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### ARTICLE

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Synthesis and photophysical properties of selenopheno[2,3b]quinoxaline and selenopheno[2,3-b]pyrazine heteroacenes

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In this paper, we report the novel synthesis of three different heterocycles namely 2arylselenopheno[2,3-*b*]quinoxaline, 3-(aryl/alkylselanyl)-2-arylselenopheno[2,3-*b*]quinoxaline and 6-phenyl-7-(arylselanyl)selenopheno[2,3-*b*]pyrazine derivatives from the corresponding 2,3-dichloroquinoxaline and 2,3-dichloropyrazine derivatives. Further, photophysical properties were investigated to study the effect of heteroatoms on UV-absorbance and fluorescence properties.

#### Introduction

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Electrophilic cyclization is widely used for the synthesis of biologically important novel heterocycles.<sup>1</sup> Among the Ncontaining heterocycles, quinoxaline belongs to the benzodiazine family with its 1,4-nitrogens as heteroatoms.<sup>2</sup> Quinoxaline core system is an attractive nucleus for medicinal chemists due to diverse biological activities i.e. anticancer,<sup>3</sup> antitubercular,<sup>4</sup> antifungal,<sup>5</sup> antibacterial,<sup>6</sup> antimalarial,<sup>7</sup> antitumor,<sup>8</sup> antiamoebic,<sup>9</sup> antiproliferative,<sup>10</sup> anti-HCV<sup>11</sup> and anti-inflammatory etc.<sup>12</sup> Synthesis of various quinoxaline fused heterocycles was successfully achieved by electrophilic cyclization.<sup>13</sup> To the best of our knowledge, selenopheno[2,3-b]quinoxaline heterocycles have never been described due to difficulties in their synthesis. Therefore, the development of new synthetic methodologies to access guinoxaline-fused selenoheterocycles becomes an important objective. In our ongoing research toward the synthesis of various N-heterocycles, recently, we used this electrophilic cyclization methodology for the synthesis of selenophene-fused. quinoline-based heteroacenes.14 thieno[2,3-b]quinoline and selenopheno[2,3-b]quinoline,<sup>15</sup> thieno/furo[2,3-c]acridine,<sup>16</sup> pyrano[4,3-b]quinoline<sup>17</sup> and isoquinoline-fused quinazolinones.<sup>18</sup> Herein, we are going to report the synthesis of three different heterocycles namely 2-arylselenopheno[2,3-b]quinoxaline, 3-(aryl/alkylselanyl)-2-

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arylselenopheno[2,3-*b*]quinoxaline and 6-phenyl-7-(arylselanyl)selenopheno[2,3-*b*]pyrazine derivatives from the corresponding 2,3-dichloroquinoxaline and 2,3dichloropyrazine derivatives. Further, UV-absorbance and fluorescence studies were investigated.

#### **Result and Discussion**

The synthesis of 2-chloro-3-(methylselanyl)quinoxaline **2a** and 2-chloro-3-(methylselanyl)pyrazine **2b** in 92% and 85% yields were successfully achieved *via* the intermediate **A** using a literature procedure<sup>15,16</sup>, successfully affording starting compounds **2a-2b** (Scheme 1).

Scheme 1. Synthesis of starting compounds 2a-2b.



With these two starting materials **1a-1b** and **2a-2b** in hand, we proceeded for Sonogashira coupling reactions of **1a-1b** with different alkynes. The Sonogashira coupling reactions<sup>13b</sup>

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of **1a** with substituted arylalkynes was successfully achieved at room temperature, the crude products **3a-3f** were purified by silica gel chromatography using hexane/ethyl acetate (20:1) as eluent to afford the 2-chloro-3-(arylethynyl)quinoxaline derivatives **3a-3f** in 37-77% yields (Table 1).

**Table 1.** Synthesis of 2-chloro-3-(arylethynyl)quinoxalinederivatives 3



Entry	Ar	Time (h)	Yield (%) <sup>a, b</sup> <b>3</b>
1	Ph-	3	59 <b>(3a)</b>
2	<i>p</i> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> -	22	59 <b>(3b)</b>
3	p-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> -	18	60 <b>(3c)</b>
4	<i>p</i> -FC <sub>6</sub> H <sub>4</sub> -	22	37 <b>(3d)</b>
5	<i>m</i> -FC <sub>6</sub> H <sub>4</sub> -	21	77 <b>(3e)</b>
6	<i>o</i> -FC <sub>6</sub> H <sub>4</sub> -	19	60 <b>(3f)</b>

<sup>a</sup>All reactions were carried out under nitrogen atmosphere using **1a** (1.0 equiv.), arylacetylene (1.0 equiv.), Pd-catalyst (0.035 equiv.), Cul (0.007 equiv.), NEt<sub>3</sub> (3 mL) and a DMF solvent for 3 h at rt. <sup>b</sup>Isolated yield.

Further, NaSeH was prepared *in situ* by reactions of elemental selenium (1.0 equiv.) and sodium borohydride (2.0 equiv.) in ethanol (0.75 mL) / water (1.5 mL) mixture at 0°C for 15 min, after confirming that the solution changed from black to colorless and transparent (white), to this freshly prepared NaSeH solution, compounds **3a-3f** (1.0 equiv.) and ethanol (1 mL) was added, and the mixture was stirred under reflux conditions for 1 hour. Successfully affording the corresponding 2-arylselenopheno[2,3-*b*]quinoxaline derivatives **4a-4f** in 69-95% yields (Table 2).

**Table 2.** Synthesis of 2-arylselenopheno[2,3-b]quinoxalinederivatives 4



1	Ph-	83 (44) rticle Online DOI: 10.1039/D00B00718H
2	<i>p</i> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> -	77 <b>(4b)</b>
3	p-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> -	83 <b>(4c)</b>
4	<i>p</i> -FC <sub>6</sub> H <sub>4</sub> -	95 <b>(4d)</b>
5	<i>m</i> -FC <sub>6</sub> H <sub>4</sub> -	69 <b>(4e)</b>
6	<i>o</i> -FC <sub>6</sub> H <sub>4</sub> -	95 <b>(4f)</b>

<sup>a</sup>Reactions were carried out using NaSeH (1.0 equiv.) and compound **4a** (1 equiv.) in ethanol / water (1:1) solvent for 1 h at reflux conditions. <sup>b</sup>Isolated yield.

