

Piperazine-based simple structure for selective sensing of Hg²⁺ and glutathione and construction of logic circuit mimicking INHIBIT gate

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1. Change in emission of receptor 1 with various metal ions in THF

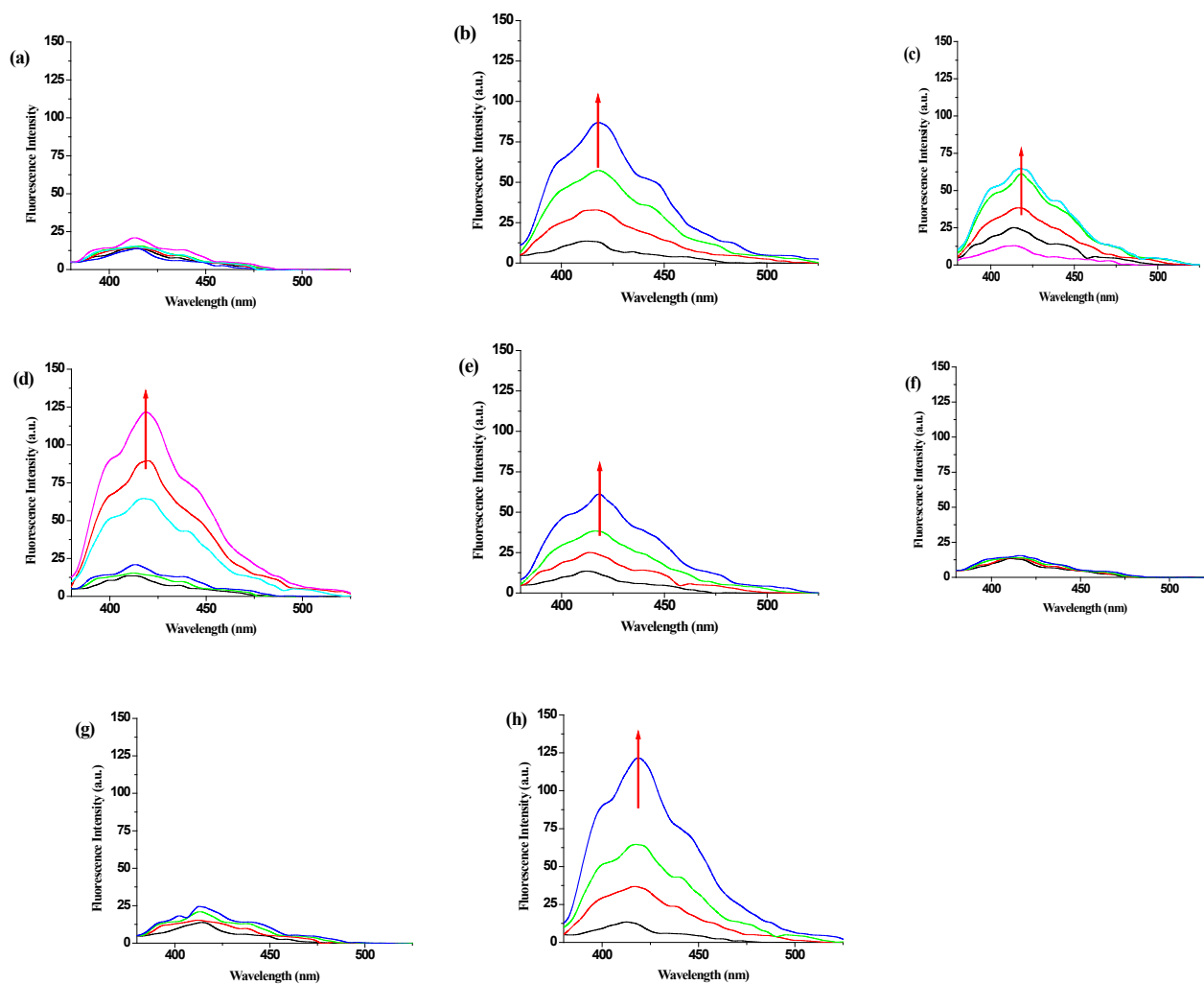


Figure 1S. Change in emission of **1** ($c = 2.5 \times 10^{-5}$ M) in THF upon addition of (a) AgClO₄, (b) Zn(ClO₄)₂, (c) Cd(ClO₄)₂, (d) Co(ClO₄)₂, (e) Cu(ClO₄)₂, (f) Mg(ClO₄)₂, (g) Ni(ClO₄)₂, (h) Pb(ClO₄)₂, [concentration of metal salts were 1×10^{-3} M].

