Efficient and Highly Selective Method for the Synthesis of 4-Iodo-3-substituted 1*H*-Isoselenochromenes and -isothiochromenes

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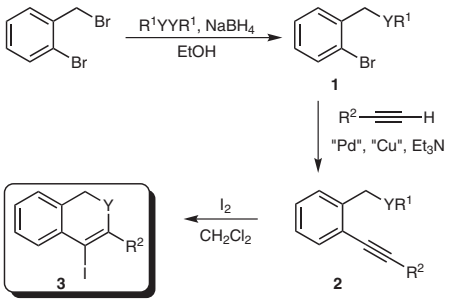
Abstract: We present here our results on the preparation of 2-alkynylbenzyl selenide and sulfide derivatives via Sonogashira cross-coupling of benzyl chalcogenides with different alkynes. This cross-coupling reaction proceeded cleanly under mild conditions and was performed with propargyl alcohol as well as alkyl- and arylalkynes. Subsequent electrophilic-cyclization reaction of the 2-alkynylbenzyl selenide and sulfide derivatives using iodine as an electrophilic source gave 4-iodo-3-substituted 1*H*-isoselenochromenes and -isothiochromenes in moderate yields. The unique product obtained during the course of this cyclization contained a six-membered ring which was confirmed by X-ray diffraction analysis.

Key words: selenides, isochromenes, electrophilic cyclization, heterocycles

In recent years there has been increased interest in the synthesis of heterocycles since they are of great importance in organic and medicinal chemistry.[1] The literature contains a variety of synthetic approaches to heterocycle ring structures, much of which has been compiled into comprehensive reviews.[2,3] A great number of selenium heterocycles have been synthesized and their chemistry has attracted a good deal of interest and activity from a variety of standpoints, such as structure, stereochemistry, reactivity, and their application in organic synthesis.[4] Selenophenes, as important selenium heterocycles, are widely studied agents with a diverse array of biological effects that include antioxidant,[5] antinociceptive,[6] and anti-inflammatory properties,[7] as well as efficacy as maturation-inducing agents.[8] Electrophilic cyclization is an alternative route for the generation of highly functionalized chalcogen heterocycles employing electrophiles, like iodine or iodine monochloride, and chalcogen derivatives.[9] The synthetic study of six-membered ring containing selenium has been surprisingly limited.[10] Among them, benzo[*c*]selenocoumarins were prepared in good yields by Christiaens and co-workers.[10b] More recently, Akiba and co-workers reported the synthesis of isotellurochromenes and isoselenochromenes together with (*Z*)-1-methylene-2-tellura- and -2-selenaindanes by an intramolecular cyclization reaction. The isochromenes were transformed into the corresponding 2-benzotelluropyrylium and 2-benzoselenopyrylium salts in good yields.[9c] As a result of combining our knowledge of the synthesis of heterocycles containing a chalcogen[11] with the unexplored iodide-promoted cyclization of 2-alkynylbenzyl chalcogenide derivatives, in this paper we reported a synthetic method for isochalcogenochromenes starting from 2-alkynylbenzyl chalcogenides. Our idea is outlined in Scheme 1, which consisted of (i) preparation of 2-bromobenzyl selenides and sulfides **1** from 2-bromobenzyl bromide, (ii) Sonogashira cross-coupling the 2-bromobenzyl selenides and sulfides **1** with terminal alkynes to obtain 2-alkynylbenzyl selenides and sulfides **2**, and (iii) electrophilic cyclization of 2-alkynylbenzyl selenides and sulfides **2** to form isoselenochromenes **3** (Y = Se) and isothiochromenes **3** (Y = S), respectively (Scheme 1).



