Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Nickel-Catalyzed Cyanation of Phenol Derivatives Activated by 2,4,6-Trichloro-1,3,5-triazine

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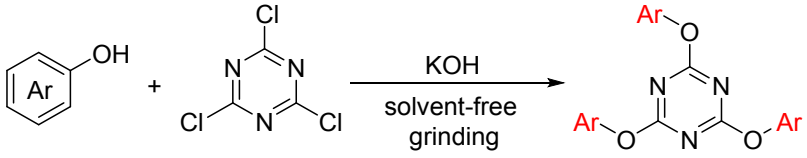
1 General experimental details

Chemicals were used as received without special purification unless stated otherwise. $Ni(cod)_2$, $NiBr_2$, Zn powder and ligands were obtained from Sigma-Aldrich. All reactions were performed with dry solvents under N_2. Thin-layer chromatography (TLC) was visualized using UV light. Column chromatography was generally performed on silica gel (300−400 mesh). ^1H and ^{13}C NMR were recorded in $CDCl_3$ or DMSO-d_6 at ambient temperature on a 300 or 500 MHz NMR spectrometer. Chemical shifts are reported in δ units, parts per million (ppm). The coupling constants J are given in Hz. GC analyses are performed on an Agilent 7890A instrument (Column: Agilent 19091J-413: 30 m × 320 μm × 0.25 μm, carrier gas: H_2, FID detection. GC/MS data was recorded on a 5975C Mass Selective Detector, coupled with a 7890A Gas Chromatograph (Agilent Technologies). Liquid Chromatograph-Mass Spectrometer (LCMS) was performed on a Shimadzu LCMS-2020 instrument with an ESI source.

1.1 Preparation of TAT derivatives

Using the reaction between phenol and TCT as example: the mixture of KOH (2.02 g, 36 mmol), phenol (1.69 g, 18 mmol) and TCT (0.92 g, 5 mmol) was grinded in a mortar. The reaction immediately released the hydrogen chloride gas and heat. After 5 mins, the color of the mixture turned into white from light yellow. The crude mixture was poured into water, stirred, filtrated, washed with water, and dried to provide the desired pure product in 81% yield (1.45 g, m.p. 232~235 °C). The white powder product could be further purified by recrystallization in DCM/ethanol if necessary.

The TAT derivatives can be also be prepared in acetone/water medium[1] using NaOH as the base or in organic solvents using NaH as the base.[2]



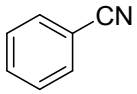
1.2 General procedure for synthesis of arylnitriles 3

Phenol derivatives **1** (0.10 mmol = aryl 0.3 mmol), 2-morpholinoacetonitrile **2** (75.7 mg, 0.60 mmol), $NiBr_2$ (6.6 mg, 0.03 mmol, 10 mol%), dcype (25.4 mg, 0.06 mmol, 20 mol%), K_3PO_4 (127.4 mg, 0.6 mmol), Zn powder (11.8 mg, 0.18 mmol, 60 mol%) and dry dioxane (1.5 mL) were added to a 10-mL glass vessel containing a magnetic stirring bar in a glovebox. The reaction was heated at 130 °C for 24 h. After cooling the reaction mixture to room temperature, the mixture was passed through a silica gel pad with EtOAc as the eluent. The filtrate was then concentrated, and purified using column chromatography on silica gel using *n*-hexane/EtOAc as eluent.

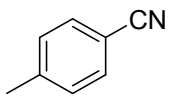
1.3 One-pot synthesis of arylnitriles 3a and 3b

NaH (24 mg, 0.6 mmol, 60% dispersion in mineral oil) was added to a stirring mixture of phenol **1a** or **1b** (0.3 mmol) in dry 1,4-dioxane (1.5 mL) at room temperature and stirred for 1h. Then, TCT (0.1 mmol) was added and the mixture was stirred at 100 °C for 12 h. After that, the reaction mixture was cooled down to room temperature, and 2-morpholinoacetonitrile **2**, $NiBr_2$, dcype, K_3PO_4 and Zn powder were added in a glovebox (see above reaction conditions). The reaction was then heated at 130 °C for 24 h. After cooling the reaction mixture to room temperature, the mixture was passed through a silica gel pad with EtOAc as the eluent. The filtrate was then concentrated, and purified using column chromatography on silica gel using *n*-hexane/EtOAc as eluent.

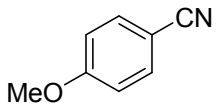
2 Characterization data of compounds



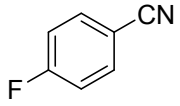
Benzonitrile **3a**.[3] Colorless oil (25.0 mg, 81%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46-7.49 (m, 2H), 7.60-7.66 (m, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 111.4, 117.9, 128.2, 131.1, 131.8. MS (ESI) *m/z*: 103 [M^+].



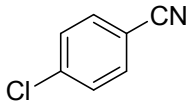
4-Methylbenzonitrile **3b**.[4] Yellow liquid (29.1 mg, 81%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.43 (s, 3H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 20.8, 108.3, 118.1, 128.9, 131.0, 142.7. MS (ESI) *m/z*: 117 [M^+].



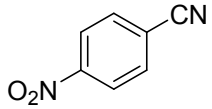
4-Methoxybenzonitrile **3c**.[3] Yellow solid (33.9 mg, 85%), m.p. 61-62 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.86 (s, 3H), 6.95 (d, J = 9.0 Hz, 2H), 7.58 (d, J = 9.0 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 54.6, 103.0, 113.8, 118.2, 133.0, 161.9. MS (ESI) *m/z*: 133 [M^+].



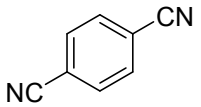
4-Fluorobenzonitrile **3d**.[5] Yellow solid (27.2 mg, 75%), m.p. 29-31 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.08-7.12 (m, 2H), 7.59-7.62 (m, 2H). ^{1}H NMR (75 MHz, $CDCl_3$) δ 109.4 (d, $J_{C\text{-}F}$ = 3.8 Hz), 117.6 (d, $J_{C\text{-}F}$ = 22.7 Hz), 118.1, 135.5 (d, $J_{C\text{-}F}$ = 9.3 Hz), 166.1 (d, $J_{C\text{-}F}$ = 253 Hz). MS (ESI) *m/z*: 121 [M^+].



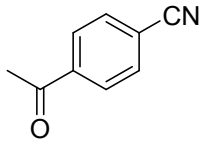
4-Chlorobenzonitrile **3e**.[4] Yellow solid (28.7 mg, 70%), m.p. 91-93 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47 (d, J = 8.5 Hz, 2H), 7.61 (d, J = 8.5 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 109.8, 117.0, 128.7, 132.4, 138.6. MS (ESI) *m/z*: 137 [M^+].



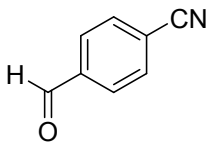
4-Nitrobenzonitrile **3f**.[3] Yellow solid (32.8 mg, 74%), m.p. 141-143 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78 (d, J = 8.5 Hz, 2H), 8.25 (d, J = 9.0 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 115.8, 117.4, 123.3, 132.5, 149.1. MS (ESI) *m/z*: 148 [M^+].



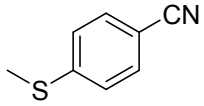
Terephthalonitrile **3g**.[6] Yellow solid (27.6 mg, 72%), m.p. 214-216 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.08 (s, 4H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 115.7, 117.5, 133.2. MS (ESI) *m/z*: 128 [M^+].



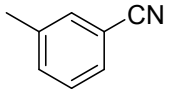
4-Acetylbenzonitrile **3h**.[7] Yellow solid (33.9 mg, 78%), m.p. 55-57 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.64 (s, 3H), 7.77 (d, J = 8.7 Hz, 2H), 8.04 (d, J = 8.7 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 26.7, 116.3, 117.9, 128.6, 132.4, 139.8, 196.5. MS (ESI) *m/z*: 145 [M^+].



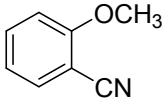
4-Formylbenzonitrile **3i.**[6] Light yellow solid (27.5 mg, 70%), m.p. 98-100 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.2 Hz, 2H), 8.00 (d, *J* = 8.5 Hz, 2H), 10.10 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 117.5, 117.6, 129.8, 132.8, 138.7, 190.6. MS (ESI) *m/z*: 131 [M^+].



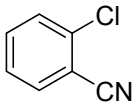
4-(Methylthio)benzonitrile **3j**.[8] Yellow solid (35.7 mg, 80%), m.p. 57-59 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.50 (s, 3H), 7.25 (d, *J* = 8.6 Hz, 2H), 7.52 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.6, 107.6, 118.9, 125.4, 132.1, 146.1. MS (ESI) *m/z*: 149 [M^+].



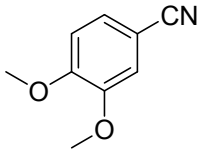
3-Methylbenzonitrile **3k**.[9] Yellow liquid (29.5 mg, 84%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.39 (s, 3H), 7.43 – 7.32 (m, 2H), 7.49 – 7.43 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.1,112.2, 119.0, 128.9, 129.2, 132.4, 133.6, 139.1. MS (ESI) *m/z*: 117 [M^+].



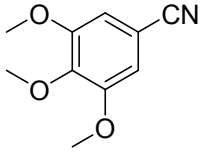
2-Methoxybenzonitrile **3l**.[5] Yellow liquid (24.7 mg, 62%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.87 (s, 3H), 6.90-6.95 (m, 2H), 7.46-7.50 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.0, 100.8, 110.3, 115.5, 119.8, 132.8, 133.4, 160.3. MS (ESI) *m/z*: 133 [M^+].



2-Chlorobenzonitrile **3m**.[10] Yellow solid (26.7 mg, 65%), m.p. 43-45 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 – 7.35 (m, 1H), 7.59 – 7.49 (m, 2H), 7.71 – 7.65 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 113.3, 115.9, 127.1, 130.0, 133.8, 133.9, 136.8. (s. MS (ESI) *m/z*: 137 [M^+].

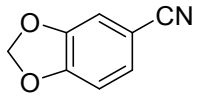


3,4-Dimethoxybenzonitrile **3n**.[4] Yellow solid (37.2 mg, 76%), m.p. 62-65 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.91 (s, 3H), 3.94 (s, 3H), 6.91 (d, *J* = 8.5 Hz, 1H), 7.09 (d, *J* = 1.5 Hz, 1H), 7.29 – 7.31 (dd, *J* = 8.3, 1.8 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.1, 102.9, 110.3, 113.0, 118.2, 125.5, 148.2, 151.9. MS (ESI) *m/z*: 163 [M^+].

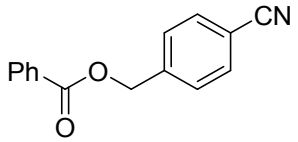


3,4,5-Trimethoxybenzonitrile **3o**.[11] Yellow solid (41.7 mg, 72%), m.p. 89-90 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.88 (s, 6H), 3.90 (s, 3H), 6.86 (s, 2H). ^{13}C NMR (75 MHz,

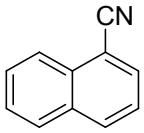
$CDCl_3$) δ 55.4, 60.1, 105.7, 108.5, 118.0, 141.4, 152.6. MS (ESI) *m/z*: 193 [M^+].



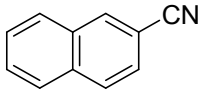
Benzo[d][1,3]dioxole-5-carbonitrile **3p**.[12] Yellow solid (33.1 mg, 75%), m.p. 90-92 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.07 (s, 2H), 6.86 (d, *J* = 8.1 Hz, 1H), 7.02 (d, *J* = 1.5 Hz, 1H), 7.20 (dd, *J* = 8.1, 1.6 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 102.2, 104.8, 109.0, 111.3, 118.8, 128.1, 147.9, 151.4. MS (ESI) *m/z*: 147 [M^+].



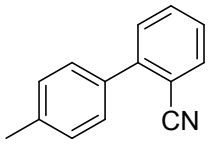
4-Cyanobenzyl benzoate **3q**.[13] Yellow liquid (51.9 mg, 73%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.34 (s, 2H), 5.37 – 5.41 (t, *J* = 7.5 Hz, 2H), 7.47 – 7.53 (m, 3H), 7.60 (d, *J* = 8.5 Hz, 2H), 8.09 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 64.5, 111.1, 117.6, 127.3, 127.6, 128.6, 128.7, 131.5, 132.4, 140.4, 165.1. MS (ESI) *m/z*: 237 [M^+].



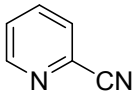
1-Naphthonitrile **3r**.[3] White solid (32.1 mg, 70%), m.p. 34-35 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 – 7.56 (t, *J* = 7.8 Hz, 1H), 7.62 – 7.65 (t, *J* = 7.5 Hz, 1H), 7.70 – 7.73 (t, *J* = 7.5 Hz, 1H), 7.92 – 7.95 (t, *J* = 6.3 Hz, 2H), 8.09 (d, *J* = 8.5 Hz, 1H), 8.25 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 109.3, 116.8, 123.9, 124.2, 126.6, 127.6, 131.4, 131.6, 132.0, 132.3. MS (ESI) *m/z*: 153 [M^+].



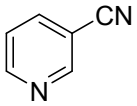
2-Naphthonitrile **3s**.[3] White solid (31.2 mg, 68%), m.p. 62-63 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62 – 7.69 (m, 3H), 7.91 – 7.95 (m, 3H), 8.26 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 108.4, 118.2, 125.4, 126.7, 127.1, 127.4, 128.0, 128.2, 131.3, 133.2, 133.7. MS (ESI) *m/z*: 153 [M^+].



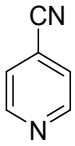
4'-Methylbiphenyl-2-carbonitrile **3t**.[14] White solid (26.6 mg, 46%), m.p. 50-52 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.35 (s, 3H), 7.23 (d, 2H, *J* = 8.0 Hz), 7.33 – 7.36 (t, 1H, *J* =7.5 Hz), 7.39 (d, *J* = 8.0 Hz, 2H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.54 – 7.57 (t, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 7.5 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 20.3, 110.2, 117.9, 126.3, 127.6, 128.5, 129.0, 131.8, 132.7, 134.3, 137.7, 144.6. MS (ESI) *m/z*: 193 [M^+].



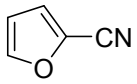
2-Cyanopyridine **3u**.[15] Light yellow solid (13.1 mg, 42%), m.p. 26-28 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.67 (d, *J* = 4.6 Hz, 1H), 7.83 (td, *J* = 7.8, 1.3 Hz, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.51 (dd, *J* = 7.7, 4.9 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 117.0, 126.9, 128.4, 133.6, 137.0, 150.9. MS (ESI) *m/z*: 104 [M^+].



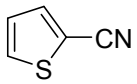
3-Cyanopyridine **3v**.[14] White solid (22.8 mg, 73%), m.p. 50-52 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 – 7.45 (m, 1H), 7.95 – 7.98 (m, 1H), 8.81-8.88 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 109.2, 115.5, 122.7, 138.3, 151.5, 152.0. MS (ESI) *m/z*: 104 [M^+].



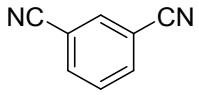
4-Cyanopyridine **3w**.[16] Light yellow solid (20.3 mg, 65%), m.p. 86-88 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.77 (d, *J* = 5.8 Hz, 2H), 7.50 (d, *J* = 5.9 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 116.2, 120.3, 125.1, 150.6. MS (ESI) *m/z*: 104 [M^+].



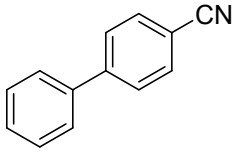
Furan-2-carbonitrile **3x**.[17] Light yellow liquid (11.4 mg, 41%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 1.4 Hz, 1H), 7.10 (d, *J* = 3.5 Hz, 1H), 6.53 (dd, *J* = 3.6, 1.8 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 113.3, 113.4, 121.9, 126.2, 147.3. MS (ESI) *m/z*: 93 [M^+].



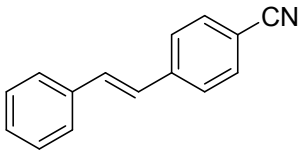
Thiophene-2-carbonitrile **3y**.[17] Light yellow liquid (16.4 mg, 50%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (t, *J* = 4.5 Hz, 2H), 7.14 – 7.09 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 109.6, 114.1, 127.5, 132.5, 137.3. MS (ESI) *m/z*: 109 [M^+].



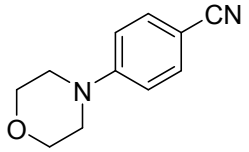
Isophthalonitrile **3z**.[18] White solid (18.4 mg, 48%), m.p. 163-165 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.66 (t, *J* = 7.9 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 114.0, 116.5, 130.2, 135.3, 135.9. MS (ESI) *m/z*: 128 [M^+].



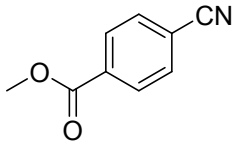
[1,1'-Biphenyl]-4-carbonitrile **4**.[19] Yellow solid (34.4 mg, 64%), m.p. 85-87 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 – 7.55 (m, 3H), 7.57 – 7.64 (m, 2H), 7.66 – 7.78 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 110.8, 118.9, 127.1, 127.6, 128.6, 129.0, 132.5, 139.1, 145.6. MS (ESI) *m/z*: 179 [M^+].



(*E*)-4-styrylbenzonitrile **5**.[20] Yellow solid (40.6 mg, 66%), m.p. 113-115 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.95 (d, *J* = 16.3 Hz, 1H), 7.09 (d, *J* = 16.3 Hz, 1H), 7.30 – 7.16 (m, 3H), 7.54 – 7.37 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 110.5, 119.0, 126.7, 126.8, 126.9, 128.6, 128.8, 132.3, 132.4, 136.2, 141.8. MS (ESI) *m/z*: 205 [M^+].



