

## Supporting Information

### **Hg<sup>2+</sup> induced hydrolysis of pentaquinone based Schiff Base: A new chemodosimeter for Hg<sup>2+</sup> ions in aqueous media**

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Sharma,<sup>b</sup> and Tandeep Kaur<sup>b</sup>

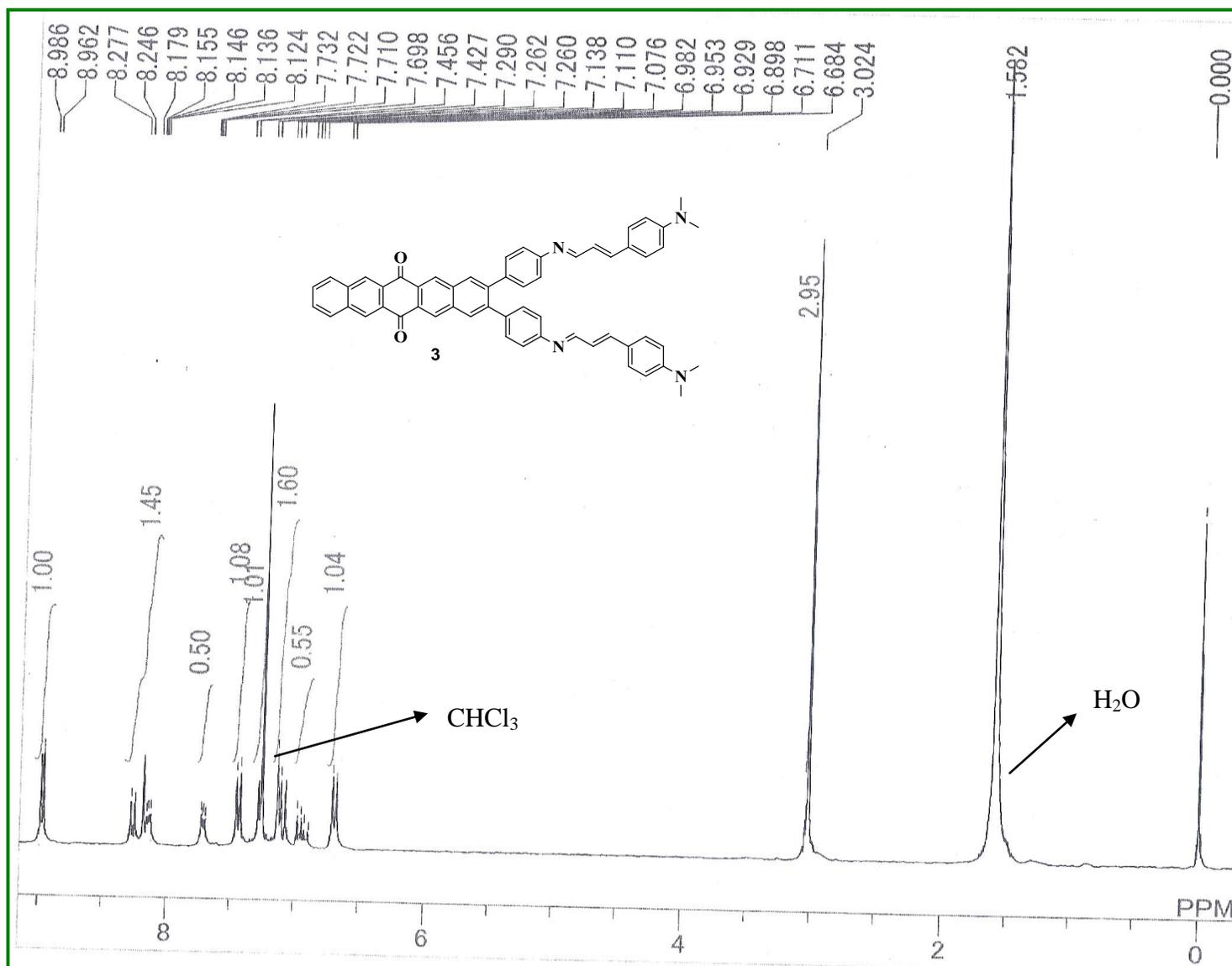
