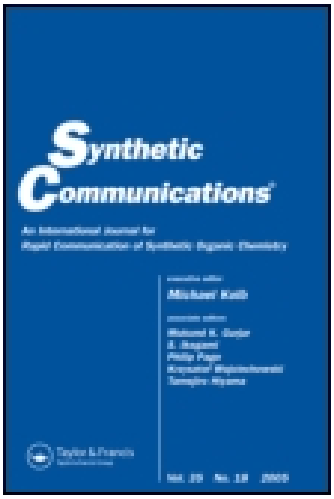

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Facile One-Pot Synthesis of 1,2,3-Triazoles Featuring Oxygen, Nitrogen, and Sulfur Functionalized Pendant Arms

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FACILE ONE-POT SYNTHESIS OF 1,2,3-TRIAZOLES FEATURING OXYGEN, NITROGEN, AND SULFUR FUNCTIONALIZED PENDANT ARMS

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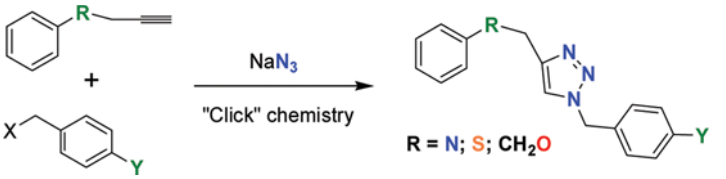
GRAPHICAL ABSTRACT



Abstract *A practical and efficient one-pot synthesis of novel 1,2,3-triazoles featuring nitrogen, oxygen, and sulfur functionalized pendant arms has been developed. The click reaction of mono-propargyl derivatives supported by aniline, thiophenol, and benzyl alcohol, with sodium azide and* p*-substituted benzyl halogenides, renders a series of* N*-substituted-1,2,3-triazoles in good yields under mild reaction conditions. The catalyst system was based in* $Cu(OAc)_2 \cdot H_2O$*, sodium L-ascorbate, and 1,10-phenanthroline monohydrate, and all reactions were performed in a mixture* H_2O*–ethanol (4:1* v/v*). Additionally, the preparation of bis-1,2,3-triazoles supported by di-propargylated aniline was carried out, demonstrating the versatility of the present methodology.*

[Supplementary materials are available for this article. Go to the publisher's online edition of Synthetic Communications® *for the following free supplemental resource(s): Full experimental and spectral details.]*

Keywords Catalysis; click chemistry; cycloaddition; multicomponent synthesis; 1,2,3-triazoles

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INTRODUCTION

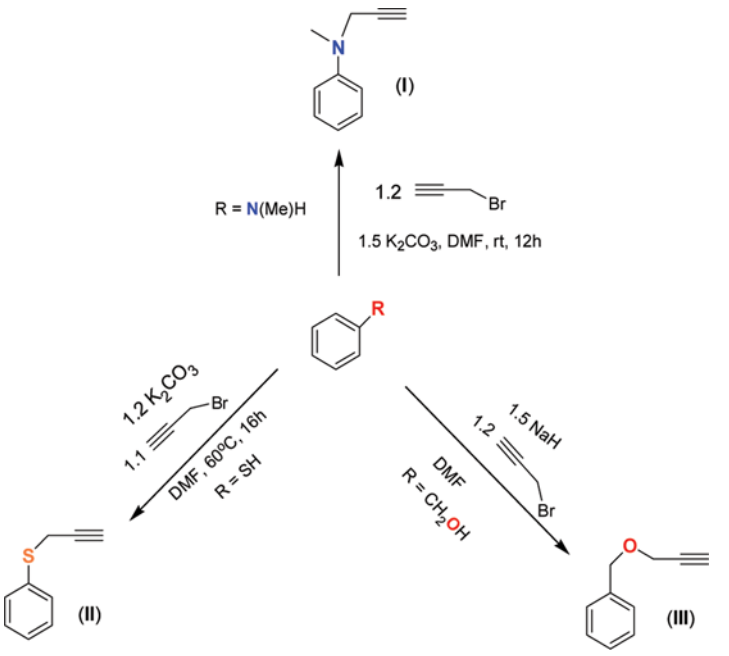
1,2,3-Triazoles and its derivatives have found numerous applications in areas such as agrochemicals, polymers, dyes, materials, and pharmaceuticals.[1] Ever since Sharpless and coworkers' pivotal report[2] on the concept of "click" chemistry, an enormous amount of papers based on copper(I)-catalyzed alkyne–azide cycloaddition (CuAAC) have been published. This metal-catalyzed reaction constitutes a substantial improvement on the classical Huisgen-type thermal 1,3-dipolar cycloaddition,[3] as it allows the regioselective preparation of 1,4-disubstituted 1,2,3-triazoles.[4]