Y = Se, S; R^1 = Me, *n*-Bu; R^2 = alkyl, aryl

Scheme 1

To prepare 2-bromobenzyl selenides **1** (Y = Se), we chose the alkylation of selenolates.[12] In this way, the reaction of 2-bromobenzyl bromide with the alkylselenolate anion, generated from dialkyl diselenide and sodium borohydride in ethanol, at room temperature, gave the desired product **1** (Y = Se) in good yield. For the introduction of the terminal alkyne, we used the Sonogashira cross-coupling.[13] Thus the reaction of 2-bromobenzyl selenide **1** (Y = Se, 0.5 mmol) with terminal alkyne (2.5 equiv) using $PdCl_2(PPh_3)_2$ (2 mol%) as the palladium source, copper(I) iodide (1 mol%) as co-catalyst and triethylamine (5 mL) as solvent and base, at reflux for 12 hours, gave the desired 2-alkynylbenzyl selenides **2** (Y = Se). Using this sequence, we were able to prepare a number of novel 2-alkynylbenzyl selenides **2** (Y = Se) and the analogous sul-

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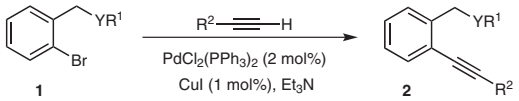
fides **2** (Y = S) to illustrate the generality and scope of the reaction (Table 1).

We gained a good understanding of this process by studying the scope and limitations of this reaction. First, to determine the real influence of the terminal alkyne, we kept the butyl benzyl selenide **1** (YR^1 = SeBu) invariant (Table 1). Interestingly, all entries provided the corresponding 2-alkynylbenzyl selenides **2** (Y = Se) in acceptable yields. Both alkyl- and bulky alkyl-substituted alkynes gave the products in similar yields, e.g. **2a** and **2b** (entries 1 and 2). Our experiments showed that the reaction with propargyl or homopropargyl alcohols gave the corresponding products **2c–e** in good yields, although the yield was lower for the propargyl alcohol itself (entries 3–5). In addition to alkylalkynes and propargyl alcohols, the reaction took place with arylalkynes and we observed that the reaction was not sensitive to electronic effects in the aromatic ring of the arylalkynes. For example, arylalkynes having either an electron-donating (Me) or an electron-withdrawing (Cl) group delivered the products **2h** and **2j** in comparable yields (entries 8 and 10). Finally, we then explored the possibility of expanding our methodology to 2-alkynylbenzyl sulfides. It was found that the reaction worked well, affording the 2-alkynylbenzyl sulfides **2l–s** in moderate to excellent yields, under the same reaction conditions.

After the success in the synthesis of 2-alkynylbenzyl chalcogenides **2**, we next focused our attention on the development of an optimum set of conditions for the electrophilic cyclization. For this purpose, the reaction of **2f** with iodine was chosen as a model system.

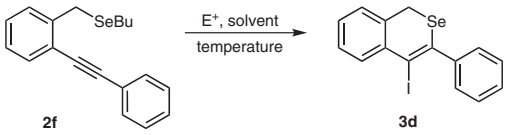
Table 1 Synthesis of 2-Alkynylbenzyl Selenides **2** (Y = Se) and Sulfides **2** (Y = S)[a]



Entry	YR^1	R^2	Product	Yield[a] (%)
1	SeBu	$(CH_2)_4Me$	**2a**	51
2	SeBu	*t*-Bu	**2b**	60
3	SeBu	$C(OH)Me_2$	**2c**	83
4	SeBu	CH_2OH	**2d**	61
5	SeBu	$(CH_2)_2OH$	**2e**	85
6	SeBu	Ph	**2f**	69
7	SeBu	2-$MeOC_6H_4$	**2g**	67
8	SeBu	4-MeC_6H_4	**2h**	50
9	SeBu	3-MeC_6H_4	**2i**	54
10	SeBu	4-ClC_6H_4	**2j**	55
11	SeBu	1-naphthyl	**2k**	80
12	SMe	$(CH_2)_4Me$	**2l**	75
13	SMe	*t*-Bu	**2m**	61
14	SMe	$C(OH)Me_2$	**2n**	92
15	SMe	CH_2OH	**2o**	59
16	SMe	Ph	**2p**	75
17	SMe	4-MeC_6H_4	**2q**	85
18	SMe	4-ClC_6H_4	**2r**	76
19	SMe	1-naphthyl	**2s**	85

[a] Isolated yields.

