

**An Electrochemical Method for Deborylative Seleno/thiocyanation of  
Arylboronic Acids under Catalyst- and Oxidant-free Conditions**

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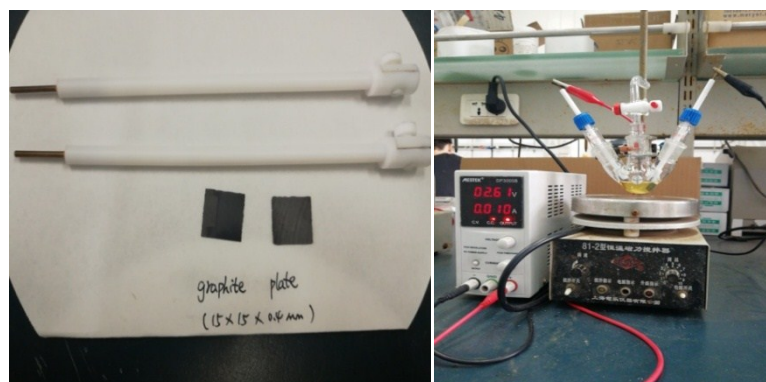
**General considerations.** The reagents used for experiments were commercially available and used as received unless otherwise noted. CH<sub>3</sub>CN was distilled from CaH<sub>2</sub> under reduced pressure and stored under nitrogen. The instrument for electrolysis is dual display potentiostat (DJS-292B) (made in China). Cyclic voltammograms were obtained on a IVIUMSTAT potentiostat. Column chromatography was performed on silica gel 300 - 400 mesh. The yields reported are the isolated yields and the average of two runs. <sup>1</sup>H and <sup>13</sup>C NMR spectra of all compounds were recorded at 400 and 100 MHz with CDCl<sub>3</sub> as solvent respectively. All coupling constants (*J* values) were reported in Herz (Hz). HRMS were performed by Analysis and Testing Center, Nanchang University. GC-MS analysis was conducted on a Shimadzu GCMS-QP2010 instrument equipped with a Restec-5HT column (30 m × 0.25 mm, Hewlett-Packard).

### **General procedure for metal-free electrocatalytic selenocyanation of arylboronic acids**

**Procedure A:** Arylboronic acid (0.2 mmol), KSeCN (0.8 mmol, 4.0 equiv), CH<sub>3</sub>CN (10 mL) and H<sub>2</sub>O (50 μL) were combined and added into oven-dried three-necked flask (25 mL) with a stir bar. The flask was equipped with two graphite felts (15 mm × 15 mm × 0.4 mm) as the cathode and anode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under room temperature for 80 min. When the reaction was finished, the reaction mixture was filtered through a short plug of silica gel that was then washed with EtOAc and concentrated in vacuo. The resulting residue was purified by flash chromatography on silica gel to provide corresponding product.

### **General procedure for metal-free electrocatalytic thiocyanation of arylboronic acids**

**Procedure B:** Arylboronic acid (0.2 mmol), TMSNCS (0.6 mmol, 3.0 equiv), CH<sub>3</sub>CN (10 mL) and H<sub>2</sub>O (30 μL) were combined and added into oven-dried three-necked flask (25 mL) with a stir bar. The flask was equipped with two graphite felts (15 mm × 15 mm × 0.4 mm) as the cathode and anode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under room temperature for 3 h. When the reaction was finished, the reaction mixture was filtered through a short plug of silica gel that was then washed with EtOAc and concentrated in vacuo. The resulting residue was purified by flash chromatography on silica gel to provide corresponding product.



**1-Methoxy-4-selenocyanatobenzene (1a).** Procedure A was followed using (4-methoxyphenyl)boronic acid (30.4 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). With stirring, the reaction mixture was performed for 3 hours instead of 80 minutes. The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 36.0 mg (85%) of the product as a colorless liquid. Exhibited spectral data in accordance with previous report.<sup>[1]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.60 (d,  $J$  = 8.8 Hz, 2 H), 6.92 (d,  $J$  = 8.8 Hz, 2 H), 3.82 (s, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  161.3, 136.0, 116.0, 111.0, 102.1, 55.5.

**1-Methoxy-2-selenocyanatobenzene (2a).** Procedure A was followed using (2-methoxyphenyl)boronic acid (30.4 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 80 minutes. The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 31.0 mg (73%) of the product as a colorless liquid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.63 (d,  $J$  = 7.6 Hz, 1 H), 7.34 (t,  $J$  = 7.6 Hz, 1 H), 7.03 (t,  $J$  = 7.6 Hz, 1 H), 6.90 (d,  $J$  = 8.4 Hz, 1 H), 3.90 (s, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  155.7, 130.0, 129.8, 122.8, 112.6, 110.9, 101.5, 56.2. HRMS (ESI-TOF)  $m/z$ : [M+H]<sup>+</sup> Calcd. for C<sub>8</sub>H<sub>7</sub>NOSe: 213.9773; Found: 213.9755.

**2,4-Dimethoxy-1-selenocyanatobenzene (3a).** Procedure A was followed using (2,4-dimethoxyphenyl)boronic acid (36.4 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 39.2 mg (81%) of the product as a colorless liquid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.50 (d,  $J$  = 8.4 Hz, 1 H), 6.54 (dd,  $J$  = 8.8 Hz, 2.4 Hz, 1 H), 6.48 (s, 1 H), 3.87 (s, 1 H), 3.81 (s, 1 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  162.4, 157.8, 132.9, 106.7, 101.9, 101.7, 99.3, 56.2, 55.7. HRMS (ESI-TOF)  $m/z$ : [M+H]<sup>+</sup> Calcd. for C<sub>9</sub>H<sub>9</sub>NO<sub>2</sub>Se: 243.9879; Found: 243.9863.

