Supporting Information

Colorimetric detection of iron and fluorescent detection of zinc and cadmium by a chemosensor having a bio-friendly octopamine

Ji Hye Kang and Cheal Kim

Department of Fine Chemistry and Department of Interdisciplinary Bio IT Materials, Seoul National University of Science and Technology, Seoul 139-743, Korea. Fax: +82-2-973-9149; Tel: +82-2-970-6693; E-mail: chealkim@seoultech.ac.kr (C. Kim).
Fig. S1. $^{13}$C NMR spectrum of 1.
Fig. S2. UV-vis absorption spectra of 1 (20 µM) in MeOH.
Fig. S3. Job plot for the binding ratio of 1 (80 μM) toward $\text{Fe}^{3+}$ (80 μM).
Fig. S4. Positive-ion ESI-mass spectrum of 1 (100 μM) in the presence of 1 equiv of Fe(NO$_3$)$_3$. 
Fig. S5. The association constant of 1 toward Fe$^{3+}$ using non-linear equation on the basis of UV-vis titration.
Fig. S6. The detection limit (via 3σ/slope) of 1 (40 μM) with Fe$^{3+}$ on the basis of UV-vis titrations. σ means the average of the standard deviations.
Fig. S7. Absorbance (at 500 nm) of **I** (40 μM) and **1-Fe**$^{3+}$ complex (0.75 equiv) at pH range of 2-12.
**Fig. S8.** The calibration curve (at 500 nm) of 1 upon the addition of Fe$^{3+}$. [1] = 40 $\mu$M and [Fe$^{3+}$] = 0.0–10.0 $\mu$M in buffer (bis-tris, 10 mM, pH = 7.0).
Fig. S9. UV-vis spectral changes of 1 (40 μM) as the different concentrations of Fe^{2+}. Inset: Plot of absorbance at 500 nm vs Fe^{2+} concentration.
Fig. S10. Job plot for the binding ratio of 1 (80 μM) toward Fe²⁺ (80 μM).
Fig. S11. Positive-ion ESI-mass spectrum of 1 (100 μM) in the presence of 1 equiv of Fe(ClO$_4$)$_2$. 
Fig. S12. The association constant of 1 toward Fe$^{2+}$ using non-linear equation on the basis of UV-vis titration.
**Fig. S13.** The detection limit (via 3σ/slope) of 1 (40 μM) with Fe$^{2+}$ on the basis of UV-vis titrations. σ means the average of the standard deviations.
Fig. S14. Bar graphs of 1 (40 μM) for detection of Fe$^{2+}$ in the presence of various metal ions in buffer (bis-tris, 10 mM, pH = 7.0).
**Fig. S15.** Absorbance (at 500 nm) of 1 (40 μM) and 1-Fe$^{2+}$ complex (0.75 equiv) at pH range of 2-12.
**Fig. S16.** UV-vis titrations of 1 (20 μM) in the change of Zn$^{2+}$ concentrations. Inset: Plot of absorbance at 374 nm vs Zn$^{2+}$ concentration.
Fig. S17. Job plot for the binding ratio of 1 (100 μM) toward Zn$^{2+}$ (100 μM).
Fig. S18. Positive-ion ESI-mass spectrum of 1 (100 μM) in the presence of 1 equiv of Zn(NO₃)₂.
Fig. S19. The binding constant of 1 toward Zn^{2+} using Benesi-Hilderbrand equation on the basis of fluorescence titration.
Fig. S20. The detection limit (\textit{via} 3\textit{σ}/slope) of 1 (20 \textmu{}M) with Zn\textsuperscript{2+} on the basis of fluorescence titrations. \textit{σ} means the average of the standard deviations.
Fig. S21. Bar graphs (at 493 nm) of 1 (20 μM) for detection of Zn$^{2+}$ in the presence of various metal ions.
Fig. S22. UV-vis titrations of 1 (20 μM) in the change of Cd$^{2+}$ concentrations. Inset: Plot of absorbance at 327 nm vs Cd$^{2+}$ concentration.
Fig. S23. Job plot for the binding ratio of 1 (100 μM) toward Cd²⁺ (100 μM).
Fig. S24. Positive-ion ESI-mass spectrum of 1 (100 μM) in the presence of 1 equiv of Cd(NO₃)₂.
Fig. S25. $^1$H NMR titrations of 1 with Cd$^{2+}$ (0, 1, 5 and 10 equiv).
**Fig. S26.** The binding constant of 1 toward Cd\(^{2+}\) using Benesi-Hilderbrand equation on the basis of fluorescence titration.
**Fig. S27.** The detection limit (via 3σ/slope) of 1 (20 μM) with Cd^{2+} on the basis of fluorescence titrations. σ means the average of the standard deviations.
Fig. S28. Bar graphs (at 465 nm) of 1 (20 μM) for detection of Cd$^{2+}$ in the presence of various metal ions.
Fig. S29. (a) The theoretical excitation energies and the experimental UV-vis spectrum of 1. (b) The major electronic transition energy and molecular orbital contributions for 1 (H = HOMO and L = LUMO).
Fig. S30. (a) The theoretical excitation energies and the experimental UV-vis spectrum of 1-Zn<sup>2+</sup>. (b) The major electronic transition energy and molecular orbital contributions for 1-Zn<sup>2+</sup> (H = HOMO and L = LUMO).
Fig. S31. (a) The theoretical excitation energies and the experimental UV-vis spectrum of 1-Cd\(^{2+}\). (b) The major electronic transition energy and molecular orbital contributions for 1-Cd\(^{2+}\) (H = HOMO and L = LUMO).
Fig. S32. MO diagrams and excitation energies of 1, 1-Zn$^{2+}$ and 1-Cd$^{2+}$ by TD-DFT methods.