Supplementary Material

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

Junjun Wang, Qingpeng Rao, Haiyan Wang, Qiong Zhang, Gang Liu, Zhichao Wu, Jianhua Yu, Xiaojiao Zhu*, Yupeng Tian, Hongping Zhou*

College of Chemistry and Chemical Engineering, Anhui University and Key Laboratory of Functional Inorganic Materials Chemistry of Anhui Province, Anhui Province Key Laboratory of Chemistry for Inorganic/Organic Hybrid Functionalized Materials, 230601, Hefei, PR China.

Corresponding author Fax: +86-551-63861279; Tel: +86-551-63861279

E-mail: zhpzhp@263.net, xiaojzhu@ahu.edu.cn.

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. ^{1}H NMR spectra (400 MHz, 600 MHz) and ^{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, δ 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.

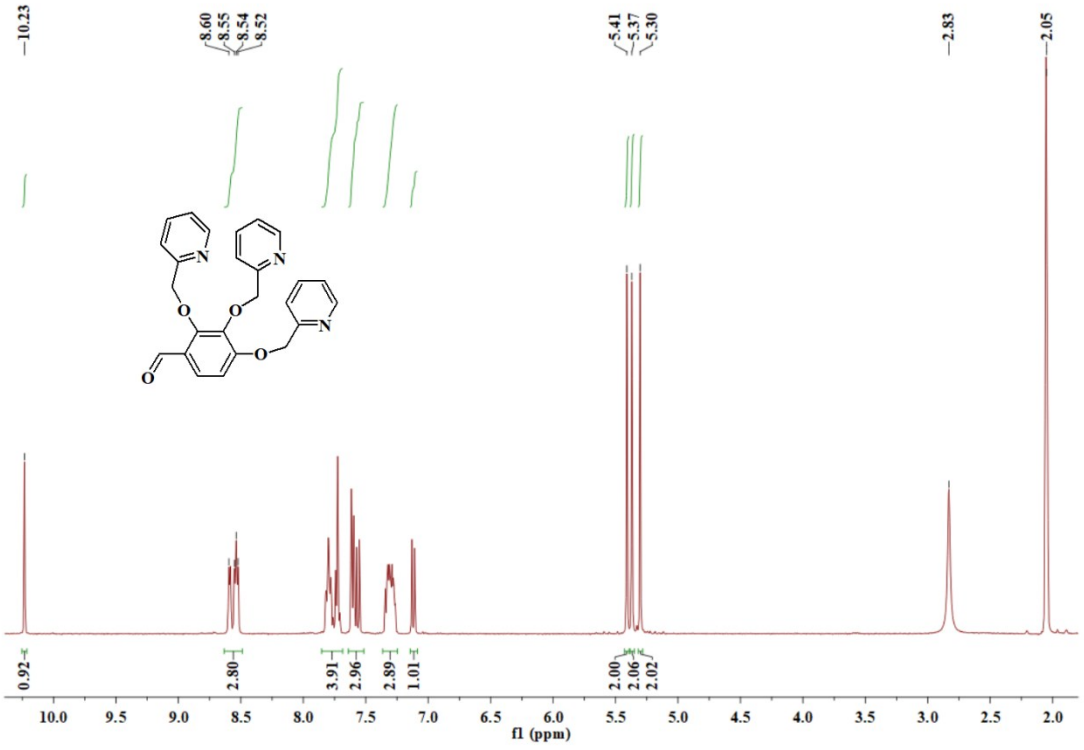

Fig. S1. ^{1}H NMR (400MHz) spectrum of **M1 (**in Acetone-d_6 **)**

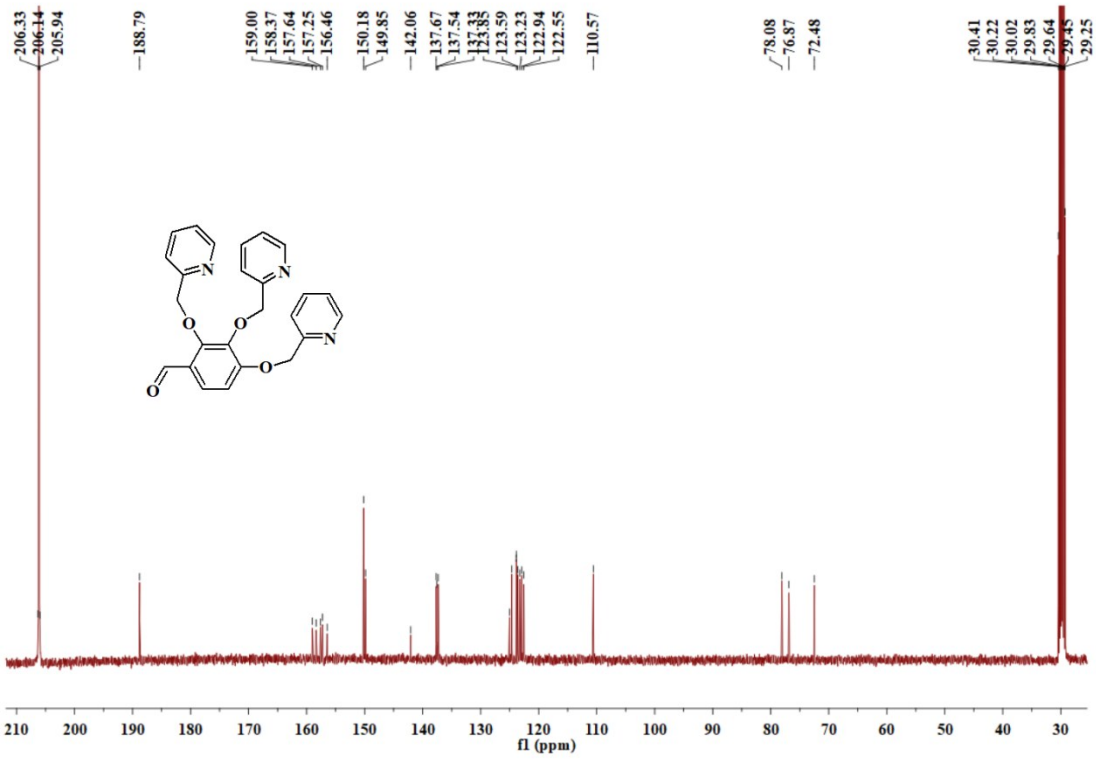

Fig. S2. ^{13}C NMR (100 MHz) spectrum of **M1 (**in Acetone -d_6**)**

