Supplementary Material

A terpyridine-based test strip for detection of Hg2+ in various water samples and drinks

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EXPERIMENTAL SECTION

Materials and instruments

All chemical regents and solvents, unless otherwise noted, were purchased from commercial suppliers and used as received without further purification. Aqueous solutions (1.0×10^{-2} M) of Hg^{2+} was prepared from its bromate salt, and the other metal ions were prepared from their nitrate salts, an aqueous solution of TPI (1.0×10^{-5} M) was prepared (1% DMSO served as co-solvent), respectively. \textsuperscript{1}H NMR spectra (400 MHz, 600 MHz) and \textsuperscript{13}C NMR spectra (100 MHz) were recorded on Bruker Avance with deuterated acetone, DMSO, chloroform or methyl alcohol solvent, and tetramethylsilane (TMS) as the internal standard, respectively. All coupling constants (\(J\)) are given in Hz, \(\delta\) values are reported in parts per million. Mass spectra were obtained on a Thermo Fisher Scientific LTO-Orbitrap mass spectrometer. IR spectra were collected on Nicolet FT-IR NEXUS 870 spectrometer by KBr pellet method, in the region of 4000-400 cm^{-1}. Ultraviolet-visible (UV-vis) spectra were taken on a UV-265 spectrophotometer. Fluorescence spectra were recorded on a Hitachi F-7000 fluorescence spectrophotometer.

\textbf{Fig. S1.} \textsuperscript{1}H NMR (400MHz) spectrum of M1 (in Acetone-\textit{d}_6)
**Fig. S2.** $^{13}$C NMR (100 MHz) spectrum of M1 (in Acetone -$d_6$)

**Fig. S3.** ESI-Mass spectrum of M1
Fig. S4. FT-IR of M1 in KBr

Fig. S5. $^1$H NMR (400MHz) spectrum of TPI (in DMSO-$d_6$)
Fig. S6. $^{13}$C NMR (100MHz) spectrum of TPI (in DMSO-$d_6$)

Fig. S7. ESI-Mass spectrum of TPI
**Fig. S8.** FT-IR of TPI in KBr

![FT-IR spectrum of TPI in KBr](image)

**Fig. S9.** The table of total energy (E) and binding energy (E)

<table>
<thead>
<tr>
<th></th>
<th>Binding Energy(E)</th>
<th>Total Energy(E)</th>
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<tbody>
<tr>
<td>Hg(NO₃)₂</td>
<td>(-15.5358)</td>
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<tr>
<td>Zn(NO₃)₂</td>
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<tr>
<td>Cd(NO₃)₂</td>
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<td>Cu(NO₃)₂</td>
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<tr>
<td>AgNO₃</td>
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<tr>
<td><strong>TPI</strong></td>
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</table>

*Note: The last row indicates the binding energy (E) for TPI, which is significantly lower than the other metal nitrate complexes.*

**Fig. S9.** Wavelength absorbance for different metal ions.
Fig. S10. Absorbance spectra of TPI (10 µM) in aqueous medium upon addition of 1.0 equiv. of different metal ions.

Fig. S11. Calibration curve of TPI-Hg$^{2+}$

Fig. S12. Job’s plot of the complexation between the probe TPI and Hg$^{2+}$. 
Fig. S13. ESI-Mass spectrum of $\text{TPI}^+\text{[HgBr]}^+$

Fig. S14. Absorbance spectra of TPI (10 µM) in CHCl$_3$ upon addition of 1.0 equiv. of Hg$^{2+}$. 
**Fig. S15.** Fluorescence spectra of TPI (10 µM) in CHCl₃ upon addition of 1.0 equiv. of Hg²⁺. Inset: color of TPI and TPI-Hg²⁺ under UV lamp at 365 nm.