Because of the versatility of the CuAAC methodology, significant progress has been achieved on applying 1,2,3-triazole building blocks as either biologically active motifs in drug discovery[5] or designed functional groups employed in new materials preparation.[6] For instance, the functionalization tolerance of the "click" technique has allowed for the preparation of a wide variety of biological model structures or applications such as DNA labeling,[7] oligonucleotide synthesis,[8] and selective modification of enzymes[9] and cells.[10] Furthermore, the functionalization of 1,2,3-triazoles has been applied to the design of ligands for transition-metal complexes with potential applications in areas such as catalysts, sensors, and light-emitting devices.[11]

Our group has a long-standing interest in the preparation of 1,2,3-triazoles featuring diverse functional groups as they present potential as steel corrosion inhibitors or suitable ligands for transition-metal chemistry. In this regard, we have recently reported the successful synthesis of mono-, bis-, and tris-1,2,3-triazoles supported by hydroxy benzenes moieties featuring a wide variety of structural topologies.[12] As an expansion of that work, we describe herein the use of monopropargylated derivatives supported by aniline, thiophenol, and benzylalcohol scaffolds, which after the "click" reaction conditions render a series of 1,2,3-triazoles featuring oxygen, nitrogen, and sulfur functionalized pendant arms. The modular one-pot synthesis utilizes only 5 mol% of the copper active catalyst system and room-temperature conditions, and permits the incorporation of several electron-donor and electron-attractor groups. Additionally, the scope of the methodology is further expanded by the preparation of bis-1,2,3-triazoles supported by *N,N*-dipropargylated aniline, demonstrating the versatility of the procedure.

RESULTS AND DISCUSSION

The selected approach to install oxygen, sulfur, and nitrogen moieties in the 1,2,3-triazole framework was based in the preparation of monopropargyl derivatives supported by methylaniline, thiophenol, and benzyl alcohol. Monopropargylated methylaniline,[13] and thiophenol,[14] were achieved following the literature procedure through deprotonation of the respective S-H and N-H groups with excess of potassium carbonate in dimethylformamide (DMF) or MeCN, followed by slow addition of equimolar amounts of propargyl bromide (Scheme 1). The propargylation of methylaniline (**I**) proceeds at room temperature under stirring for 12 h, while thiophenol mono-propargyl derivative (**II**) requires heating at 60 °C for half an hour before addition of propargyl bromide. After purification through column chromatography



Scheme 1. Synthesis of monopropargylated derivatives. (Figure is provided in color online.)

on silica gel, the desired products are obtained in 81 and 70% yields, respectively. In the case of benzyl alcohol, deprotonation of the O-H group using K_2CO_3 proved inefficient as the yield of the product was not greater than 45%. In this case, excess of NaH in DMF and addition of excess of propargyl bromide yielded 2-propynyl benzyl ether (**III**) in 76% yield after purification (Scheme 1).

