– Electronic Supplementary Material (ESI) –

Iron Catalyzed Oxidative Cyanation of Tertiary Amines

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General. All reactions were carried out under an atmosphere of dry nitrogen. ^{1}H and ^{13}C NMR spectra of solutions in $CDCl_3$ were recorded on 200, 300, or 400 MHz NMR spectrometers. Chemical shifts were expressed in parts per million (ppm) downfield from tetramethylsilane and refer to the solvent signals (δ_H 7.24 and δ_C 77.0 ppm). Abbreviations for signal couplings are: s, singlet; d, doublet; t, triplet; m, multiplet. HRMS was performed on a Finnigan MAT 95Q mass spectrometer. Infrared spectra of neat substances were recorded on a Perkin-Elmer Spectrum BX II FT-IR spectrometer equipped with an ATR probe (diamond).

Materials. Commercially available tertiary amines were used as received. *N*,*N*-Dimethyl-*p*-anisidine,[S1] 1-phenylpiperidine,[S2] 2-phenyl-1,2,3,4-tetrahydroisoquinoline[S2] and 2-(4-methoxyphenyl)-1,2,3,4-tetrahydroisoquinoline[S2] were prepared according to literature procedures.

The following iron and copper salts were used: Iron(II) acetate (anhydrous, 97 %, Strem), iron(III) acetylacetonate (99.9 %, Aldrich), iron(III) bromide (99 %, ABCR), iron(II) chloride (98 %, Aldrich), iron(III) chloride (anhydrous, 97 %, Grüssing), iron(III) chloride hexahydrate (99 %), iron(II) fluoride (anhydrous, 99 %, Strem), iron(II) gluconate hydrate (purum p.a., Fluka), iron(II) sulfate (99 %), copper(I) bromide (98 %, Acros), and copper(II) bromide (> 99%, Acros).

Trimethylsilyl cyanide (98 %, Acros) and *tert.*-butyl hydroperoxide (5.5 M solution in decane, purum, Aldrich) were purchased.

Typical Procedure for Iron-Catalyzed Cyanation of Tertiary Amines. Under an atmosphere of dry N_2, a 25 mL Schlenk flask was charged with iron(II) chloride (10 mol-%, 13 mg). The tertiary amine (1.0 mmol), trimethylsilyl cyanide (2.0 mmol, 0.27 mL), and MeOH (2.0 mL) were added successively by syringe. To the mixture was added dropwise *tert.*-butyl hydroperoxide (2.5 mmol, 0.470 mL, 5.5 M solution in decane) over a period of 5 min. The mixture was stirred at room temperature for the indicated time. At the end of the reaction, the reaction mixture was poured into a saturated aqueous NaCl solution (20 mL) and extracted with CH_2Cl_2 (3 × 20 mL). The organic phases were combined, and the volatile components were evaporated in a rotary evaporator. The crude product was purified by column chromatography on silica gel (*n*-pentane/diethyl ether = 15:2, v/v).

(S1) J. A. Hodges and R. T. Raines, *Org. Lett.*, 2006, **8**, 4695-4697.

(S2) Z. P. Li, S. D. Bohle and C. J. Li, *Proc. Natl. Acad. Sci. USA*, 2006, **103**, 8928–8933.

[(4-Methoxyphenyl)-methyl-amino]acetonitrile

Known compound; the NMR spectroscopic data agree with those given in lit.[S3]. δ_H($CDCl_3$, 400 MHz) 2.90 (s, 3 H), 3.76 (s, 3 H), 4.06 (s, 2 H), 6.86 ppm (s, 4 H); δ_C($CDCl_3$, 100 MHz) 39.9, 43.9, 55.5, 114.7, 115.4, 117.8, 142.1, 154.3 ppm; HRMS *m/z* (EI) 176.0944, $C_{10}H_{12}N_2O$ requires 176.0950.

(Methyl-*p*-tolyl-amino)acetonitrile

Known compound; the NMR spectroscopic data agree with those given in lit.[S3]. δ_H($CDCl_3$, 300 MHz) 2.29 (s, 3 H), 2.96 (s, 3 H), 4.12 (s, 2 H), 6.80 (d, *J* 8.5 Hz, 2 H), 7.12 ppm (d, *J* 8.5 Hz, 2 H); δ_C($CDCl_3$, 100 MHz) 20.3, 39.4, 42.7, 115.3, 115.4, 129.8, 129.9, 145.6 ppm; HRMS *m/z* (EI) 160.0990, $C_{10}H_{12}N_2$ requires 160.1001.

(Methyl-*m*-tolyl-amino)acetonitrile

Known compound; the NMR spectroscopic data agree with those given in lit.[S3]. δ_H($CDCl_3$, 300 MHz) 2.31 (s, 3 H), 2.98 (s, 3 H), 4.25 (s, 2 H), 6.66-6.68 (m, 2 H), 6.74 (d, *J* 6.0 Hz, 1 H)), 7.16-7.22 ppm (m, 1 H); δ_C($CDCl_3$, 100 MHz) 21.8, 39.2, 42.3, 112.0, 115.5, 115.6, 121.1, 129.2, 139.2, 147.8 ppm; HRMS *m/z* (EI) 160.0990, $C_{10}H_{12}N_2$ requires 160.1001.

(Methyl-*o*-tolyl-amino)acetonitrile

Known compound; the NMR spectroscopic data agree with those given in lit.[S3]. δ_H($CDCl_3$, 300 MHz) 2.29 (s, 3 H), 2.85 (s, 3 H), 3.84 (s, 2 H), 7.03-7.09 (m, 1 H), 7.17-7.22 ppm (m, 3 H); δ_C($CDCl_3$, 100 MHz) 17.7, 41.0, 45.0, 115.6, 120.6, 124.9, 126.8, 131.3, 132.8, 148.4 ppm; HRMS *m/z* (EI) 160.0995, $C_{10}H_{12}N_2$ requires 160.1001.

(Methyl-phenyl-amino)acetonitrile

Known compound; the NMR spectroscopic data agree with those given in lit.[S3]. δ_H($CDCl_3$, 300 MHz) 3.00 (s, 3 H), 4.16 (s, 2 H), 6.85-6.94 (m, 3 H), 7.28-7.33 ppm (m, 2 H); δ_C($CDCl_3$, 100 MHz) 39.3, 42.3, 114.9, 115.4, 120.2, 129.4, 147.7 ppm; HRMS *m/z* (EI) 146.0841, $C_9H_{10}N_2$ requires 146.0844.

(S3) S. I. Murahashi, T. Nakae, H. Terai and N. Komiya, *J. Am. Chem. Soc*., 2008, **130**, 11005–11012.

[(4-Bromophenyl)-methyl-amino]acetonitrile. The reaction mixture was heated to reflux. Known compound; the NMR spectroscopic data agree with those given in lit.[S3]. δ_H($CDCl_3$, 300 MHz) 2.98 (s, 3 H), 4.13 (s, 2 H), 6.72 (d, *J* 9.0 Hz, 2 H), 7.37-7.40 ppm (m, 2 H); δ_C($CDCl_3$, 100 MHz) 39.3, 42.2, 112.6, 115.1, 116.4, 132.2, 146.7 ppm; HRMS *m/z* (EI) 223.9943, $C_9H_9BrN_2$ requires 223.9949.

[(2-Bromophenyl)-methyl-amino]acetonitrile

Viscous oil; ν_{max}(neat/ATR probe)/cm^{-1} 2956, 2887, 2802, 2232 (C≡N), 1586, 1473, 1439, 1415, 1337, 1325, 1222, 1177, 1111, 1023, 987, 919, 871, 766, 752, 272, 722 and 653; δ_H($CDCl_3$, 300 MHz) 2.92 (s, 3 H), 4.07 (s, 2 H), 6.98-7.04 (m, 1 H), 7.25-7.35 (m, 2 H) , 7.55-7.58 ppm (m, 1 H); δ_C($CDCl_3$, 100 MHz) 40.6, 44.8, 115.1, 119.7, 122.8, 126.3, 128.5, 133.9, 147.3 ppm; HRMS *m/z* (EI) 223.9942, $C_9H_9BrN_2$ requires 223.9949; Anal. Calcd for $C_9H_9BrN_2$: C, 48.03; H, 4.03; N, 12.45. Found: C, 48.10; H, 3.70; N, 12.41.

[(4-Ethynylphenyl)-methyl-amino]acetonitrile. The reaction mixture was heated to reflux. Viscous oil; ν_{max}(neat/ATR probe)/cm^{-1} 3279 (≡C-H), 3042, 2916, 2823, 2240 (C≡N), 2101 (C≡C), 1671, 1605, 1512, 1360, 1332, 1246, 1181, 1113, 997, 924 and 819; δ_H($CDCl_3$, 200 MHz) 2.99 (s, 1 H), 3.03 (s, 3 H), 4.18 (s, 2 H), 6.75 (d, *J* 9.0 Hz, 2 H), 7.42 ppm (d, *J* 9.0 Hz, 2 H); δ_C($CDCl_3$, 100 MHz) 37.7, 40.5, 76.0, 84.7, 113.5, 113.9, 115.1, 133.5, 148.5 ppm; HRMS *m/z* (EI) 170.0839, $C_{11}H_{10}N_2$ requires 170.0844.

[Methyl-(4-nitrophenyl)-amino]acetonitrile. The reaction mixture was heated to reflux. Known compound; the NMR spectroscopic data agree with those given in lit.[S4]. Solid, mp 112.5-113.4 °C (lit.,[S4] 114 °C); δ_H($CDCl_3$, 400 MHz) 3.17 (s, 3 H), 4.26 (s, 2 H), 6.79 (d, *J* 8.0 Hz, 2 H), 8.19 ppm (d, *J* 8.0 Hz, 2 H); δ_C($CDCl_3$, 100 MHz) 39.3, 41.1, 112.3, 114.5, 126.0, 139.9, 152.0 ppm; HRMS *m/z* (EI) 191.0691, $C_9H_9N_3O_2$ requires 191.0695.

[Methyl-(3-nitrophenyl)-amino]acetonitrile

Solid, mp 99.3-99.5 °C (from Et_2O/pentane); ν_{max}(neat/ATR probe)/cm^{-1} 3099, 3042, 2920, 2240 (C≡N), 1617, 1520, 1337, 1259, 1221, 1132, 1015, 881, 860, 789, 782, 737 and 667; δ_H($CDCl_3$, 300 MHz) 3.11 (s, 3 H), 4.25 (s, 2 H), 7.09-7.13 (m, 1 H), 7.45 (t, *J* 8.3 Hz, 1 H),

(S4) M. Barzoukas, D. Josse, P. Fremaux, J. Zyss, J. F. Nicoud and J. O. Morley, *J. Opt. Soc. Am. B*, 1987, **4**, 977–986.

7.65-7.76 ppm (m, 2 H); δ_C($CDCl_3$, 100 MHz) 39.3, 41.7, 108.7, 114.4, 114.7, 119.6, 130.3, 148.3, 149.3 ppm; HRMS *m/z* (EI) 191.0689, $C_9H_9N_3O_2$ requires 191.0695; Anal. Calcd for $C_9H_9N_3O_2$: C, 56.54; H, 4.74; N, 21.98. Found: C, 56.40; H, 4.73; N, 21.45.

2-Phenyl-1,2,3,4-tetrahydroisoquinoline-1-carbonitrile

Known compound; the NMR spectroscopic data agree with those given in lit.[S3]. δ_H($CDCl_3$, 200 MHz) 2.91-3.24 (m, 2 H), 3.41-3.55 (m, 1 H), 3.71-3.82 (m, 1 H), 5.50 (s, 1 H), 6.97-7.10 (m, 3 H), 7.24-7.39 ppm (m, 6 H); δ_C($CDCl_3$, 100 MHz) 28.1, 44.1, 53.4, 117.6, 117.7, 121.9, 126.8, 127.1, 128.8, 129.3, 129.5, 129.6, 134.1, 148.1 ppm; HRMS *m/z* (EI) 234.1146, $C_{16}H_{14}N_2$ requires 234.1157.

2-(4-Methoxyphenyl)-1,2,3,4-tetrahydroisoquinoline-1-carbonitrile

Solid; ν_{max}(neat/ATR probe)/cm^{-1} 2996, 2933, 2837, 2221 (C≡N), 1647, 1510, 1465, 1454, 1259, 1245, 1206, 1179, 1030, 829 and 733; δ_H($CDCl_3$, 400 MHz) 2.91-2.96 (m, 1 H), 3.12-3.21 (m, 1 H), 3.40-3.47 (m, 1 H), 3.55-3.59 (m, 1 H), 3.80 (s, 3 H), 5.36 (s, 1 H), 6.90-6.94 (m, 2 H), 7.07-7.11 (m, 2 H), 7.22-7.33 ppm (m, 4 H); δ_C($CDCl_3$, 100 MHz) 28.7, 44.9, 55.5, 55.6, 114.8, 117.6, 121.0, 126.7, 127.1, 128.6, 129.4, 129.6, 134.3, 142.6, 155.7 ppm; HRMS *m/z* (EI) 264.1250, $C_{17}H_{16}N_2O$ requires 264.1263; Anal. Calcd for $C_{17}H_{16}N_2O$: C, 77.25; H, 6.10; N, 10.60. Found: C, 76.88; H, 6.51; N, 10.43.

1-Phenylpiperidine-2-carbonitrile from the reaction without methanol.

