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 N₂ 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 ¹H-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 %), PCy₃ (22 mg, 8.0 mol %), K₂CO₃ (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 N₂ for 22 h at 120 °C. Et₂O (75 mL) and H₂O (75 mL) were added to the cold reaction mixture. The separated aqueous phase was extracted with Et₂O (2 × 75 mL). The combined organic layers were washed with aqueous NH₄Cl (50 mL), H₂O (50 mL) and brine (50 mL), dried over Na₂SO₄ 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%).
[4-(5-Butyl-3-o-tolyl-3H-1,2,3-triazol-4-yl)-phenyl]-phenyl-methanone (3av): ¹H-NMR (300 MHz, CDCl₃): 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). ¹³C-NMR (75 MHz, CDCl₃): δ = 195.8 (Cₐ), 145.8 (Cₐ), 137.4 (Cₐ), 137.0 (Cₐ), 135.8 (Cₐ), 135.0 (Cₐ), 133.9 (Cₐ), 132.7 (CH), 131.5 (Cₐ), 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 (CH₂), 25.1 (CH₂), 22.5 (CH₂), 17.6 (CH₃), 13.8 (CH₃). 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 C₂₆H₂₆N₃O 396.2070, found 396.2072. The spectral data were in accordance with those reported in the literature.[⁵]

1-Benzyl-5-(4-methoxyphenyl)-4-phenyl-1H-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/Et₂O 3:1 → 2:1 → 1:1) yielded 3aa (315 mg, 92%) as yellow oil. \(^1\)H-NMR (600 MHz, CDCl₃): \(\delta = 7.60-7.59\) (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, CDCl₃): \(\delta = 160.5\) (C₉), 144.4 (C₉), 135.5 (C₉), 133.7 (C₉), 131.7 (CH), 131.1 (C₉), 128.6 (CH), 128.4 (CH), 128.1 (CH), 127.5 (CH), 127.4 (CH), 126.6 (CH), 119.6 (C₉), 114.6 (CH), 55.3 (CH₃), 51.8 (CH₂). IR (ATR): 1613, 1514, 1485, 1455, 1440, 1290, 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\(_{3}\)O 341.1528, found 341.1529.

\[\text{3ab}\]

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/Et₂O 5:1) yielded 3ab (131 mg, 74%) as a white solid. M.p.: 115-116 °C. \(^1\)H-NMR (600 MHz, CDCl₃): \(\delta = 7.49\) (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, CDCl₃): \(\delta = 159.2\) (C₉), 144.3 (C₉), 139.6 (C₉), 135.6 (C₉), 133.2 (C₉), 130.0 (CH), 129.8 (CH), 128.7 (CH), 128.0 (CH), 127.9 (CH), 127.5 (CH), 125.1 (C₉), 123.9 (C₉), 113.9 (CH), 55.2 (CH₃), 51.9 (CH₂), 21.4 (CH₃). 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\(_{3}\)O 355.1685, found 355.1667.
1-(4-Methoxybenzyl)-4-phenyl-5-p-tolyl-1H-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/Et2O 2:1) yielded 3ac (285 mg, 80%) as yellow viscous oil. $^1$H-NMR (600 MHz, CDCl3): $\delta$ = 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, CDCl3): $\delta$ = 159.4 (Cq), 144.4 (Cq), 139.7 (Cq), 133.8 (Cq), 131.1 (Cq), 130.0 (CH), 129.8 (CH), 129.0 (CH), 128.3 (CH), 127.6 (Cq), 127.5 (CH), 126.6 (CH), 124.8 (Cq), 114.0 (CH), 55.2 (CH3), 51.4 (CH2), 21.4 (CH3). 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 C23H22N3O 356.1747, found 356.1760.

1-Octyl-4-phenyl-5-p-tolyl-1H-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/Et2O 3:1) yielded 3ad (122 mg, 70%) as a colourless
oil. $^1$H-NMR (600 MHz, CDCl$_3$): $\delta$ = 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$_3$): $\delta$ = 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.

1-Benzyl-4-pentyl-5-p-tolyl-1H-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$_2$O 2:1) yielded 3ae (105 mg, 66%) as a pale-yellow oil. $^1$H-NMR (600 MHz, CDCl$_3$): $\delta$ = 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$_3$): $\delta$ = 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.

