Synthesis of [(Arylselanyl)alkyl]-1,2,3-triazoles by Copper-Catalyzed 1,3-Dipolar Cycloaddition of (Arylselanyl)alkynes with Benzyl Azides

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Abstract: In the presence of catalytic amounts of copper salts and sodium ascorbate, various (arylselanyl)alkynes underwent click-type 1,3-dipolar cycloaddition reactions with a range of benzyl azides bearing electron-withdrawing or electron-donating groups to give a series of novel [(arylselanyl)alkyl]-1,2,3-triazoles. This click chemistry protocol is an efficient method for synthesizing new selenium–nitrogen compounds that are potentially useful in biological studies.

Key words: heterocycles, azides, alkynes, click reactions, selenium, cycloadditions, catalysis, copper

The versatility and usefulness of organoselenium compounds in organic chemistry is well described in many reviews[1] and books.[2] Organoselenium compounds are attractive synthetic targets because of their use as ionic liquids,[3] their applications in asymmetric catalysis,[1b,e,4] their fluorescence properties,[5] and their interesting biological activities.[6] Nitrogen-containing organoselenium compounds form a particular class of molecules that have been used in various organic transformations, particularly in asymmetric synthesis.[1b,e,4] Consequently, the search for new and efficient protocols for the synthesis of nitrogen-functionalized organoselenium compounds, especially selenium-containing heterocycles, remains an interesting challenge in organic chemistry.

Functionalized 1,2,3-triazoles are an important category of molecules that display a wide spectrum of biological activities[7] and that are widely used in various fields of chemistry, for example, in the discovery and modulation of drug candidates,[8] in the development of new materials,[9] and in the design of new catalysts,[10] among others.[11] Various methods are available for the preparation of 1,2,3-triazoles, the most attractive of which involves a thermal 1,3-dipolar cycloaddition of an azide with an alkyne. This reaction was pioneered by Huisgen[12] and was popularized, independently, by Sharpless[13] and by Meldal,[14] who discovered a copper-catalyzed protocol for the reaction. The development of the copper-catalyzed azide–alkyne cycloaddition (CuAAC) represents a definitive advance in triazole synthesis and is the most effective reaction of the type known as click chemistry.[15] There remains, however, a need for an in-depth study of various combinations of substrates for the synthesis of more highly functionalized and complex 1,2,3-triazoles. Although sulfur-functionalized 1,2,3-triazoles have been synthesized in high yields by CuAAC reactions of alkynyl sulfides as the alkyne precursors,[16] the use of alkynyl selenides as substrates in CuAAC-based syntheses of selenium-containing 1,2,3-triazoles has not been previously described. Alkynyl selenides have, however, been widely used in many reactions, such as syntheses of functionalized heterocycles[17] or alkenes.[18]

Many selenium-containing 1,2,3-triazoles have been synthesized[17a,19] and, very recently, a CuAAC protocol was reported for the synthesis of arylseleno-1,2,3-triazoles in excellent yields under mild conditions from the corresponding azido aryl selenides.[19c] However, few methods based on CuAAC have been reported for the synthesis of organoselenium-functionalized triazoles and this type of reaction has not been explored in detail. With this background, and with our interest in applying the CuAAC protocol for the synthesis of organoselenium-functionalized triazoles, we examined the copper-catalyzed 1,3-dipolar cycloaddition reactions of alkynylselenium compounds **1** with benzyl azides **2** to give the corresponding [(arylselanyl)alkyl]-1,2,3-triazoles **3** (Scheme 1).

The normal experimental procedures for reactions of this type require the generation in situ of copper(I) species from copper(II) sulfate pentahydrate and sodium ascorbate in a 1:2 mixture of *tert*-butyl alcohol and water.[13a] For this reason, we began by studying the reaction of (prop-2-yn-1-ylselanyl)benzene (**1a**; 0.3 mmol) with benzyl azide (**2a**; 0.3 mmol) in the presence of copper(II) sulfate pentahydrate (1 mol%) and sodium ascorbate (2 mol%) in 1:2 *tert*-butyl alcohol–water at room temperature. Under these standard conditions, the desired 1,2,3-triazole **3a** was obtained in 35% yield after 12 hours (Table 1; entry 1). In an attempt to improve the yield of product **3a**, we examined the effects of various copper salts and solvent systems on the reaction of alkyne **1a**, azide **2a**, and sodium ascorbate under air for 12 hours (Table 1). We obtained triazole **3a** in 89% by using 3 mol% of copper(II) acetate monohydrate in a 1:1 mixture of *tert*-butyl alcohol

