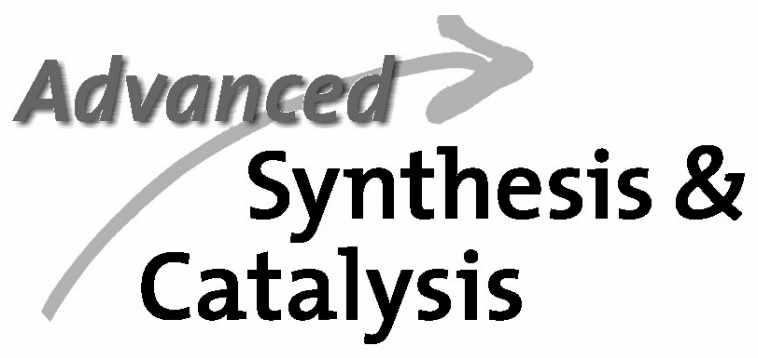

Supporting Information

Palladium-Catalyzed Direct Arylations of 1,2,3-Triazoles with Aryl Chlorides Using Conventional Heating

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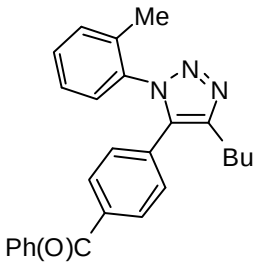
General remarks

Catalytic reactions were carried out under a N_2 atmosphere using pre-dried glassware. Triazoles **1** were prepared in analogy to previously described methodologies.[1-4] Additional starting materials 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, unless otherwise indicated. Flash chromatography: Macherey-Nagel silica gel 60 (70-230 mesh). NMR: Spectra were recorded on Varian-NMR 300, 500 or 600 instruments in the solvent indicated; chemical shifts (δ) are given in ppm.

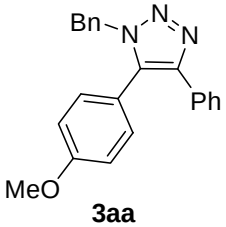
Representative Procedure for Palladium-Catalyzed Direct Arylations: Preparation of Triazole 3av (Table 3, entry 9).

A suspension of $Pd(OAc)_2$ (9.0 mg, 4.0 mol %), PCy_3 (22 mg, 8.0 mol %), K_2CO_3 (276 mg, 2.00 mmol), **1i** (215 mg, 1.00 mmol) and **2k** (325 mg, 1.50 mmol) in PhMe (2 mL) was stirred under N_2 for 22 h at 120 °C. Et_2O (75 mL) and H_2O (75 mL) were added to the cold reaction mixture. The separated aqueous phase was extracted with Et_2O (2 × 75 mL). The combined organic layers were washed with aqueous NH_4Cl (50 mL), H_2O (50 mL) and brine (50 mL), dried over Na_2SO_4 and concentrated in vacuum. The remaining residue was purified by column chromatography on silica gel (*n*-hexane/EtOAc 5:1) to yield **3av** as a colourless oil (382 mg, 95%).



3av

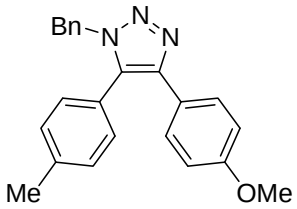
[4-(5-Butyl-3-*o*-tolyl-3*H*-1,2,3-triazol-4-yl)-phenyl]-phenyl-methanone (3av): ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.76-7.69 (m, 4H), 7.60-7.53 (m, 1H), 7.48-7.42 (m, 2H), 7.36-7.29 (m, 1H), 7.24-7.17 (m, 5H), 2.82 (t, *J* = 8.0 Hz, 2H), 1.95 (s, 3H), 1.77 (quint, *J* = 7.9 Hz, 2H), 1.39 (tq, *J* = 7.5, 7.5 Hz, 2H), 0.91 (t, *J* = 7.3 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 195.8 (C_q), 145.8 (C_q), 137.4 (C_q), 137.0 (C_q), 135.8 (C_q), 135.0 (C_q), 133.9 (C_q), 132.7 (CH), 131.5 (C_q), 131.2 (CH), 130.3 (CH), 130.0 (CH), 129.9 (CH), 128.8 (CH), 128.4 (CH), 127.6 (CH), 126.8 (CH), 31.7 (CH_2), 25.1 (CH_2), 22.5 (CH_2), 17.6 (CH_3), 13.8 (CH_3). IR (NaCl): 2957, 2860, 1660, 1610, 1498, 1447, 1317, 1177, 996, 939, 924, 857, 766, 668 cm^{-1}. MS (EI) *m/z* (relative intensity) 395 (3) [M^+], 367 (65), 324 (100), 207 (31), 179 (8), 158 (8), 118 (9), 105 (29), 91 (15), 77 (12), 65 (8). HR-MS (ESI) *m/z* calcd for $C_{26}H_{26}N_3O$ 396.2070, found 396.2072. The spectral data were in accordance with those reported in the literature.[5]



3aa

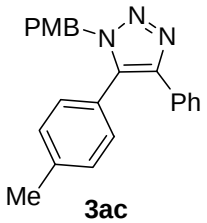
1-Benzyl-5-(4-methoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole (3aa, Table 1, entry 14): The representative procedure was followed using **1a** (235 mg, 1.00 mmol) and **2a** (175 mg, 1.22 mmol) in 1,4-dioxane (2.0 mL) at 105 °C. After 24 h, purification by chromatography (*n*-

pentane/Et_2O 3:1 → 2:1 → 1:1) yielded **3aa** (315 mg, 92%) as yellow oil. ^{1}H-NMR (600 MHz, $CDCl_3$): δ = 7.60-7.59 (m, 2H), 7.29-7.23 (m, 6H), 7.08-7.06 (m, 4H), 6.95 (md, *J* = 8.8 Hz, 2H), 5.41 (s, 2H), 3.88 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 160.5 (C_q), 144.4 (C_q), 135.5 (C_q), 133.7 (C_q), 131.7 (CH), 131.1 (C_q), 128.6 (CH), 128.4 (CH), 128.1 (CH), 127.5 (CH), 127.4 (CH), 126.6 (CH), 119.6 (C_q), 114.6 (CH), 55.3 (CH_3), 51.8 (CH_2). IR (ATR): 1613, 1514, 1485, 1455, 1440, 1290, 1248, 1175, 1023, 982, 836, 732, 719, 692 cm^{-1}. MS (EI) *m/z* (relative intensity) 341 (43) [M^+], 222 (100), 195 (5), 190 (4), 178 (4), 91 (10). HR-MS (EI) *m/z* calcd for $C_{22}H_{19}N_3O$ 341.1528, found 341.1529.



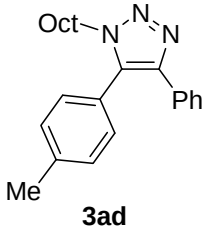
3ab

1-Benzyl-4-(4-methoxyphenyl)-5-*p*-tolyl-1*H*-1,2,3-triazole (3ab, Table 2, entry 1): The representative procedure was followed using **1b** (132 mg, 0.50 mmol) and **2b** (98 mg, 0.75 mmol). After 17 h, purification by chromatography (*n*-pentane/Et_2O 5:1) yielded **3ab** (131 mg, 74%) as a white solid. M.p.: 115-116 °C. ^{1}H-NMR (600 MHz, $CDCl_3$): δ = 7.49 (d, *J* = 8.8 Hz, 2H), 7.27-7.24 (m, 3H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.06-7.03 (m, 2H), 7.02 (d, *J* = 7.9 Hz, 2H), 6.80 (d, *J* = 8.8 Hz, 2H), 5.38 (s, 2H), 3.77 (s, 3H), 2.42 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 159.2 (C_q), 144.3 (C_q), 139.6 (C_q), 135.6 (C_q), 133.2 (C_q), 130.0 (CH), 129.8 (CH), 128.7 (CH), 128.0 (CH), 127.9 (CH), 127.5 (CH), 125.1 (C_q), 123.9 (C_q), 113.9 (CH), 55.2 (CH_3), 51.9 (CH_2), 21.4 (CH_3). IR (ATR): 3034, 2971, 2937, 1615, 1520, 1489, 1451, 1301, 1254, 1240, 1175, 1108, 1027, 1018, 984, 836, 728, 694 cm^{-1}. MS (EI) *m/z* (relative intensity) 355 [M^+] (48), 119 (5), 90 (5). HR-MS (EI) *m/z* calcd for $C_{23}H_{21}N_3O$ 355.1685, found 355.1667.



3ac

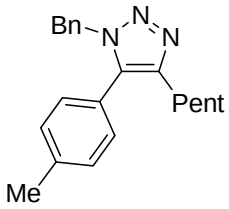
1-(4-Methoxybenzyl)-4-phenyl-5-*p*-tolyl-1*H*-1,2,3-triazole (3ac, Table 2, entry 2): The representative procedure was followed using **1c** (265 mg, 1.00 mmol) and **2b** (206 mg, 1.52 mmol). After 22 h, purification by chromatography (*n*-pentane/Et_2O 2:1) yielded **3ac** (285 mg, 80%) as yellow viscous oil. ^{1}H-NMR (600 MHz, $CDCl_3$): δ = 7.58-7.56 (m, 2H), 7.27-7.21 (m, 5H), 7.05 (md, *J* = 8.0 Hz, 2H), 7.00 (md, *J* = 8.7 Hz, 2H), 6.79 (md, *J* = 8.7 Hz, 2H), 5.33 (s, 2H), 3.78 (s, 3H), 2.45 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 159.4 (C_q), 144.4 (C_q), 139.7 (C_q), 133.8 (C_q), 131.1 (C_q), 130.0 (CH), 129.8 (CH), 129.0 (CH), 128.3 (CH), 127.6 (C_q), 127.5 (CH), 126.6 (CH), 124.8 (C_q), 114.0 (CH), 55.2 (CH_3), 51.4 (CH_2), 21.4 (CH_3). IR (NaCl): 1613, 1515, 1486, 1444, 1351, 1252, 1178, 1028, 985, 825, 778 cm^{-1}. MS (EI) *m/z* (relative intensity) 355 (13) [M^+], 206 (30), 121 (100), 103 (4), 89 (6), 77 (13), 57 (2), 41 (4). HR-MS (ESI) *m/z* calcd for $C_{23}H_{22}N_3O$ 356.1747, found 356.1760.



3ad

1-Octyl-4-phenyl-5-*p*-tolyl-1*H*-1,2,3-triazole (3ad, Table 2, entry 3): The representative procedure was followed using **1d** (129 mg, 0.50 mmol) and **2b** (99 mg, 0.75 mmol). After 22 h, purification by chromatography (*n*-pentane/Et_2O 3:1) yielded **3ad** (122 mg, 70%) as a colourless

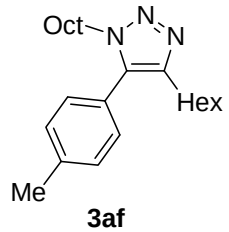
oil. ^{1}H-NMR (600 MHz, $CDCl_3$): δ = 7.57 (dd, J = 8.4, 1.3 Hz, 2H), 7.31 (dd, J = 7.5 Hz, 2H), 7.26 (tt, J = 7.1, 1.8 Hz, 2H), 7.23 (tt, J = 7.1, 1.3 Hz, 1H), 7.20 (d, J = 7.9 Hz, 2H), 4.18 (t, J = 7.5 Hz, 2H), 2.45 (s, 3H), 1.78 (quint, J = 7.1 Hz, 2H), 1.28-1.19 (m, 10H), 0.86 (t, J = 7.1 Hz, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 124.1 (C_q), 139.7 (C_q), 133.7 (C_q), 131.3 (C_q), 130.1 (CH), 129.8 (CH), 128.4 (CH), 127.5 (CH), 126.7 (CH), 125.2 (C_q), 43.2 (CH_2), 31.7 (CH_2), 30.1 (CH_2), 29.0 (CH_2), 28.9 (CH_2), 26.4 (CH_2), 22.6 (CH_2), 21.4 (CH_3), 14.1 (CH_3). IR (ATR): 2922, 2854, 1515, 1484, 1456, 1354, 1018, 981, 824, 775, 730, 693 cm^{-1}. MS (EI) *m/z* (relative intensity) 347 (35) [M^+], 319 (8), 206 (100), 179 (5), 165 (9). HR-MS (EI) *m/z* calcd for $C_{23}H_{29}N_3$ 347.2361, found 347.2343.



3ae

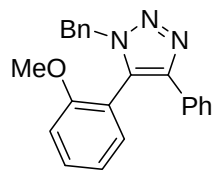
1-Benzyl-4-pentyl-5-*p*-tolyl-1*H*-1,2,3-triazole (3ae, Table 2, entry 4): The representative procedure was followed using **1e** (114 mg, 0.50 mmol), **2b** (99 mg, 0.75 mmol) and pivalic acid (31 mg, 30 mol %). After 24 h, purification by chromatography (*n*-pentane/Et_2O 2:1) yielded **3ae** (105 mg, 66%) as a pale-yellow oil. ^{1}H-NMR (600 MHz, $CDCl_3$): δ = 7.25-7.22 (m, 3H), 7.21 (d, J = 7.5 Hz, 2H), 7.01 (dd, J = 7.1, 3.5 Hz, 2H), 6.99 (d, J = 7.9 Hz, 2H), 5.38 (s, 2H), 2.59 (t, J = 7.9 Hz, 2H), 2.40 (s, 3H), 1.62 (quint, J = 7.5 Hz, 2H), 1.27-1.22 (m, 4H), 0.82 (t, J = 7.1 Hz, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 146.0 (C_q), 139.2 (C_q), 135. 8 (C_q), 134.4 (C_q), 129.6 (CH), 129.5 (CH), 128.6 (CH), 127.9 (CH), 127.3 (CH), 124.5 (C_q), 51.8 (CH_2), 31.5 (CH_2), 29.3 (CH_2), 25.1 (CH_2), 22.3 (CH_2), 21.4 (CH_3), 14.0 (CH_3). IR (ATR): 3029, 2925, 2856, 1506, 1496, 1454, 1215, 1011, 827, 715, 692 cm^{-1}. MS (EI) *m/z* (relative intensity) 319 (82) [M^+], 273 (12),

260 (99), 200 (42), 130 (24), 105 (16), 91 (100). HR-MS (EI) *m/z* calcd for $C_{21}H_{25}N_3$ 319.2048, found 319.2051.



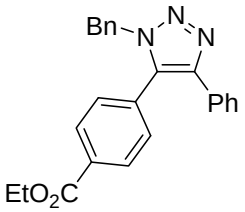
3af

4-Hexyl-1-octyl-5-*p*-tolyl-1*H*-1,2,3-triazole (3af, Table 2, entry 5): The representative procedure was followed using **1f** (133 mg, 0.50 mmol), **2b** (99 mg, 0.75 mmol) and pivalic acid (31 mg, 30 mol %). After 24 h, purification by chromatography (*n*-pentane/Et_2O 2:1) yielded **3af** (120 mg, 68%) as a colourless oil. ^{1}H-NMR (600 MHz, $CDCl_3$): δ = 7.28 (d, *J* = 8.4 Hz, 2H), 7.13 (d, *J* = 8.4 Hz, 2H), 4.15 (t, *J* = 7.8 Hz, 2H), 2.57 (t, *J* = 7.2 Hz, 2H), 2.42 (s, 3H), 1.71 (quint, *J* = 6.6 Hz, 2H), 1.60 (quint, *J* = 7.2 Hz, 2H), 1.26-1.12 (m, 16H), 0.84 (t, *J* = 6.6 Hz, 3H), 0.81 (d, *J* = 8.4 Hz, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 145.6 (C_q), 139.1 (C_q), 134.0 (C_q), 129.6 (CH), 129.4 (CH), 125.0 (C_q), 48.2 (CH_2), 31.7 (CH_2), 31.5 (CH_2), 30.1 (CH_2), 29.7 (CH_2), 29.0 (CH_2), 26.4 (CH_2), 25.1 (CH_2), 22.6 (CH_2), 22.5 (CH_2), 21.3 (CH_2), 14.1 (CH_3), 14.0 (CH_3). IR (ATR): 2922, 2854, 1505, 1456, 1376, 1011, 823, 721 cm^{-1}. MS (EI) *m/z* (relative intensity) 355 (85) [M^+], 326 (9), 312 (9), 298 (29), 285 (100), 256 (11), 215 (19), 144 (27), 16 (13), 43 (7). HR-MS (EI) *m/z* calcd for $C_{23}H_{37}N_3$ 355.2987, found 355.2978.



3ag

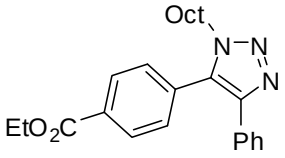
1-Benzyl-5-(2-methoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole (3ag, Table 2, entry 6): The representative procedure was followed using **1a** (235 mg, 1.00 mmol) and **2c** (216 mg, 1.51 mmol). After 22 h, purification by chromatography (*n*-pentane/Et_2O 3:1 → 2:1 → 1:1) yielded **3ag** (326 mg, 95%) as an off-white solid. M.p.: 129-131 °C. ^{1}H-NMR (600 MHz, $CDCl_3$): δ = 7.57-7.56 (m, 2H), 7.46-7.43 (m, 1H), 7.25-7.18 (m, 6H), 6.98-6.93 (m, 5H), 5.39 (d, *J* = 15.0 Hz, 1H), 5.28 (d, *J* = 15.0 Hz, 1H), 3.53 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 157.5 (C_q), 144.9 (C_q), 135.2 (C_q), 131.8 (CH), 131.6 (CH), 131.3 (C_q), 130.7 (C_q), 128.4 (CH), 128.3 (CH), 127.8 (CH), 127.7 (CH), 127.4 (CH), 126.3 (CH), 121.0 (CH), 116.6 (C_q), 111.2 (CH), 55.2 (CH_3), 52.3 (CH_2). IR (ATR): 1505, 1480, 1454, 1246, 1018, 983, 781, 749, 729, 695 cm^{-1}. MS (EI) *m/z* (relative intensity) 341 (69) [M^+], 222 (96), 206 (9), 194 (13), 165 (10), 116 (7), 91 (100), 65 (7). HR-MS (EI) *m/z* calcd for $C_{22}H_{19}N_3O$ 341.1528, found 341.1510.



3ah

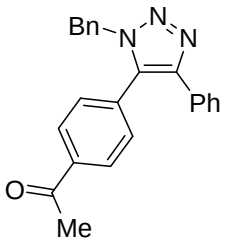
Ethyl 4-(1-benzyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)benzoate (3ah, Table 2, entry 7): The representative procedure was followed using **1a** (235 mg, 1.00 mmol) and **2d** (287 mg, 1.55 mmol). After 22 h, purification by chromatography (*n*-pentane/Et_2O 3:1 → 2:1) yielded **3ah** (271 mg, 70%) as a white solid. M.p.:114-115 °C. ^{1}H-NMR (600 MHz, $CDCl_3$): δ = 8.10-8.08 (md, *J* = 8.5 Hz, 2H), 7.53-7.51 (m, 2H), 7.28-7.23 (m, 8H), 7.04-7.02 (m, 2H), 5.44 (s, 2H), 4.43 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 165.8 (C_q), 144.9 (C_q), 135.1 (C_q), 132.8 (C_q), 132.4 (C_q), 131.6 (C_q), 130.5 (C_q), 130.2 (CH), 130.1 (CH), 128.8 (CH), 128.5 (CH), 128.3 (CH), 127.9 (CH), 127.4 (CH), 126.8 (CH), 61.4 (CH_2), 52.2 (CH_2), 14.3

(CH_3). IR (ATR): 1713, 1286, 1276, 1129, 1018, 855, 780, 767, 733, 707, 696 cm^{-1}. MS (EI) *m/z* (relative intensity) 383 (49) [M^+], 338 (5), 264 (100), 236 (9), 191 (6), 165 (7), 91 (74). HR-MS (EI) *m/z* calcd for $C_{24}H_{21}N_3O_2$ 383.1634, found 383.1632. The spectral data were in accordance with those reported in the literature.[5]



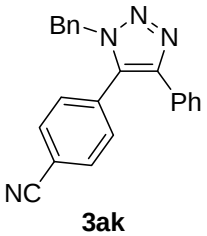
3ai

Ethyl 4-(1-octyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)benzoate (3ai, Table 2, entry 8): The representative procedure was followed using **1d** (128 mg, 0.50 mmol) and **2d** (138 mg, 0.75 mmol). After 23 h, purification by chromatography (*n*-hexane/EtOAc 5:1) yielded **3ai** (128 mg, 63%) as colourless oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.11 (d, *J* = 8.2 Hz, 2H), 7.45-7.20 (m, 2H), 7.35 (d, *J* = 8.2 Hz, 2H), 7.20-7.16 (m, 3H), 4.36 (q, *J* = 7.1 Hz, 2H), 4.14 (t, *J* = 7.2 Hz, 2H), 1.69 (quint, *J* = 7.2 Hz, 2H), 1.36 (t, *J* = 7.2 Hz, 3H), 1.16-1.05 (m, 10H), 0.77 (t, *J* = 6.6 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.8 (C_q), 144.5 (C_q), 132.7 (C_q), 132.6 (C_q), 131.6 (C_q), 130.6 (C_q), 130.4 (CH), 130.0 (CH), 128.5 (CH), 127.8 (CH), 126.8 (CH), 61.4 (CH_2), 48.4 (CH_2), 31.6 (CH_2), 30.0 (CH_2), 28.9 (CH_2), 28.7 (CH_2), 26.3 (CH_2), 22.5 (CH_2), 14.3 (CH_3), 14.0 (CH_3). IR (film): 2929, 2857, 1717, 1653, 1616, 1559, 1457, 1368, 1179, 1110, 1019, 983, 865, 778 cm^{-1}. MS (EI) *m/z* (relative intensity) 405 (39) [M^+], 377 (9), 265 (100), 237 (8), 165 (10), 43 (11). HR-MS (ESI) *m/z* calcd for $C_{25}H_{32}N_3O_2$ 406.2489, found 406.2490.



3aj

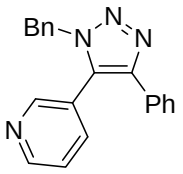
1-(4-(1-Benzyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)phenyl)ethanone (3aj, Table 2, entry 11): The representative procedure was followed using **1a** (235 mg, 1.00 mmol), **2e** (235 mg, 1.52 mmol) and pivalic acid (31 mg, 30.5 mol %) as additive. After 22 h, purification by chromatography (*n*-pentane/Et_2O 2:1 → 1:1) yielded **3aj** (236 mg, 67%) as an off-white solid. M.p.:122-123 °C. ^{1}H-NMR (600 MHz, $CDCl_3$): δ = 8.00 (dt, J = 8.4, 1.8 Hz, 2H), 7.53-7.51 (m, 2H), 7.28-7.26 (m, 8H), 7.04-7.02 (m, 2H), 5.44 (s, 2H), 2.66 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 197.2 (C_q), 145.0 (C_q), 137.7 (C_q), 135.1 (C_q), 132.7 (C_q), 132.6 (C_q), 130.5 (C_q), 130.4 (CH), 128.9 (CH), 128.8 (CH), 128.5 (CH), 128.3 (CH), 128.0 (CH), 127.3 (CH), 126.8 (CH), 52.2 (CH_2), 26.7 (CH_3). IR (ATR): 1685, 1352, 1258, 1242, 848, 836, 775, 735, 724, 699 cm^{-1}. MS (EI) *m/z* (relative intensity) 353 (46) [M^+], 234 (100), 190 (5), 165 (5), 91 (65). HR-MS (EI) *m/z* calcd for $C_{23}H_{19}N_3O$ 353.1528, found 353.1503.



