

## Supplementary Information (SI)

# A fluorescent chemosensor for Sn<sup>2+</sup> and Cu<sup>2+</sup> based on a carbazole-containing diarylethene

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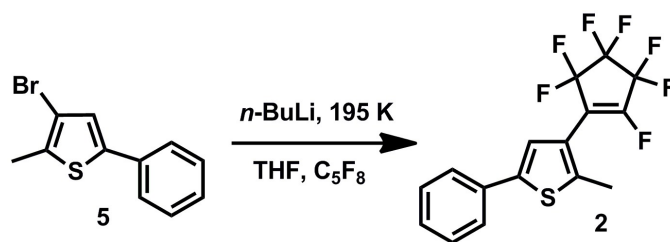
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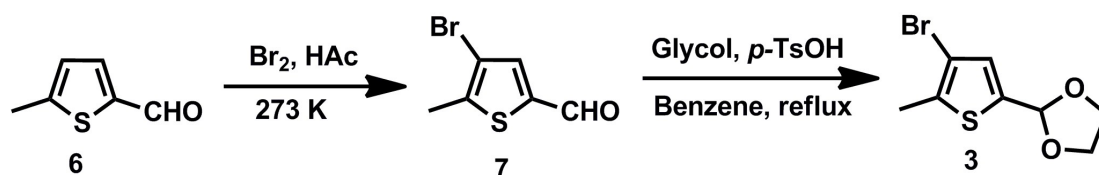
## 1. Synthesis and characterization data



Scheme S1 Synthesis of intermediate 2.

### (2-Methyl-5-phenyl)-3-thienyl-perfluorocyclopentene (2)

To a stirred of **5** (2.52 g, 10 mmol) in THF solution (50 mL),  $n\text{-BuLi}$ /hexane solution (2.5 mol L<sup>-1</sup>) was slowly added under a nitrogen atmosphere at 195 K. After 30 min,  $\text{C}_5\text{F}_8$  (2.33 g, 11 mmol) was added and the mixture was stirred for 2 h at this temperature. The reaction mixture was extracted with diethyl ether and evaporated in vacuo, then purified by column chromatography to give compound **2** (2.34 g) in 64.1 % yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 2.41 (s, 3H, -CH<sub>3</sub>), 7.22 (s, 1H, thienyl-H), 7.28 (s, 1H, phenyl-H), 7.32 (d, 2H, phenyl-H,  $J = 8.0$  Hz), 7.48 (d, 2H, phenyl-H,  $J = 8.0$  Hz); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz),  $\delta$  (ppm): 14.4, 120.1, 122.7, 125.7, 128.6, 129.6, 132.8, 142.5, 143.8.



Scheme S2 Synthesis of intermediate 3.

### 2-Methyl-3-bromo-5-formaldehyde-thiophene (7)

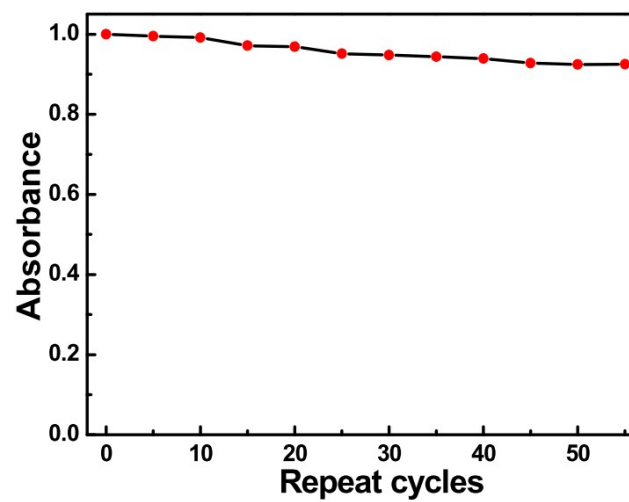
To a stirred solution of compound **6** (24.0 g, 190.5 mmol) in acetic acid (100 mL) at 273 K was slowly added  $\text{Br}_2$  (25 mL). The reaction mixture was stirred overnight at this temperature. The reaction was stopped by the addition of water. The mixture was neutralized by  $\text{Na}_2\text{CO}_3$  and

extracted with ether. The ether extract was dried, filtrated, and concentrated. The residue was purified by distillation in vacuo. Compound **7** was obtained as a yellow solid of 32.3 g in 81.2 % yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 2.47 (s, 3H, -CH<sub>3</sub>), 7.62 (s, 1H, thiophene-H), 9.75 (s, 1H, -CHO); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz), δ (ppm): 15.4, 101.7, 139.6, 140.0, 145.3, 183.1