Table 2 Influence of Reaction Conditions on the Iodo Cyclization of Butyl 2-Phenylbenzyl Selenide (**2f**)[a]



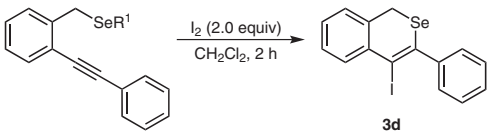
Entry	E^+ (equiv)	Solvent	Temp	Yield (%)
1	I_2 (2.0)	CH_2Cl_2	r.t.	69
2	I_2 (2.0)	Et_2O	r.t.	32
3	I_2 (2.0)	MeCN	r.t.	35
4	I_2 (2.0)	THF	r.t.	41
5	I_2 (2.0)	EtOH	r.t.	47
6	I_2 (1.1)	CH_2Cl_2	r.t.	47
7	I_2 (3.0)	CH_2Cl_2	r.t.	45
8	ICl (1.1)	CH_2Cl_2	r.t.	35
9	ICl (2.0)	CH_2Cl_2	r.t.	55
10	ICl (3.0)	CH_2Cl_2	r.t.	n.r.
11	ICl (2.0)	CH_2Cl_2	–20 C	n.r.

[a] Reactions performed using **2f** (0.25 mmol), 2 h.

Thus, the reaction of substrate **2f** (0.25 mmol) with iodine (2.0 equiv) was performed at room temperature using different solvents (Table 2). A comparison of the effectiveness of the solvents showed that all of them yielded cyclized product **3d** (entries 1–5), but dichloromethane was the most efficient since the product was obtained in 69% yield after two hours (entry 1). It is important to note that when the amount of the electrophile was changed from 2.0 to 1.1 or 3.0 equivalents the yield of **3d** decreased (entry 1 vs entries 6 and 7). Examining the electrophile source showed that 1.1 to 3.0 equivalents of iodine monochloride gave the target product **3d** in unacceptable yield (entries 8–11). Thus, the optimum conditions for this electrophilic cyclization were identified as 2-alkynylbenzyl chalcogenide **2** (1.0 equiv), iodine (2.0 equiv) as the electrophilic source, dichloromethane as the solvent, at room temperature for two hours.

Since the success of this reaction probably is dependent on the nature of the group directly linked to the selenium atom,[13] we decided to explore this influence by using different alkyl, aryl, and benzyl groups; the results are shown in Table 3. Inspection of these results revealed that butyl and propyl selenides **2t**,**u** resulted in the formation of **3d** in high yields (entries 1 and 2). Benzyl 2-phenylbenzyl selenide (**2v**) also gave the product **3d**, but in moderate yield (entry 3). Performing the reaction with phenyl 2-phenylbenzyl selenide (**2x**) did not give the desired product even after a long reaction time (entry 4). These results demonstrated that the efficiency of the cyclization reaction significantly depends on steric effects and that it only occurs with 2-alkynylbenzyl selenide that contain a Se–Csp^3 bond.

Table 3 Influence of the Group Bonded to the Selenium Atom[a]



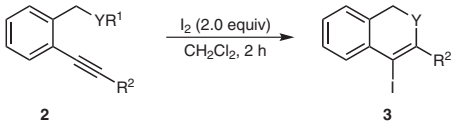
Entry	Substrate		Yield (%)
	2	R^1	
1	**2t**	Pr	70
2	**2u**	Bu	69
3	**2v**	Bn	56
4	**2x**	Ph	n.r.

[a] Reactions performed with **2t–x** (0.25 mmol), I_2 (2.0 equiv), CH_2Cl_2, 2 h.

In order to demonstrate the efficiency of this reaction, we explored the generality of our method by extending these conditions to various 2-alkynylbenzyl chalcogenides **2**; the results are summarized in Table 4. In most cases, the corresponding 4-iodo-3-substituted-1*H*-isoselenochromenes **3** (Y = Se) and -isothiochromenes (Y = S) were obtained in moderate yields. Table 4 shows the limitations in this methodology; 2-alkynylbenzyl selenides **2a** and **2g** containing a pentyl or anisyl group (entries 1 and 5) and 2-alkynylbenzyl sulfides **2n** and **2o** containing a propargyl or homopropargyl alcohol (entries 10 and 11) did not give the desired products.