4-Hexyl-1-octyl-5-p-toly1-1H-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_{2}O 2:1) yielded 3af (120 mg, 68%) as a colourless oil. \(^1\)H-NMR (600 MHz, CDCl\(_3\)): \(\delta = 7.28 \text{ (d, } J = 8.4 \text{ Hz, 2H)}, \ 7.13 \text{ (d, } J = 8.4 \text{ Hz, 2H)}, \ 4.15 \text{ (t, } J = 7.8 \text{ Hz, 2H)}, \ 2.57 \text{ (t, } J = 7.2 \text{ Hz, 2H)}, \ 2.42 \text{ (s, 3H)}, \ 1.71 \text{ (quint, } J = 6.6 \text{ Hz, 2H)}, \ 1.60 \text{ (quint, } J = 7.2 \text{ Hz, 2H)}, \ 1.26-1.12 \text{ (m, 16H)}, \ 0.84 \text{ (t, } J = 6.6 \text{ Hz, 3H)}, \ 0.81 \text{ (d, } J = 8.4 \text{ Hz, 3H}). \ ^{13}\text{C-NMR (150 MHz, CDCl}\(_3\)): \(\delta = 145.6 \text{ (C\_q)}, \ 139.1 \text{ (C\_q)}, \ 134.0 \text{ (C\_q)}, \ 129.6 \text{ (CH)}, \ 129.4 \text{ (CH)}, \ 125.0 \text{ (C\_q)}, \ 48.2 \text{ (CH\_2)}, \ 31.7 \text{ (CH\_2)}, \ 31.5 \text{ (CH\_2)}, \ 30.1 \text{ (CH\_2)}, \ 29.7 \text{ (CH\_2)}, \ 29.0 \text{ (CH\_3)}, \ 26.4 \text{ (CH\_2)}, \ 25.1 \text{ (CH\_2)}, \ 22.6 \text{ (CH\_2)}, \ 22.5 \text{ (CH\_2)}, \ 21.3 \text{ (CH\_2)}, \ 14.1 \text{ (CH\_3)}, \ 14.0 \text{ (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.
1-Benzyl-5-(2-methoxyphenyl)-4-phenyl-1H-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/Et₂O 3:1 → 2:1 → 1:1) yielded 3ag (326 mg, 95%) as an off-white solid. M.p.: 129-131 °C. ¹H-NMR (600 MHz, CDCl₃): 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). ¹³C-NMR (150 MHz, CDCl₃): δ = 157.5 (Cq), 144.9 (Cq), 135.2 (Cq), 131.8 (CH), 131.6 (CH), 131.3 (Cq), 130.7 (Cq), 128.4 (CH), 128.3 (CH), 127.8 (CH), 127.7 (CH), 127.4 (CH), 126.3 (CH), 121.0 (CH), 116.6 (Cq), 111.2 (CH), 55.2 (CH₃), 52.3 (CH₂). 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 C₂₂H₁₉N₃O 341.1528, found 341.1510.

![Chemical Structure](image)

**Ethyl 4-(1-benzyl-4-phenyl-1H-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/Et₂O 3:1 → 2:1) yielded 3ah (271 mg, 70%) as a white solid. M.p.:114-115 °C. ¹H-NMR (600 MHz, CDCl₃): 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). ¹³C-NMR (150 MHz, CDCl₃): δ = 165.8 (Cq), 144.9 (Cq), 135.1 (Cq), 132.8 (Cq), 132.4 (Cq), 131.6 (Cq), 130.5 (Cq), 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 (CH₂), 52.2 (CH₂), 14.3
(CH₃). IR (ATR): 1713, 1286, 1276, 1129, 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 C₂₄H₂₁N₃O₂ 383.1634, found 383.1632. The spectral data were in accordance with those reported in the literature.[5]

![Chemical structure](image)

**Ethyl 4-(1-octyl-4-phenyl-1H-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. ¹H-NMR (300 MHz, CDCl₃): 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). ¹³C-NMR (75 MHz, CDCl₃): δ = 165.8 (Cq), 144.5 (Cq), 132.7 (Cq), 132.6 (Cq), 131.6 (Cq), 130.6 (Cq), 130.4 (CH), 130.0 (CH), 128.5 (CH), 127.8 (CH), 126.8 (CH), 61.4 (CH₂), 48.4 (CH₂), 31.6 (CH₂), 30.0 (CH₂), 28.9 (CH₂), 28.7 (CH₂), 26.3 (CH₂), 22.5 (CH₂), 14.3 (CH₃), 14.0 (CH₃). 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 C₂₅H₃₂N₃O₂ 406.2489, found 406.2490.
1-(4-(1-Benzyl-4-phenyl-1H-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/Et₂O 2:1 → 1:1) yielded 3aj (236 mg, 67%) as an off-white solid. M.p.: 122-123 °C. ¹H-NMR (600 MHz, CDCl₃): 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). ¹³C-NMR (150 MHz, CDCl₃): 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 (CH₂), 26.7 (CH₃). 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 C₂₃H₁₉N₃O 353.1528, found 353.1503.