Owing to the fact that 1,4-disubstitued 1,2,3-triazoles prepared through "click" chemistry may be regarded as potential *N*-donor structures, a series of functionalized mono-, bis-, and poly-1,2,3-triazoles have been synthesized during recent years.[15] For instance, a variety of 1(pyridine-2-yl)-1,2,3-triazoles have been prepared by base-promoted substitution between 1,2,3-triazole and 2-halopyridines,[16] or by thermal 1,3-dipolar cyclo-additions[17] and some other multistep procedures.[18] The one-pot preparation of bi- and tridentate pyridil-1,2,3-triazole molecules from their corresponding halides, sodium azide, and alkynes have been reported as well.[19] To a lesser extent, sulfur-linked triazoles have also been prepared. Some examples include heterocycles featuring groups such as sulfonyl, sulfonamides, and 1-sulfamoyl- that have been achieved through multistep preparations[20] and "click" methodologies that permitted the synthesis of novel bis-heterocycles incorporating 2-mercaptobenzothiazoles and 1,2,3-triazoles.[21]

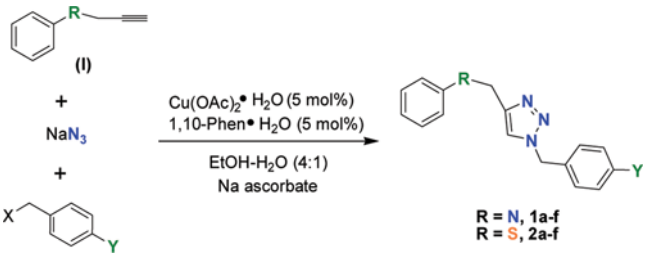
Even though CuAAC has proven the most efficient method for the assembly and functionalization of the triazole motif,[4] some drawbacks related to the instability of the in situ–generated azides or alkynes have decreased the overall process performance, sometimes forcing multistep syntheses. Because we are interested in the development of environmentally friendly processes and the easy functionalization

of the triazole motif, we decided to test the click methodology for the preparation of 1,2,3-triazoles featuring nitrogen and sulfur pendant arms. We hypothesized that by using stable alkyne derivatives, the performance of the process could be enhanced.

Experimentally, the click reaction of alkynes (**I**) and (**II**) with sodium azide in the presence of *p*-substituted benzyl halogenides yields a series of mono-1,2,3--triazoles **1a–f** and **2a–f**, displaying several electron-donor and electron-attractor groups (Table 1). The crude products precipitated out from the reaction mixtures, and after purification by chromatography column on silica gel using mixtures of dichloromethane and methanol, all pure heterocycles presented a white crystalline appearance. As described previously, the catalyst system employed relied on the use of $Cu(OAc)_2 \cdot H_2O$ as the metal source, sodium ascorbate as the reducing agent, and 1,10-phenanthroline to stabilize the Cu(I) active center. Optimal reaction times for both nitrogen and sulfur derivatives ranged between 16 and 18 h, and room-temperature conditions provided good yields in most cases (Table I). Through the series preparation, we noticed that slower reaction rates and yields were obtained when the *p*-methoxy benzylchloride substrate was used.

Triazoles **1a–f** and **2a–f** were fully characterized by ^{1}H and ^{13}C NMR and Fourier transform infrared (FT-IR). In ^{1}H NMR, the triazolyl protons are observed as single sharp peaks in the region of $\delta = 7.18$–7.21 ppm and $\delta = 7.19$–7.36 ppm for nitrogen and sulfur substituted triazoles, respectively. In ^{13}C NMR, the *C*H and quaternary triazole signals show single peaks in the range of $\delta = 120.9$–121.4 and $\delta = 145.6$–146.2 ppm, respectively, for **1a–f**, and peaks in the range of

Table 1. Synthesis of mono-1,2,3-triazoles **1a–f** and **2a–f**



Entry	X	Y	Product	Yield (%)	Product	Yield (%)
1	Cl	H	**1a**	70	**2a**	79
2	Cl	F	**1b**	72	**2b**	75
3	Cl	Cl	**1c**	71	**2c**	81
4	Br	Br	**1d**	77	**2d**	80
5	Br	I	**1e**	83	**2e**	87
6	Cl	OMe	**1f**	63	**2f**	70