Known compound; the NMR spectroscopic data agree with those given in lit.[S3,S5]. δ_H($CDCl_3$, 400 MHz) 1.66-1.73 (m, 2 H), 1.84-1.87 (m, 2 H), 1.99-2.03 (m, 2 H), 3.00-3.06 (m, 1 H), 3.46 (d, *J* 12 Hz, 1 H), 4.63 (s, 1 H), 6.98-7.02 (m, 3 H), 7.25-7.34 ppm (m, 2 H); δ_C($CDCl_3$, 100 MHz) 20.1, 25.0, 29.1, 46.4, 51.9, 117.1, 118.1, 122.0, 129.2, 149.6 ppm; HRMS *m/z* (EI) 186.1153, $C_{12}H_{14}N_2$ requires 186.1157.

Additional NMR signals of unidentified byproducts: δ_H($CDCl_3$, 400 MHz) 1.3-1.5 (m), 5.93 (s), 6.80-6.82 (m); δ_C($CDCl_3$, 100 MHz) 16.0, 21.6, 22.3, 69.4, 86.9, 113.1, 117.4, 121.9, 129.4, 146.5, 150.6 ppm. One of the byproducts is tentatively assigned to the dicyanation product 1-phenylpiperidine-2,6-dicarbonitrile[S6] based on HRMS [*m/z* (EI) 211.1106,

(S5) E. Le Gall, J.-P. Hurvois, T. Renaud, C. Moinet, A. Tallec, P. Uriac, S. Sinbandhit and L. Toupet, *Liebigs Ann./Recueil*, 1997, 2089–2101.

(S6) K. Takahashi, T. Mikajiri, H. Kurita, K. Ogura and H. Iida, *J. Org. Chem.*, 1985, **50**, 4372–4375.

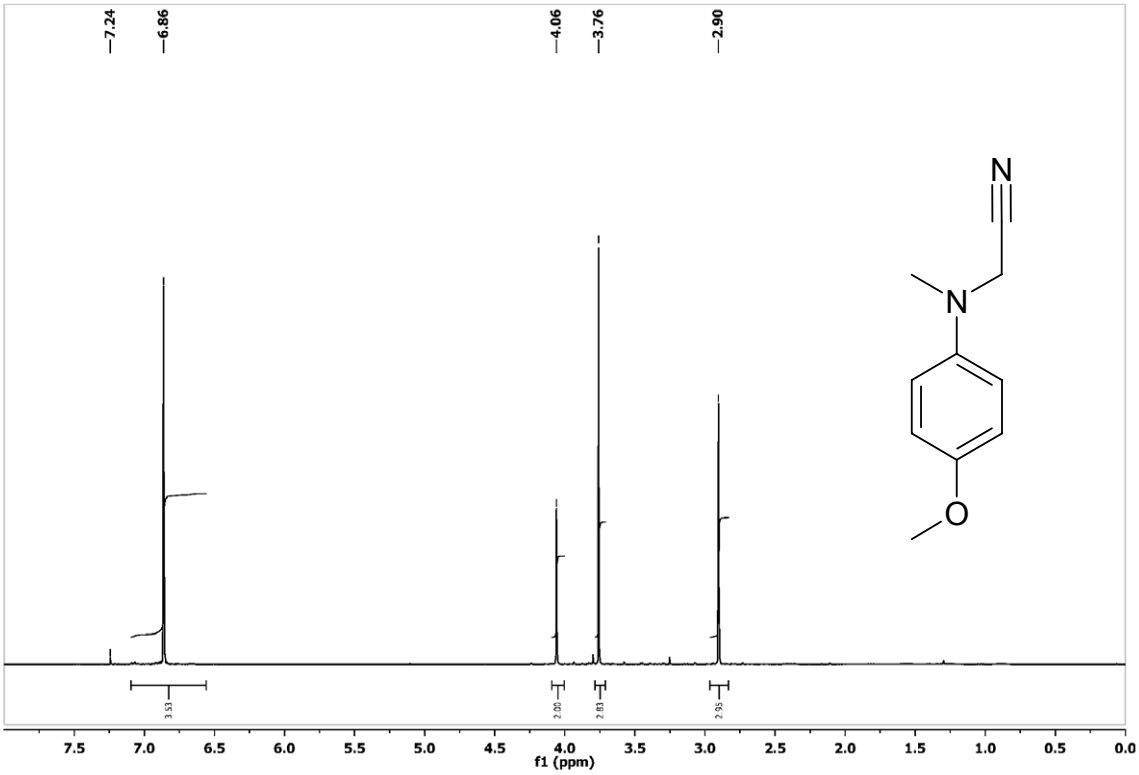
$C_{13}H_{13}N_3$ requires 211.1109]. Because of superimposition of resonances, however, an unambiguous assignment of the signals in the NMR spectra was not possible.

1-Phenylpyrrolidine-2-carbonitrile from the reaction without methanol.
Known compound; the NMR spectroscopic data agree with those given in lit.[S7]. δ_H($CDCl_3$, 200 MHz) 2.07-2.34 (m, 4 H), 3.26-3.38 (m, 2 H), 4.33-4.37 (m, 1 H), 6.58-6.63 (m, 2 H), 6.74 (t, *J* 7.4 Hz, 1 H), 7.16-7.25 ppm (m, 2 H); δ_C($CDCl_3$, 100 MHz) 23.9, 31.5, 47.4, 49.0, 112.6, 118.1, 119.2, 129.4, 145.1 ppm; HRMS *m/z* (EI) 172.0991, $C_{11}H_{12}N_2$ requires 172.1000.

1-Phenylpyrrolidine-2,5-dicarbonitrile from the reaction in the presence of TMSCN (4.0 mmol). The Typical Procedure was followed to obtain the crude product which was purified by column chromatography (SiO_2, *n*-pentane/diethyl ether = 3:1, v/v).
Known compound (lit.[S8]); ν_{max}(neat/ATR probe)/cm^{-1} 3075, 3050, 3003, 2930, 2233, 1597, 1504, 1347, 1338, 1323, 1269, 1251, 1180, 1160, 966, 818, 745 and 693; δ_H($CDCl_3$, 400 MHz) 2.56-2.63 (m, 4 H), 4.57 (t, *J* 2.8 Hz, 2 H), 6.78-6.81 (m, 2 H), 6.96-6.99 (m, 1 H), 7.35-7.39 ppm (m, 2 H); δ_C($CDCl_3$, 100 MHz) 30.4, 48.9, 113.4, 117.9, 120.5, 129.9, 141.8 ppm. Attempts to elucidate the stereochemistry of the product were not made.

(S7) W. Liu, Y. Ma, Y. W. Yin and Y. F. Zhao, *Bull. Chem. Soc. Jpn.*, 2006, **79**, 577–579.