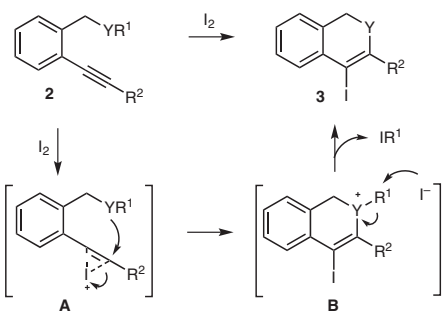
We believe that the mechanism of this cyclization reaction involves; (i) coordination of the C≡C bond to iodine to generate the iodonium intermediate **A**, which activates the triple bond towards nucleophilic attack, (ii) *anti*-nucleophilic attack of the selenium atom on the activated iodonium intermediate to produce the salt **B**, and (iii) facile removal of the alkyl group via S_N2 displacement by the iodide anion present in the reaction mixture to generate the 4-iodoisochalcogenochromene product **3** and one molecule of R^1I (Scheme 2). This cyclization could give a mixture of two isomers, one being the expected isochalcogenochromene product and the other possible product contains a five-membered ring, e.g. a dihydrobenzo[*c*]selenophene. In order to determine the nature of the co- and/or byproducts formed in addition to the isolated iodoisochalcogenochromenes **3**, we analyzed the crude reaction mixture, which showed that only one product was formed. This encouraged us to confirm the structure of our cyclized product using X-ray crystallography, which indeed proved to be the isochalcogenochromene **3** (Figure 1).

Table 4 Synthesis of Isoselenochromenes **3** (Y = Se) and Isothiochromenes **3** (Y = S) via Electrophilic Cyclization of 2-Alkynylbenzyl Chalcogenides **2**[a]



Entry	Substrate				Product	Yield (%)
	2	Y	R^1	R^2		
1	**2a**	Se	Bu	$(CH_2)_4Me$	**3a**	–
2	**2b**	Se	Bu	*t*-Bu	**3b**	52
3	**2e**	Se	Bu	$(CH_2)_2OH$	**3c**	32
4	**2f**	Se	Bu	Ph	**3d**	69
5	**2g**	Se	Bu	2-$MeOC_6H_4$	**3e**	–[b]
6	**2h**	Se	Bu	4-MeC_6H_4	**3f**	62
7	**2i**	Se	Bu	3-MeC_6H_4	**3g**	70
8	**2k**	Se	Bu	1-naphthyl	**3h**	65
9	**2m**	S	Me	*t*-Bu	**3i**	30
10	**2n**	S	Me	$C(OH)Me_2$	**3j**	–
11	**2o**	S	Me	CH_2OH	**3k**	–
12	**2p**	S	Me	Ph	**3l**	48
13	**2q**	S	Me	4-MeC_6H_4	**3m**	55
14	**2s**	S	Me	1-naphthyl	**3n**	60

[a] Reactions performed using **2** (0.25 mmol), I_2 (2.0 equiv), CH_2Cl_2, 2 h.
[b] A complex inseparable mixture of products was observed.



Scheme 2

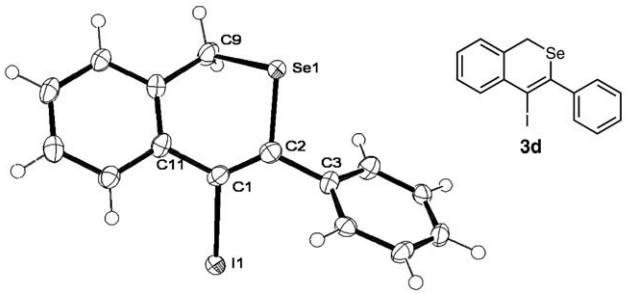


Figure 1 ORTEP view of the compound **3d**

We described herein efficient methodology for the synthesis of 2-alkynylbenzyl chalcogenide derivatives via Sonogashira cross-coupling of 2-bromobenzyl chalcogenides with different alkynes. This cross-coupling reaction proceeded cleanly under mild conditions and was performed with propargyl alcohols, as well as alkyl- and arylalkynes. The product obtained subsequent underwent an efficient electrophilic cyclization reaction using iodine as electrophilic source, giving the corresponding 4-iodo-1*H*-isochalcogenochromenes in moderate yields. Regarding the five- versus six-membered ring, it is important to point out that the unique product obtained during the course of this cyclization contained a six-membered ring, which was determined by X-ray diffraction analysis.