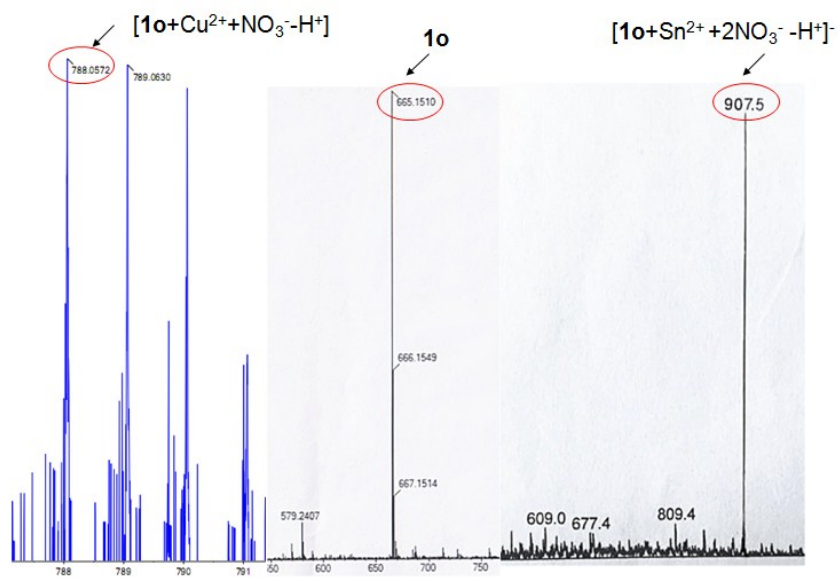
**2-Methyl-3-bromo-5-(1,3-dioxolane)-thiophene (3)**

Compound **7** (2.04 g, 10 mmol), glycol (3.2 g, 50 mmol), and *p*-toluenesulfonic acid (0.02 g, 4.27 mmol) was dissolved in benzene (120 mL). Under the Dean–Stark condition, the reaction mixture was refluxed overnight, and then washed with NaHCO<sub>3</sub> (5 % (w/v), 2 × 50 mL) aqueous. The combined benzene layers were dried, filtered, and evaporated in vacuum to give 2.31 g **3** as a solid in 93 % yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 2.37 (s, 3H, -CH<sub>3</sub>), 3.98–4.15 (m, 4H, -CH<sub>2</sub>), 6.04 (s, 1H, -CH), 6.95 (s, 1H, thiophene-H); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz), δ (ppm): 15.3, 60.6, 63.2, 111.2, 139.2, 139.6.0, 145.5.