2. Change in emission of receptor 1 with various metal ions in (THF-H₂O, 3:1 v/v) .

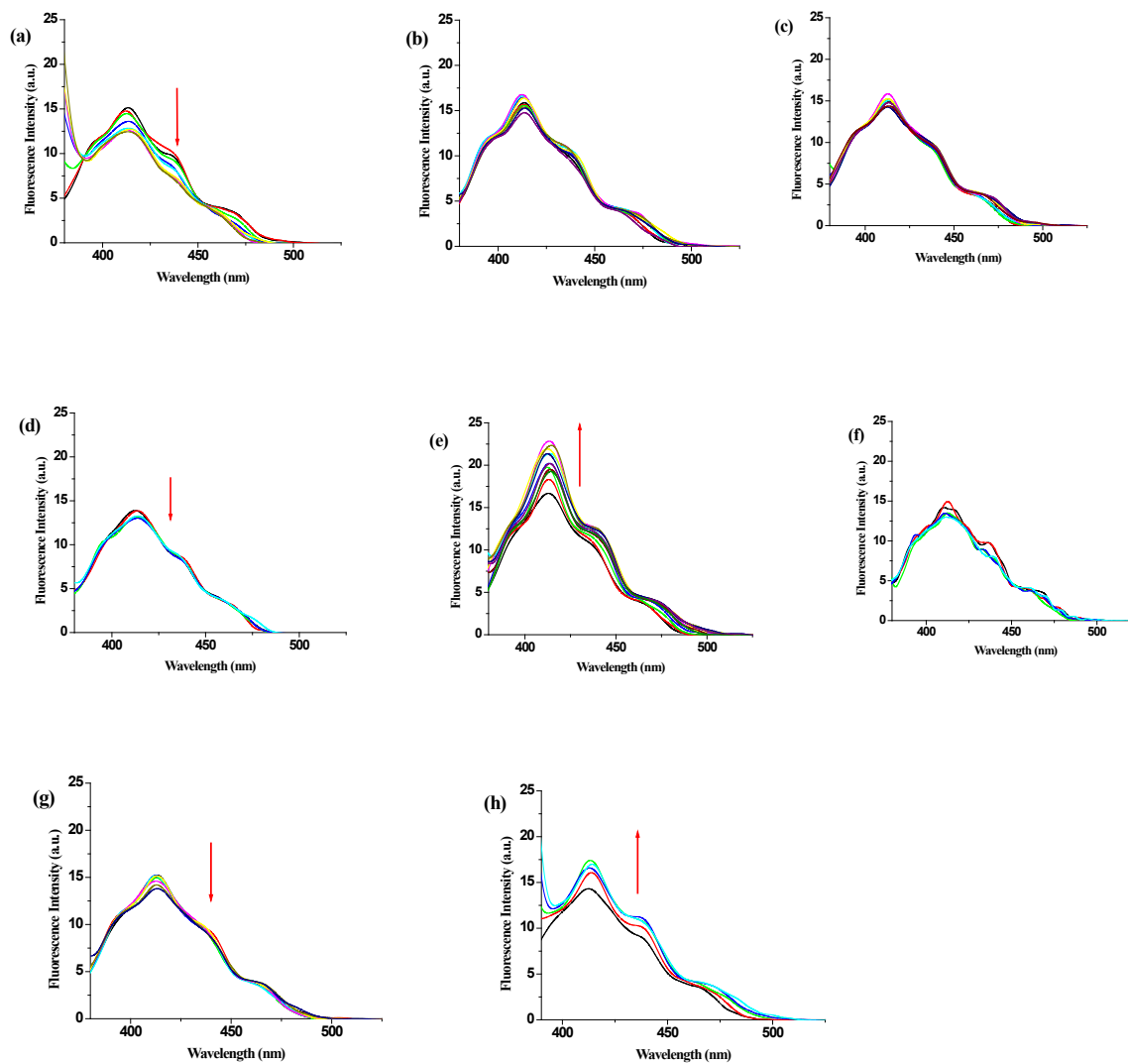


Figure 2S. Change in emission of 1 ($c = 2.5 \times 10^{-5}$ M) in THF-Water (3:1 v/v) upon addition of (a) AgClO₄ (b) Zn(ClO₄)₂, (c) Cd(ClO₄)₂, (d) Co(ClO₄)₂ (e) Cu(ClO₄)₂, (f) Mg(ClO₄)₂, (g) Ni(ClO₄)₂, (h) Pb(ClO₄)₂, [concentration of metal salts were 1×10^{-3} M].

