Electronic Supplementary Material

A rhodamine-based dual chemosensors for the naked-eyes detection of Hg²⁺ and enhancement of the fluorescence emission

for Fe³⁺

Jian-Peng Hu, ^a Hao-Hang Yang, ^a Qi Lin, ^a Hong Yao, ^a You-Ming Zhang, ^{a, b} Tai-Bao Wei ^{a,*} and Wen-Juan Qu ^{a,*}

^a Key Laboratory of Polymer Materials of Gansu Province, Research Center of Gansu Military and Civilian Integration Advanced Structural Materials, College of Chemistry and Chemical Engineering, Northwest Normal University, Anning East Road 967, Lanzhou, Gansu, 730070, P. R. China.

^b Deputy Director-General of Gansu Natural Energy Research Institute, Renmin Road 23, Lanzhou, Gansu, 730000, P. R. China.

Content

The synthetic route of TR	3
¹ H NMR spectrum of RBA	5
¹³ C NMR spectrum of RBA	6
ESI/MS of RBA	7
¹ H NMR spectrum of TR	8
ESI/MS of TR	9
UV-vis of sensor (TR) for different aqueous systems of Hg ²⁺	10
Fluorescence spectra of sensor TR for different aqueous syste	ems of
Fe ³⁺	11
Determine of the UV-vis detection limit for Hg ²⁺	12
Determine of the fluorescent detection limit for Fe ³⁺	13
Fluorescence spectra of TR in various pH values EtOH $/H_2O$ (9)	1, v/v)
HEPES buffer solution	14
Mass spectrum between TR and Hg ²⁺	15
Mass spectrum between TR and Fe ³⁺	16
IR spectra of compound TR、TR+Hg ²⁺ and TR+Fe ³⁺	17

The synthetic route of **TR**.



Scheme S1. The synthesis of TR.

Synthesis of **RBA**. Rhodamine B (1.20 g, 2.5 mmol) was placed in a 100mL flask and subsequently dissolved in 30 mL ethanol. Stirred at room temperature for 30 min and dropped 3.0 mL of hydrazine hydrate (85%) into it. The stirred mixture was heated at 85 °C and refluxed for 8 h. The solution changed from dark purple to light orange and became clear. The mixture was cooled and the solvent was removed under reduced pressure. Add 1 mol/L (about 50 mL) to the flask to produce a clear red solution. On this basis, 1mol/L (about 70 mL) was added and stirred until the

solution pH reached 9~10. The resulting precipitate was filtered and washed 3 times with 15 mL of water. Then thoroughly dried under vacuum and the reaction afforded 0.83 g (75%) as pink solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.94 (s, 1H), 7.44 (d, *J* = 6.9 Hz, 2H), 7.11 (s, 1H), 6.46 (s, 2H), 6.41 (s, 2H), 3.61 (s, 2H), 3.33 (s, 8H), 1.16 (t, *J* = 7.0 Hz, 12H). ¹³C NMR (400 MHz, CDCl₃) δ 166.1, 153.8, 151.5, 148.9, 132.5, 128.1, 123.8, 122.9, 108.0, 104.6, 99.98, 65.9. ESI-MS m/z:(M + H)⁺ calculated C₂₈H₃₃N₄O₂ 457.2595; Found 457.2597.

¹H NMR spectrum of **RBA**



Figure S1. ¹H NMR spectrum of RBA in CDCl₃

¹³C NMR spectrum of **RBA**



Figure S2. ¹³C NMR spectrum of RBA in CDCl₃

ESI/MS of RBA



Figure S3. The ESI/MS of RBA in CH₃CN

¹H NMR spectrum of **TR**



Figure S4. ¹H NMR spectrum of TR in DMSO- d_6 .

ESI/MS of TR



Figure S5. The ESI/MS of TR in CH₃CN.

UV-vis of sensor (**TR**) for different aqueous systems of Hg^{2+} .



Figure S6. UV-vis of sensor TR for different aqueous systems of Hg²⁺.

Fluorescence spectra of sensor \mathbf{TR} for different aqueous systems of Fe^{3+} .



Figure S7. Fluorescence spectra of sensor TR for different aqueous systems of Fe³⁺.

Determine of the UV-vis detection limit for Hg²⁺



Linear Equation: $Y = 0.3013 \text{ X} \cdot 0.2341$ R = 0.97669

S = 0.3013×10⁶
$$\delta = \sqrt{\frac{\Sigma(A-\overline{A})2}{(N-1)}} = 0.002473(N = 20)$$
 K = 3
LOD = K × $\delta/S = 2.46 \times 10^{-8}$ M

Figure S8. The photograph of the UV-vis absorption spectral linear range for Hg²⁺.

Determine of the fluorescent detection limit for Fe³⁺



Figure S9. The photograph of the fluorescent spectrum linear range for Fe³⁺.

Fluorescence spectra of **TR** in various pH values EtOH / H_2O (9:1,

v/v) HEPES buffer solution



Figure S10. Fluorescence spectra of TR in various pH values EtOH / H_2O (9:1, v/v) HEPES buffer solution

Mass spectrum between **TR** and Hg^{2+} .



Figure S11. Mass spectrum between TR and Hg²⁺.

Mass spectrum between **TR** and Fe^{3+} .



Figure S12. Mass spectrum between **TR** and Fe^{3+} .



IR spectra of compound TR、TR+Hg²⁺and TR+Fe³⁺

Figure S13. IR spectra of compound TR TR+Hg²⁺ and TR+Fe³⁺.