**2-Methoxy-5-selenocyanatobenzaldehyde (4a).** Procedure A was followed using (3-formyl-4-methoxyphenyl)boronic acid (36.0 mg, 0.2 mmol), KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv) and H<sub>2</sub>O (10  $\mu$ L) instead of H<sub>2</sub>O (50  $\mu$ L). With stirring, the reaction mixture was performed for 5 hours instead of 80 minutes. The reaction mixture was purified by flash column chromatography on silica gel (22:3, petroleum ether: EtOAc) to afford 31.7 mg (66%) of the product as a white solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  10.41 (s, 1 H), 8.09 (s, 1 H), 7.87 (d,  $J$  = 8.4 Hz, 1 H), 7.06 (d,  $J$  = 8.8 Hz, 1 H), 3.98 (s, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  188.1, 162.9, 141.5, 134.4, 125.9, 114.1, 112.2, 101.4, 56.2. HRMS (ESI-TOF)  $m/z$ : [M+H]<sup>+</sup> Calcd. for C<sub>9</sub>H<sub>7</sub>NO<sub>2</sub>Se: 241.9722; Found: 241.9710.

**4-Selenocyanatophenol (5a).** Procedure A was followed using (4-hydroxyphenyl)boronic acid (27.6 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (22:3, petroleum ether: EtOAc) to afford 31.7 mg (80%) of the product as a colorless liquid. Exhibited spectral data in accordance with previous report.<sup>[2]</sup> <sup>1</sup>H

NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.52 (d,  $J$  = 8.8 Hz, 2 H), 6.84 (d,  $J$  = 8.0 Hz, 2 H), 6.38 (s, 1 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  158.1, 136.5, 117.6, 110.3, 103.2.

**2-Selenocyanatoaniline (6a).** Procedure A was followed using (2-aminophenyl)boronic acid (27.4 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (9:1, petroleum ether: EtOAc) to afford 29.2 mg (74%) of the product as a white solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.55 (d,  $J$  = 8.0 Hz, 1 H), 7.26 (t,  $J$  = 8.0 Hz, 1 H), 6.82 (d,  $J$  = 8.0 Hz, 1 H), 6.72 (t,  $J$  = 7.6 Hz, 1 H), 4.34 (s, 2 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  148.2, 137.4, 132.9, 119.5, 116.2, 105.0, 100.5. HRMS (ESI-TOF)  $m/z$ : [M+H]<sup>+</sup> Calcd. for C<sub>7</sub>H<sub>6</sub>N<sub>2</sub>Se: 198.9762; Found: 198.9776.

***N,N*-dimethyl-4-selenocyanatoaniline (7a).** Procedure A was followed using (4-(dimethylamino)phenyl)boronic acid (33.0 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 40.0 mg (89%) of the product as a yellow solid. Exhibited spectral data in accordance with previous report.<sup>[2]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.51 (d,  $J$  = 8.8 Hz, 2 H), 6.64 (d,  $J$  = 8.8 Hz, 2 H), 2.99 (s, 6 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  151.6, 136.4, 113.3, 104.3, 102.8, 40.1.

**1-Isopropyl-4-selenocyanatobenzene (8a).** Procedure A was followed using (4-isopropylphenyl)boronic acid (32.8 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 80 minutes. The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 35.9 mg (80%) of the product as a colorless liquid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.55 (d,  $J$  = 8.0 Hz, 2 H), 7.25 (d,  $J$  = 8.0 Hz, 2 H), 2.99 - 2.85 (m, 1 H), 1.24 (d,  $J$  = 6.8 Hz, 6 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  151.3, 133.4, 128.6, 118.2, 101.8, 33.9, 23.8. HRMS (ESI-TOF)  $m/z$ : [M+H]<sup>+</sup> Calcd. for C<sub>10</sub>H<sub>11</sub>NSe: 226.0137; Found: 226.0122.

**1-Methyl-4-selenocyanatobenzene (9a).** Procedure A was followed using *p*-tolylboronic acid (27.2 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 80 minutes. The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 25.5 mg (65%) of the product as a light yellow liquid. Exhibited spectral data in accordance with previous report.<sup>[1]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.53 (d,  $J$  = 8.0 Hz, 2 H), 7.21 (d,  $J$  = 7.6 Hz, 2 H), 2.38 (s, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  140.4, 133.3, 131.1, 117.9, 101.7, 21.2.

**1-Methyl-2-selenocyanatobenzene (10a).** Procedure A was followed using *o*-tolylboronic acid (27.2 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 80 minutes. The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 30.1 mg (78%) of the product as a colorless liquid.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.72 (d, *J* = 7.6 Hz, 1 H), 7.35 (t, *J* = 7.6 Hz, 1 H), 7.31 (t, *J* = 7.2 Hz, 1 H), 7.22 (t, *J* = 7.6 Hz, 1 H), 2.49 (s, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 139.9, 134.0, 131.2, 130.3, 127.8, 123.0, 101.2, 22.3. HRMS (ESI-TOF) *m/z*: [M+H]<sup>+</sup> Calcd. for C<sub>8</sub>H<sub>7</sub>NSe: 197.9824; Found: 197.9810.