4-Morpholinobenzonitrile **6**.[21] White solid (34.4 mg, 61%), m.p. 74-76 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.22 – 3.33 (m, 4H), 3.79 – 3.90 (m, 4H), 6.81– 6.92 (m, 2H), 7.46 – 7.57 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 47.2, 66.4, 100.8, 114.0, 119.8, 133.4, 153.4. MS (ESI) *m/z*: 188 [M^+].



Methyl 4-cyanobenzoate **7**.[21] White solid (25.1 mg, 52%), m.p. 63-65 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.96 (s, 3H), 7.74 (d, *J* = 8.5 Hz, 2H), 8.14 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 52.7, 116.3, 117.9, 130.0, 132.2, 133.8, 165.4. MS (ESI) *m/z*: 161 [M^+].

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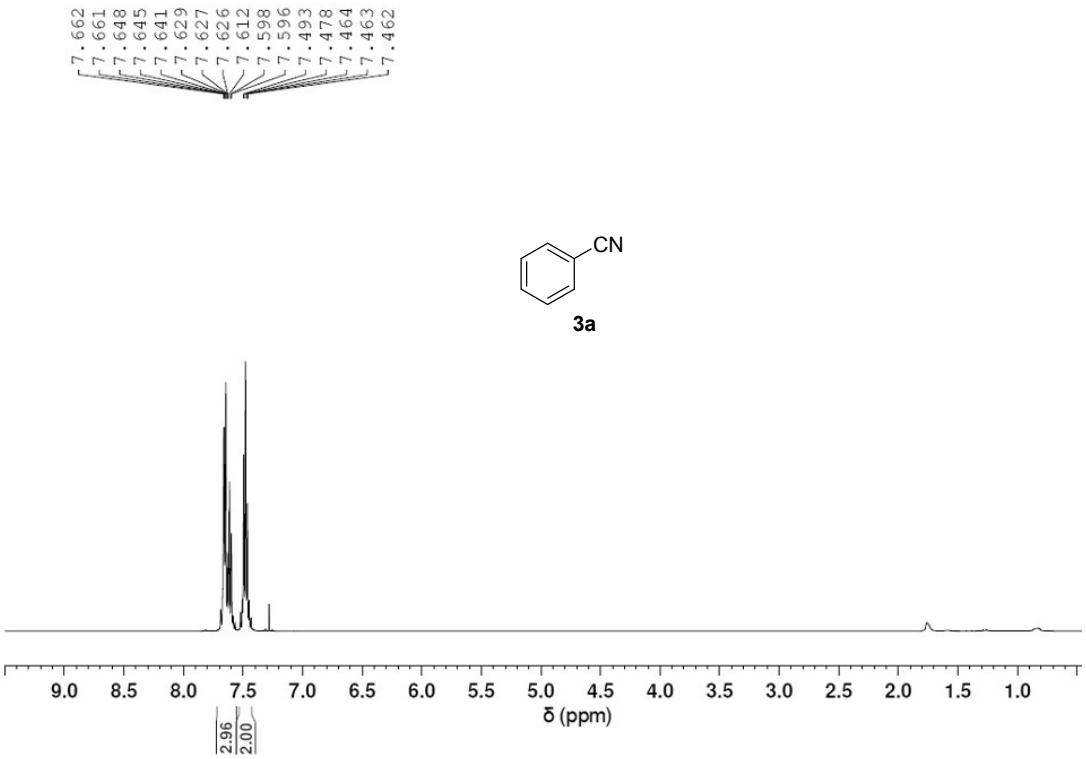
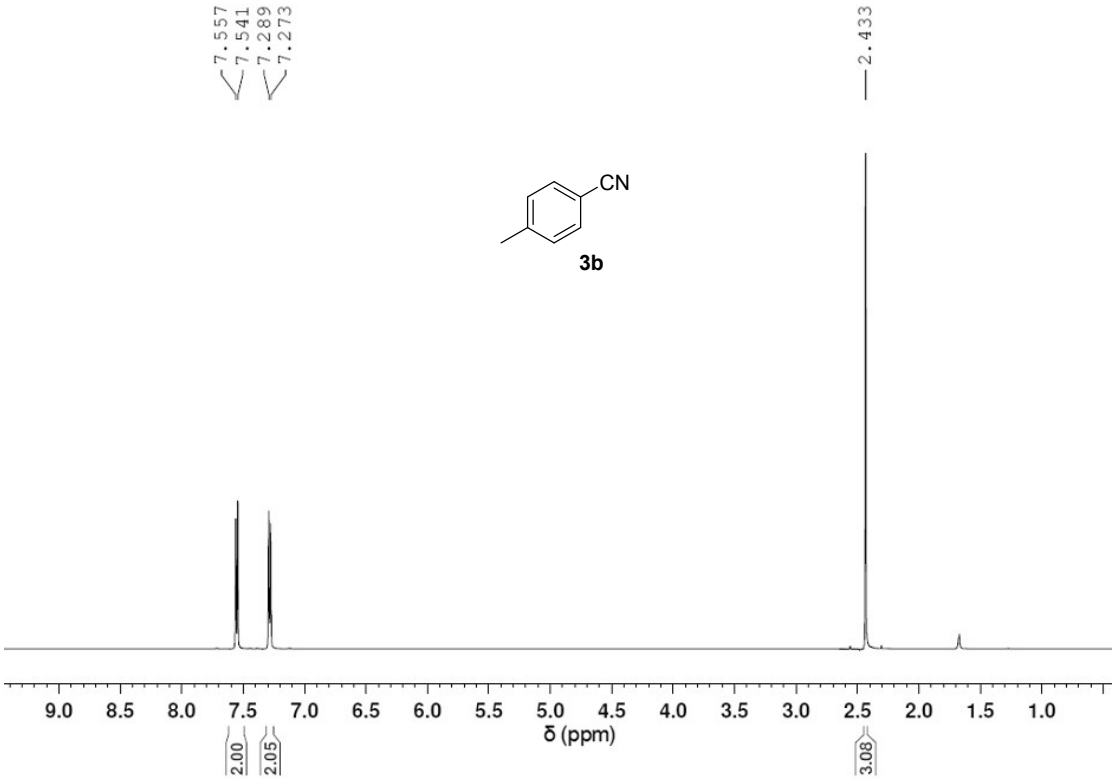
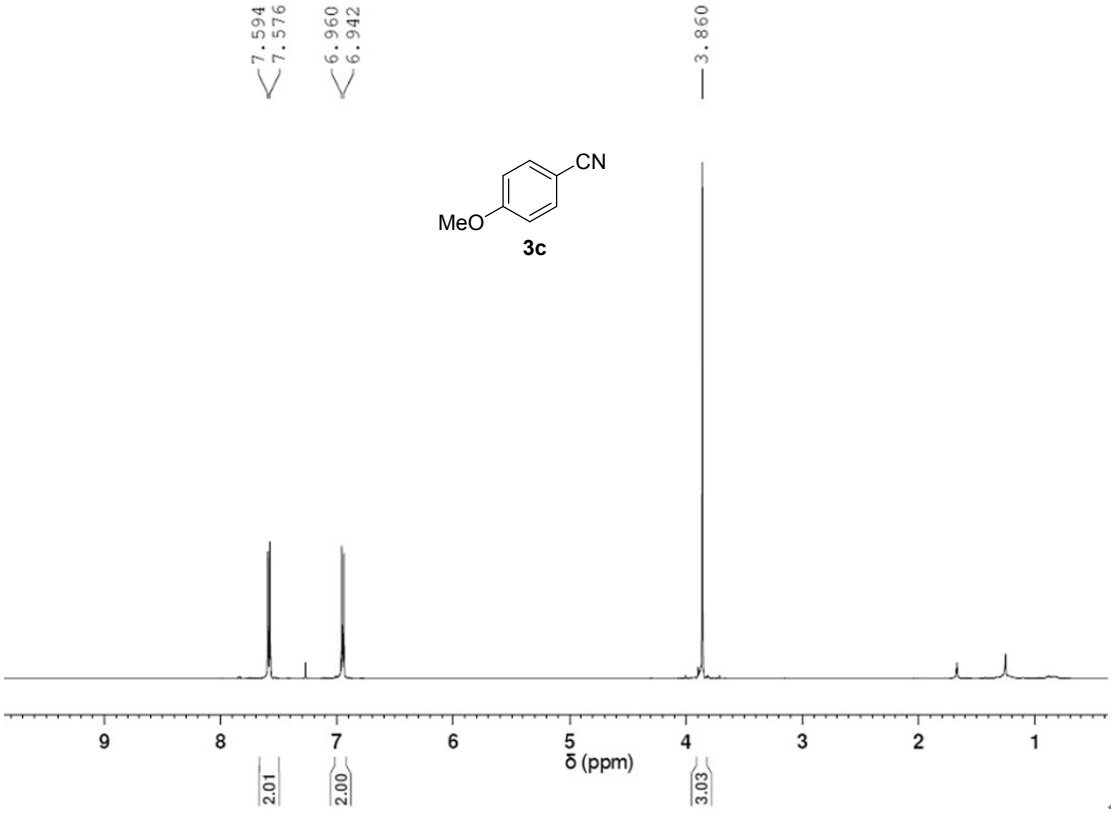
3 Selected Copies of ^{1}H NMR and ^{13}C NMR spectra