4-(1-Benzyl-4-phenyl-1H-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/Et₂O 2:1 → 1:1) yielded 3ak (238 mg, 71%) as an off-white solid. M.p.: 146-148 °C. ¹H-
NMR (600 MHz, CDCl₃): 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). ¹³C-NMR (150 MHz, CDCl₃): δ = 145.3 (Cₐq), 134.8 (Cₐq), 132.8 (Cₐq), 132.7 (CH), 131.9 (Cₐq), 130.9 (CH), 130.1 (Cₐq), 128.9 (CH), 128.6 (CH), 128.5 (CH), 128.2 (CH), 127.2 (CH), 126.9 (CH), 117.9 (Cₐq), 113.6 (Cₐq), 52.5 (CH₂). 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 C₂₂H₁₆N₄ 336.1375, found 336.1375.

3-(1-Benzyl-4-phenyl-1H-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/Et₂O 1:2) yielded 3al (90 mg, 58%) as an off-white solid. M.p.: 110-112 °C. ¹H-NMR (600 MHz, CDCl₃): 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). ¹³C-NMR (150 MHz, CDCl₃): δ = 150.8 (CH), 150.5 (CH), 145.9 (Cₐq), 137.6 (CH) 134.9 (Cₐq), 130.5 (Cₐq), 130.3 (Cₐq), 128.9 (CH), 128.7 (CH), 128.5 (CH), 128.1 (CH), 127.3 (CH), 126.8 (CH), 124.5 (Cₐq), 123.7 (CH), 52.5 (CH₂). 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 C₂₀H₁₆N₄ 312.1375, found 312.1362. The spectral data were in accordance with those reported in the literature.⁶
2-(1-Benzyl-4-phenyl-1H-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/Et₂O 1:1) yielded 3am (125 mg, 82%) as a white solid. M.p.: 93-95 °C. ¹H-NMR (600 MHz, CDCl₃): 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). ¹³C-NMR (150 MHz, CDCl₃): δ = 150.1 (CH), 148.0 (Cq), 145.7 (Cq), 136.7 (CH), 135.5 (Cq), 132.2 (Cq), 130.9 (Cq), 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 (CH₂). 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 C₂₀H₁₆N₄ 312.1375, found 312.1377.

Ethyl 4-(4-butyl-1-phenyl-1H-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$_3$): $\delta$ = 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$_3$): $\delta$ = 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) $m/z$ calcld for C$_{21}$H$_{24}$N$_3$O$_2$ 350.1863, found 350.1864.

**Ethyl 4-(4-butyl-1-m-tolyl-1H-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$_3$): $\delta$ = 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$_3$): $\delta$ = 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 (CH₂), 31.7 (CH₂), 24.8 (CH₂), 22.4 (CH₂), 21.2 (CH₃), 14.2 (CH₃),
13.7 (CH₃). 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

Methyl 3-(4-butyl-1-m-tolyl-1H-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, CDCl₃): \(\delta = 8.02\) (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). \(^1^3\)C-NMR (75 MHz, CDCl₃):
\(\delta = 166.2\) (C₄), 146.5 (C₄), 139.5 (C₄), 136.4 (C₄), 133.9 (CH), 132.8 (C₄), 130.8 (C₄), 130.5
(CH), 129.9 (CH), 129.7 (CH), 128.9 (CH), 128.5 (C₄), 128.3 (CH), 125.5 (CH), 121.9 (CH),
52.3 (CH₃), 31.7 (CH₂), 24.8 (CH₂), 22.4 (CH₂), 21.2 (CH₃), 13.7 (CH₃). 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 C₂₁H₂₄N₃O₂ 350.1863, found 350.1864.
4-Butyl-5-(3-methoxyphenyl)-1-m-tolyl-1H-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$_3$): $\delta$ = 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$_3$): $\delta$ = 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$_3$O 322.1914, found 322.1912.