Next, compounds 2a was transformed via Sonogashira coupling reaction conditions used for Scheme 2, but reaction did not proceed. Further, we attempted different reaction conditions (See supporting information Table S1); it is found that the reaction proceeded when compound 2-chloro-3-(methylselanyl)guinoxaline **2a** reacted with substituted aryl alkynes (2.5 equiv.), Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> (0.2 equiv.), Na<sub>2</sub>CO<sub>3</sub> (2M, 4 mL) and DME (2 mL) solvent was heated at 90°C, after completion of the reactions, the crude products 5a-5f was purified by silica gel chromatography using hexane/ethyl acetate (20:1) as eluent, successfully affording the 2-(methylselanyl)-3-(arylethynyl)quinoxaline derivatives 5a-5f in 19-41% yields (Table 3). Further, the same reaction conditions from compound 2b is used for the synthesis of corresponding 2-(methylselanyl)-3-(arylethynyl)pyrazine derivatives 6a-6f in 7-25% yields (Table 4).

Table	3.	Synthesis	of	2-(methylselanyl)-3-
(arylethy	nyl)qui	noxaline deriva	tives 5	

		<u></u> —A	r	A
$\bigwedge$	× <sup>N</sup> × <sup>CI</sup>	Pd(PPh <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub> , Na	<sub>2</sub> CO <sub>3</sub>	N N
Ļ	N Se 2a	DME, 90°	C, Time	N Se 5
	Entry	Ar	Time (h)	Yield (%) <b>5</b>
	1	Ph-	28	41 <b>(5a)</b>
	2	<i>p</i> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> -	22	32 <b>(5b)</b>
	3	p-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> -	18	36 <b>(5c)</b>
	4	<i>p</i> -FC <sub>6</sub> H <sub>4</sub> -	22	19 <b>(5d)</b>
	5	<i>m</i> -FC <sub>6</sub> H <sub>4</sub> -	23	37 <b>(5e)</b>
	6	<i>o</i> -FC <sub>6</sub> H <sub>4</sub> -	22	40 <b>(5f)</b>

<sup>a</sup>All reactions were carried out using **2a** (1.0 equiv.), arylacetylene (2.5 equiv.), Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> (20 mol%),

 $Na_2CO_3$  (2M, 4mL), NEt<sub>3</sub> (2 mL) and a DMF solvent for 3 h at 90°C. <sup>b</sup>Isolated yield.

**Table4.**Synthesisof2-(methylselanyl)-3-(arylethynyl)pyrazinederivatives**6** 

	<u> </u>	Ar	Ar
N CI	Pd(PPh <sub>3</sub> ) <sub>2</sub> C	N	
N Se 2b	DME, 90°C, Time		N Se 6
Entry	Ar	Time (h)	Yield (%) <b>6</b>
1	Ph-	18	16 <b>(6a)</b>
2	<i>p</i> -CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> -	22	14 <b>(6b)</b>
3	<i>p</i> -CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> -	18	25 <b>(6c)</b>
4	<i>p</i> -FC <sub>6</sub> H <sub>4</sub> -	19	7 <b>(6d)</b>
5	<i>m</i> -FC <sub>6</sub> H <sub>4</sub> -	18	12 <b>(6e)</b>
6	<i>o</i> -FC <sub>6</sub> H <sub>4</sub> -	20	20 <b>(6f)</b>

<sup>a</sup>All reactions were carried out using **2b** (1.0 equiv.), arylacetylene (2.5 equiv.),  $Pd(PPh_3)_2Cl_2$  (20 mol%),  $Na_2CO_3$  (2M, 4mL), NEt<sub>3</sub> (2 mL) and a DMF solvent for 3 h at 90°C. <sup>b</sup>Isolated yield.

The electrophilic cyclizations of alkynes using diorganyl diselenides are gaining considerable attention due to the synthesis of seleno-heterocycles<sup>19</sup> and further applications of these seleno-heterocycles in the preparation of physical materials that show different optical properties.<sup>20</sup> Herein, the electrophilic cascade cyclization of 2-(methylselanyl)-3-(arylethynyl)quinoxaline 5 and 2-(methylselanyl)-3-(arylethynyl)pyrazine 6 derivatives were successfully achieved by using diorganyl diselenides and diorganyl disulfides as electrophilic source. To a stirred mixture of diorganyl diselenides (1.0 equiv.) and FeCl<sub>3</sub>·6H<sub>2</sub>O (2.0 equiv.) in dichloromethane solvent was added the of 2-(methylselanyl)-3-(arylethynyl)quinoxaline 5 (1.0 equiv.) and heated at 45°C, successfully affording the 3-(arylselanyl/sulfanyl)-2-arylselenopheno[2,3-b]quinoxaline derivatives 7a-7j in 57-92% yields, respectively (Scheme 2). The reactions was less facile with dimethyl disulfide and formation of 3-(methylthio)-2-phenylselenopheno[2,3b]quinoxaline 7i was relatively lower yield (52%), while reactions with diphenyl disulfide, the formation of 2-phenyl-3-(phenylthio)selenopheno[2,3-b]quinoxaline 7j was only 5% yield. On the other hand, to a stirred mixture of diorganyl diselenides (1.0 equiv.) and FeCl<sub>3</sub>·6H<sub>2</sub>O (2.0 equiv.) in dichloromethane solvent the 2-(methylselanyl)-3-(arylethynyl)pyrazine 6 (1.0 equiv.) at 45°C was added, to afford the 6-aryl-7-(phenylselanyl)selenopheno[2, 3e b]pyrazine derivatives **8a-8e** in 47-70% yields (Scherrers)).718H

**Scheme 2.** Synthesis of 3-(arylselanyl/sulfanyl)-2-arylselenopheno[2,3-*b*]quinoxaline derivatives **7** 







Next, the compounds **9a** and **9b** were synthesized to study the effect of heteroatoms (O, S, Se) on fluorescence and UVabsorbance properties. The 2-chloro-3-(phenylethynyl) quinoxaline **3a** reacted with sodium hydroxide (5 equiv.) in presence of DMSO /  $H_2O$  (1 : 4) mixture and refluxed for 2 h, successfully affording the 2-phenylfuro[2,3-*b*]quinoxaline **9a**. While, 2-chloro-3-(phenylethynyl)quinoxaline **3a** reacted with NaSH·xH<sub>2</sub>O (5 equiv.) in DMF solvent and refluxed for 2 h, successfully affording 2-phenylthieno[2,3-*b*]quinoxaline **9b** (Scheme 4).