**1,3-Dimethyl-2-selenocyanatobenzene (11a).** Procedure A was followed using (2,6-dimethylphenyl)boronic acid (30.0 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 80 minutes and 15 mA instead of 10 mA. The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 17.7 mg (42%) of the product as a colorless liquid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.24 - 7.22 (m, 1 H), 7.16 (d, *J* = 7.2 Hz, 2 H), 2.60 (s, 6 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 143.1, 130.9, 128.8, 123.9, 101.1, 24.5. HRMS (ESI-TOF) *m/z*: [M+H]<sup>+</sup> Calcd. for C<sub>9</sub>H<sub>9</sub>NSe: 211.9980; Found: 211.9970.

**Selenocyanatobenzene (12a).** Procedure A was followed using phenylboronic acid (24.4 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 80 minutes and 15 mA instead of 10 mA. The reaction mixture was purified by flash column chromatography on silica gel (99:1, petroleum ether: EtOAc) to afford 17.4 mg (48%) of the product as a colorless liquid. Exhibited spectral data in accordance with previous report.<sup>[1]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.64 (dd, *J* = 6.8 Hz, 0.8 Hz, 2 H), 7.43 - 7.38 (m, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 132.8, 130.4, 129.8, 121.8, 101.6.

**1-Selenocyanatonaphthalene (17a).** Procedure A was followed using naphthalen-1-ylboronic acid (34.4 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 80 minutes. The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 37.6 mg (81%) of the product as a white solid. Exhibited spectral data in accordance with previous report.<sup>[1]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.16 (d, *J* = 8.4 Hz, 1 H), 7.98 (d, *J* = 7.2 Hz, 1 H), 7.95 (d, *J* = 8.0 Hz, 1 H), 7.88 (d, *J* = 8.0 Hz, 1 H), 7.66 (t, *J* = 7.2 Hz, 1 H), 7.58 (t, *J* = 7.2 Hz, 1 H), 7.43 (t, *J* = 8.0 Hz, 1 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 134.6, 134.4, 133.1, 131.7, 129.0, 128.2, 127.1, 126.6, 126.1, 120.5, 101.2.

**2-Selenocyanatonaphthalene (18a).** Procedure A was followed using naphthalen-2-ylboronic acid (34.4 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv), H<sub>2</sub>O (30 μL) instead of H<sub>2</sub>O (50 μL). With stirring, the reaction mixture was performed for 3 hours instead of 80 minutes. The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 24.6 mg (53%) of the product as a white solid. Exhibited spectral data in accordance with previous report.<sup>[1]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.09 (s, 1 H), 7.85 - 7.76 (m, 3 H), 7.61 (dd, *J* = 8.4, 1.6 Hz, 1 H), 7.57 - 7.52 (m, 2 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 133.8, 133.1, 132.6, 130.2, 128.8, 127.9, 127.7, 127.4, 118.8, 101.6.

**4-Selenocyanatodibenzo[b,d]furan (19a).** Procedure A was followed using dibenzo[b,d]furan-4-ylboronic acid (42.4 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 80 minutes and 15 mA instead of 10 mA. The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 23.4 mg (43%) of the product as a yellow solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.93 (dd, *J* = 8.0, 0.8 Hz, 1 H), 7.89 (dd, *J* = 7.6, 0.4 Hz, 1 H), 7.68 (dd, *J* = 7.6, 0.8 Hz, 1 H), 7.59 (d, *J* = 8.4 Hz, 1 H), 7.48 (td, *J* = 8.4, 1.2 Hz, 1 H), 7.35 (t, *J* = 7.2 Hz, 1 H), 7.31 (t, *J* = 8.0 Hz, 1 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 156.0, 154.7, 131.4, 128.2, 125.5, 124.3, 123.6, 122.7, 121.1, 112.1, 103.5, 100.1. HRMS (ESI-TOF) *m/z*: [M+H]<sup>+</sup> Calcd. for C<sub>13</sub>H<sub>7</sub>NOSe: 273.9773; Found: 273.9761.

**3-Selenocyanatobenzo[b]thiophene (20a).** Procedure A was followed using benzo[b]thiophen-3-ylboronic acid (35.6 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 38.6 mg (81%) of the product as a red solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.97 (d, *J* = 8.0 Hz, 1 H), 7.91 (d, *J* = 5.2 Hz, 2 H), 7.54 (t, *J* = 7.2 Hz, 1 H), 7.47 (t, *J* = 7.2 Hz, 1 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 139.4, 138.5, 135.3, 125.73, 125.72, 123.3, 123.0, 109.1, 100.1. HRMS (ESI-TOF) *m/z*: [M+H]<sup>+</sup> Calcd. for C<sub>9</sub>H<sub>5</sub>NSSe: 239.9388; Found: 239.9382.

**2-Selenocyanatobenzo[b]thiophene (21a).** Procedure A was followed using benzo[b]thiophen-2-ylboronic acid (35.6 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 80 minutes. The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 31.4 mg (66%) of the product as a red solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.87 - 7.80 (m, 2 H), 7.69 (s, 1 H), 7.45 - 7.39 (m, 2 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 144.0, 139.1, 135.1, 126.2, 125.2, 124.2, 122.0, 115.3, 100.2. HRMS (ESI-TOF) *m/z*: [M+H]<sup>+</sup> Calcd. for C<sub>9</sub>H<sub>5</sub>NSSe: 239.9388; Found: 239.9377.

