Electronic Supplementary Material (ESI) for RSC Advances

Electronic Supporting information:

Development of Pyrene based "Turn On" Fluorescent Chemosensor for Hg^{2+}

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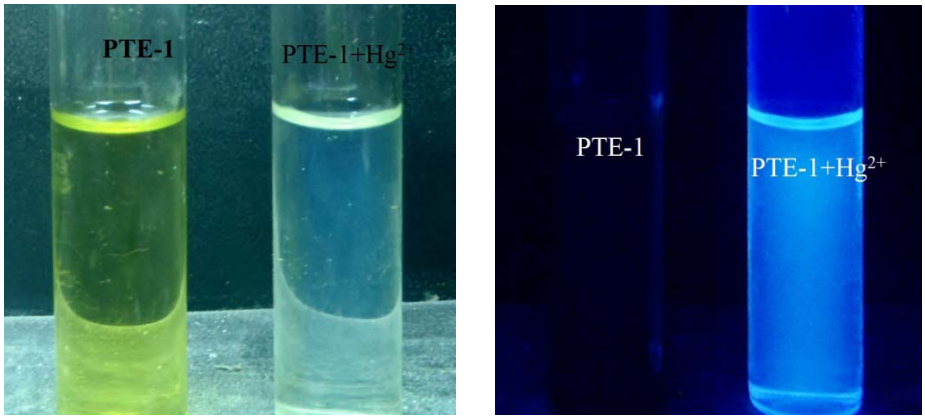

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Fig-S1: ^{1}H-NMR spectrum of PTE-1 .