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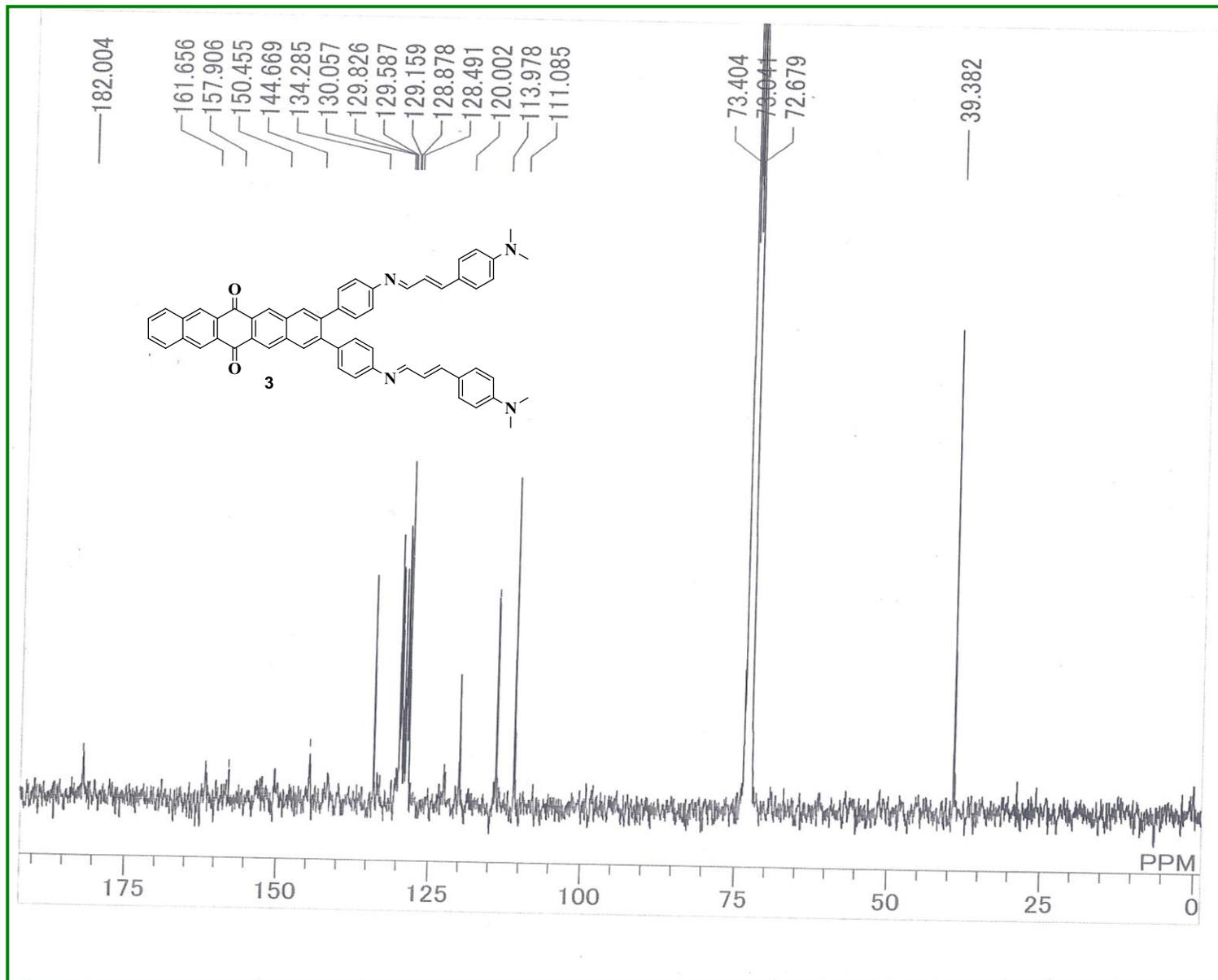
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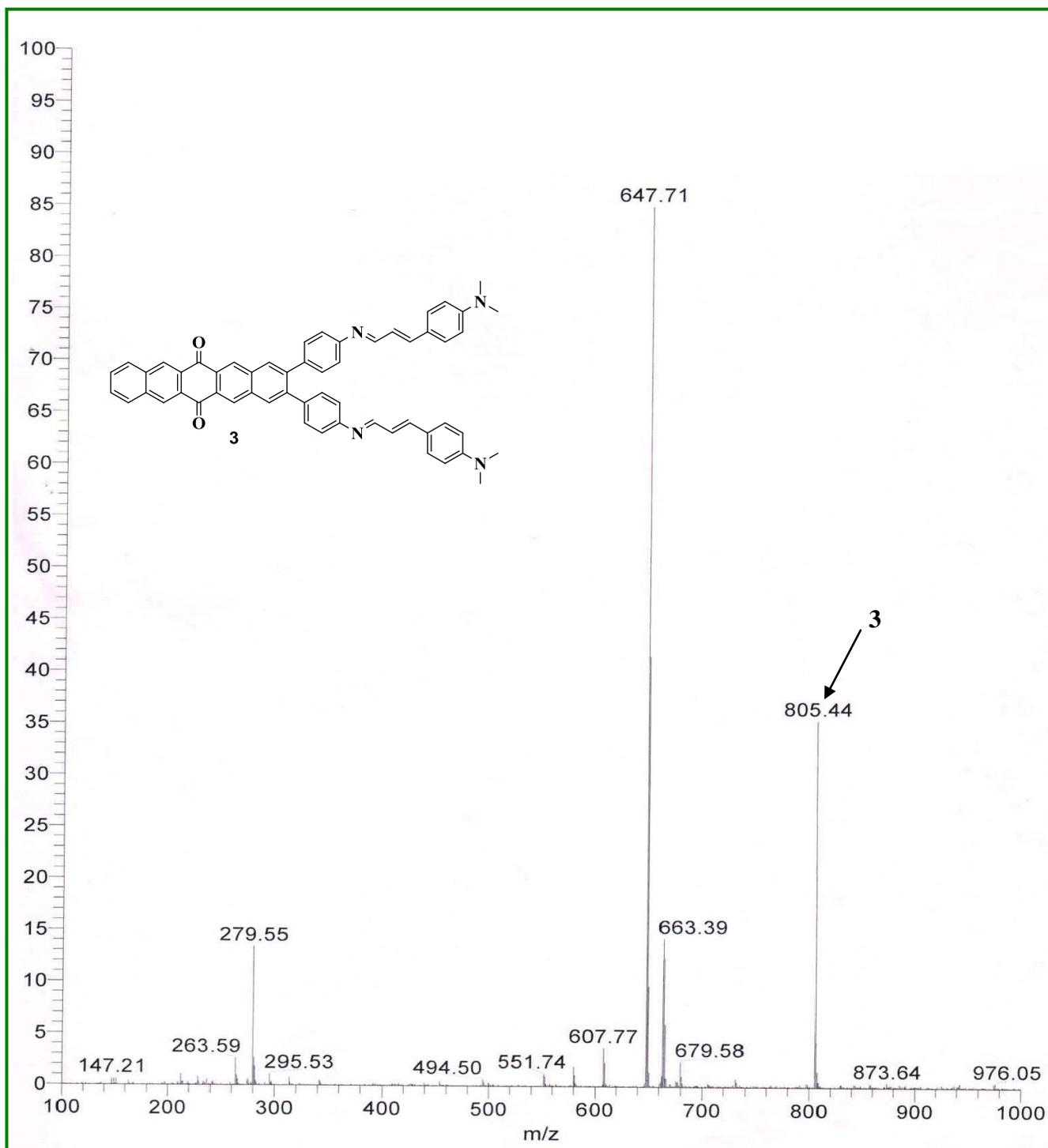
Figure S1.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz, ppm) spectrum of **3**.



