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### **Supporting Information (SI)**

# Ag-NHC supported on silica: An efficient ultra-low loading catalyst for regioselective 1,2,3triazole synthesis

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## **General information**

All reactions were carried out in oven dried glassware under atmospheric conditions otherwise noted. Starting materials and solvents were obtained from common commercial sources and used without further purification. All reported yields are isolated yields. TLC was carried out using aluminium sheets pre-coated with silica gel 60F<sub>254</sub> (Merck) and was visualized under 254 nm UV light. <sup>1</sup>H NMR (600 MHz), <sup>13</sup>C NMR (150 MHz) were measured on JEOL 600 MHz spectrometer in deuterated CDCl<sub>3</sub> and DMSO. Chemical shifts are reported in parts per million (ppm), downfield from residual solvents peaks and coupling constants are reported as Hertz (Hz). Splitting patterns are designated as singlet (s), doublet (d), triplet (t) etc., splitting patterns that could not be interpreted or easily

visualized are designated as multiplet (m). Melting points of the isolated products were determined using BUCHI B450 melting point apparatus and reported uncorrected. N<sub>2</sub> adsorption/desorption isotherms were measured using Quantachrome Instrument, Micromeritics, 3FLEX-3500 at liquid  $N_2$ temperature. The surface area of the samples was calculated according to the BET equation and pore size distribution was evaluated using BJH algorithm. Silver loading in the catalyst and its leaching after catalytic cycle was determined using inductively coupled plasma-atomic emission spectrometry (ICP-AES) on a Thermo Electron IRIS INTERPID II XSP DUO instrument. ESI-MS spectra were recorded on a Thermo Fischer Endura LC/MS MS mass spectrometer whereas HRMS spectra are recorded on Xevo XS QTof mass spectrometer. Transmission electron microscopic (TEM) images are taken in Jeol JEM 2100 Transmission Electron Microscope. XPS experiments were carried out on PHI 5000 Versa Prob II, X-Ray photoelectron spectrometer and binding energies ( $\pm$  0.1 eV) were determined with respect to the position C 1s peak at 282.95 eV. Calibration of the binding energy (BE) scale was done by using the C 1s (BE = 284.8 eV) signal. SEM and EDX analyses are carried out on Jeol JSM-IT300 Scanning electron microscope. TGA and DTG analyses are carried out with Perkin Elmer STA 8000 instrument at a ramp rate or scanning rate of 20 °C/min under nitrogen atmosphere (N<sub>2</sub> gas flow rate: 20 mL/min) taking empty alumina as reference.

#### General procedure for the preparation of 1-iodo-4-(prop-2-yn-1-yloxy)benzene

To the stirred solution of 4-Iodophenol (1.1g, 5 mmol) in N,N-dimethylformamide (DMF) (10 mL), were added  $K_2CO_3$  (1.04g, 7.5 mmol) and propargyl bromide (0.6g, 5 mmol) at room temperature. The progress of the reaction was monitored by TLC. After completion of the reaction, the reaction mixture was poured into water and extracted with ethyl acetate (2 x 20 mL). The combined organic extracts were washed with  $H_2O$ , dried over  $Na_2SO_4$  and concentrated under reduced pressure. The residual crude product was used directly without purification.

#### **Preparation of catalyst:**

The supported catalyst was prepared from commercial chromatography grade silica gel (60-120 Mesh). 2 gm of silica (dried at 120°C for 12h) was suspended on 50 ml dry toluene and treated with 3 mmol of (3-Chloropropyl)trimethoxysilane at 80°C under  $N_2$  atmosphere. After cooling, the solids were separated by filtration and repeatedly washed through soxhlet extraction with dry toluene. The resulting material was dried at 100°C for 12 hour. 1.5 gm of the silane functionalized silica is then treated with 2 mmol 1-methyl imidazole in refluxing toluene for 8 hour under nitrogen atmosphere to get silica immobilized ionic liquid. After filtration, washing through soxhlet extraction with dry toluene and drying the functionalized silica support, 1 gm of the material was treated with 0.25 mmol AgBr in presence of 1 mmol of KO'Bu in THF and magnetically stirred for 24 hour under light protection. The material obtained was again cooled, filtered and alternatively washed with THF and water for 3 cycles. After drying, Ag-NHC@SiO<sub>2</sub> catalyst was obtained as light grey coloured solid.