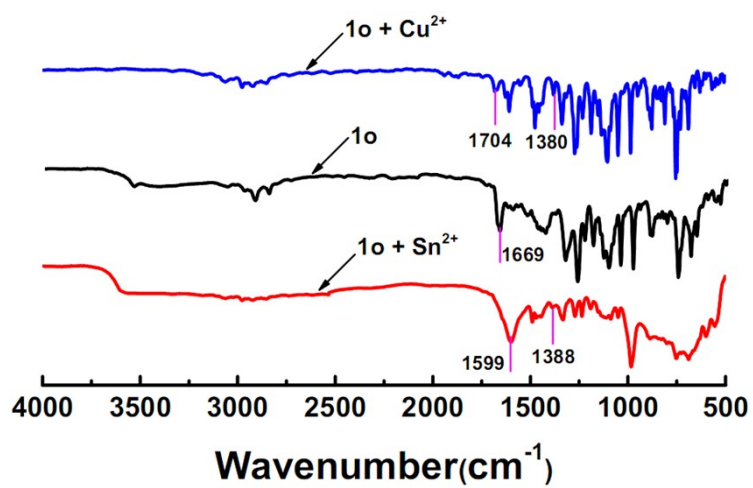
## 2. Supplementary data



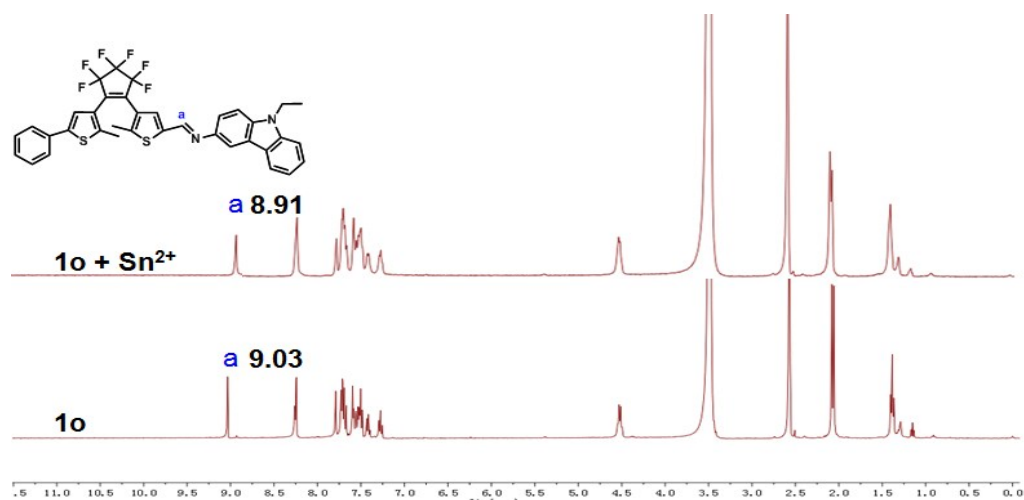
**Fig. S1.** The stability of **1o**. Initial absorbance of the sample was fixed to 1.0.



**Fig. S2.** Mass spectra of  $1\mathbf{o}$ ,  $1\mathbf{o} + \text{Sn}^{2+}$  and  $1\mathbf{o} + \text{Cu}^{2+}$ .



**Fig. S3.** Changes in IR spectra of **1o** induced by Sn<sup>2+</sup> and Cu<sup>2+</sup>.



**Fig. S4.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectral changes of **1o** with Sn<sup>2+</sup> ions.

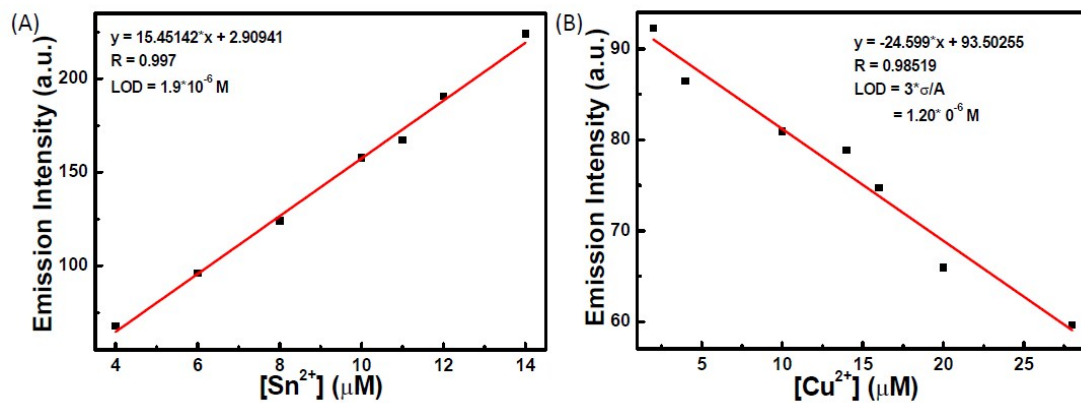
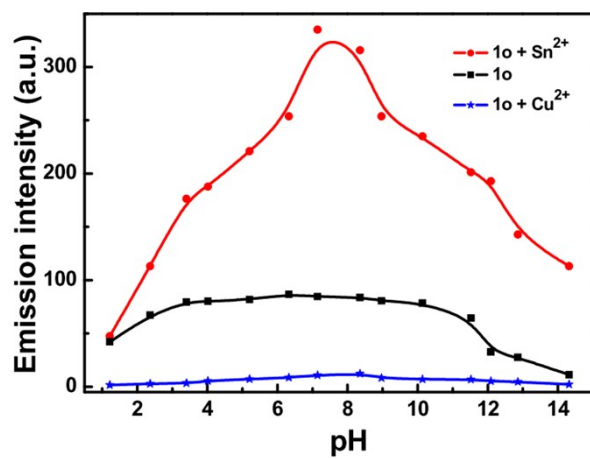


Fig. S5. Detection limit plot: intensity verse concentration of  $\text{Sn}^{2+}$  and  $\text{Cu}^{2+}$ : (A)  $\text{Sn}^{2+}$ ; and (B)  $\text{Cu}^{2+}$ .