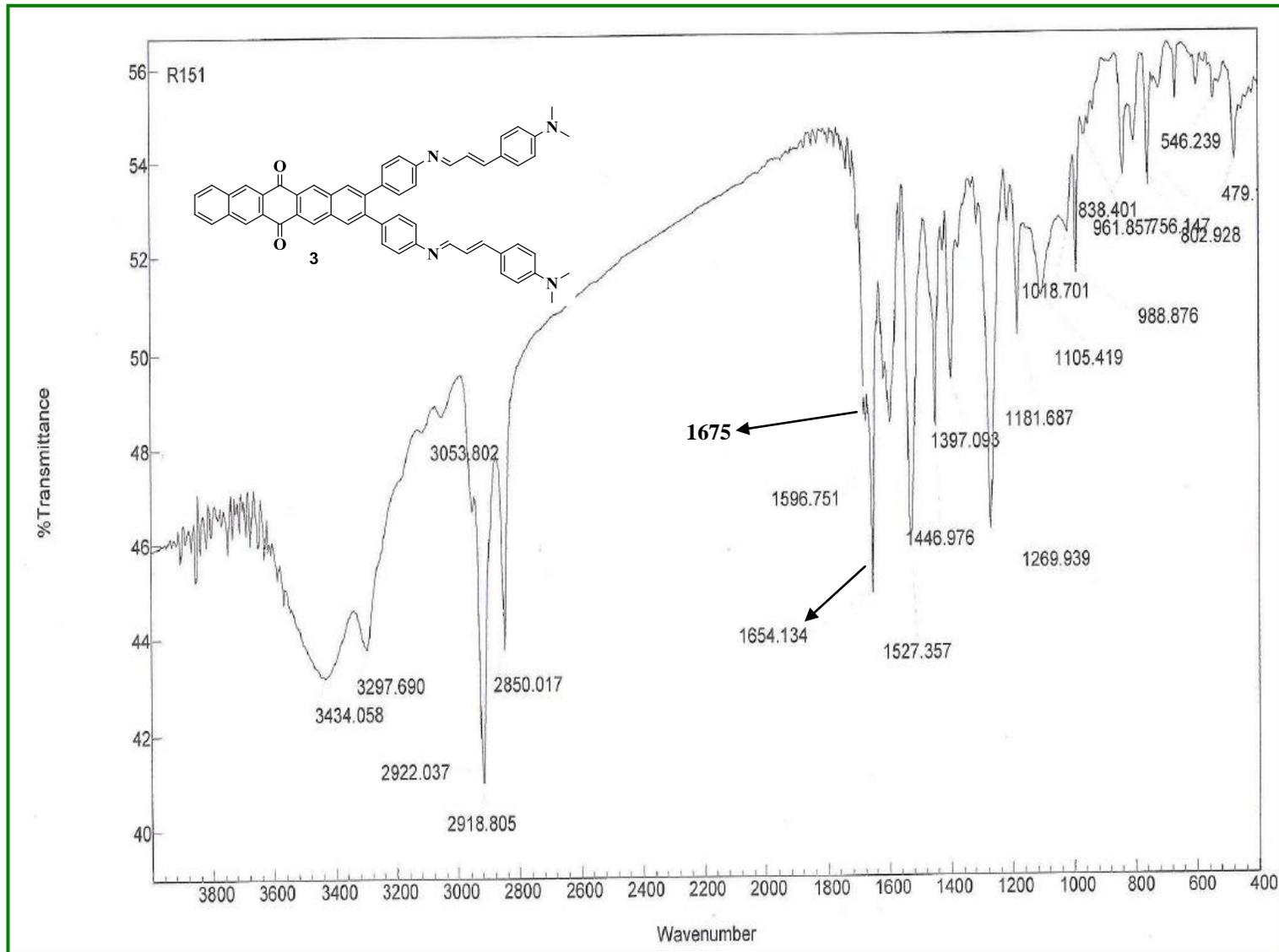
**Figure S2.**  $^{13}\text{C}$  NMR (1,1,2,2-tetrachloroethane- $d_2$ , 75.45 MHz, ppm) spectrum of **3**.

