# **Supporting Information**

### Copper-Catalyzed Diarylation of Se with Aryl Iodides and Heterocycles

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## **General Information**

5-aryl-1,3,4-oxadiazole<sup>1</sup> and 5-aryl-1,3-azole<sup>2</sup> were prepared according to the reported procedures. <sup>1</sup>H and <sup>13</sup>C spectra of known compounds were in accordance with those described in the literatures. All other reagents were purchased from TCI, Sigma-Aldrich, Alfa Aesar, Acros, and Meryer and used without further purification. Toluene was distilled from Na under nitrogen and stored under nitrogen. <sup>1</sup>H NMR (500 MHz), <sup>13</sup>C NMR (125 MHz) and <sup>19</sup>F NMR (470 MHz) spectra were recorded in CDCl<sub>3</sub> or (CD<sub>3</sub>)<sub>2</sub>SO solutions using a Burker AVANCE 500 spectrometer. Highresolution mass spectra were recorded on an ESI-Q-TOF mass spectrometer. Analysis of crude reaction mixture was done on the Varian 4000 GC/MS and 1200 LC. All conducted using standard Schlenk techniques. reactions were Column chromatography was performed using EM silica gel 60 (300-400 m).

### **General Experimental Procedures:**

General Procedure for C-H arylselenation of 2-Aryl-1,3,4-oxadiazoles: In a 25 mL Schlenk tube equipped with a stir bar were placed 2-aryl-1,3,4-oxadiazoles (0.2 mmol), iodobenzene (0.6 mmol), Se (0.6 mmol), CuCl<sub>2</sub> (10 mol %), and Na<sub>2</sub>CO<sub>3</sub> (0.8 mmol) in DMF (2 mL). The tube was evacuated and refilled with N<sub>2</sub> three times. The reaction mixture was stirred at 140 °C for 24 h. After it was cooled, the reaction mixture was diluted with 10 mL of ethyl ether, and filtered through a pad of silica gel, followed by washing the pad of silica gel with the same solvent (20 mL). The filtrate was washed with water (3×15 mL). The organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The residue was then purified by flash chromatography on silica gel to provide the corresponding product.

General Procedure for C-H arylselenation of 5-Aryl-1,3-azoles: In a 25 mL Schlenk tube equipped with a stir bar were placed 5-aryl-1,3-azoles (0.2 mmol), iodobenzene (0.6 mmol), Se (0.6 mmol), CuCl<sub>2</sub> (10 mol %), and Cs<sub>2</sub>CO<sub>3</sub> (1.4 mmol) in DMF (2 mL). The tube was evacuated and refilled with N<sub>2</sub> three times. The reaction mixture was stirred at 140 °C for 24 h. After it was cooled, the reaction mixture was diluted with 10 mL of ethyl ether, and filtered through a pad of silica gel, followed by washing the pad of silica gel with the same solvent (20 mL). The filtrate was washed with water (3×15 mL). The organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The residue was then purified by flash chromatography on silica gel to provide the corresponding product.

**Procedure for C-H arylselenation of quinoline N-Oxide:** In a 25 mL Schlenk tube equipped with a stir bar were placed quinoline N-Oxide (0.2 mmol), iodobenzene 2 (0.6 mmol), Se (0.6 mmol), CuI (10 mol %), 1,10-Phen (10 mol%) and Ag<sub>2</sub>CO<sub>3</sub> (0.4

mmol) in toluene (2 mL). The tube was evacuated and refilled with  $O_2$  three times. The reaction mixture was stirred at 140 °C for 24 h. After it was cooled, the reaction mixture was diluted with 10 mL of ethyl ether, and filtered through a pad of silica gel, followed by washing the pad of silica gel with the same solvent (20 mL). The filtrate was washed with water (3×15 mL). The organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The residue was then purified by flash chromatography on silica gel to provide the corresponding product.

### **Characterization of Products in Details :**

2-Phenyl-5-(phenylselanyl)-1,3,4-oxadiazole<sup>3</sup>



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (85 % yield), mp 52-53  $^{\circ}$ C. The <sup>1</sup>H, <sup>13</sup>C NMR spectra were in accordance with those described in the literature.