#### General procedure for the synthesis of 1,4-disubstituted-1H-1,2,3-triazole

To a mixture of catalyst (15 mg, 0.006 mmol%) benzyl azide (0.5 mmol) and phenylacetylene (1.2 eq.) quinine (1eq.) was added in 1 mL water and stirred at 60 °C for 5 h. After completion of the reaction it was extracted with ethyl acetate ( $2 \times 10$  mL), washed with brine, dried over anhydrous sodium sulphate and concentrated under vacuum, which on column chromatography (ethyl acetate: hexanes) afforded the desired product. The products were then characterized by NMR and ESI-MS spectra.

## **PXRD** pattern of reused catalyst

The PXRD pattern of the reused catalyst after 5<sup>th</sup> cycle of reuse shows practically no change in diffraction pattern only intensity of the peaks got decreased which clearly indicates strong anchoring and rule out possibility of leaching during the course of reuse.



#### Solid UV-Visible spectra

Solid UV-Visible spectrum of the catalyst which do not possess peak at around 420 nm is an indication that the silver is in +1 oxidation state and no metallic silver in nanoparticle form exists.



## Spectral data of products

**1-Benzyl-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 1)**<sup>[1]</sup>: White solid; mp 128-130 °C, 98% yield.<sup>1</sup>H NMR (600 MHz, ) δ 7.80 (d, J = 8.1 Hz, 2H), 7.66 (s, 1H), 7.44 – 7.35 (m, 5H), 7.31 (t, J = 6.5 Hz, 3H), 5.58 (s, 2H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): δ148.32, 130.61, 129.25, 128.88, 128.25, 128.15, 125.78, 119.56, 54.32. MS (ESI) *m/z*: 236.17 [M + H]<sup>+</sup>, cal. 236.11.

1-(4-Diphenyl)-1H-1,2,3-triazole (Table 3, Entry 2)<sup>[1]</sup>: Pale yellow solid, mp 183–184 °C, 89% yield. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  8.08 (s, 1H), 7.67 (d, J= 7.89 Hz, 2H), 7.49–7.19 (m, 8H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>):  $\delta$  149.0, 135.6, 132.6, 129.8, 128.9, 128.9, 128.56, 127.9, 125.7, 120.5; MS (ESI) *m/z*: 222.07 [M + H]<sup>+</sup>, cal. 222.10.

1-(4-Chlorophenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 3)<sup>[1]</sup>: Yellow solid; mp 225–227



°C, 85% yield. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  8.11 (s, 1H), 7.84 (d, J = 7.2 Hz, 2H), 7.68 (d, J = 8.8 Hz, 2H), 7.46 (d, J = 8.8 Hz, 2H), 7.40 (t, J = 7.6 Hz, 2H), 7.32 (t, J = 7.4 Hz, 1H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  148.58,

135.41, 134.44, 129.87, 128.86, 128.48, 127.46, 125.41, 121.55, 117.40. MS (ESI) *m/z*: 256.14 [M + H]<sup>+</sup>, cal. 256.06.

**1-(4-Fluorophenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 4)**<sup>[2]</sup>: White Solid; mp 221-222 °C, 91% yield. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  8.05 (s, 1H), 7.74 (dd, J = 9.1, 4.6 Hz, 2H), 7.58 (t, J = 5.4 Hz, 4H), 7.45 (t, J = 7.7 Hz, 2H), 7.25 (t, J = 7.7 Hz, 2H), 7.2 8.7 Hz, 1H).<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 157.35, 145.01, 134.39, 128.66, 128.18, 126.72, 126.64, 122.56, 121.12, 114.94. MS (ESI) *m/z*: 240.04 [M + H]<sup>+</sup>, cal. 240.09.