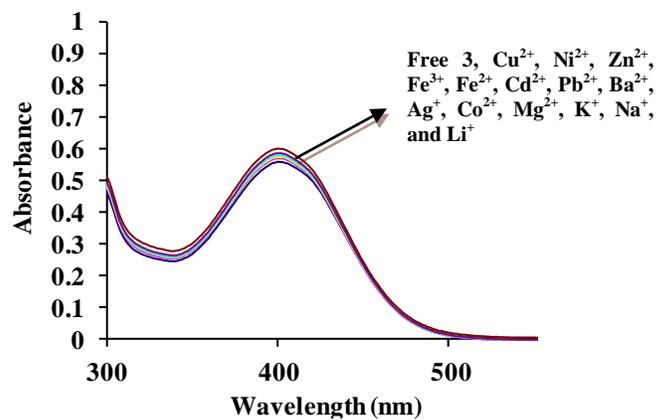


**Figure S3.** Mass spectrum of **3**.

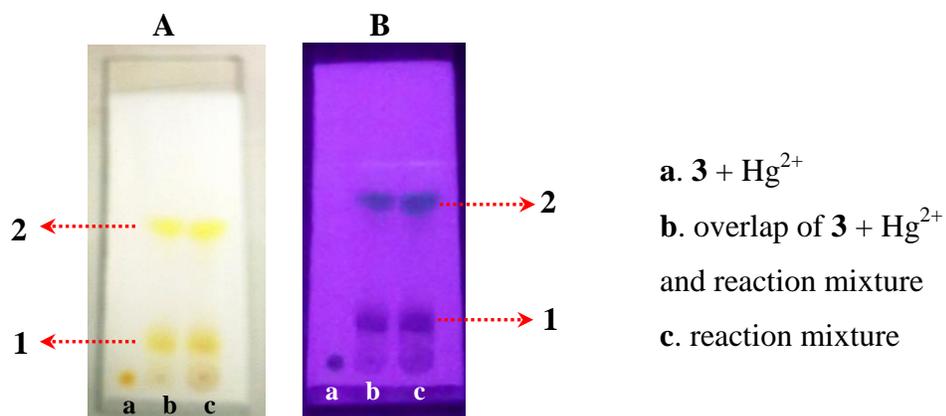


**Figure S4.** IR spectrum of **3**.

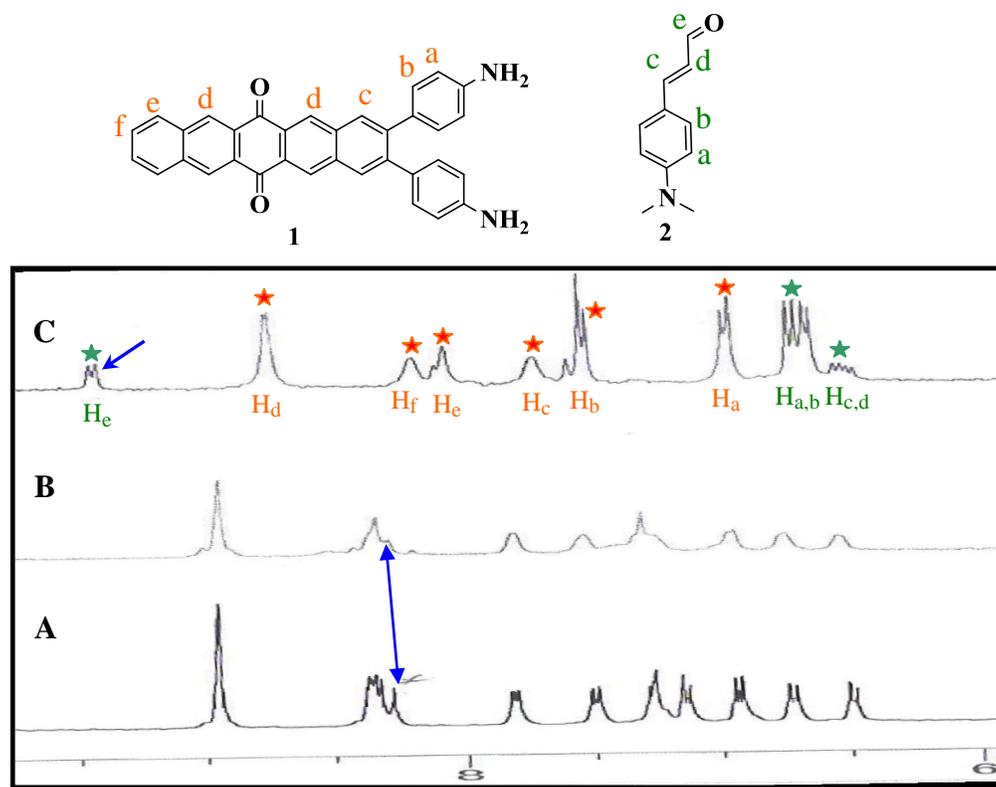




**Figure S5.** UV-vis spectra of **3** (5 μM) in the presence of various metal ions (0-200 equiv) in THF/H<sub>2</sub>O (9.5:0.5, v:v) buffered with HEPES, pH = 7.