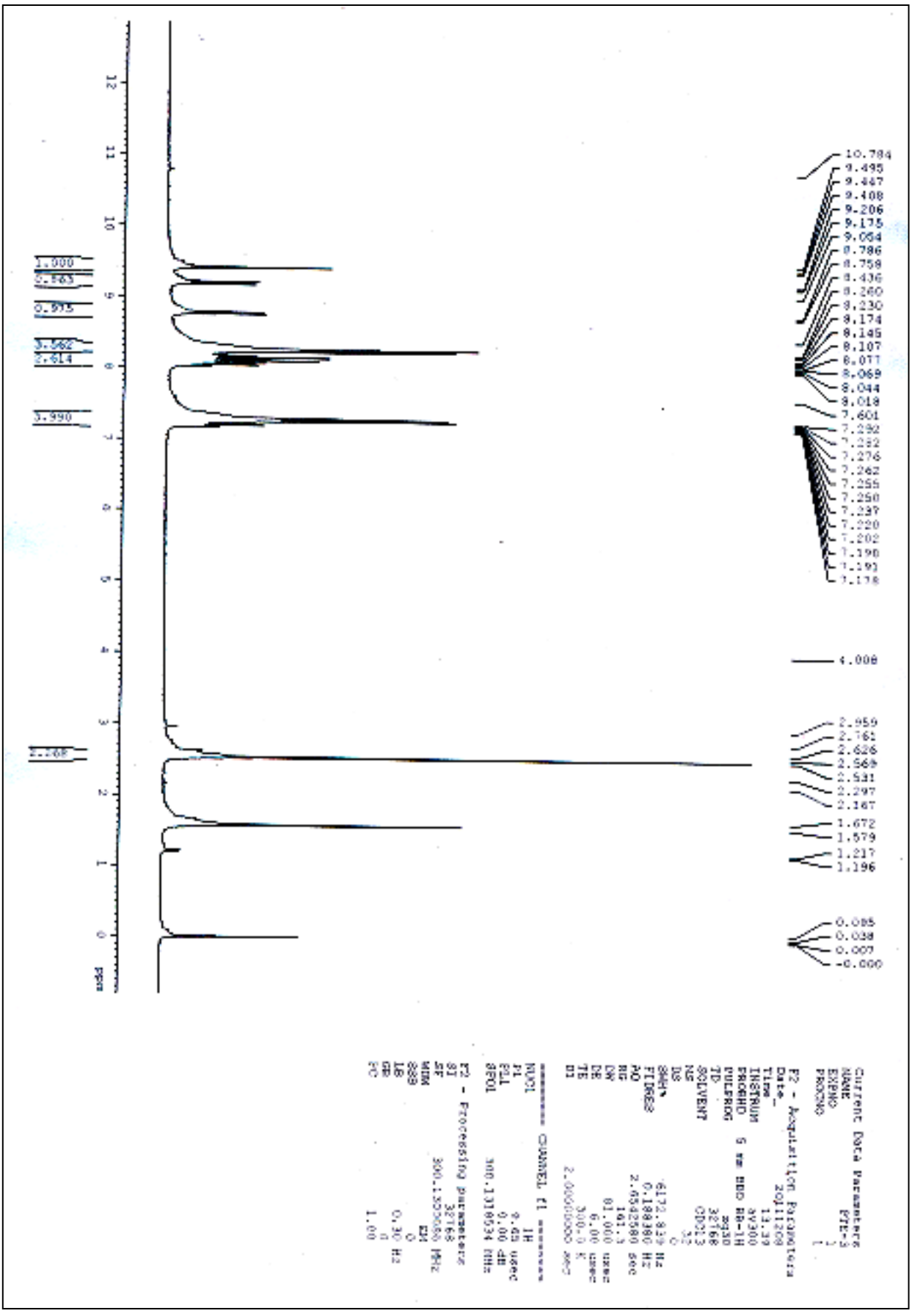


Fig-S2: ^{13}C-NMR spectrum of PTE-1 .

