Rhodamine-based Chemosensor for Hg^{2+} in Aqueous Solution with a Broad pH Range and Its Application in Live Cell Imaging

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Electronic Supplementary Information (ESI†)

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1. IR spectra of 1 and 1–Hg$^{2+}$ complex in KBr disks

![IR spectra of 1 and 1–Hg$^{2+}$ complex in KBr disks](image)

Fig. S1 IR spectra of 1 (a) and 1–Hg$^{2+}$ (b) were taken in KBr disks, respectively.

2. $^1$H NMR-titration experiments (Fig. S2).

![$^1$H NMR-titration experiments](image)

Fig. S2 Hg$^{2+}$ $^1$H NMR-titration of 1 (10.0 mM) with Hg$^{2+}$ (5 equiv.) in CDCl$_3$. 
3. Effects of water content on the fluorescence of 1–Hg$^{2+}$ system.

![Figure S3](image.png)

**Fig. S3** Effects of water content on the fluorescence of 1–Hg$^{2+}$ system in aqueous acetonitrile solution. [$1] = 20 \text{ µM}$, [Hg$^{2+}$] = 100µM.

4. Time-dependent change in fluorescence intensity of 1 after Hg$^{2+}$ addition

![Figure S4](image.png)

**Fig. S4** Time course of the response of 1 (20 µM) in MeCN-water solution (95/5, v/v, pH=7.2) upon addition of 5 equiv. of Hg(NO$_3$)$_2$.

5. Determination of binding constant of the complex

The data obtained from fluorescence titration profile were fitted to be a 1:1 binding model according to following equation.

$$
\Delta F = \frac{1}{2} \left\{ \alpha \left[ H J_0 + [G] + \frac{1}{K} \right] - \sqrt{\frac{\alpha^2}{2} \left[ [H J_0 + [G] + \frac{1}{K} \right]^2 - 4[H J_0][G]} \right\}
$$

The binding constant (K) is an important parameter, indicating the inclusion
capacity of the host-guest complex. The binding constants \( (K) \) can thus be obtained by a nonlinear least's squares analysis of \( \Delta F \) versus \([\text{Hg}^{2+}]\), fitting to the experimental data obtained from the absorption and fluorescence titrations. Where \([\text{H}]_0\) and \([\text{G}]_0\) are the initial concentrations of host sensor 1 and guest \text{Hg}^{2+}, respectively. \( \Delta F \) denotes the change of the absorption and fluorescence intensity of sensor 1 with the addition of \text{Hg}^{2+}. \( \alpha \) is a sensitive factor of the structure change of the complex 1-Hg\(^{2+}\) at the interactive course \( (\alpha = (F_{\text{max}}-F_0)/[\text{G}]_0) \).

**Fig. S5** UV/VIS titration profile of 1 (20µM) in MeCN-water solution (95:5, v/v, Ph=7.2), from which the association constant was determined, \( K_a = 2.18 \times 10^6 \text{ M}^{-1} \) \( (R^2 = 0.9916) \).

**Fig. S6** Fluorescence titration profile (\( \lambda_{\text{em}} = 530 \text{ nm} \)) of 1 (20µM) in MeCN-water solution (95:5, v/v, Ph=7.2), from which the association constant was determined, \( K_a = 1.27 \times 10^6 \text{ M}^{-1} \) \( (R^2 = 0.9898) \).
6. Selectivity investigation by absorption spectra

Fig. S7 (a) The absorption spectra of 1 (20 μM) upon addition of 100 μM of Hg²⁺ and various other metal ions in a MeCN-water solution (95/5, v/v, pH 7.2). (b) Absorption change of 1 (20 μM) to 100 μM of Hg²⁺ in a MeCN-water solution (95/5, v/v, pH 7.2) containing 100 μM of various metal ions.

7. Reversibility investigation by introduction of iodide anion.
**Fig. S8** Reversibility of Hg$^{2+}$ coordination to probe 1 by I$^-$. Slash denotes the sequence of addition. [I] = 2.0 × 10$^{-5}$ M, in aqueous acetonitrile solution (95/5, v/v, pH=7.2). [Hg$^{2+}$](1st) = 1.0 × 10$^{-4}$ M, [I$^-$] = 4.0 × 10$^{-4}$ M, [Hg$^{2+}$] (2nd) = 6.0 × 10$^{-4}$ M, [I$^-$] = 2.4 × 10$^{-3}$ M, [Hg$^{2+}$](3rd) = 1.8 × 10$^{-3}$ M, [I$^-$] = 7.2 × 10$^{-2}$ M.
Fig. S9 $^1$H NMR chart of 1 (CDCl$_3$, 300MHz)
Fig. S10 $^{13}$C NMR chart of 1 (CDCl$_3$, 75MHz)
Fig. S11 EI-MS chart of 1