
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77.097
76.779
44.935
11.832
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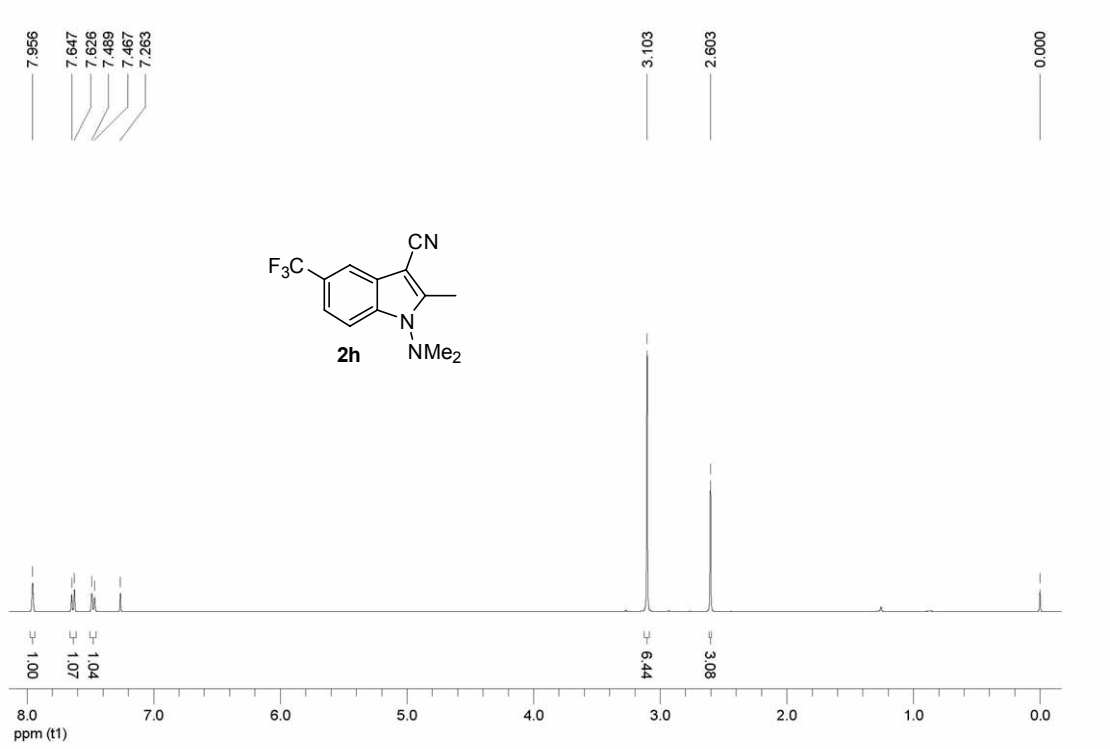
CN
N
NMe2
2g
150
100
50
ppm (t1)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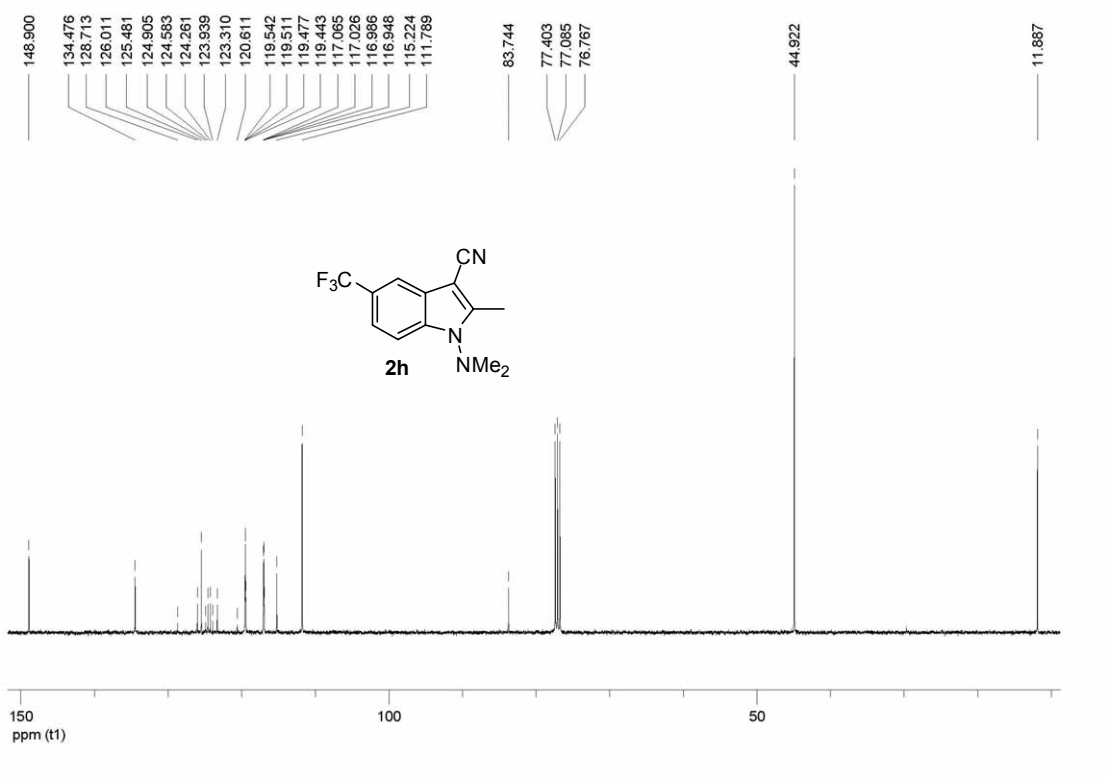
7.647
7.626
7.489
7.467
7.263
3.103
2.603
0.000
CN
F3C
N
NMe2
2h
1.00
1.07
1.04
6.44
3.08
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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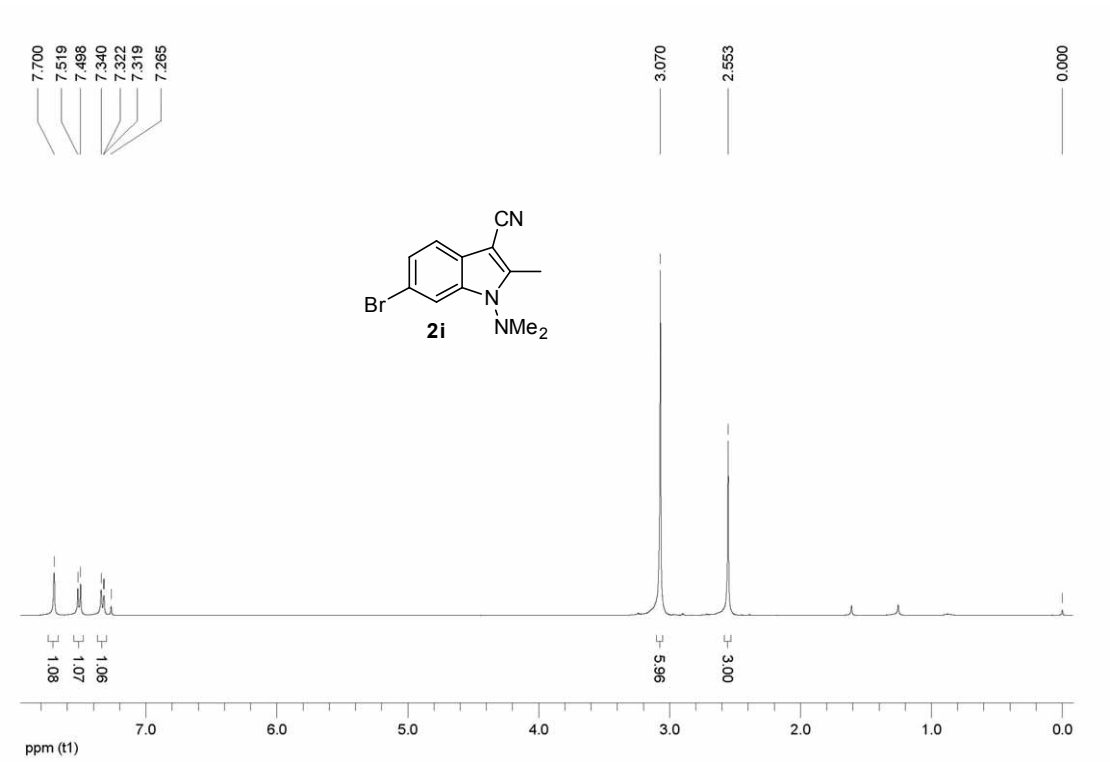
128.713
126.011
125.481
124.905
124.583
124.261
123.939
123.310
120.611
119.542
119.511
119.477
119.443
117.065
117.026
116.986
116.948
115.224
111.789
83.744
77.403
77.085
76.767
44.922
11.887
CN
F3C
N
NMe2
2h
150
100
50
ppm (t1)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7.519
7.498
7.340
7.322
7.319
7.265
3.070
2.553
0.000
CN
Br
N
NMe2
2i
1.08
1.07
1.06
5.96
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7.0
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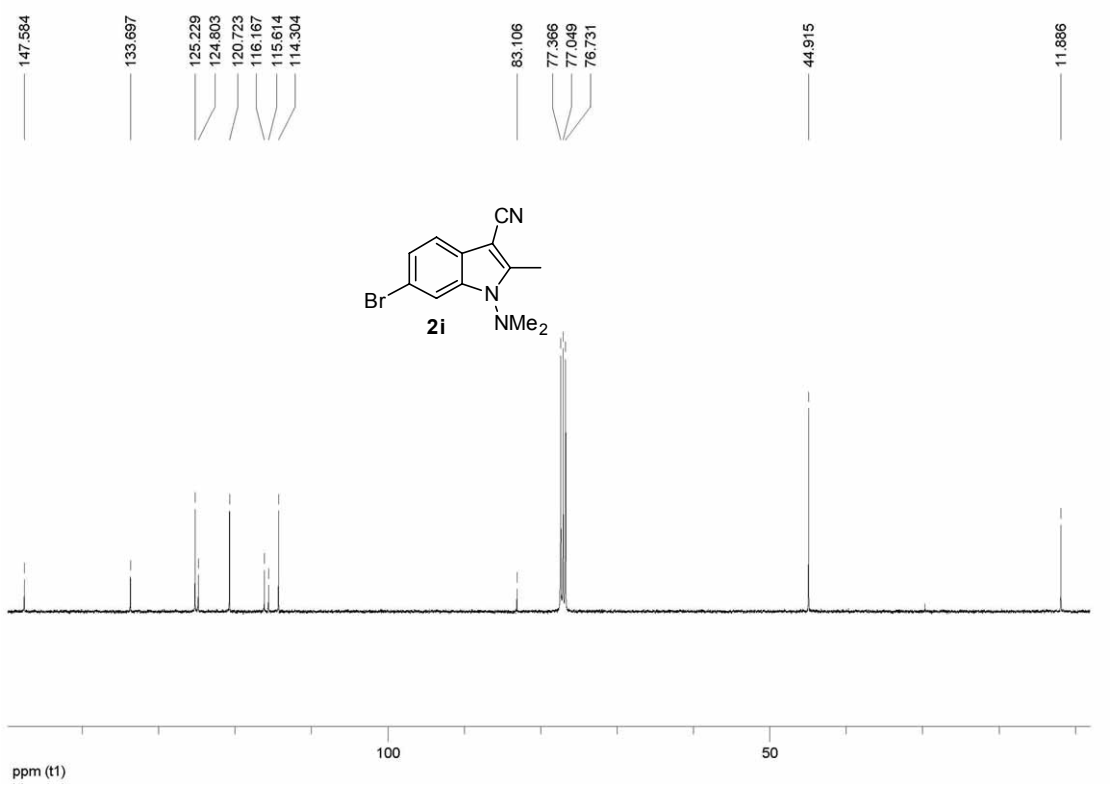
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


