Supporting Information

Versatile Ruthenium(II)-Catalyzed C–H Cyanations of Benzamides

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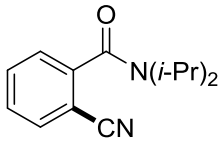
General Remarks

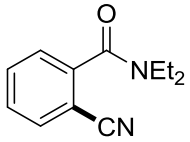
1,2-Dichloroethane (DCE), 1,4-dioxane and toluene were distilled over CaH_2. The following starting materials were synthesized according to previously described methods: **1a-x**[1], $[D]_5$-**1a**[1] and **2**[2]. Other chemicals were obtained from commercial sources and were used without further purification. Yields refer to isolated compounds, estimated to be > 95% pure as determined by ^{1}H-NMR and GC. TLC: Macherey-Nagel, TLC plates Alugram® Sil G/UV254. Detection under UV light at 254 nm. Chromatography: Separations were carried out on Merck Silica 60 (0.040–0.063 mm, 70–230 mesh ASTM). All IR spectra were recorded on a BRUKER ALPHA-P spectrometer. MS: EI-MS: Finnigan MAT 95, 70eV; ESI-MS: Finnigan LCQ. High resolution mass spectrometry (HRMS): APEX IV 7T FTICR, Bruker Daltonic. M. p. Stuart® Melting Point Apparatus SMP3 melting point apparatus, values are uncorrected. ^{1}H, ^{13}C, ^{19}F NMR-spectra were recorded at 300 (^{1}H), 600 (^{1}H), 75 {^{13}C, APT (Attached Proton Test)} and 283 MHz (^{19}F), respectively, on Varian Unity-300 (600) and AMX 300 instruments in $CDCl_3$ solutions. If not otherwise specified, chemical shifts (δ) are given in ppm.

General Procedure for Direct Cyanation of Benzamides:

Benzamides **(1)** (0.50 mmol), *N*-cyano-*N*-phenyl-4-methylbenzenesulfonamide **(2)** (272 mg, 1.0 mmol), $[RuCl_2(p\text{-cymene})]_2$ (15.4 mg, 5.0 mol %), $AgSbF_6$ (34.4 mg, 20 mol %), NaOAc (8.2 mg, 20 mol %) and DCE (2.0 mL) were placed in a 20 mL sealed tube under N_2 and stirred at 120 °C for 24 h. At ambient temperature, the reaction mixture was diluted with H_2O (15 mL) and extracted with EtOAc (3 x 15 mL). The combined organic layer was dried with Na_2SO_4 and concentrated under reduced pressure. The crude products were purified by column chromatography on silica gel to afford the desired products.

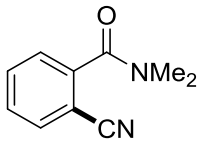


2-Cyano-*N*,*N*-diisopropylbenzamide (3a): The representative procedure was followed using *N*,*N*-diisopropylbenzamide **(1a)** (103 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 5/1→2/1) yielded **3a** (97 mg, 84%) as a colorless solid. M.p. = 109–111 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.62 (ddd, *J* = 7.7, 1.3, 0.6 Hz, 1H), 7.57 (ddd, *J* = 7.7, 7.7, 1.3 Hz, 1H), 7.40 (ddd, *J* = 7.7, 7.7, 1.3 Hz, 1H), 7.29 (ddd, *J* = 7.7, 1.3, 0.6 Hz, 1H), 3.52 (hept, *J* = 6.7 Hz, 2H), 1.56 (d, *J* = 6.7 Hz, 6H), 1.15 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.7 (C_q), 142.4 (C_q), 133.0 (CH), 132.8 (CH), 128.5 (CH), 125.7 (CH), 116.8 (C_q), 108.9 (C_q), 51.4 (CH), 46.1 (CH), 20.6 (CH_3), 20.2 (CH_3). IR (neat): 2964, 2225, 1625, 1437, 1341, 1031, 788, 552 cm^{-1}. MS (EI) *m/z* (relative intensity) 230 (5) [M^+], 187 (24), 173 (25), 130 (100), 102 (36). HR-MS (EI) *m/z* calcd for $C_{14}H_{18}N_2O$ [M^+] 230.1419, found 230.1424. The spectral data are in accordance with those reported in the literature.[3]

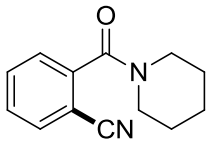


2-Cyano-*N*,*N*-diethylbenzamide (3b): The representative procedure was followed using *N*,*N*-diethylbenzamide **(1b)** (89 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 5/1→2/1) yielded **3b** (75 mg, 74%) as a colorless oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.63 (ddd, *J* = 7.7, 1.3, 0.6 Hz, 1H), 7.58 (ddd, *J* = 7.7, 7.7, 1.3 Hz, 1H), 7.42 (ddd, *J* = 7.7, 7.7, 1.3 Hz, 1H), 7.35 (ddd, *J* = 7.7, 1.3, 0.6 Hz, 1H), 3.53 (q, *J* = 7.1 Hz, 2H), 3.12 (q, *J* = 7.1 Hz, 2H), 1.22 (t, *J* = 7.1 Hz, 3H), 1.03 (t, *J* = 7.1 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 167.0 (C_q), 140.9 (C_q), 132.8 (CH), 132.7 (CH), 129.0 (CH), 126.6 (CH), 116.5 (C_q), 109.6 (C_q), 43.0 (CH_2), 39.1 (CH_2), 13.9 (CH_3), 12.4 (CH_3). IR (neat): 2976, 2228, 1628, 1429, 1292, 1080, 762, 546 cm^{-1}. MS (EI) *m/z* (relative intensity) 202 (20) [M^+], 173 (15), 130 (100), 102 (40). HR-MS (ESI) *m/z* calcd for $C_{12}H_{14}N_2NaO$ [M + Na^+] 225.1004, found

225.0998.

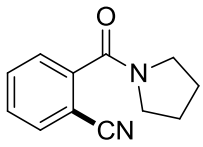


2-Cyano-*N*,*N*-dimethylbenzamide (3c): The representative procedure was followed using *N*,*N*-dimethylbenzamide **(1c)** (75 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 5/1→1/1) yielded **3c** (58 mg, 67%) as a colorless oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.66–7.57 (m, 2H), 7.47–7.39 (m, 2H), 3.10 (s, 3H), 2.88 (s, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 167.5 (C_q), 140.3 (C_q), 133.0 (CH), 132.7 (CH), 129.4 (CH), 127.4 (CH), 116.7 (C_q), 109.7 (C_q), 38.5 (CH_3), 34.9 (CH_3). IR (neat): 2933, 2228, 1632, 1396, 1069, 760, 542 cm^{-1}. MS (EI) *m/z* (relative intensity) 174 (35) [M^+], 130 (100), 102 (65), 75 (23). HR-MS (ESI) *m/z* calcd for $C_{10}H_{11}N_2O$ [M + H^+] 175.0871, found 175.0866. The spectral data are in accordance with those reported in the literature.[4]

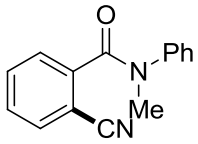


2-(Piperidine-1-carbonyl)benzonitrile (3d): The representative procedure was followed using phenyl(piperidin-1-yl)methanone **(1d)** (95 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 5/1→2/1) yielded **3d** (81 mg, 76%) as a colorless solid. M.p. = 108–110 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.64 (d, *J* = 7.7 Hz, 1H), 7.59 (dd, *J* = 7.7, 7.6 Hz, 1H), 7.43 (dd, *J* = 7.6, 7.6 Hz, 1H), 7.38 (d, *J* = 7.6 Hz, 1H), 3.72–3.69 (m, 2H), 3.18 (t, *J* = 5.6 Hz, 2H), 1.64–1.62 (m, 4H), 1.54–1.48 (m, 2H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.0 (C_q), 140.5 (C_q), 132.9 (CH), 132.8 (CH), 129.2 (CH), 127.1 (CH), 116.8 (C_q), 109.6 (C_q), 48.1 (CH_2), 42.9 (CH_2), 26.2 (CH_2), 25.2 (CH_2), 24.2 (CH_2). IR (neat): 2928, 2228, 1621, 1437, 1292, 1254, 779, 554 cm^{-1}. MS (EI) *m/z* (relative intensity) 214 (45) [M^+], 213 (100), 130 (100), 102 (50), 84 (23). HR-MS (ESI) *m/z* calcd for $C_{13}H_{15}N_2O$ [M + H^+] 215.1184,

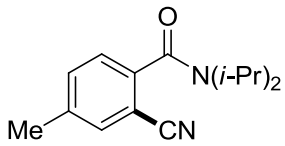
found 215.1179.



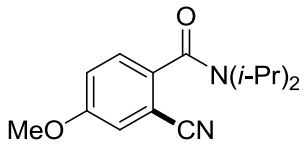
2-(Pyrrolidine-1-carbonyl)benzonitrile (3e): The representative procedure was followed using phenyl(pyrrolidin-1-yl)methanone **(1e)** (88 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 5/1→1/1) yielded **3e** (67 mg, 66%) as a colorless oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.68–7.52 (m, 2H), 7.46–7.40 (m, 2H), 3.60 (t, J = 6.8 Hz, 2H), 3.22 (t, J = 6.4 Hz, 2H), 1.96–1.79 (m, 4H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.7 (C_q), 141.2 (C_q), 132.9 (CH), 132.8 (CH), 129.4 (CH), 127.1 (CH), 116.9 (C_q), 109.5 (C_q), 48.3 (CH_2), 45.8 (CH_2), 25.9 (CH_2), 24.1 (CH_2). IR (neat): 2973, 2879, 2228, 1623, 1594, 1448, 760, 650 cm^{-1}. MS (EI) *m/z* (relative intensity) 200 (55) [M^+], 171 (35), 130 (100), 102 (65), 70 (50). HR-MS (EI) *m/z* calcd for $C_{12}H_{12}N_2O$ [M^+] 200.0950, found 200.0951.



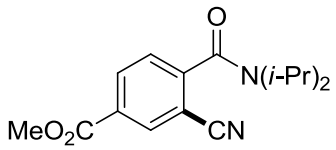
2-Cyano-*N*-methyl-*N*-phenylbenzamide (3f): The representative procedure was followed using *N*-methyl-*N*-phenylbenzamide **(1f)** (106 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 10/1→2/1) yielded **3f** (63 mg, 53%) as a colorless solid. M.p. = 75–77 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.48–7.08 (m, 9H), 3.49 (s, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 167.4 (C_q), 142.8 (C_q), 140.8 (C_q), 132.7 (CH), 132.0 (CH), 129.2 (CH), 129.1 (CH), 128.4 (CH), 127.3 (CH), 127.0 (CH), 117.1 (C_q), 110.5 (C_q), 37.7 (CH_3). IR (neat): 3053, 2227, 1632, 1592, 1495, 1380, 769, 699, 553 cm^{-1}. MS (EI) *m/z* (relative intensity) 236 (35) [M^+], 143 (22), 130 (100), 102 (35), 77 (18). HR-MS (EI) *m/z* calcd for $C_{15}H_{12}N_2O$ [M^+] 236.0950, found 236.0946.



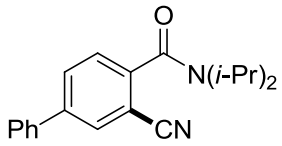
2-Cyano-*N*,*N*-diisopropyl-4-methylbenzamide (3g): The representative procedure was followed using *N*,*N*-diisopropyl-4-methylbenzamide **(1g)** (110 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 10/1→2/1) yielded **3g** (98 mg, 80%) as a colorless solid. M.p. = 92–94 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.42 (s, 1H), 7.36 (d, J = 7.9 Hz, 1H), 7.17 (d, J = 7.9 Hz, 1H), 3.52 (hept, J = 6.8 Hz, 2H), 2.34 (s, 3H), 1.52 (d, J = 6.8 Hz, 6H), 1.12 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 167.0 (C_q), 139.7 (C_q), 138.8 (C_q), 133.7 (CH), 133.0 (CH), 125.6 (CH), 116.9 (C_q), 108.8 (C_q), 51.3 (CH), 46.0 (CH), 20.8 (CH_3), 20.6 (CH_3), 20.2 (CH_3). IR (neat): 2970, 1617, 1440, 1342, 1037, 822, 597 cm^{-1}. MS (EI) *m/z* (relative intensity) 244 (10) [M^+], 201 (50), 187 (22), 144 (100), 116 (20), 89 (18). HR-MS (EI) *m/z* calcd for $C_{15}H_{20}N_2O$ [M^+] 244.1576, found 244.1571.



2-Cyano-*N*,*N*-diisopropyl-4-methoxybenzamide (3h): The representative procedure was followed using *N*,*N*-diisopropyl-4-methoxybenzamide **(1h)** (118 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 5/1→1/1) yielded **3h** (117 mg, 90%) as a colorless solid. M.p. = 118–120 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.19 (d, J = 8.0 Hz, 1H), 7.08 (d, J = 2.6 Hz, 1H), 7.07 (dd, J = 8.0, 2.6 Hz, 1H), 3.78 (s, 3H), 3.53 (s_{br}, 2H), 1.50 (s_{br}, 6H), 1.12 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.8 (C_q), 159.0 (C_q), 134.9 (C_q), 127.2 (CH), 119.2 (CH), 117.3 (CH), 116.7 (C_q), 109.9 (C_q), 55.6 (CH_3), 51.3 (CH), 46.0 (CH), 20.4 (CH_3), 20.3 (CH_3). IR (neat): 2978, 2228, 1622, 1441, 1372, 1248, 1026, 848, 593 cm^{-1}. MS (EI) *m/z* (relative intensity) 260 (10) [M^+], 217 (50), 160 (100), 117 (15), 77 (10). HR-MS (EI) *m/z* calcd for $C_{15}H_{20}N_2O_2$ [M^+] 260.1525, found 260.1532.

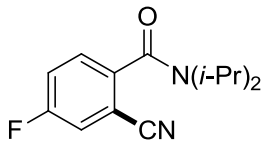


Methyl 3-cyano-4-(diisopropylcarbamoyl)benzoate (3i): The representative procedure was followed using methyl 4-(diisopropylcarbamoyl)benzoate **(1i)** (132 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 10/1→2/1) yielded **3i** (94 mg, 65%) as a colorless solid. M.p. = 81–83 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.28 (d, J = 1.6 Hz, 1H), 8.20 (dd, J = 8.0, 1.6 Hz, 1H), 7.38 (d, J = 8.0 Hz, 1H), 3.89 (s, 3H), 3.52 (hept, J = 6.7 Hz, 1H), 3.44 (hept, J = 6.7 Hz, 1H), 1.52 (d, J = 6.8 Hz, 6H), 1.13 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.8 (C_q), 164.5 (C_q), 145.8 (C_q), 134.0 (CH), 133.9 (CH), 130.6 (C_q), 126.0 (CH), 115.9 (C_q), 109.5 (C_q), 52.6 (CH_3), 51.5 (CH), 46.3 (CH), 20.5 (CH_3), 20.1 (CH_3). IR (neat): 2958, 2231, 1719, 1635, 1433, 1295, 1261, 1107, 769, 555 cm^{-1}. MS (EI) *m/z* (relative intensity) 288 (10) [M^+], 245 (65), 231 (50), 188 (100), 101 (10). HR-MS (ESI) *m/z* calcd for $C_{16}H_{21}N_2O_3$ [M + H^+] 289.1552, found 289.1547.

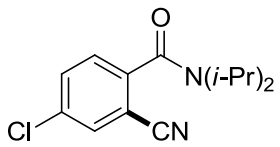


3-Cyano-*N*,*N*-diisopropyl-[1,1'-biphenyl]-4-carboxamide (3j): The representative procedure was followed using *N*,*N*-diisopropyl-[1,1'-biphenyl]-4-carboxamide **(1j)** (141 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc/Et_3N: 200/10/1→200/60/1) yielded **3j** (140 mg, 92%) as a colorless solid. M.p. = 114–116 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.81 (d, J = 1.8 Hz, 1H), 7.77 (dd, J = 8.0, 1.8 Hz, 1H), 7.53–7.34 (m, 6H), 3.64 (hept, J = 6.7 Hz, 1H), 3.56 (hept, J = 6.7 Hz, 1H), 1.58 (d, J = 6.8 Hz, 6H), 1.18 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.6 (C_q), 141.7 (C_q), 140.8 (C_q), 138.0 (C_q), 131.5 (CH), 131.1 (CH), 129.0 (CH), 128.4 (CH), 126.8 (CH), 126.2 (CH), 116.8 (C_q), 109.5 (C_q), 51.4 (CH), 46.1 (CH), 20.6 (CH_3), 20.2 (CH_3). IR (neat): 2970, 1627, 1442, 1342, 1034, 753, 695 cm^{-1}. MS (EI) *m/z* (relative intensity) 306 (10) [M^+], 263 (60), 206 (100), 151 (15). HR-MS (EI)

m/z calcd for $C_{20}H_{22}N_2O$ [M^+] 306.1732, found 306.1730.

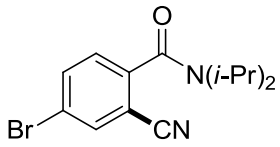


2-Cyano-4-fluoro-*N*,*N*-diisopropylbenzamide (3k): The representative procedure was followed using 4-fluoro-*N*,*N*-diisopropylbenzamide **(1k)** (112 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 10/1→5/1) yielded **3k** (101 mg, 81%) as a colorless solid. M.p. = 129–131 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.37–7.29 (m, 3H), 3.54 (hept, J = 6.7 Hz, 2H), 1.55 (d, J = 6.7 Hz, 6H), 1.17 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.8 (C_q), 161.3 ($^1J_{C–F}$ = 256 Hz, C_q), 138.9 ($^4J_{C–F}$ = 4 Hz, C_q), 128.0 ($^3J_{C–F}$ = 8 Hz, CH), 120.7 ($^2J_{C–F}$ = 21 Hz, CH), 119.7 ($^2J_{C–F}$ = 24 Hz, CH), 115.6 ($^4J_{C–F}$ = 3 Hz, C_q), 110.7 ($^3J_{C–F}$ = 9 Hz, C_q), 51.6 (CH), 46.4 (CH), 20.8 (CH_3), 20.3 (CH_3). ^{19}F-NMR (283 MHz, $CDCl_3$): δ = –(110.0–110.1) (m). IR (neat): 2973, 2231, 1617, 1443, 1372, 1342, 1156, 1032, 829, 597 cm^{-1}. MS (EI) *m/z* (relative intensity) 248 (5) [M^+], 205 (35), 191 (40), 148 (100), 120 (25), 58 (17). HR-MS (EI) *m/z* calcd for $C_{14}H_{17}FN_2O$ [M^+] 248.1325, found 248.1323.

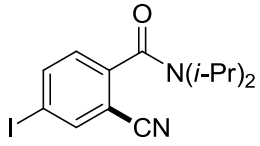


4-Chloro-2-cyano-*N*,*N*-diisopropylbenzamide (3l): The representative procedure was followed using 4-chloro-*N*,*N*-diisopropylbenzamide **(1l)** (120 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc/Et_3N: 100/10/1→100/20/1) yielded **3l** (91 mg, 68%) as a colorless solid. M.p. = 131–133 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.64 (d, J = 1.6 Hz, 1H), 7.57 (dd, J = 8.2, 1.6 Hz, 1H), 7.28 (d, J = 8.2 Hz, 1H), 3.53 (hept, J = 6.0 Hz, 2H), 1.55 (d, J = 6.0 Hz, 6H), 1.17 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.7 (C_q), 140.7 (C_q), 134.5 (C_q), 133.3 (CH), 132.4 (CH), 127.2 (CH), 115.5 (C_q), 110.7 (C_q), 51.6 (CH), 46.4 (CH), 20.8 (CH_3), 20.3 (CH_3). IR (neat): 2981, 2231, 1626, 1442, 1339, 1033, 847, 589 cm^{-1}. MS (EI)

m/z (relative intensity) 264 (5) [M^+], 221 (48), 207 (45), 164 (100), 136 (20), 100 (10). HR-MS (EI) *m/z* calcd for $C_{14}H_{17}ClN_2O$ [M^+] 264.1029, found 264.1028.