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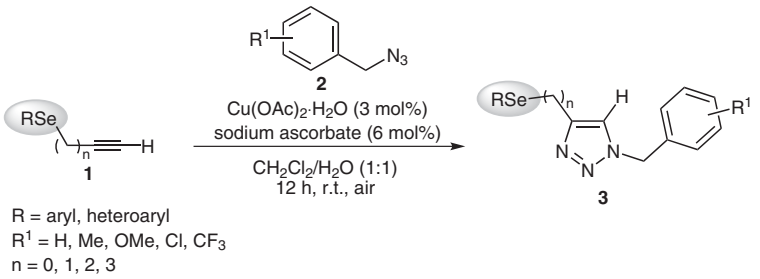
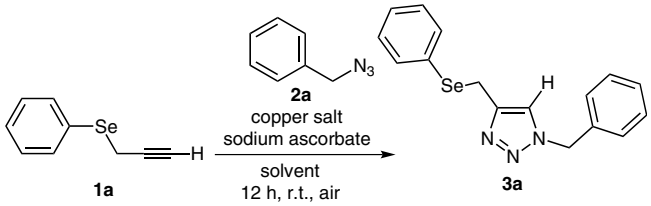


Scheme 1 General scheme for the reaction

and water (entry 5), and when we used the same catalyst in a 1:1 mixture of dichloromethane and water,[20] we obtained triazole **3a** in 94% yield (entry 7).

Table 1 Optimization of the Conditions for the Reaction of Alkyne **1a** and Azide **2a**



Entry[a]	Catalyst (mol%)	Solvent	Yield (%)
1	$CuSO_4·5H_2O$ (1%)	*t*-BuOH–H_2O (1:2)	35
2	$CuSO_4·5H_2O$ (1%)	*t*-BuOH–H_2O (1:1)	55
3[b]	$CuSO_4·5H_2O$ (3%)	*t*-BuOH–H_2O (1:1)	64
4[b]	$Cu(OTf)_2$ (3%)	*t*-BuOH–H_2O (1:1)	51
5[b]	$Cu(OAc)_2·H_2O$ (3%)	*t*-BuOH–H_2O (1:1)	89
6[b]	$Cu(OAc)_2·H_2O$ (3%)	THF–H_2O (1:1)	70
7[b]	$Cu(OAc)_2·H_2O$ (3%)	CH_2Cl_2–H_2O (1:1)	94
8	$Cu(OAc)_2·H_2O$ (1%)	CH_2Cl_2–H_2O (1:1)	75

[a] Reaction conditions: alkyne **1a** (0.3 mmol), BnN_3 (**2a**; 0.3 mmol), sodium ascorbate (2 mol%), mixed solvent (2 mL), r.t., under air, 12 h.
[b] 6 mol% of sodium ascorbate was used.

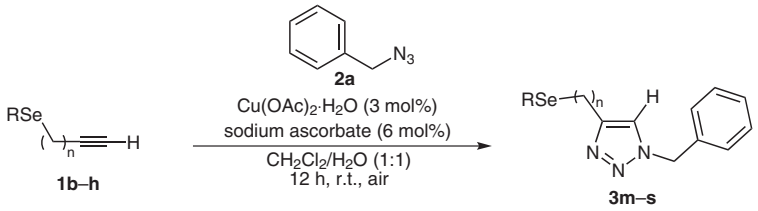
An analysis of our results indicated that the best yield of product **3a** was obtained in the presence of copper(II) acetate (3 mol%) and sodium ascorbate (6 mol%) in a 1:1 mixture of dichloromethane and water at room temperature under air for 12 hours. To extend the scope of the reaction of (prop-2-yn-1-ylselanyl)benzene (**1a)** as a precursor of triazoles, we examined its reactions with several substituted benzyl azides under the optimized reaction conditions (Table 2). We found that our protocol worked well for a wide variety of substituted benzylic and alkyl azides, giving excellent yields of the desired triazoles.

