Supporting Information

One pot 'click' reaction: Cu^{II}–hydrotalcite catalyzed tandem synthesis of *β*–hydroxy triazoles via regioselective opening of epoxide followed by [3+2] cycloaddition

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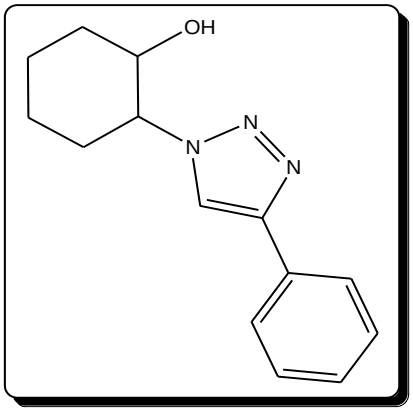
1. General Information: ^{1}H NMR spectra were recorded on Varian VXR-Unity 200 MHz, Bruker UXNMR/XWIN-NMR Avance-300 MHz, and GEMINI spectrometers. Chemical shifts (δ) are given in ppm relative to tetramethylsilane (TMS), which is used as an internal standard, and the coupling constants (J) are reported in Hz. Splitting patterns of proton are described as s, d, dd, t, q, br s, and m, which stand for the resonance multiplicities singlet, doublet, doublet of doublet, triplet, quartet, broad singlet, and multiplet, respectively. Only the most important IR absorptions (cm^{-1}) and the molecular ions and/or base peaks in MS are given.

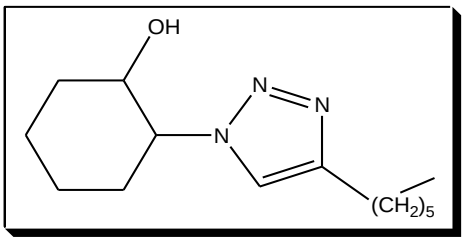
2. ^{1}H NMR, FTIR, MS data of Isolated Products:

Table 2, Entry 1: 2-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)cyclohexanol:



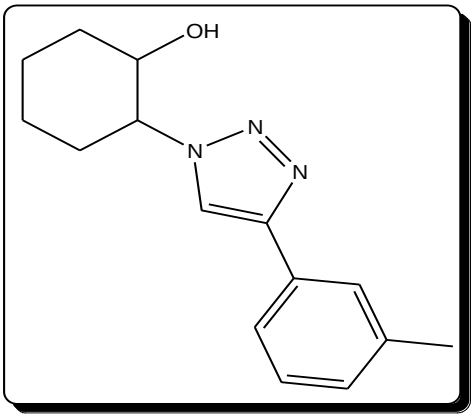
^{1}H NMR ($CDCl_3$) δ 1.23–1.29 (m, 2H), 1.46–1.51 (m, 2H), 1.87–1.94 (m, 2H), 2.17–2.27 (m, 2H), 3.56 (br s, 1H), 4.04–4.08 (m, 1H), 4.09–4.14 (m, 1H), 7.26–7.36 (m, 3H), 7.62–7.65 (m, 2H), 7.68 (s, 1H). IR (KBr) ν/cm^{-1} 3306, 3117, 2933, 2857, 1448, 1231, 1083, 964, 765, 695, 556. MS (ESI) *m*/*z*: 244 [M^{+}+1].

Table 2, Entry 2: 2-(4-Hexyl-1*H*-1,2,3-triazol-1-yl)cyclohexanol:



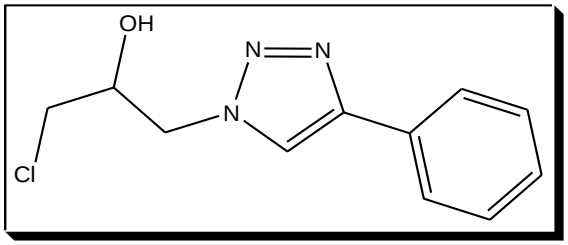
^{1}H NMR ($CDCl_3$) δ 0.90 (t, *J* = 7.72 Hz, 3H), 0.93 (t, *J* = 7.72 Hz, 2H) 1.30–1.38 (m, 12H), 1.45–1.52 (m, 2H), 1.64–1.74 (m, 2H), 2.49–2.55 (m, 1H), 2.63–2.68 (m, 1H), 7.26 (s, 1H). IR (KBr ν/cm^{-1} 3296, 3142, 2931, 2855, 1551, 1457, 1359, 1209, 1083, 957, 806, 639. MS (ESI) *m*/*z*: 251 [M^++1].