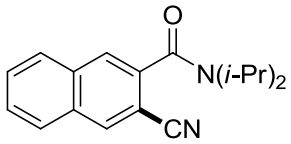


4-Bromo-2-cyano-*N*,*N*-diisopropylbenzamide (3m): The representative procedure was followed using 4-bromo-*N*,*N*-diisopropylbenzamide **(1m)** (142 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc/Et_3N: 100/10/1→100/20/1) yielded **3m** (110 mg, 71%) as a colorless solid. M.p. = 121–123 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.78 (d, *J* = 2.0 Hz, 1H), 7.72 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.20 (d, *J* = 8.2 Hz, 1H), 3.53 (hept, *J* = 6.7 Hz, 2H), 1.55 (d, *J* = 6.7 Hz, 6H), 1.16 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.8 (C_q), 141.2 (C_q), 136.3 (CH), 135.3 (CH), 127.3 (CH), 122.1 (C_q), 115.5 (C_q), 110.9 (C_q), 51.6 (CH), 46.4 (CH), 20.7 (CH_3), 20.3 (CH_3). IR (neat): 2966, 2218, 1630, 1443, 1344, 1037, 850, 554 cm^{-1}. MS (EI) *m/z* (relative intensity) 310 (10) [M^+] (^{81}Br), 308 (10) [M^+] (^{79}Br), 267 (55) (^{81}Br), 265 (55) (^{79}Br), 210 (100) (^{81}Br), 208 (100) (^{79}Br), 182 (20) (^{81}Br), 180 (20) (^{79}Br). HR-MS (EI) *m/z* calcd for $C_{14}H_{17}BrN_2O$ [M^+] 308.0524, found 308.0529.

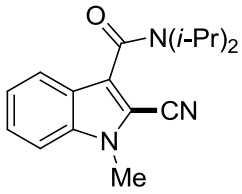


2-Cyano-4-iodo-*N*,*N*-diisopropylbenzamide (3n): The representative procedure was followed using 4-iodo-*N*,*N*-diisopropylbenzamide **(1n)** (166 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/CH_2Cl_2: 1/1) yielded **3n** (162 mg, 91%) as a colorless solid. M.p. = 157–159 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.94 (d, *J* = 1.6 Hz, 1H), 7.88 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.03 (d, *J* = 8.1 Hz, 1H), 3.50 (hept, *J* = 6.6 Hz, 2H), 1.50 (d, *J* = 6.6 Hz, 6H), 1.12 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.8 (C_q), 141.9 (CH), 141.5 (C_q), 140.8 (CH), 127.1 (CH), 115.1 (C_q), 110.8 (C_q), 92.8 (C_q), 51.4 (CH), 46.2 (CH), 20.6 (CH_3), 20.1 (CH_3). IR (neat): 2966, 2223, 1631,

1439, 1338, 1034, 825, 557 cm^{-1}. MS (EI) *m/z* (relative intensity) 356 (15) [M^+], 313 (80), 299 (40), 256 (100), 227 (12), 101 (17). HR-MS (EI) *m/z* calcd for $C_{14}H_{17}IN_2O$ [M^+] 356.0386, found 356.0388.

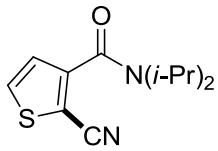


3-Cyano-*N*,*N*-diisopropyl-2-naphthamide (3o): The representative procedure was followed using *N*,*N*-diisopropyl-2-naphthamide **(1o)** (128 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 10/1→2/1) yielded **3o** (109 mg, 78%) as a colorless solid. M.p. = 133–135 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.20 (s, 1H), 7.83 (d, *J* = 8.5 Hz, 2H), 7.74 (s, 1H), 7.64–7.53 (m, 2H), 3.36–3.54 (m, 2H), 1.60 (d, *J* = 6.0 Hz, 6H), 1.16 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 167.0 (C_q), 136.5 (C_q), 135.1 (CH), 134.1 (C_q), 131.4 (C_q), 129.6 (CH), 128.2 (CH), 128.0 (CH), 127.9 (CH), 124.9 (CH), 117.1 (C_q), 106.7 (C_q), 51.4 (CH), 46.1 (CH), 20.5 (CH_3), 20.3 (CH_3). IR (neat): 2972, 2229, 1617, 1474, 1342, 1152, 901, 756, 481 cm^{-1}. MS (EI) *m/z* (relative intensity) 280 (20) [M^+], 237 (45), 180 (100), 152 (40). HR-MS (EI) *m/z* calcd for $C_{18}H_{20}N_2O$ [M^+] 280.1576, found 280.1576.

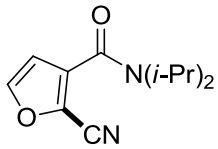


2-Cyano-*N*,*N*-diisopropyl-1-methyl-1*H*-indole-3-carboxamide (3p): The representative procedure was followed using *N*,*N*-diisopropyl-1-methyl-1*H*-indole-3-carboxamide **(1p)** (129 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 10/1→10/3) yielded **3p** (122 mg, 86%) as a colorless solid. M.p. = 202–204 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.56 (d, *J* = 8.1 Hz, 1H), 7.38 (dd, *J* = 8.3, 6.7 Hz, 1H), 7.30 (d, *J* = 8.3 Hz, 1H), 7.20 (dd, *J* = 8.1, 6.7 Hz, 1H), 3.83 (s, 3H), 3.73 (hept, *J* = 6.7 Hz, 2H), 1.39 (s_{br}, 12H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 163.2

(C_q), 137.2 (C_q), 126.4 (CH), 124.0 (C_q), 123.9 (C_q), 121.9 (CH), 120.9 (CH), 112.2 (C_q), 110.2 (CH), 107.1 (C_q), 48.8 (CH), 31.5 (CH_3), 20.9 (CH_3). IR (neat): 2979, 2224, 1616, 1536, 1371, 1311, 1045, 745 cm^{-1}. MS (EI) *m/z* (relative intensity) 283 (10) [M^+], 240 (15), 183 (100), 128 (10). HR-MS (EI) *m/z* calcd for $C_{17}H_{21}N_3O$ [M^+] 283.1685, found 283.1679.

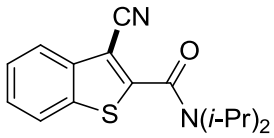


2-Cyano-*N*,*N*-diisopropylthiophene-3-carboxamide (3q): The representative procedure was followed using *N*,*N*-diisopropylthiophene-3-carboxamide **(1q)** (106 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 10/1→3/1) yielded **3q** (91 mg, 77%) as a colorless solid. M.p. = 76–78 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.58 (d, *J* = 5.0 Hz, 1H), 7.05 (d, *J* = 5.0 Hz, 1H), 3.59 (s_{br}, 2H), 1.52 (s_{br}, 6H), 1.20 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 163.0 (C_q), 148.3 (C_q), 132.8 (CH), 126.1 (CH), 112.7 (C_q), 106.2 (C_q), 51.4 (CH), 46.4 (CH), 20.7 (CH_3), 20.5 (CH_3). IR (neat): 3072, 2221, 1629, 1444, 1323, 1203, 1038, 776 cm^{-1}. MS (EI) *m/z* (relative intensity) 236 (5) [M^+], 221 (15), 193 (25), 179 (45), 136 (100), 58 (8). HR-MS (EI) *m/z* calcd for $C_{12}H_{16}N_2OS$ [M^+] 236.0983, found 236.0981.

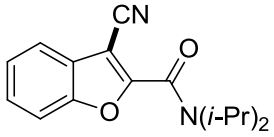


2-Cyano-*N*,*N*-diisopropylfuran-3-carboxamide (3r): The representative procedure was followed using *N*,*N*-diisopropylfuran-3-carboxamide **(1r)** (98 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 10/1→5/1) yielded **3r** (89 mg, 81%) as a colorless oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.51 (d, *J* = 1.9 Hz, 1H), 6.50 (d, *J* = 1.9 Hz, 1H), 3.66 (s_{br}, 2H), 1.29 (s_{br}, 12H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 160.6 (C_q), 146.9 (CH), 133.8 (C_q), 123.2 (C_q), 110.7 (CH), 110.2 (C_q), 51.3 (CH), 46.5 (CH), 20.6 (CH_3). IR (neat): 2973, 2229, 1628, 1484, 1372, 1336, 1026, 1019,

754 cm^{-1}. MS (EI) *m/z* (relative intensity) 220 (10) [M^+], 205 (20), 177 (23), 163 (70), 120 (100), 64 (8). HR-MS (EI) *m/z* calcd for $C_{12}H_{16}N_2O_2$ [M^+] 220.1212, found 220.1207.

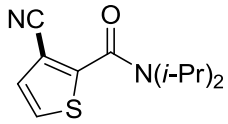


3-Cyano-*N*,*N*-diisopropylbenzo[*b*]thiophene-2-carboxamide (3s): The representative procedure was followed using *N*,*N*-diisopropylbenzo[*b*]thiophene-2-carboxamide **(1s)** (131 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/CH_2Cl_2: 1/1) yielded **3s** (129 mg, 90%) as a colorless solid. M.p. = 134–136 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.93 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.85 (dd, *J* = 7.4, 1.3 Hz, 1H), 7.55–7.45 (m, 2H), 3.72 (s_{br}, 2H), 1.40 (s_{br}, 12H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 160.5 (C_q), 149.2 (C_q), 137.3 (C_q), 136.8 (C_q), 126.7 (CH), 126.4 (CH), 122.8 (CH), 122.7 (CH), 113.0 (C_q), 104.0 (C_q), 20.6 (CH_3). $\underline{C}H(CH_3)_2$ is not detectable. IR (neat): 2969, 2224, 1633, 1452, 1343, 1316, 1037, 751, 611 cm^{-1}. MS (EI) *m/z* (relative intensity) 286 (8) [M^+], 271 (10), 243 (15), 186 (75), 158 (13), 114 (15), 43 (100). HR-MS (EI) *m/z* calcd for $C_{16}H_{18}N_2OS$ [M^+] 286.1140, found 286.1149.

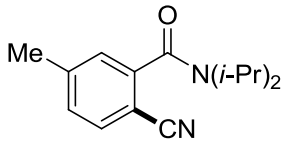


3-Cyano-*N*,*N*-diisopropylbenzofuran-2-carboxamide (3t): The representative procedure was followed using *N*,*N*-diisopropylbenzofuran-2-carboxamide **(1t)** (123 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc/Et_3N: 100/5/1→100/20/1) yielded **3t** (105 mg, 78%) as a colorless solid. M.p. = 99–101 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.70–7.67 (m, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.48–7.36 (m, 2H), 3.80 (s_{br}, 2H), 1.40 (s_{br}, 12H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 157.6 (C_q), 156.9 (C_q), 153.1 (C_q), 127.5 (CH), 125.2 (CH), 125.1 (C_q), 120.5 (CH),

112.2 (CH), 111.7 (C_q), 94.1 (C_q), 50.7 (CH), 47.4 (CH), 20.5 (CH_3). IR (neat): 2972, 2233, 1626, 1440, 1321, 1181, 1036, 738 cm^{-1}. MS (EI) *m/z* (relative intensity) 270 (10) [M^+], 227 (30), 213 (45), 170 (100), 114 (30), 43 (45). HR-MS (EI) *m/z* calcd for $C_{16}H_{18}N_2O_2$ [M^+] 270.1368, found 270.1368.

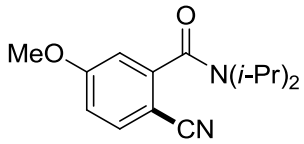


3-Cyano-*N*,*N*-diisopropylthiophene-2-carboxamide (3u): The representative procedure was followed using *N*,*N*-diisopropylthiophene-2-carboxamide **(1u)** (106 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 10/1→5/1) yielded **3u** (100 mg, 85%) as a colorless solid. M.p. = 99–101 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.35 (d, *J* = 5.2 Hz, 1H), 7.16 (d, *J* = 5.2 Hz, 1H), 3.71–3.62 (m, 2H), 1.36 (s_{br}, 12H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 160.5 (C_q), 148.1 (C_q), 128.4 (CH), 126.3 (CH), 113.8 (C_q), 108.2 (C_q), 49.6 (CH), 20.6 (CH_3). IR (neat): 2980, 2227, 1627, 1455, 1328, 1207, 1029, 766 cm^{-1}. MS (EI) *m/z* (relative intensity) 236 (5) [M^+], 221 (18), 193 (23), 179 (50), 136 (100), 58 (10). HR-MS (EI) *m/z* calcd for $C_{12}H_{16}N_2OS$ [M^+] 236.0983, found 236.0982.

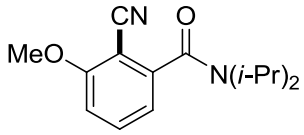


2-Cyano-*N*,*N*-diisopropyl-5-methylbenzamide (3v): The representative procedure was followed using *N*,*N*-diisopropyl-3-methylbenzamide **(1v)** (110 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 10/1→3/1) yielded **3v** (95 mg, 78%) as a colorless solid. M.p. = 147–149 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.53 (d, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 1H), 7.12 (s, 1H), 3.57 (hept, *J* = 7.0 Hz, 1H), 3.54 (hept, *J* = 7.0 Hz, 1H), 2.40 (s, 3H), 1.57 (d, *J* = 6.7 Hz, 6H), 1.17 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 167.0 (C_q), 144.2 (C_q), 142.4 (C_q), 132.7 (CH), 129.3 (CH), 126.3 (CH), 117.1 (C_q), 105.9 (C_q), 51.4 (CH), 46.1 (CH), 21.8 (CH_3), 20.7 (CH_3), 20.3 (CH_3). IR (neat): 2978, 2228, 1628, 1443, 1338, 1038, 843, 550 cm^{-1}. MS

(EI) *m/z* (relative intensity) 244 (20) [M^+], 229 (20), 201 (60), 187 (35), 144 (100), 116 (23), 89 (17). HR-MS (EI) *m/z* calcd for $C_{15}H_{20}N_2O$ [M^+] 244.1576, found 244.1566.

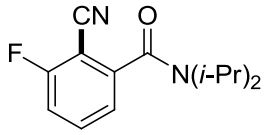


2-Cyano-*N*,*N*-diisopropyl-3-methoxybenzamide (3w): The representative procedure was followed using *N*,*N*-diisopropyl-3-methoxybenzamide **(1w)** (118 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 5/1→1/1) yielded **3w** (45 mg, 34%) and **3w'** (72 mg, 55%) as colorless solids. M.p. = 163–165 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.55 (d, *J* = 8.7 Hz, 1H), 6.89 (dd, *J* = 8.7, 2.5 Hz, 1H), 6.77 (d, *J* = 2.5 Hz, 1H), 3.83 (s, 3H), 3.56 (hept, *J* = 6.8 Hz, 1H), 3.52 (hept, *J* = 6.8 Hz, 1H), 1.54 (d, *J* = 6.8 Hz, 6H), 1.15 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.6 (C_q), 162.9 (C_q), 144.3 (C_q), 134.7 (CH), 117.2 (C_q), 114.4 (CH), 111.4 (CH), 100.5 (C_q), 55.7 (CH_3), 51.4 (CH), 46.2 (CH), 20.7 (CH_3), 20.2 (CH_3). IR (neat): 2964, 2224, 1630, 1457, 1337, 1242, 1027, 850, 680 cm^{-1}. MS (EI) *m/z* (relative intensity) 260 (20) [M^+], 217 (50), 203 (35), 160 (100), 117 (14). HR-MS (EI) *m/z* calcd for $C_{15}H_{20}N_2O_2$ [M^+] 260.1525, found 260.1523.



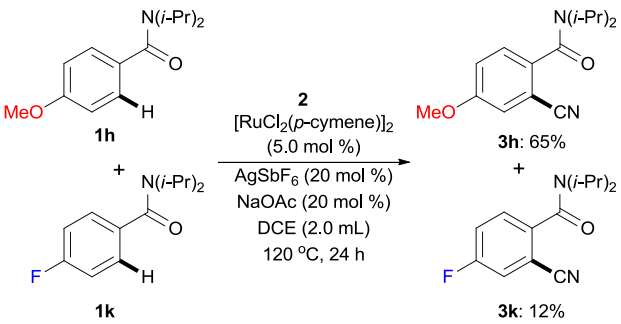
2-Cyano-*N*,*N*-diisopropyl-5-methoxybenzamide (3w'): M.p. = 165–167 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.49 (dd, *J* = 8.6, 7.6 Hz, 1H), 6.90 (d, *J* = 8.6 Hz, 1H), 6.81 (d, *J* = 7.6 Hz, 1H), 3.88 (s, 3H), 3.56 (hept, *J* = 6.8 Hz, 1H), 3.49 (hept, *J* = 6.8 Hz, 1H), 1.52 (d, *J* = 6.8 Hz, 6H), 1.12 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.5 (C_q), 161.4 (C_q), 143.8 (C_q), 134.5 (CH), 117.2 (CH), 114.3 (C_q), 110.7 (CH), 98.3 (C_q), 56.1 (CH_3), 51.3 (CH), 46.0 (CH), 20.5 (CH_3), 20.1 (CH_3). IR (neat): 2971, 2227, 1625, 1461, 1342, 1276, 1030, 800, 605 cm^{-1}. MS (EI) *m/z* (relative intensity)

260 (13) [M^+], 217 (50), 203 (25), 160 (100), 117 (18). HR-MS (EI) *m/z* calcd for $C_{15}H_{20}N_2O_2$ [M^+] 260.1525, found 260.1523.



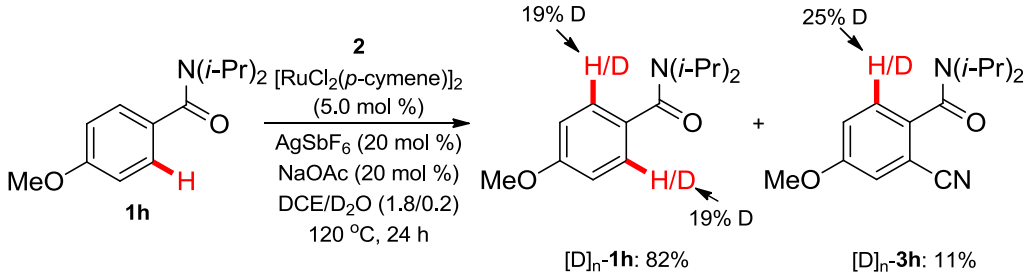
2-Cyano-3-fluoro-*N*,*N*-diisopropylbenzamide (3x): The representative procedure was followed using 3-fluoro-*N*,*N*-diisopropylbenzamide **(1x)** (112 mg, 0.50 mmol). Isolation by column chromatography (*n*-hexane/EtOAc: 5/1→1/1) yielded **3x** (100 mg, 80%) as a colorless solid. M.p. = 148–150 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.58 (ddd, *J* = 8.5, 7.6, 5.4 Hz, 1H), 7.15 (td, *J* = 8.5, 1.0 Hz, 1H), 7.08 (dd, *J* = 7.6, 0.9 Hz, 1H), 3.52 (hept, *J* = 6.7 Hz, 2H), 1.52 (d, *J* = 6.7 Hz, 6H), 1.14 (s_{br}, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.3 ($^4J_{C–F}$ = 2 Hz, C_q), 163.1 ($^1J_{C–F}$ = 261 Hz, C_q), 143.9 (C_q), 135.2 ($^3J_{C–F}$ = 9 Hz, CH), 121.3 ($^4J_{C–F}$ = 3 Hz, CH), 115.8 ($^2J_{C–F}$ = 19 Hz, CH), 111.9 (C_q), 98.5 ($^2J_{C–F}$ = 16 Hz, (C_q), 51.5 (CH), 46.2 (CH), 20.5 (CH_3), 20.1 (CH_3). ^{19}F-NMR (283 MHz, $CDCl_3$): δ = –105.0 (q). IR (neat): 2980, 1629, 1442, 1344, 1256, 809, 583 cm^{-1}. MS (EI) *m/z* (relative intensity) 248 (8) [M^+], 205 (50), 191 (70), 148 (100), 120 (28). HR-MS (EI) *m/z* calcd for $C_{14}H_{17}FN_2O$ [M^+] 248.1325, found 248.1333.

Intermolecular Competition Experiment between 1h and 1k



N,*N*-Diisopropyl-4-methoxybenzamide **(1h)** (118 mg, 0.50 mmol), 4-fluoro-*N*,*N*-diisopropylbenzamide **(1k)** (112 mg, 0.50 mmol), **2** (136 mg, 0.50 mmol), $[RuCl_2(p\text{-cymene})]_2$ (15.4 mg, 5.0 mol %), $AgSbF_6$ (34.4 mg, 20 mol %), NaOAc (8.2 mg, 20 mol %) and DCE (2.0 mL) were placed into a 20 mL sealed tube under N_2 and stirred at 120 °C for 24 h. At ambient temperature, the reaction mixture was diluted with H_2O (15 mL) and extracted with EtOAc (3 x 15 mL). The combined organic layer was dried with Na_2SO_4 and concentrated under reduced pressure, purified by column chromatography on silica gel (*n*-hexane/EtOAc: 20/1→1/1) to afford the products **3h** (84 mg, 65%) and **3k** (15 mg, 12%).