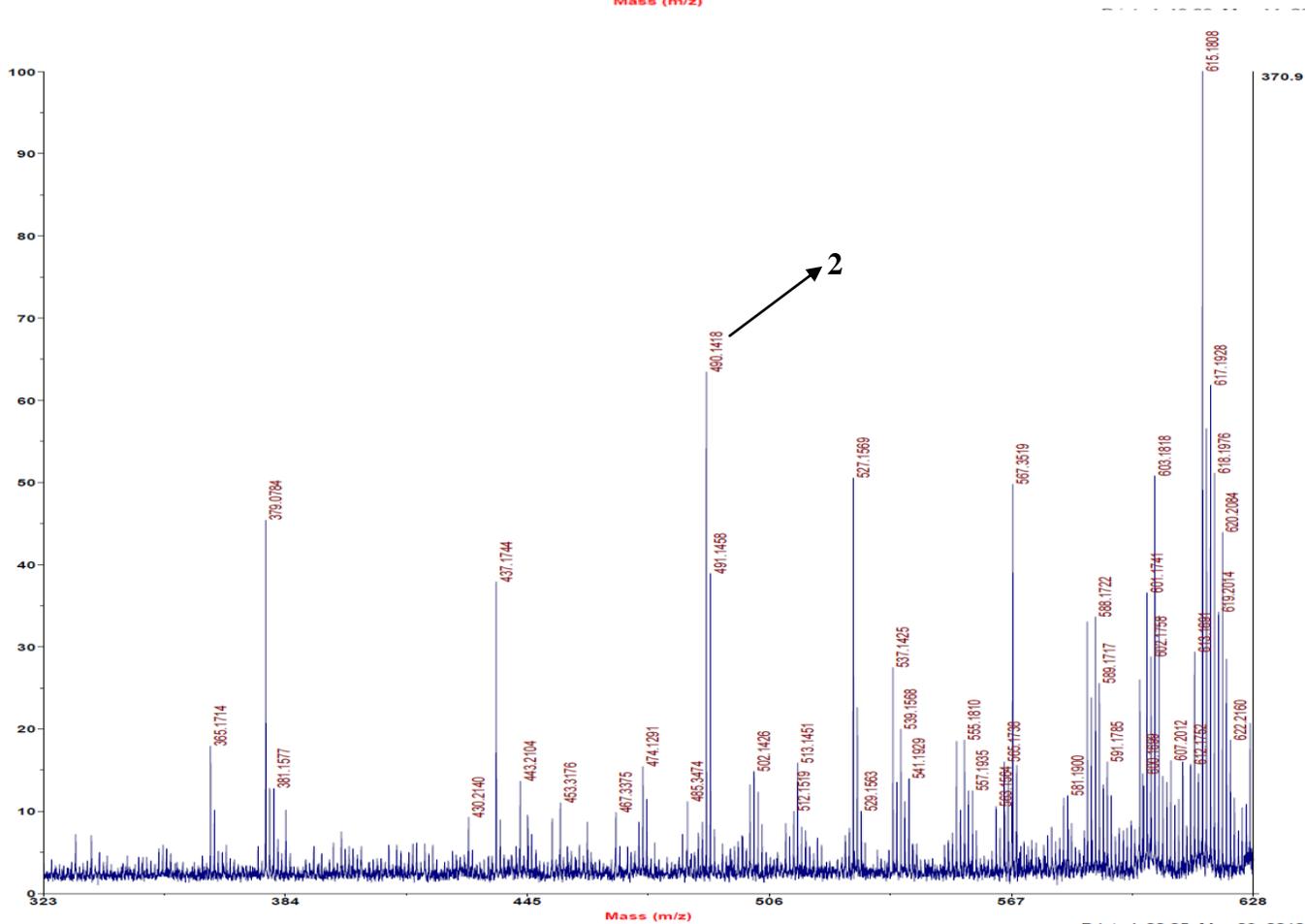
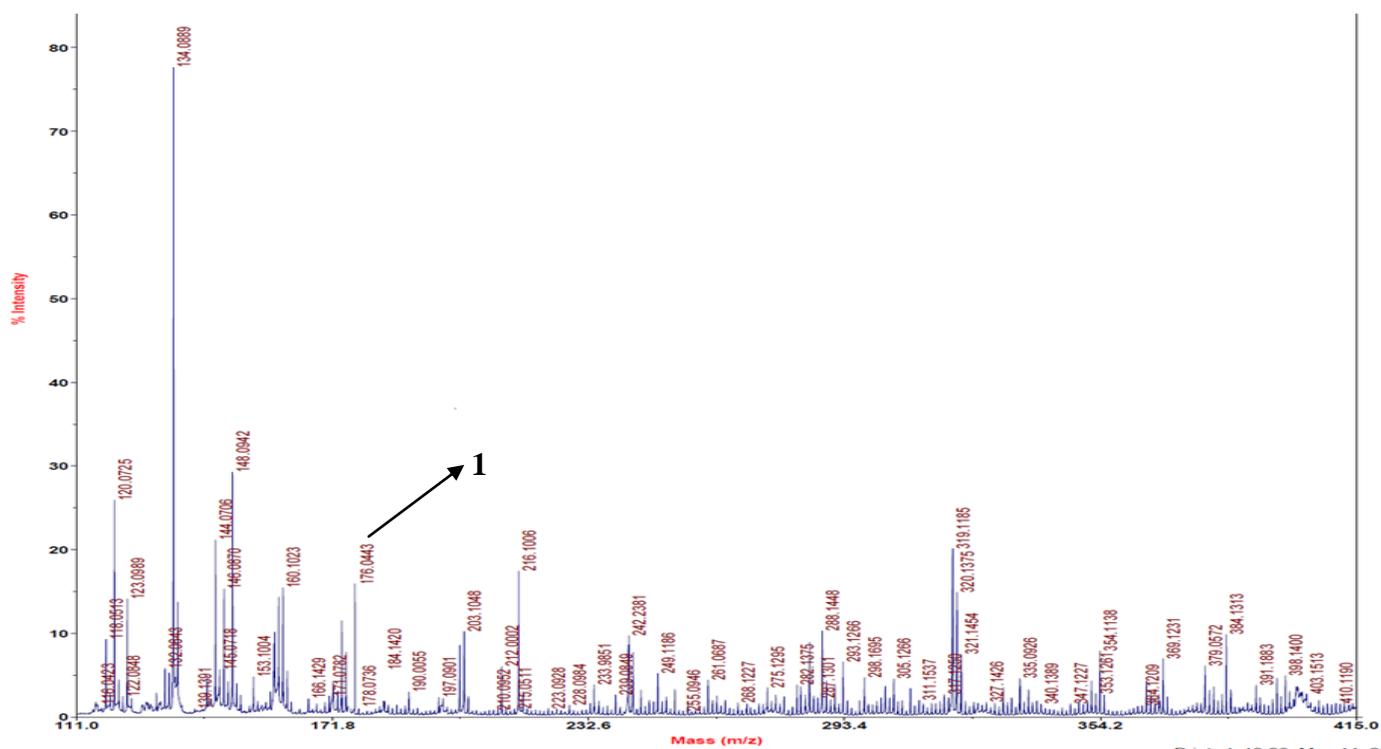