147.584
133.697
125.229
124.803
120.723
116.167
115.614
114.304
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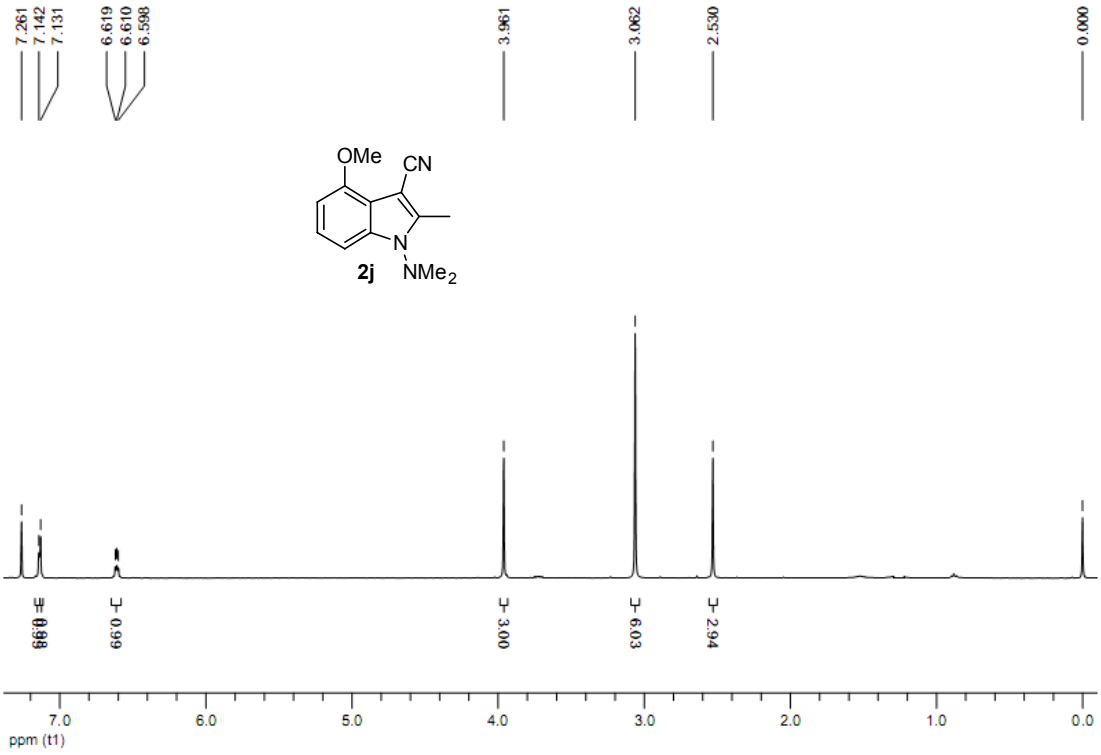
77.049
76.731
44.915
11.886
CN
Br
N
NMe2
2i
100
50
ppm (t1)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7.142
7.131
6.619
6.610
6.598
3.961
3.062
2.530
0.000
OMe
CN
N
NMe2
2j
0.99
3.00
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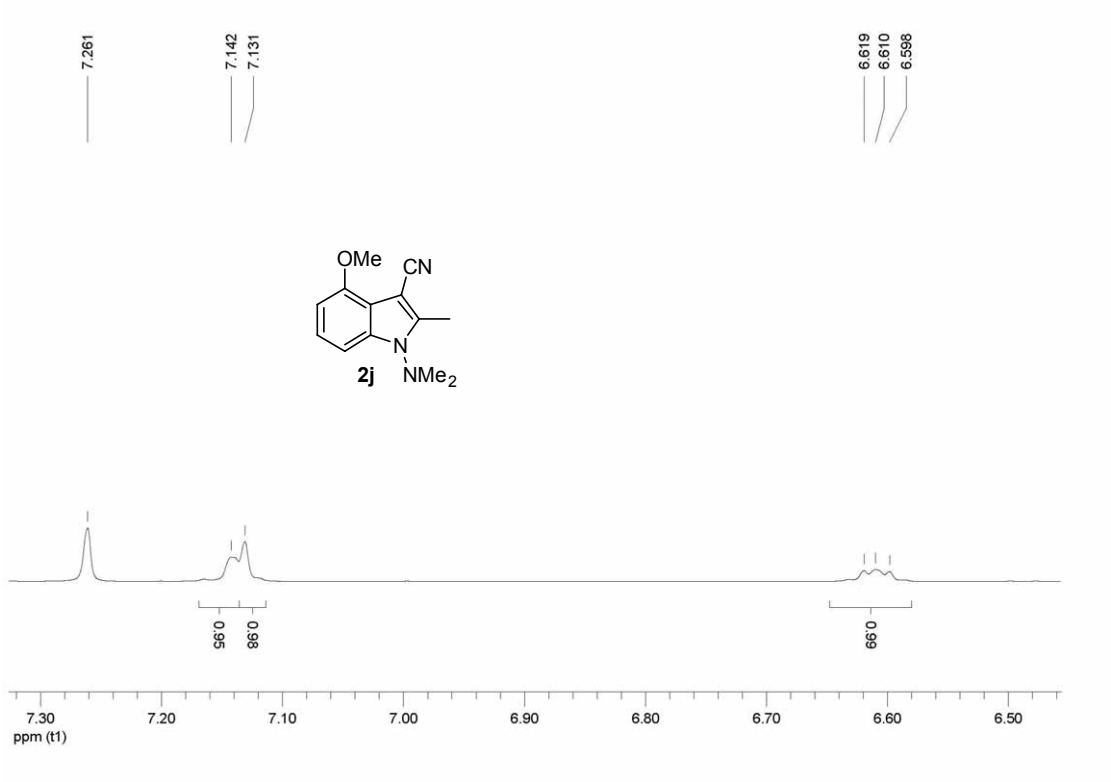
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


7.261
7.142
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6.619
6.610
6.598
OMe
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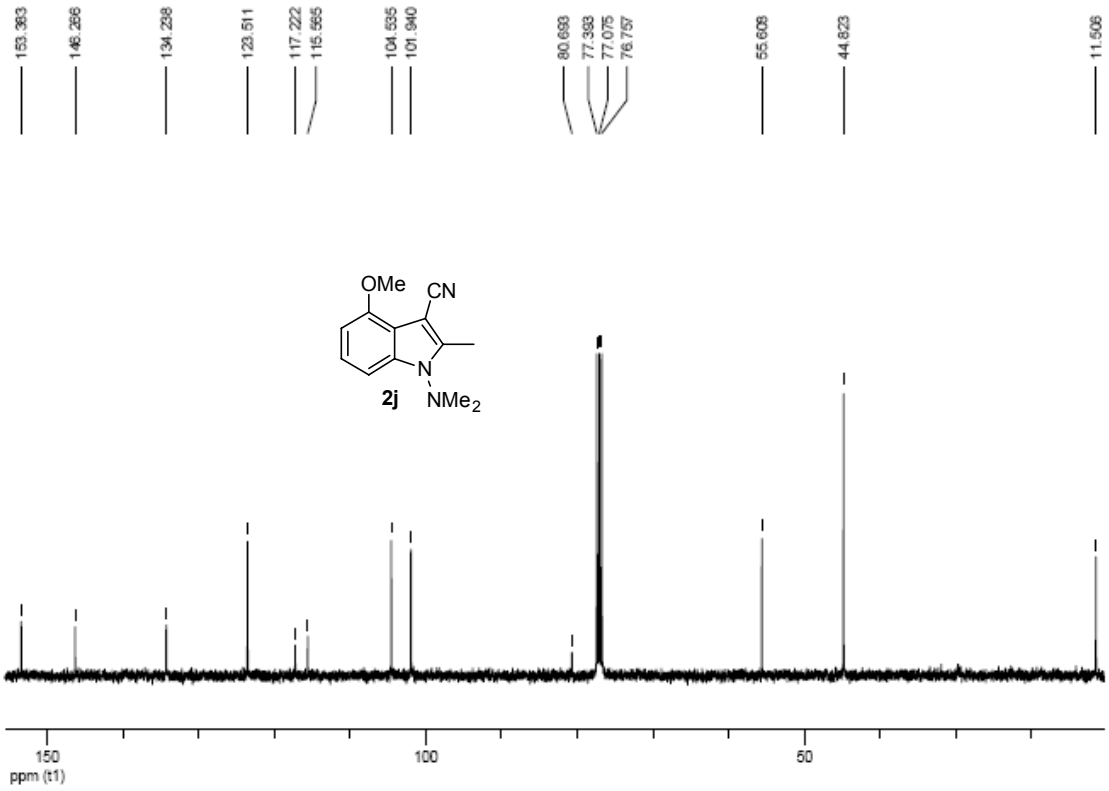
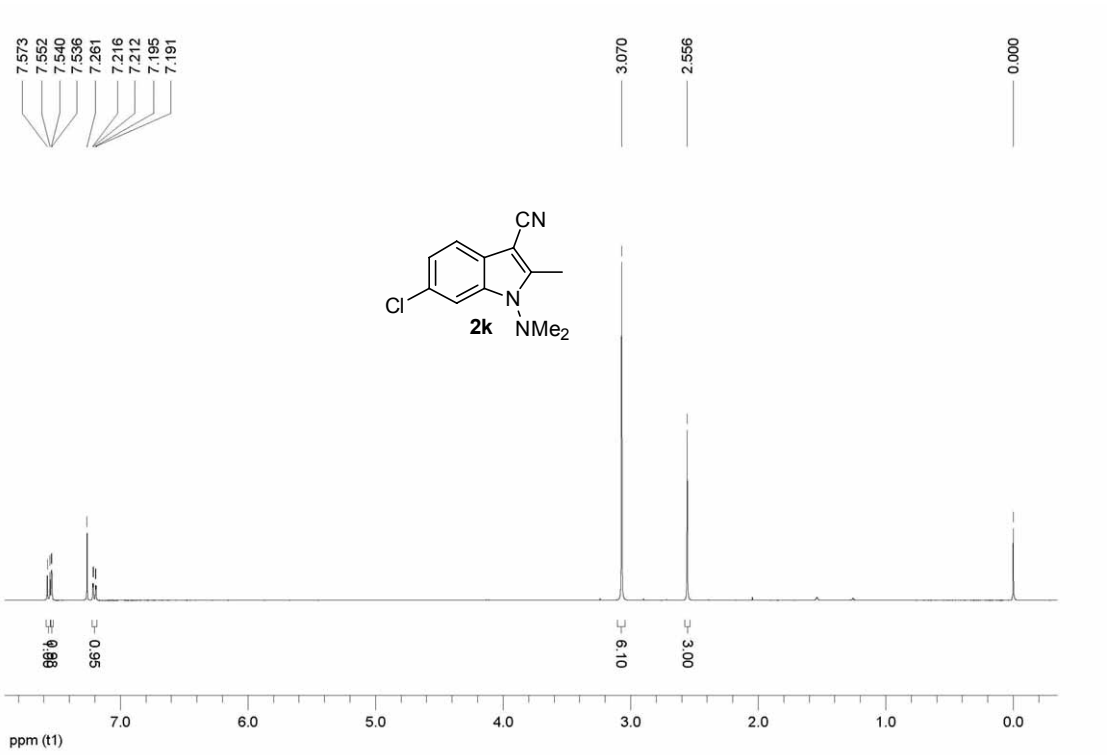
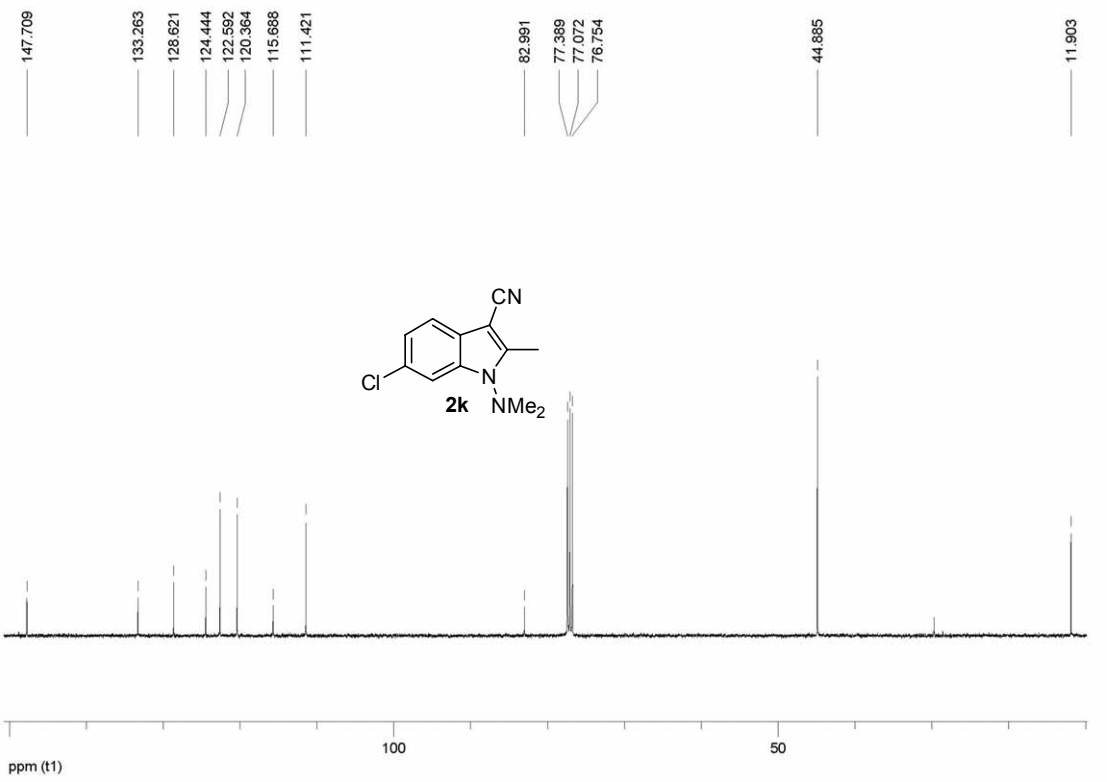
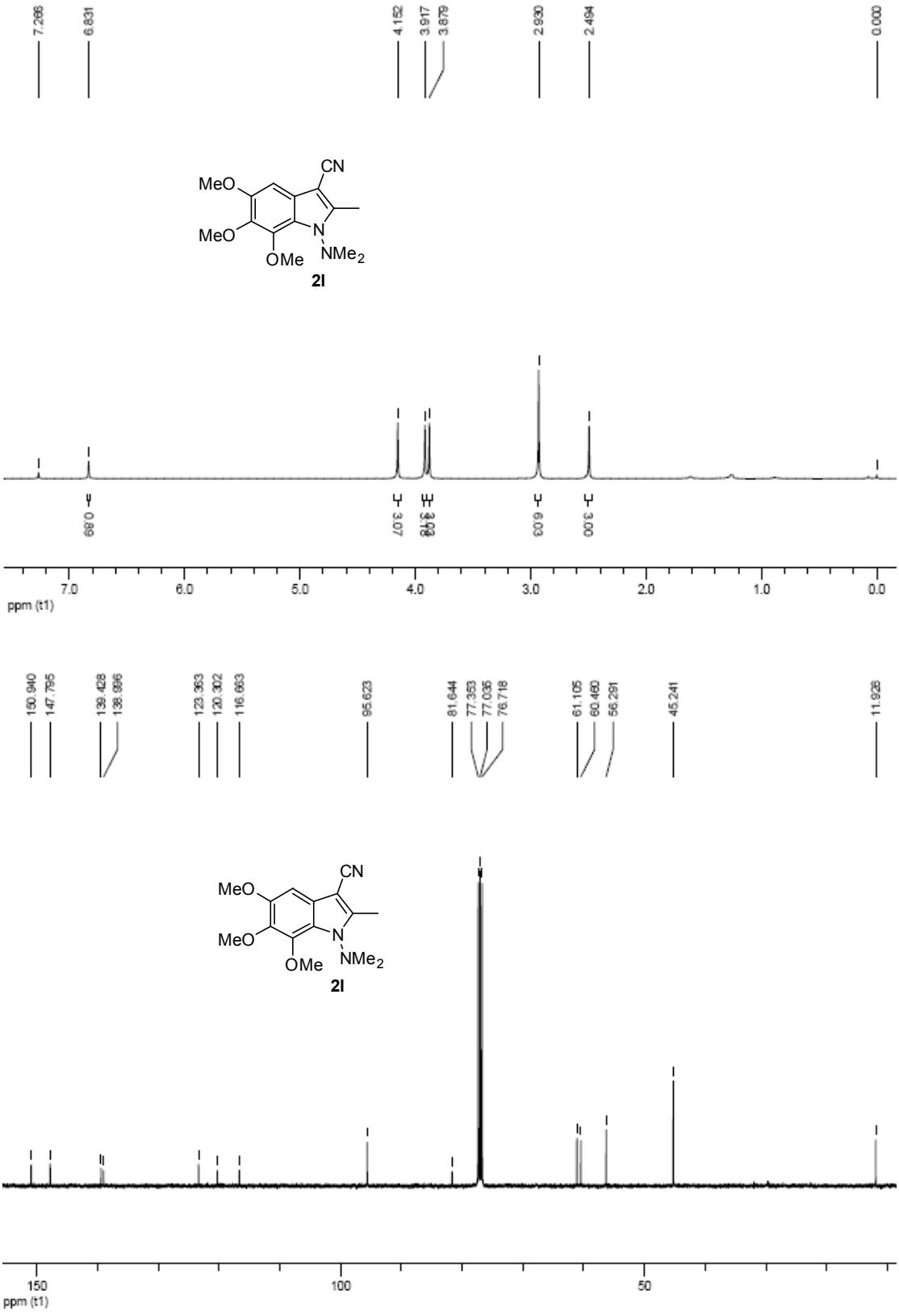
NMe2
2j
0.95
0.98
0.99
7.30
7.20
7.10
7.00
6.90
6.80
6.70
6.60
6.50
ppm (t1)