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7.576
6.960
6.942
3.860
CN
MeO
3c
9
8
7
6
5
4
3
2
1
δ (ppm)
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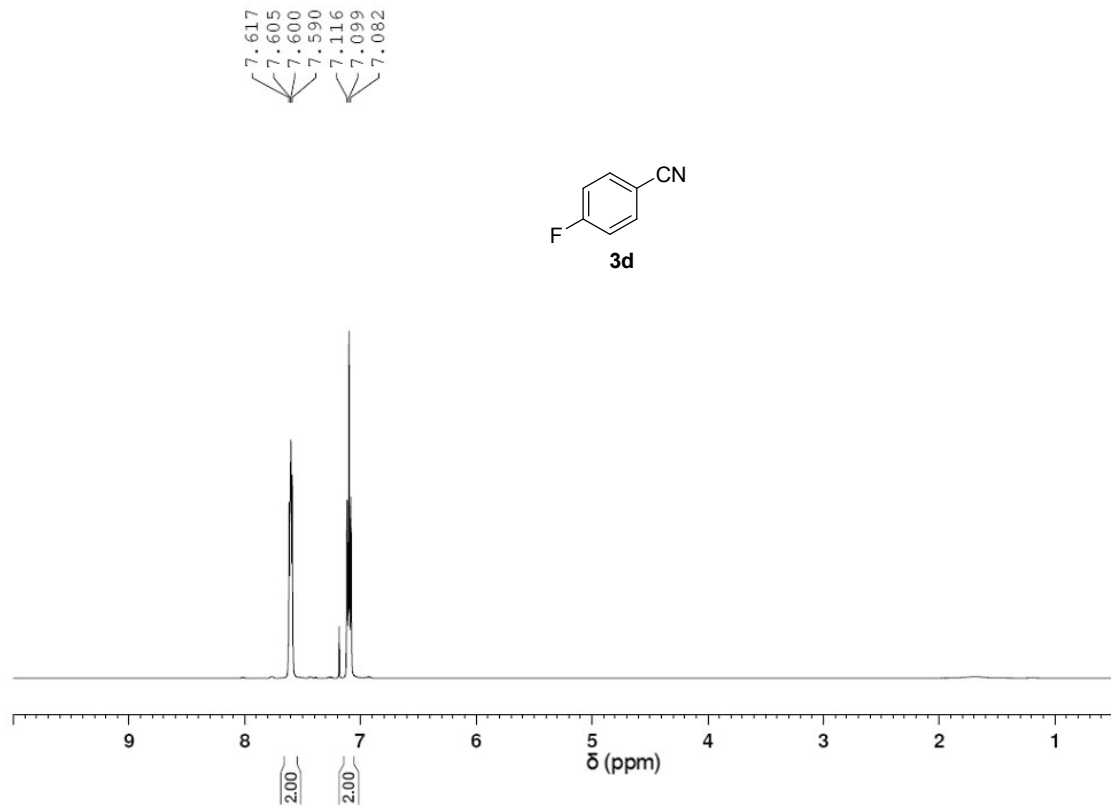
2.00
3.03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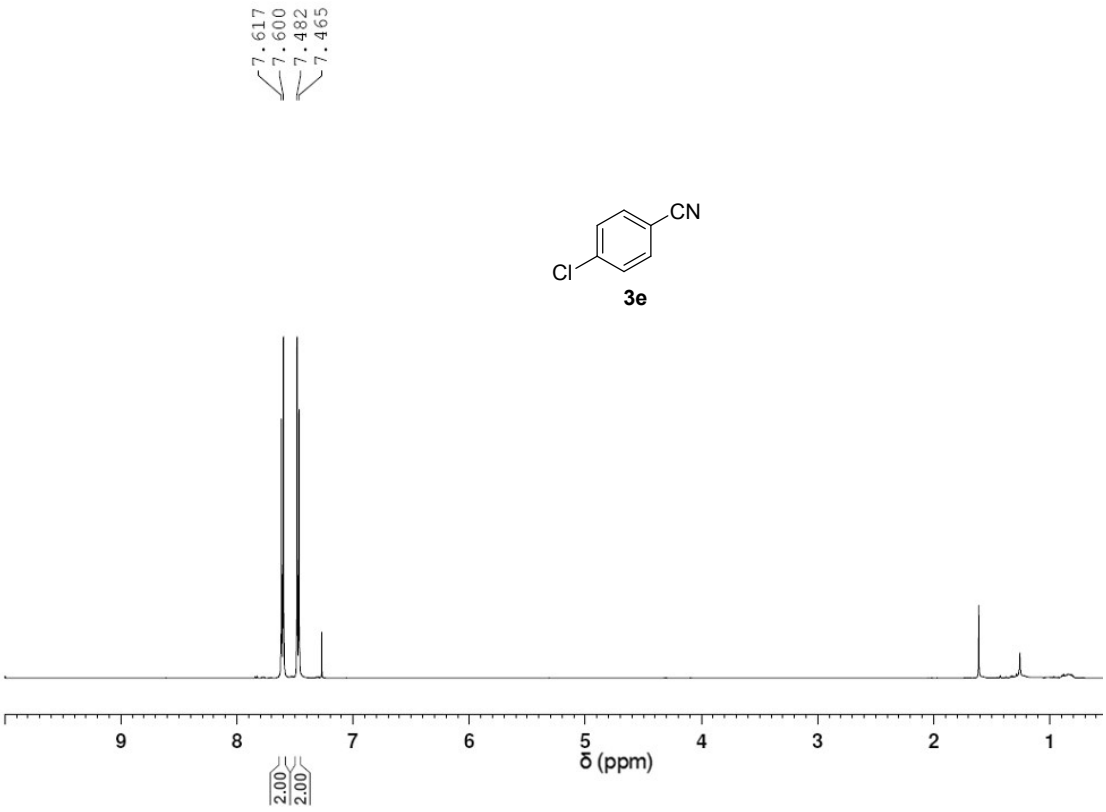
7.605
7.600
7.590
7.116
7.099
7.082
CN
F
3d
9
8
7
6
5
4
3
2
1
δ (ppm)
2.00
2.00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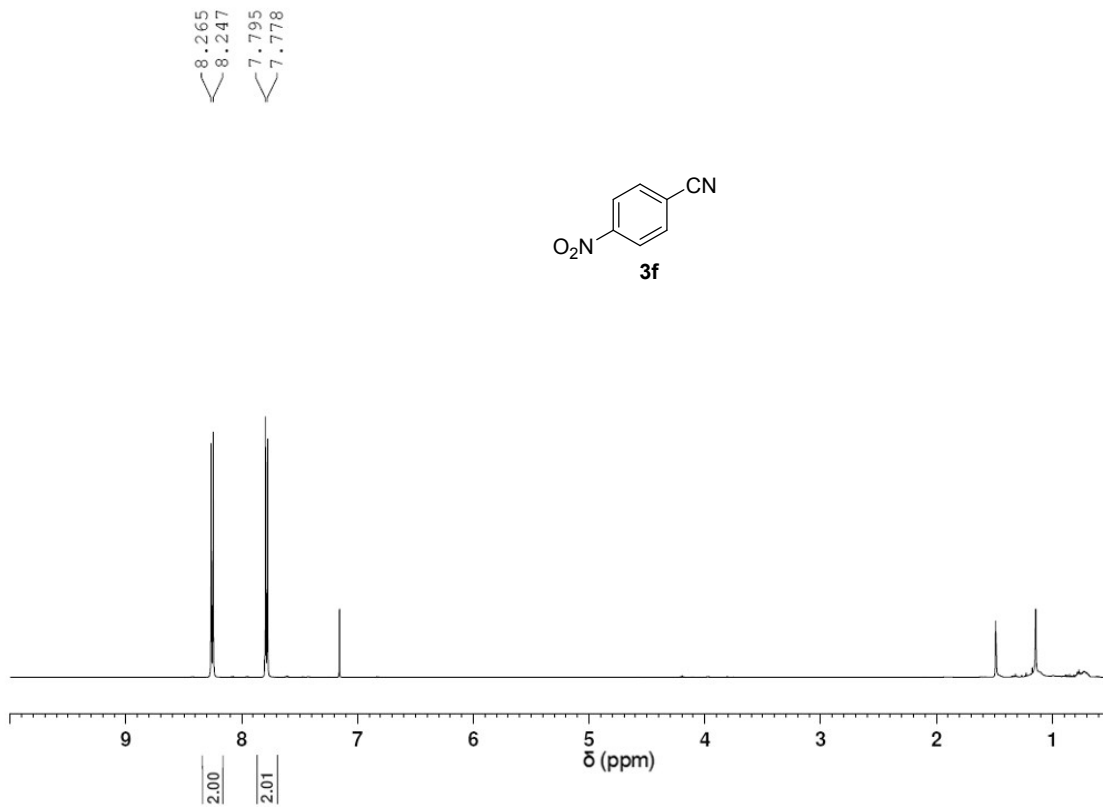
Cl
3e
9
8
7
6
5
4
3
2
1
δ (ppm)
2.00
2.00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8.247
7.795
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3f
9
8
7
6
5
4
3
2
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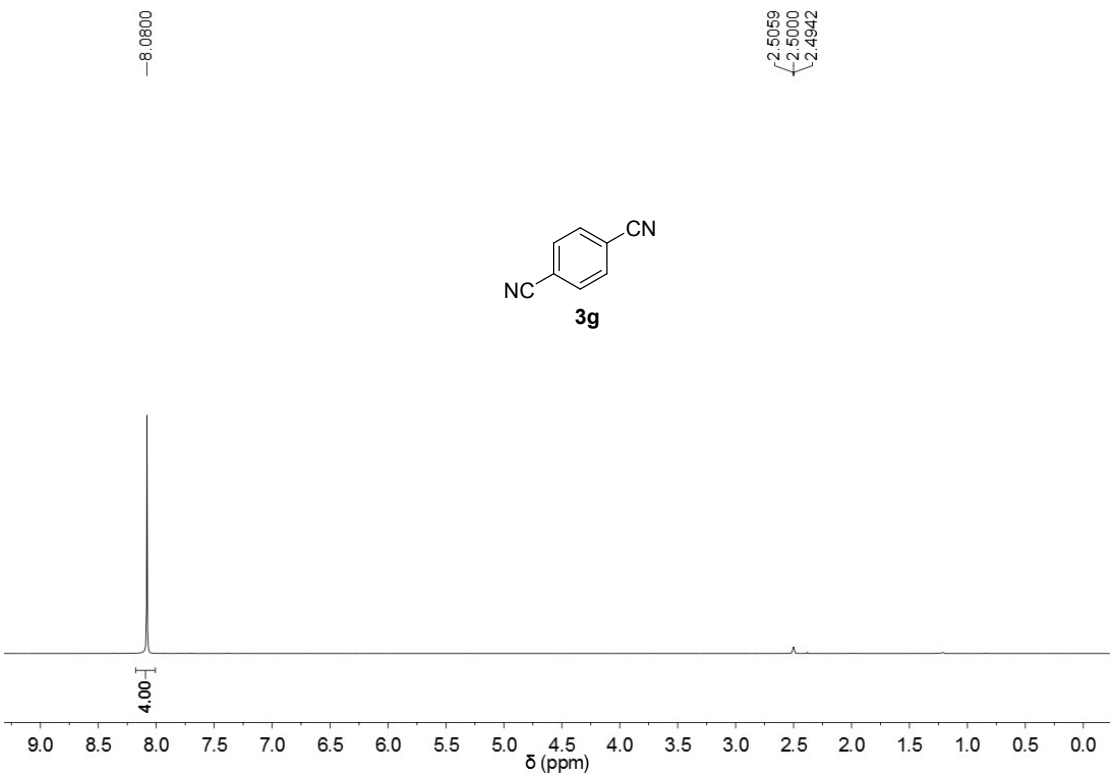
δ (ppm)
2.00
2.01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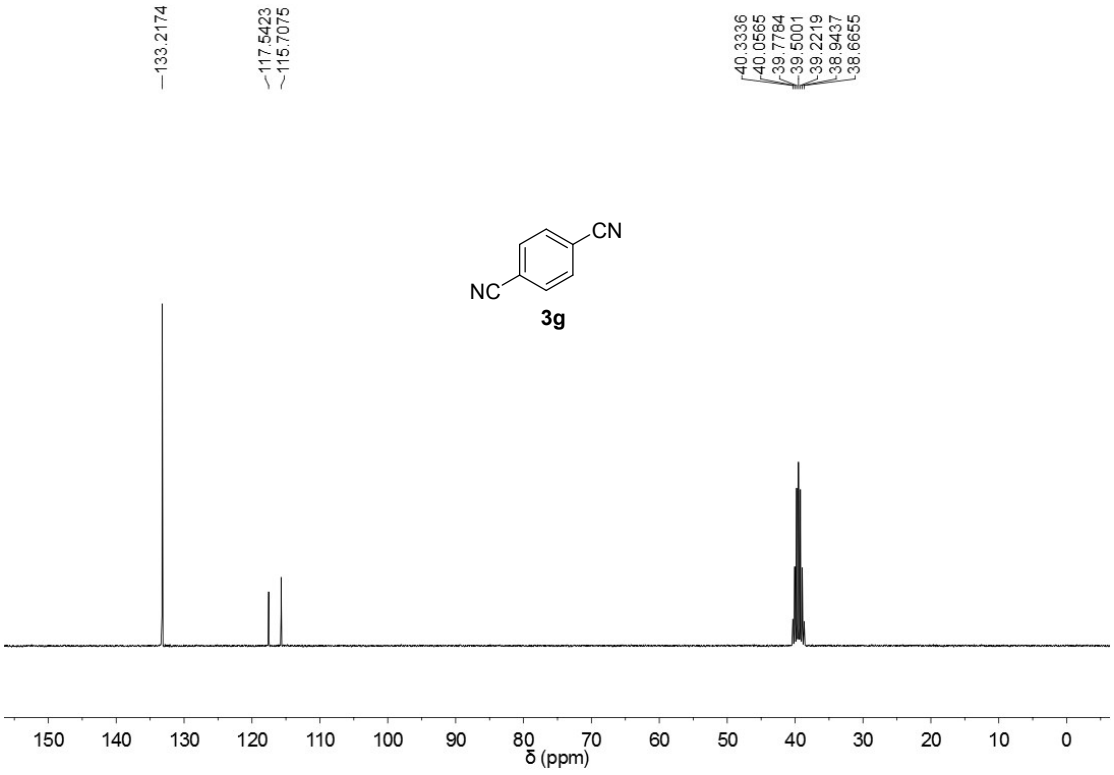
2.5059
2.5000
2.4942
CN
NC
3g
4.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)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117.5423
115.7075
40.3336
40.0565
39.7784
39.5001
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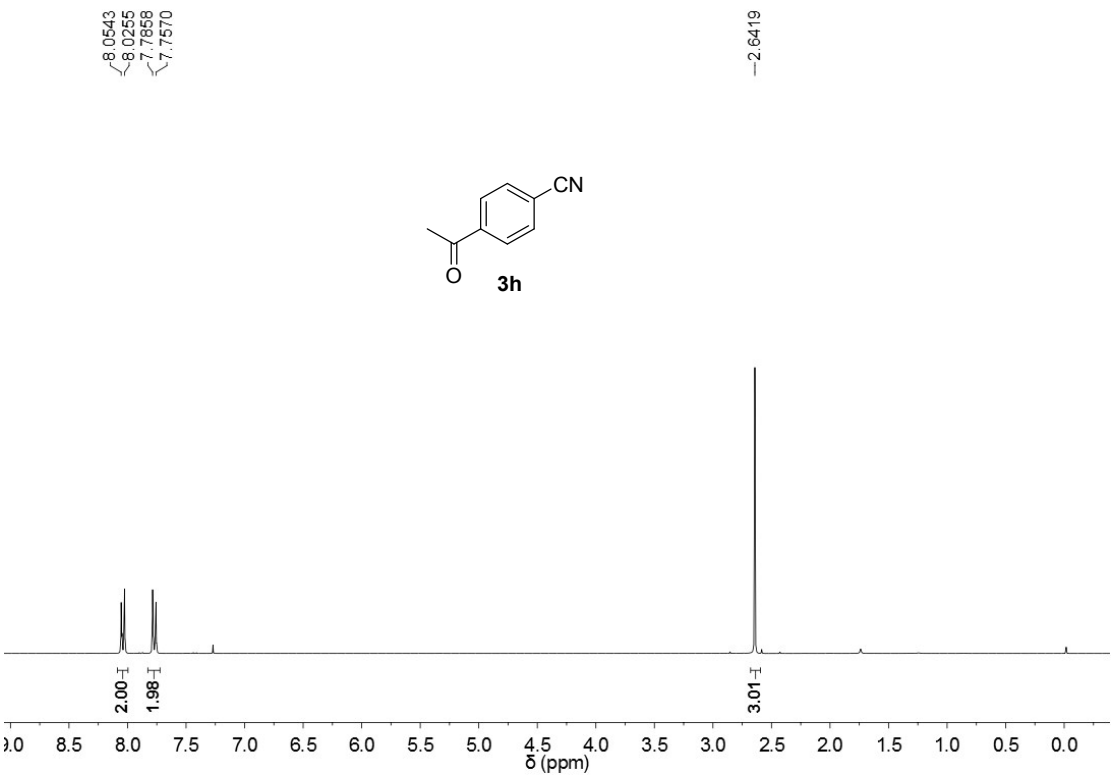
CN
NC
3g
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)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CN
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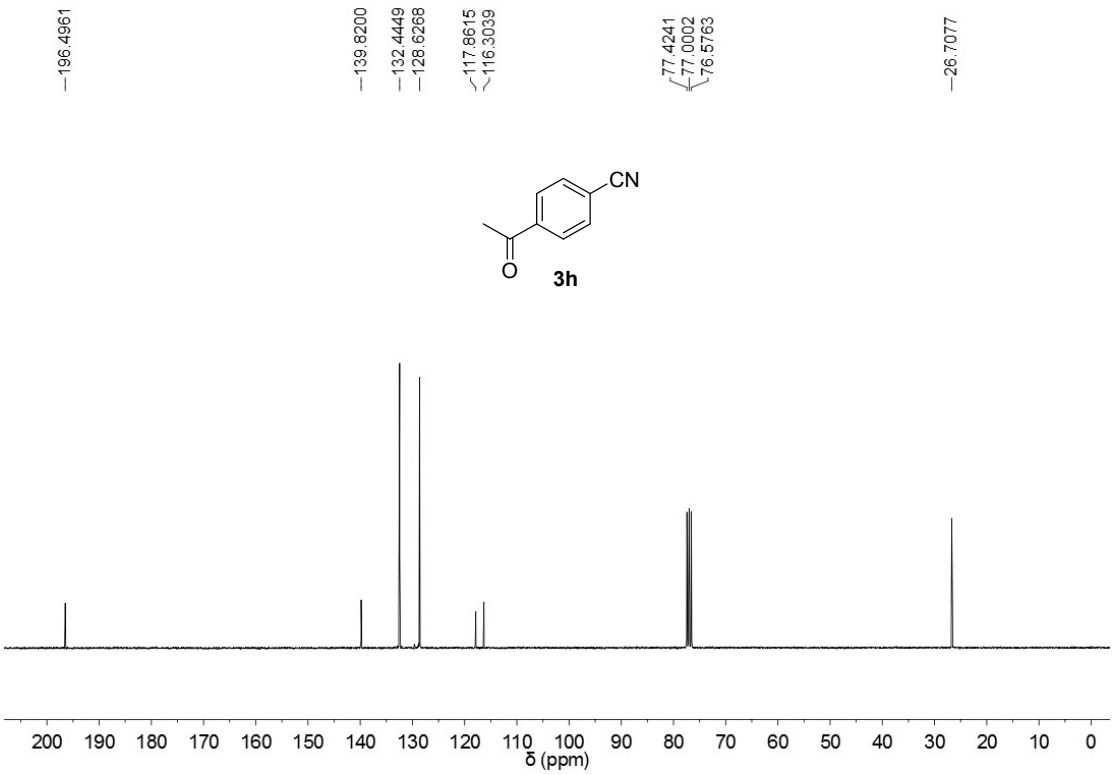
3.01
δ (ppm)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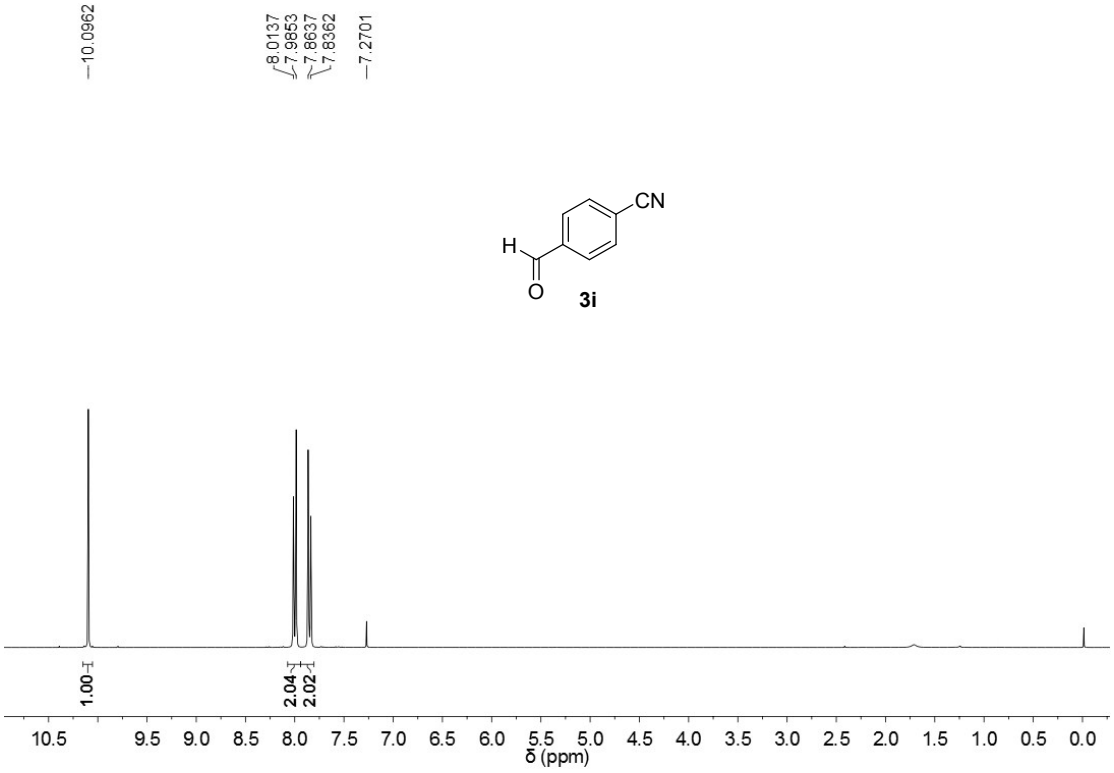
O
3h
δ (ppm)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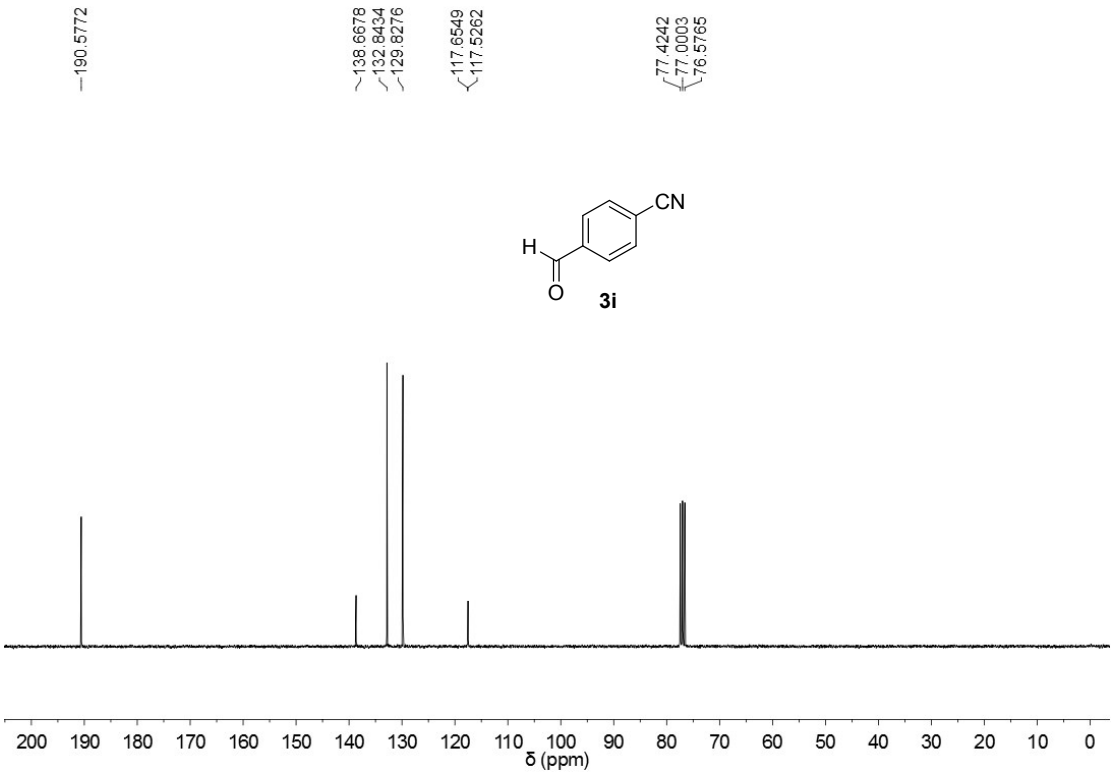
CN
H
O
3i
1.00
2.04
2.02
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)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129.8276
117.6549
117.5262
77.4242
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CN
H
O
3i
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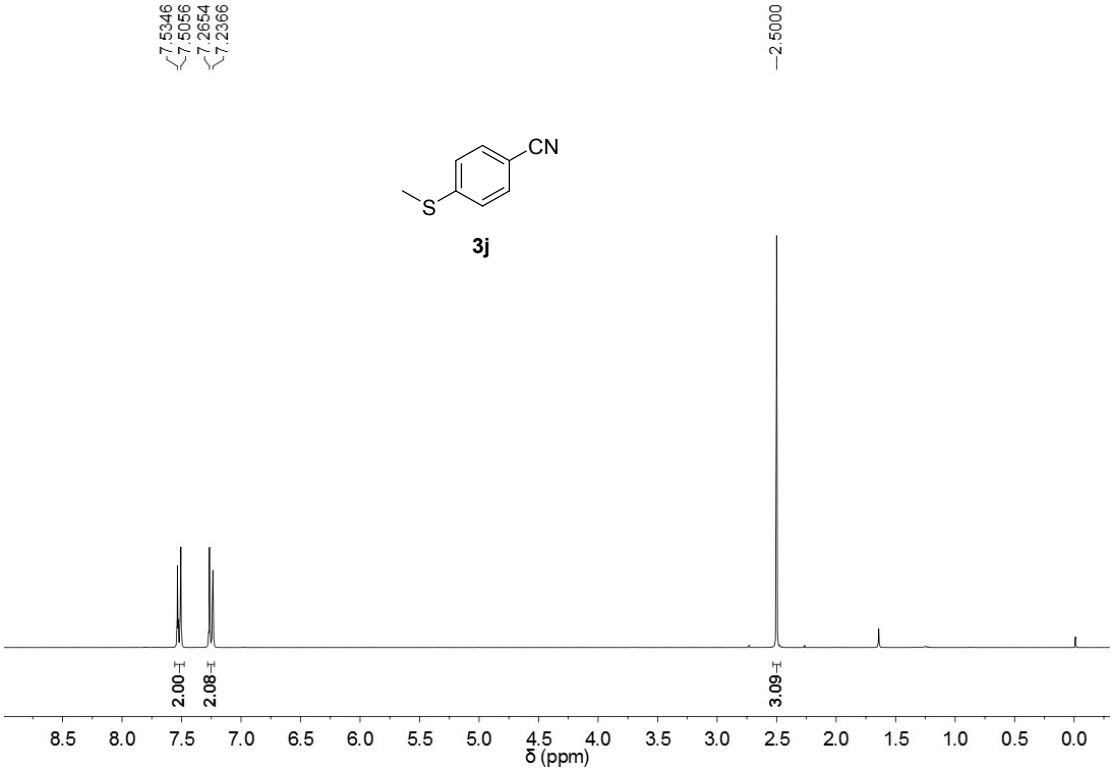
δ (ppm)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3j
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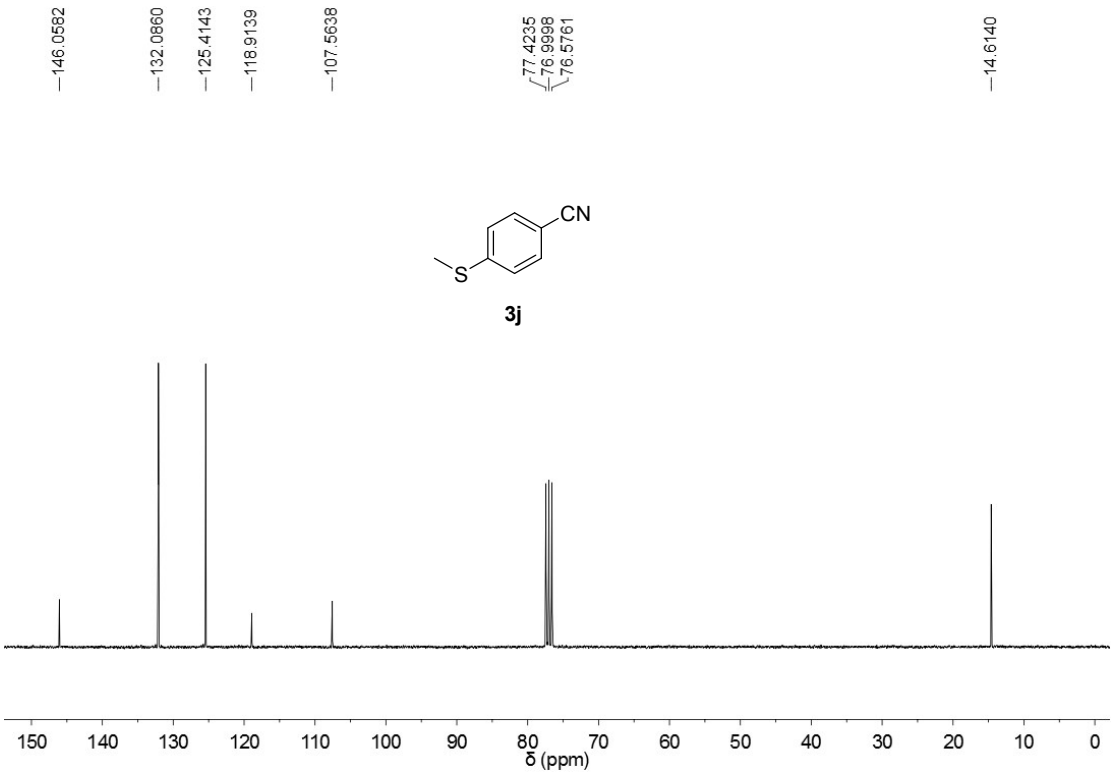
2.08
3.09