**3-Selenocyanatobenzofuran (22a).** Procedure A was followed using benzofuran-3-ylboronic acid (32.4 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 31.0 mg (70%) of the product as a white solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.89 (s, 1 H), 7.70 (d, *J* = 6.8 Hz, 1 H), 7.56 (d, *J* = 8.0 Hz, 1 H), 7.45 - 7.36 (m, 2 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 155.1, 145.0, 127.3, 126.1, 124.4, 120.2, 112.1, 99.6, 97.2. HRMS (ESI-TOF) *m/z*: [M-H]<sup>-</sup> Calcd. for C<sub>9</sub>H<sub>5</sub>NOSe: 221.9426; Found: 221.9524.

**2-Selenocyanatobenzofuran (23a).** Procedure A was followed using benzofuran-2-ylboronic acid (32.4 mg, 0.2 mmol) and KSeCN (115.3 mg, 0.8 mmol, 4.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (49:1, petroleum ether: EtOAc) to afford 23.5 mg (53%) of the product as a white solid. <sup>1</sup>H

NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.59 (d,  $J$  = 8.0 Hz, 1 H), 7.53 (d,  $J$  = 8.4 Hz, 1 H), 7.38 (t,  $J$  = 8.0 Hz, 1 H), 7.28 (t,  $J$  = 7.6 Hz, 1 H), 7.23 (s, 1 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  157.8, 132.0, 127.5, 126.6, 123.8, 121.5, 119.0, 111.7, 98.5. HRMS (ESI-TOF)  $m/z$ : [M+H]<sup>+</sup> Calcd. for C<sub>9</sub>H<sub>5</sub>NOSe: 223.9614; Found: 223.9604.

**1-Methoxy-4-thiocyanatobenzene (1b).** Procedure B was followed using 4-methoxyphenylboronic acid (30.4 mg, 0.2 mmol) and TMSNCS (84.5  $\mu$ L, 0.6 mmol, 3.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 27.6 mg (83%) of the product as a light yellow liquid. Exhibited spectral data in accordance with previous report.<sup>[6]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.48 (d,  $J$  = 8.8 Hz, 2 H), 6.94 (d,  $J$  = 8.8 Hz, 2 H), 3.82 (s, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  161.3, 133.9, 115.8, 113.7, 111.7, 55.5.

**1-Methoxy-2-thiocyanatobenzene (2b).** Procedure B was followed using (2-methoxyphenyl)boronic acid (30.4 mg, 0.2 mmol) and TMSNCS (84.5  $\mu$ L, 0.6 mmol, 3.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 21.6 mg (65%) of the product as a colorless liquid. Exhibited spectral data in accordance with previous report.<sup>[8]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.56 (d,  $J$  = 8.0 Hz, 1 H), 7.36 (t,  $J$  = 8.0 Hz, 1 H), 7.06 (t,  $J$  = 7.6 Hz, 1 H), 6.94 (d,  $J$  = 8.0 Hz, 1 H), 3.92 (s, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  156.5, 130.5, 129.9, 122.0, 113.1, 111.4, 110.4, 56.2.

**2,4-Dimethoxy-1-thiocyanatobenzene (3b).** Procedure B was followed using (2,4-dimethoxyphenyl)boronic acid (36.4 mg, 0.2 mmol) and TMSNCS (84.5  $\mu$ L, 0.6 mmol, 3.0 equiv). With stirring, the reaction mixture was performed for 80 minutes instead of 3 hours. The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 33.3 mg (85%) of the product as a yellow liquid. Exhibited spectral data in accordance with previous report.<sup>[3]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.45 (d,  $J$  = 8.4 Hz, 1 H), 6.53 (dd,  $J$  = 8.4, 2.4 Hz, 1 H), 6.50 (d,  $J$  = 2.4 Hz, 1 H), 3.90 (s, 3 H), 3.82 (s, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  163.0, 159.0, 133.9, 111.4, 106.1, 102.3, 99.5, 56.2, 55.7.

**2-Methoxy-5-thiocyanatobenzaldehyde (4b).** Procedure B was followed using (3-formyl-4-methoxyphenyl)boronic acid (36.0 mg, 0.2 mmol) and TMSNCS (84.5  $\mu$ L, 0.6 mmol, 3.0 equiv), H<sub>2</sub>O (10  $\mu$ L) instead of H<sub>2</sub>O (30  $\mu$ L). With stirring, the reaction mixture was performed for 5 hours instead of 3 hours. The reaction mixture was purified by flash column chromatography on silica gel (22:3, petroleum ether: EtOAc) to afford 23.3 mg (60%) of the product as a white solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  10.42 (s, 1 H), 8.00 (d,  $J$  = 2.8 Hz, 1 H), 7.77 (dd,  $J$  = 8.8 Hz, 2.4 Hz, 1 H), 7.10 (d,  $J$  = 8.8 Hz, 1 H), 3.99 (s, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  187.9, 162.8, 138.9, 132.2, 125.9, 115.4, 114.0, 110.7, 56.2. HRMS (ESI-TOF)  $m/z$ : [M+H<sub>3</sub>O]<sup>+</sup> Calcd. for C<sub>8</sub>H<sub>7</sub>NSO<sub>2</sub>: 212.0381; found: 212.0800.