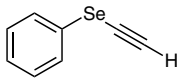
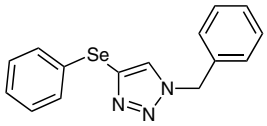
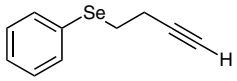
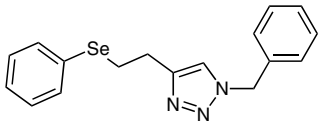
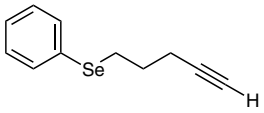
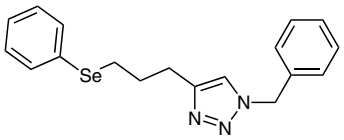
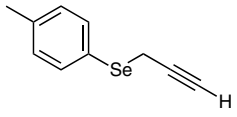
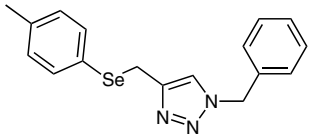
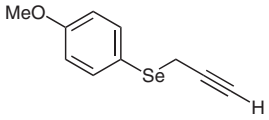
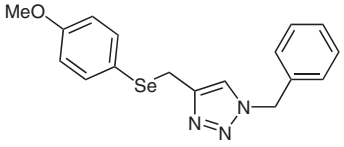
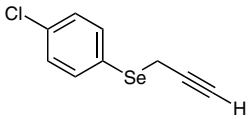
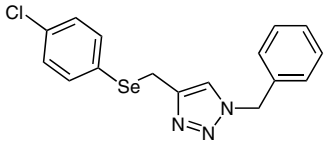
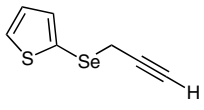
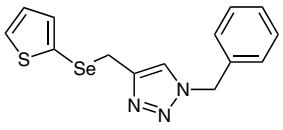
In general, the reactions were insensitive to electronic effects in the aromatic ring of the azide partner. Benzylic azides containing electron-donating groups (Me or OMe) or electron-withdrawing groups (Cl or CF_3) on the aromatic ring gave excellent yields of the corresponding triazoles **3b**–**h** (Table 2, entries 2–8). When the reaction was performed with 2-(azidomethyl)naphthalene (**2i**), the corresponding product **3i** was obtained in 86% yield (entry 9). Furthermore, selenide **1a** reacted smoothly with azidomethyl phenyl selenide (**2j**) to give 1,4-bis[(phenylselanyl)methyl]-1*H*-1,2,3-triazole (**3j**) in 80% yield (entry 10). Octyl azide and dodecyl azide also reacted efficiently with selenide **1a** to give good yields of the corresponding triazoles **3k** and **3l** (entries 11 and 12).

We also examined the possibility of performing the reaction with benzyl azide (**2a**) and various alkynes (Table 3). (Ethynylselanyl)benzene (**1b**) reacted efficiently with azide **2a** to give triazole **3m** in 84% yield (Table 3; entry 1). When the reaction was performed with the homopropargylic selenide **1c** or its homologue **1d**, the corresponding products **3n** and **3o** were each obtained in 90% yield (entries 2 and 3). High yields of the substituted [(arylselanyl)methyl]-1,2,3-triazoles **3p**–**s** were obtained from the corresponding substituted aryl propargyl selenides **1e**–**h** (entries 4–7).

In conclusion, we have demonstrated that (arylselanyl)alkynes undergo a copper-catalyzed 1,3-dipolar click cycloaddition reaction with benzyl azides to give a novel series of arylselanyl-containing 1,2,3-triazoles selectively and in high yields under mild conditions. This atom-economic method provides an efficient way of synthesizing new selenium-containing triazoles, the biological proprieties of which we are currently evaluating.

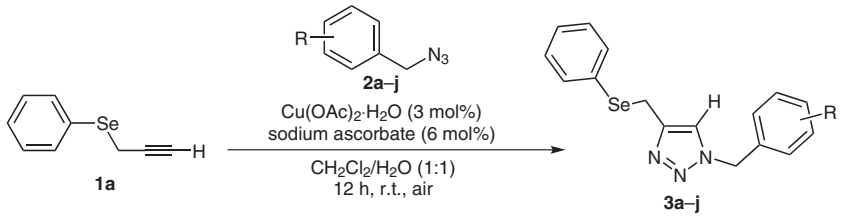
Table 3 Syntheses of Triazoles **3m–s**



Entry	Alkyne	Product (yield)
1[a]	 **1b**	 **3m** (84%)
2	 **1c**	 **3n** (90%)
3	 **1d**	 **3o** (90%)
4	 **1e**	 **3p** (88%)
5	 **1f**	 **3q** (89%)
6	 **1g**	 **3r** (85%)
7	 **1h**	 **3s** (81%)

[a] Reaction conditions: alkynes **1a–h** (0.3 mmol), BnN_3 (**2a**; 0.3 mmol), $Cu(OAc)_2·H_2O$ (3 mol%), sodium ascorbate (6 mol%), (1:1) CH_2Cl_2/H_2O (2 mL), r.t., under air, 12 h.

Table 2 Syntheses of 1-Benzyl-4-(phenylselanylmethyl)-1*H*-1,2,3-triazoles **3a–j**