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)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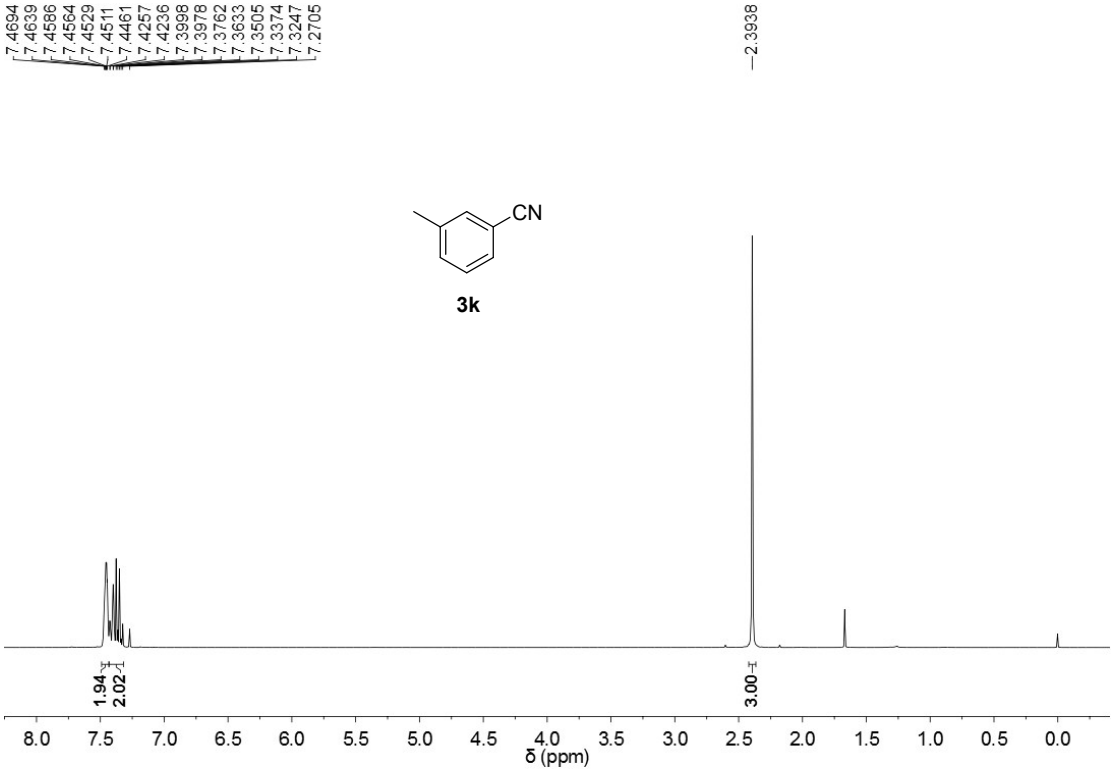
δ (ppm)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7.3505
7.3374
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7.2705
2.3938
CN
3k
1.94
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3.00
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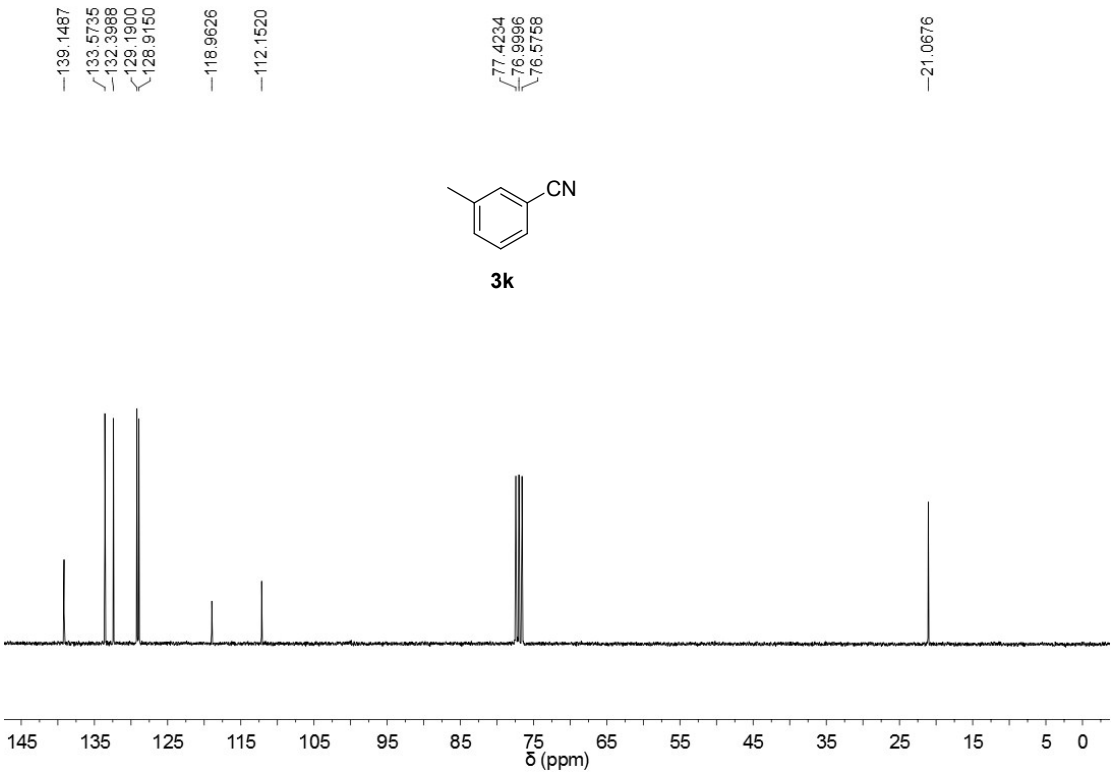
δ (ppm)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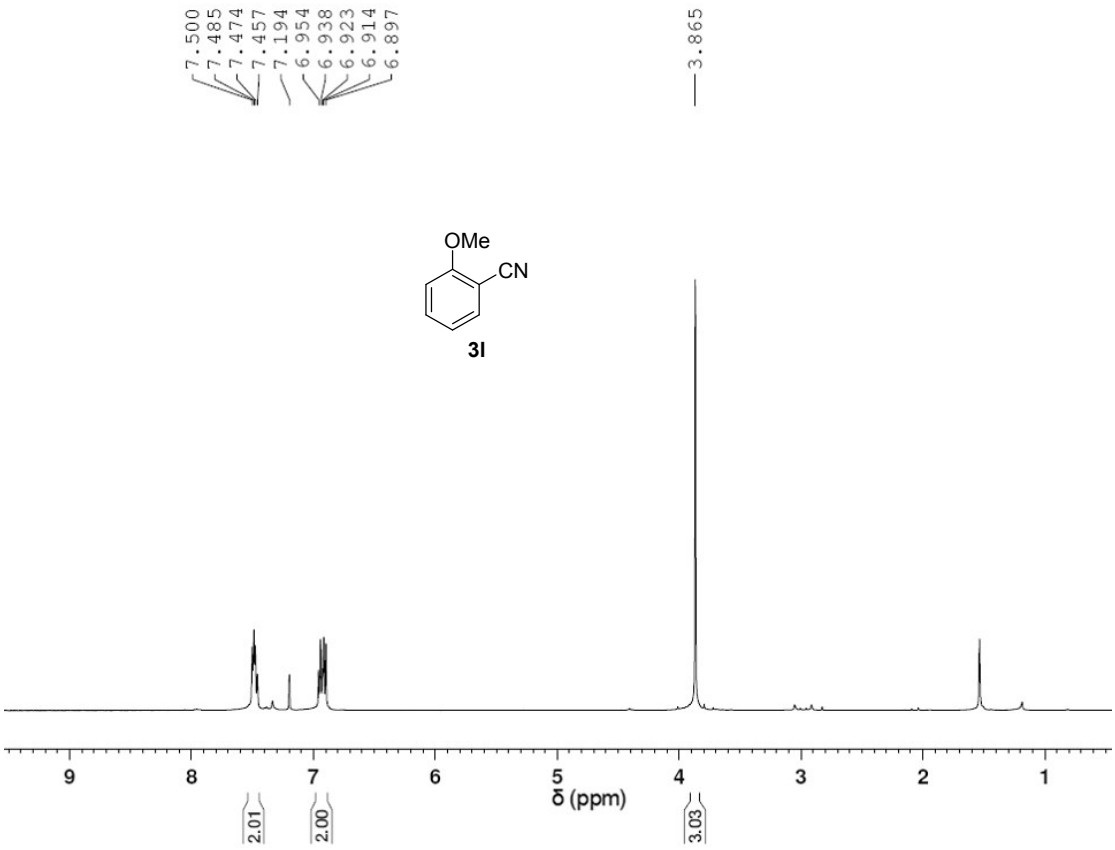
145 135 125 115 105 95 85 75 65 55 45 35 25 15 5 0
δ (ppm)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OMe
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9
8
7
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δ (ppm)
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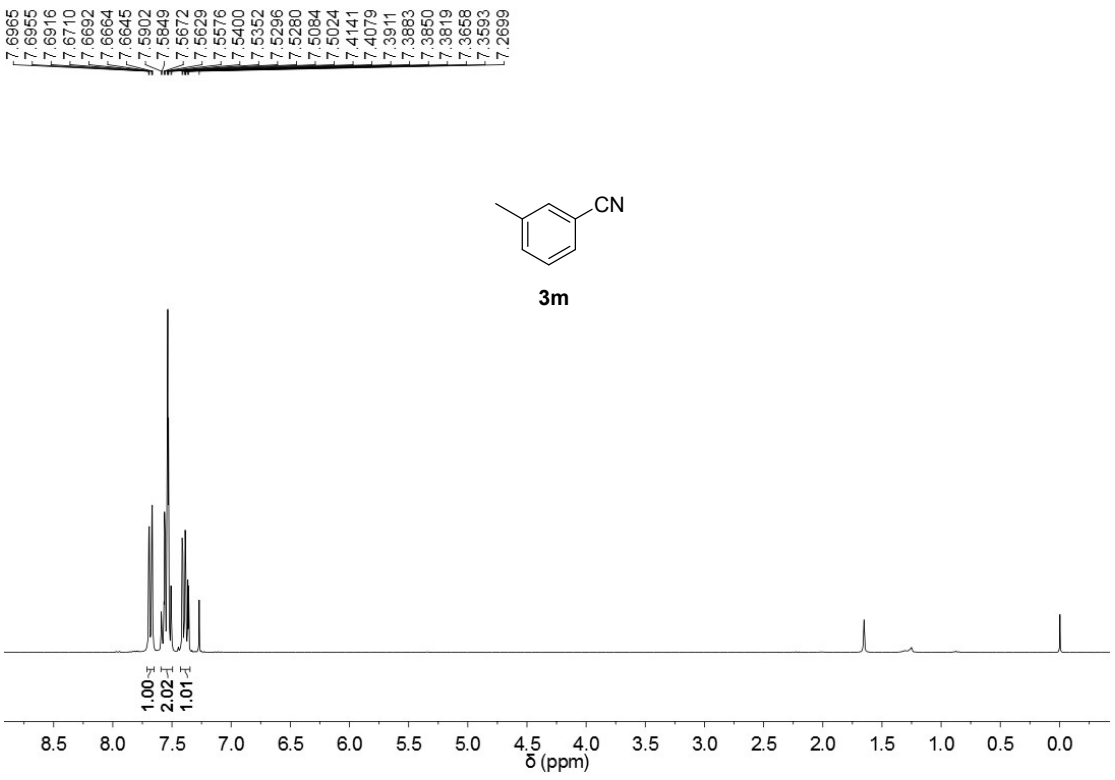
2.00
3.03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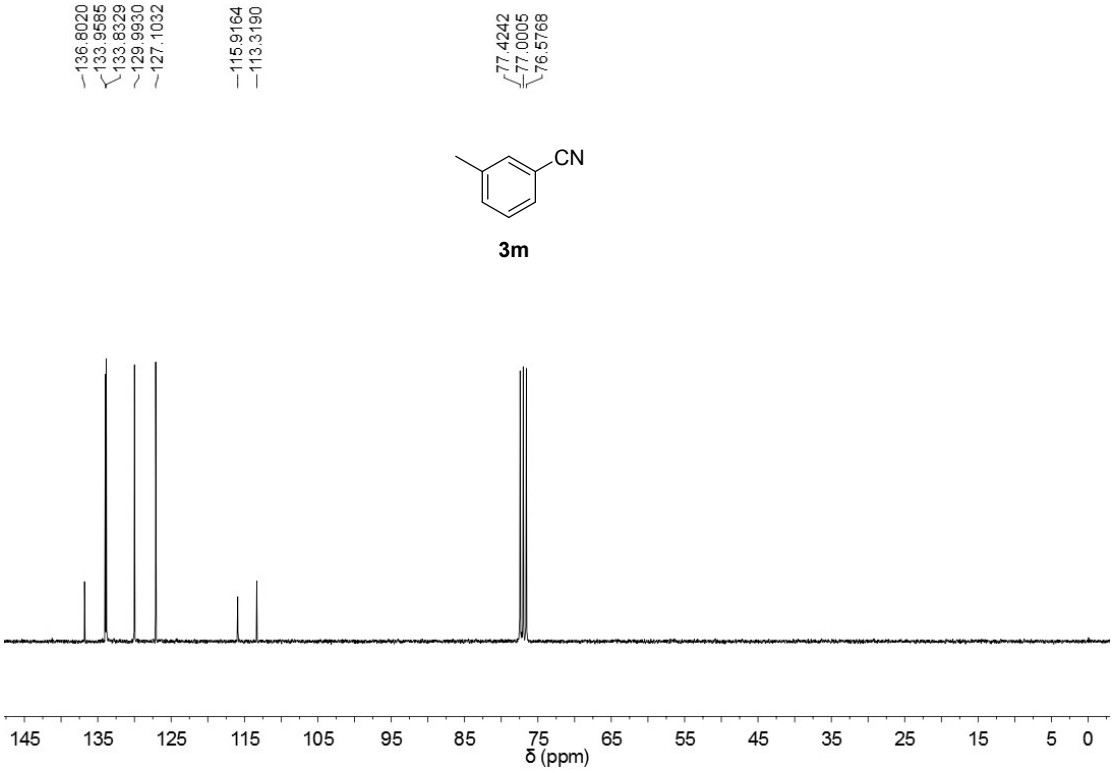
δ (ppm)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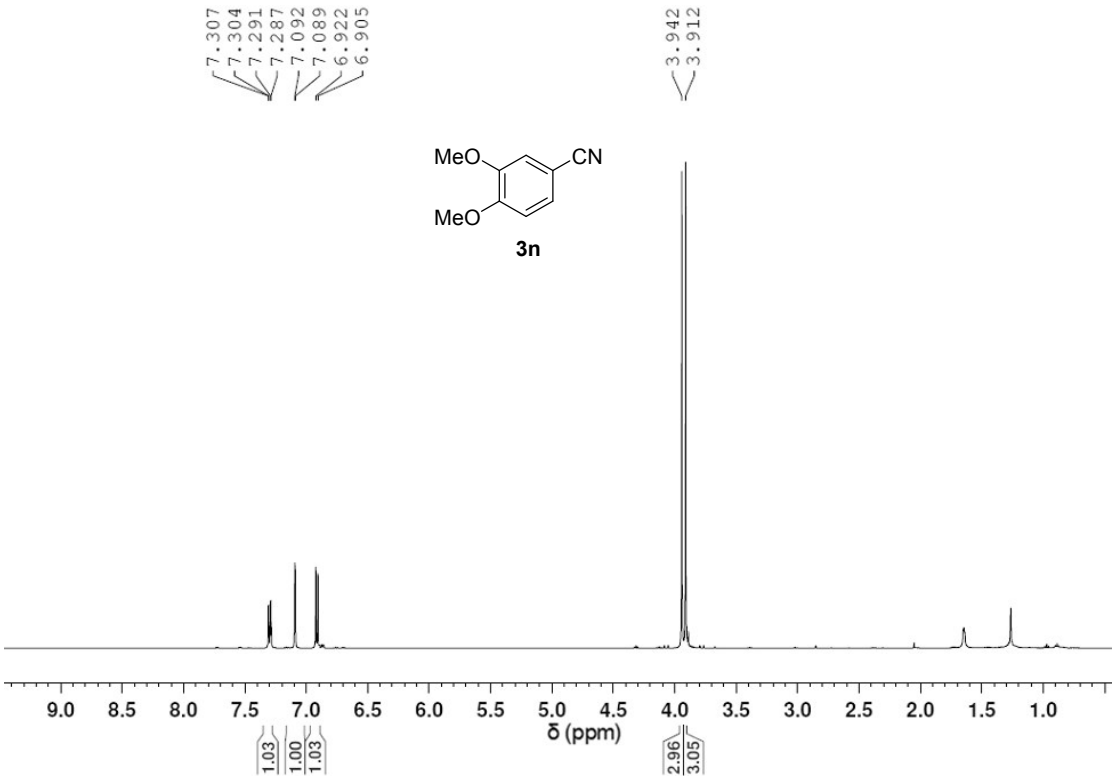
δ (ppm)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7.291
7.287
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7.089
6.922
6.905
3.942
3.912
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CN
MeO
3n
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
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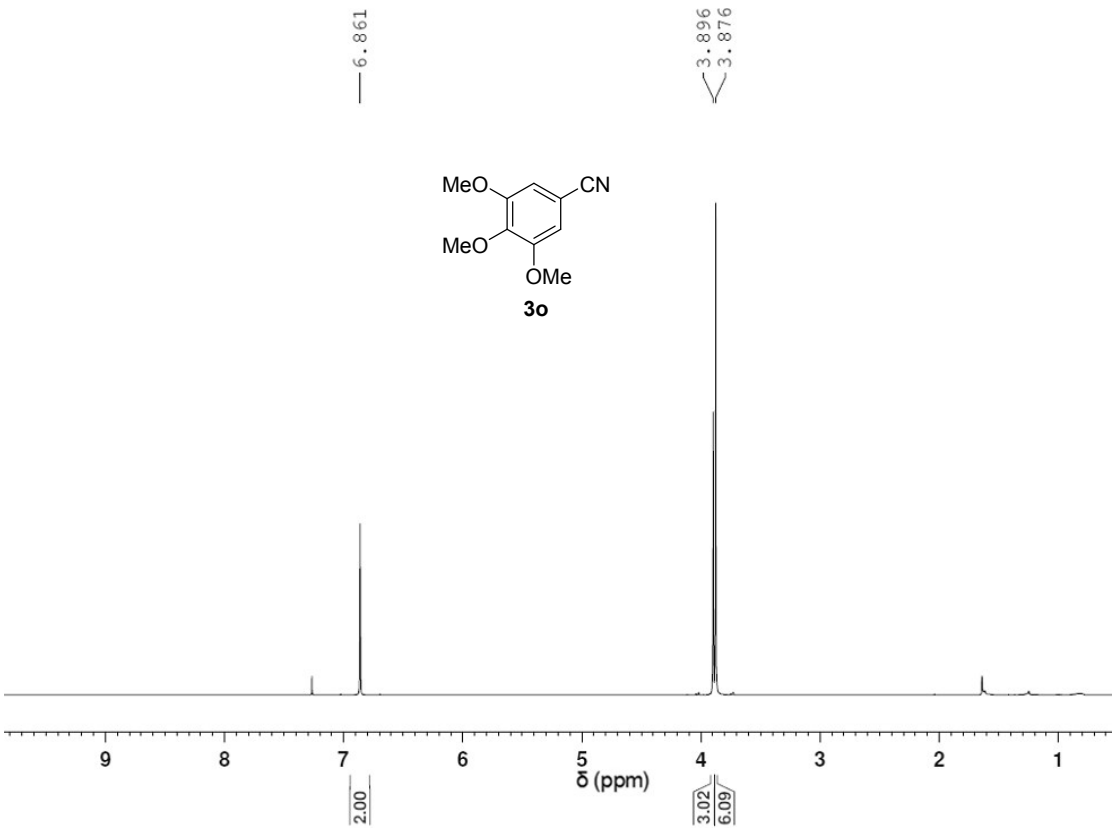
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δ (ppm)
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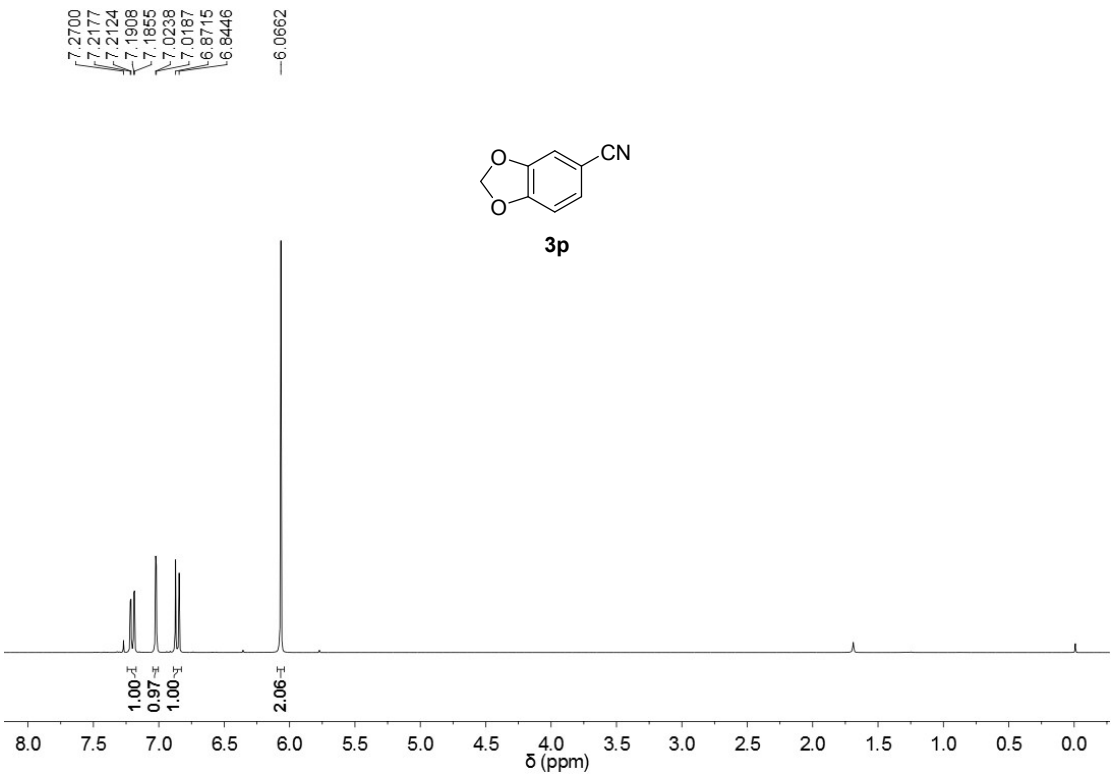
6.09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O
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1.00
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7.0
6.5
6.0
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5.0
4.5
4.0
3.5
3.0
2.5
2.0
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1.0
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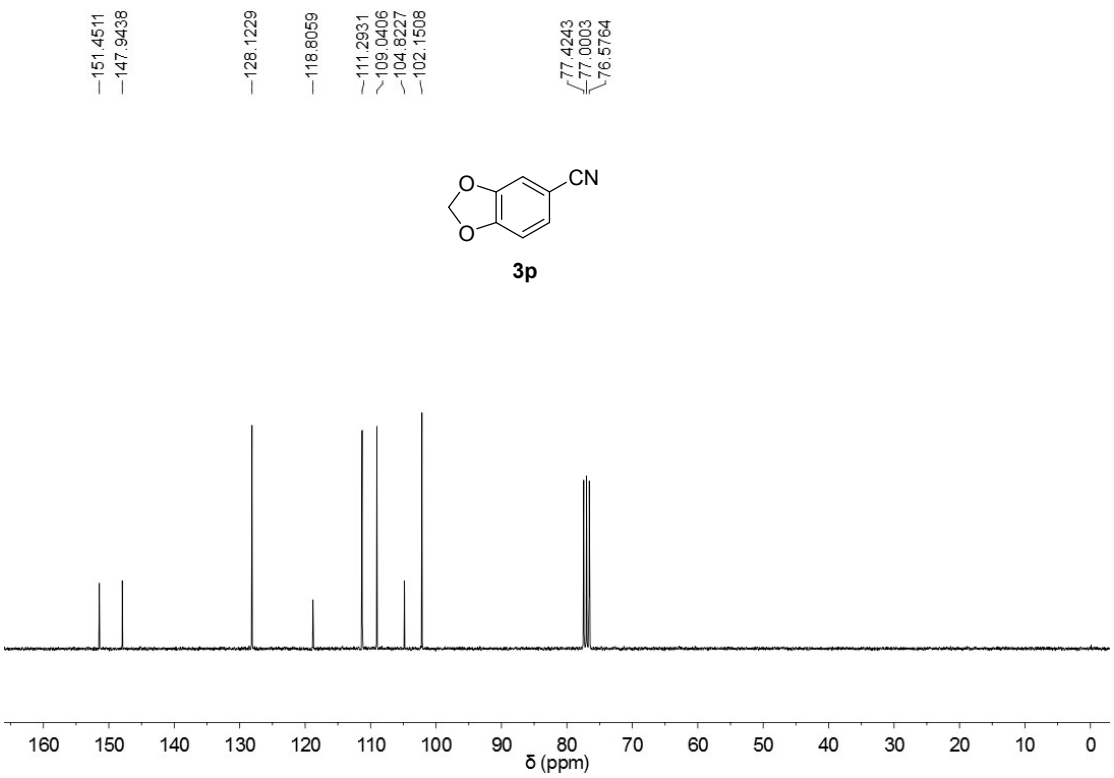
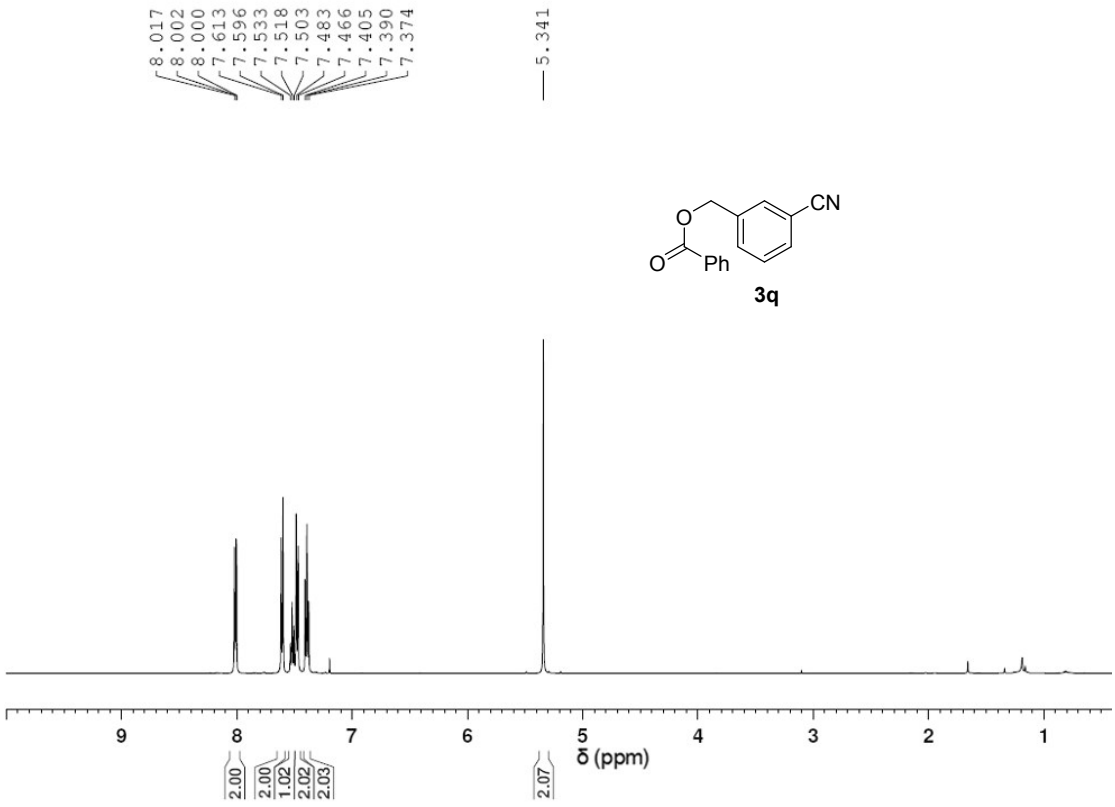
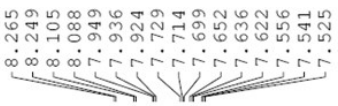
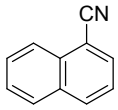
0.0
δ (ppm)