**4-Thiocyanatophenol (5b).** Procedure B was followed using (4-hydroxyphenyl)boronic acid (27.6 mg, 0.2 mmol), TMSNCS (84.5  $\mu$ L, 0.6 mmol, 3.0 equiv). With stirring, the reaction mixture was performed for 80 minutes instead of 3 hours. The reaction mixture was purified by flash column chromatography on silica gel (22:3, petroleum ether: EtOAc) to afford 23.7 mg (78%) of the product as a colorless liquid. Exhibited spectral data in accordance with previous report.<sup>[6]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.43 (d,  $J$  = 8.4 Hz, 2 H), 6.88 (d,  $J$  = 8.4 Hz, 2 H), 6.29 (s, 1 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  158.0, 134.2, 117.5, 113.1, 112.3.

***N,N*-Dimethyl-4-thiocyanatoaniline (7b).** Procedure B was followed using (4-(dimethylamino)phenyl)boronic acid (33.0 mg, 0.2 mmol) and TMSNCS (84.5  $\mu$ L, 0.6 mmol, 3.0 equiv). With stirring, the reaction mixture was performed for 80 minutes instead of 3 hours. The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 31.1 mg (87%) of the product as a white solid. Exhibited spectral data in accordance with previous report.<sup>[5]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.42 (d,  $J$  = 8.4 Hz, 2 H), 6.67 (d,  $J$  = 8.4 Hz, 2 H), 3.00 (s, 6 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  151.6, 134.5, 113.1, 112.7, 106.3, 40.2.

**1-Isopropyl-4-thiocyanatobenzene (8b).** Procedure B was followed using 4-isopropylphenylboronic acid (32.8 mg, 0.2 mmol) and TMSNCS (84.5  $\mu$ L, 0.6 mmol, 3.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 3 hours. The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 19.6 mg (55%) of the product as a colorless liquid. Exhibited spectral data in accordance with previous report.<sup>[6]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.45 (d,  $J$  = 8.0 Hz, 2 H), 7.28 (d,  $J$  = 8.0 Hz, 2 H), 2.98 - 2.95 (m, 1 H), 1.23 (d,  $J$  = 6.8 Hz, 6 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  151.1, 130.8, 128.4, 120.7, 111.1, 33.4, 23.8.

**1-Methyl-4-thiocyanatobenzene (9b).** Procedure B was followed using p-tolylboronic acid (27.2 mg, 0.2 mmol) and TMSNCS (84.5  $\mu$ L, 0.6 mmol, 3.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 18.3 mg (62%) of the product as a colorless liquid. Exhibited spectral data in accordance with previous report.<sup>[6]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.42 (d,  $J$  = 8.0 Hz, 2 H), 7.24 (d,  $J$  = 8.0 Hz, 2 H), 2.38 (s, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  140.2, 130.9, 130.7, 120.5, 111.0, 21.1.

**2-Methylphenyl thiocyanate (10b).** Procedure B was followed using o-tolylboronic acid (27.2 mg, 0.2 mmol) and TMSNCS (84.5  $\mu$ L, 0.6 mmol, 3.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 17.4 mg (58%) of the product as a colorless liquid. Exhibited spectral data in accordance with previous report.<sup>[8]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.63 (d,  $J$  = 8.0 Hz, 1 H), 7.35 (t,  $J$  = 7.2 Hz, 1 H), 7.29 (t,  $J$  = 5.6 Hz, 2 H),



2.48 (s, 3 H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  139.3, 131.9, 131.4, 130.2, 127.7, 123.6, 110.4, 20.4.

**1,3-Dimethyl-2-thiocyanatobenzene (11b).** Procedure B was followed using (2,6-dimethylphenyl)boronic acid (30.0 mg, 0.2 mmol) and TMSNCS (84.5  $\mu\text{L}$ , 0.6 mmol, 3.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 3 hours and 15 mA instead of 10 mA. The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 20.3 mg (60%) of the product as a colorless solid. Exhibited spectral data in accordance with previous report.<sup>[4]</sup>  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.28 (t,  $J = 7.2$  Hz, 1 H), 7.19 (d,  $J = 7.2$  Hz, 2 H), 2.60 (s, 6 H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  142.9, 131.1, 129.2, 122.6, 110.6, 22.1.

**Thiocyanatobenzene (12b).** Procedure B was followed using phenylboronic acid (24.4 mg, 0.2 mmol) and TMSNCS (84.5  $\mu\text{L}$ , 0.6 mmol, 3.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 3 hours and 15 mA instead of 10 mA. The reaction mixture was purified by flash column chromatography on silica gel (99:1, petroleum ether: EtOAc) to afford 6.8 mg (25%) of the product as a colorless liquid. Exhibited spectral data in accordance with previous report.<sup>[7]</sup>  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.53 - 7.50 (m, 2 H), 7.42 - 7.40 (m, 3 H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  130.2, 130.0, 129.5, 124.4, 110.4.

**1-Bromo-4-thiocyanatobenzene (13b).** Procedure B was followed using (4-bromophenyl)boronic acid (40.2 mg, 0.2 mmol) and TMSNCS (84.5  $\mu\text{L}$ , 0.6 mmol, 3.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 3 hours and 15 mA instead of 10 mA. The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 9.1 mg (21%) of the product as a white solid. Exhibited spectral data in accordance with previous report.<sup>[7]</sup>  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.55 (d,  $J = 8.8$  Hz, 2 H), 7.38 (d,  $J = 8.8$  Hz, 2 H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  133.4, 131.5, 124.1, 123.4, 109.8.