3. Change in absorbance of receptor 1 with various metal ions in THF.

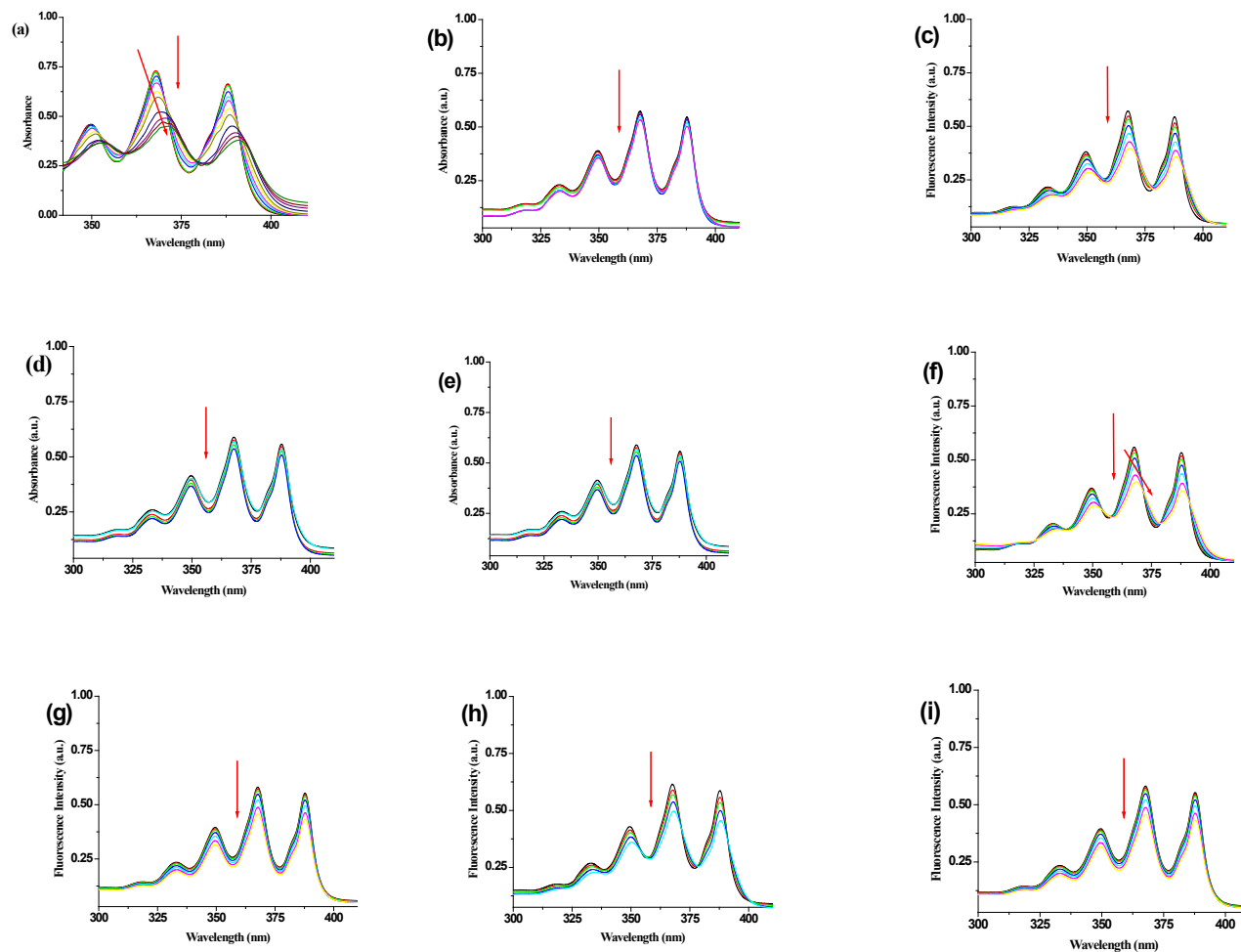


Figure 3S. Change in absorbance of **1** ($c = 2.5 \times 10^{-5}$ M) in THF upon addition of (a) Hg(ClO₄)₂, (b) AgClO₄, (c) Zn(ClO₄)₂, (d) Cd(ClO₄)₂, (e) Cu(ClO₄)₂, (f) Co(ClO₄)₂, (g) Mg(ClO₄)₂, (h) Pb(ClO₄)₂, (i) Ni(ClO₄)₂ [concentration of metal salts were 1×10^{-3} M].

4. UV-Vis Job plot of receptor 1 with $\text{Hg}(\text{ClO}_4)_2$ in (THF- H_2O , 3:1 v/v).

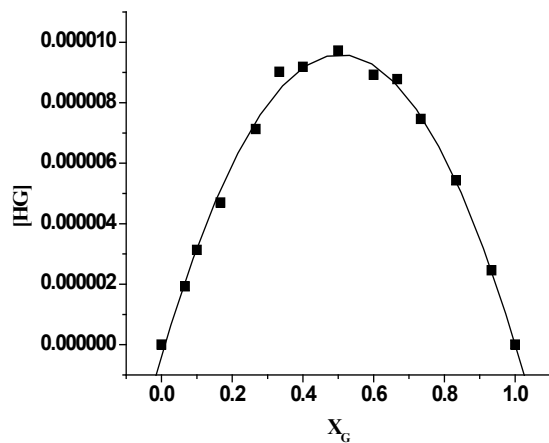


Figure 4S. UV-vis Job plot for receptor 1 with Hg^{2+} ($[\text{H}] = [\text{G}] = 2.5 \times 10^{-5} \text{ M}$).

5. Binding constant curve for 1 with Hg^{2+} .

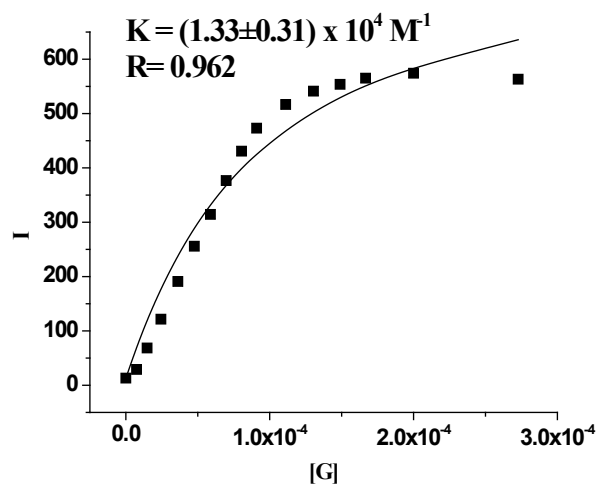


Figure 5S. Non linear binding constant curve for receptor 1 ($c = 2.5 \times 10^{-5} \text{ M}$) with Hg^{2+} ($c = 1 \times 10^{-3} \text{ M}$).

6. Comparison of IR- Sepctra.

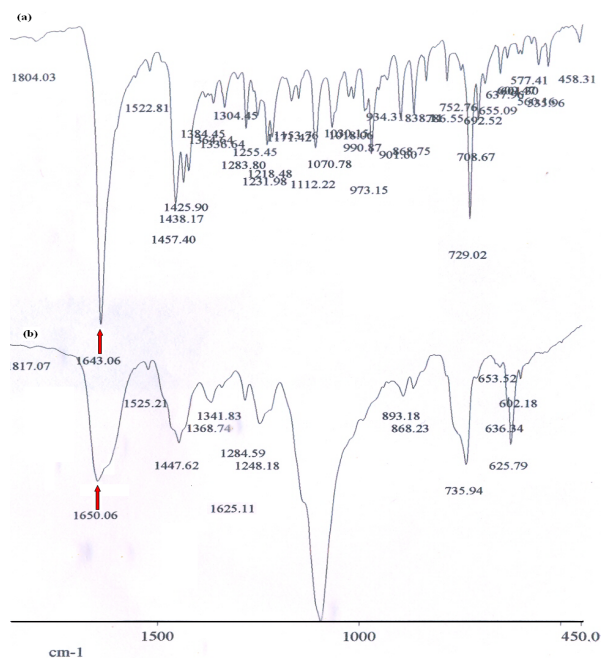


Figure 6S. Partial IR spectrum of (a) **1** and (b) **1** in presence of equivalent amounts of Hg(ClO₄)₂.