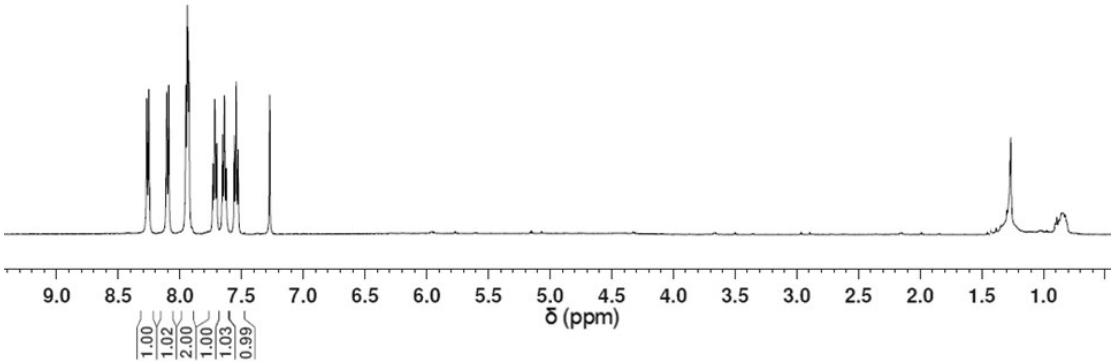

151.4511
147.9438
128.1229
118.8059
111.2931
109.0406
104.8227
102.1508
77.4243
77.0003
76.5764
O
O
CN
3p
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ (ppm)