Proton nuclear magnetic resonance spectra (^{1}H NMR) were obtained at 200 MHz on a DPX-200 NMR spectrometer or at 400 MHz on DPX-400 NMR spectrometer. Spectra were recorded in $CDCl_3$ solutions. Chemical shifts are reported in ppm, referenced to the solvent peak of $CDCl_3$ or tetramethylsilane (TMS) as the external reference. Data are reported as follows: chemical shift (δ), multiplicity, coupling constant (*J*) in Hz and integrated intensity. Carbon-13 nuclear magnetic resonance spectra (^{13}C NMR) were obtained either at 50 MHz on a DPX-200 NMR spectrometer or at 100 MHz on a DPX-400 NMR spectrometer. Spectra were recorded in $CDCl_3$ solutions. Chemical shifts are reported in ppm, referenced to the solvent peak of $CDCl_3$. Abbreviations to denote the multiplicity of a particular signal are s (singlet), d (doublet), t (triplet), q (quartet), quint (quintet), sex (sextet) and m (multiplet). High-resolution mass spectra were recorded on a MS50TC double focusing magnetic sector mass spectrometer using EI at 70 eV. Column chromatography was performed using silica gel (230–400 mesh) following the methods described by Still. Thin-layer chromatography (TLC) was performed using silica gel GF254, 0.25 mm thickness. For visualization, TLC plates were either placed under ultraviolet light, or stained with iodine vapour or acidic vanillin. Most reactions were monitored by TLC for disappearance of starting material. Air- and moisture-sensitive reactions were conducted in flame-dried or oven-dried glassware equipped with tightly fitted rubber septa and under a positive atmosphere of dry argon. Reagents and solvents were handled using standard syringe techniques. Temperatures above room temperature were maintained by use of a mineral oil bath with an electrically heated coil connected to a Variac controller.

Selected spectral and analytical data are given. The characterization of additional new products is provided in the Supporting Information.

Alkyl 2-Bromobenzyl Chalcogenides 1; General Procedure

To a soln of alkyl dichalcogenide (5 mmol) in EtOH (50 mL), under argon was added $NaBH_4$ (30 mmol) at r.t. with vigorous stirring. To this soln was added 2-bromobenzyl bromide (10 mmol) and the mixture was stirred at r.t. for 5 h. The mixture was diluted with EtOAc (20 mL) and washed with brine (2 × 30 mL). The organic phase was separated, dried ($MgSO_4$), and concentrated under vacuum. The residue was purified by flash chromatography (hexane).

Alkyl 2-(Substituted-ethynyl)benzyl Chalcogenides 2; General Procedure

To a Schlenck tube, under argon, containing $Pd(PPh_3)_2Cl_2$ (2 mol%) and Et_3N (5 mL) was added the 2-bromobenzyl chalcogenide **1** (0.5 mmol) and the resulting soln was stirred at r.t. for 5 min. After this time, the terminal alkyne (2.5 equiv) dissolved in Et_3N (0.5 mL) was then added dropwise, and the mixture was stirred for an additional 5 min. CuI (1 mol%) was added and the soln was stirred at reflux for 12 h. The mixture was diluted with CH_2Cl_2 (10 mL), and washed with brine (3 × 10 mL). The organic phase was separated, dried ($MgSO_4$), and concentrated under vacuum. The residue was purified by flash chromatography (silica gel, EtOAc–hexane).

Butyl 2-(Phenylethynyl)benzyl Selenide (2f)

Yield: 0.225 g (69%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.55–7.48 (m, 3 H), 7.36–7.30 (m, 4 H), 7.24 (t, *J* = 7.3 Hz, 1 H), 7.17 (t, *J* = 7.6 Hz, 1 H), 4.01 (s, 2 H), 2.57 (t, *J* = 7.3 Hz, 2 H), 1.62 (quint, *J* = 7.6 Hz, 2 H), 1.33 (sextet, *J* = 7.3 Hz, 2 H), 0.83 (t, *J* = 7.3 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 142.05, 132.24, 131.41, 129.01, 128.36, 128.28, 128.24, 126.44, 123.24, 122.41, 94.30, 87.70, 32.58, 25.34, 23.99, 23.03, 13.47.