153.383
146.266
134.298
123.511
117.222
115.565
104.535
101.940
80.693
77.393
77.075
76.757
55.608
44.823
11.506
OMe
CN
N
NMe2
2j
150
100
50
ppm (t1)


7.573
7.552
7.540
7.536
7.261
7.216
7.212
7.195
7.191
3.070
2.556
0.000
CN
Cl
N
NMe2
2k
0.95
6.10
3.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


147.709
133.263
128.621
124.444
122.592
120.364
115.688
111.421
82.991
77.389
77.072
76.754
44.885
11.903
CN
Cl
N
NMe2
2k
100
50
ppm (t1)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6.831
4.152
3.917
3.879
2.930
2.494
0.000
CN
MeO
MeO
OMe
N
NMe2
2l
0.89
3.07
3.08
6.03
3.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
150.940
147.795
139.428
138.996
123.363
120.302
116.663
95.623
81.644
77.353
77.035
76.718
61.105
60.460
56.291
45.241
11.926
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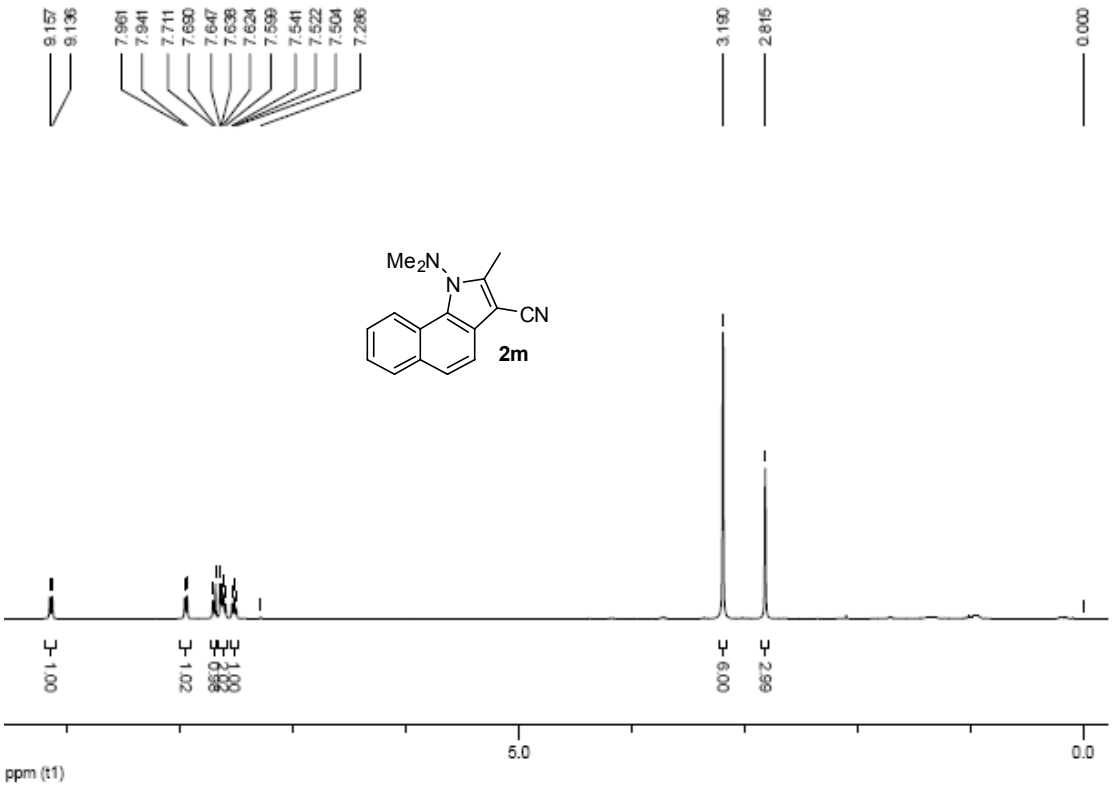
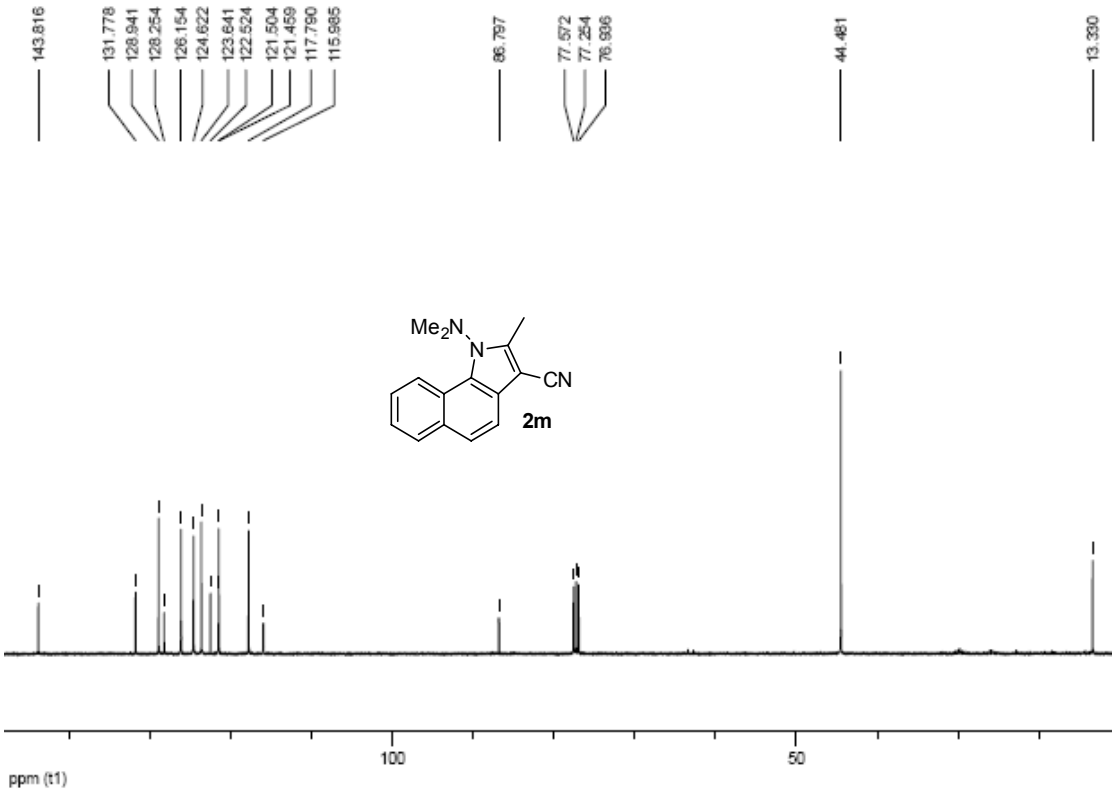
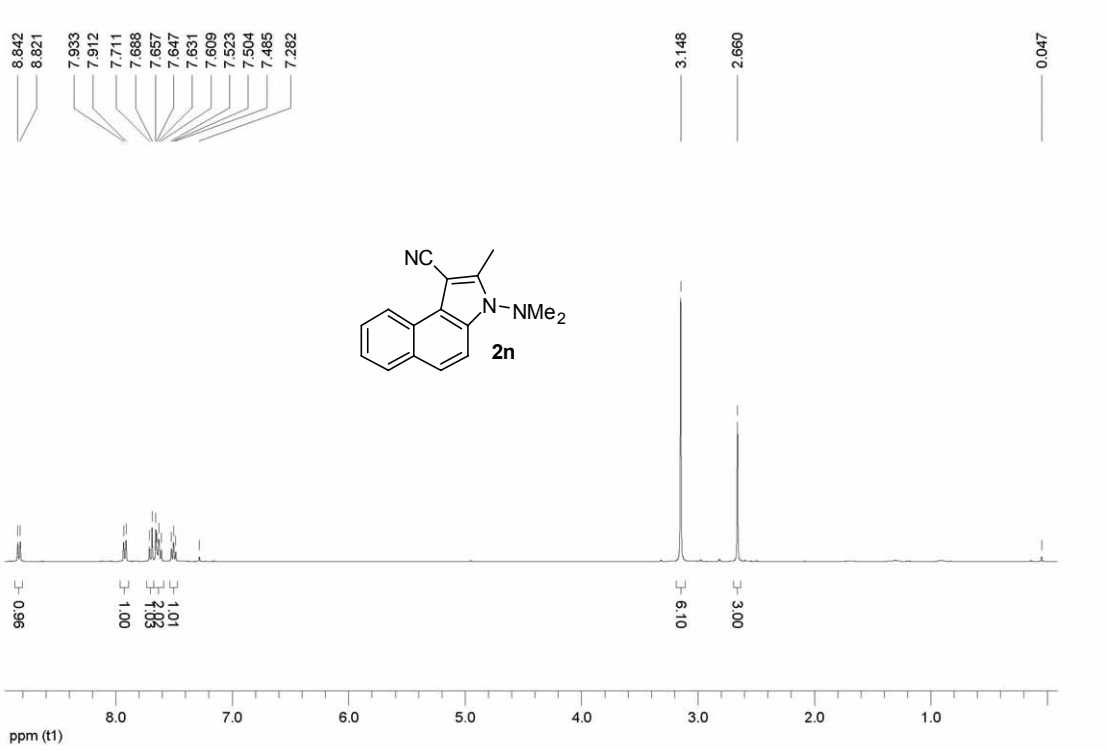
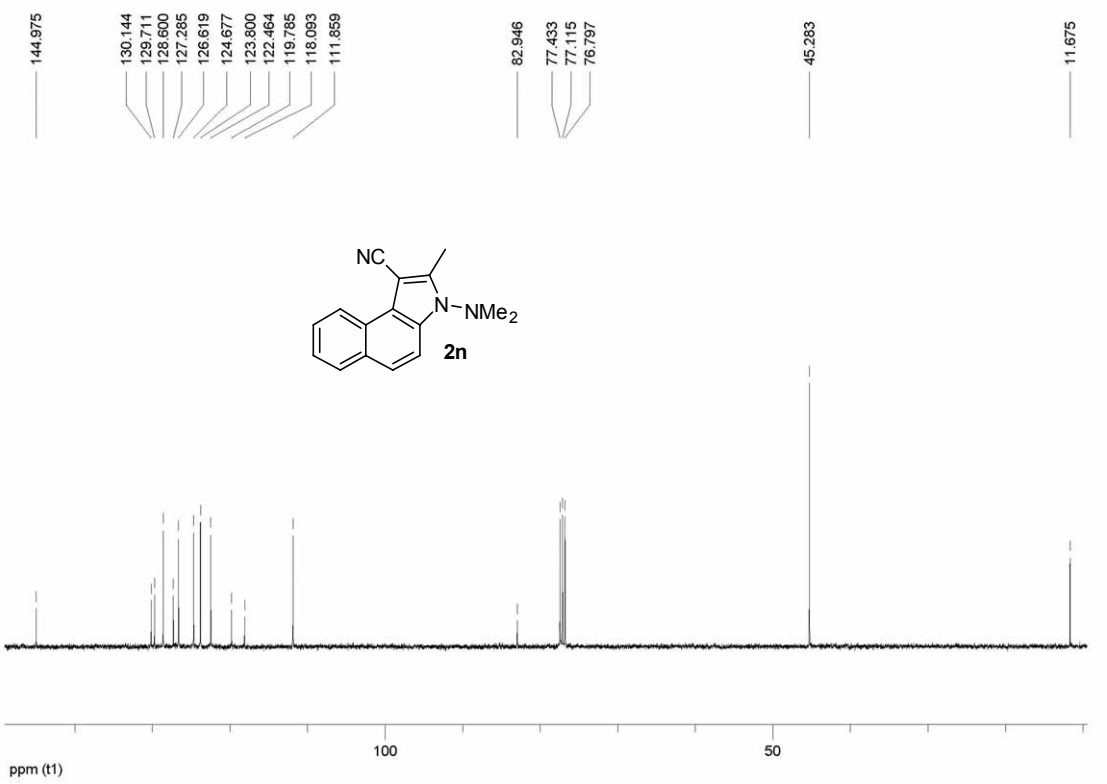
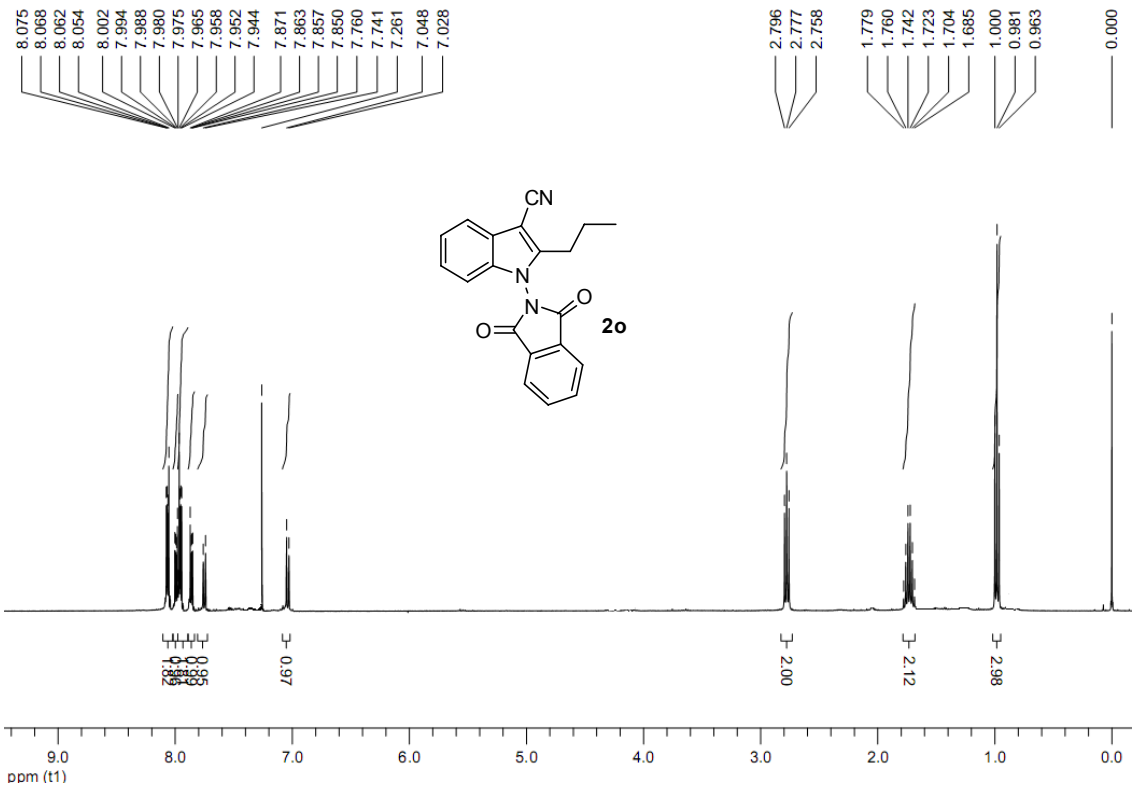
MeO
OMe
N
NMe2
2l
150
100
50
ppm (t1)