**1-Chloro-4-thiocyanatobenzene (14b).** Procedure B was followed using (4-chlorophenyl)boronic acid (31.3 mg, 0.2 mmol) and TMSNCS (84.5  $\mu\text{L}$ , 0.6 mmol, 3.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 3 hours and 15 mA instead of 10 mA. The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 7.5 mg (22%) of the product as a white solid. Exhibited spectral data in accordance with previous report.<sup>[6]</sup>  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.45 (d,  $J = 8.4$  Hz, 2 H), 7.39 (d,  $J = 8.4$  Hz, 2 H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  136.1, 131.4, 130.4, 122.7, 110.0.

**Methyl-4-thiocyanatobenzoate (15b).** Procedure B was followed using (4-methoxycarbonylphenyl)boronic acid (36.0 mg, 0.2 mmol) and TMSNCS (84.5  $\mu\text{L}$ , 0.6 mmol, 3.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 3 hours and 15 mA instead of 10 mA. The reaction mixture was purified by

flash column chromatography on silica gel (22:3, petroleum ether: EtOAc) to afford 12.4 mg (32%) of the product as a white solid. Exhibited spectral data in accordance with previous report.<sup>[3]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.08 (d,  $J$  = 8.4 Hz, 2 H), 7.55 (d,  $J$  = 8.4 Hz, 2 H), 3.93 (s, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  165.7, 131.1, 130.8, 130.4, 128.3, 109.0, 52.5.

**4-Thiocyanatobenzonitrile (16b).** Procedure B was followed using (4-cyanophenyl)boronic acid (29.4 mg, 0.2 mmol) and TMSNCS (84.5  $\mu$ L, 0.6 mmol, 3.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 3 hours and 15 mA instead of 10 mA. The reaction mixture was purified by flash column chromatography on silica gel (22:3, petroleum ether: EtOAc) to afford 10.6 mg (33%) of the product as a white solid. Exhibited spectral data in accordance with previous report.<sup>[7]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.73 (d,  $J$  = 8.4 Hz, 2 H), 7.61 (d,  $J$  = 8.4 Hz, 2 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  133.5, 131.3, 128.8, 117.4, 113.0, 108.1.

**1-Thiocyanatonaphthalene (17b).** Procedure B was followed using naphthalen-1-ylboronic acid (34.4 mg, 0.2 mmol) and TMSNCS (84.5  $\mu$ L, 0.6 mmol, 3.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 23.4 mg (63%) of the product as a white solid. Exhibited spectral data in accordance with previous report.<sup>[6]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.25 (d,  $J$  = 8.4 Hz, 1 H), 7.99 (d,  $J$  = 8.4 Hz, 1 H), 7.94 (d,  $J$  = 7.6 Hz, 2 H), 7.71 (t,  $J$  = 7.2 Hz, 1 H), 7.62 (t,  $J$  = 7.2 Hz, 1 H), 7.52 (t,  $J$  = 8.0 Hz, 1 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  134.3, 132.4, 132.2, 131.6, 129.0, 128.1, 127.2, 125.9, 124.2, 120.7, 110.7.

**2-Thiocyanatonaphthalene (18b).** Procedure B was followed using naphthalen-2-ylboronic acid (34.4 mg, 0.2 mmol) and TMSNCS (84.5  $\mu$ L, 0.6 mmol, 3.0 equiv). With stirring, the reaction mixture was performed for 5 hours instead of 3 hours. The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 11.5 mg (31%) of the product as a white solid. Exhibited spectral data in accordance with previous report.<sup>[6]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.01 (s, 1 H), 7.92 - 7.78 (m, 3 H), 7.59 - 7.51 (m, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  133.6, 133.0, 130.3, 129.8, 127.9, 127.7, 127.6, 127.5, 126.2, 121.2, 110.6.

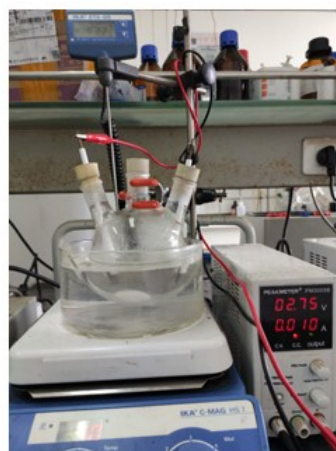
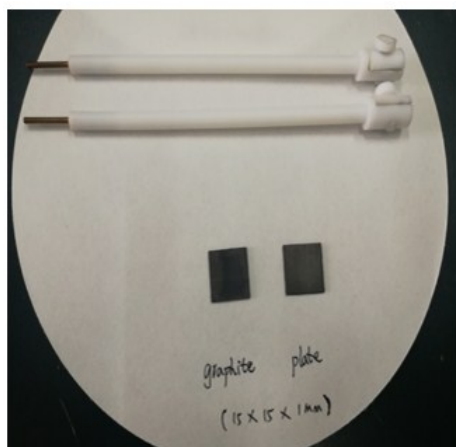
**3-Thiocyanatobenzo[b]thiophene (20b).** Procedure B was followed using benzo[b]thiophen-3-ylboronic acid (35.6 mg, 0.2 mmol) and TMSNCS (84.5  $\mu$ L, 0.6 mmol, 3.0 equiv). With stirring, the reaction mixture was performed for 80 minutes instead of 3 hours. The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 31.9 mg (83%) of the product as a white solid. Exhibited spectral data in accordance with previous report.<sup>[5]</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.99 (d,  $J$  = 7.2 Hz, 1 H), 7.90 (d,  $J$  = 6.8 Hz,

2 H), 7.55 (t,  $J = 8.0$  Hz, 1 H), 7.47 (d,  $J = 7.6$  Hz, 1 H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  139.5, 137.2, 134.3, 125.9, 125.7, 123.2, 122.2, 112.0, 109.7.

**3-Thiocyanatobenzofuran (22b).** Procedure B was followed using benzofuran-3-ylboronic acid (32.4 mg, 0.2 mmol) and TMSNCS (84.5  $\mu\text{L}$ , 0.6 mmol, 3.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 25.6 mg (73%) of the product as a yellow solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.94 (s, 1 H), 7.81 - 7.76 (m, 1 H), 7.58 (dd,  $J = 8.0, 1.6$  Hz, 1 H), 7.46 - 7.42 (m, 2 H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  155.3, 149.1, 126.3, 126.2, 124.4, 119.6, 112.3, 109.3, 101.3. HRMS (ESI-TOF)  $m/z$ :  $[\text{M}-\text{H}]^-$  Calcd. for  $\text{C}_9\text{H}_5\text{NSO}$ : 174.0024; found: 173.9630.

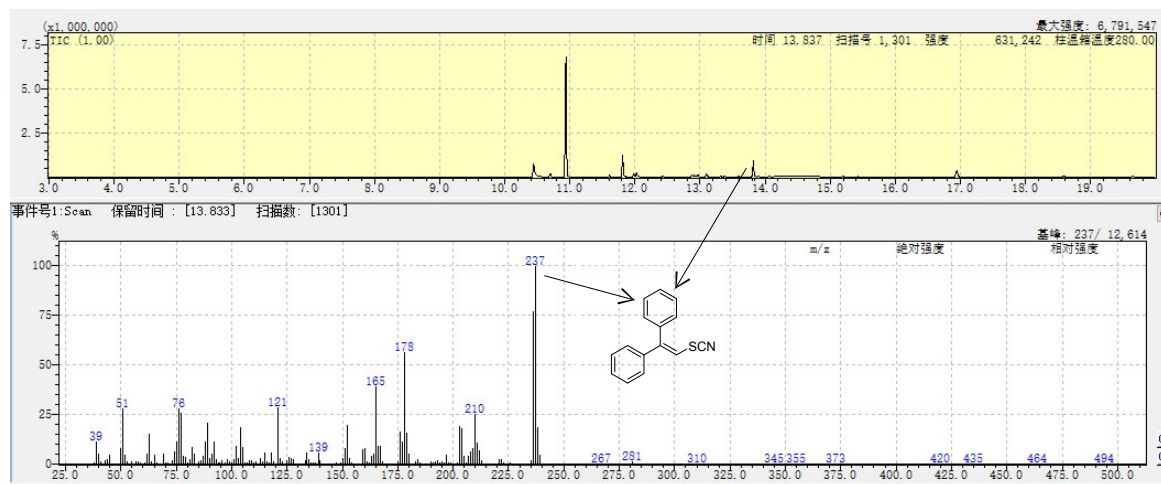
**2-Thiocyanatobenzofuran (23b).** Procedure B was followed using benzofuran-2-ylboronic acid (32.4 mg, 0.2 mmol) and TMSNCS (84.5  $\mu\text{L}$ , 0.6 mmol, 3.0 equiv). The reaction mixture was purified by flash column chromatography on silica gel (97:3, petroleum ether: EtOAc) to afford 22.9 mg (65%) of the product as a yellow solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.61 (d,  $J = 8.0$  Hz, 1 H), 7.55 (d,  $J = 8.0$  Hz, 1 H), 7.43 (t,  $J = 8.0$  Hz, 1 H), 7.31 (t,  $J = 7.6$  Hz, 1 H), 7.22 (s, 1 H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  157.2, 134.9, 127.4, 126.9, 123.9, 121.6, 117.1, 111.8, 107.4. HRMS:  $[\text{M}+\text{H}]^+$  calcd. for  $\text{C}_9\text{H}_5\text{NSO}$ : 176.0153; found: 176.0170.

**Gram-scale synthesis of *p*-hydroxyphenyl selenocyanate (5a).** (4-hydroxyphenyl)boronic acid (4.0 mmol),  $\text{KSeCN}$  (16.0 mmol) and MeCN (200 mL),  $\text{H}_2\text{O}$  (1 mL) were combined and added into an oven-dried three-necked flask (500 mL) with a stir bar. The flask was equipped with graphite felts (15 mm  $\times$  15 mm  $\times$  1 mm) as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA (The dual display potentiostat was operating in constant current mode) under room temperature for 23 h. When the reaction was finished, the solution was filtered and washed with EtOAc. The solvent was removed with a rotary evaporator. The pure product was obtained by flash column chromatography on silica gel (22:3, petroleum ether: EtOAc) to afford 0.66 g (84%) of the **5a**.