4-(5-Butyl-3-o-tolyl-3H-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$_3$): $\delta$ = 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$_3$): $\delta$ = 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$_3$O$_2$ 364.2020, found 364.2021.

4-[5-Butyl-3-(2-methoxyphenyl)-3H-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$_3$): $\delta$ = 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$_3$): $\delta$ = 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$_q$), 128.0 (CH), 126.6 (CH), 126.4 (CH), 125.7 (CH), 124.8 (CH), 124.4 (CH), 122.1 (CH), 120.0 (CH), 118.0 (CH), 115.0 (CH), 111.0 (CH), 106.1 (CH), 102.8 (CH), 31.7 (CH$_2$), 25.1 (CH$_2$), 22.8 (CH$_2$), 17.7 (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$_3$O$_2$ 364.2020, found 364.2021.
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, 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 C₂₂H₂₆N₃O₃ 380.1914, found 380.1914.

![3at](image)

3-(5-Butyl-3-ο-tolyl-3Η-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. ¹H-NMR (300 MHz, CDCl₃): 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). ¹³C-NMR (75 MHz, CDCl₃): 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 C₂₁H₂₄N₃O₂ 350.1863, found 350.1862.
**Ethyl 4-(1-o-tolyl-4-((trimethylsilyl)methyl)-1H-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$_3$): $\delta = 7.94$ (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$_3$): $\delta = 165.8$ (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$_3$O$_2$Si 394.1945, found 394.1946.

**[3-(5-Butyl-3-o-tolyl-3H-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\(_3\)): \(\delta = 7.81 \text{ (dt, } J = 7.7, 1.4 \text{ Hz, 1H)}, 7.59-7.56 \text{ (m, 3H)}, 7.50-7.34 \text{ (m, 6H)}, 7.28-7.17 \text{ (m, 3H)}, 2.79 \text{ (t, } J = 7.8 \text{ Hz, 2H)}, 1.96 \text{ (s, 3H)}, 1.80-1.69 \text{ (m, 2H)}, 1.37 \text{ (tq, } J = 7.4, 7.4 \text{ Hz, 2H)}, 0.89 \text{ (t, } J = 7.3 \text{ Hz, 3H}). \(^{13}\)C-NMR (75 MHz, CDCl\(_3\)): \(\delta = 195.5 \text{ (C\(_\text{q}\))}, 145.6 \text{ (C\(_\text{q}\))}, 137.9 \text{ (C\(_\text{q}\))}, 136.8 \text{ (C\(_\text{q}\))}, 135.7 \text{ (C\(_\text{q}\))}, 135.1 \text{ (C\(_\text{q}\))}, 134.0 \text{ (C\(_\text{q}\))}, 132.7 \text{ (CH)}, 132.6 \text{ (CH)}, 131.2 \text{ (CH)}, 130.7 \text{ (CH)}, 130.1 \text{ (CH)}, 129.9 \text{ (CH)}, 129.8 \text{ (CH)}, 129.0 \text{ (CH)}, 128.4 \text{ (CH)}, 127.7 \text{ (CH)}, 127.5 \text{ (C\(_\text{q}\))}, 126.8 \text{ (CH)}, 31.7 \text{ (CH\(_2\))}, 25.0 \text{ (CH\(_2\))}, 22.5\text{(CH\(_2\))}, 17.6 \text{ (CH\(_3\))}, 13.8 \text{ (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\(_3\)O 396.2070, found 396.2071.

**1-(4-(4-Butyl-1-o-tolyl-1H-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\(_3\)): \(\delta = 7.59 \text{ (d, } J = 8.5 \text{ Hz, 2H)}, 7.33-7.28 \text{ (m, 1H)}, 7.24-7.15 \text{ (m, 3H)}, 7.11 \text{ (d, } J = 8.5 \text{ Hz, 2H)}, 2.77 \text{ (t, } J = 7.6 \text{ Hz, 2H)}, 1.90 \text{ (s, 3H)}, 1.73 \text{ (quint, } J = 7.8 \text{ Hz, 2H)}, 1.35 \text{ (tq, } J = 7.6, 7.6 \text{ Hz, 2H)}, 1.27 \text{ (s, 9H)}, 0.87 \text{ (t, } J = 7.3 \text{ Hz, 3H}). \(^{13}\)C-NMR (75 MHz, CDCl\(_3\)): \(\delta = 208.3 \text{ (C\(_\text{q}\))}, 145.5 \text{ (C\(_\text{q}\))}, 138.3 \text{ (C\(_\text{q}\))}, 135.7 \text{ (C\(_\text{q}\))}, 134.9 \text{ (C\(_\text{q}\))}, \)
133.9 (C₉), 131.1 (CH), 129.9 (CH), 129.8 (C₉), 128.5 (CH), 128.1 (CH), 127.5 (CH), 126.7 (CH), 44.1 (C₉), 31.6 (CH₂), 27.8 (CH₃), 25.0 (CH₂), 22.4 (CH₂), 17.5 (CH₃), 13.7 (CH₃). 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 C₂₄H₃₀N₃O 376.2383, found 376.2385.