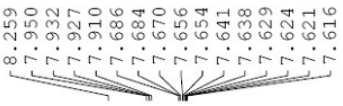

8.017
8.002
8.000
7.613
7.596
7.533
7.518
7.503
7.483
7.466
7.405
7.390
7.374
5.341
O
O
Ph
CN
3q
9
8
7
6
5
4
3
2
1
δ (ppm)
2.00
2.00
1.02
2.02
2.03
2.07


8.265
8.249
8.105
8.088
7.949
7.936
7.924
7.729
7.714
7.699
7.652
7.636
7.622
7.556
7.541
7.525


CN

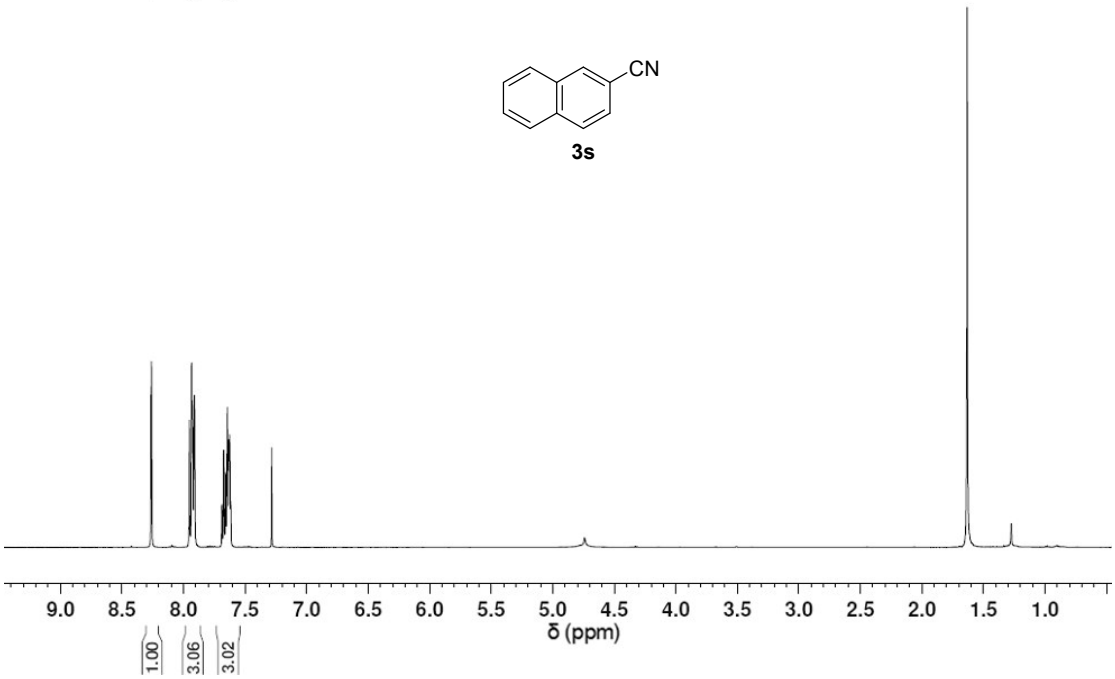
3r

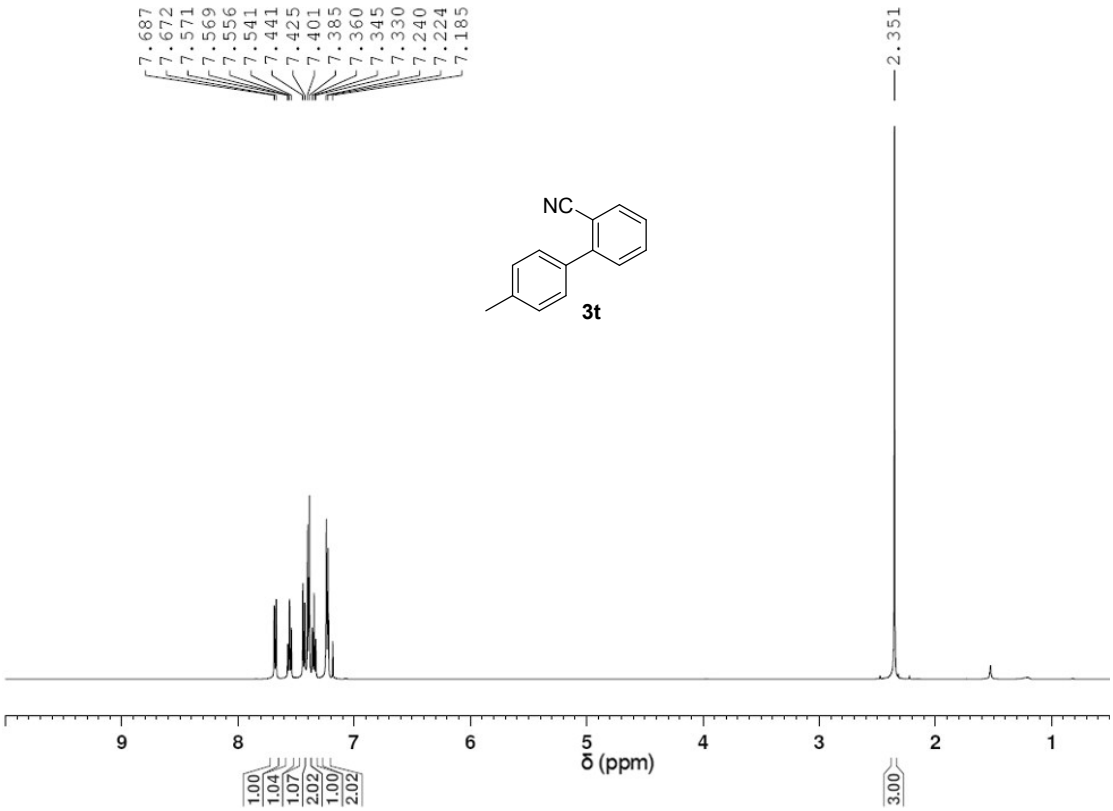

9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
δ (ppm)
1.00
1.02
2.00
1.00
1.03
0.99

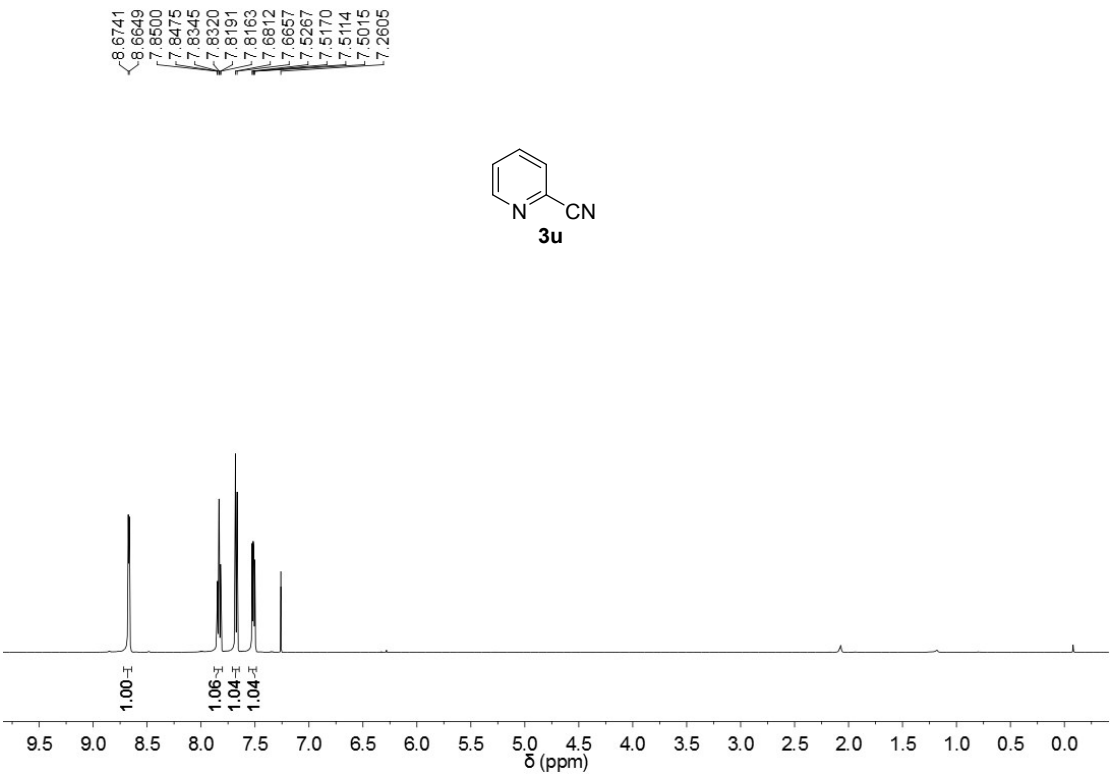

8.259
7.950
7.932
7.927
7.910
7.686
7.684
7.670
7.656
7.654
7.641
7.638
7.629
7.624
7.621
7.616

