Supporting Information

Multiple target chemosensor: a fluorescent sensor for Zn(II) and Al(III) and chromogenic sensor for Fe(II) and Fe(III)

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### Table S1. Determination of Zn(II) in Tap water

<table>
<thead>
<tr>
<th>Sample</th>
<th>Zn(II) added (μmol/L)</th>
<th>Zn(II) found (μmol/L)</th>
<th>Recovery (%)</th>
<th>R.S.D. (n = 3) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tap water</td>
<td>0.00</td>
<td>0.00</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>110.00</td>
<td>113.11</td>
<td>102.8</td>
<td>0.8</td>
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</table>

Conditions: [1] = 10 μmol/L in DMF-buffer solution (95:5, v/v, 10 mM, bis-tris, pH 7.0).
Table S2. Determination of Fe(III) in water samples

<table>
<thead>
<tr>
<th>Sample</th>
<th>Fe(III) added (μmol/L)</th>
<th>Fe(III) found (μmol/L)</th>
<th>Recovery (%)</th>
<th>R.S.D. (n = 3) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tap water</td>
<td>0.00</td>
<td>0.00</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>15.00</td>
<td>14.58</td>
<td>97.2</td>
<td>3.1</td>
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<td>Water sample[a]</td>
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<td>0.00</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>15.00</td>
<td>14.52</td>
<td>96.8</td>
<td>1.8</td>
</tr>
</tbody>
</table>

[a] Synthesized by deionized water, 6.00 μmol/L Zn(II), 10 μmol/L Cd(II), Pb(II), Na(I), K(I), Ca(II), Mg(II). Conditions: [I] = 10 μmol/L in 10 mM MeOH-bis-tris buffer solution (9:1, pH 7.0).
Figure S1. (a) UV-vis spectral changes of \( \textbf{1} \) (10 \( \mu \text{M} \)) after addition of zinc ions (0, 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8, and 1.9 equiv) in DMF. Inset: Plot of the UV-vis absorbance at 375 nm as a function of \( \text{Zn}^{2+} \) concentration. (b) UV-vis spectral changes of \( \textbf{1} \) (10 \( \mu \text{M} \)) after addition of aluminium ions (0, 0.4, 0.8, 1.2, 1.6, 2.0, 2.4, 2.8, 3.2, 3.6, 4.0, 4.4 and 5.2 equiv) in DMF. Inset: Plot of the UV-vis absorbance at 400 nm as a function of \( \text{Al}^{3+} \) concentration.
Figure S2. (a) Benesi-Hildebrand equation plot (fluorescence intensity at 448 nm) of 1, assuming 1:1 stoichiometry for association between 1 and Zn$^{2+}$. (b) Benesi-Hildebrand equation plot (fluorescence intensity at 418 nm) of 1, assuming 1:1 stoichiometry for association between 1 and Al$^{3+}$. 
Figure S3. (a) Detection limit of 1 (10 μM) for Zn\(^{2+}\) through change of absorbance intensity (fluorescence intensity at 448 nm). (b) Detection limit of 1 (10 μM) for Al\(^{3+}\) through change of absorbance intensity (fluorescence intensity at 418 nm).
Figure S4. Effect of competitive metal ions (10 μM) on the interaction between 1 (110 μM) and Al$^{3+}$ ion (110 μM) in DMF ($\lambda_{\text{ex}} = 355$ nm and $\lambda_{\text{em}} = 456$ nm).
Figure S5. $^1$H NMR titration of 1 with Al$^{3+}$ in DMF-$d_7$: (a) only 1; (b) 1+Al$^{3+}$ (0.6 equiv); (c) 1+ Al$^{3+}$ (1 equiv).
Figure S6. (a) Positive-ion electrospray ionization mass spectrum of 1 (100 μM) upon addition of 1 equiv of Zn(NO$_3$)$_2$. (b) Positive-ion electrospray ionization mass spectrum of 1 (100 μM) upon addition of 1 equiv of Al(NO$_3$)$_3$. 
Figure S7. Benesi-Hildebrand equation plot (fluorescence intensity at 446 nm) of 1, assuming 1:1 stoichiometry for association between 1 and Zn$^{2+}$. 