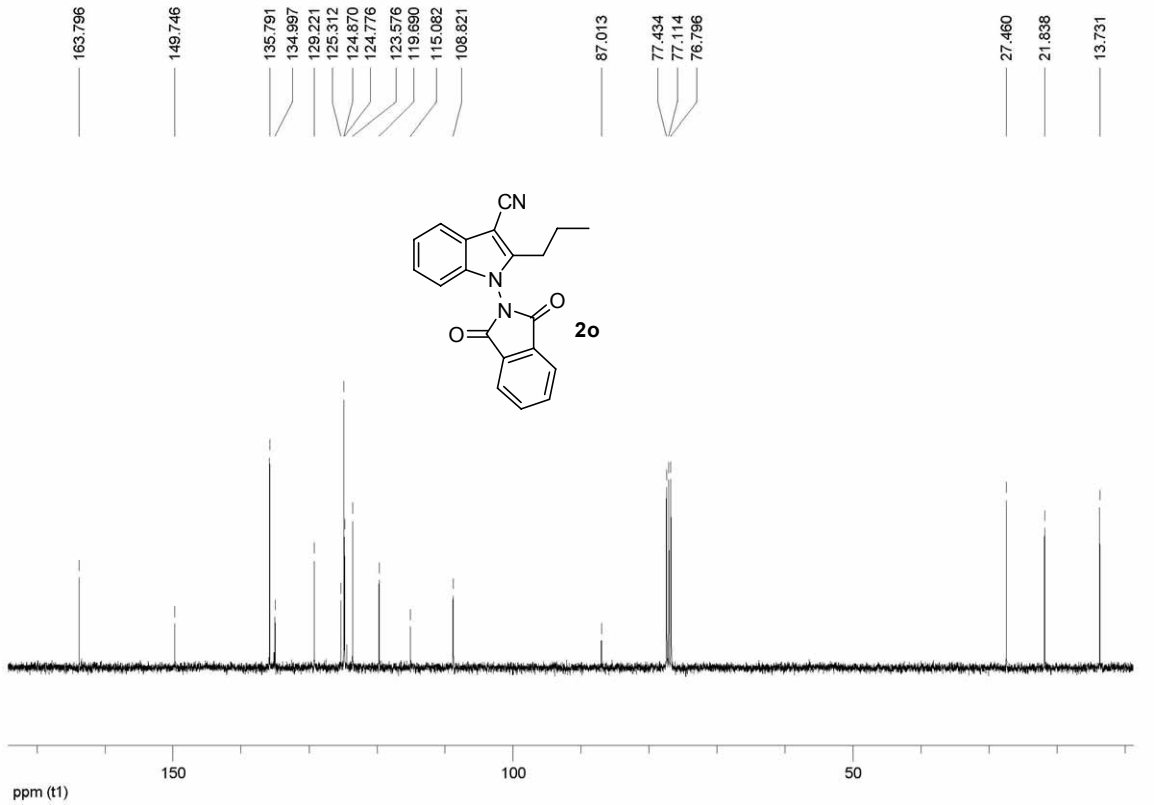

9.157
9.136
7.961
7.941
7.711
7.690
7.647
7.638
7.624
7.599
7.541
7.522
7.504
7.286
3.190
2.815
0.000
Me2N
N
CN
2m
1.00
1.02
6.00
2.99
5.0
0.0
ppm (t1)

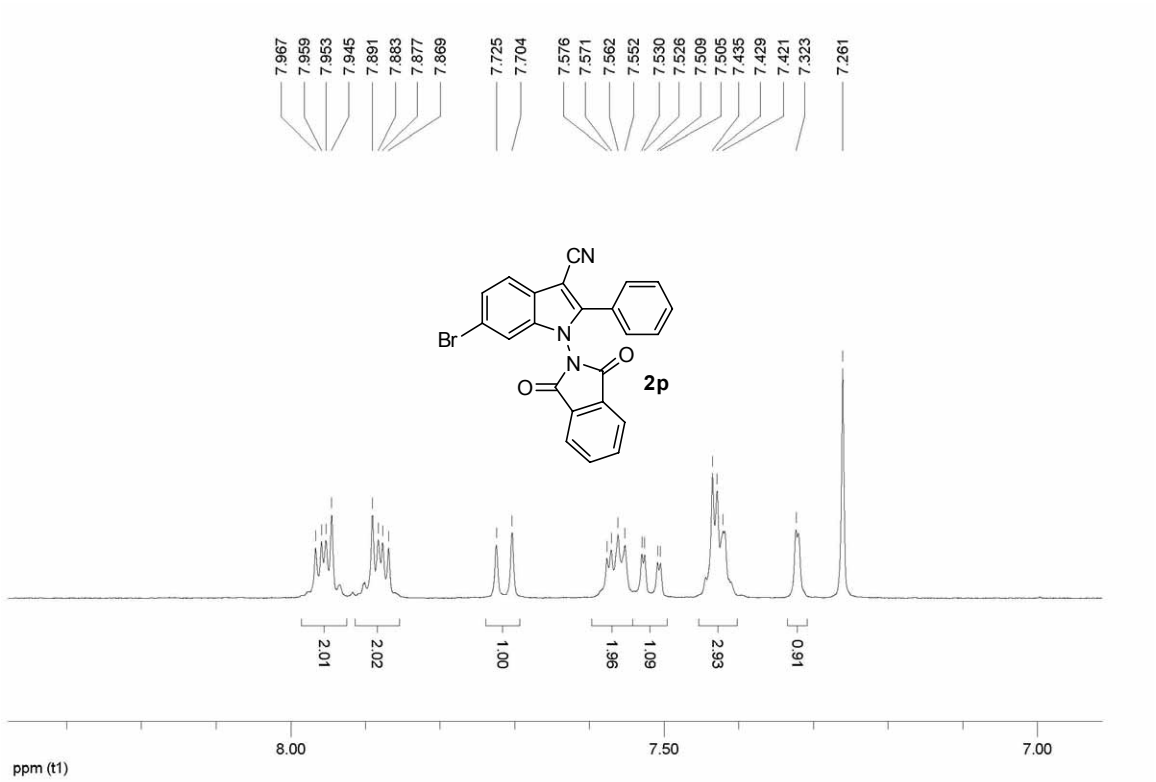

143.816
131.778
128.941
128.254
126.154
124.622
123.641
122.524
121.504
121.459
117.790
115.885
86.797
77.572
77.254
76.936
44.481
13.390
Me2N
N
CN
2m
100
50
ppm (t1)

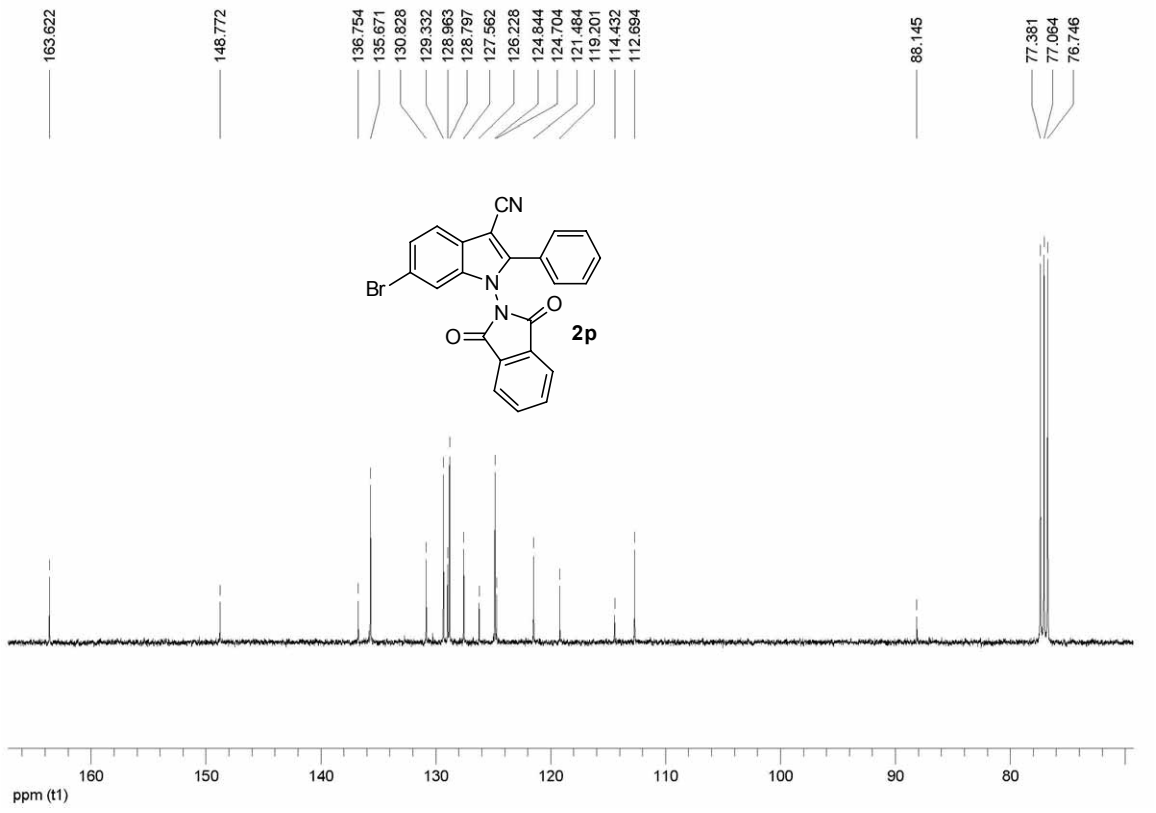

8.842
8.821
7.933
7.912
7.711
7.688
7.657
7.647
7.631
7.609
7.523
7.504
7.485
7.282
3.148
2.660
0.047
NC
N
NMe2
2n
0.96
1.00
1.01
6.10
3.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)

