Supporting Information

Chemosensor for micro to nano-molar detection of Ag$^+$ and Hg$^{2+}$ ions in pure aqueous media and its applications in cell imaging

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Figure S-3: $^{13}$C-NMR spectrum of sensor PTB-1

Figure S-4: HRMS spectrum of sensor PTB-1.
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Figure S-6: Linear fitting curve for LOD and LOQ determination of PTB-1 for Ag$^+$.

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**Figure S-11:** Mole ratio plot/change in emission spectra ($\Delta F$) as a function of concentration of Hg$^{2+}$ ion.
Figure S-12: Mass spectrum of PTB-1 in the presence of Hg$^{2+}$.

Figure S-13: Benesi-Hildebrand plot of $1/\Delta F$ against $1/[\text{Hg}^{2+}]$. 

$y = -3\times 10^{-11}x + 3\times 10^{-6}$

$R^2 = 0.9905$
Figure S14: Plots of the fluorescence intensity of PTB-1 vs. the increasing concentration of (A) Hg$^{2+}$ and (B) Ag$^+)$. 

![Figure S14](image1.png)

Figure S15: Selectivity and reversibility measurement of PTB-1 to Hg$^{2+}$ and Ag$^+)$. Changes in fluorescence emission intensity of PTB-1 [2 mL, 4 x 10$^{-5}$ M, in CH$_3$OH:H$_2$O (20:80, v/v)] upon the sequential addition of (A, B) Hg$^{2+}$ and EDTA; (C, D) Ag$^+$ and EDTA at $\lambda_{ex} = 290$ nm. 

![Figure S15](image2.png)
**Figure S16:** The DFT computed molecular structure of PTB-1 and its PTB-1.\((\text{Ag}^+)_2\) and \((\text{PTB-1})_2.\text{Hg}^{2+}\) complexes.

**Figure S-17:** Partial \(^1\text{H}\) NMR spectra (aromatic region) of receptor PTB-1 (a), PTB-1 in the presence of 0.25 equiv. \(\text{HgCl}_2\) (b), 0.5 equiv. \(\text{HgCl}_2\) (c) and 1.0 equiv. \(\text{HgCl}_2\) (d) taken in CDCl\(_3\).
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Figure S-19: FT-IR overlap spectra of PTB-1 (blue color) and PTB-1+Hg$^{2+}$ complex (green color).
**Figure 20:** Photographs of PTB-1 loaded test strips with varying concentration of Ag⁺

A = PTB-1 (1x10⁻² M) loaded test strip and [Ag⁺]: B = 1 x 10⁻⁴ M, C = 5 x 10⁻⁵ M, D = 1 x 10⁻⁵ M, E = 5 x 10⁻⁶ M, F = 1 x 10⁻⁶ M.

**Figure S21:** Fluorescence stability of PTB-1 [(2 mL, 4 x 10⁻⁵ M) in CH₃OH:H₂O (20:80, v/v)] upon 0 - 3 h. λₓₑₓ = 290 nm, λₑₘₑ = 420 nm. The data were shown as mean (± s.d.) (n = 7).
Figure S22: MTT assay of HepG2 cells with different concentrations of PTB-1. The data were shown as mean (± s.d.) (n = 7).

Figure S-23: Hydrogen-bonded centrosymmetric dimers in the structure of PTB-1.
Table S-1 Comparison of PTB-1 with previously reported sensors.

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<th>Research Group</th>
<th>Selectivity for</th>
<th>Solvent for analysis</th>
<th>Detection limit</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>Patil, U.D. et. al.</td>
<td>Ag(^+) and Hg(^{2+})</td>
<td>Methanol:water (20:80)</td>
<td>For Ag(^+): 3.67 x 10(^{-6}) M</td>
<td>Cell Imaging, Paper Strips, Supported Silica</td>
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<tr>
<td>Fu, Y. et. al.</td>
<td>Only Ag(^+)</td>
<td>THF:water (80:20)</td>
<td>2.92 x 10(^{-7}) M and 6.5 x 10(^{-7}) M</td>
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<tr>
<td>Hatai, J. et. al.</td>
<td>Only Hg(^{2+})</td>
<td>Methanol:water (80:20)</td>
<td>1.03 x 10(^{-7}) M</td>
<td>--</td>
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<tr>
<td>Hatai, J. et. al.</td>
<td>Only Ag(^+)</td>
<td>DMSO:water (1:99)</td>
<td>1.0 x 10(^{-7}) M</td>
<td>Cell Imaging, Paper Strips</td>
</tr>
<tr>
<td>Hu, Z.Q. et. al.</td>
<td>Only Hg(^{2+})</td>
<td>Ethanol:water (11:89)</td>
<td>4.2 x 10(^{-8}) M</td>
<td>Cell Imaging</td>
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<tr>
<td>Mahapatra, A.K. et. al.</td>
<td>Only Hg(^{2+})</td>
<td>Acetonitrile:water (20:80)</td>
<td>4.0 x 10(^{-7}) M</td>
<td>Cell Imaging</td>
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<tr>
<td>Tang, B. et. al.</td>
<td>Only Hg(^{2+})</td>
<td>Acetonitrile</td>
<td>1.39 x 10(^{-8}) M</td>
<td>Cell Imaging</td>
</tr>
<tr>
<td>Vedamalai, M. et. al.</td>
<td>Only Hg(^{2+})</td>
<td>Acetonitrile:water (90:10)</td>
<td>0.226 x 10(^{-6}) M</td>
<td>Cell Imaging</td>
</tr>
<tr>
<td>Wang, Y. et. al.</td>
<td>Only Ag(^+)</td>
<td>Ethanol:water (10:90)</td>
<td>2.79 x 10(^{-7}) M</td>
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<tr>
<td>Xiang, G. et. al.</td>
<td>Only Ag(^+)</td>
<td>THF</td>
<td>5 x 10(^{-8}) M</td>
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<tr>
<td>Ye, J.H. et. al.</td>
<td>Only Ag(^+)</td>
<td>THF:water (33:66)</td>
<td>0.2 x 10(^{-6}) M</td>
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<tr>
<td>Zhang, D. et. al.</td>
<td>Only Hg(^{2+})</td>
<td>Ethanol:water (50:50)</td>
<td>0.067 x 10(^{-6}) M</td>
<td>Cell Imaging</td>
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<tr>
<td>Zheng, H. et. al.</td>
<td>Only Ag(^+)</td>
<td>Methanol:water (20:80)</td>
<td>34 x 10(^{-9}) M</td>
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</tr>
</tbody>
</table>

References