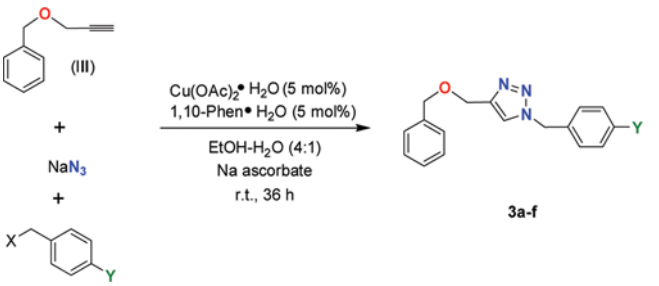
Notes. Reagents and conditions: For *methylaniline*: 1.03 mmol of (**I**), $Cu(OAc)_2 \cdot H_2O$ 5 mol%, 1,10-phenanthroline 5 mol%, sodium ascorbate 1.03 mmol, 1.24 mmol of sodium azide, 1.24 mmol of *p*-substituted benzyl halogenide, stirring at room temperature for 18 h, $EtOH/H_2O$ (4:1). For *thiophenol*: 0.61 mmol of **I**, $Cu(OAc)_2 \cdot H_2O$ 5 mol%, 1,10-phenanthroline monohydrate 5 mol%, sodium L-ascorbate 0.76 mmol, 0.83 mmol of sodium azide, 0.83 mmol of *p*-substituted benzyl halogenide, stirring at room temperature for 16 h, $EtOH/H_2O$ (4:1).

$\delta = 121.7–122.0$ and $\delta = 145.2–145.6$ ppm for **2a–f**. Purity of all compounds was validated by high-resolution mass spectrometry (HRMS) analyses.

Having previously synthesized monotriazoles supported by phenol,[11] we decided to explore the reactivity of 2-propynyl benzyl ether (**III**), as the oxygen atom in this molecule was not directly connected to the aromatic ring. At first glance, when using the same "click" conditions as in the sulfur and nitrogen cases, we noticed that the resulting 1,2,3-triazoles did not precipitate from the reaction mixtures. In all these cases, the products were extracted from the reaction mixtures with dichloromethane and further purified by column chromatography using dichloromethane and ethanol. Overall, the "click" process yielded the desired triazoles **3a–f** in yields ranging from 35 to 59%. Because of the lower yield observed in these series, several optimization trials were performed. While monitoring by thin-layer chromatography (TLC), we noticed that after 24 h of reaction, a considerable amount of starting material was still present. By increasing the reaction time to 36 h (all starting material was consumed) and after purification, triazoles **3a–f** were obtained in greater yields (Table 2). Attempts to improve the process efficiency or reduce reaction times by increasing amount of active catalyst were unsuccessful even with catalyst loads of 10 mol%.

Triazoles **3a–f** were isolated as white waxy solids featuring high solubility in chloroform, dichloromethane, and ethanol. The ^{1}H NMR spectra showed the expected triazolyl protons as single sharp peaks in the range from 7.41 to 7.51 ppm. The *C*H and quaternary carbons presented chemical shifts at 122.1–122.5 and 145.5–145.9 ppm, respectively, all consistent with the formation of the monocyclic structures.