**Scheme 4.** Synthesis of 2-phenylthieno/furo[2,3-*b*]quinoxalines **9a** and **9b**.



The UV-vis absorption spectra for the compounds 4a, 9a, 9b, 7a, 7g, 7i and 8a was measured in DCM solvent (Fig. 1). In 2-phenylfuro/thio/seleno-fused the cases of [2,3b]quinoxaline derivatives 4a, 9a and 9b, the absorption maximum ( $\lambda_{max}$ ) and molar extinction coefficient ( $\mathcal{E}$ ) values of 2-phenylfuro[2,3-b]quinoxaline (4a:  $\lambda_{max}$  = 368 nm,  $\mathcal{E}$  = 23,694), 2-phenylthieno[2,3-b]quinoxaline (**9a**:  $\lambda_{max}$  = 369 nm, *E* = 40,194), 2-phenylselenopheno[2,3-*b*]quinoxaline (9b:  $\lambda_{\text{max}}$  = 380 nm,  $\mathcal{E}$  = 25,192) derivatives (Fig. 1a, Table 5) were higher 3-(aryl/alkylselanyl/sulfanyl)-2observed than phenylselenopheno[2,3-b]quinoxaline derivatives (**7a**:  $\lambda_{max}$  = 363 nm,  $\mathcal{E}$  = 17,455) (**7g**:  $\lambda_{max}$  = 365 nm,  $\mathcal{E}$  = 16,992), (**7i**:  $\lambda_{max}$ = 322 nm,  $\mathcal{E}$  = 11,327) and 6-phenyl-7-(phenylselanyl) selenopheno[2,3-b]pyrazine (8a:  $\lambda_{max}$  = 368 nm,  $\mathcal{E}$  = 17,057) derivative (Fig. 1b, Table 5).





The fluorescence spectra for the compounds **4a**, **9a**, **9b**, **7a**, **7g**, **7i** and **8a** was measured in DCM solvent (**Fig. 2**). The fluorescence maximum ( $F_{max}$ ) and Stokes shift values were in the range of 404 to 522 nm and 35 to 142 nm, respectively (**Table 5**) for 2-phenylfuro/thio/seleno-fused[2,3-*b*]quinoxaline derivatives **4a**, **9a** and **9b**. While, the 3-(aryl/alkylselanyl/sulfanyl)-2-phenylselenopheno[2,3-

*b*]quinoxaline derivatives **7a**, **7g**, **7i** and 6-phenyl-7-(phenylselanyl) selenopheno[2,3-*b*] pyrazine **8a** are nonfluorescent due to heavy atom present (S, Se) as phenylselanyl/sulfanyl substituents. The fluorescence quantum yield values ( $\Phi_f$ ) of 2-phenylfuro/thio/seleno-fused [2,3-*b*]quinoxaline derivatives **4a**, **9a** and **9b** were ( $\Phi_f$ : 0.002-0.171), while the fluorescence quantum yield values ( $\Phi_f$ ) of 3-(aryl/alkylselanyl/sulfanyl)-2-phenylselenopheno[2,3-

*b*]quinoxaline derivatives **7a**, **7g**, **7i** and 6-phenyl-7-(phenylselanyl)selenopheno[2,3-*b*]pyrazine **8a** were relatively low ( $\mathcal{D}_{f}$ : 0.002-0.004) due to heavy atom effect <sup>21</sup> The fluorescence spectra of 2-phenylfuro[2,3-b]quinoxaline **9a** (**Fig. 2a**) showed the higher fluorescence than the 2phenylthieno[2,3-b]quinoxaline **4a** and 2phenylselenopheno[2,3-b]quinoxaline **9b** (**Fig. 2b**). The difference in fluorescence intensity clearly showed the heavy atom effect.



Fig. 2. Fluorescence spectra in DCM.



Compound	$\lambda_{\max}(c) / nm$	$F_{\rm max}$ / nm	Stokes shift / nm	$\phi_{\rm f}^{\ b}$
4a	293 (39,532), 368 (23,694), 381 (21,110)	434	66	0.004
7a	287 (27,837), 363 (17,455)			0.002
7g	283 (28,549), 365 (16,992)			0.002
7i	262 (15,041), 322 (11,327)			0.001
8a	288 (27,767), 368 (17,057)			0.002
9a	279 (17,172), 369 (40,194), 383 (33,847)	404	35	0.171
9b	287 (39,892), 380 (25,192)	522	142	0.009
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In this study, we proposed the plausible mechanism for novel seleno-cascade cyclization. In the first step, iron salt and diphenyl diselenide are allowed to react which promoting the cleavage of Se-Se bond to give an organoselenyl cation and an organoselenyl anionic spacies<sup>22</sup>. The Fe(III) coordinates with one selenium atom from diphenyl diselenide, which results in the intermediate I, further the nucleophilic anti-attack on activated seleniranium ion I by intramolecular Se-nucleophile results into the intermediate II is achieved *via*  $S_N$ 2 displacement by the phenyl selenolate anion present in the reaction mixture to afford the corresponding 2-phenyl-3-(phenylselanyl)selenopheno[2,3-b]quinoxaline **7a**.

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Fig. 3. Plausible mechanism

#### **Conclusion:**

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In conclusion, we report the novel synthesis of three different heterocycles namely 2-arylselenopheno[2,3b]quinoxaline, 3-(aryl/alkylselanyl)-2-arylselenopheno[2,3b]quinoxaline and 6-phenyl-7-(arylselanyl)selenopheno[2,3b]pyrazine derivatives from the corresponding 2,3dichloroquinoxaline and 2,3-dichloropyrazine derivatives. Further, photophysical properties were investigated to study the effect of heteroatoms on UV-absorbance and fluorescence properties.

#### **Experimental: General**

All solvents and reagents were purchased from the suppliers and used without further purification. IR spectra were recorded on a JASCO FT/IR-460 Plus spectrophotometer. Reactions were monitored by TLC on silica plates using UVlight or lodine chamber for visualization. Evaporation and condensation were carried out in vacuo. NMR spectra were recorded with JEOL JNM-ECS 400 spectrometers with tetramethylsilane as an internal standard. Chemical shifts  $\delta$ and coupling constants J are given in ppm (parts per million) and Hz (hertz), respectively. The abbreviations were used as follows: s: singlet, d: doublet, t: triplet, m: multiplet. All known compound data are in consistent with the given literature reports. Scale up reactions also performed as per the given general procedure without any deviation. Melting points were measured by a Yanaco micromelting point apparatus. The HRMS were recorded with the Acquity XEVO QTof MS analyzer. UV-vis spectra were taken on a Hitachi U4100 spectrophotometer. Fluorescence spectra were measured on a FP-8600 spectrofluorometer. Fluorescence quantum yields were recorded on a Quantaurus-QY.

General procedure and spectral data for compounds 4a-4f.

NaSeH was prepared in situ by reactions of elemental selenium (1.0 equiv.) and sodium borohydride (2.0 equiv.) and ethanol (0.75 mL) / water (1.5 mL) mixture at 0°C for 15 min, after confirming that the solution changed from black to colorless and transparent (white), to this freshly prepared NaSeH solution, compounds 3a-3f (1.0 equiv.) and ethanol (1 mL) was added, and the mixture was stirred under reflux for 1 hour. After confirming the completion of the reaction by TLC (Hexane:EtOAc = 7:3), the reaction mixture was cooled to room temperature, and the obtained solution was extracted with ethyl acetate and water. Thereafter, the organic layer was washed with a brine solution and dried over anhydrous sodium sulphate. The residue was purified by silica gel column chromatography (Hexane:EtOAc = 19:1) afforded the corresponding 2-arylselenopheno[2,3b]quinoxaline derivatives **4a-4f** in 69-95% yields

#### 2-Phenylselenopheno[2,3-b]quinoxaline (4a)

Yield: 83%; Melting point: 134-135°C; IR (ATR): 1442, 1330, 1044, 753 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.14-8.08 (2H, m, H-5 and H-8), 7.88 (1H, s, H-3), 7.79-7.72 (4H, m, H-6, H-7, H-2' and H-6'), 7.50-7.44 (3H, m, H-3', H-4' and H-5'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  159.4, 155.2, 155.1, 141.2, 140.2, 135.0, 130.3, 129.3 (2C), 129.26, 129.23, 128.3, 127.1 (2C), 120.2; <sup>77</sup>Se NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  488.9; HRESIMS: *m/z* 311.0065 [M+H]<sup>+</sup> (calcd. for C<sub>16</sub>H<sub>11</sub>N<sub>2</sub>Se, 311.0087).

#### 2-(p-Tolyl)selenopheno[2,3-b]quinoxaline (4b)

Yield: 77%; Melting point: 174-175°C; IR (ATR): 3039, 2910, 1555, 1138, 1043, 801, 751, 461 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.11-8.06 (2H, m, H-5 and H-8), 7.80 (1H, s, H-3), 7.75-7.71 (2H, m, H-6 and H-7), 7.58 (2H, d, *J* = 8.2 Hz, H-2' and H-6'), 7.23 (2H, d, *J* = 8.2 Hz, H-3' and H-5'), 2.37 (3H, s, H-7'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  159.5, 155.4, 141.3, 140.8, 140.2, 132.3, 130.0 (2C), 129.3, 129.1, 128.4, 127.1 (2C), 119.5, 21.5; <sup>77</sup>Se NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  486.9; HRESIMS: *m/z* 325.0226 [M+H]<sup>+</sup> (calcd. for C<sub>17</sub>H<sub>13</sub>N<sub>2</sub>Se, 325.0244).

#### 2-(4-Methoxyphenyl)selenopheno[2,3-b]quinoxaline (4c)

Yield: 83%; Melting point: 140-142°C; IR (ATR): 1601, 1505, 1258, 1182, 1036, 748 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.11-8.10 (2H, m, H-5 and H-8), 7.78-7.69 (5H, m, H-3, H-6, H-7, H-2' and H-6'), 7.03-7.00 (2H, m, H-3' and H-5'), 3.89 (3H, s, H-7'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  161.5, 159.5, 155.7, 155.1, 141.3, 140.1, 129.3, 129.0, 128.7, 128.6, 128.4, 127.8, 118.63, 118.58, 114.8, 114.7, 55.6; <sup>77</sup>Se NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  484.8; HRESIMS: *m/z* 341.0182 [M+H]<sup>+</sup> (calcd. for C<sub>17</sub>H<sub>13</sub>N<sub>2</sub>OSe, 341.0193).

#### 2-(4-Fluorophenyl)selenopheno[2,3-b]quinoxaline (4d)

Yield: 95%; Melting point: 179-180°C; IR (ATR): 3053, 1560, 1503, 1229, 1045, 828, 750 cm  $^{-1}$ .  $^{1}\text{H}$  NMR (400 MHz, CDCl\_3):  $\delta$ 

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8.10-8.04 (2H, m, H-5 and H-8), 7.73 (1H, s, H-3), 7.76-7.71 (2H, m, H-6 and H-7), 7.65-7.62 (2H, m, H-3' and H-5'), 7.12 (2H, t, *J* = 8.5 Hz, H-2' and H-6'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  165.2, 162.6, 159.4, 155.1, 153.8, 141.2, 140.2, 131.4, 129.40, 129.36, 129.3, 129.27, 129.02, 128.4, 120.3, 116.5, 116.3; <sup>77</sup>Se NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  489.9; <sup>19</sup>F-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  -109.63; HRESIMS: *m/z* 328.9970 [M+H]<sup>+</sup> (calcd. for C<sub>16</sub>H<sub>10</sub>N<sub>2</sub>SeF, 328.9993).

#### 2-(3-Fluorophenyl)selenopheno[2,3-b]quinoxaline (4e)

Yield: 69%; Melting point: 169-170°C; IR (ATR): 3047, 1583, 1476, 1329, 1161, 1045, 780 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.11-8.105 (2H, m, H-5 and H-8), 7.82 (1H, s, H-3), 7.76-7.71 (2H, m, H-6 and H-7), 7.46-7.36 (3H, m, H-2', H-4' and H-6'), 7.13-7.09 (1H, m, H-5'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  164.4, 161.9, 159.3, 154.8, 153.4, 141.3, 140.4, 137.24, 137.16, 131.0, 130.8, 129.6, 129.5, 129.4, 128.4, 123.0, 121.3, 117.2, 117.0, 114.1, 113.8; <sup>77</sup>Se NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  492.8; <sup>19</sup>F-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  -111.57; HRESIMS: *m/z* 328.9970 [M+H]<sup>+</sup> (calcd. for C<sub>16</sub>H<sub>10</sub>N<sub>2</sub>SeF, 328.9993).

#### 2-(2-Fluorophenyl)selenopheno[2,3-b]quinoxaline (4f)

Yield: 95%; Melting point: 125-126°C; IR (ATR): 3053, 1447, 1102, 1046, 747 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.14-8.08 (2H, m, H-5 and H-8), 8.06 (1H, s, H-3), 7.78-7.74 (2H, m, H-6 and H-7), 7.71-7.67 (1H, m, H-4'), 7.40-7.37 (1H, m, H-5'), 7.27-7.18 (2H, m, H-4' and H-6'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  161.0, 159.61, 159.55, 158.5, 154.6, 147.4, 141.3, 140.4, 131.6, 131.5, 129.8, 129.8, 129.5, 129.41, 129.38, 128.4, 125.0, 124.9, 124.07, 124.00, 123.1, 123.0, 116.9, 116.7; <sup>77</sup>Se NMR (75 MHz, CDCl<sub>3</sub>): 512.5; <sup>19</sup>F-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  -111.66; HRESIMS: *m/z* 328.9966 [M+H]<sup>+</sup> (calcd. for C<sub>16</sub>H<sub>10</sub>N<sub>2</sub>SeF, 328.9993).

#### General procedure and spectral data for compounds 7a-7i.

To a stirred mixture of diorganyl diselenides (1.0 equiv.) and  $FeCl_3 \cdot 6H_2O$  (2.0 equiv.) in dichloromethane solvent was added the compounds 2-(methylselanyl)-3- (arylethynyl)quinoxaline **5** (1.0 equiv.) and heated at 45°C, successfully affording the corresponding 3- (arylselanyl/sulfanyl)-2-arylselenopheno[2,3-*b*]quinoxaline derivatives **7a-7i** in 57-92% yields.

## 2-Phenyl-3-(phenylselanyl)selenopheno[2,3-b]quinoxaline (7a)

Yield: 74%; Melting point: 155-156°C; IR (ATR): 2920, 1474, 1437, 1063, 1020, 759, 743, 690 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.23 (1H, dd, *J* = 6.9 and 2.9 Hz, H-5 or H-8), 8.13 (1H, dd, *J* = 7.2 and 2.6 Hz, H-5 or H-8), 7.80-7.75 (2H, m, H-6 and H-7), 7.66 (2H, dd, *J* = 6.6 and 3.2 Hz, H-2" and H-6"), 7.44-7.43 (3H, m, H-3", H-4" and H-5"), 7.36-7.34 (2H, m, H-2' and H-6'), 7.10-7.09 (3H, m, H-3', H-4' and H-5'); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  159.1, 158.4, 154.3, 141.6, 140.9, 135.8,

#### (calcd. for C<sub>22</sub>H<sub>15</sub>N<sub>2</sub>Se<sub>2</sub>, 466.9566). **3-(Phenylselanyl)-2-(***p***-tolyl)selenopheno[2,3-***b***]quinoxaline (7b)**

MHz, CDCl<sub>3</sub>): δ 556.7, 303.9; HRESIMS: *m/z* 466.9581 [M+H]<sup>+</sup>

Yield: 81%; Melting point: 155-157°C; IR (ATR): 2922, 1474, 1436, 1185, 1065, 1019, 814, 762, 736, 720, 689 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.13 (1H, dd, *J* = 7.2 and 3.2 Hz, H-5 or H-8), 8.04 (1H, dd, *J* = 6.9 and 2.9 Hz, H-5 or H-8), 7.71-7.66 (2H, m, H-6 and H-7), 7.50 (2H, d, *J* = 8.0 Hz, H-2' and H-6'), 7.28-7.27 (2H, m, H-2" and H-6"), 7.19-7.17 (2H, m, H-3' and H-5'), 7.03-7.01 (3H, m, H-3", H-4" and H-5"), 2.33 (3H, s, H-7'); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  159.1, 158.9, 154.5, 141.6, 140.8, 140.3, 133.0, 132.0, 131.2 (2C), 130.1, 129.9 (2C), 129.8, 129.33 (2C), 129.25, 129.1 (2C), 128.2, 126.7, 118.1, 21.5; <sup>77</sup>Se NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  553.7, 302.1; HRESIMS: *m/z* 480.9746 [M+H]<sup>+</sup> (calcd. for C<sub>23</sub>H<sub>17</sub>N<sub>2</sub>Se<sub>2</sub>, 480.9722).

#### 2-(4-Methoxyphenyl)-3-(phenylselanyl)selenopheno[2,3b]quinoxaline (7c)

Yield: 92%; Melting point: 142-144°C; IR (ATR): 2928, 2832, 1600, 1571, 1473, 1254, 1171, 1025, 829, 822, 764, 742 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.22-8.19 (1H, m, H-5 or H-8), 8.13-8.10 (1H, m, H-5 or H-8), 7.77-7.74 (2H, m, H-6 and H-7), 7.66 (2H, d, *J* = 8.7 Hz, H-2' and H-6'), 7.36-7.33 (2H, m, H-2" and H-6"), 7.11-7.09 (3H, m, H-3", H-4" and H-5"), 6.96 (2H, d, *J* = 8.7 Hz, H-3' and H-5'), 3.86 (3H, s, H-7'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  161.0, 159.0, 158.7, 154.7, 141.6, 140.8, 132.1 (2C), 131.6, 130.9 (2C), 130.0, 129.7, 129.2, 129.1 (2C), 128.2, 128.1, 126.7, 117.4, 114.1 (2C), 55.5; <sup>77</sup>Se NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  550.4, 300.7; HRESIMS: *m/z* 494.9670 [M+H]<sup>+</sup> (calcd. for C<sub>23</sub>H<sub>17</sub>N<sub>2</sub>OSe<sub>2</sub>, 494.9700).