2-(Naphthalen-2-ylselanyl)-5-phenyl-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a white solid (88 % yield) , mp 106-107 °C. **<sup>1</sup>H NMR** (500 MHZ, CDCl<sub>3</sub>):  $\delta$  8.28 (s, 1H), 7.94-7.92 (m, 2H), 7.85-7.80 (m, 3H), 7.76 (dd, J = 8.6, 1.7 Hz, 1H), 7.55-7.51 (m, 2H), 7.49-7.46 (m, 1H), 7.44-7.41 (m, 2H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  167.3, 156.2, 134.8, 133.9, 133.3, 131.8, 131.3, 129.5, 129.0, 127.9, 127.8, 127.4, 126.9, 126.8, 123.5, 121.4. HRMS (ESI): calcd for C<sub>18</sub>H<sub>12</sub>Cl<sub>2</sub>OSe [M + H]<sup>+</sup> 353.0188, found 353.0165.

2-Phenyl-5-(p-tolylselanyl)-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a white solid (93 % yield), mp 83-84 °C. <sup>1</sup>H NMR (500 MHZ, CDCl<sub>3</sub>):  $\delta$  7.93 (d, *J* = 7.2 Hz, 2H), 7.64 (d, J = 8.0 Hz, 2H), 7.49-7.42 (m, 3H), 7.18 (d, *J* = 8.0 Hz, 2H), 2.35 (s, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  167.1, 156.6, 140.1, 135.3, 135.2, 131.8, 130.7, 129.0, 126.8, 123.6, 120.4, 21.3. HRMS (ESI): calcd for C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>OSe [M + H]<sup>+</sup> 317.0188, found 317.0188.

2-(4-Methoxyphenylselanyl)-5-phenyl-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (83 % yield), mp 94-95 °C. <sup>1</sup>H NMR (500 MHZ, CDCl<sub>3</sub>):  $\delta$  7.92 (d, *J* = 7.0 Hz, 2H), 7.69 (d, J = 8.8 Hz, 2H), 7.49-7.42 (m, 3H), 6.90 (d, *J* = 8.8 Hz, 2H), 3.80 (s, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  167.0, 161.0, 156.9, 137.5, 131.7, 126.7, 123.6, 115.5, 113.9, 55.4. HRMS (ESI): calcd for C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>Se [M + H]<sup>+</sup> 333.0137, found 333.0104.

2-(Mesitylselanyl)-5-phenyl-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a white solid (95 % yield), mp 115-116 °C. **<sup>1</sup>H NMR** (500 MHZ, CDCl<sub>3</sub>):  $\delta$  7.91-7.90 (m, 2H), 7.48-7.42 (m, 3H), 7.01 (s, 2H), 2.56 (s, 6H), 2.30 (s, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  166.8, 156.6, 143.6, 140.6, 131.6, 129.3, 128.9, 126.7, 123.7, 122.7, 24.4, 21.1. **HRMS** (ESI): calcd for C<sub>17</sub>H<sub>16</sub>N<sub>2</sub>OSe [M + H]<sup>+</sup> 345.0501, found 345.0531.

2-(4-Fluorophenylselanyl)-5-phenyl-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (76 % yield), mp 73-74 °C. <sup>1</sup>H NMR (500 MHZ, CDCl<sub>3</sub>):  $\delta$  7.95-7.93 (m, 2H), 7.79-7.75 (m, 2H), 7.52-7.44 (m, 3H), 7.11-7.08 (m, 2H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  167.2, 163.7 (d, *J* = 251.0 Hz), 156.2, 137.7 (d, *J* = 8.3 Hz), 131.9, 129.0, 126.8, 123.5, 118.6 (d, *J* = 3.3 Hz), 117.2 (d, *J* = 22.2 Hz); <sup>19</sup>F NMR (470 MHz, CDCl<sub>3</sub>):  $\delta$  -110.2 (s, 1F). HRMS (ESI): calcd for

 $C_{14}H_9FN_2OSe [M + H]^+ 320.9937$ , found 320.9943.

2-(4-Chlorophenylselanyl)-5-phenyl-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (74 % yield), mp 86-87 °C. <sup>1</sup>H NMR (500 MHZ, CDCl<sub>3</sub>):  $\delta$  7.95 (d, *J* = 7.3 Hz, 2H), 7.70 (d, *J* = 8.5 Hz, 2H), 7.52-7.49 (m, 1H), 7.48-7.45 (m, 2H), 7.36 (d, J = 8.4 Hz, 2H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  167.3, 155.8, 136.4, 136.3, 131.9, 130.1, 129.1, 126.8, 123.4, 122.2. HRMS (ESI): calcd for C<sub>14</sub>H<sub>9</sub>ClN<sub>2</sub>OSe [M + H]<sup>+</sup> 336.9642, found 336.9662.

