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Accessory Publication

New Highly Selective Colorimetric and Fluorescent Chemodosimeters for Mercury Ion

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Additional spectra

Fig. SI-1. UV absorption responses of **1** to various metal ions in aqueous solution (DMSO/H₂O = 4/1, v/v).

Fig. SI-2. Fluorescene intensity responses of **1** to various metal ions in aqueous solution (DMSO/H₂O = 4/1, v/v).

Fig. SI-3. ¹³C NMR spectrum of (a) **1**, (b) **1** with 1.0 equiv of Hg^{2+} , and (c) **4** in DMSO-d₆.

Fig. SI-4. Family of spectra taken in the course of the titration of a solution in **2** with a standard solution of Hg^{2+} at 25 °C.

Fig. SI-5. Family of spectra taken in the course of the titration of a solution in **3** with a standard solution of Hg^{2+} at 25 °C.

Fig. SI-6. Absorbance responses of 2 to various metal ions in aqueous solution (DMSO/H₂O = 4/1, v/v).

Fig. SI-7. Absorbance responses of 3 to various metal ions in aqueous solution (DMSO/H₂O = 4/1, v/v).

Fig. SI-8. (a) Fluorescence spectra of 2 in response to the metal ions. (b) Photograps of 2 upon addition of miscellaneous cations in aqueous solution (DMSO/H₂O = 4/1, v/v).

Fig. SI-9. (a) Fluorescence spectra of **3** in response to the metal ions. (b) Photograps of **3** upon addition of miscellaneous cations in aqueous solution (DMSO/H₂O = 4/1, v/v).



Fig. SI-1. UV absorption responses of **1** (30 μ M) to various metal ions (300 μ M) in aqueous solution (DMSO/H₂O = 4/1, v/v). Bars represent the intensity ratios of absorption at 360 nm. A₀ represents the responses of **1**+Hg²⁺, A represents either the responses of **1**+Mⁿ⁺ or the responses of **1**+(Hg²⁺+Mⁿ⁺).



 $\mathbf{1} + Cation$

Fig. SI-2. Fluorescene intensity responses of **1** (0.5 μ M) to various metal ions (5.0 μ M) in aqueous solution (DMSO/H₂O = 4/1, v/v). Bars represent the intensity ratios of absorption at 395 nm. I₀ represents the responses of **1**+Hg²⁺, I represents either the responses of **1**+Mⁿ⁺ or the responses of **1**+(Hg²⁺+Mⁿ⁺).



Fig. SI-3. ¹³C NMR spectrum of (a) **1**, (b) **1** with 1.0 equiv of Hg^{2+} , and (c) **4** in DMSO-d₆.



Fig. SI-4. Family of spectra taken in the course of the titration of a solution in **2** (30 μ M, DMSO/H₂O = 4/1, v/v) with a standard solution of Hg²⁺ at 25 °C. Titration profile (insert) indicates the formation of a 1:1 complex.



Fig. SI-5. Family of spectra taken in the course of the titration of a solution in **3** (30 μ M, DMSO/H₂O = 4/1, v/v) with a standard solution of Hg²⁺ at 25 °C. Titration profile (insert) indicates the formation of a 1:1 complex.



2 + Cation

Fig. SI-6. Absorbance responses of **2** (30 μ M) to various metal ions (300 μ M) in aqueous solution (DMSO/H₂O = 4/1, v/v). Bars represent the intensity ratios of absorption at 372 nm. A₀ represents the responses of **2**+Hg²⁺, A represents either the responses of **2**+Mⁿ⁺ or the responses of **2**+(Hg²⁺+Mⁿ⁺).



Fig. SI-7. Absorbance responses of **3** (30 μ M) to various metal ions (300 μ M) in aqueous solution (DMSO/H₂O = 4/1, v/v). Bars represent the intensity ratios of absorption at 360 nm. A₀ represents the responses of **3**+Hg²⁺, A represents either the responses of **3**+Mⁿ⁺ or the responses of **3**+(Hg²⁺+Mⁿ⁺).



Fig. SI-8. (a) Fluorescence spectra of **2** in response to the metal ions. [**2**] = 0.5 μ M, [Mⁿ⁺] = 5.0 μ M, in DMSO/H₂O = 4/1. λ_{ex} = 372 nm. (b) Photograps of **2** (0.5 μ M) upon addition of miscellaneous cations (X) including Na⁺, K⁺, Mg²⁺, Ca²⁺, Cr³⁺, Mn²⁺, Fe³⁺, Co²⁺, Ni²⁺, Cu²⁺, Ag⁺, Pb²⁺, Zn²⁺, Cd²⁺ and Hg²⁺ (1.0 equiv) in aqueous solution (DMSO/H₂O = 4/1, v/v).



Fig. SI-9. (a) Fluorescence spectra of **3** in response to the metal ions. [**3**] = 0.5 μ M, [Mⁿ⁺] = 5.0 μ M, in DMSO/H₂O = 4/1. λ_{ex} = 349 nm. (b) Photograps of **3** (0.5 μ M) upon addition of miscellaneous cations (X) including Na⁺, K⁺, Mg²⁺, Ca²⁺, Cr³⁺, Mn²⁺, Fe³⁺, Co²⁺, Ni²⁺, Cu²⁺, Ag⁺, Pb²⁺, Zn²⁺, Cd²⁺ and Hg²⁺ (1.0 equiv) in aqueous solution (DMSO/H₂O = 4/1, v/v).