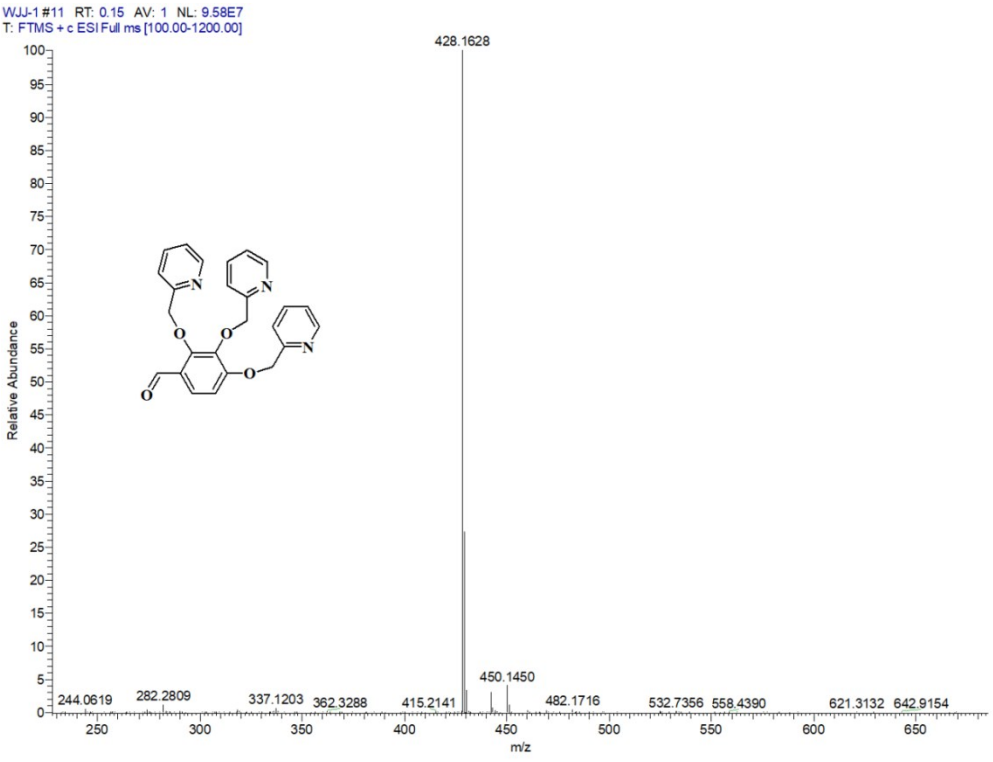

Fig. S3. ESI-Mass spectrum of **M1**

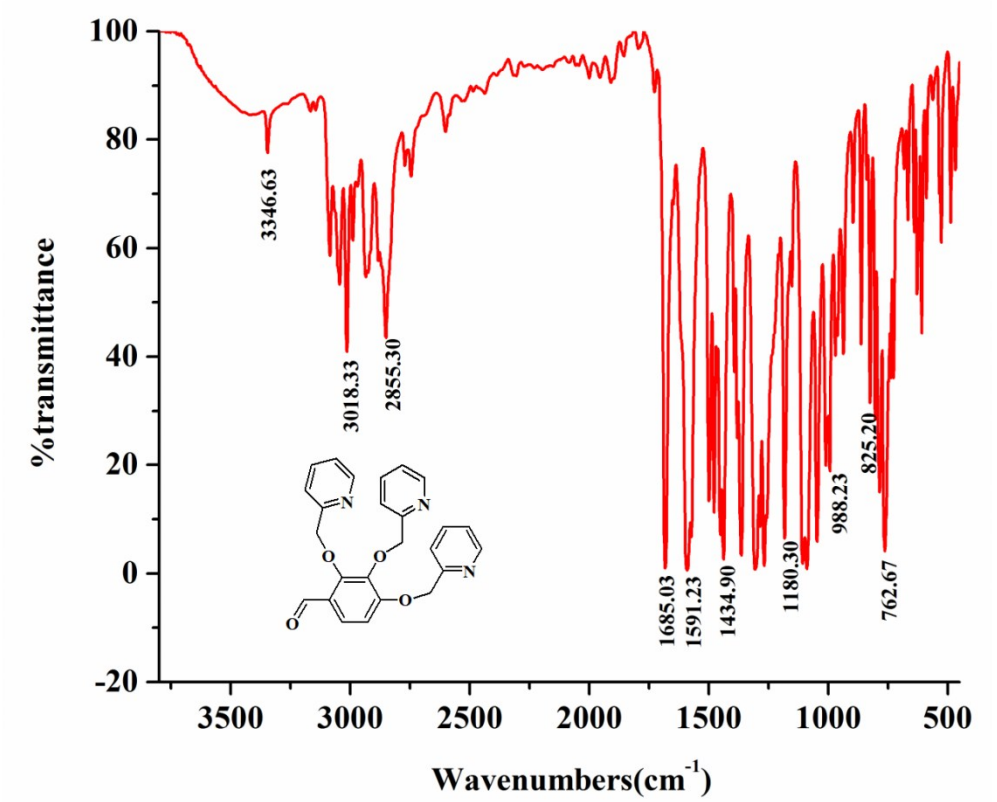

Fig. S4. FT-IR of **M1** in KBr

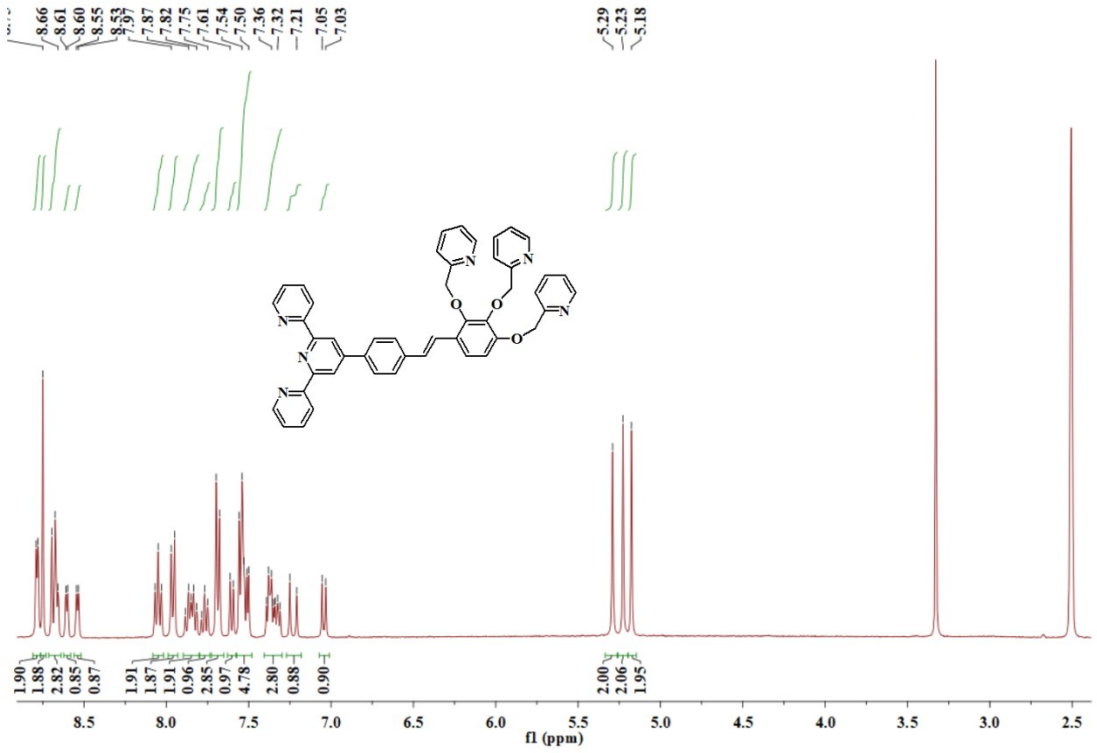

Fig. S5. ^{1}H NMR (400MHz) spectrum of **TPI (**in DMSO-d_6 **)**

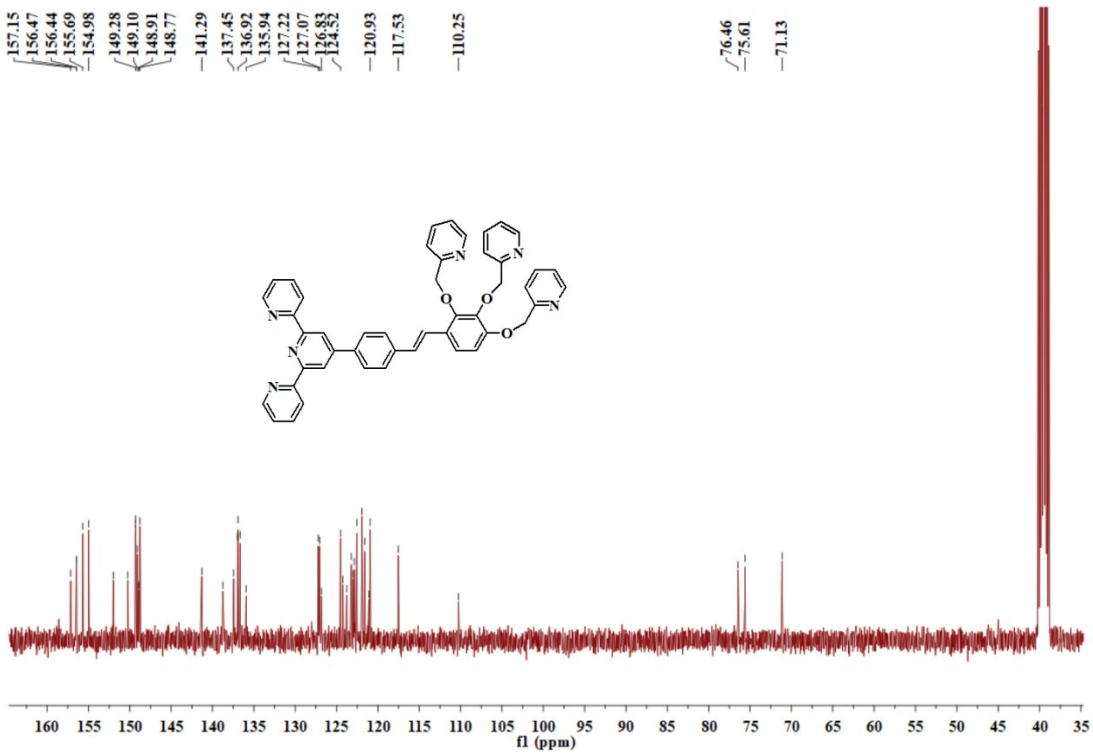