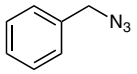
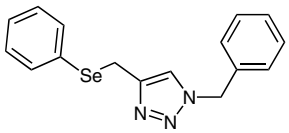
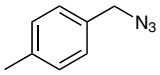
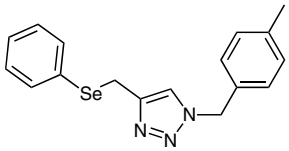
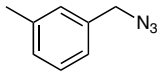
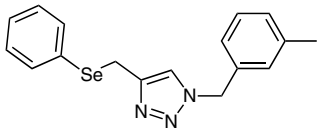
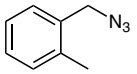
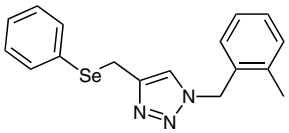
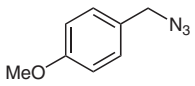
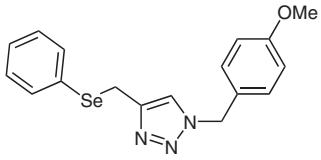
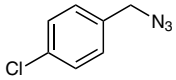
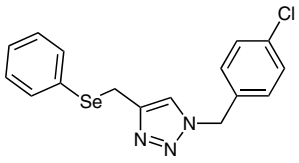
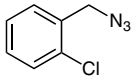
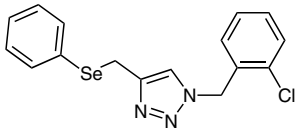
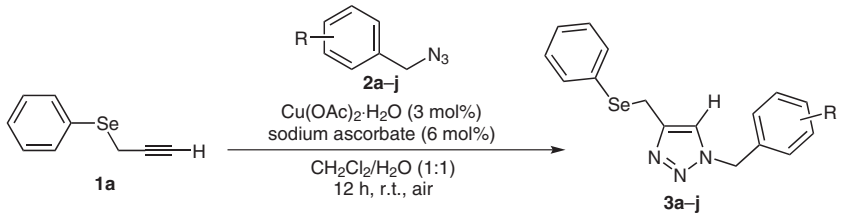
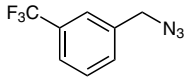
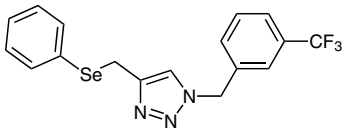
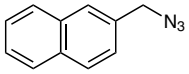
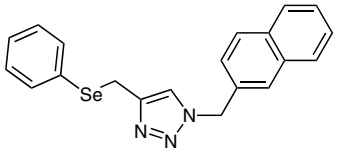
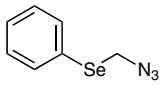
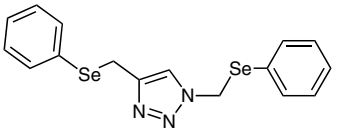
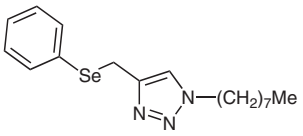
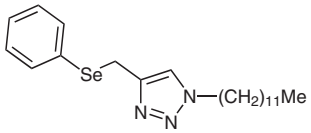
Entry[a]	Azide	Product (yield)
1[b]	 **2a**	 **3a** (94%)
2	 **2b**	 **3b** (96%)
3	 **2c**	 **3c** (94%)
4	 **2d**	 **3d** (91%)
5	 **2e**	 **3e** (95%)
6	 **2f**	 **3f** (92%)
7	 **2g**	 **3g** (91%)

Table 2 Syntheses of 1-Benzyl-4-(phenylselanylmethyl)-1*H*-1,2,3-triazoles **3a–j** (continued)



Entry[a]	Azide	Product (yield)
8	 **2h**	 **3h** (85%)
9	 **2i**	 **3i** (86%)
10	 **2j**	 **3j** (80%)
11	$Me(CH_2)_7N_3$ **2k**	 **3k** (77%)
12	$Me(CH_2)_{11}N_3$ **2l**	 **3l** (74%)

[a] Reaction conditions: alkyne **1a** (0.3 mmol), azide **2a–l** (0.3 mmol), $Cu(OAc)_2·H_2O$ (3 mol%), sodium ascorbate (6 mol%), 1:1 CH_2Cl_2–H_2O (2 mL), r.t., under air, 12 h.
[b] At the 5-mmol scale, this reaction gave **3a** in 90% yield.

^1H NMR spectra were recorded in $CDCl_3$ at 400 MHz on a Bruker DPX-400 NMR spectrometer. Chemical shifts are reported in ppm relative to TMS as an external standard. ^{13}C NMR spectra were recorded in $CDCl_3$ at 100 MHz on a Bruker DPX-400 NMR spectrometer. Chemical shifts are reported in ppm relative to the solvent peak of $CDCl_3$. Mass spectra were recorded on a Shimadzu GCMS-QP2010 mass spectrometer. Column chromatography was performed on Merck silica gel (230–400 mesh). TLC was performed on Merck silica gel GF_{254} (0.25 mm thickness) and the plates were visualized by UV radiation or by staining with I_2 vapor or acidic vanillin. All solvents were used as purchased unless otherwise noted. Arylselanyl alkynes[17b,21] and organic azides[22] were prepared according to the methods reported in the literature.

4-[(Arylselanyl)alkyl]-1-benzyl-1,2,3-triazoles 3a–s; General Method

Azide **2** (0.3 mmol) and H_2O (0.5 mL) were added to a soln of alkyne **1** (0.3 mmol) in CH_2Cl_2 (1.0 mL). A fresh soln of sodium ascorbate (6 mol%) and $Cu(OAc)_2·H_2O$ (3 mol%) in H_2O (0.5 mL) was added and the mixture was stirred under air for 12 h. Brine (3 mL) was then added and the mixture was extracted with CH_2Cl_2 (3 × 5 mL). The organic layers were combined, washed with brine (3 mL), and dried ($MgSO_4$). The solvent was removed under vacuum and the product was isolated by column chromatography (silica gel, hexane–EtOAc).