(S8) K. Takahashi, H. Saitoh, K. Ogura and H. Iida, *Heterocycles*, 1986, **24**, 2905–2910.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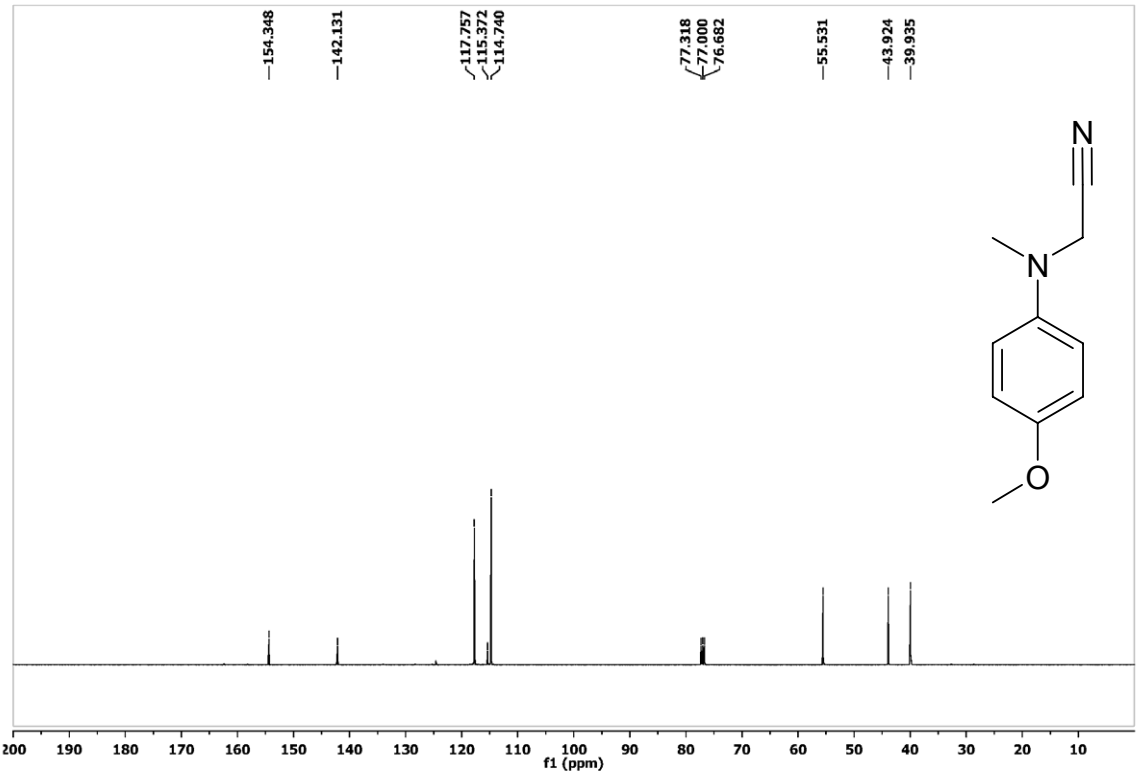
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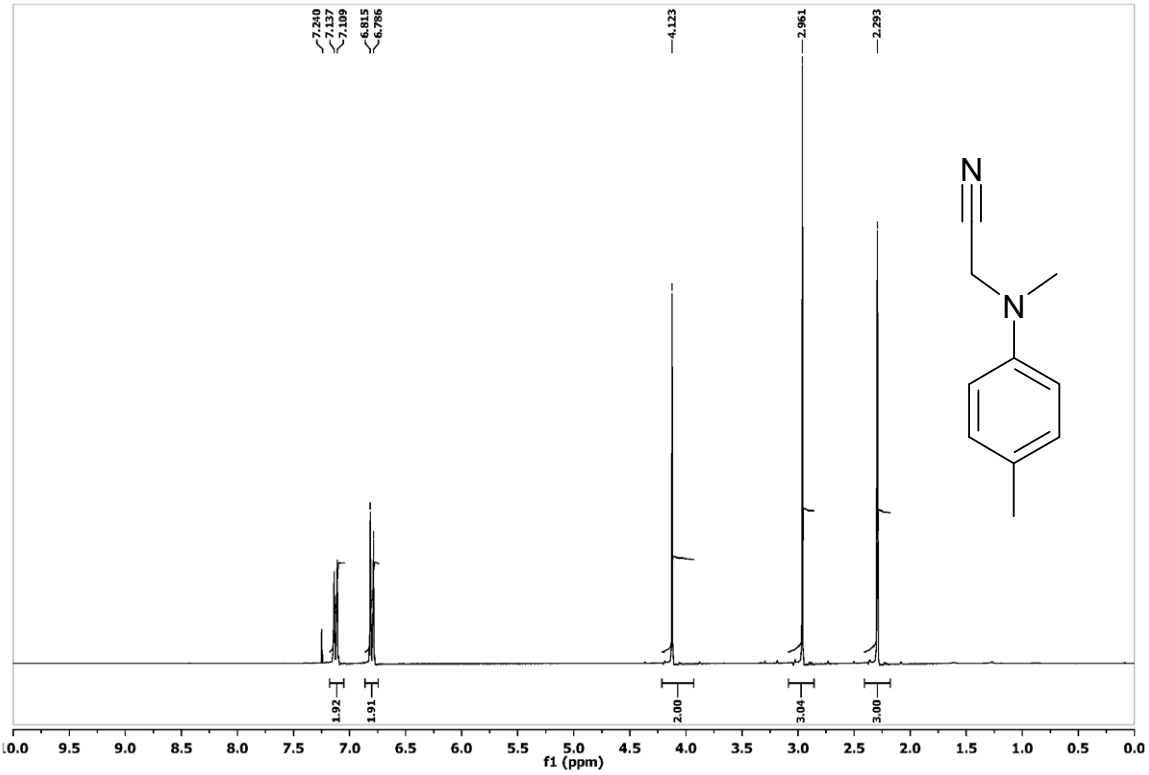
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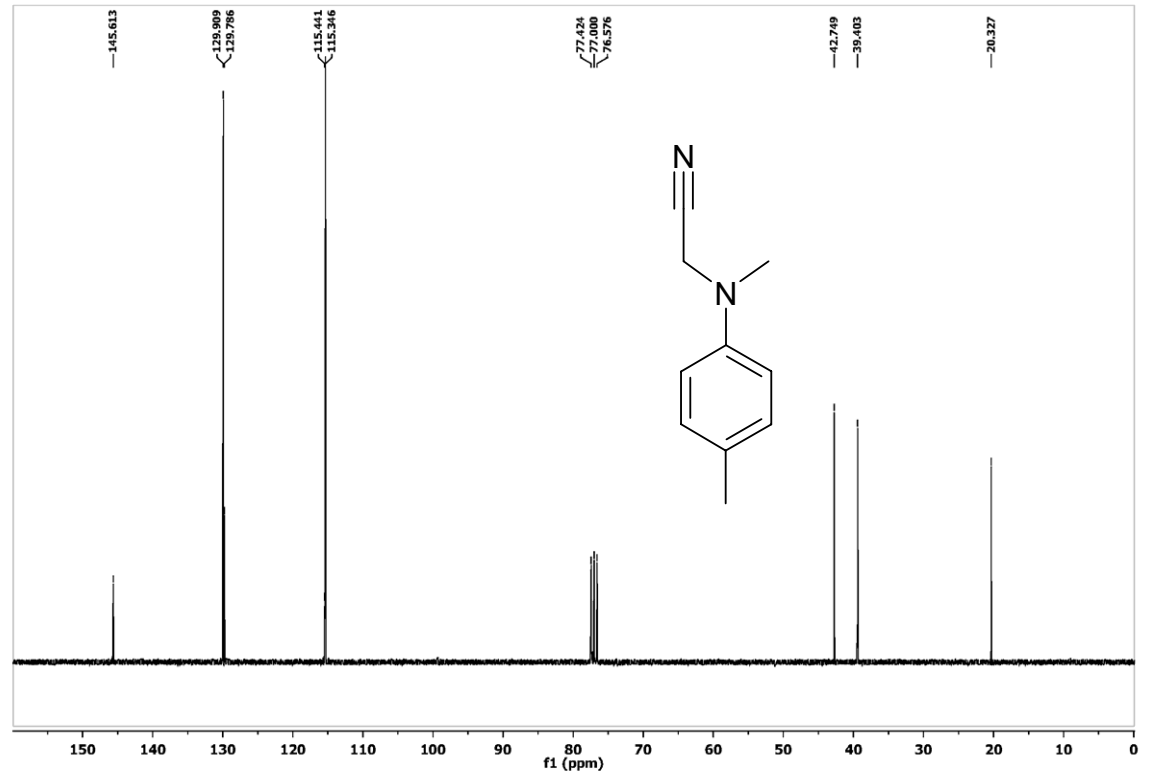
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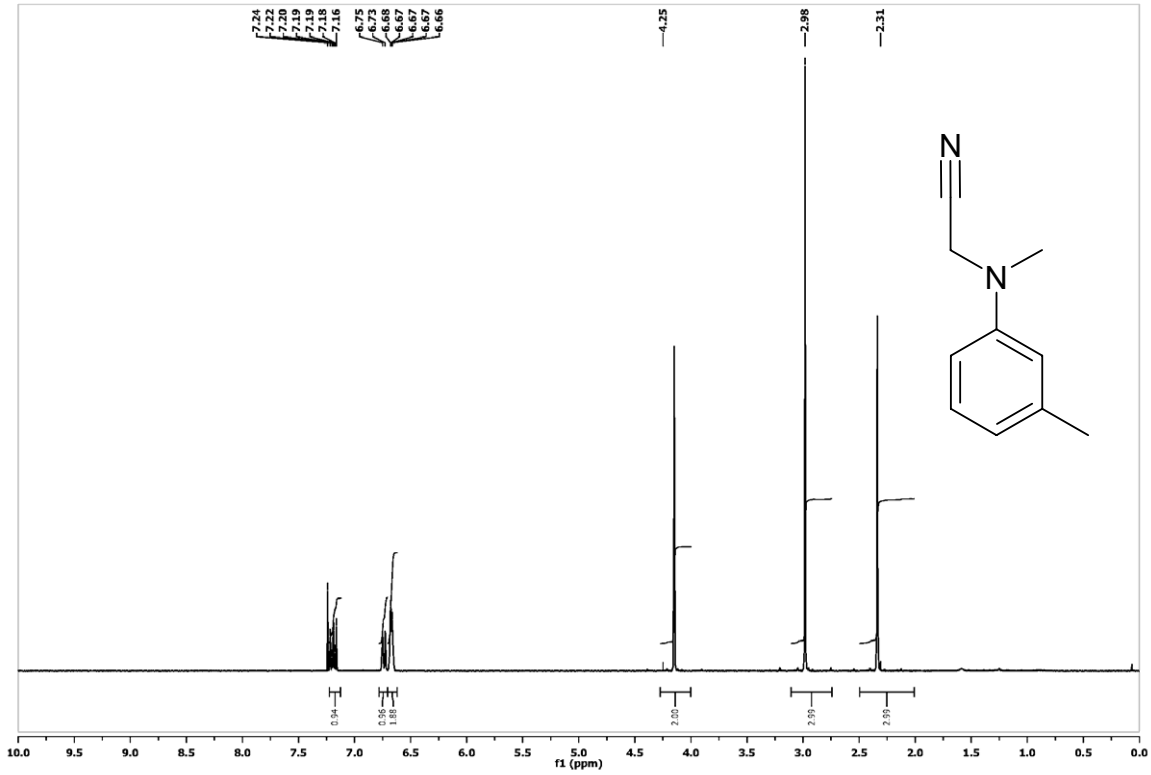
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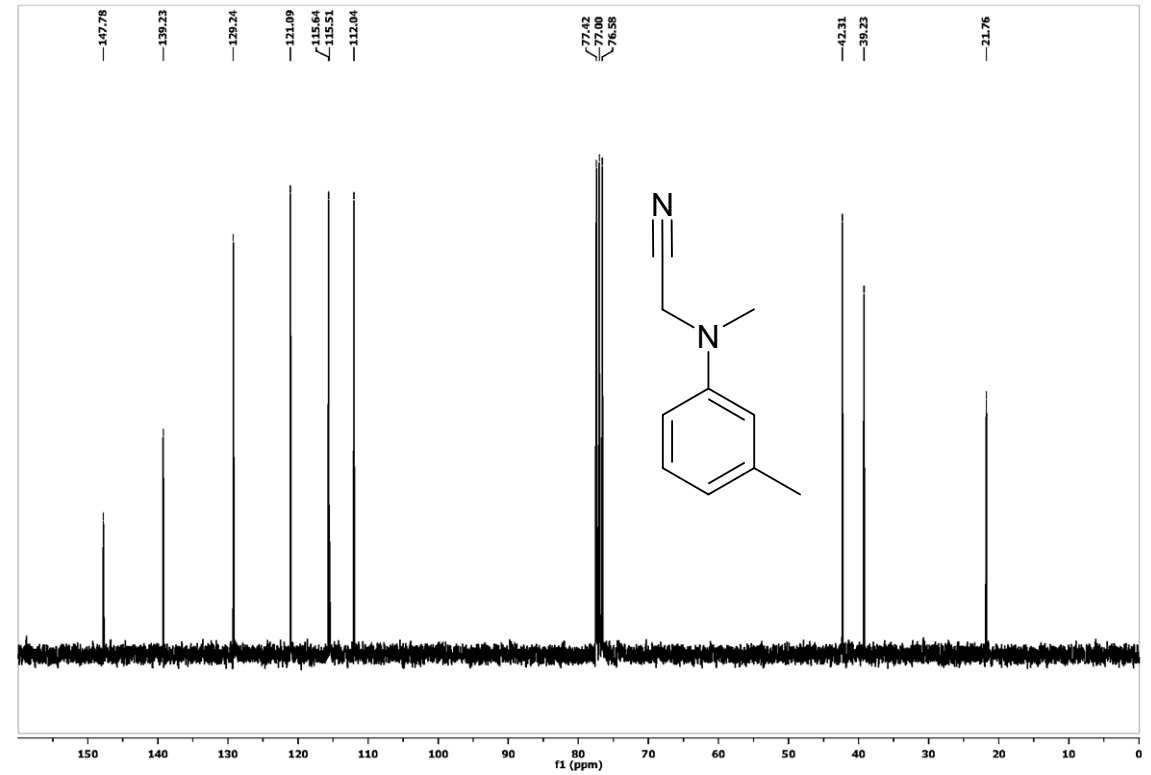