Fig. S6. ^{13}C NMR (100MHz) spectrum of **TPI (**in DMSO-d_6 **)**

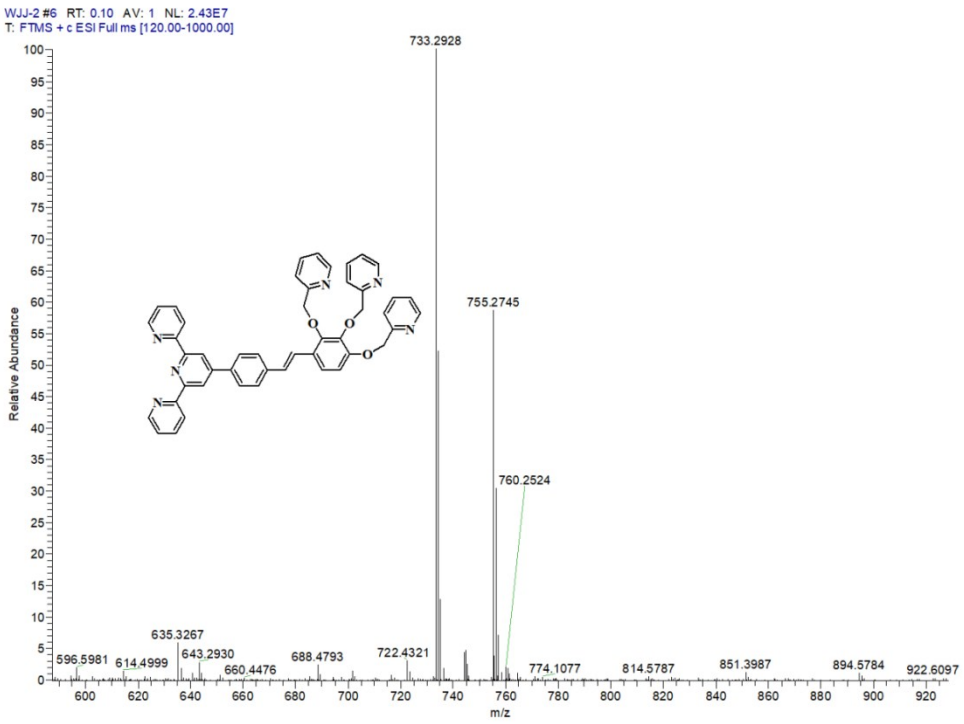

Fig. S7. ESI-Mass spectrum of **TPI**

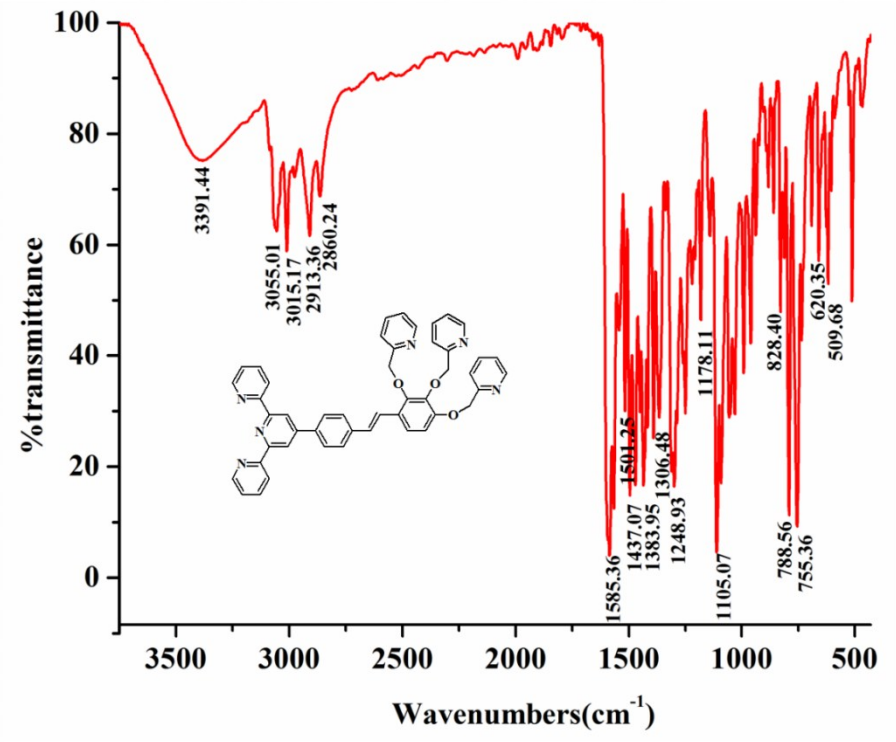

Fig. S8. FT-IR of **TPI** in KBr

Binding Energy(E) / Total Energy(E)	$Hg(NO_3)_2$ (-15.5358)	$Zn(NO_3)_2$ (-46.5682)	$Cd(NO_3)_2$ (-45.2850)	$Cu(NO_3)_2$ (-46.2897)	$AgNO_3$ (5.4899)
TPI (-2365.3105)	-2349.7747	-2318.7432	-2320.0255	-2319.0208	×

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

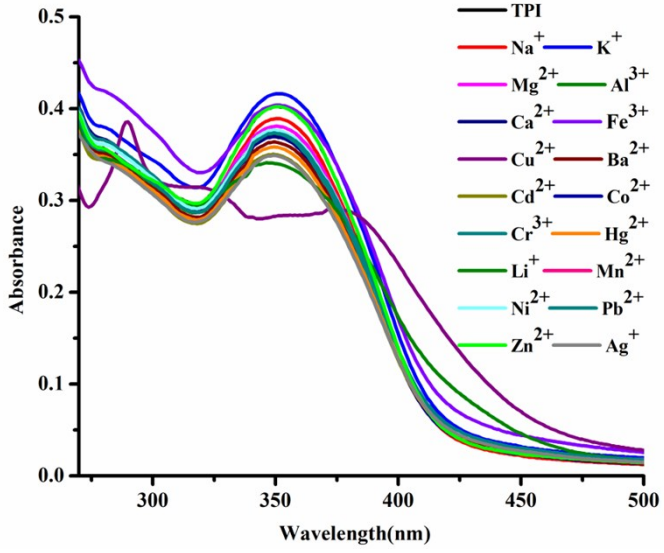

Fig. S10. Absorbance spectra of **TPI** (10 μM) in aqueous medium upon addition of 1.0 equiv. of different metal ions.