MS: *m*/*z* (%) = 328 (7), 272 (20), 191 (100), 165 (25).

Butyl 2-[(2-Methoxyphenyl)ethynyl]benzyl Selenide (2g)

Yield: 0.239 g (67%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.54 (td, *J* = 7.6, 1.4 Hz, 2 H), 7.32–7.26 (m, 2 H), 7.23 (td, *J* = 7.6, 1.4 Hz, 1 H), 7.17 (td, *J* = 7.3, 1.4 Hz, 1 H), 6.92 (td, *J* = 7.3, 1.2 Hz, 1 H), 6.88 (d, *J* = 8.3 Hz, 1 H), 4.08 (s, 2 H), 3.90 (s, 3 H), 2.57 (t, *J* = 7.6 Hz, 2 H), 1.61 (quint, *J* = 7.6 Hz, 2 H), 1.32 (sextet, *J* = 7.6 Hz, 2 H), 0.81 (t, *J* = 7.3 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.99, 142.23, 133.05, 132.03, 129.67, 128.97, 128.14, 126.32, 122.80, 120.35, 112.59, 110.56, 91.85, 90.82, 55.68, 32.52, 25.22, 23.67, 23.05, 13.47.

MS: *m*/*z* (%) = 358 (11), 301 (25), 221 (22), 206 (100), 178 (70), 115 (31).

Butyl 2-(4-Tolylethynyl)benzyl Selenide (2h)

Yield: 0.170 g (50%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.43 (d, *J* = 8.0 Hz, 2 H), 7.31–7.13 (m, 6 H), 4.00 (s, 2 H), 2.57 (t, *J* = 7.6 Hz, 2 H), 2.35 (s, 3 H), 1.62 (quint, *J* = 7.3 Hz, 2 H), 1.33 (sextet, *J* = 7.6 Hz, 2 H), 0.83 (t, *J* = 7.3 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 141.94, 138.37, 132.16, 131.31, 129.05, 128.98, 128.17, 126.41, 122.62, 120.18, 94.52, 87.05, 32.59, 25.37, 23.98, 23.02, 21.43, 13.48.

MS: *m*/*z* (%) = 342 (5), 286 (16), 205 (100), 190 (36).

Anal. Calcd for $C_{20}H_{22}Se$: C, 70.37; H, 6.50. Found: C, 70.51; H, 6.60.

Butyl 2-(3-Tolylethynyl)benzyl Selenide (2i)

Yield: 0.184 g (54%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.49 (dd, *J* = 7.6,1.2 Hz, 1 H), 7.36–7.30 (m, 3 H), 7.26–7.13 (m, 4 H), 4.01 (s, 2 H), 2.58 (t, *J* = 7.6 Hz, 2 H), 2.35 (s, 3 H), 1.63 (quint, *J* = 7.3 Hz, 2 H), 1.34 (sextet, *J* = 7.6 Hz, 2 H), 0.84 (t, *J* = 7.6 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 142.06, 138.00, 132,28, 132.01, 129.20, 129.05, 128.57, 128.33, 128.23, 126.48, 123.08, 122.55, 94.53, 87.36, 32.64, 25.39, 24.04, 23.09, 21.21, 13.52.

MS: *m*/*z* (%) = 342 (4), 284 (9), 205 (100), 190 (46).

Anal. Calcd for $C_{20}H_{22}Se$: C, 70.37; H, 6.50. Found: C, 70.61; H, 6.69.

Butyl 2-[(4-Chlorophenyl)ethynyl]benzyl Selenide (2j)
Yield: 0.199 g (55%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.49–7.44 (m, 3 H), 7.32–7.16 (m, 5 H), 3.98 (s, 2 H), 2.57 (t, *J* = 7.6 Hz, 2 H), 1.62 (quint, *J* = 7.3 Hz, 2 H), 1.34 (sextet, *J* = 7.3 Hz, 2 H), 0.84 (t, *J* = 7.6 Hz, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 142.10, 134.27, 132,61, 132.29, 129.05, 128.65, 128.58, 126.52, 122.09, 121.74, 93.18, 88.66, 32.57, 25.34, 24.03, 23.02, 13.50.