7. Change in emission of **1** upon addition of Hg²⁺ in THF-HEPES buffer (10 mmol, pH 7.4) 3:1, v/v.

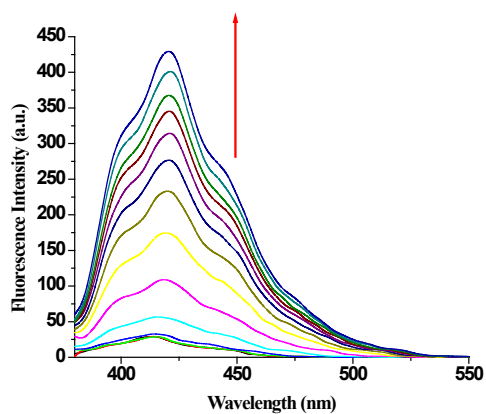


Figure 7S. Change in emission of receptor **1** (c = 2.5 × 10⁻⁵ M) in THF-HEPES buffer (10 mmol, pH 7.4) 3:1, v/v. upon addition of 10 equiv. amounts of Hg(ClO₄)₂.

8. Detection sensitivity level of 1 for $\text{Hg}(\text{ClO}_4)_2$.

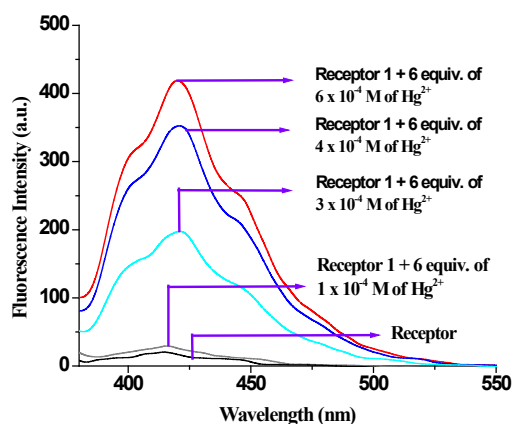


Figure 8S. Change in emission of receptor 1 upon addition of 6 equiv. of different concentrations of Hg^{2+} .

9. Change in emission of 2 upon addition of Hg^{2+} in (THF- H_2O , 3:1 v/v) and fluorescence Job plot of receptor 2 with $\text{Hg}(\text{ClO}_4)_2$ in (THF- H_2O , 3:1 v/v).

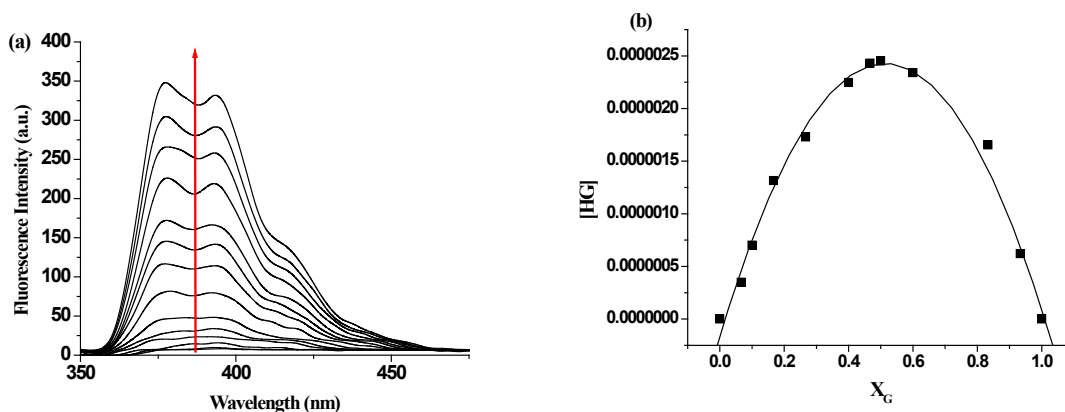


Figure 9S. (a) Change in emission of 2 ($c = 2.5 \times 10^{-5}$ M) in THF-Water (3:1 v/v) upon addition of 10 equiv. of $\text{Hg}(\text{ClO}_4)_2$ ($c = 1 \times 10^{-3}$ M); (b) fluorescence Job plot for 2 with Hg^{2+} ($[\text{H}] = [\text{G}] = 2.5 \times 10^{-5}$ M).

10. Binding constant curve for 2 with Hg^{2+} .

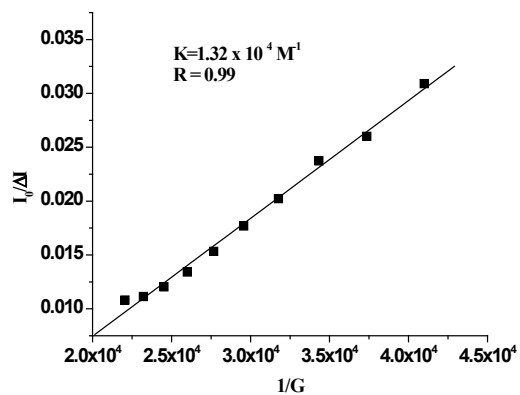


Figure 10S. linear fittings for binding constant curve of 2 ($c = 2.5 \times 10^{-5}$ M) with Hg^{2+} ($c = 1 \times 10^{-3}$ M).

11. Selectivity experiment on 2 towards sensing of Hg^{2+} over other metal ions.

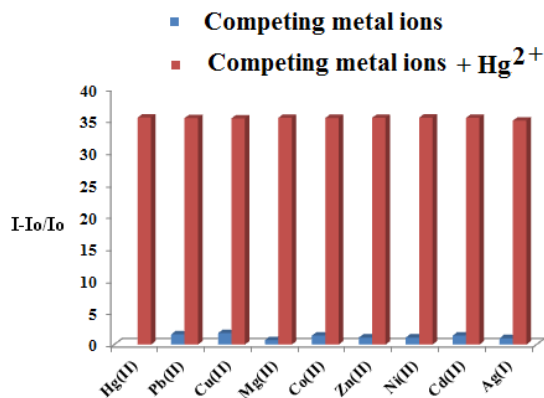


Figure 11S. Selectivity of 2 ($c = 2.5 \times 10^{-5}$ M) towards Hg^{2+} ($c = 1 \times 10^{-3}$ M) in presence of different cations in THF- H_2O (3:1, v/v). 7 equiv.

