

Supplementary Material (ESI) for New Journal of Chemistry

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## Supporting Information for

# Fluorescence sensing of iodide and bromide in aqueous solution: anion ligand exchanging and metal ion removing

Lin Xu, Yufang Xu, Weiping Zhu, Zheng Xu, Mengjie Chen and Xuhong Qian\*

Shanghai Key Laboratory of Chemical Biology,

State Key Laboratory of Bioreactor Engineering, School of Pharmacy,

East China University of Science and Technology, Shanghai, 200237, China.

Fax: +86 21 6425 2603; Tel: +86 21 6425 3589; E-mail: xhqian@ecust.edu.cn

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## **1. Materials and Apparatus**

Unless otherwise mentioned, all the reagents were of analytic grade.  $^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR spectras were measured on a Bruker AM-400 spectrometer with chemical shifts reported as ppm (in  $\text{CDCl}_3$ , TMS as internal standard). Mass spectrometry were obtained with a HP 5989A spectrometer. All pH measurements were made with a Sartorius basic pH-Meter PB-20. Absorption spectra were determined on a Varian Cary 100 Spectrophotometer. Fluorescence spectra were determined on a Varian Cary Eclipse.

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## 2. The characterization data of chemosensor RSP

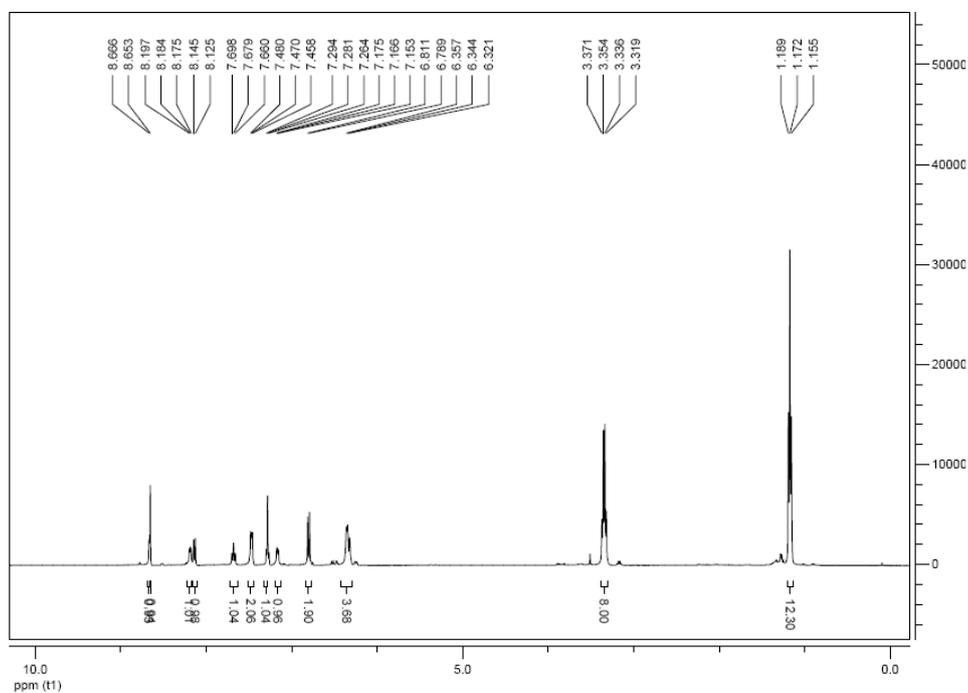


Fig. S1 (a) The  $^1\text{H}$  NMR spectra of RSP

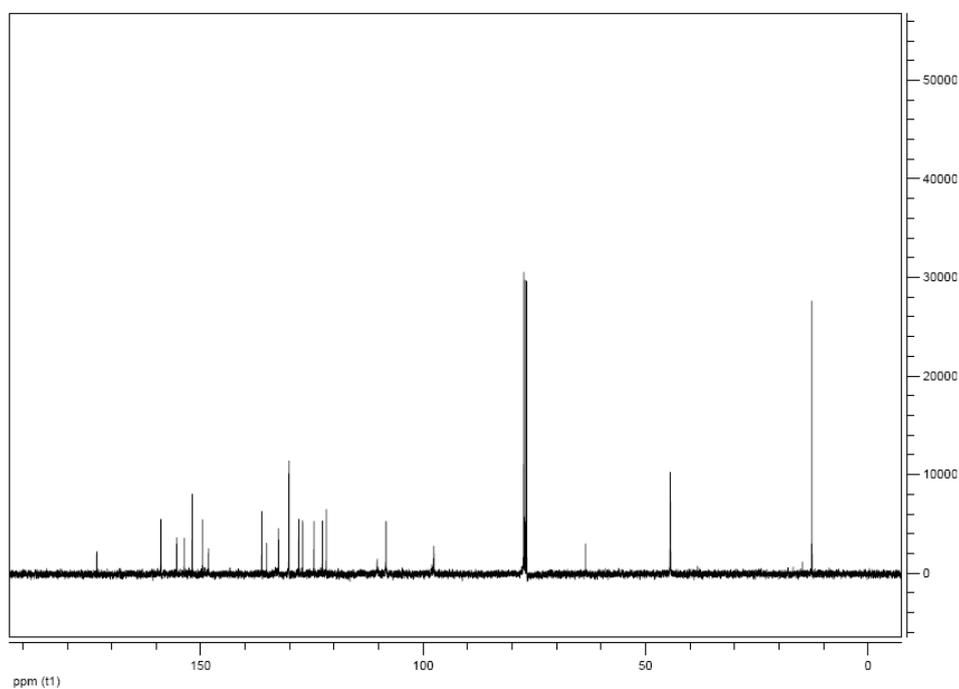
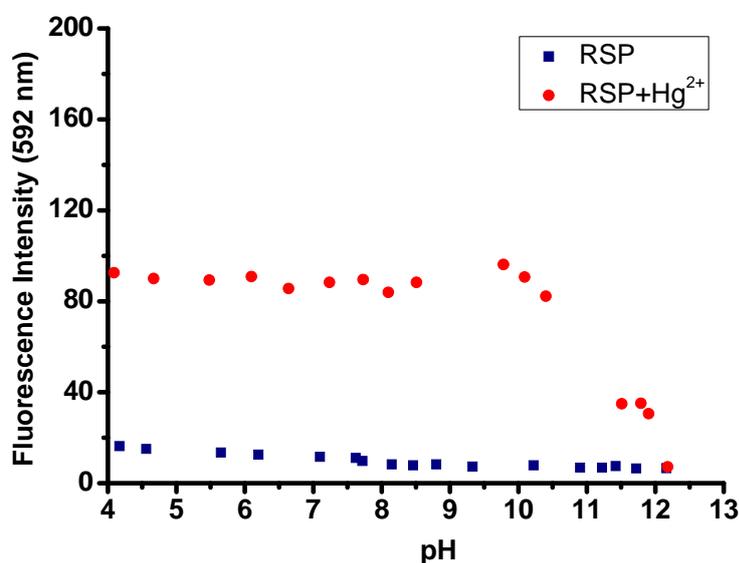


Fig. S1 (b) The  $^{13}\text{C}$  NMR spectra of RSP

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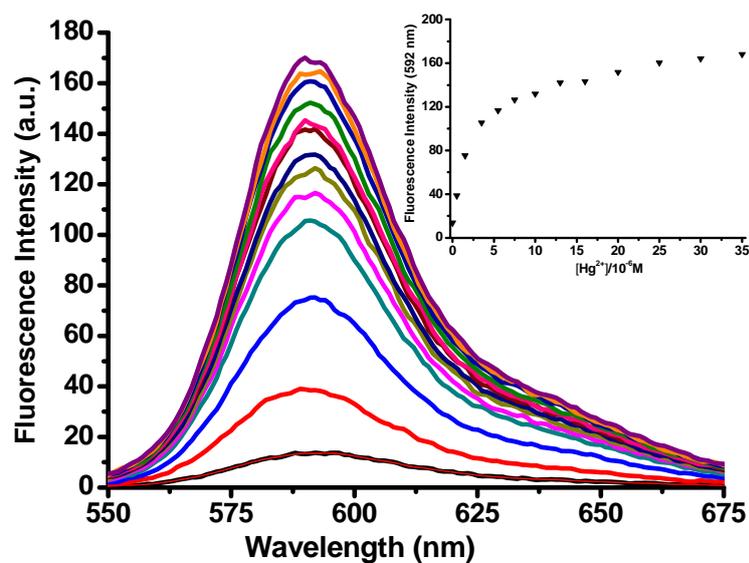
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### 3. The pH-titration of free RSP and [RSP@Hg<sup>2+</sup>]



**Fig. S2** The influence of pH on the fluorescence of **RSP** (10  $\mu$ M) without Hg<sup>2+</sup> and with 10  $\mu$ M Hg<sup>2+</sup> in EtOH/water solution (4:6, v/v), the pH of the solution was adjusted by adding 10% HClO<sub>4</sub> or 2.0 M NaOH. Excitation was performed at 530 nm.

### 4. Fluorescence titration spectra of RSP with Hg<sup>2+</sup>

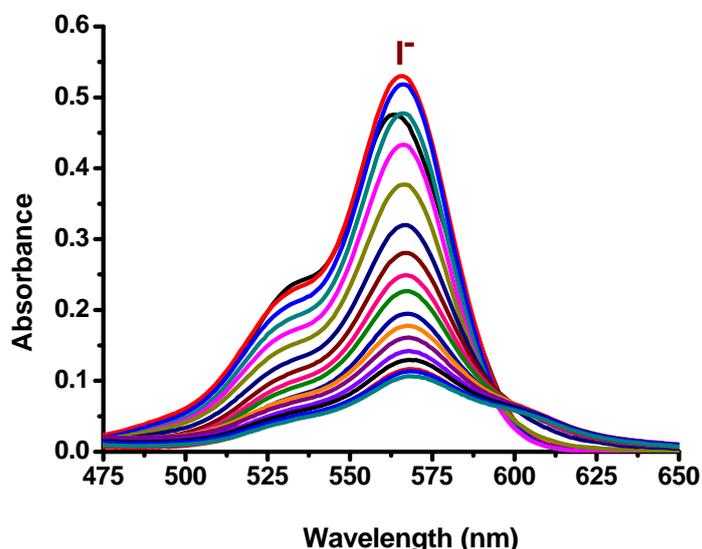


**Fig. S3** Fluorescence spectra of **RSP** (10  $\mu$ M) upon addition of Hg<sup>2+</sup> (0.5~35  $\mu$ M) in Tris-HClO<sub>4</sub> aqueous buffer (10 mM, pH 7.4, containing 40% ethanol as a co-solvent), ( $\lambda_{\text{ex}}$  = 530 nm, slits: 2.5 nm, 5 nm).

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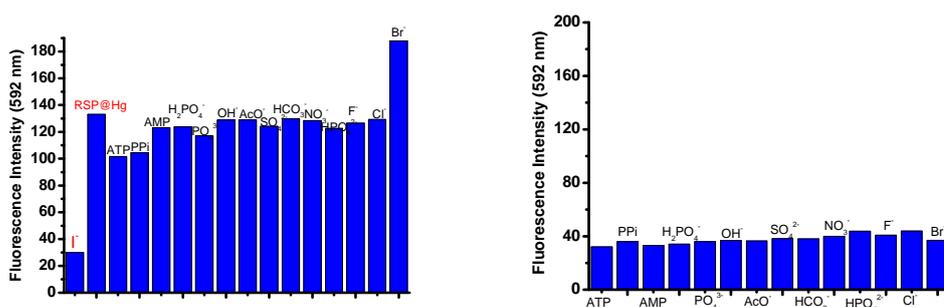
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## 5. Absorption titration spectra of RSP-Hg<sup>2+</sup> with I<sup>-</sup>



**Fig. S4** The absorption spectra of RSP-Hg<sup>2+</sup> (10 μM RSP and 10 μM Hg<sup>2+</sup>) upon addition of I<sup>-</sup> (10–300 μM) in Tris-HClO<sub>4</sub> aqueous buffer (10 mM, pH 7.4, containing 40% ethanol as a co-solvent).