#### 2-(4-Fluorophenyl)-3-(phenylselanyl)selenopheno[2,3b]quinoxaline (7d)

Yield: 69%; Melting point: 155-157°C; IR (ATR): 3051, 1474, 1062, 1019, 759, 743, 690, 604 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.24-8.22 (1H, m, H-5 or H-8), 8.15-8.12 (1H, m, H-5 or H-8), 7.79-7.76 (2H, m, H-6 and H-7), 7.67-7.65 (2H, m, H-2' and H-6'), 7.45-7.43 (2H, m, H-2" and H-6"), 7.36-7.34 (2H, m, H-3' and H-6'), 7.10-7.09 (3H, m, H-3", H-4" and H-5"); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  159.1, 158.4, 154.3, 148.2, 141.5, 140.9, 135.8, 133.5, 131.8, 131.3 (2C), 130.1, 130.0 (2C), 129.9, 129.8, 129.5, 129.3, 129.1 (2C), 128.6 (2C), 128.2, 126.8, 118.8, 72.7; <sup>77</sup>Se NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  556.7, 303.6; <sup>19</sup>F-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  -109.75; HRESIMS: *m/z* 484.9472 [M+H]<sup>+</sup> (calcd. for C<sub>22</sub>H<sub>14</sub>N<sub>2</sub>FSe<sub>2</sub>, 484.9471).

#### 2-(3-Fluorophenyl)-3-(phenylselanyl)selenopheno[2,3b]quinoxaline (7e)

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Yield: 61%; Melting point: 127-128°C; IR (ATR): 3063, 1576, 1474, 1068, 763, 733, 722, 684 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.26-8.23 (1H, m, H-5 or H-8), 8.15-8.12 (1H, m, H-5 or H-8), 7.81-7.78 (2H, m, H-6 and H-7), 7.41-7.34 (5H, m, H-2", H-3", H-4", H-5" and H-6"), 7.14-7.09 (4H, m, H-2', H-4', H-5' and H-6'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  163.7, 161.2, 158.8, 155.8, 154.1, 141.6, 141.0, 137.8, 137.7, 131.7 (2C), 131.3, 130.2, 130.10, 130.07, 129.5, 129.2 (2C), 128.2, 127.0, 125.7, 119.9, 117.1, 116.8, 116.7, 116.5; <sup>77</sup>Se NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  560.2, 308.7; <sup>19</sup>F-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  -112.07; HRESIMS: *m/z* 484.9500 [M+H]<sup>+</sup> (calcd. for C<sub>22</sub>H<sub>14</sub>N<sub>2</sub>FSe<sub>2</sub>, 484.9471).

#### 2-(2-Fluorophenyl)-3-(phenylselanyl)selenopheno[2,3b]quinoxaline (7f)

Yield: 88%; Melting point: 110-111°C; IR (ATR): 3065, 1476, 1437, 1065, 757, 748, 738, 727 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.25-8.22 (1H, m, H-5 or H-8), 8.14-8.12 (1H, m, H-5 or H-8), 7.81-7.77 (2H, m, H-6 and H-7), 7.47-7.35 (4H, m, H-3', H-4', H-5' and H-6'), 7.22-7.05 (5H, m, H-2", H-3", H-4", H-5" and H-6"); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  160.3, 159.3, 157.8, 153.3, 150.1, 141.4, 140.8, 133.5, 132.3 (2C), 131.7, 131.6, 130.8, 130.10, 130.06, 129.4, 128.9 (2C), 128.2, 127.0, 124.19, 124.16, 123.9, 123.8, 122.5, 116.3, 116.1; <sup>77</sup>Se NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  569.5, 319.6; <sup>19</sup>F-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  -110.428; HRESIMS: *m/z* 484.9482 [M+H]<sup>+</sup> (calcd. for C<sub>22</sub>H<sub>14</sub>N<sub>2</sub>FSe<sub>2</sub>, 484.9471).

## 3-(Methylselanyl)-2-phenylselenopheno[2,3-b]quinoxaline (7g)

Yield: 66%; Melting point: 118-120°C; IR (ATR): 3064, 3012, 2924, 1478, 1061.9, 756, 716, 691, 505 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.32 (1H, dd, *J* = 6.4 and 3.2 Hz, H-5 or H-8), 8.14 (1H, dd, *J* = 6.4 and 3.2 Hz, H-5 or H-8), 7.82-7.79 (2H, m, H-6 and H-7), 7.73-7.71 (2H, m, H-2' and H-6'), 7.54-7.48 (3H, m, H-3', H-4' and H-5'), 2.38 (3H, s, H-7'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  159.2, 154.7, 153.8, 141.3, 140.6, 136.1, 130.0 (2C), 129.79, 129.75, 129.3, 128.7 (2C), 128.2, 119.0, 8.6; <sup>77</sup>Se NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  551.4, 128.9; HRESIMS: *m/z* 404.9413 [M+H]<sup>+</sup> (calcd. for C<sub>17</sub>H<sub>13</sub>N<sub>2</sub>Se<sub>2</sub>, 404.9409).

## 3-(Butylselanyl)-2-phenylselenopheno[2,3-*b*]quinoxaline (7h)

Yield: 80%; Sticky; IR (ATR): 3058, 3021, 2954, 2924, 1478, 1440, 1263, 1063, 755, 708, 690 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.32 (1H, dd, *J* = 7.3 and 2.7 Hz, H-5 or H-8), 8.15 (1H, dd, *J* = 7.3 and 2.7 Hz, H-5 or H-8), 7.82-7.79 (2H, m, H-6 and H-7), 7.73-7.70 (2H, m, H-2' and H-6'), 7.51-7.47 (3H, m, H-3', H-4' and H-5'), 3.05 (2H, t, *J* = 7.6 Hz, H-1"), 1.55-1.48 (2H, m, H-2"), 1.30-1.21 (2H, m, H-3"), 0.77 (3H, t, *J* = 7.3 Hz, H-4"); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  159.1, 154.8, 154.4, 141.2, 140.5, 136.1, 129.91 (2C), 129.85, 129.6, 129.5, 129.1,

128.5 (2C), 128.1, 118.3, 32.2, 27.7, 22.6, 13.5;  $\sqrt[7]{Se}$  NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  551.1, 204.3; HRESIMS:  $m/z^{1}446.9882$  [M74H]<sup>4</sup> (calcd. for C<sub>20</sub>H<sub>19</sub>N<sub>2</sub>Se<sub>2</sub>, 446.9879).

