Electronic supplementary information (ESI)

for

Rhodamine Thiospirolactone. Highly Selective and Sensitive Reversible Sensing of Hg (II)

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Instruments and Materials

NMR spectra in CDCl₃ were recorded on Bruker AV400 NMR and Bruker AV300 NMR. Mass spectra were measured with a JEOL JMS-T100LC mass spectrometer (ESI⁺). Single crystal data were obtained by a Bruker Smart Apex CCD Area Detector. Uncorrected fluorescence emission spectra were conducted on a Perkin Elmer LS55 luminescence spectrometer. Absorption spectra were determined on a Varian CARY 300 and Thermo Genesys 5 spectrophotometer. Dry benzene was distilled from CaH₂. Doubly distilled water was used throughout the experiments. All the materials for synthesis were purchased from commercial suppliers and used without further purification. The solutions of metal ions were prepared from their nitrate salts. Reactions were monitored by TLC with visual observation of the dye spots. Products were purified by column chromatography, or by recrystallization.

General Procedure

A 1.0×10^{-3} M stock solution of compound **1** was prepared in absolute CH₃CN with the aid of a touch mixer for 15 min. To 10-mL glass tubes containing 10 mM NaAc-HAc buffer of pH 4.0 and different amounts of metal ions, proper amounts of the solution of compound **1** was added directly with a micropipette. The solutions were diluted with water to 10 mL and mixed, then the absorption and fluorescence sensing of metal ions were run immediately.



Fig. S1 ¹H-NMR spectra of 1 in CDCl₃.



Fig. S2 ¹³C-NMR spectra of 1

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Fig. S4 Effect of pH on the absorption response of **1** to Hg^{2+} at 559 nm. [**1**] =10 μ M, $[Hg^{2+}] = 10.0 \ \mu$ M.



Fig. S5 Effect of pH on the fluorescence response of **1** to Hg^{2+} . [**1**] =10 μ M, [Hg²⁺] = 10.0 μ M. λ ex = 530 nm. Slit: 5nm / 5nm.



Fig. S6 Job's plot of the complexation between **1** and Hg^{2+} in 99:1 (v/v) H_2O :MeCN solutions at pH 4.0 (in a 10 mM NaAc-HAc buffer). Total concentration of **1** and Hg^{2+} was kept constant at 10.0 μ M.

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Fig. S7 ESI-MS of 1 in the presence of 1eq HgCl₂ in a H₂O-CH₃CN solution.



Fig. S8 Absorption spectra of **1** $(1.0 \times 10^{-5} \text{ M})$ in 99:1 H₂O:MeCN aqueous solution in the presence of 1.0×10^{-5} M metal ions, respectively.



Fig.S9 Spectrometric response of probe **1** toward 1eq Hg²⁺ in the presence of 10 eq competitive background metal ions in 99:1 (v/v) H₂O:CH₃CN solutions. None: no competitive ions except Hg²⁺. [**1**]=10 μ M.