1-Benzyl-4-[(phenylselanyl)methyl]-1*H*-1,2,3-triazole (3a)

Yield: 0.093 g (94%); pale yellow solid; mp 35–36 °C.

^1H NMR (400 MHz, $CDCl_3$): δ = 7.42–7.40 (m, 2 H), 7.36–7.32 (m, 3 H), 7.20–7.14 (m, 5 H), 7.08 (s, 1 H), 5.41 (s, 2 H), 4.12 (s, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.88, 134.63, 133.43, 129.65, 128.98 (2 C), 128.59, 127.87, 127.35, 121.64, 53.99, 20.66.

MS: *m/z* (%) = 329 (7), 157 (3), 144 (38), 117 (8), 104 (10), 91 (100), 77 (10), 65 (13).

Anal. Calcd for $C_{16}H_{15}N_3Se$: C, 58.54; H, 4.61; N, 12.80. Found: C, 58.94; H, 4.59; N, 12.54.

1-(4-Methylbenzyl)-4-[(phenylselanyl)methyl]-1*H*-1,2,3-triazole (3b)
Yield: 0.099 g (96%); white solid; mp 43–44 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.42–7.40 (m, 2 H), 7.19–7.12 (m, 5 H), 7.07–7.05 (m, 3 H), 5.35 (s, 2 H), 4.11 (s, 2 H), 2.33 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.82, 138.51, 133.43, 131.75, 129.65, 129.67, 128.97, 127.96, 127.29, 121.53, 53.85, 20.99, 20.74.

MS: *m/z* (%) = 343 (10), 341 (5), 158 (35), 105 (100), 79 (9), 77 (13), 51 (3), 43 (2).

Anal. Calcd for $C_{17}H_{17}N_3Se$: C, 59.65; H, 5.01; N, 12.28. Found: C, 59.90; H, 5.03; N, 12.17.

1-(3-Methylbenzyl)-4-[(phenylselanyl)methyl]-1*H*-1,2,3-triazole (3c)
Yield: 0.097 g (94%); white solid; mp 41–43 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.42–7.40 (m, 2 H), 7.26–7.14 (m, 5 H), 7.08 (s, 1 H), 7.00 (s, 1 H), 6.97 (d, *J* = 7.5 Hz, 1 H), 5.37 (s, 2 H), 4.13 (s, 2 H), 2.33 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.79, 138.79, 134.49, 133.36, 129.69, 129.33, 128.96, 128.86, 128.61, 127.31, 124.96, 121.62, 53.99, 21.23, 20.67.

MS: *m/z* (%) = 343 (11), 341 (6), 158 (46), 143 (7), 131 (6), 106 (9), 105 (100), 91 (9), 79 (12), 77 (16).

Anal. Calcd for $C_{17}H_{17}N_3Se$: C, 59.65; H, 5.01; N, 12.28. Found: C, 59.54; H, 5.18; N, 12.58.

1-(2-Methylbenzyl)-4-[(phenylselanyl)methyl]-1*H*-1,2,3-triazole (3d)
Yield: 0.094 g (91%); white solid; mp 32–34 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.41–7.39 (m, 2 H), 7.28–7.25 (m, 1 H), 7.20–7.14 (m, 5 H), 7.02 (d, *J* = 7.6 Hz, 1 H), 6.95 (s, 1 H), 5.41 (s, 2 H), 4.11 (s, 2 H), 2.20 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.61, 136.73, 133.39, 132.45, 130.89, 129.62, 129.20, 128.95 (2 C), 127.32, 126.52, 121.44, 52.17, 20.66, 18.81.

MS: *m/z* (%) = 343 (10), 341 (5), 158 (39), 118 (8), 105 (100), 91 (7), 79 (12), 77 (16), 65 (3), 51 (4).

Anal. Calcd for $C_{17}H_{17}N_3Se$: C, 59.65; H, 5.01; N, 12.28. Found: C, 59.62; H, 5.21; N, 12.34.

1-(4-Methoxybenzyl)-4-[(phenylselanyl)methyl]-1*H*-1,2,3-triazole (3e)
Yield: 0.102 g (95%); white solid; mp 61–63 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.42–7.40 (m, 2 H), 7.21–7.15 (m, 3 H), 7.13 (d, *J* = 8.6 Hz, 2 H), 7.05 (s, 1 H), 6.87 (d, *J* = 8.6 Hz, 2 H), 5.35 (s, 2 H), 4.12 (s, 2 H), 3.80 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.88, 145.75, 133.37, 129.76, 129.46, 128.99, 127.32, 126.62, 121.42, 114.42, 55.30, 53.56, 20.69.

MS: *m/z* (%) = 359 (4), 174 (11), 121 (100), 91 (5), 78 (6), 77 (9), 65 (2), 57 (3), 43 (4).