Table 2. Synthesis of 1,2,3-triazoles **3a–f**



Entry	X	Y	Product	Yield (%)
1	Cl	H	**3a**	77
2	Cl	F	**3b**	73
3	Cl	Cl	**3c**	73
4	Br	Br	**3d**	85
5	Br	I	**3e**	79
6	Cl	OMe	**3f**	67

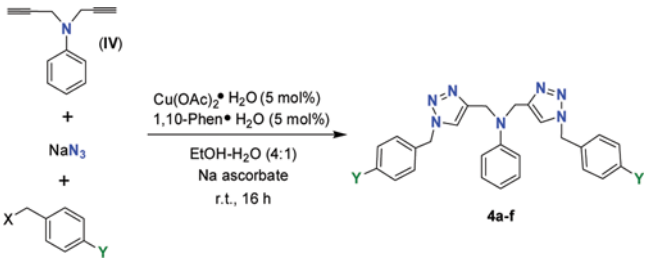
Notes. Reagents and conditions: 0.7 mmol of **III**, $Cu(OAc)_2 \cdot H_2O$ 5 mol%, 1,10-phenanthroline 5 mol%, sodium ascorbate 0.7 mmol, 0.77 mmol of sodium azide, 0.83 mmol of *p*-substituted benzyl halogenide, stirring at room temperature for 36 h, $EtOH/H_2O$ (4:1).

Nitrogen functionalized 1,2,3-triazoles are important scaffolds with application in areas such as biochemistry, materials, and transition-metal chemistry.[22] With the target of extending the scope of the multicomponent one-pot methodology, we envisioned the preparation of a series of bis-triazoles utilizing *N,N*-diprop-2-ynylaniline (**IV**) as precursor. The preparation of this bis-alkyne was accomplished by the addition of propargyl bromide to aniline in the presence of potassium carbonate, according to a literature procedure.[23]

The preparation of bis-1,2,3-triazoles **4a–f** followed similar "click" reaction conditions as those for the monotriazoles, only differing in longer reaction times (24 h). The crude materials precipitate out from the reaction mixture after water addition, and their purification is accomplished through chromatography column on silica gel using a mixture of DCM and methanol as eluent. As depicted in Table 3, the reaction scope permits the installation of several electron attractor and donor groups and provides good yields, employing only 2.5 mol% of the copper catalyst per each triazole formed (5 mol% overall).

Regardless of the complex topology of bis-1,2,3-triazoles **4a–f,** they display excellent solubility in dichloromethane or chloroform and their purification can be performed by column chromatography on silica gel using DCM/MeOH as mobile phase. In solution, the ^{1}H and ^{13}C NMR spectra of **4a–f** feature C_2 symmetry patterns displaying a single sharp peak for the two triazolyl-CH groups in the region of $\delta = 7.24$–7.31 ppm, and singlets for the two nonequivalent series of methylene bridges at $\delta = 3.78$–4.65 ppm (ArCH_2N) and $\delta = 4.60$–5.45 ppm (C-CH_2N). Similarly, a single set of aromatic patterns is displayed in all cases, corroborating the high symmetry of the bis-1,2,3-triazole system (see the experimental section).

Table 3. Synthesis of bis-1,2,3-triazoles **4a–f**



Entry	X	Y	Product	Yield (%)
1	Cl	H	**4a**	72
2	Cl	F	**4b**	73
3	Cl	Cl	**4c**	78
4	Br	Br	**4d**	75
5	Br	I	**4e**	84
6	Cl	OMe	**4f**	65

Notes. Reagents and conditions: 0.59 mmol of **IV**, $Cu(OAc)_2 \cdot H_2O$ 5 mol%, 1,10-phenanthroline 5 mol%, sodium L-ascorbate 0.59 mmol, 1.42 mmol of sodium azide, 1.42 mmol of *p*-substituted benzyl halogenide, stirring at room temperature for 24 h, EtOH/H_2O (4:1).

Besides the wide variety of structural topologies and the rational functionalization, an appealing feature of the synthesized 1,2,3-triazoles is the presence of halogens at the *para* position of the benzylic groups, which carries a reactive position that could be explored in further transformations.