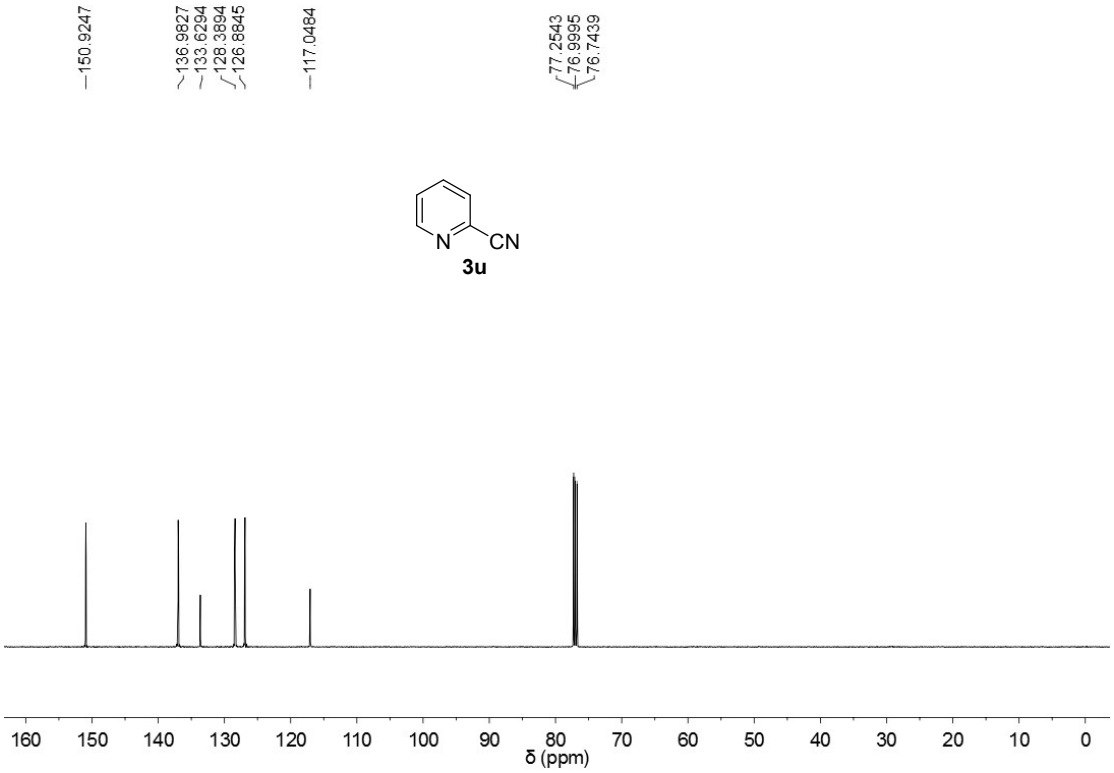
CN

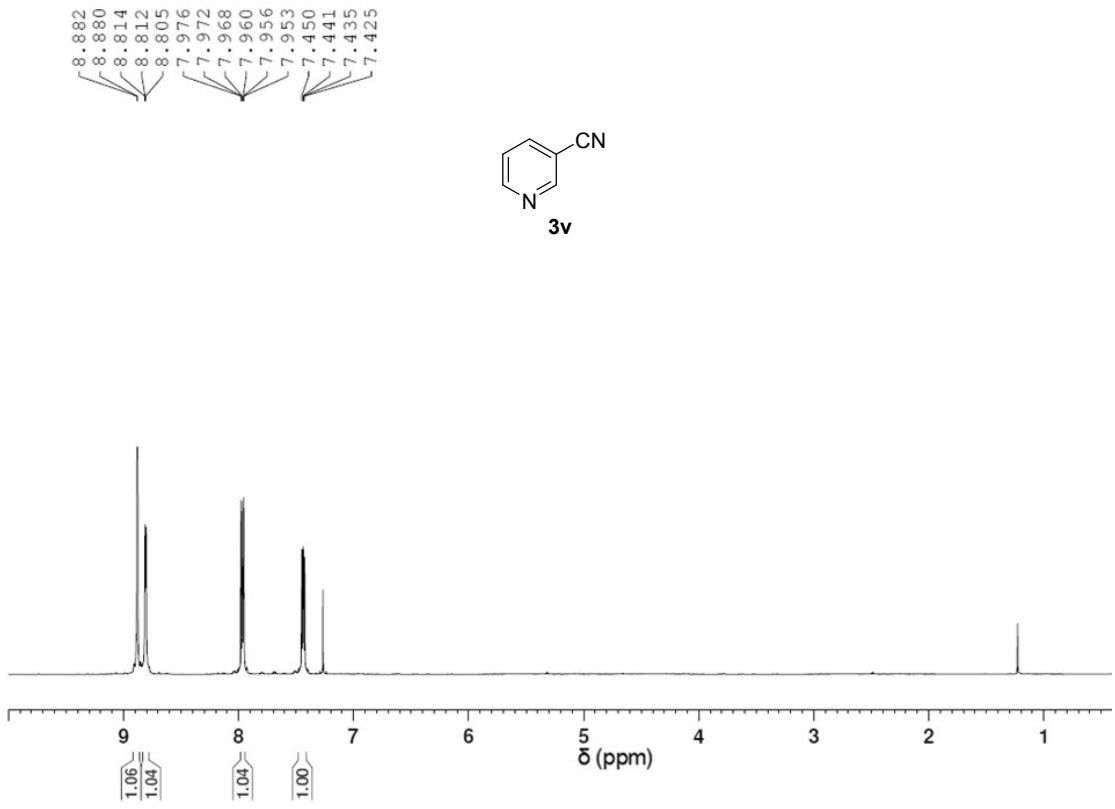
3s

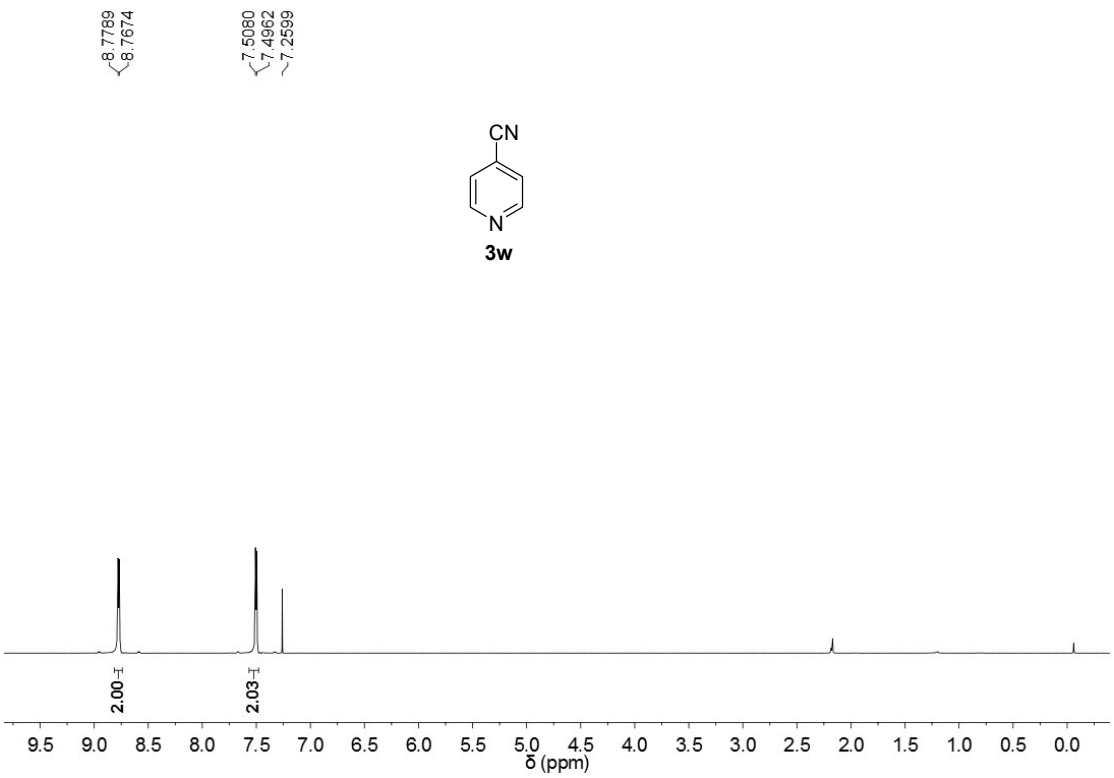

9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
δ (ppm)
1.00
3.06
3.02

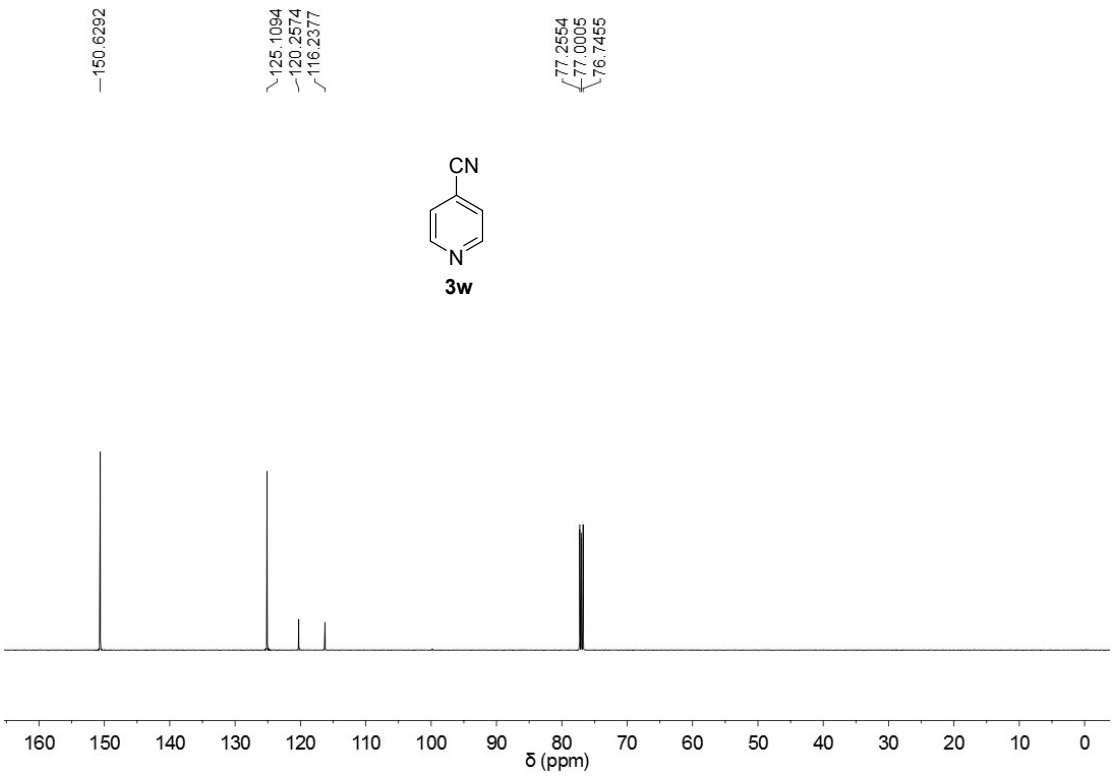

7.687
7.672
7.571
7.569
7.556
7.541
7.441
7.425
7.401
7.385
7.360
7.345
7.330
7.240
7.224
7.185
2.351
NC
3t
9
8
7
6
5
4
3
2
1
δ (ppm)
1.00
1.04
1.07
2.02
1.00
2.02
3.00

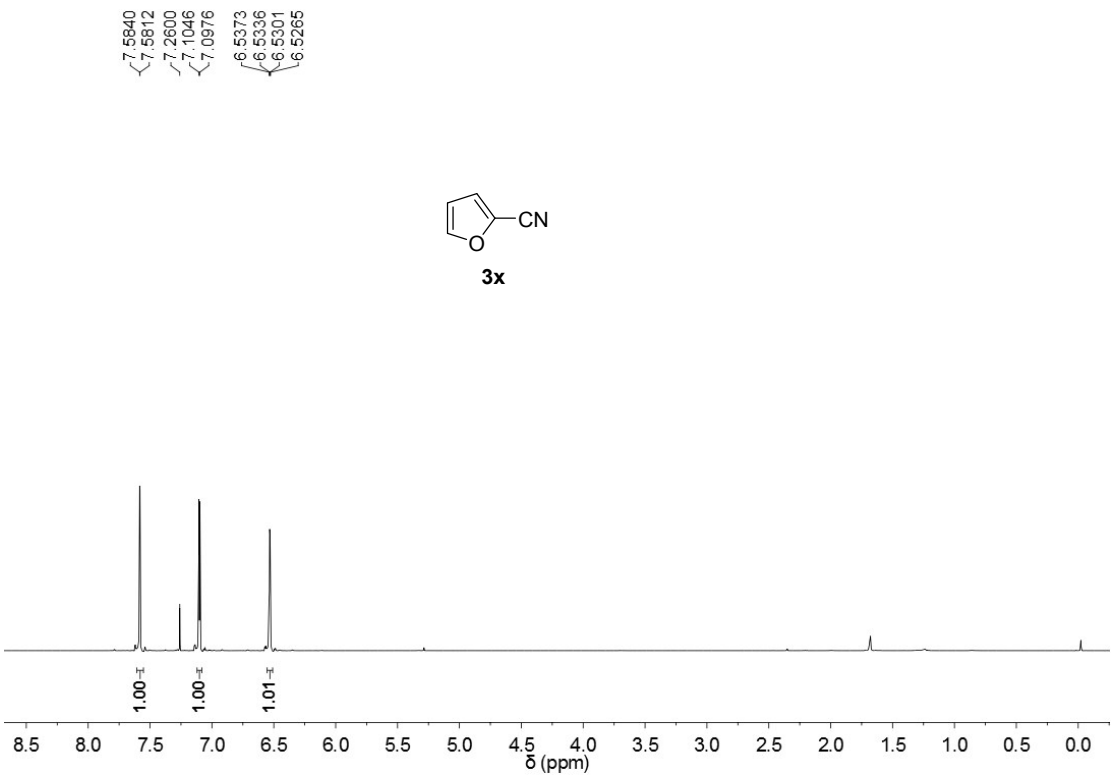

8.6741
8.6649
7.8500
7.8475
7.8345
7.8320
7.8191
7.8163
7.6812
7.6657
7.5267
7.5170
7.5114
7.5015
7.2605
N
CN
3u
1.00
1.06
1.04
1.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ (ppm)

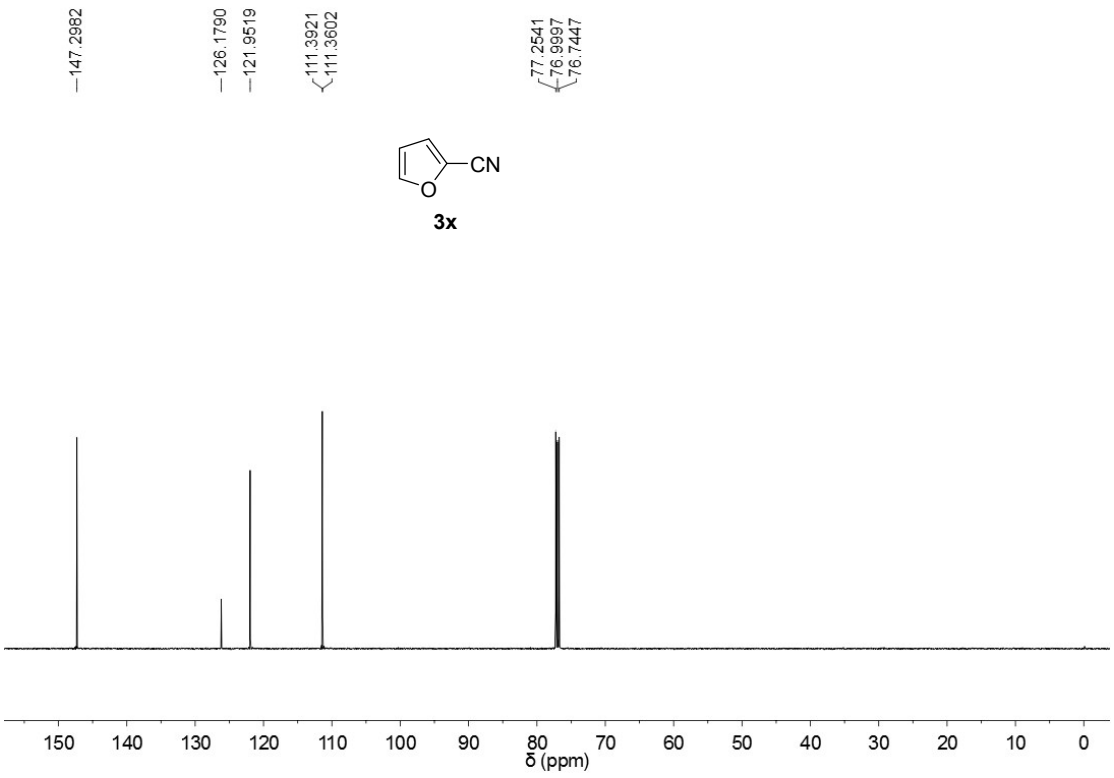

150.9247
136.9827
133.6294
128.3894
126.8845
117.0484
77.2543
76.9995
76.7439
N
CN
3u
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ (ppm)

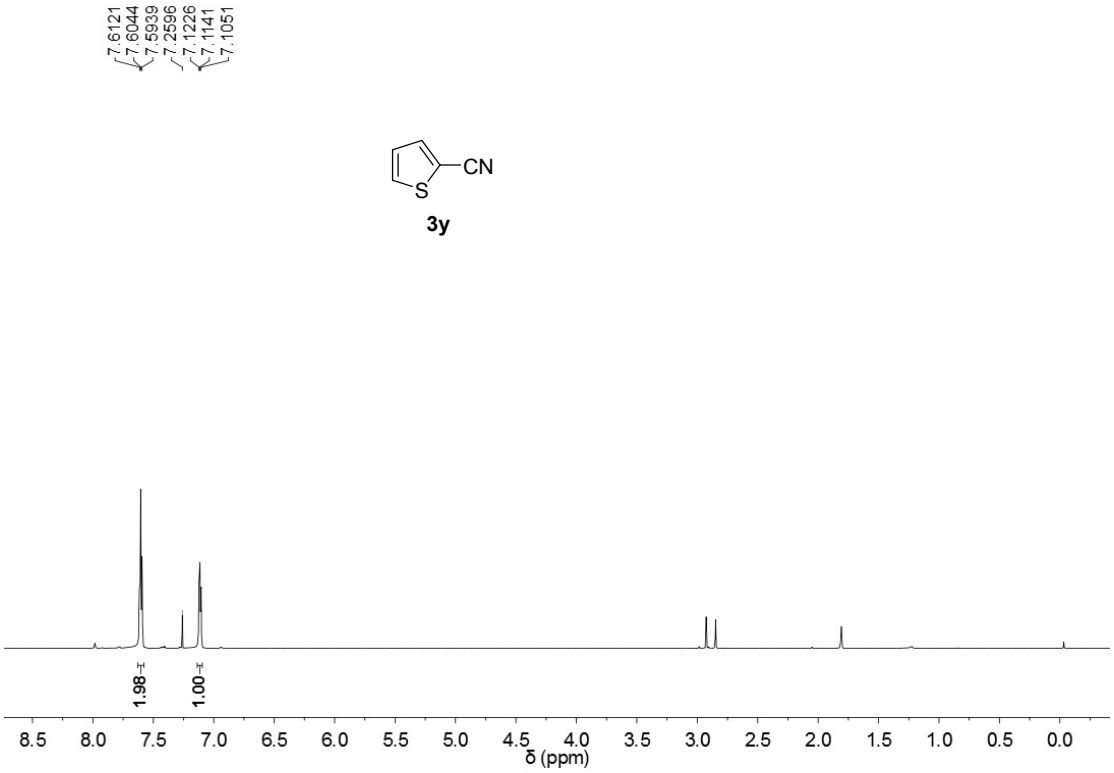

8.882
8.880
8.814
8.812
8.805
7.976
7.972
7.968
7.960
7.956
7.953
7.450
7.441
7.435
7.425
CN
N
3v
9
8
7
6
5
4
3
2
1
δ (ppm)
1.06
1.04
1.04
1.00

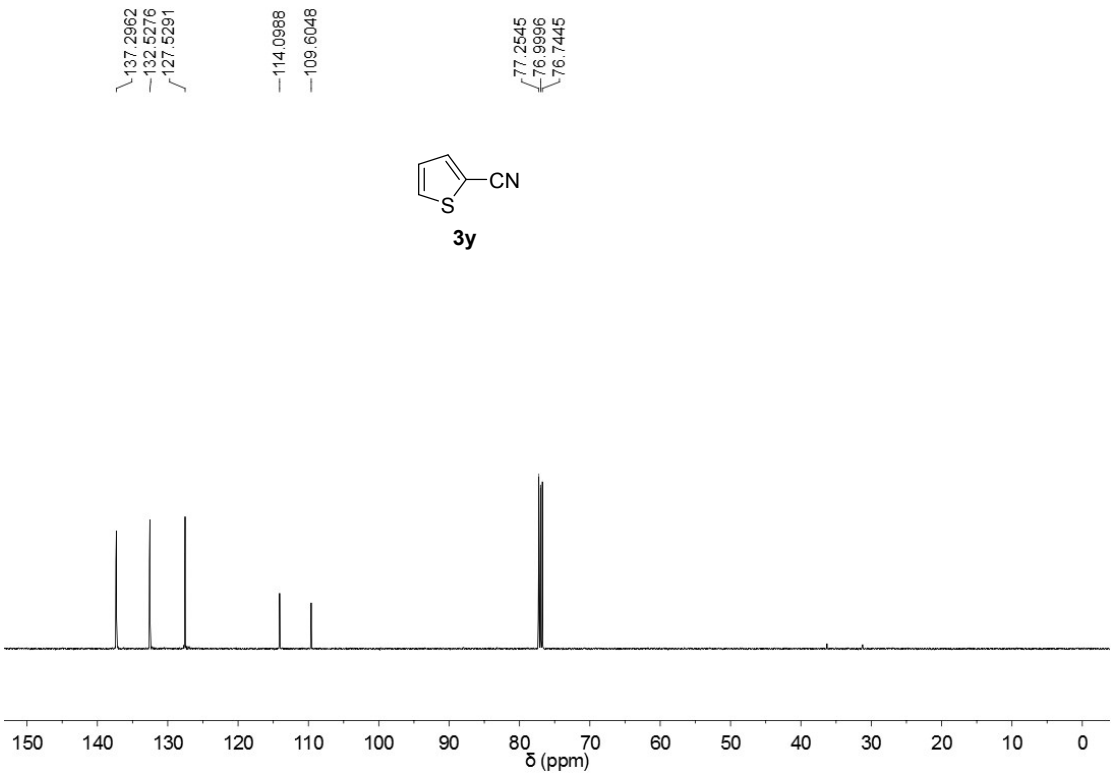

8.7789
8.7674
7.5080
7.4962
7.2599
CN
N
3w
2.00
2.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)


150.6292
125.1094
120.2574
116.2377
77.2554
77.0005
76.7455
CN
N
3w
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)

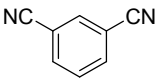

7.5840
7.5812
7.2600
7.1046
7.0976
6.5373
6.5336
6.5301
6.5265
CN
O
3x
1.00
1.00
1.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)


147.2982
126.1790
121.9519
111.3921
111.3602
77.2541
76.9997
76.7447
CN
O
3x
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)

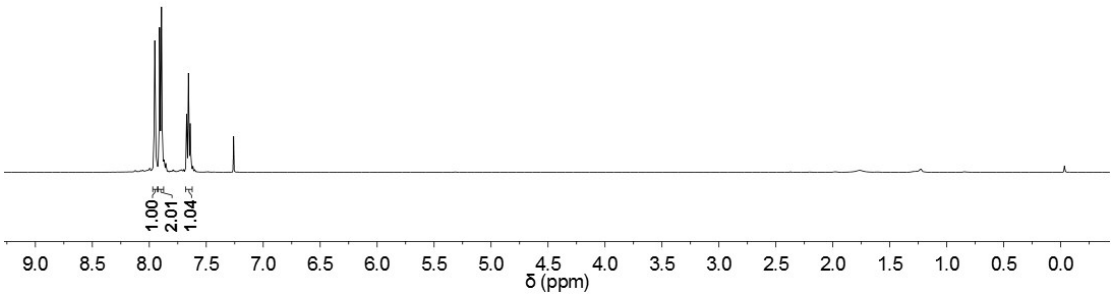

7.6121
7.6044
7.5939
7.2596
7.1226
7.1141
7.1051
CN
S
3y
1.98
1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)


137.2962
132.5276
127.5291
114.0988
109.6048
77.2545
76.9996
76.7445
CN
S
3y
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)

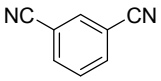

7.9522
7.9095
7.8927
7.8710
7.8548
7.6718
7.6561
7.6403
7.6173
7.2598


NC
CN

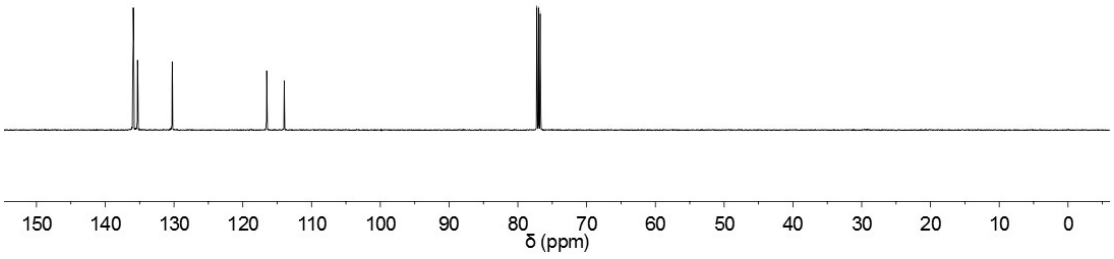
3z


1.00
2.01
1.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)