3ak

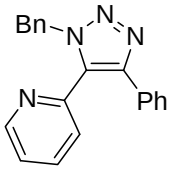
4-(1-Benzyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)benzonitrile (3ak, Table 2, entry 13): The representative procedure was followed using **1a** (235 mg, 1.00 mmol), **2f** (206 mg, 1.50 mmol) and pivalic acid (31 mg, 30.5 mol %) as additive. After 22 h, purification by chromatography (*n*-pentane/Et_2O 2:1 → 1:1) yielded **3ak** (238 mg, 71%) as an off-white solid. M.p.: 146-148 °C. ^{1}H-

NMR (600 MHz, $CDCl_3$): δ = 7.68 (dt, *J* = 8.3, 1.8 Hz, 2H), 7.48-7.47 (m, 2H), 7.30-7.24 (m, 8H), 7.00-6.99 (m, 2H), 5.45 (s, 2H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 145.3 (C_q), 134.8 (C_q), 132.8 (C_q), 132.7 (CH), 131.9 (C_q), 130.9 (CH), 130.1 (C_q), 128.9 (CH), 128.6 (CH), 128.5 (CH), 128.2 (CH), 127.2 (CH), 126.9 (CH), 117.9 (C_q), 113.6 (C_q), 52.5 (CH_2). IR (ATR): 2228, 1445, 1357, 983, 856, 846, 778, 738, 733, 725, 695, 691 cm^{-1}. MS (EI) *m/z* (relative intensity) 336 (33) [M^+], 217 (100), 91 (42). HR-MS (EI) *m/z* calcd for $C_{22}H_{16}N_4$ 336.1375, found 336.1375.



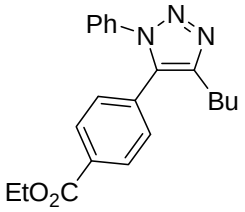
3al

3-(1-Benzyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)pyridine (3al, Table 2, entry 14): The representative procedure was followed using **1a** (118 mg, 0.50 mmol) and **2g** (88 mg, 0.75 mmol). After 22 h, purification by chromatography (*n*-pentane/Et_2O 1:2) yielded **3al** (90 mg, 58%) as an off-white solid. M.p.: 110-112 °C. ^{1}H-NMR (600 MHz, $CDCl_3$): δ = 8.68 (dd, *J* = 4.9, 1.8 Hz, 1H), 8.39 (d, *J* = 1.8 Hz, 1H), 7.50-7.47 (m, 2H), 7.38 (td, *J* = 7.9, 1.8 Hz, 1H), 7.30 (ddd, *J* = 7.9, 4.9, 0.9 Hz, 1H), 7.26-7.21 (m, 6H), 6.98 (dd, *J* = 7.5, 1.8 Hz, 2H), 5.43 (s, 2H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 150.8 (CH), 150.5 (CH), 145.9 (C_q), 137.6 (CH) 134.9 (C_q), 130.5 (C_q), 130.3 (C_q), 128.9 (CH), 128.7 (CH), 128.5 (CH), 128.1 (CH), 127.3 (CH), 126.8 (CH), 124.5 (C_q), 123.7 (CH), 52.5 (CH_2). IR (ATR): 3029, 1564, 1493, 1455, 1443, 1408, 1351, 1325, 1217, 1072, 1019, 981, 828, 774, 739, 732, 713, 702, 691 cm^{-1}. MS (EI) *m/z* (relative intensity) 312 (35) [M^+], 193 (100), 90 (40). HR-MS (EI) *m/z* calcd for $C_{20}H_{16}N_4$ 312.1375, found 312.1362. The spectral data were in accordance with those reported in the literature.[6]



3am

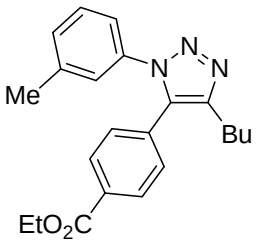
2-(1-Benzyl-4-phenyl-1*H*-1,2,3-triazol-5-yl)pyridine (3am, Table 2, entry 15): The representative procedure was followed using **1a** (118 mg, 0.50 mmol) and **2h** (88 mg, 0.75 mmol). After 18 h, purification by chromatography (*n*-pentane/Et_2O 1:1) yielded **3am** (125 mg, 82%) as a white solid. M.p.: 93-95 °C. ^{1}H-NMR (600 MHz, $CDCl_3$): δ = 8.78 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 7.55 (dt, *J* = 7.9, 1.8 Hz, 1H), 7.53-7.51 (m, 2H), 7.32-7.28 (m, 4H), 7.18-7.15 (m, 3H), 7.07 (td, *J* = 7.9, 0.9 Hz, 1H), 7.04-7.02 (m, 2H), 5.82 (s, 2H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 150.1 (CH), 148.0 (C_q), 145.7 (C_q), 136.7 (CH), 135.5 (C_q), 132.2 (C_q), 130.9 (C_q), 128.53 (CH), 128.48 (CH), 128.1 (CH), 127.9 (CH), 127.8 (CH), 127.7 (CH), 125.6 (CH), 123.6 (CH), 52.7 (CH_2). IR (ATR): 3048, 2916, 2847, 1595, 1578, 1557, 1505, 1497, 1456, 1446, 1422, 1353, 1280, 1249, 1215, 1143, 1002, 992, 819, 769, 700, 687 cm^{-1}. MS (EI) *m/z* (relative intensity) 312 (10) [M^+], 283 (70), 207 (6), 193 (100), 180 (8), 90 (31). HR-MS (EI) *m/z* calcd for $C_{20}H_{16}N_4$ 312.1375, found 312.1377.



3an

Ethyl 4-(4-butyl-1-phenyl-1*H*-1,2,3-triazol-5-yl)benzoate (3an, Table 3, entry 1): The representative procedure was followed using **1g** (201 mg, 1.00 mmol) and **2d** (277 mg, 1.50 mmol). After 22 h, purification by chromatography (*n*-hexane/EtOAc 5:1) yielded **3an** (230 mg,

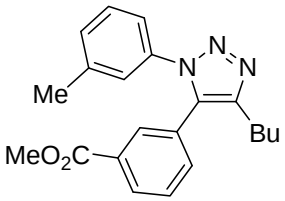
65%) as a colourless oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.02 (d, J = 8.7 Hz, 2H), 7.37-7.31 (m, 3H), 7.18-7.19 (m, 4H), 4.35 (t, J = 6.9 Hz, 2H), 2.37 (t, J = 7.8 Hz, 2H), 1.69 (quint, J = 7.5 Hz, 2H), 1.36 (t, J = 7.2 Hz, 3H), 1.34 (tq, J = 7.2, 7.2 Hz, 2H), 0.86 (t, J = 7.5 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.8 (C_q), 146.6 (C_q), 136.6 (C_q), 132.8 (C_q), 132.2 (C_q), 130.8 (C_q), 129.9 (CH), 129.5 (CH), 129.3 (CH), 128.9 (CH), 124.8 (CH), 61.3 (CH_2), 31.7 (CH_2), 24.8 (CH_2), 22.4 (CH_2), 14.3 (CH_3), 13.7 (CH_3). IR (film): 2957, 2931, 2871, 1718, 1614, 1598, 1500, 1462, 1403, 1367, 1309, 1275, 1180, 1109, 1072, 1016, 995, 862, 779, 763, 701 cm^{-1}. MS (EI) *m/z* (relative intensity) 349 (1) [M^+], 321 (26), 304 (7), 278 (100), 205 (6), 175 (49), 147 (21), 130 (12), 104 (19), 77 (39), 51 (8). HR-MS (ESI) *m/z* calcd for $C_{21}H_{24}N_3O_2$ 350.1863, found 350.1864.



3ao

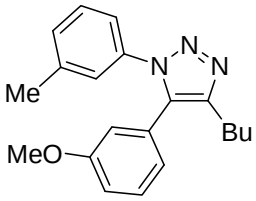
Ethyl 4-(4-butyl-1-*m*-tolyl-1*H*-1,2,3-triazol-5-yl)benzoate (3ao, Table 3, entry 2): The representative procedure was followed using **1h** (215 mg, 1.00 mmol) and **2d** (277 mg, 1.50 mmol). After 22 h, purification by chromatography (*n*-hexane/EtOAc 5:1) yielded **3ao** (236 mg, 65%) as a colourless oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.03 (d, J = 8.4 Hz, 2H), 7.23 (d, J = 8.4 Hz, 2H), 7.20-7.16 (m, 3H), 6.93 (td, J = 6.4, 2.5 Hz, 1H), 4.37 (q, J = 7.1 Hz, 2H), 2.74 (t, J = 7.6 Hz, 2H), 2.32 (s, 3H), 1.70 (quint, J = 7.8 Hz, 2H), 1.38 (t, J = 7.1 Hz, 3H), 1.35-1.30 (m, 2H), 0.87 (t, J = 7.3 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.9 (C_q), 146.5 (C_q), 139.5 (C_q), 136.4 (C_q), 132.8 (C_q), 132.2 (C_q), 130.6 (C_q), 129.8 (CH), 129.7 (CH), 129.4 (CH), 128.9 (CH),

125.5 (CH), 121.9 (CH), 61.2 (CH_2), 31.7 (CH_2), 24.8 (CH_2), 22.4 (CH_2), 21.2 (CH_3), 14.2 (CH_3), 13.7 (CH_3). IR (film): 2958, 2870, 1717, 1612, 1494, 1467, 1368, 1180, 1109, 867, 777 cm^{-1}. MS (EI) *m/z* (relative intensity) 363 (1) [M^+], 335 (27), 292 (100), 175 (18), 144 (34), 118 (11), 91 (32), 65 (15). HR-MS (ESI) *m/z* calcd for $C_{22}H_{26}N_3O_2$ 364.2020, found 364.2020.



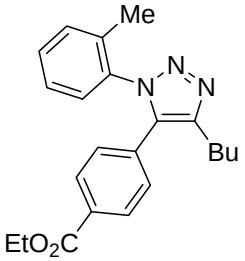
3ap

Methyl 3-(4-butyl-1-*m*-tolyl-1*H*-1,2,3-triazol-5-yl)benzoate (3ap, Table 3, entry 3): The representative procedure was followed using **1h** (215 mg, 1.00 mmol) and **2i** (256 mg, 1.50 mmol). After 22 h, purification by chromatography (*n*-hexane/EtOAc 4:1) yielded **3ap** (236 mg, 69%) as a light brown oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.02 (dt, *J* = 7.7, 1.5 Hz, 1H), 7.90 (t, *J* = 1.8 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.25 (dt, *J* = 7.7, 1.3 Hz, 1H), 7.21-7.12 (m, 3H), 6.92 (dt, *J* = 6.9, 2.1 Hz, 1H), 3.89 (s, 3H), 2.71 (t, *J* = 7.5 Hz, 2H), 2.30 (s, 3H), 1.69 (quint, *J* = 7.9 Hz, 2H), 1.33 (tq, *J* = 7.5, 7.5 Hz, 2H), 0.86 (t, *J* = 7.3 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.2 (C_q), 146.5 (C_q), 139.5 (C_q), 136.4 (C_q), 133.9 (CH), 132.8 (C_q), 130.8 (C_q), 130.5 (CH), 129.9 (CH), 129.7 (CH), 128.9 (CH), 128.5 (C_q), 128.3 (CH), 125.5 (CH), 121.9 (CH), 52.3 (CH_3), 31.7 (CH_2), 24.8 (CH_2), 22.4 (CH_2), 21.2 (CH_3), 13.7 (CH_3). IR (film): 2954, 2860, 1727, 1610, 1592, 1495, 1437, 1285, 1110, 1084, 969, 916, 861, 788, 760, 696 cm^{-1}. MS (EI) *m/z* (relative intensity) 349 (3) [M^+], 321 (33), 278 (100), 161 (25), 119 (19), 91 (16). HR-MS (ESI) *m/z* calcd for $C_{21}H_{24}N_3O_2$ 350.1863, found 350.1864.



3aq

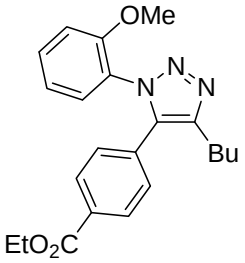
4-Butyl-5-(3-methoxyphenyl)-1-*m*-tolyl-1*H*-1,2,3-triazole (3aq, Table 3, entry 4): The representative procedure was followed, using **1h** (233 mg, 1.04 mmol) and **2j** (224 mg, 1.57 mmol). After 22 h, purification by chromatography (*n*-hexane/EtOAc 10:1 → 7:1) yielded **3aq** (202 mg, 60%) as an off-white solid. M.p.: 77-79 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.30-7.15 (m, 4H), 6.98 (md, *J* = 7.4 Hz, 1H), 6.90 (md, *J* = 8.3 Hz, 1H), 6.74-6.68 (m, 2H), 3.72 (s, 3H), 2.74 (t, *J* = 7.8 Hz, 2H), 2.33 (s, 3H), 1.77-1-67 (m, 2H), 1.37 (tq, *J* = 7.5, 7.5 Hz, 2H), 0.89 (t, *J* = 7.4 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 159.5 (C_q), 146.1 (C_q), 139.3 (C_q), 136.8 (C_q), 133.6 (C_q), 129.8 (CH), 129.4 (CH), 129.0 (C_q), 128.7 (CH), 125.4 (CH), 122.0 (CH), 121.8 (CH), 115.1 (CH), 114.3 (CH), 55.2 (CH_3), 31.8 (CH_2), 24.8 (CH_2), 22.5 (CH_2), 21.3 (CH_3), 13.8 (CH_3). IR (NaCl): 2956, 1610, 1592, 1495, 1466, 1288, 1230, 1022, 786, 736, 696 cm^{-1}. MS (EI) *m/z* (relative intensity) 321 (4) [M^+], 293 (43), 278 (4), 250 (100), 144 (4), 133 (35), 118 (19), 91 (10), 77 (3), 65 (6). HR-MS (ESI) *m/z* calcd for $C_{20}H_{24}N_3O$ 322.1914, found 322.1912.



3ar

4-(5-Butyl-3-*o*-tolyl-3*H*-1,2,3-triazol-4-yl)-benzoic acid ethyl ester (3ar, Table 3, entry 5): The representative procedure was followed, using **1i** (213 mg, 0.989 mmol) and **2d** (284 mg, 1.54

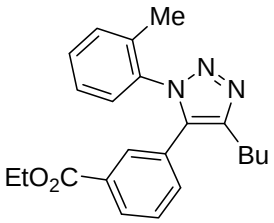
mmol). After 22 h, purification by chromatography (*n*-hexane/EtOAc 10:1 → 5:1 → 4:1) yielded **3ar** (245 mg, 68%) as a yellow oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.92 (dt, *J* = 8.4, 1.7 Hz, 2H), 7.31-7.27 (m, 1H), 7.21-7.11 (m, 5H), 4.29 (q, *J* = 7.1 Hz, 2H), 2.75 (t, *J* = 7.8 Hz, 2H), 1.89 (s, 3H), 1.75-1.65 (m, 2H), 1.39-1.26 (m, 5H), 0.85 (t, *J* = 7.3 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.8 (C_q), 145.7 (C_q), 135.8 (C_q), 135.0(C_q), 134.0 (C_q), 131.9 (C_q), 131.2 (CH), 130.6 (C_q), 130.0 (CH), 129.8 (CH), 128.9 (CH), 127.6 (CH), 126.7 (CH), 61.2 (CH_2), 31.6 (CH_2), 25.1 (CH_2), 22.5 (CH_2), 17.5 (CH_3), 14.3 (CH_3), 13.8 (CH_3). IR (NaCl): 2957, 1717, 1615, 1499, 1465, 1367, 1275, 1180, 1016, 996, 767 cm^{-1}. MS (EI) *m/z* (relative intensity) 363 (1) [M^+], 335 (5), 292 (13), 220 (2), 187 (7), 172 (9), 158 (6), 144 (100), 131 (9), 118 (8), 91 (32), 65 (8). HR-MS (ESI) *m/z* calcd for $C_{22}H_{26}N_3O_2$ 364.2020, found 364.2021.



3as

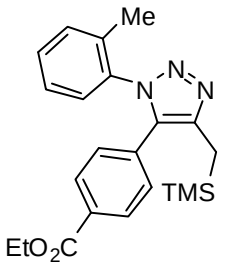
4-[5-Butyl-3-(2-methoxyphenyl)-3*H*-1,2,3-triazol-4-yl]-benzoic acid ethyl ester (3as, Table 3, entry 6): The representative procedure was followed, using **1j** (116 mg, 0.50 mmol) and **2d** (138 mg, 0.75 mmol). After 22 h, purification by chromatography (*n*-hexane/EtOAc 3:1) yielded **3as** (118 mg, 62%) as a colourless oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.95 (d, *J* = 8.3 Hz, 2H), 7.41 (dd, *J* = 6.1, 1.7 Hz, 1H), 7.40-7.32 (m, 1H), 7.18 (d, *J* = 8.5 Hz, 2H), 7.02 (td, *J* = 7.6, 1.0 Hz, 1H), 6.82 (d, J = 7.6 Hz, 1H), 4.33 (q, *J* = 7.1 Hz, 2H), 3.40 (s, 3H), 2.75 (t, *J* = 7.7 Hz, 2H), 1.71 (quint, *J* = 8.0 Hz, 2H), 1.38-1.31 (m, 5H), 0.87 (t, *J* = 7.5 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.3 (C_q), 153.5 (C_q), 145.6 (C_q), 134.9 (C_q), 133.1 (C_q), 131.5 (CH), 130.5 (C_q),

129.7 (CH), 128.7 (CH), 128.6 (CH), 125.9 (C_q), 121.2 (CH), 112.4 (CH), 61.4 (CH_2), 55.5 (CH_3), 32.0 (CH_2), 25.2 (CH_2), 22.7 (CH_2), 14.5 (CH_3), 14.0 (CH_3). IR (NaCl): 2956, 2860, 1653, 1610, 1598, 1579, 1499, 1457, 1447, 1317, 1178, 1105, 1072, 995, 939, 925, 858, 795, 658 cm^{-1}. MS (EI) *m/z* (relative intensity) 379 (2) [M^+], 353 (66), 310 (100), 207 (35), 179 (11), 105 (22), 77 (26). HR-MS (ESI) *m/z* calcd for $C_{22}H_{26}N_3O_3$ 380.1914, found 380.1914.



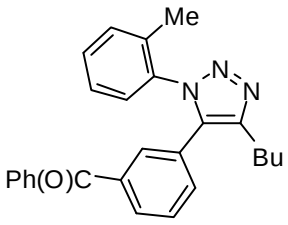
3at

3-(5-Butyl-3-*o*-tolyl-3*H*-1,2,3-triazol-4-yl)-benzoic acid methyl ester (3at, Table 3, entry 7): The representative procedure was followed, using **1i** (225 mg, 1.05 mmol) and **2i** (254 mg, 1.49 mmol). After 22 h, purification by chromatography (*n*-hexane/EtOAc, 7:1 → 5:1) yielded **3at** (354 mg, 96%) as a yellow oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.97 (md, *J* = 7.8 Hz, 1H), 7.86-7.85 (m, 1H), 7.39-7.30 (m, 2H), 7.25-7.21 (m, 4H), 3.88 (s, 3H), 2.79 (t, *J* = 7.8 Hz, 2H), 1.95 (s, 3H), 1.81-1.71 (m, 2H), 1.38 (tq, *J* = 7.4, 7.4 Hz, 2H), 0.90 (t, *J* = 7.4 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.1 (C_q), 145.5 (C_q), 135.7 (C_q), 135.0 (C_q), 134.0 (C_q), 133.1 (CH), 131.1 (CH), 130.7 (C_q), 130.1 (CH), 129.9 (CH), 129.7 (CH), 128.8 (CH), 127.8 (C_q), 127.7 (CH), 126.7 (CH), 52.3 (CH_3), 31.6 (CH_2), 24.9 (CH_2), 22.4 (CH_2), 17.5 (CH_3), 13.8 (CH_3). IR (NaCl): 2955, 1726, 1500, 1437, 1286, 1258, 1112, 1084, 1003, 764, 718 cm^{-1}. MS (EI) *m/z* (relative intensity) 349 (1) [M^+], 321 (21), 278 (100), 218 (7), 161 (29), 144 (7), 118 (27), 115 (9), 91 (41), 65 (25), 41 (10). HR-MS (ESI) *m/z* calcd for $C_{21}H_{24}N_3O_2$ 350.1863, found 350.1862.



3au

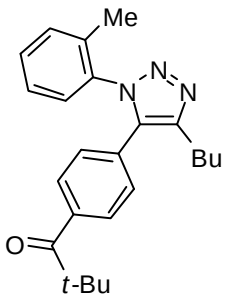
Ethyl 4-(1-*o*-tolyl-4-((trimethylsilyl)methyl)-1*H*-1,2,3-triazol-5-yl)benzoate (3au, Table 3, entry 8): The representative procedure was followed using **1k** (129 mg, 0.50 mmol) and **2d** (138 mg, 0.75 mmol). After 23 h, purification by chromatography (*n*-hexane/EtOAc 5:1) yielded **3au** (92 mg, 47%) as a colourless oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.94 (d, J = 8.4 Hz, 2H), 7.35-7.27 (m, 1H), 7.25-7.17 (m, 3H), 7.15 (d, J = 8.4 Hz, 2H), 4.32 (q, J = 7.1 Hz, 2H), 2.23 (s, 2H), 1.93 (s, 3H), 1.34 (t, J = 7.1 Hz, 3H), -0.03 (s, 9H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.8 (C_q), 144.0 (C_q), 135.9 (C_q), 135.0 (C_q), 132.9 (C_q), 132.3 (C_q), 131.1 (CH), 130.3 (C_q), 129.8 (CH), 129.7 (CH), 128.9 (CH), 127.5 (CH), 126.7 (CH), 61.2 (CH_2), 17.5 (CH_3), 14.6 (CH_2), 14.2 (CH_3), -1.4 (CH_3). IR (film): 2956, 1716, 1614, 1499, 1368, 1351, 1180, 1109, 1015, 995, 852 cm^{-1}. MS (EI) *m/z* (relative intensity) 393 (9) [M^+], 378 (28), 365 (89), 350 (44), 292 (100), 266 (29), 219 (14), 190 (34), 175 (16), 118 (10), 91 (30), 73 (66), 65 (13), 45 (9). HR-MS (ESI) *m/z* calcd for $C_{22}H_{28}N_3O_2Si$ 394.1945, found 394.1946.



3aw

[3-(5-Butyl-3-*o*-tolyl-3*H*-1,2,3-triazol-4-yl)-phenyl]-phenylmethanone (3aw, Table 3, entry 10): The representative procedure was followed, using **1i** (218 mg, 1.01 mmol) and **2l** (327 mg,

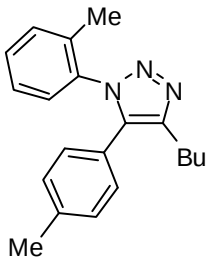
1.51 mmol). After 22 h, purification by chromatography (*n*-hexane/EtOAc 5:1 → 4:1 → 3:1) yielded **3aw** (320 mg,80 %) as a yellow oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.81 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.59-7.56 (m, 3H), 7.50-7.34 (m, 6H), 7.28-7.17 (m, 3H), 2.79 (t, *J* = 7.8 Hz, 2H), 1.96 (s, 3H), 1.80-1.69 (m, 2H), 1.37 (tq, *J* = 7.4, 7.4 Hz, 2H), 0.89 (t, *J* = 7.3 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 195.5 (C_q), 145.6 (C_q), 137.9 (C_q), 136.8 (C_q), 135.7 (C_q), 135.1 (C_q), 134.0 (C_q), 132.7 (CH), 132.6 (CH), 131.2 (CH), 130.7 (CH), 130.1 (CH), 129.9 (CH), 129.8 (CH), 129.0 (CH), 128.4 (CH), 127.7 (CH), 127.5 (C_q), 126.8 (CH), 31.7 (CH_2), 25.0 (CH_2), 22.5(CH_2), 17.6 (CH_3), 13.8 (CH_3). IR (NaCl): 2958, 1662, 1598, 1559, 1499, 1447, 1319, 1003, 946, 766, 700 cm^{-1}. MS (EI) *m/z* (relative intensity) 395 (1) [M^+], 367 (54), 324 (99), 218 (4), 207 (40), 178 (14), 144 (14), 118 (15), 105 (100), 91 (49), 77 (54), 65 (31), 41 (7). HR-MS (ESI) *m/z* calcd for $C_{26}H_{26}N_3O$ 396.2070, found 396.2071.