CONCLUSION

In conclusion, we have successfully synthesized a series of 1,2,3-triazoles featuring nitrogen, sulfur, and oxygen functionalized pendant arms utilizing "click" chemistry. The use of stable propargyl derivatives allowed for the easy assembly of 1,2,3-triazoles that feature a wide variety of structural topologies under mild reaction conditions that involved room temperature, reaction periods of 16–36 h, and catalyst loads of 5 mol%. Reactions involving propargylated benzyl alcohol presented slower conversion rates to products, while the use of *p*-methoxy benzyl chloride provided lower yields in all the triazole series. Furthermore, the versatility of the procedure was demonstrated by the straightforward preparation of bis-1,2,3-triazoles constructed over *N,N*-diprop-2-ynylaniline. The potential of the synthetized triazoles as corrosion inhibitors and transition-metal ligands is a focus of current research in our laboratory.

EXPERIMENTAL

Commercially available reagents and solvents were used as received. Alkynes **I**,[13] **II**,[14] **III**,[24] and **IV**[23] were synthesized as reported in the literature. Flash column chromatography was performed on Kieselgel silica gel 60 (230–400 mesh). Melting points were determined on a Fisher-Johns apparatus and are uncorrected. IR spectra were recorded on a Bruker Alpha FT-IR/ATR spectrometer. NMR spectra were obtained with a Jeol ECA-500 (500-MHz) spectrometer. Chemical shifts (δ) are given in parts per million (ppm) downfield from Me_4Si as an internal reference; coupling constants are given in hertz. High-resolution mass spectra (HRMS) were recorded on a Jeol JMS-SX 102a and Agilent-MSD-TOF-1069A 41 spectrometers.

Typical Procedure for the Synthesis of 1,2,3-Triazoles Derived from Methylaniline

To a 20-mL, round-bottomed flask equipped with a magnetic stirrer were charged 11 mg (0.053 mmol, 5 mol%) of $Cu(OAc)_2 \cdot H_2O$, 10 mg (0.053 mmol, 5 mol%) of 1,10-phenanthroline monohydrate, and 204 mg (1.03 mmol) of sodium L-ascorbate. After addition of 7 mL of a mixture of EtOH–H_2O (4:1 *v*/*v*), the resulting suspension was stirred for 5 min at room temperature. Subsequently, 150 mg (1.03 mmol) of **I**, 81 mg (1.24 mmol) of sodium azide, and 0.14 mL (1.24 mmol) of benzyl chloride were added to the reaction mixture, which was stirred for 18 h at room temperature. Then 5 mL of H_2O were added to the reaction mixture and the precipitate was filtered off, washed thoroughly with H_2O and petroleum ether, and dried under vacuum. The crude product was purified by column chromatography (CH_2Cl_2) to afford 200 mg (70% yield) of **3a** as a white solid. Mp = 82–84 °C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 2.96 (s, 3H, NCH_3), 4.61 (s, 2H,

ArCH_2N), 5.45 (s, 2H, NCH_2C=C), 6.72 (t, 7.9 Hz, 1H, CH_{ar}), 6.76 (d, 7.8 Hz, 2H, CH_{ar}), 7.18–7.22 (m, 4H, CH_{ar}), 7.21 (s, 1H, $CH_{triazole}$), 7.33–7.35 (m, 3H, CH_{ar}). ^{13}C NMR ($CDCl_3$, 125.76 MHz): $\delta = 38.5$ (NCH_3), 48.8 (ArCH_2N), 54.1 (NCH_2C=C), 113.0 (CH_{ar}), 117.2 (CH_{ar}), 121.4 ($CH_{triazole}$), 127.8 (CH_{ar}), 128.6 (CH_{ar}), 129.0 (CH_{ar}), 129.2 (CH_{ar}), 134.7 (C_{ar}), 145.9 ($C_{triazole}$), 149.1 (C_{ar}). FT-IR/ATR ν_{max} cm^{-1}: 3124, 3059, 3032, 2944, 2900, 1820, 1726, 1598, 1570. HRMS (ESI-TOF) calculated for $C_{17}H_{18}N_4$ +H$^+$: 279.1610; found: 279.1608.