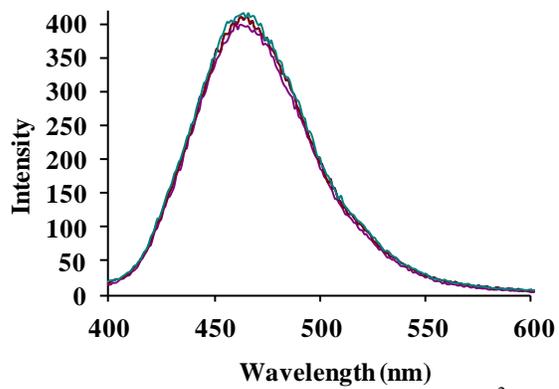
**Figure S6.** TLC showing the formation of pentaquinone diamine (**1**) and *N,N*-dimethylaminocinnamaldehyde (**2**). (**A**) naked eye (**B**) under UV lamp (excited at 365 nm).



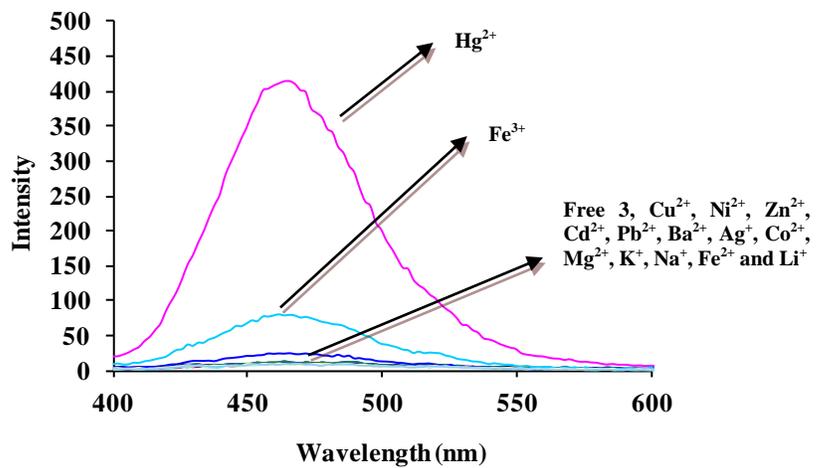
**Figure S7.** Partial <sup>1</sup>H NMR spectra of (A) **3** in DMSO-d<sub>6</sub> (B) **3** + Hg<sup>2+</sup> in DMSO-d<sub>6</sub> (C) reaction of **3** with Hg<sup>2+</sup> was carried out in DMSO-D<sub>2</sub>O (9:1, v/v) for 5 min and then <sup>1</sup>H NMR spectrum of the resulting solution was recorded. ★ Protons of *N,N*-dimethylaminocinnamaldehyde (**2**) ★ Protons of pentaquinone diamine (**1**).