Table 2, Entry 3: 2-(4-*m*-Tolyl-1*H*-1,2,3-triazol-1yl)cyclohexanol:



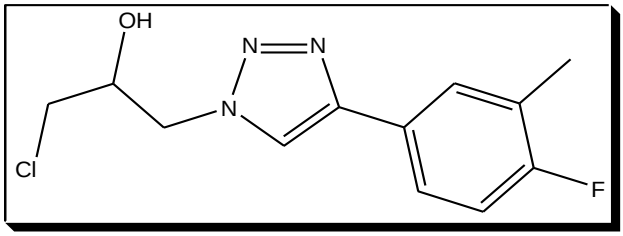
^{1}H NMR ($CDCl_3$) δ 1.42–1.48 (m, 4H), 1.85–1.95 (m, 2H), 2.16–2.25 (m, 2H), 2.35 (s, 3H), 3.87 (br s, 1H), 3.97–4.00 (m, 1H), 4.01–4.04 (m, 1H), 7.02–7.08 (m, 1H), 7.18–7.23 (m, 1H), 7.38–7.45 (m, 2H), 7.65 (s, 1H). IR (KBr) ν/cm^{-1} 3301, 3117, 2928, 2856, 1609, 1450, 1232, 1083, 844, 789, 696. MS (ESI) *m*/*z*: 257 [M^++1].

Table 2, Entry 4: 1-Chloro-3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propan-2-ol:



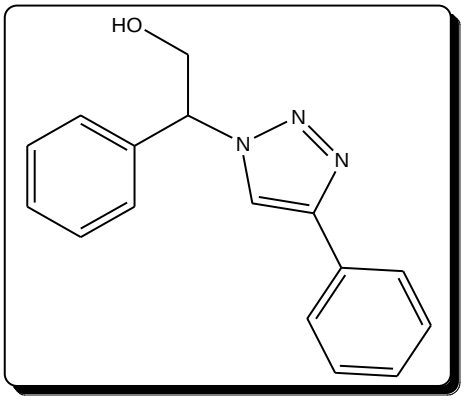
^{1}H NMR ($CDCl_3$) δ 2.50–2.55 (m, 1H), 2.87–2.92 (m, 1H), 3.34–3.39 (m, 1H) 4.35 (dd, *J* = 6.04, 8.49 Hz, 1H), 4.84 (dd, *J* = 2.64, 12.08 Hz, 1H), 7.27–7.31(m, 1H), 7.36–7.41 (m, 2H), 7.78–7.82 (m, 2H), 7.84 (s, 1H). IR (KBr) ν/cm^{-1} 3322, 2923, 2853, 1734, 1459, 1260, 1089, 1025, 800, 696. MS (ESI) *m*/*z*: 238 [M$^+$+1].

Table 2, Entry 5: 1-Chloro-3-(4-(4-fluoro-3-methyl-phenyl)-1*H*-1,2,3-triazol-1-yl)propan-2-ol:



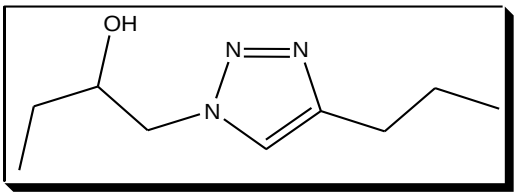
^{1}H NMR ($CDCl_3$) δ 2.34 (s, 3H), 2.89–2.93 (m, 1H), 3.34–3.39 (m, 1H), 4.29–4.36 (m, 1H), 4.82–4.88 (m, 1H), 6.99–7.05 (m, 1H), 7.54–7.59 (m, 1H), 7.66–7.71 (m, 1H), 7.79 (s, 1H). IR (KBr) ν/cm^{-1} 3346, 2925, 2854, 1737, 1461, 1236, 1176, 1078, 759, 592. MS (ESI) *m*/*z*: 270 [M$^+$+1].