12. Detection sensitivity level of **2** for $\text{Hg}(\text{ClO}_4)_2$

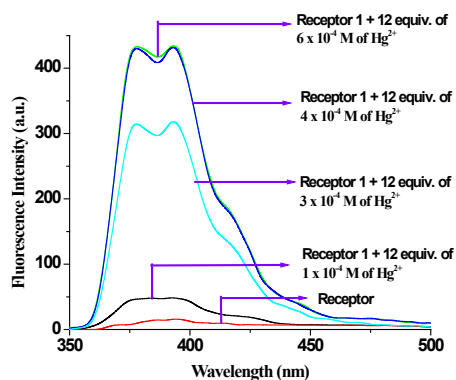


Figure 12S. Change in emission of **2** upon addition of 6 equiv. of different concentrations of Hg^{2+} .

13. Change in emission of “**1**- Hg^{2+} ” ensemble upon addition of Cys and Hcy in THF: H_2O (pH 7.4, HEPES buffer 10 mmol, 3:1, v/v)

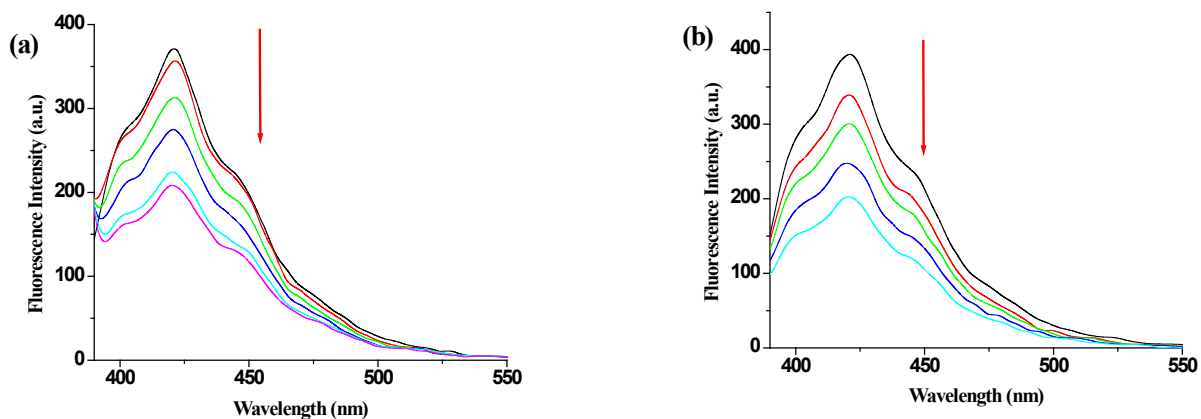


Figure 13S. Fluorescence emission spectra of **1**- Hg^{2+} complex in THF- H_2O (10 mmol HEPES, pH 7.4, 3:1, v/v) upon addition of 30 equiv. amounts of (a) Cysteine and (b) Homocysteine.

14. Fluorescence emission spectra of 1.Hg²⁺.GSH upon various additions of Hg²⁺

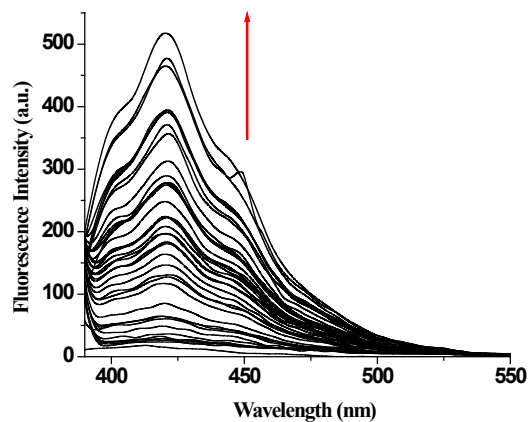


Figure 14S. Change in emission from solution of 1.Hg²⁺.GSH upon gradual addition of Hg²⁺.

15. Change in fluorescence ratio of “2.Hg²⁺” ensemble upon addition of Cys, Hcy and GSH

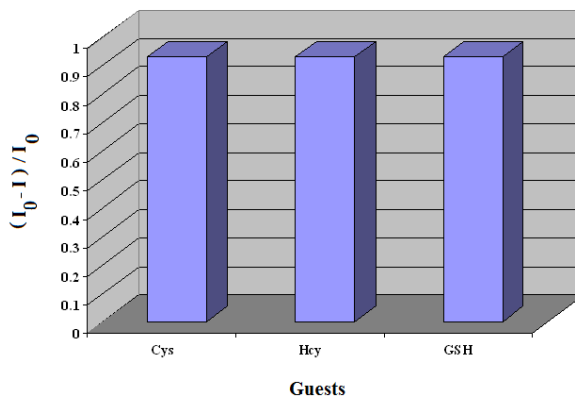


Figure 15S. Change in fluorescence ratio at 385 nm for ‘2-Hg²⁺’ ensemble upon addition of 30 equiv. of various thiols ($c = 1 \times 10^{-3}$ M) in THF-H₂O (3:1, v/v; 10 mmol HEPES buffer, pH 7.4; $\lambda_{ex} = 340$ nm).