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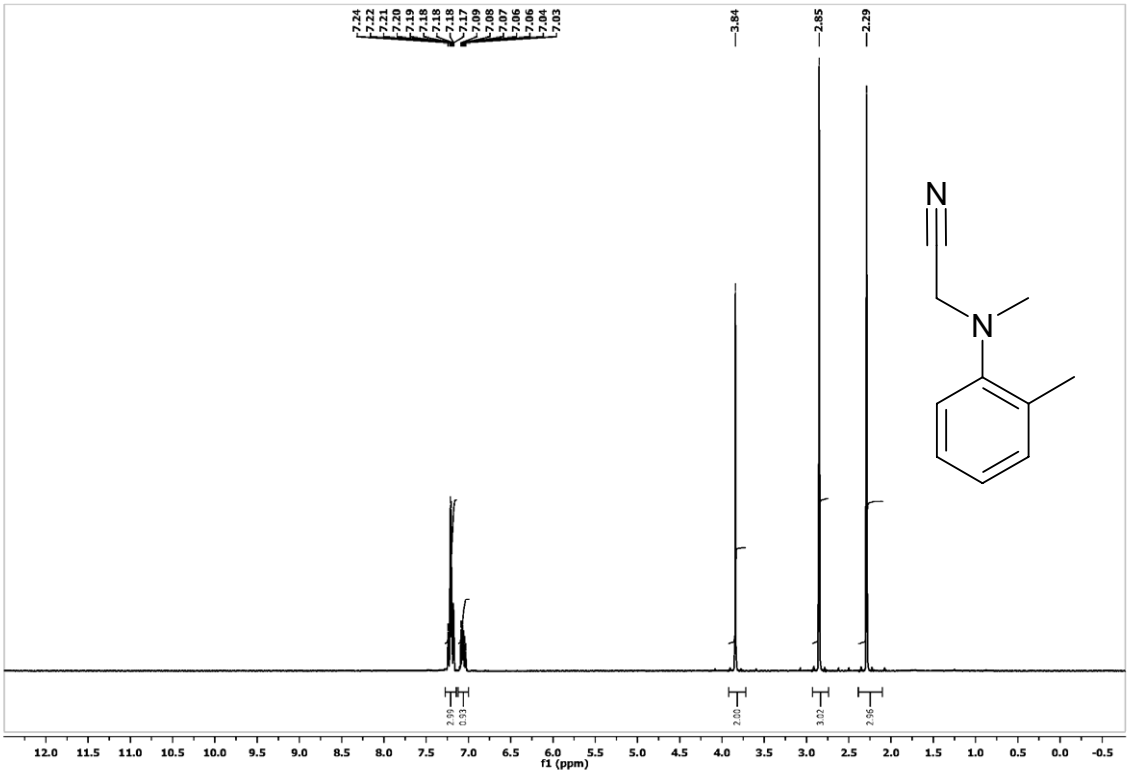
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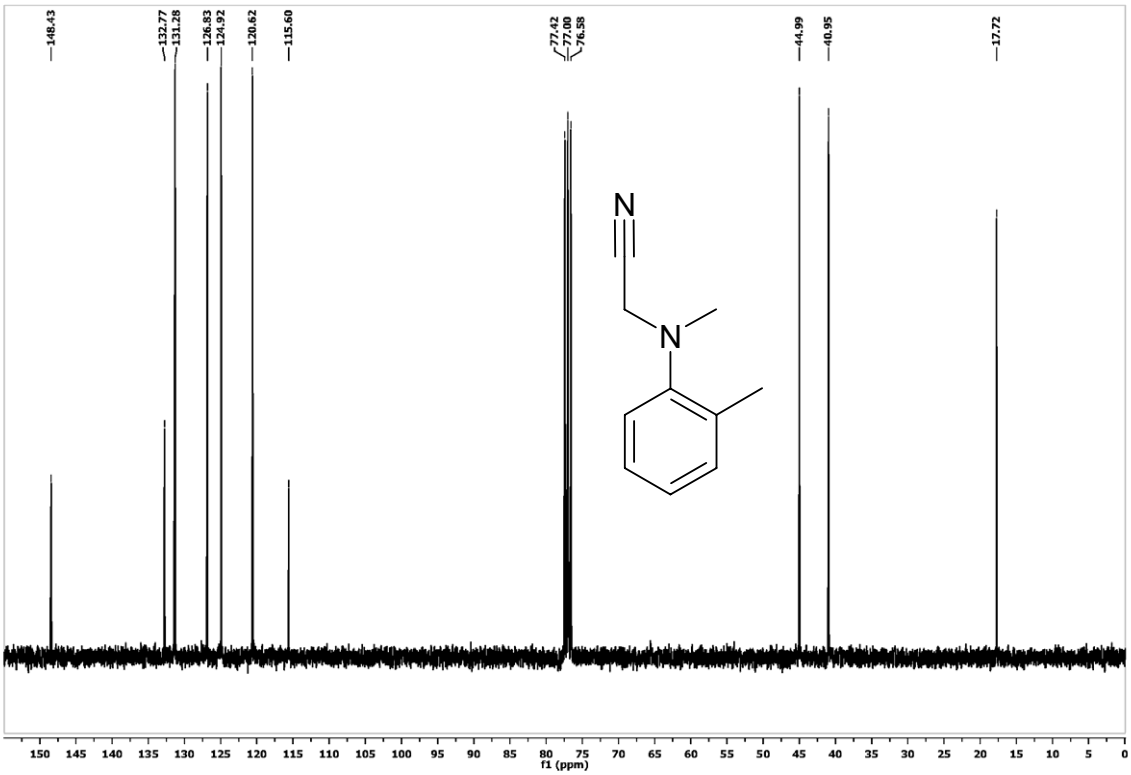
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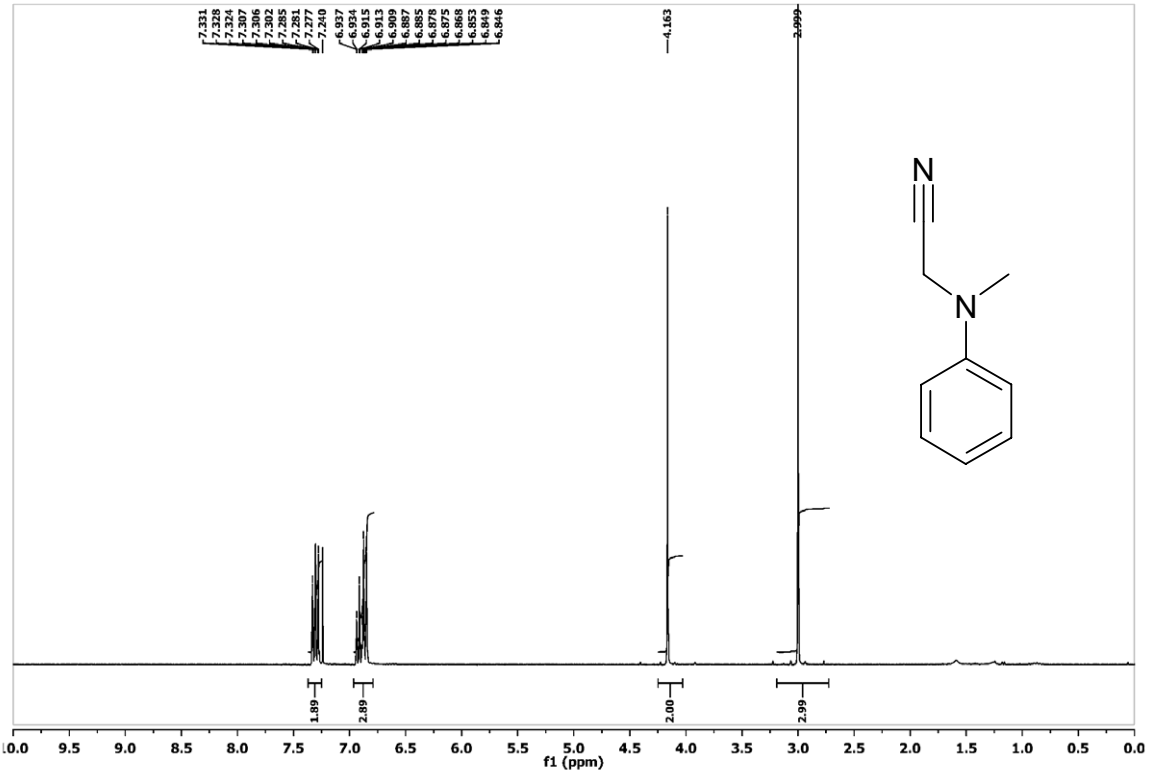
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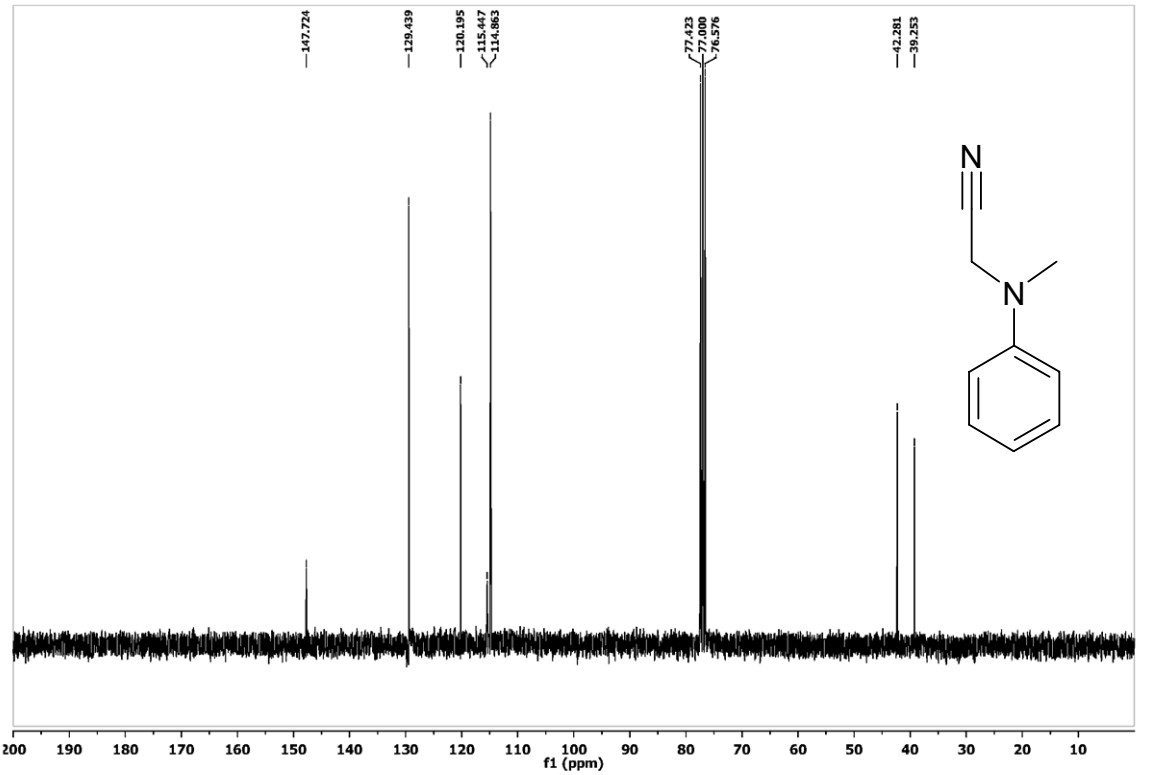
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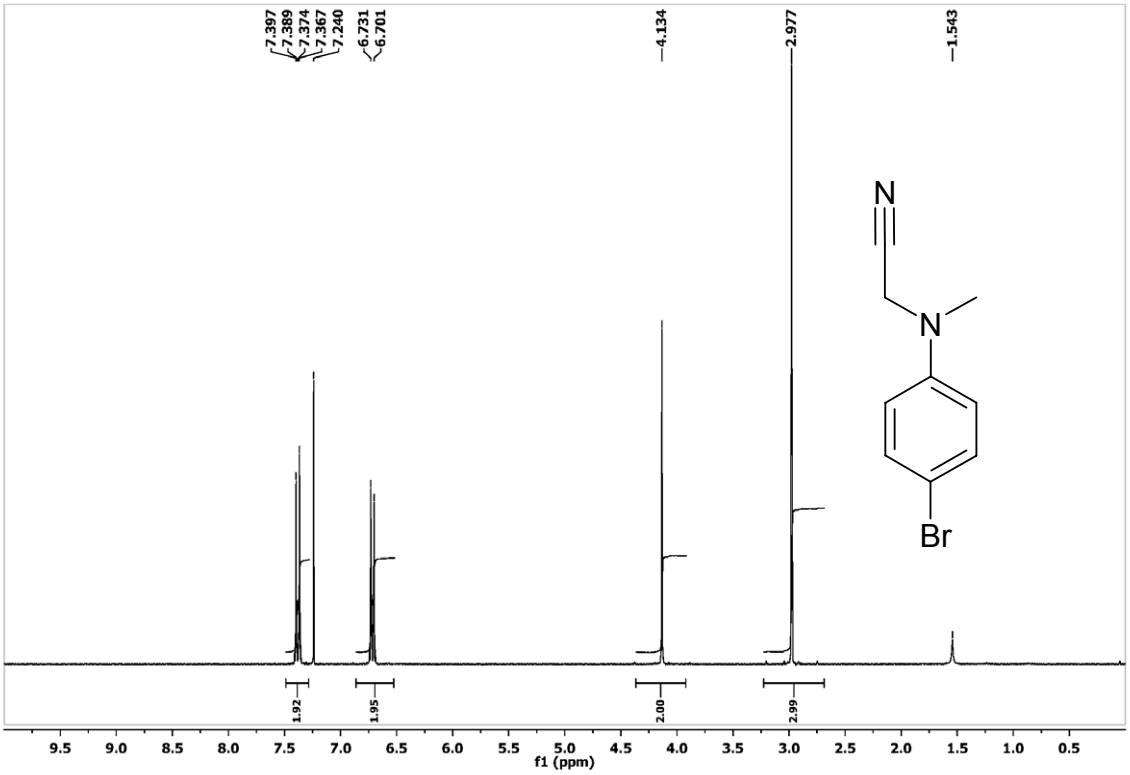