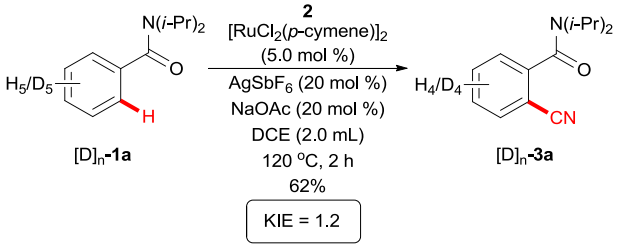
Ruthenium-Catalyzed H/D Exchange in 1h with D_2O as the Cosolvent



N,*N*-Diisopropyl-4-methoxybenzamide **(1h)** (0.50 mmol), **2** (272 mg, 1.0 mmol), $[RuCl_2(p\text{-cymene})]_2$ (15.4 mg, 5.0 mol %), $AgSbF_6$ (34.4 mg, 20 mol %), NaOAc (8.2 mg, 20 mol %), DCE (1.8 mL) and D_2O (0.2 mL) were placed into a 20 mL sealed tube under N_2 and stirred at 120 °C for 24 h. At ambient temperature, the reaction

mixture was diluted with H_2O (15 mL) and extracted with EtOAc (3 x 15 mL). The combined organic layer was dried with Na_2SO_4 and concentrated under reduced pressure. The crude products were purified by flash column chromatography on silica gel to afford $[D]_n$-**1h** (97 mg, 82%) and $[D]_n$-**3h** (15 mg, 11%). The deuterium incorporation was estimated by ^{1}H-NMR spectroscopy.

Kinetic Isotope Effect



N,*N*-Diisopropylbenzamide **(1a)** (51 mg, 0.25 mmol), $[D]_5$-*N*,*N*-diisopropylbenzamide **(**$[D]_5$**-1a)** (53 mg, 0.25 mmol), **2** (68 mg, 0.25 mmol), $[RuCl_2(p\text{-cymene})]_2$ (7.7 mg, 5.0 mol %), $AgSbF_6$ (17 mg, 20 mol %), NaOAc (4.1 mg, 20 mol %) and DCE (2.0 mL) were placed into a 20 mL sealed tube under N_2 and stirred at 120 °C for 2 h. At ambient temperature, the reaction mixture was diluted with H_2O (15 mL) and extracted with EtOAc (3 x 15 mL). The combined organic layer was dried with Na_2SO_4 and concentrated under reduced pressure. The crude products were purified by flash column chromatography on silica gel to afford $[D]_n$-**3a** (36 mg, 62%). The kinetic isotope effect of this reaction was determined to be $k_H/k_D \approx 1.2$ as estimated by ^{1}H-NMR spectroscopy.

References

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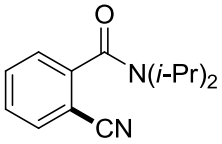
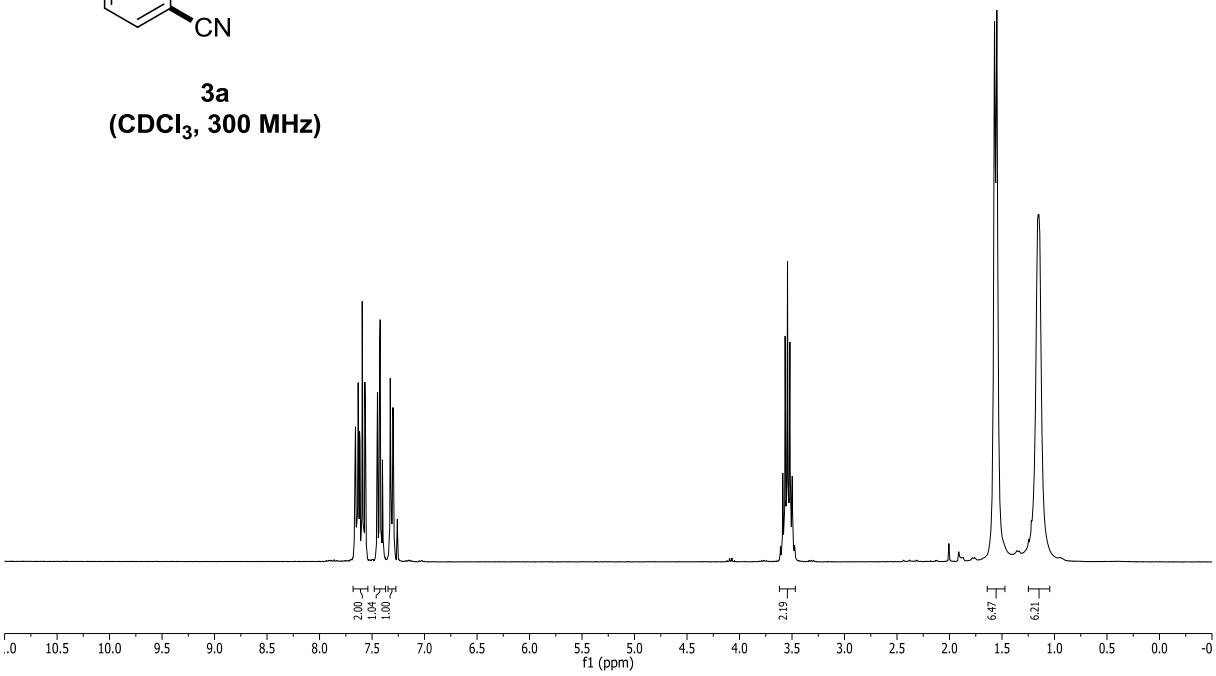
2. P. Anbarasan, H. Neumann and M. Beller, *Angew. Chem., Int. Ed.*, 2011, **50**, 519–522.

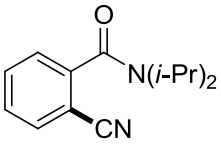
3. N. Sato and Q. Yue, *Tetrahedron*, 2003, **59**, 5831–5836.

4. Z. Liu, J. Zhang, S. Chen, E. Shi, Y. Xu, and X. Wan, *Angew. Chem., Int. Ed.*, 2012, **51**, 3231–3235.

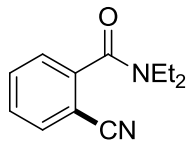


3a
($CDCl_3$, 300 MHz)

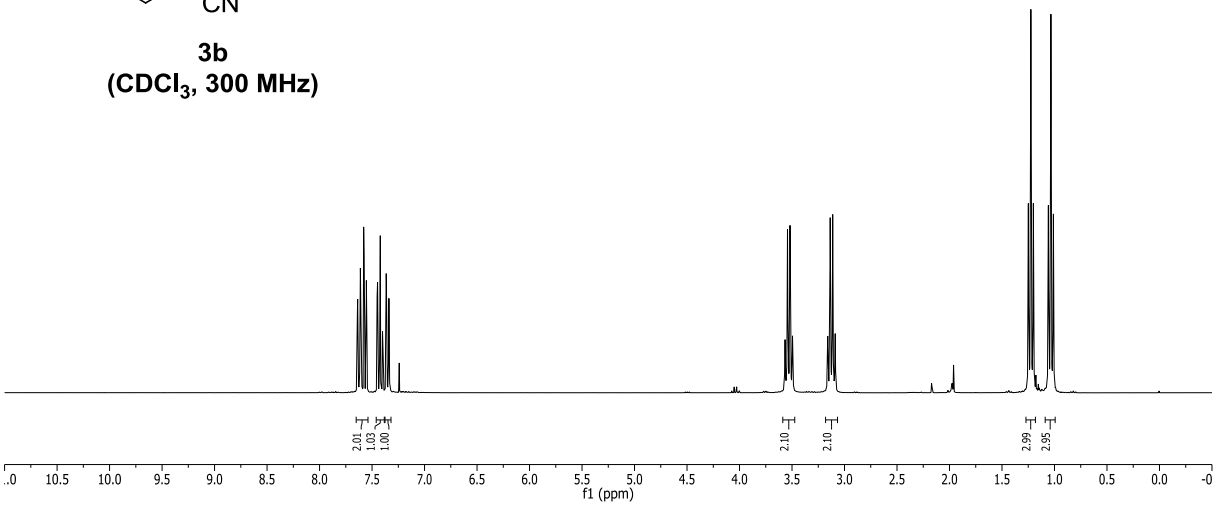


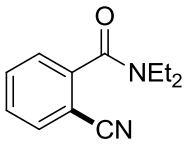


3a
($CDCl_3$, 75 MHz)

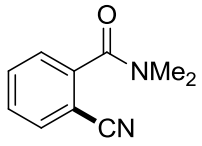


3b
($CDCl_3$, 300 MHz)

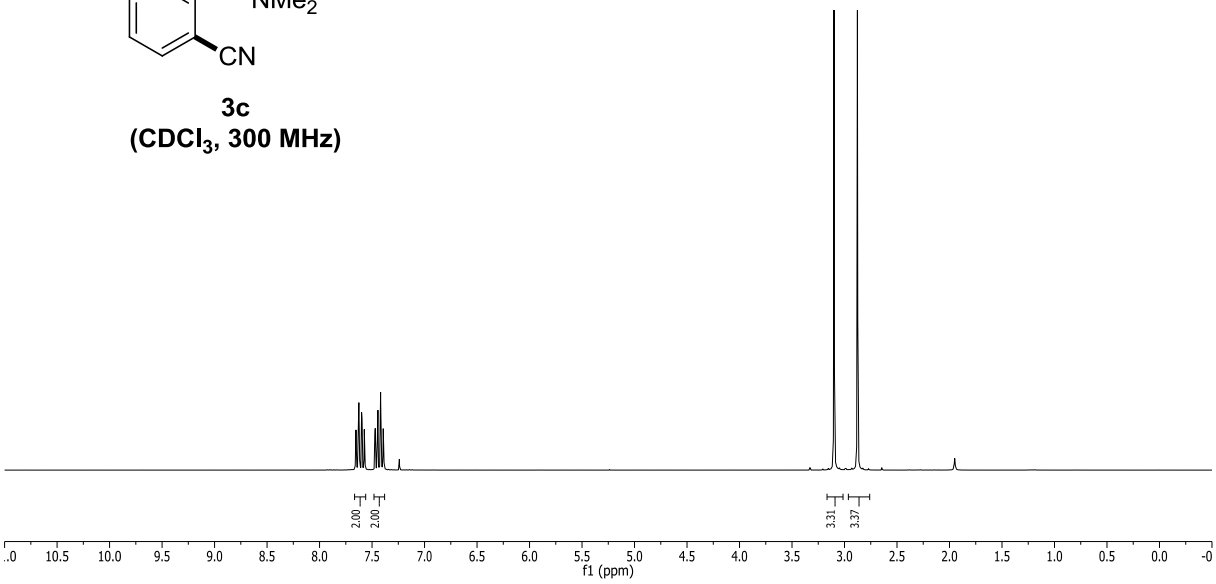


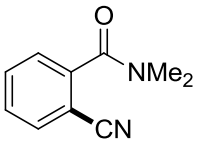


3b
($CDCl_3$, 75 MHz)

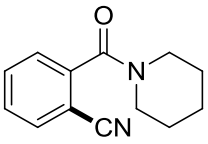


3c
($CDCl_3$, 300 MHz)

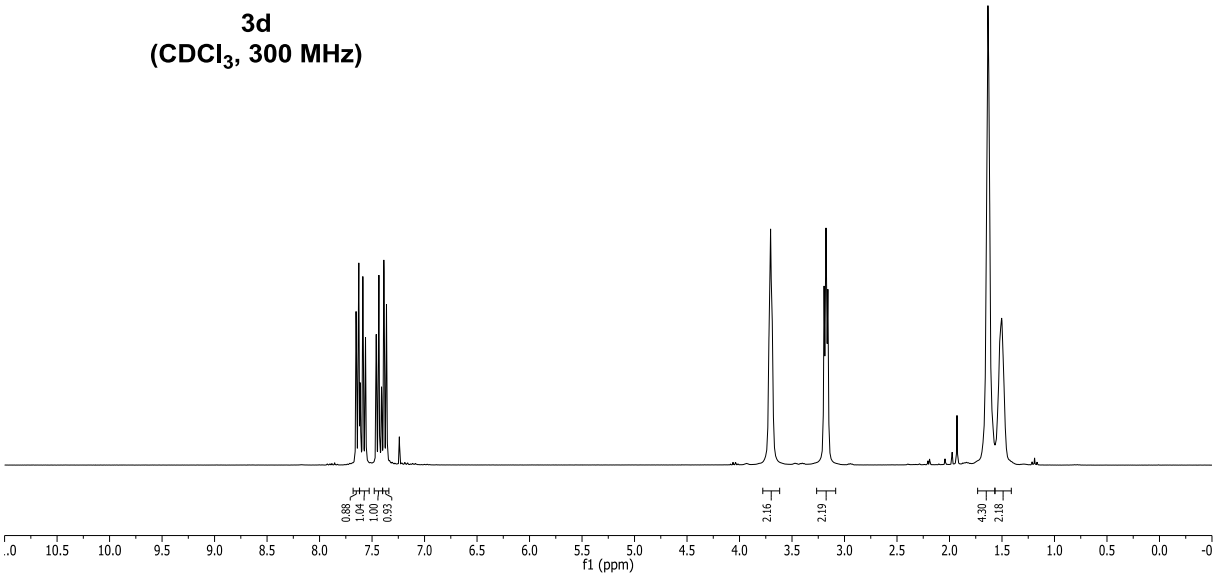


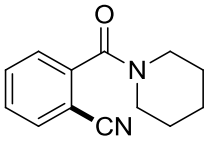


3c
($CDCl_3$, 75 MHz)

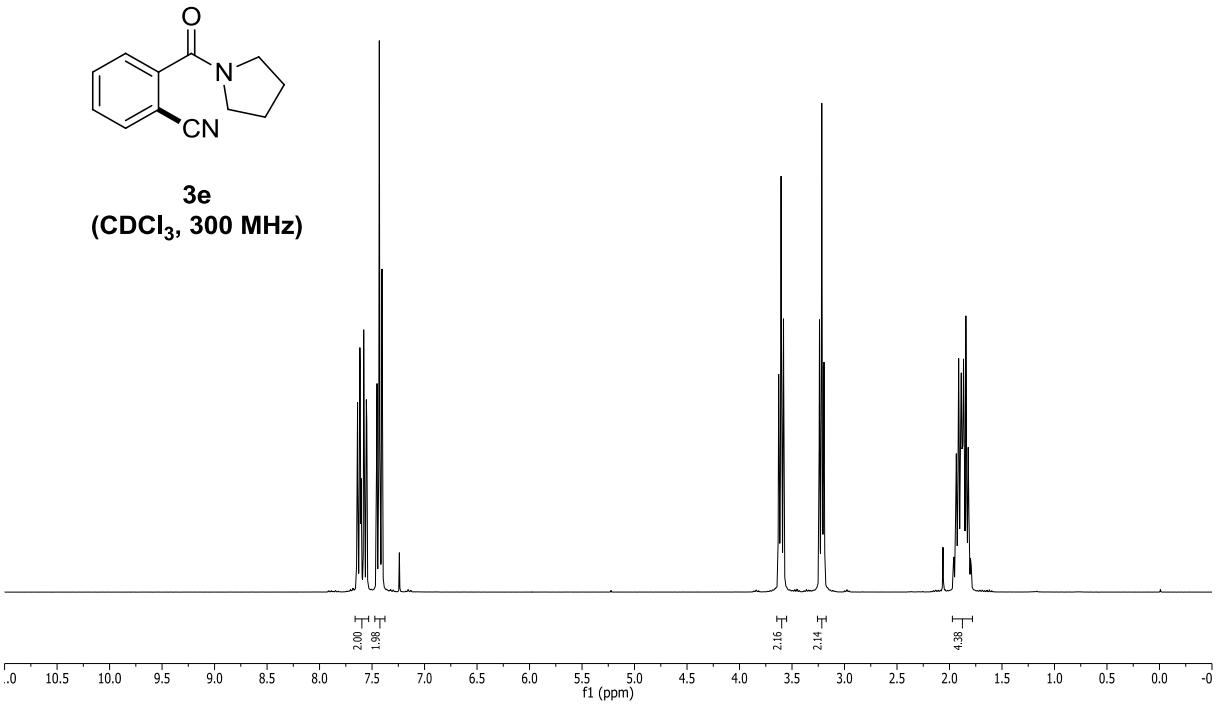


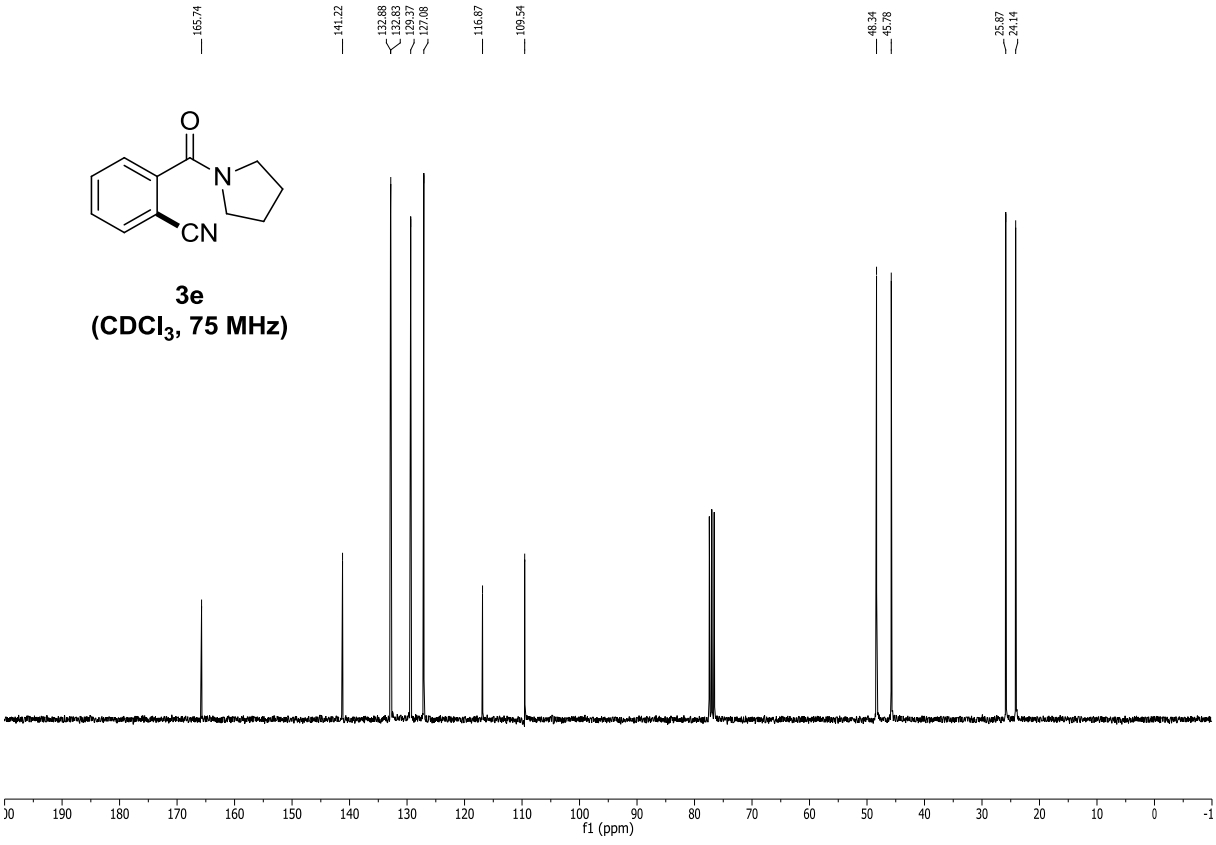
3d
($CDCl_3$, 300 MHz)