Anal. Calcd for $C_{17}H_{17}N_3OSe$: C, 56.99; H, 4.78; N, 11.73. Found: C, 56.98; H, 5.18; N, 11.79.

1-(4-Chlorobenzyl)-4-[(phenylselanyl)methyl]-1*H*-1,2,3-triazole (3f)
Yield: 0.100 g (92%); pale gray solid; mp 43–44 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.41–7.40 (m, 2 H), 7.29 (d, *J* = 8.2 Hz, 2 H), 7.20–7.15 (m, 3 H), 7.09–7.07 (m, 3 H), 5.36 (s, 2 H), 4.12 (s, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 146.00, 134.60, 133.32, 133.17, 129.61, 129.13 (2C), 128.94, 127.31, 121.60, 53.15, 20.49.

MS: *m/z* (%) = 365 (6), 363 (13), 180 (12), 178 (34), 157 (5), 143 (16), 127 (33), 125 (100), 115 (9), 89 (16), 85 (9), 77 (10), 57 (17).

Anal. Calcd for $C_{16}H_{14}ClN_3Se$: C, 52.98; H, 3.89; N, 11.58. Found: C, 52.36; H, 3.96; N, 11.80.

1-(2-Chlorobenzyl)-4-[(phenylselanyl)methyl]-1*H*-1,2,3-triazole (3g)
Yield: 0.099 g (91%); pale gray solid; mp 41–43 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.44–7.39 (m, 3 H), 7.30–7.17 (m, 6 H), 7.06 (d, *J* = 7.3 Hz, 1 H), 5.55 (s, 2 H), 4.14 (s, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.90, 133.53, 133.43, 132.59, 130.17, 130.06, 129.85, 129.76, 129.00, 127.50, 127.39, 121.96, 51.26, 20.67.

MS: *m/z* (%) = 365 (6), 363 (14), 180 (15), 178 (45), 157 (6), 143 (18), 127 (32), 125 (100), 115 (12), 89 (19), 77 (11).

Anal. Calcd for $C_{16}H_{14}ClN_3Se$: C, 52.98; H, 3.89; N, 11.58. Found: C, 52.96; H, 3.69; N, 11.52.

4-[(Phenylselanyl)methyl]-1-[3-(trifluoromethyl)benzyl]-1*H*-1,2,3-triazole (3h)
Yield: 0.101 g (85%); white solid; mp 58–60 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.62 (d, *J* = 7.8 Hz, 1 H), 7.52–7.32 (m, 5 H), 7.22–7.13 (m, 3 H), 7.10 (s, 1 H), 5.48 (s, 2 H), 4.15 (s, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 146.33, 135.71, 133.48, 131.49 (q, *J* = 32.5 Hz), 131.15, 129.67, 129.51, 129.01, 127.46, 125.53 (q, *J* = 3.7 Hz), 124.57 (q, *J* = 3.7 Hz), 123.66 (q, *J* = 272.5 Hz), 121.68, 53.37, 20.54.

MS: *m/z* (%) = 397 (19), 395 (10), 212 (62), 172 (22), 159 (100), 119 (6), 109 (19), 77 (13), 66 (1), 51 (5), 41 (3).

Anal. Calcd for $C_{17}H_{14}F_3N_3Se$: C, 51.53; H, 3.56; N, 10.60. Found: C, 51.49; H, 3.97; N, 11.32.

1-(2-Naphthylmethyl)-4-[(phenylselanyl)methyl]-1*H*-1,2,3-triazole (3i)
Yield: 0.098 g (86%); pale yellow solid; mp 82–84 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.91–7.86 (m, 3 H), 7.53–7.47 (m, 2 H), 7.42 (dd, *J* = 8.2, 7.1 Hz, 1 H), 7.30–7.28 (m, 3 H), 7.11–7.07 (m, 1 H), 7.03–7.01 (m, 2 H), 6.91 (s, 1 H), 5.85 (s, 2 H), 4.05 (s, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.73, 133.98, 133.53, 131.21, 129.93, 129.86, 129.59, 128.86, 128.84, 127.62, 127.28, 127.20, 126.34, 125.26, 122.83, 121.58, 52.14, 20.74.

MS: *m/z* (%) = 380 (3), 379 (11), 377 (6), 194 (29), 141 (100), 115 (19), 77 (4), 66 (2), 51 (2).

Anal. Calcd for $C_{20}H_{17}N_3Se$: C, 63.49; H, 4.53; N, 11.11. Found: C, 63.07; H, 4.51; N, 10.85.

1,4-Bis[(phenylselanyl)methyl]-1*H*-1,2,3-triazole (3j)
Yield: 0.098 g (80%); pale yellow solid; mp 45–47 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.46–7.43 (m, 2 H), 7.41–7.38 (m, 2 H), 7.33–7.29 (m, 1 H), 7.26–7.21 (m, 5 H), 7.19 (s, 1 H), 5.57 (s, 2 H), 4.11 (s, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 146.24, 134.57, 133.10, 129.95, 129.51, 129.09, 128.80, 127.47, 127.32, 121.55, 44.50, 20.50.