Table 2, Entry 6: 2-Phenyl-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethanol:



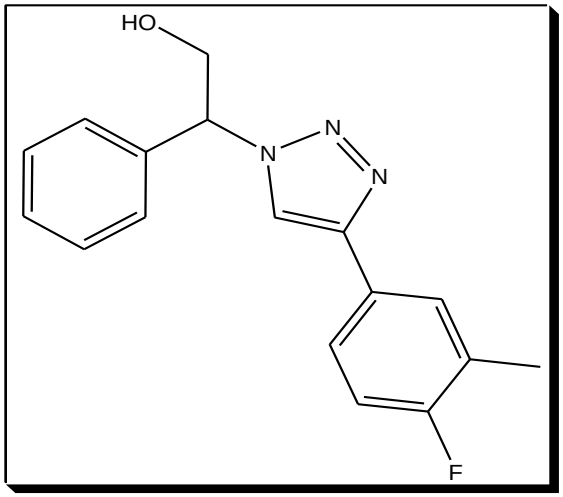
^{1}H NMR ($CDCl_3$) δ 3.42 (br s, 1H), 4.17 (dd, *J* = 3.39, 12.46 Hz, 1H), 4.62 (dd, *J* = 8.30, 12.46Hz, 1H), 5.62 (dd, *J* = 3.39, 8.30 Hz, 1H), 7.22–7.29 (m, 3H), 7.32–7.37 (m, 5H), 7.62 (s, 1H), 7.71 (d, *J* = 6.98 Hz, 2H). IR (KBr) ν/cm^{-1} 3400, 3091, 2962, 2855, 1611, 1458, 1221, 1076, 1049, 760, 694. MS (ESI) *m*/*z*: 266 [M$^+$+1].

Table 2, Entry 7: 1-(4-Propyl-1*H*-1,2,3-triazol-1-yl)-butan-2-ol:



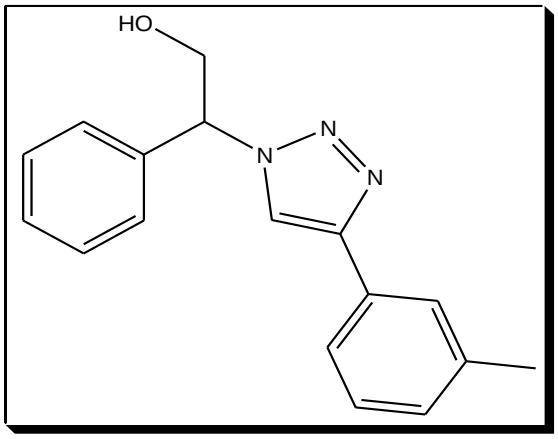
^{1}H NMR ($CDCl_3$) δ 0.96 (t, *J* = 7.55 Hz, 3H), 1.04 (t, *J* = 7.55 Hz, 3H), 1.47–1.58 (m, 2H), 1.62–1.69 (m, 2H), 2.60 (t, *J* = 7.55 Hz, 2H), 3.93–4.01 (m, 1H), 4.14 (dd, *J* = 8.30, 13.59 Hz, 1H), 4.37 (dd, *J* = 3.02, 13.59 Hz, 1H), 7.33 (s, 1H). IR (KBr) ν/cm^{-1} 3235, 2962, 2874, 1564, 1461, 1221, 1056, 798. MS (EI) *m*/*z*: 184 [M$^+$+1].