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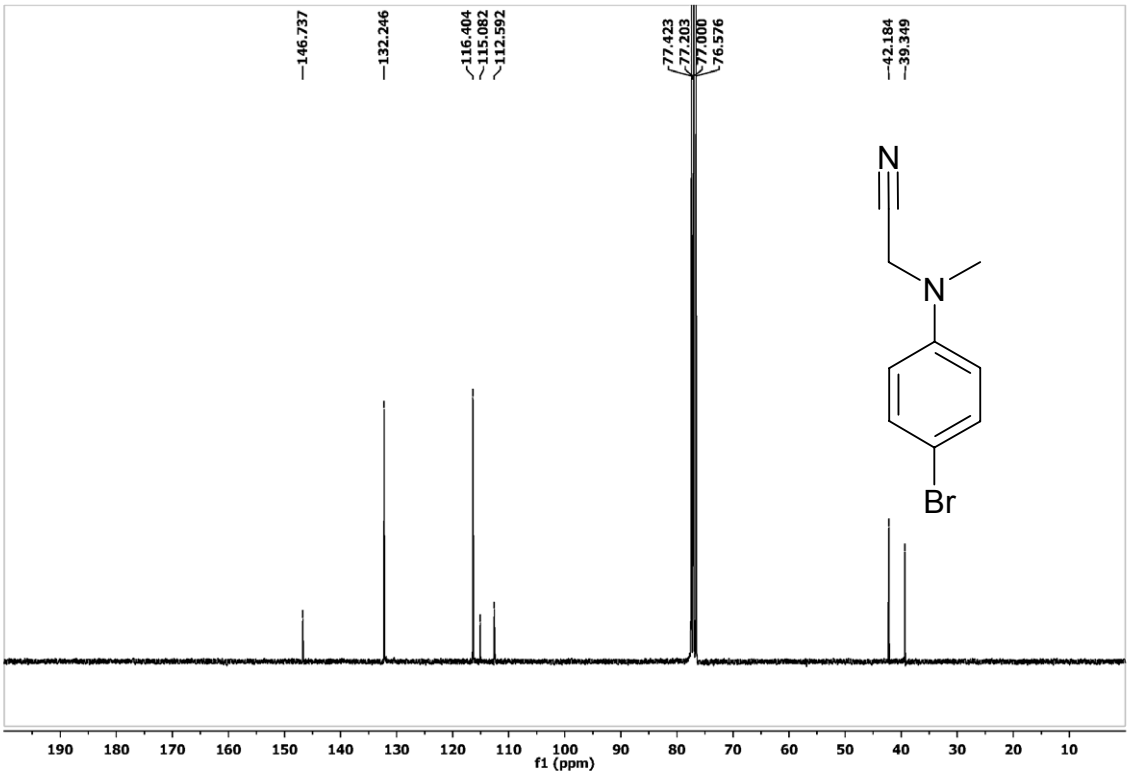
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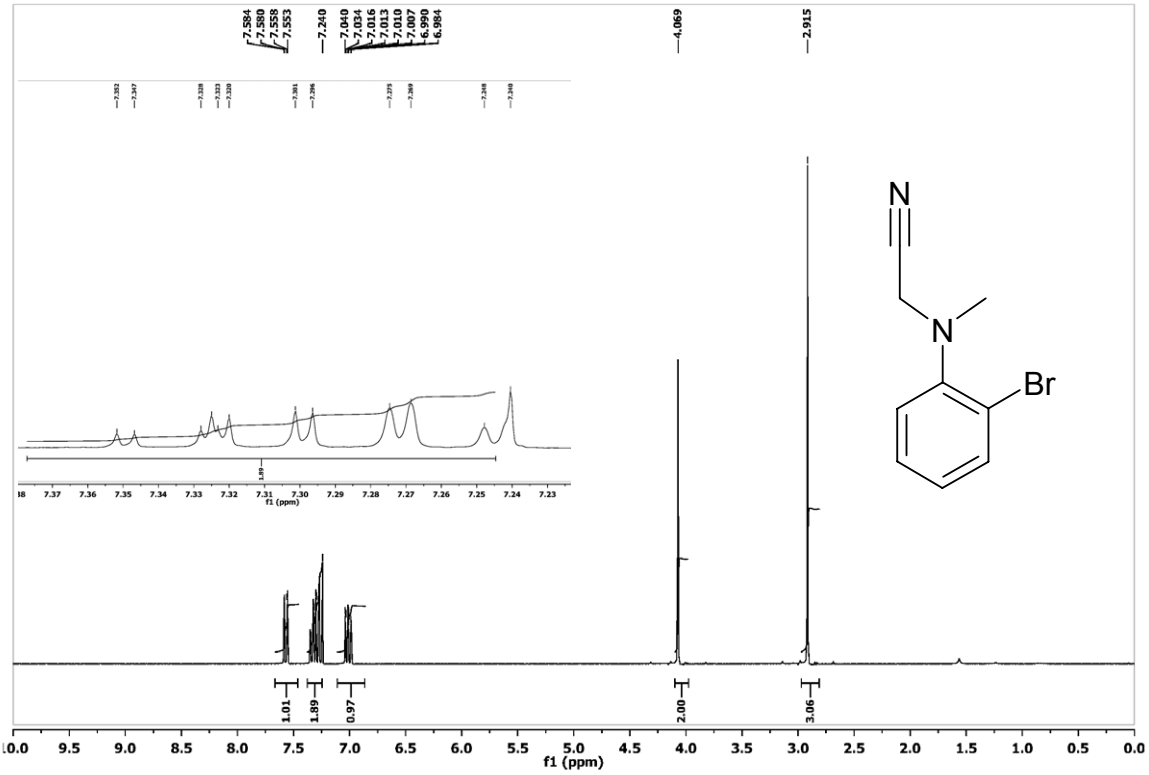
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N
Br
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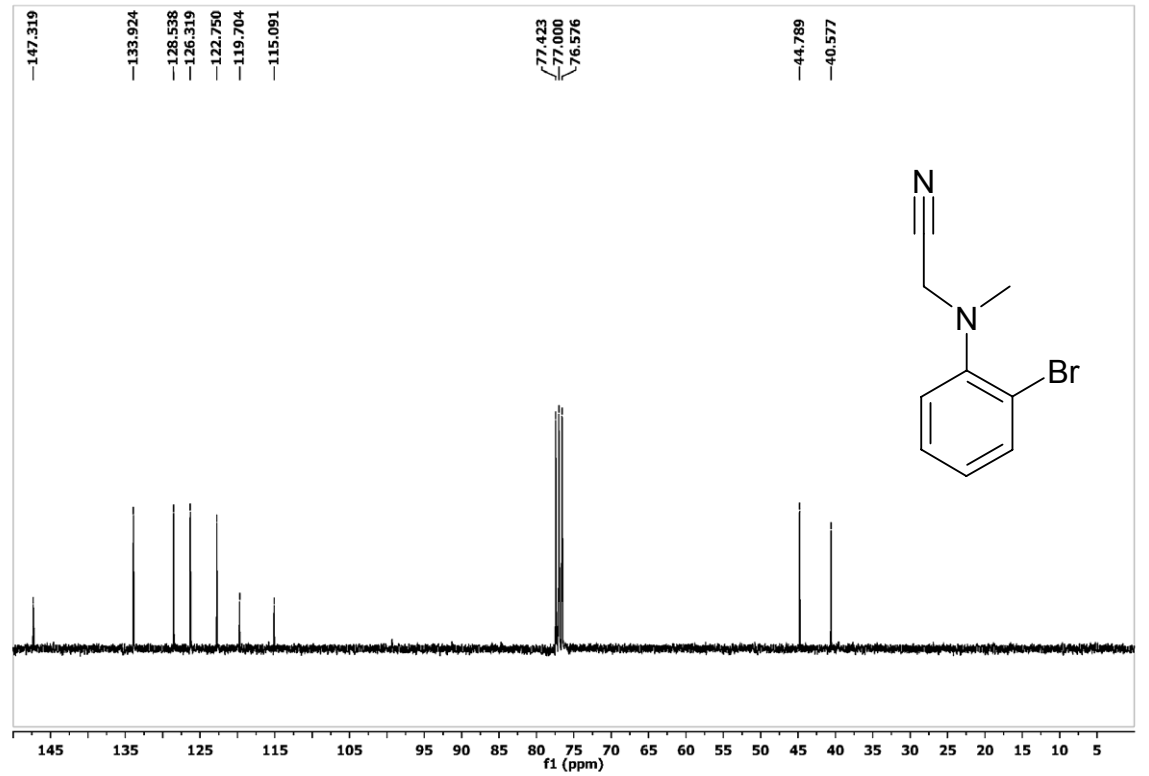
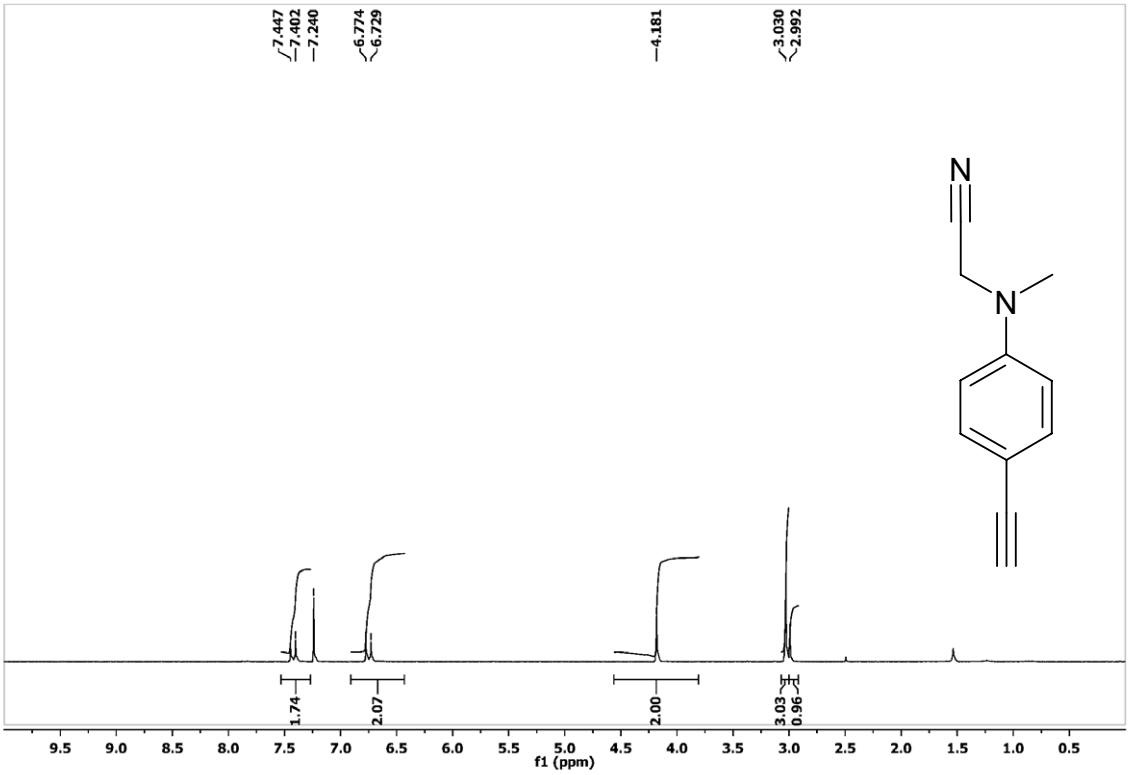
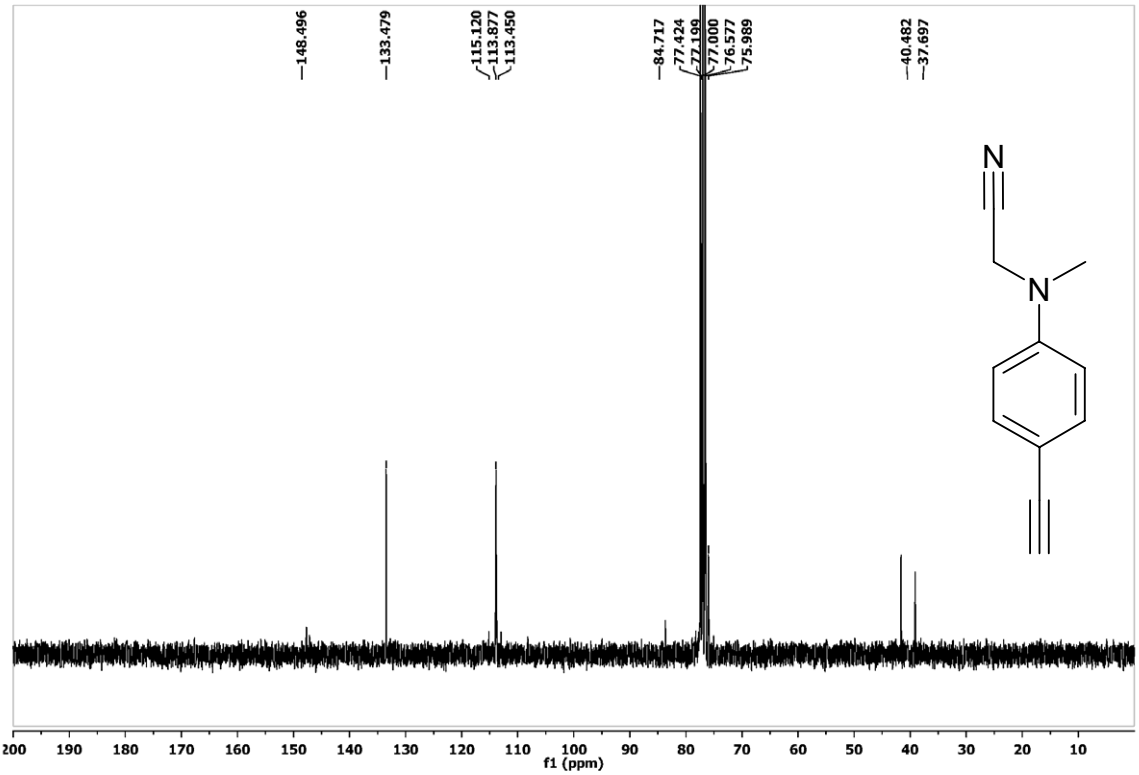
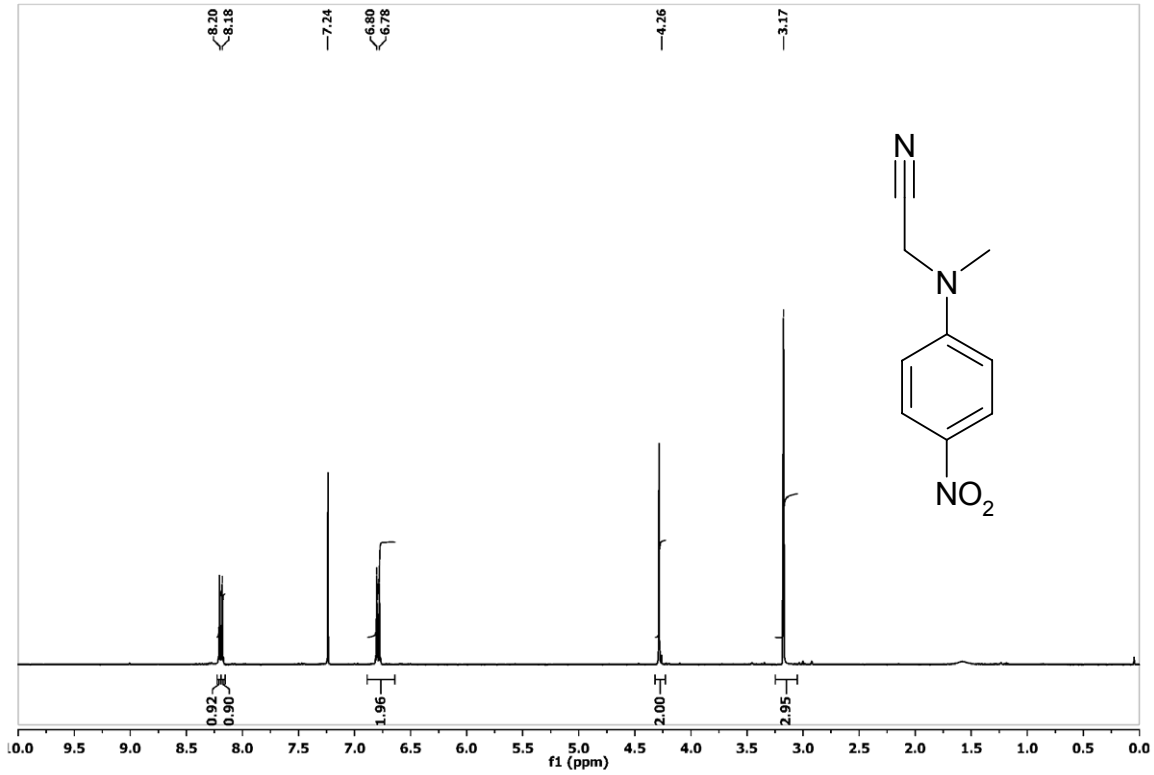
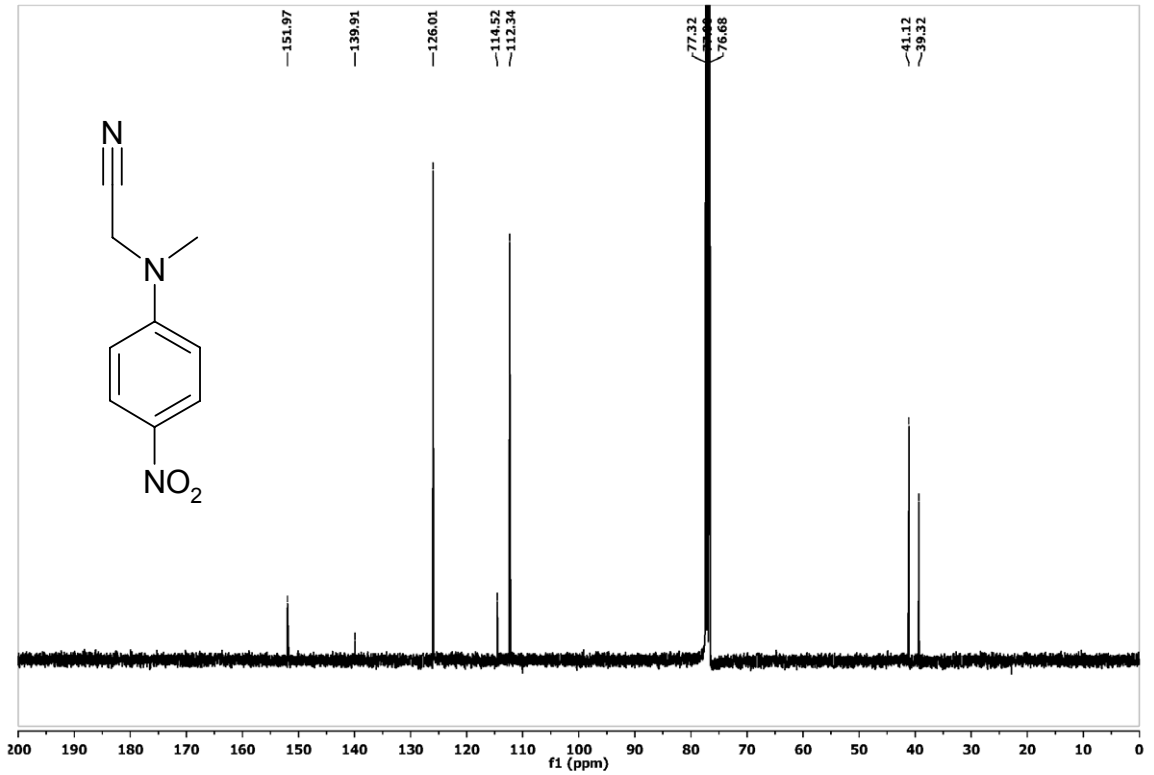
2.00
3.06
f1 (ppm)