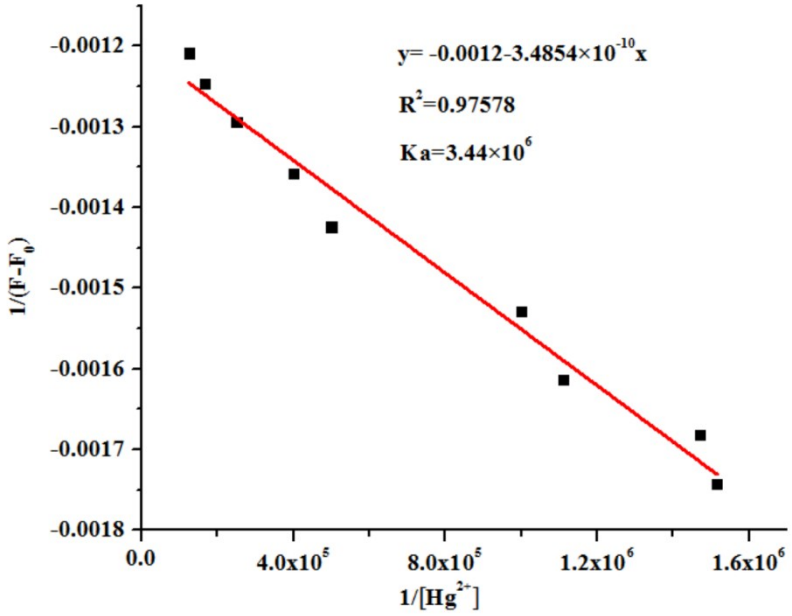

Fig. S11. Calibration curve of **TPI-Hg^{2+}**

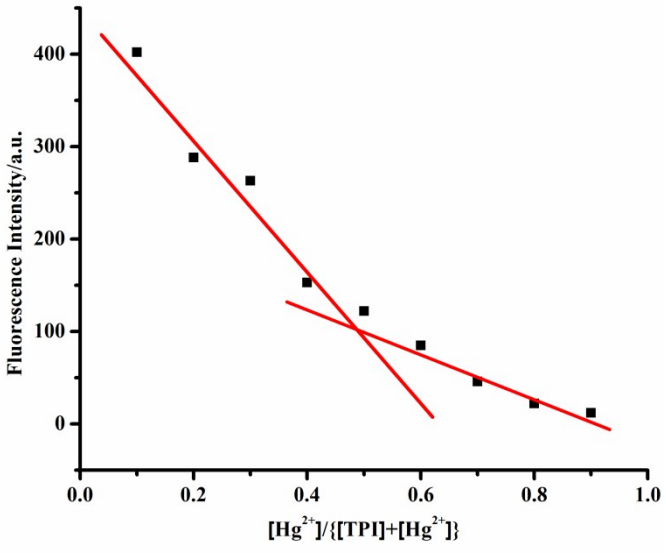

Fig. S12. Job's plot of the complexation between the probe **TPI** and Hg^{2+}.

