Supporting Information
for DOI: 10.1055/s-0036-1589157
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One-pot Synthesis of 1-Monosubstituted-1, 2, 3-Triazoles from Propargyl Alcohol

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General:

$^1$H NMR spectra were recorded with a Bruker ACF400 spectrometer (400 MHz and 500 MHz) in CDCl$_3$ with TMS as an internal standard. All reactions were monitored by TLC with HuanghaiGF 254 silica gel coated plates. Column chromatography was carried out using 300–400 mesh silica gel at medium pressure.

General Procedures for the Target Products.

\[ \text{R} - \text{N}_3 + \text{OH} \rightarrow \text{R} - \text{N} - \text{R} \]

1-Azido-4-methylbenzenes 1 (0.3 mmol), propargyl alcohol 2 (0.36 mmol), CuI (0.03 mmol), NaAsc (0.06 mmol), and 2 mL solvent were added to a 15 mL pressure tube. The tube was then sealed, and the mixture was stirred at 80 °C for 5 hours. After the reaction completed, the above system was added with KMnO$_4$ (0.75 mmol) and Na$_2$CO$_3$ (0.45 mmol), and stirred at 80 °C for 8 h until the reaction completed. Then, Ag$_2$O (0.03 mmol) and K$_2$S$_2$O$_7$ (0.6 mmol) were added to the tube and the mixture was conducted at 100 °C for 24 h until the transformation finished by TLC analysis. H$_2$O (25 mL) was added to the mixture and the system was extracted with EtOAc (3 × 20 mL). The combined organic layer was washed with brine (3 × 5 mL), dried with Na$_2$SO$_4$, and concentrated under reduced pressure to afford the crude product. Purification by column chromatography on silica gel with EtOAc-PE (1:3) afforded the desired product 3.
Spectral Data of the Compounds

1-(p-Tolyl)-1H-1, 2, 3-triazole (3a):

![Structure of 3a]

White solid; $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ = 7.96 (d, $J = 0.8$ Hz, 1H), 7.83 (s, 1H), 7.62 (d, $J = 8.4$ Hz, 2H), 7.32 (d, $J = 8.2$ Hz, 2H), 2.43 (s, 3H).

1-Phenyl-1H-1, 2, 3-triazole (3b):

![Structure of 3b]

White solid; $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ = 8.01 (s, 1H), 7.86 (s, 1H), 7.75 (d, $J = 8.0$ Hz, 2H), 7.54 (t, $J = 7.8$ Hz, 2H), 7.45 (t, $J = 7.4$ Hz, 1H).

1-(o-Tolyl)-1H-1, 2, 3-triazole (3c):

![Structure of 3c]

White solid; $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ = 7.85 (s, 1H), 7.78 (s, 1H), 7.41 (dd, $J = 5.6$, 2.5 Hz, 1H), 7.37 (d, $J = 7.4$ Hz, 1H), 7.33 (s, 2H), 2.20 (s, 3H).

1-(m-Tolyl)-1H-1, 2, 3-triazole (3d):

![Structure of 3d]

White solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ = 7.86 (s, 1H), 7.67 (s, 1H), 7.51 (s, 1H), 7.43 (d, $J = 8.1$ Hz, 1H), 7.31 (t, $J = 7.8$ Hz, 1H), 7.09 (d, $J = 7.5$ Hz, 1H), 2.41 (s, 3H).

1-(4-Methoxyphenyl)-1H-1, 2, 3-triazole (3e):

![Structure of 3e]

White solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ = 7.92 (d, $J = 0.7$ Hz, 1H), 7.83 (s, 1H), 7.68 – 7.59 (m, 2H), 7.03 (d, $J = 9.0$ Hz, 2H), 3.87 (s, 3H).

1-(2-Methoxyphenyl)-1H-1, 2, 3-triazole (3f):

![Structure of 3f]

White solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ = 8.13 (d, $J = 1.0$ Hz, 1H), 7.82 (d, $J = 1.0$ Hz, 1H), 7.79 (dd, $J = 7.9$, 1.7 Hz, 1H), 7.46 – 7.41 (m, 1H), 7.14 – 7.08 (m, 2H), 3.89 (s, 3H).