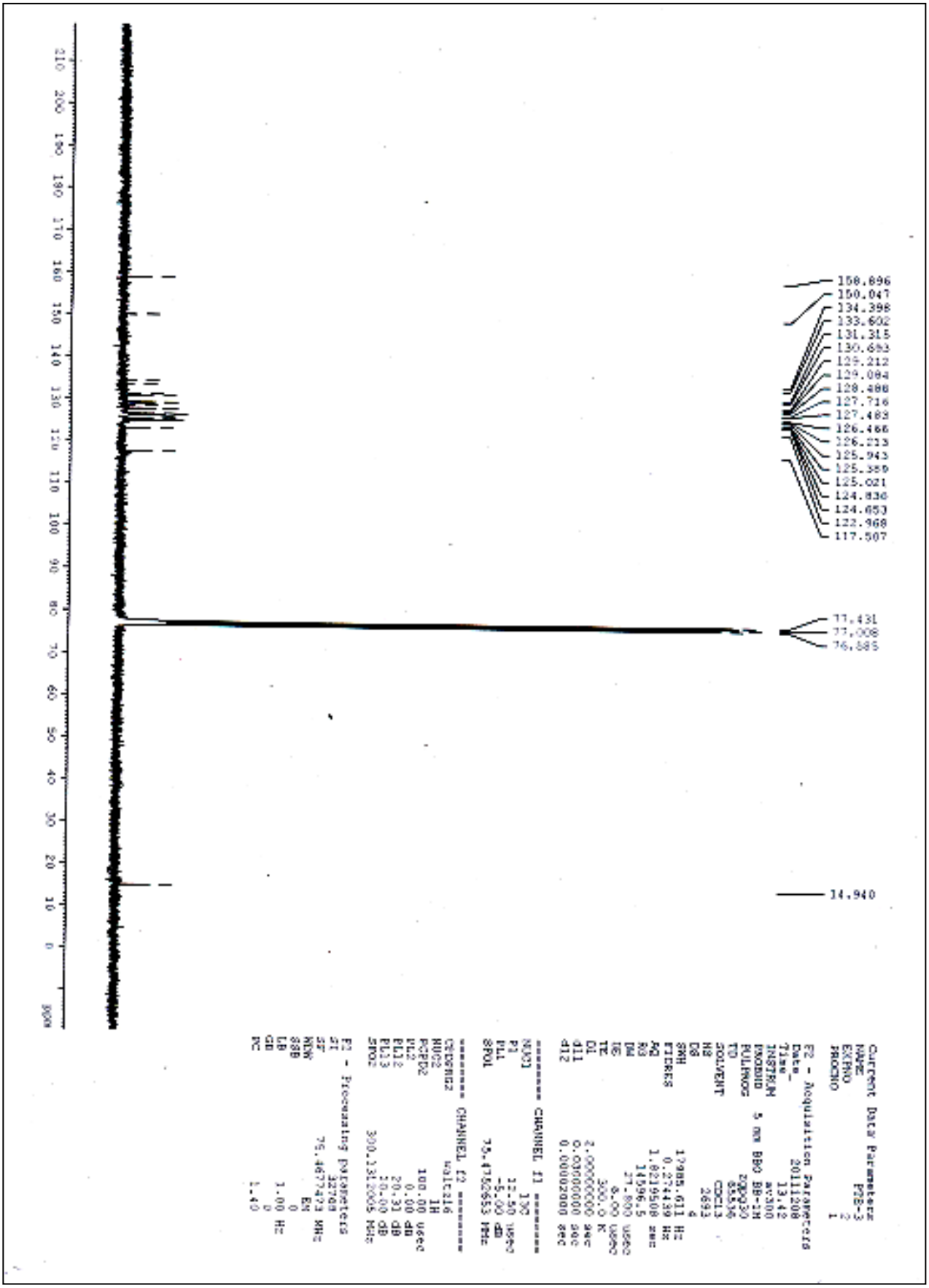


Fig-S 3: ESI-MS spectrum of PTE-1

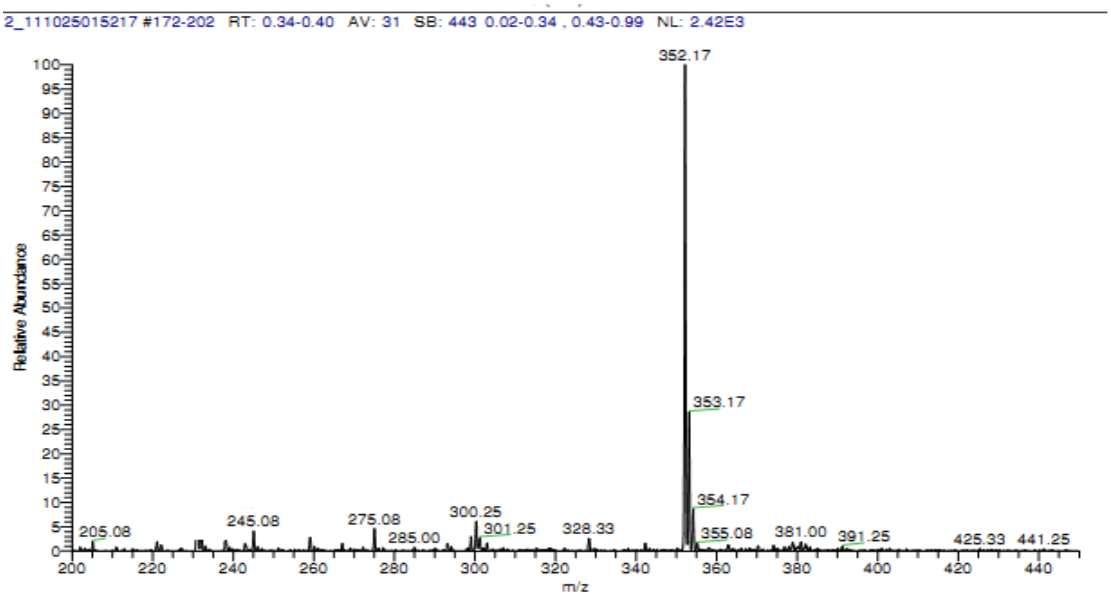


Fig-4: The absorption spectrum with several metal cations (Na^{+}, K^{+}, Ca^{2+}, Mn^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Cd^{2+}, Hg^{2+}, Pb^{2+}, and Sn^{2+}) using their chloride salts in H_2O-CH_3CN (30:70,v/v). Inset selected wavelength to show the changes.

