

## Supporting information

### **A highly sensitive and selective colorimetric probe based on a cycloruthenated complex: a Hg<sup>2+</sup>-promoted switch of thiophene coordination**

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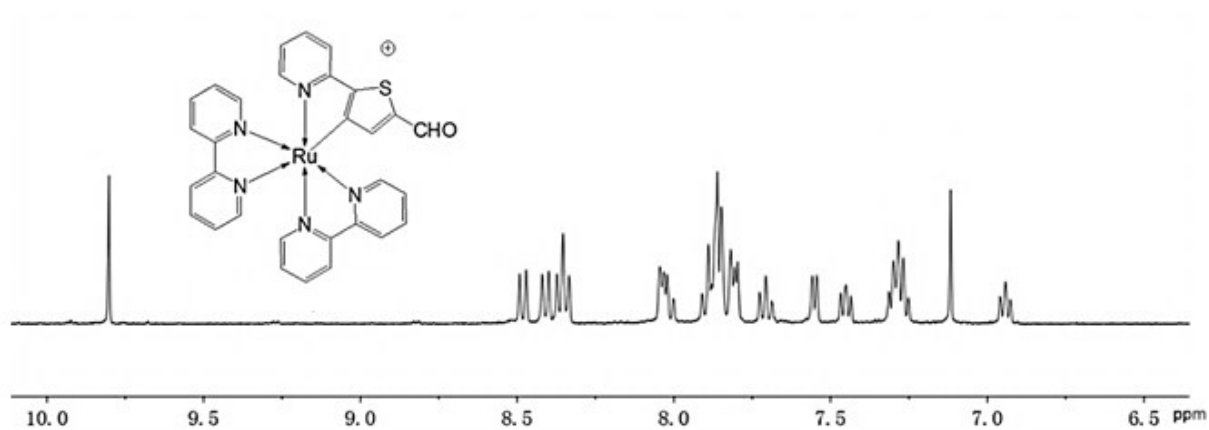


Figure S1.  $^1\text{H}$  NMR of  $[\text{Ru}(\text{fthpy})(\text{bpy})_2]^+$  in  $\text{CD}_3\text{CN}$ .

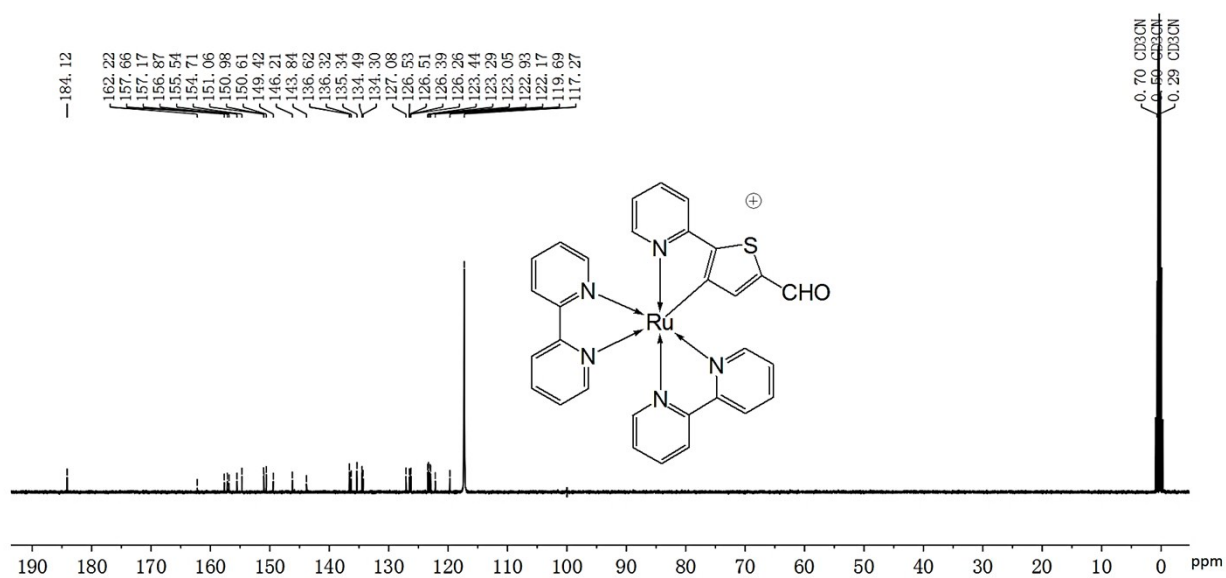


Figure S2.  $^{13}\text{C}$  NMR of  $[\text{Ru}(\text{fthpy})(\text{bpy})_2]^+$  in  $\text{CD}_3\text{CN}$ .

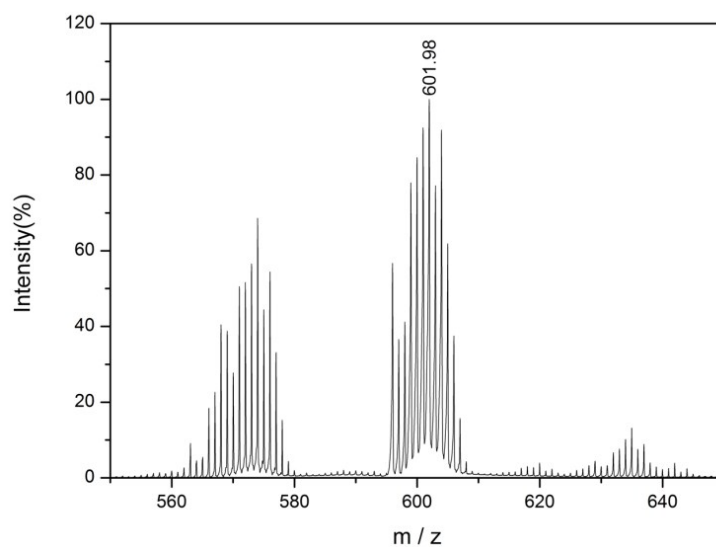


Figure S3. MS spectrum of  $[\text{Ru}(\text{fthpy})(\text{bpy})_2]^+$  in  $\text{CD}_3\text{CN}$ .

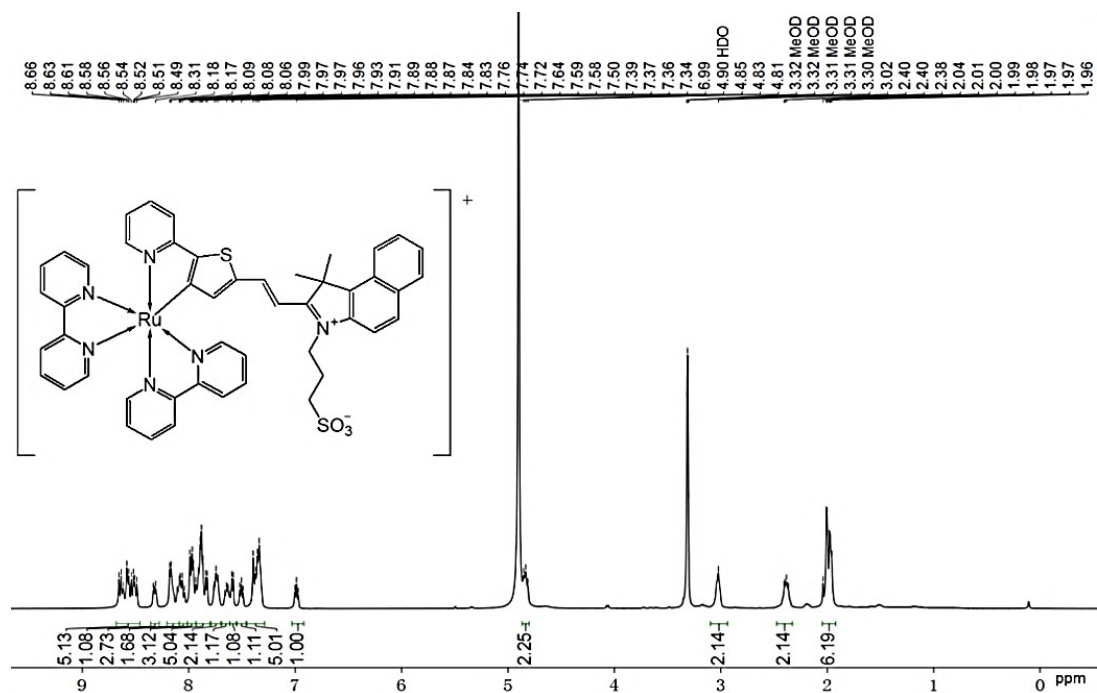


Figure S4. <sup>1</sup>H NMR spectra of **1** in CD<sub>3</sub>OD.

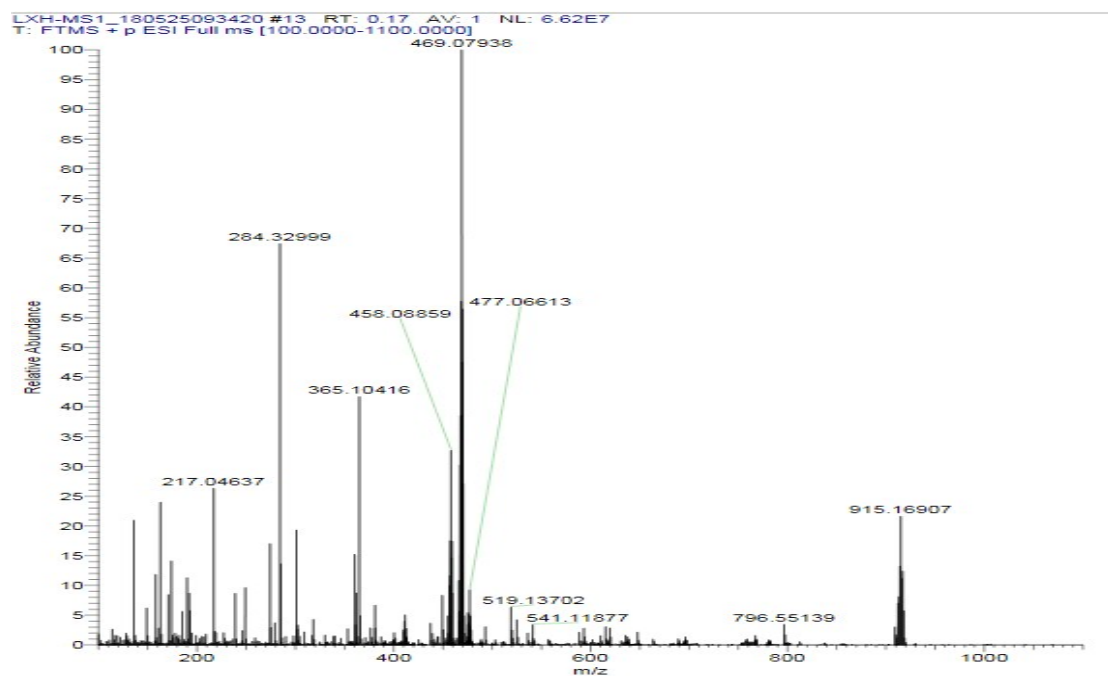


Figure S5. HRMS spectrum of the complex **1**.

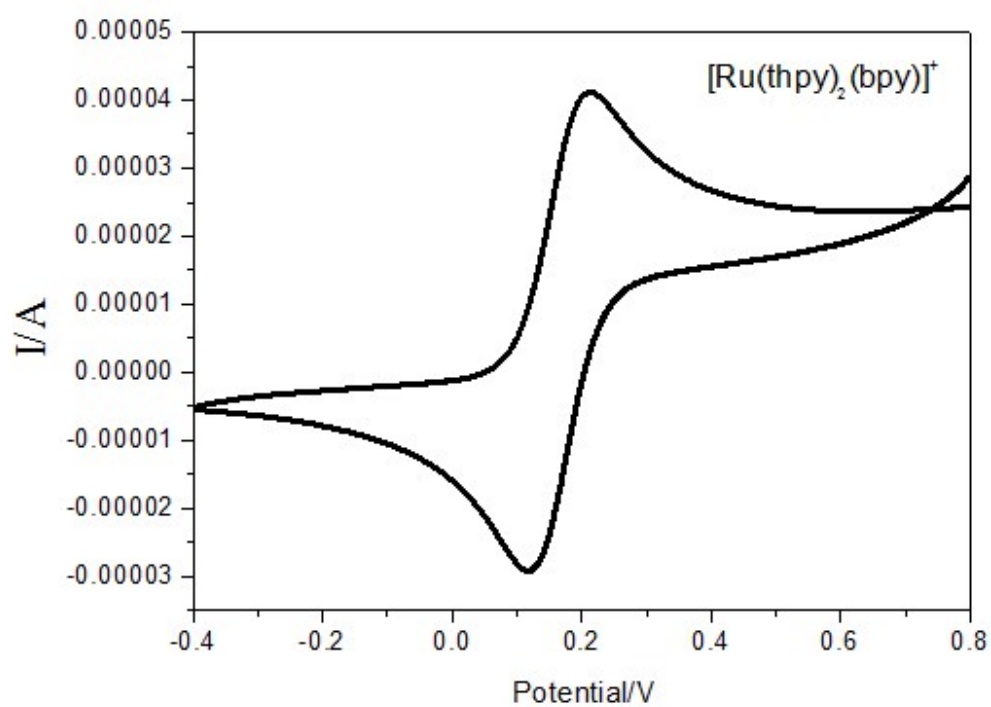
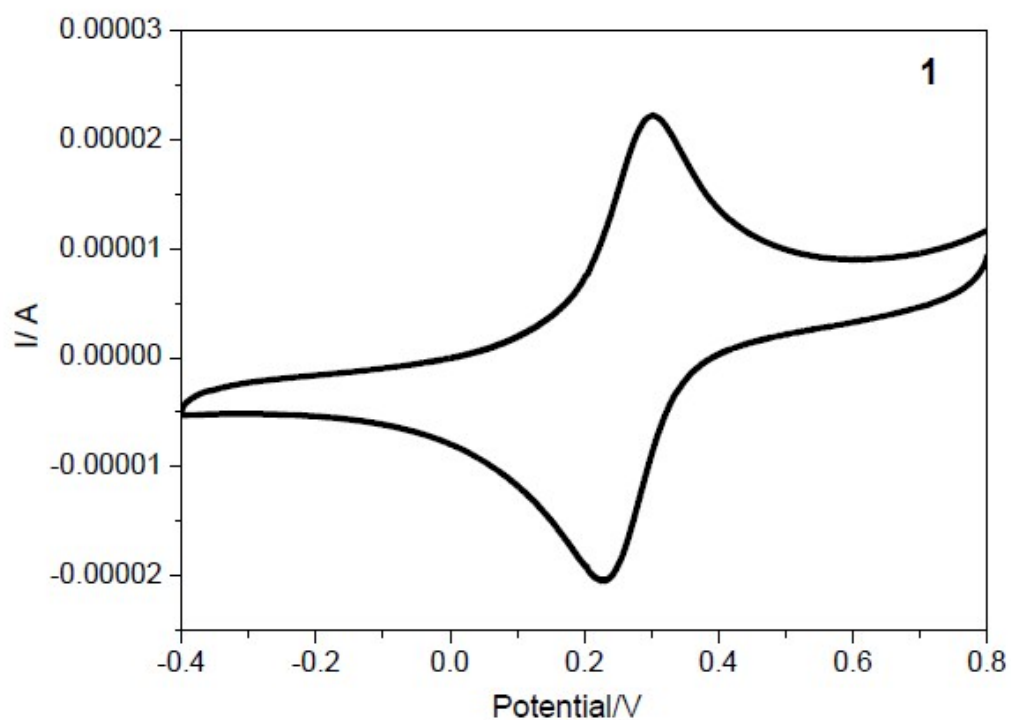


Figure S6. Cyclic voltammograms of **1** and  $[\text{Ru}(\text{thpy})_2(\text{bpy})]^+$  in the  $\text{CH}_3\text{CN}$  solution containing 0.1 M  $\text{Bu}_4\text{NBF}_4$ . The scan rate is of 100 mV/s. The working electrode is a platinum wire, the counter electrode is another platinum wire with  $\text{Ag}/\text{AgNO}_3$  used as the reference electrode.

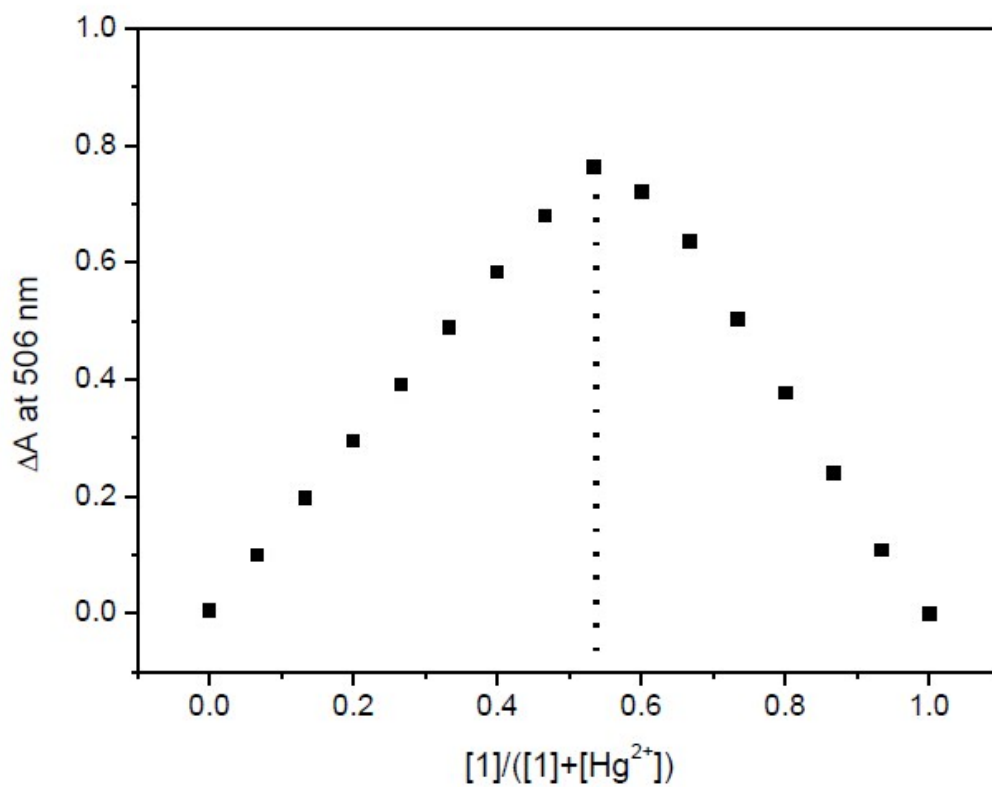


Figure S7. Job's plot for **1** and  $Hg^{2+}$  in water.  $[1] + [Hg^{2+}] = 1.0 \times 10^{-4} M$ .

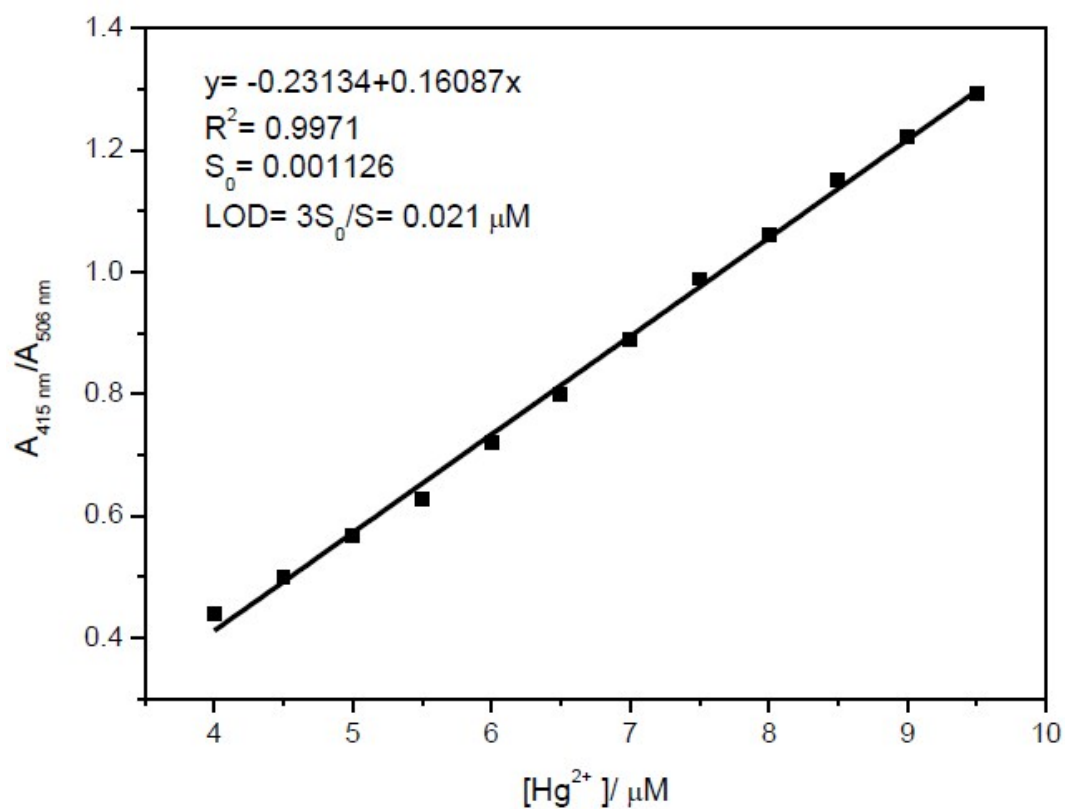


Figure S8. Sensitivity test of **1** towards  $Hg^{2+}$  by using UV-Vis absorption spectra.

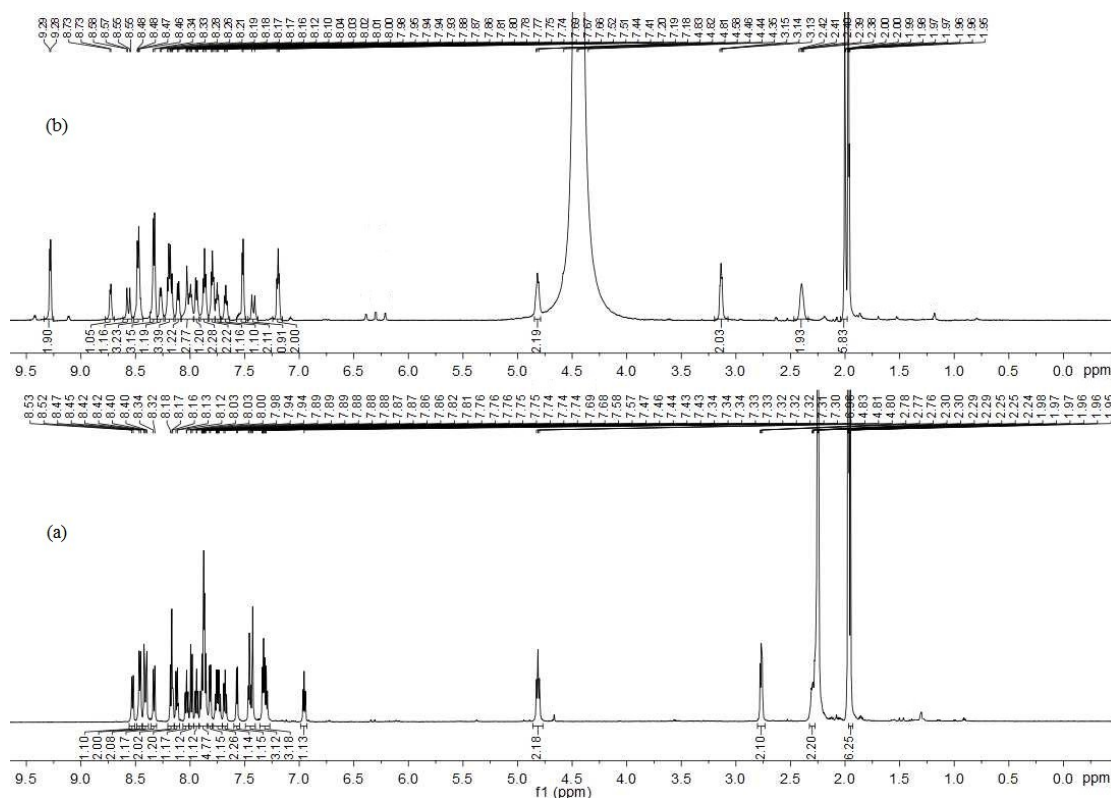


Figure S9.  $^1\text{H}$  NMR spectra of **1** in the absence (a) and presence (b) of  $\text{Hg}(\text{ClO}_4)_2$  in  $\text{CD}_3\text{CN}/\text{D}_2\text{O}$  (v/v=5:1).

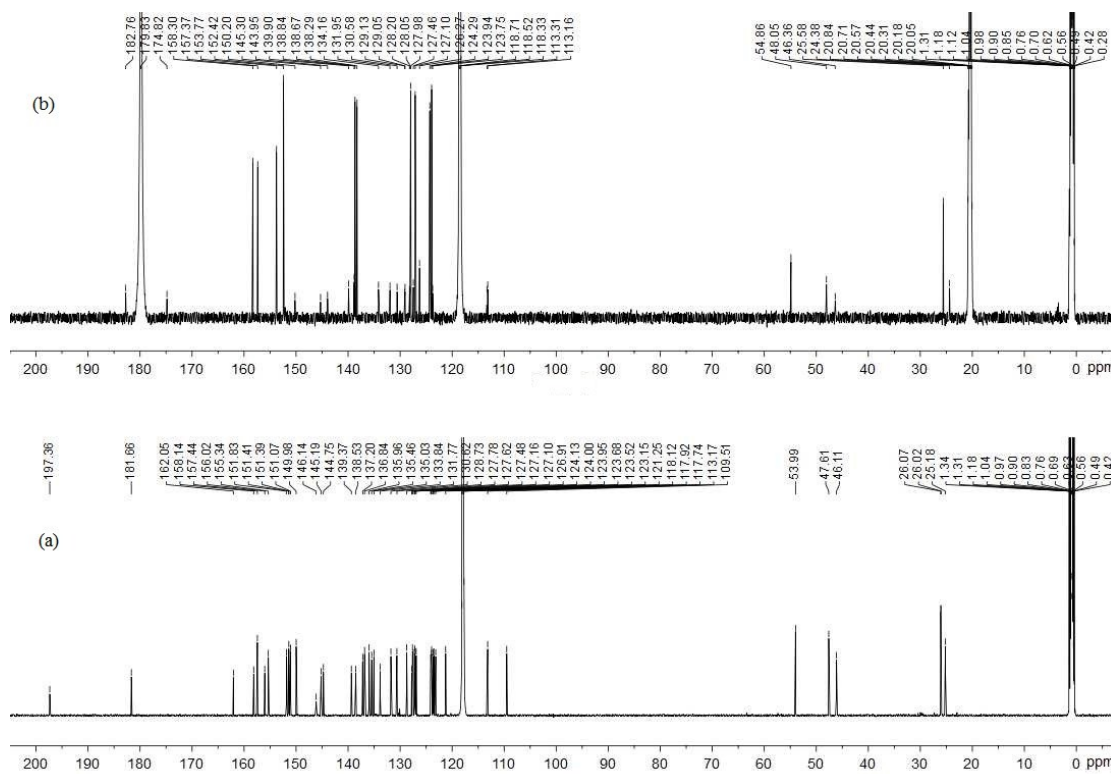


Figure S10.  $^{13}\text{C}$  NMR spectra of **1** in the absence (a) and presence (b) of  $\text{Hg}(\text{ClO}_4)_2$  in  $\text{CD}_3\text{CN}/\text{D}_2\text{O}$  (v/v=5:1).

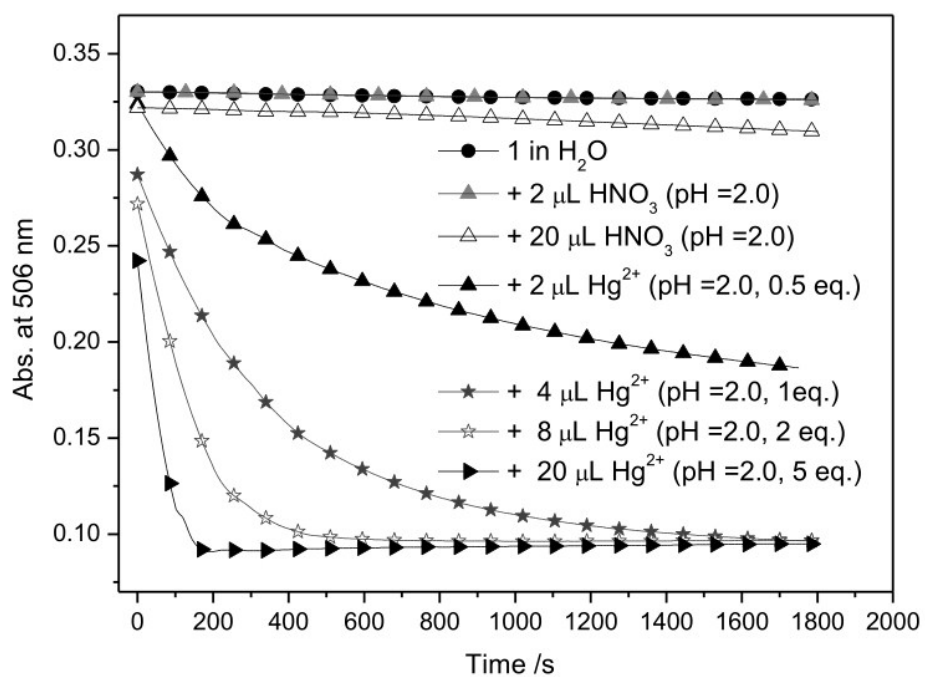


Figure S11. Time-dependent absorption spectral changes at  $\lambda_{506 \text{ nm}}$  of **1** in the presence and absence of  $\text{Hg}^{2+}$  (pH 2.0) in pure water.

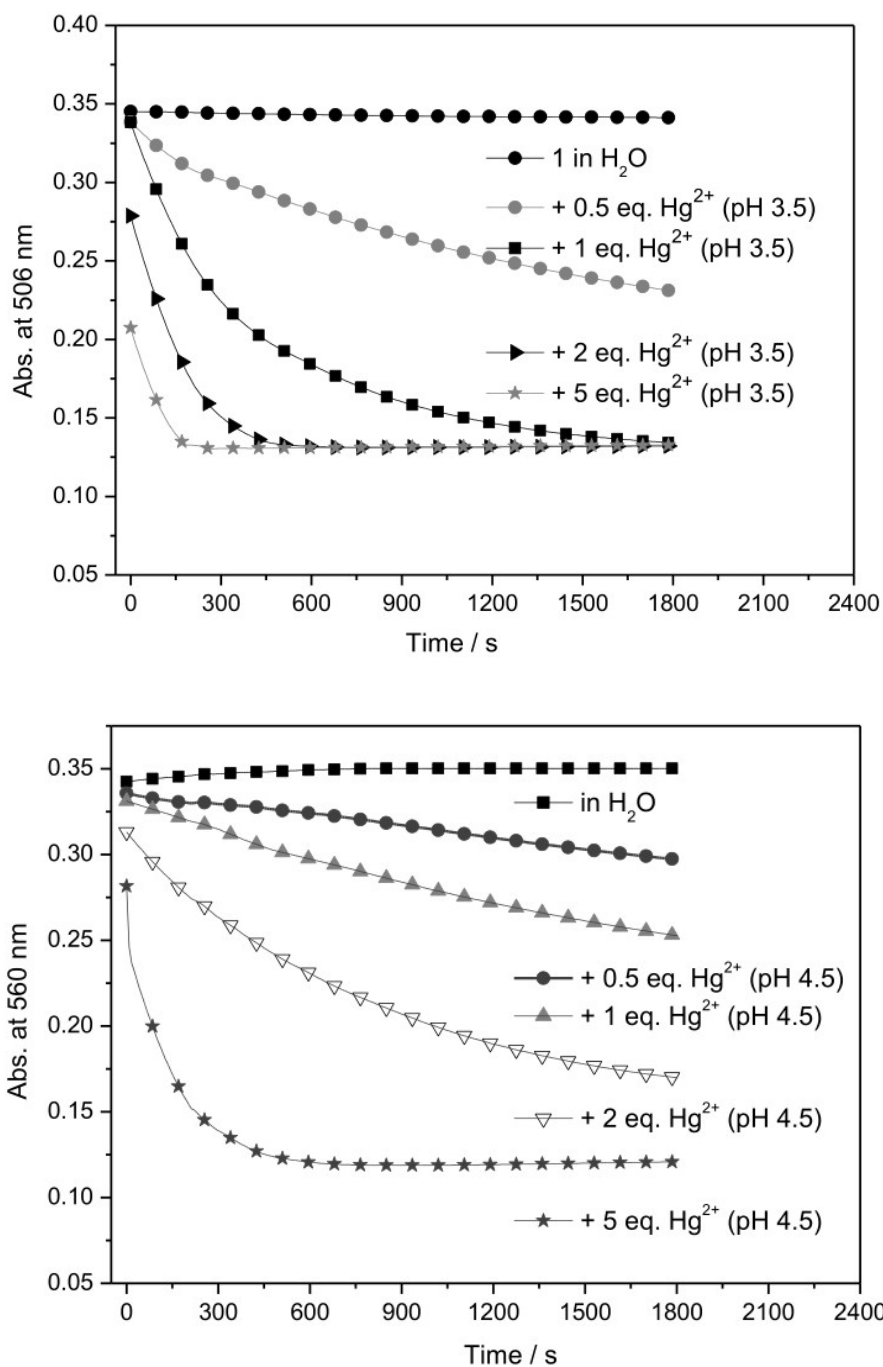


Figure S12. Time-dependent absorption spectral changes at  $A_{506 \text{ nm}}$  of **1** in the presence of  $\text{Hg}^{2+}$  (pH 3.5 and pH 4.5) in pure water.



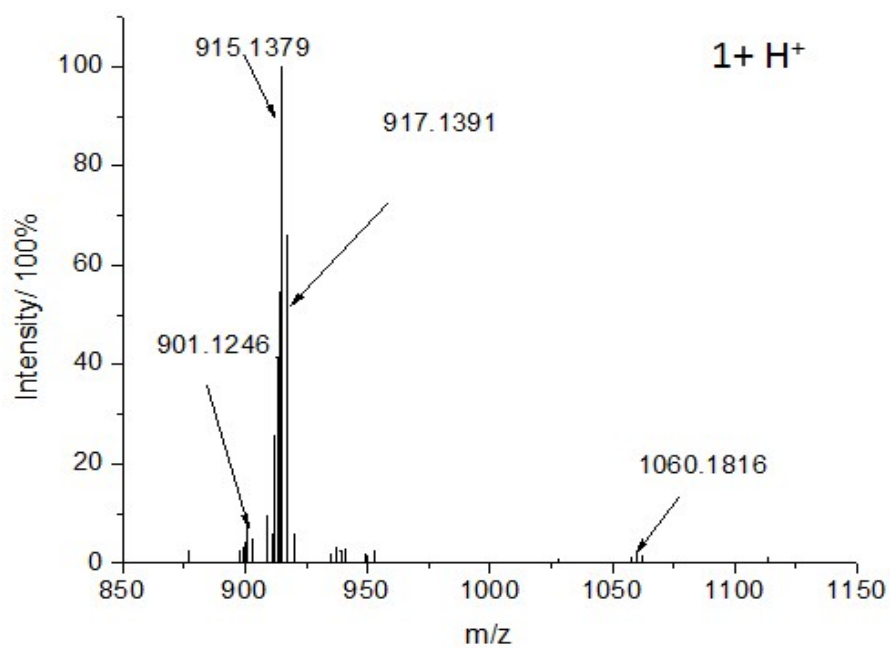


Figure S13. The mass spectrum of **1** in acid solution (pH 3.5).

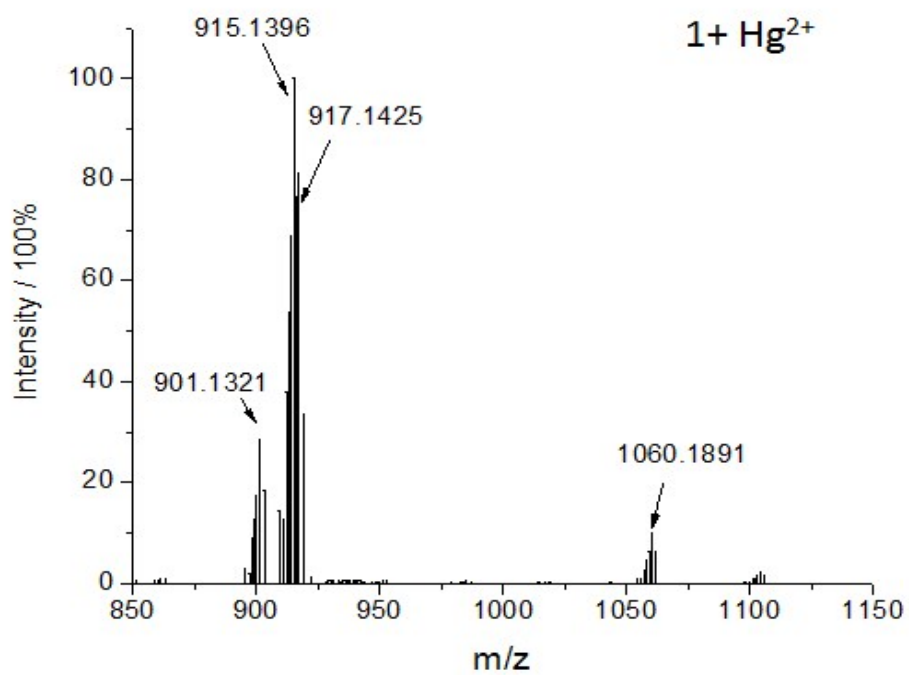


Figure S14. The mass spectrum of **1** in the presence of  $Hg^{2+}$  in  $CH_3CN/H_2O$  (v/v=5:1).

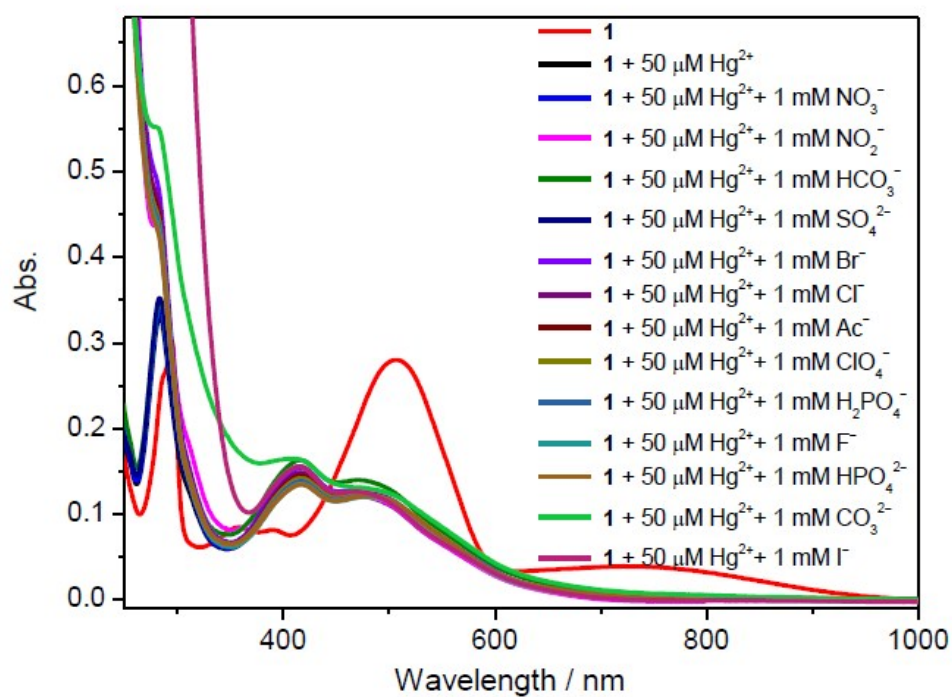


Figure S15. The absorption spectral changes upon the addition of 1mM various anions to the solutions of **1** (7  $\mu\text{M}$ ) with 50  $\mu\text{M}$   $\text{Hg}^{2+}$ .