4-Butyl-1-o-toly-5-p-toly-1H-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. ¹H-NMR (300 MHz, CDCl₃): 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). ¹³C-NMR (75 MHz, CDCl₃): δ = 145.0 (C₉), 138.6 (C₉), 136.1 (C₉), 135.1 (C₉), 135.0 (C₉), 131.0 (CH), 129.7 (CH), 129.3 (CH), 128.9 (CH), 127.7 (CH), 126.5 (CH), 124.4 (C₉), 31.7 (CH₂), 25.0 (CH₂), 22.5 (CH₂), 21.2 (CH₃), 17.6 (CH₃), 13.8 (CH₃). 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 C₂₀H₂₄N₃ 306.1965, found 306.1965.
4-Butyl-5-(4-methoxyphenyl)-1-o-tolyl-1H-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\(_3\)): \(\delta = 7.35-7.29\) (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\(_3\)): \(\delta = 159.7\) (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\(_3\)O 322.1914, found 322.1915.
4-Butyl-5-(3,5-dimethoxyphenyl)-1-o-tolyl-1H-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\(_3\)): \(\delta = 7.35-7.25\) (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). \[^1\]C-NMR (75 MHz, CDCl\(_3\)): \(\delta = 160.6\) (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\(_3\)O\(_2\) 352.2019, found 352.2020.

![3bb](image)

1-Benzyl-5-(4-chlorophenyl)-4-phenyl-1H-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\(_3\)): \(\delta = 7.53-7.48\) (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). \[^1\]C-NMR (75 MHz, CDCl\(_3\)): \(\delta = 144.7\) (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, 1266, 1093, 1016, 984, 839, 778, 740, 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$_{17}$CI$_3$N$_3$ 346.1106, found 346.1107.

Toluene-4-sulfonic acid 4-(5-butyl-3-o-tolyl-3H-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$_3$O$_3$S 462.1846, found 462.1846.
1-Benzyl-5-(4-methylphenyl)-4-phenyl-1H-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/Et₂O 3:1 → 2:1) yielded 3bd (303 mg, 93%) as an off-white solid. M.p.: 120-121 °C. ¹H-NMR (600 MHz, CDCl₃): 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). ¹³C-NMR (150 MHz, CDCl₃): δ = 144.4 (Cq), 139.7 (Cq), 135.5 (Cq), 134.0 (Cq), 131.1 (Cq), 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 (Cq), 51.8 (CH₂), 21.4 (CH₃). 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 C₂₂H₁₉N₃ 325.1579, found 325.1568. The spectral data were in accordance with those reported in the literature.[⁵]

Ethyl 4-(1-benzyl-5-phenyl-1H-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/Et₂O 3:1) yielded 3be (139 mg, 40%) as a white solid. M.p.: 106-109 °C. ¹H-NMR (300 MHz, CDCl₃): 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$_3$): $\delta = 166.5$ (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, 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) $m/z$ calc'd for C$_{24}$H$_{22}$N$_3$O$_2$ 384.1707, found 384.1708.

1-Benzyl-5-p-tolyl-1H-1,2,3-triazole (3bf) and 1-benzyl-4,5-di-p-tolyl-1H-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$_3$): $\delta = 7.68$ (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$_3$): $\delta = 139.6$ (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) $m/z$ calc'd 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$_3$): $\delta = 7.37$ (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$_3$): $\delta$ = 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.