## 6. The selectivity and competition of [RSP@Hg<sup>2+</sup>] for I<sup>-</sup>

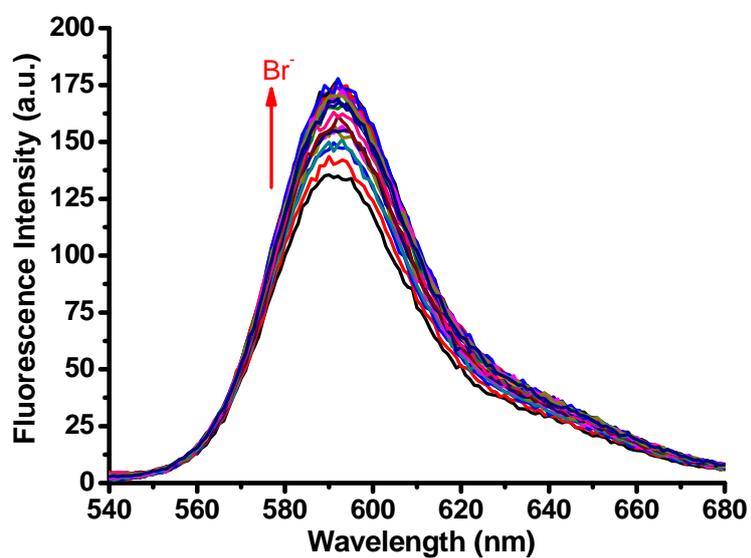


**Fig. S5** Left figure was the selective experiment and right figure was the competitive experiment. The concentration of all the anions added to [RSP@Hg<sup>2+</sup>] (10 μM RSP and 10 μM Hg<sup>2+</sup>) were 200 μM in Tris-HClO<sub>4</sub> aqueous buffer (10 mM, pH 7.4, containing 40% ethanol as a co-solvent), (λ<sub>ex</sub> = 530 nm, slits: 2.5 nm, 5 nm).

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### 7. Fluorescence titration spectra of [RSP@Hg<sup>2+</sup>] with Br<sup>-</sup>

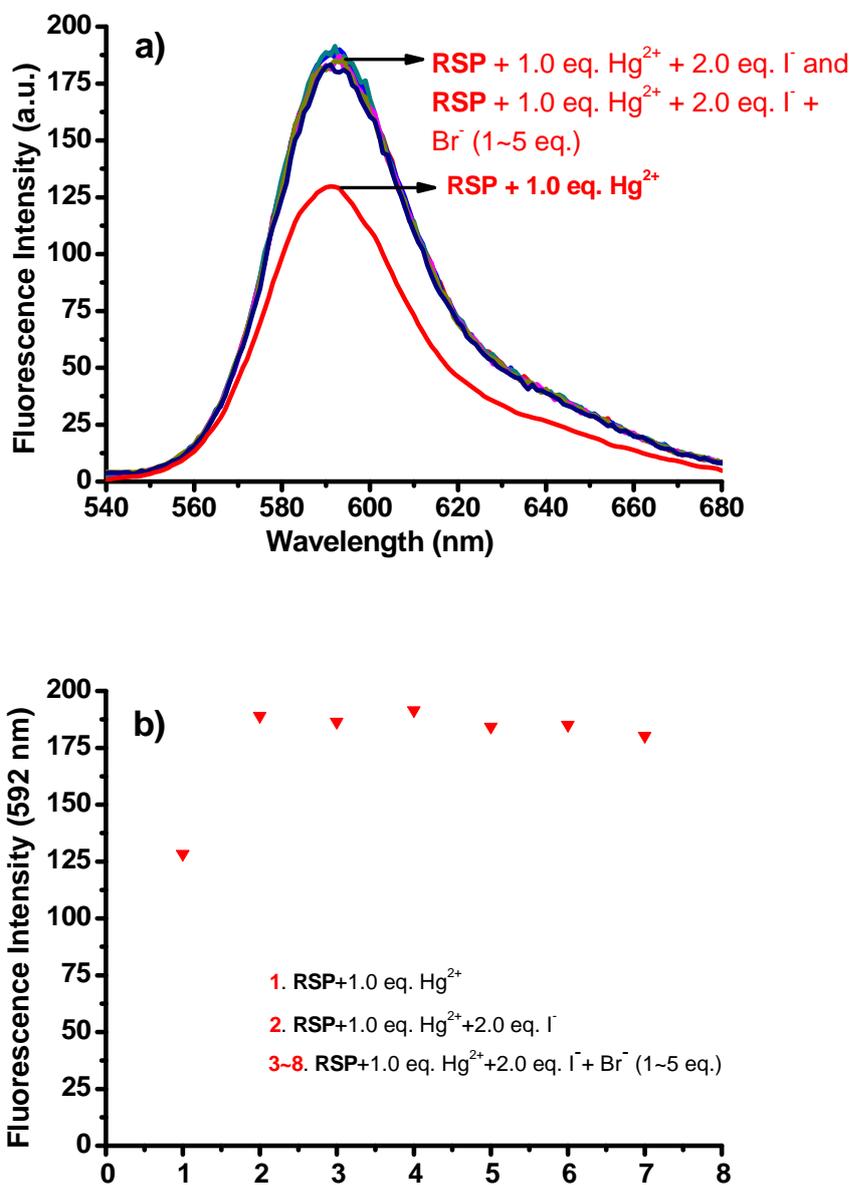


**Fig. S6** Fluorescence spectra of [RSP@Hg<sup>2+</sup>] (10 μM RSP and 10 μM Hg<sup>2+</sup>) upon addition of Br<sup>-</sup> (10–200 μM) in Tris-HClO<sub>4</sub> aqueous buffer (10 mM, pH 7.4, containing 40% ethanol as a co-solvent), (λ<sub>ex</sub> = 530 nm, slits: 2.5 nm, 5 nm).

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## 8. Fluorescence titration spectra of [RSP@Hg<sup>2+</sup>] with I<sup>-</sup> and Br<sup>-</sup>

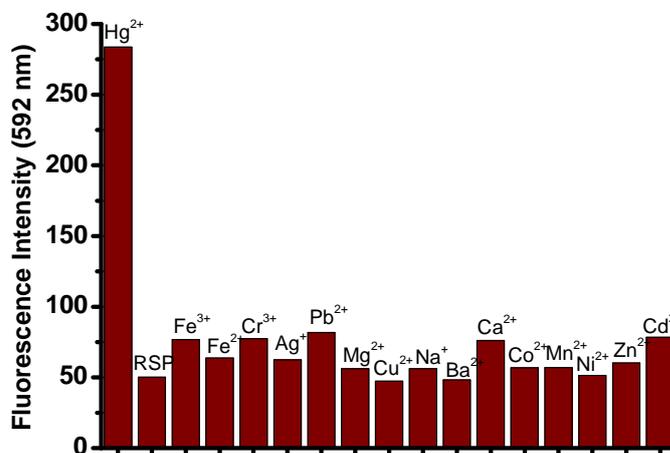


**Fig. S7** (a) Fluorescence spectra of [RSP@Hg<sup>2+</sup>] (10  $\mu$ M RSP and 10  $\mu$ M Hg<sup>2+</sup>) upon addition of I<sup>-</sup> (20  $\mu$ M), and then upon addition of Br<sup>-</sup> (10 ~ 50  $\mu$ M) in Tris-HClO<sub>4</sub> aqueous buffer (10 mM, pH 7.4, containing 40% ethanol as a co-solvent), ( $\lambda_{\text{ex}} = 530$  nm, slits: 2.5 nm, 5 nm). (b) Fluorescence intensity at 592 nm of (a).

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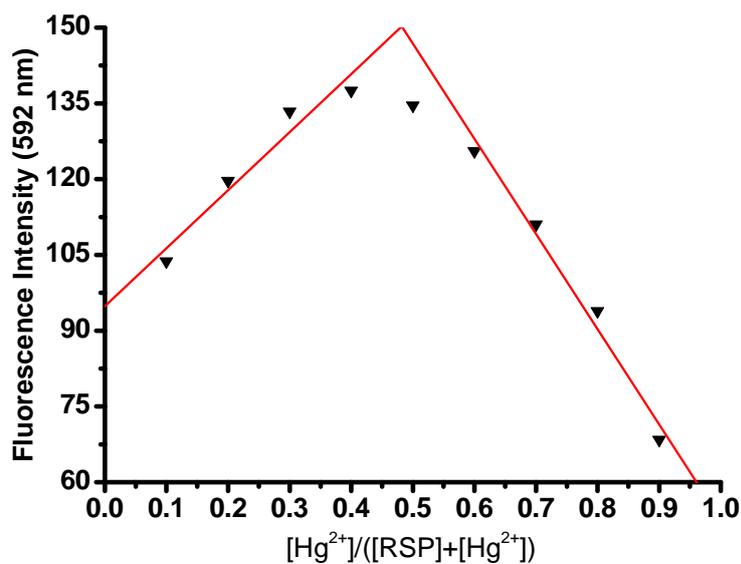
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### 9. The selectivity of RSP for $\text{Hg}^{2+}$