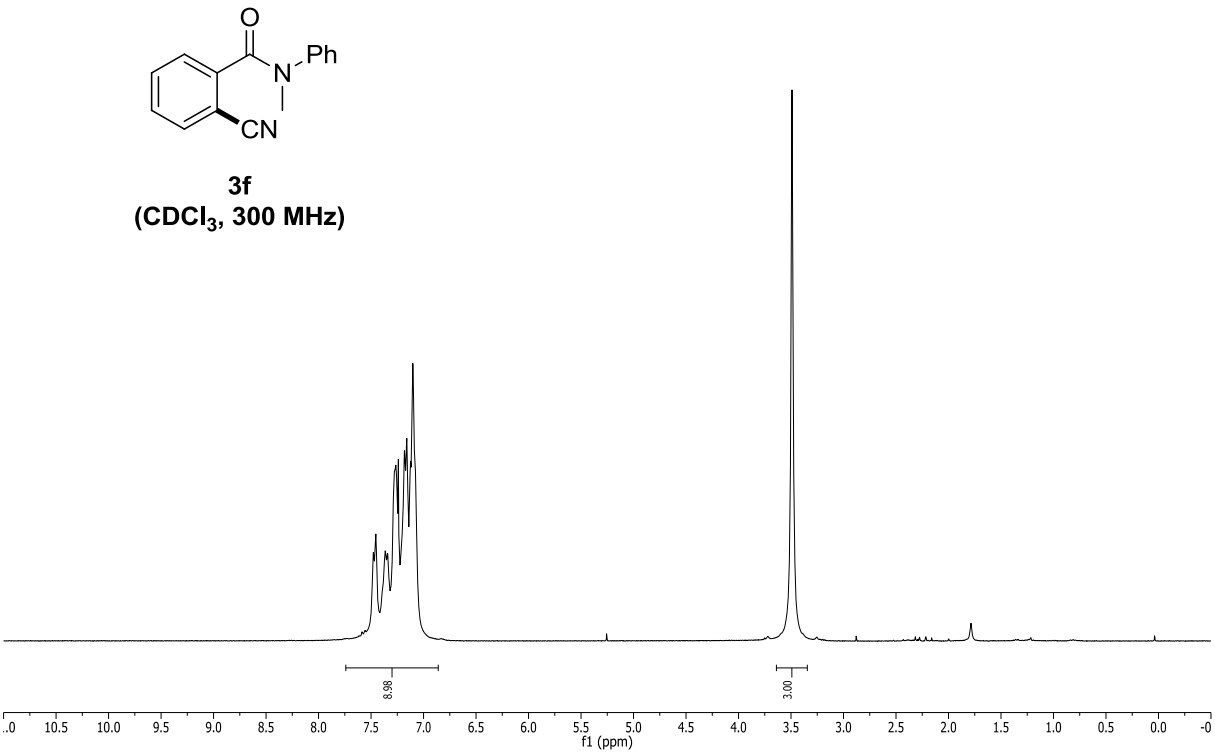




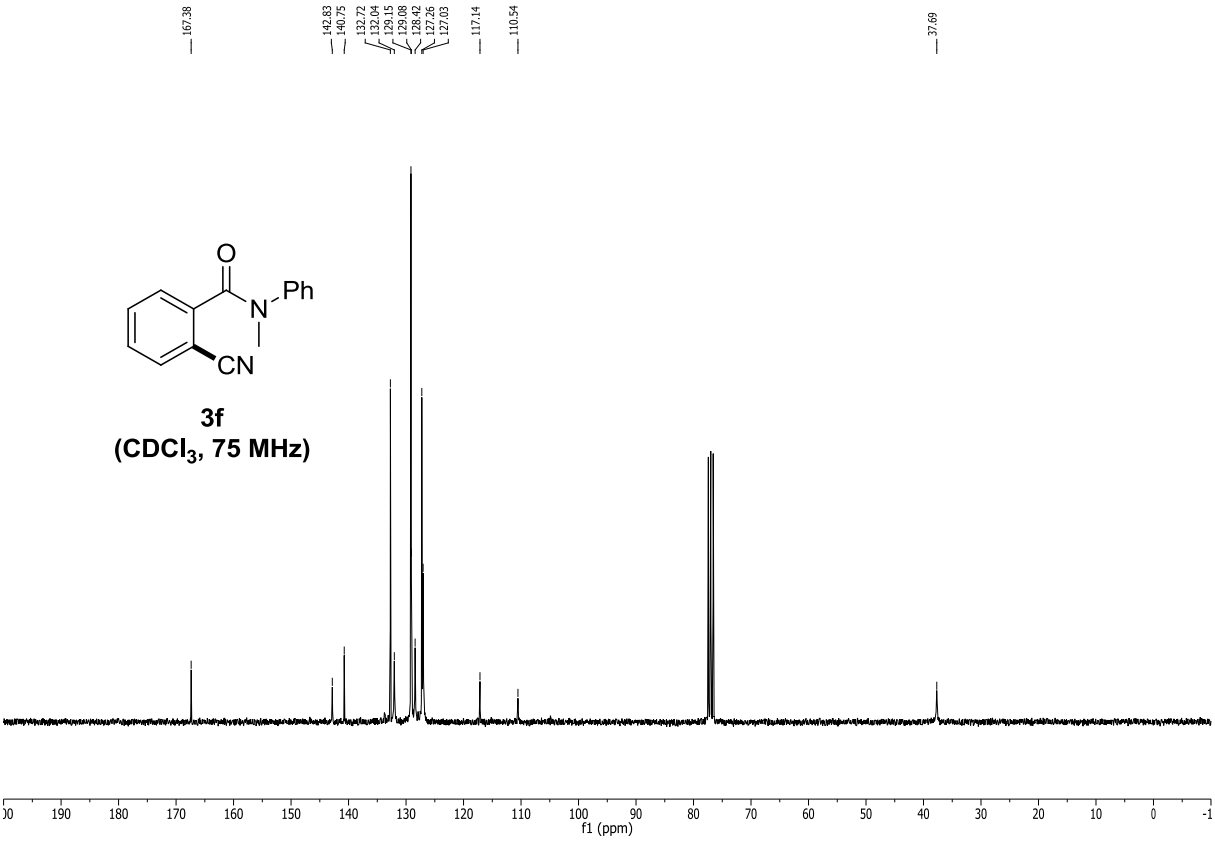
3d
($CDCl_3$, 75 MHz)


O
N
CN
3e
(CDCl3, 300 MHz)
2.00
1.98
2.16
2.14
4.38
f1 (ppm)

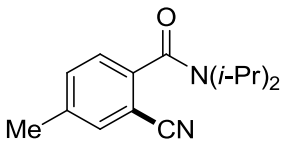

165.74
141.22
132.88
132.83
129.37
127.08
116.87
109.54
48.34
45.78
25.87
24.14
O
N
CN
3e
(CDCl3, 75 MHz)
f1 (ppm)



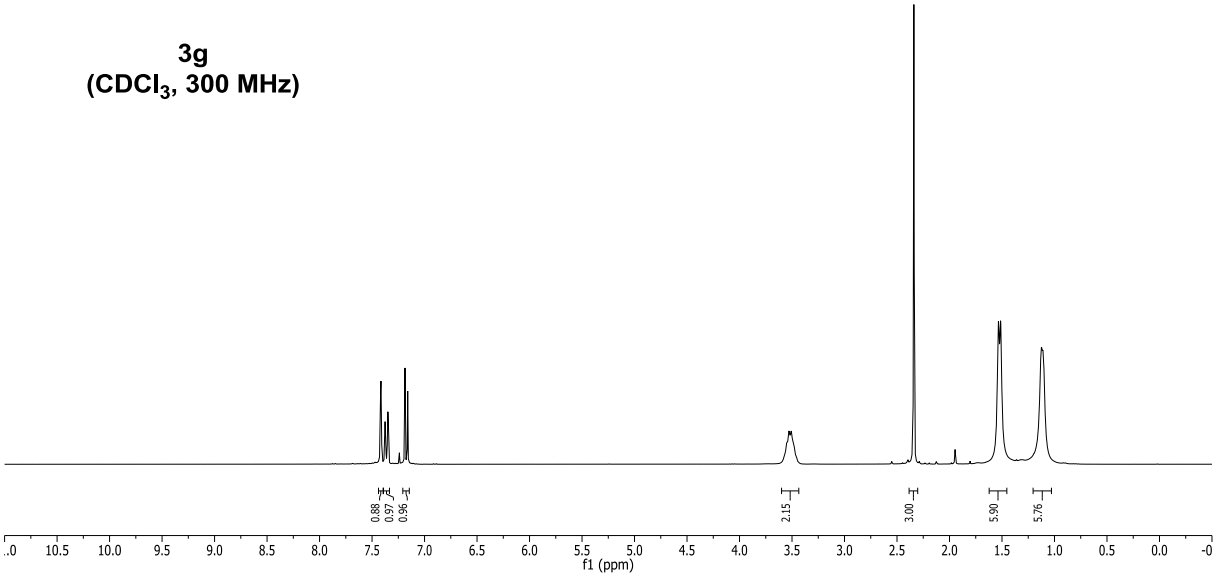
3f
($CDCl_3$, 300 MHz)

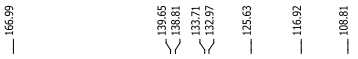


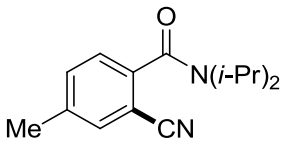
3f
($CDCl_3$, 75 MHz)



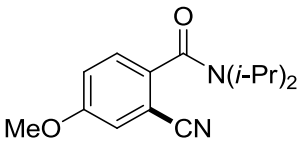
3g
($CDCl_3$, 300 MHz)







3g
($CDCl_3$, 75 MHz)



3h
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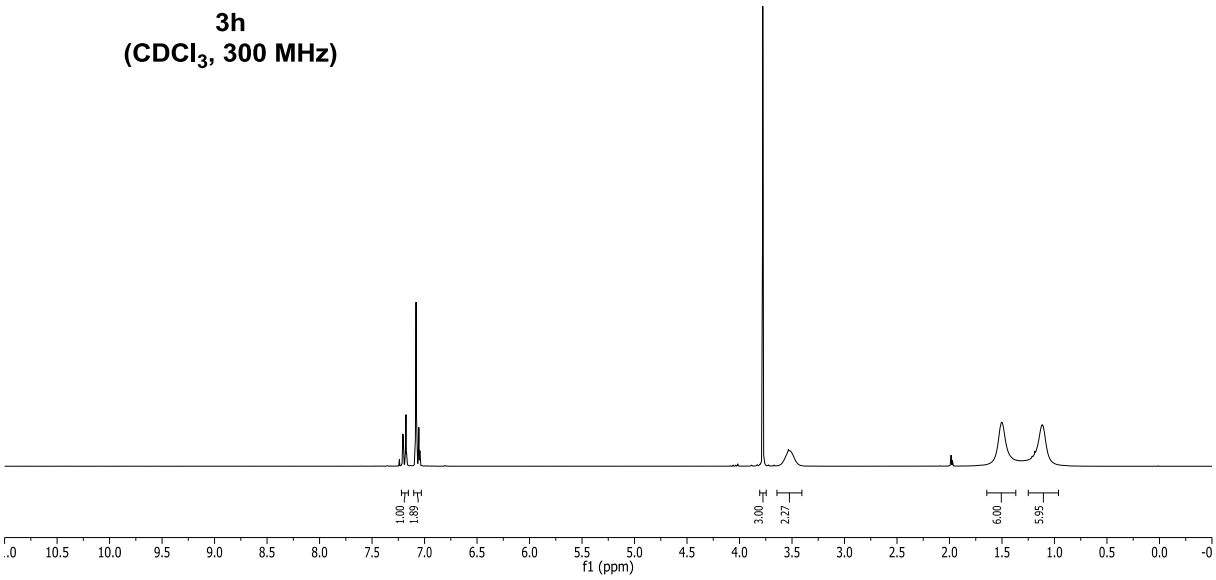
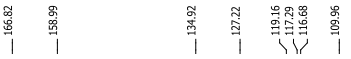
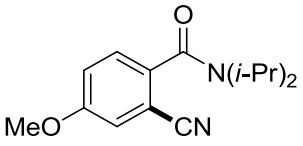
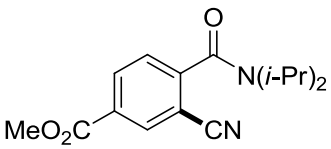


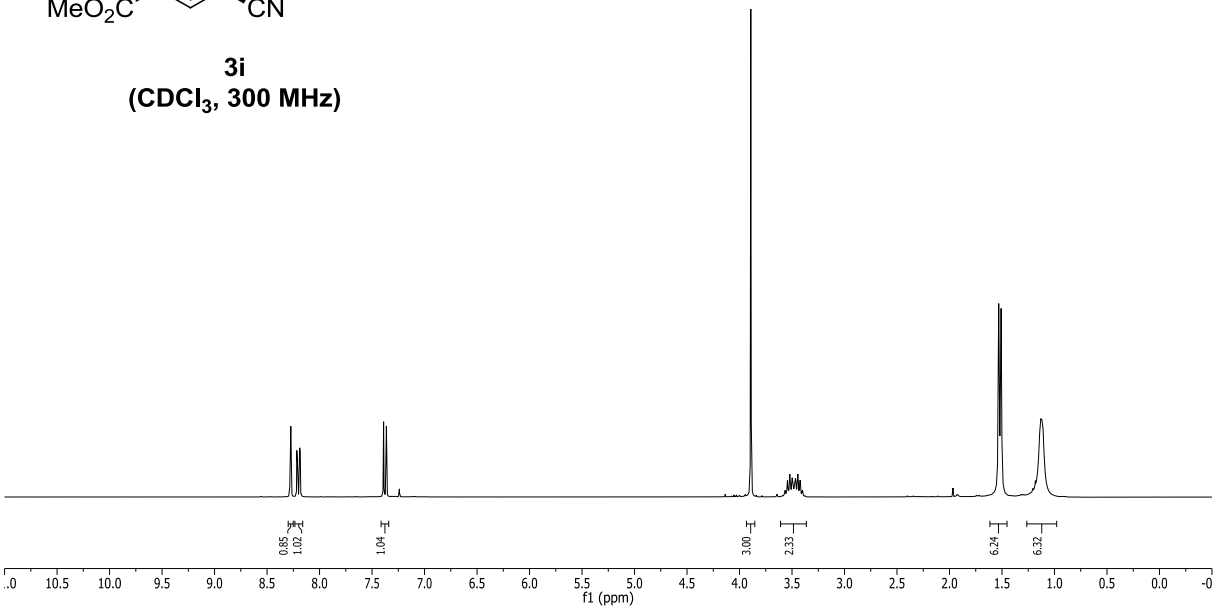


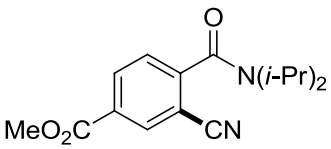


3h
($CDCl_3$, 75 MHz)



3i
($CDCl_3$, 300 MHz)





3i
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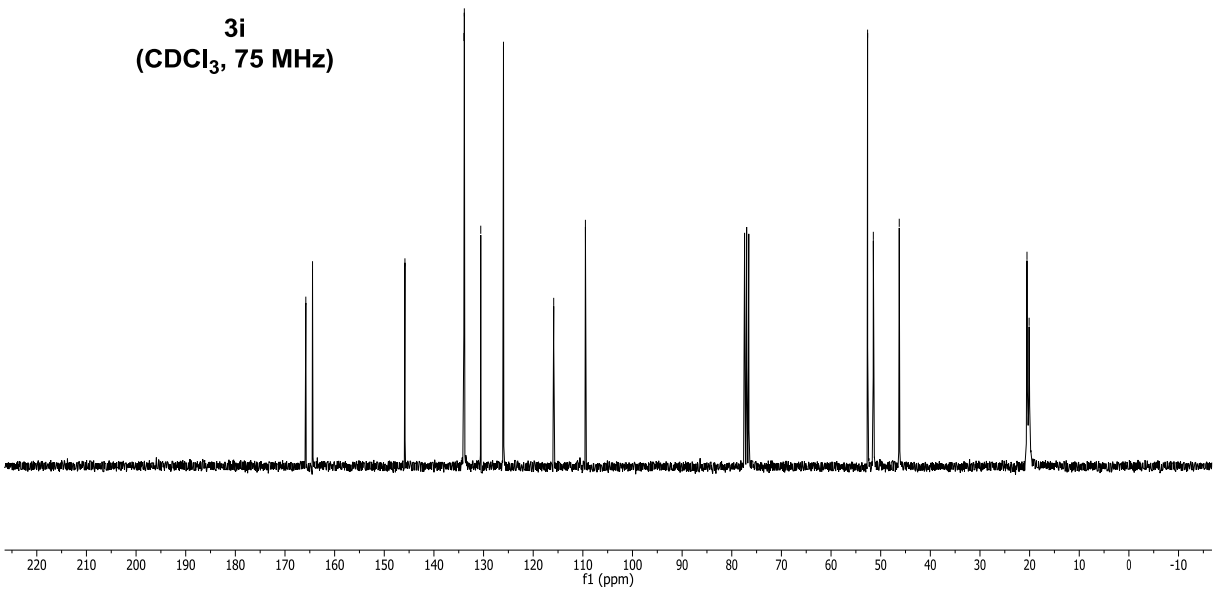