Typical Procedure for the Synthesis of 1,2,3-Triazoles Derived from Thiophenol

To a 20-mL, round-bottomed flask equipped with a magnetic stirrer were charged 6 mg (0.031 mmol, 5 mol%) of $Cu(OAc)_2 \cdot H_2O$, 6 mg (0.031 mmol, 5 mol%) of 1,10-phenanthroline monohydrate, and 150 mg (0.76 mmol) of sodium L-ascorbate. After addition of 5 mL of a mixture of EtOH–H_2O (4:1 *v*/*v*), the resulting suspension was stirred for 5 min at room temperature. Subsequently, 90 mg (0.61 mmol) of **II**, 54 mg (0.83 mmol) of sodium azide, and 0.09 mL (0.83 mmol) of benzyl chloride were added to the reaction mixture, which was stirred for 16 h at room temperature. Then 5 mL of H_2O were added to the reaction mixture, and the precipitate was filtered off, washed thoroughly with H_2O and petroleum ether, and dried under vacuum. The crude product was purified by column chromatography (CH_2Cl_2–MeOH 99:1 *v*/*v*) to afford 136 mg (79% yield) of **2a** as a white solid. Mp = 71–73 °C. ^{1}H NMR ($CDCl_3$, 500 MHz): $\delta = 4.23$ (s, 2H, ArCH_2N), 5.47 (s, 2H, ArSCH_2), 7.17–7.20 (m, 3H, CH_{ar}), 7.23–7.26 (m, 3H, CH_{ar}), 7.30–7.32 (m, 2H, CH_{ar}), 7.36–7.37 (m. 2H, CH_{ar}), 7.36 (s, 1H, $CH_{triazole}$). ^{13}C NMR ($CDCl_3$, 125.76 MHz): $\delta = 29.1$ (ArCH_2N), 54.1 (ArSCH_2), 122.0 ($CH_{triazole}$), 126.5 (CH_{ar}), 127.9 (CH_{ar}), 128.7 (CH_{ar}), 128.9 (CH_{ar}), 129.1 (CH_{ar}), 129.8 (CH_{ar}), 134.6 (C_{ar}), 135.4 (C_{ar}), 145.5 ($C_{triazole}$). FT-IR/ATR ν_{max} cm^{-1}: 3140, 3073, 3046, 3013, 2986, 2951, 2923, 1956, 1726, 1586, 1553, 1476, 1455. HRMS (ESI-TOF) calculated for $C_{16}H_{15}N_3S$ +H$^+$: 281.0987; found: 282.1058.

Typical Procedure for the Synthesis of Triazoles Derived from Benzyl Alcohol

To a 20-mL, round-bottomed flask equipped with a magnetic stirrer were charged 7 mg (0.035 mmol, 5 mol%) of $Cu(OAc)_2 \cdot H_2O$, 7 mg (0.035 mmol, 5 mol%) of 1,10-phenanthroline monohydrate, and 139 mg (0.70 mmol) of sodium L-ascorbate. After addition of 5 mL of a mixture of EtOH–H_2O (4:1 *v*/*v*), the resulting suspension was stirred for 5 min at room temperature. Subsequently, 103 mg (0.70 mmol) of **I**, 50 mg (0.77 mmol) of sodium azide, and 0.09 mL (0.83 mmol) of benzyl chloride were added to the reaction mixture, which was stirred for 36 h at room temperature. Then 5 mL of H_2O were added to the reaction mixture, and the precipitate was filtered off, washed thoroughly with H_2O and petroleum ether, and dried under vacuum. The crude product was purified by column chromatography (CH_2Cl_2–MeOH 98:2 *v*/*v*) to afford 150 mg (77% yield) of **1a** as a white solid. Mp = 53–55 °C. ^{1}H NMR ($CDCl_3$, 500 MHz): $\delta = 4.58$ (s, 2H, ArCH_2N), 4.65 (s, 2H, C-CH_2O), 5.50 (s, 2H, ArCH_2O), 7.25–7.27 (m, 3H, CH_{ar}), 7.32–7.34 (m, 4H,