**Figure S8.** Mass spectrum of receptor **3** in THF-H<sub>2</sub>O(9:1).

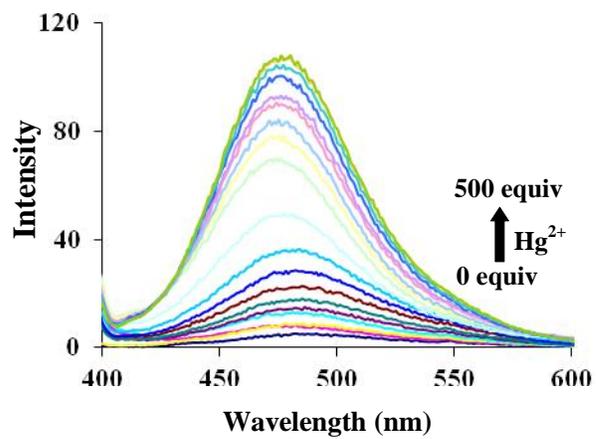




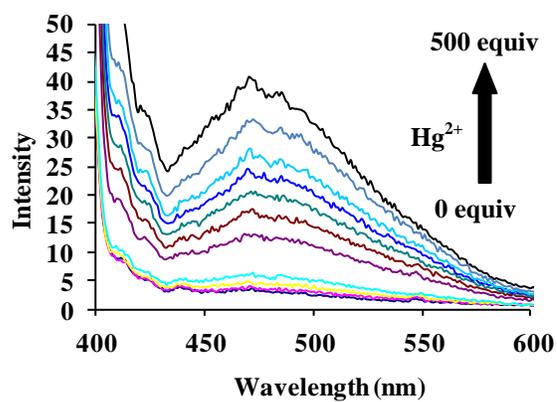
**Figure S9.** Fluorescence response of **3-Hg<sup>2+</sup>** towards TBAI (400 equiv) in THF/H<sub>2</sub>O (9.5:0.5, v:v) buffered with HEPES, pH = 7.



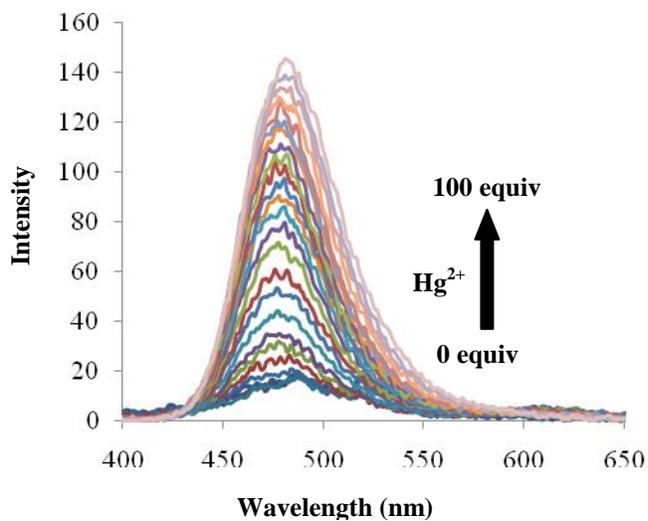
**Figure S10.** Fluorescence spectra of **3** (5 μM) in response to different metal ions (200 equiv each) in THF/H<sub>2</sub>O (9.5:0.5, v:v) buffered with HEPES, pH = 7; λ<sub>ex</sub> = 380 nm.



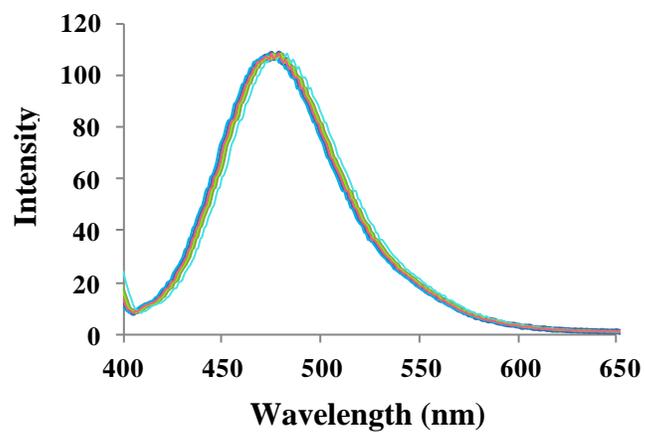
**Figure S11.** Fluorescence response of receptor **3** (5  $\mu\text{M}$ ) on addition of  $\text{Hg}^{2+}$  ions (0-500 equiv) in THF/ $\text{H}_2\text{O}$  (1:1, v:v) buffered with HEPES, pH = 7;  $\lambda_{\text{ex}}$  = 380 nm. Spectra were recorded at the interval of every 30 sec.



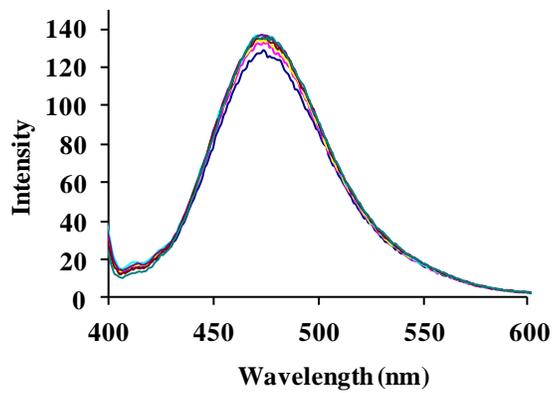
**Figure S12.** Fluorescence response of receptor **3** ( $5 \mu\text{M}$ ) on addition of  $\text{Hg}^{2+}$  ions (0-500 equiv) in THF/ $\text{H}_2\text{O}$  (0.5:9.5, v:v) buffered with HEPES,  $\text{pH} = 7$ ;  $\lambda_{\text{ex}} = 380 \text{ nm}$ . Spectra were recorded at the interval of every 30 sec.