3ax

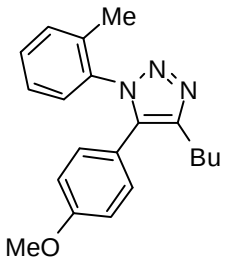
1-(4-(4-Butyl-1-*o*-tolyl-1*H*-1,2,3-triazol-5-yl)phenyl)-2,2-dimethylpropan-1-one (3ax, Table 3, entry 11): The representative procedure was followed using **1i** (107 mg, 0.50 mmol) and **2m** (147 mg, 0.75 mmol). After 22 h, purification by chromatography (*n*-hexane/EtOAc 3:1) yielded **3ax** (179 mg, 95%) as a colourless oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.59 (d, *J* = 8.5 Hz, 2H), 7.33-7.28 (m, 1H), 7.24-7.15 (m, 3H), 7.11 (d, *J* = 8.5 Hz, 2H), 2.77 (t, *J* = 7.6 Hz, 2H), 1.90 (s, 3H), 1.73 (quint, *J* = 7.8 Hz, 2H), 1.35 (tq, *J* = 7.6, 7.6 Hz, 2H), 1.27 (s, 9H), 0.87 (t, *J* = 7.3 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 208.3 (C_q), 145.5 (C_q), 138.3 (C_q), 135.7 (C_q), 134.9 (C_q),

133.9 (C_q), 131.1 (CH), 129.9 (CH), 129.8 (C_q), 128.5 (CH), 128.1 (CH), 127.5 (CH), 126.7 (CH), 44.1 (C_q), 31.6 (CH_2), 27.8 (CH_3), 25.0 (CH_2), 22.4 (CH_2), 17.5 (CH_3), 13.7 (CH_3). IR (film): 2959, 1764, 1611, 1499, 1464, 1367, 1175, 996, 964, 851, 766 cm^{-1}. MS (EI) *m/z* (relative intensity) 375 (4) [M^+], 347 (54), 304 (59), 290 (100), 219 (14), 91 (11), 57 (8). HR-MS (ESI) *m/z* calcd for $C_{24}H_{30}N_3O$ 376.2383, found 376.2385.



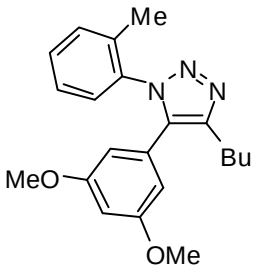
3ay

4-Butyl-1-*o*-tolyl-5-*p*-tolyl-1*H*-1,2,3-triazole (3ay, Table 3, entry 12): The representative procedure was followed using **1i** (215 mg, 1.00 mmol) and **2b** (190 mg, 1.50 mmol). After 22 h, purification by chromatography (*n*-hexane/EtOAc 2:1) yielded **3ay** (213 mg, 70%) as a colourless oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.34-7.27 (m, 1H), 7.25-7.18 (m, 3H), 7.07 (d, *J* = 8.0 Hz, 2H), 6.97 (d, *J* = 8.2 Hz, 2H), 2.76 (t, *J* = 7.6 Hz, 2H), 2.29 (s, 3H), 1.93 (s, 3H), 1.74 (quint, *J* = 7.8 Hz, 2H), 1.36 (hex, *J* = 7.6 Hz, 2H), 0.89 (t, *J* = 7.3 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 145.0 (C_q), 138.6 (C_q), 136.1 (C_q), 135.1 (C_q), 135.0 (C_q), 131.0 (CH), 129.7 (CH), 129.3 (CH), 128.9 (CH), 127.7 (CH), 126.5 (CH), 124.4 (C_q), 31.7 (CH_2), 25.0 (CH_2), 22.5 (CH_2), 21.2 (CH_3), 17.6 (CH_3), 13.8 (CH_3). IR (film): 3027, 2956, 2859, 1617, 1585, 1499, 1465, 1380, 1233, 1116, 996, 824, 756, 718 cm^{-1}. MS (EI) *m/z* (relative intensity) 305 (4) [M^+], 277 (45), 234 (100), 144 (7), 117 (67), 91 (22), 65 (12). HR-MS (ESI) *m/z* calcd for $C_{20}H_{24}N_3$ 306.1965, found 306.1965.



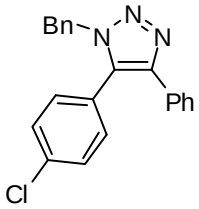
3az

4-Butyl-5-(4-methoxyphenyl)-1-*o*-tolyl-1*H*-1,2,3-triazole (3az, Table 3, entry 13): The representative procedure was followed, using **1i** (217 mg, 1.01 mmol) and **2a** (216 mg, 1.51 mmol). After 22 h, purification by chromatography (*n*-hexane/EtOAc 7:1 → 5:1 → 4:1) yielded **3az** (284 mg, 87%) as an off-white solid. M.p.: 86-88 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.35-7.29 (m, 1H), 7.26-7.22 (m, 3H), 7.02 (md, *J* = 8.8 Hz, 2H), 6.82 (md, *J* = 8.8 Hz, 2H), 3.77 (s, 3H), 2.77 (t, *J* = 7.8 Hz, 2H), 1.94 (s, 3H), 1.81-1.70 (m, 2H), 1.38 (tq, *J* = 7.4, 7.4 Hz, 2H), 0.91 (t, *J* = 7.3 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 159.7 (C_q), 144.9 (C_q), 136.1 (C_q), 135.1 (C_q), 134.8 (C_q), 131.0 (CH), 130.3(CH), 129.6 (CH), 127.8 (CH), 126.6 (CH), 119.5 (C_q), 114.1 (CH), 55.2 (CH_3), 31.7 (CH_2), 25.1 (CH_2), 22.5 (CH_2), 17.6 (CH_3), 13.8 (CH_3). IR (NaCl): 2959, 1616, 1507, 1465, 1294, 1253, 1178, 1038, 1023, 995, 837 cm^{-1}. MS (EI) *m/z* (relative intensity) 321 (6) [M^+], 293 (36), 278 (2), 250 (46), 144 (5), 133 (100), 118 (6), 91 (12), 65 (8). HR-MS (ESI) *m/z* calcd for $C_{20}H_{24}N_3O$ 322.1914, found 322.1915.



3ba

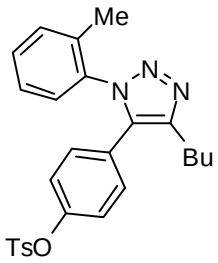
4-Butyl-5-(3,5-dimethoxyphenyl)-1-*o*-tolyl-1*H*-1,2,3-triazole (3ba, Table 3, entry 14): The representative procedure was followed, using **1i** (215 mg, 1.00 mmol) and **2n** (260 mg, 1.51 mmol). After 22 h, purification by chromatography (*n*-hexane/EtOAc 6:1) yielded **3ba** (316 mg, 90%) as a white solid. M.p.: 114-116 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.35-7.25 (m, 1H), 7.25-7.20 (m, 3H), 6.36 (t, *J* = 2.3 Hz, 1H), 6.21 (d, *J* = 2.3 Hz, 2H), 3.60 (s, 6H), 2.80 (t, *J* = 7.6 Hz, 2H), 1.94 (s, 3H), 1.76 (quint, *J* = 7.5 Hz, 2H), 1.38 (tq, *J* = 7.5, 7.5 Hz, 2H), 0.90 (t, *J* = 7.4 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 160.6 (C_q), 145.1 (C_q), 136.2 (C_q), 135.2 (C_q), 134.7 (C_q), 131.0 (CH), 129.7 (CH), 128.9 (C_q), 127.6 (CH), 126.6 (CH), 107.0 (CH), 107.0 (CH), 100.7 (CH), 55.2 (CH_3), 55.2 (CH_3), 31.7 (CH_2), 25.1 (CH_2), 22.5 (CH_2), 17.5 (CH_3), 13.8 (CH_3). IR (NaCl): 3004, 2954, 2871, 1594, 1501, 1462, 1432, 1332, 1320, 1206, 1161, 1061, 1032, 1002, 943, 841, 768, 689 cm^{-1}. MS (EI) *m/z* (relative intensity) 351 (10) [M^+], 323 (60), 280 (100), 163 (10). HR-MS (ESI) *m/z* calcd for $C_{21}H_{26}N_3O_2$ 352.2019, found 352.2020.



3bb

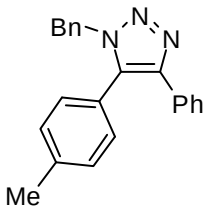
1-Benzyl-5-(4-chlorophenyl)-4-phenyl-1*H*-1,2,3-triazole (3bb, Scheme 1): The representative procedure was followed using **1a** (235 mg, 1.00 mmol) and **2o** (287 mg, 1.50 mmol). After 16 h, purification by chromatography (*n*-hexane/EtOAc 4:1) yielded **3bb** (201 mg, 73%) as white solid. M.p.: 115-117 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.53-7.48 (m, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.26-7.20 (m, 6H), 7.07-6.97 (m, 4H), 5.38 (s, 2H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 144.7 (C_q), 135.8 (C_q), 135.0 (C_q), 132.6 (C_q), 131.2 (CH), 130.5 (C_q), 129.4 (CH), 128.7 (CH), 128.4 (CH), 128.1 (CH), 127.8 (CH), 127.3 (CH), 126.6 (CH), 126.2 (C_q), 52.0 (CH_2). IR (film): 3052,

1506, 1479, 1456, 1445, 1354, 1266, 1093, 1016, 984, 839, 778, 740, 714, 698 cm^{-1}. MS (EI) *m/z* (relative intensity) 345 (14) [M^+], 226 (49), 91 (100). HR-MS (ESI) *m/z* calcd for $C_{21}H_{17}ClN_3$ 346.1106, found 346.1107.



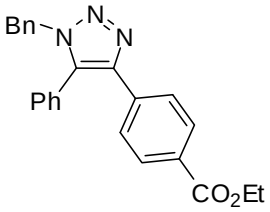
3bc

Toluene-4-sulfonic acid 4-(5-butyl-3-*o*-tolyl-3*H*-1,2,3-triazol-4-yl)-phenyl ester (3bc, Scheme 2): The representative procedure was followed, using **1i** (221 mg, 1.03 mmol) and **2p** (426 mg, 1.51 mmol). After 22 h, purification by chromatography (*n*-hexane/EtOAc 4:1) yielded **3bc** (361 mg, 76%) as an off-white solid. M.p.: 90-91 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.62 (md, *J* = 8.2 Hz, 2H), 7.37-7.14 (m, 6H), 7.02 (md, *J* = 8.6 Hz, 2H), 6.93 (md, *J* = 8.6 Hz, 2H), 2.75 (t, *J* = 7.8 Hz, 2H), 2.44 (s, 3H), 1.91 (s, 3H), 1.78-1.68 (m, 2H), 1.36 (tq, *J* = 7.4, 7.4 Hz, 2H), 0.90 (t, *J* = 7.3 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 149.5 (C_q), 145.6 (C_q), 145.3 (C_q), 135.7 (C_q), 134.9 (C_q), 133.7 (C_q), 132.0 (C_q), 131.1 (CH), 130.3 (CH), 129.9 (CH), 129.7 (CH), 128.4 (CH), 127.6 (CH), 126.7 (CH), 126.4 (C_q), 122.8 (CH), 31.6 (CH_2), 24.9 (CH_2), 22.4 (CH_2), 21.7 (CH_3), 17.5 (CH_3), 13.8(CH_3). IR (NaCl): 2959, 2361, 1498, 1376, 1201, 1179, 1156, 1093, 864, 572, 552 cm^{-1}. MS (EI) *m/z* (relative intensity) 461 (1) [M^+], 433 (6), 390 (2), 278 (100), 236 (4), 206 (2), 155 (3), 119 (6), 91 (42), 65 (16), 41 (3). HR-MS (ESI) *m/z* calcd for $C_{26}H_{28}N_3O_3S$ 462.1846, found 462.1846.



3bd

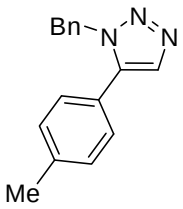
1-Benzyl-5-(4-methylphenyl)-4-phenyl-1*H*-1,2,3-triazole (3bd, Scheme 3): The representative procedure was followed using **1a** (235 mg, 1.00 mmol) and **2b** (194 mg, 1.53 mmol). After 22 h, purification by chromatography (*n*-pentane/Et_2O 3:1 → 2:1) yielded **3bd** (303 mg, 93%) as an off-white solid. M.p.:120-121 °C. ^{1}H-NMR (600 MHz, $CDCl_3$): δ = 7.57-7.55 (m, 2H), 7.26-7.20 (m, 8H), 7.05-7.02 (m, 4H), 5.38 (s, 2H), 2.42 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 144.4 (C_q), 139.7 (C_q), 135.5 (C_q), 134.0 (C_q), 131.1 (C_q), 129.9 (CH), 129.8 (CH), 128.6 (CH), 128.4 (CH), 128.0 (CH), 127.6 (CH), 127.4 (CH), 126.7 (CH), 124.7 (C_q), 51.8 (CH_2), 21.4 (CH_3). IR (ATR): 1496, 1485, 1456, 984, 830, 776, 732, 718, 694 cm^{-1}. MS (EI) *m/z* (relative intensity) 325 (48) [M^+], 206 (100), 190 (8), 179 (13), 91 (25). HR-MS (EI) *m/z* calcd for $C_{22}H_{19}N_3$ 325.1579, found 325.1568. The spectral data were in accordance with those reported in the literature.[5]



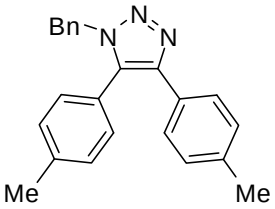
3be

Ethyl 4-(1-benzyl-5-phenyl-1*H*-1,2,3-triazol-4-yl)benzoate (3be, Scheme 4): The representative procedure was followed using **1l** (213 mg, 0.91 mmol) and **2d** (256 mg, 1.36 mmol). After 23 h, purification by chromatography (*n*-pentane/Et_2O 3:1) yielded **3be** (139 mg, 40%) as a white solid. M.p.: 106-109 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.93 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 8.8 Hz, 2H), 7.50 (tt, *J* = 7.5, 1.3 Hz, 1H), 7.43 (t, *J* = 7.9 Hz, 2H), 7.26-7.24

(m, 3H), 7.14 (dd, J = 7.1, 1.3 Hz, 2H), 7.03-7.01 (m, 2H), 5.41 (s, 2H), 4.33 (q, J = 7.5 Hz, 2H), 1.36 (t, J = 7.5 Hz, 3H).^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.5 (C_q), 143.6 (C_q), 135.3 (C_q), 135.2 (C_q), 134.8 (C_q), 130.0 (CH), 129.7 (CH), 129.4 (C_q), 129.3 (CH), 128.7 (CH), 128.2 (CH), 127.5 (CH), 127.5 (C_q), 126.3 (CH), 60.9 (CH_2), 52.1 (CH_2), 14.3 (CH_3). IR (ATR): 2986, 1697, 1607, 1455, 1352, 1275, 1243, 1107, 1021, 983, 866, 781, 760, 740, 712, 695, 677 cm^{-1}. MS (EI) *m/z* (relative intensity) 383 (47) [M^+], 338 (4), 298 (3), 264 (100), 236 (10), 190 (7), 165 (7), 91 (87). HR-MS (ESI) *m/z* calcd for $C_{24}H_{22}N_3O_2$ 384.1707, found 384.1708.



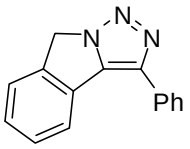
3bf



3bg

1-Benzyl-5-*p*-tolyl-1*H*-1,2,3-triazole (3bf) and 1-benzyl-4,5-di-*p*-tolyl-1*H*-1,2,3-triazole (3bg) (Scheme 5): The representative procedure was followed using **1m** (127 mg, 0.80 mmol) and **2b** (151 mg, 1.20 mmol). After 24 h, purification by chromatography (*n*-hexane/EtOAc 1:1) **3bg** as minor product (40 mg, 13%) and **3bf** (135 mg, 67%) as a colourless oil. **3bf**: ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.68 (s, 1H), 7.27-7.21 (m, 3H), 7.20-7.09 (m, 4H), 7.07-7.04 (m, 2H), 5.50 (s, 2H), 2.36 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$): δ = 139.6 (C_q), 138.2 (C_q), 135.6 (C_q), 133.1 (CH), 129.6 (CH), 128.8 (CH), 128.7 (CH), 128.1 (CH), 127.1 (CH), 123.9 (C_q), 51.7 (CH_2), 21.3 (CH_3). IR (film): 3032, 2924, 1497, 1455, 1360, 1315, 1268, 1243, 1213, 1114, 1075, 1030, 1014, 976, 820, 729, 694, 531 cm^{-1}. MS (EI) *m/z* (relative intensity) 249 (61) [M^+], 220 (18), 130 (17), 104 (16), 91 (100), 65 (9). HR-MS (ESI) *m/z* calcd for $C_{16}H_{16}N_3$ 250.1339, found 250.1340. **3bg**: White solid. M.p.: 90-91 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.37 (d, J = 8.1 Hz, 2H), 7.20-7.12 (m, 5H), 7.01-6.93 (m, 6H), 5.32 (s, 2H), 2.35 (s, 3H), 2.23 (s, 3H). ^{13}C-NMR (150

MHz, $CDCl_3$): δ = 144.5 (C_q), 139.6 (C_q), 137.4 (C_q), 135.6 (C_q), 133.6 (C_q), 129.9 (CH), 129.8 (CH), 129.1 (CH), 128.6 (CH), 128.2 (C_q), 128.0 (CH), 127.5 (CH), 126.6 (CH), 124.8 (C_q), 51.8 (CH_2), 21.4 (CH_3), 21.2 (CH_3). IR (film): 3032, 2922, 1524, 1496, 1455, 1352, 1265, 1214, 1184, 1110, 1042, 1019, 986, 826, 736, 717 cm^{-1}. MS (EI) *m/z* (relative intensity) 339 (35) [M^+], 220 (100), 193 (7), 190 (8), 103 (5), 91 (9) . HR-MS (ESI) *m/z* calcd for $C_{23}H_{22}N_3$ 340.1808, found 340.1808.



3bh

3-Phenyl-8*H*-[1,2,3]triazolo[5,1-*a*]isoindole (3bh, Scheme 6): The representative procedure was followed using **1n** (270 mg, 1.00 mmol). After 15 h, purification by chromatography (*n*-hexane/EtOAc 3:1) yielded **3bh** (194 mg, 83%) as a light brown solid. M.p.: 146-148 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.89-7.78 (m, 3H), 7.48-7.41 (m, 3H), 7.40-7.30 (m, 3H), 5.29 (s, 2H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 141.1 (C_q), 141.1 (C_q), 139.3 (C_q), 139.0 (C_q), 131.3 (C_q), 128.9 (CH), 128.8 (CH), 128.4 (CH), 128.2 (CH), 127.0 (CH), 124.2 (CH), 121.3 (CH), 50.9 (CH_2). IR (film): 3054, 2985, 1711, 1611, 1498, 1474, 1449, 1420, 1360, 1265, 1179, 1130, 1072, 1020, 985, 896, 762, 736, 700, 669 cm^{-1}. MS (EI) *m/z* (relative intensity) 233 (15) [M^+], 204 (100), 190 (10), 176 (11), 149 (12), 102 (14), 89 (8). HR-MS (ESI) *m/z* calcd for $C_{15}H_{12}N_3$ 234.1026, found 234.1026.

Literature:

[1] L. Zhang, X. Chen, P. Xue, H. H. Y. Sun, I. D. Williams, K. B. Sharpless, V. V. Fokin, G. Jia, *J. Am. Chem. Soc.* **2005**, *127*, 15998–15999.
[2] P. Appukkuttan, W. Dehaen, V. V. Fokin, E. Van der Eycken, *Org. Lett.* **2004**, *6*, 4223–4225.
[3] K. Kacprzak, *Synlett* **2005**, 943–946.
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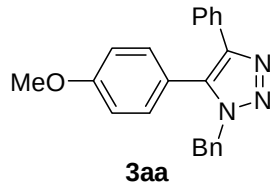
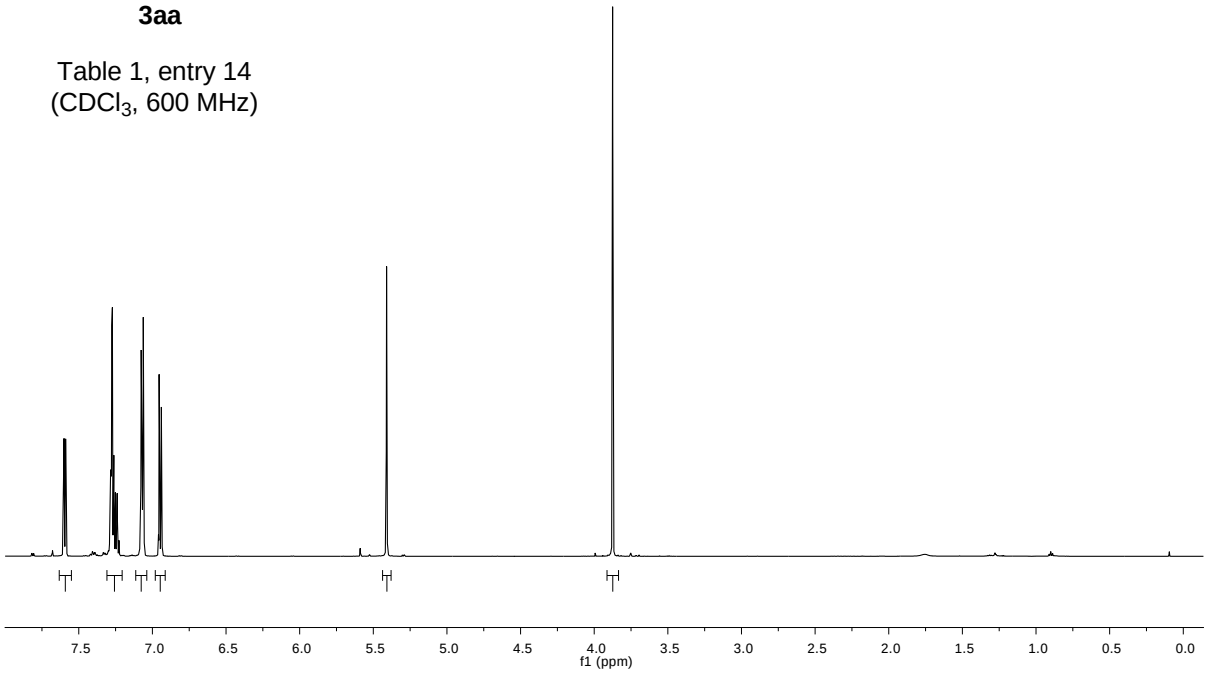
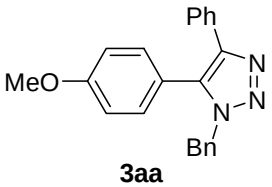
[5] M. Iwasaki, H. Yorimitsu, K. Oshima, *Chem. Asian J.* **2007**, *2*, 1430–1435.
[6] S. Chuprakov, N. Chernyak, A. S. Dudnik, V. Gevorgyan, *Org. Lett.* **2007**, *9*, 2333–2336.