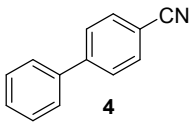

135.9215
135.3097
130.2557
116.5195
113.9759
77.2540
76.9996
76.7448


NC
CN

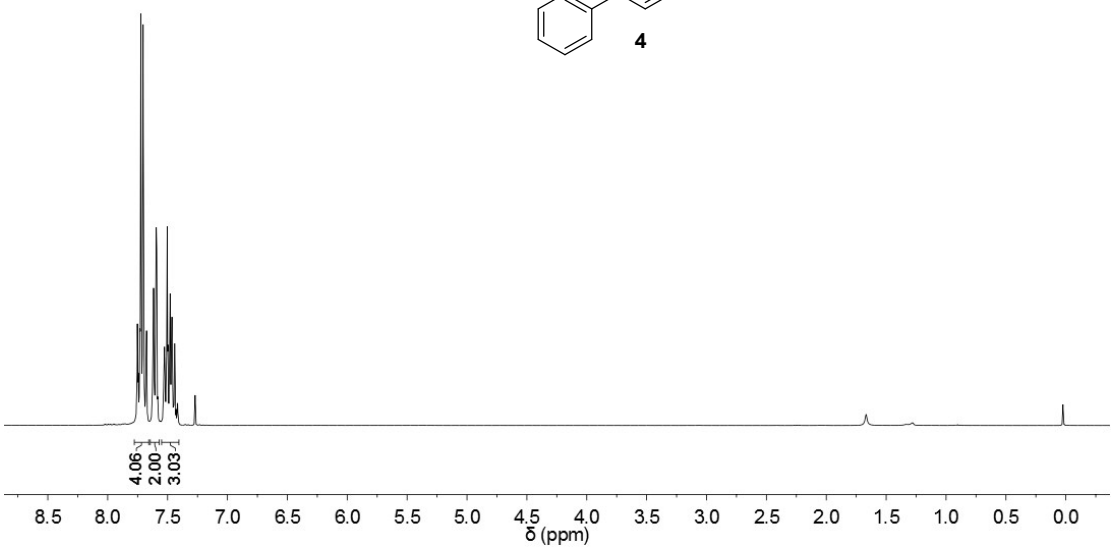
3z


150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)

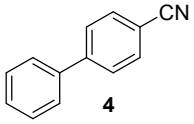

7.7522
7.7450
7.7309
7.7235
7.7045
7.6968
7.6826
7.6756
7.6225
7.6169
7.6100
7.5998
7.5946
7.5904
7.5823
7.5314
7.5255
7.5189
7.5029
7.4975
7.4827
7.4782
7.4687
7.4634
7.4583
7.4496
7.4404
7.4288
7.4207
7.4162
7.4117
7.2701


CN

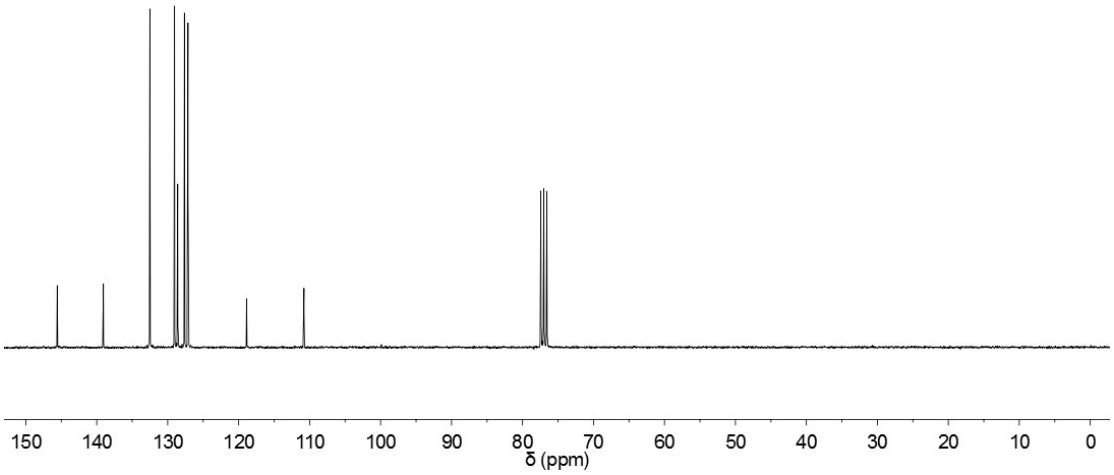
4


4.06
2.00
3.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)

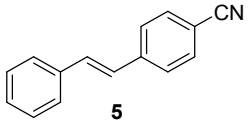

145.5632
139.0616
132.5112
129.0376
128.5904
127.6411
127.1433
118.8813
110.7963
77.4237
76.9999
76.5762


CN

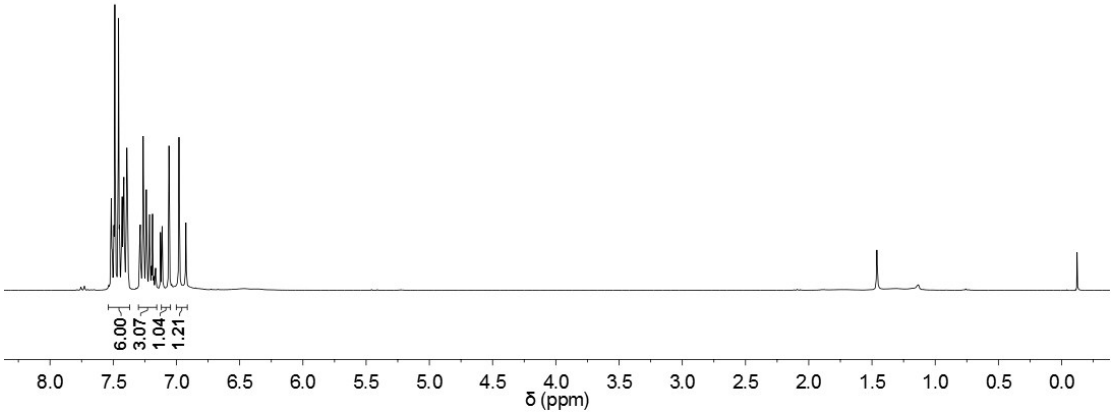
4


150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)

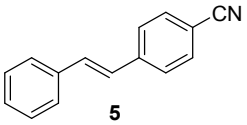

7.5157
7.5094
7.4942
7.4872
7.4577
7.4510
7.4295
7.4211
7.4156
7.3921
7.2910
7.2862
7.2801
7.2630
7.2576
7.2380
7.2174
7.2127
7.2081
7.1974
7.1891
7.1264
7.1134
7.0590
6.9798
6.9253


CN

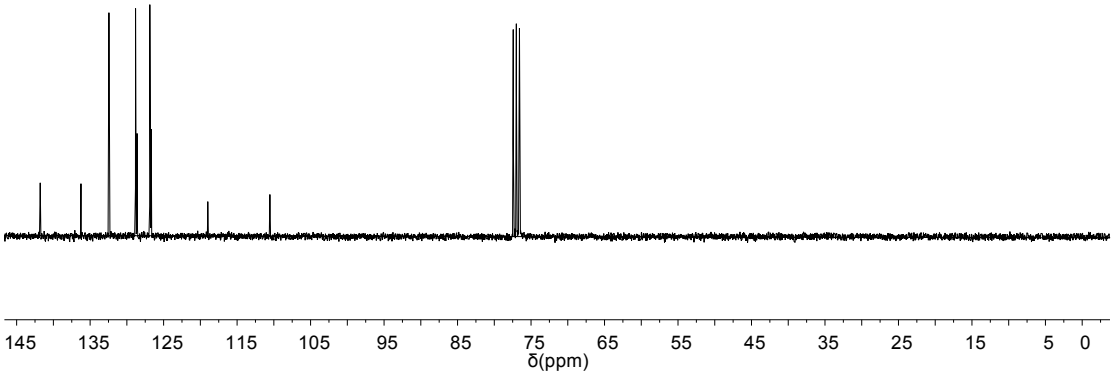
5

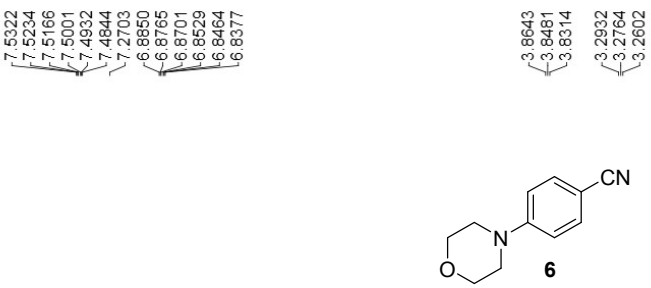

6.00
3.07
1.04
1.21
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ (ppm)

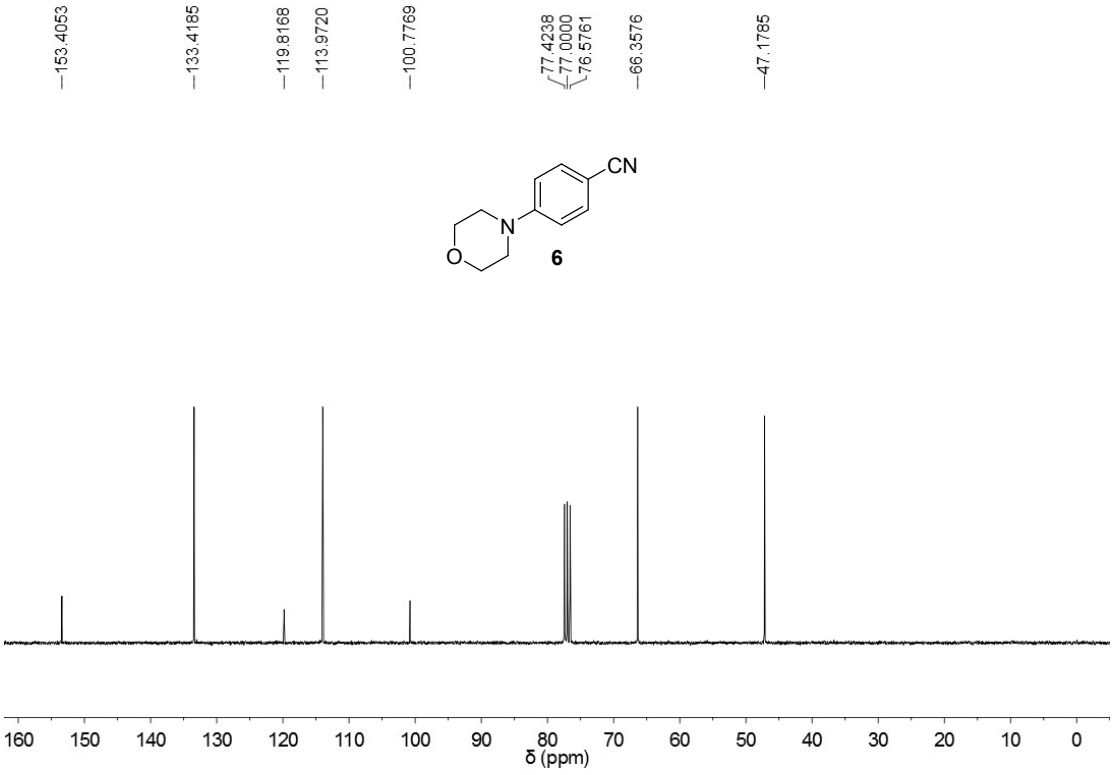

141.7913
132.4401
132.3666
128.8172
128.6031
126.8750
126.8202
110.5349
77.4232
76.9998
76.5763

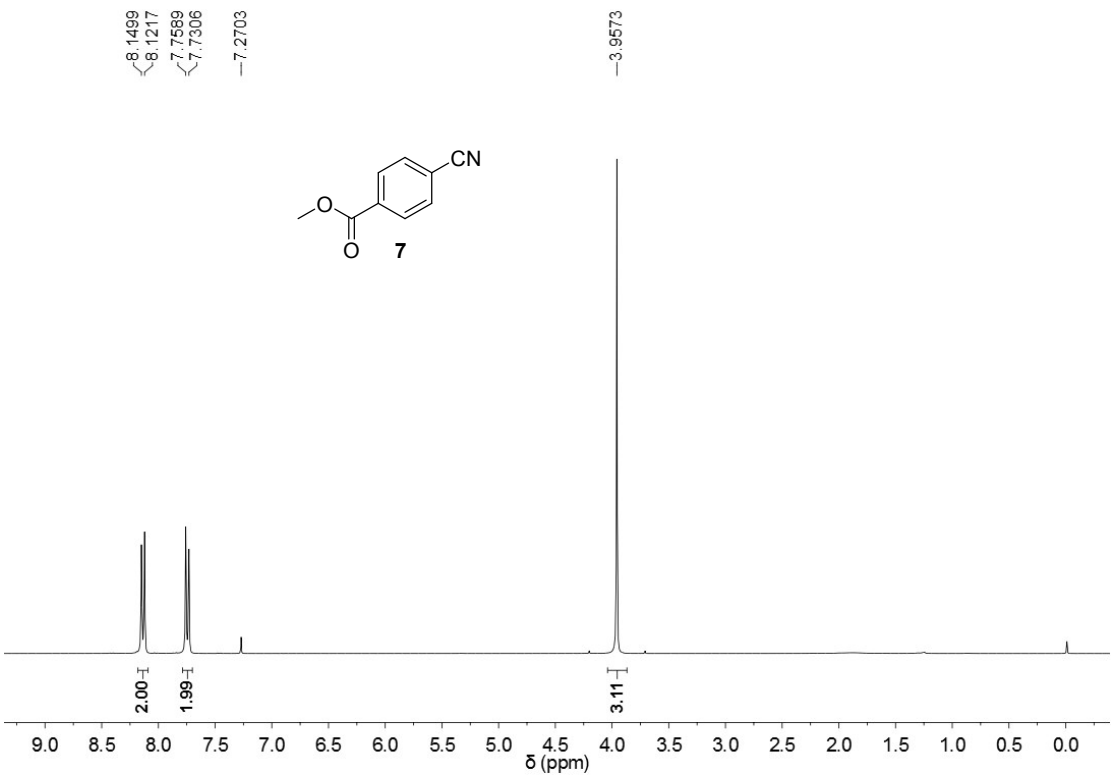

CN

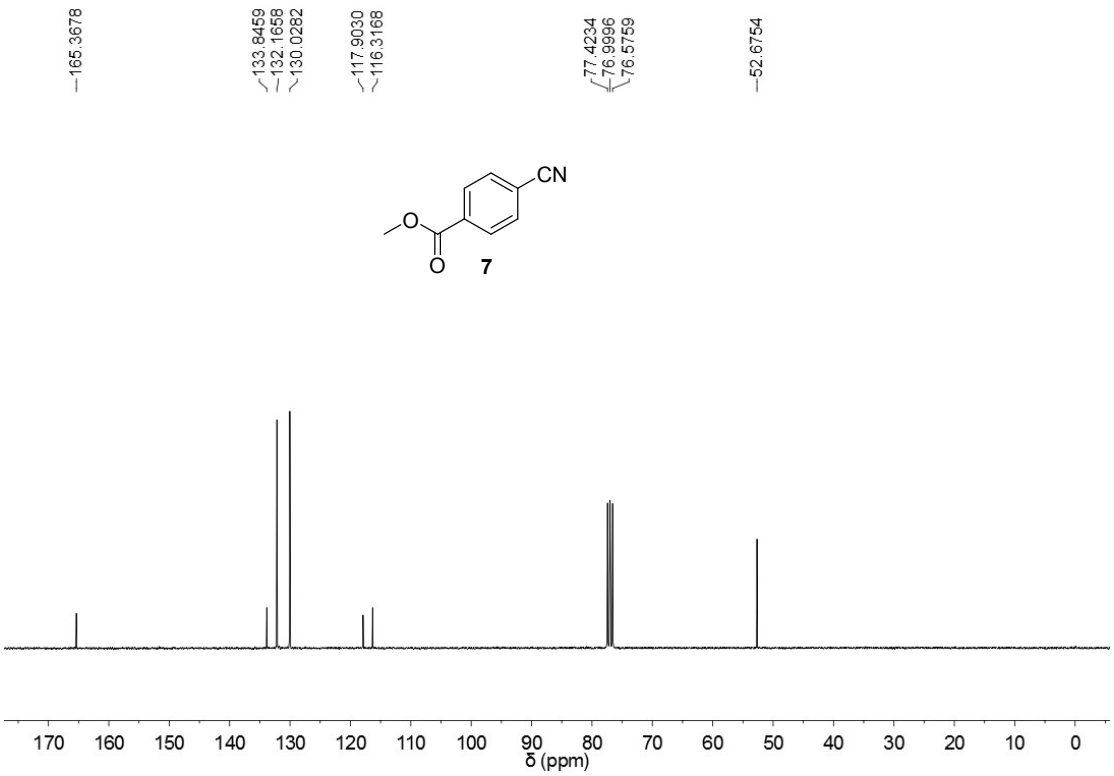
5


145
135
125
115
105
95
85
75
65
55
45
35
25
15
5
0
δ(ppm)


7.5322
7.5234
7.5166
7.5001
7.4932
7.4844
7.2703
6.8850
6.8765
6.8701
6.8529
6.8464
6.8377
3.8643
3.8481
3.8314
3.2932
3.2764
3.2602
CN
N
O
6
2.00
2.04
4.06
4.06
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ (ppm)


153.4053
133.4185
119.8168
113.9720
100.7769
77.4238
77.0000
76.5761
66.3576
47.1785
CN
N
O
6
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ (ppm)


8.1499
8.1217
7.7589
7.7306
7.2703
3.9573
CN
O
O
7
2.00
1.99
3.11
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
δ (ppm)


165.3678
133.8459
132.1658
130.0282
117.9030
116.3168
77.4234
76.9996
76.5759
52.6754
CN
O
O
7
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)