**Fig. S8** The fluorescence intensity at 592 nm of RSP (10  $\mu\text{M}$ ) in the presence of  $\text{Hg}^{2+}$  (20  $\mu\text{M}$ ) and various metal ions (100  $\mu\text{M}$ ) in 99% aqueous buffer solution (10 mM HEPES, pH 7.4). ( $\lambda_{\text{ex}}$  = 530 nm; slit widths: 10 nm, 10 nm).

### 10. Job's plot of RSP and $\text{Hg}^{2+}$

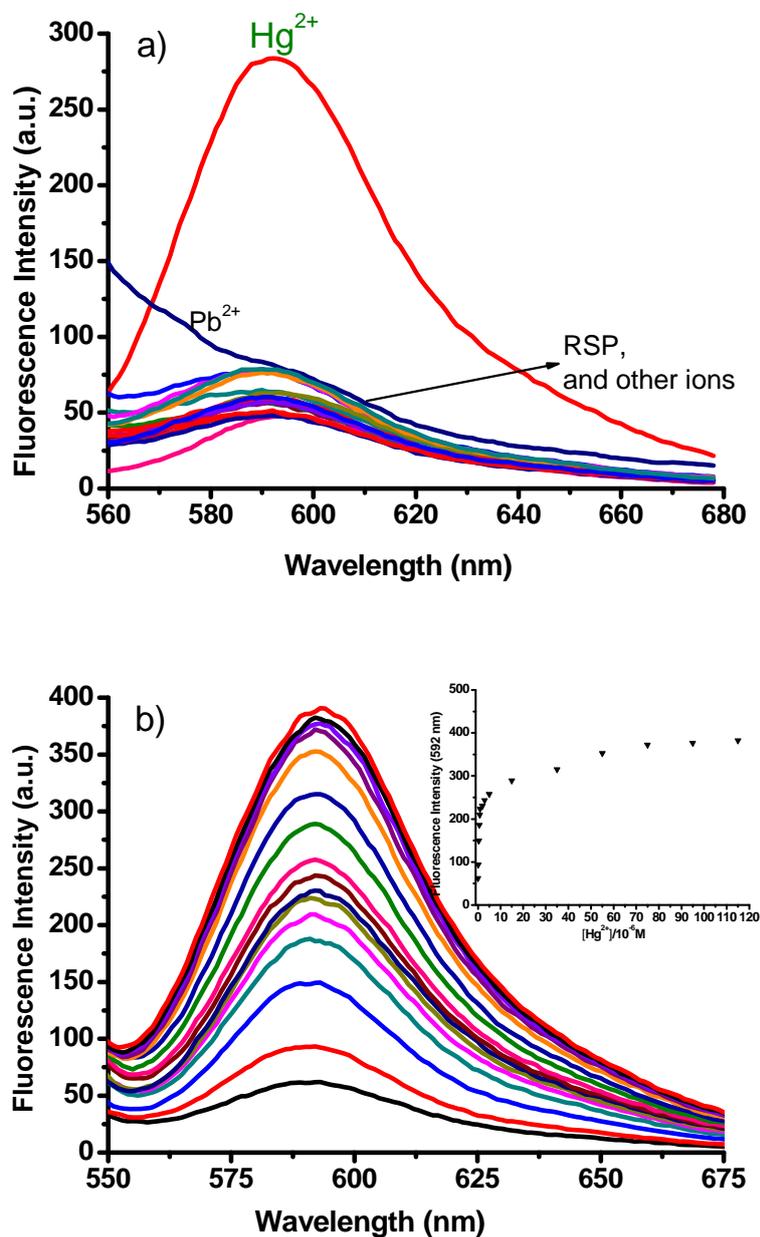


**Fig. S9** Job's plot of RSP and  $\text{Hg}^{2+}$  ( $[\text{RSP}]+[\text{Hg}^{2+}]=20 \mu\text{M}$ ) in Tris- $\text{HClO}_4$  aqueous buffer (10 mM, pH 7.4, containing 40% ethanol as a co-solvent). ( $\lambda_{\text{ex}}$  = 530 nm; slit widths: 2.5 nm, 5 nm).