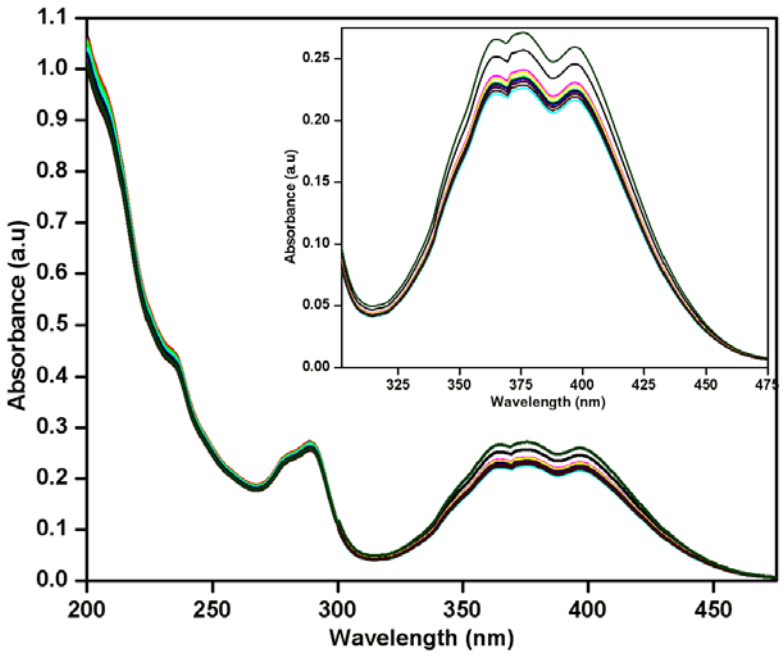


Fig-S5: Fluorescence response of 1 µM PTE-1 to various metal ions. Bars represent the final (F_f) over the initial (Fi) integrated emission. The red bars represent the addition of the corresponding metal ion to PTE-1. The blue bars represent the change of the emission that occurs upon the subsequent addition of Hg^{2+} to the above solution. Excitation at 340 nm, emission integrated over 380-560 nm (slit width = 5 nm).

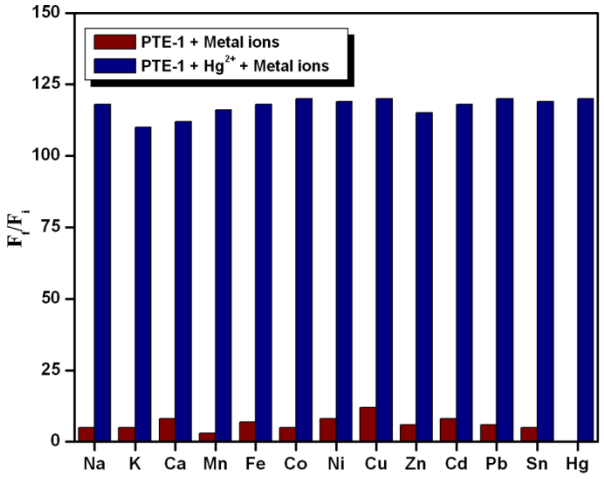


Fig-S6: Fluorescence response of PTE-1 + Hg^{2+} on addition with sodium Sulfide

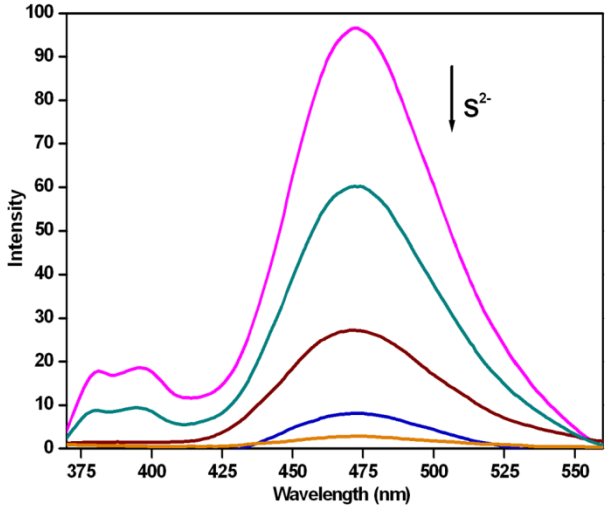


Fig-S7: Dependence of the intensity ratio of emission at 472 nm (F_f/F_i) on Hg^{2+}