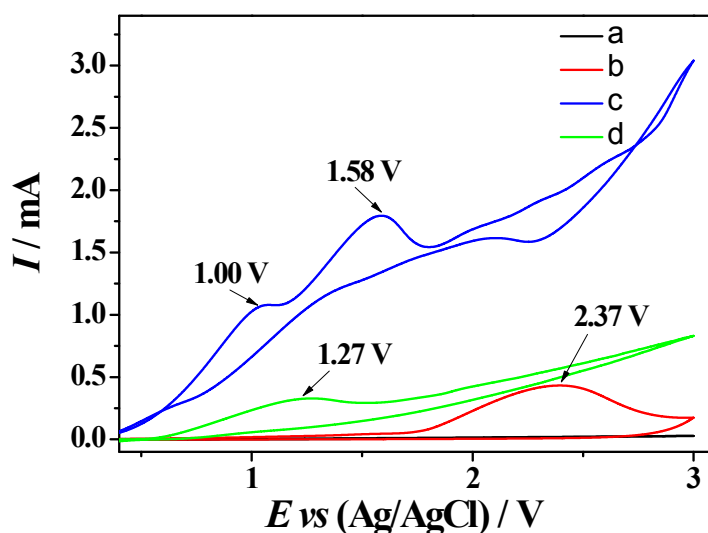


**Free radical trapping experiment**

Into a round bottom flask, (4-methoxyphenyl)boronic acid (0.2 mmol, 1.0 equiv), TMSNCS (0.6 mmol, 3.0 equiv), and DPE (0.4 mmol, 2.0 equiv) were dissolved in MeCN (10 mL), H<sub>2</sub>O (30  $\mu$ L) with KF (0.1 M) as an electrolyte. The resulting solution was electrolyzed with two graphite felts (15 mm  $\times$  15 mm  $\times$  0.4 mm) as the cathode and anode under a constant current (10 mA) at room temperature for 3 h. GC-MS analysis of the resulting crude reaction solution revealed a DPE-SCN adduct (13.833 min) (mass weight: 237).



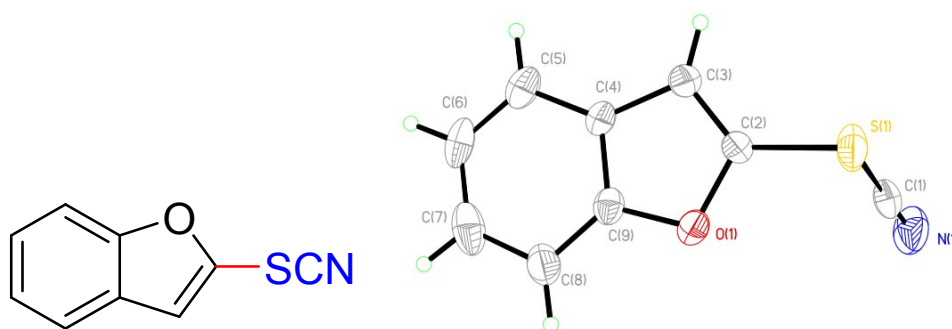
**General procedure for cyclic voltammetry (CV).** CV was performed in a threeelectrode cell connected to a schlenk line under room temperature. Glassy carbon electrode was used as working electrode, and platinum wire was employed as counter electrode. Ag/AgCl reference electrode was submerged in saturated aqueous KCl solution and separated from reaction by a salt bridge. The MeCN (10 mL), H<sub>2</sub>O (50  $\mu$ L) containing 0.25 mol/L KF was poured into the electrochemical cell in all experiments. The scan rate was 100 mV/s ranging from -1.5 V to 3.0 V.



**Figure 1.** Cyclic voltammograms of substrates: (a) background (KF 0.25 mol/L in

MeCN/H<sub>2</sub>O); (b) 4-methoxyphenylboronic acid **2** (0.05 mol/L); (c) KSeCN (0.08 mol/L); (d). TMSNCS (0.06 mmol/L).

**Crystal data and structure refinement for product 2-thiocyanatobenzofuran (23b).**



**Figure 2.** X-structure of **23b**. (CCDC 1902841)

**Table 1.** Crystallographic information for **23b**

compound	23b
CCDC numbers	1902841
Empirical formula	C <sub>9</sub> H <sub>5</sub> NOS
Formula weight	175.21
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 8.398(5) Å = 90° b = 7.421(5) Å = 90.90° c = 13.749(7) Å = 90°
Volume	844.1(9) Å <sup>3</sup>
Z	4
Density (calculated)	1.379 Mg/m <sup>3</sup>
Absorption coefficient	0.327 mm <sup>-1</sup>
F(000)	360
Crystal size	0.25 x 0.23 x 0.20 mm
Theta range for data collection	2.46 to 26.00°
Index ranges	-10 ≤ h ≤ 10, -9 ≤ k ≤ 9, -16 ≤ l ≤ 16
Reflections collected	6090
Independent reflections	1655 [R(int) = 0.0472]
Completeness to theta = 26.00°	99.9%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.937 and 0.922

Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	1655 / 0 / 109
Goodness-of-fit on F2	3.633
Final R indices [ $I > 2\sigma(I)$ ]	$R_1 = 0.0905$ , $wR_2 = 0.1814$
R indices (all data)	$R_1 = 0.1066$ , $wR_2 = 0.1828$
Absolute structure parameter	109
Largest diff. peak and hole	0.760 and -0.359 e.Å <sup>-3</sup>

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