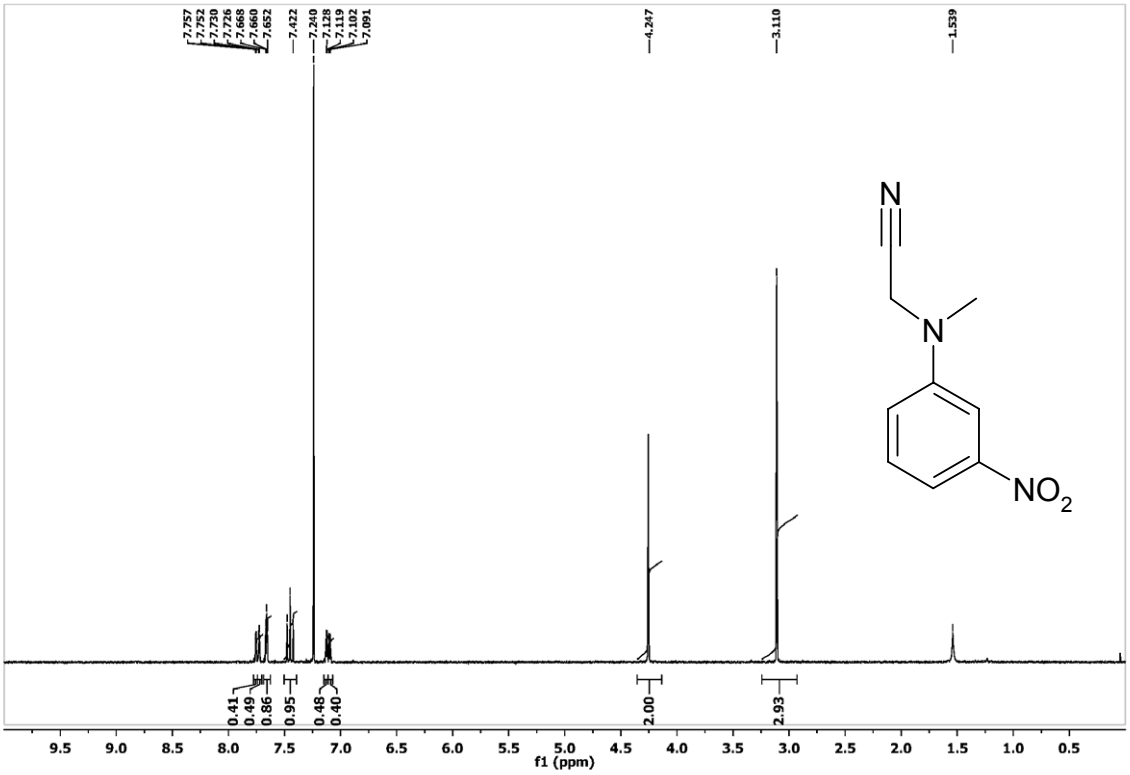

147.319
133.924
128.538
126.319
122.750
119.704
115.091
77.423
77.000
76.576
44.789
40.577
N
N
Br
f1 (ppm)

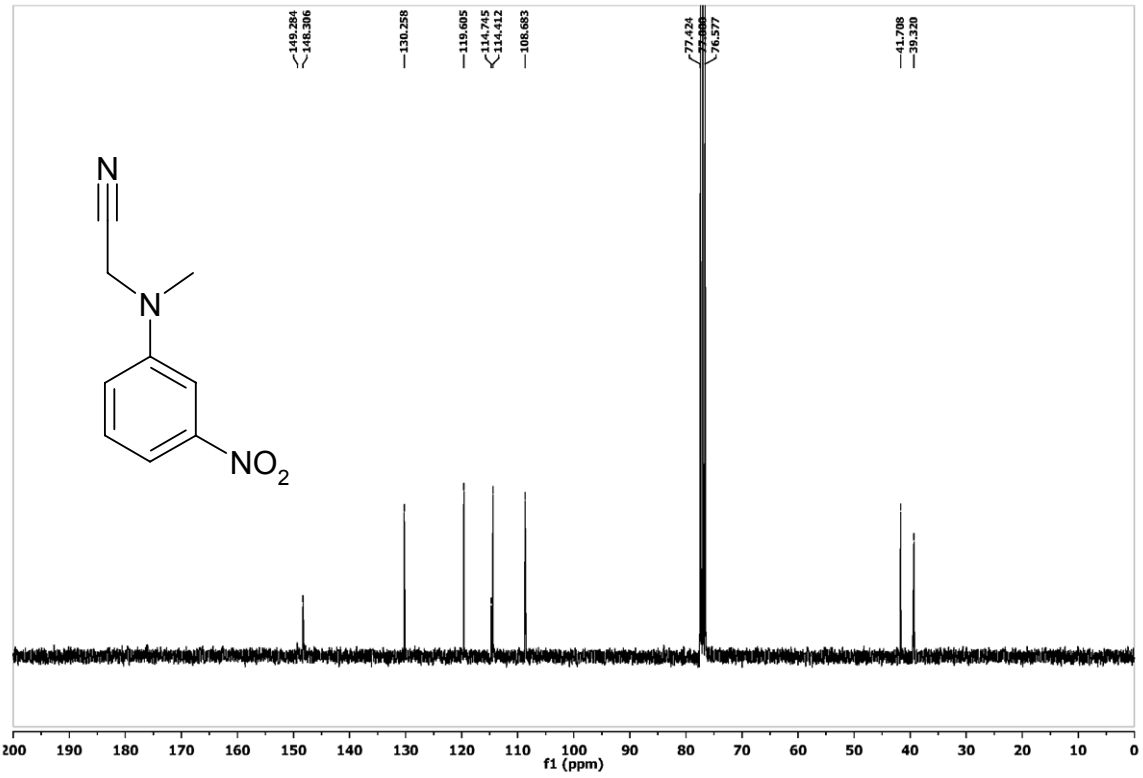

7.447
7.402
7.240
6.774
6.729
4.181
3.030
2.992
N
N
1.74
2.07
2.00
3.03
0.96
f1 (ppm)

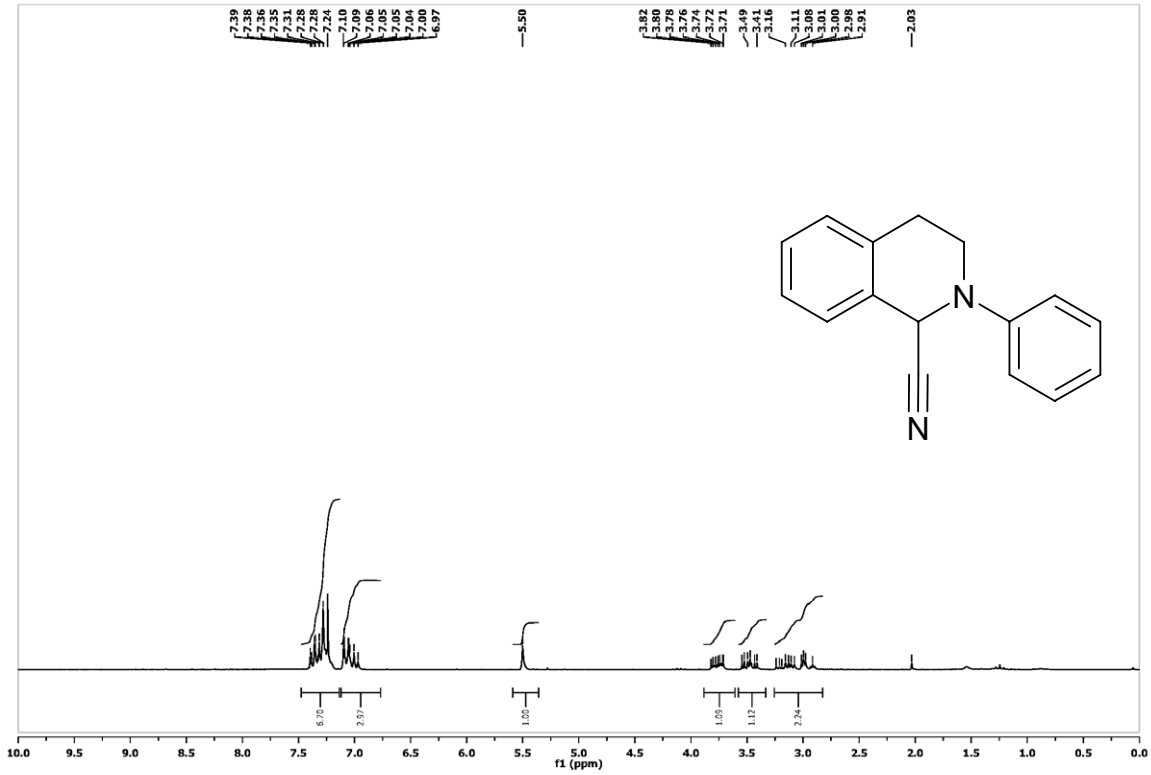

148.496
133.479
115.120
113.877
113.450
84.717
77.424
77.199
77.000
76.577
75.989
40.482
37.697
N
N
f1 (ppm)

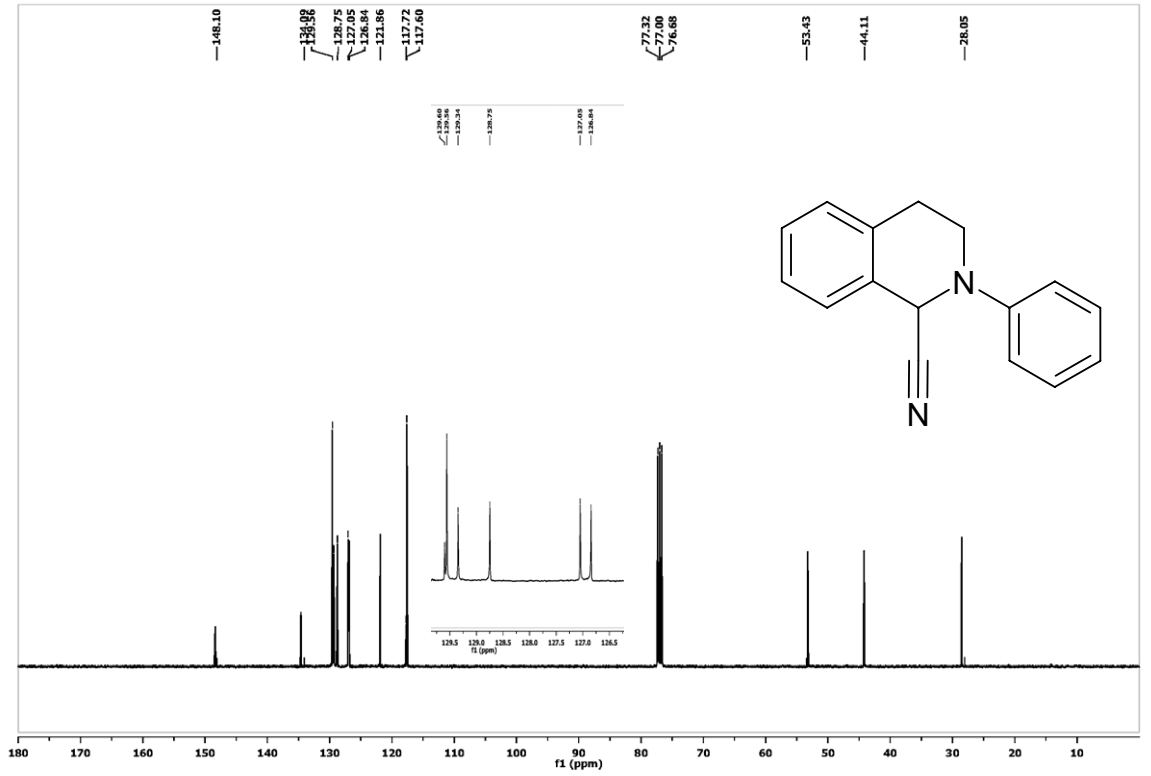

8.20
8.18
7.24
6.80
6.78
4.26
3.17
N
N
NO2
0.92
0.90
1.96
2.00
2.95
f1 (ppm)

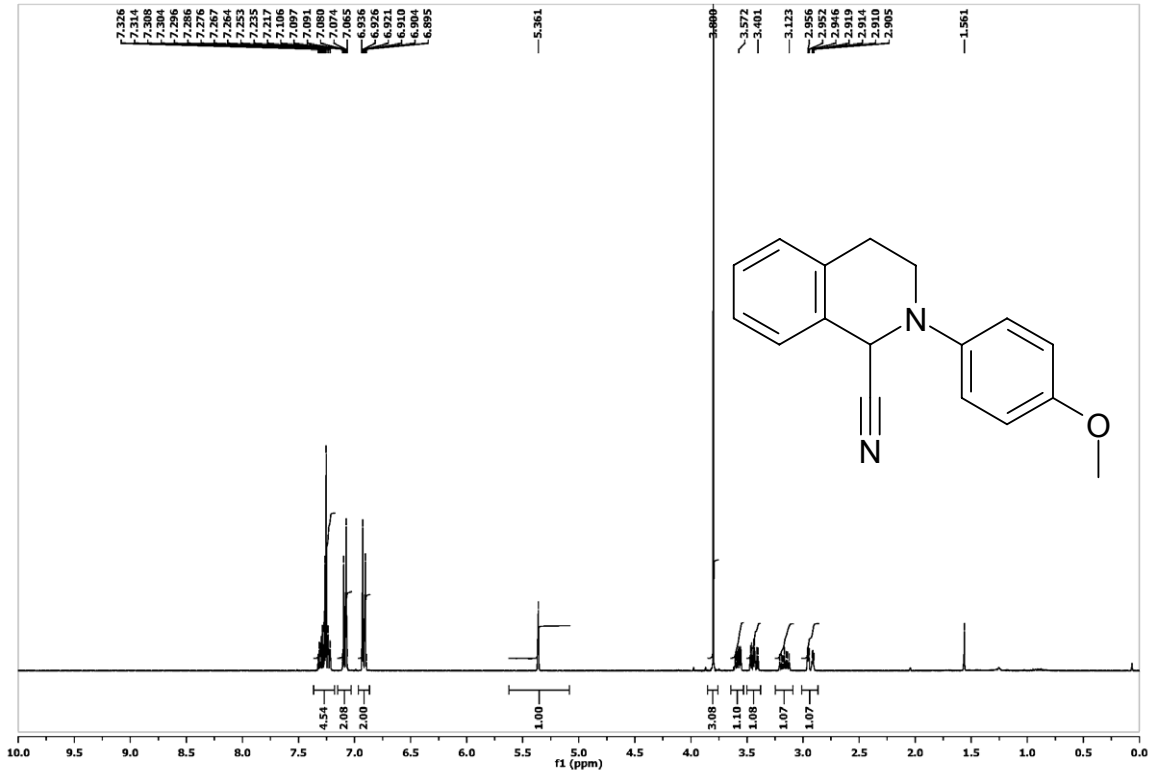

151.97
139.91
126.01
114.52
112.34
77.32
76.68
41.12
39.32
N
N
NO2
f1 (ppm)

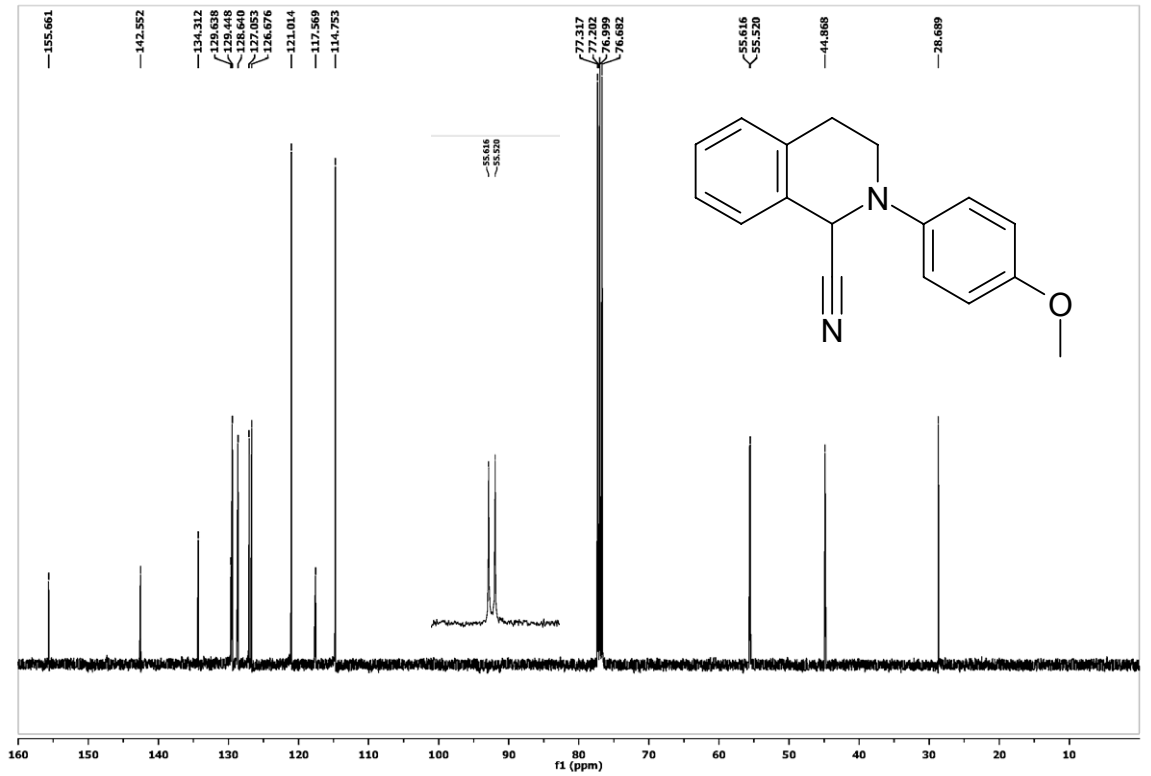

7.757
7.752
7.730
7.726
7.668
7.660
7.652
7.422
7.240
7.128
7.119
7.102
7.091
4.247
3.110
1.539
N
N
NO2
0.41
0.49
0.86
0.95
0.48
0.40
2.00
2.93
f1 (ppm)

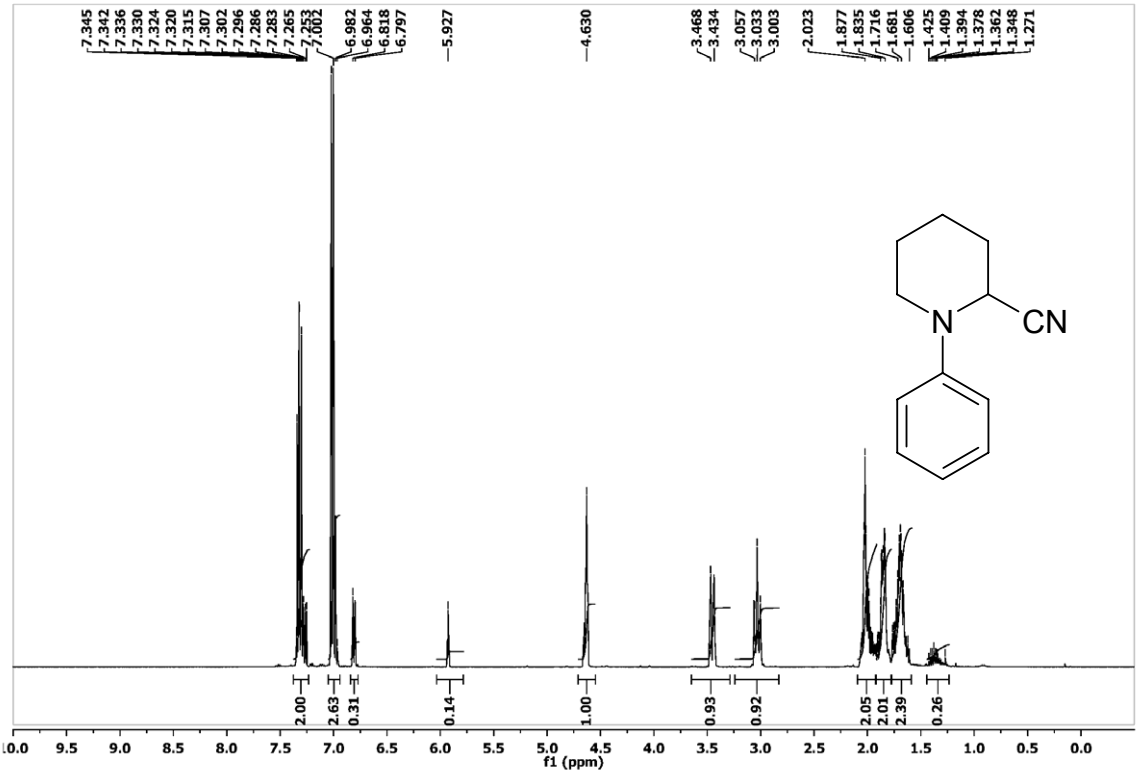

149.284
148.306
130.258
119.605
114.745
114.412
108.683
77.424
76.577
41.708
39.320
N
N
NO2
f1 (ppm)

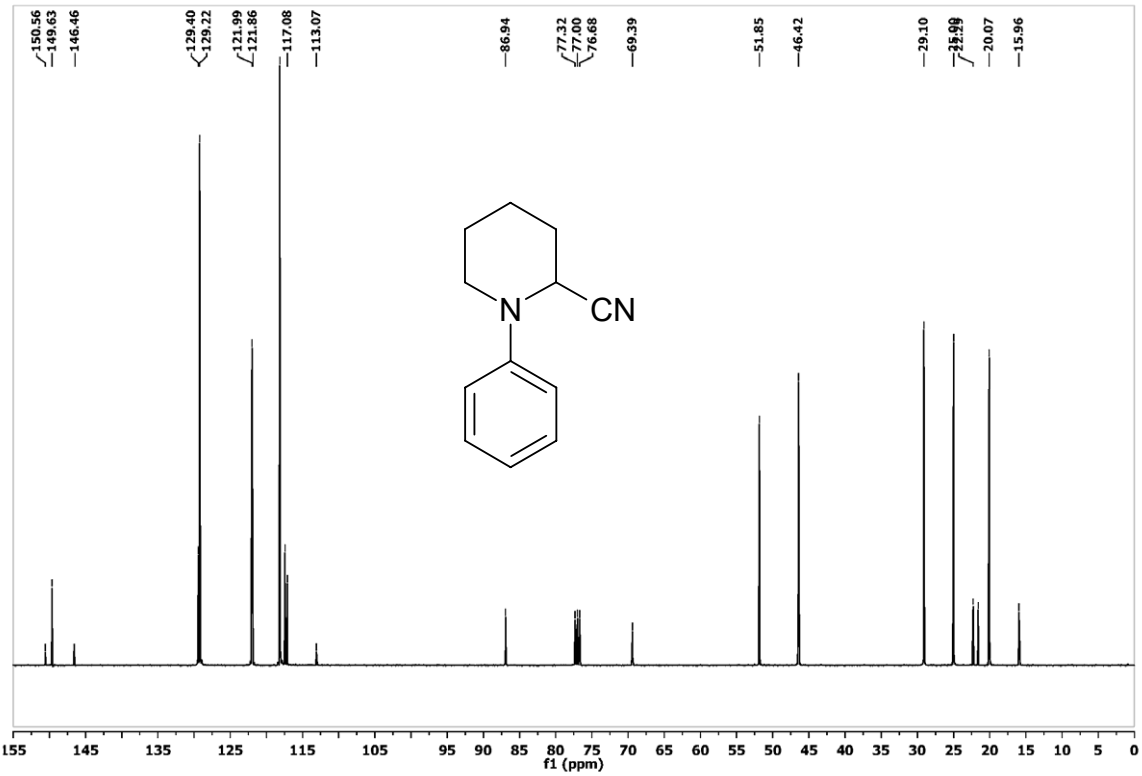

7.39
7.38
7.36
7.35
7.31
7.28
7.28
7.24
7.10
7.09
7.06
7.05
7.05
7.04
7.00
6.97
5.50
3.82
3.80
3.78
3.76
3.74
3.72
3.71
3.49
3.41
3.16
3.11
3.08
3.01
3.00
2.98
2.91
2.03
N
N
6.70
2.97
1.00
1.05
1.12
2.24
f1 (ppm)