1-(4-(difluoromethoxy)phenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 5): Yellow Solid; mp



154-156 °C, 85% yield. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  8.17 (s, 1H), 7.91 (d, *J* = 7.8 Hz, 2H), 7.81 (d, *J* = 8.3 Hz, 2H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.39 (t, *J* = 7.2 Hz, 1H), 7.32 (d, *J* = 8.9 Hz, 2H), 6.59 (t, *J* = 73.0 Hz, 1H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$ 163.24, 158.86, 144.12,

129.05, 125.96, 122.12, 121.09, 117.68, 53.51 (s). HRMS (ESI-TOF) *m/z*: 288.1015 [M + H]<sup>+</sup>, cal. 288.0949.

**4-Phenyl-1-(o-tolyl)-1H-1,2,3-triazole (Table 3, Entry 7)**<sup>[2]</sup>: Light yellow oil; 90% yield. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.85 (s, 1H), 7.82 (d, *J* = 7.1 Hz, 2H), 7.38 – 7.23 (m, 7H), 2.18 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  147.52, 144.96, 131.45, 131.07, 129.88, 128.87, 128.32, 126.70, 125.88, 125.73, 124.73, 121.16, 17.81. MS (ESI) *m/z*: 236.17 [M + H]<sup>+</sup>, cal. 236.28.

1-(4-Nitrophenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 8) <sup>[4]</sup>: light yellow solid; m.p. 151– N=N N=NN=N

4-(4-Phenyl-1H-1,2,3-triazol-1-yl)benzonitrile (Table 3, Entry 9) <sup>[4]</sup>: Pale yellow solid; mp 219-220  $^{\circ}$ C, 78% yield. <sup>1</sup>H NMR (600 MHz, DMSO-d<sub>6</sub>)  $\delta$  9.10(s, 1H), 8.14 (d, J = 9.1 Hz, 2H), 8.08 (d, J = 9.1 Hz, 2H), 7.58 (dd, J = 8.7, 4.4 Hz, 2H), 7.39 (t, J = 7.7 Hz, 2H), 7.27 (t, J = 7.4 Hz, 1H). <sup>13</sup>C NMR (150 MHz, DMSO-d<sub>6</sub>) 157.90, 144.95, 134.84, 133.60, 128.35, 127.33, 126.74,

122.88, 121.08, 118.62, 115.74. MS (ESI) *m/z*: 247.02 [M + H]<sup>+</sup>, cal. 247.09.

**1-Octyl-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 10)**<sup>[5,7]</sup>: White solid; mp 99-101 °C, 91% yield.  $\stackrel{N=N}{\longrightarrow}$   $\stackrel{IH}{\longrightarrow}$  NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.61 (s, 1H), 7.54 (t, *J* = 8.9 Hz, 2H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 4.35 (t, *J* = 7.4 Hz, 2H), 1.93 - 1.89 (m, 2H), 1.32 - 1.25 (m, 10H), 0.87 (t, J = 6.9 Hz, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  144.22, 128.81, 128.29, 126.82, 122.51, 50.57, 31.77, 30.36, 29.02, 26.57, 22.67, 14.14. MS (ESI) m/z: 258.28 [M + H]<sup>+</sup>, cal. 258.19.

1-Benzyl-4-(6-methoxynaphthalen-2-yl)-1H-1,2,3-triazole (Table 3, Entry 11)<sup>[6]</sup>: White solid; mp



206-207 °C, 87% yield. <sup>1</sup>H NMR (600 MHz, DMDO-d<sub>6</sub>)  $\delta$  8.64 (s, 1H), 8.28 (s, 1H), 7.89 (d, J = 8.2 Hz, 1H), 7.84 – 7.82 (m, 2H), 7.36-7.29 (m, 6H), 7.14 (d, J = 8.9 Hz, 1H), 5.63 (s, 2H), 3.84 (s, 3H). <sup>13</sup>C NMR (150 MHz, DMDO-d<sub>6</sub>)  $\delta$  165.90, 157.98, 136.55,

134.57, 130.05, 129.36, 129.05, 128.72, 128.48, 127.88, 126.40, 124.62, 123.99, 121.96, 119.65, 106.54, 55.75, 53.60. MS (ESI) *m/z*: 316.09 [M + H]<sup>+</sup>, cal. 316.14.