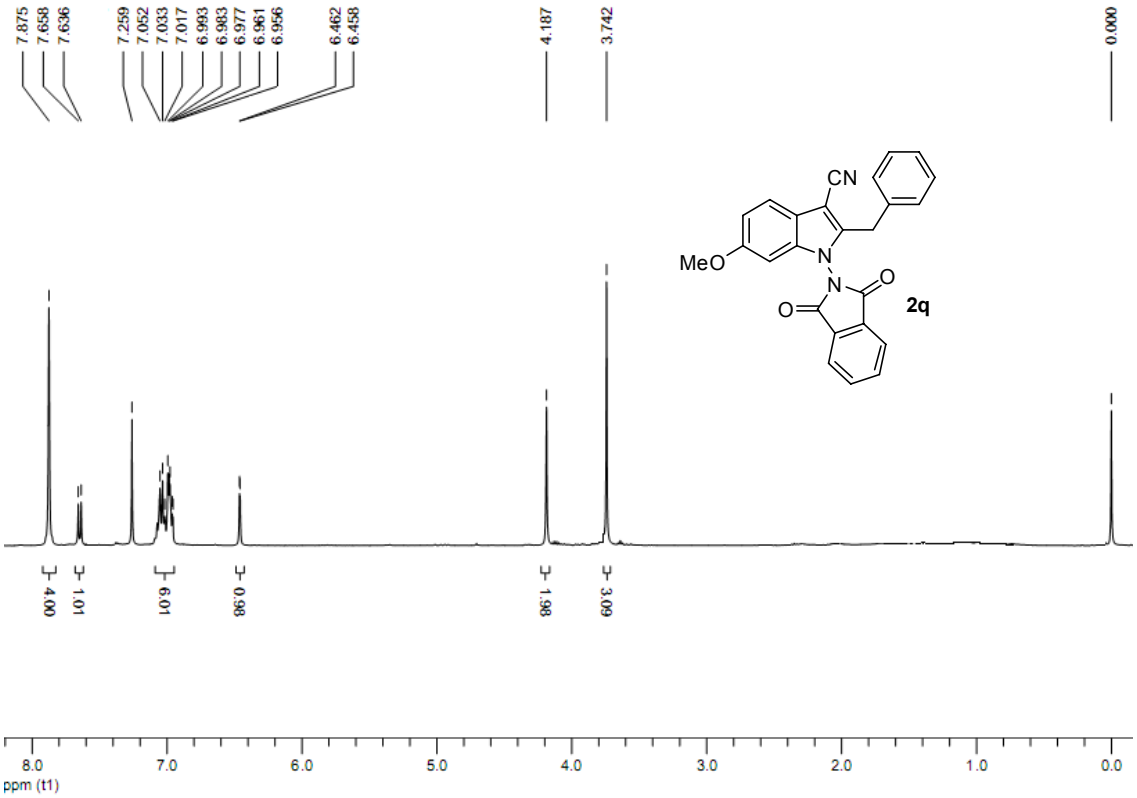

144.975
130.144
129.711
128.600
127.285
126.619
124.677
123.800
122.464
119.785
118.093
111.859
82.946
77.433
77.115
76.797
45.283
11.675
NC
N
NMe2
2n
100
50
ppm (t1)

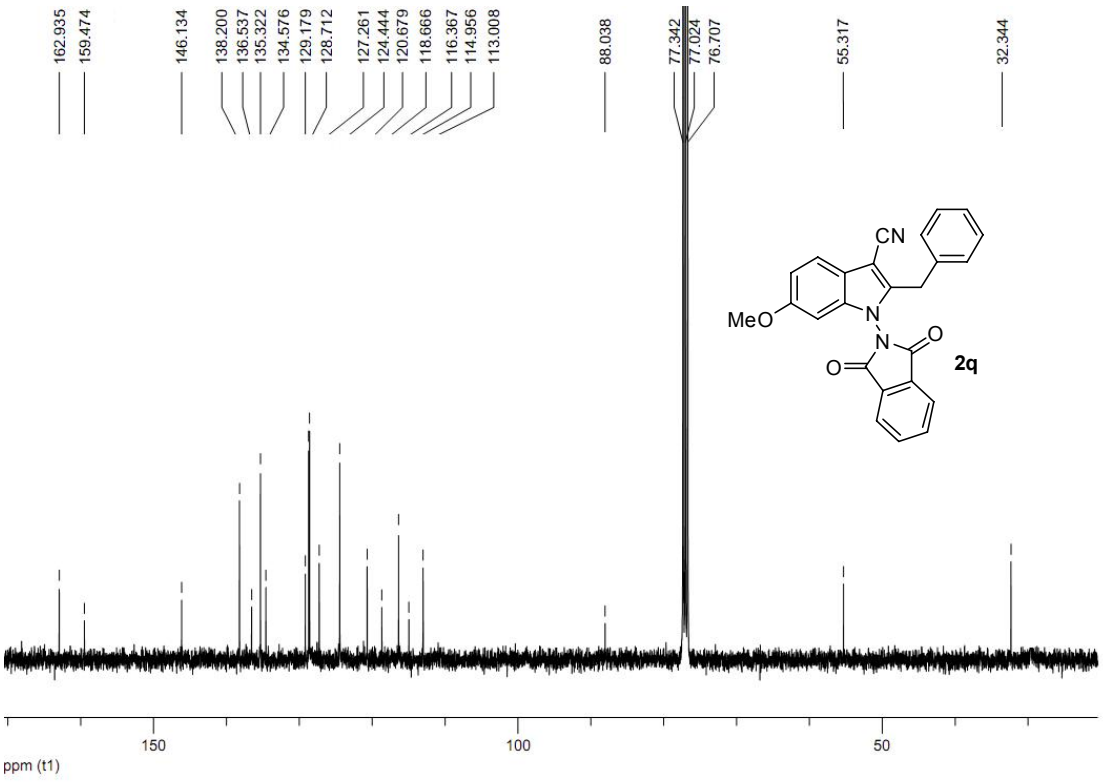

8.075
8.068
8.062
8.054
8.002
7.994
7.988
7.980
7.975
7.965
7.958
7.952
7.944
7.871
7.863
7.857
7.850
7.760
7.741
7.261
7.048
7.028
2.796
2.777
2.758
1.779
1.760
1.742
1.723
1.704
1.685
1.000
0.981
0.963
0.000
CN
N
N
O
O
2o
0.97
2.00
2.12
2.98
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

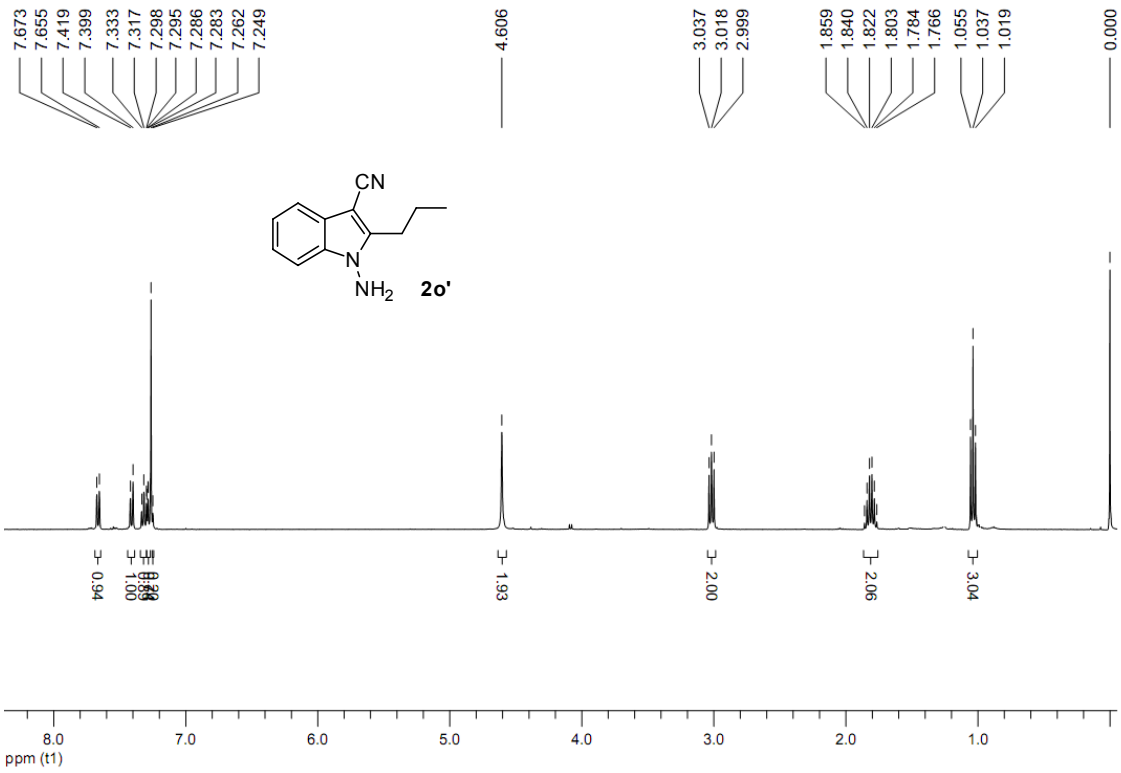

163.796
149.746
135.791
134.997
129.221
125.312
124.870
124.776
123.576
119.690
115.082
108.821
87.013
77.434
77.114
76.796
27.460
21.838
13.731
CN
N
N
O
O
2o
150
100
50
ppm (t1)


7.967
7.959
7.953
7.945
7.891
7.883
7.877
7.869
7.725
7.704
7.576
7.571
7.562
7.552
7.530
7.526
7.509
7.505
7.435
7.429
7.421
7.323
7.261
CN
Br
N
N
O
O
2p
2.01
2.02
1.00
1.96
1.09
2.83
0.91
8.00
7.50
7.00
ppm (t1)


163.622
148.772
136.754
135.671
130.828
129.332
128.963
128.797
127.562
126.228
124.844
124.704
121.484
119.201
114.432
112.694
88.145
77.381
77.064
76.746
CN
Br
N
N
O
O
2p
160
150
140
130
120
110
100
90
80
ppm (t1)


7.875
7.658
7.636
7.259
7.052
7.033
7.017
6.993
6.983
6.977
6.961
6.956
6.462
6.458
4.187
3.742
0.000
CN
MeO
N
N
O
O
2q
4.00
1.01
6.01
0.98
1.98
3.09
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


162.935
159.474
146.134
138.200
136.537
135.322
134.576
129.179
128.712
127.261
124.444
120.679
118.666
116.367
114.956
113.008
88.038
77.342
77.024
76.707
55.317
32.344
CN
MeO
N
N
O
O
2q
150
100
50
ppm (t1)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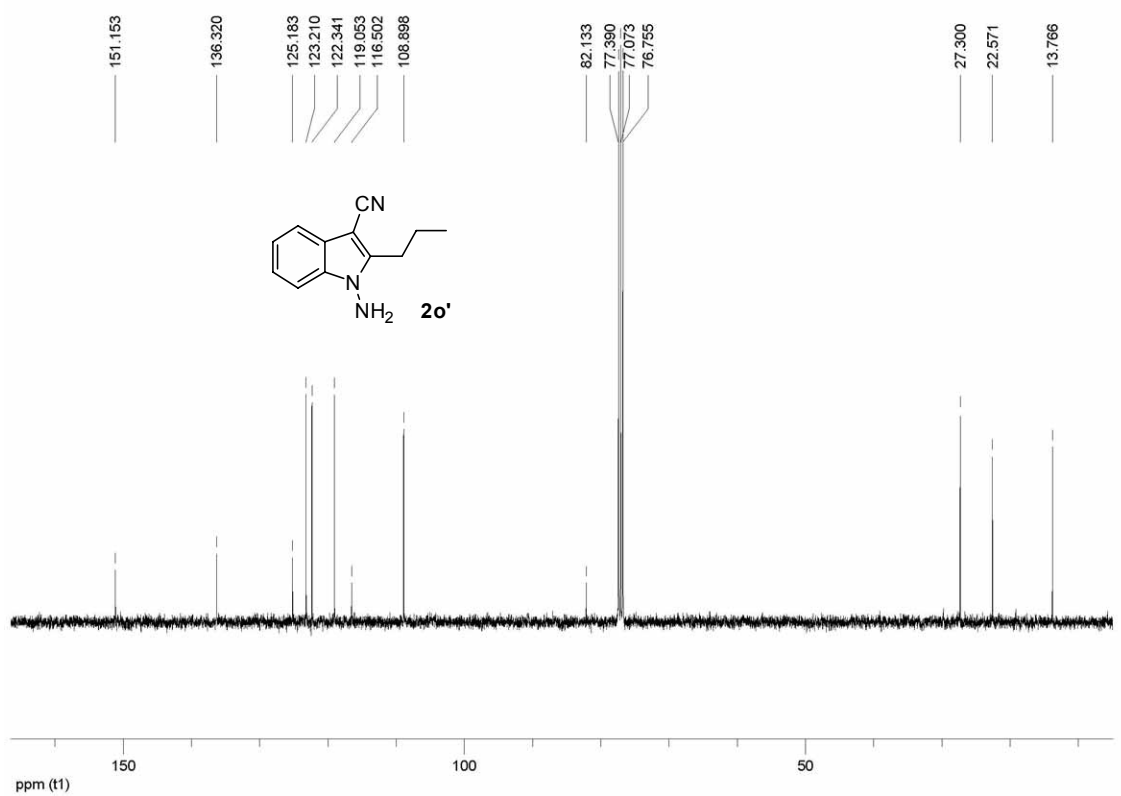
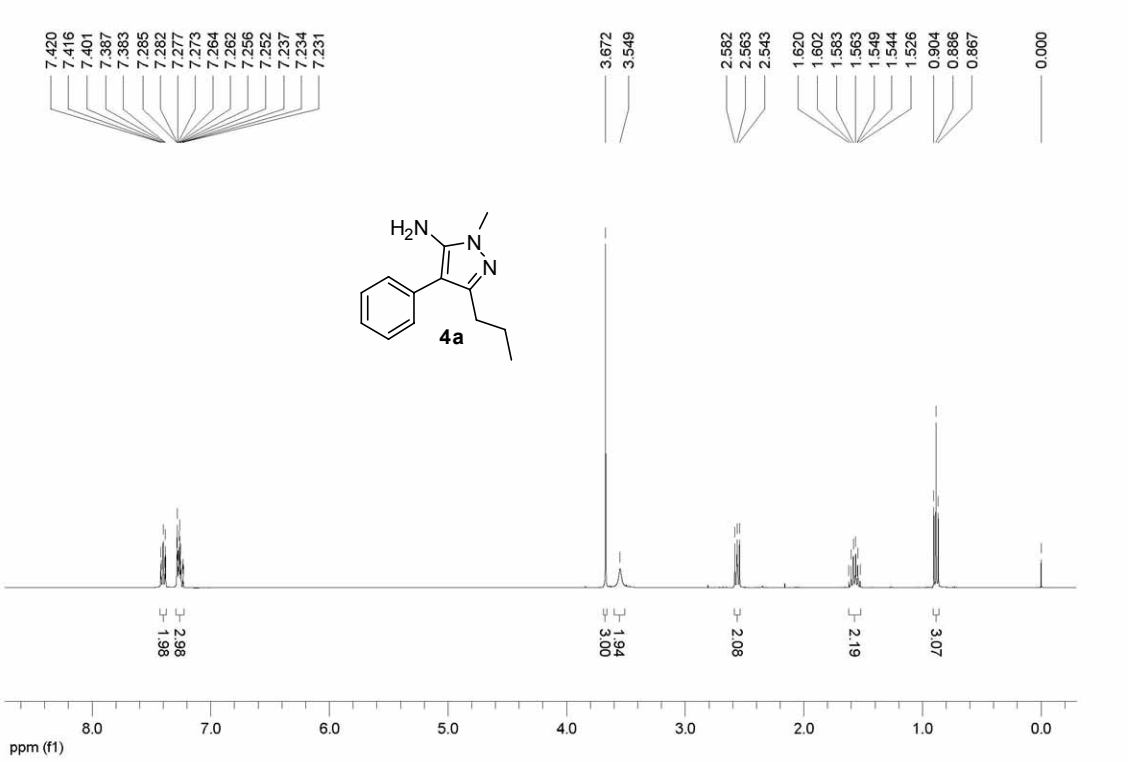
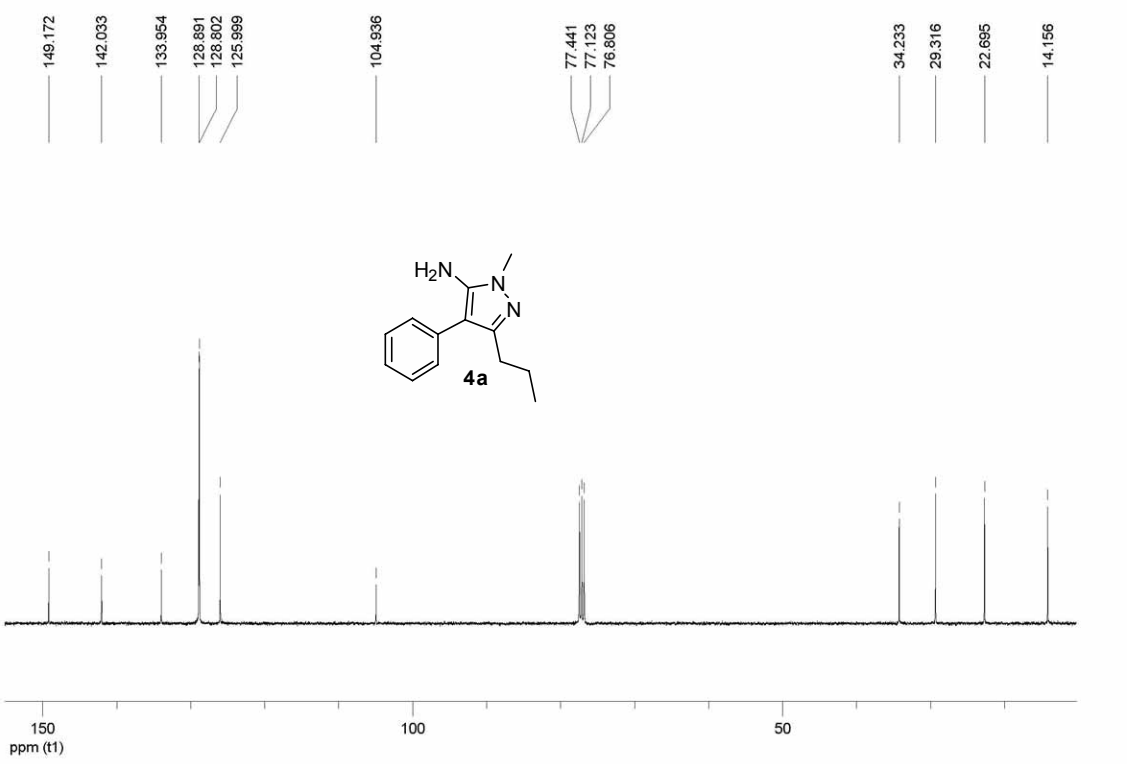
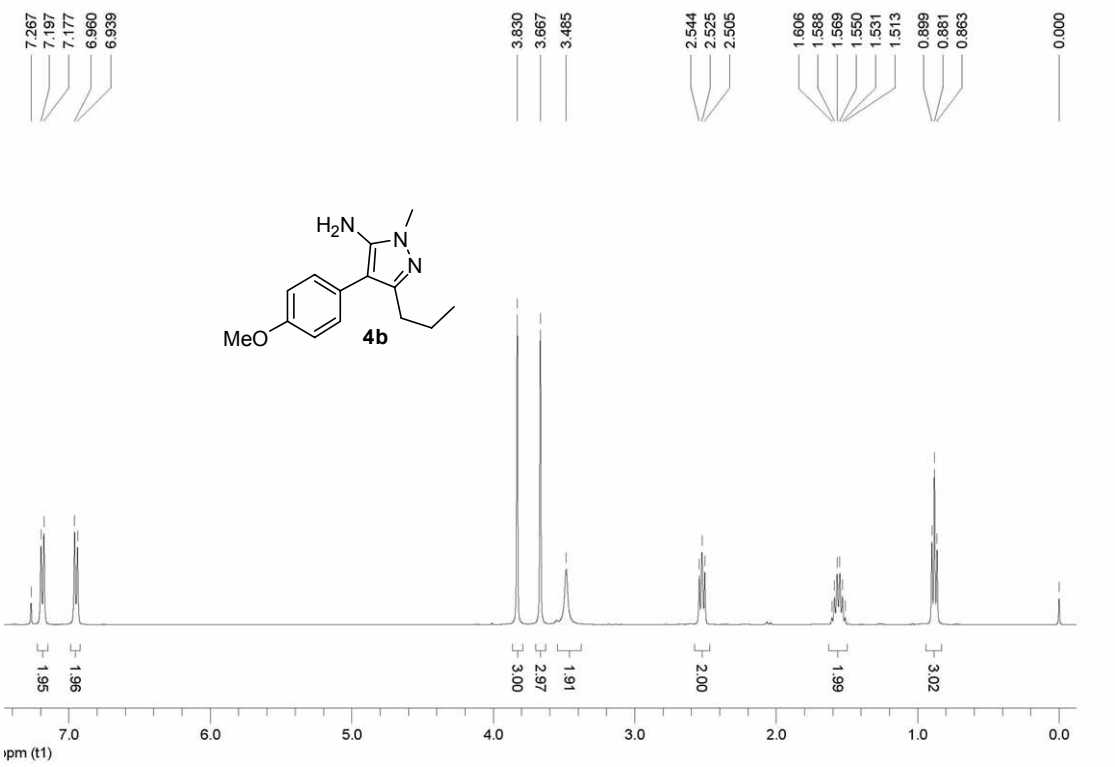
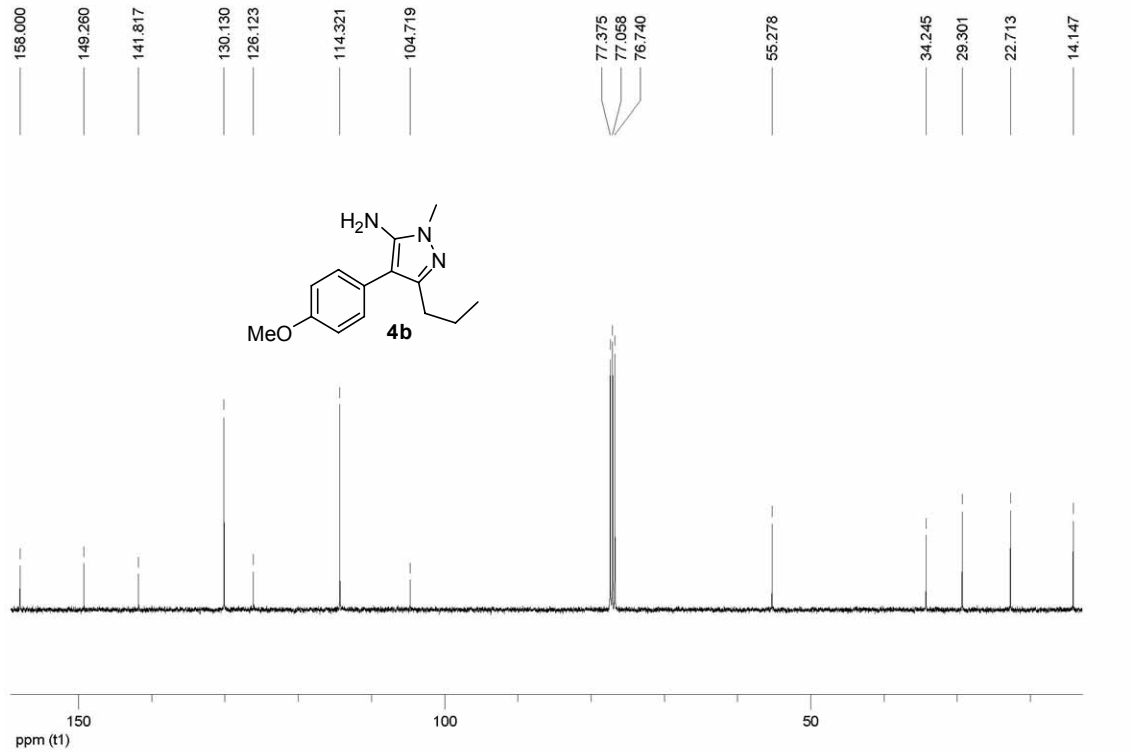
7.655
7.419
7.399
7.333
7.317
7.298
7.295
7.286
7.283
7.262
7.249
4.606
3.037
3.018
2.999
1.859
1.840
1.822
1.803
1.784
1.766
1.055
1.037
1.019
0.000
CN
N
NH2
2o'
0.94
1.00
1.93
2.00
2.06
3.04
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)

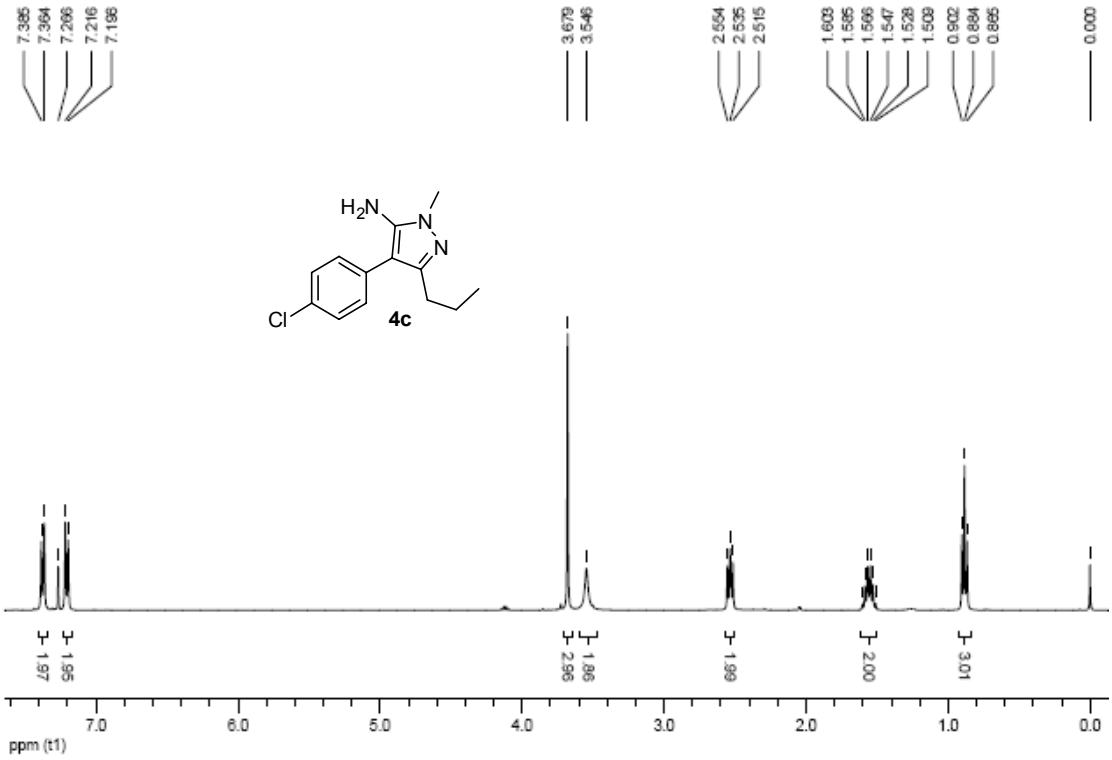

151.153
136.320
125.183
123.210
122.341
119.053
116.502
108.898
82.133
77.390
77.073
76.755
27.300
22.571
13.766
CN
N
NH2
2o'
150
100
50
ppm (t1)

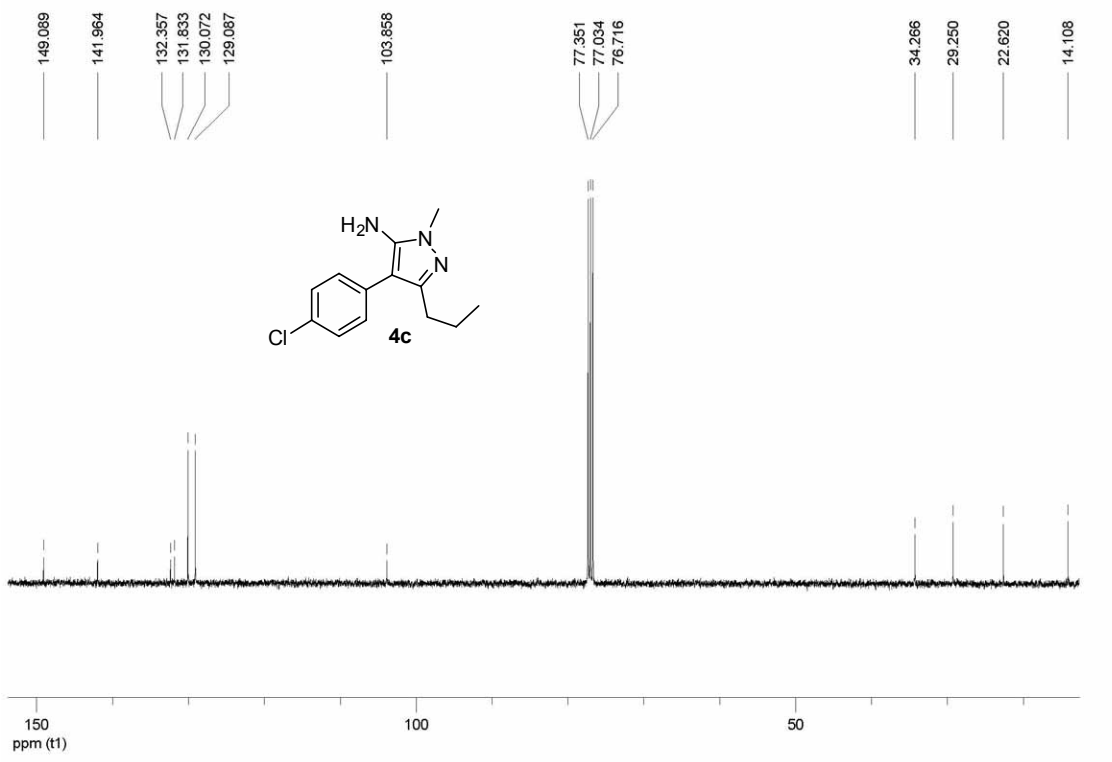

7.420
7.416
7.401
7.387
7.383
7.285
7.282
7.277
7.273
7.264
7.262
7.256
7.252
7.237
7.234
7.231
3.672
3.549
2.582
2.563
2.543
1.620
1.602
1.583
1.563
1.549
1.544
1.526
0.904
0.886
0.867
0.000
H2N
N
N
4a
1.98
2.98
3.00
1.94
2.08
2.19
3.07
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)


149.172
142.033
133.954
128.891
128.802
125.999
104.936
77.441
77.123
76.806
34.233
29.316
22.695
14.156
H2N
N
N
4a
150
100
50
ppm (t1)


7.267
7.197
7.177
6.960
6.939
3.830
3.667
3.485
2.544
2.525
2.505
1.606
1.588
1.569
1.550
1.531
1.513
0.899
0.881
0.863
0.000
H2N
N
N
MeO
4b
1.95
1.96
3.00
2.67
1.91
2.00
1.99
3.02
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


158.000
149.260
141.817
130.130
126.123
114.321
104.719
77.375
77.058
76.740
55.278
34.245
29.301
22.713
14.147
H2N
N
N
MeO
4b
150
100
50
ppm (t1)


7.385
7.364
7.206
7.216
7.198
3.679
3.546
2.554
2.535
2.515
1.603
1.585
1.566
1.547
1.528
1.509
0.902
0.884
0.865
0.000
H2N
N
N
Cl
4c
1.97
1.96
2.96
1.86
1.99
2.00
3.01
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


149.089
141.964
132.357
131.833
130.072
129.087
103.858
77.351
77.034
76.716
34.266
29.250
22.620
14.108
H2N
N
N
Cl
4c
150
100
50
ppm (t1)

X-ray structure and data of 2a

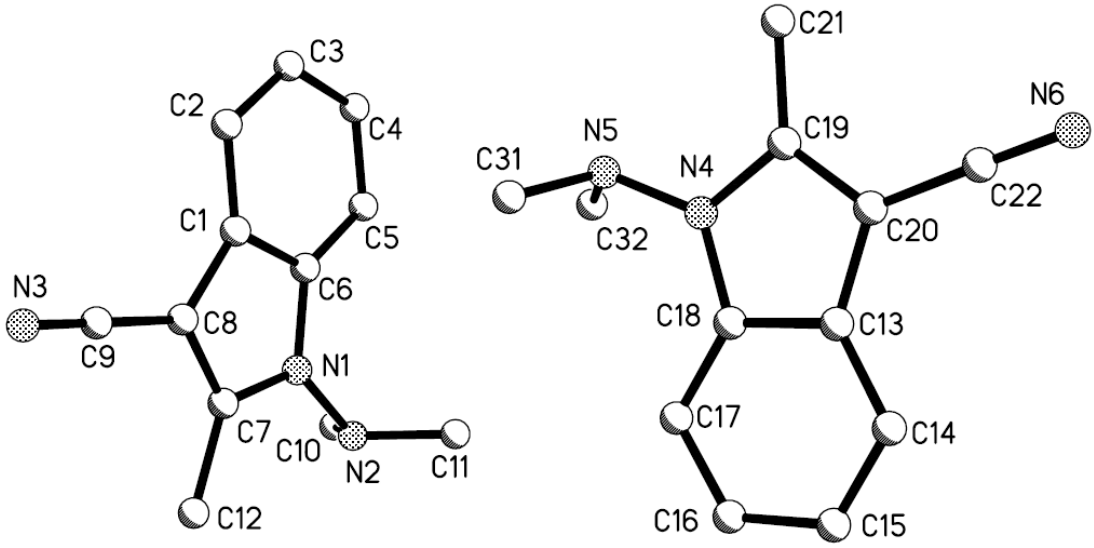


Table 1. Crystal data and structure refinement for **2a**.

The crystal of **2a** has been depostited in CCDC with number 772745.

Identification code	**2a**
Empirical formula	C_{12} H_{13} N_3
Formula weight	199.25
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 8.8268(18) A alpha = 99.27(3) deg. b = 8.9764(18) A beta = 96.72(3) deg. c = 16.501(3) A gamma = 118.09(3) deg.
Volume	1110.1(4) A^3
Z, Calculated density	4, 1.192 Mg/m^3
Absorption coefficient	0.074 mm^-1
F(000)	424.0
Crystal size	0.30 x 0.27 x 0.21 mm

Theta range for data collection	2.99 to 25.20 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -19<=l<=19
Reflections collected / unique	10965/3982 [R(int) = 0.0291]
Completeness to theta = 25.20	99.7 %
Absorption correction	Multi-scan
Max. and min. transmission	0.9847 and 0.9782
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3982 / 0 / 277
Goodness-of-fit on F^2	1.069
Final R indices [I>2sigma(I)]	R1 = 0.0535, wR2 = 0.1461
R indices (all data)	R1 = 0.1123, wR2 = 0.2100
Largest diff. peak and hole	0.22 and -0.20 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2a**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	1519(3)	-803(4)	939.2(18)	660(7)
C(2)	560(4)	-2202(4)	1288(2)	778(9)
C(3)	37(4)	-1861(4)	2018(2)	808(9)
C(4)	433(4)	-189(4)	2408(2)	771(8)
C(5)	1373(4)	1203(4)	2078(18)	711(8)
C(6)	1914(3)	879(4)	1342(18)	635(7)
C(7)	3015(3)	1074(4)	168(18)	664(7)
C(8)	2236(4)	-640(4)	200(18)	681(7)
C(9)	2163(4)	-1991(4)	-417(2)	796(9)
C(10)	2355(4)	4390(4)	984(2)	848(9)
C(11)	5031(4)	4657(4)	1800(2)	820(9)
C(12)	3881(4)	1916(4)	-479(2)	857(9)
C(13)	11012(4)	3684(4)	4366(17)	659(7)
C(14)	12663(4)	4905(4)	4271(2)	796(9)
C(15)	12759(5)	5705(4)	3623(2)	889(10)
C(16)	11229(5)	5282(4)	3063(2)	884(10)
C(17)	9578(5)	4037(4)	3115	(19)
C(18)	9496(4)	3248(4)	3777(17)	653(7)
C(19)	8629(4)	1649(4)	4744(17)	653(7)
C(20)	10431(4)	2676(4)	4970(17)	656(7)
C(21)	7397(4)	406(4)	5168(19)	802(9)
C(22)	11500(4)	2739(4)	5698(19)	714(8)
C(31)	6034(5)	-50(5)	2778(2)	1002(11)
C(32)	5509(4)	2178(5)	3562(2)	1022(12)
N(1)	2845(3)	1994(3)	8634(14)	664(6)
N(2)	3642(3)	3815(3)	1036(15)	691(6)
N(3)	2110(4)	-3083(4)	-908(2)	1043(10)
N(4)	8065(3)	1981(3)	4019(14)	680(6)
N(5)	6279(3)	1037(3)	3596(15)	763(7)
N(6)	12393(4)	2807(4)	6286(18)	955(9)

Table 3. Bond lengths [A] and angles [deg] for **2a**.

C(1)-C(6)	1.404(4)
C(1)-C(2)	1.404(4)
C(1)-C(8)	1.436(4)
C(2)-C(3)	1.380(4)
C(2)-H(2)	0.9300
C(3)-C(4)	1.389(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.376(4)
C(4)-H(4)	0.9300
C(5)-C(6)	1.393(4)
C(5)-H(5)	0.9300
C(6)-N(1)	1.390(3)
C(7)-N(1)	1.369(3)
C(7)-C(8)	1.371(4)
C(7)-C(12)	1.484(4)
C(8)-C(9)	1.422(4)
C(9)-N(3)	1.145(4)
C(10)-N(2)	1.452(4)
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-N(2)	1.457(4)
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-C(14)	1.398(4)
C(13)-C(18)	1.404(4)
C(13)-C20)	1.430(4)
C(14)-C(15)	1.369(4)
C(14)-H(14)	0.9300
C(15)-C(16)	1.391(4)
C(15)-H(15)	0.9300
C(16)-C(17)	1.380(4)
C(16)-H(16)	0.9300
C(17)-C(18)	1.386(4)
C(17)-H(17)	0.9300
C(18)-N(4)	1.400(3)
C(19)-C(20)	1.374(4)
C(19)-N(4)	1.372(3)

C(19)-C(21)	1.484(4)
C(20)-C(22)	1.414(4)
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-N(6)	1.150(3)
C(31)-N(5)	1.459(4)
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(32)-N(5)	1.476(4)
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
N(1)-N(2)	1.403(3)
N(4)-N(5)	1.409(3)
C(6)-C(1)-C(2)	119.3(3)
C(6)-C(1)-C(8)	106.2(3)
C(2)-C(1)-C(8)	134.5(3)
C(3)-C(2)-C(1)	118.2(3)
C(3)-C(2)-H(2)	120.9
C(1)-C(2)-H(2)	120.9
C(2)-C(3)-C(4)	121.8(3)
C(2)-C(3)-H(3)	119.1
C(4)-C(3)-H(3)	119.1
C(5)-C(4)-C(3)	121.0(3)
C(5)-C(4)-H(4)	119.5
C(3)-C(4)-H(4)	119.5
C(4)-C(5)-C(6)	117.8(3)
C(4)-C(5)-H(5)	121.1
C(6)-C(5)-H(5)	121.1
C(5)-C(6)-N(1)	130.9(3)
C(5)-C(6)-C(1)	121.8(3)
N(1)-C(6)-C(1)	107.2(3)
N(1)-C(7)-C(8)	108.0(3)
N(1)-C(7)-C(12)	122.1(3)
C(8)-C(7)-C(12)	130.0(3)
C(7)-C(8)-C(9)	124.2(3)
C(7)-C(8)-C(1)	108.5(3)
C(9)-C(8)-C(1)	127.4(3)
N(3)-C(9)-C(8)	179.5(4)
N(2)-C(10)-H(10A)	109.5
N(2)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5

N(2)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(2)-C(11)-H(11A)	109.5
N(2)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
N(2)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(7)-C(12)-H(12A)	109.5
C(7)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(7)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	119.4(3)
C(14)-C(13)-C(20)	134.0(3)
C(18)-C(13)-C(20)	106.6(3)
C(15)-C(14)-C(13)	119.2(3)
C(15)-C(14)-H(14)	120.4
C(13)-C(14)-H(14)	120.4
C(14)-C(15)-C(16)	120.1(3)
C(14)-C(15)-H(15)	120.0
C(16)-C(15)-H(15)	120.0
C(17)-C(16)-C(15)	122.7(3)
C(17)-C(16)-H(16)	118.7
C(15)-C(16)-H(16)	118.7
C(16)-C(17)-C(18)	116.7(3)
C(16)-C(17)-H(17)	121.6
C(18)-C(17)-H(17)	121.6
C(17)-C(18)-N(4)	131.4(3)
C(17)-C(18)-C(13)	121.9(3)
N(4)-C(18)-C(13)	106.7(3)
C(20)-C(19)-N(4)	107.5(3)
C(20)-C(19)-C(21)	129.9(3)
N(4)-C(19)-C(21)	122.6(3)
C(19)-C(20)-C(22)	124.6(3)
C(19)-C(20)-C(13)	108.8(3)
C(22)-C(20)-C(13)	126.6(3)
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5

H(21B)-C(21)-H(21C)	109.5
N(6)-C(22)-C(20)	178.9(4)
N(5)-C(31)-H(31A)	109.5
N(5)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
N(5)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
N(5)-C(32)-H(32A)	109.5
N(5)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
N(5)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(7)-N(1)-C(6)	110.2(2)
C(7)-N(1)-N(2)	120.8(2)
C(6)-N(1)-N(2)	128.9(2)
N(1)-N(2)-C(10)	112.1(2)
N(1)-N(2)-C(11)	111.6(2)
C(10)-N(2)-C(11)	115.7(2)
C(19)-N(4)-C(18)	110.4(2)
C(19)-N(4)-N(5)	121.1(2)
C(18)-N(4)-N(5)	128.4(2)
N(4)-N(5)-C(31)	111.0(2)
N(4)-N(5)-C(32)	111.8(2)
C(31)-N(5)-C(32)	114.1(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **2a**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	59(15)	70(18)	65(18)	18(15)	9(14)	29(14)
C(2)	71(18)	72(19)	86(2)	27(17)	13(17)	32(16)
C(3)	68(18)	89(2)	88(2)	45(19)	22(17)	34(17)
C(4)	71(18)	93(2)	74(2)	34(18)	24(16)	40(18)
C(5)	69(17)	75(19)	67(19)	19(16)	17(15)	34(16)
C(6)	58(15)	68(18)	62(17)	21(14)	15(13)	27(14)
C(7)	58(15)	74(19)	59(18)	15(15)	11(13)	27(15)
C(8)	61(16)	69(18)	63(18)	10(15)	8(14)	27(14)
C(9)	66(18)	82(2)	78(2)	5(18)	8(16)	33(17)
C(10)	76(19)	93(2)	94(2)	36(19)	19(17)	45(18)
C(11)	70(18)	75(19)	81(2)	15(17)	3(16)	26(16)
C(12)	84(2)	105(2)	68(2)	28(18)	25(17)	43(19)
C(13)	71(18)	71(18)	57(17)	10(14)	12(14)	38(15)
C(14)	75(2)	83(2)	76(2)	15(17)	17(16)	37(17)
C(15)	92(2)	86(2)	87(2)	25(19)	32(2)	40(19)
C(16)	115(3)	92(2)	79(2)	37(19)	38(2)	60(2)
C(17)	94(2)	92(2)	66(2)	26(17)	23(17)	55(2)
C(18)	70(17)	71(17)	59(17)	15(14)	15(14)	38(15)
C(19)	73(18)	77(18)	53(16)	16(14)	12(14)	44(16)
C(20)	68(17)	74(18)	55(16)	11(14)	7(13)	38(15)
C(21)	81(2)	92(2)	74(2)	30(18)	24(17)	44(18)
C(22)	70(18)	77(19)	60(18)	11(15)	7(15)	34(16)
C(31)	95(2)	96(2)	80(2)	-4(2)	-1(19)	37(2)
C(32)	88(2)	134(3)	105(3)	30(2)	12(2)	73(2)
N(1)	68(14)	62(14)	63(15)	18(12)	17(12)	26(12)
N(2)	62(13)	60(14)	74(16)	16(12)	9(12)	24(11)
N(3)	95(2)	105(2)	103(2)	-4(19)	15(18)	54(19)
N(4)	65(14)	81(15)	59(14)	15(12)	8(11)	39(13)
N(5)	66(14)	92(18)	67(16)	14(14)	4(12)	40(14)
N(6)	93(19)	113(2)	75(19)	23(16)	3(16)	50(18)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **2a**.

	x	y	z	U(eq)
H(2)	284	-3328	1033	930
H(3)	-598	-2775	2257	970
H(4)	57	-7	2899	930
H(5)	1639	2322	2338	850
H(10A)	1661	3963	419	1270
H(10B)	2953	5640	1135	1270
H(10C)	1601	3946	1363	1270
H(11A)	4517	4448	2281	1230
H(11B)	5683	5888	1848	1230
H(11C)	5809	4189	1776	1230
H(12A)	3080	2100	-838	1290
H(12B)	4208	1177	-809	1290
H(12C)	4915	3016	-207	1290
H(14)	13684	5170	4642	960
H(15)	13848	6532	3558	1070
H(16)	11322	5862	2636	1060
H(17)	8571	3742	2724	950
H(21A)	8056	232	5612	1200
H(21B)	6625	-688	4766	1200
H(21C)	6713	869	5399	1200
H(31A)	6607	680	2417	1500
H(31B)	4799	-766	2527	1500
H(31C)	6535	-778	2850	1500
H(32A)	6117	3018	3254	1530
H(32B)	5624	2771	4124	1530
H(32C)	4286	1487	3286	1530

Table 6. Torsion angles [deg] for **2a**.

C(6)-N(1)-N(2)-C(10)	-69.51
C(6)-N(1)-N(2)-C(11)	62.16
C(7)-N(1)-N(2)-C(10)	114.66
C(7)-N(1)-N(2)-C(11)	-113.67
C(6)-C(1)-C(2)-C(3)	0.14
C(8)-C(1)-C(2)-C(3)	-178.20
C(2)-C(1)-C(6)-N(1)	-179.44
C(2)-C(1)-C(6)-C(5)	-0.29
C(8)-C(1)-C(6)-N(1)	-0.67
C(8)-C(1)-C(6)-C(5)	178.47
C(2)-C(1)-C(8)-C(7)	178.21
C(2)-C(1)-C(8)-C(9)	-1.08
C(6)-C(1)-C(8)-C(7)	-0.28
C(6)-C(1)-C(8)-C(9)	-179.58
C(1)-C(2)-C(3)-C(4)	0.08
C(2)-C(3)-C(4)-C(5)	-0.16
C(3)-C(4)-C(5)-C(6)	0.00
C(4)-C(5)-C(6)-N(1)	179.14
C(4)-C(5)-C(6)-C(1)	0.22
C(1)-C(6)-N(1)-N(2)	-174.78
C(1)-C(6)-N(1)-C(7)	-1.41
C(5)-C(6)-N(1)-N(2)	6.19
C(5)-C(6)-N(1)-C(7)	-177.63
C(8)-C(7)-N(1)-N(2)	174.95
C(8)-C(7)-N(1)-C(6)	-1.59
C(12)-C(7)-N(1)-N(2)	-6.32
C(12)-C(7)-N(1)-C(6)	177.13
N(1)-C(7)-C(8)-C(1)	1.14
N(1)-C(7)-C(8)-C(9)	-179.54
C(12)-C(7)-C(8)-C(1)	-177.46
C(12)-C(7)-C(8)-C(9)	1.87
C(6)-C(1)-C(2)-H(2)	-180
C(8)-C(1)-C(2)-H(2)	2
C(1)-C(2)-C(3)-H(3)	-180
H(2)-C(2)-C(3)-C(4)	-180
H(2)-C(2)-C(3)-H(3)	0
C(2)-C(3)-C(4)-H(4)	180
H(3)-C(3)-C(4)-C(5)	180
H(3)-C(3)-C(4)-H(4)	0
C(3)-C(4)-C(5)-H(5)	-180
H(4)-C(4)-C(5)-C(6)	-180

H(4)-C(4)-C(5)-H(5)	0
H(5)-C(5)-C(6)-N(1)	-1
H(5)-C(5)-C(6)-C(1)	-180
N(1)-C(7)-C(12)-H(12A)	-78
N(1)-C(7)-C(12)-H(12B)	162
N(1)-C(7)-C(12)-H(12C)	42
C(8)-C(7)-C(12)-H(12A)	100
C(8)-C(7)-C(12)-H(12B)	-20
C(8)-C(7)-C(12)-H(12C)	-140
H(10A)-C(10)-N(2)-N(1)	-63
H(10A)-C(10)-N(2)-C(11)	167
H(10B)-C(10)-N(2)-N(1)	177
H(10B)-C(10)-N(2)-C(11)	47
H(10C)-C(10)-N(2)-N(1)	57
H(10C)-C(10)-N(2)-C(11)	-73
H(11A)-C(11)-N(2)-N(1)	-70
H(11A)-C(11)-N(2)-C(10)	60
H(11B)-C(11)-N(2)-N(1)	170
H(11B)-C(11)-N(2)-C(10)	-60
H(11C)-C(11)-N(2)-N(1)	50
H(11C)-C(11)-N(2)-C(10)	180
C(18)-N(4)-N(5)-C(31)	62.80
C(18)-N(4)-N(5)-C(32)	-65.95
C(19)-N(4)-N(5)-C(31)	-113.14
C(19)-N(4)-N(5)-C(32)	118.10
C(18)-C(13)-C(14)-C(15)	2.78
C(20)-C(13)-C(14)-C(15)	-177.23
C(14)-C(13)-C(18)-N(4)	178.54
C(14)-C(13)-C(18)-C(17)	-2.20
C(20)-C(13)-C(18)-N(4)	-1.45
C(20)-C(13)-C(18)-C(17)	177.81
C(14)-C(13)-C(20)-C(19)	-179.06
C(14)-C(13)-C(20)-C(22)	2.64
C(18)-C(13)-C(20)-C(19)	0.93
C(18)-C(13)-C(20)-C(22)	-177.36
C(13)-C(14)-C(15)-C(16)	-0.99
C(14)-C(15)-C(16)-C(17)	-1.54
C(15)-C(16)-C(17)-C(18)	2.12
C(16)-C(17)-C(18)-N(4)	178.82
C(16)-C(17)-C(18)-C(13)	-0.23
C(13)-C(18)-N(4)-N(5)	-174.79
C(13)-C(18)-N(4)-C(19)	1.50
C(17)-C(18)-N(4)-N(5)	6.05
C(17)-C(18)-N(4)-C(19)	-177.66

C(20)-C(19)-N(4)-N(5)	175.68
C(20)-C(19)-N(4)-C(18)	-0.92
C(21)-C(19)-N(4)-N(5)	-5.57
C(21)-C(19)-N(4)-C(18)	177.83
N(4)-C(19)-C(20)-C(13)	-0.03
N(4)-C(19)-C(20)-C(22)	178.32
C(21)-C(19)-C(20)-C(13)	-178.65
C(21)-C(19)-C(20)-C(22)	-0.31
C(18)-C(13)-C(14)-H(14)	-177
C(20)-C(13)-C(14)-H(14)	3
C(13)-C(14)-C(15)-H(15)	179
H(14)-C(14)-C(15)-C(16)	179
H(14)-C(14)-C(15)-H(15)	-1
C(14)-C(15)-C(16)-H(16)	178
H(15)-C(15)-C(16)-C(17)	178
H(15)-C(15)-C(16)-H(16)	-2
C(15)-C(16)-C(17)-H(17)	-178
H(16)-C(16)-C(17)-C(18)	-178
H(16)-C(16)-C(17)-H(17)	2
H(17)-C(17)-C(18)-N(4)	-1
H(17)-C(17)-C(18)-C(13)	180
N(4)-C(19)-C(21)-H(21A)	172
N(4)-C(19)-C(21)-H(21B)	52
N(4)-C(19)-C(21)-H(21C)	-68
C(20)-C(19)-C(21)-H(21A)	-10
C(20)-C(19)-C(21)-H(21B)	-130
C(20)-C(19)-C(21)-H(21C)	110
H(31A)-C(31)-N(5)-N(4)	-66
H(31A)-C(31)-N(5)-C(32)	62
H(31B)-C(31)-N(5)-N(4)	174
H(31B)-C(31)-N(5)-C(32)	-58
H(31C)-C(31)-N(5)-N(4)	54
H(31C)-C(31)-N(5)-C(32)	-178
H(32A)-C(32)-N(5)-N(4)	62
H(32A)-C(32)-N(5)-C(31)	-65
H(32B)-C(32)-N(5)-N(4)	-58
H(32B)-C(32)-N(5)-C(31)	175
H(32C)-C(32)-N(5)-N(4)	-178
H(32C)-C(32)-N(5)-C(31)	55

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **2a** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)