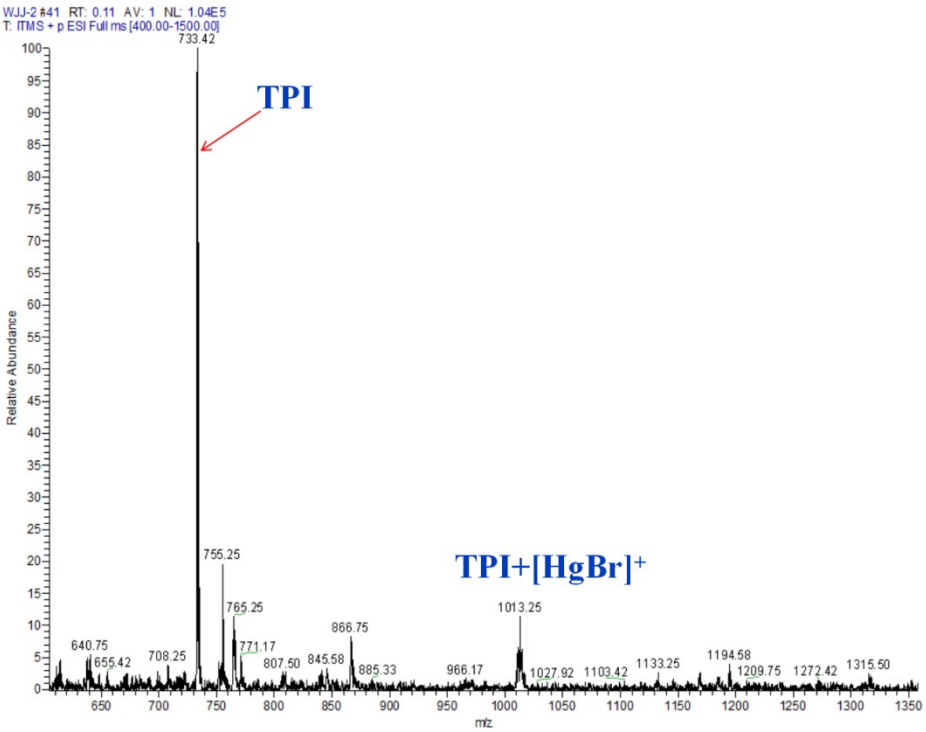

Fig. S13. ESI-Mass spectrum of **TPI**+[**HgBr**]$^{+}$

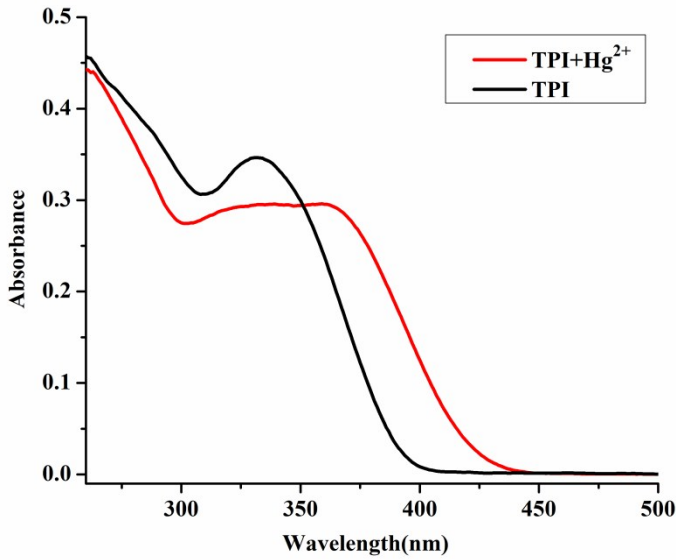

Fig. S14. Absorbance spectra of **TPI** (10 μM) in $CHCl_3$ upon addition of 1.0 equiv. of Hg^{2+}.

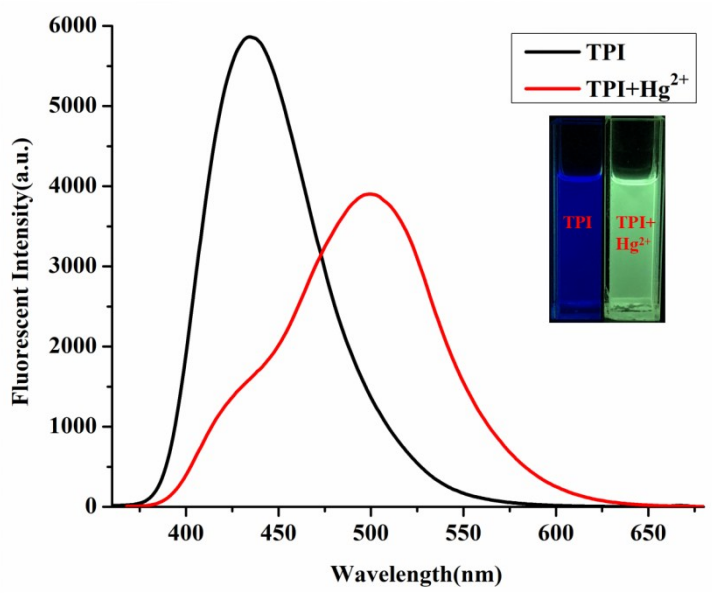

Fig. S15. Fluorescence spectra of **TPI** (10 μM) in $CHCl_3$ upon addition of 1.0 equiv. of Hg^{2+}.Inset: color of **TPI** and **TPI-Hg^{2+}** under UV lamp at 365 nm.