**1-Benzyl-4-((4-iodophenoxy)methyl)-1H-1,2,3-triazole (Table 3, Entry 12):** White solid; mp 132-134 °C, 98% yield. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.54 (d, *J* = 8.5 Hz, 2H), 7.51 (s, 1H), 7.40 – 7.36 (m, 3H), 7.27 (d, *J* = 8.1 Hz, 2H), 6.74 (d, *J* = 8.5 Hz, 2H), 5.53 (s, 2H), 5.14 (s, 2H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  158.13, 144.23, 138.37, 134.45, 129.26, 128.95, 128.21,

122.72, 117.30, 83.55, 62.18, 54.37. HRMS (ESI-TOF) *m/z*: 392.0787 [M + H]<sup>+</sup>, cal. 392.0261.

#### 1-benzyl-4-(4-methoxy-2-methylphenyl)-1H-1,2,3-triazole (Table 3, Entry 13):



White solid; mp 97-99 °C, 75% yield. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.66 (d, *J* = 8.1 Hz, 1H), 7.49 (s, 1H), 7.39 – 7.35 (m, 3H), 7.30 (d, *J* = 7.1 Hz, 2H), 6.79 (d, *J* = 8.3 Hz, 2H), 5.58 (s, 2H), 3.81 (s, 3H), 2.39

(s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 159.43, 147.50, 137.17, 134.98, 130.25, 129.20, 128.77, 128.03, 122.74, 121.19, 116.28, 111.47, 55.31, 54.18, 21.64. HRMS (ESI-TOF) *m/z*: 280.1544 [M + H]<sup>+</sup>, cal. 280.1451.

(1-Benzyl-1H-1,2,3-triazol-4-yl) methanol (Table 3, Entry 14) <sup>[5]</sup>: White solid, mp 76-78 °C, 91% yield. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.44 (s, 3H), 7.39–7.28 (m, 5H), 5.52 (s, 2H), 4.77 (s, 2H), 3.74 (s, br, 1H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 142.90, 137.11, 129.17, 128.85, 128.15, 125.31, 54.24, 48.46. MS (ESI) *m/z*: 190.15 [M + H]<sup>+</sup>, cal. 190.09.



Ethyl 1-benzyl-1H-1,2,3-triazole-4-carboxylate (Table 3, Entry 15) <sup>[5]</sup>: Pale white solid; mp 64-66 °C, 93% yield. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.91 (s, 1H), 7.37 – 7.27 (m, 3H), 7.25 – 7.12 (m, 2H), 5.51 (s, 2H), 4.32 (q, *J* = 7.1 Hz, 2H), 1.31 (t, *J* = 7.1 Hz, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 160.59, 140.50, 133.61, 129.21, 129.04, 128.17, 127.23, 61.22, 54.35, 14.19. MS (ESI) *m/z*: 232.17 [M + H]<sup>+</sup>, cal. 232.10.

(1-phenyl-1H-1,2,3-triazol-4-yl)methyl benzoate (Table 3, Entry 16)<sup>[8]</sup>: Pale white solid; 84-86 °C, 91% yield. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  8.15 (s, 1H), 8.07 (d, J = 7.2N=N Hz, 2H), 7.74 (d, J = 7.6 Hz, 2H), 7.58-7.52 (m, 3H), 7.48-7.43 (m, 3H),

N O Ph

Hz, 2H), 7.74 (d, J = 7.6 Hz, 2H), 7.58-7.52 (m, 3H), 7.48-7.43 (m, 3H), 5.53 (s, 2H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  166.54, 143.34, 136.86, 133.29, 129.78, 129.77, 128.95, 128.42, 122.34, 120.65, 57.82. MS (ESI)

*m*/*z*: 280.16 [M + H]<sup>+</sup>, cal. 280.10.