16. MTT assays for 1 and 2

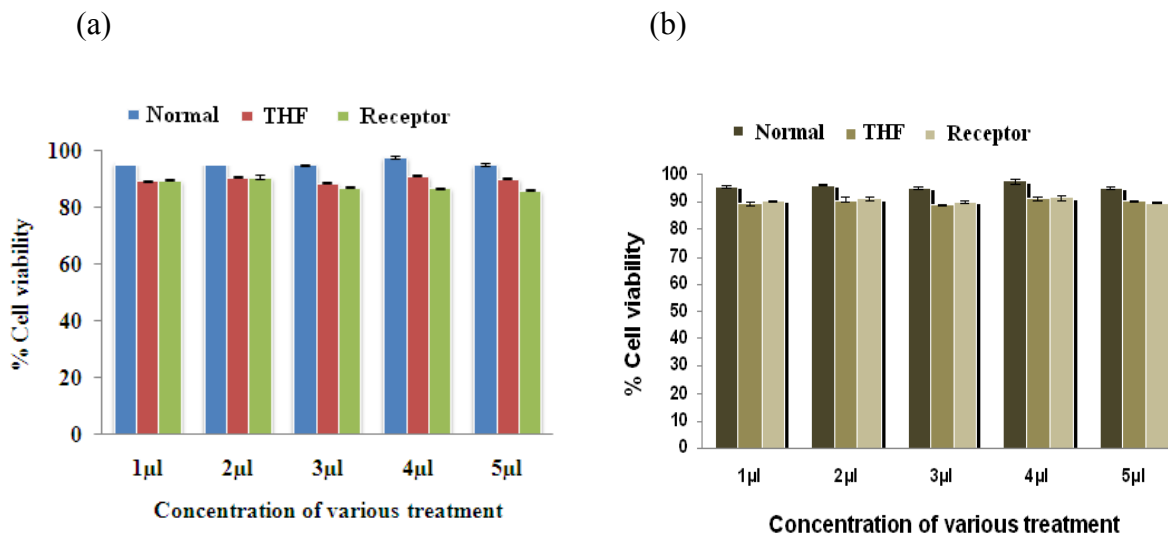


Figure 16S. MTT assays for (a) 1 and (b) 2.

17. Fluorescence and bright field images of HeLa cells upon incubation with 2 and $\text{Hg}(\text{ClO}_4)_2$

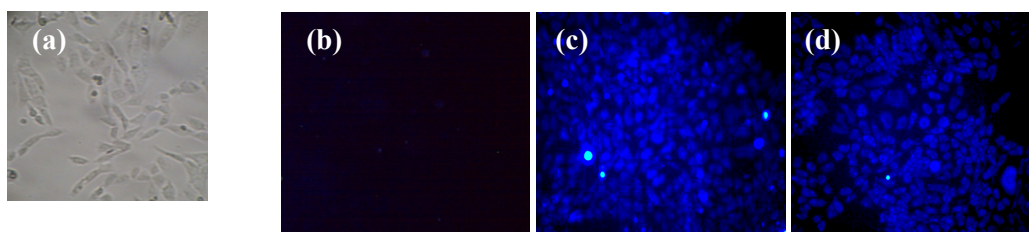
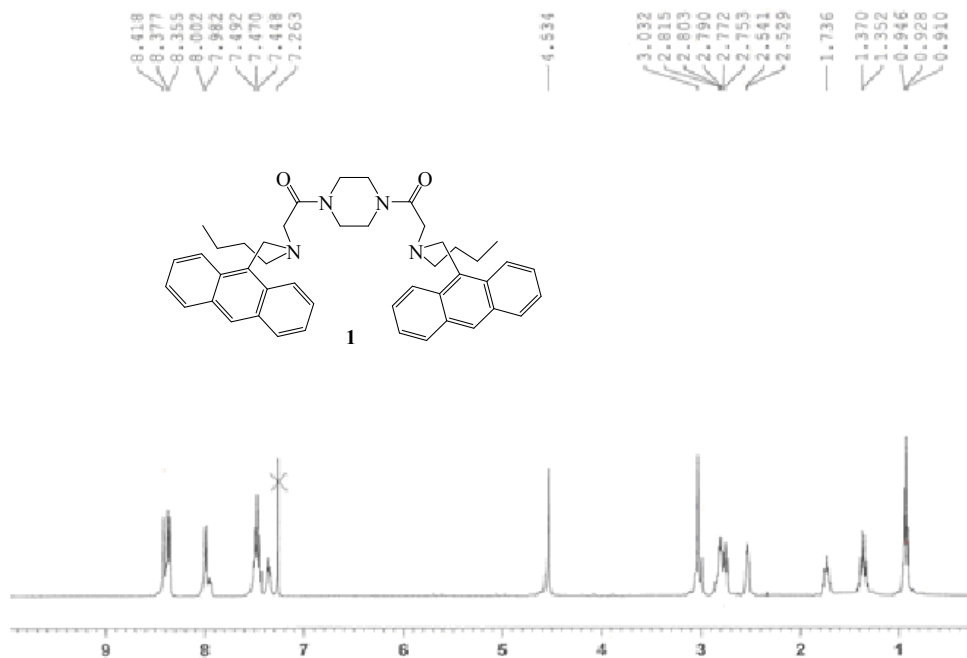
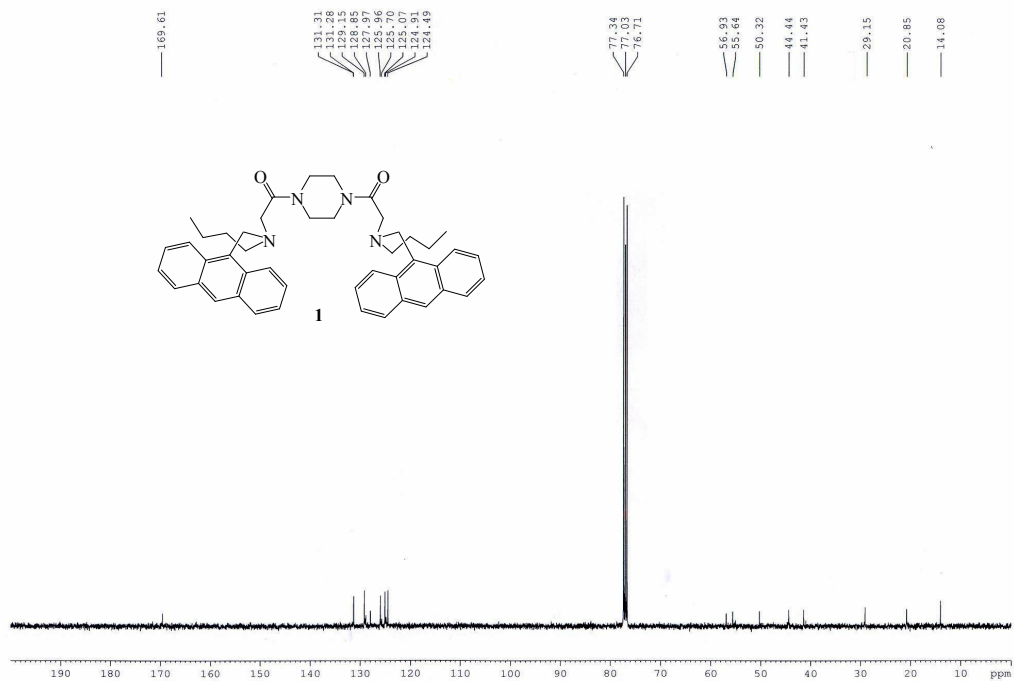