The equation of the line is:

\[ y = 3 \times 10^{-7}x + 0.0023 \]

\[ R^2 = 0.9832 \]

\[ K = 7.7 \times 10^3 \]
Figure S8. Detection limit of 1 (10 μM) for Zn$^{2+}$ through change of fluorescence intensity (fluorescence intensity at 446 nm).
Figure S9. Effect of competitive metal ions (12 equiv) on the interaction between 1 (10 µM) and Zn$^{2+}$ ion (120 µM) in DMF-buffer solution (95:5, v/v, 10 mM, bis-tris, pH 7.0) ($\lambda_{ex} = 355$ nm and $\lambda_{em} = 456$ nm).
**Figure S10.** Fluorescence spectra of sensor 1 in the presence of Zn$^{2+}$ ion and EDTA in DMF-buffer solution (95:5, v/v, 10 mM, bis-tris, pH 7.0). $\lambda_{\text{ex}}$ = 355 nm and $\lambda_{\text{em}}$ = 456 nm.
Figure S11. Fluorescence intensity (at 446 nm) of 1 as a function of Zn(II) concentration. [I] = 10 μM, [Zn(II)] = 0-120.00 μM; Conditions: the sample was conducted in DMF-buffer solution (95:5, v/v, 10 mM, bis-tris, pH 7.0). $\lambda_{ex} = 355$ nm and $\lambda_{em} = 456$ nm.
Figure S12. (a) UV-vis titration of 1 (10 μM) with Zn$^{2+}$ (0-1.9 equiv) in MeOH-buffer solution (9:1, v/v, 10 mM, bis-tris, pH 7.0). (b) UV-vis titration of 1 (10 μM) with Al$^{3+}$ (0-1.2 equiv) in MeOH-buffer solution (9:1, v/v, 10 mM, bis-tris, pH 7.0).
Figure S13. (a) Job plot of 1 and Fe$^{2+}$ in MeOH-buffer solution (9:1, v/v, 10 mM, bis-tris, pH 7.0). The total concentration of 1 and Fe$^{2+}$ was 40 μM (absorbance at 461 nm). (a) Job plot of 1 and Fe$^{3+}$ in MeOH-buffer solution (9:1, v/v, 10 mM, bis-tris, pH 7.0). The total concentration of 1 and Fe$^{3+}$ was 40 μM (absorbance at 450 nm).
Figure S14. (a) Positive-ion electrospray ionization mass spectrum of 1 (100 μM) upon addition of 1 equiv of Fe(NO$_3$)$_3$. (b) Positive-ion electrospray ionization mass spectrum of 1 (100 μM) upon addition of 1 equiv of Fe(ClO$_4$)$_2$. 
Figure S15. (a) Benesi-Hildebrand plot (absorbance at 457 nm) of 1, assuming 1:1 stoichiometry for association between 1 and Fe$^{2+}$. (b) Benesi-Hildebrand plot (absorbance at 457 nm) of 1, assuming 1:1 stoichiometry for association between 1 and Fe$^{3+}$. 
Figure S16. (a) Detection limit of $1$ ($10 \, \mu\text{M}$) for Fe$^{2+}$ through change of absorption intensity (absorbance at 457 nm). (b) Detection limit of $1$ ($10 \, \mu\text{M}$) for Fe$^{3+}$ through change of absorption intensity (absorbance at 457 nm).
Figure S17. UV-vis spectra (at 457 nm) of 1 as a function of Fe(III) concentration. [1] = 10 μM, [Fe(III)] = 0-15.00 μM; Conditions: the sample was conducted in MeOH-buffer solution (9:1, v/v, 10 mM, bis-tris, pH 7.0).