4-(1H-1, 2, 3-Triazol-1-yl)benzenesulfonamide (3g):

![Structure of 3g]

White solid; $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ = 8.93 (s, 1H), 8.14 (d, $J = 8.6$ Hz, 2H), 8.04 (d, $J = 6.1$ Hz, 3H), 7.55 (s, 2H).
1-(4-Nitrophenyl)-1H-1, 2, 3-triazole (3h):
White solid; \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta = 9.01\) (s, 1H), 8.43 (d, \(J = 8.7\) Hz, 2H), 8.22 (d, \(J = 8.6\) Hz, 2H), 8.04 (s, 1H).

1-(2-Nitrophenyl)-1H-1, 2, 3-triazole (3i):
White solid; \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta = 8.71\) (d, \(J = 0.8\) Hz, 1H), 8.22 (dd, \(J = 8.1, 1.0\) Hz, 1H), 8.01 (d, \(J = 0.8\) Hz, 1H), 7.96 (td, \(J = 7.9, 1.2\) Hz, 1H), 7.89 – 7.82 (m, 2H).

1-(2-Fluorophenyl)-1H-1, 2, 3-triazole (3j):
White solid; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta = 8.11\) (d, \(J = 2.2\) Hz, 1H), 7.99 (td, \(J = 7.7, 1.6\) Hz, 1H), 7.88 (s, 1H), 7.49 – 7.41 (m, 1H), 7.37 – 7.28 (m, 2H).

1-(4-Fluorophenyl)-1H-1, 2, 3-triazole (3k):
White solid; \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta = 7.99\) (s, 1H), 7.84 (s, 1H), 7.73 (dd, \(J = 8.9, 4.6\) Hz, 2H), 7.23 (t, \(J = 8.4\) Hz, 2H).

1-(2-Chlorophenyl)-1H-1, 2, 3-triazole (3l):
White solid; \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta = 8.03\) (s, 1H), 7.87 (s, 1H), 7.64 – 7.55 (m, 2H), 7.50 – 7.42 (m, 2H).

1-(3-Chlorophenyl)-1H-1, 2, 3-triazole (3m):
White solid; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta = 8.02\) (d, \(J = 1.1\) Hz, 1H), 7.86 (d, \(J = 1.0\) Hz, 1H), 7.80 (t, \(J = 2.0\) Hz, 1H), 7.66 (ddd, \(J = 7.9, 2.0, 1.3\) Hz, 1H), 7.51 – 7.40 (m, 2H).

1-(4-Chlorophenyl)-1H-1, 2, 3-triazole (3n):
White solid; \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta = 8.01\) (s, 1H), 7.85 (s, 1H), 7.70 (d, \(J = 8.7\) Hz, 2H), 7.50 (d, \(J = 8.7\) Hz, 2H).
1-(2-Bromophenyl)-1H-1, 2, 3-triazole (3o):
White solid; $^1$H NMR (500 MHz, CDCl$_3$) $\delta = 8.01$ (s, 1H), 7.85 (s, 1H), 7.70 (d, $J = 8.7$ Hz, 2H), 7.50 (d, $J = 8.7$ Hz, 2H).

1-(3-Bromophenyl)-1H-1, 2, 3-triazole (3p):
White solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta = 8.00$ (d, $J = 1.1$ Hz, 1H), 7.95 (t, $J = 1.9$ Hz, 1H), 7.86 (d, $J = 0.9$ Hz, 1H), 7.71 (ddd, $J = 8.1$, 2.0, 0.9 Hz, 1H), 7.58 (ddd, $J = 8.0$, 1.7, 0.9 Hz, 1H), 7.41 (t, $J = 8.1$ Hz, 1H).

1-(4-Bromophenyl)-1H-1, 2, 3-triazole (3q):
White solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta = 7.85$ (s, 1H), 7.69 (s, 1H), 7.56 (s, 4H).

(1-(p-Tolyl)-1H,1,2,3-triazol-4-yl)methanol (4a):
White solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta 7.95$ (s, 1H), 7.58 (d, $J = 8.4$ Hz, 2H), 7.30 (d, $J = 8.2$ Hz, 2H), 4.88 (d, $J = 5.2$ Hz, 2H), 3.14 (t, $J = 5.6$ Hz, 1H), 2.42 (s, 3H).

1-(p-Tolyl)-1H-1,2,3-triazole-4-carboxylic acid (5a):
White solid; $^1$H NMR (600 MHz, DMSO-$d_6$) $\delta 9.33$ (s, 1H), 7.86 (d, $J = 8.4$ Hz, 2H), 7.42 (d, $J = 8.1$ Hz, 2H), 2.39 (s, 3H).
$^1$H NMR spectra of the compounds

3a

3b