MS: *m*/*z* (%) = 362 (4), 306 (20), 225 (94), 189 (100).

Anal. Calcd for $C_{19}H_{19}ClSe$: C, 63.08; H, 5.29. Found: C, 63.25; H, 5.35.

4-Iodo-3-substituted Isoselenochromenes 3 (Y = Se) and Isothiochromenes 3 (Y = S); General Procedure
To a soln of the alkyne **2** (0.25 mmol) and CH_2Cl_2 (2 mL) was gradually added I_2 (2.0 equiv) dissolved in CH_2Cl_2 (6 mL). The mixture was allowed to stir at r.t. for 2 h. The excess I_2 was removed by washing with sat. aq $Na_2S_2O_3$. The mixture was then extracted with EtOAc (3 × 10 mL). The combined organic extracts were dried ($MgSO_4$ and concentrated under vacuum.

4-Iodo-3-phenyl-1*H*-isoselenochromene (3d)
Yield: 0.273g (69%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.80–7.78 (m, 1 H), 7.42–7.32 (m, 5 H), 7.29–7.22 (m, 2 H), 7.11–7.09 (m, 1 H), 3.93 (s, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 143.86, 138.12, 133.61, 131.48, 130.04, 128.82, 128.57, 128.06, 127.48, 125.92, 91.41, 26.81.

MS: *m*/*z* (%) = 397 (44), 269 (17), 191 (100).

Anal. Calcd for $C_{15}H_{11}ISe$: C, 45.37; H, 2.79. Found: C, 45.52; H, 2.87.

4-Iodo-3-(4-tolyl)-1*H*-isoselenochromene (3f)
Yield: 0.254 g (62%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.79 (dd, *J* = 7.8, 1.7 Hz, 1 H), 7.33 (d, *J* = 7.8 Hz, 2 H), 7.30–7.25 (m, 2 H), 7.20 (d, *J* = 7.8 Hz, 2 H), 7.12 (d, *J* = 7.0 Hz, 1 H), 3.95 (s, 2 H), 2.38 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 140.91, 138.70, 138.12, 133.64, 130.12, 129.53, 128.77, 128.73, 127.88, 127.44, 125.90, 90.88, 26.83, 21.39.

MS: *m*/*z* (%) = 411 (100), 285 (39), 270 (53), 205 (90), 189 (45).

Anal. Calcd for $C_{16}H_{13}ISe$: C, 46.74; H, 3.19. Found: C, 46.85; H, 3.28.

3-Iodo-3-(3-tolyl)-1*H*-isoselenochromene (3g)
Yield: 0.287 g (70%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.79 (d, *J* = 7.3 Hz, 1 H), 7.29–7.16 (m, 6 H), 7.11 (d, *J* = 7.3 Hz, 1 H), 3.93 (s, 2 H), 2.38 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 143.80, 138.33, 137.96, 137.73, 133.60, 131.51, 130.64, 129.35, 128.77, 127.96, 127.46, 127.05, 125.91, 91.18, 26.81, 21.37.

MS: *m*/*z* (%) = 411 (100), 285 (32), 270 (57), 205 (93), 189 (49).

4-Iodo-3-(naphthalen-1-yl)-1*H*-isoselenochromene (3h)
Yield: 0.290 g (65%).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.95–7.93 (m, 1 H), 7.88–7.81 (m, 3 H), 7.52–7.46 (m, 3 H), 7.37–7.35 (m, 1 H), 7.30–7.26 (m, 2 H), 7.15–7.13 (m, 1 H), 4.12 (d, *J* = 12.5 Hz, 1 H), 3.98 (d, *J* = 12.5 Hz, 1 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 142.12, 137.14, 135.95, 133.73, 133.43, 131.27, 129.75, 129.13, 128.73, 128.43, 127.65, 126.50, 126.43, 126.19, 125.50, 125.42, 95.47, 27.00.

MS: *m*/*z* (%) = 447 (20), 321 (20), 240 (100), 119 (44).

Anal. Calcd for $C_{16}H_{13}ISe$: C, 46.74; H, 3.19. Found: C, 46.90; H, 3.27.

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

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