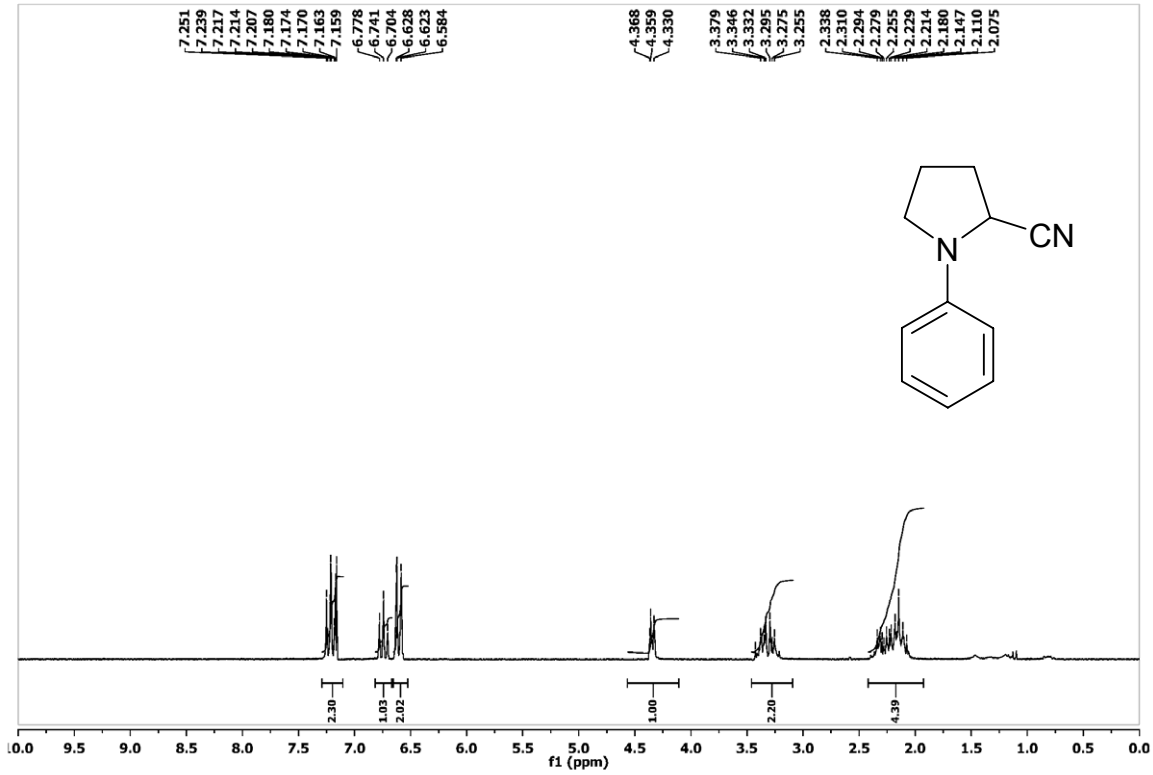

148.10
134.09
129.96
129.34
128.75
127.05
126.84
121.86
117.72
117.60
77.32
77.00
76.68
53.43
44.11
28.05
N
N
f1 (ppm)


7.326
7.314
7.308
7.304
7.296
7.286
7.276
7.267
7.264
7.253
7.235
7.217
7.106
7.097
7.091
7.080
7.074
7.065
6.936
6.926
6.921
6.910
6.904
6.895
5.361
3.880
3.572
3.401
3.123
2.956
2.932
2.926
2.919
2.914
2.910
2.905
1.561
4.54
2.08
2.00
1.00
3.08
1.10
1.08
1.07
1.07
N
N
O
f1 (ppm)


155.661
142.552
134.312
129.638
129.448
128.640
127.053
126.676
121.014
117.569
114.753
77.317
77.202
76.999
76.682
55.616
55.520
44.868
28.689
55.616
55.520
N
N
O
f1 (ppm)


7.345
7.342
7.336
7.330
7.324
7.320
7.315
7.307
7.302
7.296
7.286
7.283
7.265
7.253
7.002
6.982
6.964
6.818
6.797
5.927
4.630
3.468
3.434
3.057
3.033
3.003
2.023
1.877
1.835
1.716
1.681
1.606
1.425
1.409
1.394
1.378
1.362
1.348
1.271
2.00
2.63
0.31
0.14
1.00
0.93
0.92
2.05
2.01
2.39
0.26
N
CN
f1 (ppm)


150.56
149.63
146.46
129.40
129.22
121.99
121.86
117.08
113.07
86.94
77.32
77.00
76.68
69.39
51.85
46.42
29.10
20.07
15.96
N
CN
f1 (ppm)


7.251
7.239
7.217
7.214
7.207
7.180
7.174
7.170
7.163
7.159
6.778
6.741
6.704
6.628
6.623
6.584
4.368
4.359
4.330
3.379
3.346
3.332
3.295
3.275
3.255
2.338
2.310
2.294
2.279
2.255
2.229
2.214
2.180
2.147
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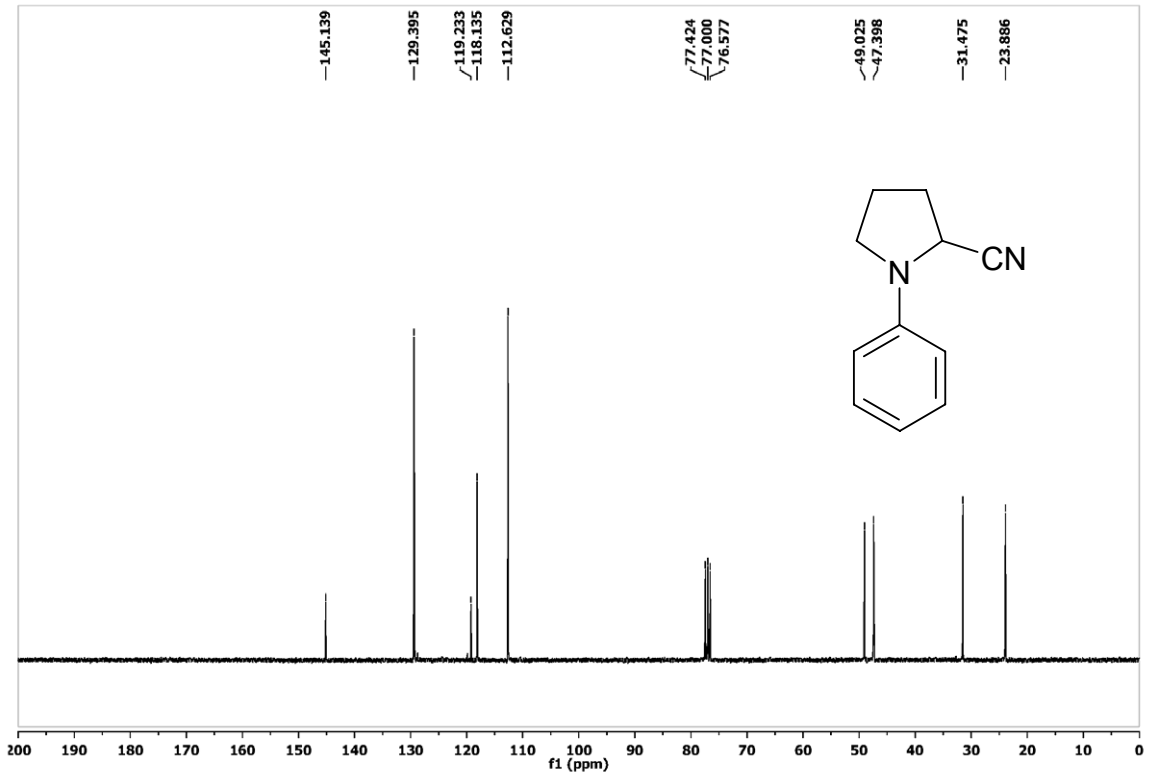
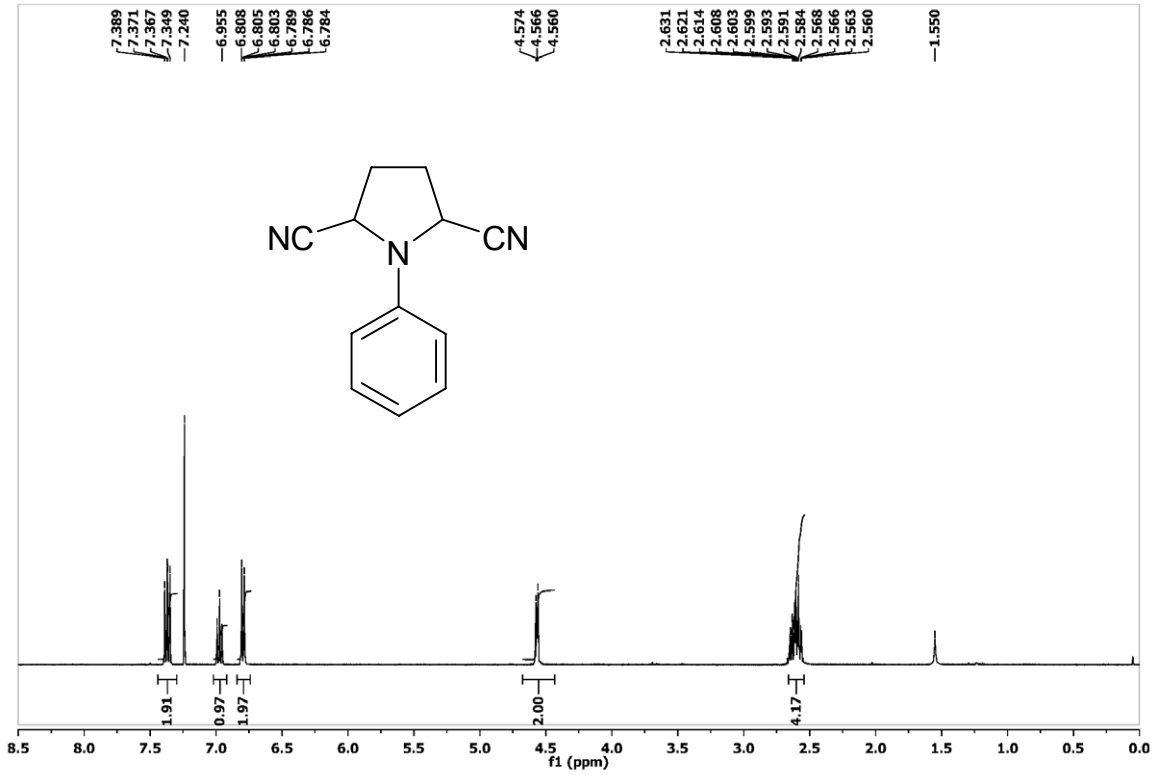
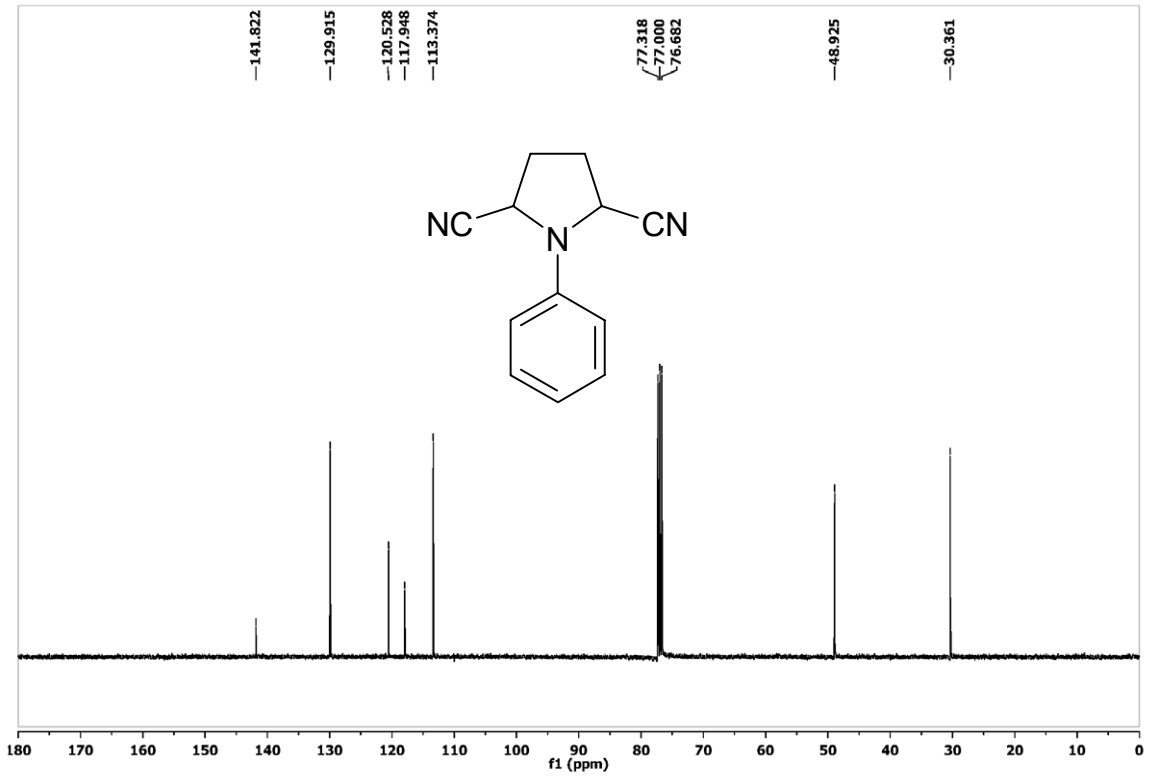
2.075
CN
N
2.30
1.03
2.02
1.00
2.20
4.39
f1 (ppm)


145.139
129.395
119.233
118.135
112.629
77.424
77.000
76.577
49.025
47.398
31.475
23.886
CN
N
f1 (ppm)


7.389
7.371
7.367
7.349
7.240
6.955
6.808
6.805
6.803
6.789
6.786
6.784
4.574
4.566
4.560
2.631
2.621
2.614
2.608
2.603
2.599
2.593
2.591
2.584
2.568
2.566
2.563
2.560
1.550
NC
N
CN
1.91
0.97
1.97
2.00
4.17
f1 (ppm)


141.822
129.915
120.528
117.948
113.374
77.318
77.000
76.682
48.925
30.361
NC
N
CN
f1 (ppm)