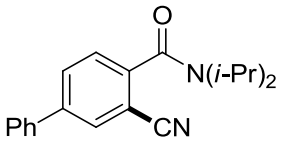

3j
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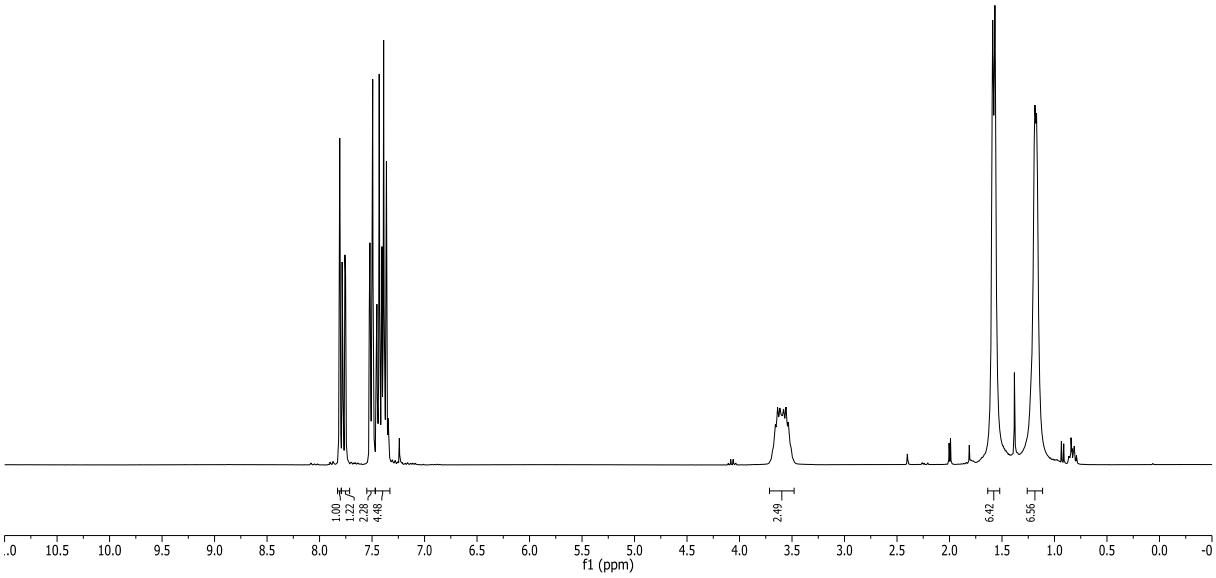
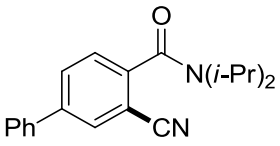
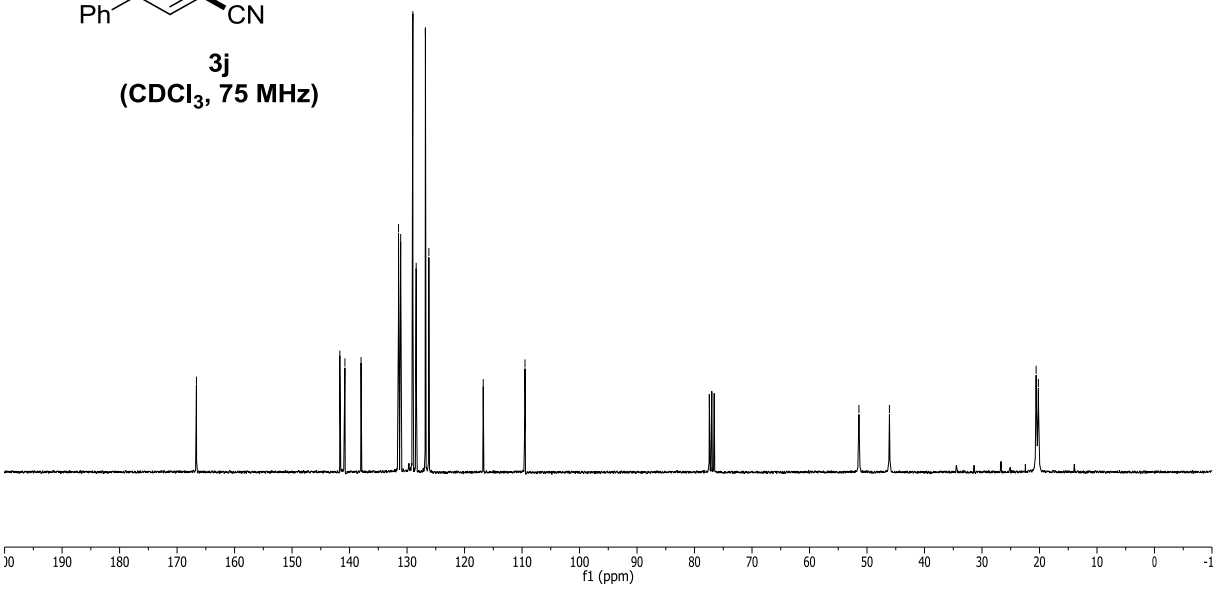
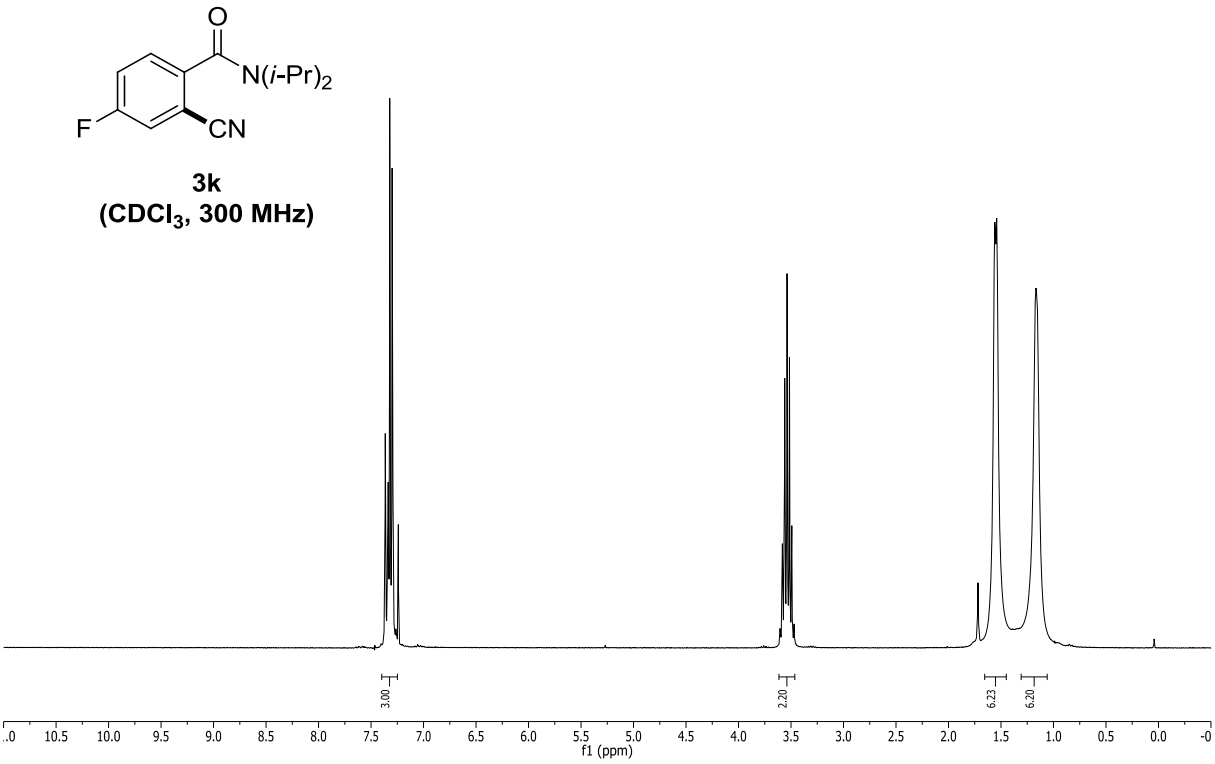
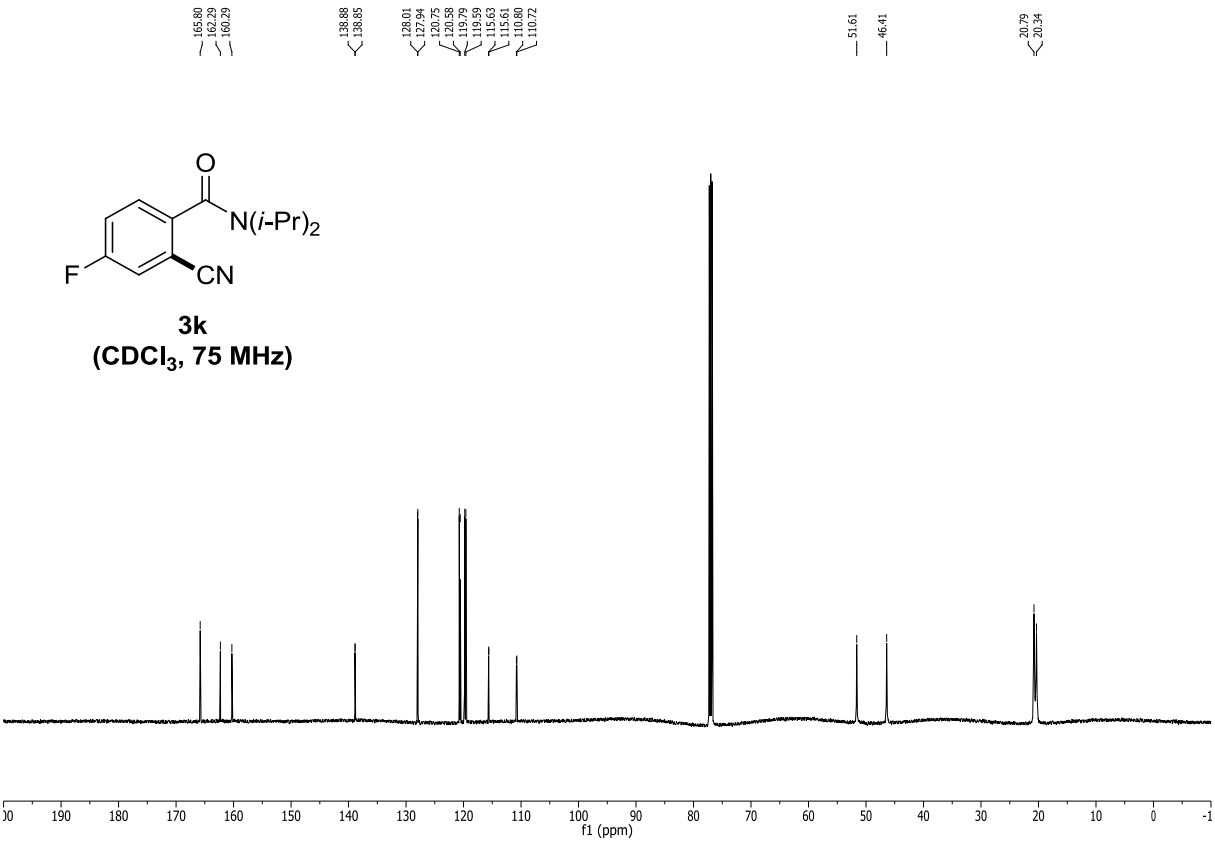


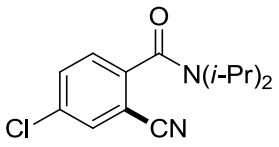


3j
($CDCl_3$, 75 MHz)

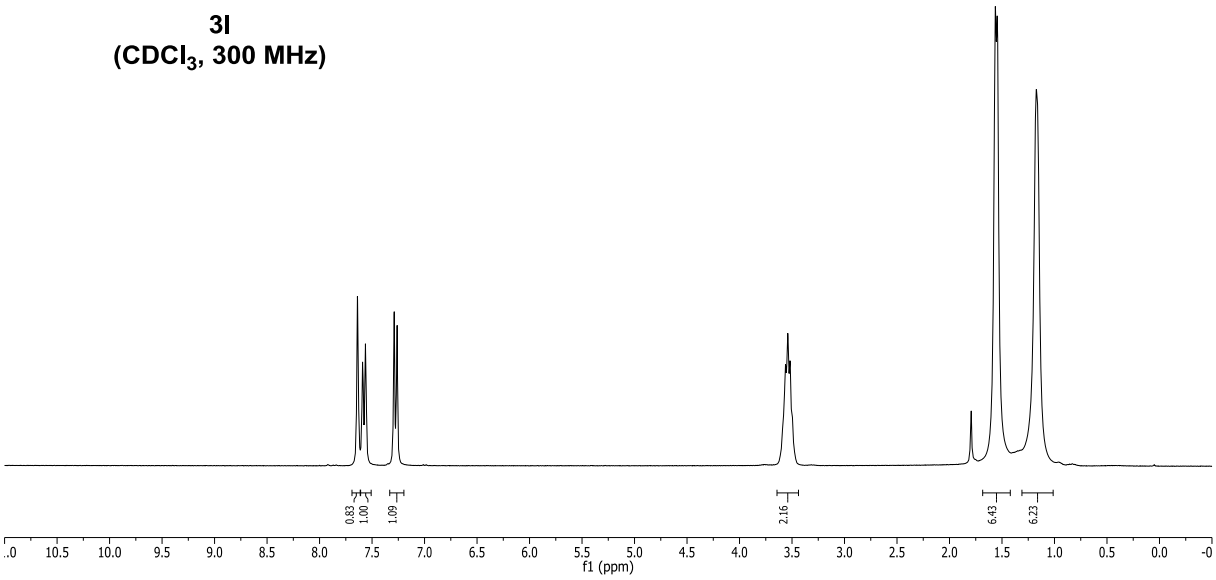


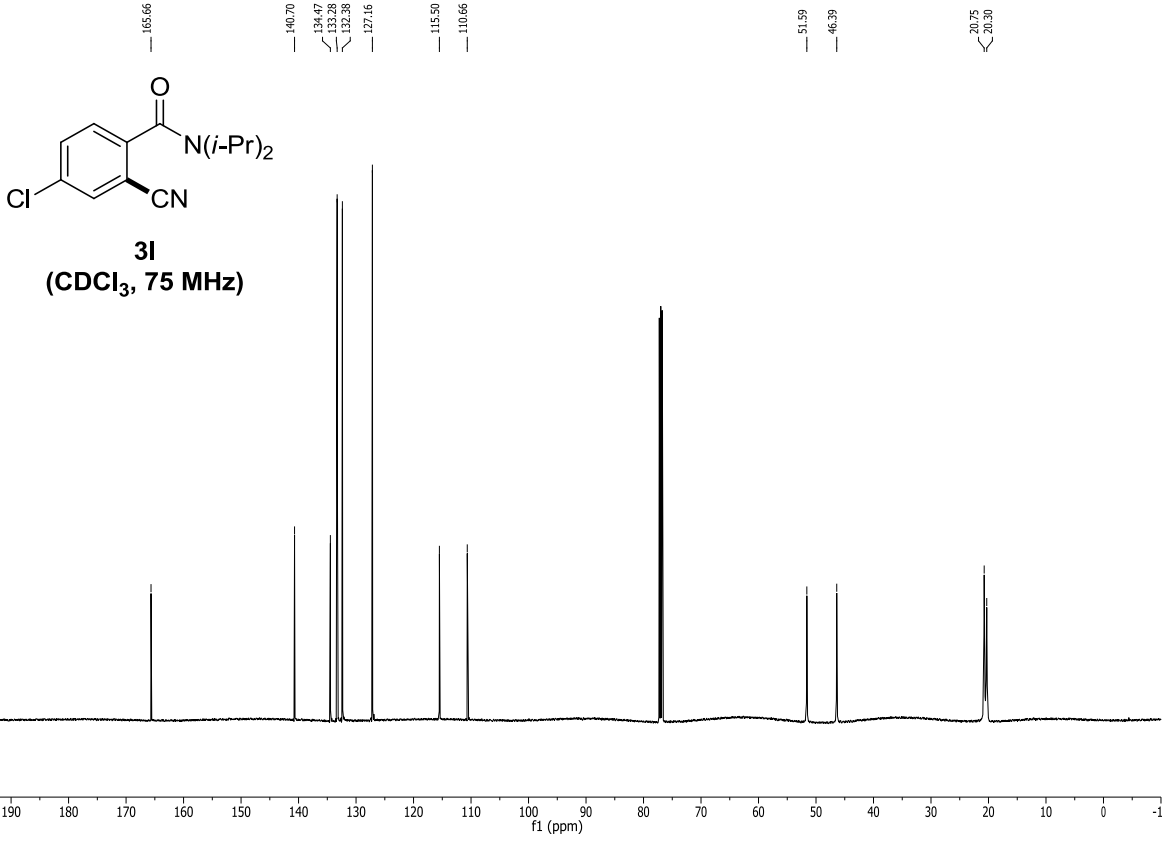

O
N(i-Pr)2
F
CN
3k
(CDCl3, 300 MHz)
3.00
2.20
6.23
6.20
f1 (ppm)


165.80
162.29
160.29
138.88
138.85
128.01
127.94
120.75
120.58
119.79
119.59
115.63
115.61
110.80
110.72
51.61
46.41
20.79
20.34
O
N(i-Pr)2
F
CN
3k
(CDCl3, 75 MHz)
f1 (ppm)



3l
($CDCl_3$, 300 MHz)





3l
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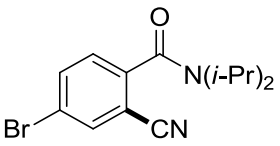
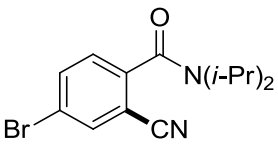
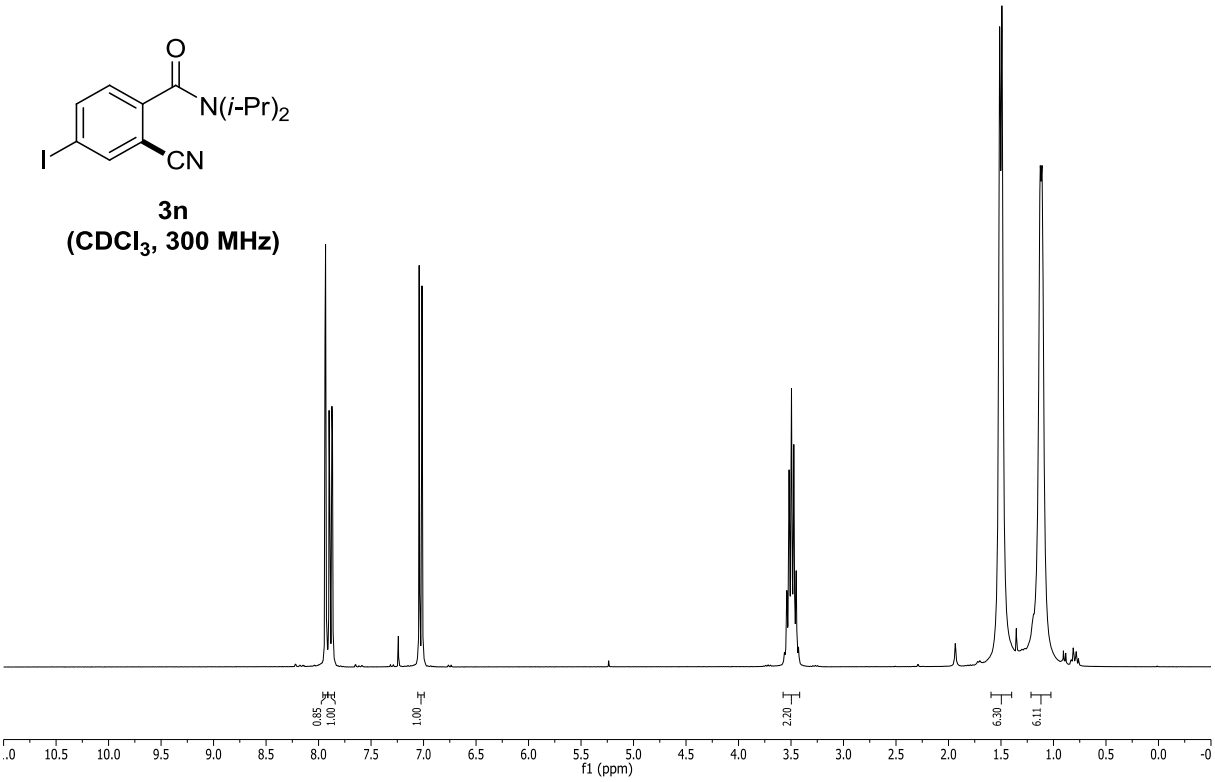
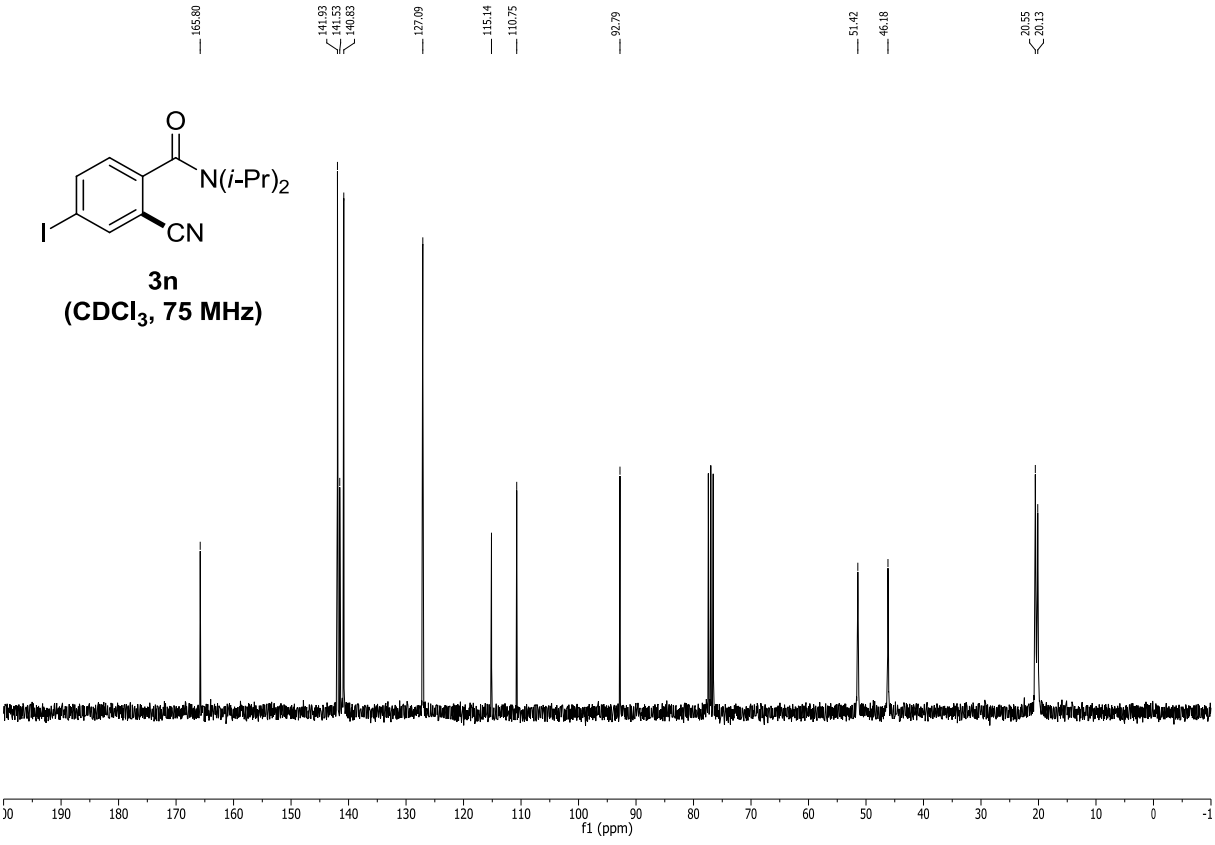


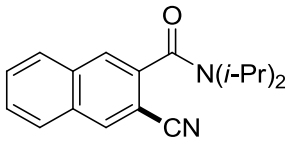
3m
($CDCl_3$, 300 MHz)



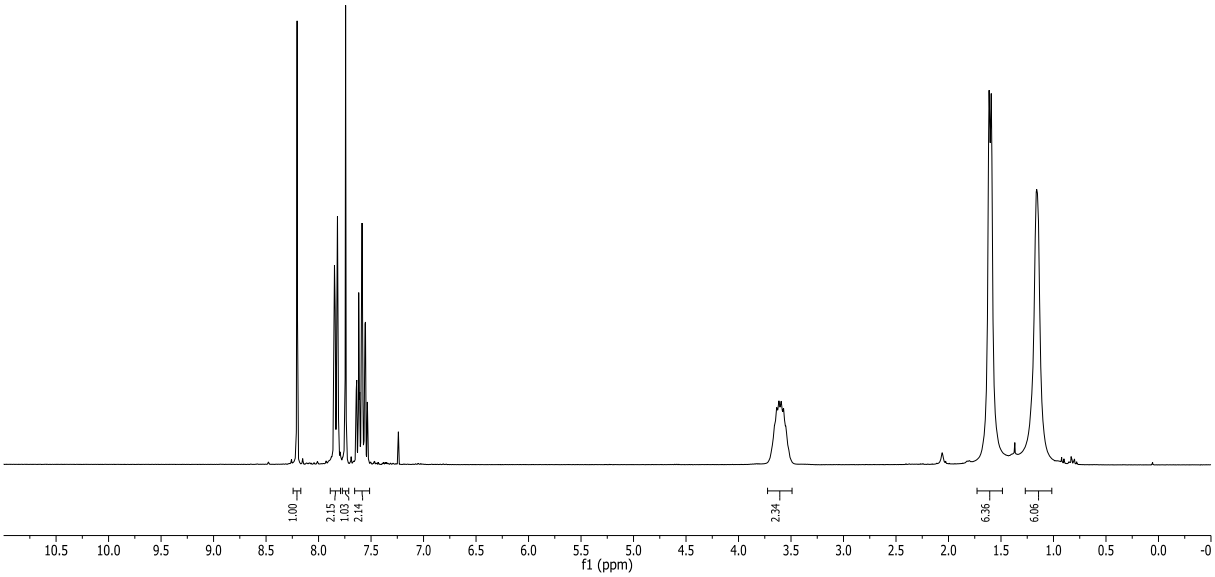
3m
($CDCl_3$, 75 MHz)

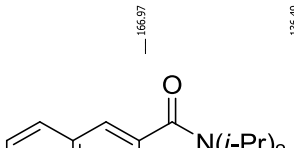

O
N(i-Pr)2
I
CN
3n
(CDCl3, 300 MHz)
0.85
1.00
1.00
2.20
6.30
6.11
f1 (ppm)


165.80
141.93
141.53
140.83
127.09
115.14
110.75
92.79
51.42
46.18
20.55
20.13
O
N(i-Pr)2
I
CN
3n
(CDCl3, 75 MHz)
f1 (ppm)

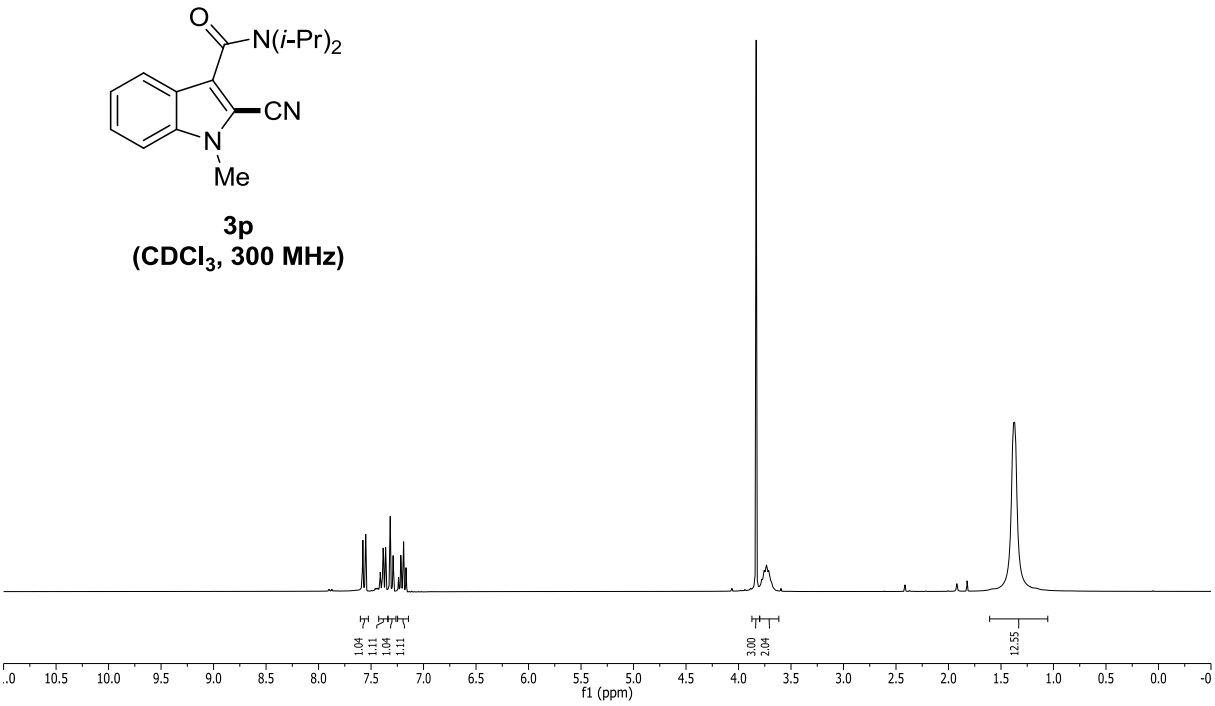


3o
($CDCl_3$, 300 MHz)

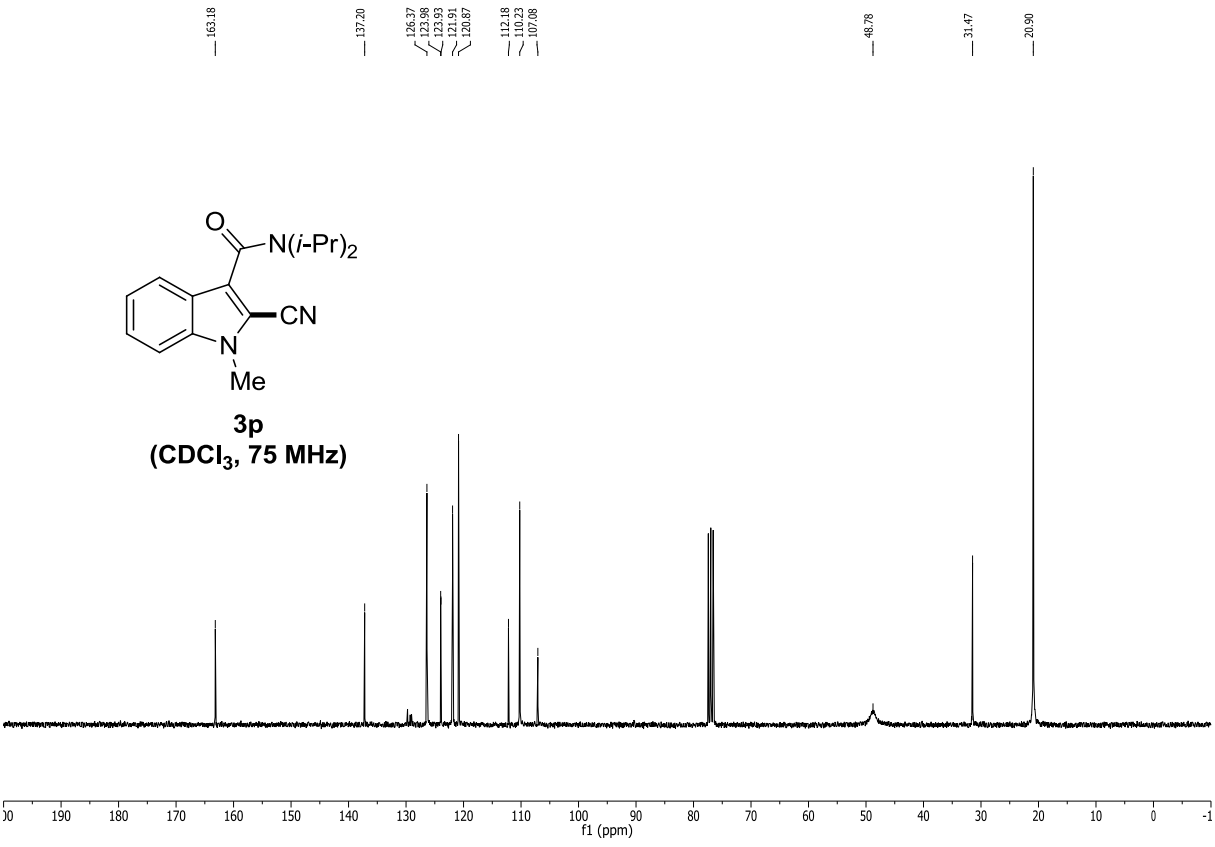




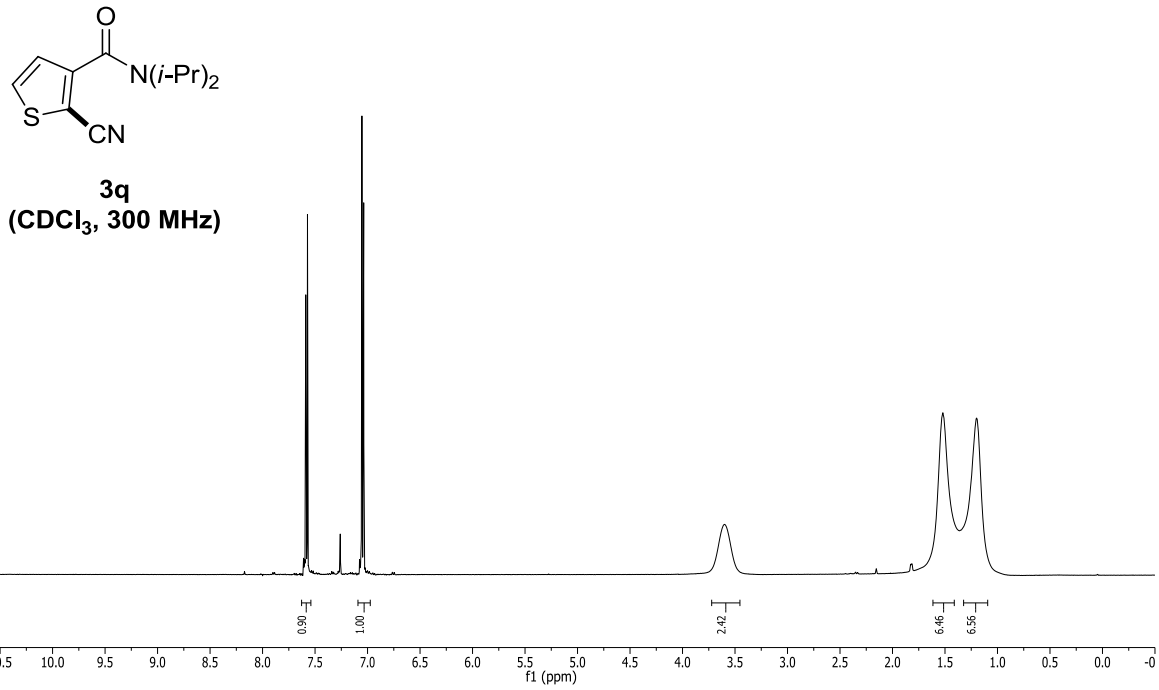
3o
($CDCl_3$, 75 MHz)



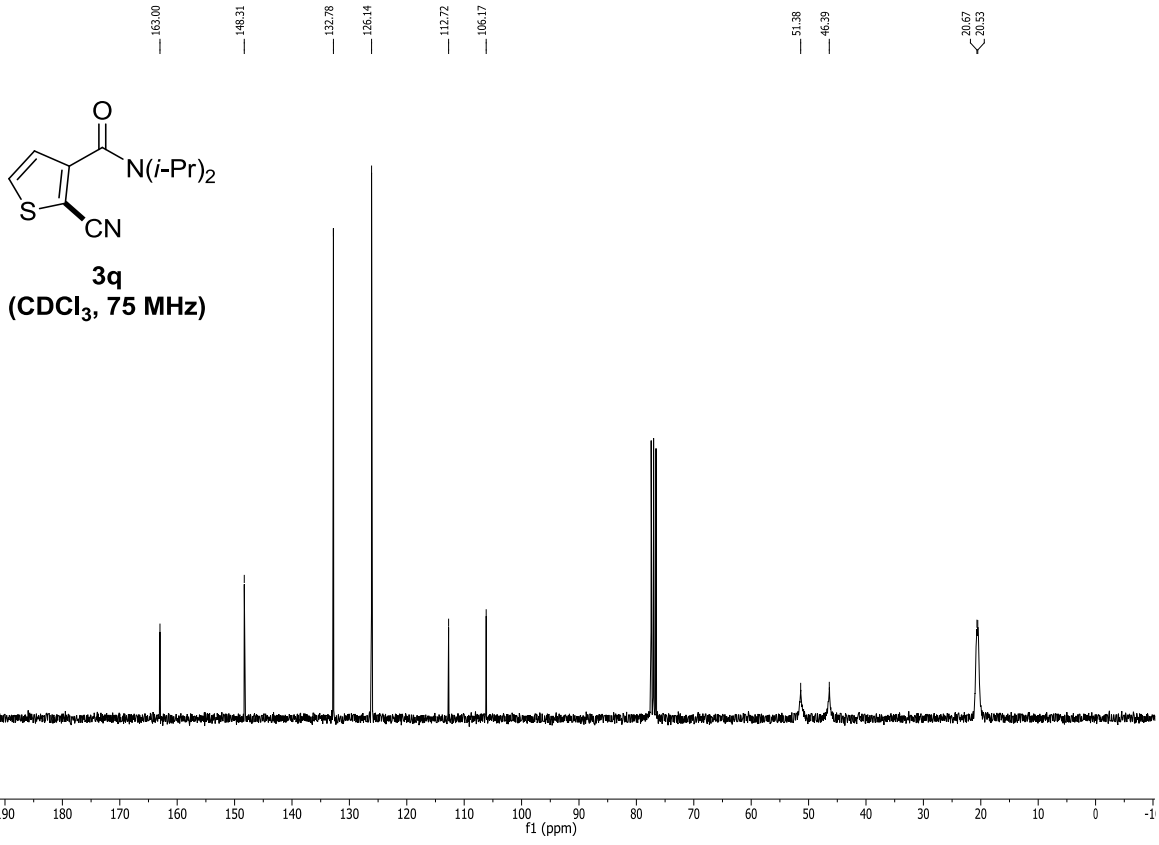
3p
($CDCl_3$, 300 MHz)



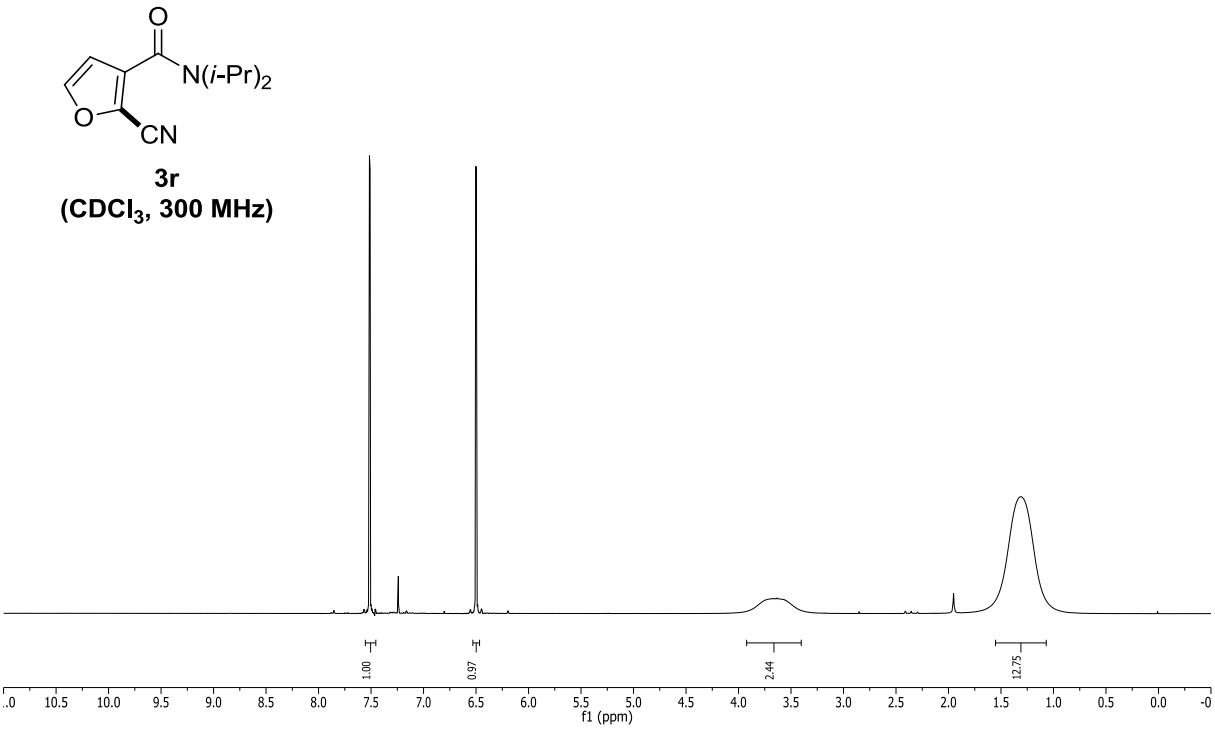
3p
($CDCl_3$, 75 MHz)

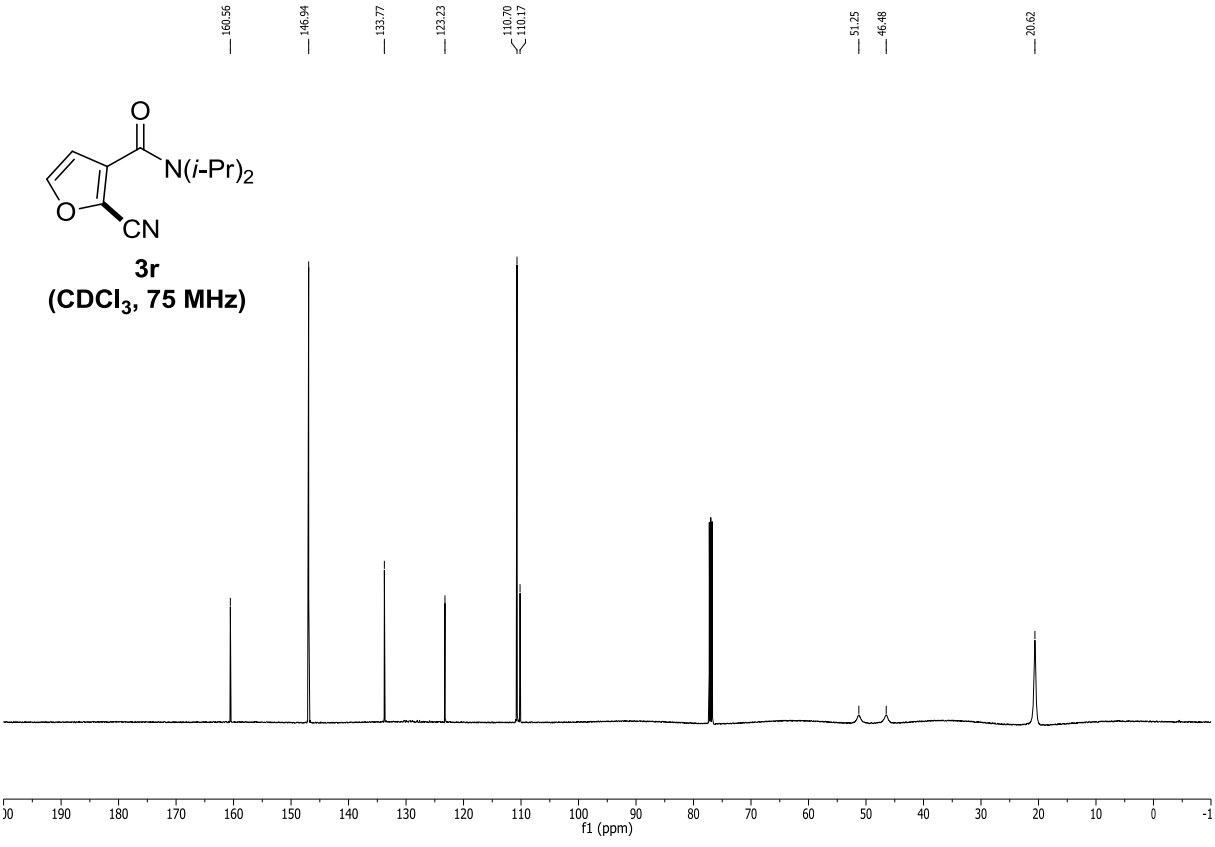


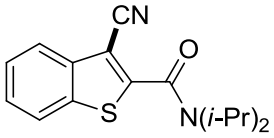
3q
($CDCl_3$, 300 MHz)



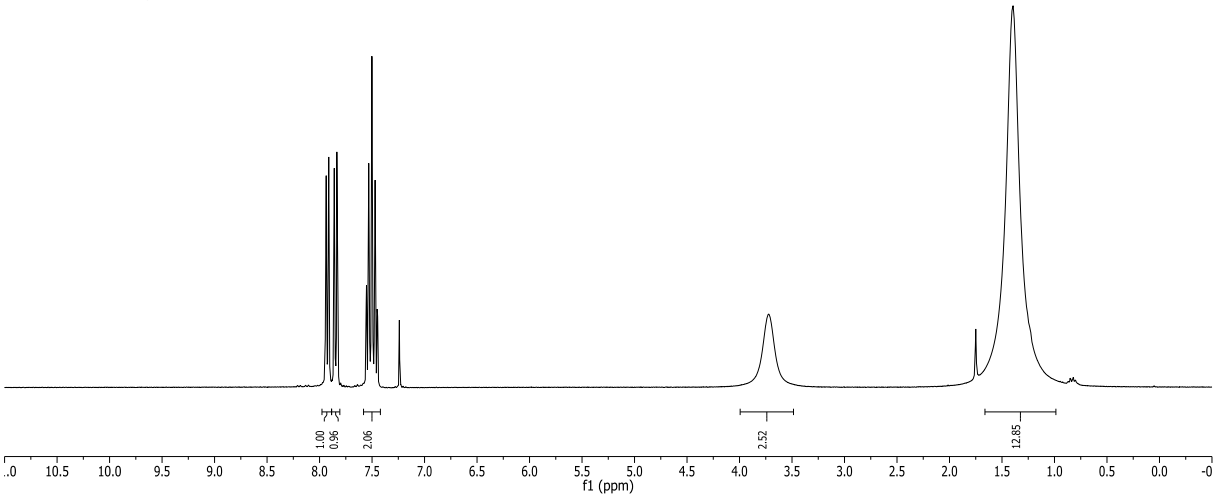
3q
($CDCl_3$, 75 MHz)

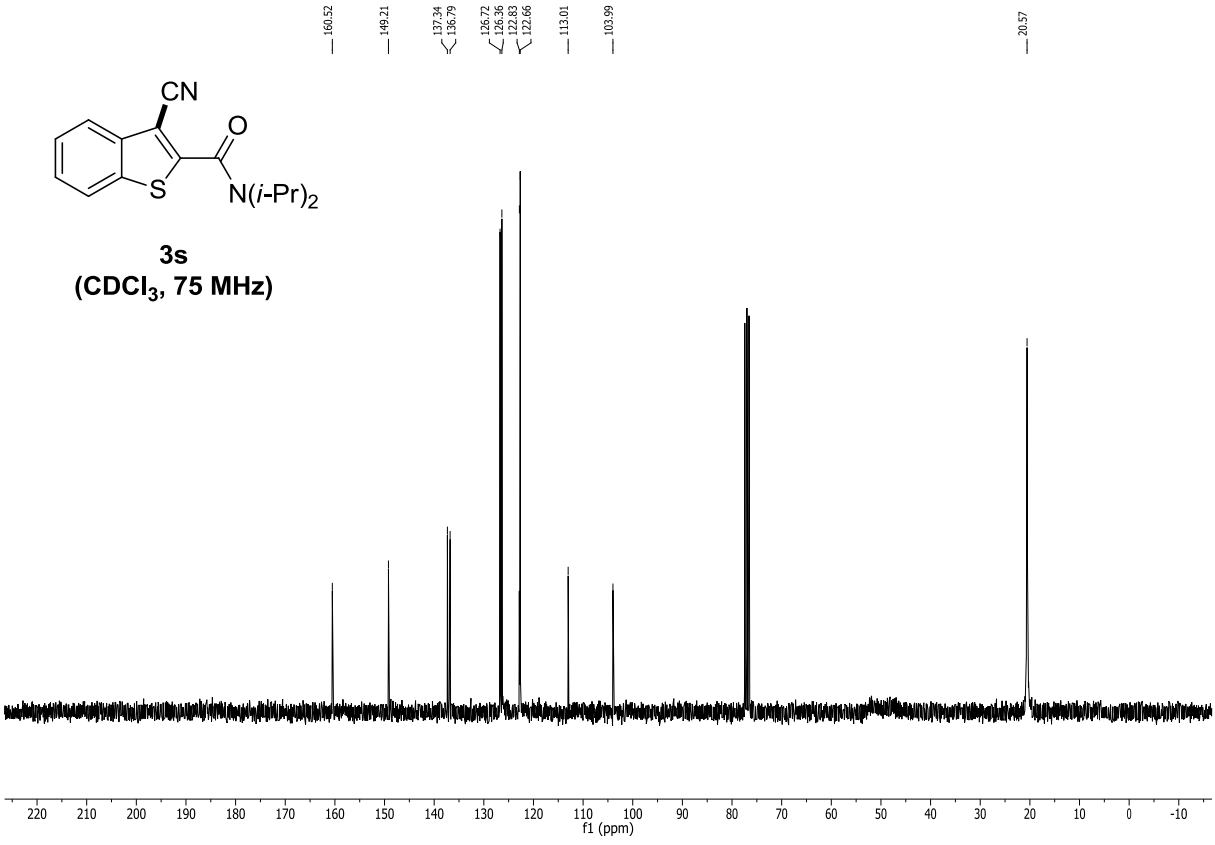

O
N(i-Pr)2
O
CN
3r
(CDCl3, 300 MHz)
1.00
0.97
2.44
12.75
f1 (ppm)


160.56
146.94
133.77
123.23
110.70
110.17
51.25
46.48
20.62
O
N(i-Pr)2
O
CN
3r
(CDCl3, 75 MHz)
f1 (ppm)

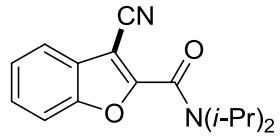


3s
($CDCl_3$, 300 MHz)

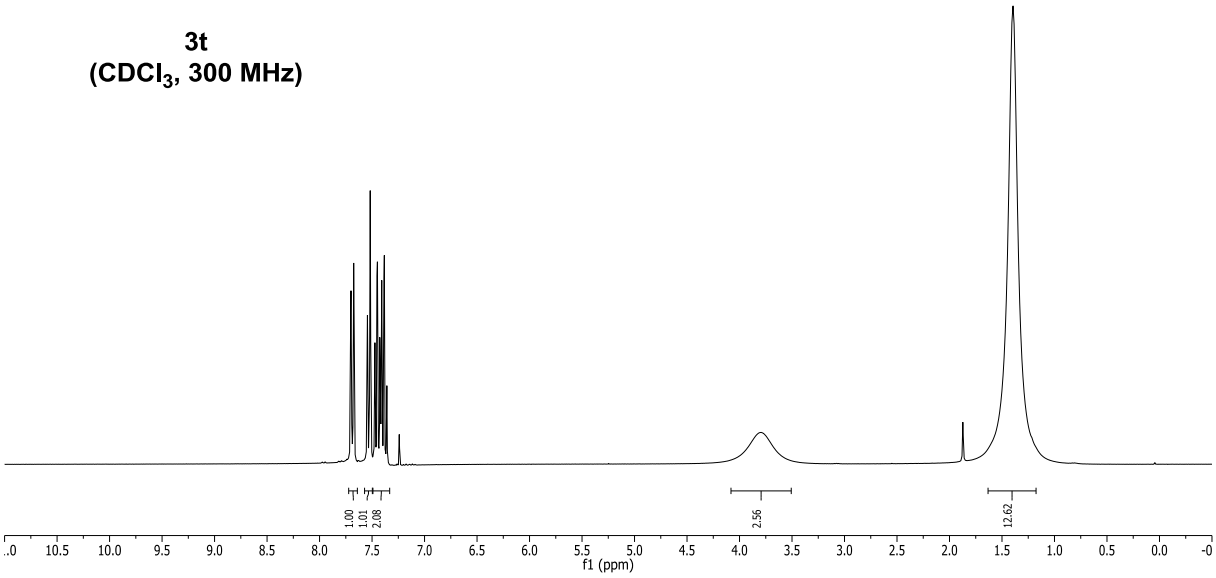


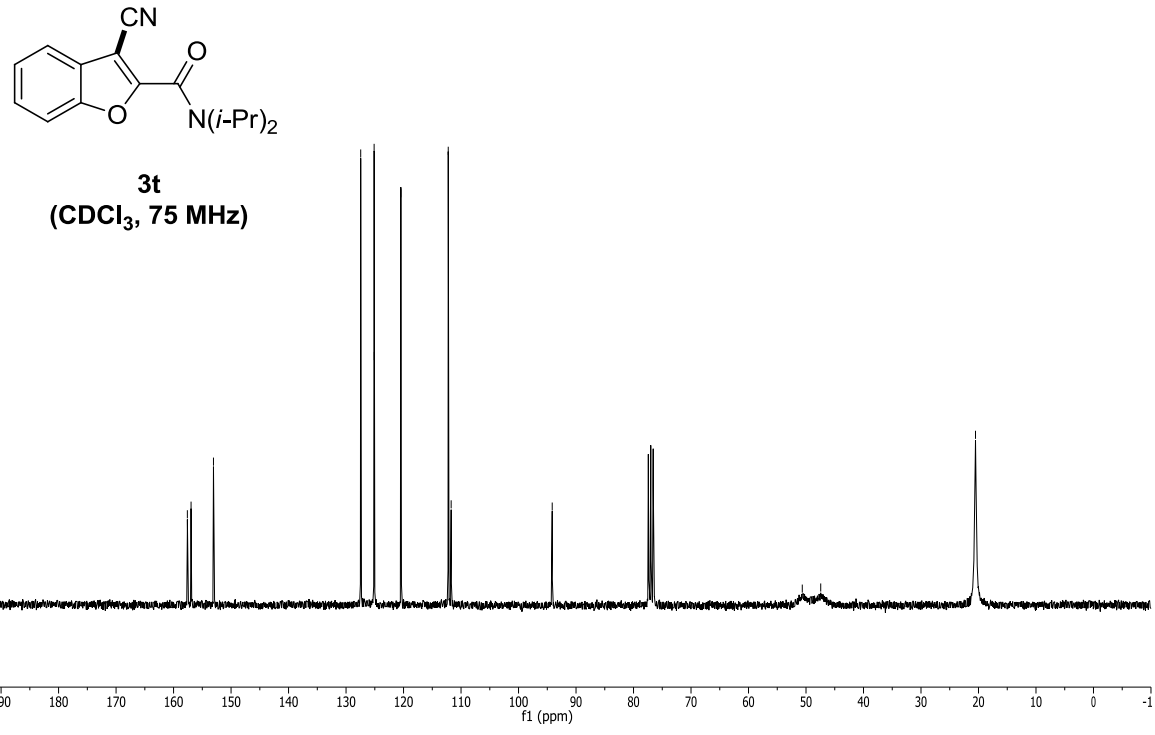


3s
($CDCl_3$, 75 MHz)

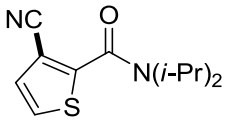


3t
($CDCl_3$, 300 MHz)

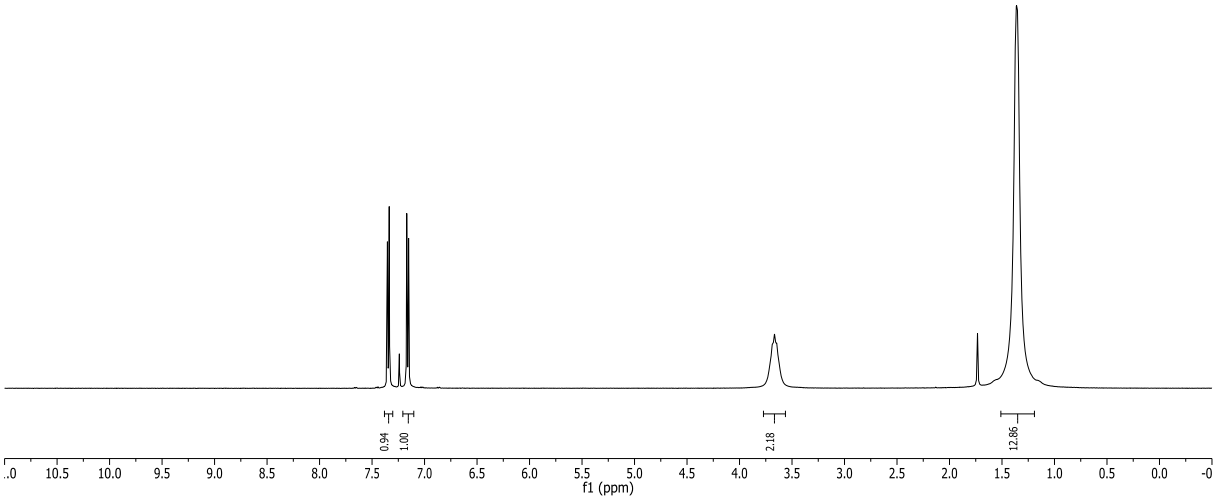


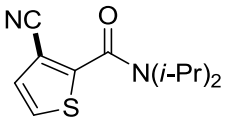


3t
($CDCl_3$, 75 MHz)

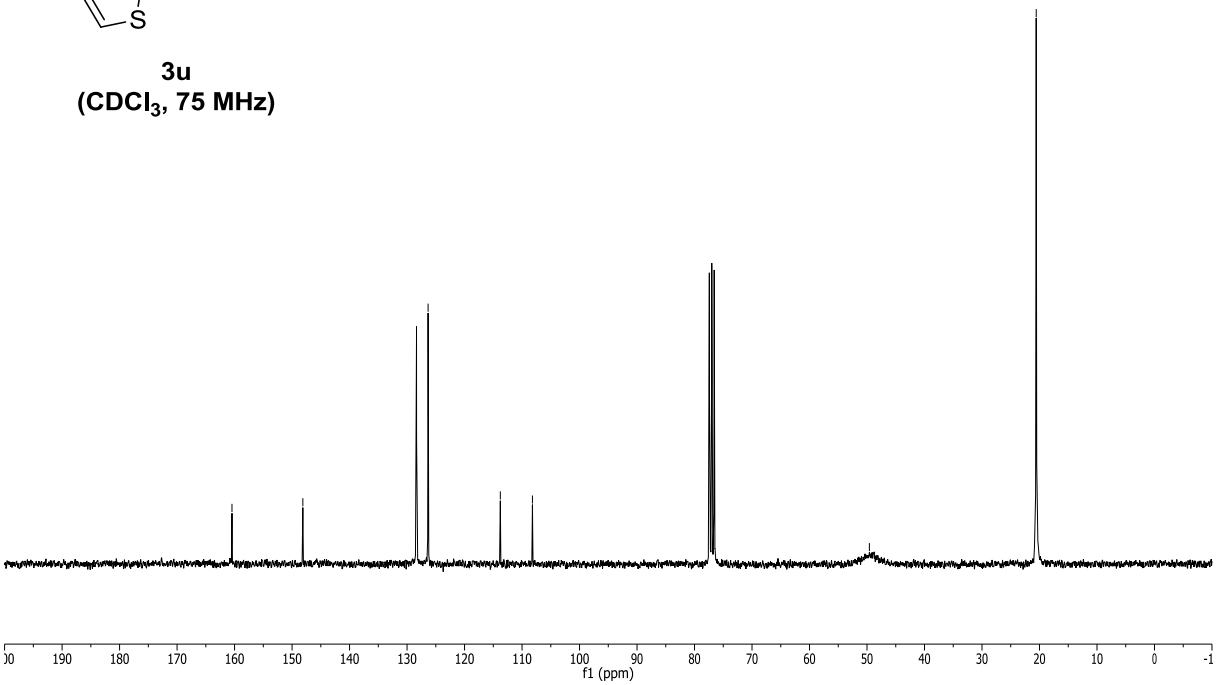


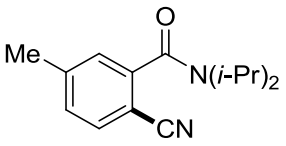
3u
($CDCl_3$, 300 MHz)



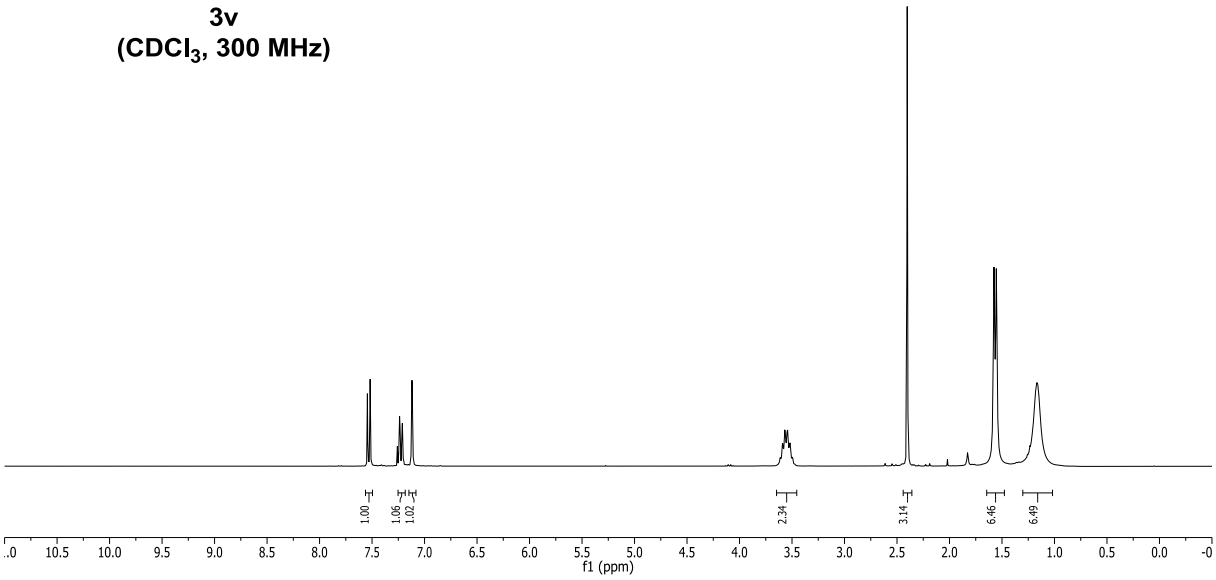


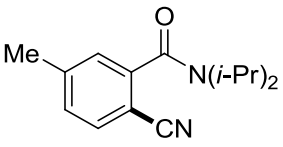
3u
($CDCl_3$, 75 MHz)



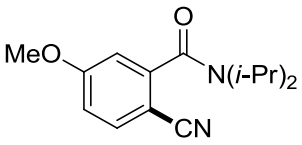


3v
($CDCl_3$, 300 MHz)

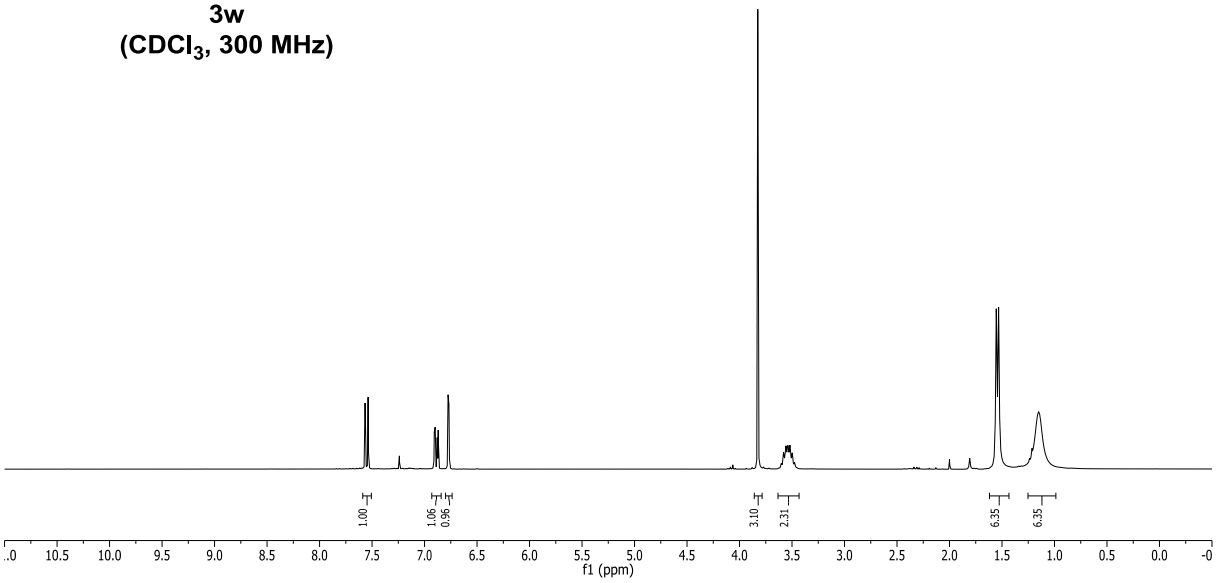


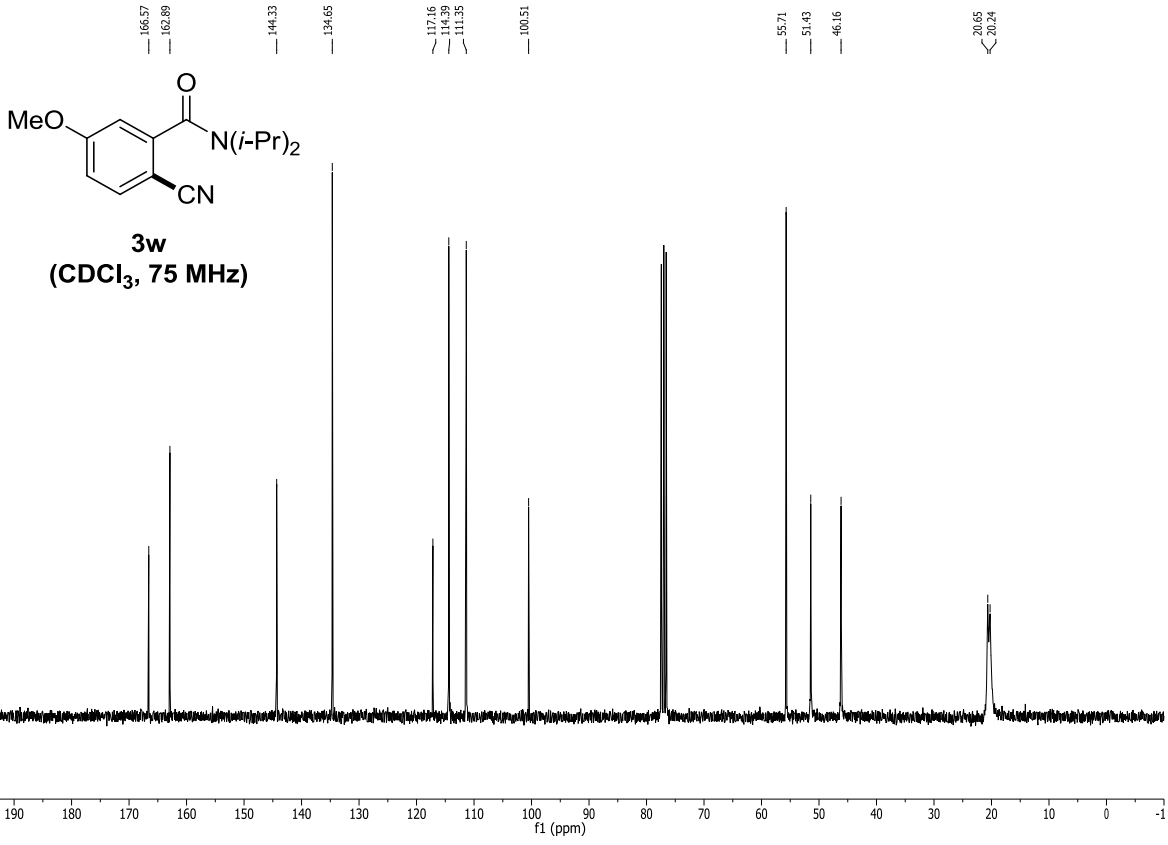


3v
($CDCl_3$, 75 MHz)

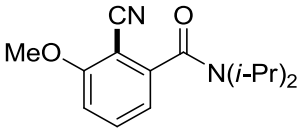


3w
($CDCl_3$, 300 MHz)

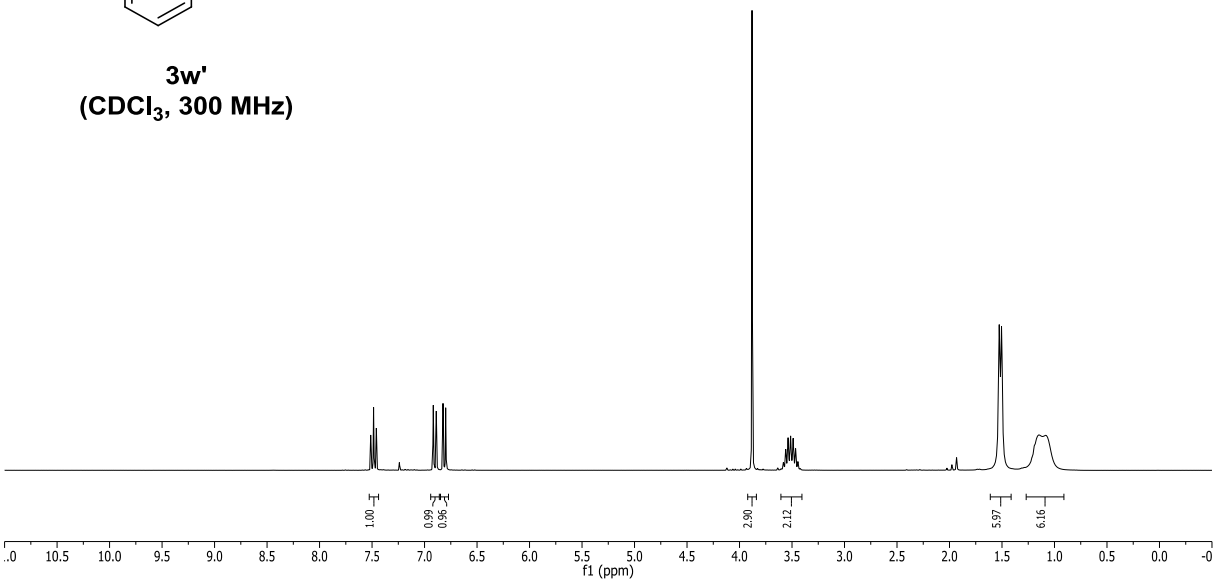


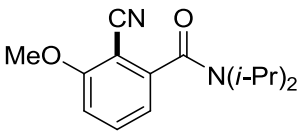


3w
($CDCl_3$, 75 MHz)

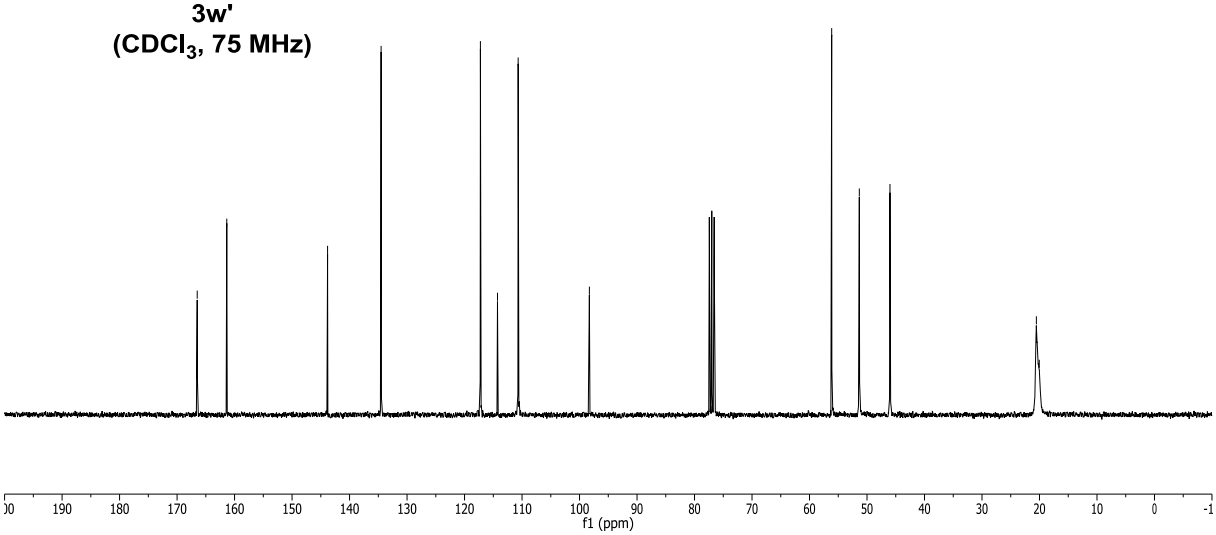


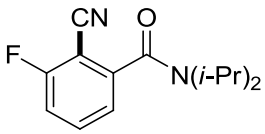
3w'
($CDCl_3$, 300 MHz)



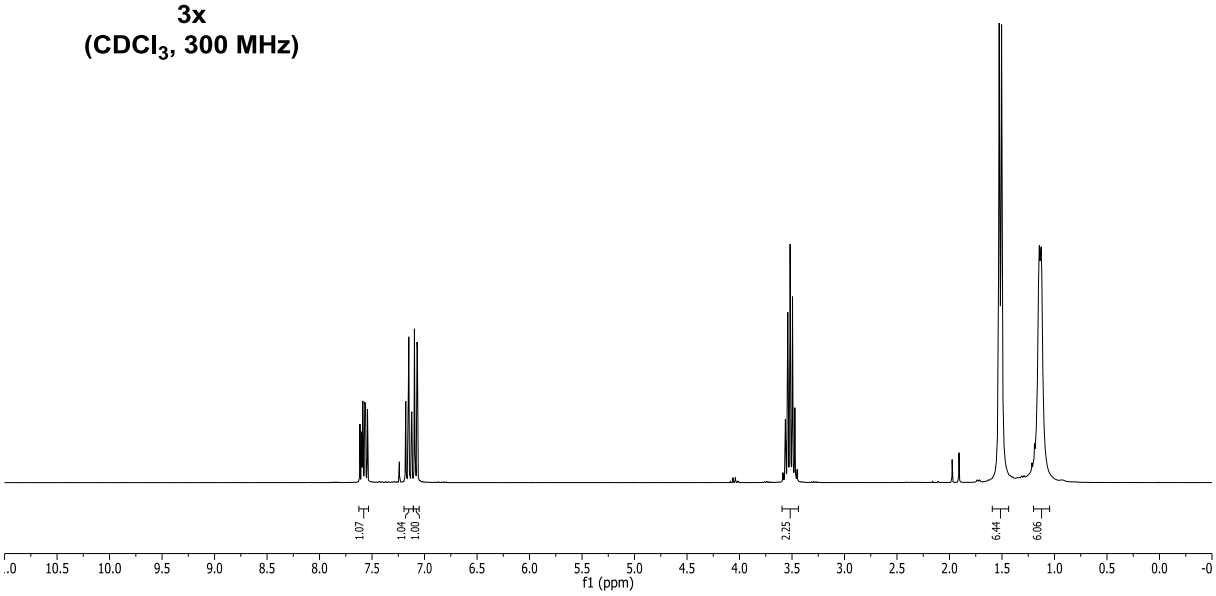


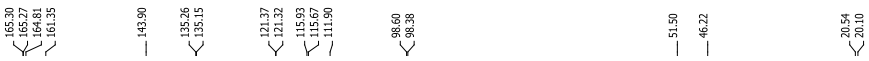
3w'
($CDCl_3$, 75 MHz)

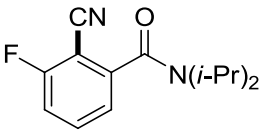




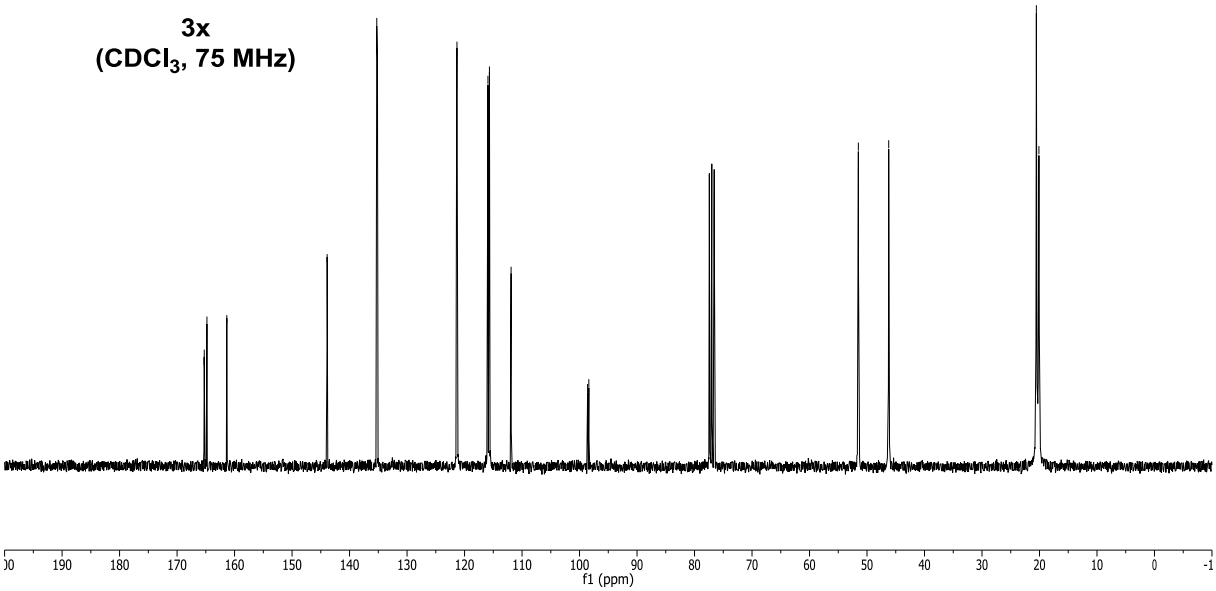
3x
($CDCl_3$, 300 MHz)

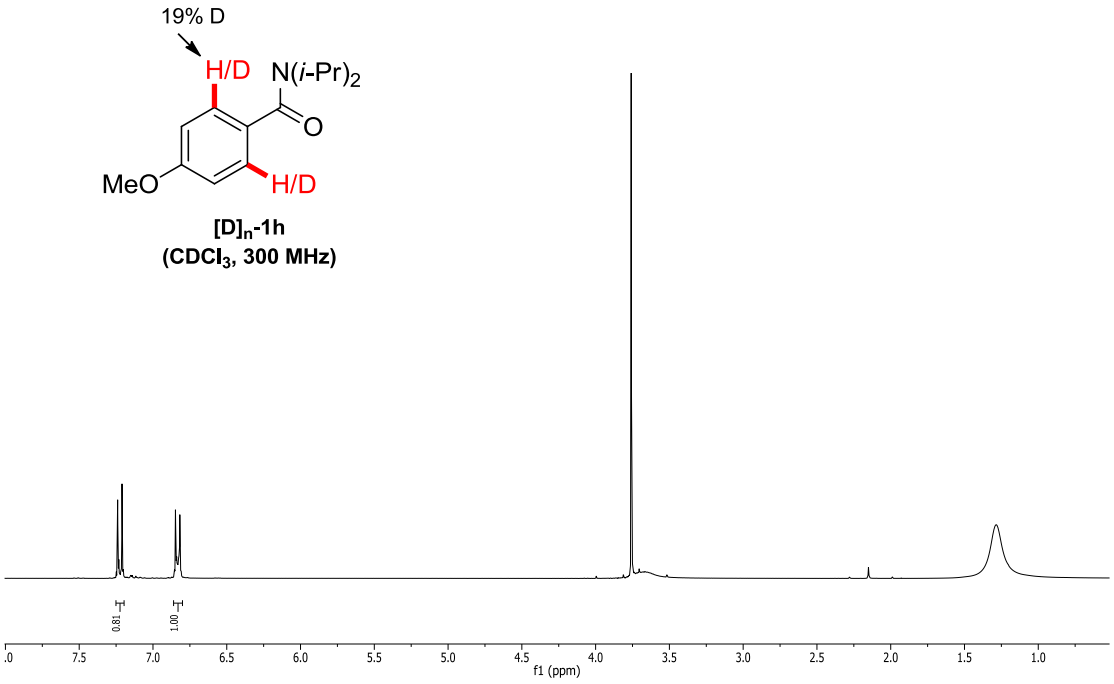




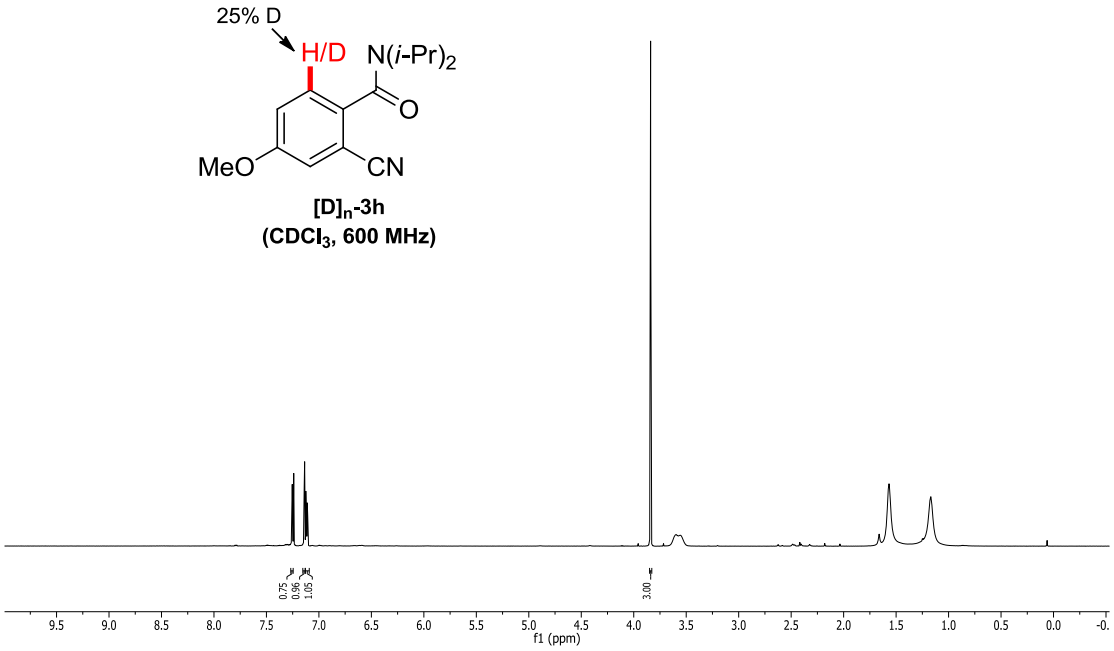


3x
($CDCl_3$, 75 MHz)

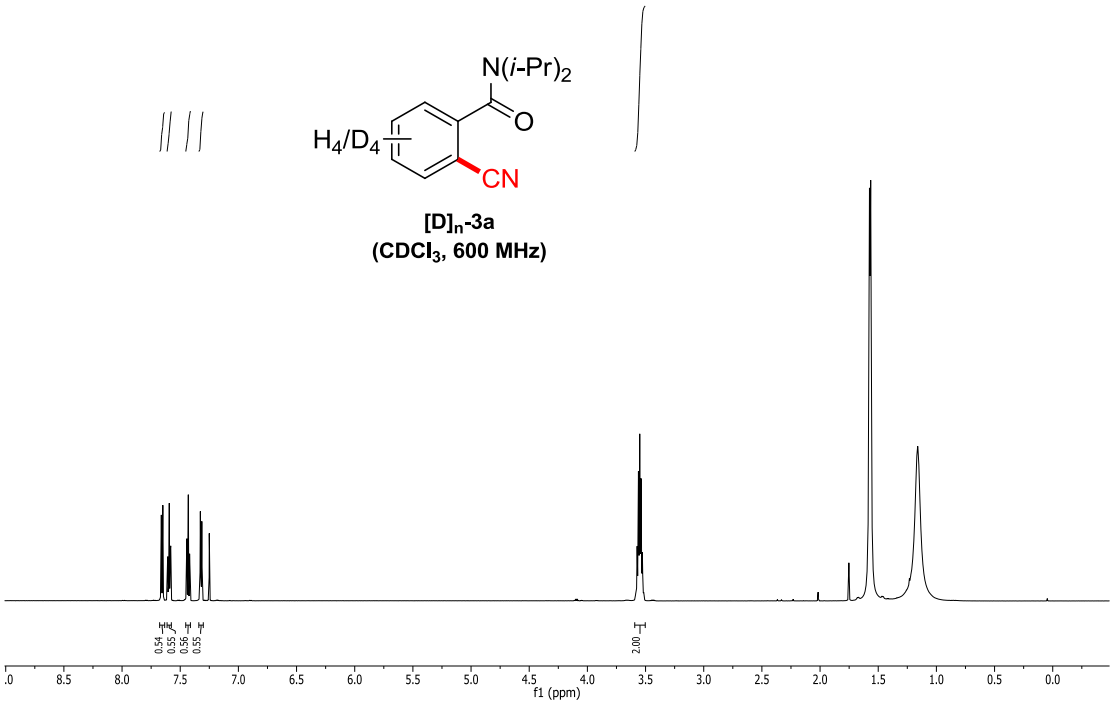




$[D]_n$-1h
($CDCl_3$, 300 MHz)



$[D]_n$-3h
($CDCl_3$, 600 MHz)


N(i-Pr)2
O
H4/D4
CN
[D]n-3a
(CDCl3, 600 MHz)
0.54
0.55
0.56
0.55
2.00
f1 (ppm)