Figure 17S. (a) Bright field image of cells treated with receptor 2 (10 μM) for 1 h at 37 $^\circ\text{C}$, (b) Fluorescence image of cells treated with 2 (10 μM) for 1 h at 37 $^\circ\text{C}$, (c) Blue fluorescence image of cells upon treatment with receptor 2 (10 μM) and then $\text{Hg}(\text{ClO}_4)_2$ (30 μM) for 30 min at 37 $^\circ\text{C}$, (d) Blue fluorescence image of cells upon treatment with 2 (10 μM) and then $\text{Hg}(\text{ClO}_4)_2$ (30.0 μM) for 1 h at 37 $^\circ\text{C}$.

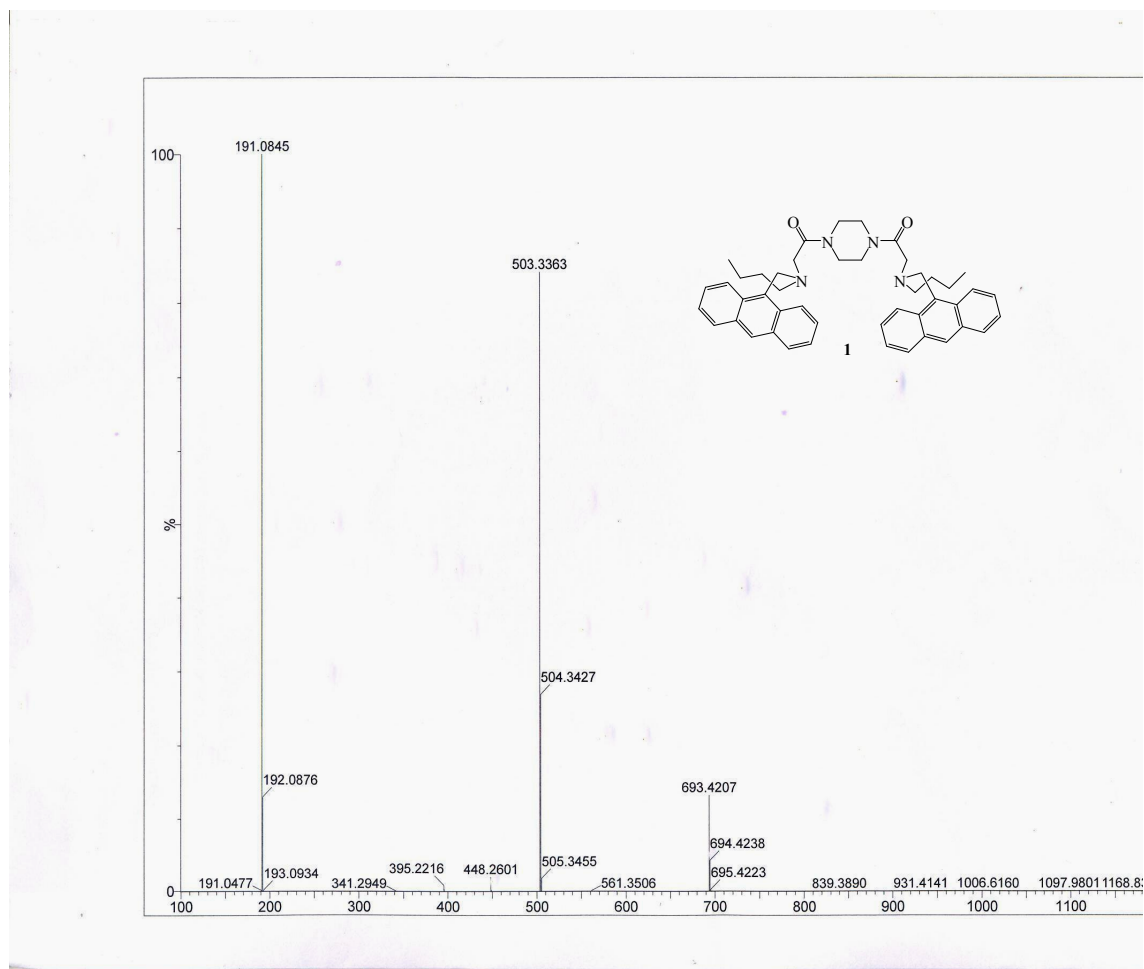
¹H NMR of 1 (400 MHz, CDCl₃):



