Supporting Information

Rhodamine-labelled simple architectures for fluorometric and colorimetric sensing of Hg$^2$ and Pb$^2$ ions in semi-aqueous and aqueous environments

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1. Spectral data of compounds

$^1$H NMR of 3 (CDCl$_3$, 400 MHz):

![NMR spectrum of compound 3](image)
$^1$H NMR of 1 (CDCl$_3$, 400 MHz):
$^{13}$C NMR of 1 (CDCl$_3$, 100 MHz):
Mass of 1:
2. Change in emission of receptor 1 with Zn\(^{2+}\), Fe\(^{3+}\), Cd\(^{2+}\), Co\(^{2+}\), Pb\(^{2+}\), Mg\(^{2+}\), Ni\(^{2+}\), Ag\(^{+}\) in MeCN/Water (4/1,v/v; 10 \(\mu\)M tris HCl buffer; pH 7).

![Fluorescence intensity spectra for different ions](image)

**Figure S1.** Change in emission of receptor 1 \((c = 2.25 \times 10^{-5} \text{ M})\) upon addition of (a) Zn\(^{2+}\), (b) Fe\(^{3+}\), (c) Cd\(^{2+}\), (d) Co\(^{2+}\), (e) Cu\(^{2+}\), (f) Mg\(^{2+}\), (g) Ni\(^{2+}\), (h) Ag\(^{+}\) in MeCN/Water (4/1, v/v; 10 \(\mu\)M tris HCl buffer; pH 7) (in all cases [cation] \(4.5 \times 10^{-4} \text{ M}\) \(\lambda_{\text{exc}} = 490 \text{ nm}\).
3. Change in absorbance of receptor 1 with various metal ions in MeCN/water (4/1, v/v; 10 μM tris HCl buffer; pH = 7)

![AbsorptionTitrationSpectra](image)

**Figure S2.** Absorption titration spectra for 1 (c = 2.25 x 10^{-5} M) with (a) Cu^{2+}, (b) Fe^{3+}, (c) Zn^{2+}, (d) Cd^{2+}, (e) Mg^{2+}, (f) Ni^{2+}, (g) Co^{2+} and (h) Ag^{+} in MeCN/water (4/1,v/v; 10 μM tris HCl buffer; pH =7 ) (in all cases [cation] =4.5 x 10^{-4} M).
4. $^1$H NMR study, UV and Fluorescence Job plots for 1 with Hg$^{2+}$ and Pb$^{2+}$ measured at 556 nm.

Figure S3a. Partial $^1$H NMR (400 MHz, CDCl$_3$) of (A) 1 (5.21 x 10$^{-3}$ M); (B) with 1 equiv. amount of Pb(ClO$_4$)$_2$ and (c) with 1 equiv. Hg(ClO$_4$)$_2$.

Figure S3b. Fluorescence Job plots for 1 with (a) Hg$^{2+}$; (b) Pb$^{2+}$; UV Job plots for 1 with (c) Hg$^{2+}$, (d) Pb$^{2+}$ in MeCN/Water (4/1,v/v; 10 μM tris HCl buffer; pH = 7 ) ([H] = [G] = 4.5 x 10$^{-5}$ M).
5. Change in fluorescence spectra of (a) 1- Hg$^{2+}$, (b) 1- Pb$^{2+}$ complex upon addition of KI

![Fluorescence Spectrum](image)

**Figure S4:** (a) Change in fluorescence spectra of (a) 1- Hg$^{2+}$, (b) 1- Pb$^{2+}$ complex ($c = 4.1 \times 10^{-5}$ M) in MeCN/Water (4/1, v/v) 10 μM tris HCl buffer (pH 7) upon addition of (a) KI ($c = 2.1 \times 10^{-3}$ M).

6. Colorimetric change of 1 with Pb$^{2+}$:

![Colorimetric Change](image)

**Figure S5:** Change in fluorescence spectra of 1 ($c = 2.25 \times 10^{-5}$ M) in CH$_2$CN/water (4/1, v/v; 10 μM tris HCl buffer, pH = 7.0) upon addition of (a) Hg$^{2+}$ and (b) Pb$^{2+}$ of different concentrations.
7. MTT assay.

![MTT assay graph](image)

**Figure S6.** Cell viability of HeLa cells treated with different concentrations (1 µM-100 µM) of chemosensor 1 for six hrs determined by MTT assay.

8. FTIR spectra of 1, Merrifield resin and 2:

![FTIR spectra](image)

**Figure S7.** FTIR spectra of 1, Merrifield resin and 2.
9. FTIR spectra of 2, 2- Hg$^{2+}$ and 2- Pb$^{2+}$ complex:

![FTIR spectra of 2, 2- Hg$^{2+}$ and 2- Pb$^{2+}$ complex](image)

**Figure S8.** FTIR spectra of 2 and 2- Hg$^{2+}$, 2- Pb$^{2+}$ complexes.

10. Reuse study:

![Reuse study of 2 for Hg$^{2+}$ ions](image)

**Figure S9.** Reuse study of 2 for Hg$^{2+}$ ions.