MS: *m/z* (%) = 410 (7), 409 (22), 408 (5), 407 (21), 224 (16), 197 (12), 195 (40), 171 (15), 157 (88), 155 (46), 144 (28), 143 (28), 116 (30), 115 (33), 91 (69), 77 (61), 67 (66), 66 (100), 65 (12), 51 (23), 41 (29).

Anal. Calcd for $C_{16}H_{15}N_3Se_2$: C, 47.19; H, 3.71; N, 10.32. Found: C, 46.83; H, 3.57; N, 10.48.

1-Octyl-4-[(phenylselanyl)methyl]-1*H*-1,2,3-triazole (3k)
Yield: 0.081 g (77%); white solid; mp 40–42 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.49–7.46 (m, 2 H), 7.26–7.24 (m, 3 H), 7.17 (s, 1 H), 4.24 (t, *J* = 7.2 Hz, 2 H), 4.17 (s, 2 H), 1.81 (quin, *J* = 7.2 Hz, 2 H), 1.31–1.26 (m, 10 H), 0.88 (t, *J* = 7.2 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.14, 132.97, 129.63, 128.75, 127.04, 121.18, 49.95, 31.36, 29.90, 28.68, 28.60, 26.09, 22.25, 20.37, 13.69.

MS: *m/z* (%) = 352 (28), 351 (62), 349 (35), 166 (100), 157 (22), 155 (12), 126 (11), 110 (10).

Anal. Calcd for $C_{17}H_{25}N_3Se$: C, 58.28; H, 7.19; N, 11.99. Found: C, 58.93; H, 7.55; N, 12.19.

1-Dodecyl-4-[(phenylselanyl)methyl]-1*H*-1,2,3-triazole (3l)
Yield: 0.091 g (74%); white solid; mp 52–53 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.49–7.46 (m, 2 H), 7.26–7.24 (m, 3 H), 7.17 (s, 1 H), 4.24 (t, *J* = 7.2 Hz, 2 H), 4.17 (s, 2 H), 1.81 (quin, *J* = 7.2 Hz, 2 H), 1.32–1.26 (m, 18 H), 0.88 (t, *J* = 7.2 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.46, 133.30, 129.96, 129.08, 127.36, 121.51, 50.28, 31.89, 30.23, 29.58 (2 C), 29.50, 29.36, 29.31, 28.97, 26.43, 22.66, 20.70, 14.07.

MS: *m/z* (%) = 407 (39), 406 (16), 405 (24), 182 (6), 223 (17), 222 (100), 158 (10), 157 (16), 110 (12).

Anal. Calcd for $C_{21}H_{33}N_3Se$: C, 62.05; H, 8.18; N, 10.34. Found: C, 62.22; H, 8.27; N, 10.34.

1-Benzyl-4-(phenylselanyl)-1*H*-1,2,3-triazole (3m)
Yield: 0.079 g (84%); yellow solid; mp 56–58 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.52 (s, 1 H), 7.44–7.41 (m, 2 H), 7.36–7.32 (m, 3 H), 7.25–7.22 (m, 2 H), 7.20–7.17 (m, 3 H), 5.50 (s, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 134.39, 132.71, 131.59, 130.70, 129.22, 129.17, 128.86, 128.26, 128.09, 127.21, 54.34.

MS: *m/z* (%) = 315 (8), 286 (23), 284 (13), 206 (14), 169 (13), 130 (29), 103 (20), 91 (100), 77 (21), 65 (27), 51 (13).

Anal. Calcd for $C_{15}H_{13}N_3Se$: C, 57.33; H, 4.17; N, 13.37. Found: C, 57.58; H, 4.26; N, 13.19.

1-Benzyl-4-[2-(phenylselanyl)ethyl]-1*H*-1,2,3-triazole (3n)
Yield: 0.093 g (90%); white solid; mp 64–65 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.46–7.44 (m, 2 H), 7.37–7.32 (m, 3 H), 7.23–7.20 (m, 6 H), 5.45 (s, 2 H), 3.18 (t, *J* = 7.4 Hz, 2 H), 3.08 (t, *J* = 7.4 Hz, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 146.97, 134.78, 132.70, 129.69, 128.99, 128.97, 128.54, 127.87, 126.88, 121.01, 53.91, 26.72, 26.63.

MS: *m/z* (%) = 343 (6), 263 (8), 262 (38), 91 (100), 83 (6), 83 (6), 71 (11), 65 (11), 57 (8), 43 (9).

Anal. Calcd for $C_{17}H_{17}N_3Se$: C, 59.65; H, 5.01; N, 12.28. Found: C, 58.96; H, 4.60; N, 12.68.

