Supporting Information

A fluorescence “turn-on” chemosensor for Hg\(^{2+}\) and Ag\(^{+}\) based on NBD (7-nitrobenzo-2-oxa-1,3-diazolyl)

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Table S1. Examples of chemosensors for simultaneous detection of Hg$^{2+}$ and Ag$^+$. 

<table>
<thead>
<tr>
<th>Sensor</th>
<th>Detection limit (Hg$^{2+}$/Ag$^+$, μM)</th>
<th>Binding constant (Hg$^{2+}$/Ag$^+$, M$^{-1}$)</th>
<th>Percent of water in solution (%)</th>
<th>Method of detection (Hg$^{2+}$/Ag$^+$)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Chemical structure 1" /></td>
<td>0.29 / 0.4</td>
<td>2.3 x 10$^5$ / 5.1 x 10$^7$</td>
<td>50</td>
<td>Fluorescence</td>
<td>1</td>
</tr>
<tr>
<td><img src="image2" alt="Chemical structure 2" /></td>
<td>140 / 650</td>
<td>No data</td>
<td>15</td>
<td>Fluorescence, Colorimetric</td>
<td>2</td>
</tr>
<tr>
<td><img src="image3" alt="Chemical structure 3" /></td>
<td>0.21 / 0.009</td>
<td>2.2 x 10$^5$ / No data</td>
<td>40</td>
<td>Fluorescence</td>
<td>3</td>
</tr>
<tr>
<td><img src="image4" alt="Chemical structure 4" /></td>
<td>0.25 / No data</td>
<td>7.4 x 10$^7$ / No data</td>
<td>80</td>
<td>Fluorescence</td>
<td>4</td>
</tr>
<tr>
<td><img src="image5" alt="Chemical structure 5" /></td>
<td>No data</td>
<td>1.0 x 10$^5$ / 4.1 x 10$^6$</td>
<td>0.5</td>
<td>Fluorescence</td>
<td>5</td>
</tr>
<tr>
<td><img src="image6" alt="Chemical structure 6" /></td>
<td>0.37 / 0.34</td>
<td>2.6 x 10$^3$ / No data</td>
<td>67</td>
<td>Fluorescence</td>
<td>6</td>
</tr>
<tr>
<td><img src="image7" alt="Chemical structure 7" /></td>
<td>0.19 / 0.59</td>
<td>1.0 x 10$^7$ / 9.4 x 10$^7$</td>
<td>10</td>
<td>Fluorescence</td>
<td>7</td>
</tr>
<tr>
<td><img src="image8" alt="Chemical structure 8" /></td>
<td>0.13 / No data</td>
<td>3.1 x 10$^7$ / 1.2 x 10$^9$</td>
<td>50</td>
<td>Fluorescence, Colorimetric</td>
<td>8</td>
</tr>
<tr>
<td><img src="image9" alt="Chemical structure 9" /></td>
<td>0.05 / 0.12</td>
<td>5.0 x 10$^7$ / 3.5 x 10$^9$</td>
<td>70</td>
<td>Fluorescence</td>
<td>This work</td>
</tr>
</tbody>
</table>

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References
Fig. S1 $^1$H NMR spectrum of 2.
Fig. S2 $^1$H NMR spectrum of 1.
Fig. S3 \(^{13}\text{C}\) NMR spectrum of 1.
Fig. S4 Job plot of 1 and Hg$^{2+}$. The total concentrations of 1 and Hg$^{2+}$ were 20 μM.
**Fig. S5** $^1$H NMR titration of 1 with Hg$^{2+}$ ions.
**Fig. S6** Benesi-Hildebrand plot (at 520 nm) of 1 based on fluorescence titration, assuming 1:1 stoichiometry for association between 1 and Hg$^{2+}$. 

\[ y = 8 \times 10^{-9}x + 0.0004 \]

\[ R^2 = 0.9976 \]

\[ K = 5.0 \times 10^4 \]
Fig. S7 Determination of the detection limit based on change in the ratio of 1 (5 μM) with Hg$^{2+}$.

\[ y = 97.179x + 41.19 \]
\[ R^2 = 0.9998 \]
\[ \text{LOD} = 0.05 \text{ μM} \]
Fig. S8 Fluorescence intensities (520 nm) of 1 (5 μM) and 1-Hg\(^{2+}\) complex, respectively, at pH 2-12 in a mixture of buffer-CH\(_3\)CN (7:3, v/v) at room temperature.
Fig. S9 Absorption spectral changes of 1 (5 μM) in the presence of different concentrations of Ag⁺ ions in a mixture of buffer-CH₂CN (7:3, v/v) at room temperature.
Fig. S10 Job plot of 1 and Ag⁺. The total concentrations of 1 and Ag⁺ were 20 μM.
Fig. S11 Positive-ion electrospray ionization mass spectrum of 1 (10 μM) upon addition of AgNO₃ (1.0 equiv).
Fig. S12 $^1$H NMR titration of 1 with Ag$^+$ ions.
Fig. S13 Benesi-Hildebrand plot (at 520 nm) of 1 based on fluorescence titration, assuming 1:1 stoichiometry for association between 1 and Ag\(^+\).
Fig. S14 Determination of the detection limit based on change in the ratio of 1 (5 μM) with Ag$^+$. 

\[
y = 51.636x + 31.985 \\
R^2 = 0.9996 \\
LOD = 0.12 \mu M
\]
Fig. S15 Competitive selectivity of 1 (5 μM) toward Ag⁺ (2.6 equiv) in the presence of other metal ions (2.6 equiv).
Fig. S16 Fluorescence intensities (520 nm) of 1 (5 μM) and 1-Ag$^+$ complex, respectively, at pH 2-12 in a mixture of buffer-CH$_3$CN (7:3, v/v) at room temperature.
Fig. S17 Fluorescence spectral changes of 1 (5 µM) after the sequential addition of (a) Ag⁺ and Cl⁻, and (b) Hg²⁺ and Cl⁻.
**Fig. S18** Emission intensity (520 nm) of 1 as a function of Ag$^+$ concentration. [1] = 5 μmol/L and [Ag$^+$] = 0.0-12.0 μmol/L in buffer-CH$_3$CN mixture (7:3, v/v).
Fig. S19 (a) The theoretical excitation energies and the experimental UV-vis spectrum of 1.
(b) The major electronic transition energies and molecular orbital contributions for 1 (H = HOMO and L = LUMO).
(a) The theoretical excitation energies and the experimental UV-vis spectrum of 1-Hg\(^{2+}\). (b) The major electronic transition energies and molecular orbital contributions for 1-Hg\(^{2+}\) (H = HOMO and L = LUMO).

<table>
<thead>
<tr>
<th>Excited state 3</th>
<th>Wavelength (nm)</th>
<th>Percent (%)</th>
<th>Main character</th>
<th>Oscillator strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>H → L + 2</td>
<td>337.73</td>
<td>83</td>
<td>Inhibited PET, (\pi \rightarrow \pi^*)</td>
<td>0.5289</td>
</tr>
</tbody>
</table>
Fig. S21 Molecular orbital diagrams and excitation energies of 1 and 1-Hg$^{2+}$ complex.
Fig. S22 (a) The theoretical excitation energies and the experimental UV-vis spectrum of 1-Ag⁺. (b) The major electronic transition energies and molecular orbital contributions for 1-Ag⁺ (H = HOMO and L = LUMO).
Fig. S23 Molecular orbital diagrams and excitation energies of 1 and 1-Ag⁺ complex.