Table 2, Entry 8: 2-(4-(4-Fluoro-3-methylphenyl)-1*H*-1,2,3-triazol-1-yl)-2-phenylethanol:



^{1}H NMR ($CDCl_3$) δ 2.31 (s, 3H), 4.12–4.20 (m, 1H), 4.56–4.65 (m, 1H), 5.60 (dd, *J* = 3.77, 8.30 Hz, 1H), 6.95–7.02 (m, 1H), 7.18–7.24 (m, 2H), 7.33–7.38 (m, 3H), 7.49–7.54 (m, 1H), 7.56 (s, 1H), 7.58–7.61 (m, 1H). IR (KBr) ν/cm^{-1} 3404, 3138, 2927, 1612, 1490, 1196, 1060, 809, 705, 626. MS (ESI) *m*/*z*: 298 [M$^+$+1].

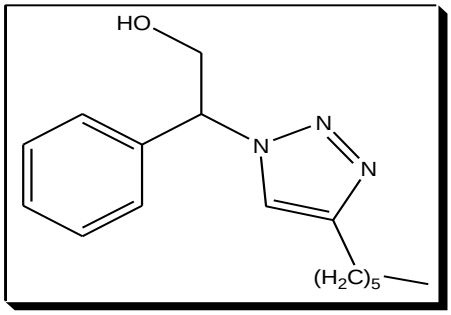
Table 2, Entry 9: 2-Phenyl-2-(4-*m*-tolyl-1*H*-1,2,3-triazol-1-yl)ethanol:



^{1}H NMR ($CDCl_3$) δ 2.37 (s, 3H), 3.47 (br s, 1H), 4.12–4.20 (m, 1H), 4.57–4.65 (m, 1H), 5.61 (dd, *J* = 4.53, 8.30 Hz, 1H), 7.06–7.10 (m, 1H), 7.22–7.26 (m, 3H), 7.33–7.37 (m,

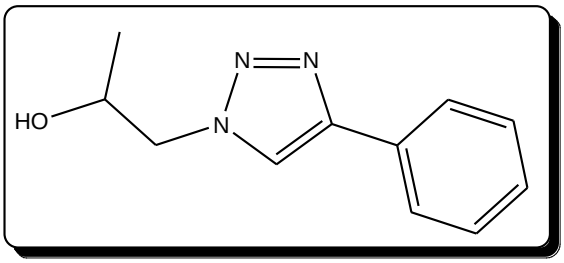
2H), 7.49–7.54 (m, 2H), 7.59 (s, 1H). IR (KBr) ν/cm^{-1} 3421, 3131, 2926, 1590, 1454, 1215, 1153, 1049, 782, 704, 547. MS (ESI) *m*/*z*: 280 [M^{+}+1].

Table 2, Entry 10: 2-(4-Hexyl-1*H*-1,2,3-triazol-1-yl)-2-phenylethanol:



^{1}H NMR ($CDCl_3$) δ 0.87 (t, *J* = 6.79 Hz, 3H), 1.25–1.32 (m, 6H), 1.57–1.64 (m, 2H), 2.46 (t, *J* = 7.55 Hz, 2H), 3.59 (br s, 1H), 4.10 (dd, *J* = 3.02, 12.27 Hz, 1H), 4.54 (dd, *J* = 8.49, 12.27 Hz, 1H), 5.52 (dd, *J* = 3.77, 12.27 Hz, 1H), 7.14–7.19 (m, 3H), 7.30–7.35 (m, 3H). IR (KBr) ν/cm^{-1} 3381, 3069, 2923, 2850, 1557, 1459, 1217, 1145, 1055, 848, 754, 539. MS (ESI) *m*/*z*: 274 [M^{+}+1].

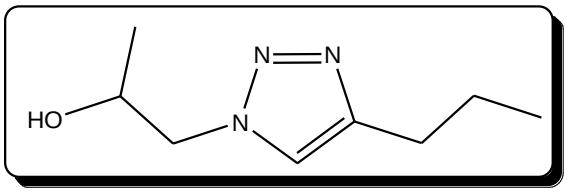
Table 2, Entry 11: 1-(4-Phenyl -1*H*-1,2,3-triazol-1-yl)propan-2-ol:



^{1}H NMR ($CDCl_3$) δ 1.32 (d, *J* = 6.23 Hz, 3H), 4.19 (dd, *J* = 5.66, 7.74 Hz, 1H), 4.30–4.37 (m, 1H), 4.42 ν/cm^{-1} 4.47 (m, 1H), 7.26–7.37 (m, 3H), 7.66–7.71 (m, 2H), 7.75 (s,

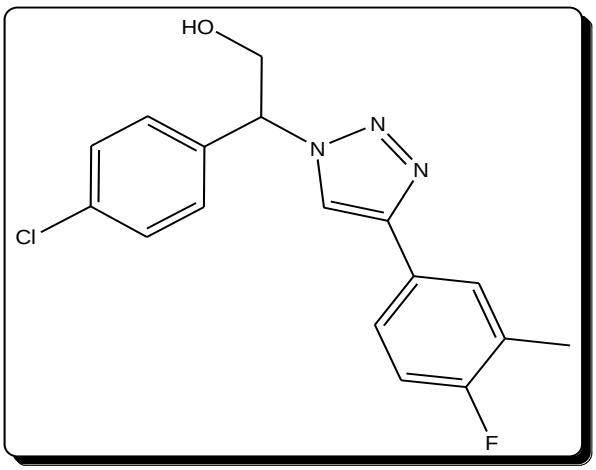
1H). IR (KBr): 3260, 2923, 2854, 1610, 1431, 1261, 1088, 813, 695. MS (ESI) *m*/*z*: 204 [M^++1].

Table 2, Entry 12; 1-(4-Propyl-1*H*-1,2,3-triazol-1-yl)propan-2-ol:



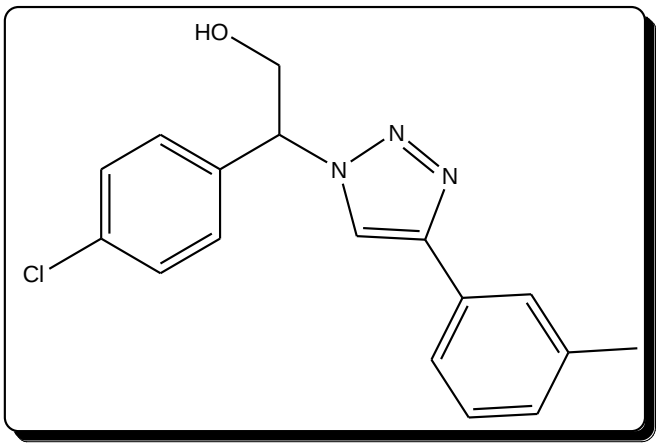
^{1}H NMR ($CDCl_3$) δ 0.95 (t, *J* = 7.55 Hz, 3H), 1.22 (d, *J* = 6.04 Hz, 3H), 1.65 (m, 2H), 2.59 (t, *J* = 7.55 Hz, 2H), 4.14 (dd, *J* = 5.28, 7.55 Hz, 1H), 4.19–4.24 (m, 1H), 4.32 (dd, *J* = 2.26, 10.57 Hz, 1H), 7.37 (s, 1H). IR (KBr) ν/cm^{-1} 3260, 3141, 2923, 2854, 1610, 1431, 1261, 1088, 813, 764, 695. MS (EI) *m*/*z*:170 [M^++1].

Table 2, Entry 13; 2-(4-Chlorophenyl)-2-(4-(4-fluoro 3-methylphenyl)-1*H*-1,2,3-triazol-1-yl)ethanol:



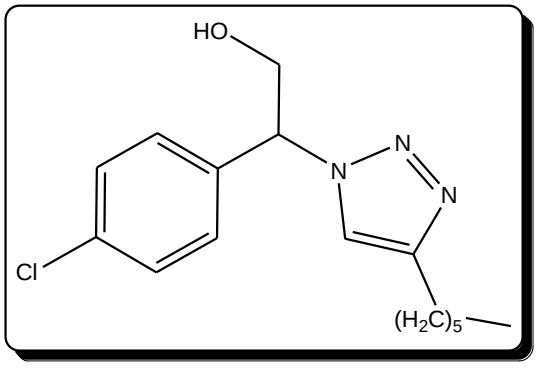
^{1}H NMR ($CDCl_3$) δ 2.35 (s, 3H), 3.90 (br s, 1H), 4.17 (dd, *J* = 3.02, 9.06 Hz, 1H), 4.58 (dd, *J* = 3.96, 8.12 Hz, 1H), 5.58 (dd, *J* = 3.02, 4.15 Hz, 1H), 7.19–7.25 (m, 3H), 7.27–7.34 (m, 2H), 7.43–7.48 (m, 2H), 7.59 (s, 1H). IR (KBr) ν/cm^{-1} 3326, 2925, 1710, 1493, 1237, 1091, 800, 508. MS (ESI) *m*/*z*: 332 [M$^+$+1].