**2-Phenyl-3-(methylthio)selenopheno[2,3-***b***]quinoxaline (7i) Yield: 57%; Melting point: 115-117°C; IR (ATR): 2918, 2849, 1124, 1066, 756, 733, 726, 691 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.33 (1H, dd,** *J* **= 6.6 and 3.4 Hz, H-5 or H-8), 8.15 (1H, dd,** *J* **= 6.6 and 3.4 Hz, H-5 or H-8), 7.83-7.77 (4H, m, H-6, H-7, H-2' and H-6'), 7.55-7.48 (3H, m, H-3', H-4' and H-5'), 2.55 (3H, s, H-7'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 158.5, 154.9, 153.5, 141.1, 140.8, 135.3, 130.02 (2C), 129.96, 129.8, 129.4, 128.8 (2C), 128.3, 124.8, 18.1; <sup>77</sup>Se NMR (75 MHz, CDCl<sub>3</sub>): δ 529.3; HRESIMS:** *m/z* **356.9951 [M+H]<sup>+</sup> (calcd. for C<sub>17</sub>H<sub>13</sub>N<sub>2</sub>SSe, 356.9965).** 

#### General procedure and spectral data for compounds 8a-8e.

To a stirred mixture of diorganyl diselenides (1.0 equiv.) and  $FeCl_3 \cdot 6H_2O$  (2.0 equiv.) in dichloromethane solvent was added the 2-(methylselanyl)-3-(arylethynyl)quinoxaline **6** (1.0 equiv.) at 45°C, successfully affording the corresponding 6-phenyl-7-(arylselanyl)selenopheno[2,3-*b*]pyrazine derivatives **8a-e** in 47-70% yields.

#### Phenyl-7-(phenylselanyl)selenopheno[2,3-b]pyrazine (8a)

Yield: 62%; Melting point: 57-58°C; IR (ATR): 3052, 3023, 1575, 1475, 1437, 1345, 1180, 732, 706, 687, 667, 629 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.70 (1H, d, *J* = 2.3 Hz, H-5 or H-6), 8.45 (1H, d, *J* = 2.3 Hz, H-5 or H-6), 7.60 (2H, dd, *J* = 6.3 and 3.4 Hz, H-2" and H-6"), 7.43-7.41 (3H, m, H-3", H-4" and H-5"), 7.21-7.20 (2H, m, H-2' and H-6'), 7.11-7.10 (3H, m, H-3', H-4' and H-5'); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  159.8, 157.8, 153.9, 142.6, 140.8, 135.6, 132.1, 130.3 (2C), 130.0 (2C), 129.6, 129.2 (2C), 128.6 (2C), 126.5, 118.5; <sup>77</sup>Se NMR (95 MHz, CDCl<sub>3</sub>):  $\delta$  575.4, 293.2; HRESIMS: *m/z* 416.9402 [M+H]<sup>+</sup> (calcd. for C<sub>18</sub>H<sub>13</sub>N<sub>2</sub>Se<sub>2</sub>, 416.9409).

#### 6-(p-Tolyl)-7-(phenylselanyl)selenopheno[2,3-b]pyrazine (8b)

Yield: 69%; Melting point: 67-68°C; IR (ATR): 3054, 2916, 1475, 1346, 1185, 1098, 811, 732 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  8.68 (1H, d, *J* = 2.7 Hz, H-5 or H-6), 8.43 (1H, d, *J* = 2.7 Hz, H-5 or H-6), 7.51 (2H, d, *J* = 7.6 Hz, H-2' and H-6'), 7.26-7.20 (4H, m, H-3', H-5', H-2" and H-6"), 7.11-7.10 (3H, m, H-3", H-4" and H-5"), 2.40 (3H, s, H-7'); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>):  $\delta$  159.7, 158.4, 154.1, 142.5, 140.6, 140.0, 132.7, 132.3, 130.1 (2C), 129.9 (2C), 129.3 (2C), 129.2 (2C), 126.4, 117.9, 21.5; <sup>77</sup>Se NMR (115 MHz, CDCl<sub>3</sub>):  $\delta$  572.8, 291.6; HRESIMS: *m/z* 430.9554 [M+H]<sup>+</sup> (calcd. for C<sub>19</sub>H<sub>15</sub>N<sub>2</sub>Se<sub>2</sub>, 430.9566).

#### 6-(4-Methoxyphenyl)-7-(phenylselanyl)selenopheno[2,3b]pyrazine (8c)

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Yield: 70%; Melting point: 118-119°C; IR (ATR): 2924, 2850, 1601, 1474, 1347, 1291, 1250, 1171, 1020, 831, 741, 690 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  8.66 (1H, d, *J* = 2.7 Hz, H-5 or H-6), 8.41 (1H, d, *J* = 2.1 Hz, H-5 or H-6), 7.58 (2H, d, *J* = 8.9 Hz, H-3' and H-5'), 7.21-7.20 (2H, m, H-2" and H-6"), 7.11-7.10 (3H, m, H-3", H-4" and H-5"), 6.94 (2H, d, *J* = 8.9 Hz, H-2' and H-6'), 3.84 (3H, s, H-7'); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>):  $\delta$  160.8, 159.6, 158.1, 154.2, 142.5, 140.6, 132.3, 131.5 (2C), 130.0 (2C), 129.2 (2C), 128.0, 126.4, 117.3, 114.1 (2C), 55.5; <sup>77</sup>Se NMR (114MHz, CDCl<sub>3</sub>):  $\delta$  570.0, 290.8; HRESIMS: *m/z* 446.9516 [M+H]<sup>+</sup> (calcd. for C<sub>19</sub>H<sub>15</sub>N<sub>2</sub>OSe<sub>2</sub>, 446.9515).