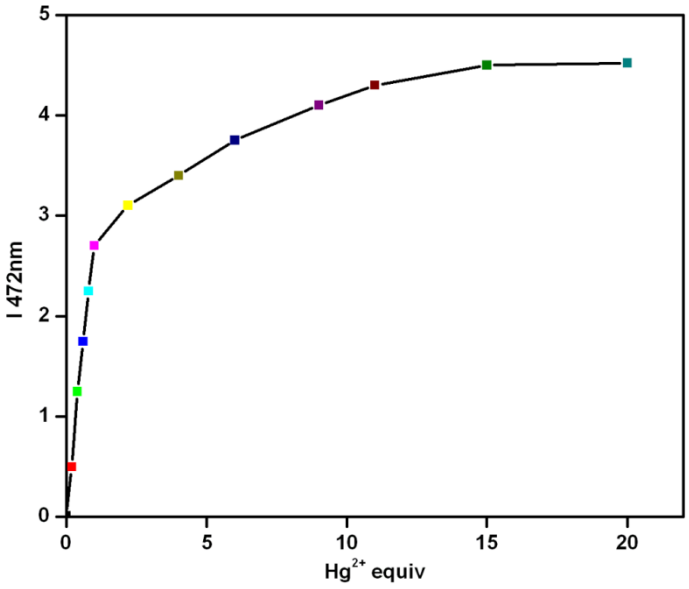


Fig-S8: Fluorescence intensity *vs* mole fraction of Hg^{2+} Job's plot

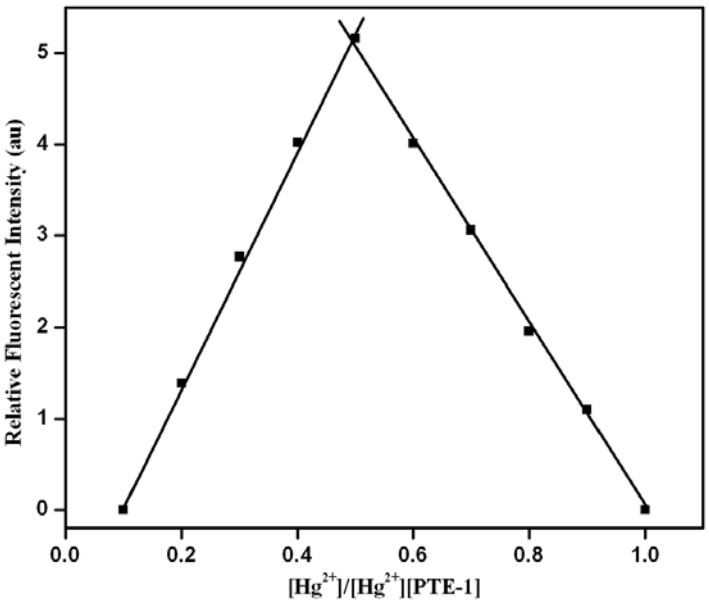


Fig-S9: ESI-MS spectrum of PTE-1+Hg^{2+}

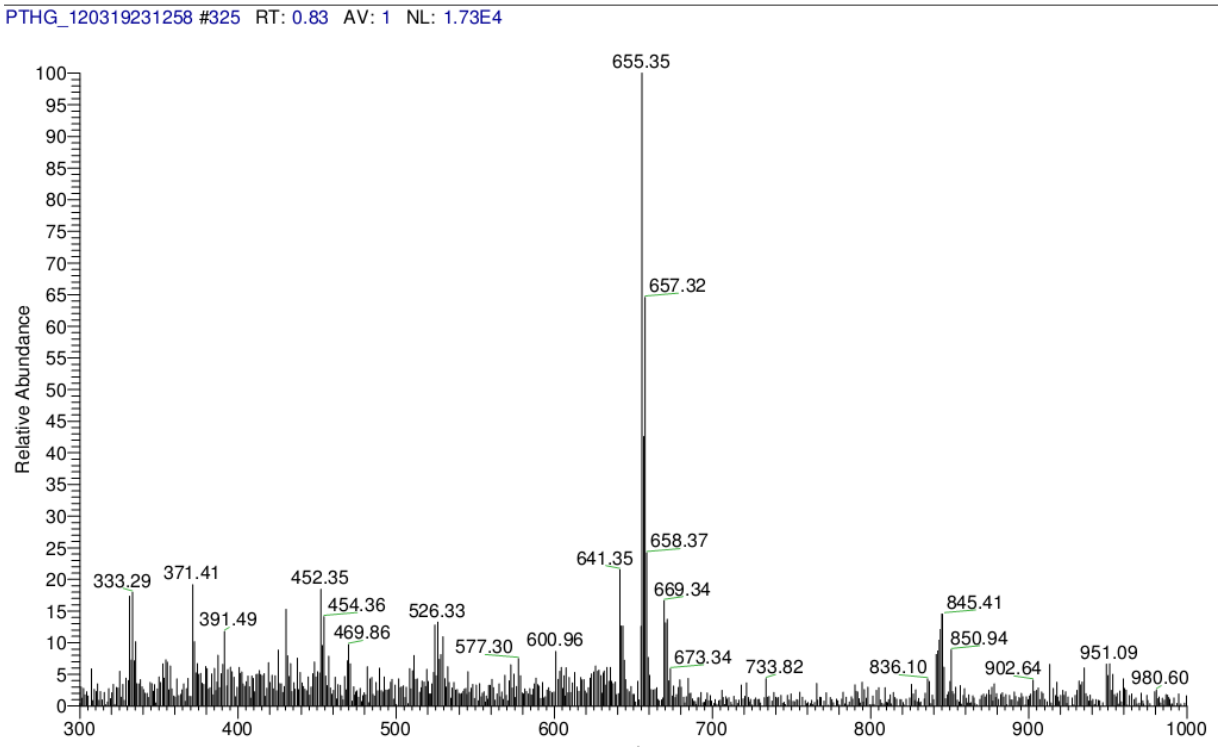


Fig-S10: Emission spectra of metal ions with PTE-2 and Emission spectra comparison of PTE-1 with PTE-1+Hg^{2+} and PTE-2.