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### 11. Fluorescence spectra of the selectivity and titration spectra of RSP for $\text{Hg}^{2+}$ in 99% aqueous solution

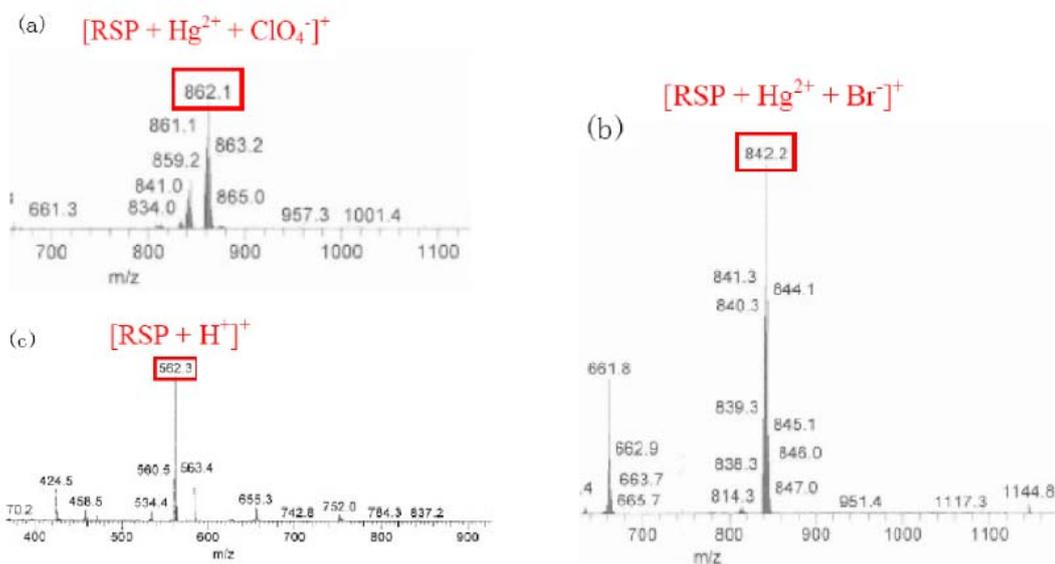


**Fig. S10** (a) The fluorescence spectra of **RSP** (10  $\mu\text{M}$ ) in the presence of  $\text{Hg}^{2+}$  (20  $\mu\text{M}$ ) and 100  $\mu\text{M}$  of various metal ions such as  $\text{Hg}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Ag}^{+}$ ,  $\text{Pb}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Na}^{+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Li}^{+}$ ,  $\text{Zn}^{2+}$  in HEPES aqueous buffer (10 mM, pH 7.4). (b) The fluorescence spectra of **RSP** (10  $\mu\text{M}$ ) upon addition of  $\text{Hg}^{2+}$  in HEPES aqueous buffer (10 mM, pH 7.4). ( $\lambda_{\text{ex}} = 530$  nm; slit widths: 10 nm, 10 nm). Inset: Fluorescence intensity at 592 nm of [**RSP**] as a function of  $[\text{Hg}^{2+}]$ .

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## 12. ESI-MS of RSP in the presence of $\text{Hg}^{2+}$ and $[\text{RSP}@\text{Hg}^{2+}]$ in the presence of $\text{Br}^-$ or $\text{I}^-$



**Fig. S11** (a) ESI-MS of **RSP** in the presence of  $\text{Hg}(\text{ClO}_4)_2$  in DMSO;

(b) ESI-MS of (a) in the presence of  $\text{Br}^-$  in DMSO;

(c) ESI-MS of (a) in the presence of  $\text{I}^-$  in DMSO.