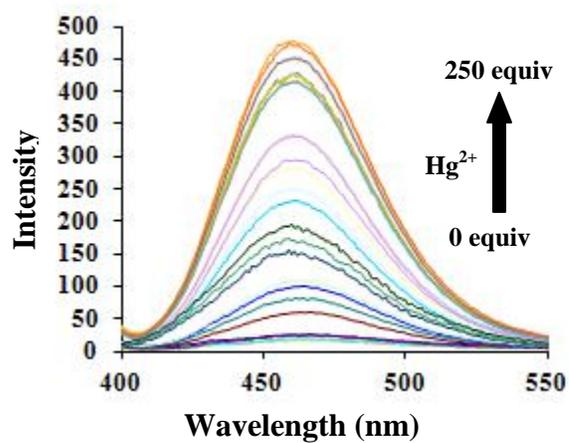
**Figure S13.** Fluorescence response of receptor **3** (5  $\mu$ M) on addition of Hg<sup>2+</sup> ions (0-100 equiv) in DMSO/H<sub>2</sub>O (9.5: 0.5, v:v),  $\lambda_{\text{ex}} = 380$  nm. Spectra were recorded at the interval of every 30 sec.



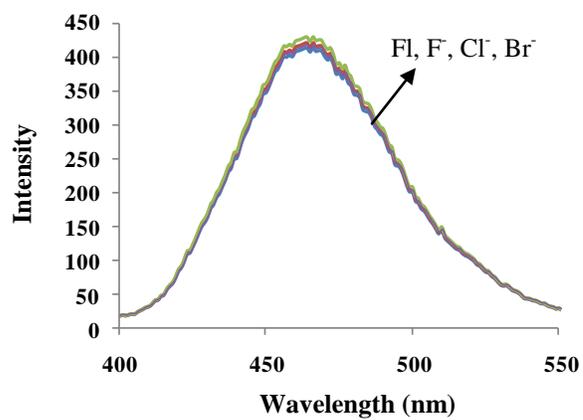
**Figure S14.** Fluorescence response of **3** + Hg<sup>2+</sup> system on addition of human blood serum in THF/H<sub>2</sub>O (1:1, v:v) buffered with HEPES, pH = 7;  $\lambda_{\text{ex}} = 380$  nm.



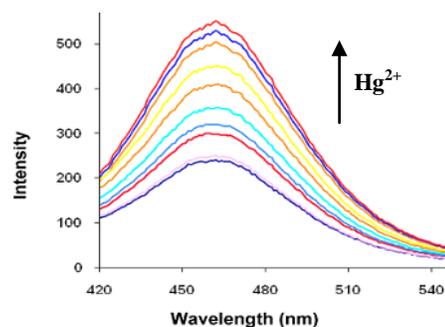
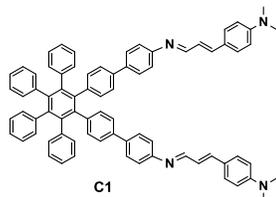
**Figure S15.** Fluorescence response of **3** + Hg<sup>2+</sup> system on addition of cystein in THF/H<sub>2</sub>O (1:1, v:v) buffered with HEPES, pH = 7;  $\lambda_{\text{ex}} = 380$  nm.



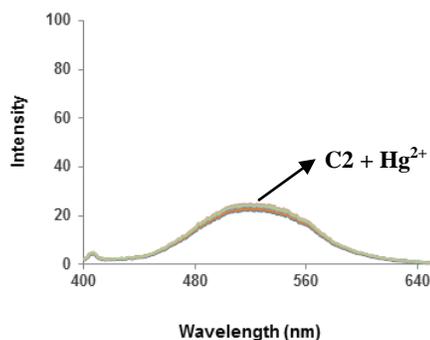
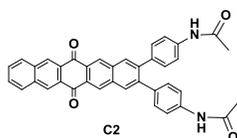
**Figure S16.** Fluorescence response of **3** upon addition of incremental amount of Hg(NO<sub>3</sub>)<sub>2</sub> (250 equiv) in drinking water;  $\lambda_{\text{ex}} = 380$  nm.



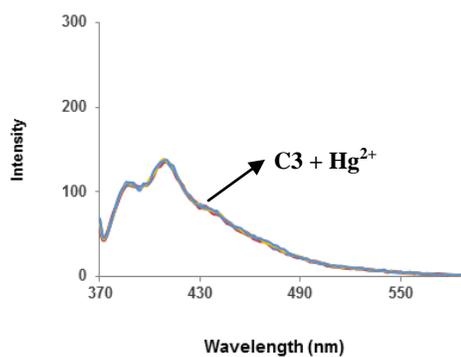
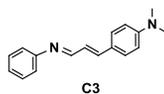
**Figure S17.** Fluorescence response of **3**-Hg<sup>2+</sup> towards TBAX (400 equiv) in THF/H<sub>2</sub>O (9.5:0.5, v:v) buffered with HEPES, pH = 7. TBAX (X = F<sup>-</sup>, Cl<sup>-</sup> and Br<sup>-</sup>)



**Figure S18.** Fluorescence spectra of C1 (5 μM) in the presence of Hg<sup>2+</sup> ions (0–150 μM) in THF:H<sub>2</sub>O (6:4); λ<sub>EX</sub> = 380 nm.



**Figure S19.** Fluorescence response of C2 in the presence of Hg<sup>2+</sup> ions (200 equiv) in THF/H<sub>2</sub>O (9.5:0.5, v:v) buffered with HEPES, pH = 7; λ<sub>EX</sub> = 380 nm.



**Figure S20.** Fluorescence response of C3 in the presence of Hg<sup>2+</sup> ions (200 equiv) in THF/H<sub>2</sub>O (9.5:0.5, v:v) buffered with HEPES, pH = 7; λ<sub>EX</sub> = 380 nm.