

## Supporting Information

### A novel rhodamine-based Hg<sup>2+</sup> sensor with simple structure and fine performance

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#### 1. Materials and instruments

Thiobisethylamine was supplied by TCI (Shanghai). Rhodamine B (RB) was bought from Shanghai SSS Reagent Co., Ltd. *N,N*-Diisopropylethylamine (DIPEA) was purchased from Jiande New Delhi Chemical Co., Ltd. NaCl, KCl, MgCl<sub>2</sub>, CaCl<sub>2</sub>, FeCl<sub>3</sub>·6H<sub>2</sub>O, FeCl<sub>2</sub>·7H<sub>2</sub>O, CuSO<sub>4</sub>·5H<sub>2</sub>O, Zn(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O, CrCl<sub>3</sub>·6H<sub>2</sub>O, Pb(NO<sub>3</sub>)<sub>2</sub>, Ni(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O, MnSO<sub>4</sub>·H<sub>2</sub>O, CoCl<sub>2</sub>·6H<sub>2</sub>O, CdCl<sub>2</sub>·2.5H<sub>2</sub>O, AgNO<sub>3</sub>, HgCl<sub>2</sub>, ethylene diamine tetraacetic acid (EDTA), KI, Na<sub>2</sub>S and 4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid (HEPES) were provided by Sinopharm Chemical Reagent Co., Ltd. The solvents used in synthesis were of analytical grade, others were spectroscopic grade. All reagents were used as commercially received without further purifications.

<sup>1</sup>H NMR and <sup>13</sup>C NMR were performed on 400 MHz and 300 MHz Varian Unity Inova spectrometers (Varian, America) respectively with CDCl<sub>3</sub> as solvent. Mass spectrum was recorded on a Bruker micro TOF-QIII LC/MS (Bruker Daltonics Co., Germany) in ESI positive mode. IR spectra were carried out on a TENSOR 27 Fourier transform infrared spectrometer (Bruker, Germany) using KBr pellet. Elemental analysis was done on a Carlo-Erba EA1110 CHNO-S elemental analyzer (Carlo-Erba Co., Italy). Absorption and fluorescence spectra were tested on a TU-1901

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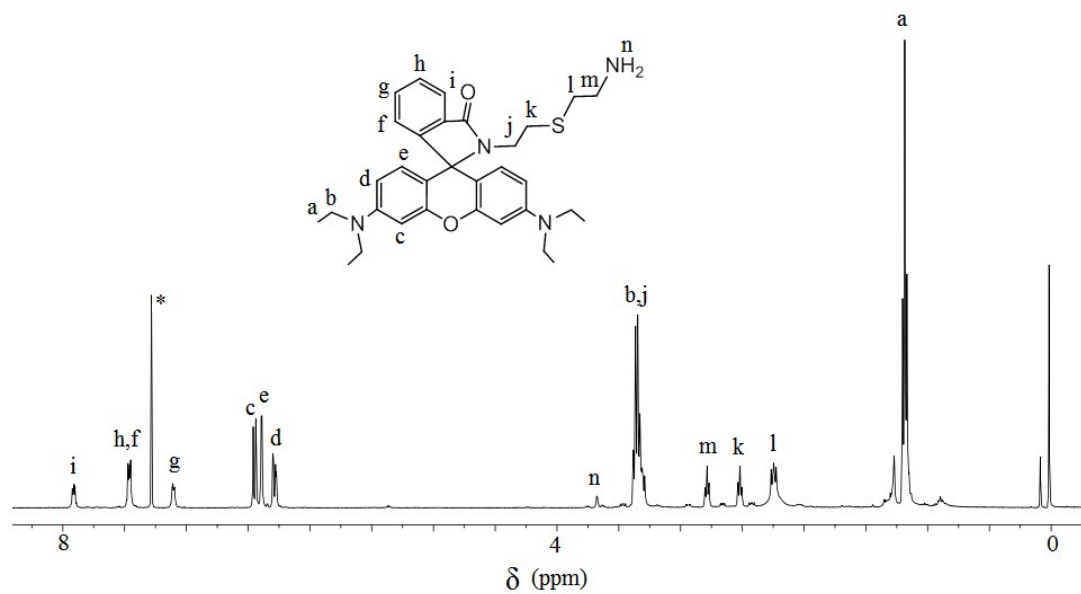
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spectrophotometer (Beijing general instrument Co., Ltd., China) and a F-2500 spectrofluorometer (HITACHI, Japan), respectively. pH values were measured with a Mettler-Toledo FE20 pH meter (Mettler-Toledo Co., America). Melting point was determined on an X-6 Microscopic melting point tester (Beijing Taike Instrument Co., Ltd., China). Atomic absorption spectroscopy (AAS) was performed on a PinAAcle900T atomic absorption spectrometer (Perkin Elmer instrument Co., Ltd., USA). Cell viability was tested by a MUSE Smart Touch cell analyzer (Nikon Merck Drugs & Biotechnology Inc., Germany). Cell fluorescence images were collected on a Nikon EOS 700D inverted fluorescence microscope (Nikon Instruments Inc., Japan).