3aa

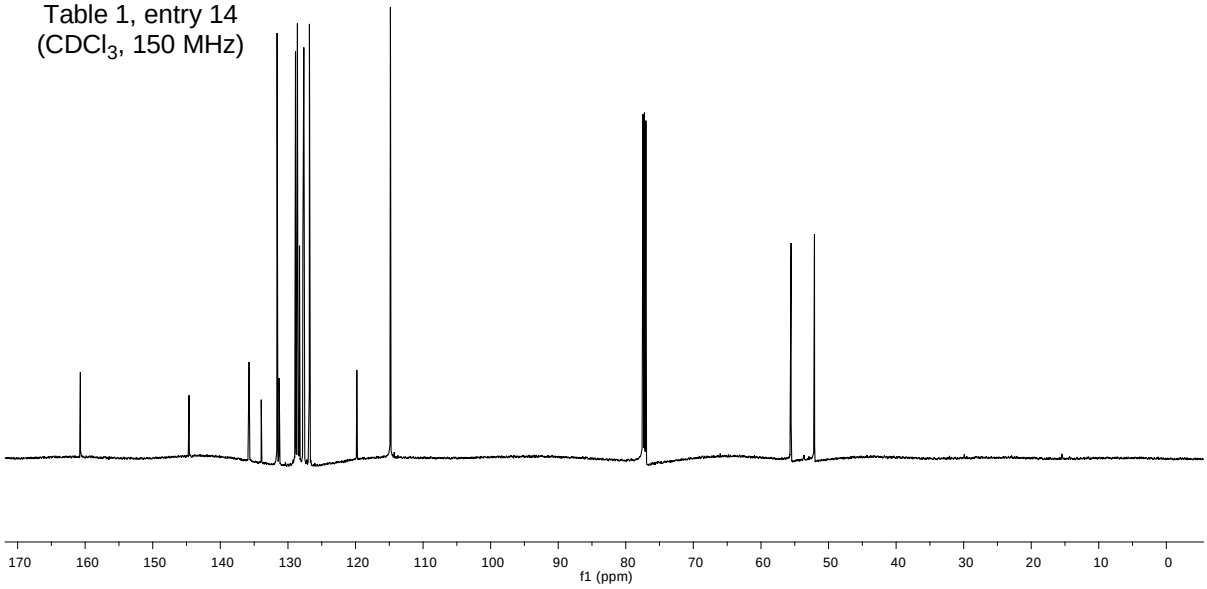
Table 1, entry 14
($CDCl_3$, 600 MHz)

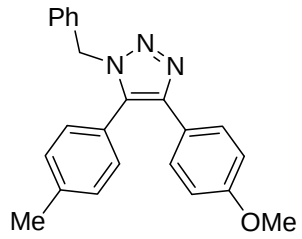




3aa

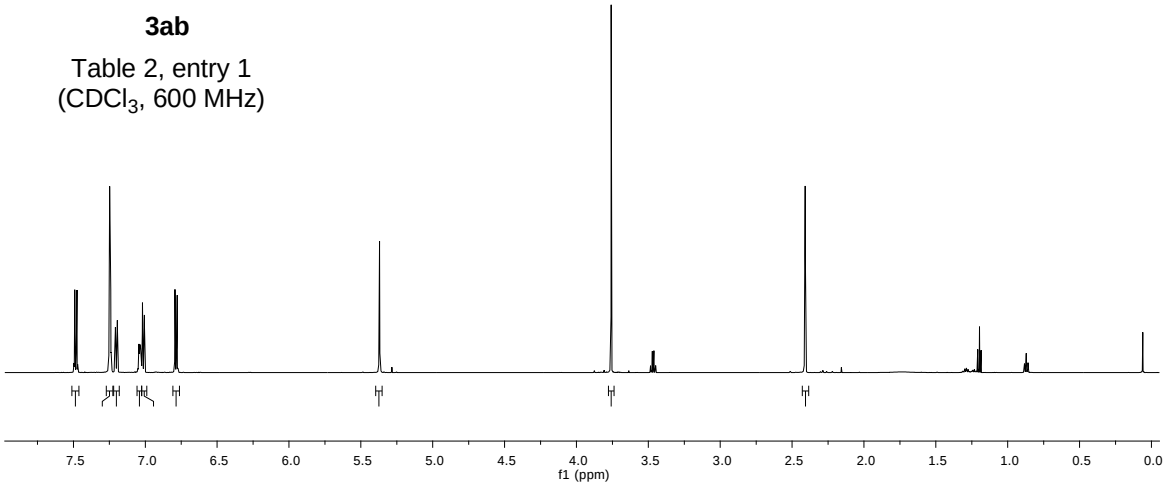
Table 1, entry 14
($CDCl_3$, 150 MHz)

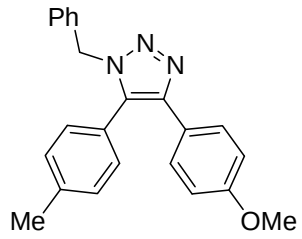




3ab

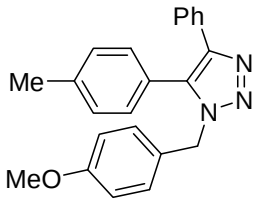
Table 2, entry 1
($CDCl_3$, 600 MHz)





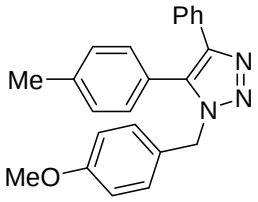
3ab

Table 2, entry 1
($CDCl_3$, 150 MHz)



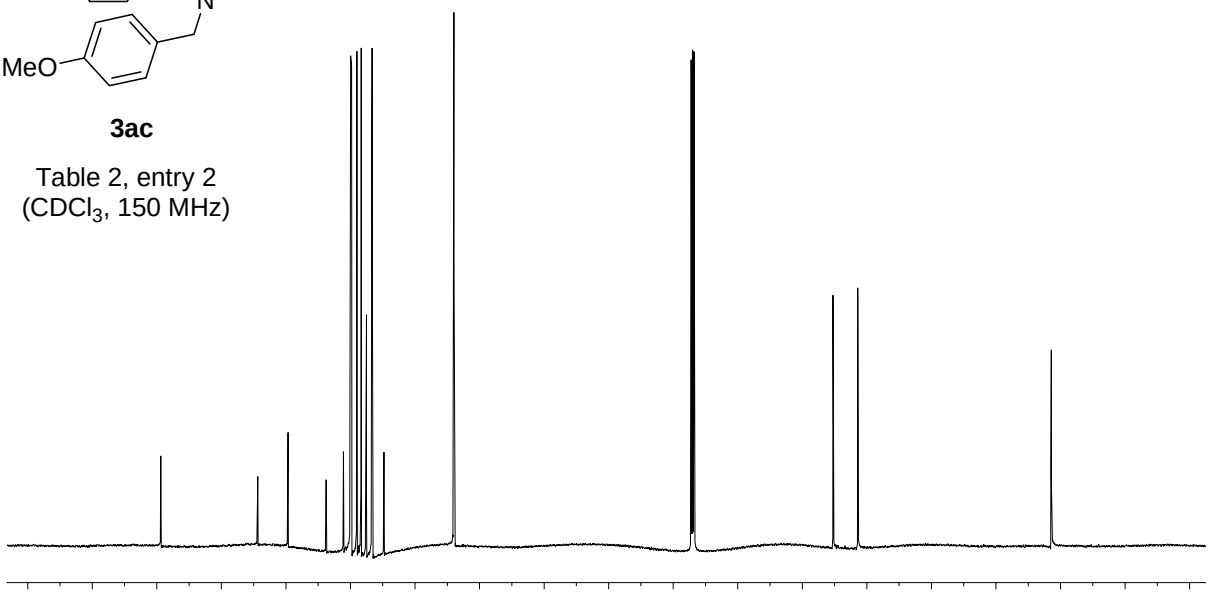
3ac

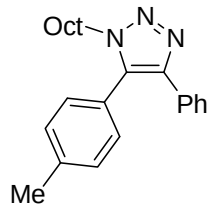
Table 2, entry 2
($CDCl_3$, 600 MHz)



3ac

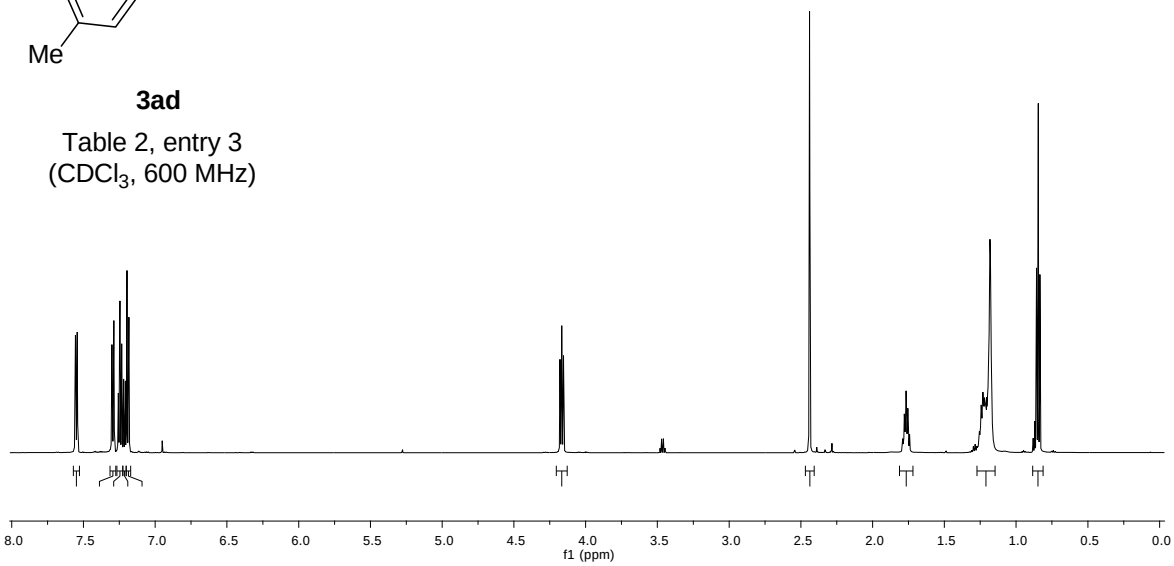
Table 2, entry 2
($CDCl_3$, 150 MHz)

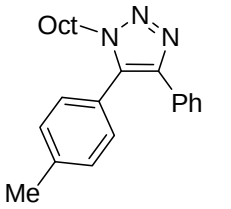




3ad

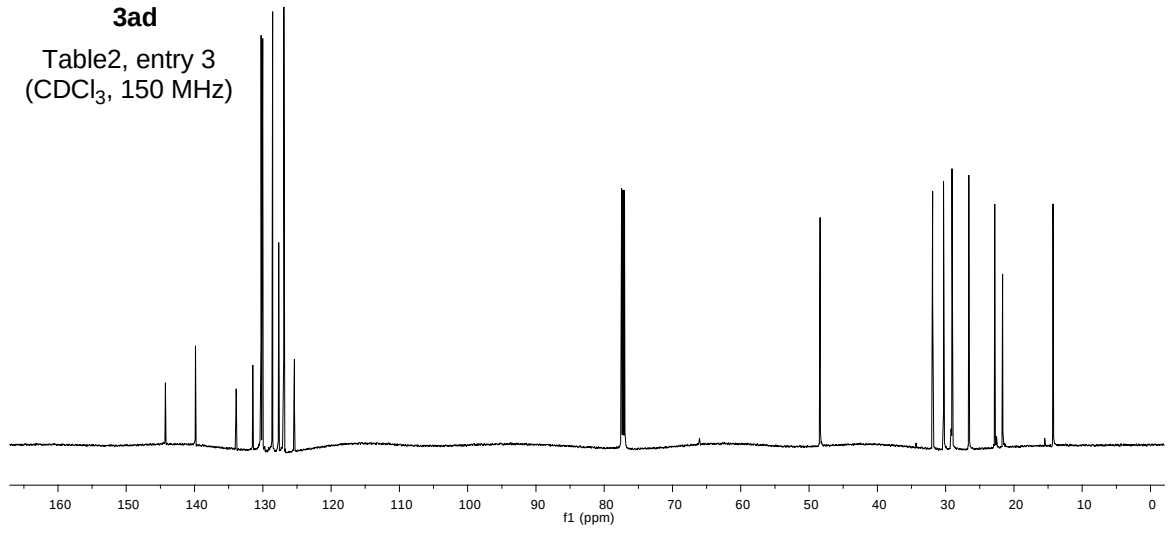
Table 2, entry 3
($CDCl_3$, 600 MHz)

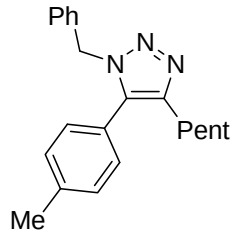




3ad

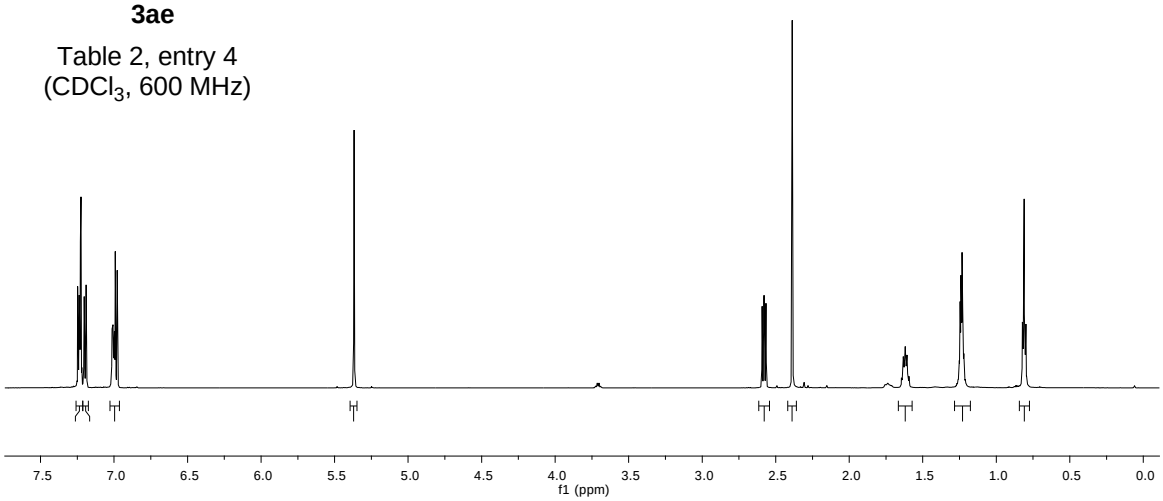
Table2, entry 3
($CDCl_3$, 150 MHz)

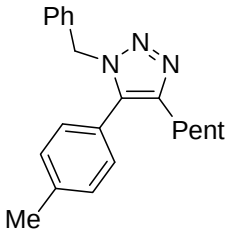




3ae

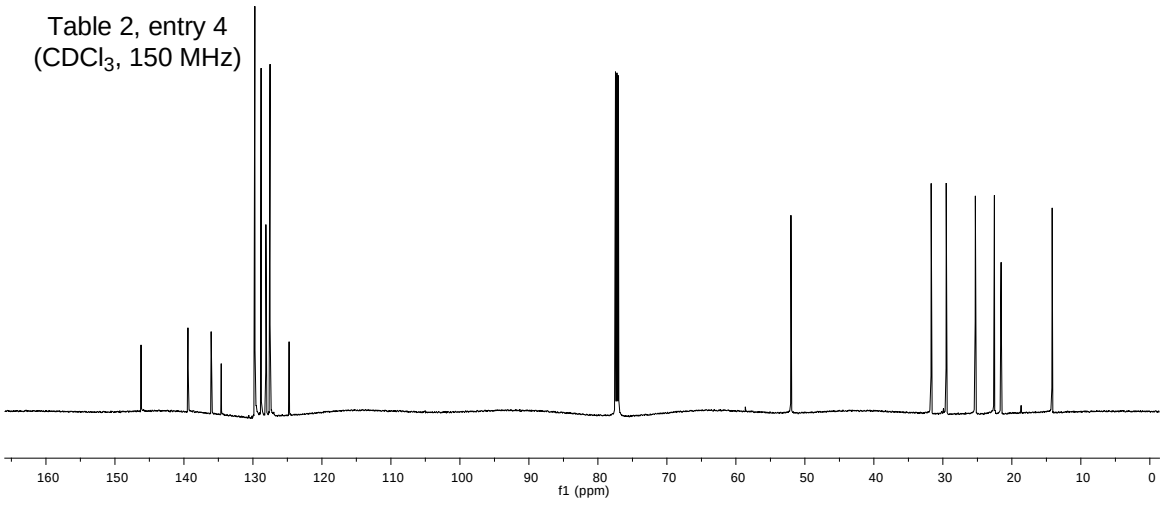
Table 2, entry 4
($CDCl_3$, 600 MHz)

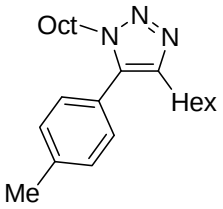




3ae

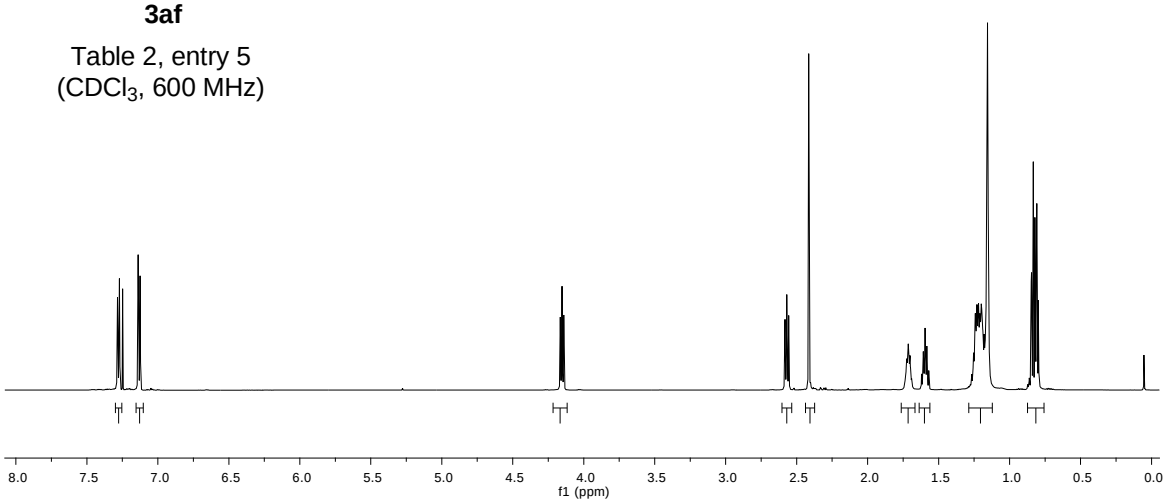
Table 2, entry 4
($CDCl_3$, 150 MHz)

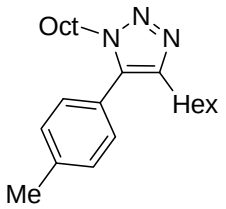




3af

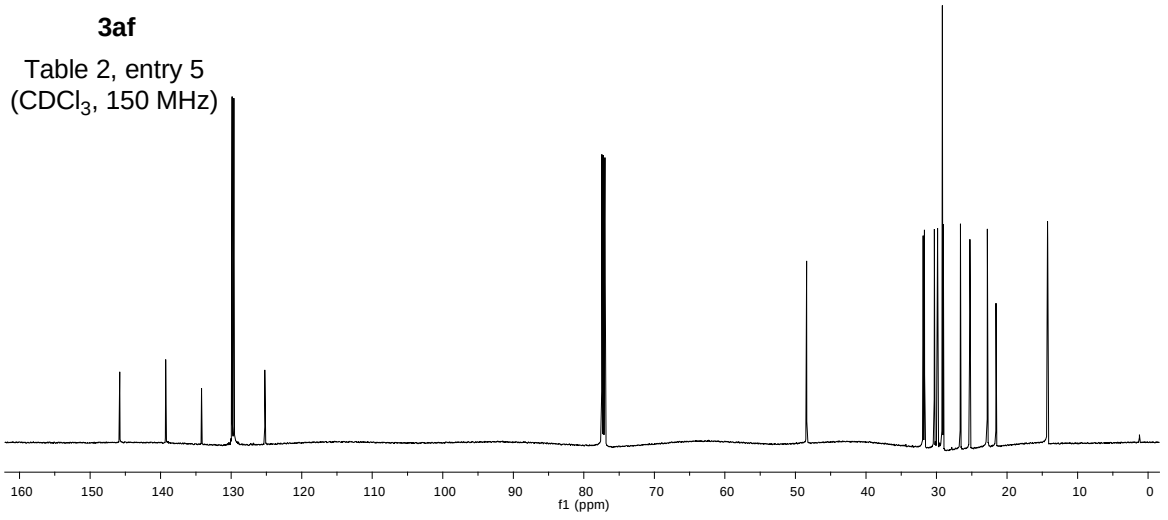
Table 2, entry 5
($CDCl_3$, 600 MHz)

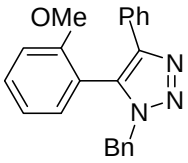




3af

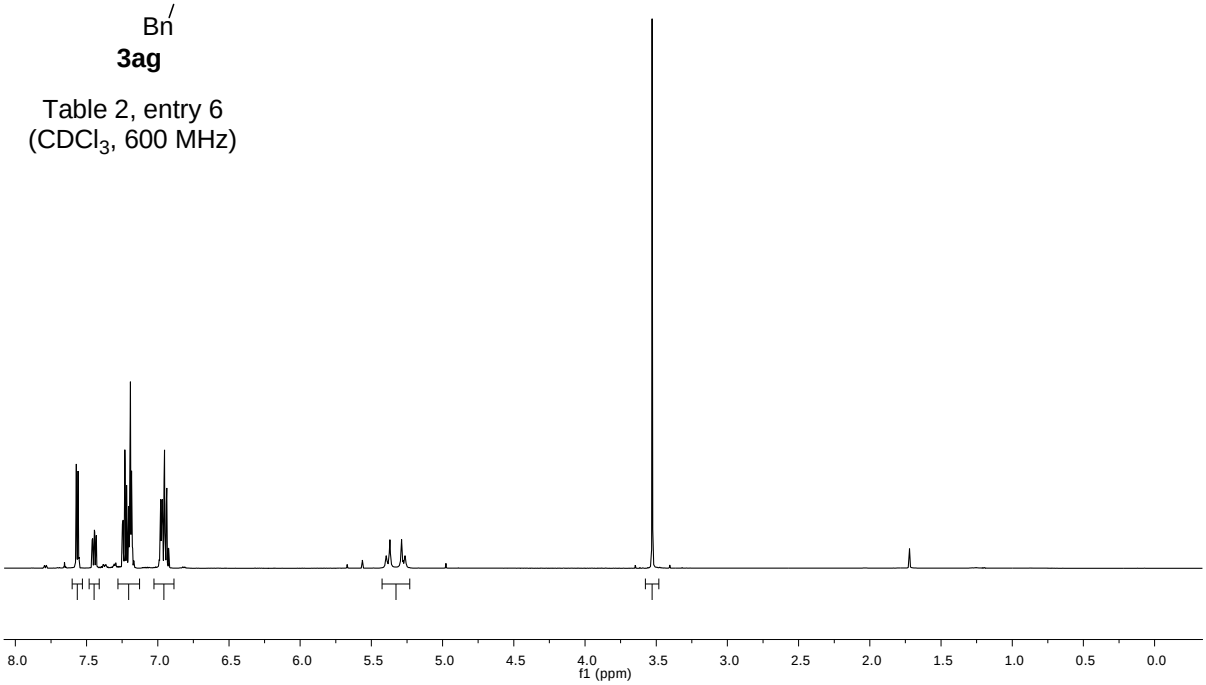
Table 2, entry 5
($CDCl_3$, 150 MHz)

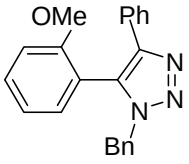




3ag

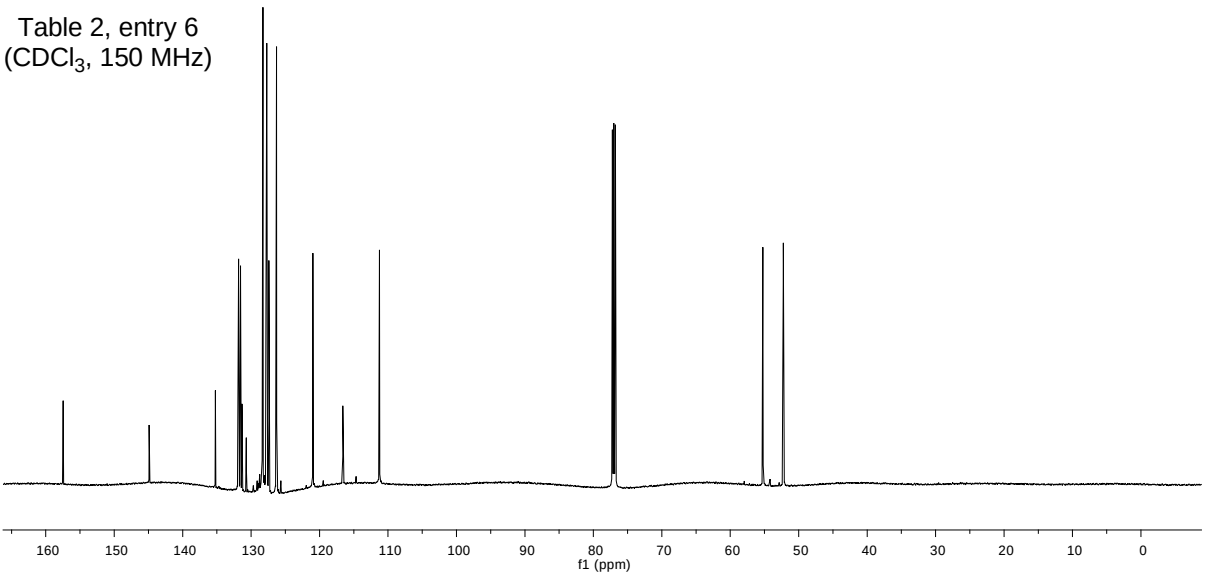
Table 2, entry 6
($CDCl_3$, 600 MHz)

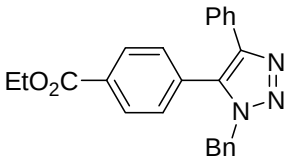




3ag

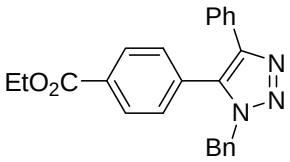
Table 2, entry 6
($CDCl_3$, 150 MHz)





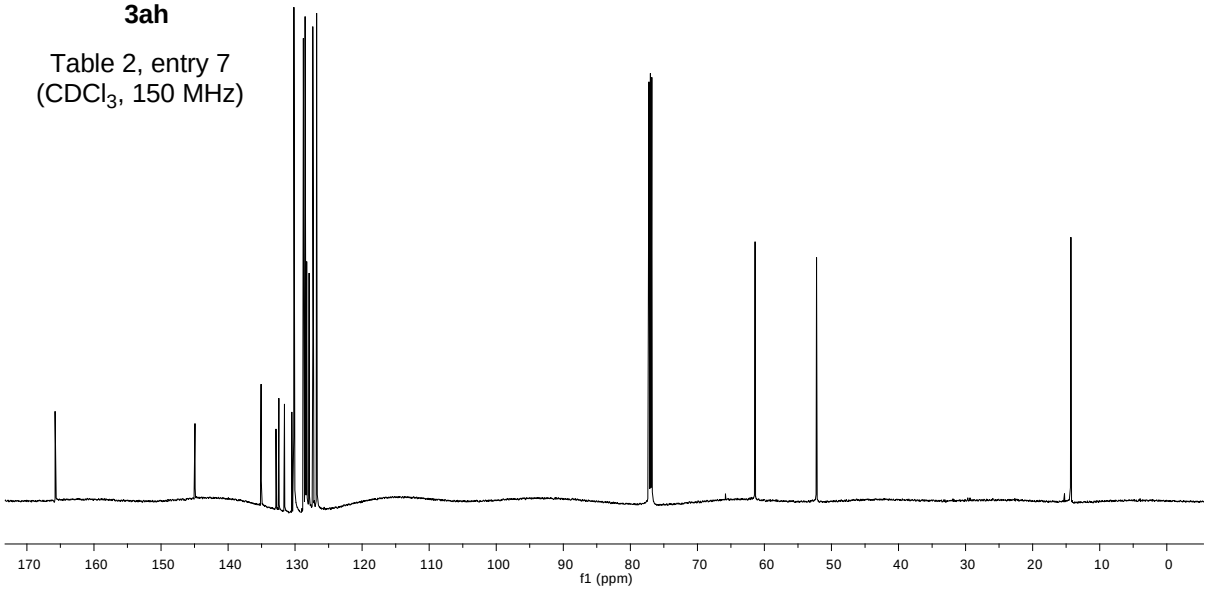
3ah

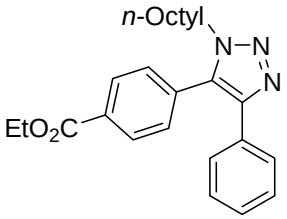
Table 2, entry 7
($CDCl_3$, 600 MHz)



3ah

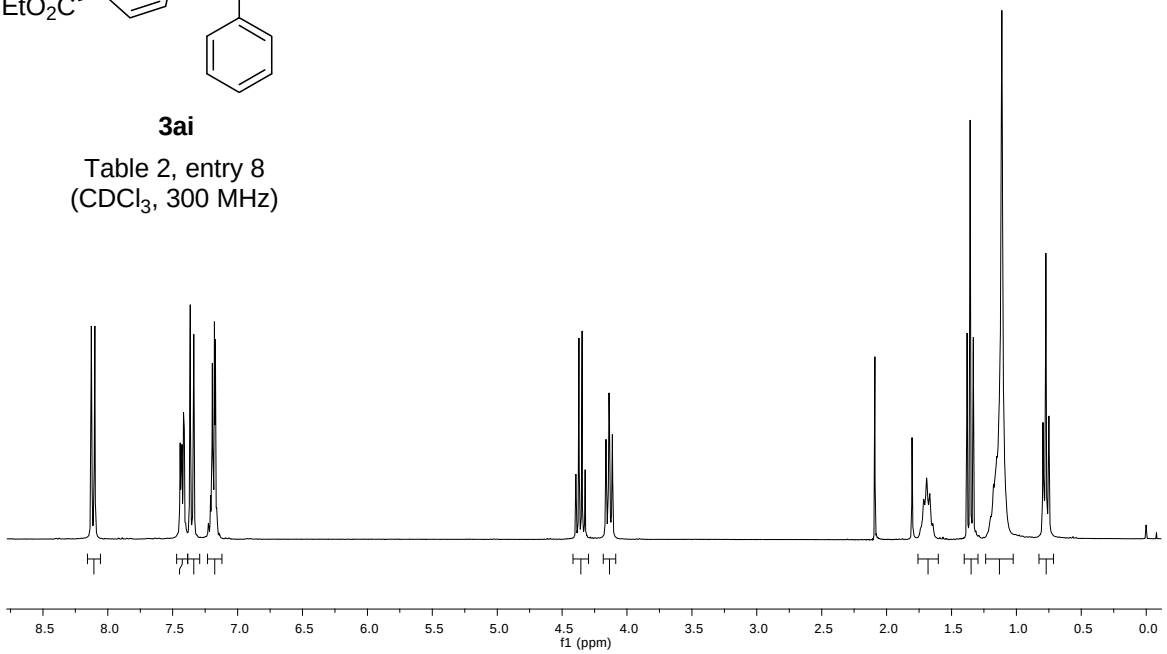
Table 2, entry 7
($CDCl_3$, 150 MHz)

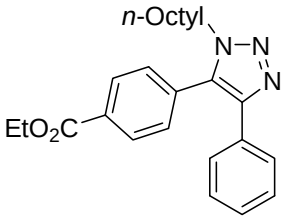




3ai

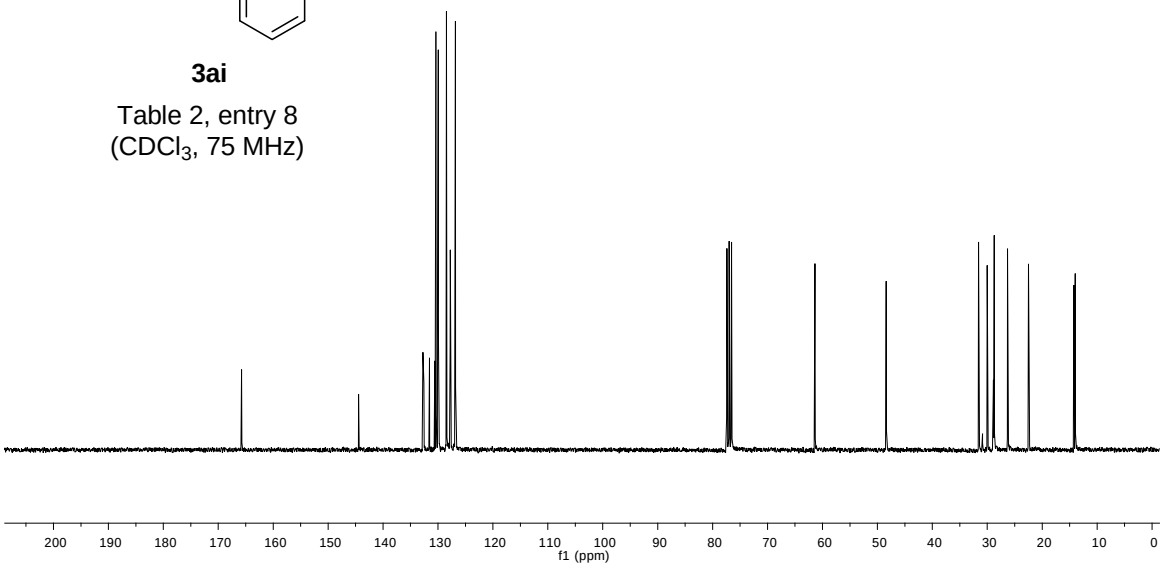
Table 2, entry 8
($CDCl_3$, 300 MHz)

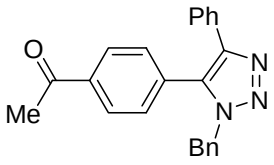




3ai

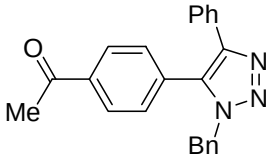
Table 2, entry 8
($CDCl_3$, 75 MHz)





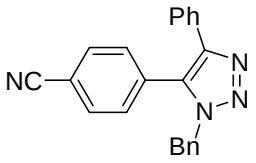
3aj

Table 2, entry 11
($CDCl_3$, 600 MHz)



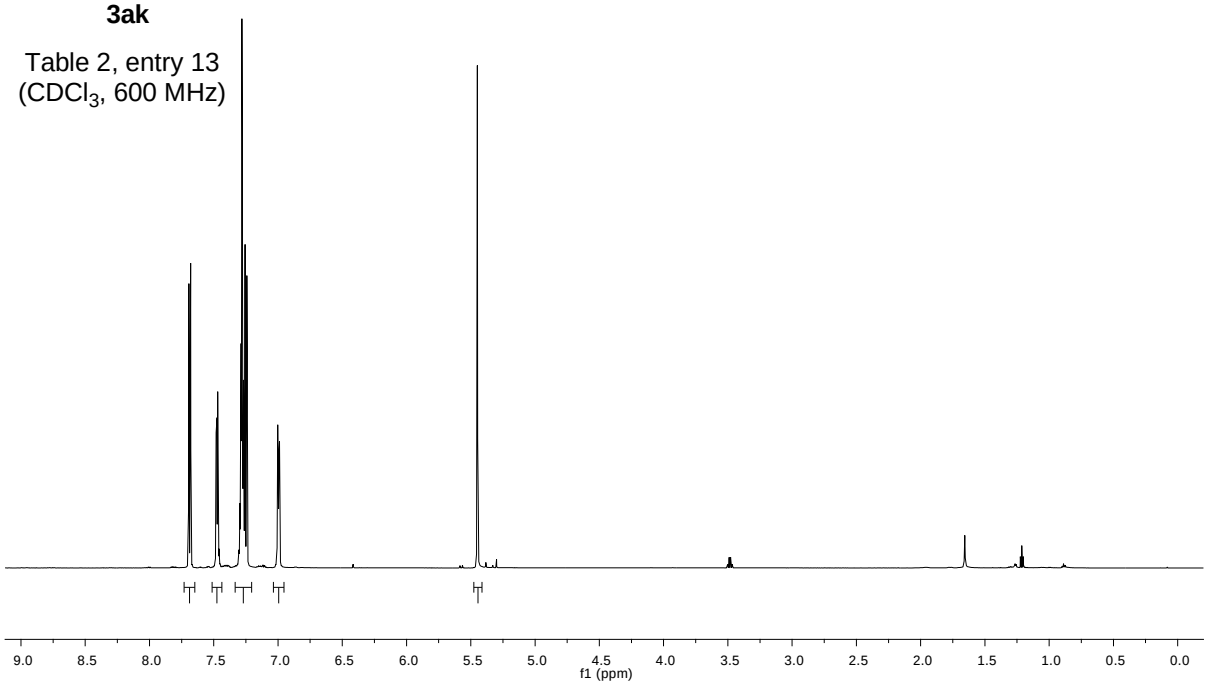
3aj

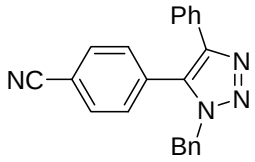
Table 2, entry11
($CDCl_3$, 150 MHz)



3ak

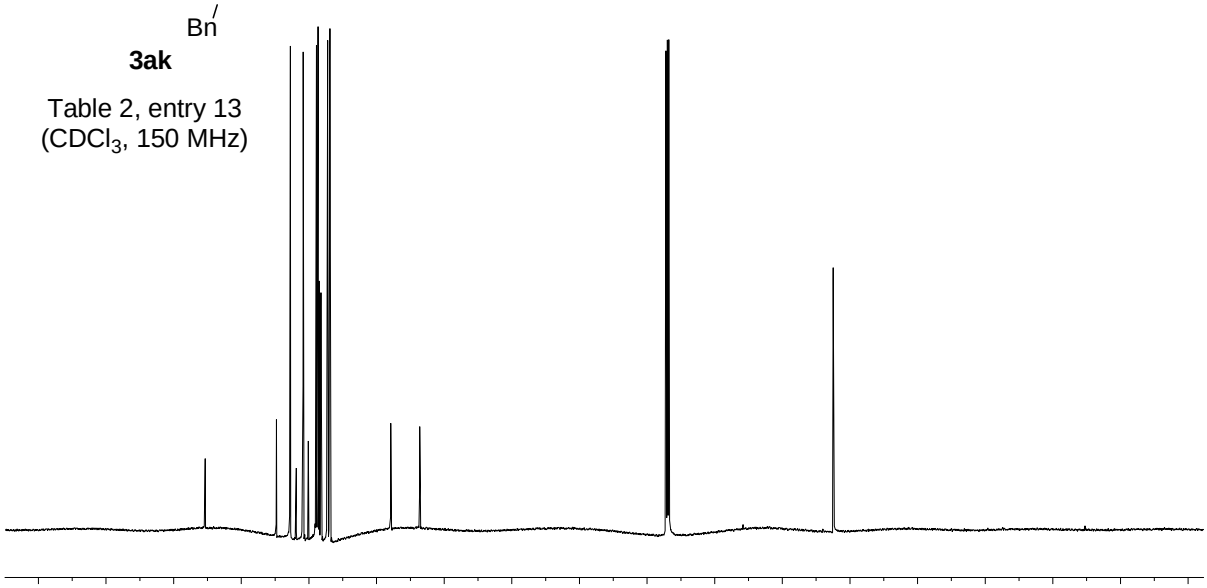
Table 2, entry 13
($CDCl_3$, 600 MHz)

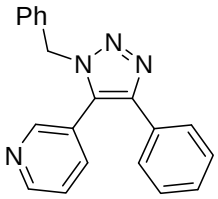




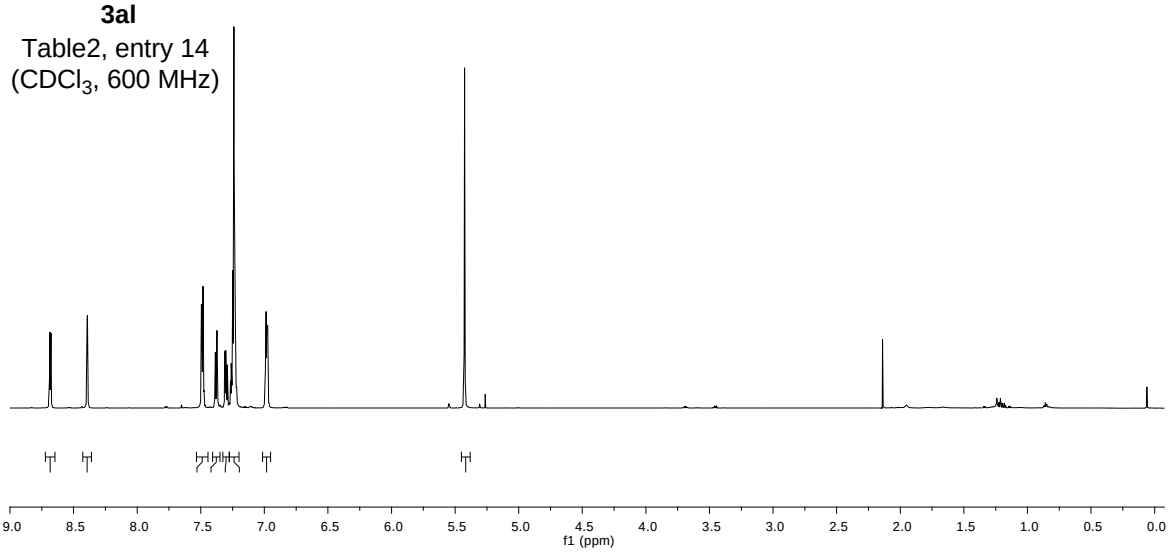
3ak

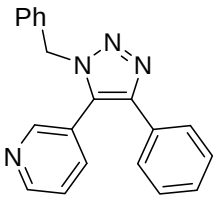
Table 2, entry 13
($CDCl_3$, 150 MHz)



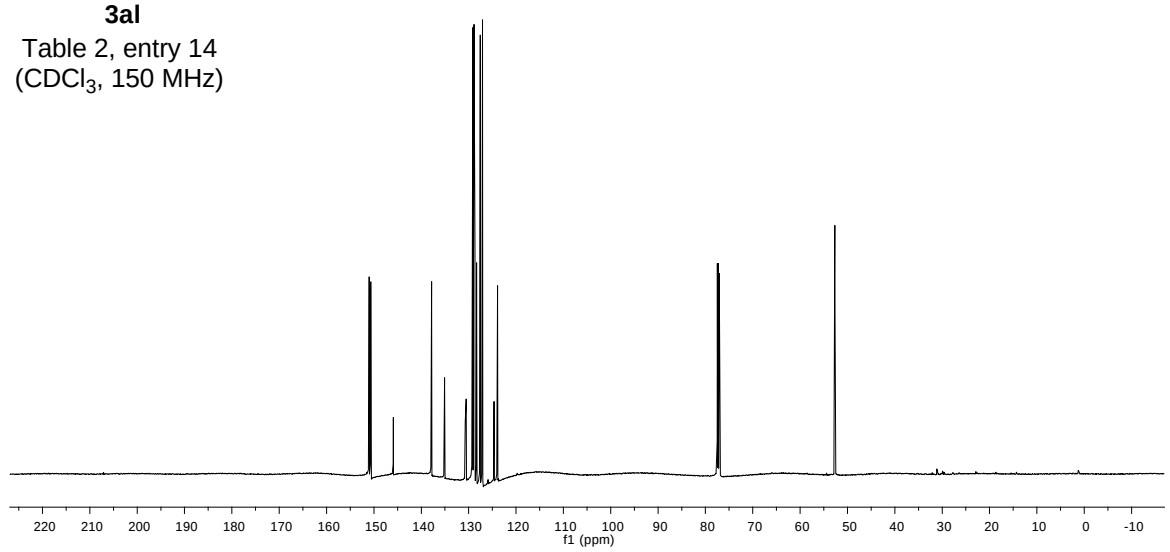


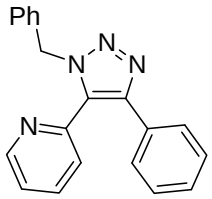
3al
Table2, entry 14
($CDCl_3$, 600 MHz)



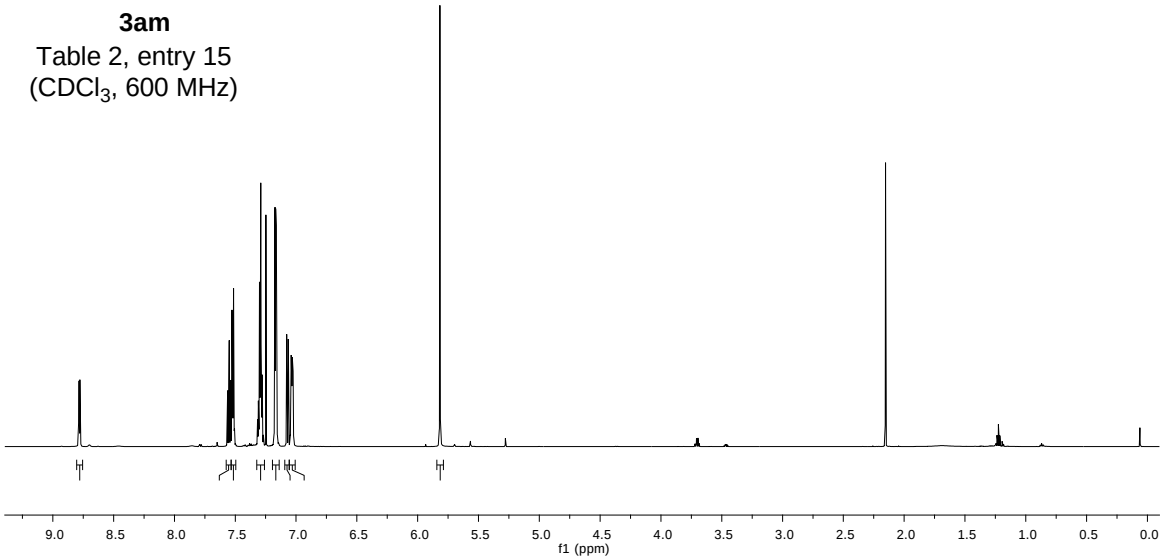


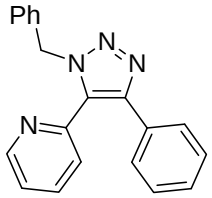
3al
Table 2, entry 14
($CDCl_3$, 150 MHz)



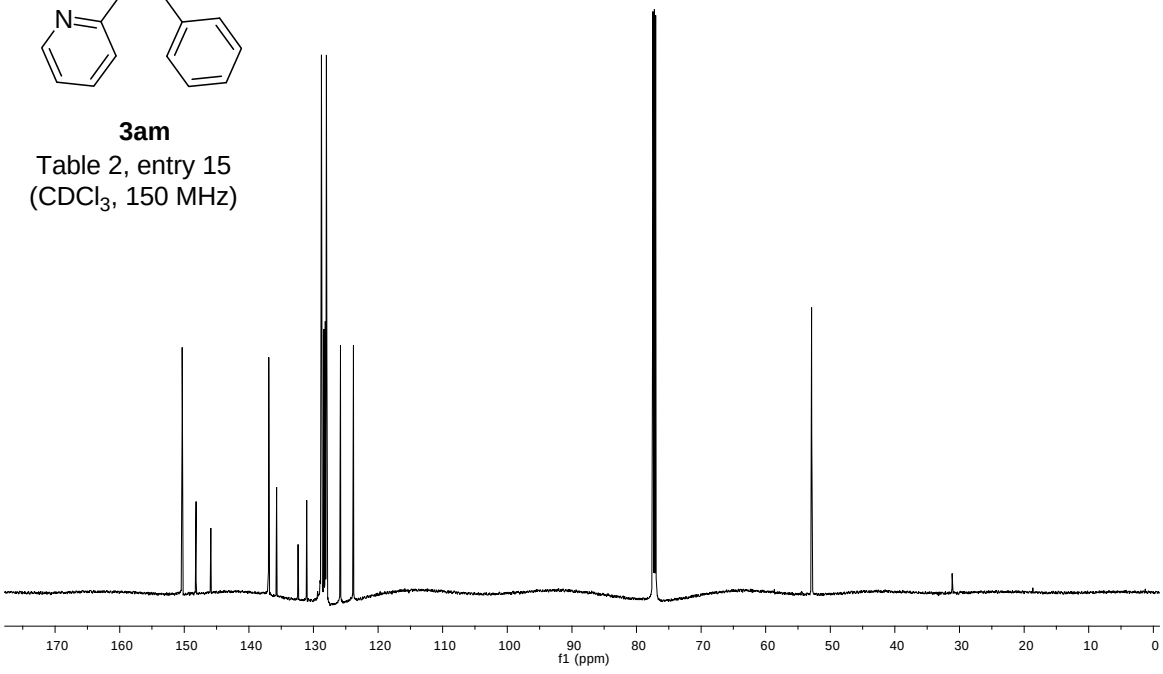


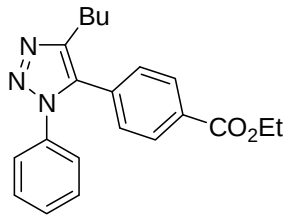
3am
Table 2, entry 15
($CDCl_3$, 600 MHz)





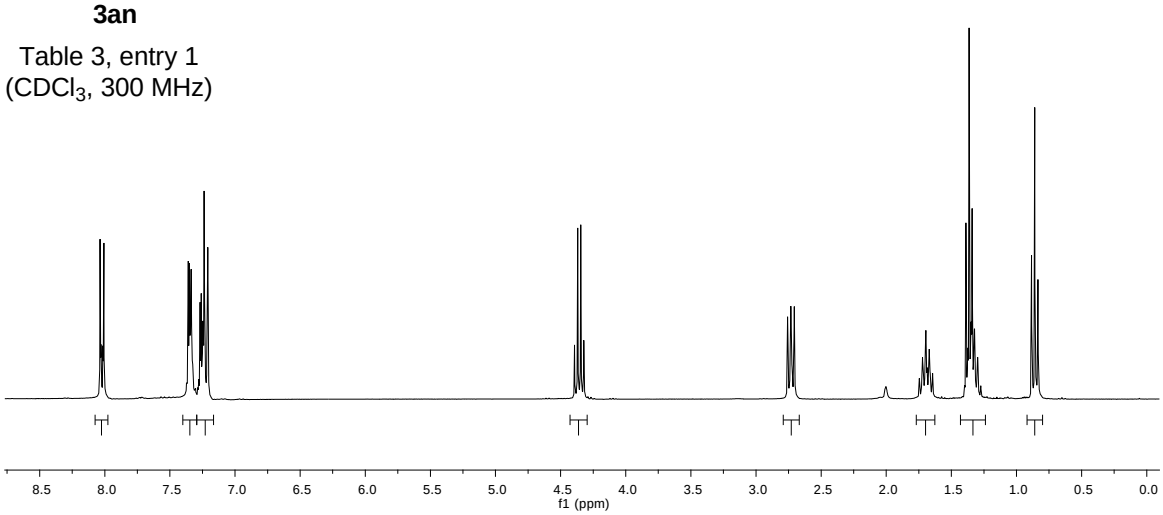
3am
Table 2, entry 15
($CDCl_3$, 150 MHz)

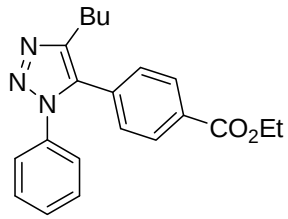




3an

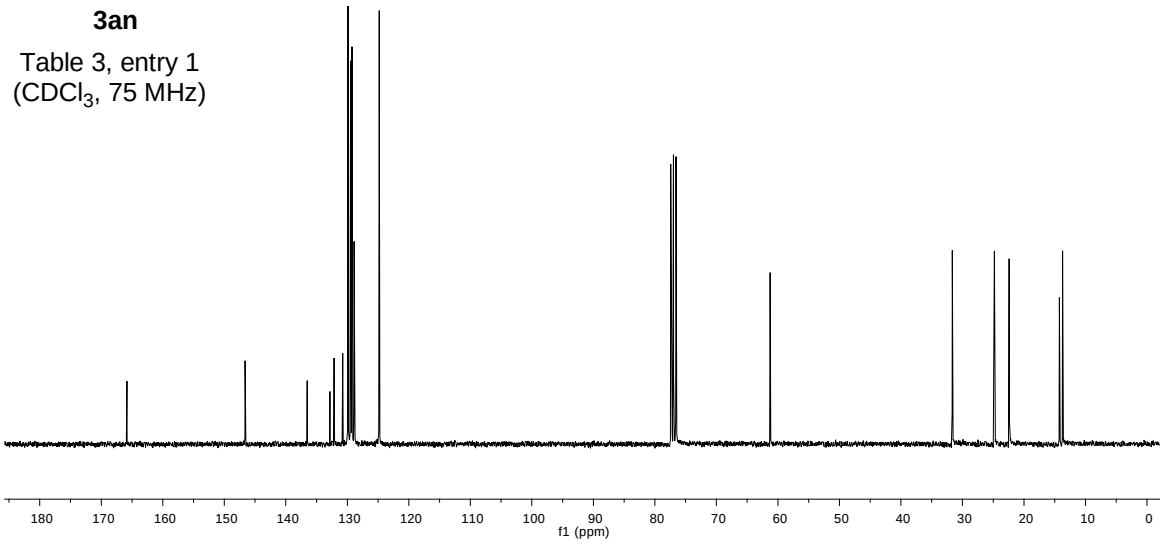
Table 3, entry 1
($CDCl_3$, 300 MHz)

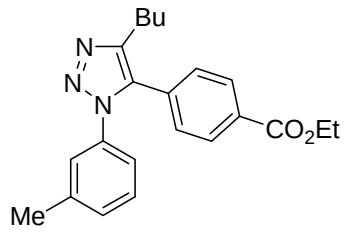




3an

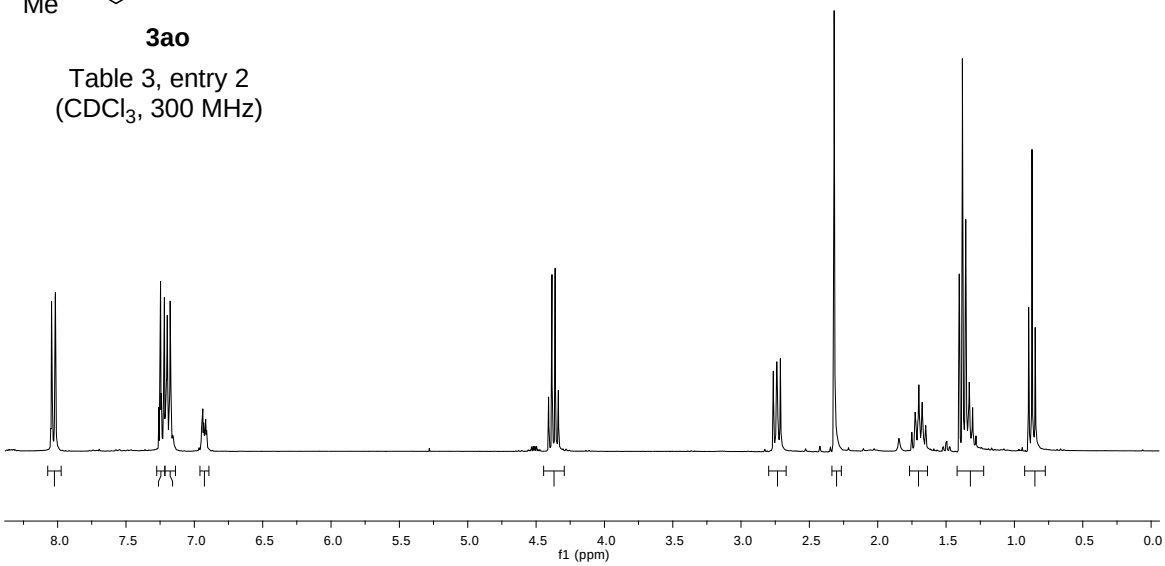
Table 3, entry 1
($CDCl_3$, 75 MHz)

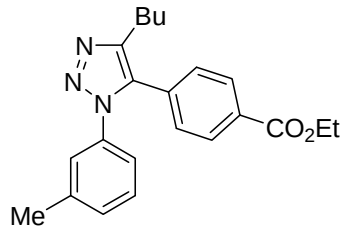




3ao

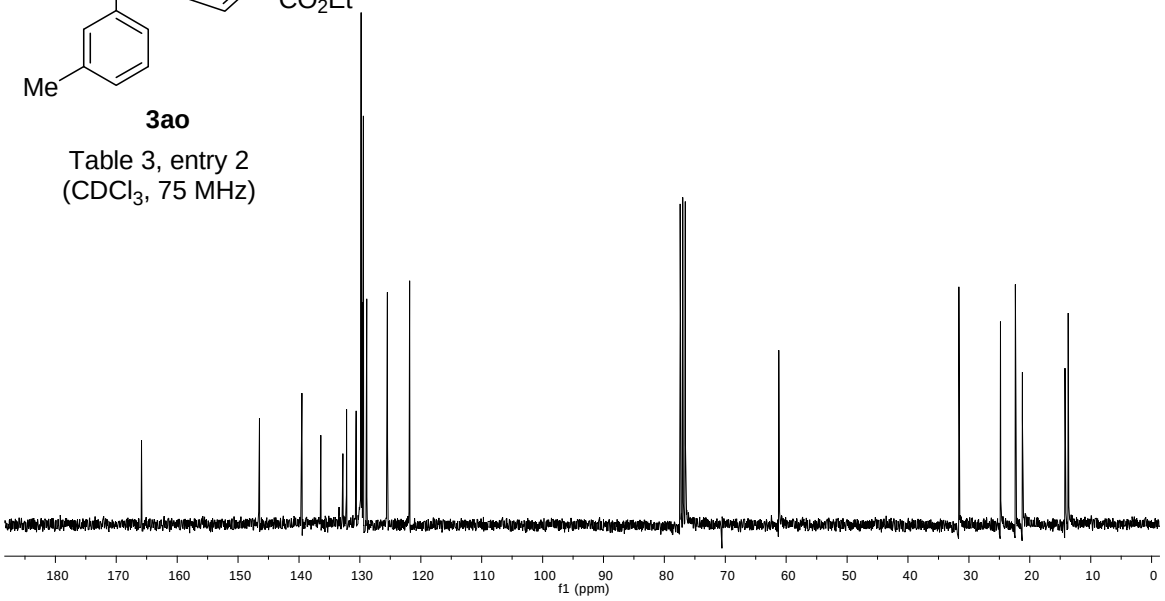
Table 3, entry 2
($CDCl_3$, 300 MHz)

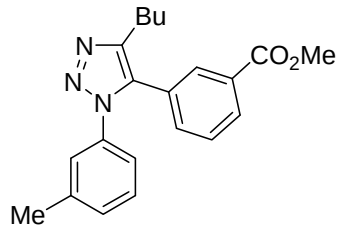




3ao

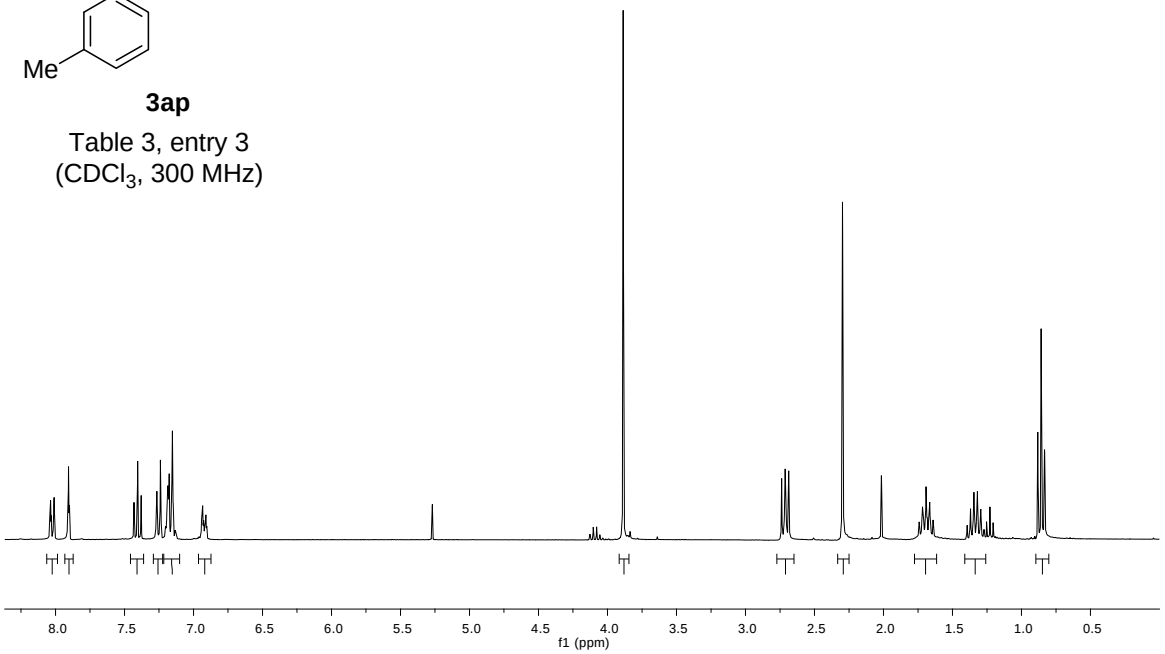
Table 3, entry 2
($CDCl_3$, 75 MHz)

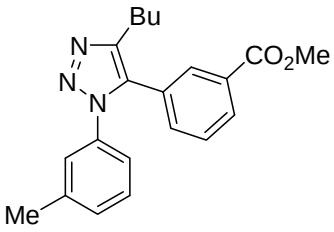




3ap

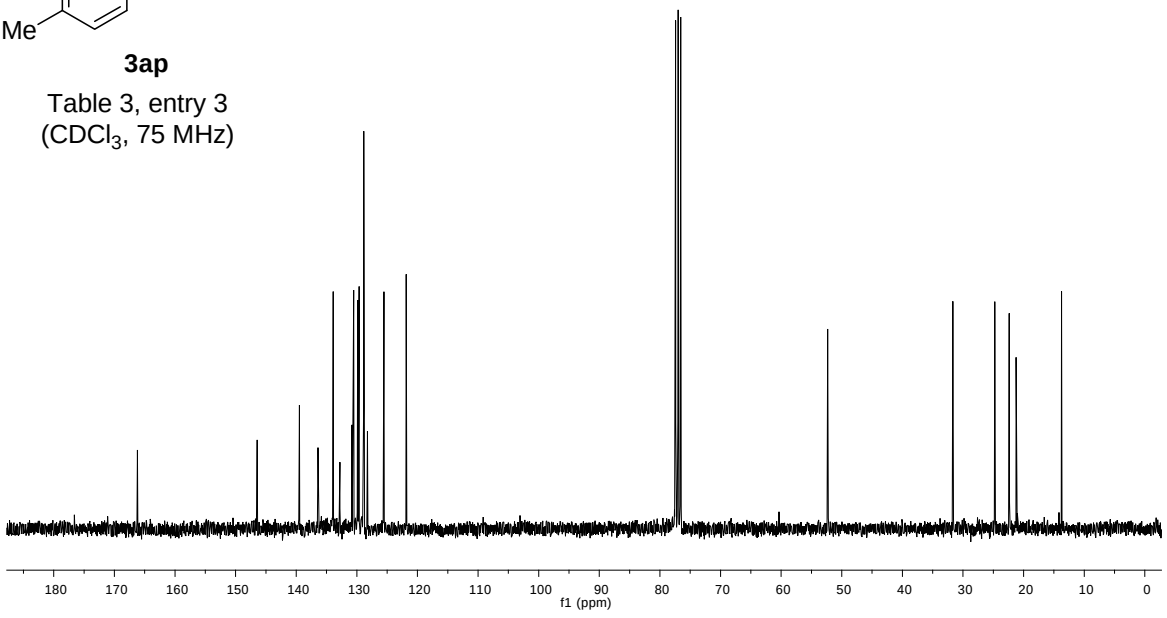
Table 3, entry 3
($CDCl_3$, 300 MHz)

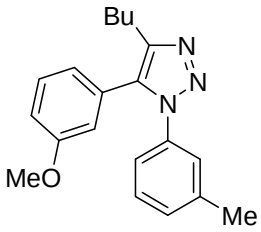




3ap

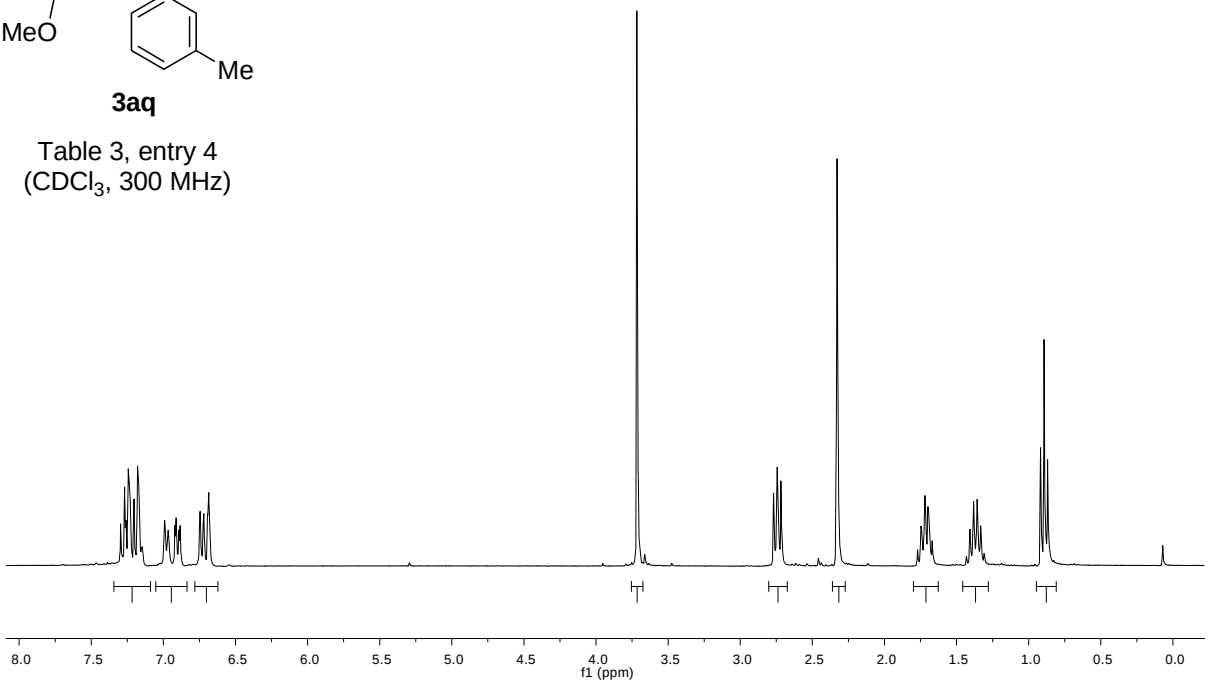
Table 3, entry 3
($CDCl_3$, 75 MHz)

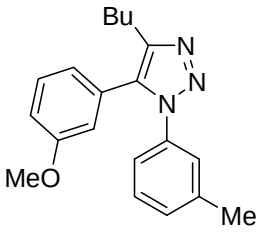




3aq

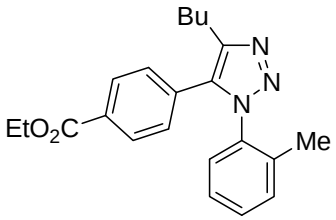
Table 3, entry 4
($CDCl_3$, 300 MHz)





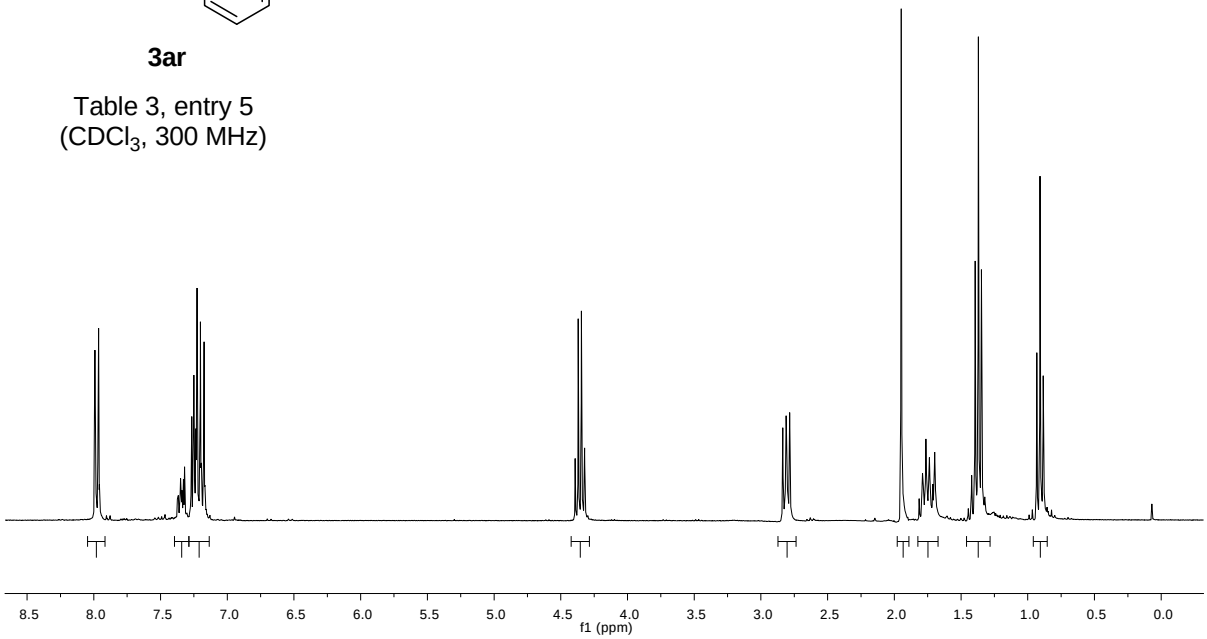
3aq

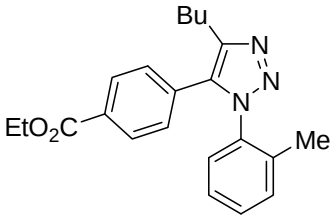
Table 3, entry 4
($CDCl_3$, 75 MHz)



3ar

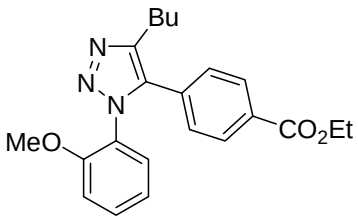
Table 3, entry 5
($CDCl_3$, 300 MHz)





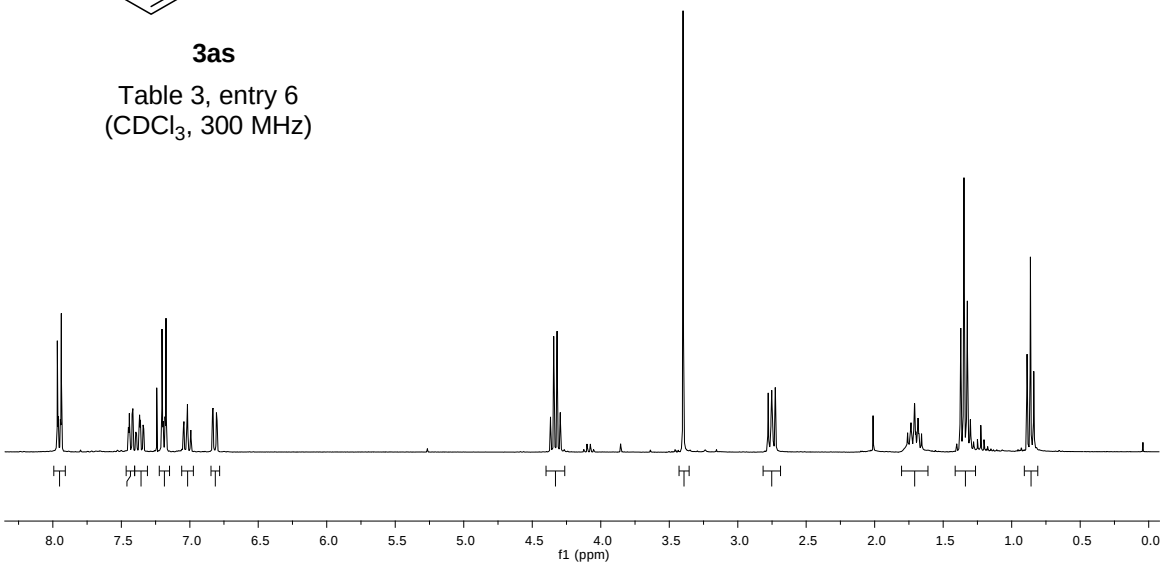
3ar

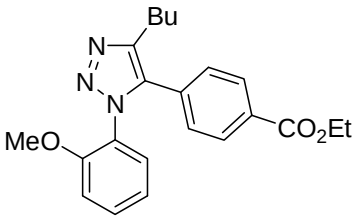
Table 3, entry 5
($CDCl_3$, 75 MHz)



3as

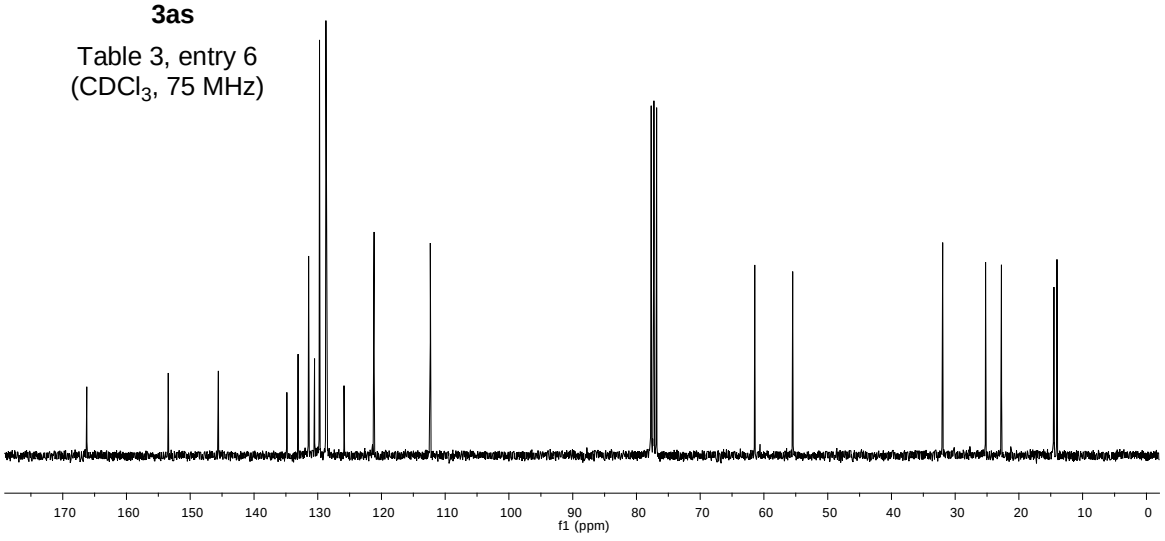
Table 3, entry 6
($CDCl_3$, 300 MHz)

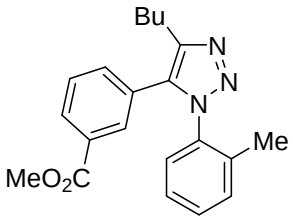




3as

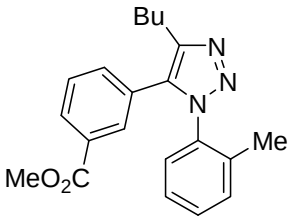
Table 3, entry 6
($CDCl_3$, 75 MHz)





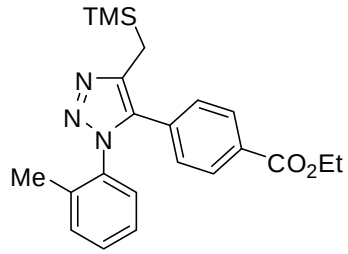
3at

Table 3, entry 7
($CDCl_3$, 300 MHz)



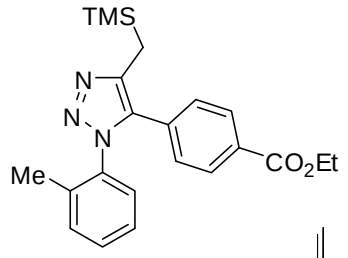
3at

Table 3, entry 7
($CDCl_3$, 75 MHz)



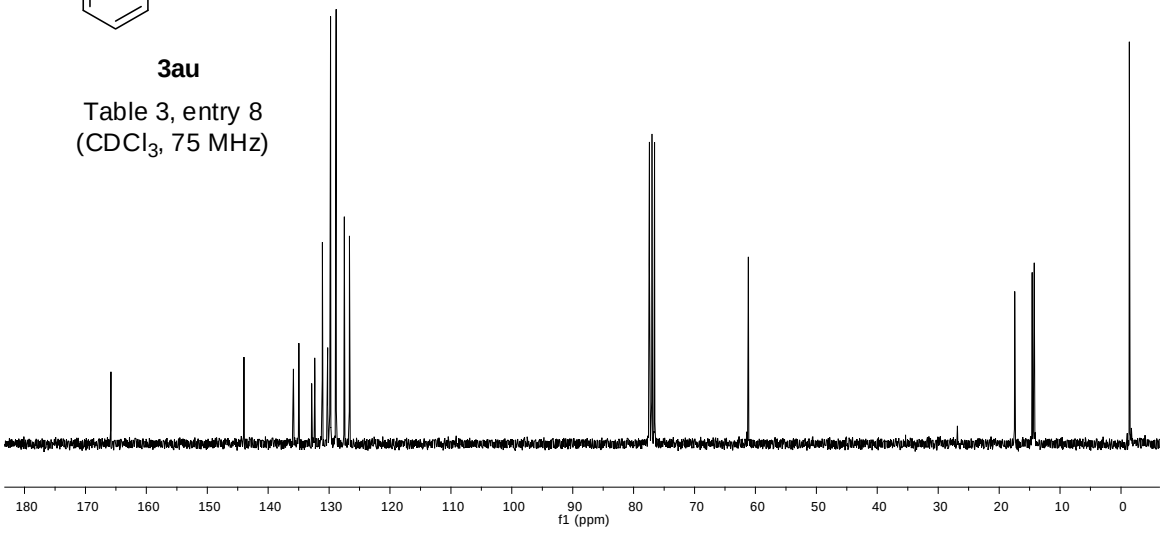
3au

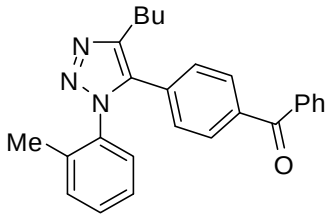
Table 3, entry 8
($CDCl_3$, 300 MHz)



3au

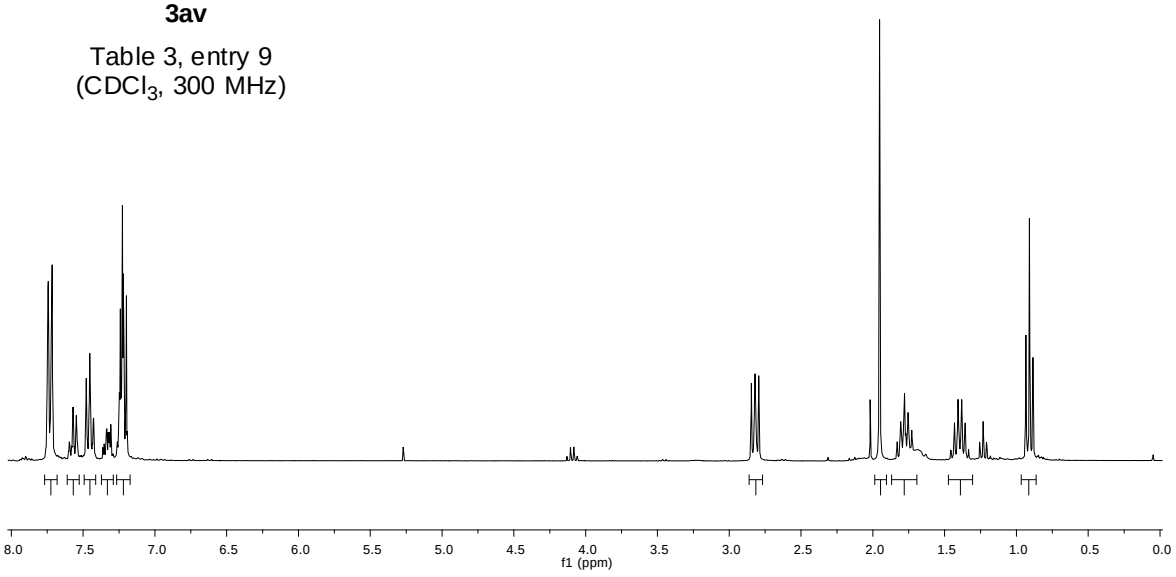
Table 3, entry 8
($CDCl_3$, 75 MHz)

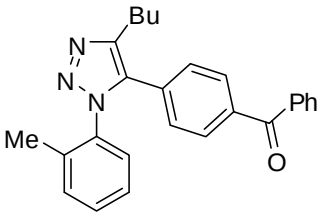




3av

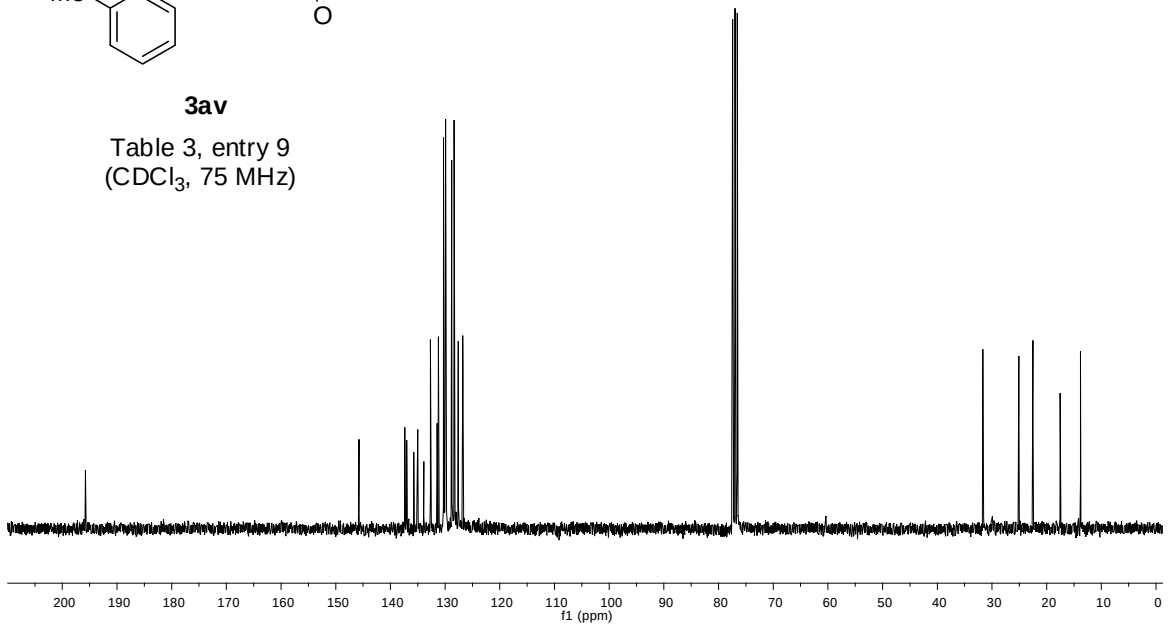
Table 3, entry 9
($CDCl_3$, 300 MHz)

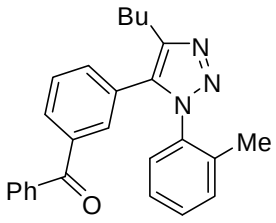




3av

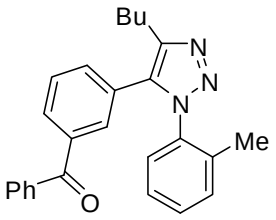
Table 3, entry 9
($CDCl_3$, 75 MHz)





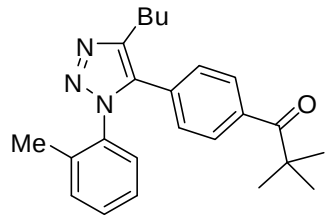
3aw

Table 3, entry 10
($CDCl_3$, 300 MHz)



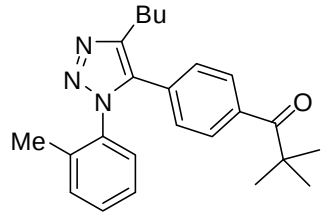
3aw

Table 3, entry 10
($CDCl_3$, 75 MHz)



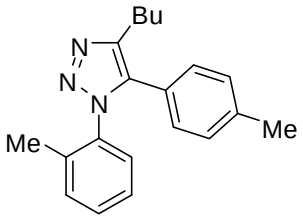
3ax

Table 3, entry 11
($CDCl_3$, 300 MHz)



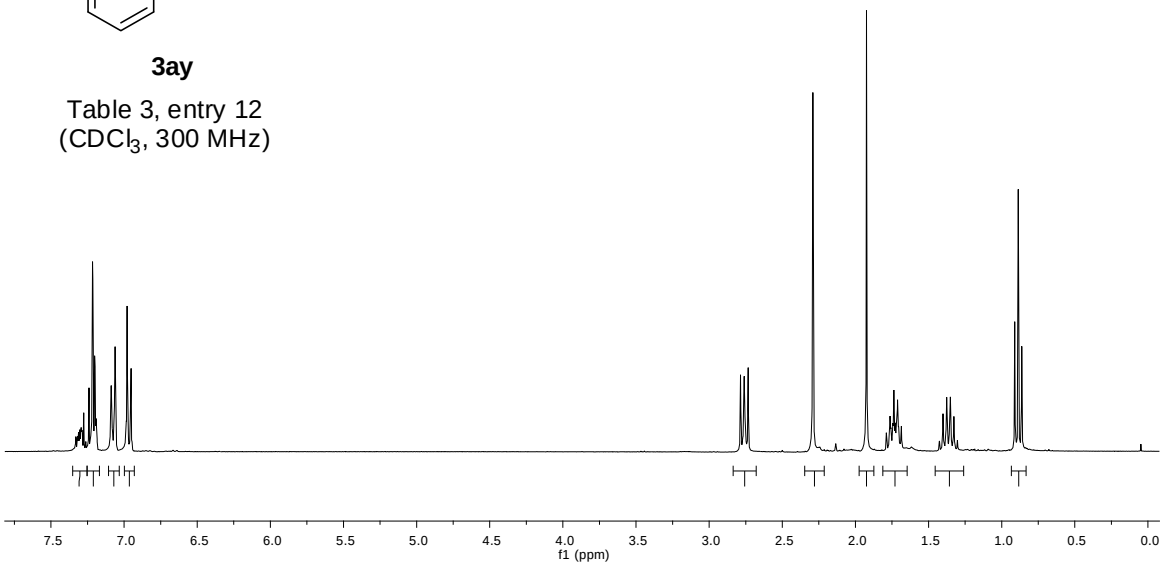
3ax

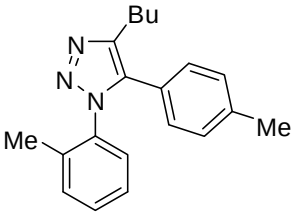
Table3, entry 11
($CDCl_3$, 75 MHz)



3ay

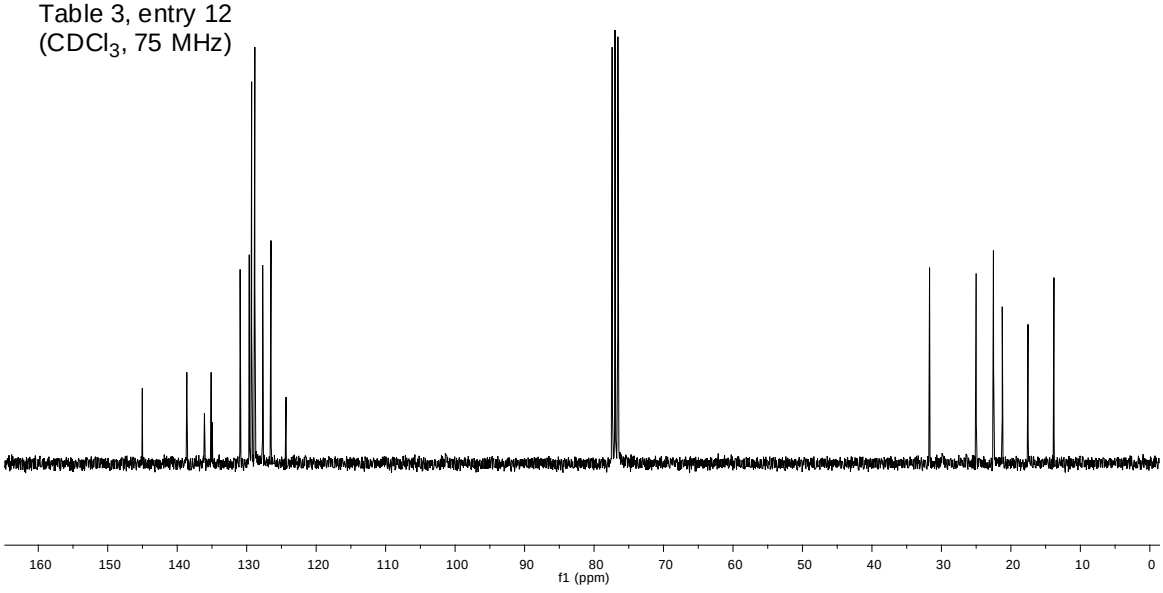
Table 3, entry 12
($CDCl_3$, 300 MHz)

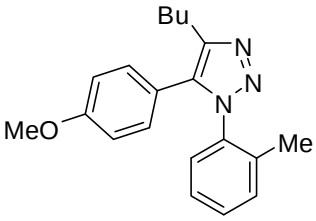




3ay

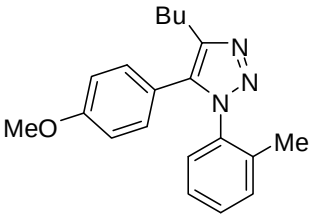
Table 3, entry 12
($CDCl_3$, 75 MHz)





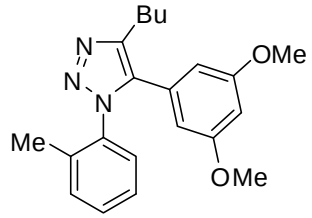
3az

Table 3, entry 13
($CDCl_3$, 300 MHz)



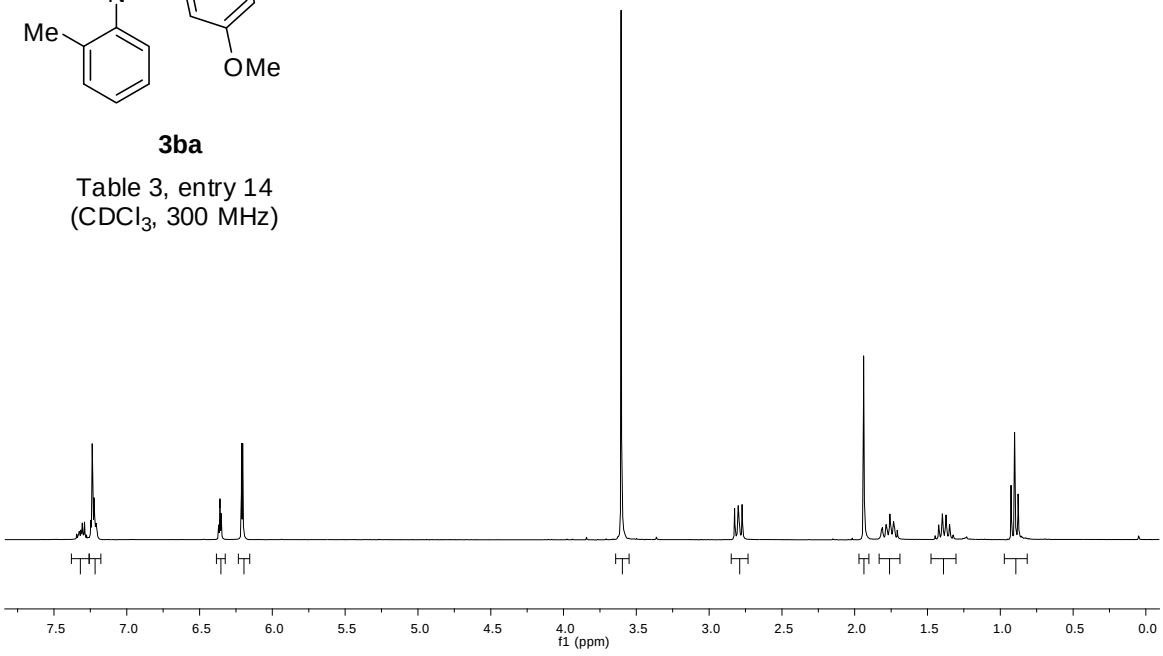
3az

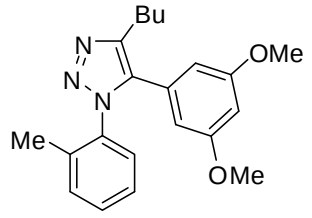
Table 3, entry 13
($CDCl_3$, 75 MHz)



3ba

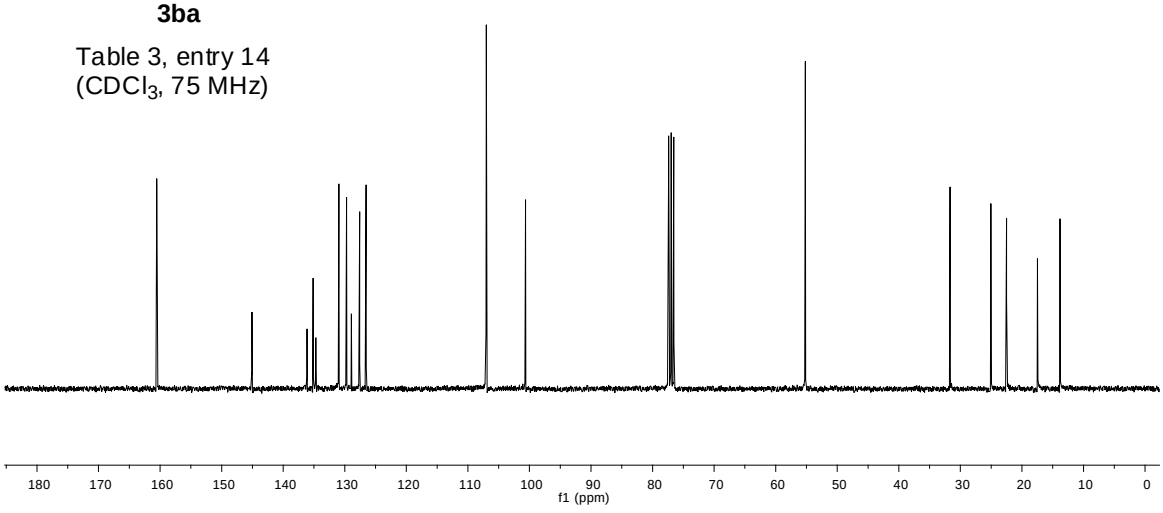
Table 3, entry 14
($CDCl_3$, 300 MHz)

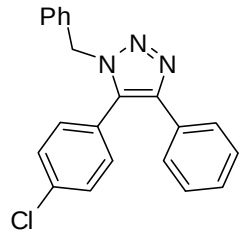




3ba

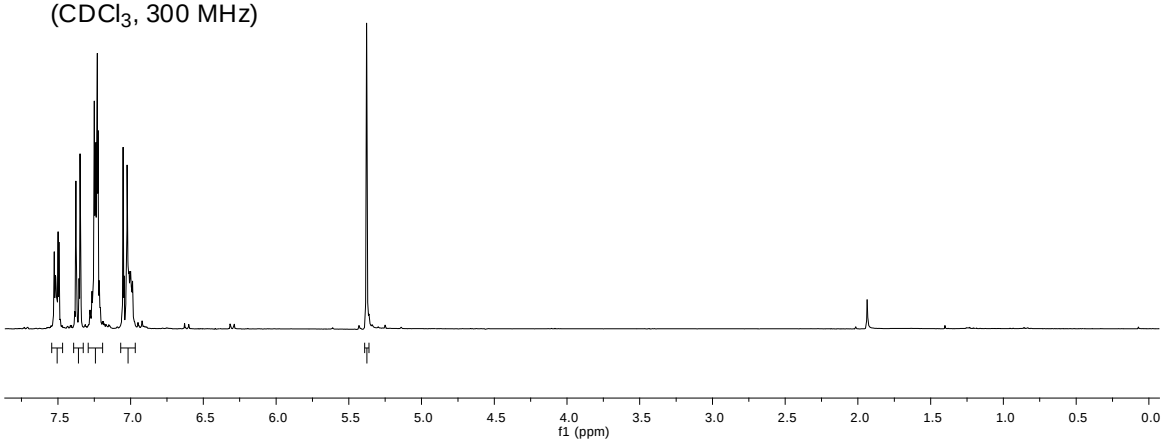
Table 3, entry 14
($CDCl_3$, 75 MHz)

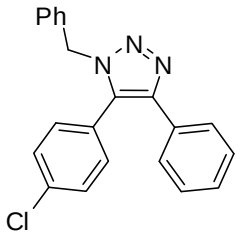




3bb

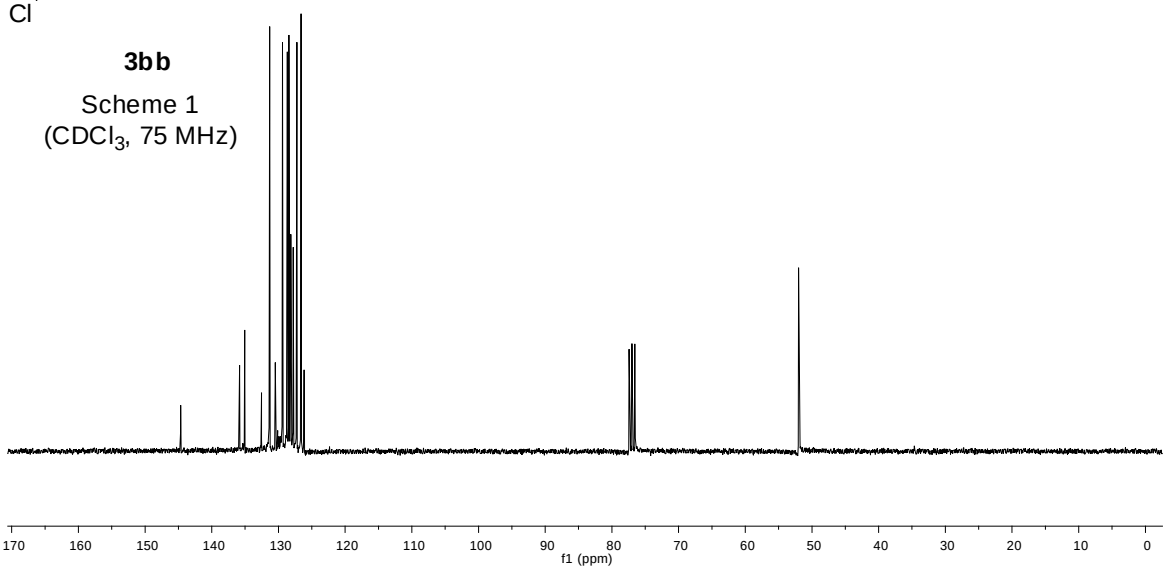
Scheme 1
($CDCl_3$, 300 MHz)

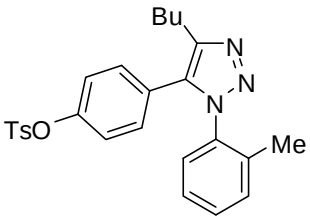




3bb

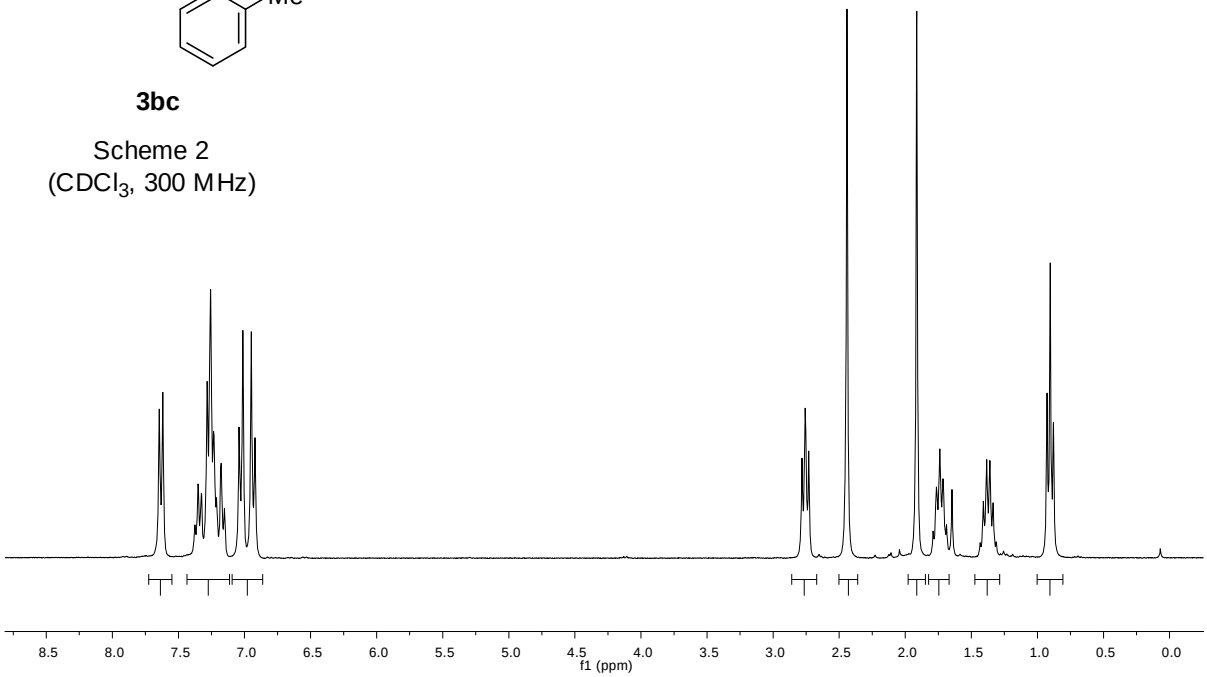
Scheme 1
($CDCl_3$, 75 MHz)

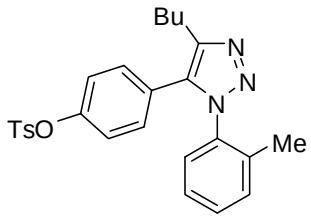




3bc

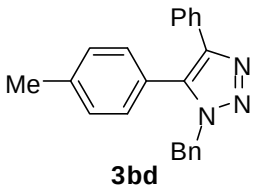
Scheme 2
($CDCl_3$, 300 MHz)





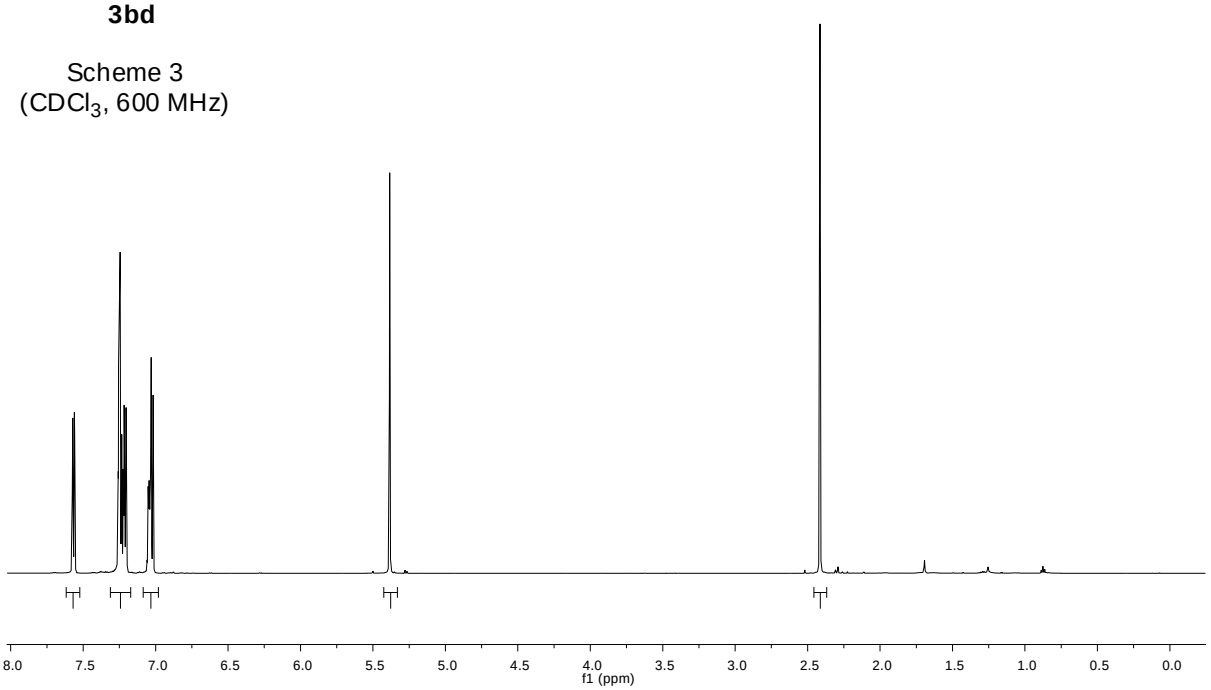
3bc

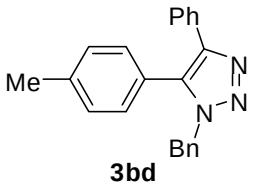
Scheme 2
($CDCl_3$, 75 MHz)



3bd

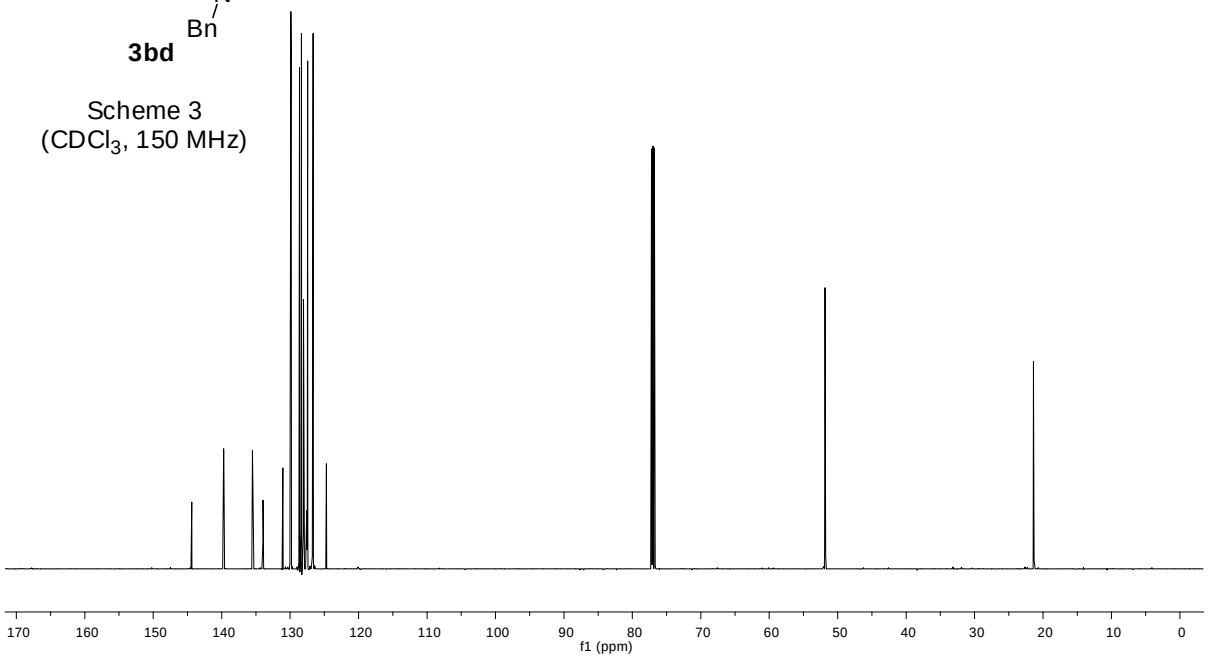
Scheme 3
($CDCl_3$, 600 MHz)

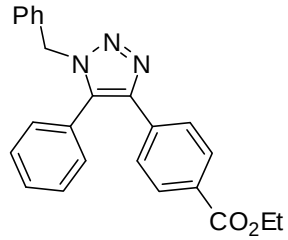




3bd

Scheme 3
($CDCl_3$, 150 MHz)

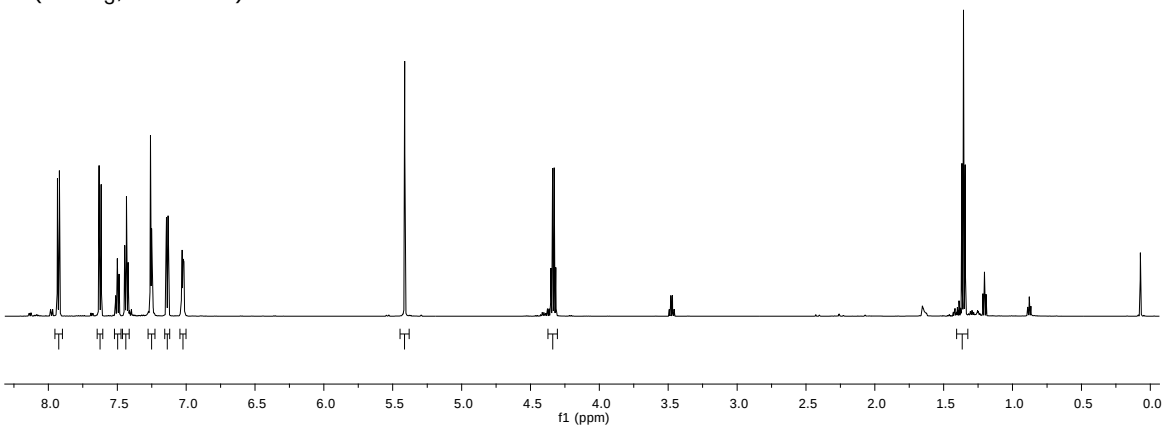


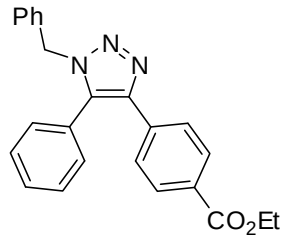


3be

Scheme 4

($CDCl_3$, 600 MHz)

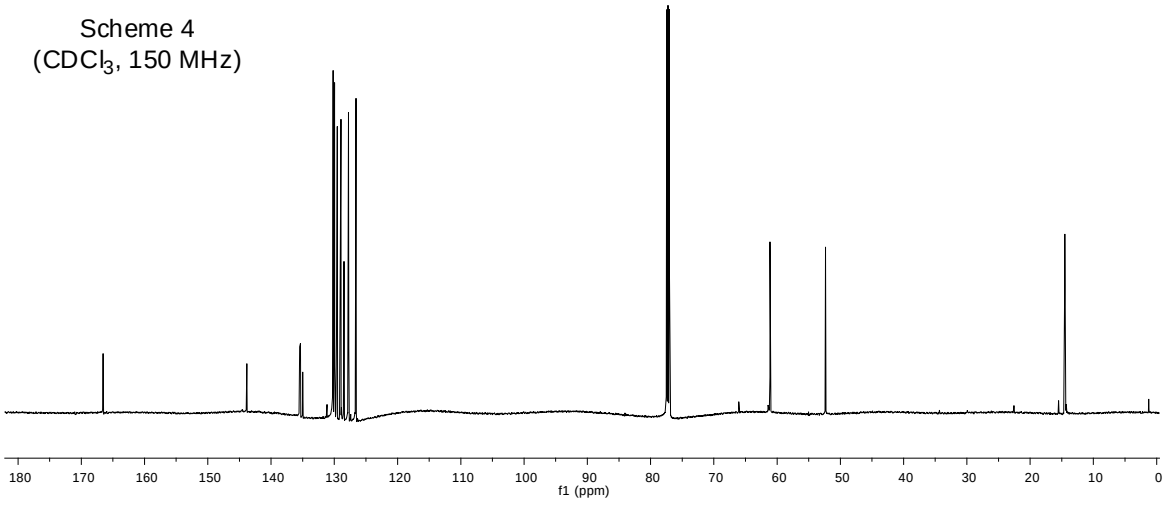


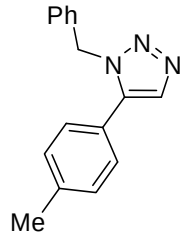


3be

Scheme 4

($CDCl_3$, 150 MHz)

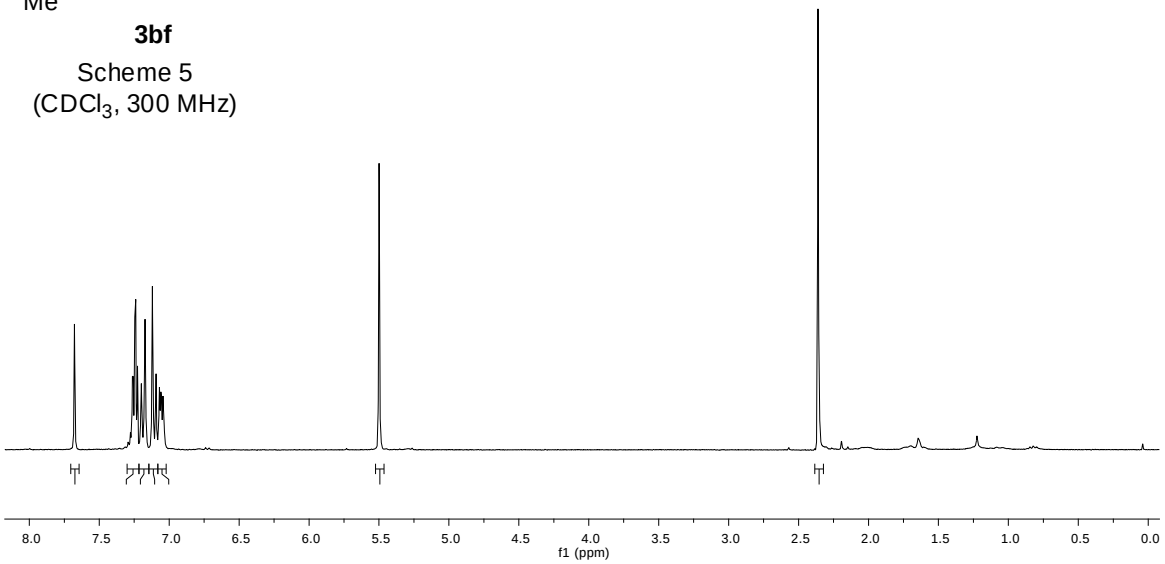


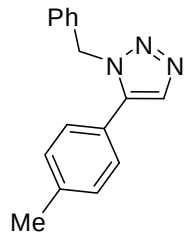


3bf

Scheme 5

($CDCl_3$, 300 MHz)

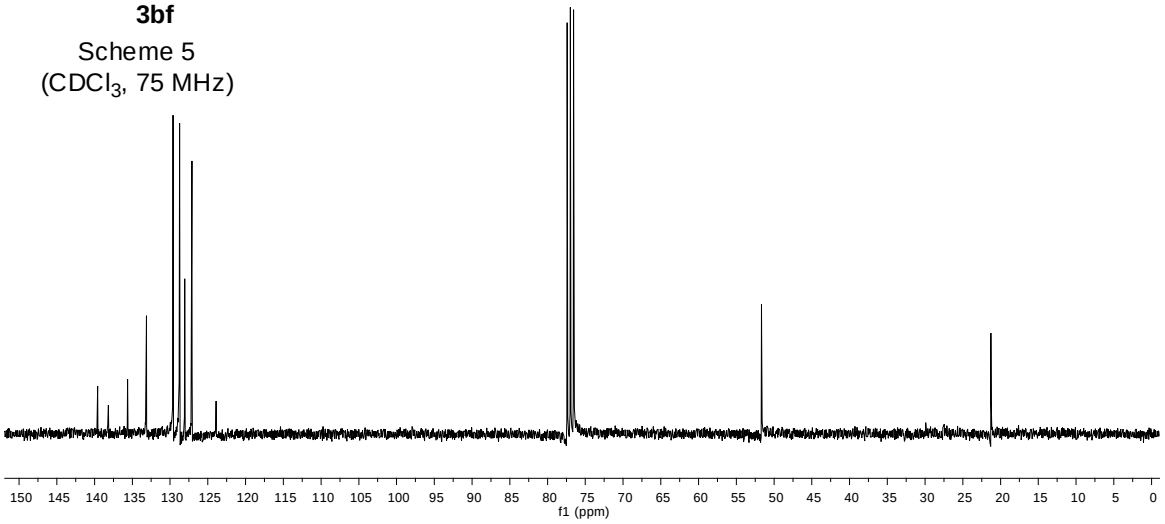


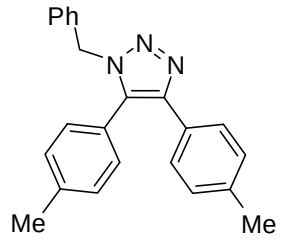


3bf

Scheme 5

($CDCl_3$, 75 MHz)

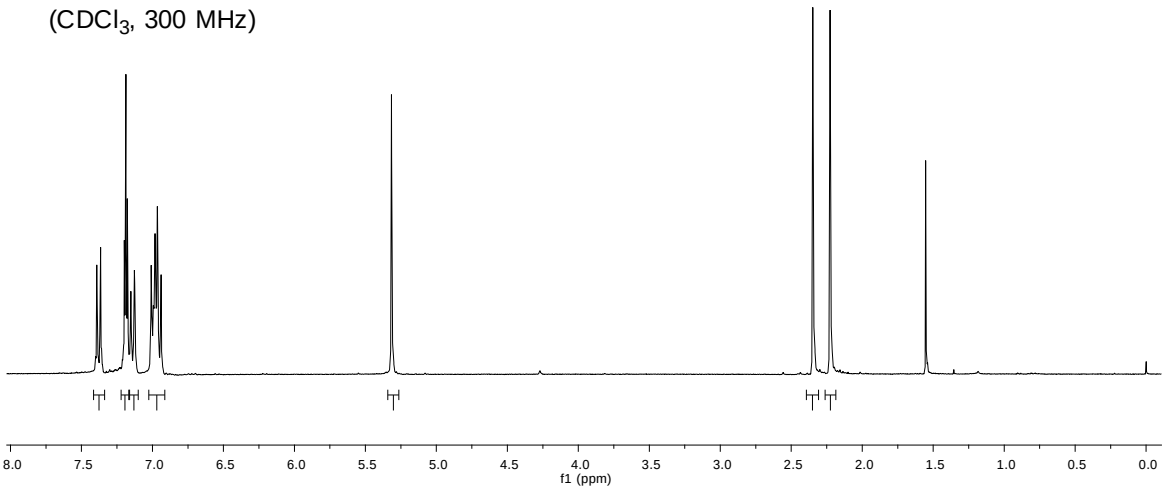


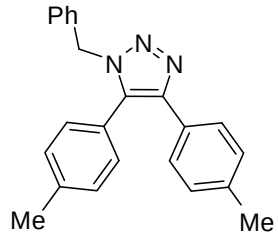


3bg

Scheme 5

($CDCl_3$, 300 MHz)

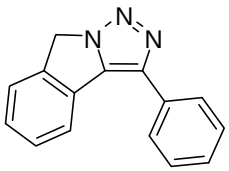




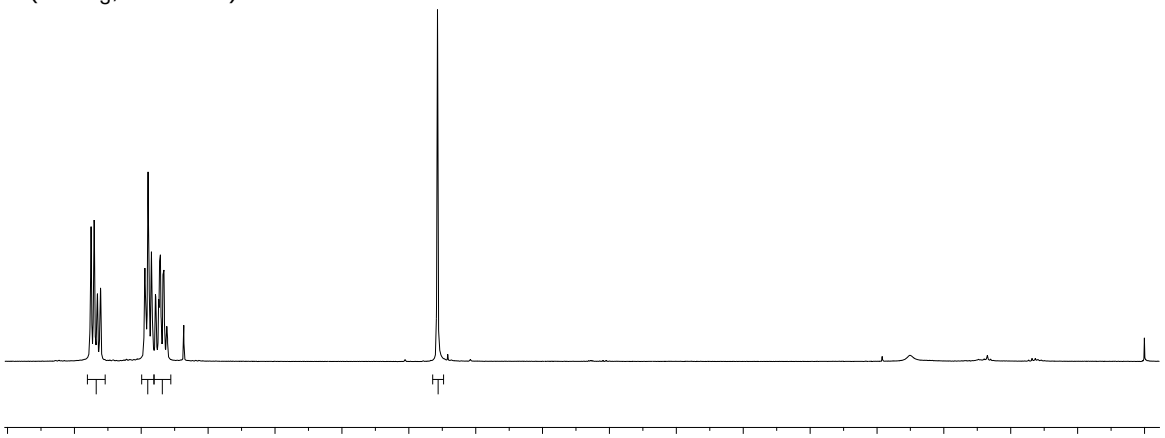
3bg

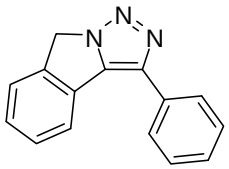
Scheme 5

($CDCl_3$, 75 MHz)



3bh
Scheme 6
($CDCl_3$, 300 MHz)





3bh
Scheme 6
($CDCl_3$, 75 MHz)