Supporting Information

Multimodal Ion Sensing by Structurally Simple Pyridine-end oligo p-Phenylenevinylenes for Sustainable Detection of Toxic Industrial Waste

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ADDITIONAL SPECTRA

Figure S1. (a) UV-vis spectra of **1** (1×10^{-5} M) with different metal ions (2 equiv. Ag^+ , Cd^{2+} , Cu^{2+} , Co^{2+} , Hg^{2+} , Mg^{2+} , Ni^{2+} , Pb^{2+} , Zn^{2+} , Mn^{2+} , Cr^{3+} , Al^{3+} , Au^{3+} and Fe^{3+} etc.) in THF. (b) Fluorescence spectra of **1** (1×10^{-5} M, $\lambda_{\text{ex}} = 400$ nm) with different metal ions (2 equiv. Ag^+ , Cd^{2+} , Cu^{2+} , Co^{2+} , Hg^{2+} , Mg^{2+} , Ni^{2+} , Pb^{2+} , Zn^{2+} , Mn^{2+} , Cr^{3+} , Al^{3+} , Au^{3+} and Fe^{3+} etc.) in THF.

Figure S2. (a) Determination of the stoichiometry for the binding of Hg^{2+} with **1** using Job's plot. (b) Calculation of binding constant of **1** with Hg^{2+} ion based on 1:1 Benesi-Hildebrand model.

Figure S3. (a) Change in absorbance of **1** (at 460/400 nm) and **2** (at 510/450 nm) (1×10^{-5} M) upon addition of Hg^{2+} in THF. (b) Change in fluorescence intensity of **1** (1×10^{-5} M, $\lambda_{\text{ex}} = 400$ nm) and **2** (1×10^{-5} M, $\lambda_{\text{ex}} = 440$ nm) at 460 and 520 nm respectively upon addition of Hg^{2+} in THF.

Figure S4. (a) UV-vis spectra of **2** (1×10^{-5} M) with different metal ions (2 equiv., Ag^+ , Cd^{2+} , Cu^{2+} , Co^{2+} , Hg^{2+} , Mg^{2+} , Ni^{2+} , Pb^{2+} , Zn^{2+} , Mn^{2+} , Cr^{3+} , Al^{3+} , Au^{3+} and Fe^{3+} etc.) in THF. (b) Fluorescence spectra of **2** (1×10^{-5} M, $\lambda_{\text{ex}} = 440$ nm) with different metal ions (2 equiv., Ag^+ , Cd^{2+} , Cu^{2+} , Co^{2+} , Hg^{2+} , Mg^{2+} , Ni^{2+} , Pb^{2+} , Zn^{2+} , Mn^{2+} , Cr^{3+} , Al^{3+} , Au^{3+} and Fe^{3+} etc.) in THF.

Figure S5. (a) Determination of the stoichiometry for the binding of Hg^{2+} with **2** using Job's plot. (b) Calculation of binding constant of **2** with Hg^{2+} ion based on 1:1 Benesi-Hildebrand model.

Figure S6. (a) UV-vis spectra of **3** (1×10^{-5} M) with different metal ions (3 equiv. Ag^+ , Cd^{2+} , Cu^{2+} , Co^{2+} , Hg^{2+} , Mg^{2+} , Ni^{2+} , Pb^{2+} , Zn^{2+} , Mn^{2+} , Cr^{3+} , Al^{3+} , Au^{3+} and Fe^{3+} etc.) in THF. (b) Fluorescence spectra of **3** (1×10^{-5} M, $\lambda_{\text{ex}} = 395$ nm) with different metal ions (3 equiv. Ag^+ , Cd^{2+} , Cu^{2+} , Co^{2+} , Hg^{2+} , Mg^{2+} , Ni^{2+} , Pb^{2+} , Zn^{2+} , Mn^{2+} , Cr^{3+} , Al^{3+} , Au^{3+} and Fe^{3+} etc.) THF.

Figure S7. (a) UV-vis spectra of **3** (1×10^{-5} M) with different anions (3 equiv., F^- , Br^- , I^- , CN^- , Cl^- , AcO^- , H_2PO_4^- , PF_6^- , CO_3^{2-} , HSO_3^- etc.) in THF. (b) Fluorescence spectra of **3** (1×10^{-5} M, $\lambda_{\text{ex}} = 395$ nm) with different anions (3 equiv., F^- , Br^- , I^- , CN^- , Cl^- , AcO^- , H_2PO_4^- , PF_6^- , CO_3^{2-} , HSO_3^- etc.) in THF.

Figure S8. (a) Fluorescence titration of **3** (1×10^{-5} M, $\lambda_{\text{ex}} = 400$ nm) with Hg^{2+} (0-2.2 equiv.) in THF. (b) Fluorescence titration of **3** (1×10^{-5} M, $\lambda_{\text{ex}} = 400$ nm) with CN^- (0-2.2 equiv.) in THF.

Figure S9. (a) Change in absorbance of **3** (1×10^{-5} M) upon addition of CN^- and Hg^{2+} ion in THF. (b) Change in absorbance of **3** (1×10^{-5} M) upon addition of Hg^{2+} ion in THF. (c) Change in fluorescence intensity of **3** (1×10^{-5} M, $\lambda_{\text{ex}} = 400$ nm) at 445 nm upon addition of CN^- ion in THF. (d) Change in fluorescence intensity of **3** (1×10^{-5} M, $\lambda_{\text{ex}} = 400$ nm) at 445 nm upon addition of Hg^{2+} ion in THF.