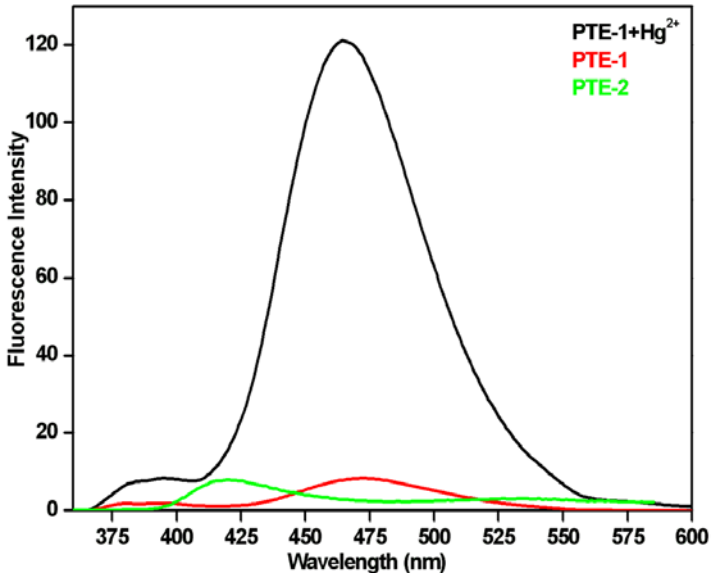


Fig-S11: Optimized geometry of the PTE-1 by DFT-B3LYP/6-31G (d, p) basis set

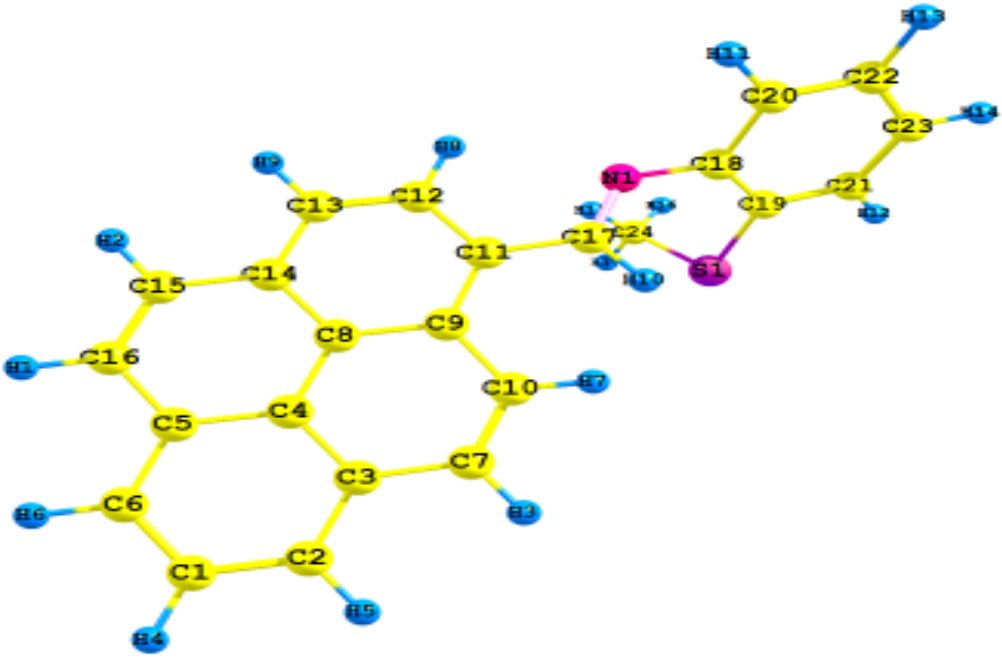


Fig-S12: Optimized geometry of the PTE-1+ Hg^{2+} by DFT-B3LYP /LANL2DZ basis set

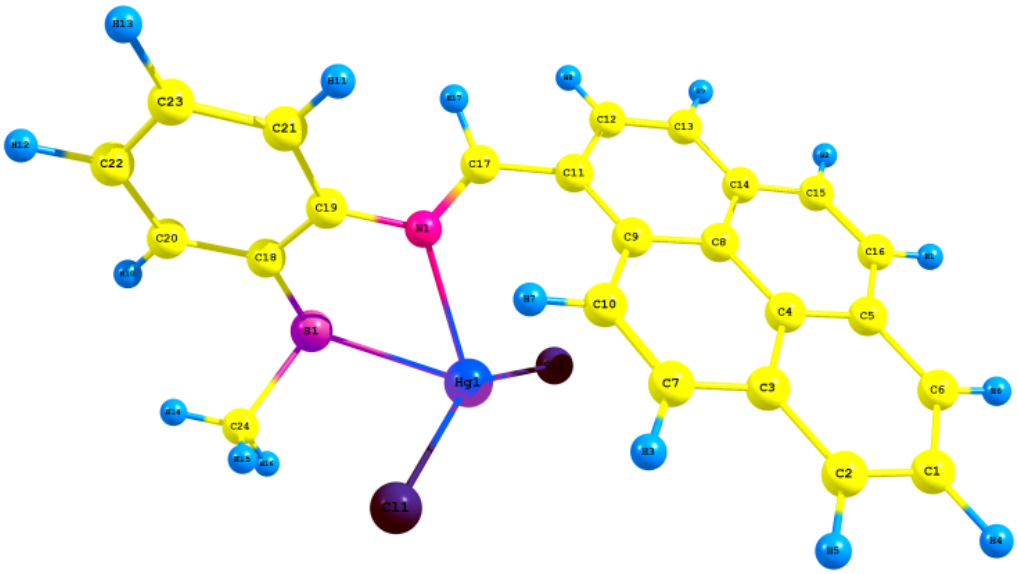


Table-S1: Frontier molecular orbital plots of PTE-1 and PTE-1 +Hg^{2+}

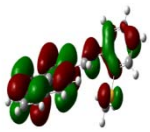
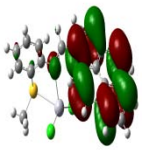
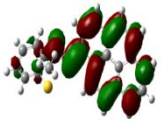
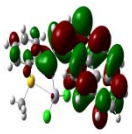
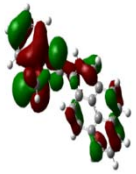
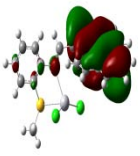
	PTE-1	PTE-1+Hg^{2+}
HOMO		
LUMO		
HOMO -1		