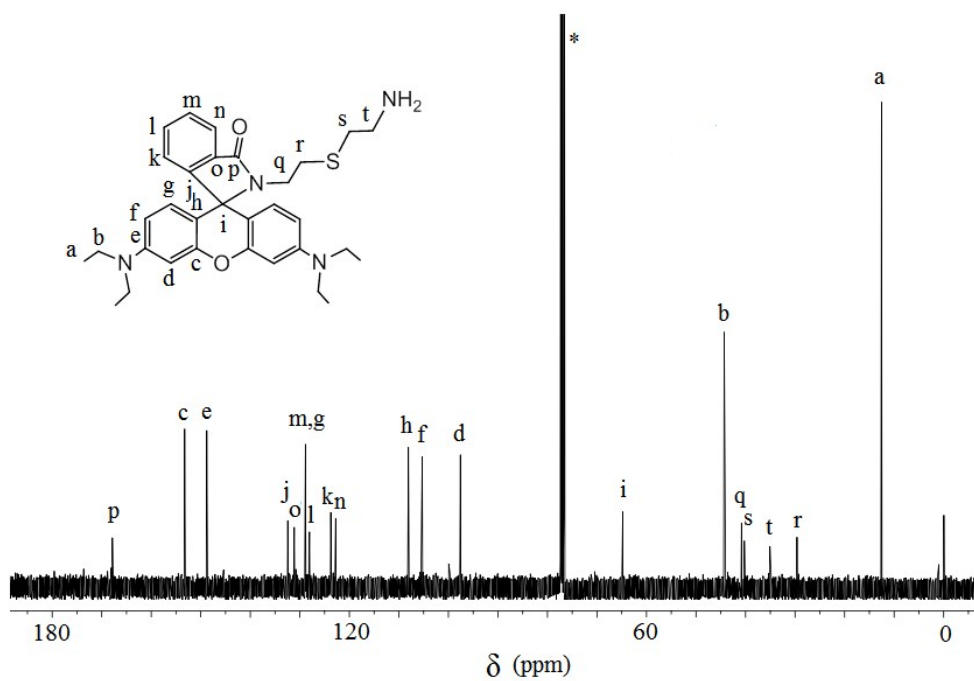
## 2. Synthesis and characterization data of RMTE

Under the protection of nitrogen, thiobisethylamine (36  $\mu$ L, 0.311 mmol) and DIPEA (160  $\mu$ L, 0.97 mmol) were dissolved in dichloromethane ( $\text{CH}_2\text{Cl}_2$ ) (4 mL). After stirring for 10 min, dichloromethane solution of RB (0.05 g, 0.104 mmol) was added dropwise and the mixture was refluxed for 24 h. Subsequently, the mixture was washed with water and purified by column chromatography using methanol/chloroform/petroleum ether (1/12/2) as the eluent to afford 0.031 g yellow solid in the yield of 54.5%, m.p. 167.4  $^\circ\text{C}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) (Fig. S1),  $\delta$  1.16 (*t*, 12H,  $J=6.8$  Hz), 2.23 (*t*, 2H,  $J=8$  Hz), 2.50 (*t*, 2H,  $J=6.4$  Hz), 2.77 (*t*, 2H,  $J=6.4$  Hz), 3.27–2.37 (*m*, 10H), 3.66 (*s*, 2H), 6.27 (*d*, 2H,  $J=6.4$  Hz), 6.37 (*d*, 2H,  $J=2.4$  Hz), 6.44 (*s*, 2H), 7.08–7.10 (*m*, 1H), 7.43–7.46 (*m*, 2H), 7.89–7.91 (*m*, 1H).  $^{13}\text{C}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (Fig. S2),  $\delta$  12.35, 29.37, 34.71, 40.24, 40.83, 44.31, 64.69, 97.34, 105.62, 107.96, 122.63, 123.74, 128.02, 128.89, 131.11, 132.33, 148.82, 153.13, 167.90. LC-MS (Fig. S3):  $[\text{M}+\text{H}]^+$  545.2944,  $[\text{M}+\text{Na}]^+$  567.2755. FTIR ( $\text{cm}^{-1}$ ) (Fig. S4):  $\nu$  (NH) 3431;  $\nu$  ( $\text{CH}_3$ ,  $\text{CH}_2$ ) 2972, 2925, 2854;  $\nu$  (C=O) 1695;  $\nu$  (ArH) 1548, 1519, 1463;  $\nu$  (C-O-C) 1118. Elemental analysis: Calculated for  $\text{C}_{32}\text{H}_{40}\text{N}_4\text{O}_2\text{S}_3$  (%): C, 70.55; N, 10.28; H, 7.40. Found (%): C, 70.34; N, 10.04; H, 7.42.