**1-Phenyl-1H-1,2,3-triazole-4-carboxylic acid (Table 3, Entry 17)** <sup>[9]</sup>: White solid; mp 89–91 °C, N=N N=N

**1-Phenyl-1H-1,2,3-triazole-4,5-dicarboxylic acid dimethyl ester (Table 3, Entry 18)** <sup>[8]</sup>: White solid; mp 106–108 °C, 94% yield. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): d 7.58–7.54 (m, 5H), 4.01–3.92(m, 6H); <sup>13</sup>CNMR (150 MHz, CDCl<sub>3</sub>): 160.0, 159.3, 138.6, 135.4, 129.8, 129.7, 129.6, 129.5, 52.6, 52.2. <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  160.20, 159.45, 138.76, 135.47, 132.50, 130.58, 130.02, 124.26, 53.90, 52.79. MS (ESI) *m/z*: 262.13 [M + H]<sup>+</sup>, cal. 262.07.

139.56, 136.16, 130.60, 121.17, 112.05, 60.94, 14.17. MS (ESI) *m/z*: 290.08 [M + H]<sup>+</sup>, cal. 290.11.

**4-Butyl-1-phenyl-1H-1,2,3-triazole (Table 3, Entry 20)** <sup>[9]</sup>: Colourless liquid; 95% yield. <sup>1</sup>H NMR N=N (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.66 (s, 1H), 7.65 (d, J = 2.3 Hz, 2H), 7.44 (t, J = 7.8 Hz, 2H), 7.36 – 7.33 (m, 1H), 2.75 – 2.72 (m, 2H), 1.68-1.62 (m, 2H), 1.40 – 1.33 (m, 2H), 0.89 (t, J = 7.4 Hz, 3H). <sup>13</sup>C NMR (150

MHz, CDCl<sub>3</sub>) 149.07, 137.06, 129.56, 128.32, 120.30, 118.70, 31.39, 25.23, 22.21, 13.73. MS (ESI) *m/z*: 202.20 [M + H]<sup>+</sup>, cal.202.13.



29.40, 28.95, 25.69, 22.58, 14.09. MS (ESI) *m/z*: 230.27 [M + H]<sup>+</sup>, cal. 230.16.

**1-phenyl-4-(thiophen-3-yl)-1H-1,2,3-triazole (Table 3, Entry 22)** <sup>[10]</sup>: Light brown solid; mp 172– 174 °C, 87% yield. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  8.11 (s, 1H), 7.90 (d, J =7.3 Hz, 2H), 7.62 (d, J = 1.8 Hz, 1H), 7.53 (d, J = 5.2 Hz, 1H), 7.51 – 7.44 (m, 3H), 7.38 (t, J = 7.4 Hz, 1H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  148.07, 135.86, 130.06, 129.03, 128.47, 127.34, 125.86, 120.82, 117.95, 114.15. MS (ESI)

m/z: 228.18 [M + H]<sup>+</sup>, cal. 228.05.

### Copies of <sup>1</sup>H and <sup>13</sup>C NMR Spectra for Compounds

# <sup>1</sup>H NMR of 1-Benzyl-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 1)





<sup>1</sup>H NMR of 1-(4-Chlorophenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 3)



<sup>13</sup>C NMR of 1-(4-Chlorophenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 3)



<sup>1</sup>H NMR of 1-(4-Fluorophenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 4)



<sup>13</sup>C NMR of 1-(4-Fluorophenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 4)



<sup>1</sup>H NMR of 1-(4-(difluoromethoxy)phenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 5)



<sup>13</sup>C NMR of 1-(4-(difluoromethoxy)phenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 5)



<sup>1</sup>H NMR of 1-(3-Chlorophenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 6)



<sup>13</sup>C NMR of 1-(3-Chlorophenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 6)



<sup>1</sup>H NMR of 4-Phenyl-1-(o-tolyl)-1H-1,2,3-triazole (Table 3, Entry 7)



<sup>13</sup>C NMR of 4-Phenyl-1-(o-tolyl)-1H-1,2,3-triazole (Table 3, Entry 7)



<sup>1</sup>H NMR of 1-(4-Nitrophenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 8)



<sup>13</sup>C NMR of 1-(4-Nitrophenyl)-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 8)









# <sup>1</sup>H NMR of 1-Octyl-4-phenyl-1H-1,2,3-triazole (Table 3, Entry 10)

<sup>1</sup>H NMR of 1-Benzyl-4-(6-methoxynaphthalen-2-yl)-1H-1,2,3-triazole (Table 3, Entry 11)