Table-S2: Calculated dominant electronic transition wavelength with oscillator strength of PTE-1 and PTE-1+Hg^{2+}

Transition	PTE-1 Wavelength (nm) (oscillator strength)	PTE-1+Hg^{2+} Wavelength (nm) (oscillator strength)
HOMO - LUMO	427.72 (0.2138)	397.14 (0.5446)
HOMO-1 - LUMO	388.26(0.4329)	357.04(0.0163)
HOMO-3 - LUMO	290.18(0.2065)	244.44(0.0249)

Fig-S13: The cell viability studies were done from lower to higher concentration.

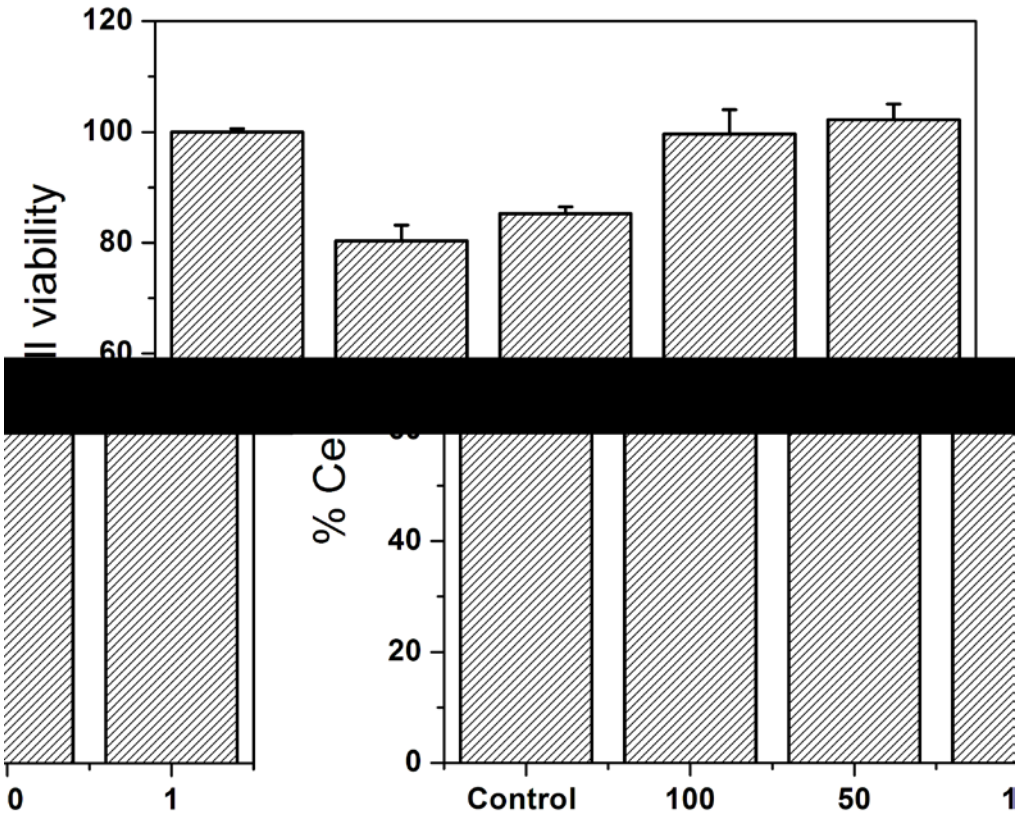


Fig-S14 : ^{1}H NMR Spectra of PTE-2.