1-Benzyl-4-[3-(phenylselanyl)propyl]-1*H*-1,2,3-triazole (3o)
Yield: 0.096 g (90%); white solid; mp 69–70 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.48–7.43 (m, 2 H), 7.40–7.33 (m, 3 H), 7.26–7.20 (m, 5 H), 7.12 (s, 1 H), 5.47 (s, 2 H), 2.92 (t, *J* = 7.4 Hz, 2 H), 2.81 (t, *J* = 7.4 Hz, 2 H), 2.05 (quin, *J* = 7.4 Hz, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 147.41, 134.81, 132.52, 130.09, 129.03, 128.99, 128.61, 127.92, 126.74, 120.76, 53.95, 29.61, 27.04, 25.46.

MS: *m/z* (%) = 357 (5), 200 (25), 173 (21), 91 (100), 77 (5), 65 (9), 53 (3).

Anal. Calcd for $C_{18}H_{19}N_3Se$: C, 60.67; H, 5.37; N, 11.79. Found: C, 60.99; H, 5.73; N, 11.95.

1-Benzyl-4-[(4-tolylselanyl)methyl]-1*H*-1,2,3-triazole (3p)
Yield: 0.091 g (88%); pale yellow solid; mp 65–67 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.35–7.16 (m, 7 H), 7.04–6.95 (m, 3 H), 5.42 (s, 2 H), 4.08 (s, 2 H), 2.29 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.97, 137.47, 134.63, 133.93, 129.77, 128.95, 128.56, 127.86, 125.72, 121.60, 53.95, 21.02, 20.91.

MS: *m/z* (%) = 343 (9), 172 (5), 144 (37), 117 (9), 92 (11), 91 (100), 85 (13), 71 (20), 57 (27).

Anal. Calcd for $C_{17}H_{17}N_3Se$: C, 59.65; H, 5.01; N, 12.28. Found: C, 59.31; H, 5.65; N, 12.40.

1-Benzyl-4-{[(4-methoxyphenyl)selanyl]methyl}-1*H*-1,2,3-triazole (3q)
Yield: 0.096 g (89%); white solid; mp 70–72 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.37–7.29 (m, 5 H), 7.19–7.15 (m, 2 H), 7.00 (s, 1 H), 6.69 (d, *J* = 8.7 Hz, 2 H), 5.42 (s, 2 H), 4.03 (s, 2 H), 3.75 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.54, 145.90, 136.30, 134.63, 128.90, 128.50, 127.79, 121.52, 119.31, 114.61, 55.11, 53.87, 21.43.

MS: *m/z* (%) = 359 (15), 149 (17), 144 (46), 127 (10), 108 (13), 97 (15), 91 (100), 83 (16), 77 (6), 57 (66).

Anal. Calcd for $C_{17}H_{17}N_3OSe$: C, 56.99; H, 4.78; N, 11.73. Found: C, 56.56; H, 5.69; N, 11.69.

1-Benzyl-4-{[(4-chlorophenyl)selanyl]methyl}-1*H*-1,2,3-triazole (3r)
Yield: 0.093 g (85%); white solid; mp 68–70 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.39–7.30 (m, 5 H), 7.21–7.10 (m, 4 H), 7.07 (s, 1 H), 5.44 (s, 2 H), 4.11 (s, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.57, 135.01, 134.49, 133.77, 129.16, 129.08, 128.75, 127.94, 127.52, 121.60, 54.08, 20.92.

MS: *m/z* (%) = 365 (3), 363 (8), 144 (54), 117 (9), 104 (10), 91 (100), 77 (4), 65 (11).

Anal. Calcd for $C_{16}H_{14}ClN_3Se$: C, 52.98; H, 3.89; N, 11.58. Found: C, 53.50; H, 3.94; N, 11.81.

1-Benzyl-4-[(2-thienylselanyl)methyl]-1*H*-1,2,3-triazole (3s)
Yield: 0.081 g (81%); pale yellow solid; mp 63–65 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.38–7.34 (m, 3 H), 7.29–7.18 (m, 3 H), 6.98–6.94 (m, 2 H), 6.82 (dd, *J* = 5.3, 3.5 Hz, 1 H), 5.43 (s, 2 H), 4.01 (s, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.05, 136.35, 134.54, 131.25, 128.88, 128.51, 127.88, 127.85, 122.84, 121.62, 53.88, 23.87.

MS: *m/z* (%) = 335 (5), 256 (3), 172 (13), 144 (48), 117 (9), 104 (9), 99 (12), 91 (100), 85 (27), 71 (85), 69 (17), 57 (58).

Anal. Calcd for $C_{14}H_{13}N_3SSe$: C, 50.30; H, 3.92; N, 12.57, S 9.59. Found: C, 49.84; H, 3.65; N, 12.87, S 9.98.

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Supporting Information for this article is available online at http://www.thieme-connect.com/ejournals/toc/synthesis.

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