<sup>13</sup>C NMR of 1-Benzyl-4-(6-methoxynaphthalen-2-yl)-1H-1,2,3-triazole (Table 3, Entry 11)



<sup>1</sup>H NMR of 1-Benzyl-4-((4-iodophenoxy)methyl)-1H-1,2,3-triazole (Table 3, Entry 12)



<sup>13</sup>C NMR of 1-Benzyl-4-((4-iodophenoxy)methyl)-1H-1,2,3-triazole (Table 3, Entry 12)



<sup>1</sup>H NMR of 1-benzyl-4-(4-methoxy-2-methylphenyl)-1H-1,2,3-triazole (Table 3, Entry 13)



<sup>13</sup>C NMR of 1-benzyl-4-(4-methoxy-2-methylphenyl)-1H-1,2,3-triazole (Table 3, Entry 13)



# <sup>1</sup>H NMR of (1-Benzyl-1H-1,2,3-triazol-4-yl) methanol (Table 3, Entry 14)



<sup>13</sup>C NMR of (1-Benzyl-1H-1,2,3-triazol-4-yl) methanol (Table 3, Entry 14)







<sup>13</sup>C NMR of Ethyl 1-benzyl-1H-1,2,3-triazole-4-carboxylate (Table 3, Entry 15)



100 90 f1 (ppm) 

<sup>1</sup>H NMR of (1-phenyl-1H-1,2,3-triazol-4-yl)methyl benzoate (Table 3, Entry 16)





<sup>13</sup>C NMR of 1-Phenyl-1H-1,2,3-triazole-4-carboxylic acid (Table 3, Entry 17)







<sup>13</sup>C NMR of 1-Phenyl-1H-1,2,3-triazole-4,5-dicarboxylic acid dimethyl ester (Table 3, Entry 18)





# <sup>1</sup>H NMR of 1-Phenyl-1H-1,2,3-triazole-4,5-dicarboxylic acid diethyl ester (Table 3, Entry 19)





<sup>13</sup>C NMR of 4-Butyl-1-phenyl-1H-1,2,3-triazole (Table 3, Entry 20)



# <sup>1</sup>H NMR of 4-Hexyl-1-phenyl-1H-1,2,3-triazole (Table 3, Entry 21)







<sup>13</sup>C NMR of 1-phenyl-4-(thiophen-3-yl)-1H-1,2,3-triazole (Table 3, Entry 22)



### References

- [1] A. Aziz Ali, M. Chetia, P. J. Saikia, D. Sarma, RSC Adv., 2014, 4, 64388
- [2] Z. Chen, Q. Yan, Z. Liu, Y. Zhang, Chem. Eur. J. 2014, 20, 1-6.
- [3] X. Meng, X. Xu, T. Gao, B. Chen, Eur. J. Org. Chem. 2010, 5409-5414
- [4] M. A. Morozova, M. S. Yusubov, B. Kratochvil, V. Eigner, A. A. Bondarev, A. Yoshimura, A.
- Saito, V. V. Zhdankin, M. E. Trusova, P. S. Postnikov, Org. Chem. Front., 2017,4, 978-985
- [5] A.Aziz Ali, M. Chetia, B.Saikia, P. J. Saikia, D. Sarma, Tetrahedron Lett., 2015, 56, 5892–5895
- [6] A. N. Semakin, D. P. Agababyan, S. Kim, S.Lee, A. Y. Sukhorukov, K. G. Fedina, J. Oh, S. L.
- Ioffe, Tetrahedron Lett., 2015, 56, 6335-6339.
- [7] J.-A. Shin, Y.-G. Lim, K.-H. Lee, J. Org. Chem. 2012, 77, 4117-4122.
- [8] A. Garg, A. A. Ali, K. Damarla, A. Kumar, D. Sarma, Tetrahedron Lett., 2018, 59, 4031–4035.
- [9] B. Kaboudin, Y. Abedia and T. Yokomatsu Org. Biomol. Chem., 2012, 10, 4543.
- [10] L. Luciani, E. Goff, D. Lanari, S. Santoro, L. Vaccaro, Green Chem., 2018,20, 183-187.