#### 6-(3-Fluorophenyl)-7-(phenylselanyl)selenopheno[2,3-

#### b]pyrazine (8d)

Yield: 60%; Sticky; IR (ATR): 3056, 2924, 1578, 1474, 1344, 1146, 1096, 785, 732, 713, 682 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.72 (1H, d, *J* = 2.7 Hz, H-5 or H-6), 8.48 (1H, d, *J* = 2.3 Hz, H-5 or H-6), 7.39-7.30 (3H, m, H-3", H-4" and H-5"), 7.23-7.21 (2H, m, H-2" and H-6"), 7.12-7.11 (4H, m, H-2', H-4', H-5' and H-6'); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  163.4, 161.5, 159.7, 155.3, 153.7, 142.7, 141.0, 137.6, 137.5, 131.6, 130.7 (2C), 130.2, 130.1, 129.2 (2C), 126.8, 125.8, 119.7, 117.1, 116.9, 116.5, 116.3; <sup>77</sup>Se NMR (95 MHz, CDCl<sub>3</sub>):  $\delta$  579.1, 297.8; <sup>19</sup>F-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  -112.10; HRESIMS: *m/z* 434.9307 [M+H]<sup>+</sup> (calcd. for C<sub>18</sub>H<sub>12</sub>N<sub>2</sub>FSe<sub>2</sub>, 434.9315).

#### 6-(2-Fluorophenyl)-7-(phenylselanyl)selenopheno[2,3b]pyrazine (8e)

Yield: 47%; Melting point: 73-75°C; IR (ATR): 3071, 2921, 1468, 1354, 1097, 851, 747, 688, 472 cm<sup>-1</sup>; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.71 (1H, d, *J* = 2.3 Hz, H-5 or H-6), 8.48 (1H, d, *J* = 2.3 Hz, H-5 or H-6), 7.41 (2H, t, *J* = 7.2 Hz, H-2" and H-6"), 7.22-7.08 (7H, m, H-3', H-4', H-5', H-6', H-3", H-4" and H-5"); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  160.4, 160.1, 158.1, 153.0, 149.4, 142.5, 140.9, 131.9, 131.52, 131.45, 131.2 (2C), 129.0 (2C), 126.8, 124.12, 124.09, 123.5, 122.2, 116.2, 116.0; <sup>77</sup>Se NMR (75 MHz, CDCl<sub>3</sub>):  $\delta$  587.8, 307.6; <sup>19</sup>F-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  -110.95; HRESIMS: *m/z* 434.9309 [M+H]<sup>+</sup> (calcd. for C<sub>18</sub>H<sub>12</sub>N<sub>2</sub>FSe<sub>2</sub>, 434.9315).

#### General procedure and spectral data for 2-phenylfuro[2,3b]quinoxaline (9a)

To the solution of 2-chloro-3-(phenylethynyl)quinoxaline **3a** (1.0 equiv.) in dimethyl sulfoxide (0.6 mL) and water (2.4 mL) was added NaOH (5.0 equiv.) are refluxed for 2 hours. After completion of the reaction, monitored by TLC (Hexane: EtOAc = 20: 1), the reaction mixture was cooled to room temperature, and the obtained solution was extracted with ethyl acetate and water. Thereafter, the organic layer was washed with a saturated saline solution and dried over anhydrous sodium sulphate. The residue was isolated and purified by silica gel column chromatography (Hexane:EtOAc

= 20:1), successfully affording the yellow-white Asolid nize phenylfuro [2,3-*b*] quinoxaline **9a** in 34% yield.

Yield: 34%; Melting point: 188-190°C; IR (ATR): 3102, 1563, 1386, 1310, 1214, 1013, 891, 767.1, 755, 741, 687, 659 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.18-8.17 (1H, m, H-5 or H-8), 8.12-8.11 (1H, m, H-5 or H-8), 8.03-8.02 (2H, m, H-6 and H-7), 7.74 (2H, dd, *J* = 5.4 and 2.6 Hz, H-2' and H-6'), 7.55-7.51 (3H, m, H-3', H-4' and H-5'), 7.28 (1H, s, H-3); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  164.1, 154.5, 144.7, 142.4, 138.9, 131.4, 129.3 (2C), 128.9, 128.8, 128.6, 128.4, 126.3 (2C), 100.9; HRESIMS: *m/z* 247.0847 [M+H]<sup>+</sup> (calcd. for C<sub>16</sub>H<sub>11</sub>N<sub>2</sub>O, 247.0871).

## General procedure and spectral data for 2-phenylthieno [2,3-*b*]quinoxaline (9b)

The mixture of 2-chloro-3-(phenylethynyl) quinoxaline 3a (1.0 equiv.) and NaSH·xH<sub>2</sub>O (5.0)equiv.) in dimethylformamide (2 mL) was refluxed for 2 hours. After completion of the reaction by TLC (Hexane: EtOAc = 20: 1), the reaction mixture was cooled to room temperature, and the reaction mixture was extracted with ethyl acetate and water. Thereafter, the organic layer was washed with a saturated saline solution and dried over anhydrous sodium sulphate. After removing the solvent with an evaporator, the residue was isolated and purified by silica gel column chromatography (Hexane:EtOAc = 20:1) successfully affording the resulting yellow-white solid 2-phenylthieno [2,3-b] quinoxaline 9b in 87% yield.

Yield: 87%; Melting point: 177-178°C; IR (ATR): 1481, 1442, 1278, 1130, 1072, 758, 713, 683, 595 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.15-8.09 (2H, m, H-5 and H-8), 7.80-7.72 (4H, m, H-6, H-7, H-2' and H-6'), 7.71 (1H, s, H-3), 7.49-7.43 (3H, m, H-3', H-4' and H-5'); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  156.6, 152.5, 152.0, 141.4, 140.3, 133.2, 130.5, 129.3 (2C), 129.2, 128.6, 126.9 (2C), 117.1; HRESIMS: *m/z* 263.0625 [M+H]<sup>+</sup> (calcd. for C<sub>16</sub>H<sub>11</sub>N<sub>2</sub>S, 263.0643).

#### **Conflicts of interest**

"There are no conflicts to declare".

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#### **Supporting Information:**

Experimental procedures, characterization data for the new compounds, and copies of <sup>1</sup>H and <sup>13</sup>C-NMR spectra. This material is available free of charge *via* the Internet at http://

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## Synthesis and photophysical properties of selenopheno[2,3-*b*]quinoxaline and selenopheno[2,3-*b*]pyrazine heteroacenes

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