Supplementary Material

A fluorescent and colorimetric chemosensor for Hg2+ based on rhodamine 6G with a two-step reaction mechanism

Cui-Bing Bai1,2, Wei-Gang Wang1, Jie Zhang1, Chang Wang1,2, Rui Qiao1,2\*, Biao Wei1,2, Lin Zhang1,2, Shui-Sheng Chen1,2, Song Yang1,2

*1School of Chemistry and Materials Engineering, Fuyang Normal University, Fuyang, Anhui Province, China*

*2Anhui Province Key Laboratory for Degradation and Monitoring of Pollution of the Environment, Fuyang, Anhui Province, China*

\*Corresponding Author

Rui Qiao, qiaorui@mail.ipc.ac.cn Tel: +86-558-2595626; Fax: +86-558-2596249



**Figure S1.** 1H NMR spectra of compound **L**



**Figure S2.** 13C NMR spectra of compound **L**



**Figure S3.** ESI-MS spectrum of **L**



**Figure S4.** Absorption response of **L** (1×10-5 M) in HEPES buffer (10 mM, pH 7.4)/CH3CN (40:60, V/V) upon addition of respective metal ions, at 526 nm, followed by addition of Hg2+.



**Figure S5.** Competitive selectivity of **L** (1.0×10-5 M) towards Cu2+ in the presence of other metal ions in HEPES buffer (10 mM, pH 7.4)/CH3CN (40:60, V/V), λex = 526 nm, fluorescent intensity at 550 nm.



**Figure S6.** Absorption response of **L** (1×10-5 M) in HEPES buffer (10 mM, pH 7.4)/CH3CN (40:60, V/V), at 526 nm, followed by addition of Hg2+. [Hg2+]/[**L**]=0, 0.5, 1, 1.5, 2 were separately tested.



**Figure S7.** Fluorescence spectra of **L** (1×10-5 M) in HEPES buffer (10 mM, pH 7.4)/CH3CN (40:60, V/V), at 550 nm, followed by addition of Hg2+. [Hg2+]/[**L**]=0, 0.5, 1, 1.5, 2 were separately tested.



**Figure S8.** ESI-MS spectrum of **LO**



**Figure S9.** ESI-MS spectrum of **LO-Hg**2+



**Figure S10.** FTIR spectra of compound **L** and **L**−Hg2**+**

(a)



(b)



**Figure S11.** (a) Absorption spectra of **L** (1.0×10-5 M) in the presence of different concentration of Hg2+ (0-3.0 equiv.) in HEPES buffer (10 mM, pH 7.4)/CH3CN (40:60, V/V). (b) A plot of absorption depending on the concentration of Hg2+ in the range from 0.1 to 3.0 equiv, at 526 nm.



**Figure S12.** Absorption of chemosensors **L** in the presence of Hg2+ with different mole ratios of [Hg2+]/ ([Hg2++**L**]) at the constant total concentration ([Hg2+] + [**L**] = 2.0×10-5 M) in HEPES buffer (10 mM, pH 7.4)/CH3CN (40:60, V/V). (b) Job’ plot for determination of the binding stoichiometry of chemosensors **L** with Hg2+, λ= 526 nm.



**Figure S13.** (a) Fluorescence spectra of chemosensor **L** in the presence of Hg2+ with different mole ratios of [Hg2+]/ ([Hg2++**L**]) at the constant total concentration ([Hg2+]+[**L**]= 2.0×10-5 M) in HEPES buffer (10 mM, pH 7.4)/CH3CN (40:60, V/V), λex= 526 nm, at 550 nm.. (b) Job’ plot for determination of the binding stoichiometry of chemosensors **L** with Hg2+.

.



**Figure S14.** Plot of the intensity at 550 nm for a mixture of the sensor **L** (1×10-5 M) and Hg2+ in HEPES buffer (10 mM, pH 7.4)/CH3CN (40:60, V/V), λex= 526 nm.

S = 2.57296× 107 δ =$\sqrt{\frac{\sum\_{}^{}(F\_{0 }– F\_{1})^{2}}{N-1}}$ = 0.01036 (N = 20) K = 3

LOD = K × δ / S = 0.012 × 10−7 M

F0 is the fluorescence intensity of **L**; F1 is the average of the F0.

**Table S1**. Fluorescence life time and quantum yield

|  |  |  |
| --- | --- | --- |
| **Probes** | **Fluorescence Life Time** | **Fluorescence quantum yield** |
| **L**-Hg2+ | 4.290913×10-9 S | 49.86 % |