Supporting information for:

Dehydration of Aldoximes Using PhSe(O)OH as the *Pre*-Catalyst in Air

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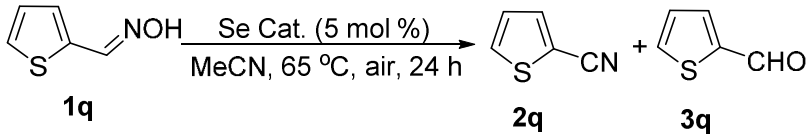
Screening of Catalysts for the Dehydration of 1q

Table S1. Screenings of the Catalysts for Dehydration of 1q.



entry	Se Cat.	**2q** / %[a]	**3q** / %[a]
1	PhSe(O)OH	25	37
2	4-$MeC_6H_4Se(O)OH$	9	18
3	3,5-$(CF_3)_2C_6H_3Se(O)OH$	17	8
4	3-$FC_6H_4Se(O)OH$	52	20

[a] Isolated yields based on **1q**.

Experimental Section

General methods

Reagents were purchased from reagent merchant with their purities more than 98% and were directly used as received. Solvents were analytical pure (AR) and directly used without any special treatment. Melting points were measured by WRS-2A digital instrument. IR spectra were measured on Bruker Tensor 27 Infrared spectrometer. ^1H and ^{13}C NMR spectra were recorded on a Bruker Avance 600/400 instrument (600 or 400 MHz for ^1H and 150 MHz for ^{13}C NMR spectroscopy) using $CDCl_3$ as the solvent and Me_4Si as the internal standard. Chemical shifts for ^1H and ^{13}C NMR were referred to internal Me_4Si (0 ppm) and *J*-values were shown in Hz. Mass spectra were measured on a Shimadzu GCMS-QP2010 Ultra spectrometer (EI).

General procedure for the synthesis of organonitriles 2

To a reaction tube, 1 mmol of aldoxime **1** and 9.5 mg of PhSe(O)OH (0.05 mmol, 5 mol %) were heated in 2 mL of MeCN at 65 °C. The reaction was monitored by TLC. When the reaction terminated, the solvent was evaporated under vacuum and the residue was isolated by flash column chromatography on silica gel using petroleum ether and ethyl acetate (12/1) as the eluent, giving the corresponding organonitriles **2**.

GC-MS Analysis for Mechanism Study

(1) Test of the Stability of MeCN in the Reaction

0.5 mmol of PhSe(O)OH was heated in 1 mL MeCN at 65 ^{o}C for 24 h. The mixture was then sent to GC-MS analysis. As shown in Fig. S1, besides the MeCN and the solvent EtOAc, no obvious oxidation product was observed.

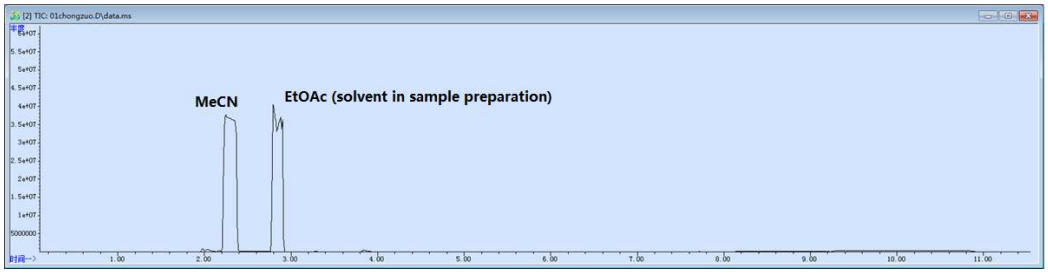


Fig. S1

(2) Test of the Stability of EtOH in the Reaction

0.5 mmol of PhSe(O)OH was heated in 1 mL EtOH at 65 ^{o}C for 24 h. The mixture was then sent to GC-MS analysis. As shown in Fig. S2 and confirmed by Fig. S3, besides EtOH and the solvent EtOAc, MeCHO, the oxidation product of EtOH was observed.

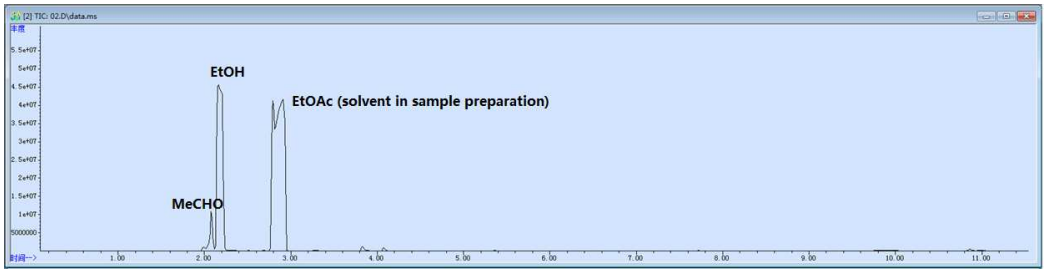


Fig. S2

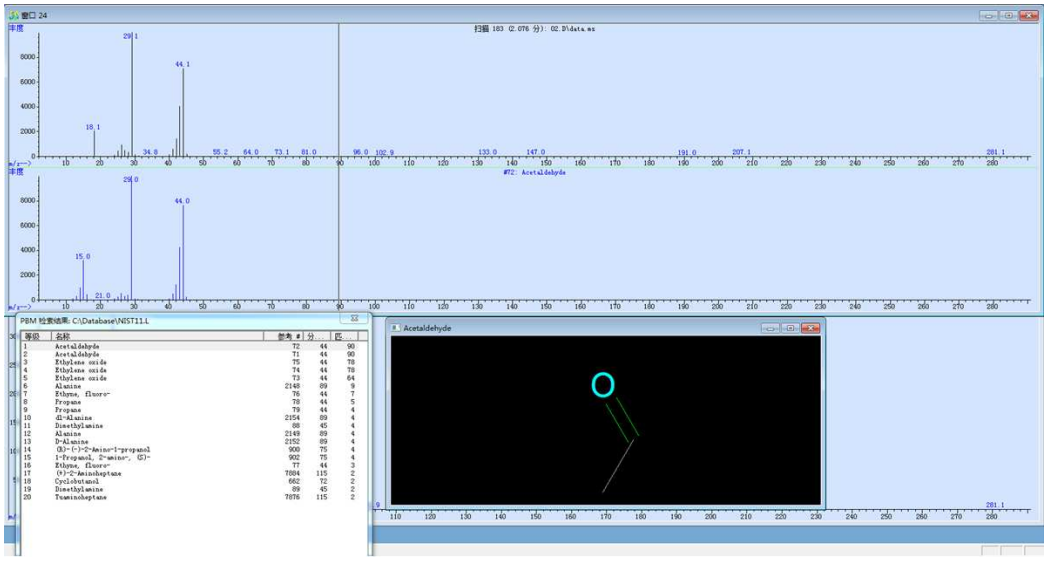
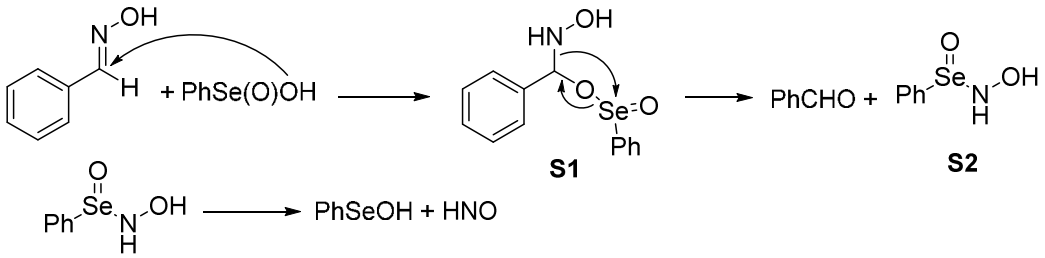


Fig. S3

(3) Test of the Stability of Aldoxime in the Reaction

0.5 mmol of PhSe(O)OH and 0.5 g of aldoxime **1a** (PhCH=NOH) were heated at 65 ^{o}C for 24 h. The mixture was then sent to GC-MS analysis. As shown in Fig. S4 and confirmed by Figs. S5-6, besides the product PhCN and the solvent EtOAc, PhCHO and PhCOOH were observed. Because there is no water in the system, we supposed that PhCHO was the **oxidation** product of aldoxime but **not** the hydration product. The possible mechanism was given in Scheme S1. The nucleophilic addition of PhSe(O)OH with aldoxime led to the intermediate **S1**, which then decomposed to PhCHO and **S2**. Further selenoxide elimination of **S2** generated the catalytic species PhSeOH and HNO. PhCHO was further oxidized by PhSe(O)OH to PhCOOH.



Scheme S1

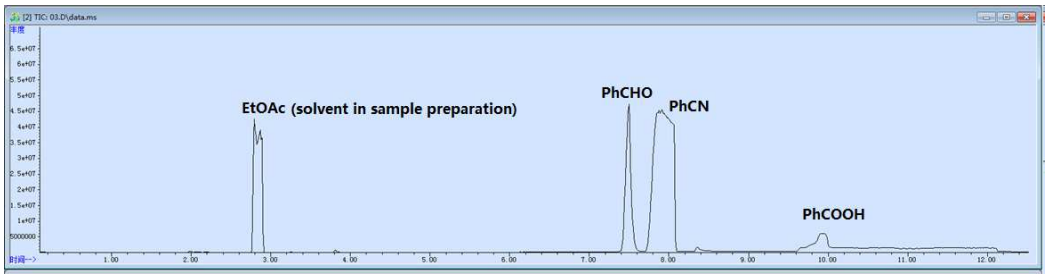


Fig. S4

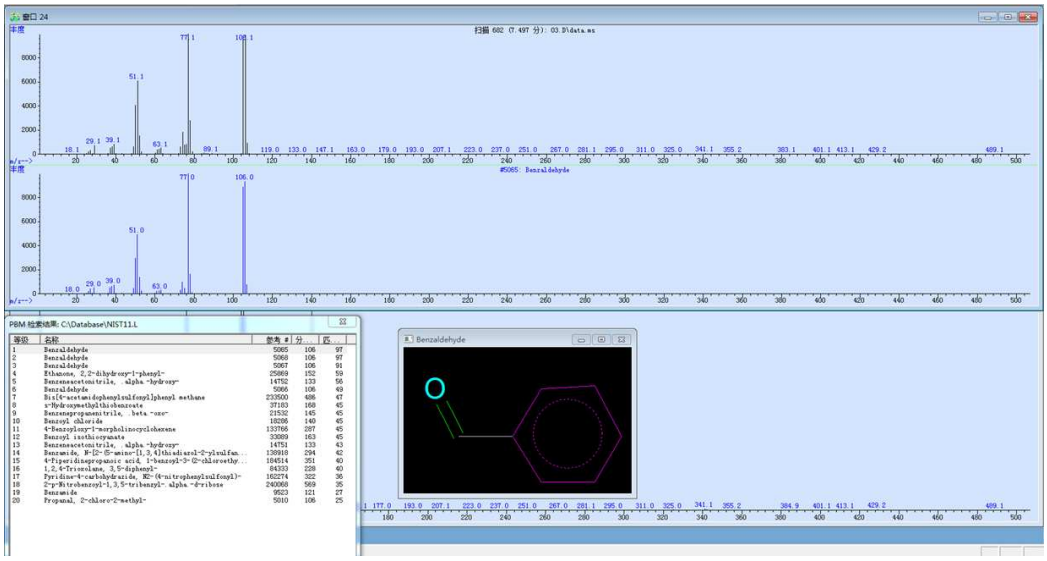


Fig. S5

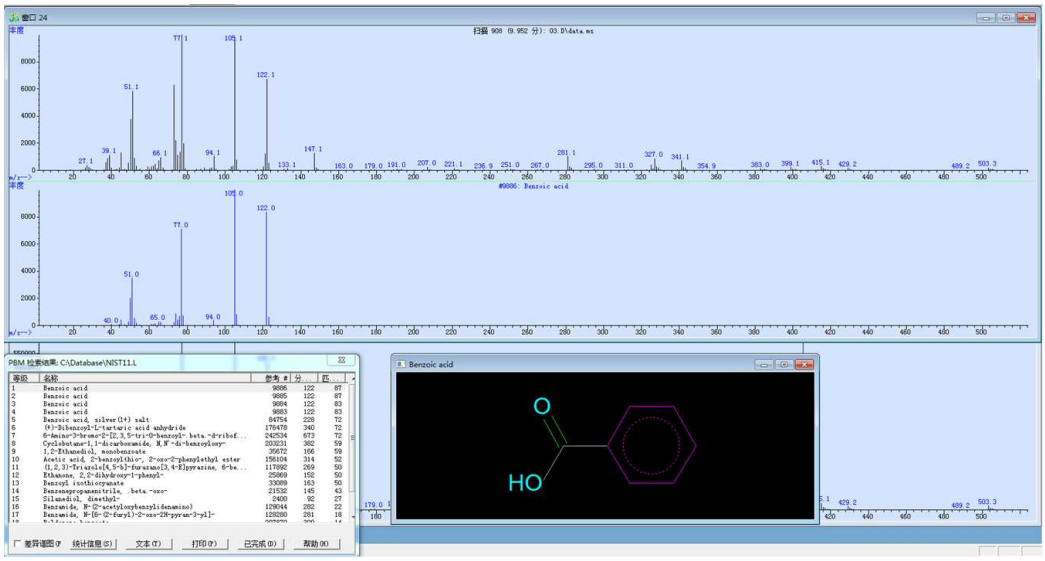


Fig. S6

(4) Test of the Stability of Nitrile in the Reaction

0.5 mmol of PhSe(O)OH was heated with 0.5 g of PhCN at 65 ^{o}C for 24 h. The mixture was then sent to GC-MS analysis. As shown in Fig. S7, besides PhCN and the solvent EtOAc, no oxidation product was observed.

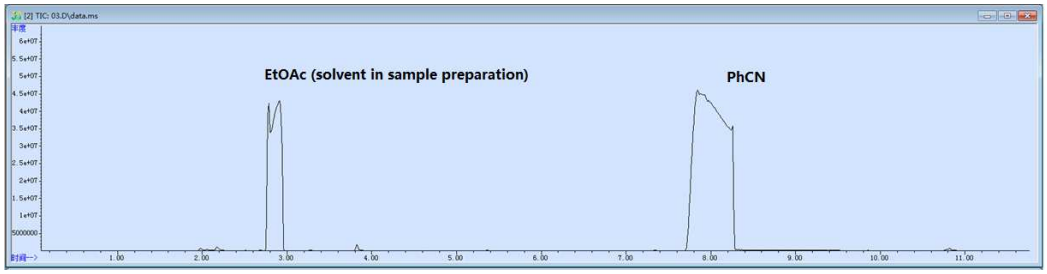
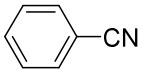
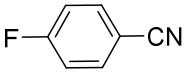


Fig. S7

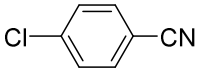
Characterization of the Products



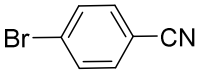
Benzonitrile 2a 438.2 mg, Oil; IR (film): 3066, 2259, 1490, 1447, 758cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$, TMS, ppm): δ 7.62 (s, 3H), 7.46 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ 132.8, 132.1, 129.2, 118.8, 112.4; MS (EI, 70 eV): m/z (%) 103 [M^+] (100), 76 (16); Known compound.[1]



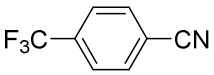
4-Fluorobenzonitrile 2b 466.2 mg, Oil; IR (film): 3076, 2232, 1603, 1508, 1240, 842, 685cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, ppm): δ 7.71-7.68 (m, 2H), 7.19 (t, J = 8.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 165.0 (d, $J_{C\text{-}F}$ = 255 Hz), 134.7 (d, $J_{C\text{-}F}$ = 9.4 Hz), 118.0, 116.8 (d, $J_{C\text{-}F}$ = 22.6 Hz), 108.5 (d, $J_{C\text{-}F}$ = 3.6 Hz); MS (EI, 70 eV): *m/z* (%) 122 [M^++1] (8), 121 [M^+] (100), 94 (33); Known compound.[1]



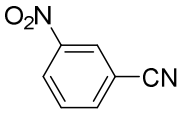
4-Chlorobenzonitrile 2c 564.2 mg, Solid, m.p. 93.3-94.1^{o}C (*lit.* 93-94 ^{o}C); IR (KBr): 3092, 3039, 2225, 1593, 1483, 1399, 1263, 830, 544cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, ppm): δ 7.61 (d, J = 8.4 Hz, 2H), 7.48 (d, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 139.5, 133.4, 129.7, 117.9, 110.8; MS (EI, 70 eV): *m/z* (%) 137 [M^+] (100), 102 (42); Known compound.[1]



4-Bromobenzonitrile 2d 800.8 mg, Solid, m.p. 112.9-113.2^{o}C (*lit.* 113-114 ^{o}C); IR (KBr): 3086, 2224, 1583, 1478, 1067, 824, 542cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$, TMS, ppm): δ 7.63 (d, J = 7.8 Hz, 2H), 7.53 (d, J = 7.8 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ 133.4, 132.7, 128.0, 118.1, 111.3; MS (EI, 70 eV): *m/z* (%) 183 (65), 181 [M^+] (70), 102 (100); Known compound.[1]

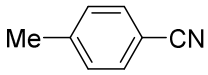


4-(Trifluoromethyl)benzonitrile 2e 718.6 mg, Oil; IR (film): 2993, 2235, 1758, 1322, 1249, 1176, 1135, 1067, 847, 731cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, ppm): δ 7.83 (d, J = 8.4 Hz, 2H), 7.77 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 134.5 (d, $J_{C\text{-}F}$ = 33.2 Hz), 132.7, 126.1 (d, $J_{C\text{-}F}$ = 3.8 Hz), 123.0 (d, $J_{C\text{-}F}$ = 271.5 Hz), 117.4, 116.0; MS (EI, 70 eV): *m/z* (%) 172 [M^++1] (11), 171 [M^+] (100), 121 (87); Known compound[1].

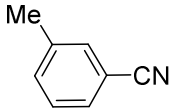


3-Nitrobenzonitrile 2f 120.0 mg, Solid, m. p. 114.2-115.1^{o}C (*lit.* 114-115 ^{o}C); IR (KBr): 3080, 2875, 2236, 1618, 1535, 1355, 817, 560cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, ppm): δ 8.50 (d, J = 11.2 Hz, 2H), 8.04 (s, 1H), 7.79 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 148.2, 137.7, 130.8, 127.6, 127.2, 116.6, 114.0; MS (EI,

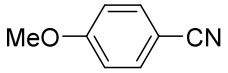
70 eV): *m/z* (%) 148 [M^+] (37), 102 (100); Known compound.[2]



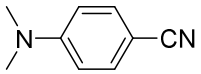
4-Methylbenzonitrile 2g 87.9 mg, Oil; IR (film): 3038, 2955, 2925, 2868, 2228, 1919, 1703, 1608, 1509, 1450, 1290, 1177, 1120, 1041, 817, 763, 706, 546cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, TMS, ppm): δ 7.53 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 143.7, 132.0, 129.8, 119.1, 109.3, 21.8; MS (EI, 70 eV): m/z (%) 118 [M^++1] (11), 117 [M^+] (100), 116 (76); Known compound.[1]



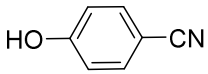
3-Methylbenzonitrile 2h 515.7 mg, Oil; IR (film): 2994, 2229, 1770, 1244, 789, 687cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, TMS, ppm): δ 7.43-7.38 (m, 3H), 7.34 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 139.2, 133.7, 132.4, 129.2, 129.0, 119.0, 112.1, 21.1; MS (EI, 70 eV): *m/z* (%) 118 [M^++1] (12), 117 [M^+] (100), 116 (78); Known compound.[1]



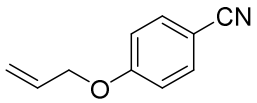
4-Methoxybenzonitrile 2i 130.5 mg, Solid, m.p. 56.3-57.2°C (*lit.* 55-57 °C); IR (KBr): 3022, 2977, 2943, 2842, 2215, 1604, 1508, 1461, 1305, 830, 547cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, TMS, ppm): δ 7.57 (d, *J* = 8.4 Hz, 2H), 6.95 (d, *J* = 8.4 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 162.8, 133.9, 119.2, 114.8, 103.8, 55.5; MS (EI, 70 eV): *m/z* (%) 134 [M^++1] (9), 133 (100) [M^+], 103 (60); Known compound.[1]



4-Dimethylaminobenzonitrile 2j 70.2 mg, Solid, m.p. 75.4-76.5 °C (*lit.* 75-76 °C); IR (KBr): 2908, 2823, 2210, 1607, 1526, 1371, 1226, 818, 545cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, TMS, ppm): δ 7.44 (d, *J* = 8.0 Hz, 2H), 6.63 (d, *J* = 8.4 Hz, 2H), 3.03 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 152.5, 133.3, 120.7, 111.4, 97.2, 39.9; MS (EI, 70 eV): *m/z* (%) 147 (8) [M^++1], 146 [M^+] (84), 145 (100), 102 (30); Known compound.[3]

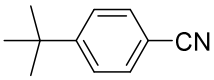


4-Hydroxybenzonitrile 2k 83.4 mg, Solid, m.p. 108.3-109.2°C (*lit.* 107-109 °C); IR (KBr): 3287, 2233, 1609, 1586, 1441, 1371, 838, 699cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, TMS, ppm): δ 7.57 (d, *J* = 8.8 Hz, 2H), 6.95 (d, *J* = 8.8 Hz, 3H, containing -OH); ^{13}C NMR (100 MHz, CDCl3, ppm): δ 160.3, 134.3, 119.3, 116.5, 102.8; MS (EI, 70 eV): *m/z* (%) 120 [M^++1] (11), 119 [M^+] (100), 91 (23); Known compound.[4]

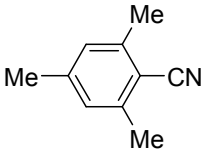


4-(Allyloxy)benzonitrile 2l 143.3 mg, Oil; IR (film): 3082, 2927, 2558, 2224, 1605,

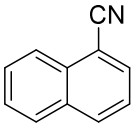
1508, 1303, 1257, 1173, 996, 835cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$, TMS, ppm): δ 7.56 (d, *J* = 7.8 Hz, 2H), 6.96 (d, *J* = 7.8 Hz, 2H), 6.05-6.00 (m, 1H), 5.42 (d, *J* = 17.4 Hz, 1H), 5.33 (d, *J* = 10.8 Hz, 1H), 4.59 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ 161.9, 133.9, 132.1, 119.2, 118.4, 115.5, 104.0, 69.0; MS (EI, 70 eV): *m/z* (%) 160 [M^++1] (9), 159 [M^+] (72), 41 (100); Known compound.[1]



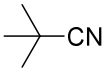
4-*tert*-Butylbenzonitrile 2m 132.1 mg, Oil; IR (film): 2966, 2228, 1606, 1505, 1465, 1366, 1270, 1106, 838cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, ppm): δ 7.59 (d, *J* = 7.8 Hz, 2H), 7.48 (d, *J* = 8.0 Hz, 2H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 156.6, 131.9, 126.2, 119.1, 109.3, 35.2, 30.9; MS (EI, 70 eV): m/z (%) 159 [M^+] (22), 144 (100), 116 (87); Known compound.[5]



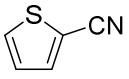
2,4,6-Trimethylbenzonitrile 2n 106.0 mg, Solid, m.p. 48.8-49.9^{o}C (*lit.* 49 ^{o}C); IR (KBr): 2975, 2921, 2857, 2215, 1608, 1471, 862, 583cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, ppm): δ 6.92 (s, 2H), 2.47 (s, 6H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 142.8, 141.9, 128.2, 117.6, 110.3, 21.5, 20.6; MS (EI, 70 eV): m/z (%) 145 [M^+] (50), 130 (100); Known compound.[6]



Naphthalene-1-carbonitrile 2o 152.1 mg, Oil; IR (film): 3060, 2970, 2221, 1943, 1849, 1699, 1653, 1590, 1508, 1457, 1375,1341, 1269, 1212, 800, 770, 689, 571, 538cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$, TMS, ppm): δ 8.19 (d, *J* = 8.4 Hz, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 7.86 (t, *J* = 10.2 Hz, 2H), 7.64 (s, 1H), 7.58 (s, 1H), 7.47 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ 133.3, 132.9, 132.6, 132.3, 128.7, 128.6, 127.6, 125.1, 124.9, 117.8, 110.2; MS (EI, 70 eV): *m/z* (%) 154 [M^++1] (19), 153 [M^+] (100), 126 (59); Known compound.[1]

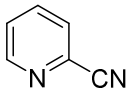


Pivalonitrile 2p 24.9 mg, Oil; IR (film): 2987, 2236, 1734, 1652, 1521, 1457, 1066, 668cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$, TMS, ppm): δ 1.38 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ 125.8, 28.3, 28.0; MS (EI, 70 eV): *m/z* (%) 84 [M^++1] (3), 42 (100), 41 (87); Known compound.[7]



Thiophene-2-carbonitrile 2q 56.8 mg, Oil; IR (film): 3118, 2228, 1608, 1511, 1482, 799, 712cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$, TMS, ppm): δ 7.61 (s, 2H), 7.12 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ 137.5, 132.9, 127.8, 114.3, 109.7; MS (EI, 70

eV): *m/z* (%) 109 [M^+] (100); Known compound.[8]



Picolinonitrile 2r 82.2 mg, Oil; IR (film): 3059, 2929, 2237, 1699, 1653, 1580, 1459, 1433, 1362, 1290, 992, 781, 737, 551cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$, TMS, ppm): δ 8.75 (s, 1H), 7.92 (s, 1H), 7.76 (s, 1H) , 7.60 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ 151.1, 137.2, 133.9, 128.6, 127.1, 117.2; MS (EI, 70 eV): *m/z* (%) 104 (100) [M^+], 78 (3); Known compound.[9]

References

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5. Wong, K.-T.; Ku, S.-Y.; Cheng, Y.-M.; Lin, X.-Y.; Hung, Y.-Y.; Pu, S.-C.; Chou, P.-T.; Lee, G.-H.; Peng, S.-M. *J. Org. Chem.* **2006**, *71*, 456.
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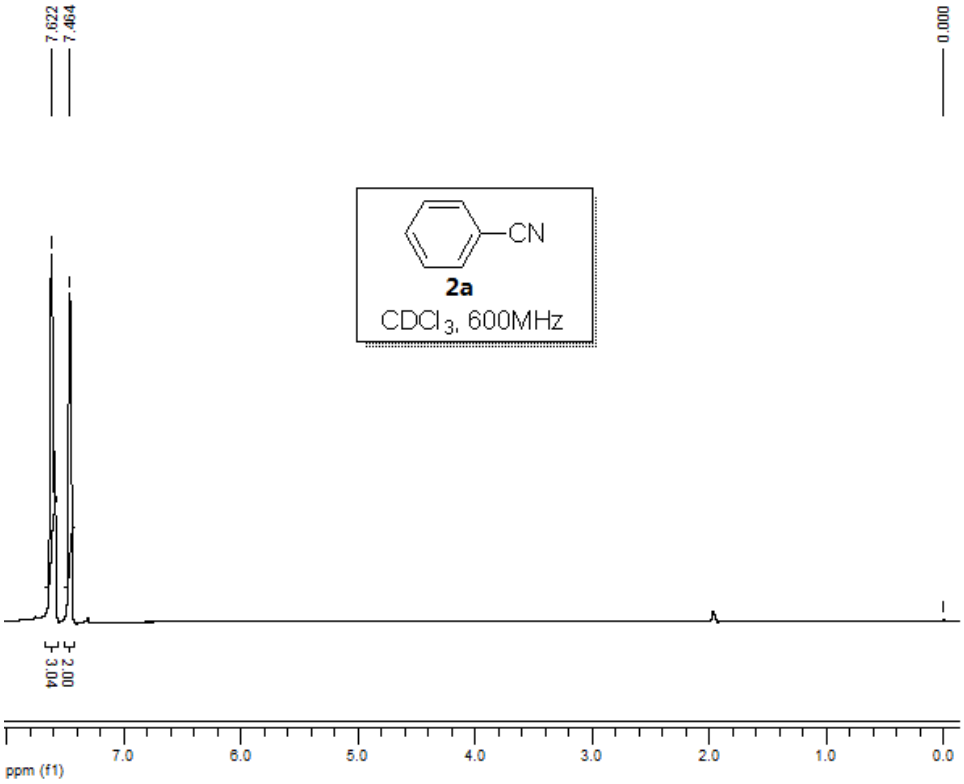
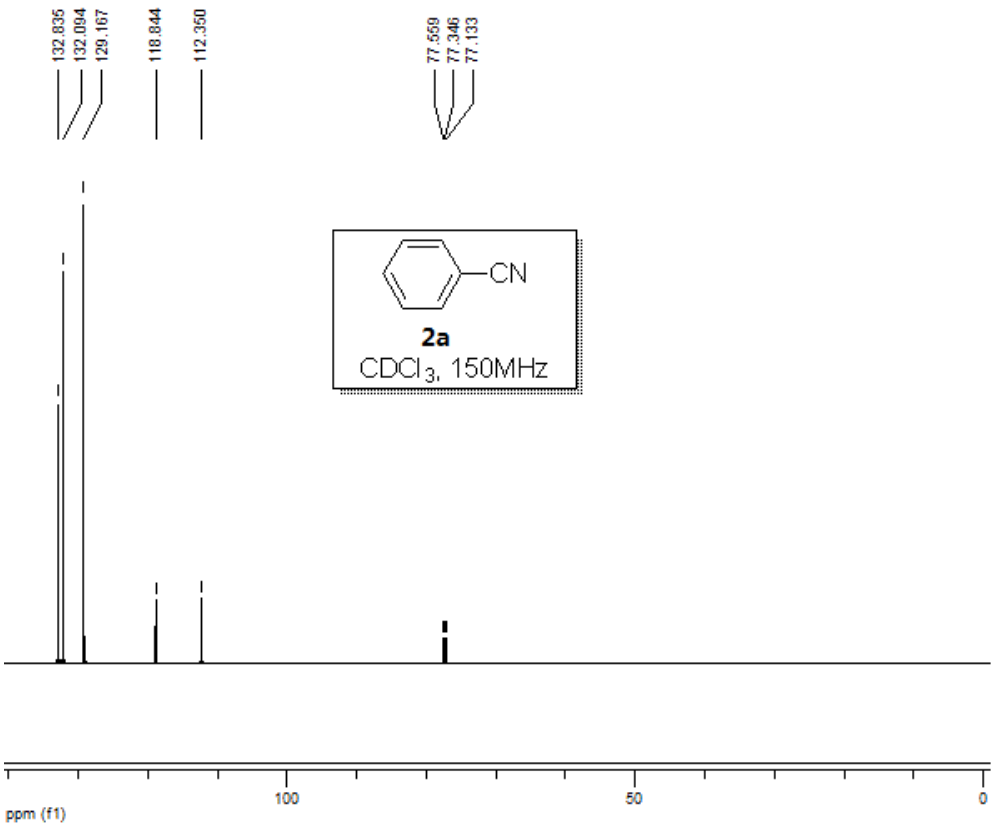
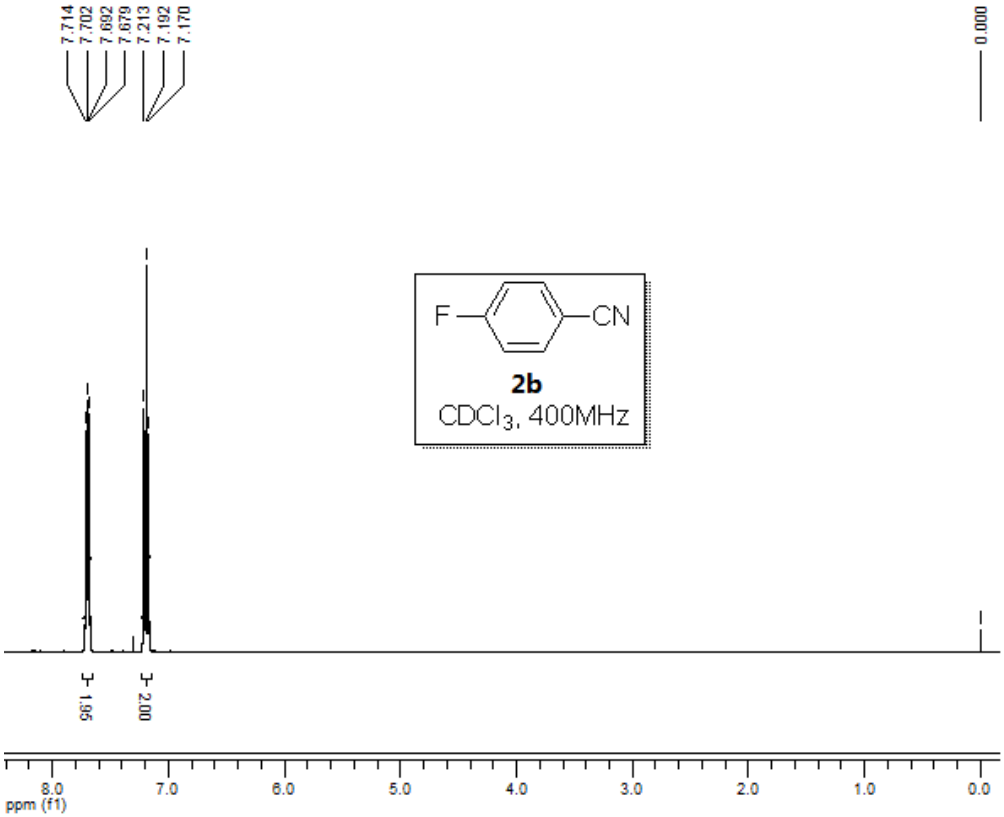
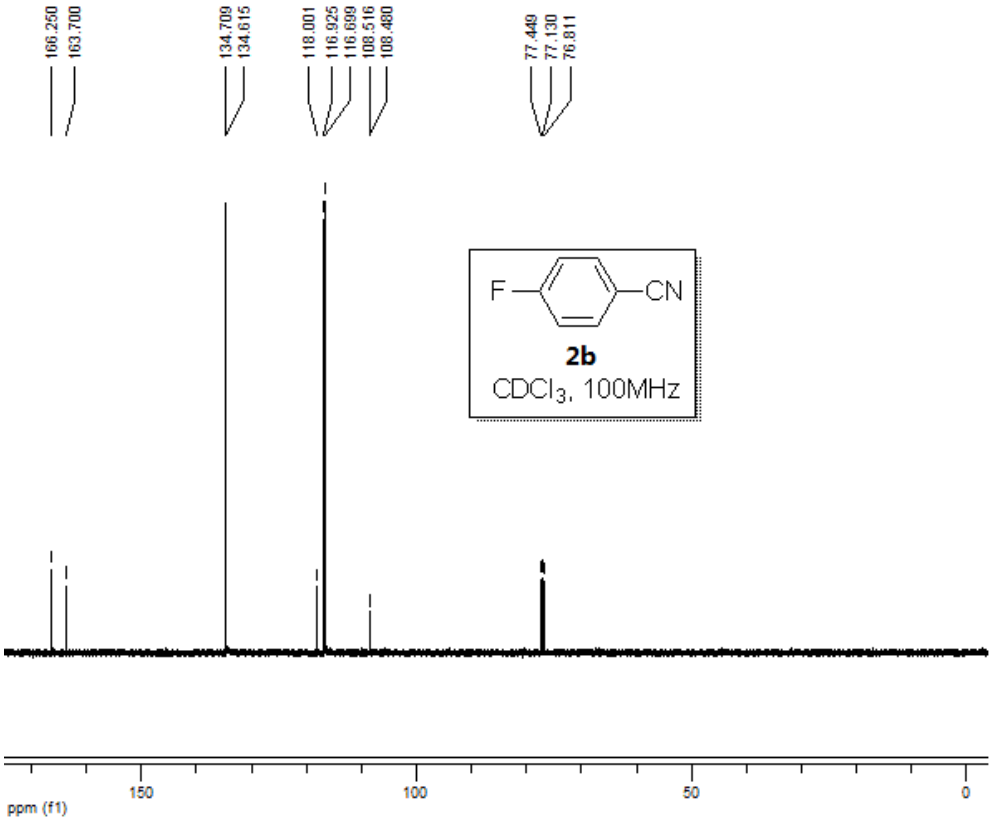
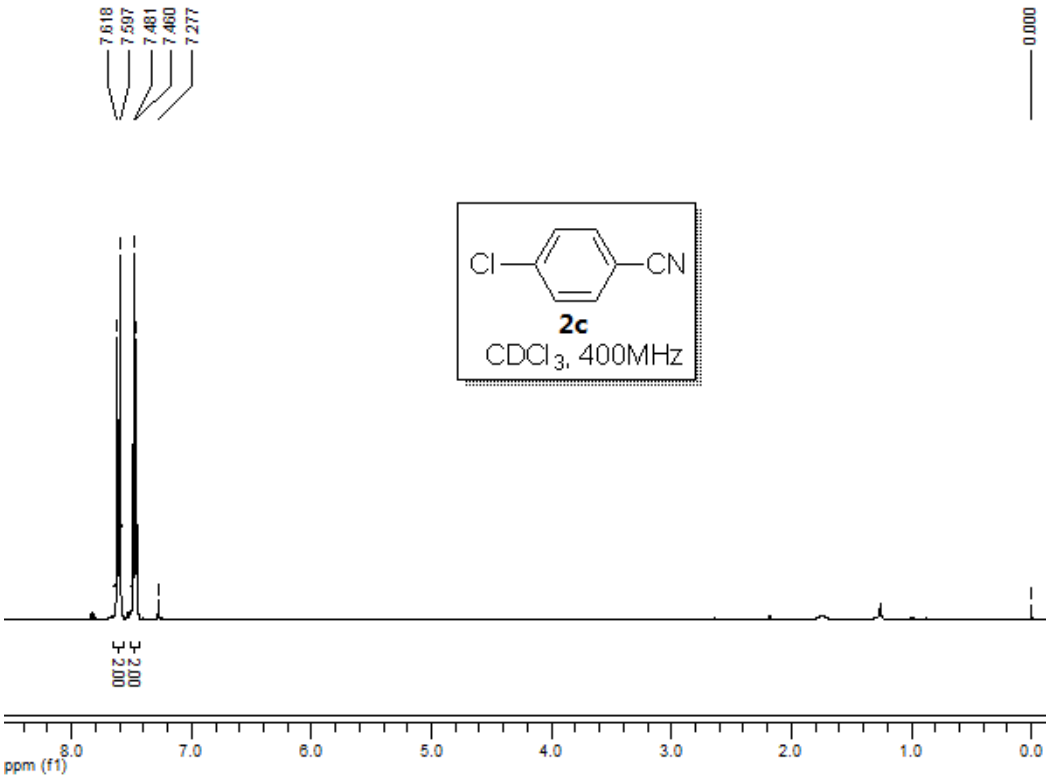
NMR Spectra

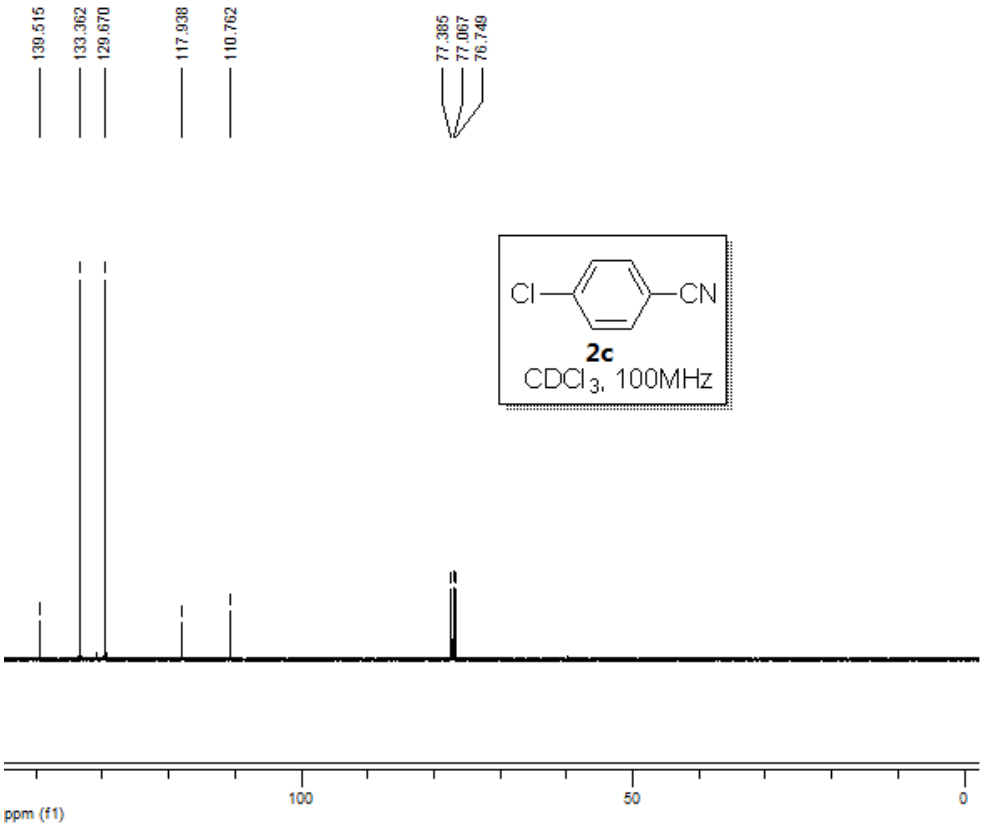

7.622
7.464
0.000
CN
2a
CDCl3, 600MHz
3.04
2.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)

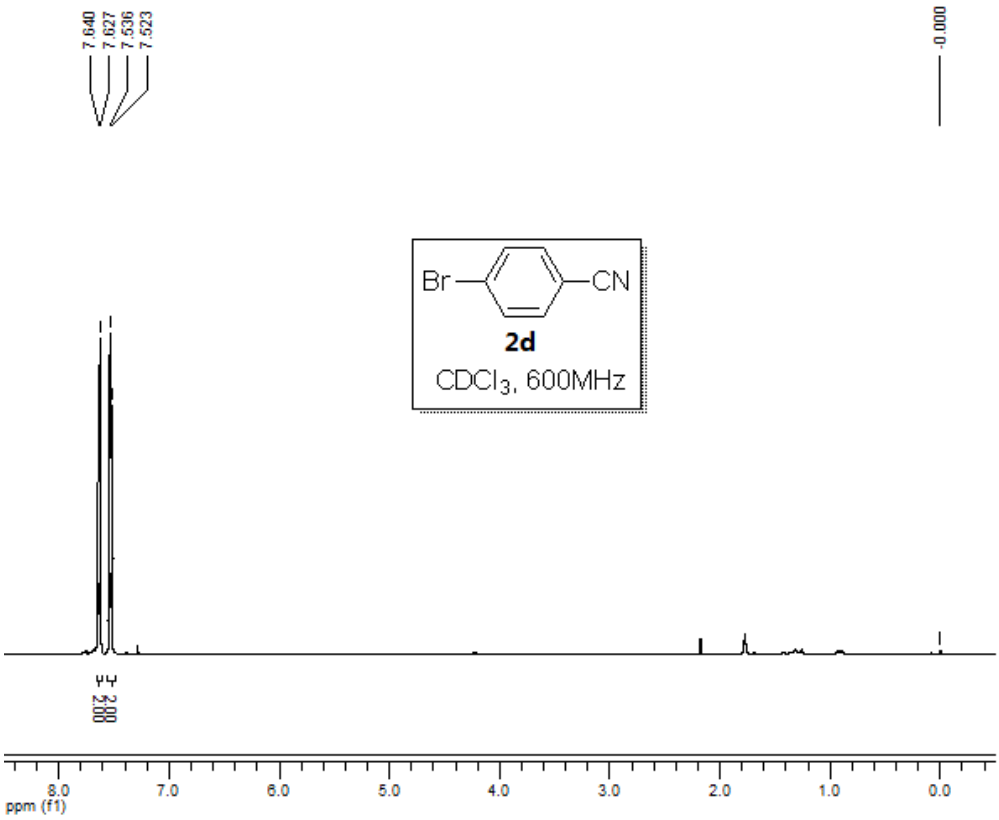

132.835
132.094
129.167
118.844
112.350
77.559
77.346
77.133
CN
2a
CDCl3, 150MHz
100
50
0
ppm (f1)

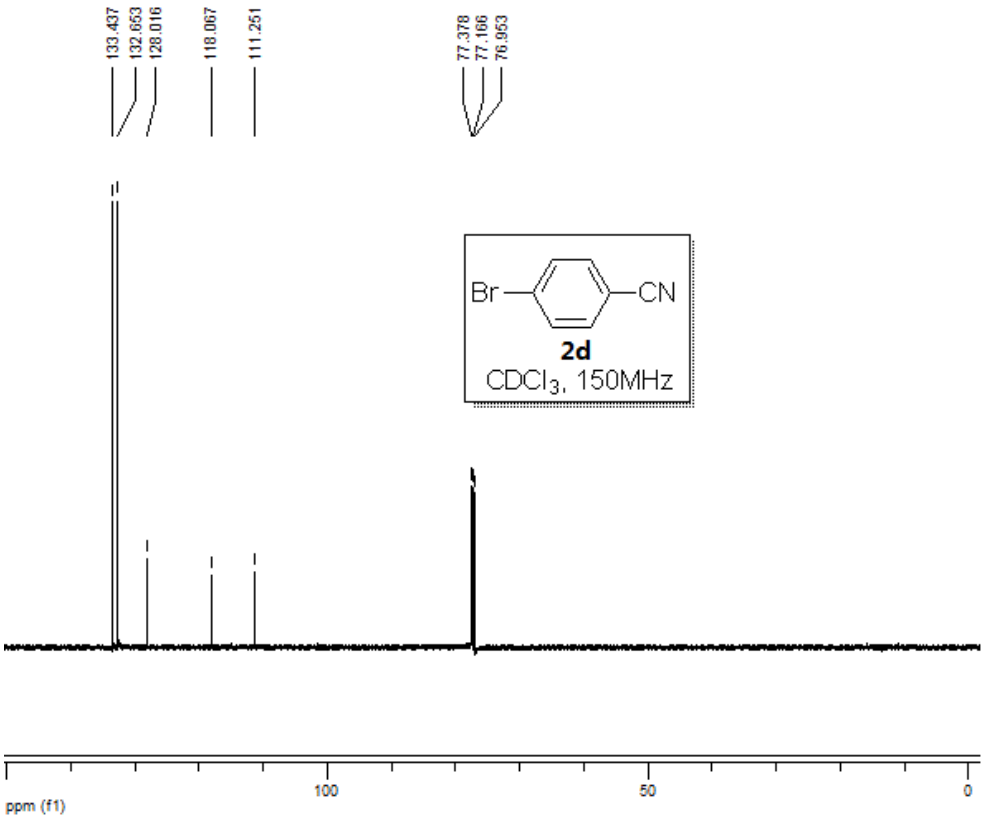

7.714
7.702
7.692
7.679
7.213
7.192
7.170
0.000
F
CN
2b
CDCl3, 400MHz
1.96
2.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)


166.250
163.700
134.709
134.615
118.001
116.925
116.699
108.516
108.480
77.449
77.130
76.811
F
CN
2b
CDCl3, 100MHz
150
100
50
0
ppm (f1)


7.618
7.597
7.481
7.460
7.277
0.000
Cl
CN
2c
CDCl3, 400MHz
3.200
3.200
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)


139.515
133.362
129.670
117.938
110.762
77.385
77.067
76.749
Cl
CN
2c
CDCl3, 100MHz
100
50
0
ppm (f1)


7.640
7.627
7.536
7.523
0.000
Br
CN
2d
CDCl3, 600MHz
2.00
2.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)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132.653
128.016
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77.166
76.953
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CN
2d
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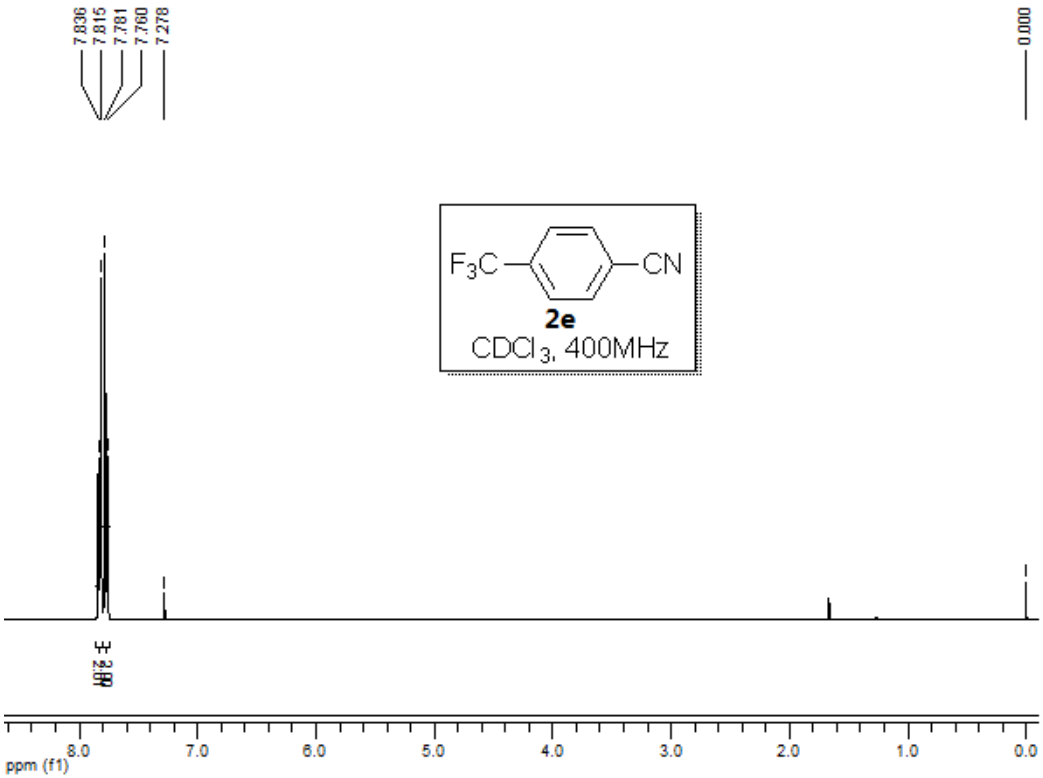
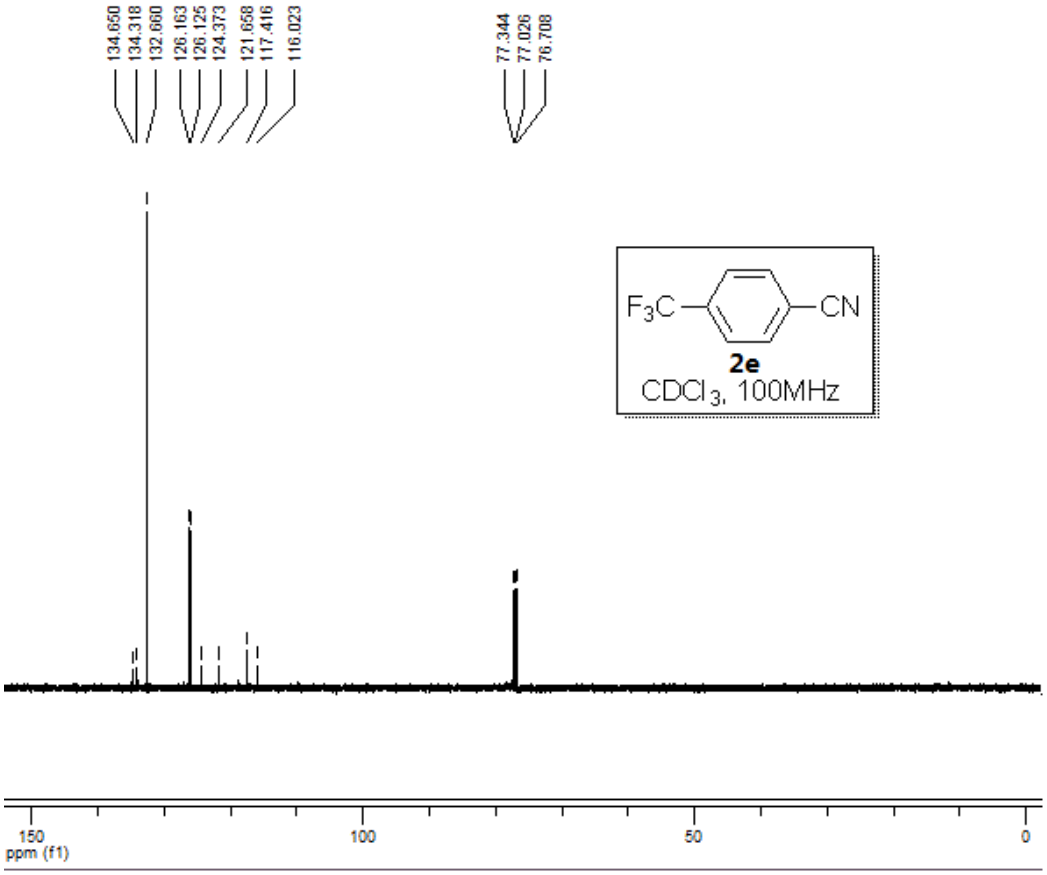
50
0
ppm (f1)


7.836
7.815
7.781
7.760
7.278
0.000
F3C
CN
2e
CDCl3, 400MHz
3.00
ppm (f1)
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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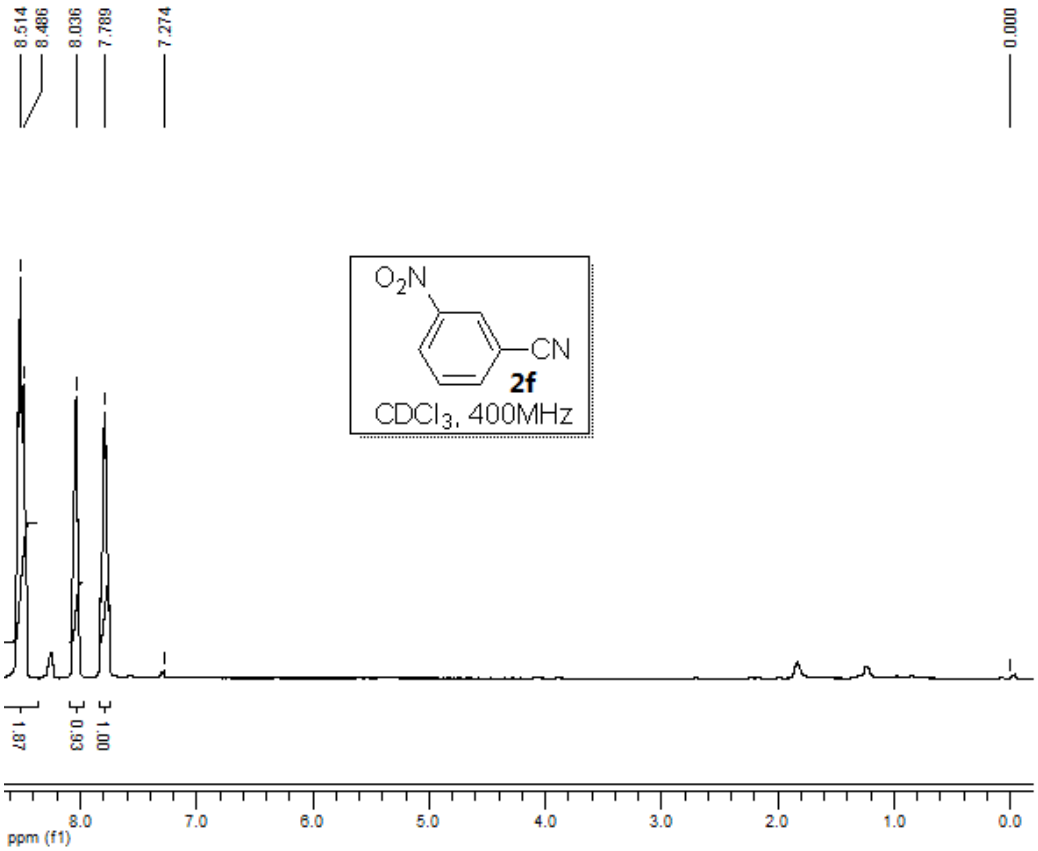
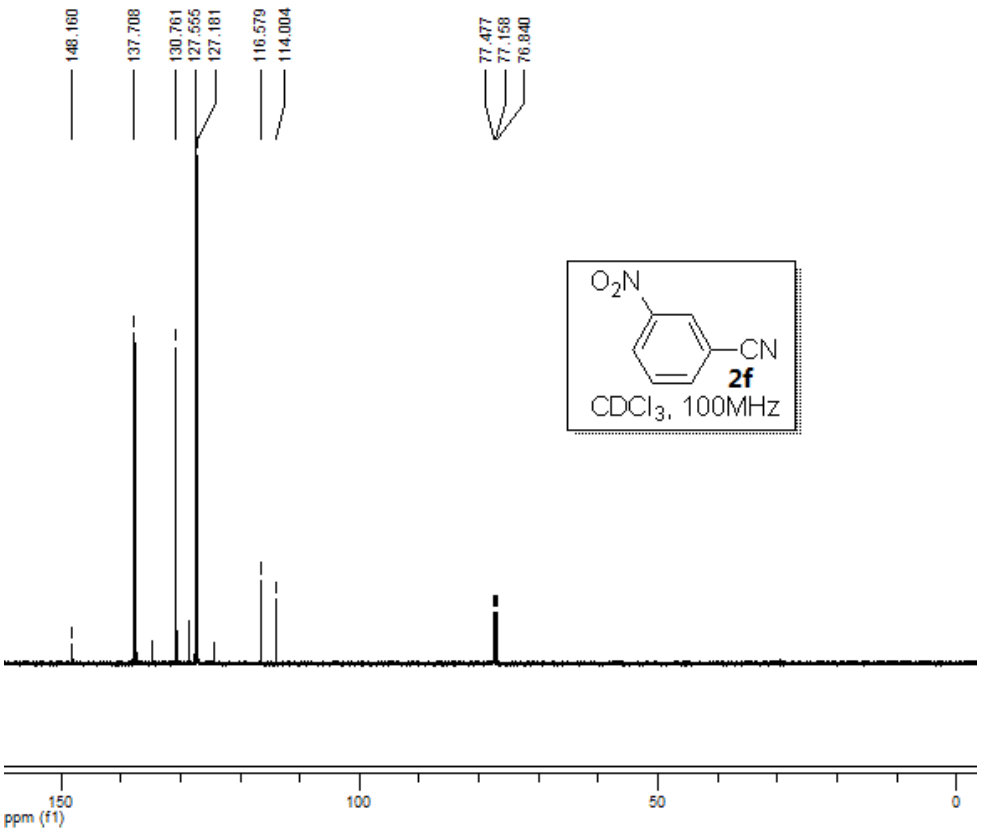
134.318
132.660
126.163
126.125
124.373
121.658
117.416
116.023
77.344
77.026
76.708
F3C
CN
2e
CDCl3, 100MHz
150
100
50
0
ppm (f1)


8.514
8.486
8.036
7.789
7.274
0.000
O_2N
CN
2f
$CDCl_3$, 400MHz
1.87
0.93
1.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)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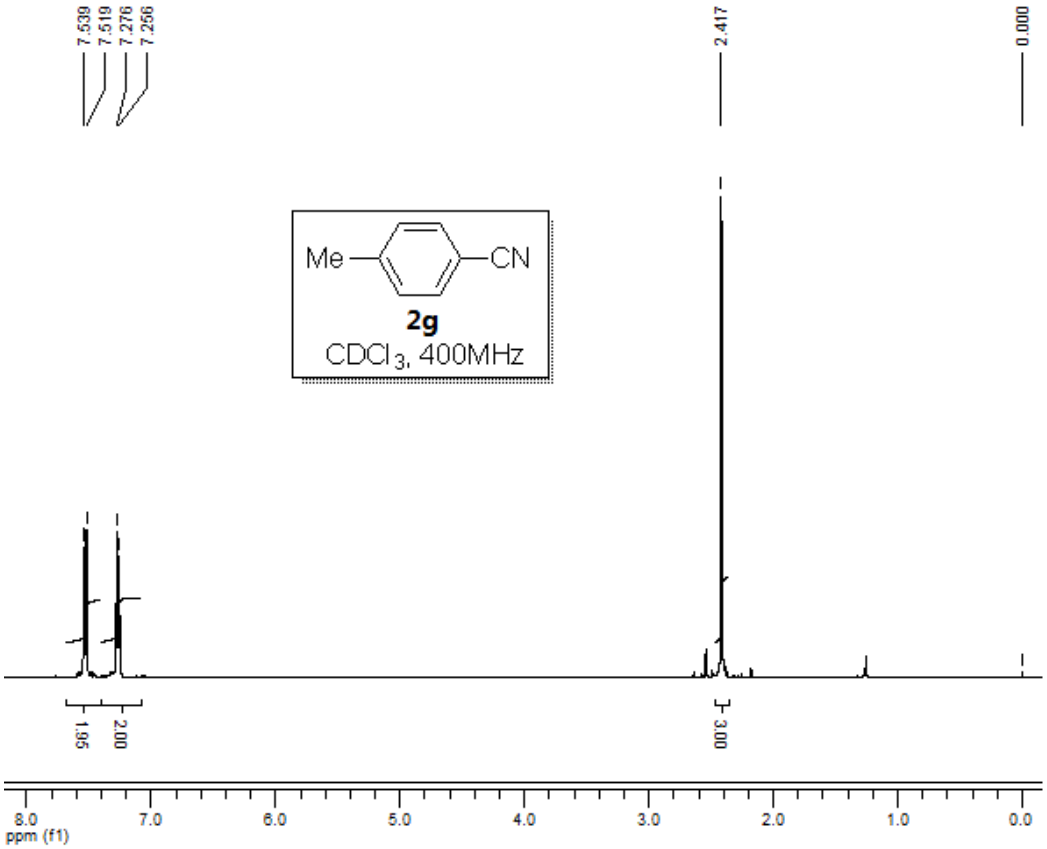
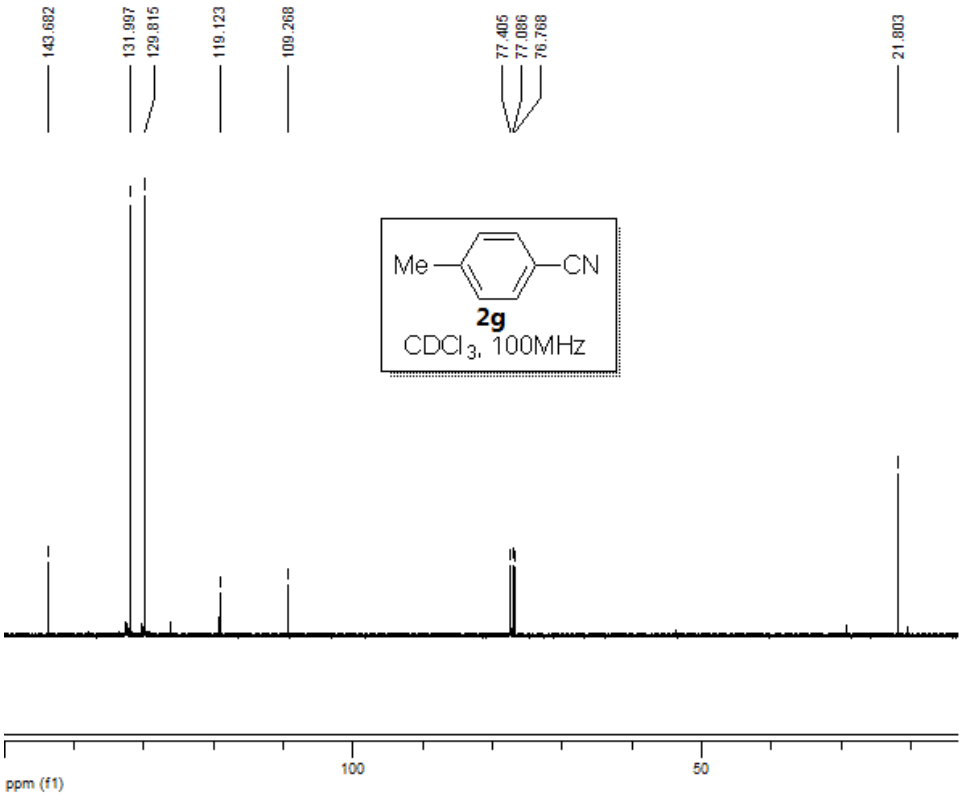
137.708
130.761
127.555
127.181
116.579
114.004
77.477
77.158
76.840
O_2N
CN
2f
$CDCl_3$, 100MHz
150
100
50
0
ppm (f1)


7.539
7.519
7.276
7.256
2.417
0.000
Me
CN
2g
CDCl3, 400MHz
1.96
2.00
3.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)


143.682
131.997
129.815
119.123
109.268
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77.086
76.768
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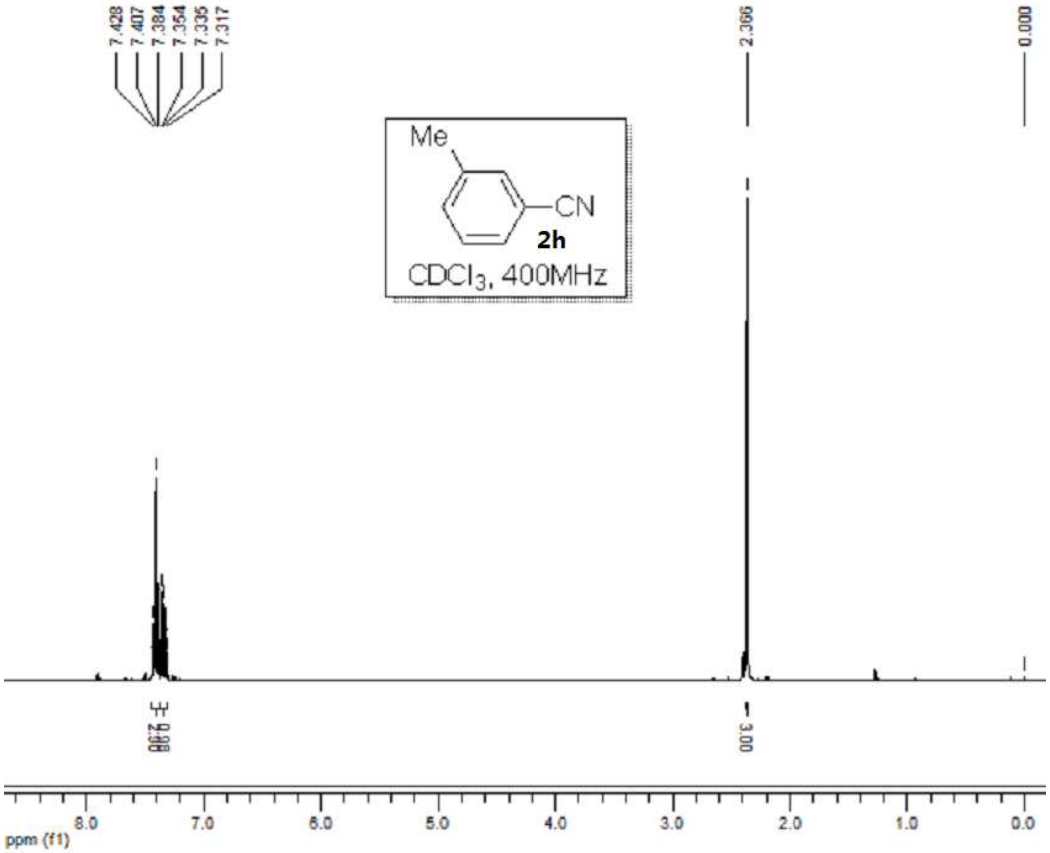
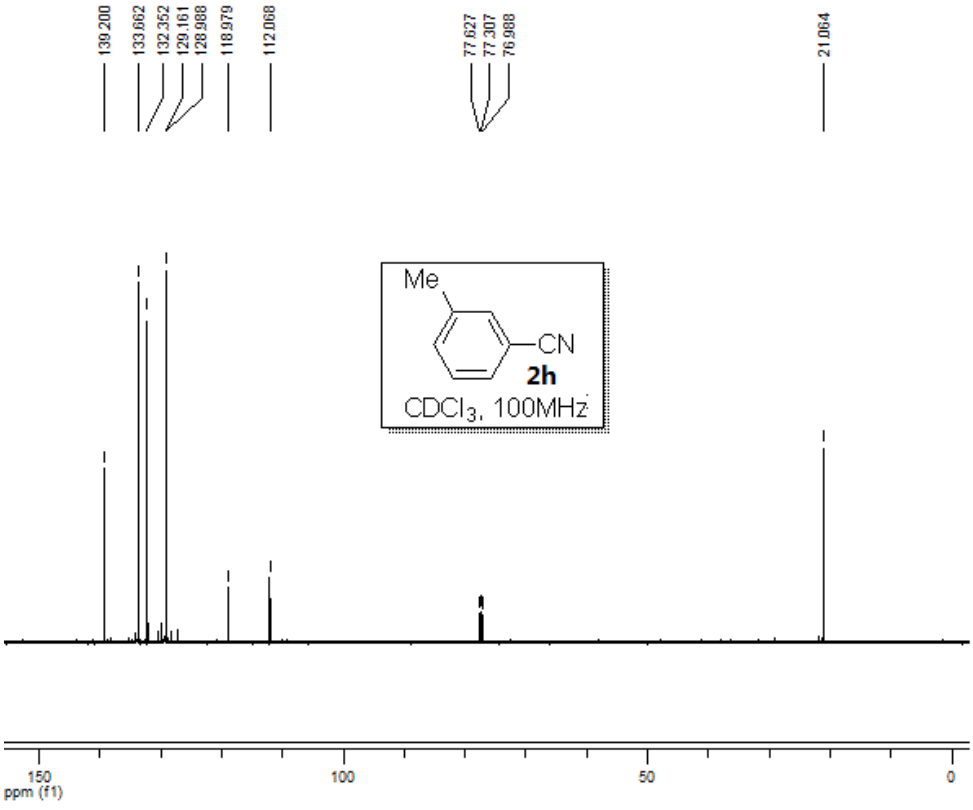
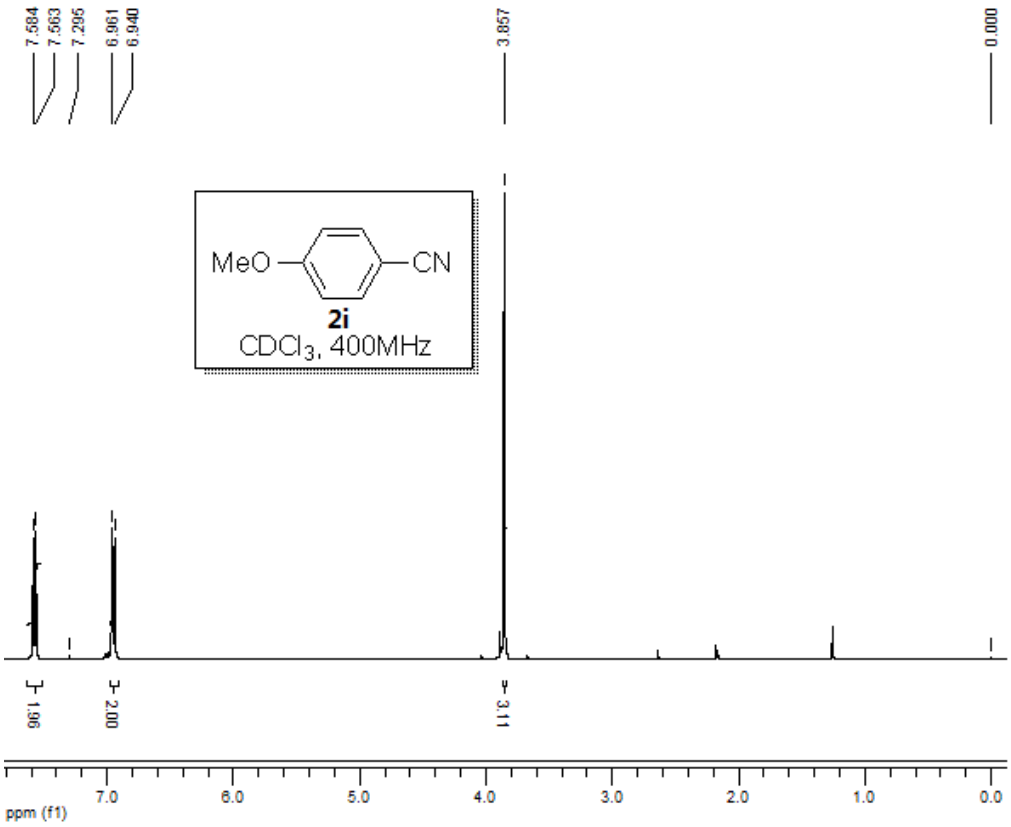
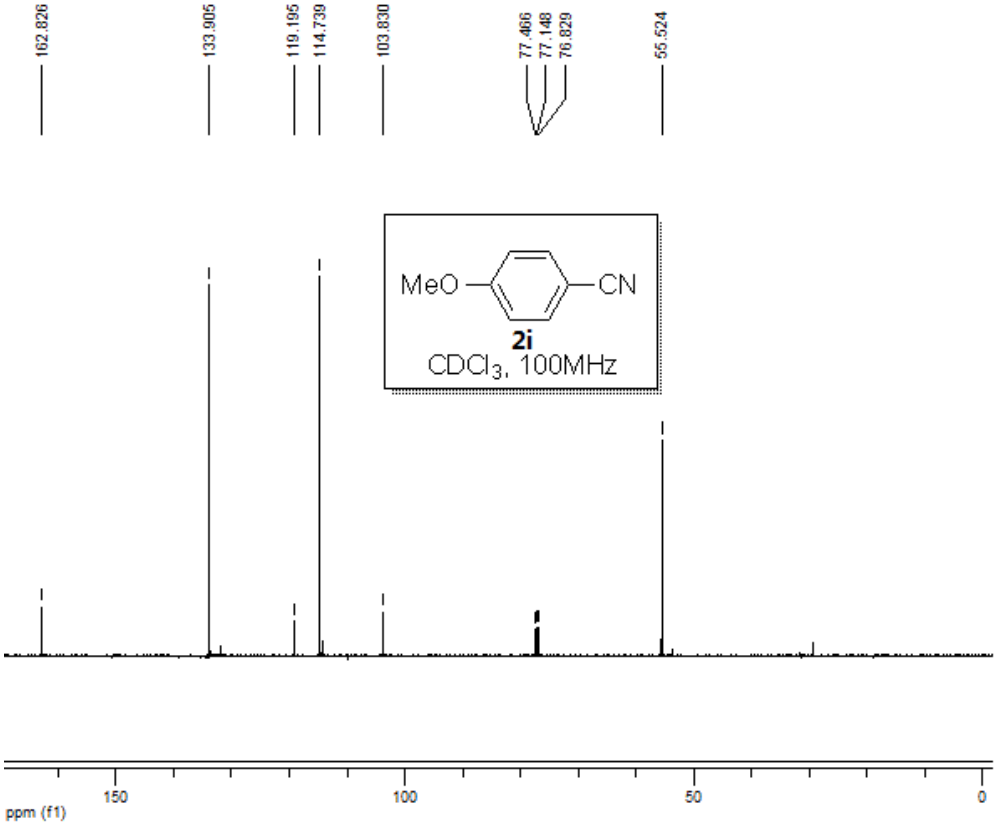
Me
CN
2g
CDCl3, 100MHz
100
50
ppm (f1)


7.428
7.407
7.384
7.354
7.335
7.317
2.366
0.000
Me
CN
2h
CDCl3, 400MHz
3.00
ppm (f1)


139.200
133.662
132.352
129.161
128.988
118.979
112.068
77.627
77.307
76.988
21.064
Me
CN
2h
CDCl3, 100MHz
ppm (f1)


7.584
7.563
7.295
6.961
6.940
3.857
0.000
MeO
CN
2i
CDCl3, 400MHz
1.96
2.00
3.11
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)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119.195
114.739
103.830
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CN
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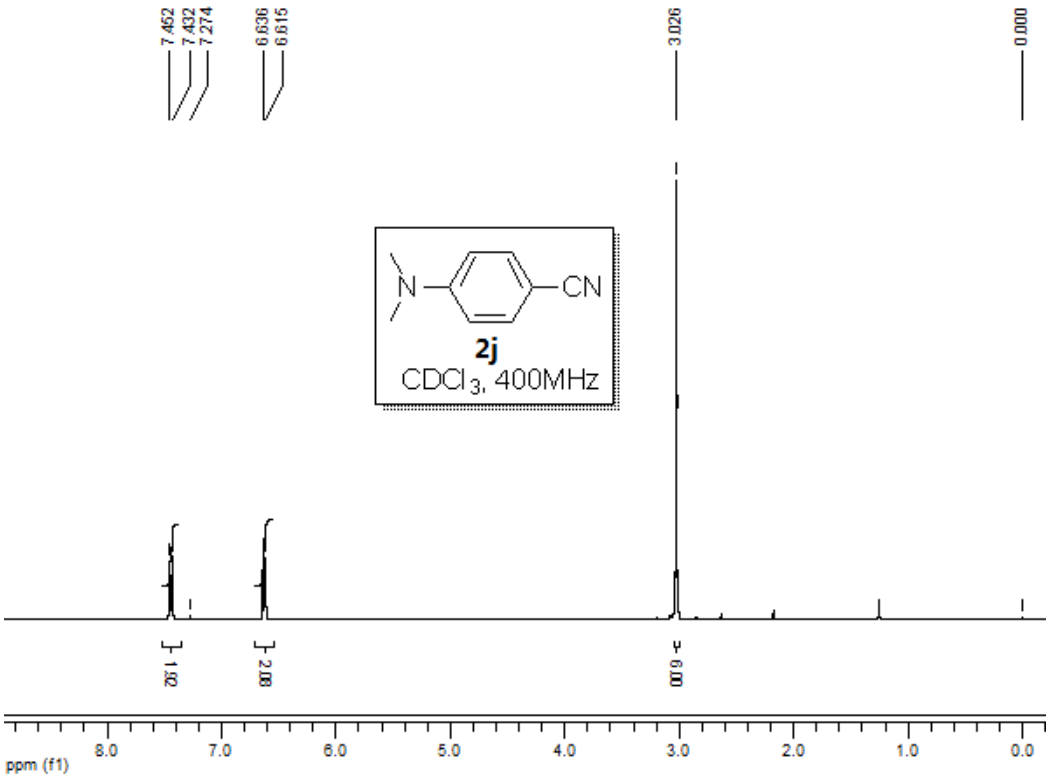
150
100
50
0
ppm (f1)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7.432
7.274
6.636
6.615
3.026
0.000
1.92
2.08
6.00
N
CN
2j
CDCl3, 400MHz
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7.0
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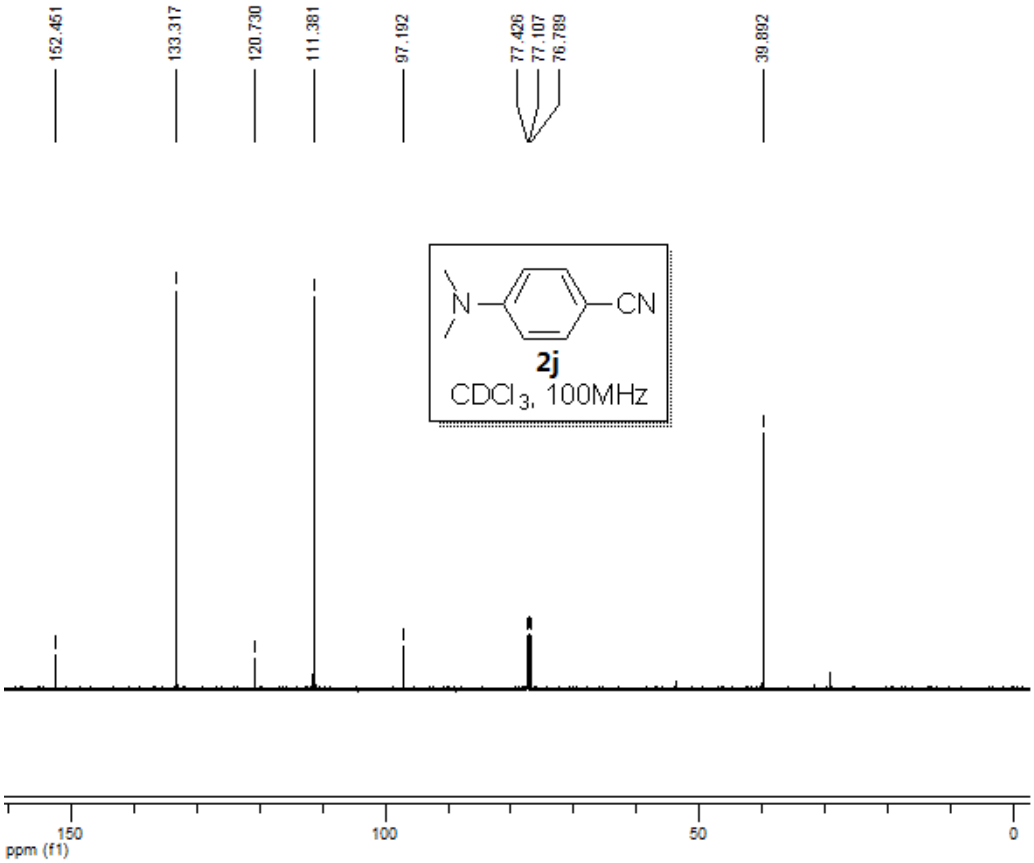
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)


152.451
133.317
120.730
111.381
97.192
77.426
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76.789
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CN
2j
CDCl3, 100MHz
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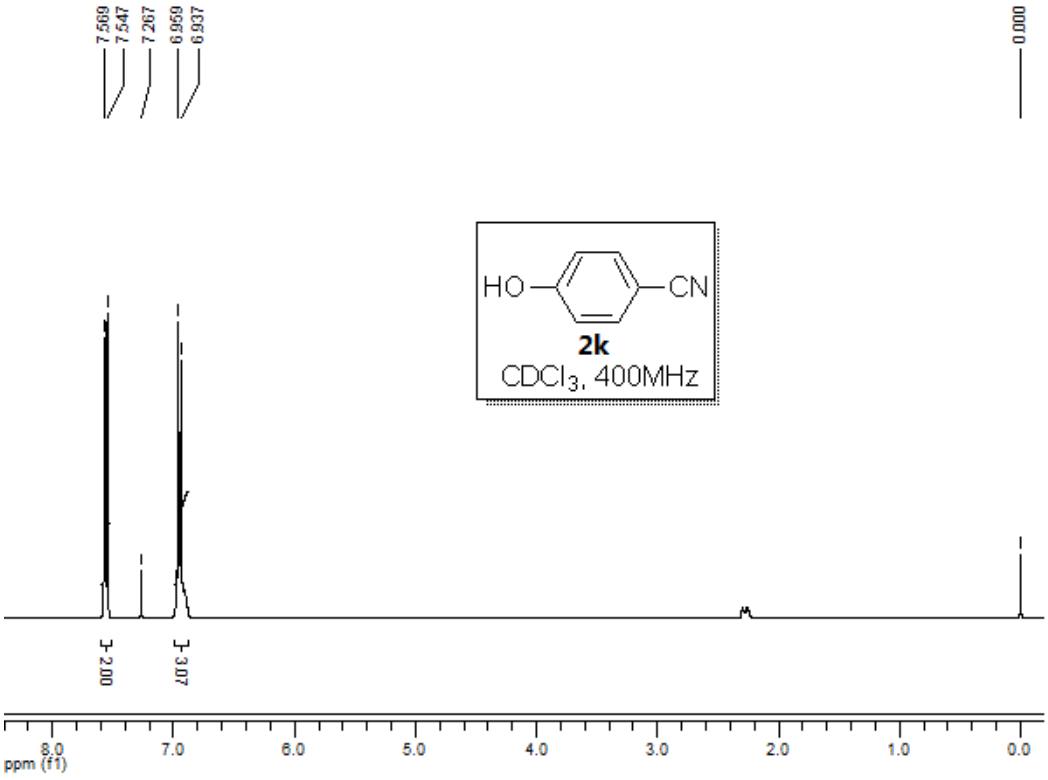
100
50
0
ppm (f1)


7.569
7.547
7.267
6.959
6.937
0.000
HO
CN
2k
CDCl3, 400MHz
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3.07
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7.0
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5.0
4.0
3.0
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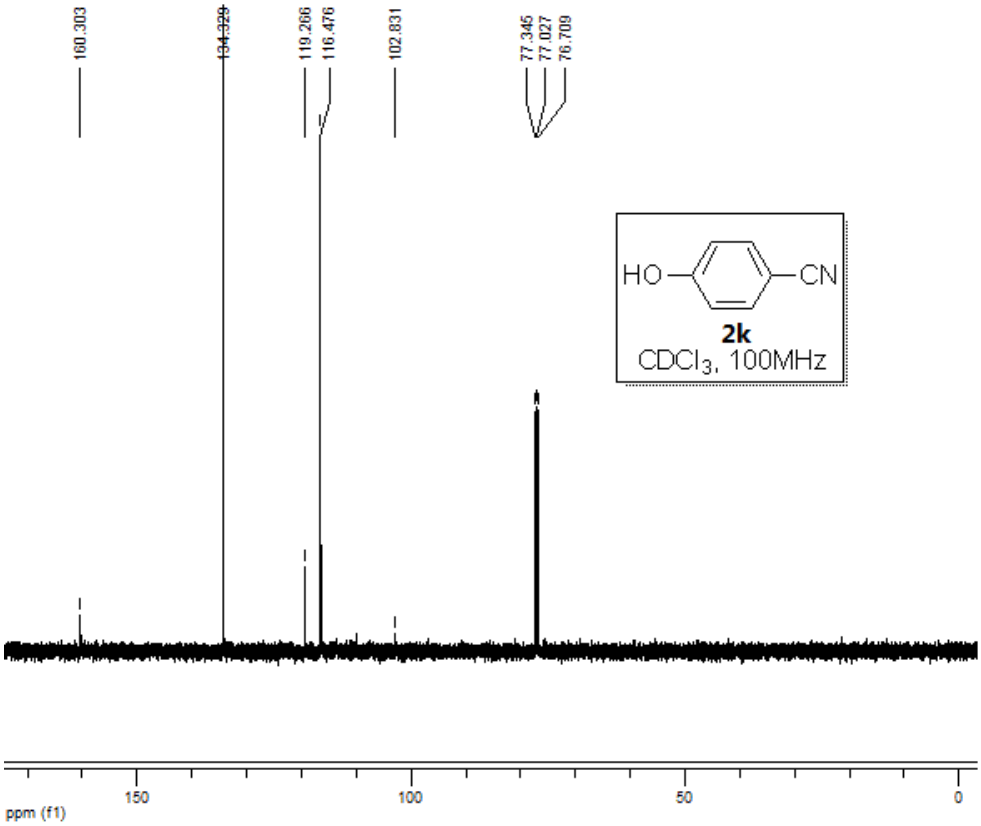
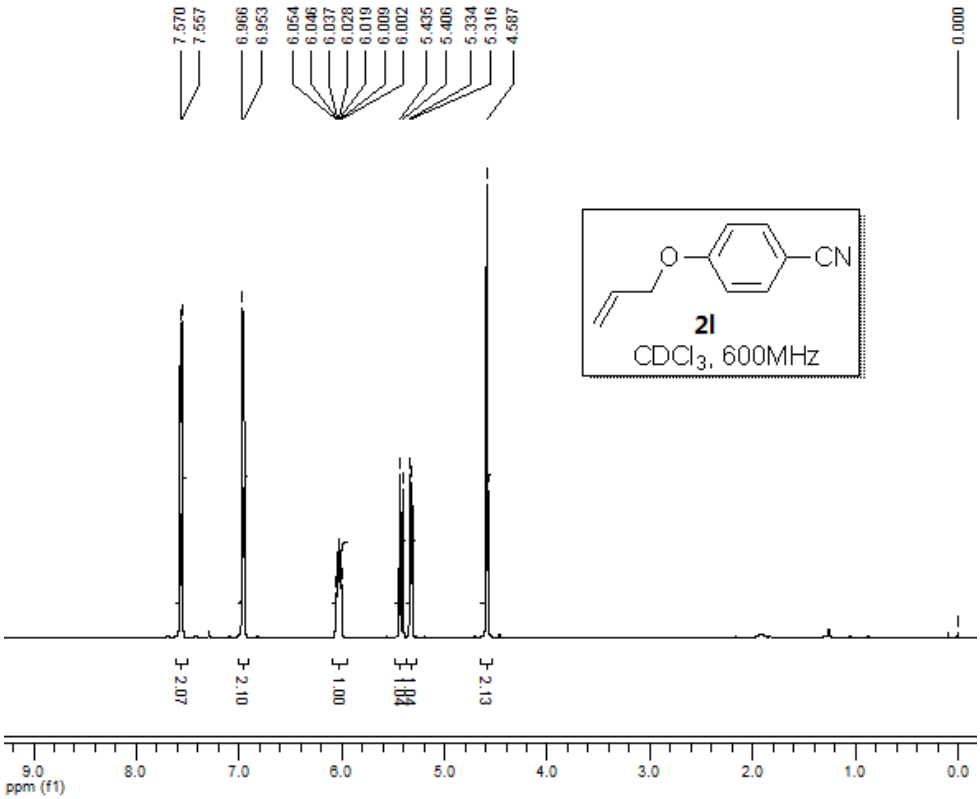
1.0
0.0
ppm (f1)


160.303
134.329
119.266
116.476
102.831
77.345
77.027
76.709
HO
CN
2k
CDCl3, 100MHz
150
100
50
0
ppm (f1)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7.557
6.966
6.953
6.054
6.046
6.037
6.028
6.019
6.009
6.002
5.435
5.406
5.334
5.316
4.587
0.000
O
CN
2l
CDCl3, 600MHz
2.07
2.10
1.00
1.84
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7.0
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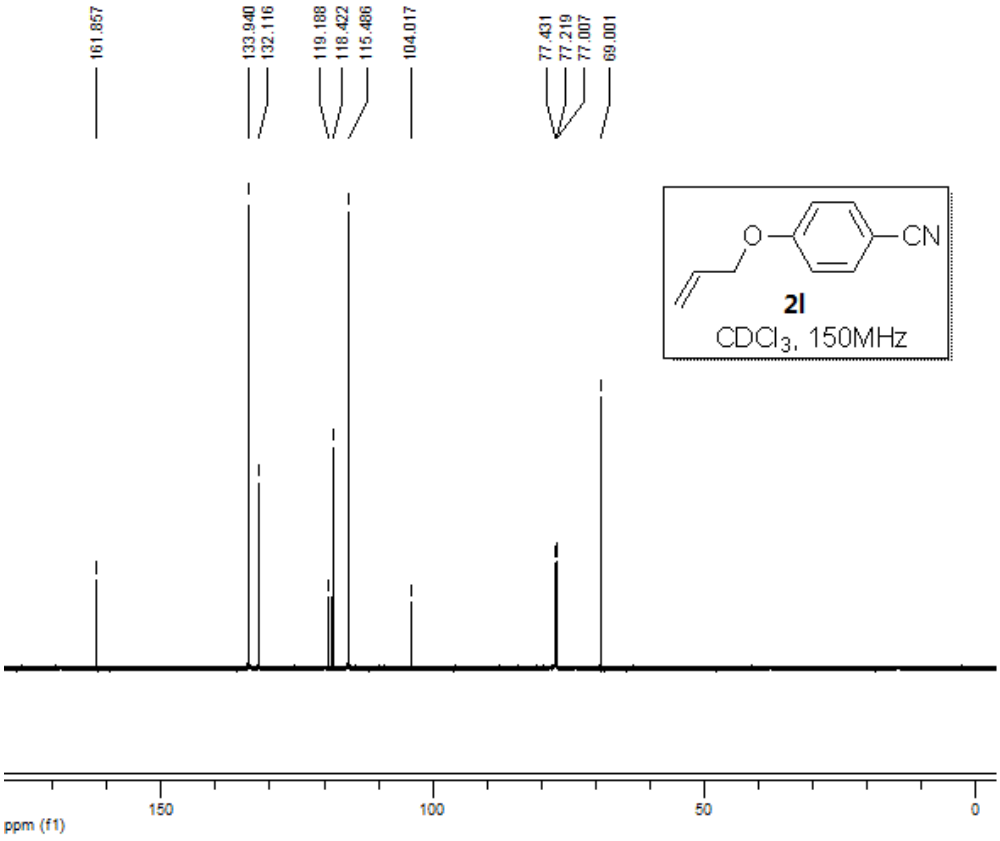
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)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118.422
115.486
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77.219
77.007
69.001
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CN
2l
CDCl3, 150MHz
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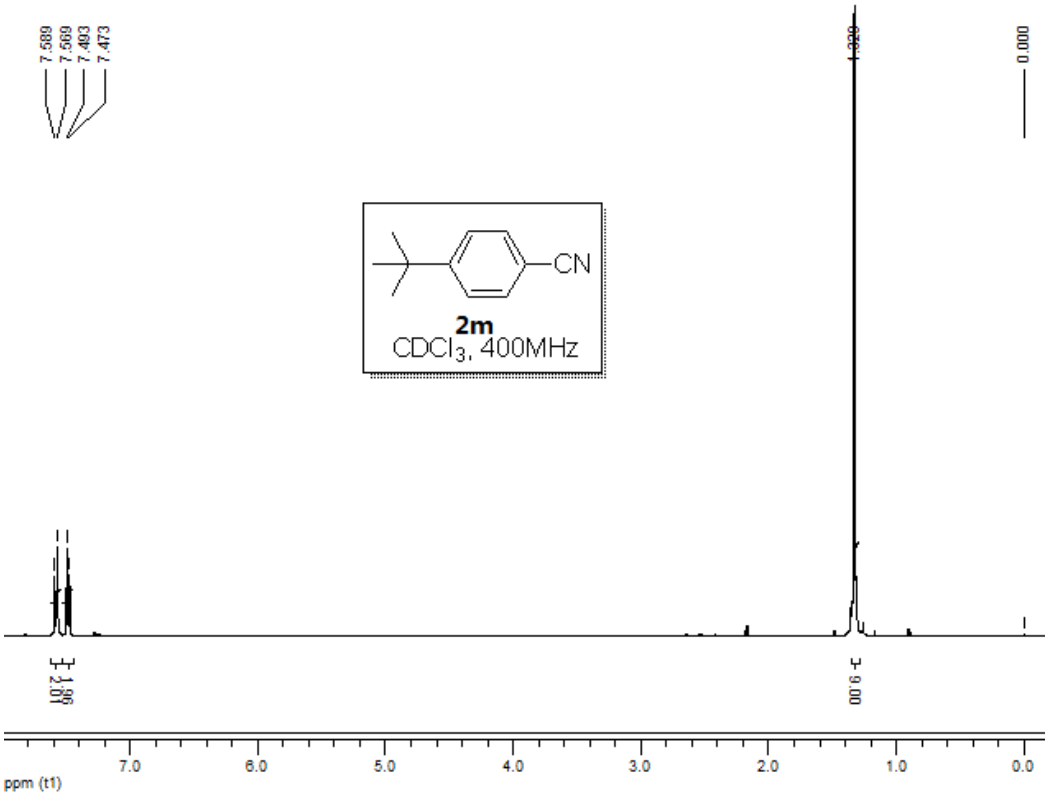
100
50
0
ppm (f1)


7.589
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7.493
7.473
1.329
0.000
CN
2m
CDCl3, 400MHz
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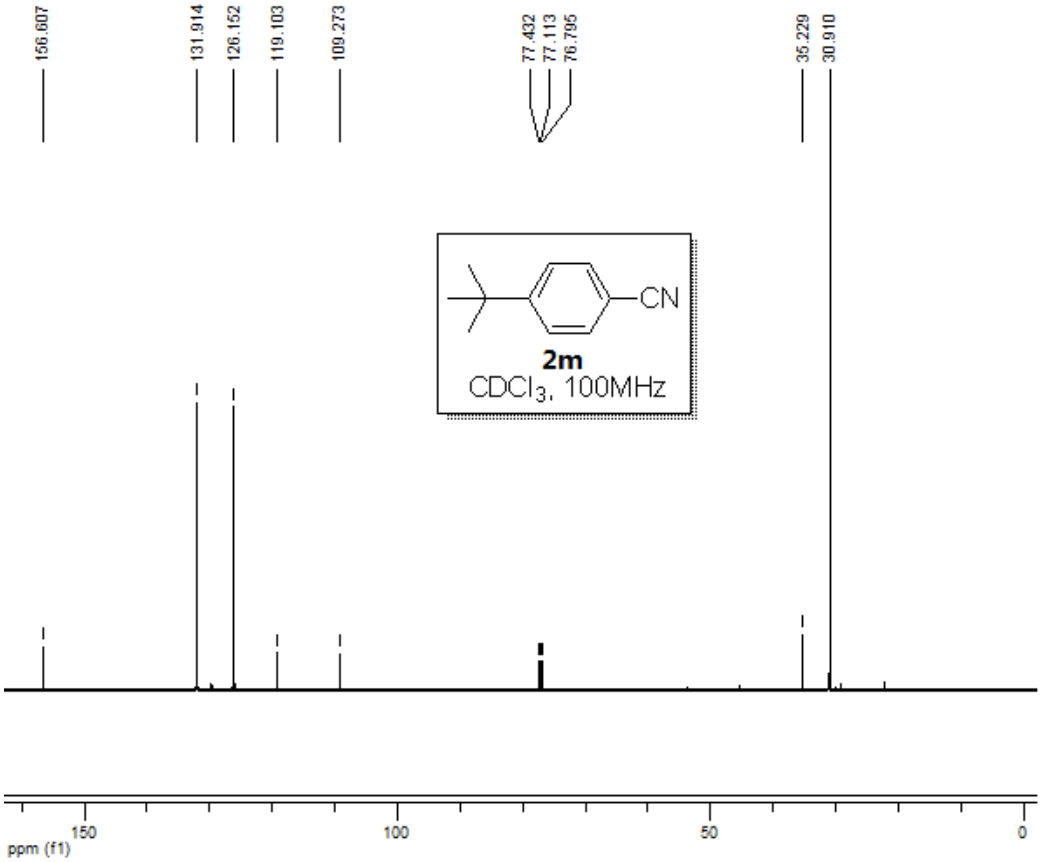
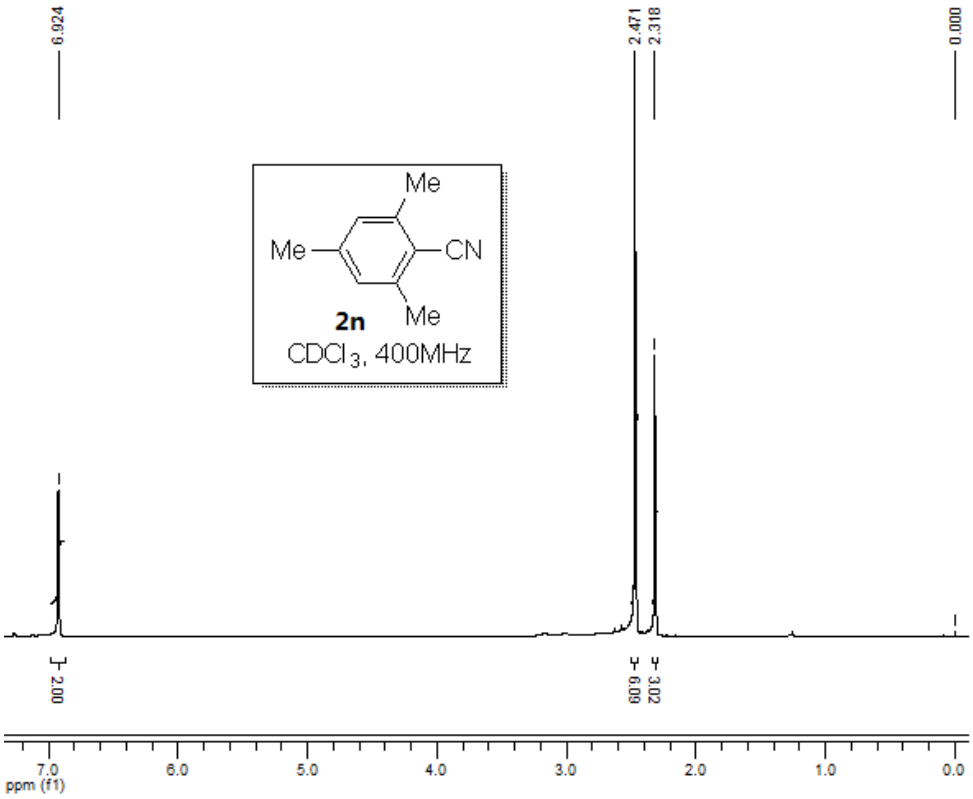
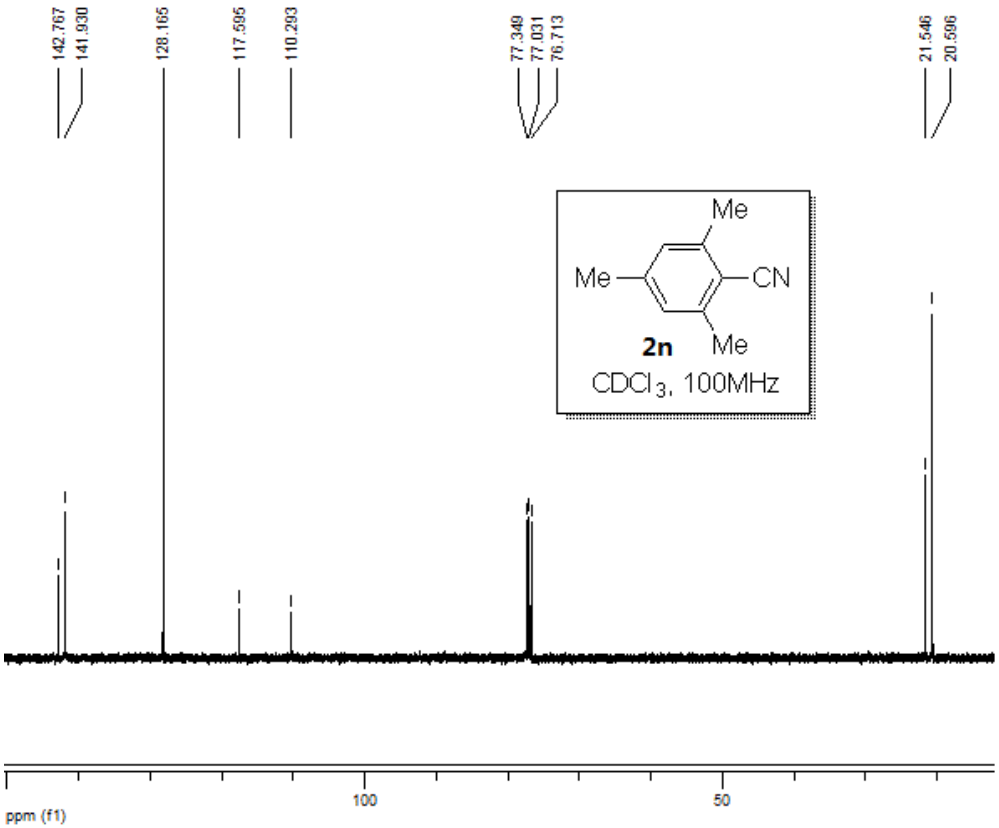
9.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


156.607
131.914
126.152
119.103
109.273
77.432
77.113
76.795
35.229
30.910
CN
2m
CDCl3, 100MHz
150
100
50
0
ppm (f1)


6.924
2.471
2.318
0.000
Me
Me
CN
Me
2n
CDCl3, 400MHz
2.00
6.09
3.02
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)


142.767
141.930
128.165
117.595
110.293
77.349
77.031
76.713
21.546
20.596
Me
Me
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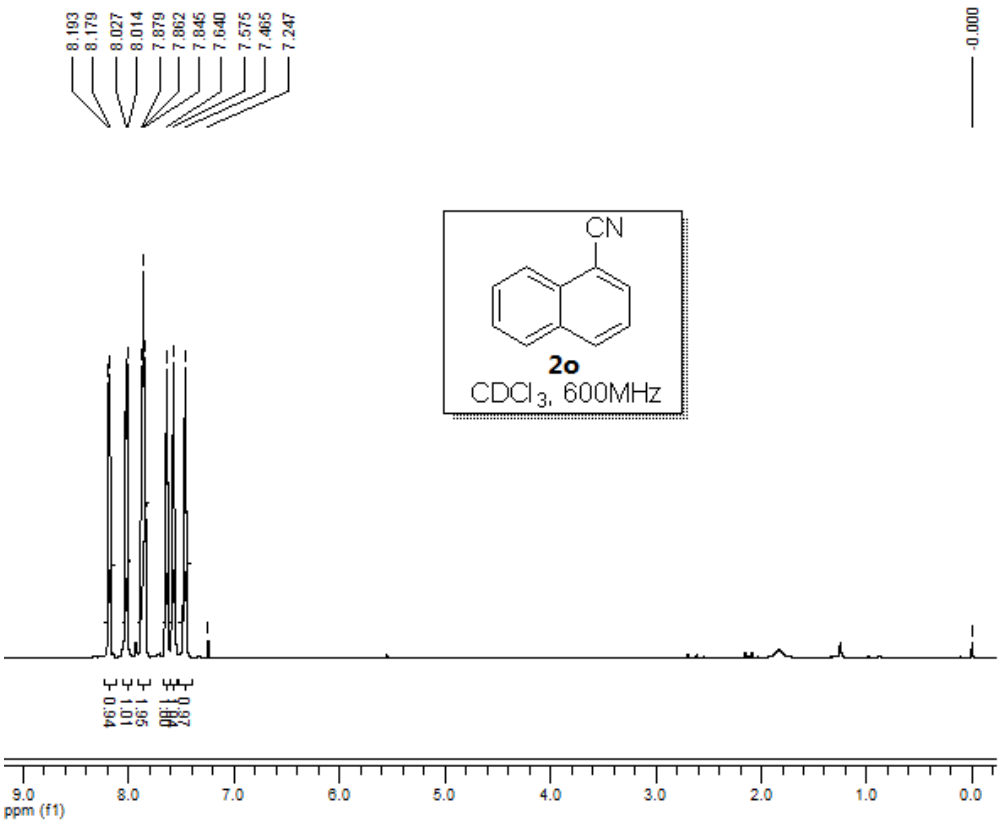
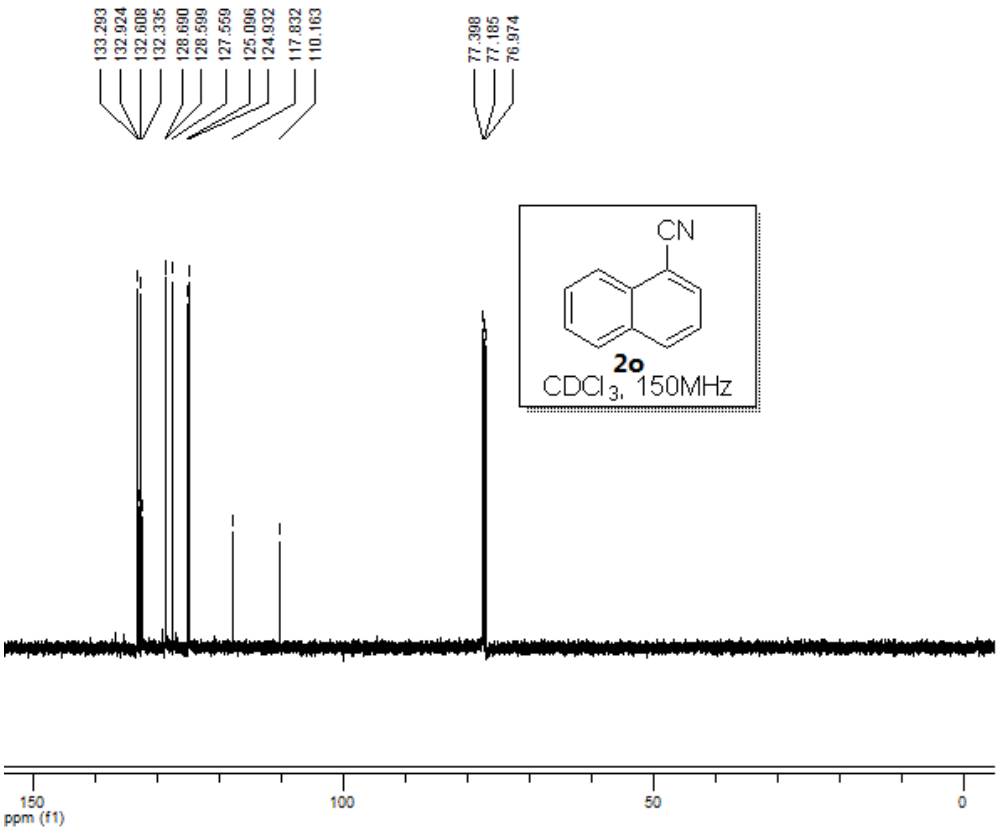
Me
2n
CDCl3, 100MHz
100
50
ppm (f1)


8.193
8.179
8.027
8.014
7.879
7.862
7.845
7.640
7.575
7.465
7.247
-0.000
CN
2o
CDCl3, 600MHz
0.94
1.01
1.96
2.00
2.10
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)


133.293
132.924
132.608
132.335
128.690
128.599
127.559
125.096
124.932
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77.185
76.974
CN
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CDCl3, 150MHz
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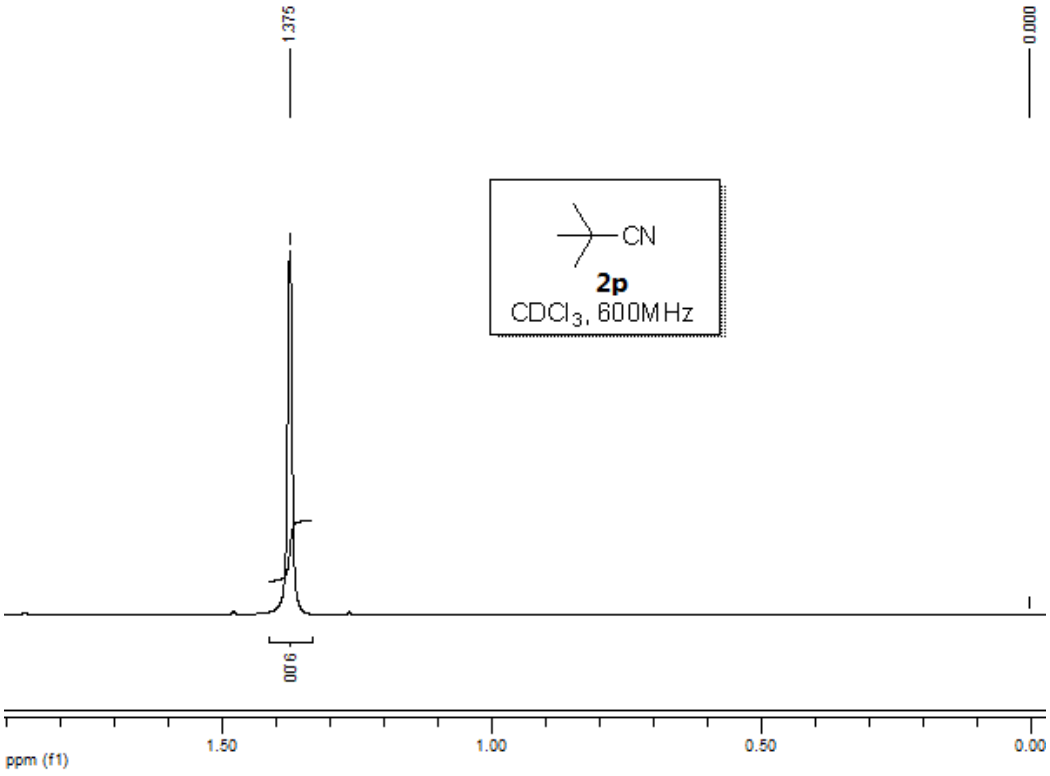
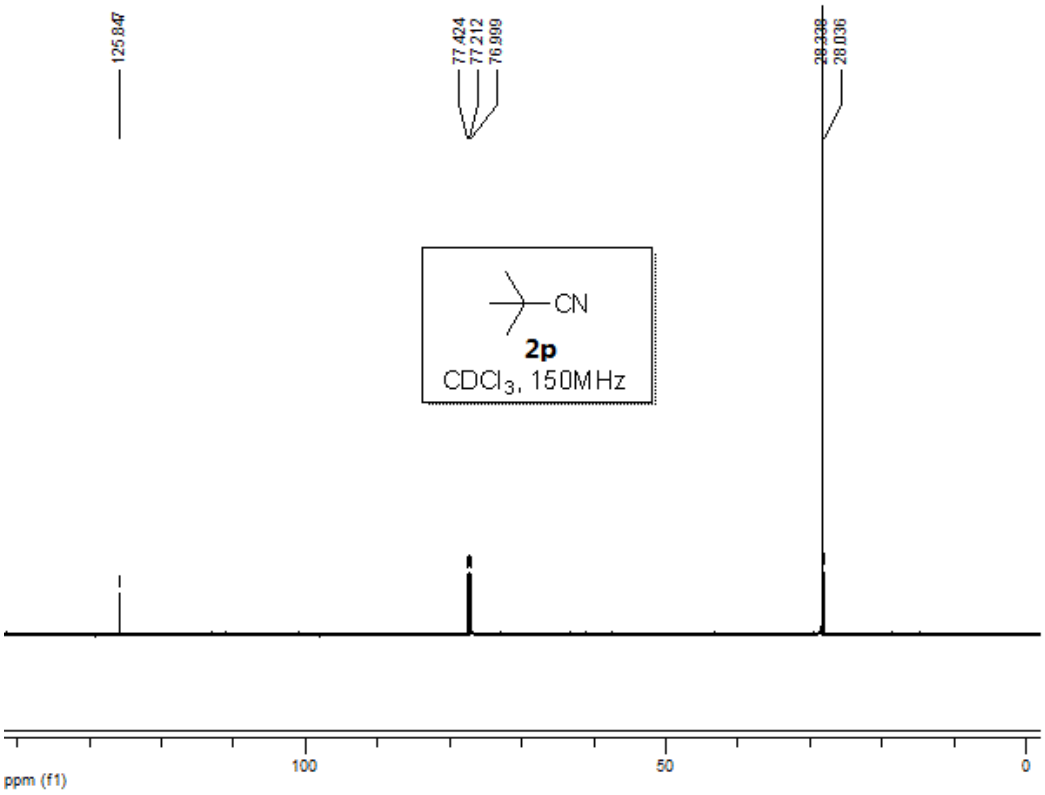
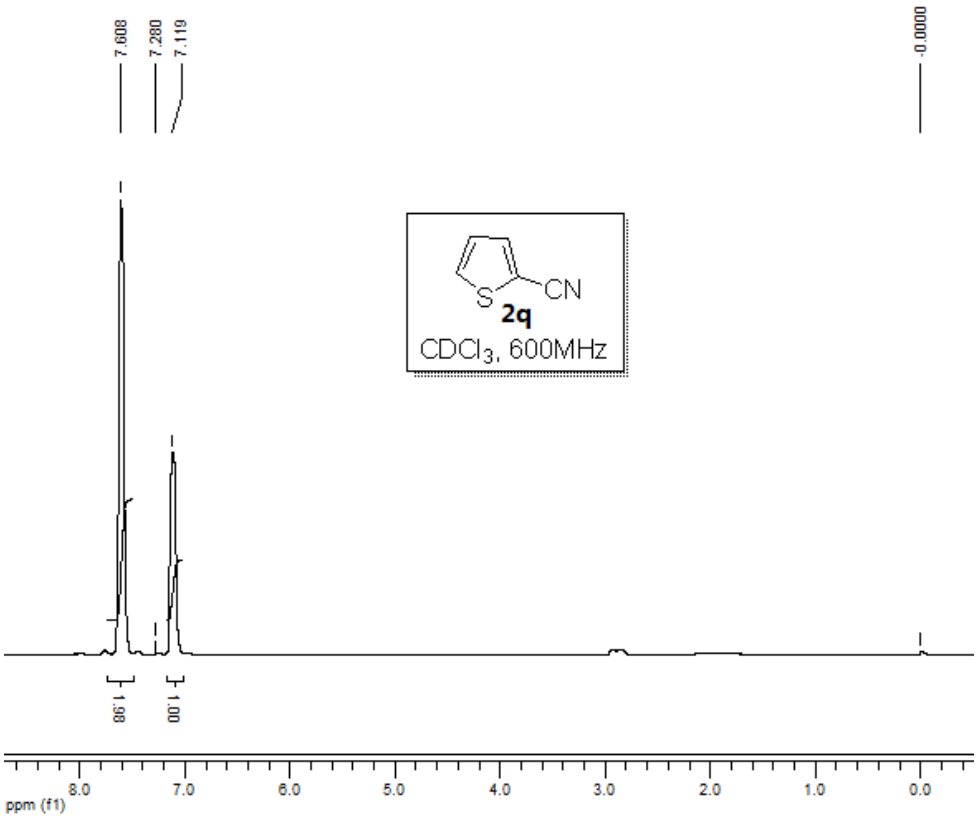
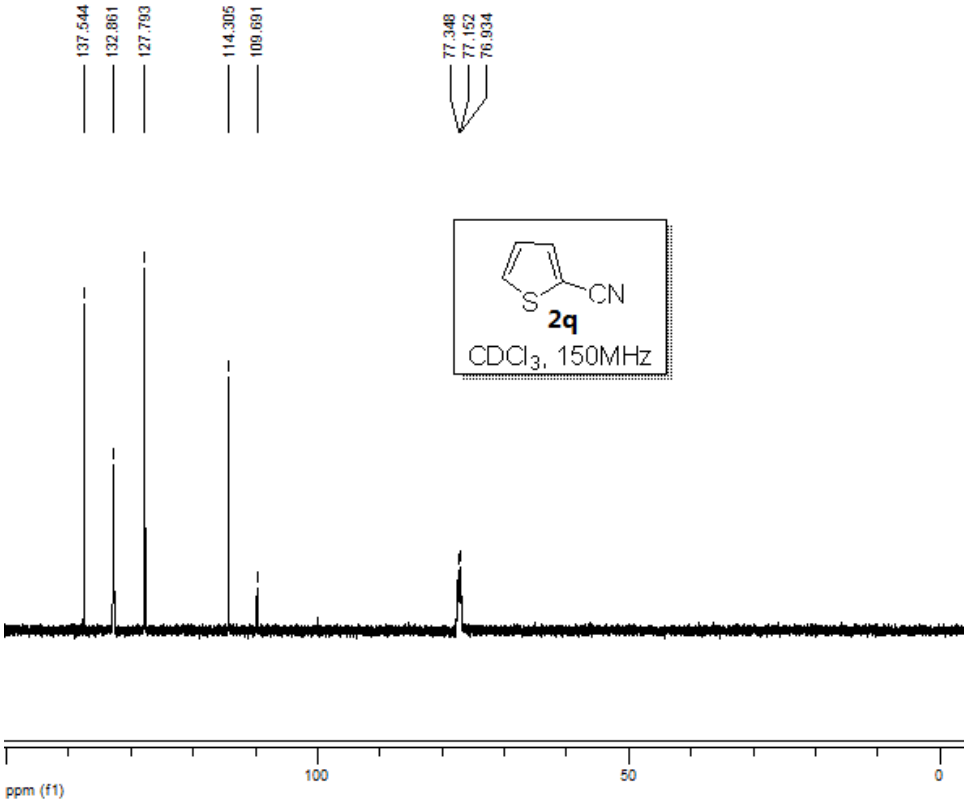
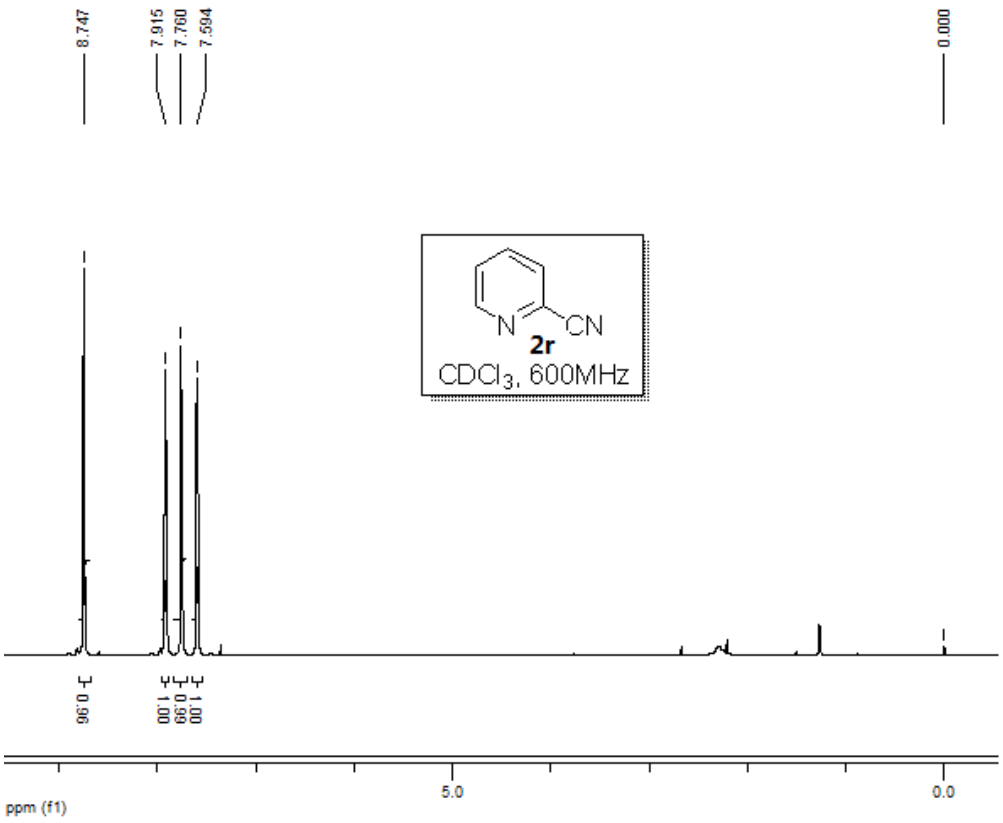
100
50
0
ppm (f1)

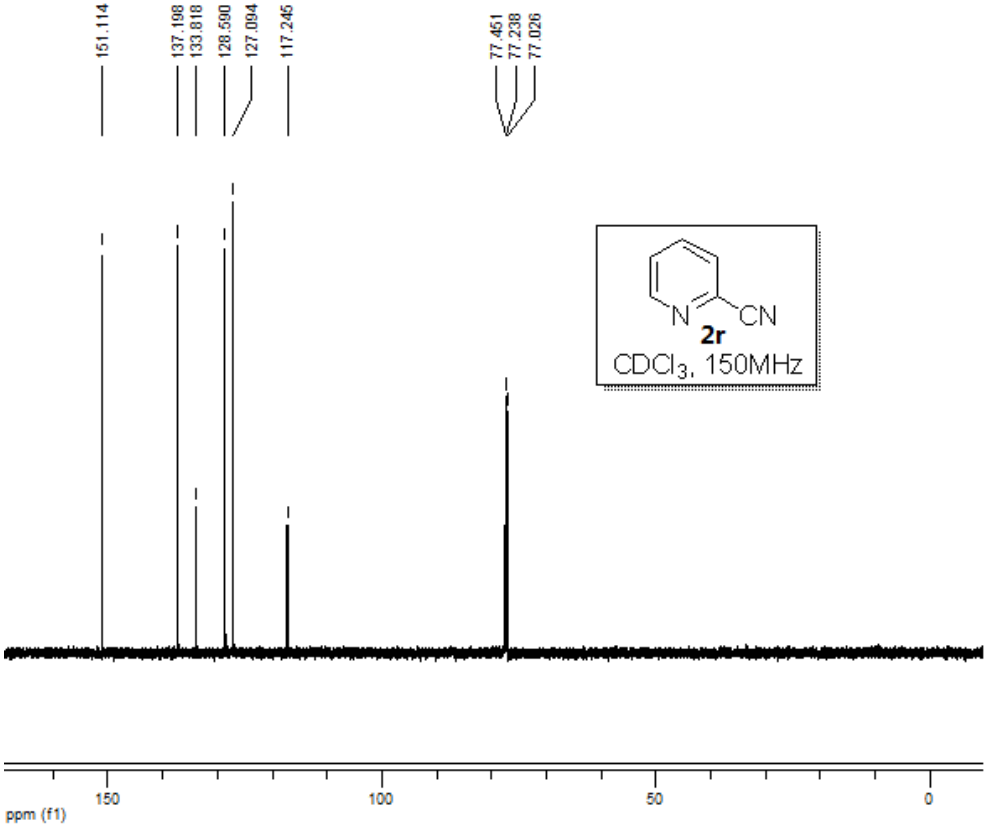

1.375
0.000
CN
2p
CDCl3, 600MHz
6.00
1.50
1.00
0.50
0.00
ppm (f1)


125.847
77.424
77.212
76.999
28.338
28.036
CN
2p
CDCl3, 150MHz
100
50
0
ppm (f1)


7.608
7.280
7.119
-0.0000
S
CN
2q
CDCl3, 600MHz
1.98
1.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)


137.544
132.861
127.793
114.305
109.691
77.348
77.152
76.934
S
CN
2q
CDCl3, 150MHz
100
50
0
ppm (f1)


8.747
7.915
7.760
7.594
0.000
N
CN
2r
CDCl3, 600MHz
0.96
1.00
0.99
1.00
5.0
0.0
ppm (f1)


151.114
137.198
133.818
128.590
127.094
117.245
77.451
77.238
77.026
N
CN
2r
CDCl3, 150MHz
150
100
50
0
ppm (f1)