Figure S10. (a) Change in emission intensity of **3** (1×10^{-5} M, $\lambda_{\text{ex}} = 400$ nm) upon addition of Hg^{2+} in presence of other metal ions in THF medium. (b) Change in emission intensity of **3** (1×10^{-5} M, $\lambda_{\text{ex}} = 400$ nm) upon addition of CN^- in presence of other metal ions in THF medium.

Figure S11. (a) Determination of the stoichiometry for the binding of Hg^{2+} with **3** using Job's plot. (b) Calculation of binding constant of **3** with Hg^{2+} ion based on 1:1 Benesi-Hildebrand model.

Figure S12. (a) Determination of the stoichiometry for the binding of CN^- with **3** using Job's plot. (b) Calculation of binding constant of **3** with CN^- ion based on 1:2 Benesi-Hildebrand model.

Figure S13. (a) UV-visible titration of **3**+CN⁻ (10 μM, [CN⁻] = 20 μM) with Hg²⁺ (0-10 μM) in THF. (b) UV-visible titration of **3**+CN⁻ (10 μM, [CN⁻] = 20 μM) with Hg²⁺ (10-40 μM) in THF.

Scheme S1. Probable mode of binding of Hg²⁺ with **1**.

Scheme S2. Concentration dependent interaction cyanide interaction with compound **3** in presence of Hg²⁺ ion in THF medium.

Figure S14. (a) Typical amplitude sweep experiment of the dioxane gel of **3** at 25 °C (Concentration = 10 mg/mL). (b) Typical angular frequency sweep experiment of the dioxane gel of **3** at 25 °C (Concentration = 10 mg/mL).

Figure S15. (a) Typical amplitude sweep experiment of the 'recovered' gel of **3** at 25 °C (Concentration = 10 mg/mL). (b) Typical angular frequency sweep experiment of the 'recovered' gel of **3** at 25 °C (Concentration = 10 mg/mL).

Figure S16. Change in emission intensity **1** (1×10^{-5} M, $\lambda_{\text{ex}} = 400$ nm) upon addition of Hg^{2+} (5 μM) in different THF-water mixture medium.

Figure S17. (a) Change in emission intensity **3** (1×10^{-5} M, $\lambda_{\text{ex}} = 400$ nm) upon addition of CN^- (5 μM) in different THF-water mixture medium. (b) Change in emission intensity **3** (1×10^{-5} M, $\lambda_{\text{ex}} = 400$ nm) upon addition of Hg^{2+} (5 μM) in different THF-water mixture medium.

Figure S18. Reversible sensing of Hg^{2+} using compound **3**-coated paper discs (using EDTA).

Comparison Table

Though the number of reports for individual sensing of Hg^{2+} and CN^- is fairly large in literature, simultaneous sensing of both these toxic analytes are rather few. Since Hg^{2+} is known to interact with multiple analytes, such as sulfides, iodide, fluoride etc, it is very difficult to achieve specific response towards CN^- using probe- Hg^{2+} conjugate. Here, we have prepared a comparison table comprising of few optical probes, which can detect Hg^{2+} and CN^- simultaneously.

Entry	medium	Limit of Detection	Optical Response	Principle of Detection	Reference
1	3:7 $\text{CH}_3\text{CN}/\text{H}_2\text{O}$ (v/v)	For Hg^{2+} : 93.3 nM For CN^- : 63.0 nM	Blank: Cyan fluorescence + Hg^{2+} : Violet fluorescence + CN^- : Cyan fluorescence	Displacement Approach	Ind. Eng. Chem. Res. 2017, 56, 6358–6368
2	$\text{CH}_3\text{CN}/\text{H}_2\text{O}$ (1 : 1 v/v)	For CN^- : 0.8 μM	Blank: colorless + CN^- : Yellow color + Hg^{2+} : colorless	Displacement Approach	Photochem. Photobiol. Sci., 2018, 17, 1450–1461
3	$\text{THF}/\text{H}_2\text{O}$ (2 : 3 v/v)	For Hg^{2+} : 19.2 nM For CN^- : 1.25 μM	Blank: Cyan fluorescence + Hg^{2+} : No fluorescence + CN^- : Cyan fluorescence	Displacement Approach	Sensors and Actuators B, 2017, 251, 729–738
4	CH_3CN	For Hg^{2+} : 5.78 μM For CN^- : 3.90 μM	Blank: Red fluorescence + Hg^{2+} : yellow fluorescence + CN^- : No fluorescence	Independent pathways	Spectrochim. Acta A, 2015, 144, 226–234
5	$\text{DMF}-\text{H}_2\text{O}$ (13:12, v/v)	For Hg^{2+} : 6.6 nM For CN^- : 0.11 μM	Blank: No fluorescence + Hg^{2+} : Red fluorescence + CN^- : No fluorescence	Independent pathways	Tetrahedron, 2016, 72, 5620-5625
6	THF and $\text{THF}-\text{water}$ (3:2)	For Hg^{2+} : 7.8 ppb For CN^- : 11.2 ppb	Blank: blue fluorescence + Hg^{2+} : cyan fluorescence + CN^- : No fluorescence	Independent pathways	Present work

Table S1. The table shows comparison of detection limit, fluorescence response, medium of for detection of different $\text{Hg}^{2+}/\text{CN}^-$ sensing systems.