Table 2, Entry 14: 2-(4-Chlorophenyl)-2-(4-*m*-tolyl-1*H*-1,2,3-triazol-1-yl)ethanol:



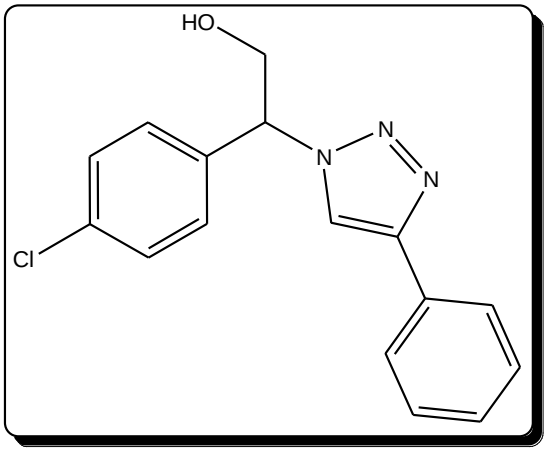
^{1}H NMR ($CDCl_3$) δ 2.35 (s, 3H), 3.90 (br s, 1H) 4.16 (dd, *J* = 3.96, 9.06 Hz, 1H), 4.55 (dd, *J* = 3.96, 8.12 Hz, 1H), 5.58 (dd, *J* = 3.02, 4.15 Hz, 1H), 7.05–7.10 (m,1H), 7.19–7.25 (m, 3H), 7.27–7.34 (m, 2H), 7.43–7.49 (m, 2H), 7.59 (s, 1H). IR (KBr) ν/cm^{-1} 3374, 2925, 1597, 1489, 1410, 1224, 1086, 784, 694, 530. MS (ESI) *m*/*z*: 314 [M$^+$+1].

Table 2, Entry 15: 2-(4-Chlorophenyl)-2-(4-hexyl-1*H*-1,2,3-triazol-1-yl)ethanol:



^{1}H NMR ($CDCl_3$) δ 0.87 (t, *J* = 6.79 Hz, 3H), 1.22–1.34 (m, 8H), 2.63 (t, *J* = 7.55 Hz, 2H), 4.10 (dd, *J* = 3.77, 5.22 Hz, 1H), 4.49 (dd, *J* = 3.96, 8.12 Hz, 1H), 5.51 (dd, *J* = 3.77, 4.34 Hz, 1H), 7.14–7.28 (m, 4H), 7.30 (s, 1H). IR (KBr) ν/cm^{-1} 3314, 2927, 1578, 1493, 1222, 1076, 1015, 765, 586. MS (ESI) *m*/*z*: 308 [M^++1].

Table 2, Entry 16: 2-(4-Chlorophenyl)-2-(4-phenyl-1*H*-1,2,3-triazole-1-yl)ethanol:



^{1}H NMR ($CDCl_3$) δ 4.14–4.22 (m, 1H), 4.53–4.61 (m, 1H), 5.55–5.61 (m, 1H), 7.20–7.25 (m, 3H), 7.33–7.38 (m, 4H), 7.61 (s, 1H), 7.69–7.74 (m, 2H). IR (KBr) ν/cm^{-1} 3347, 3084, 2925, 2854, 1597, 1489, 1459, 1223, 1088, 1048, 1019, 818, 763, 690, 512. MS (ESI) *m*/*z*: 300 [M^++1].