![Chemical Structure](image)

3-Phenyl-8H-[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$_3$): $\delta$ = 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$_3$): $\delta$ = 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:

Table 1, entry 14
(CDCl₃, 600 MHz)

Table 1, entry 14
(CDCl₃, 150 MHz)
Table 2, entry 1
(CDCl₃, 600 MHz)

Table 2, entry 1
(CDCl₃, 150 MHz)
Table 2, entry 2
(CDCl₃, 600 MHz)

Table 2, entry 2
(CDCl₃, 150 MHz)
3ad
Table 2, entry 3
(CDCl₃, 600 MHz)

3ad
Table 2, entry 3
(CDCl₃, 150 MHz)
3ae
Table 2, entry 4
(CDCl₃, 600 MHz)

3ae
Table 2, entry 4
(CDCl₃, 150 MHz)
Table 2, entry 6
(CDCl₃, 600 MHz)

Table 2, entry 6
(CDCl₃, 150 MHz)
Table 2, entry 7
(CDCl₃, 600 MHz)

Table 2, entry 7
(CDCl₃, 150 MHz)
Table 2, entry 8
(CDCl₃, 300 MHz)

3ai

Table 2, entry 8
(CDCl₃, 75 MHz)
Table 2, entry 11
(CDCl₃, 600 MHz)

Table 2, entry 11
(CDCl₃, 150 MHz)
Table 2, entry 13
(CDCl$_3$, 600 MHz)

Table 2, entry 13
(CDCl$_3$, 150 MHz)
Table 2, entry 14
(CDCl₃, 600 MHz)

Table 2, entry 14
(CDCl₃, 150 MHz)
3am
Table 2, entry 15
(CDCl₃, 600 MHz)

3am
Table 2, entry 15
(CDCl₃, 150 MHz)
3an
Table 3, entry 1
(CDCl₃, 300 MHz)

3an
Table 3, entry 1
(CDCls, 75 MHz)
Table 3, entry 2
(CDCl$_3$, 300 MHz)

Table 3, entry 2
(CDCl$_3$, 75 MHz)
3ap
Table 3, entry 3
(CDCl₃, 300 MHz)

3ap
Table 3, entry 3
(CDCl₃, 75 MHz)
Table 3, entry 5
(CDCl₃, 300 MHz)

Table 3, entry 5
(CDCl₃, 75 MHz)
Table 3, entry 6
(CDCl₃, 300 MHz)

3as

Table 3, entry 6
(CDCl₃, 75 MHz)
Table 3, entry 7
(CDCl₃, 300 MHz)

3at

Table 3, entry 7
(CDCl₃, 75 MHz)
Table 3, entry 8
(CDCl₃, 300 MHz)

3au

Table 3, entry 8
(CDCl₃, 75 MHz)
Table 3, entry 9
(CDCl₃, 300 MHz)

Table 3, entry 9
(CDCl₃, 75 MHz)
Table 3, entry 10
(CDCl₃, 300 MHz)

Table 3, entry 10
(CDCl₃, 75 MHz)
Table 3, entry 11
(CDCl₃, 300 MHz)
Table 3, entry 12
(CDCl₃, 300 MHz)

3ay

Table 3, entry 12
(CDCl₃, 75 MHz)

3ay
Table 3, entry 13 (CDCl$_3$, 300 MHz)

Table 3, entry 13 (CDCl$_3$, 75 MHz)
Table 3, entry 14
(CDCl₃, 300 MHz)

3ba

Table 3, entry 14
(CDCl₃, 75 MHz)
Scheme 1
(CDCl₃, 300 MHz)

Scheme 1
(CDCl₃, 75 MHz)
Scheme 2
(CDCl₃, 300 MHz)

\[
\begin{align*}
\text{TsO} & \quad \text{Bu} \\
\text{Me} & \quad \text{Me}
\end{align*}
\]

3bc

Scheme 2
(CDCl₃, 75 MHz)

\[
\begin{align*}
\text{TsO} & \quad \text{Bu} \\
\text{Me} & \quad \text{Me}
\end{align*}
\]
Scheme 3
(CDCl₃, 600 MHz)

Scheme 3
(CDCl₃, 150 MHz)
Scheme 4
(CDCl₃, 600 MHz)

Scheme 4
(CDCl₃, 150 MHz)
Scheme 5
(CDCl$_3$, 300 MHz)

3bf

Scheme 5
(CDCl$_3$, 75 MHz)
Scheme 5
(CDCl₃, 300 MHz)

Scheme 5
(CDCl₃, 75 MHz)
Scheme 6
(CDCl₃, 300 MHz)

3bh

Scheme 6
(CDCl₃, 75 MHz)

S61