**Fig. S6.** Fluorescence intensity of **1o** and **1o** + 10 equiv Sn<sup>2+</sup>, **1o** + 9 equiv Cu<sup>2+</sup> in water with different pH conditions.

### 3. NMR spectra

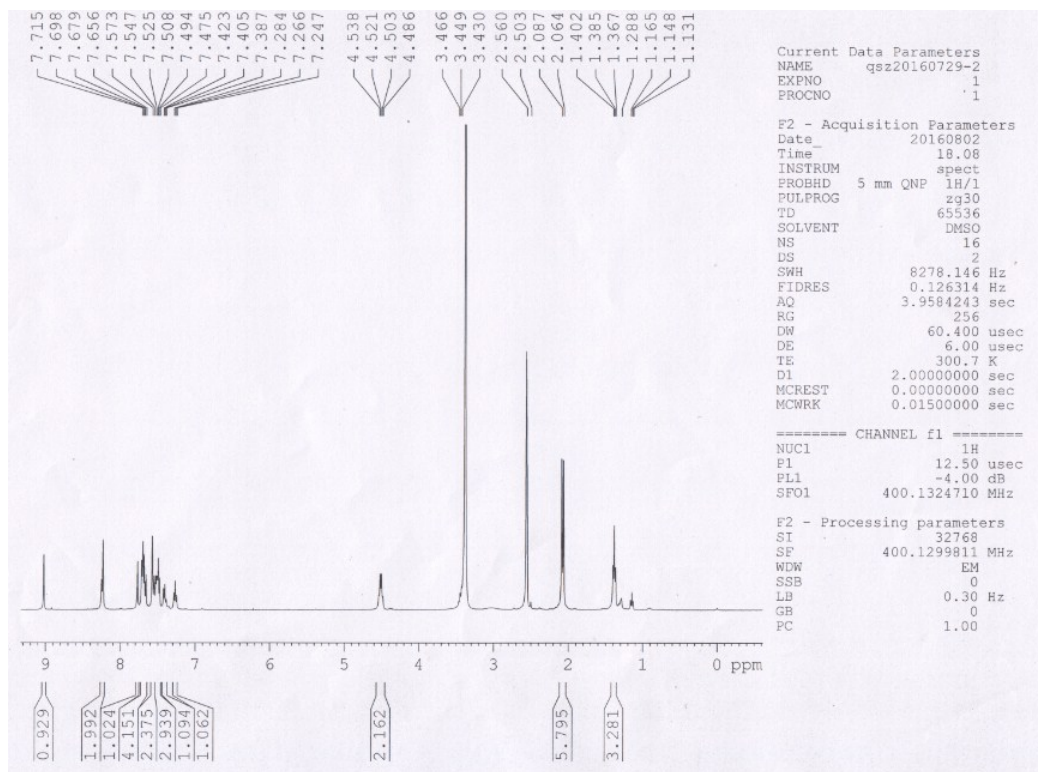
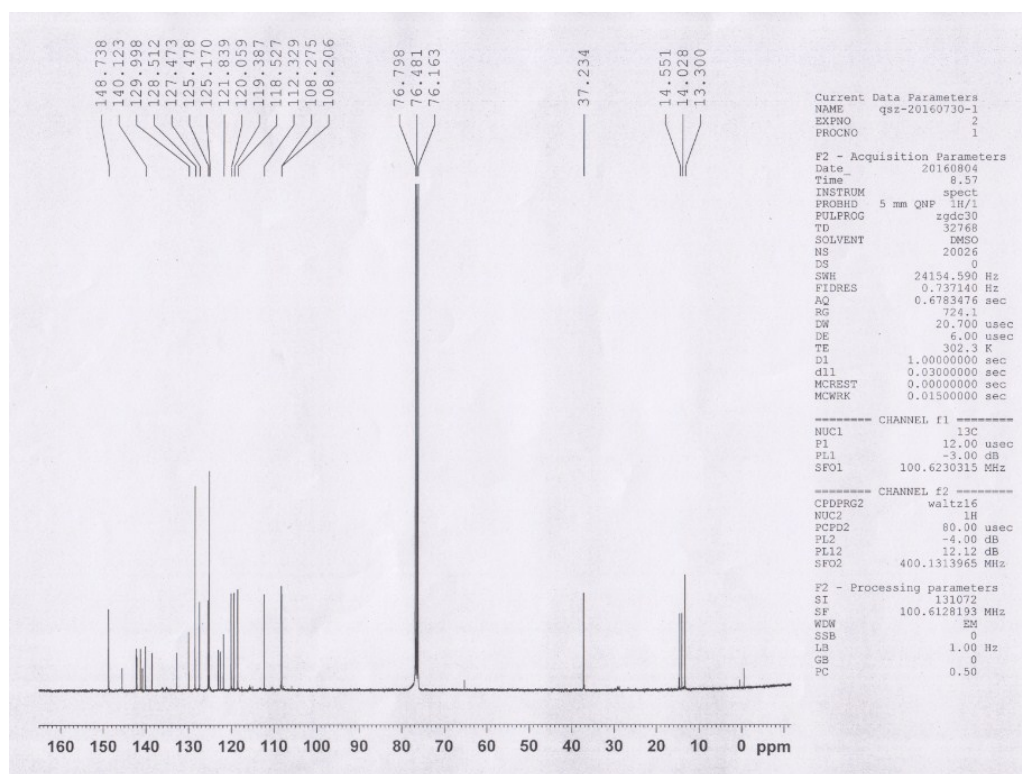