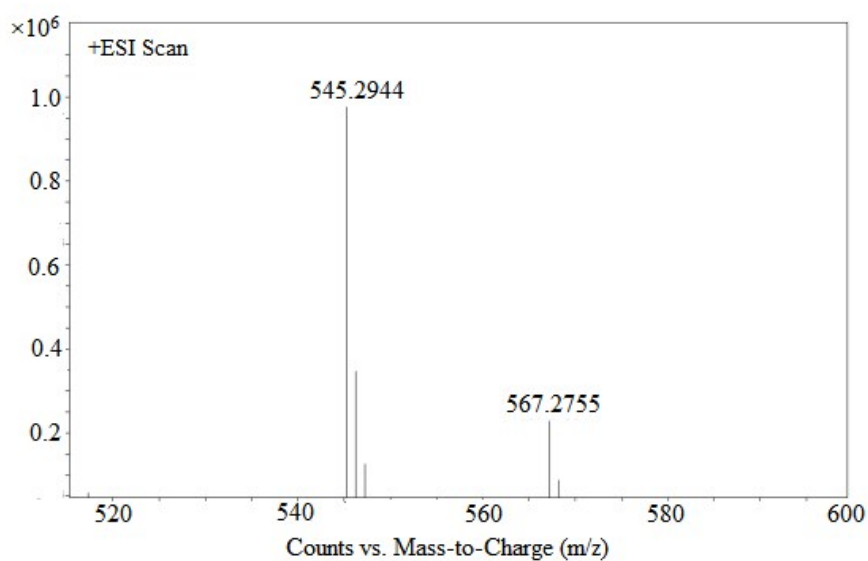
### 3. Characterization Figures



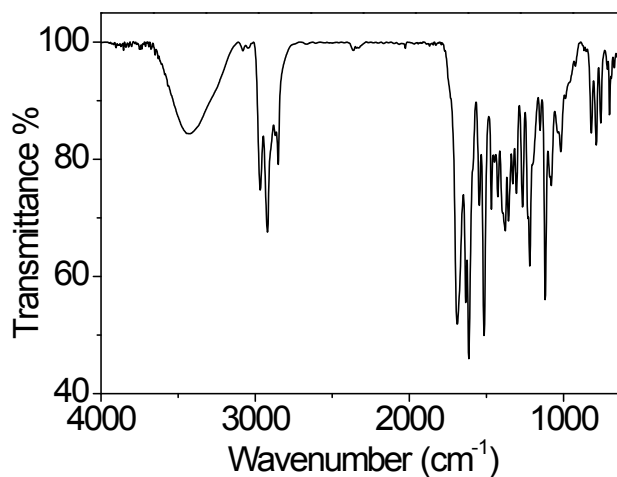
**Fig. S1.**  $^1\text{H}$  NMR spectrum of RMTE (400 MHz,  $\text{CDCl}_3$ ).



**Fig. S2.**  $^{13}\text{C}$  NMR spectrum of RMTE (300 MHz,  $\text{CDCl}_3$ ).



**Fig. S3.** LC-MS spectrum of RMTE.



**Fig. S4.** FTIR spectrum of RMTE.

#### 4. Parameter calculation methods

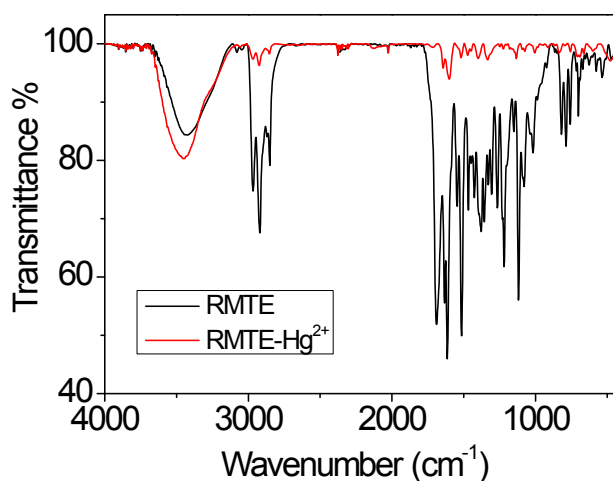
Detection limit: The detection limit was calculated on the basis of UV-vis absorption and fluorescence titration using equation (1), where,  $\delta$ : Detection limit.  $S$ : Standard deviation of 5 times testing of the absorbance and fluorescence intensity of the blank solution.  $K$ : Slope of the linear fitting lines in the UV-Vis absorption and fluorescence titration.

$$\delta = 3S/K \quad (1)$$

Binding constant: The binding constant between RMTE and  $Hg^{2+}$  was calculated by Benesi-Hildebrand equation (2). Where,  $F$ ,  $F_{min}$ ,  $F_{max}$ : Fluorescence intensity of RMTE solution with a certain concentration of  $Hg^{2+}$ , without  $Hg^{2+}$  and saturated by  $Hg^{2+}$ , respectively.  $[Hg^{2+}]$ : Concentration of  $Hg^{2+}$ .  $n$ : Binding ratio of the sensor to  $Hg^{2+}$ .  $K$ : Binding constant.

$$\log \frac{(F - F_{min})}{(F_{max} - F)} = n \log[Hg^{2+}] + \log K \quad (2)$$

#### 5. FTIR spectra of “free” ligand and in the presence of $Hg^{2+}$



**Fig. S5.** FTIR spectra of RMTE (black) and RMTE- $Hg^{2+}$  (red).