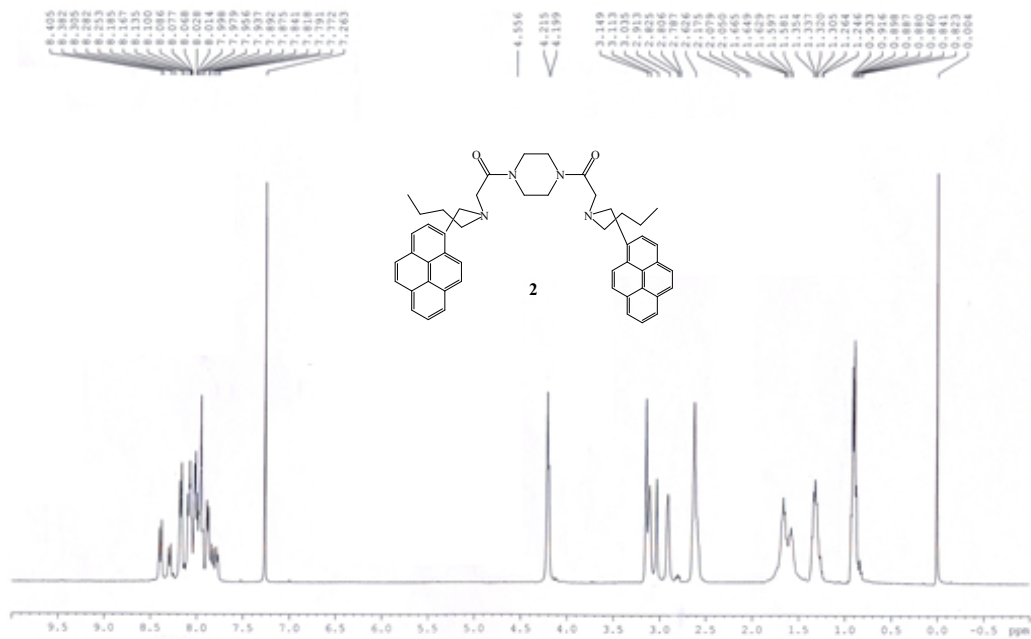
¹³C NMR of 1 (CDCl₃, 100 MHz):



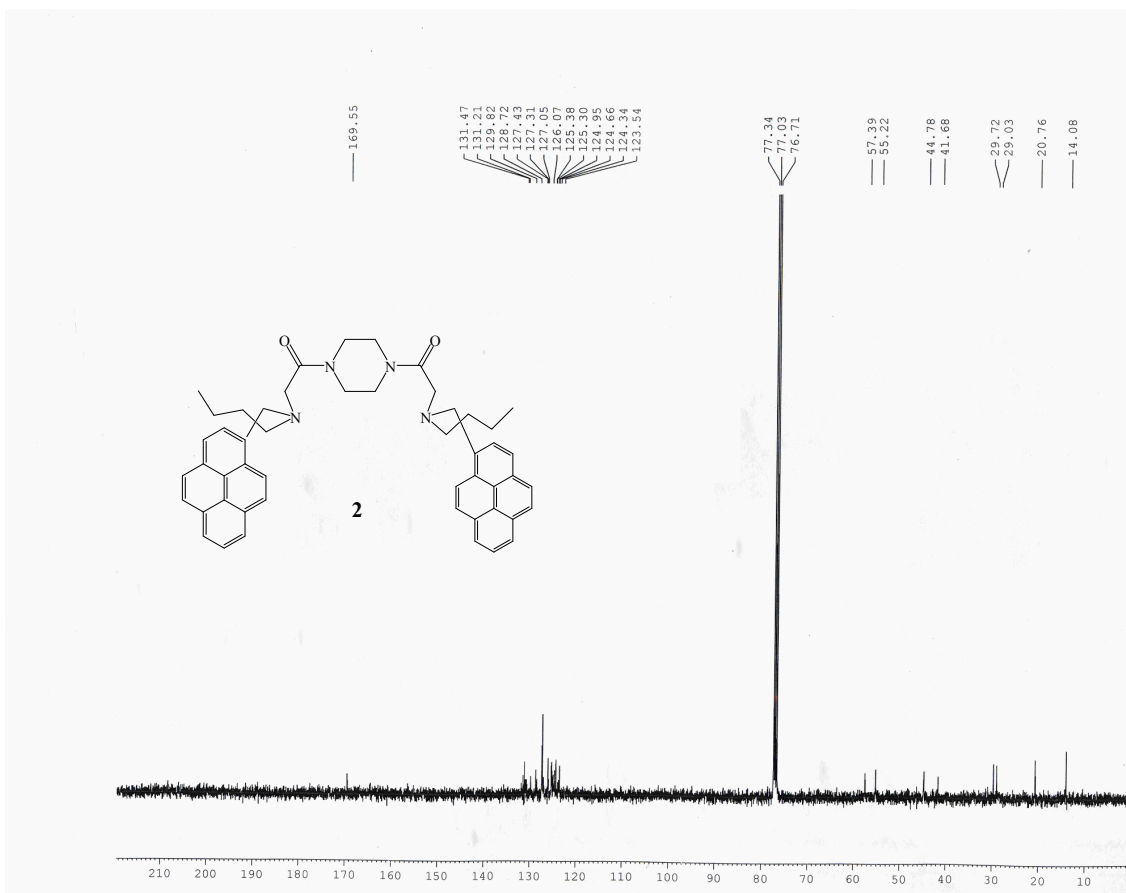
Mass of 1:



^1H NMR of 2 (400 MHz, CDCl_3):



^{13}C NMR of 2 (CDCl₃, 100 MHz):



Mass of 2:

