SUPPORTING INFORMATION

Au Nanoparticle-Catalyzed Double Hydrosilylation of Nitriles by Diethylsilane

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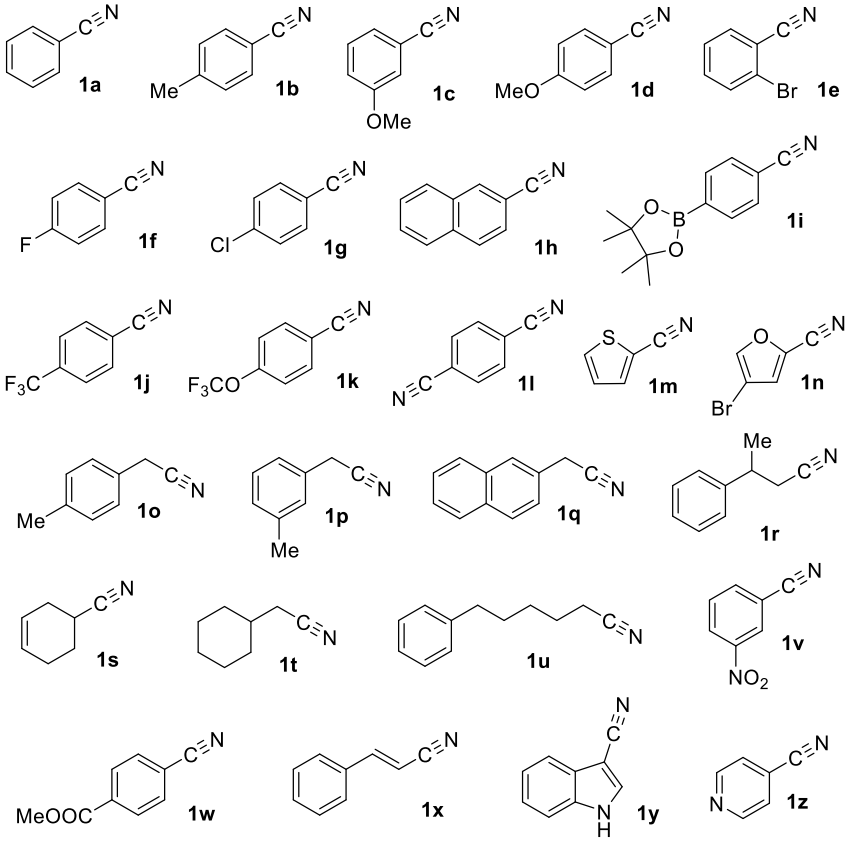
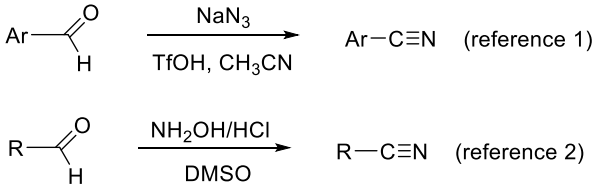
Nitriles used in this study

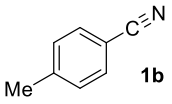


Apart from **1a**, **1i-1l**, **1o-1q** and **1y-1z** which were obtained from commercial suppliers, all aryl or heteroaryl nitriles were prepared from the corresponding aldehydes via the triflic acid-mediated Schmidt reaction,[1] while the alkyl ones via treatment of the aldehydes with hydroxylamine hydrochloride in DMSO,[2] as shown schematically below:



Spectroscopic data of synthesized nitriles

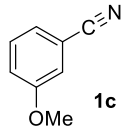
4-Methylbenzonitrile (1b)



Colorless oil (105 mg, 78% yield). Its spectroscopic data are in agreement with those of the commercially available substance. ^{1}H NMR (500 MHz, $CDCl_3$): 7.54 (d, J = 8.0 Hz, 2H),

7.27 (d, *J* = 8.0 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.7, 132.0, 129.8, 119.1, 109.3, 21.8.

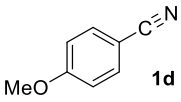
3-Methoxybenzonitrile (1c)



1c

Colorless oil (130 mg, 83% yield). Its spectroscopic data are in agreement with those of the commercially available substance. ^{1}H NMR (500 MHz, $CDCl_3$): 7.39-7.35 (m, 1H), 7.25-7.23 (m, 1H), 7.14-7.12 (m, 2H), 3.83 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 159.6, 130.3, 124.5, 119.3, 118.7, 116.8, 113.2, 55.5.

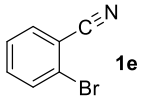
4-Methoxybenzonitrile (1d)



1d

White solid (200 mg, 91% yield). Its spectroscopic data are in agreement with those of the commercially available substance. ^{1}H NMR (500 MHz, $CDCl_3$): 7.57 (d, *J* = 9.0 Hz, 2H), 6.94 (d, *J* = 9.0 Hz, 2H), 3.84 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 162.7, 133.7, 119.0, 114.6, 103.7, 55.4.

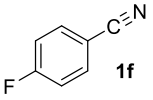
2-Bromobenzonitrile (1e)



1e

White solid (56 mg, 45% yield). Its spectroscopic data are in agreement with those of the commercially available substance. ^{1}H NMR (500 MHz, $CDCl_3$): 7.70-7.66 (m, 2H), 7.48-7.41 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): 134.3, 133.9, 133.2, 127.6, 125.3, 117.1, 115.9.

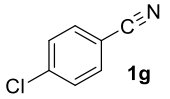
4-Fluorobenzonitrile (1f)



1f

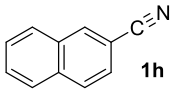
White solid (63 mg, 48% yield). Its spectroscopic data are in agreement with those of the commercially available substance. ^{1}H NMR (500 MHz, $CDCl_3$): 7.70-7.66 (m, 2H), 7.20-7.16 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): 165.0 (d, $J_{C\text{-}F}$ = 256.5 Hz), 134.7 (d, $J_{C\text{-}F}$ = 9.5 Hz), 118.0, 116.9 (d, $J_{C\text{-}F}$ = 22.0 Hz), 108.6 (d, $J_{C\text{-}F}$ = 3.5 Hz).

4-Chlorobenzonitrile (1g)



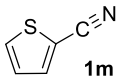
White solid (143 mg, 73% yield). Its spectroscopic data are in agreement with those of the commercially available substance. ^{1}H NMR (500 MHz, $CDCl_3$): 7.60 (d, J = 8.5 Hz, 2H), 7.47 (d, J = 8.5 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): 139.6, 133.4, 129.7, 117.9, 110.8.

2-Naphthonitrile (1h)



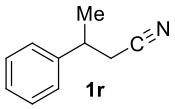
White solid (81 mg, 53% yield). Its spectroscopic data are in agreement with those of the commercially available substance. ^{1}H NMR (500 MHz, $CDCl_3$): 8.24 (s, 1H), 7.93-7.89 (m, 3H), 7.67-7.60 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 134.6, 134.1, 132.2, 129.2, 129.0, 128.4, 128.0, 127.6, 126.3, 119.2, 109.4.

Thiophene-2-carbonitrile (1m)



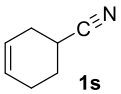
Yellow oil (66 mg, 57% yield). Its spectroscopic data are in agreement with those of the commercially available substance. ^{1}H NMR (500 MHz, $CDCl_3$): 7.64 (dd, J_1 = 3.5 Hz, J_2 = 1.0 Hz, 1H), 7.62 (dd, J_1 = 5.0 Hz, J_2 = 1.0 Hz, 1H), 7.14 (dd, J_1 = 5.0 Hz, J_2 = 3.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): 137.4, 132.5, 127.6, 114.2, 109.9.

3-Phenylbutanenitrile (1r)[3]



Colorless oil (105 mg, 72% yield). ^{1}H NMR (500 MHz, $CDCl_3$): 7.36 (t, J = 7.5 Hz, 2H), 7.29-7.24 (m, 3H), 3.17 (m, 1H), 2.62 (dd, J_1 = 16.5 Hz, J_2 = 6.5 Hz, 1H), 2.55 (dd, J_1 = 16.5 Hz, J_2 = 7.5 Hz, 1H), 1.46 (d, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 143.1, 128.8, 127.3, 126.5, 118.5, 36.5, 26.3, 20.6.

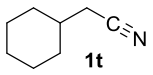
Cyclohex-3-ene-1-carbonitrile (1s)[3]



Colorless oil (72 mg, 53% yield). ^{1}H NMR (500 MHz, $CDCl_3$): 5.77-5.73 (m, 1H), 5.65-5.61 (m, 1H), 2.83-2.78 (m, 1H), 2.40-2.37 (m, 1H), 2.34-2.27 (m, 1H), 2.26-2.20 (m, 1H),

2.13-2.06 (m, 1H), 2.01-1.96 (m, 1H), 1.91-1.84 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): 127.0, 123.3, 122.4, 28.2, 25.3, 24.6, 22.9.

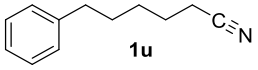
2-Cyclohexylacetonitrile (1t)[4]



1t

Colorless oil (105 mg, 49% yield). ^{1}H NMR (500 MHz, $CDCl_3$): 2.23 (d, J = 6.5 Hz, 2H), 1.84-1.81 (m, 2H), 1.77-1.73 (m, 2H), 1.69-1.62 (m, 2H), 1.32-1.03 (m, 5H). ^{13}C NMR (125 MHz, $CDCl_3$): 118.9, 34.8, 32.4, 25.7, 25.6, 24.7.

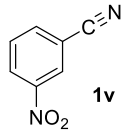
6-Phenylhexanenitrile (1u)[5]



1u

Colorless oil (142 mg, 52% yield). ^{1}H NMR (500 MHz, $CDCl_3$): 7.29 (t, J = 7.5 Hz, 2H), 7.21-7.17 (m, 3H), 2.64 (t, J = 7.5 Hz, 2H), 2.33 (t, 2H, J = 7.0 Hz), 1.72-1.63 (m, 4H), 1.53-1.46 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): 142.0, 128.3 (2C), 125.8, 119.7, 35.5, 30.6, 28.2, 25.3, 17.1.

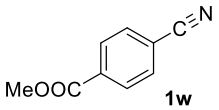
3-Nitrobenzonitrile (1v)



1v

White solid (157 mg, 80% yield). Its spectroscopic data are in agreement with those of the commercially available substance. ^{1}H NMR (500 MHz, $CDCl_3$): 8.54 (t, J = 2.0 Hz, 1H), 8.49-8.47 (m, 1H), 8.01-7.99 (m, 1H), 7.74 (t, J =8.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): 148.2, 137.6, 130.6, 127.5, 127.2, 116.5, 114.1.

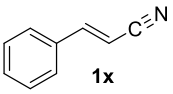
Methyl 4-cyanobenzoate (1w)



1w

White solid (123 mg, 84% yield). Its spectroscopic data are in agreement with those of the commercially available substance. ^{1}H NMR (500 MHz, $CDCl_3$): 8.13 (d, J = 8.5 Hz, 2H), 7.74 (d, J = 8.5 Hz, 2H), 3.95 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 165.4, 133.9, 132.2, 130.1, 117.9, 116.4, 52.7.

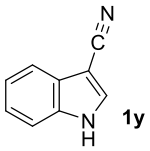
Cinnamonitrile (1x)



1x

Colorless oil (121 mg, 92% yield). Its spectroscopic data are in agreement with those of the commercially available substance. ^{1}H NMR (500 MHz, $CDCl_3$): 7.46-7.39 (m, 6H), 5.88 (d, *J* = 16.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): 150.5, 133.5, 131.2, 129.1, 127.3, 118.1, 96.3.

1*H*-indole-3-carbonitrile (1y)



1y

Yellow solid (86 mg, 59% yield). Its spectroscopic data are in agreement with those of the commercially available substance. ^{1}H NMR (500 MHz, $CDCl_3$): 8.77 (br s, 1H), 7.79 (d, *J* = 7.5 Hz, 1H), 7.74 (d, *J* = 2.5 Hz, 1H), 7.48 (d, *J* = 7.5 Hz, 1H), 7.36-7.29 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): 134.8, 131.8, 126.9, 124.3, 122.4, 119.7, 115.8, 112.0, 87.6.

References

1. B. V. Rokade and K. R. Prabhu, *J. Org. Chem.*, 2012, **77**, 5364.

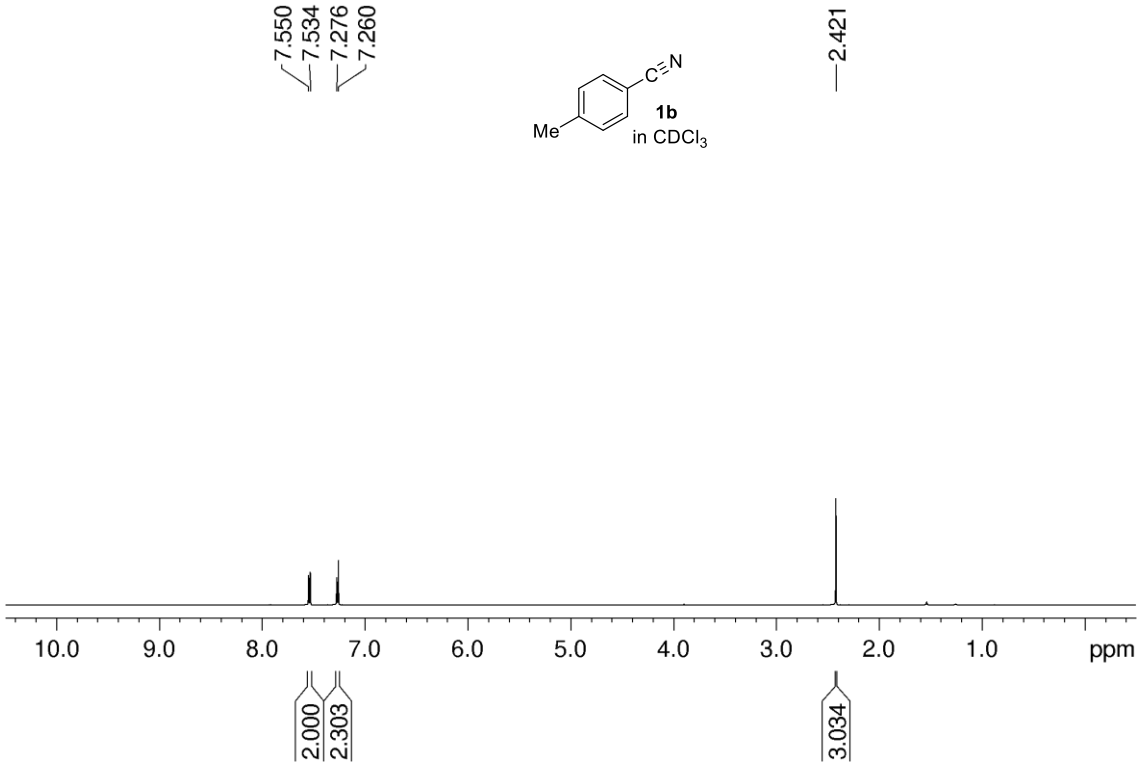
2. S. T. Chill and R. C. Mebane, *Synth. Commun.*, 2009, **39**, 3601.

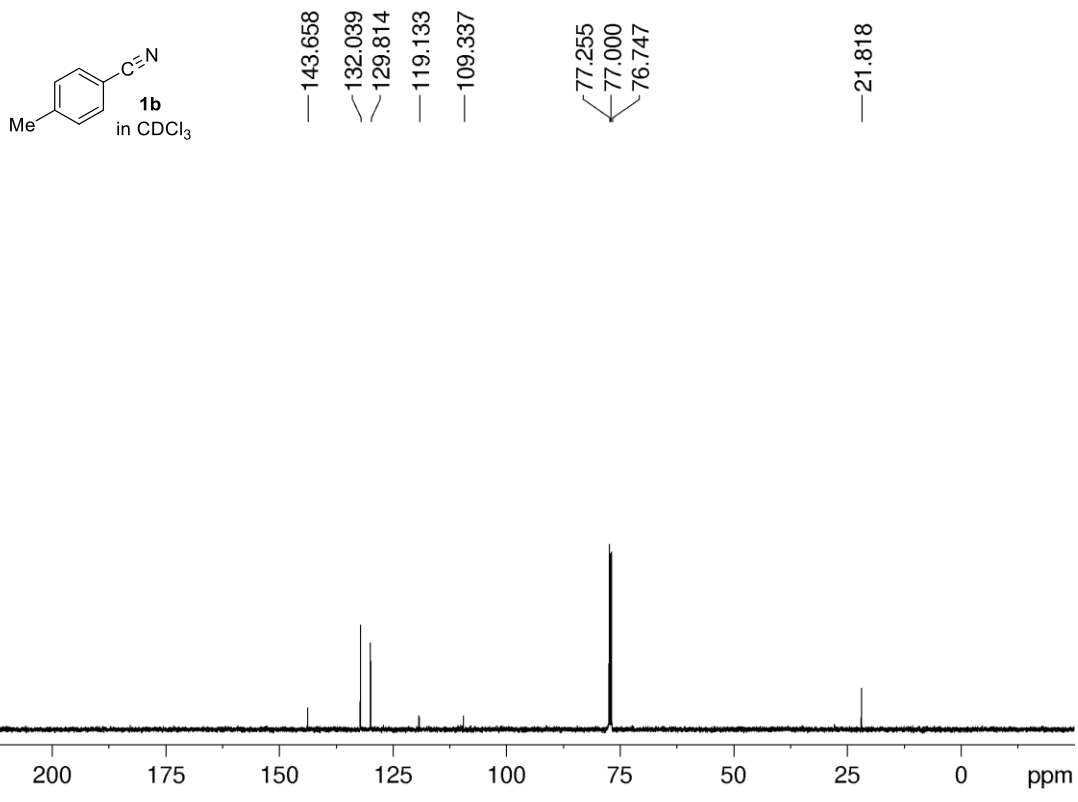
3. T. Betke, P. Rommelmann, K. Oike, Y. Asano and H. Groger, *Angew. Chem. Int. Ed.*, 2017, **56**, 12361.

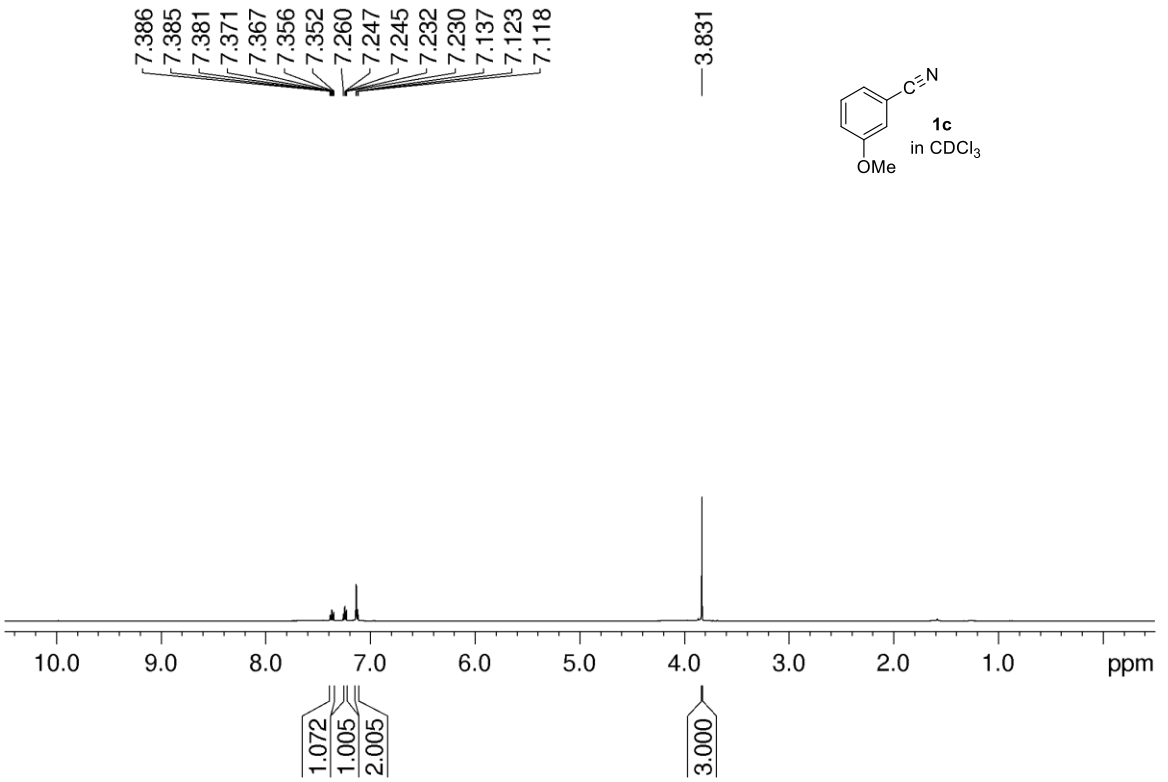
4. M. Ezawa and H. Togo, *Eur. J. Org. Chem.*, 2017, 2379.

5. B. Anxionnat, D. G. Pardo, G. Ricci and J. Cossy, *Org. Lett.*, 2011, **13**, 4084.

^{1}H and ^{13}C NMR of synthesized nitriles (500 MHz)



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7.118
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OMe
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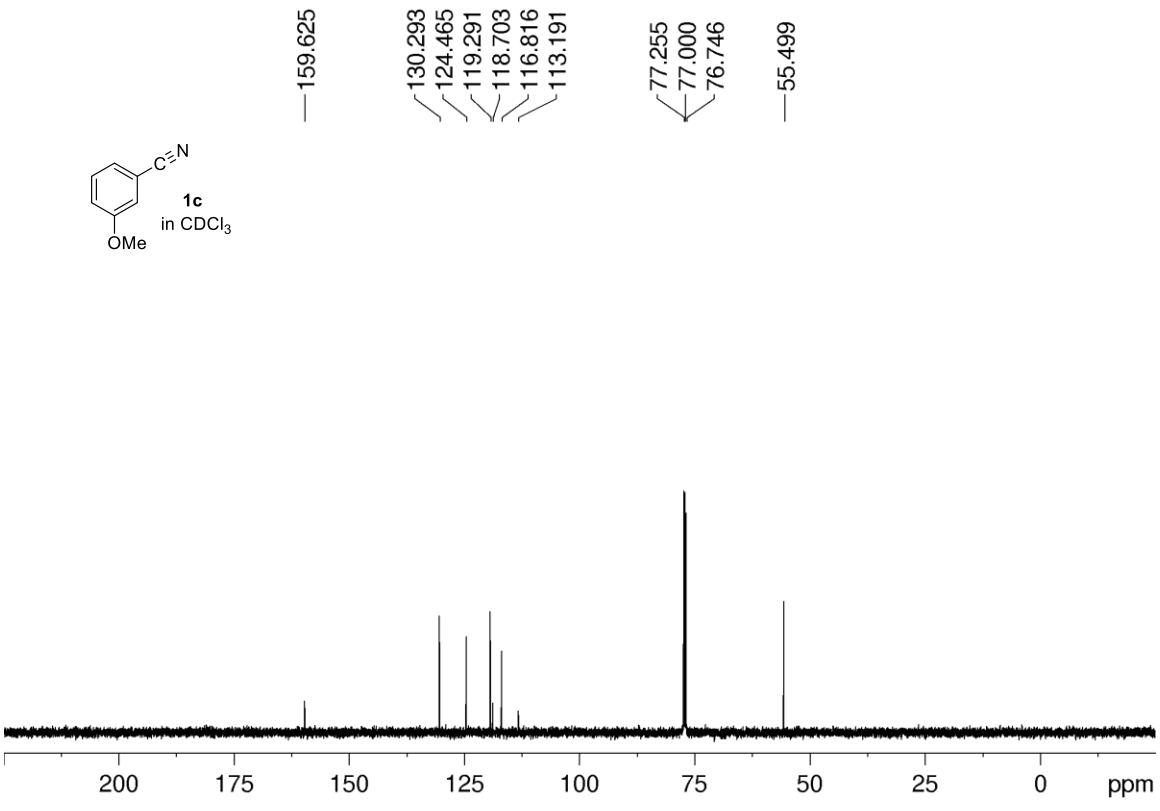
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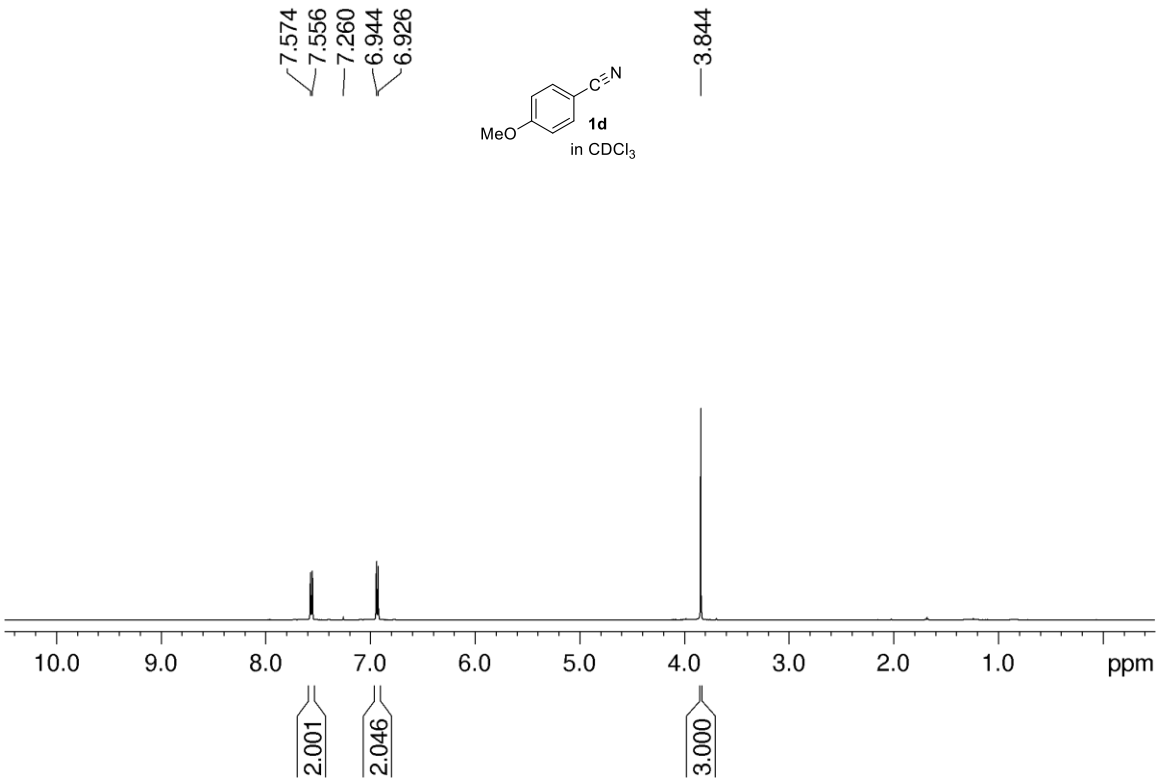
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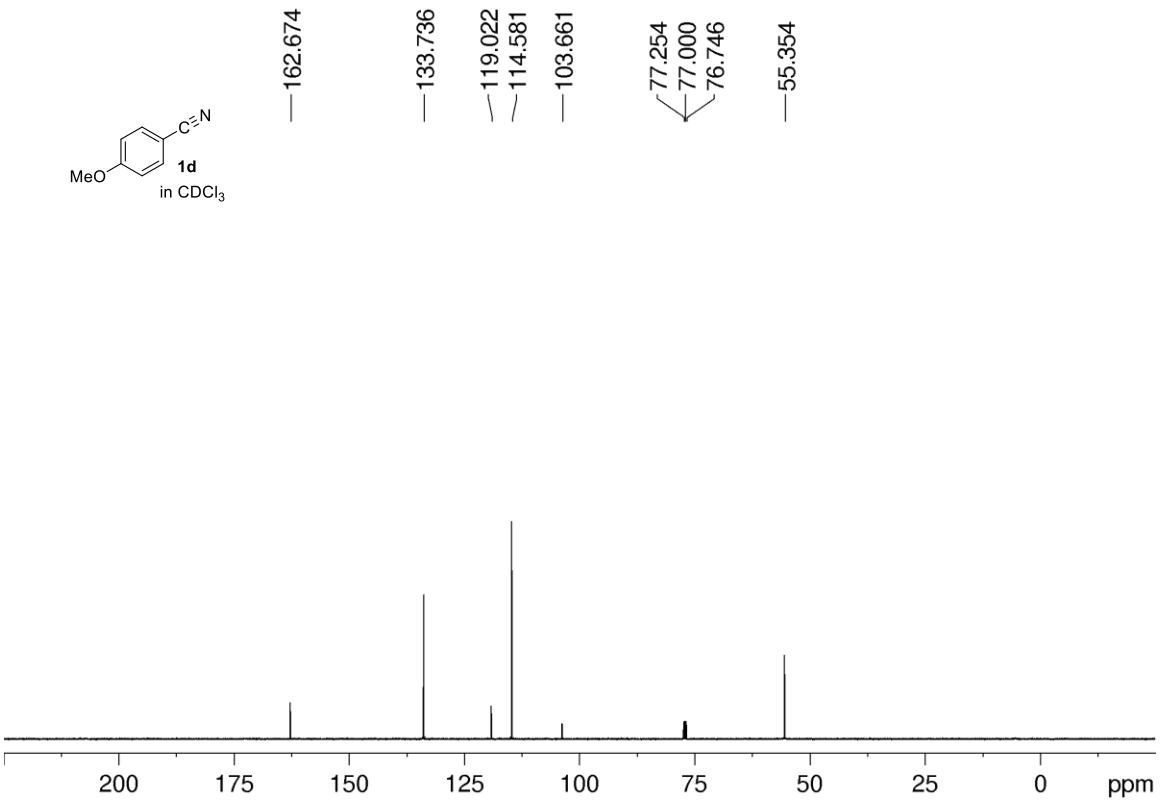
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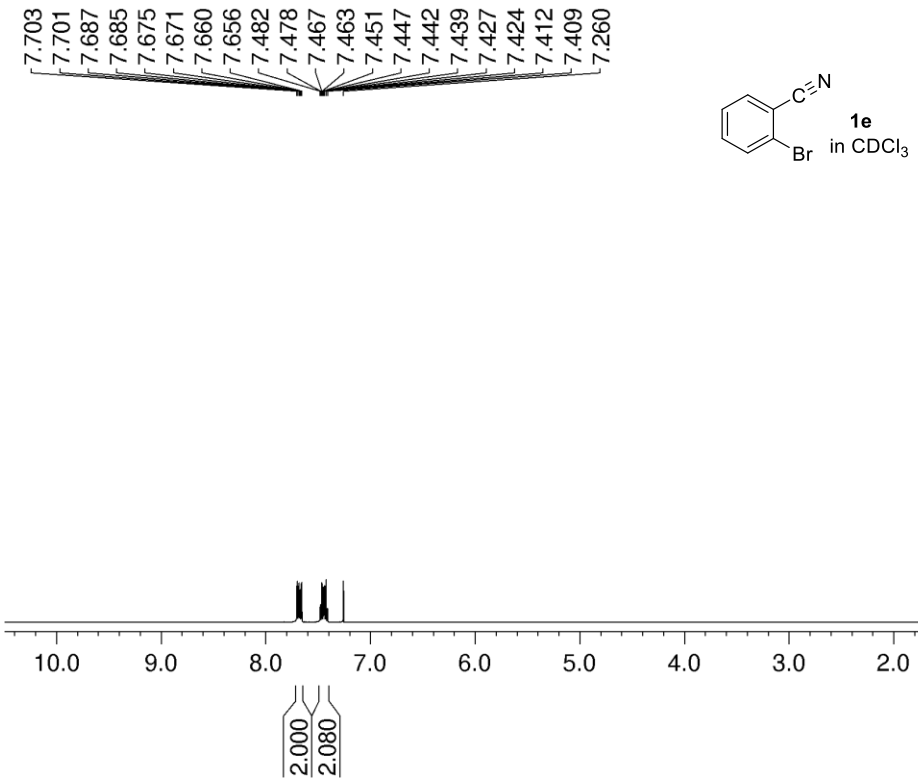
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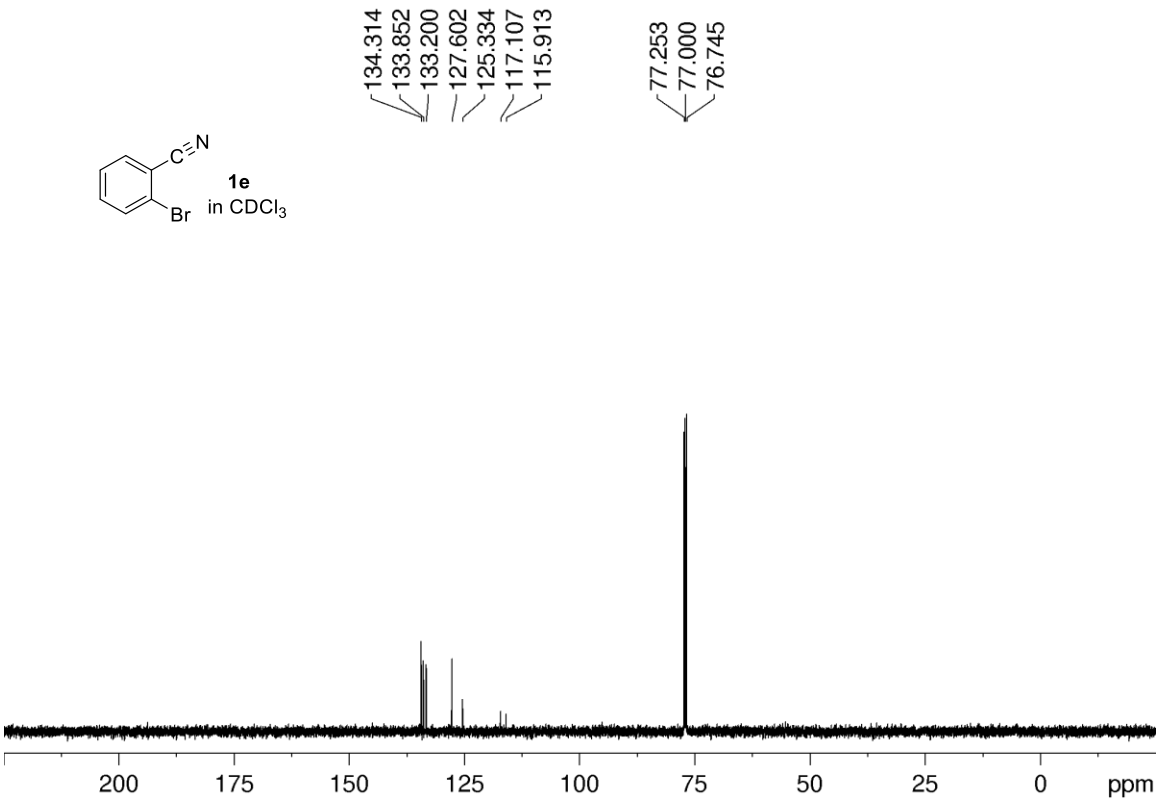
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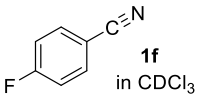
C≡N
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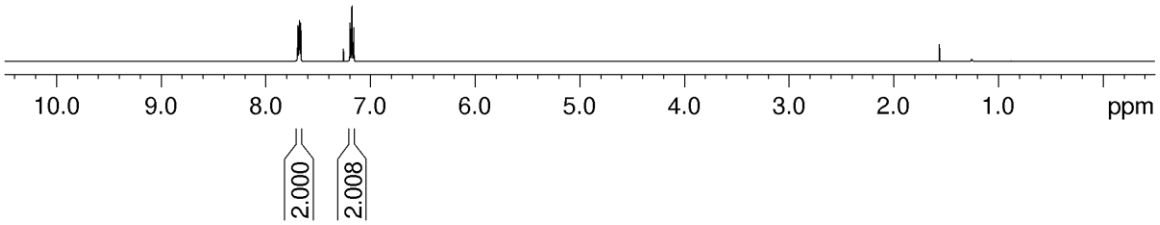
1f
in CDCl3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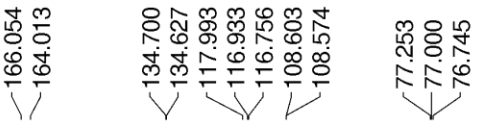
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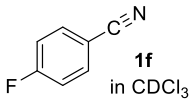
C≡N
F
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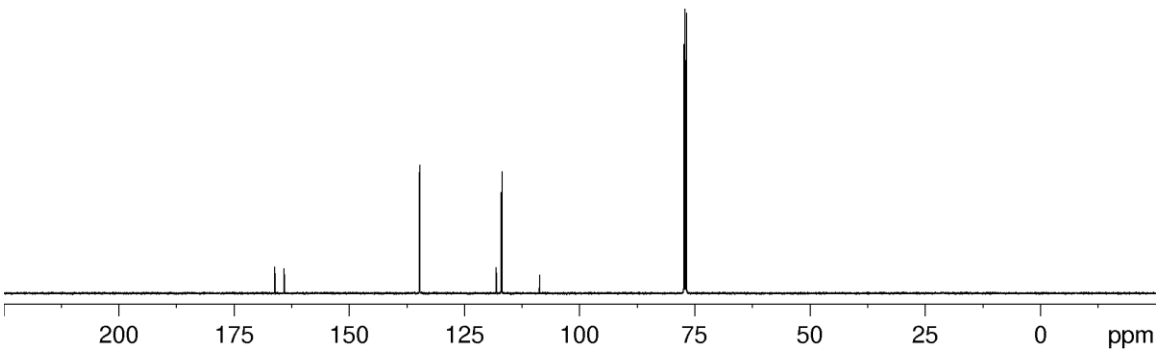
in CDCl3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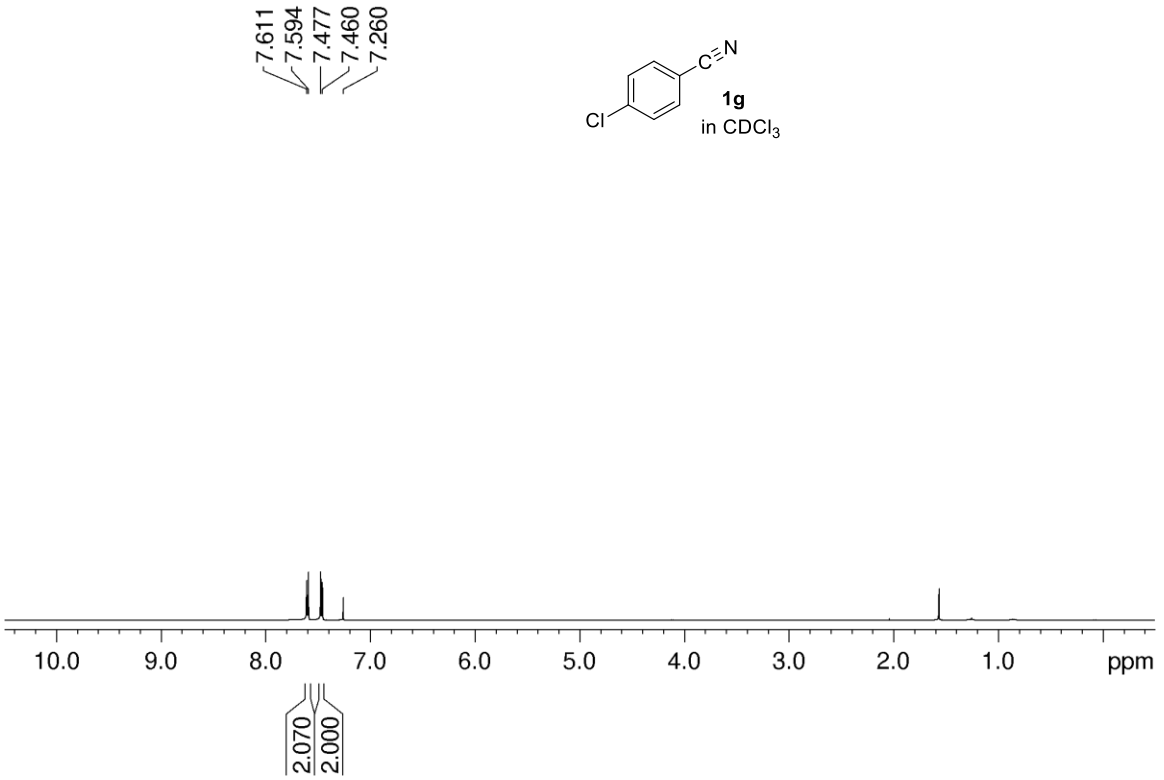
7.611
7.594
7.477
7.460
7.260
C≡N
Cl
1g
in CDCl3
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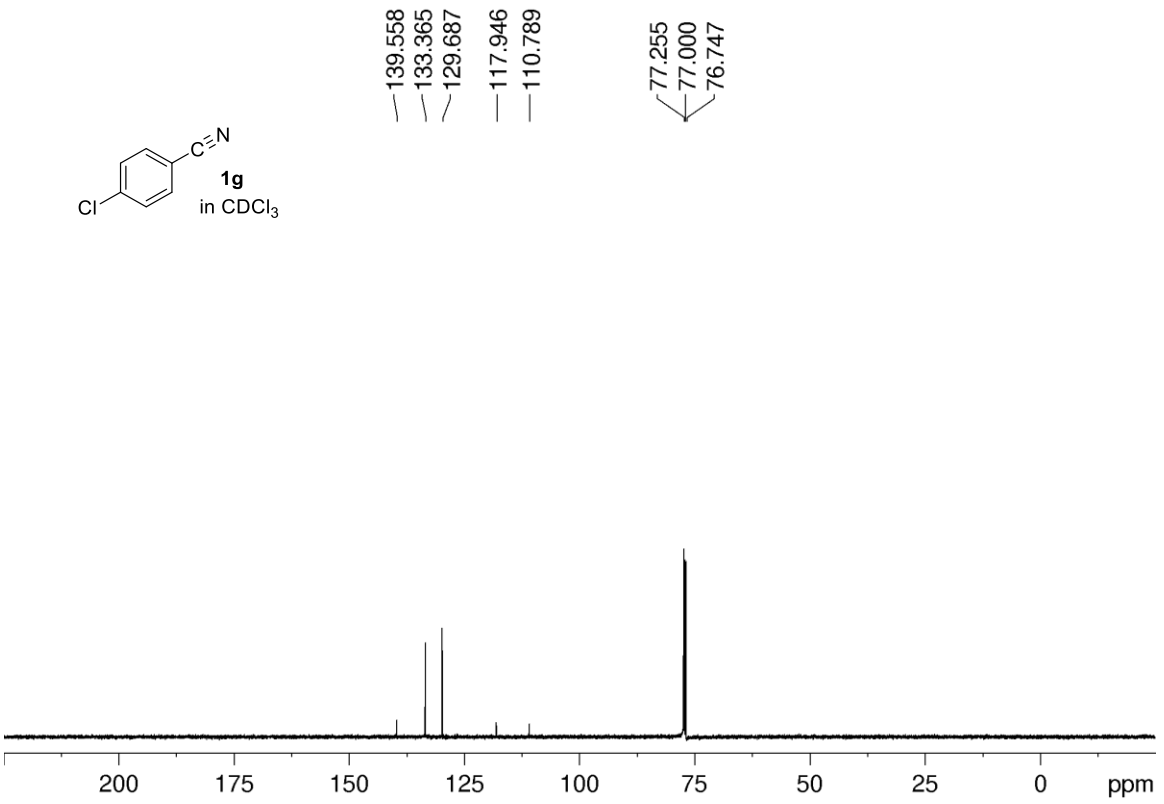
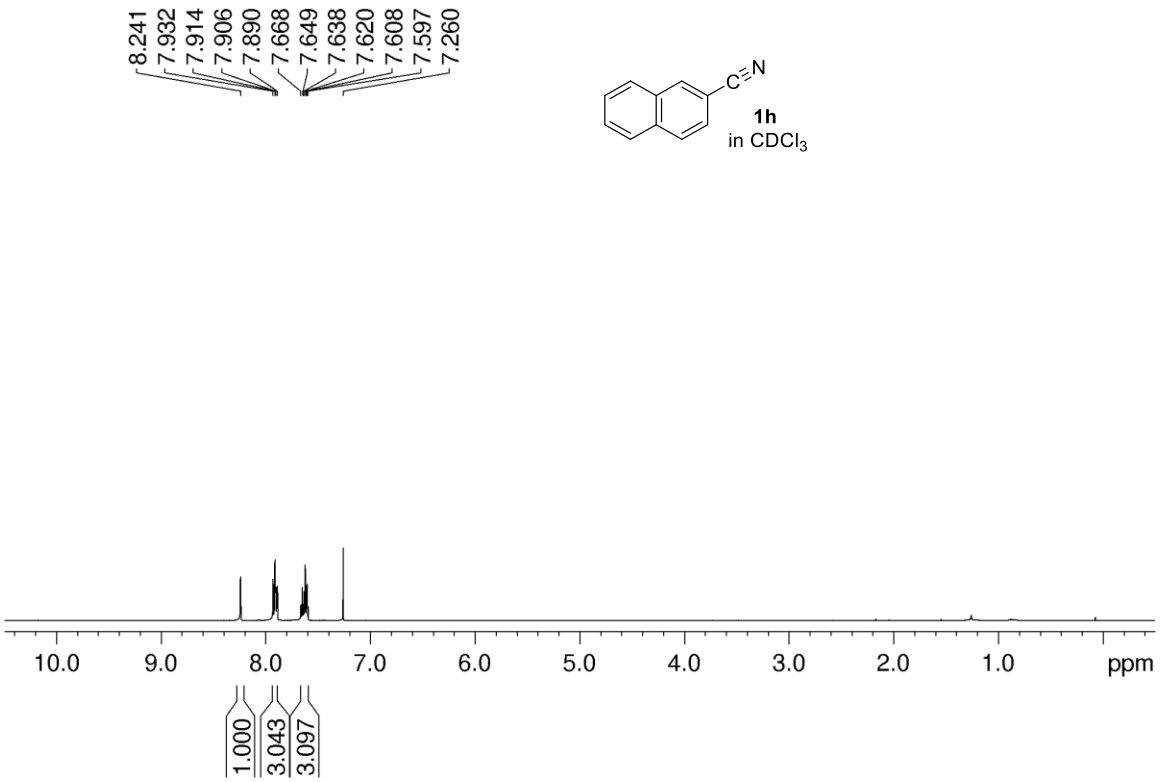
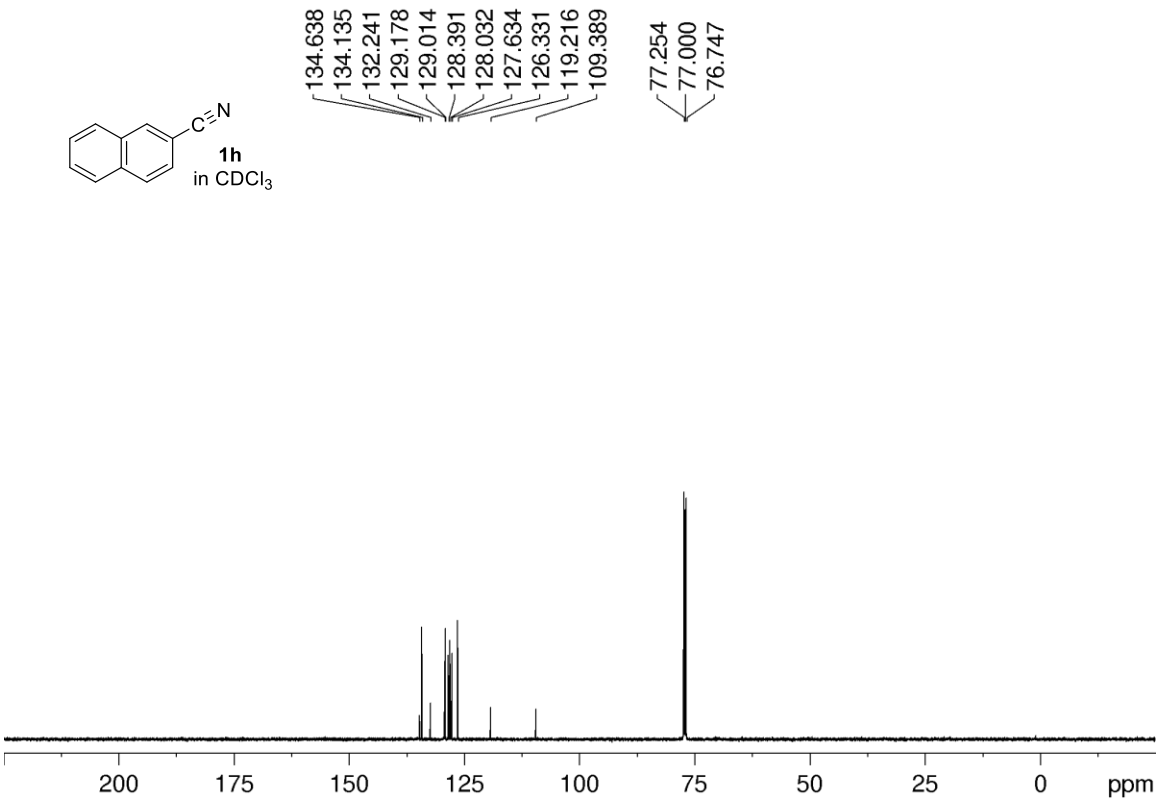
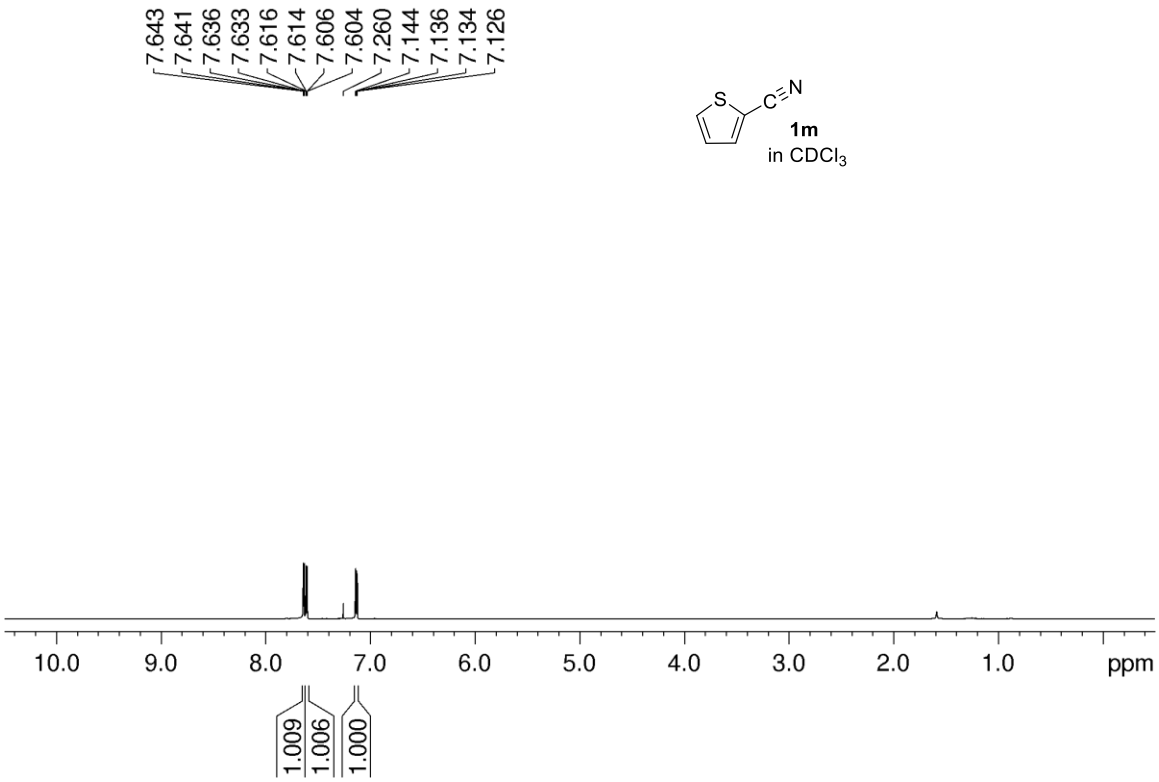
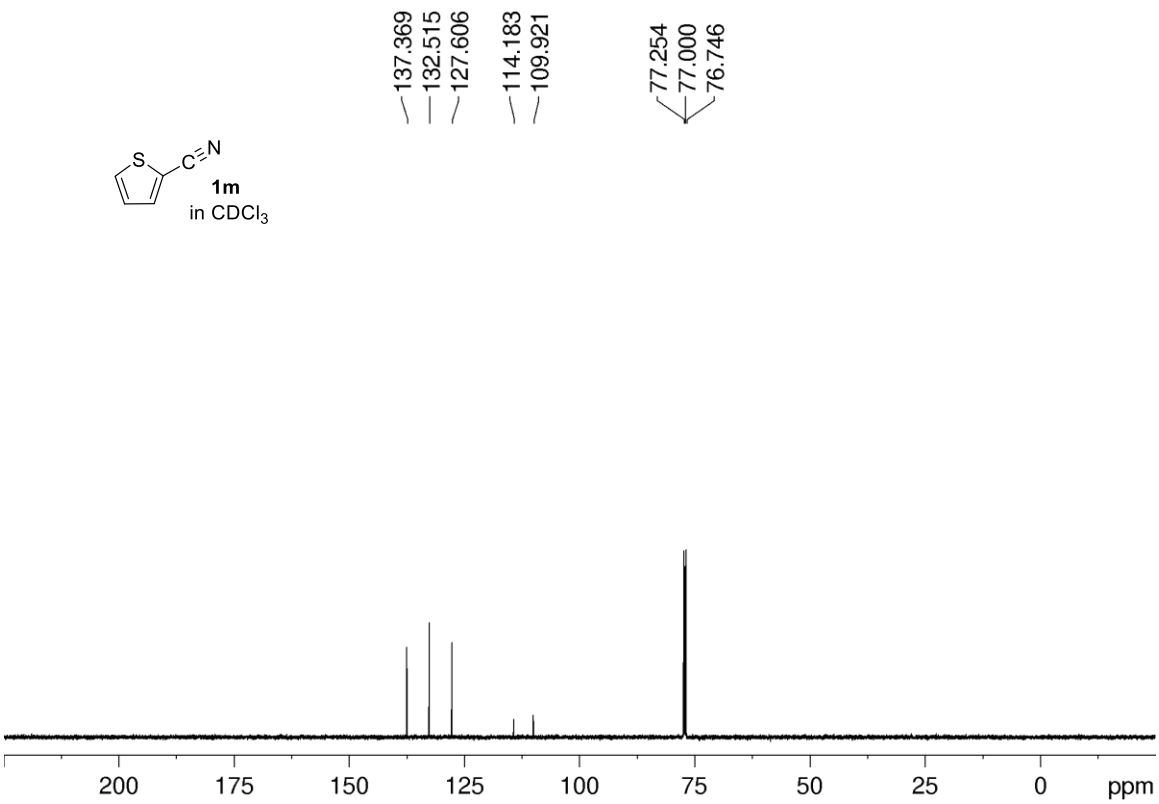
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
2.070
2.000

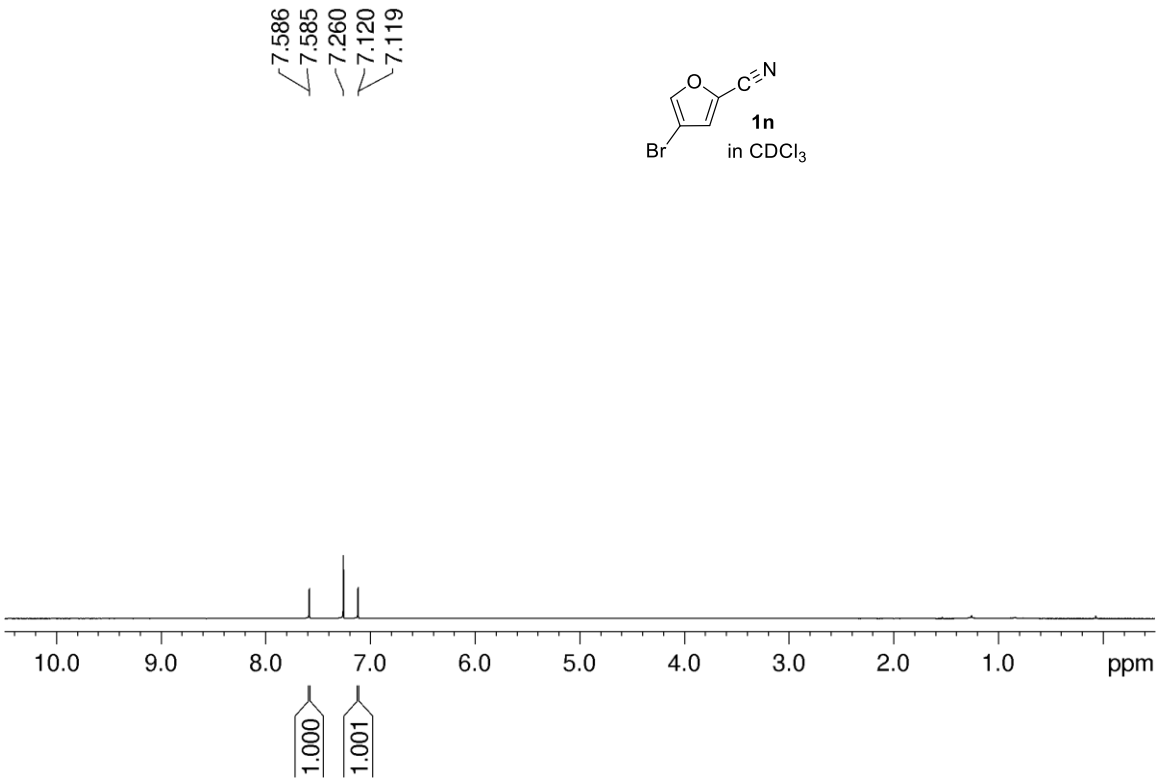

139.558
133.365
129.687
117.946
110.789
77.255
77.000
76.747
C≡N
Cl
1g
in CDCl3
200
175
150
125
100
75
50
25
0
ppm

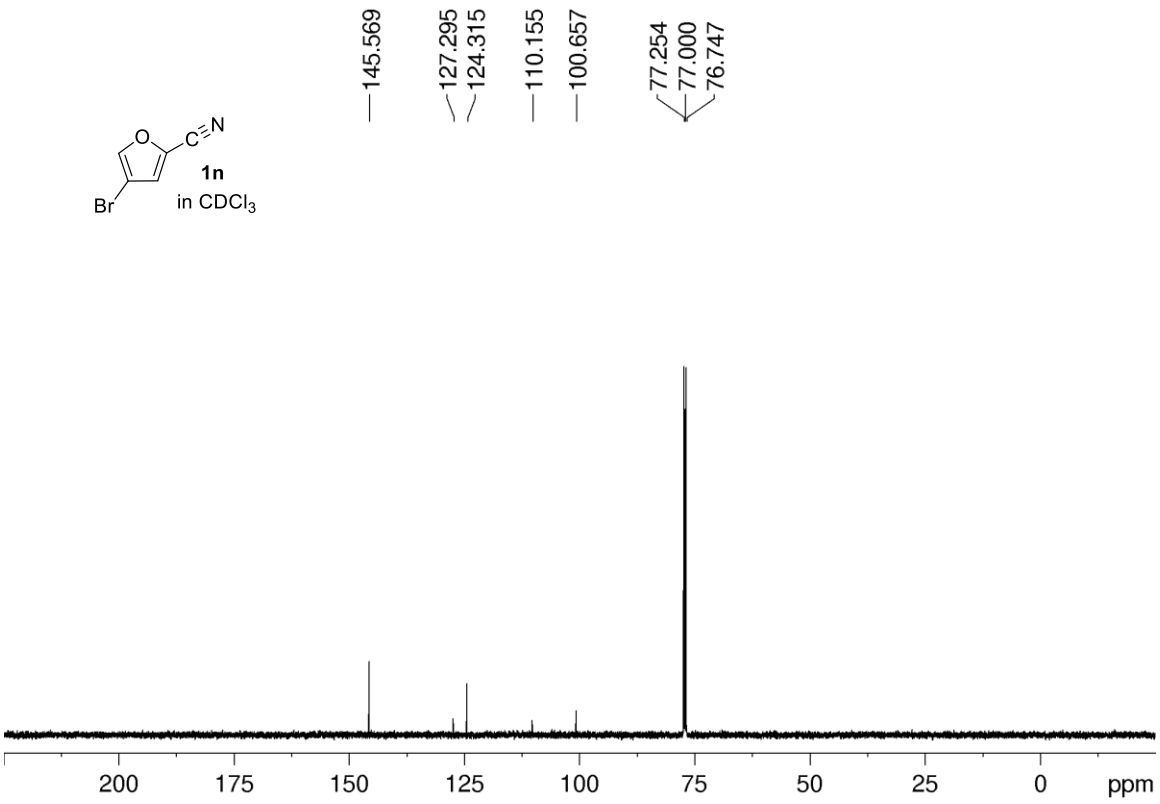

8.241
7.932
7.914
7.906
7.890
7.668
7.649
7.638
7.620
7.608
7.597
7.260
C≡N
1h
in CDCl3
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
1.000
3.043
3.097

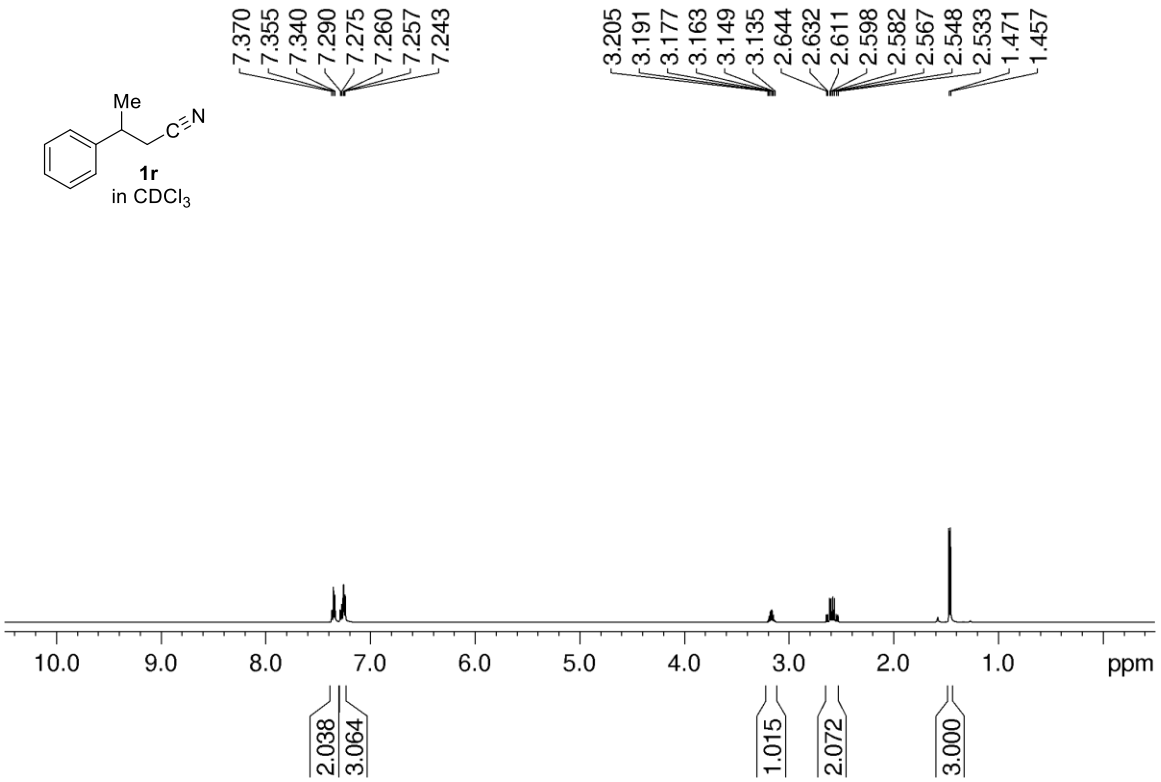

134.638
134.135
132.241
129.178
129.014
128.391
128.032
127.634
126.331
119.216
109.389
77.254
77.000
76.747
C≡N
1h
in CDCl3
200
175
150
125
100
75
50
25
0
ppm

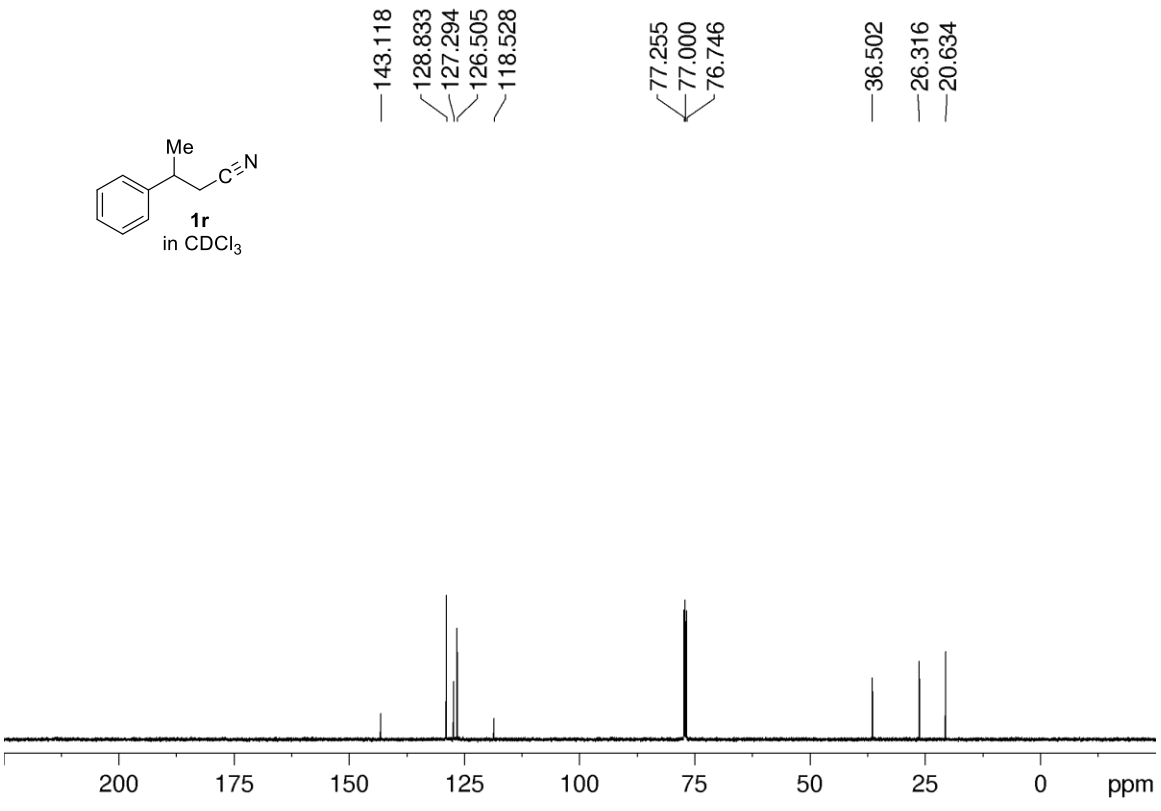

7.643
7.641
7.636
7.633
7.616
7.614
7.606
7.604
7.260
7.144
7.136
7.134
7.126
S
C≡N
1m
in CDCl3
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
1.009
1.006
1.000

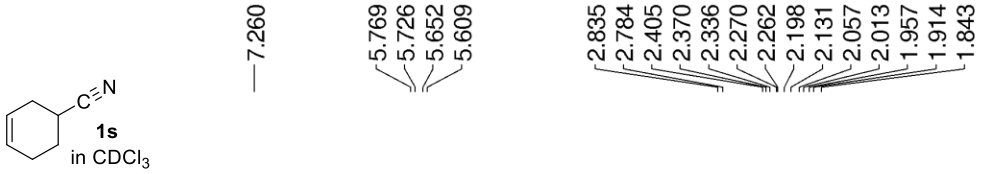

137.369
132.515
127.606
114.183
109.921
77.254
77.000
76.746
S
C≡N
1m
in CDCl3
200
175
150
125
100
75
50
25
0
ppm

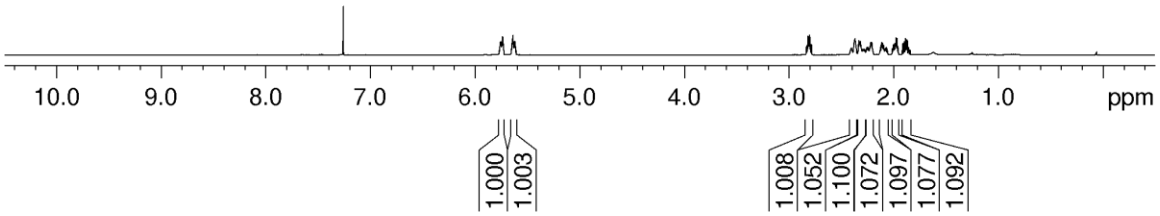

7.586
7.585
7.260
7.120
7.119
O
C≡N
Br
1n
in CDCl3
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
1.000
1.001

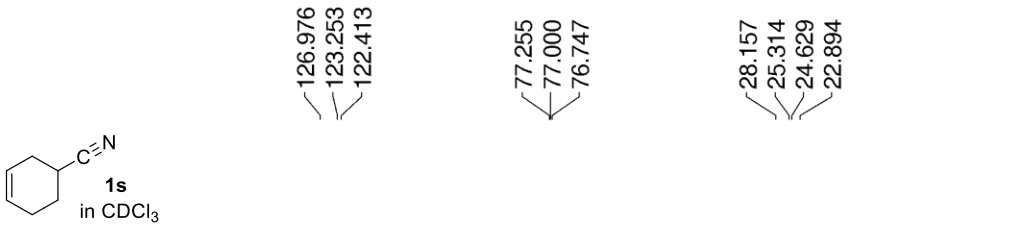

145.569
127.295
124.315
110.155
100.657
77.254
77.000
76.747
O
C≡N
Br
1n
in CDCl3
200
175
150
125
100
75
50
25
0
ppm

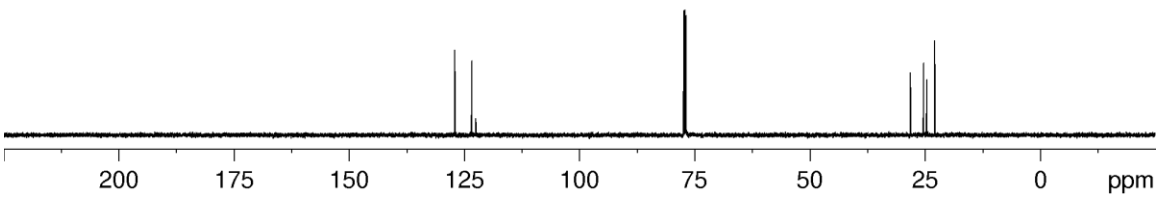

7.370
7.355
7.340
7.290
7.275
7.260
7.257
7.243
3.205
3.191
3.177
3.163
3.149
3.135
2.644
2.632
2.611
2.598
2.582
2.567
2.548
2.533
1.471
1.457
Me
C≡N
1r
in CDCl3
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
2.038
3.064
1.015
2.072
3.000

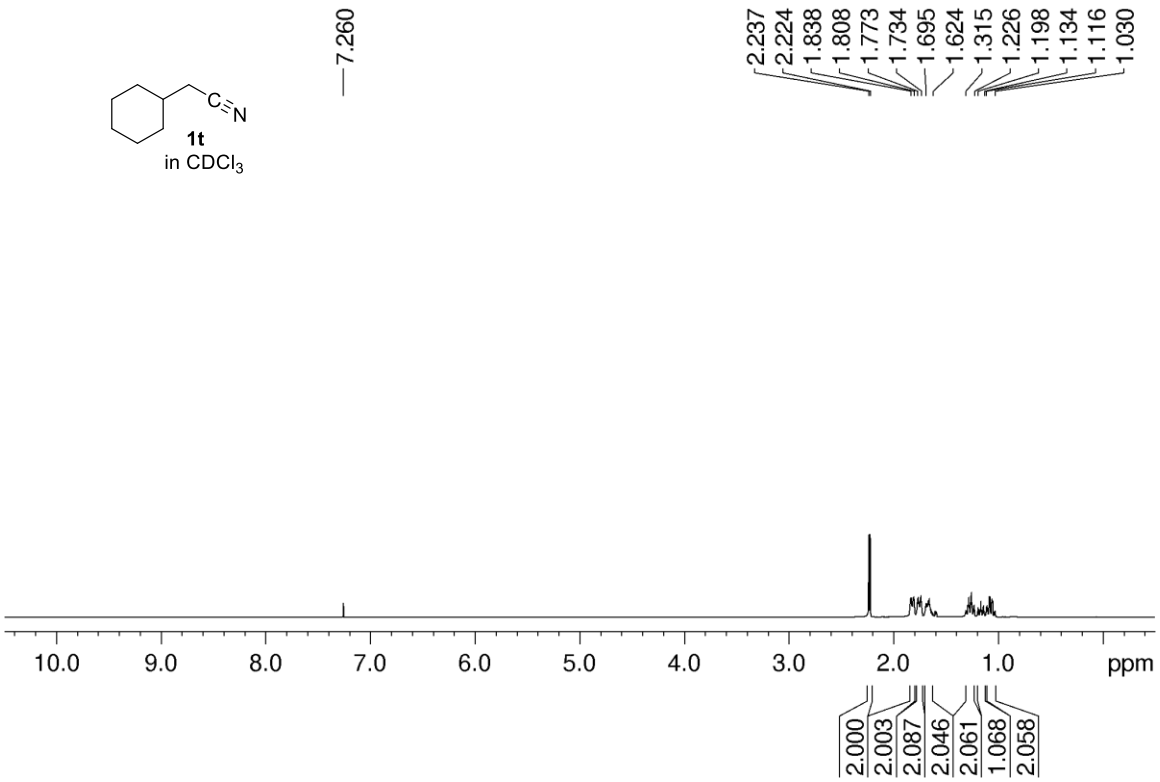

143.118
128.833
127.294
126.505
118.528
77.255
77.000
76.746
36.502
26.316
20.634
Me
C≡N
1r
in CDCl3
200
175
150
125
100
75
50
25
0
ppm

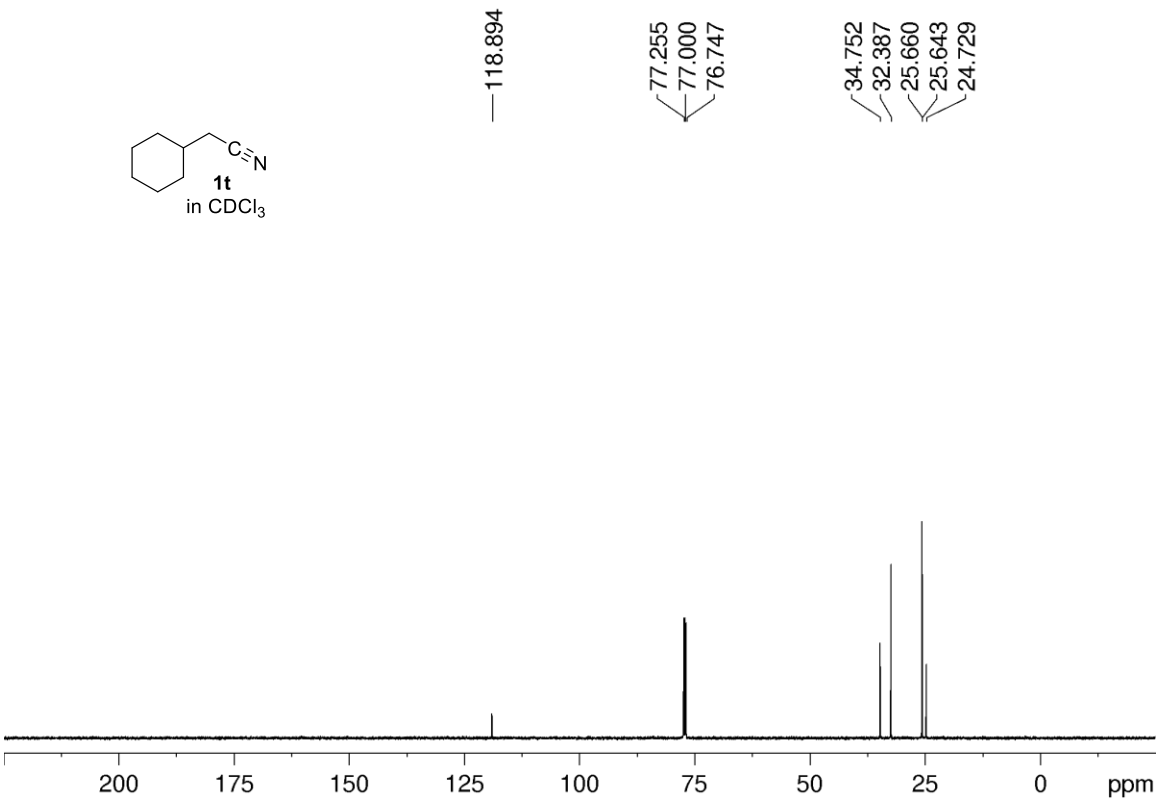

7.260
5.769
5.726
5.652
5.609
2.835
2.784
2.405
2.370
2.336
2.270
2.262
2.198
2.131
2.057
2.013
1.957
1.914
1.843
1s
in CDCl3

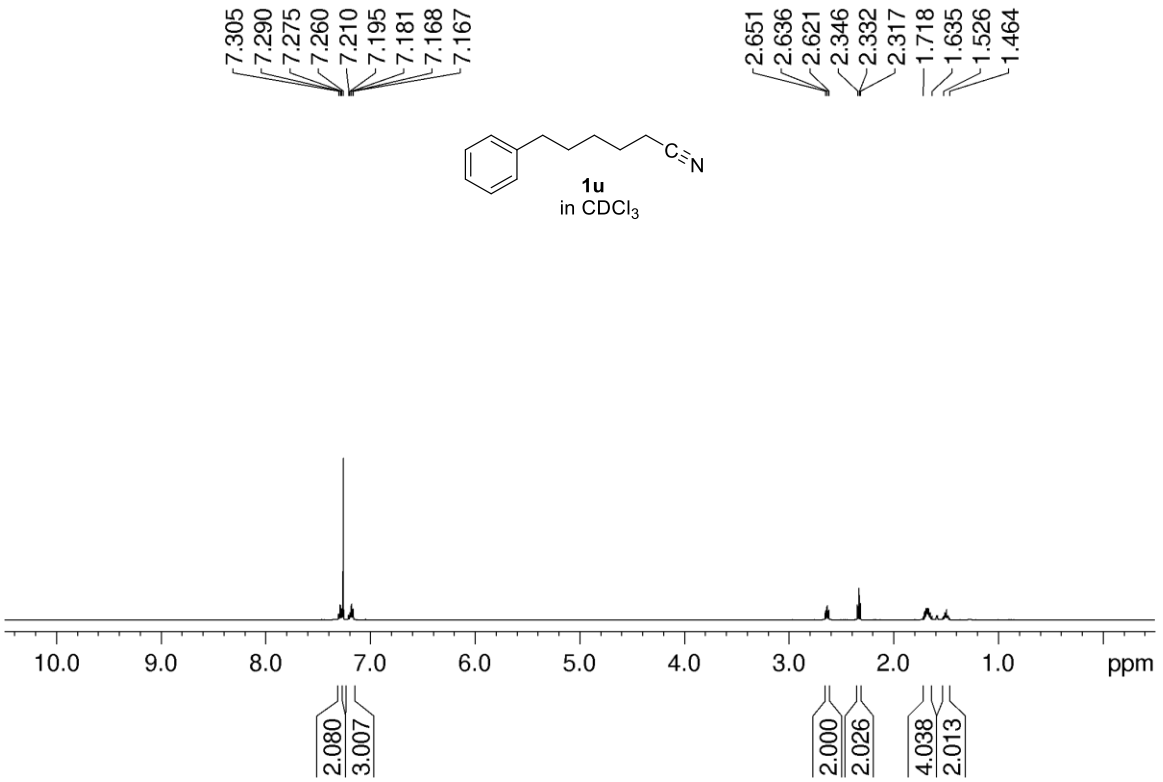

10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
1.000
1.003
1.008
1.052
1.100
1.072
1.097
1.077
1.092

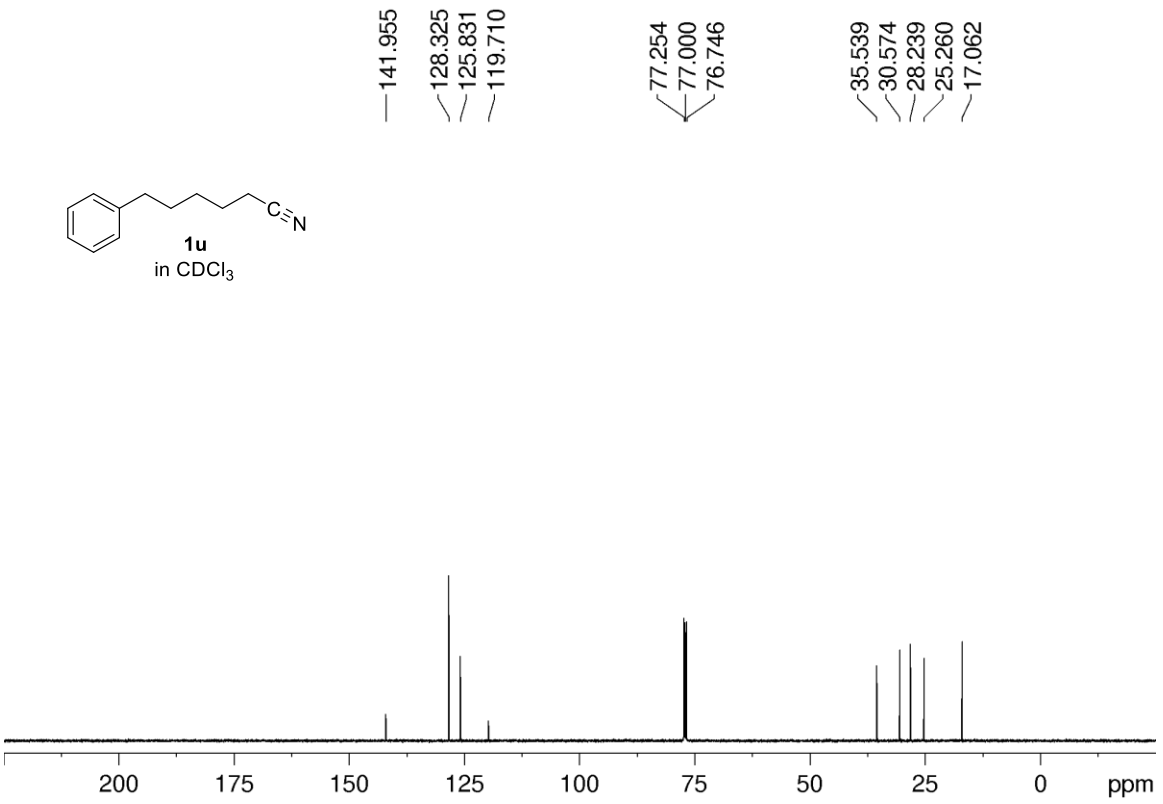

126.976
123.253
122.413
77.255
77.000
76.747
28.157
25.314
24.629
22.894
1s
in CDCl3

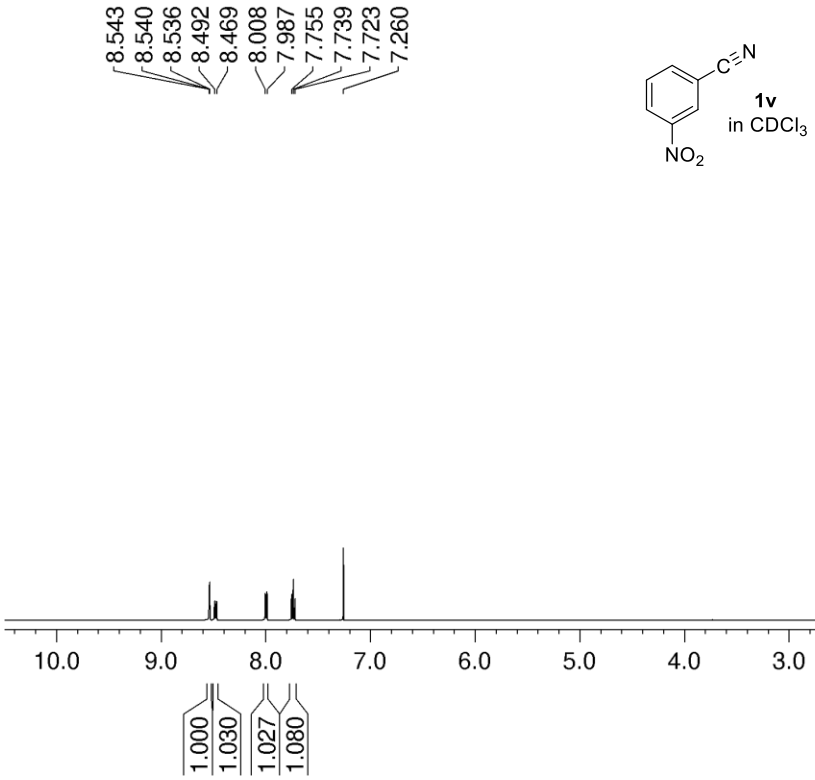

200
175
150
125
100
75
50
25
0
ppm

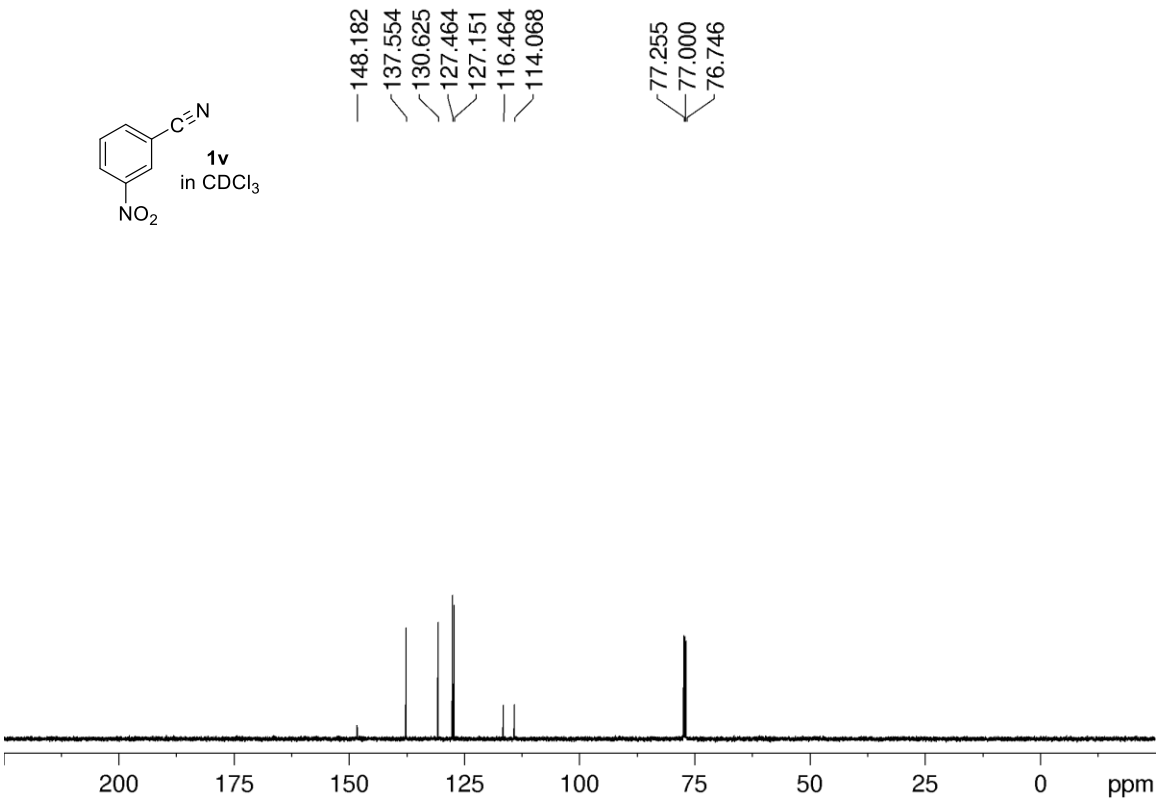

7.260
2.237
2.224
1.838
1.808
1.773
1.734
1.695
1.624
1.315
1.226
1.198
1.134
1.116
1.030
C≡N
1t
in CDCl3
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
2.000
2.003
2.087
2.046
2.061
1.068
2.058

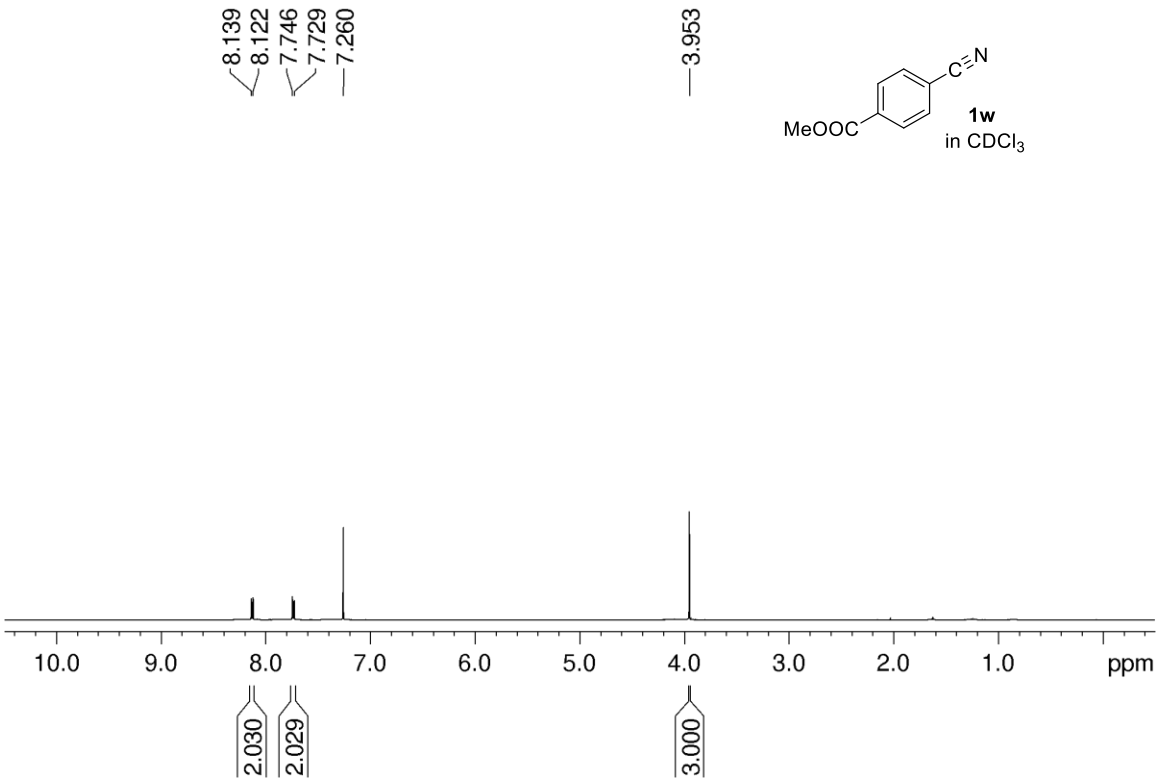

118.894
77.255
77.000
76.747
34.752
32.387
25.660
25.643
24.729
C≡N
1t
in CDCl3
200
175
150
125
100
75
50
25
0
ppm

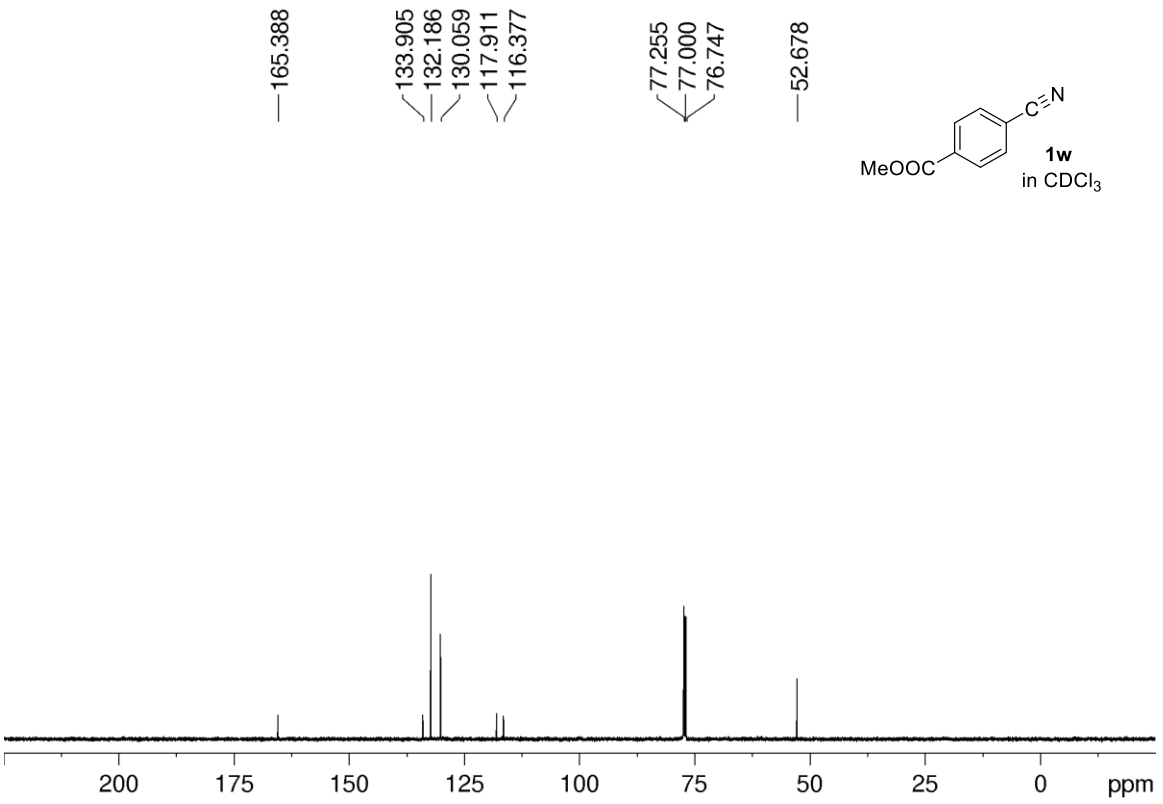

7.305
7.290
7.275
7.260
7.210
7.195
7.181
7.168
7.167
2.651
2.636
2.621
2.346
2.332
2.317
1.718
1.635
1.526
1.464
C≡N
1u
in CDCl3
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
2.080
3.007
2.000
2.026
4.038
2.013


141.955
128.325
125.831
119.710
77.254
77.000
76.746
35.539
30.574
28.239
25.260
17.062
C≡N
1u
in CDCl3
200
175
150
125
100
75
50
25
0
ppm

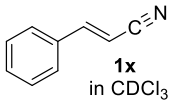

8.543
8.540
8.536
8.492
8.469
8.008
7.987
7.755
7.739
7.723
7.260
1v
in CDCl3
NO2
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
1.000
1.030
1.027
1.080

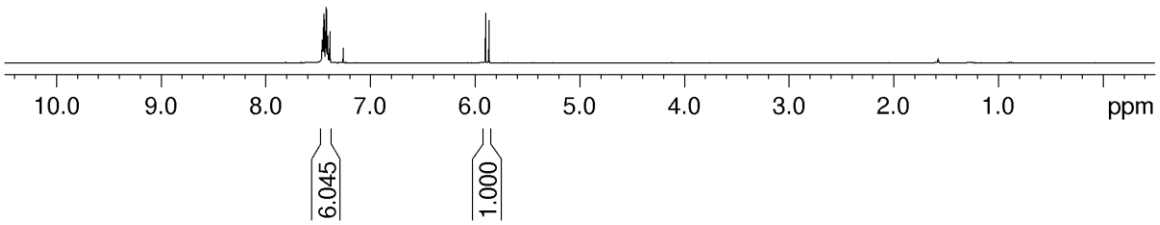

148.182
137.554
130.625
127.464
127.151
116.464
114.068
77.255
77.000
76.746
1v
in CDCl3
NO2
200
175
150
125
100
75
50
25
0
ppm

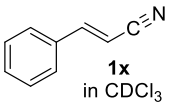

8.139
8.122
7.746
7.729
7.260
3.953
MeOOC
1w
in CDCl3
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
2.030
2.029
3.000

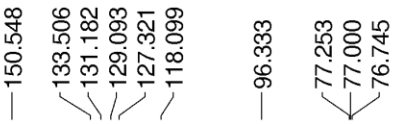

165.388
133.905
132.186
130.059
117.911
116.377
77.255
77.000
76.747
52.678
MeOOC
1w
in CDCl3
200
175
150
125
100
75
50
25
0
ppm

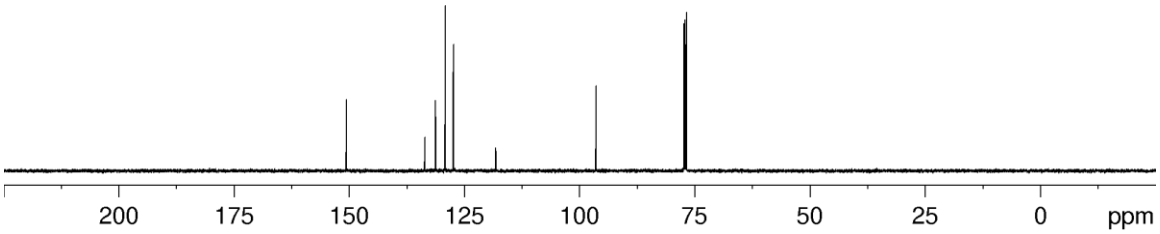

7.463
7.460
7.456
7.448
7.444
7.440
7.431
7.428
7.423
7.418
7.412
7.409
7.404
7.397
7.392
7.388
7.260
5.900
5.867

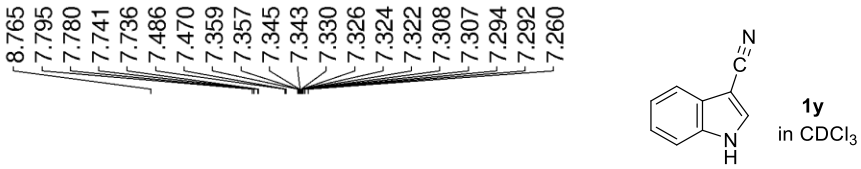

N
1x
in CDCl3


10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
6.045
1.000


N
1x
in CDCl3


150.548
133.506
131.182
129.093
127.321
118.099
96.333
77.253
77.000
76.745


200
175
150
125
100
75
50
25
0
ppm


8.765
7.795
7.780
7.741
7.736
7.486
7.470
7.359
7.357
7.345
7.343
7.330
7.326
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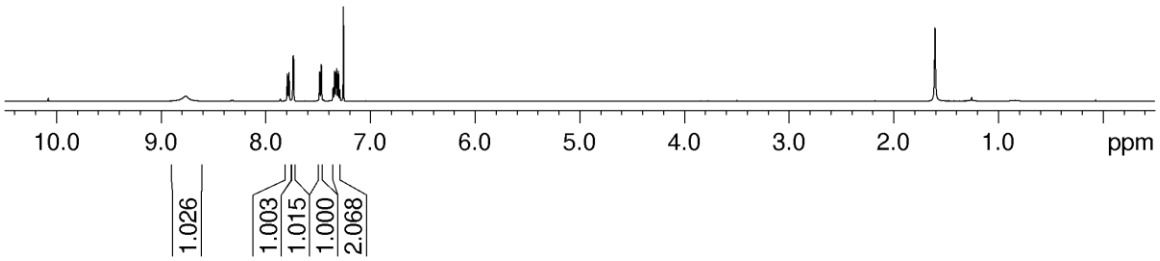
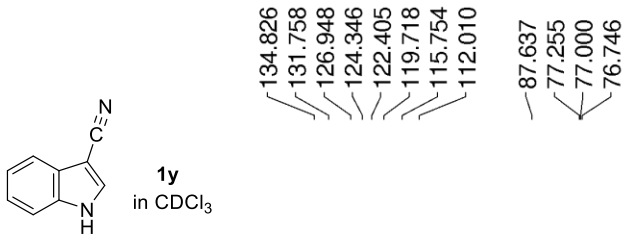
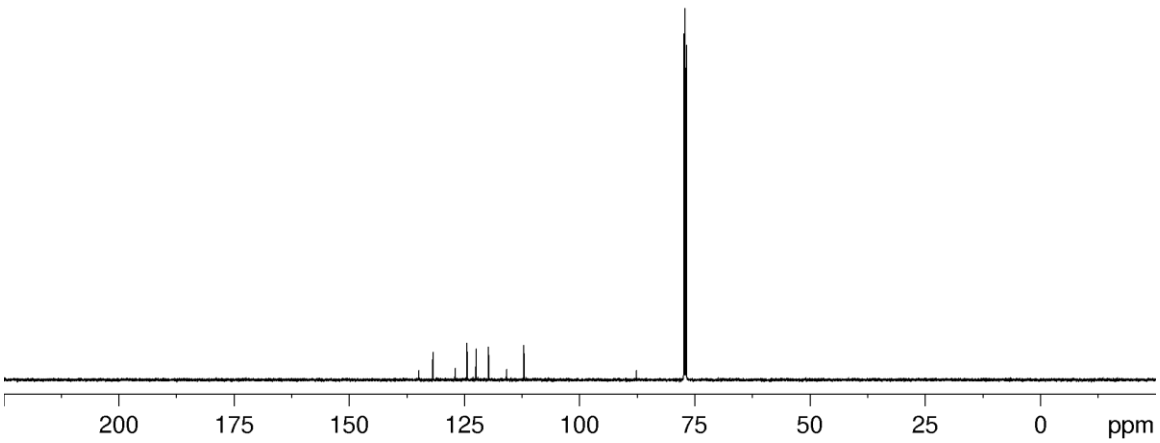
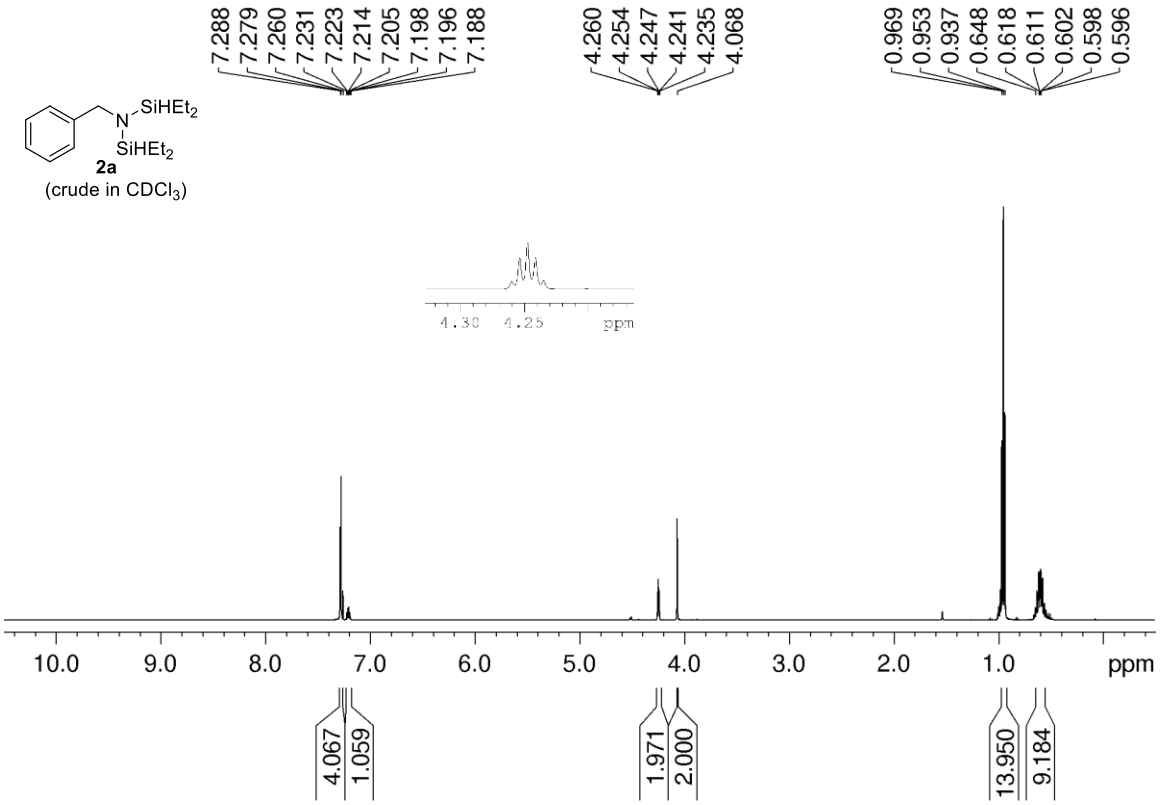
7.292
7.260
N
C
N
H
1y
in CDCl3

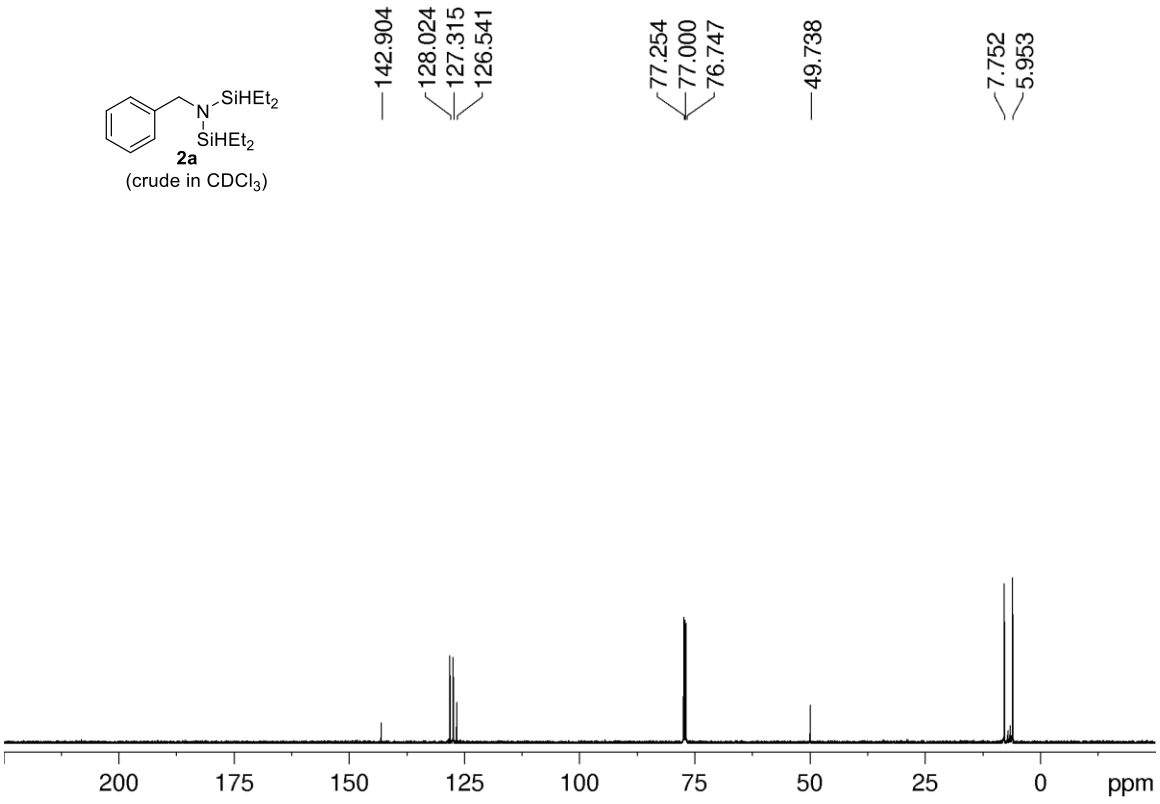

10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
1.026
1.003
1.015
1.000
2.068

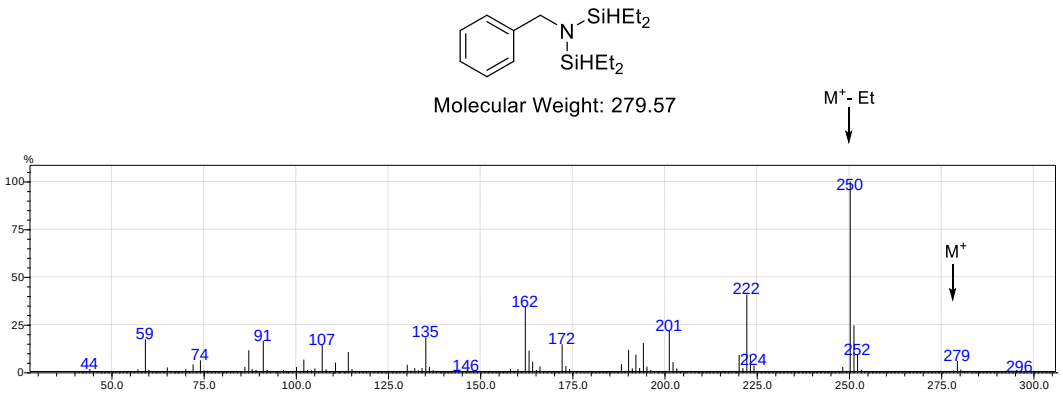

134.826
131.758
126.948
124.346
122.405
119.718
115.754
112.010
87.637
77.255
77.000
76.746
N
C
N
H
1y
in CDCl3

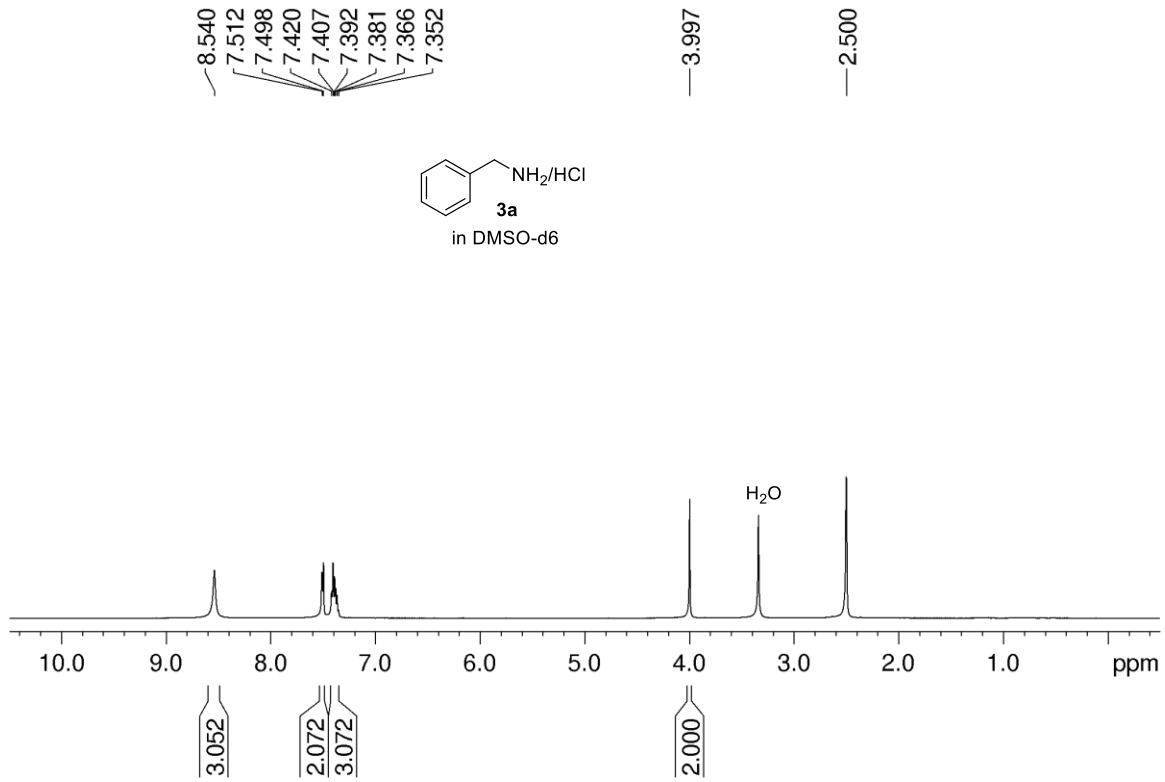

200
175
150
125
100
75
50
25
0
ppm

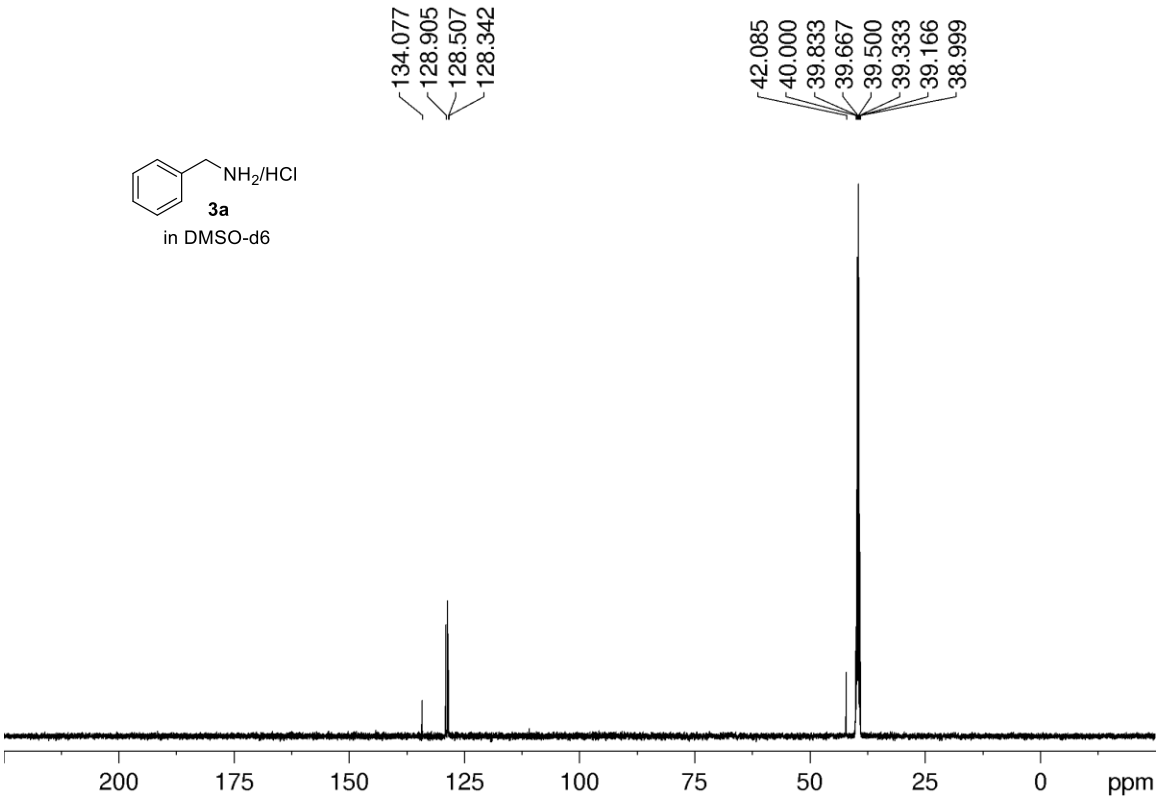
^{1}H and ^{13}C NMR spectra of products (500 MHz)

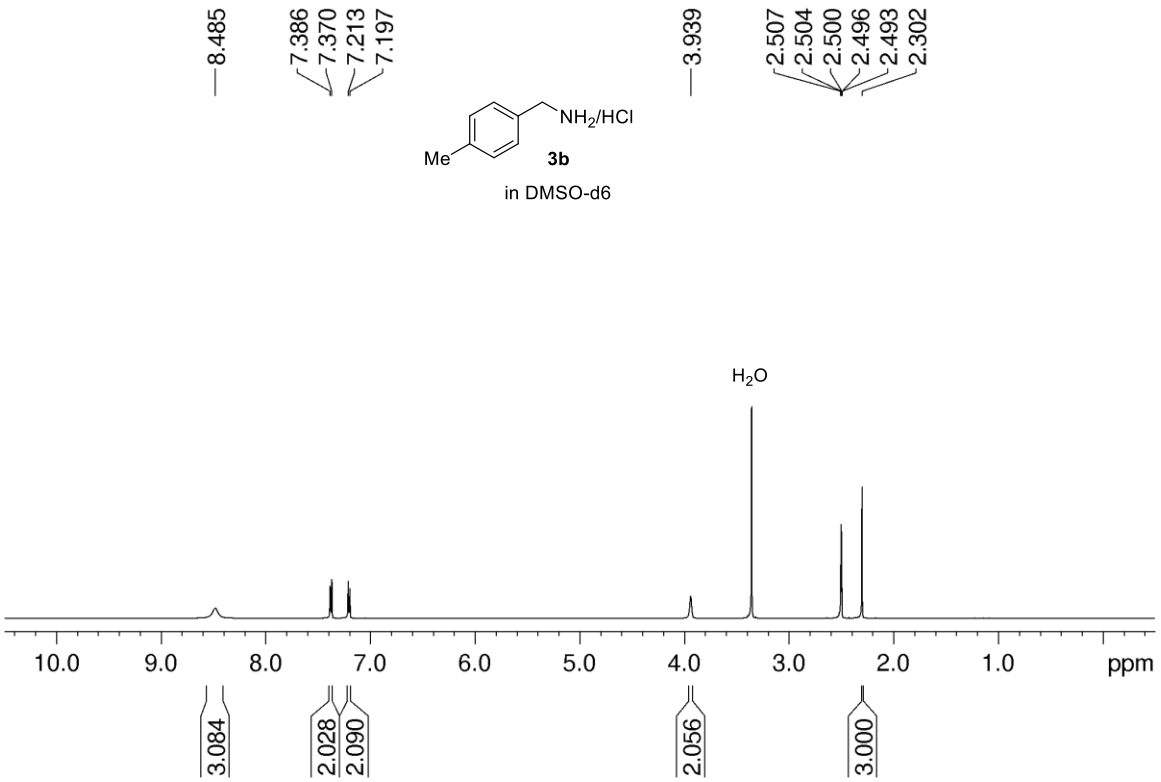


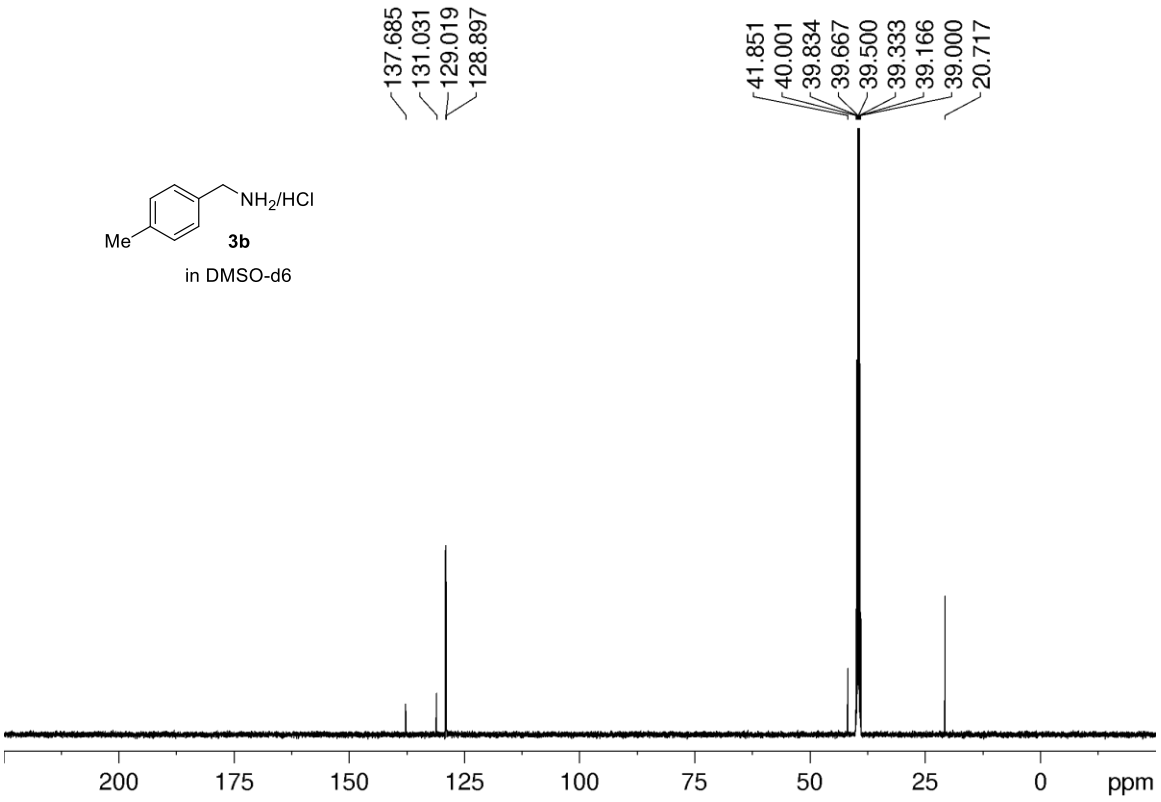



SiHEt2
N
SiHEt2
Molecular Weight: 279.57
M+- Et
M+
%
100
75
50
25
0
250
222
162
201
59
91
107
135
172
74
44
146
224
252
279
296
50.0
75.0
100.0
125.0
150.0
175.0
200.0
225.0
250.0
275.0
300.0


8.540
7.512
7.498
7.420
7.407
7.392
7.381
7.366
7.352
3.997
2.500
NH2/HCl
3a
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.052
2.072
3.072
2.000


134.077
128.905
128.507
128.342
42.085
40.000
39.833
39.667
39.500
39.333
39.166
38.999
NH2/HCl
3a
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm


8.485
7.386
7.370
7.213
7.197
3.939
2.507
2.504
2.500
2.496
2.493
2.302
NH2/HCl
Me
3b
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.084
2.028
2.090
2.056
3.000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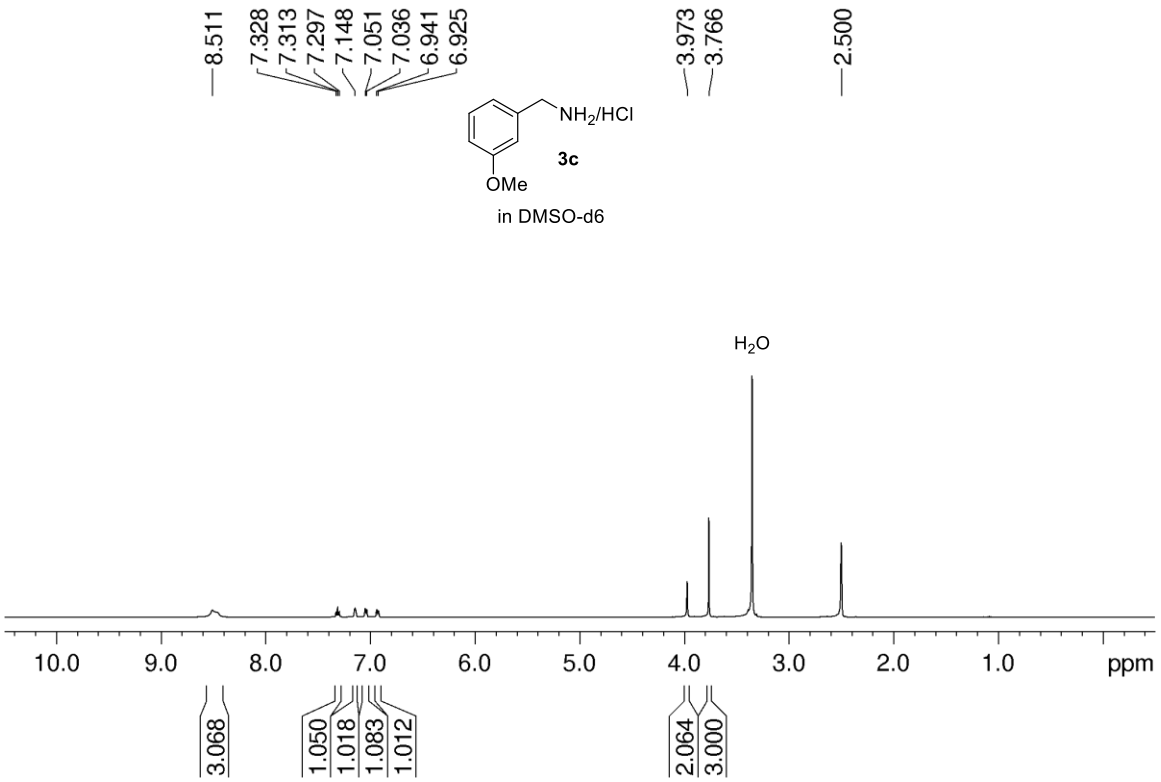
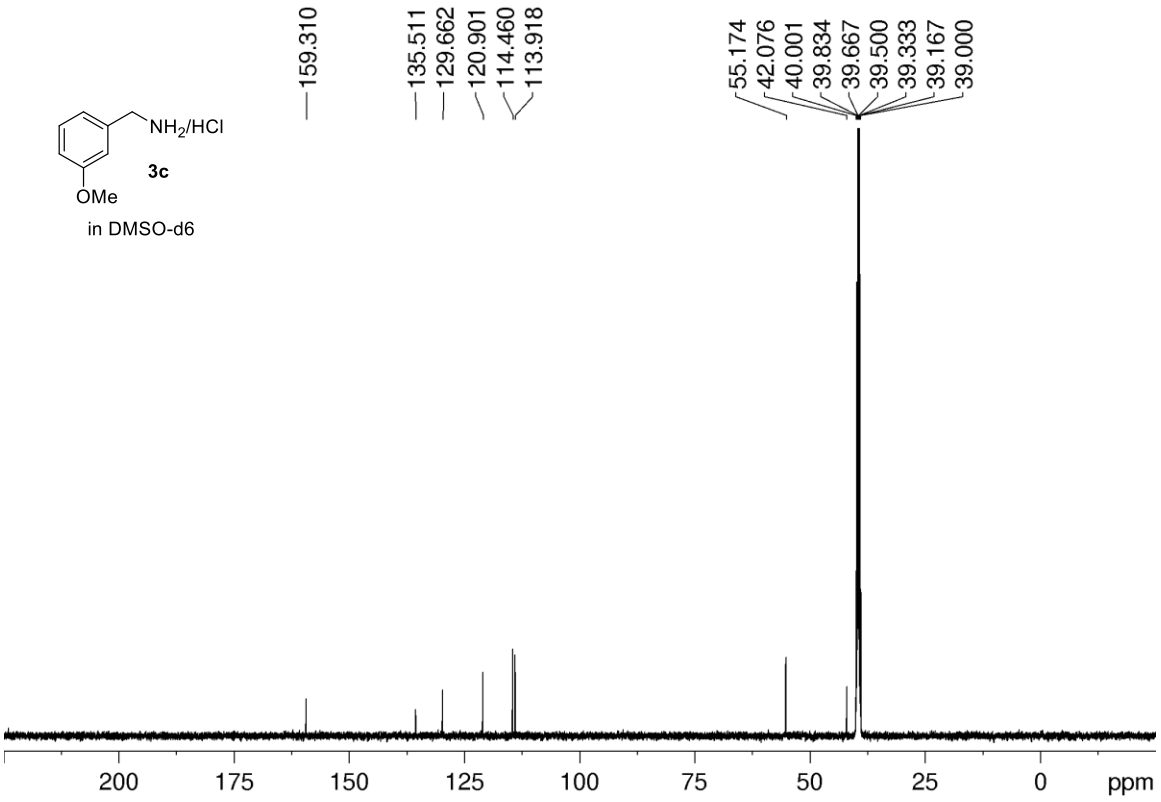
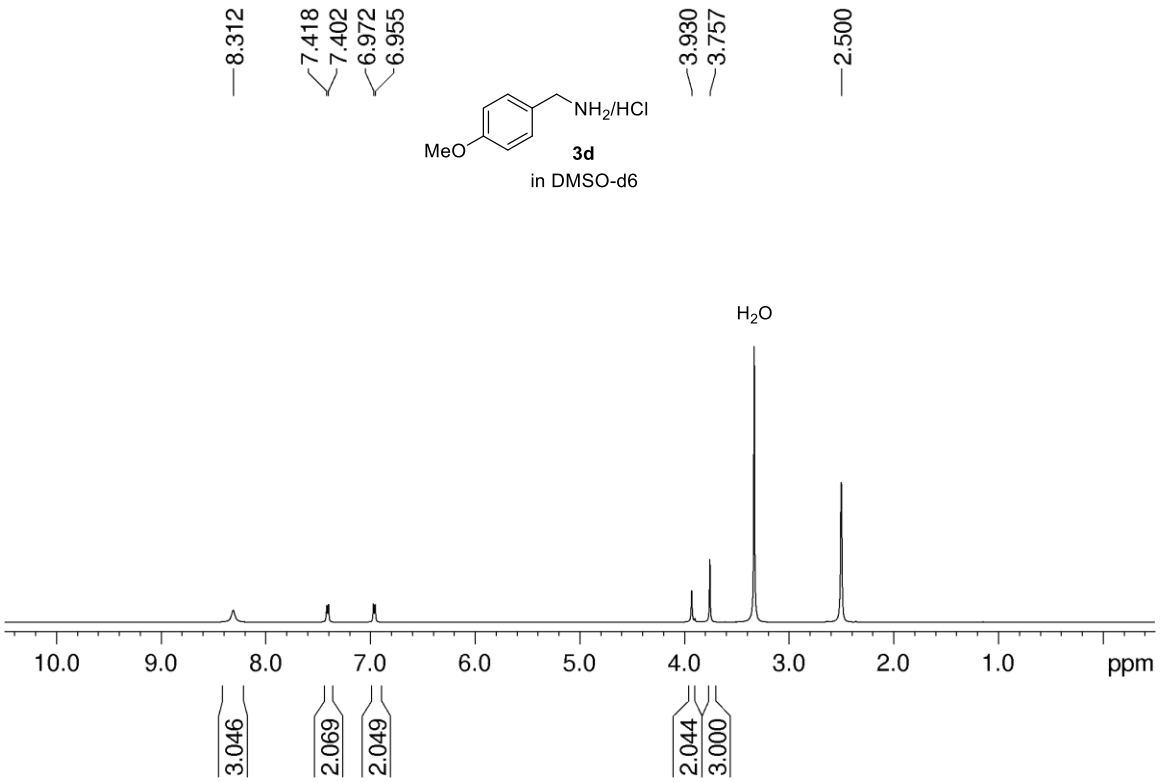
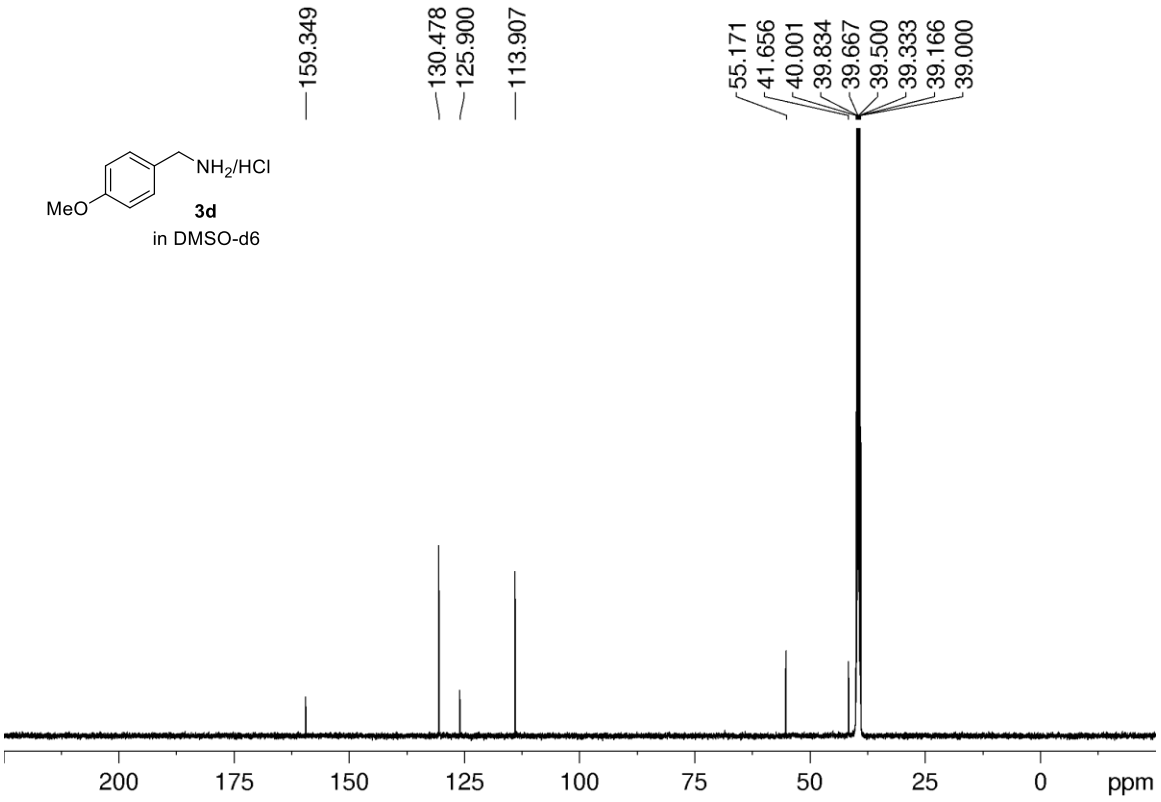
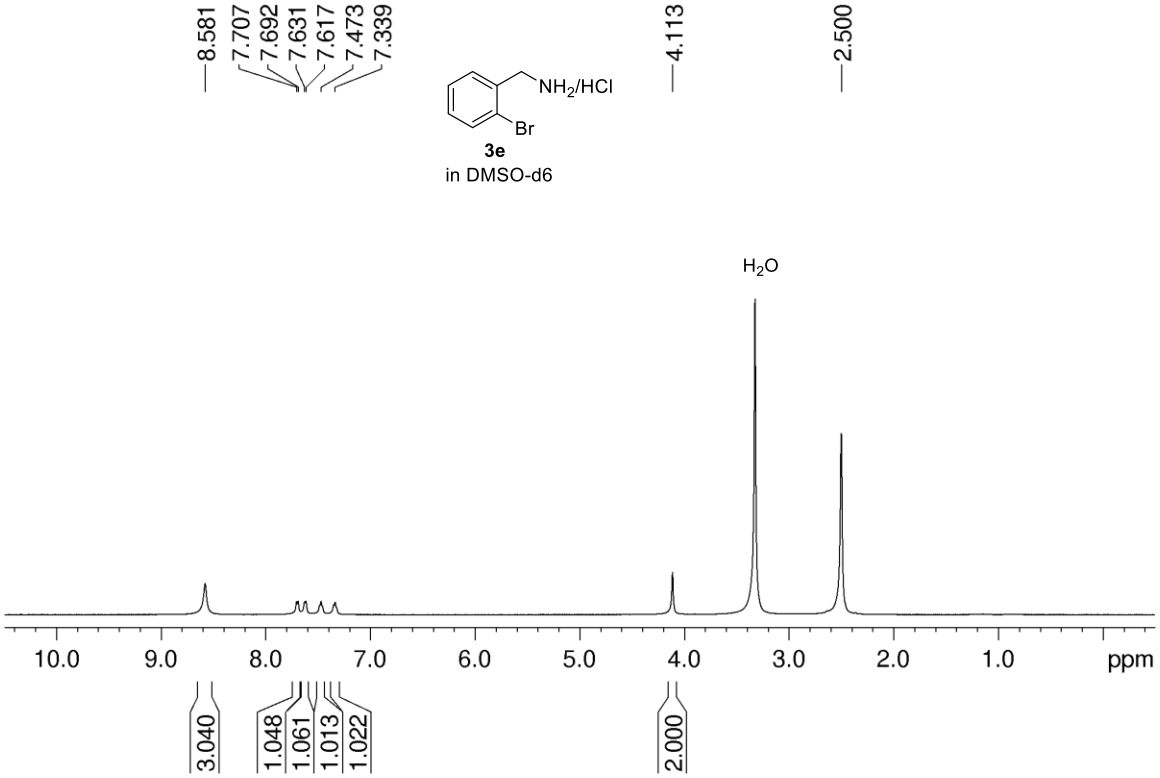
131.031
129.019
128.897
41.851
40.001
39.834
39.667
39.500
39.333
39.166
39.000
20.717
NH2/HCl
Me
3b
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

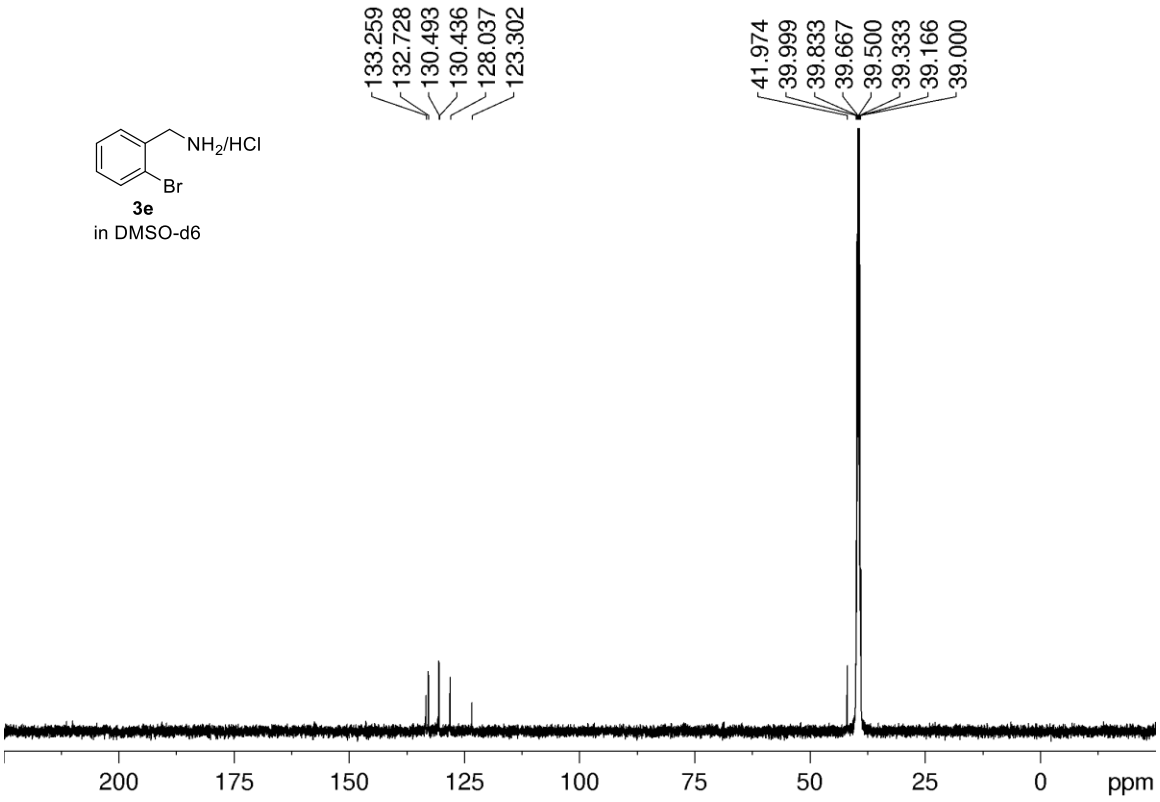

8.511
7.328
7.313
7.297
7.148
7.051
7.036
6.941
6.925
3.973
3.766
2.500
NH2/HCl
3c
OMe
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.068
1.050
1.018
1.083
1.012
2.064
3.000

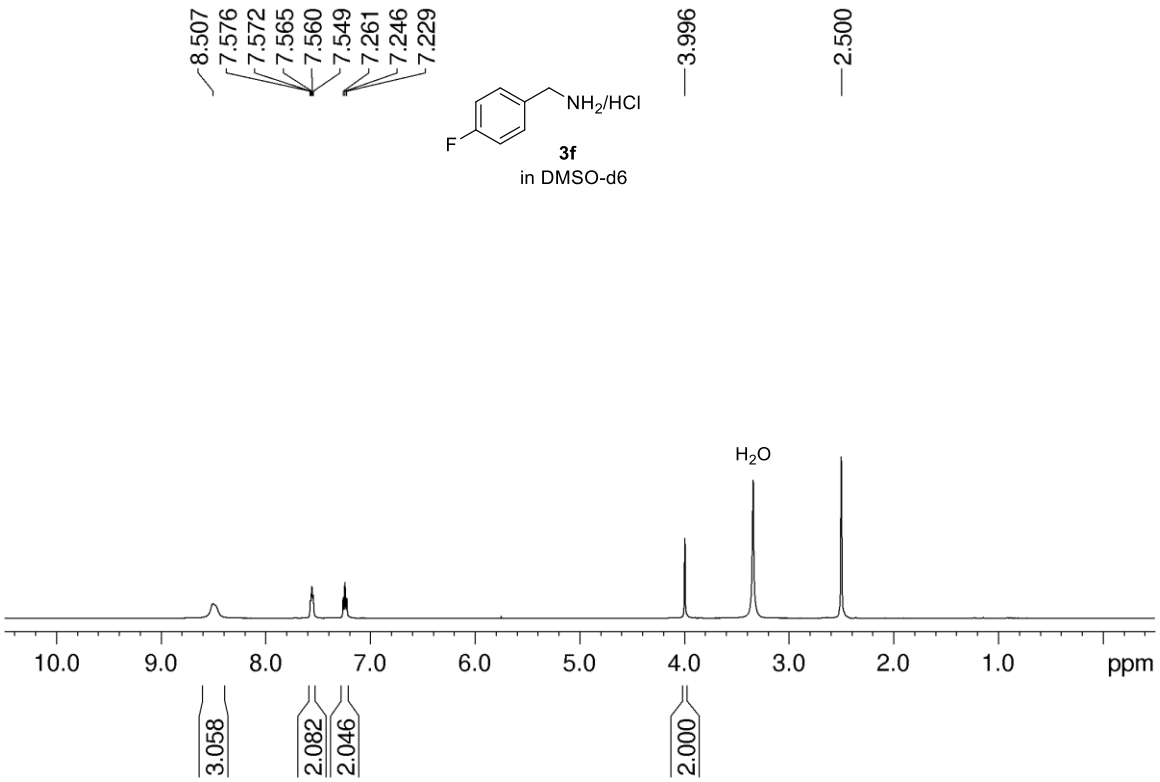

159.310
135.511
129.662
120.901
114.460
113.918
55.174
42.076
40.001
39.834
39.667
39.500
39.333
39.167
39.000
NH2/HCl
3c
OMe
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

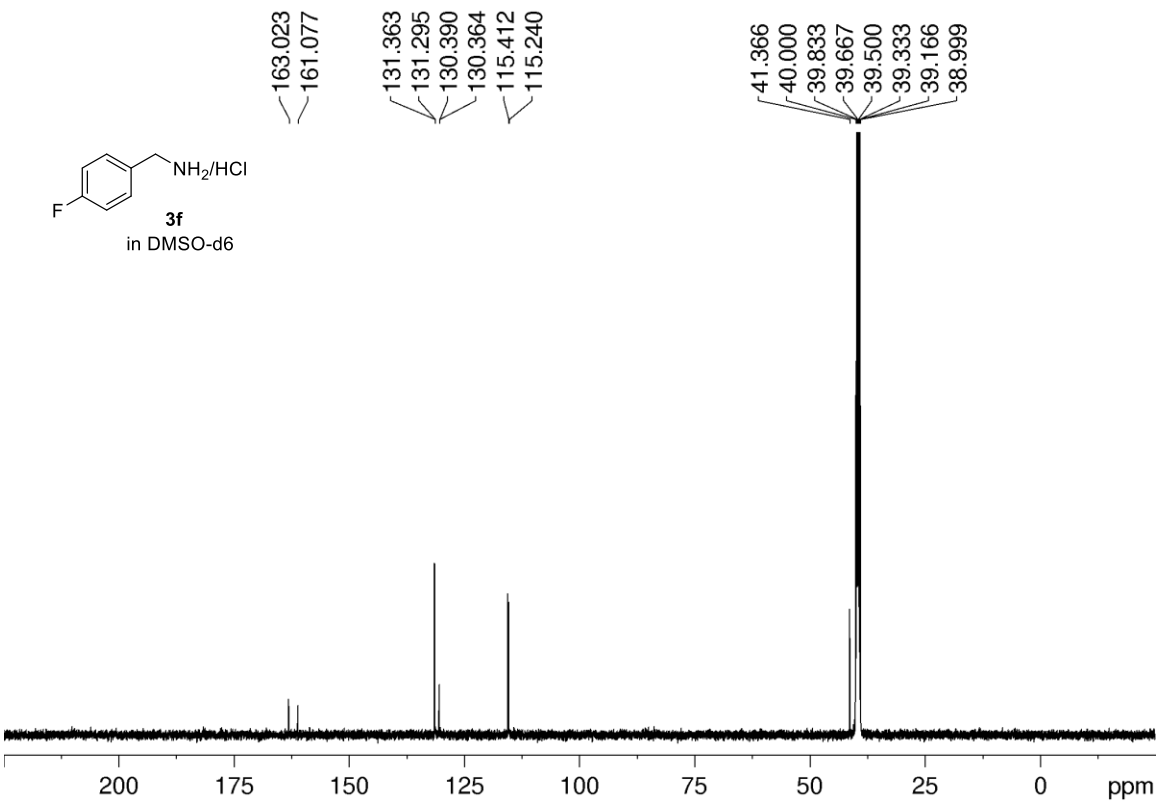

8.312
7.418
7.402
6.972
6.955
3.930
3.757
2.500
NH2/HCl
MeO
3d
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.046
2.069
2.049
2.044
3.000

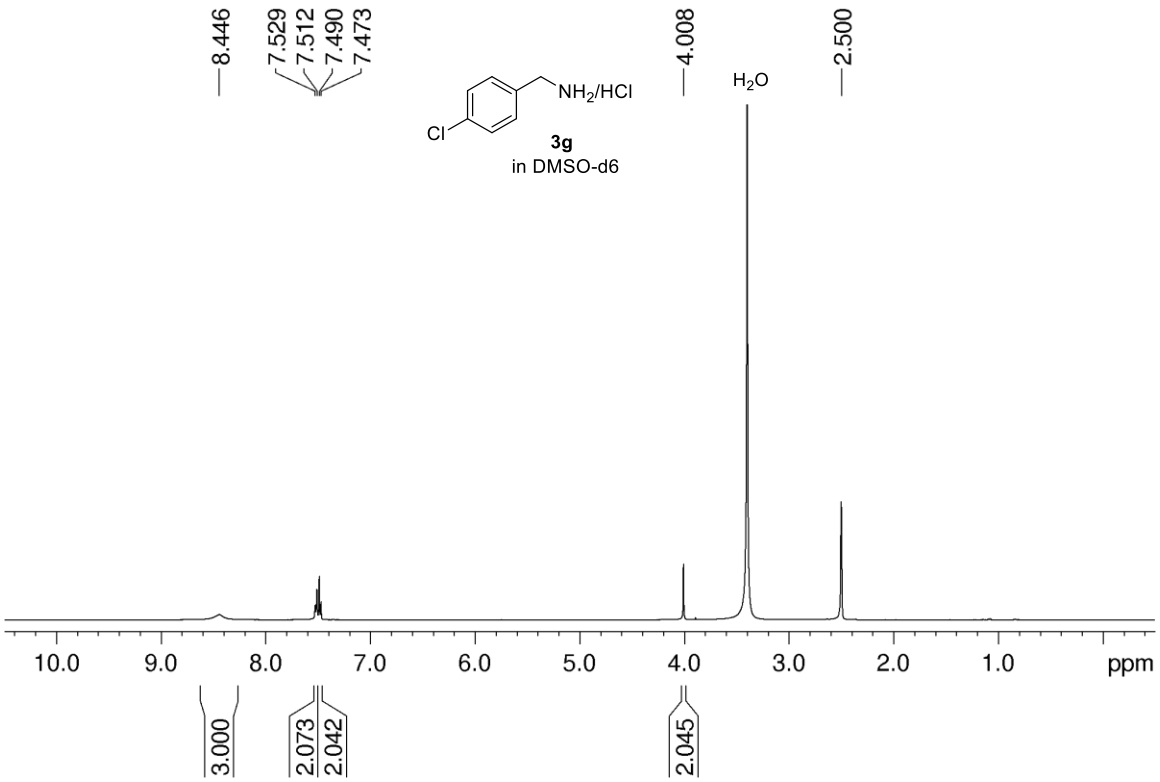

159.349
130.478
125.900
113.907
55.171
41.656
40.001
39.834
39.667
39.500
39.333
39.166
39.000
NH2/HCl
MeO
3d
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

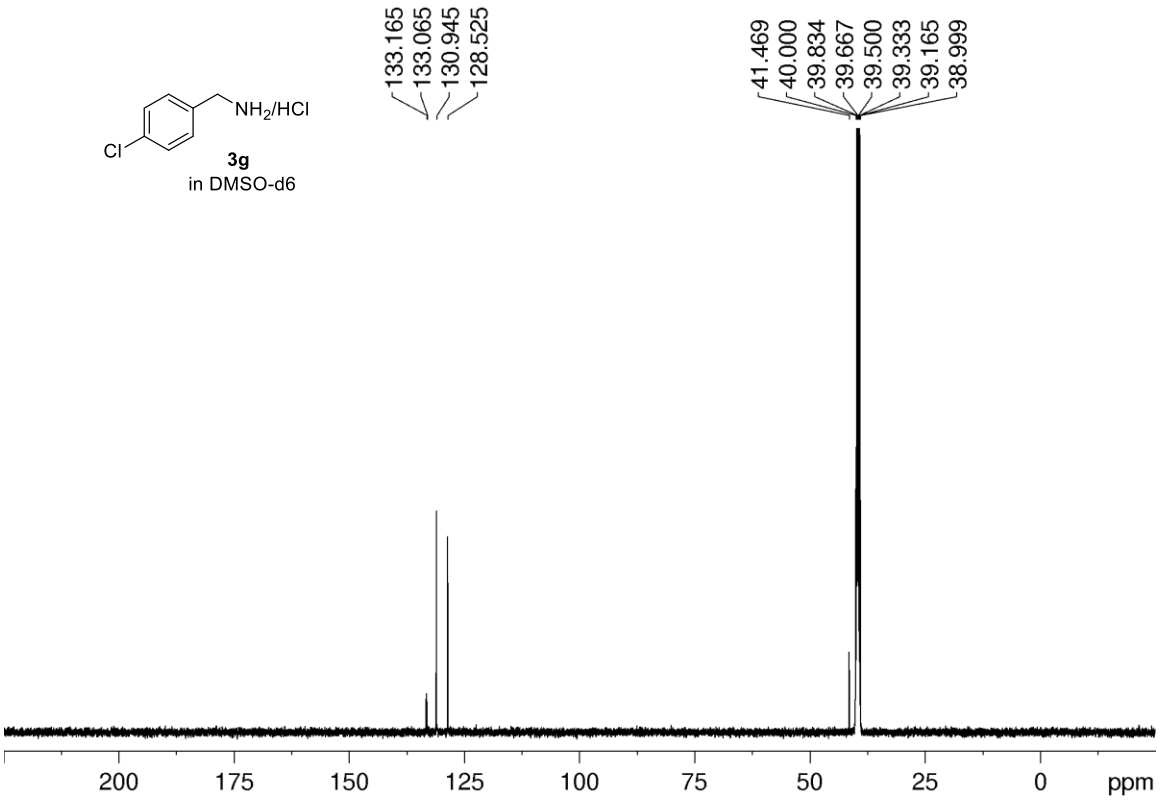

8.581
7.707
7.692
7.631
7.617
7.473
7.339
4.113
2.500
NH2/HCl
Br
3e
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.040
1.048
1.061
1.013
1.022
2.000

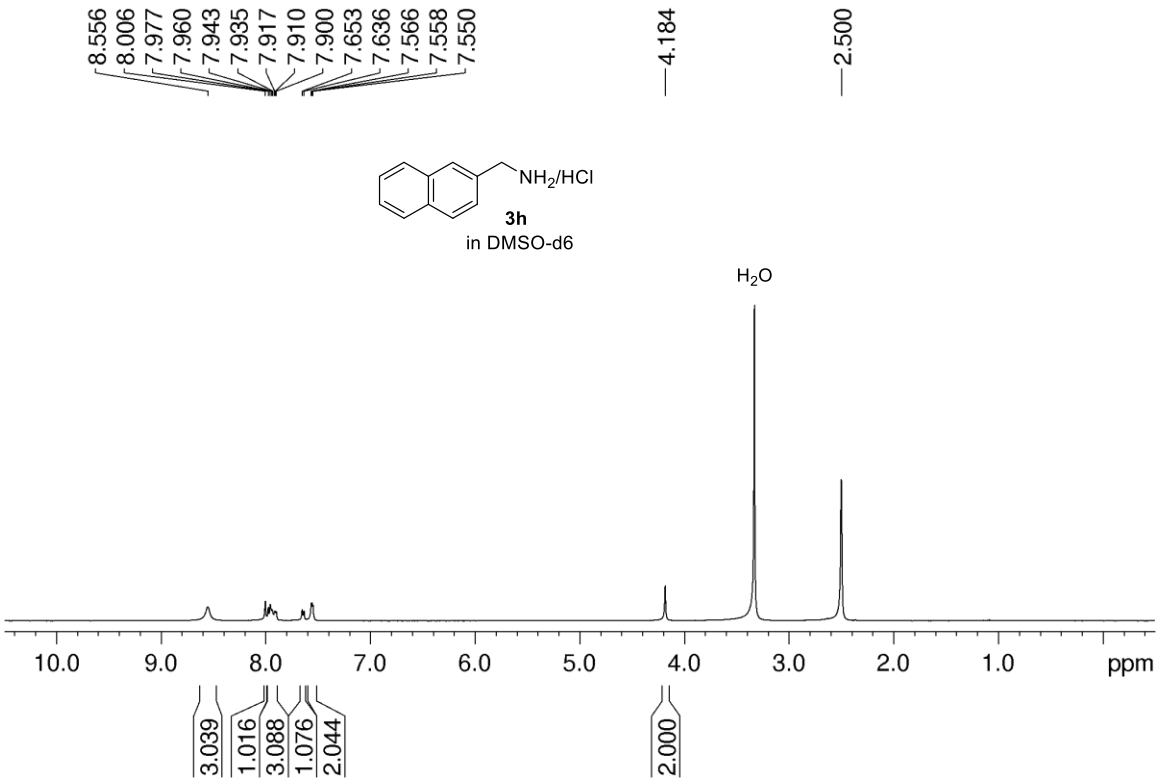

133.259
132.728
130.493
130.436
128.037
123.302
41.974
39.999
39.833
39.667
39.500
39.333
39.166
39.000
NH2/HCl
Br
3e
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

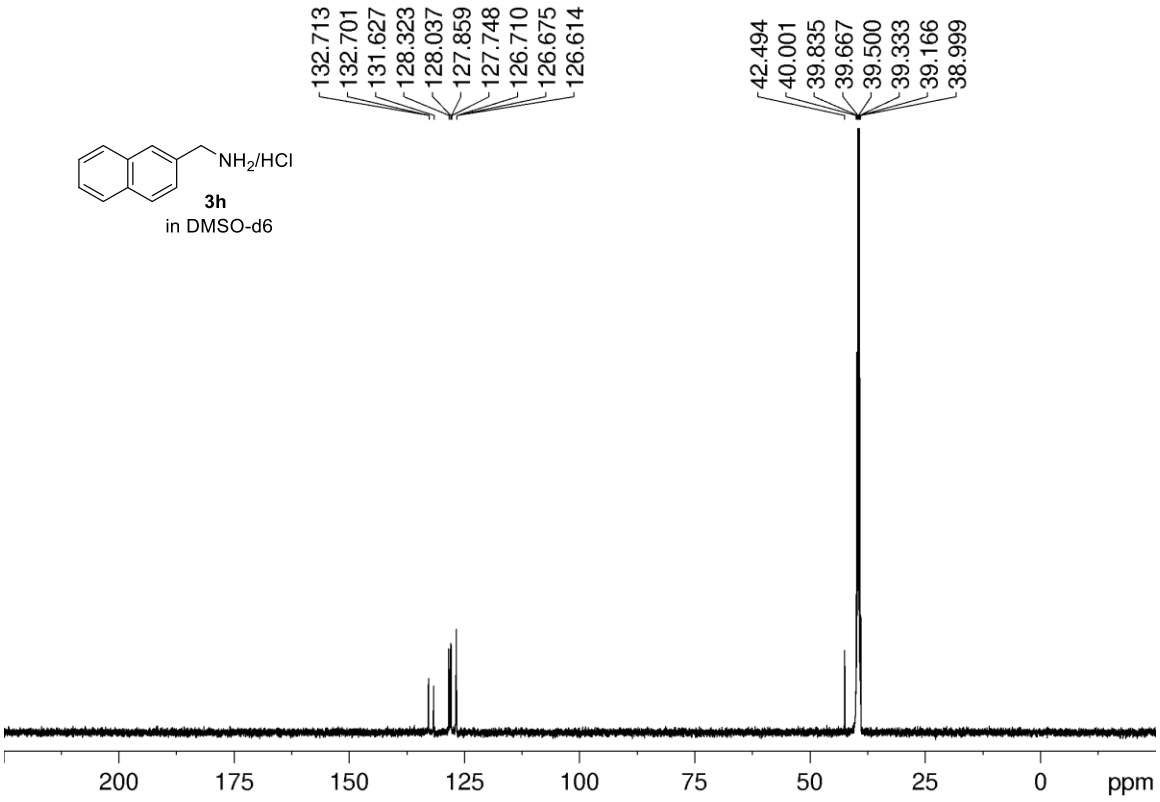

8.507
7.576
7.572
7.565
7.560
7.549
7.261
7.246
7.229
3.996
2.500
NH2/HCl
F
3f
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.058
2.082
2.046
2.000

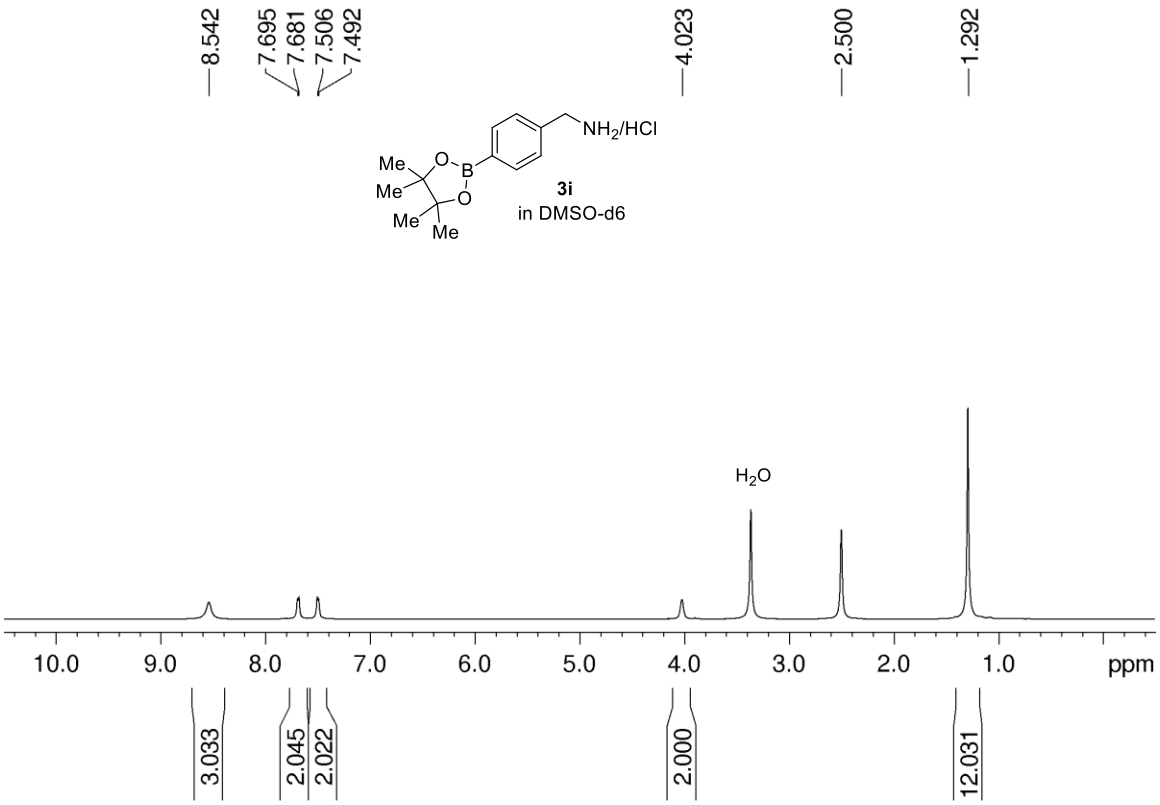

163.023
161.077
131.363
131.295
130.390
130.364
115.412
115.240
41.366
40.000
39.833
39.667
39.500
39.333
39.166
38.999
NH2/HCl
F
3f
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

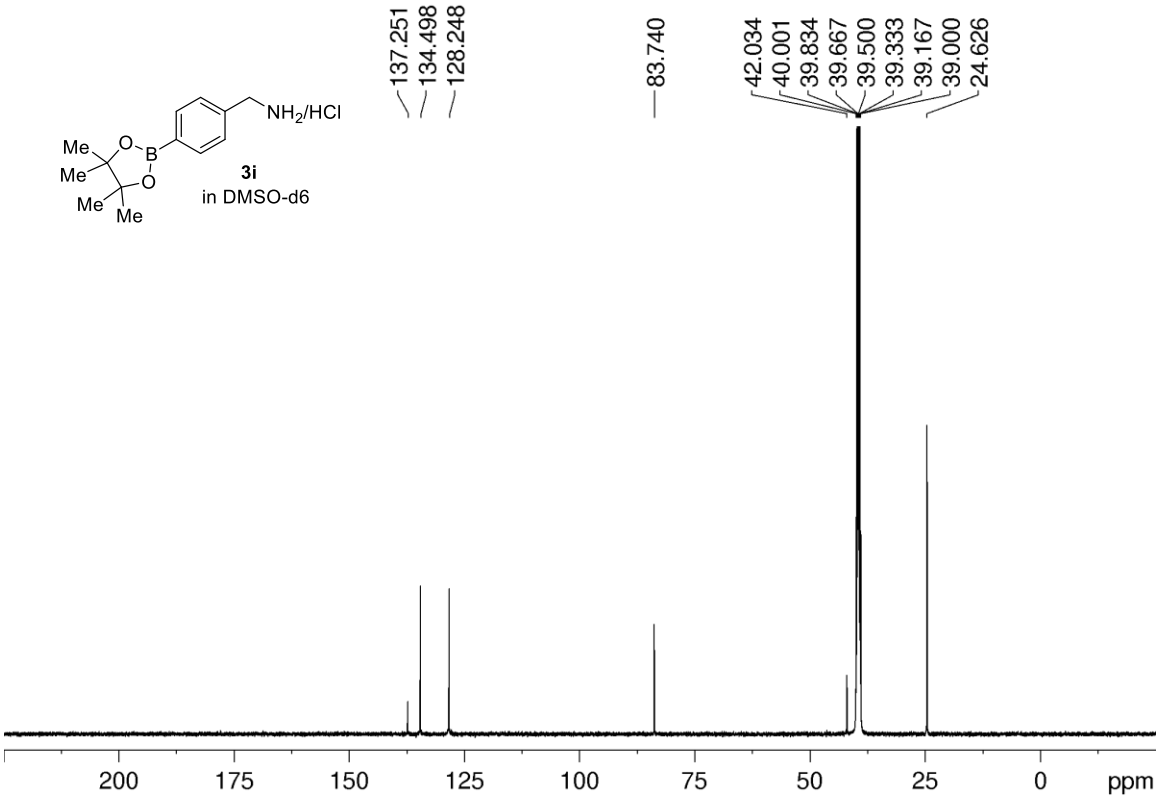

8.446
7.529
7.512
7.490
7.473
4.008
H2O
2.500
NH2/HCl
Cl
3g
in DMSO-d6
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.000
2.073
2.042
2.045

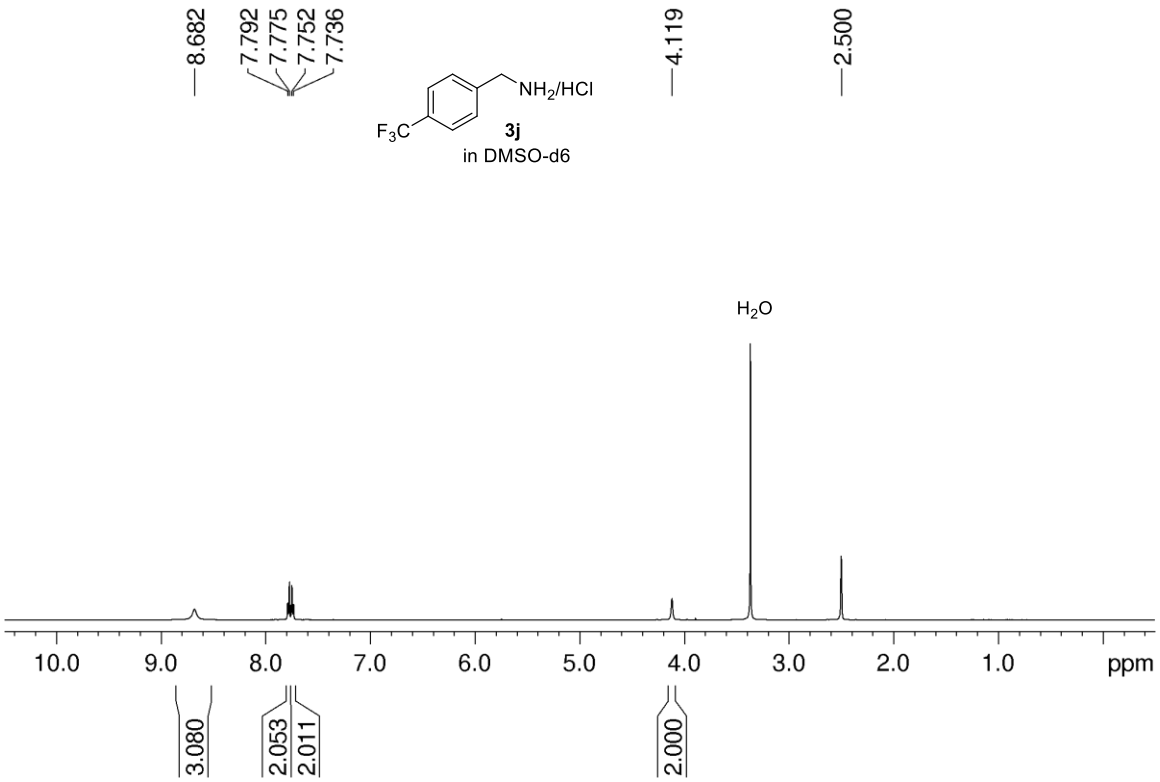

133.165
133.065
130.945
128.525
41.469
40.000
39.834
39.667
39.500
39.333
39.165
38.999
NH2/HCl
Cl
3g
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

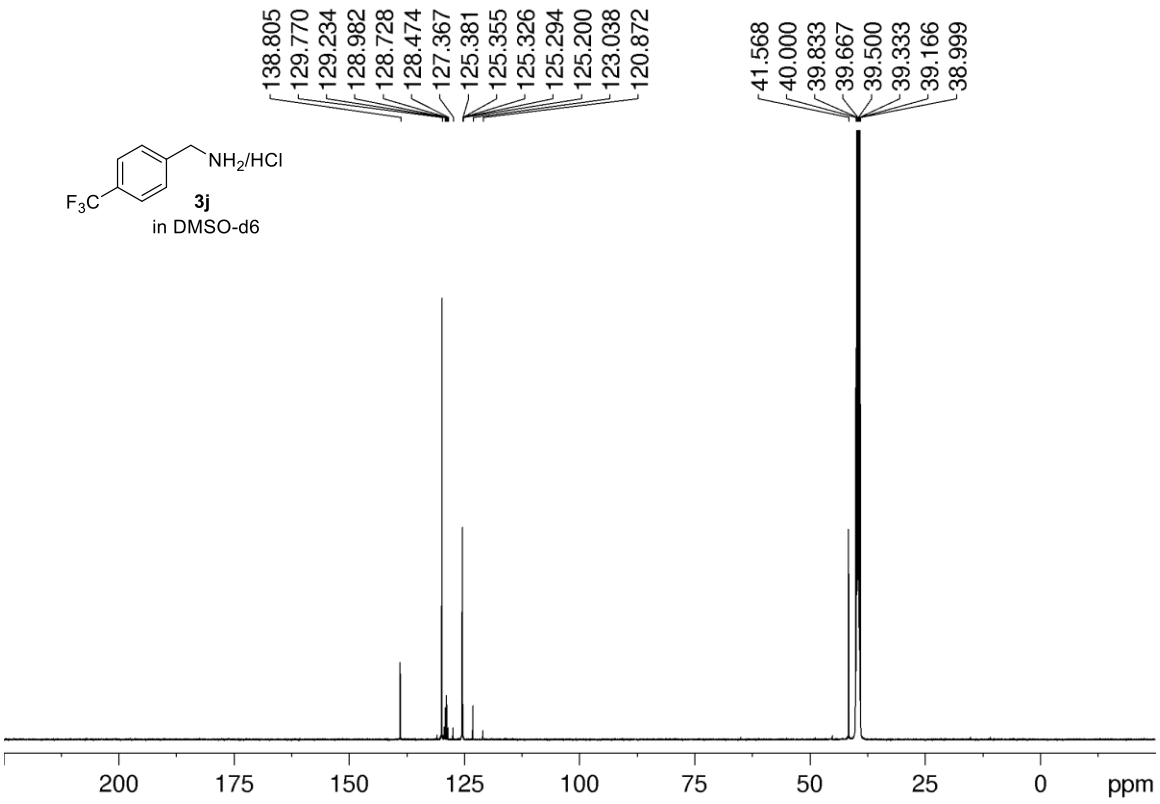

8.556
8.006
7.977
7.960
7.943
7.935
7.917
7.910
7.900
7.653
7.636
7.566
7.558
7.550
4.184
2.500
NH2/HCl
3h
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.039
1.016
3.088
1.076
2.044
2.000

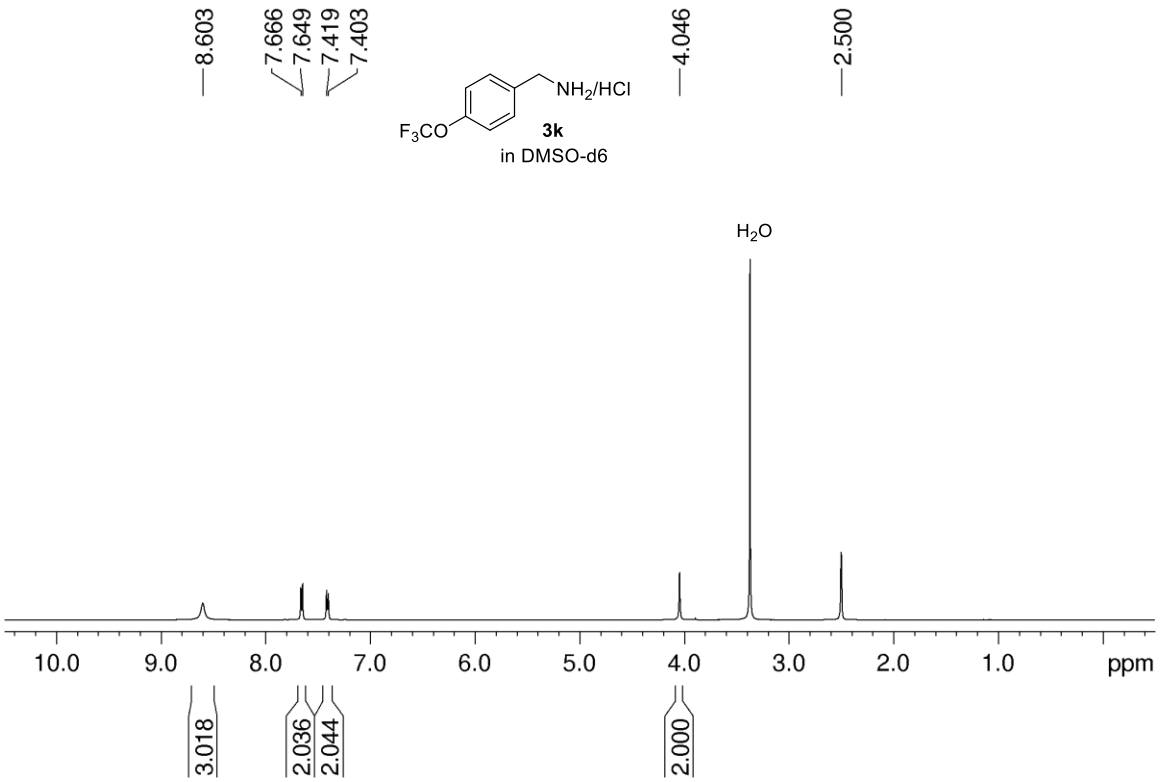

132.713
132.701
131.627
128.323
128.037
127.859
127.748
126.710
126.675
126.614
42.494
40.001
39.835
39.667
39.500
39.333
39.166
38.999
NH2/HCl
3h
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

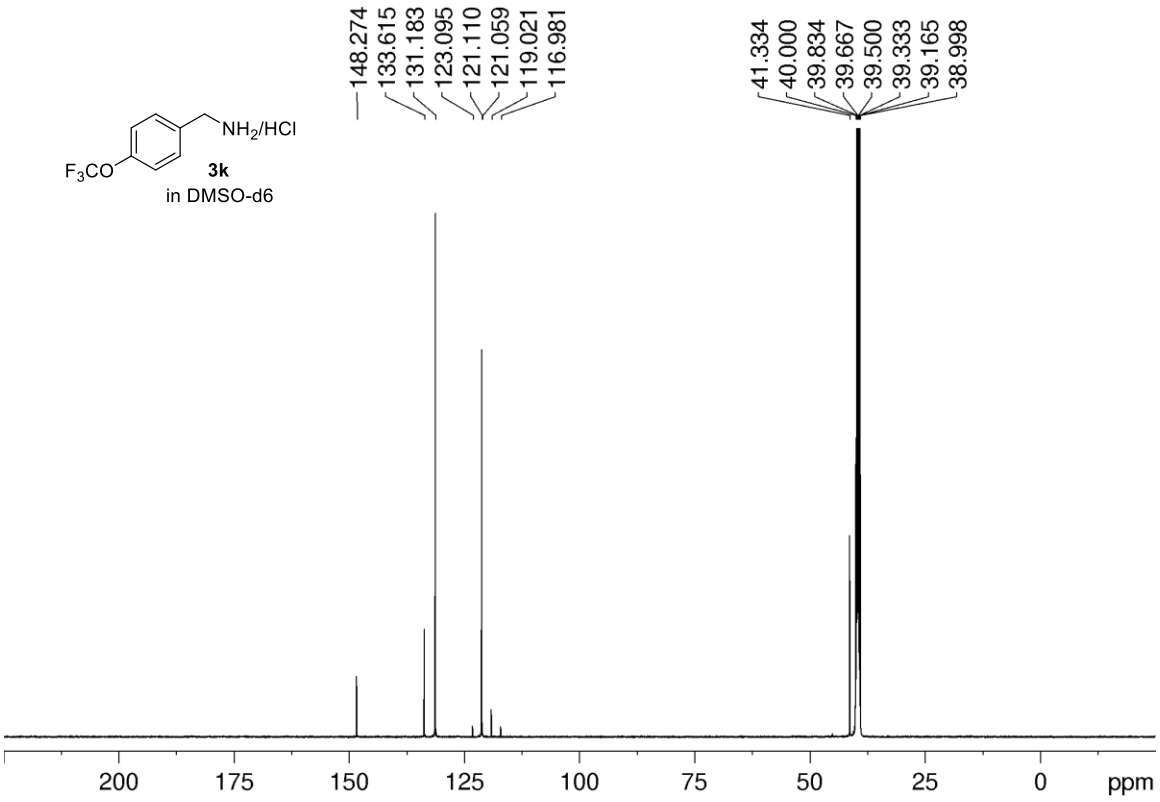

8.542
7.695
7.681
7.506
7.492
4.023
2.500
1.292
NH2/HCl
Me
Me
Me
Me
O
B
O
3i
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.033
2.045
2.022
2.000
12.031

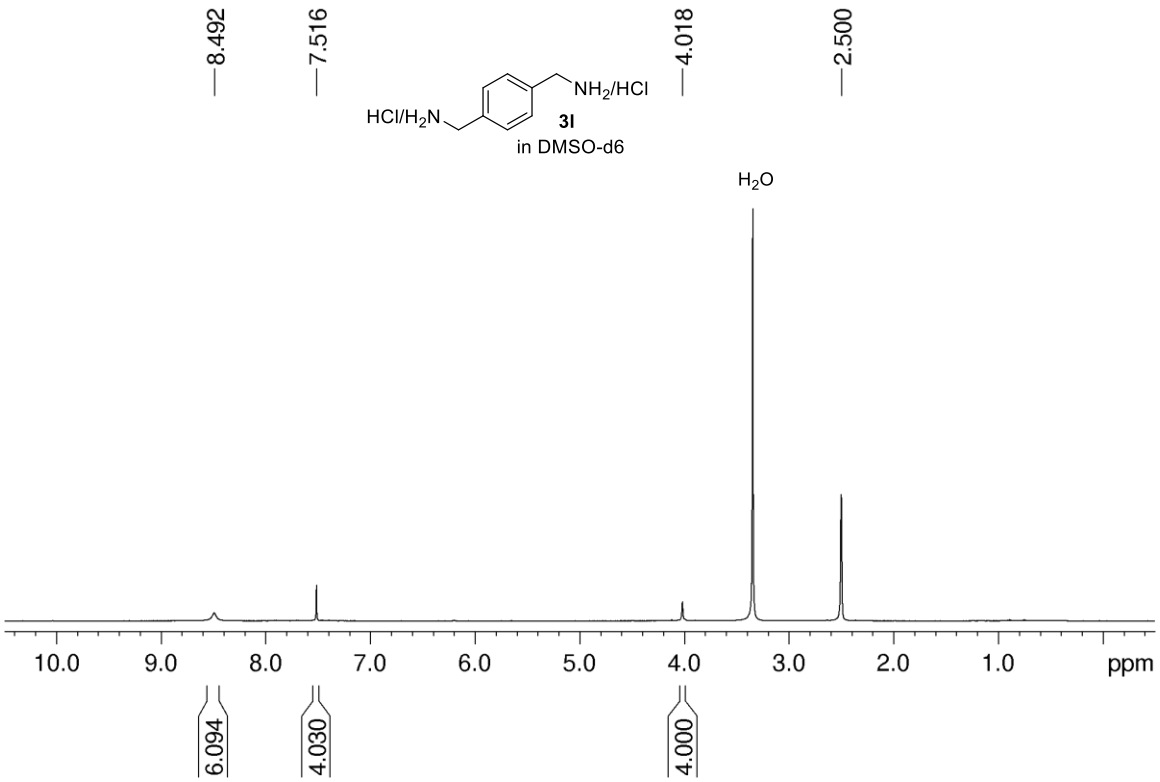

137.251
134.498
128.248
83.740
42.034
40.001
39.834
39.667
39.500
39.333
39.167
39.000
24.626
NH2/HCl
Me
Me
Me
Me
O
B
O
3i
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

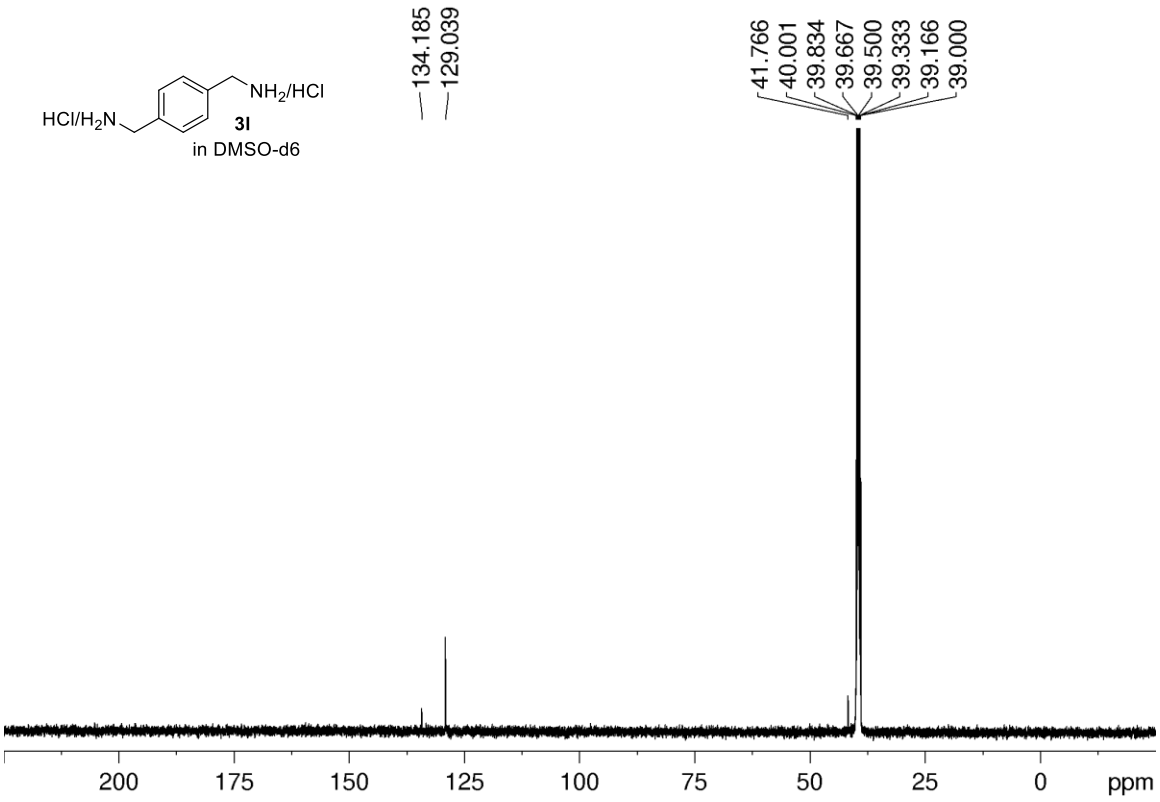

8.682
7.792
7.775
7.752
7.736
4.119
2.500
NH2/HCl
F3C
3j
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.080
2.053
2.011
2.000

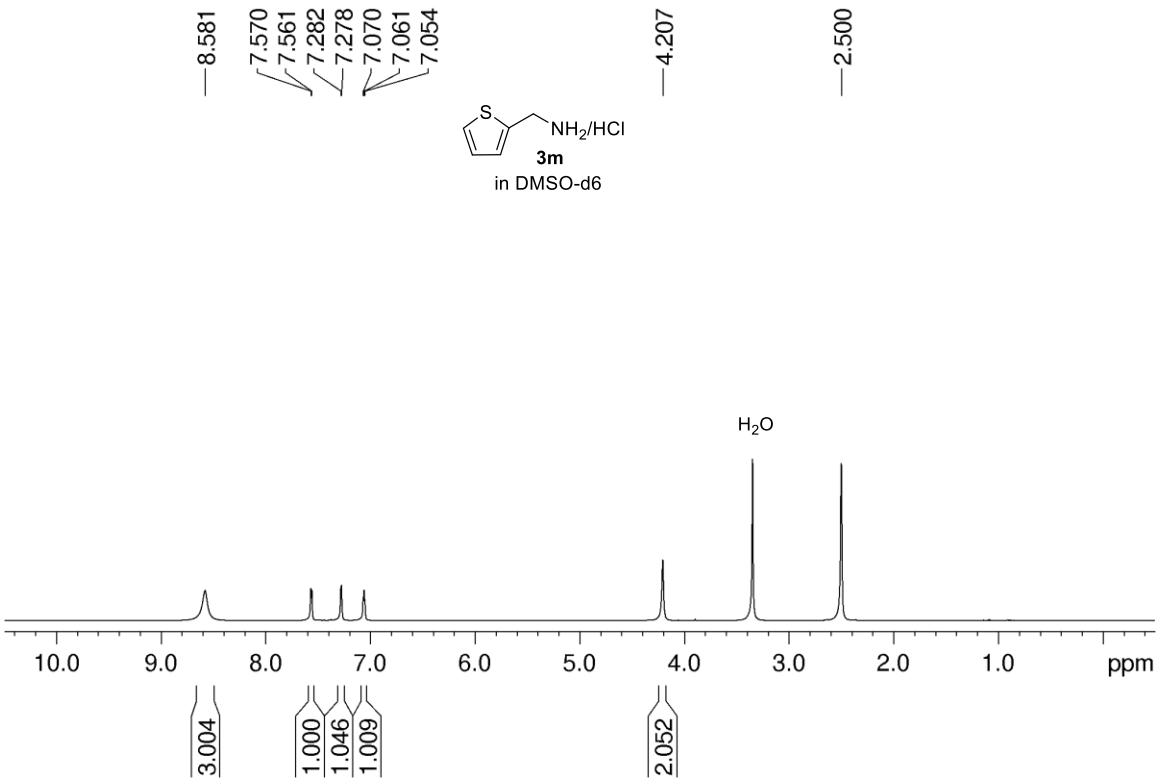

138.805
129.770
129.234
128.982
128.728
128.474
127.367
125.381
125.355
125.326
125.294
125.200
123.038
120.872
41.568
40.000
39.833
39.667
39.500
39.333
39.166
38.999
NH2/HCl
F3C
3j
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

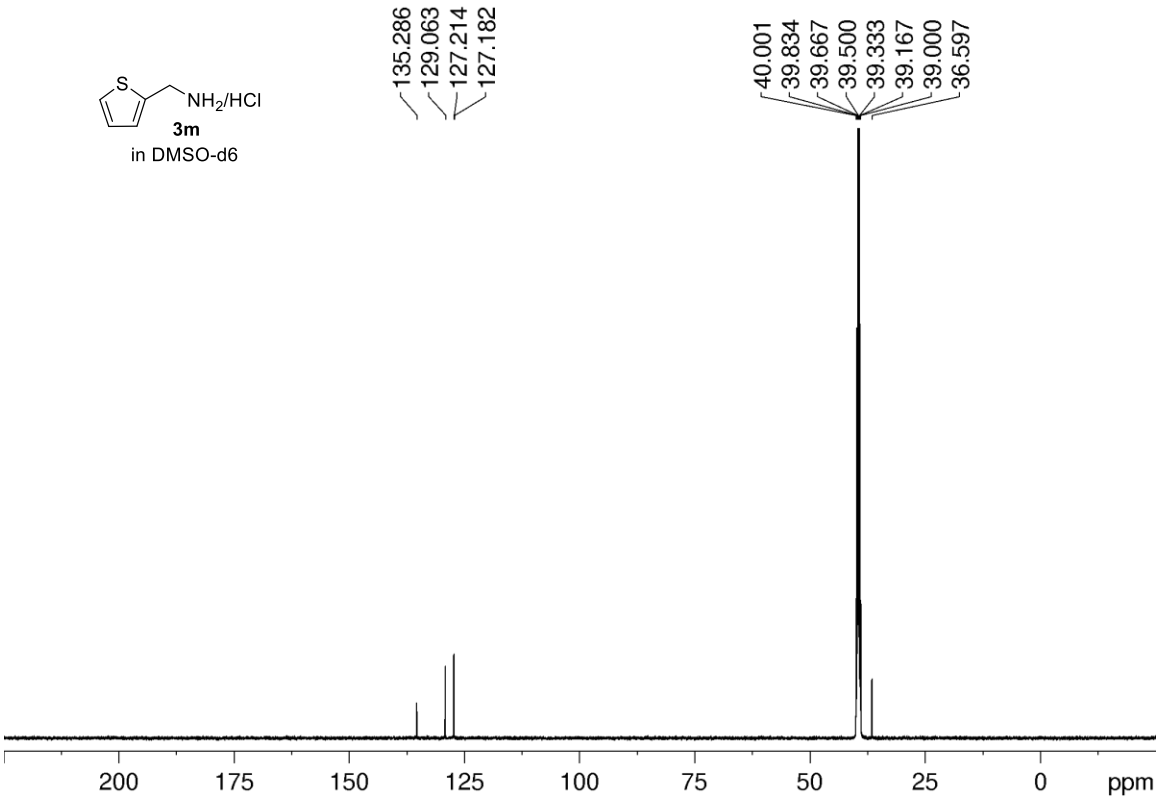

8.603
7.666
7.649
7.419
7.403
4.046
2.500
NH2/HCl
F3CO
3k
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.018
2.036
2.044
2.000

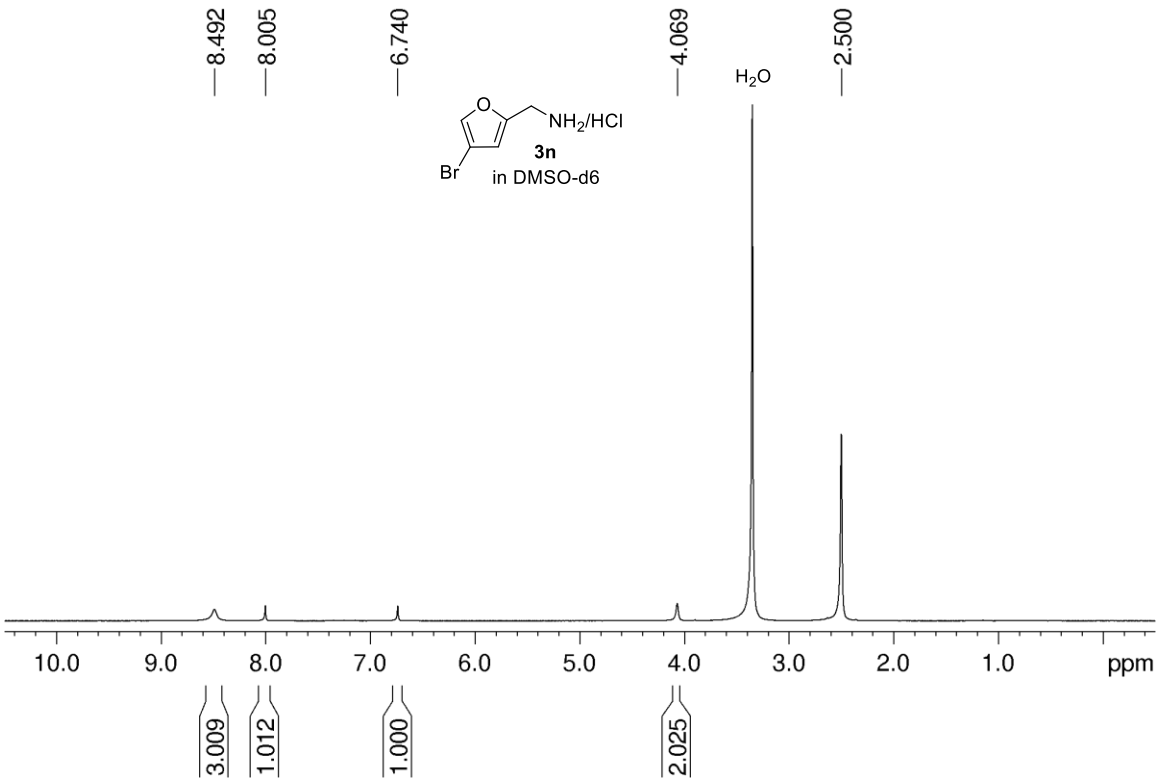

148.274
133.615
131.183
123.095
121.110
121.059
119.021
116.981
41.334
40.000
39.834
39.667
39.500
39.333
39.165
38.998
NH2/HCl
F3CO
3k
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

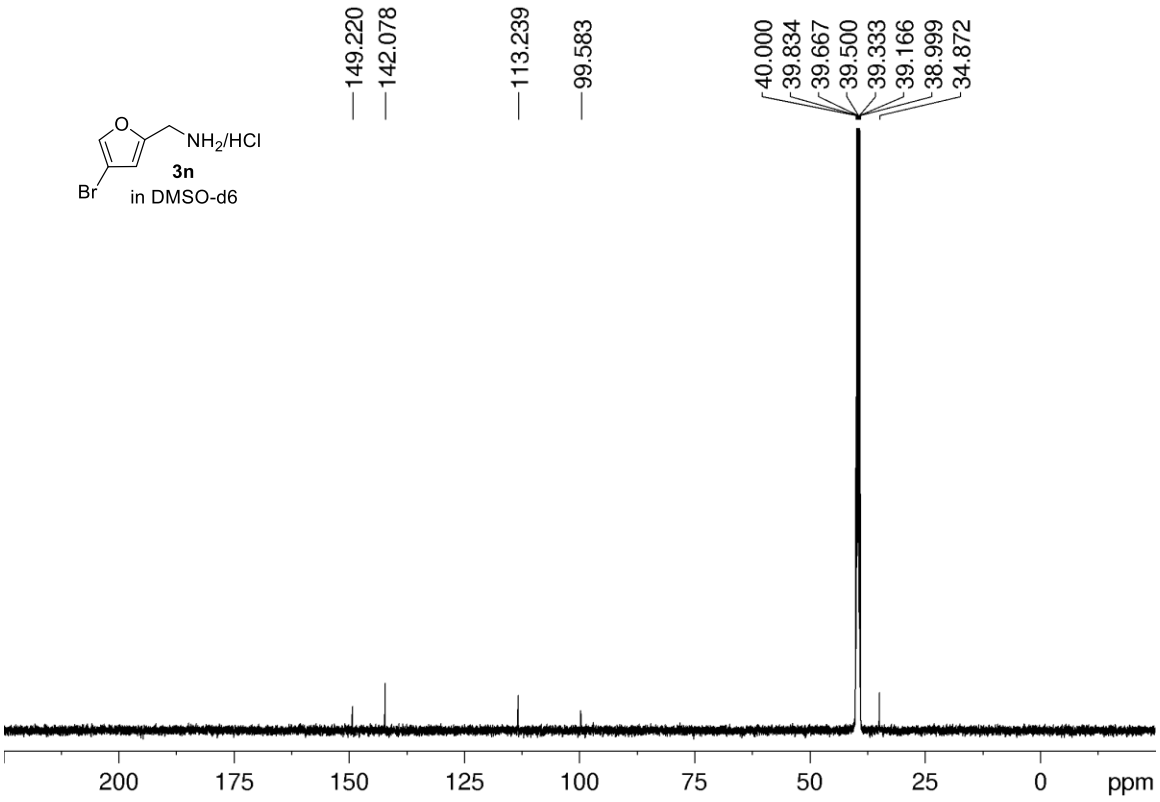

8.492
7.516
4.018
2.500
NH2/HCl
HCl/H2N
3l
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
6.094
4.030
4.000

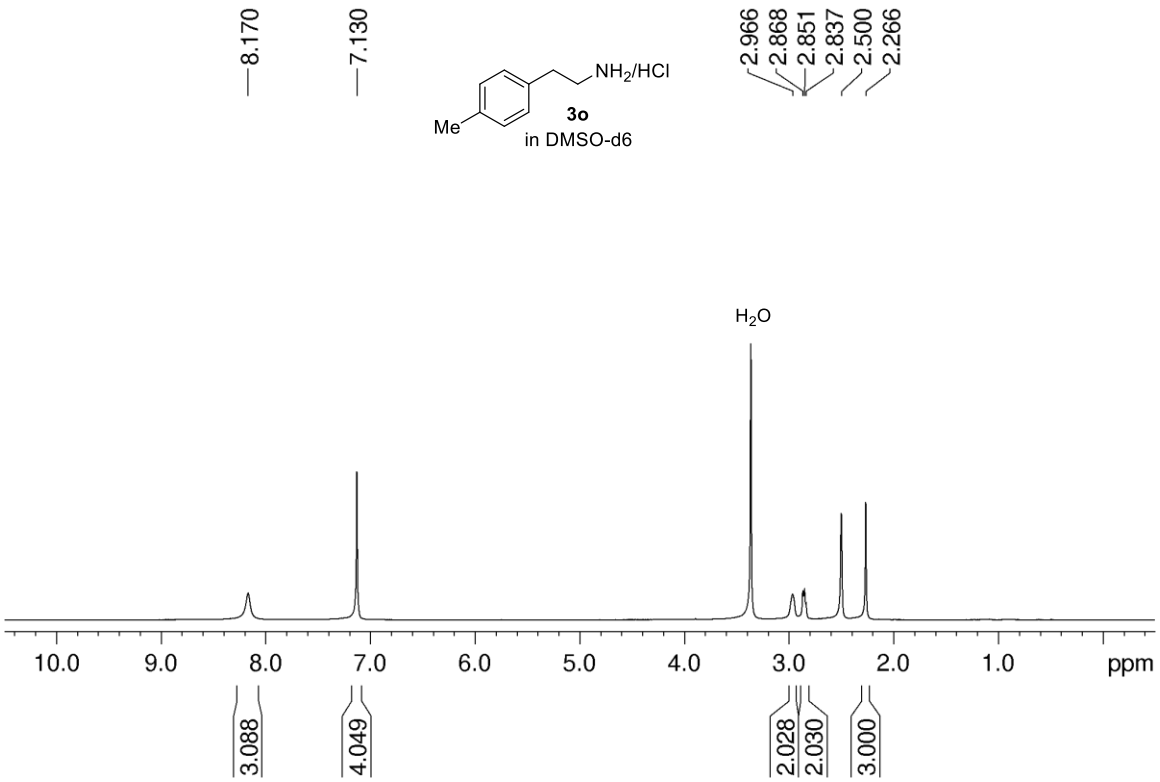

NH2/HCl
HCl/H2N
3l
in DMSO-d6
134.185
129.039
41.766
40.001
39.834
39.667
39.500
39.333
39.166
39.000
200
175
150
125
100
75
50
25
0
ppm

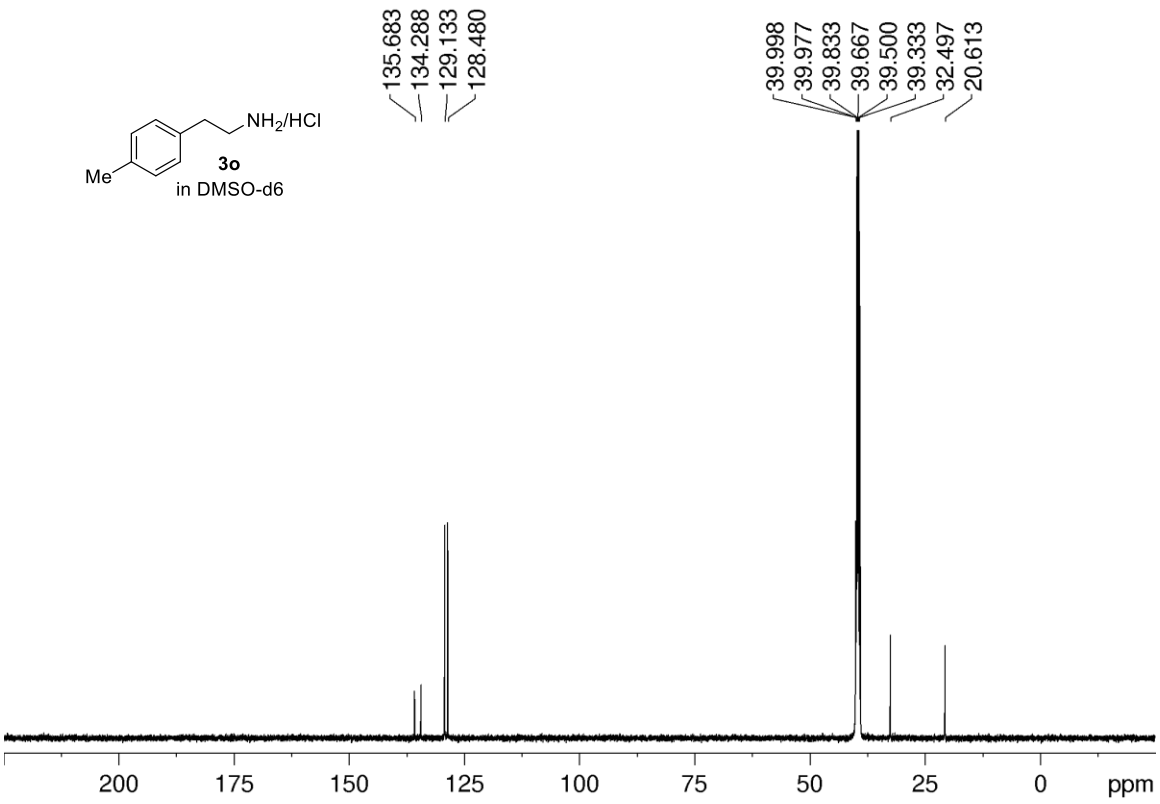

8.581
7.570
7.561
7.282
7.278
7.070
7.061
7.054
4.207
2.500
S
NH2/HCl
3m
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.004
1.000
1.046
1.009
2.052

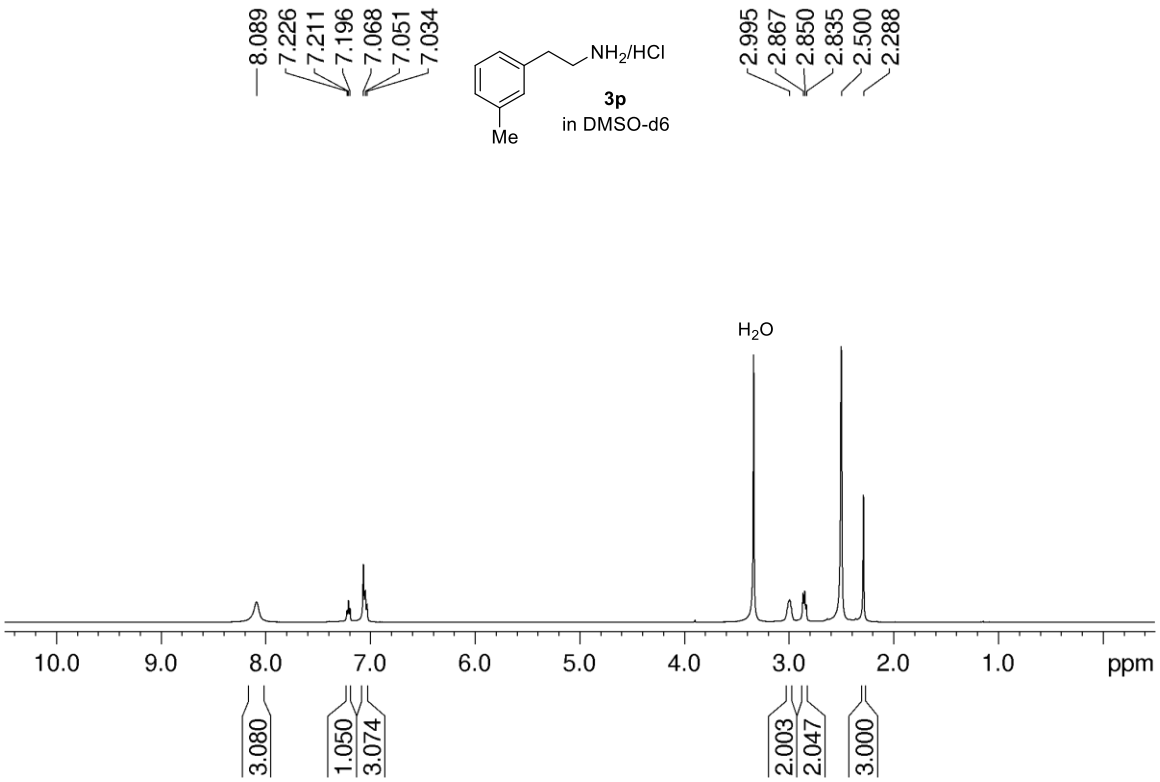

S
NH2/HCl
3m
in DMSO-d6
135.286
129.063
127.214
127.182
40.001
39.834
39.667
39.500
39.333
39.167
39.000
36.597
200
175
150
125
100
75
50
25
0
ppm

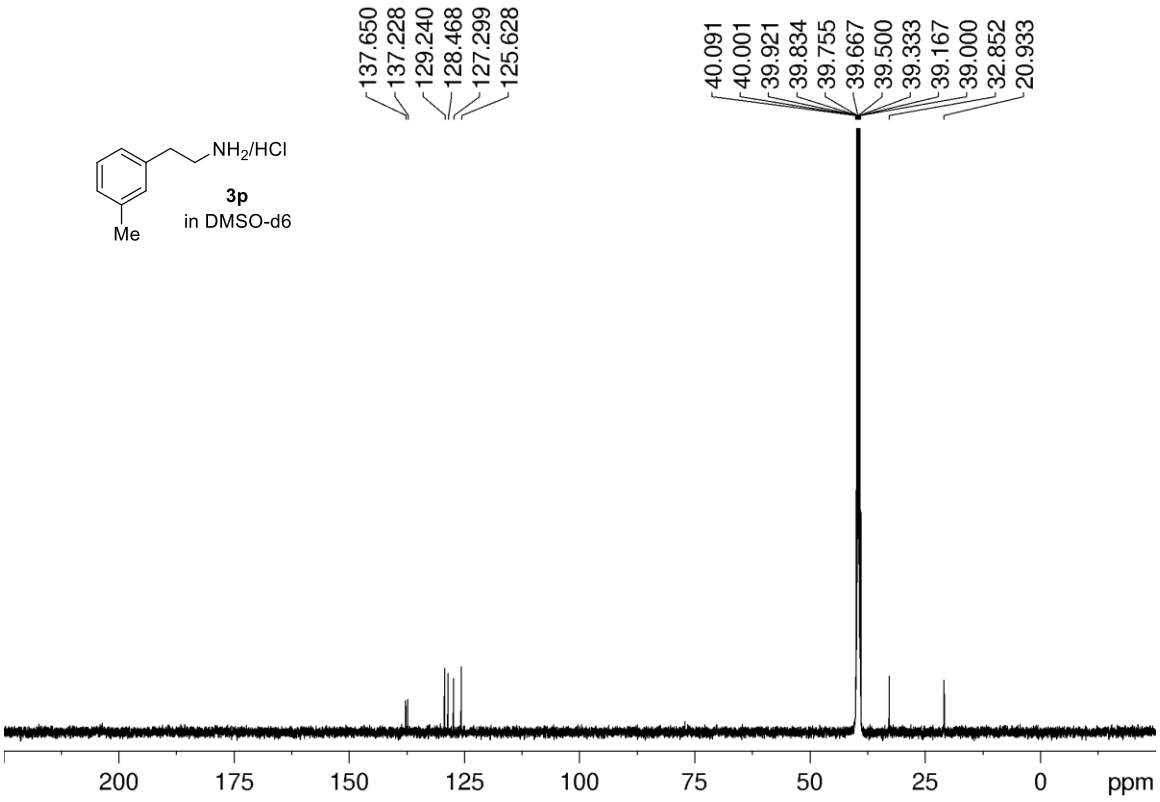

8.492
8.005
6.740
4.069
2.500
H2O
NH2/HCl
3n
in DMSO-d6
Br
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.009
1.012
1.000
2.025

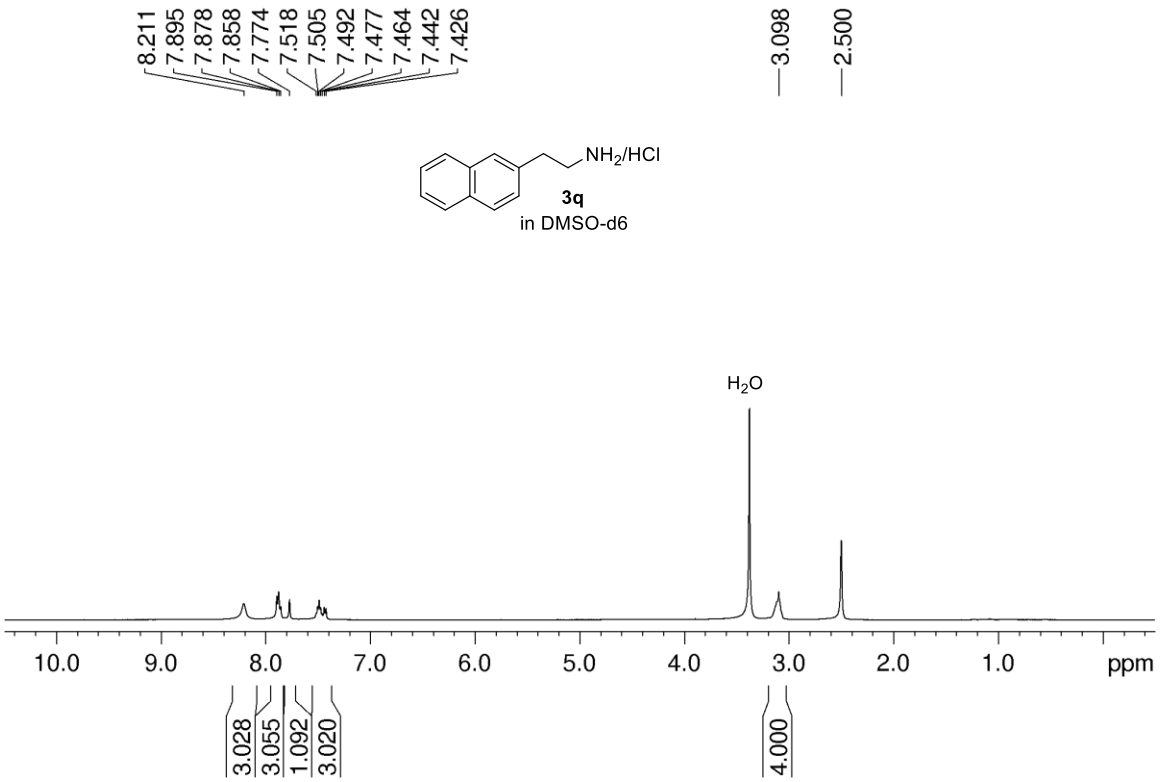

149.220
142.078
113.239
99.583
40.000
39.834
39.667
39.500
39.333
39.166
38.999
34.872
NH2/HCl
3n
in DMSO-d6
Br
200
175
150
125
100
75
50
25
0
ppm

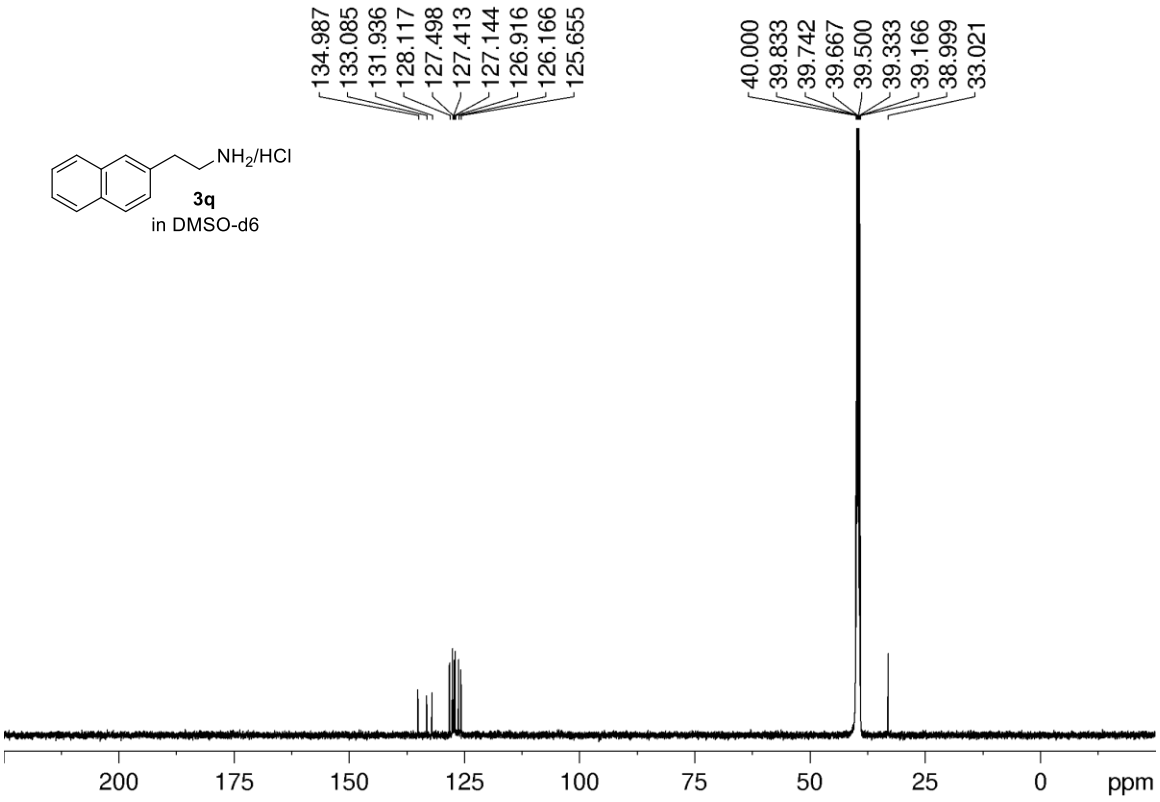

8.170
7.130
2.966
2.868
2.851
2.837
2.500
2.266
NH2/HCl
3o
Me
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.088
4.049
2.028
2.030
3.000

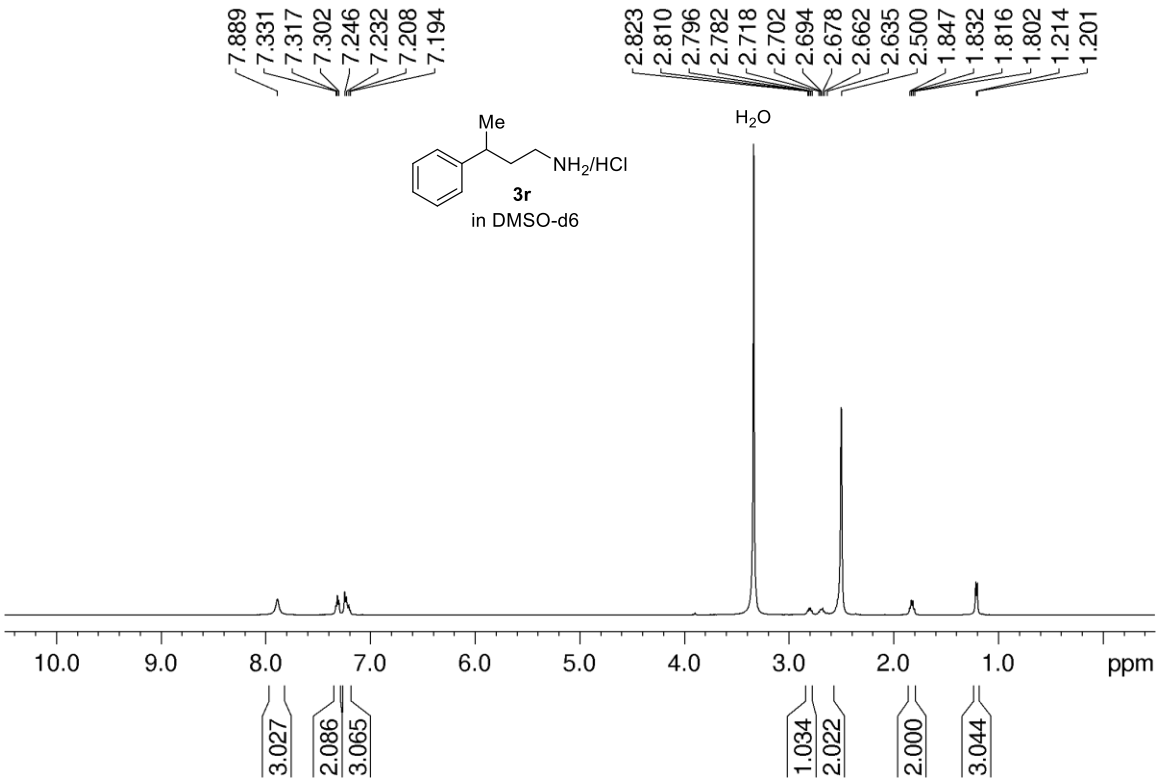

135.683
134.288
129.133
128.480
39.998
39.977
39.833
39.667
39.500
39.333
32.497
20.613
NH2/HCl
3o
Me
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

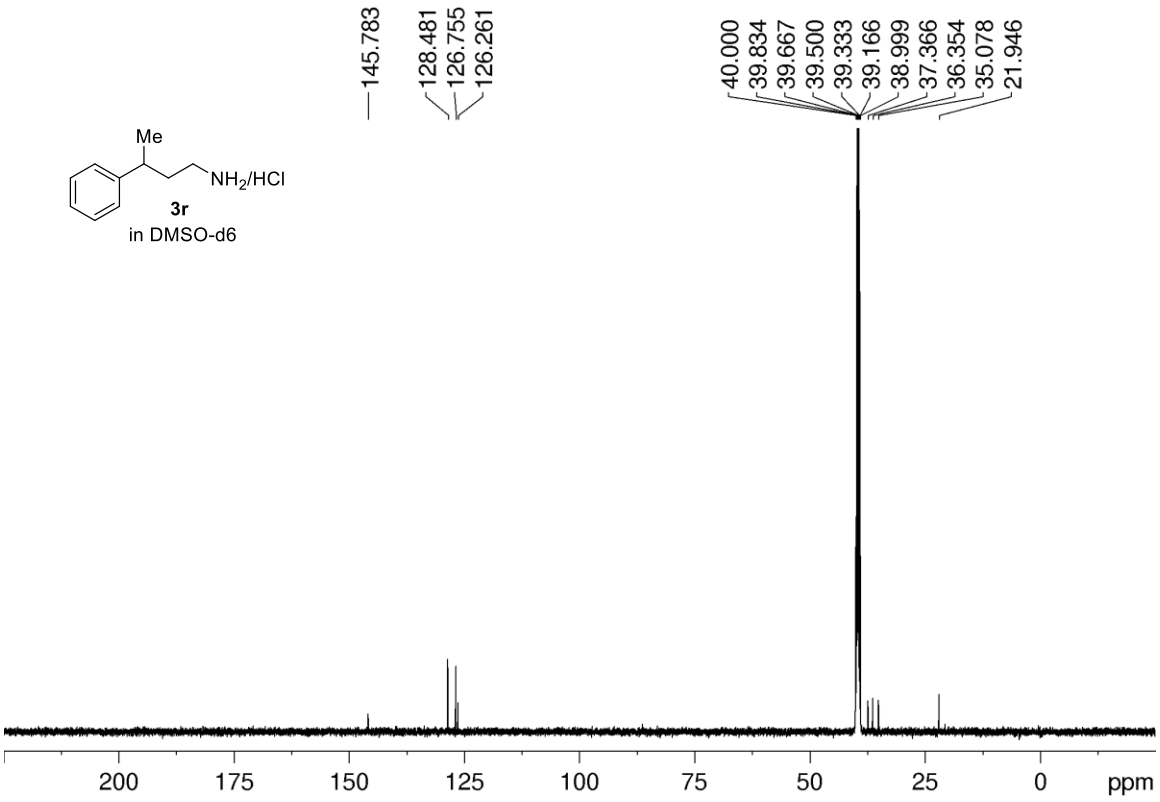

8.089
7.226
7.211
7.196
7.068
7.051
7.034
NH2/HCl
3p
in DMSO-d6
Me
2.995
2.867
2.850
2.835
2.500
2.288
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.080
1.050
3.074
2.003
2.047
3.000

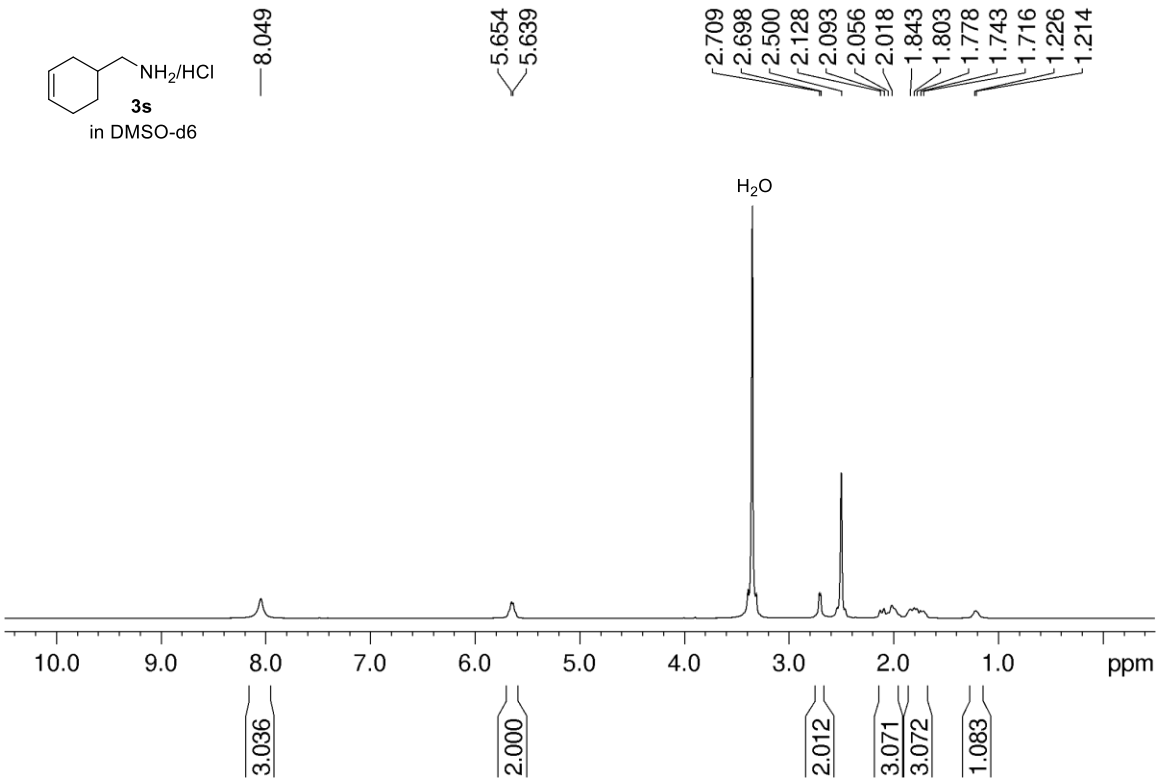

137.650
137.228
129.240
128.468
127.299
125.628
40.091
40.001
39.921
39.834
39.755
39.667
39.500
39.333
39.167
39.000
32.852
20.933
NH2/HCl
3p
in DMSO-d6
Me
200
175
150
125
100
75
50
25
0
ppm

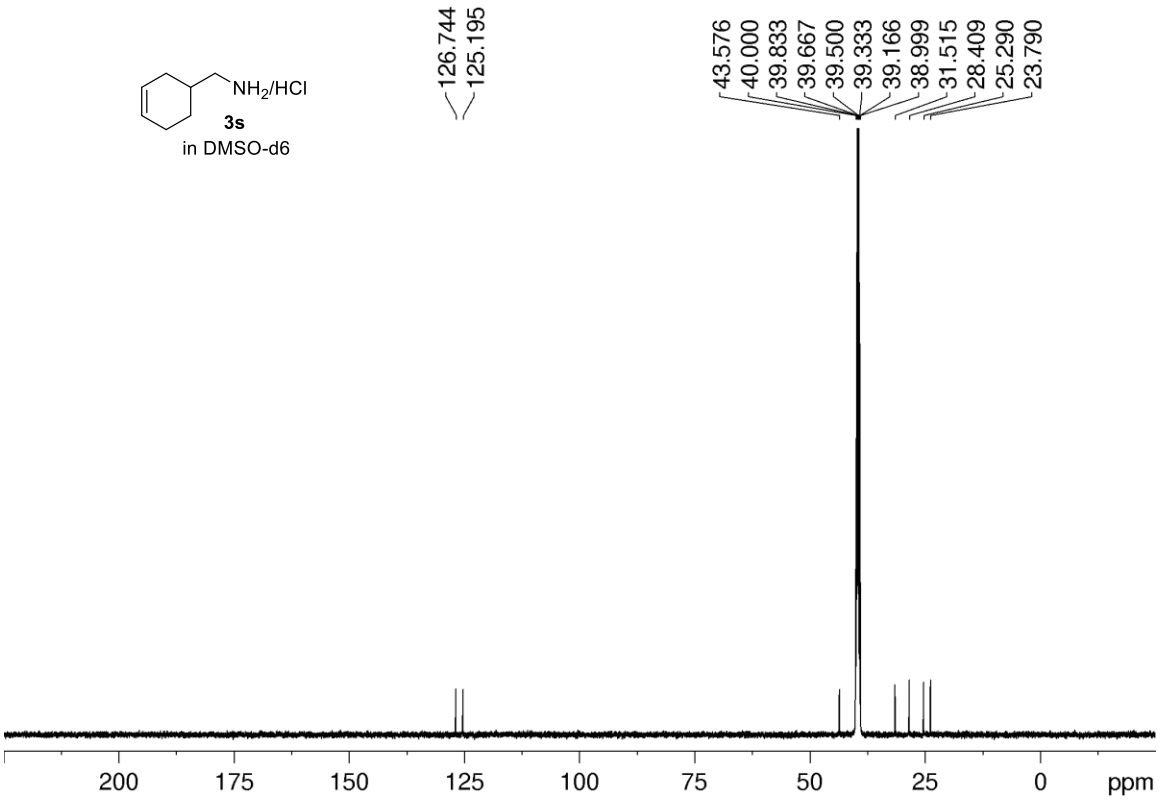

8.211
7.895
7.878
7.858
7.774
7.518
7.505
7.492
7.477
7.464
7.442
7.426
3.098
2.500
NH2/HCl
3q
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.028
3.055
1.092
3.020
4.000

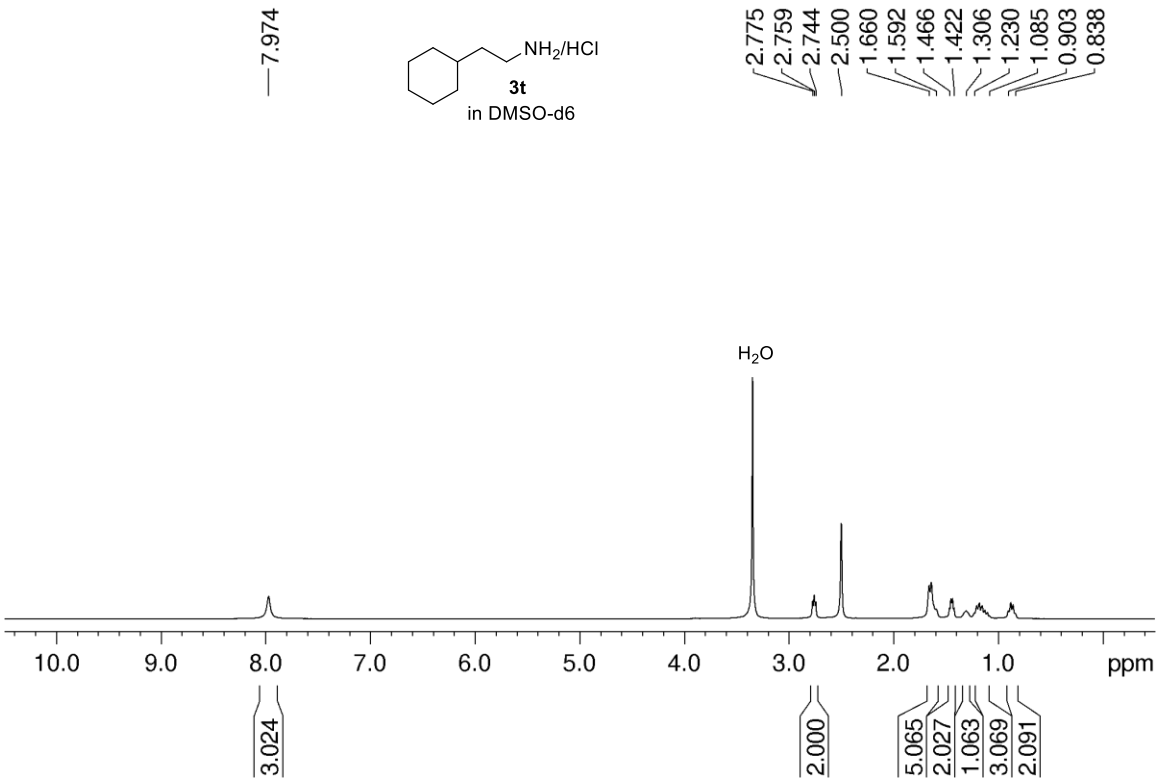

134.987
133.085
131.936
128.117
127.498
127.413
127.144
126.916
126.166
125.655
40.000
39.833
39.742
39.667
39.500
39.333
39.166
38.999
33.021
NH2/HCl
3q
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

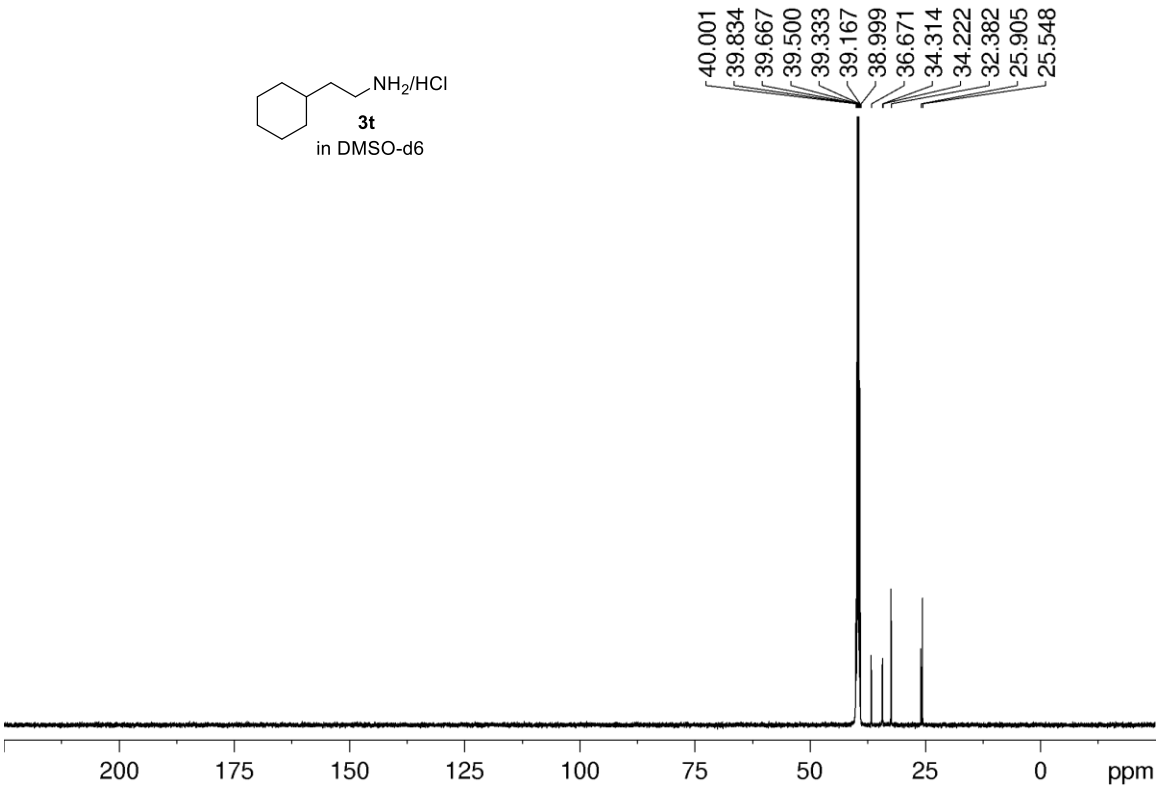

7.889
7.331
7.317
7.302
7.246
7.232
7.208
7.194
2.823
2.810
2.796
2.782
2.718
2.702
2.694
2.678
2.662
2.635
2.500
1.847
1.832
1.816
1.802
1.214
1.201
H2O
Me
NH2/HCl
3r
in DMSO-d6
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.027
2.086
3.065
1.034
2.022
2.000
3.044

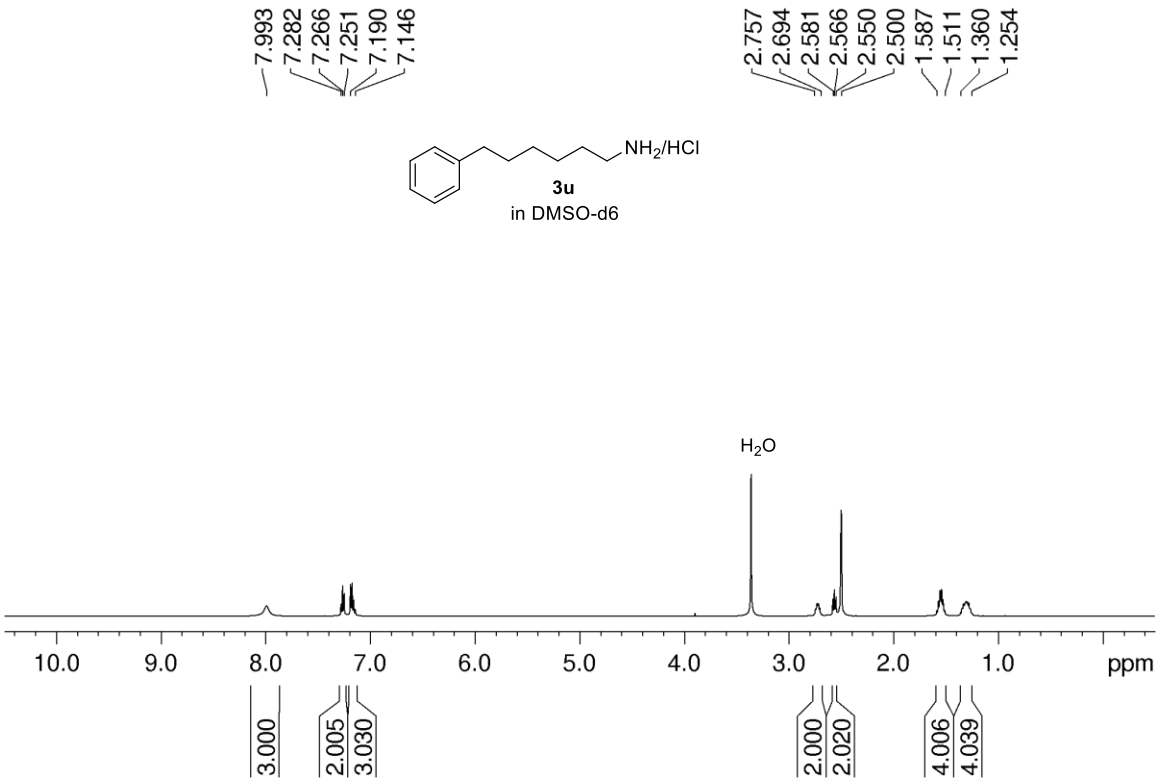

145.783
128.481
126.755
126.261
40.000
39.834
39.667
39.500
39.333
39.166
38.999
37.366
36.354
35.078
21.946
Me
NH2/HCl
3r
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

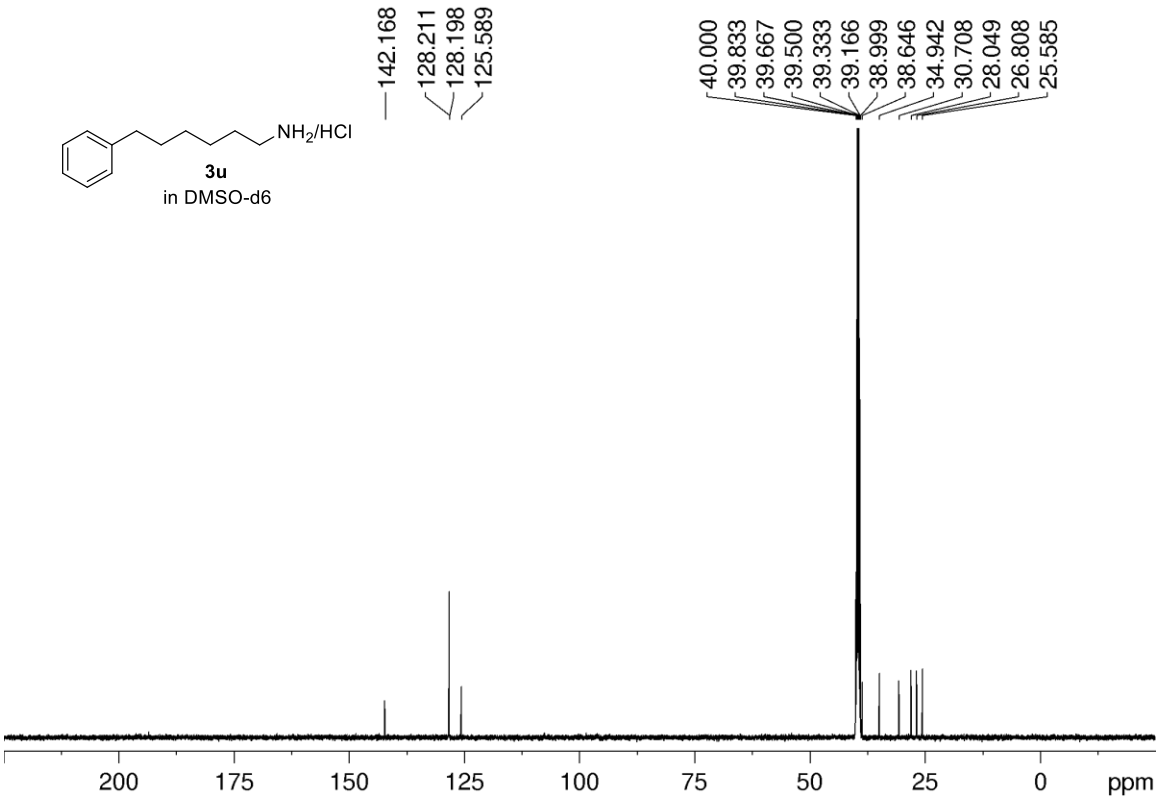

NH2/HCl
3s
in DMSO-d6
8.049
5.654
5.639
2.709
2.698
2.500
2.128
2.093
2.056
2.018
1.843
1.803
1.778
1.743
1.716
1.226
1.214
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.036
2.000
2.012
3.071
3.072
1.083

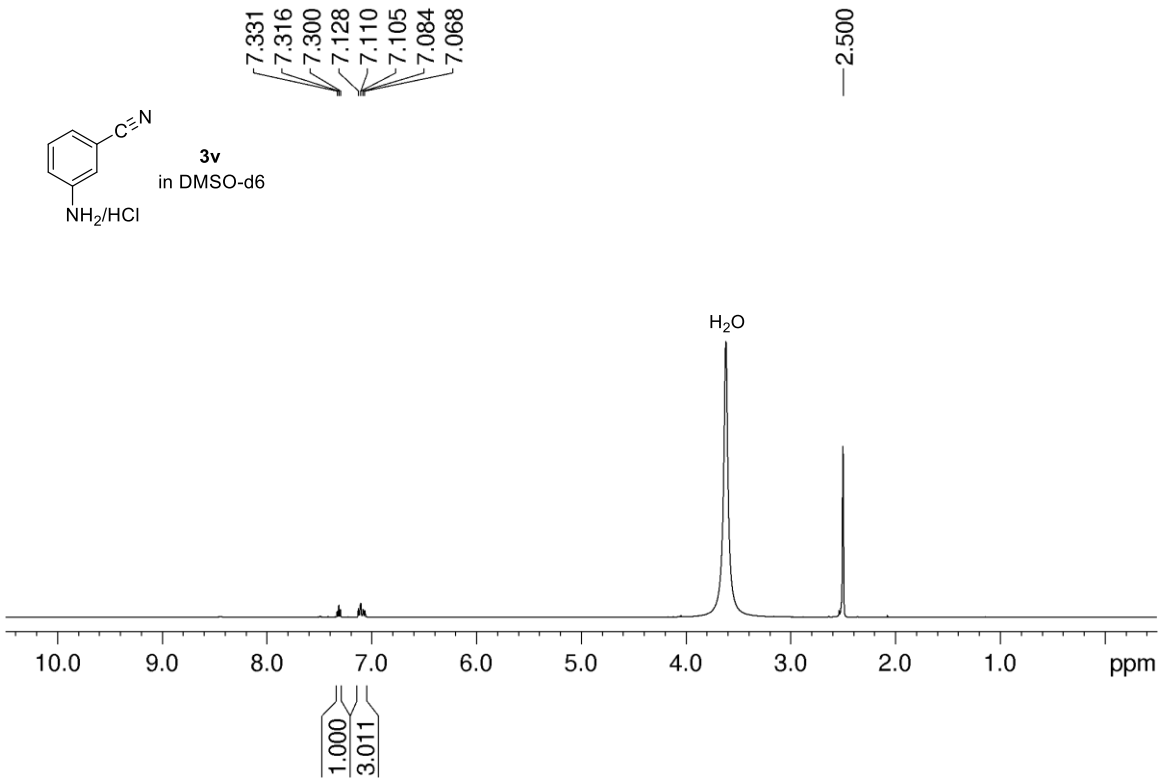

NH2/HCl
3s
in DMSO-d6
126.744
125.195
43.576
40.000
39.833
39.667
39.500
39.333
39.166
38.999
31.515
28.409
25.290
23.790
200
175
150
125
100
75
50
25
0
ppm

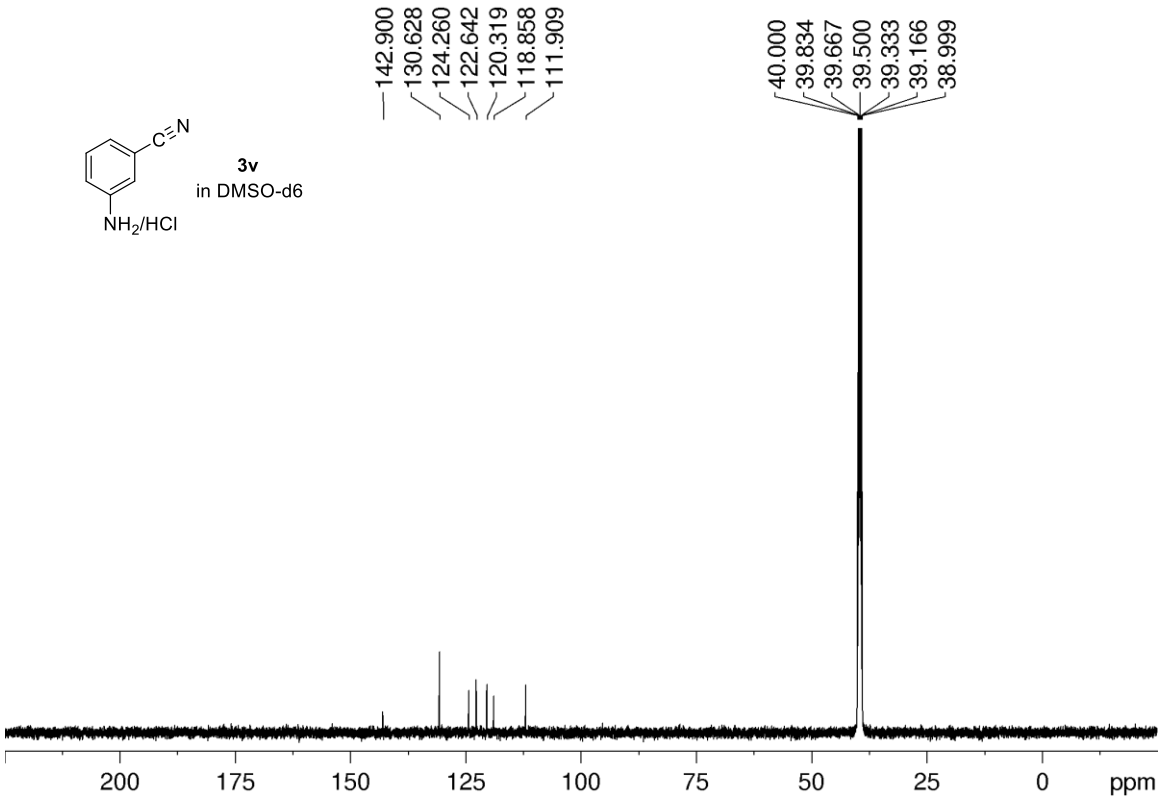

7.974
NH2/HCl
3t
in DMSO-d6
2.775
2.759
2.744
2.500
1.660
1.592
1.466
1.422
1.306
1.230
1.085
0.903
0.838
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.024
2.000
5.065
2.027
1.063
3.069
2.091

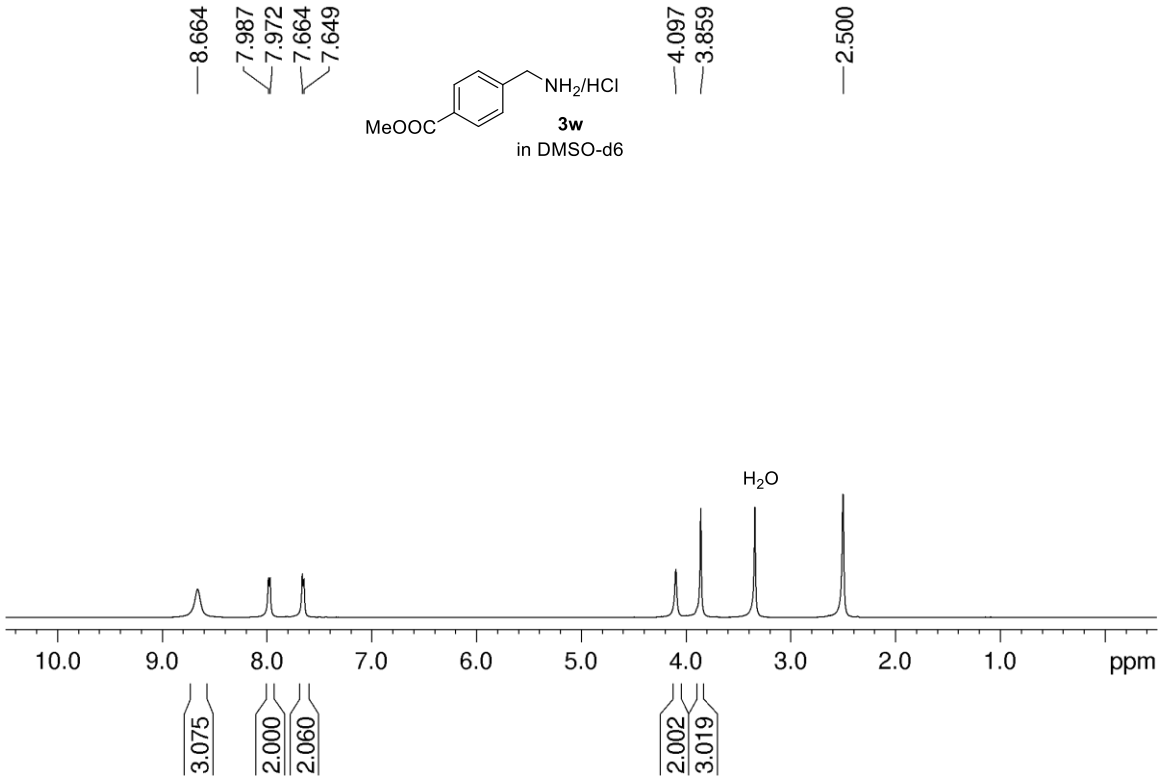

NH2/HCl
3t
in DMSO-d6
40.001
39.834
39.667
39.500
39.333
39.167
38.999
36.671
34.314
34.222
32.382
25.905
25.548
200
175
150
125
100
75
50
25
0
ppm

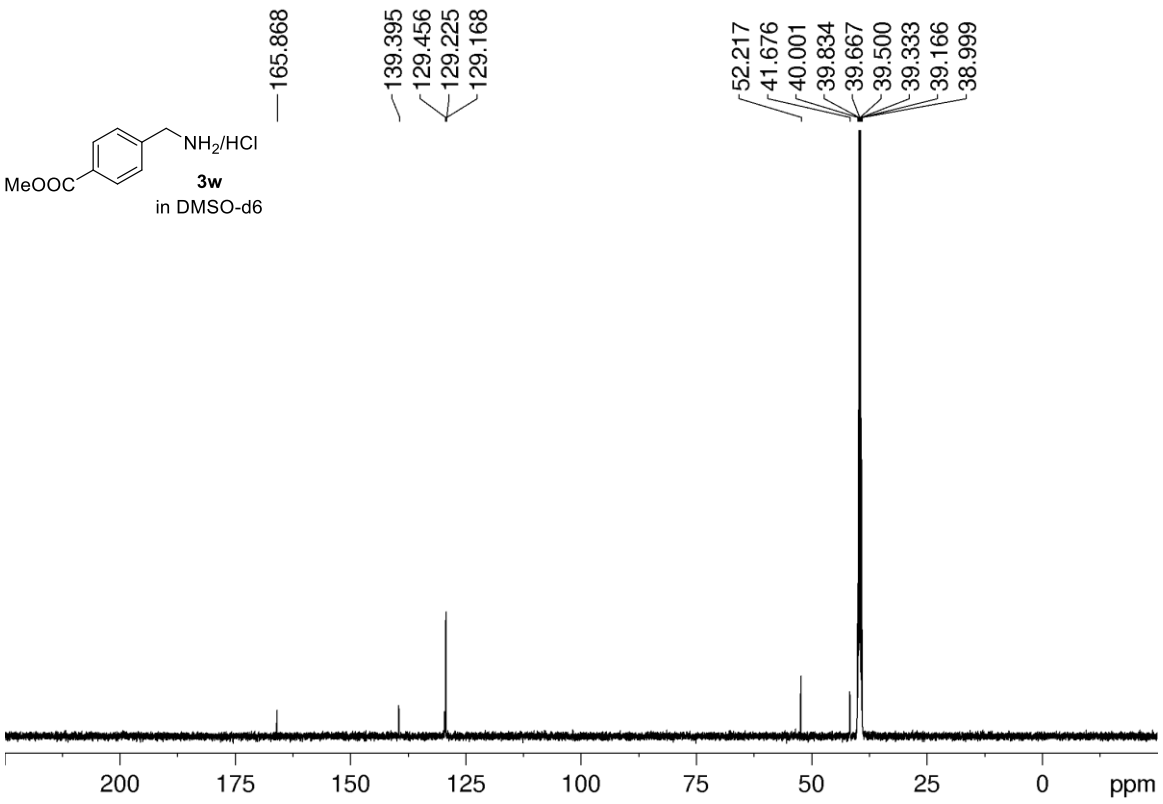

7.993
7.282
7.266
7.251
7.190
7.146
2.757
2.694
2.581
2.566
2.550
2.500
1.587
1.511
1.360
1.254
NH2/HCl
3u
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.000
2.005
3.030
2.000
2.020
4.006
4.039

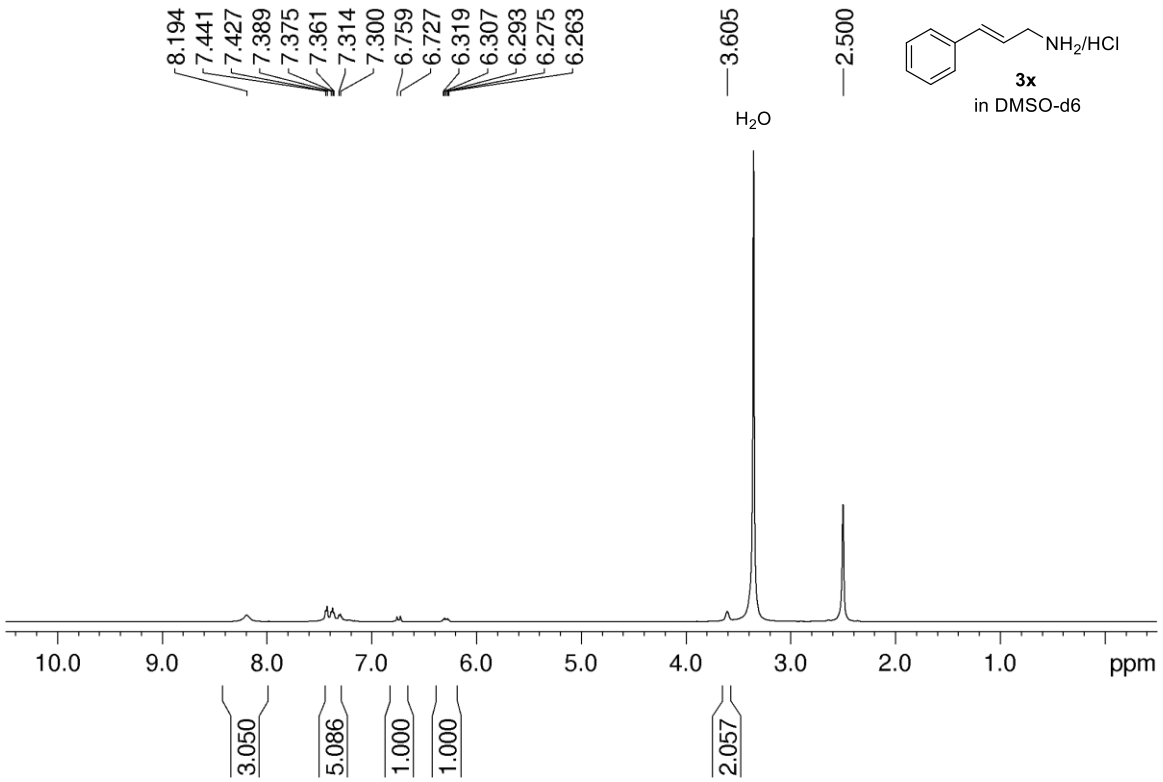

142.168
128.211
128.198
125.589
40.000
39.833
39.667
39.500
39.333
39.166
38.999
38.646
34.942
30.708
28.049
26.808
25.585
NH2/HCl
3u
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm

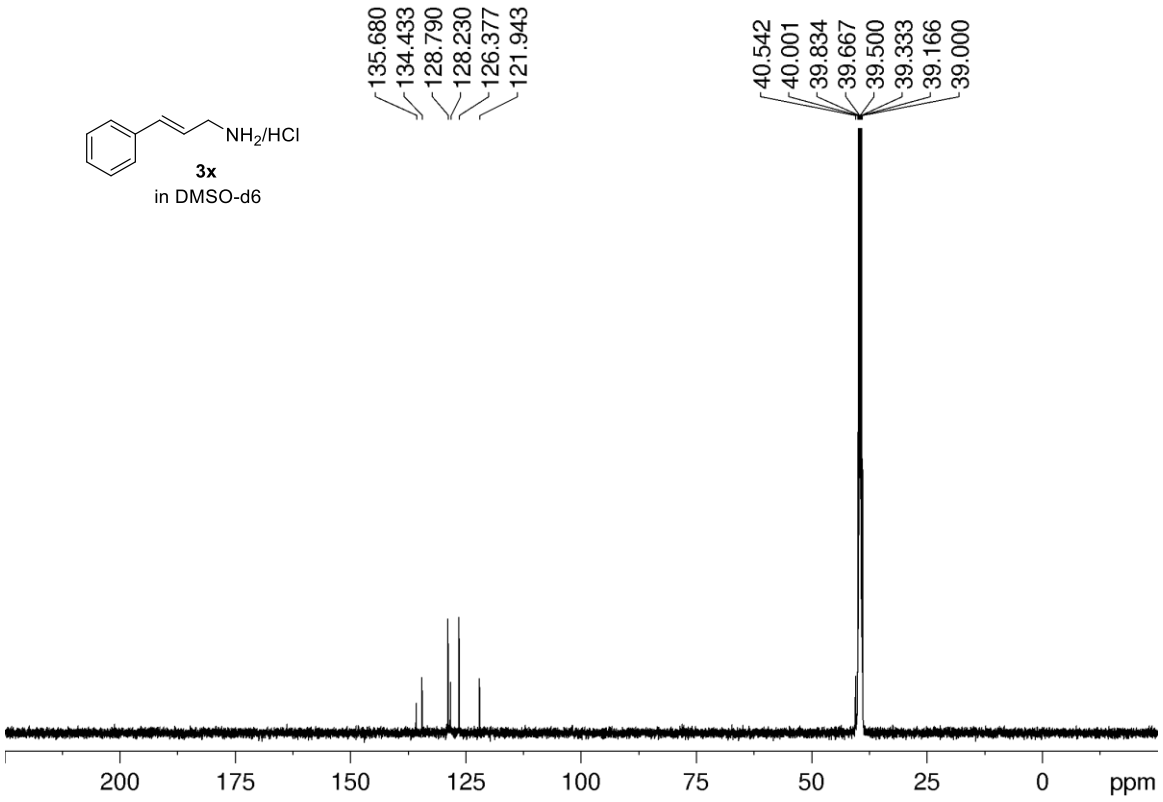

7.331
7.316
7.300
7.128
7.110
7.105
7.084
7.068
2.500
3v
in DMSO-d6
NH2/HCl
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
1.000
3.011


142.900
130.628
124.260
122.642
120.319
118.858
111.909
40.000
39.834
39.667
39.500
39.333
39.166
38.999
3v
in DMSO-d6
NH2/HCl
200
175
150
125
100
75
50
25
0
ppm


8.664
7.987
7.972
7.664
7.649
4.097
3.859
2.500
NH2/HCl
MeOOC
3w
in DMSO-d6
H2O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.075
2.000
2.060
2.002
3.019


165.868
139.395
129.456
129.225
129.168
52.217
41.676
40.001
39.834
39.667
39.500
39.333
39.166
38.999
NH2/HCl
MeOOC
3w
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm


8.194
7.441
7.427
7.389
7.375
7.361
7.314
7.300
6.759
6.727
6.319
6.307
6.293
6.275
6.263
3.605
H2O
2.500
NH2/HCl
3x
in DMSO-d6
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm
3.050
5.086
1.000
1.000
2.057


135.680
134.433
128.790
128.230
126.377
121.943
40.542
40.001
39.834
39.667
39.500
39.333
39.166
39.000
NH2/HCl
3x
in DMSO-d6
200
175
150
125
100
75
50
25
0
ppm