2-(4-Bromophenylselanyl)-5-phenyl-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (62 % yield), mp 91-92 °C. <sup>1</sup>H NMR (500 MHZ, CDCl<sub>3</sub>):  $\delta$  7.96-7.94 (m, 2H), 7.64-7.62 (m, 2H), 7.52-7.45 (m, 5H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  167.3, 155.6, 136.6, 133.0, 131.9, 129.1, 126.8, 124.5, 123.4, 122.9. HRMS (ESI): calcd for C<sub>14</sub>H<sub>9</sub>BrN<sub>2</sub>OSe [M + Na]<sup>+</sup> 402.8961, found 402.8989.

2-Phenyl-5-(4-(trifluoromethyl)phenylselanyl)-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (39 % yield), mp 82-83 °C. <sup>1</sup>H NMR (500 MHZ, CDCl<sub>3</sub>):  $\delta$  7.99-7.98 (m, 2H), 7.88 (d, *J* = 8.0 Hz, 2H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.55-7.47 (m, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$ 

167.5, 155.0, 134.4, 132.1, 131.7 (d, J = 4.0 Hz), 131.3 (d, J = 32.8 Hz), 129.1, 126.6, 126.0 (q, J = 3.7 Hz), 123.6 (q, J = 272.5 Hz), 123.3; <sup>19</sup>F NMR (470 MHz, CDCl<sub>3</sub>):  $\delta$  -62.9 (s, 3F). HRMS (ESI): calcd for C<sub>15</sub>H<sub>9</sub>F<sub>3</sub>N<sub>2</sub>OSe [M + H]<sup>+</sup> 370.9905, found 370.9903.

2-Phenyl-5-(4-(trifluoromethoxy)phenylselanyl)-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (57 % yield), mp 72-73 °C. <sup>1</sup>H NMR (500 MHZ, CDCl<sub>3</sub>):  $\delta$  7.96 (d, *J* = 8.0 Hz, 2H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.54-7.46 (m, 3H), 7.24 (d, *J* = 9.0 Hz, 2H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$ 167.4, 155.6, 150.3, 136.8, 136.7, 131.9, 129.1, 126.8, 122.2, 122.1, 120.3 (q, *J* = 258.2 Hz); <sup>19</sup>F NMR (470 MHz, CDCl<sub>3</sub>):  $\delta$  -57.8 (s, 3F). HRMS (ESI): calcd for C<sub>15</sub>H<sub>9</sub>F<sub>3</sub>N<sub>2</sub>O<sub>2</sub>Se [M + H]<sup>+</sup> 386.9854, found 386.9847.

#### Methyl 4-(5-phenyl-1,3,4-oxadiazol-2-ylselanyl)benzoate



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a white solid (41 % yield), mp 105-106 °C. **<sup>1</sup>H NMR** (500 MHZ, CDCl<sub>3</sub>):  $\delta$  8.03 (d, *J* = 8.0 Hz, 2H), 7.98 (d, *J* = 7.0 Hz, 2H), 7.80 (d, *J* = 8.5 Hz, 2H), 7.55-7.47 (m, 3H), 3.93 (s, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  167.5, 166.2, 155.1, 133.8, 132.0, 130.9, 130.7, 130.6, 129.1, 126.9, 123.3, 52.4. HRMS (ESI): calcd for C<sub>16</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>Se [M + Na]<sup>+</sup> 382.9911, found 382.9921.

#### 2-(3-nitrophenylselanyl)-5-phenyl-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (29 % yield), mp 110-111 °C. **<sup>1</sup>H NMR** (500 MHZ, CDCl<sub>3</sub>):  $\delta$  8.66 (s, 1H), 8.29 (dd, J = 8.2, 1.3 Hz, 1H), 8.11 (d, J = 7.7 Hz, 1H), 7.99 (d, J = 7.2 Hz, 2H), 7.61 (t, J = 8.0 Hz, 1H), 7.56-7.53 (m, 1H), 7.51-7.48 (m, 1H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  167.6, 154.8, 148.6, 140.5, 132.2, 130.6, 129.2, 127.1, 126.9, 126.0, 124.5, 123.2. HRMS (ESI): calcd for C<sub>14</sub>H<sub>9</sub>N<sub>3</sub>O<sub>3</sub>Se [M + H]<sup>+</sup> 347.9882, found 347.9882.

2-(1-Methyl-1H-pyrazol-4-ylselanyl)-5-phenyl-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a white solid (74 % yield), mp 107-108 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.96-7.94 (m, 2H), 7.74 (s, 1H), 7.71 (s, 1H), 7.52-7.45 (m, 3H), 3.97 (s, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  167.0, 156.3, 145.0, 136.1, 131.8, 129.0, 126.8, 123.5, 95.4, 39.4; HRMS (ESI): calcd for C<sub>12</sub>H<sub>10</sub>N<sub>4</sub>OSe [M + H]<sup>+</sup> 307.0093, found 307.0098.

2-Phenyl-5-(thiophen-3-ylselanyl)-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a white solid (80 % yield), mp 86-87 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.96-7.94 (m, 2H), 7.75-7.74 (m, 1H), 7.53-7.45 (m, 3H), 7.43-7.42 (m, 1H), 7.33 (d, *J*=4.9Hz, 1H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  167.1, 155.9, 132.8, 132.1, 131.8, 129.0, 127.4, 126.8, 123.5, 115.7; HRMS (ESI): calcd for C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>OSSe [M + H]<sup>+</sup> 308.9596, found 308.9596.

2-(9-phenyl-9H-carbazol-3-ylselanyl)-5-p-tolyl-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (72 % yield), mp 119-120 °C. <sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>Cl):  $\delta$  8.64 (s 1H), 8.20 (d, *J* = 7.8 Hz, 1H), 7.88-7.83 (m, 3H), 7.68-7.64 (m, 2H), 7.59-7.52 (m, 3H), 7.49-7.43 (m, 3H), 7.39-7.36 (m, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 2.35 (s, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  167.3, 156.9, 142.2, 141.4, 141.3, 137.0, 133.4, 130.0, 129.7, 128.6, 128.0, 127.1, 126.8, 126.7, 124.7, 122.6, 120.9, 120.7, 120.6, 113.3, 111.1, 110.1, 21.6. HRMS (ESI): calcd for C<sub>27</sub>H<sub>19</sub>N<sub>3</sub>OSe [M + H]<sup>+</sup> 482.0766, found 482.0792.

2-(quinolin-6-ylselanyl)-5-p-tolyl-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a white solid (51 % yield), mp 141-142 °C. **<sup>1</sup>H NMR** (500 MHz, CD<sub>3</sub>Cl):  $\delta$  8.98 (s 1H), 8.28 (s, 1H), 8.16-8.10 (m, 2H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.84 (d, *J* = 7.8 Hz, 2H), 7.47 (q, *J* = 4.1 Hz, 1H), 7.27-7.25 (m, 2H), 2.39 (s, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  167.6, 155.3, 151.7, 148.1, 142.6, 135.9, 134.7, 134.3, 131.1, 129.8, 128.8, 126.8, 122.8, 122.0, 120.6, 21.6. HRMS (ESI): calcd for C<sub>18</sub>H<sub>13</sub>N<sub>3</sub>OSe [M + H]<sup>+</sup> 368.0291, found 368.0279.

2-(Phenylselanyl)-5-p-tolyl-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a white solid (87 % yield), mp 65-66 °C. <sup>1</sup>H NMR (500 MHZ, CDCl<sub>3</sub>):  $\delta$  7.83 (d, J = 8.2 Hz, 2H), 7.76-7.74 (m, 2H), 7.43-7.36 (m, 3H), 7.25 (d, J = 8.2 Hz, 2H), 2.39 (m, 3H). <sup>13</sup>C NMR (125

MHz, CDCl<sub>3</sub>):  $\delta$  167.4, 155.7, 142.4, 134.9, 129.8, 129.7, 129.5, 126.8, 124.4, 120.8, 21.6. **HRMS** (ESI): calcd for C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>OSe [M + H]<sup>+</sup> 317.0188, found 317.0159.

2-(4-Tert-butylphenyl)-5-(phenylselanyl)-1,3,4-oxadiazole<sup>3</sup>



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow liquid (91 % yield). The  $^{1}$ H,  $^{13}$ C NMR spectra were in accordance with those described in the literature.

2-(4-Methoxyphenyl)-5-(phenylselanyl)-1,3,4-oxadiazole<sup>3</sup>



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (94 % yield), mp 96-97  $^{\circ}$ C. The <sup>1</sup>H, <sup>13</sup>C NMR spectra were in accordance with those described in the literature.

#### 2-(Biphenyl-4-yl)-5-(phenylselanyl)-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a white solid (81 % yield), mp 104-105 °C. <sup>1</sup>H NMR (500 MHZ, CDCl<sub>3</sub>):  $\delta$  8.0 (d, *J* = 8.0 Hz, 2H), 7.76 (d, *J* = 7.6 Hz, 2H), 7.66 (d, *J* = 8.0 Hz, 2H), 87.59 (d, *J* = 7.6 Hz, 2H), 7.45-7.37 (m, 6H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  167.1, 156.2, 144.6, 139.7, 135.1, 129.9, 129.6, 129.0, 128.2, 127.6, 127.3, 127.1, 124.3, 122.3. HRMS (ESI): calcd for C<sub>20</sub>H<sub>14</sub>N<sub>2</sub>OSe [M + H]<sup>+</sup> 379.0344, found 379.0343.



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (66 % yield), mp 86-87  $^{\circ}$ C. The <sup>1</sup>H, <sup>13</sup>C NMR spectra were in accordance with those described in the literature.

#### 2-(4-Fluorophenyl)-5-(phenylselanyl)-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (53 % yield), mp 85-86 °C. <sup>1</sup>H NMR (500 MHZ, CDCl<sub>3</sub>):  $\delta$  7.97 -7.94 (m, 2H), 7.76 (d, *J* = 7.0 Hz, 2H), 7.45-7.37 (m, 3H), 7.15 (t, *J* = 8.5 Hz, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  166.4, 165.8, 163.8, 156.3, 135.1, 129.9, 129.7, 129.2, 129.1, 124.2, 119.9, 119.9, 116.5, 116.3. <sup>19</sup>F NMR (470 MHz, CDCl<sub>3</sub>):  $\delta$  -106.5 (s, 1F). HRMS (ESI): calcd for C<sub>14</sub>H<sub>9</sub>FN<sub>2</sub>OSe [M + H]<sup>+</sup> 320.9937, found 320.9937.

2-(Benzo[d][1,3]dioxol-5-yl)-5-(phenylselanyl)-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (77 % yield), mp 91-92 °C. <sup>1</sup>H NMR (500 MHZ, CDCl<sub>3</sub>):  $\delta$  7.74-7.73 (m, 2H), 7.46 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.42 - 7.35 (m, 4H), 6.84 (d, *J* = 8.1 Hz, 1H), 6.01 (s, 2H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  166.9, 155.5, 150.7, 148.2, 134.9, 129.8, 129.6, 124.4, 121.9, 117.3, 108.8, 106.8, 101.9. HRMS (ESI): calcd for C<sub>15</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>Se [M + H]<sup>+</sup> 346.9930, found 346.9937.

2-(3-Nitrophenyl)-5-(phenylselanyl)-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (61 % yield), mp 110-111 °C. **<sup>1</sup>H NMR** (500 MHZ, CDCl<sub>3</sub>):  $\delta$  8.78 (s, 1H), 8.39 – 8.31 (m, 2H), 7.80 (d, *J* = 7.5 Hz, 2H), 7.71 (t, *J* = 8.0 Hz,1H), 7.50 - 7.42 (m, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  165.2, 157.7, 148.6, 135.4, 132.3, 130.4, 130.0, 130.0, 126.2, 125.2, 123.6, 121.7. HRMS (ESI): calcd for C<sub>14</sub>H<sub>9</sub>N<sub>3</sub>O<sub>3</sub>Se [M + H]<sup>+</sup> 347.9982, found 347.9982.

2-(Phenylselanyl)-5-(4-(trifluoromethyl)phenyl)-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (64 % yield), mp 73-74 °C. <sup>1</sup>H NMR (500 MHZ, CDCl<sub>3</sub>):  $\delta$  8.08 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 7.0 Hz, 2H), 7.74 (d, *J* = 8.5 Hz, 2H),7.48 - 7.41 (m, 3H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  166.0, 157.4, 135.3, 133.5, 129.9, 129.9, 127.1, 126.7, 126.1, 126.1, 126.1, 126.1, 124.6, 123.8, 122.4. <sup>19</sup>F NMR (470 MHz, CDCl<sub>3</sub>):  $\delta$  -63.14 (s, 3F). HRMS (ESI): calcd for C<sub>15</sub>H<sub>9</sub>F<sub>3</sub>N<sub>2</sub>OSe [M + H]<sup>+</sup> 370.9905, found 370.9903.

2-(Furan-2-yl)-5-(phenylselanyl)-1,3,4-oxadiazole<sup>3</sup>



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (89 % yield), mp 59-60  $^{\circ}$ C. The <sup>1</sup>H, <sup>13</sup>C NMR spectra were in accordance with those described in the literature.

2-(Phenylselanyl)-5-(thiophen-2-yl)-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (85 % yield), mp 63-64 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.74-7.73 (m, 2H), 7.64-7.63 (m, 1H), 7.51-7.50 (m, 1H), 7.42-7.7.35 (m, 3H), 7.11-7.09 (m, 1H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  163.4, 155.5, 135.0, 130.4, 129.9, 129.8, 129.6, 128.2, 124.7, 124.2; HRMS (ESI): calcd for C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>OSSe [M + H]<sup>+</sup> 308.9596, found 308.9598.

2-(Phenylselanyl)-5-(pyridin-4-yl)-1,3,4-oxadiazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (71 % yield), mp 87-88 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.78 (s 2H), 7.80-7.78 (m, 4H), 7.47-7.41 (m, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  165.3, 158.2, 150.8, 135.4, 135.4, 130.6, 130.0, 129.9, 123.5, 120.1; HRMS (ESI): calcd for C<sub>13</sub>H<sub>9</sub>N<sub>3</sub>OSe [M + H]<sup>+</sup> 303.9984, found 304.0015.

2-(Mesitylselanyl)-5-methylbenzo[d]oxazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (44 % yield), mp 119-120 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.38 (s 1H), 7.26-7.24 (m, 1H), 7.03 (s, 2H), 7.00 (d, *J* = 8.3 Hz, 1H), 2.51 (s, 6H), 2.41 (s, 3H), 2.32 (s, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  158.4, 150.9, 143.5, 142.6, 140.2, 133.9, 129.2, 124.8, 123.4, 118.8, 109.3, 24.4, 21.4, 21.1. HRMS (ESI): calcd for C<sub>17</sub>H<sub>17</sub>NOSe [M + H]<sup>+</sup> 332.0548, found 332.0547.

Ethyl 2-(mesitylselanyl)oxazole-5-carboxylate



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (68 % yield), mp 68-69 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.62 (s 1H), 7.01 (s, 2H), 4.34 (q, *J* = 7.1 Hz, 2H), 2.48 (s, 6H), 2.30 (s, 3H), 1.35 (t, *J* = 7.1 Hz, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  159.3, 157.4, 145.2, 143.3, 140.6, 135.5, 129.3, 129.0, 123.2, 61.3, 24.3, 21.1, 14.2. HRMS (ESI): calcd for C<sub>15</sub>H<sub>17</sub>NO<sub>3</sub>Se [M + H]<sup>+</sup> 340.0447, found 340.0463.

#### 5-(4-Chlorophenyl)-2-(phenylselanyl)oxazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (57 % yield), mp 98-99 °C. <sup>1</sup>H NMR (500 MHz, (CD<sub>3</sub>)<sub>2</sub>SO):  $\delta$  7.82 (s 1H), 7.72-7.70 (m, 2H), 7.64 (d, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 8.5 Hz, 2H), 7.45-7.43 (m, 3H); <sup>13</sup>C NMR (125MHz, (CD<sub>3</sub>)<sub>2</sub>SO):  $\delta$  153.0, 151.2, 133.6, 133.1, 129.7, 129.1, 128.8, 126.1, 125.7, 125.4, 125.2. HRMS (ESI): calcd for C<sub>15</sub>H<sub>10</sub>CINOSe [M + H]<sup>+</sup> 335.9689, found 335.9717.

#### 2-(Mesitylselanyl)-5-phenyloxazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (51 % yield), mp 65-66 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.50-7.50 (m, 1H), 7.48 (s, 1H), 7.37-7.34 (m, 2H), 7.28-7.26 (m, 1H), 7.25-7.24 (m, 1H), 7.00 (s, 2H), 2.54 (s, 6H), 2.30 (s, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$ 154.1, 152.7, 143.3, 140.0, 129.1, 128.8, 128.2, 127.8, 124.1, 123.8, 123.7, 24.4, 21.1; HRMS (ESI): calcd for C<sub>18</sub>H<sub>17</sub>NOSe [M + H]<sup>+</sup> 344.0548, found

344.0568.

5-(4-Chlorophenyl)-2-(mesitylselanyl)oxazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (54 % yield), mp 103-104 °C. **<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.42-7.40 (m, 2H), 7.33-7.31 (m, 2H), 7.24 (s, 1H), 7.00-6.99 (m, 2H), 2.53 (s, 6H), 2.30 (s, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  153.2, 153.1, 143.3, 140.1, 133.9, 129.2, 129.1, 126.3, 125.1, 124.1, 123.9, 24.4, 21.1; HRMS (ESI): calcd for C<sub>18</sub>H<sub>16</sub>CINOSe [M + H]<sup>+</sup> 378.0159, found 378.0181.

5-(4-Fluorophenyl)-2-(mesitylselanyl)oxazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (47 % yield), mp 102-103 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.47-7.44 (m, 4H), 7.19 (s, 1H), 7.05 (t, J = 7.6Hz, 2H), 7.00 (s, 2H), 2.54(s, 6H), 2.29 (s, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  162.53 (d, J = 248Hz), 153.3, 152.7, 143.3, 140.1, 129.1, 125.7 (d, J = 8.2Hz), 124.2 (d, J = 3.1Hz), 124.1, 123.3, 116.0 (d, J = 22.3Hz), 24.4, 21.1; <sup>19</sup>F NMR (470 MHz, CDCl<sub>3</sub>):  $\delta$  - 112.4 (s, 1F); HRMS (ESI): calcd for C<sub>18</sub>H<sub>16</sub>FNOSe [M + H]<sup>+</sup> 362.0454, found 362.0453.

2-(Mesitylselanyl)-5-(4-(trifluoromethyl)phenyl)oxazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a

yellow liquid (38 % yield). <sup>1</sup>**H NMR** (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.63-7.58 (m, 4H), 7.36 (s, 1H), 7.02-7.03 (m, 2H), 2.54(s, 6H), 2.31 (s, 3H); <sup>13</sup>**C NMR** (125MHz, CDCl<sub>3</sub>):  $\delta$  162.53 (d, J = 248Hz), 153.3, 152.7, 143.3, 140.1, 129.1, 125.7 (d, J = 8.2Hz), 124.2 (d, J = 3.1Hz), 124.1, 123.3, 116.0 (d, J = 22.3Hz), 24.4, 21.1; <sup>19</sup>**F NMR** (470 MHz, CDCl<sub>3</sub>):  $\delta$  -112.4 (s, 1F); **HRMS** (ESI): calcd for C<sub>19</sub>H<sub>16</sub>F<sub>3</sub>NOSe [M + H]<sup>+</sup> 412.0422, found 412.0442.

2-(Mesitylselanyl)-5-(4-(methylthio)phenyl)oxazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (58 % yield), mp 112-113 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.40 (s, 1H), 7.39 (s, 1H), 7.22 (s, 1H), 7.21-7.20 (m, 2H), 7.00 (s, 2H), 2.53(s, 6H), 2.47 (s, 3H), 2.29 (s, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  153.8, 152.4, 143.3, 140.0, 139.0, 129.1, 126.6, 124.6, 124.2, 123.3, 24.4, 21.1, 15.6; HRMS (ESI): calcd for C<sub>19</sub>H<sub>19</sub>NOSSe [M + H]<sup>+</sup> 390.0426, found 390.0439.

#### 2-(Mesitylselanyl)-5-(naphthalen-2-yl)oxazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (60 % yield), mp 103-104 °C. **<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.97 (s, 1H), 7.80-7.77 (m, 3H), 7.57 (dd, *J* = 8.5, 1.6Hz, 1H), 7.47-7.44 (m, 2H), 7.35-7.34 (m, 1H), 2.56 (s, 6H), 2.30 (s, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  154.2, 153.1, 143.4, 140.1, 133.3, 133.0, 129.2, 128.7, 128.2, 127.8, 126.7, 126.4, 125.1, 124.2, 124.1, 122.6, 121.8, 24.5, 21.1; HRMS (ESI): calcd for C<sub>22</sub>H<sub>19</sub>NOSe [M + H]<sup>+</sup> 394.0705, found 394.0729.

#### 2-(Mesitylselanyl)-1-methyl-1H-benzo[d]imidazole



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow solid (63 % yield), mp 122-123 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.67-7.65 (m, 1H), 7.22-7.15 (m, 3H), 6.94 (s, 2H), 3.57 (s, 3H), 2.43 (s, 3H), 2.26 (s, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  145.9, 144.1, 142.7, 139.3, 136.7, 129.3, 125.1, 122.2, 121.8, 119.2, 108.7, 31.2, 24.3, 21.0. HRMS (ESI): calcd for C<sub>17</sub>H<sub>18</sub>N<sub>2</sub>Se [M + H]<sup>+</sup> 331.0708, found 331.0707.

1,3-Dimethyl-8-(phenylselanyl)-1H-purine-2,6(3H,9H)-dione



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a white solid (65 % yield), mp 58-59 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  11.05 (s, 1H), 7.66-7.65 (m, 2H), 7.41-7.34 (m, 3H), 3.60 (s, 3H), 3.38 (s, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$ 154.5, 151.4, 149.7, 143.1, 134.8, 130.1, 129.5, 125.5, 109.1, 30.2, 28.3; HRMS (ESI): calcd for C<sub>13</sub>H<sub>12</sub>N<sub>4</sub>O<sub>2</sub>Se [M + H]<sup>+</sup> 337.0198, found 337.0238.





Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a white solid (74 % yield), mp 236-237 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 10.9 (s, 1H), 7.66 (s,

1H), 7.38-7.37 (m, 1H), 7.20-7.19 (m, 1H), 3.52 (s, 3H), 3.34 (s, 3H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  153.5, 150.3, 148.8 142.4, 131.8, 131.6, 127.1, 116.0, 108.0, 29.2, 27.3. **HRMS** (ESI): calcd for C<sub>11</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>SSe [M + H]<sup>+</sup> 342.9763, found 342.9798.

2-(phenylselanyl)quinoline



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a white solid (27 % yield), mp 135-136 °C. <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO):  $\delta$  8.47 (d, *J* = 8.6 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.87-7.78 (m, 4H), 7.71-7.67 (m, 1H), 7.65-7.56 (m, 3H), 6.70 (d, J = 9.1 Hz, 1H); <sup>13</sup>C NMR (125MHz, (CD<sub>3</sub>)<sub>2</sub>SO):  $\delta$  147.6, 140.4, 137.5, 131.4, 130.8, 130.6, 129.2, 128.2, 128.1, 126.3, 126.0, 120.4, 118.1. HRMS (ESI): calcd for C<sub>15</sub>H<sub>11</sub>NSe [M + H]<sup>+</sup> 286.0130, found 286.0091.

Isopropyl 2-methyl-2-(4-(4-(5-phenyl-1,3,4-oxadiazol-2-ylselanyl)benzoyl)phenoxy)propanoate



Following the general procedure, using 20 / 1 petroleum ether / EtOAc as the eluant afforded a yellow liquid (27 % yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.00 (d, *J* = 7.2 Hz, 2H), 7.84 (d, *J* = 8.2 Hz, 2H), 7.76-7.73 (m, 4H), 7.56-7.49 (m, 3H), 6.86 (d, *J* = 8.8 Hz, 2H), 5.12-5.04 (qt, J = 12.4, 6.3 Hz, 1H), 1.66 (s, 6H), 1.20 (d, *J* = 6.3 Hz, 6H); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>):  $\delta$  194.4, 173.0, 159.9, 138.9, 133.8, 132.1, 132.0, 130.8, 130.0, 129.2, 129.1, 126.9, 123.4, 117.3, 79.5, 69.3, 25.4, 21.5. HRMS (ESI): calcd for C<sub>28</sub>H<sub>26</sub>N<sub>2</sub>O<sub>5</sub>Se [M + H]<sup>+</sup> 551.1080, found 551.1106.

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## <sup>1</sup>H, <sup>13</sup>C and <sup>19</sup>F NMR spectra of products



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S24





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S44































