Fig. S7.  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) spectra of **1o**.



**Fig. S8.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectra of **1o**.

#### 4. HRMS

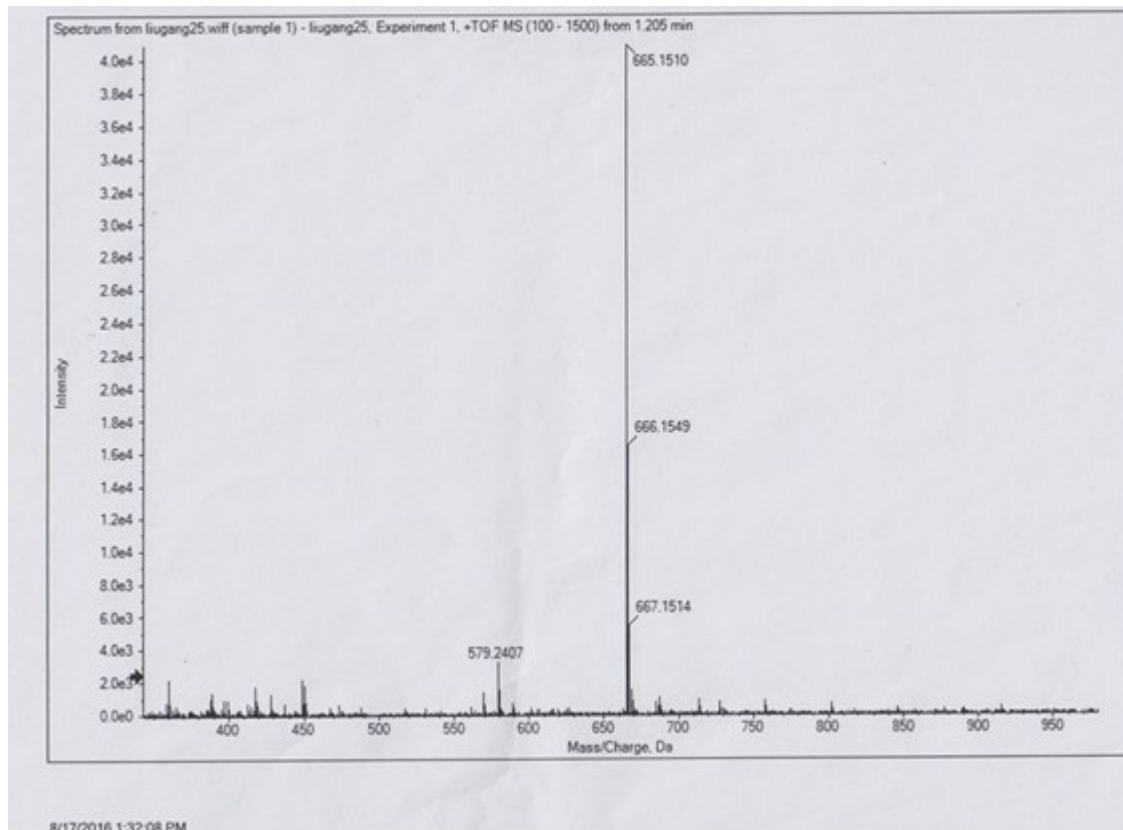


Fig. S9. HRMS for 1o.