CH_{ar}), 7.35–7.37 (m, 3H, CH_{ar}), 7.45 (s, 1H, $CH_{triazole}$). ^{13}C NMR ($CDCl_3$, 125.76 MHz): $\delta = 54.2$ (Ar*C*H_2N), 63.8 (ArO*C*H_2), 72.6 (C-*C*H_2O), 122.5 (*C*$H_{triazole}$), 127.8 (CH_{ar}), 127.9 (CH_{ar}), 128.1 (CH_{ar}), 128.4 (CH_{ar}), 128.7 (CH_{ar}), 129.1 (CH_{ar}), 134.6 (C_{ar}), 137.8(C_{ar}), 145.7 ($C_{triazole}$). FT-IR/ATR ν_{max} cm^{-1}: 3128, 3063, 3031, 2954, 2862, 1495, 1455. HRMS (ESI-TOF) calculated for $C_{17}H_{17}N_3O$ $+H^+$: 280.1450; found: 280.1443.

Typical Procedure for the Synthesis of bis-1,2,3-Triazoles Derived from Dipropargyl Aniline

To a 20-mL, round-bottomed flask equipped with a magnetic stirrer were charged 6 mg (0.030 mmol, 5 mol%) of $Cu(OAc)_2 \cdot H_2O$, 6 mg (0.030 mmol, 5 mol%) of 1,10-phenanthroline monohydrate, and 117 mg (0.59 mmol) of sodium L-ascorbate. After addition of 5 mL of a mixture of EtOH–H_2O (4:1 *v*/*v*), the resulting suspension was stirred for 5 min at room temperature. Subsequently, 100 mg (0.59 mmol) of **IV**, 92 mg (1.42 mmol) of sodium azide, and 0.16 mL (1.42 mmol) of benzyl chloride were added to the reaction mixture, which was stirred during 24 h at room temperature. Then 5 mL of H_2O were added to the reaction mixture, and the precipitate was filtered off, washed thoroughly with H_2O and petroleum ether, and dried under vacuum. The crude product was purified by column chromatography (CH_2Cl_2–MeOH 98:2 *v*/*v*) to afford 185 mg (72% yield) of **4a** as a white solid. Mp = 146–148 °C. ^1H NMR ($CDCl_3$, 500 MHz): $\delta = 4.65$ (s, 4H, ArC*H*$_2$N), 5.45 (s, 4H, NC*H*$_2$C=C), 6.75 (t, 7.9 Hz, 1H, CH_{ar}), 6.85 (d, 7.8 Hz, 2H, CH_{ar}), 7.18–7.20 (m, 3H, CH_{ar}), 7.21–7.22 (m. 3H, CH_{ar}), 7.31 (s, 2H, $CH_{triazole}$), 7.34–7.36 (m, 4H, CH_{ar}), 7.37–7.38 (m, 2H, CH_{ar}). ^{13}C NMR ($CDCl_3$, 125.76 MHz): $\delta = 46.9$ (Ar*C*H_2N), 54.1 (N*C*H_2C=C), 113.7 (CH_{ar}), 117.8 (CH_{ar}), 121.9 (*C*$H_{triazole}$), 127.8 (CH_{ar}), 128.7 (CH_{ar}), 129.0 (CH_{ar}), 129.3 (CH_{ar}), 134.7 (C_{ar}), 145.8 ($C_{triazole}$), 147.9 (C_{ar}). FT-IR/ATR ν_{max} cm^{-1}: 3116, 3066, 3027, 3003, 3027, 3003, 2960, 2894, 1719, 1597, 1503. HRMS (ESI-TOF) calculated for $C_{26}H_{25}N_7$ $+H^+$: 436.2250; found: 436.2247.

SUPPORTING INFORMATION

Full experimental detail and ^1H and ^{13}C NMR spectra can be found via the Supplementary Content section of this article's Web page.

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