Electronic Supplementary Material (ESI) for New Journal of Chemistry.

A fluorescein-based chemosensor for “turn-on” detection of Hg^{2+} and resultant complex as a fluorescent sensor for S^{2-} in semi aqueous medium with cell-Imaging application: Experimental and Computational studies

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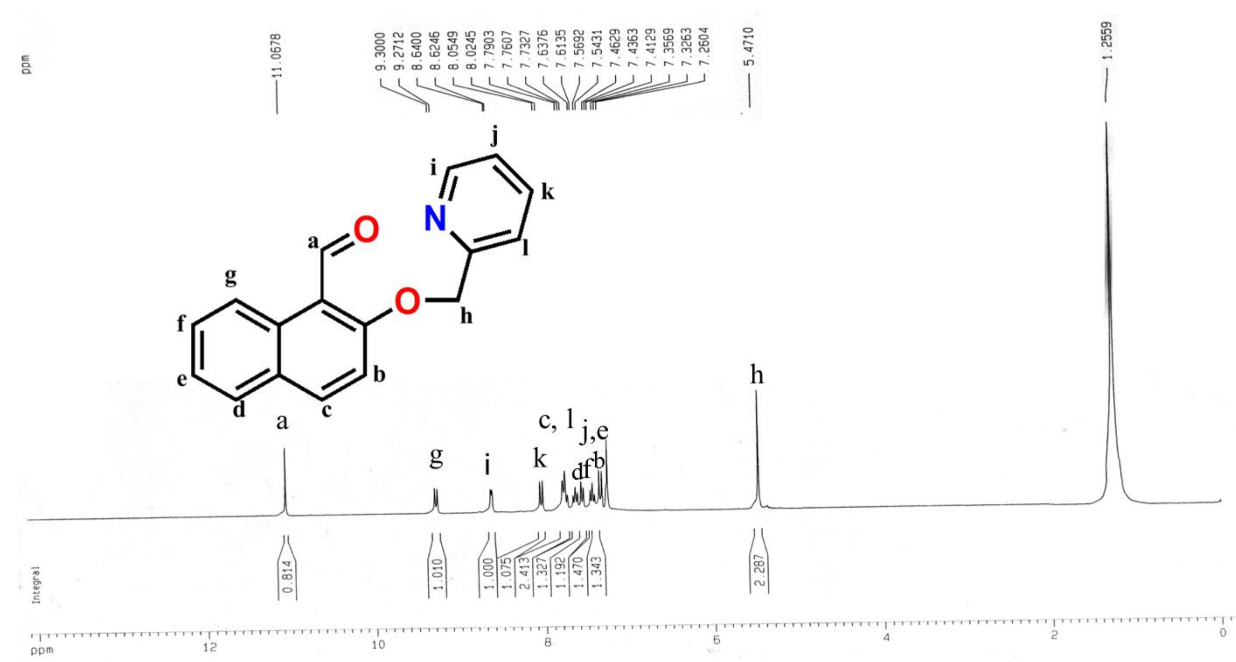


Fig. S1. ^{1}H-NMR spectrum of **L²** in DMSO-d_6.

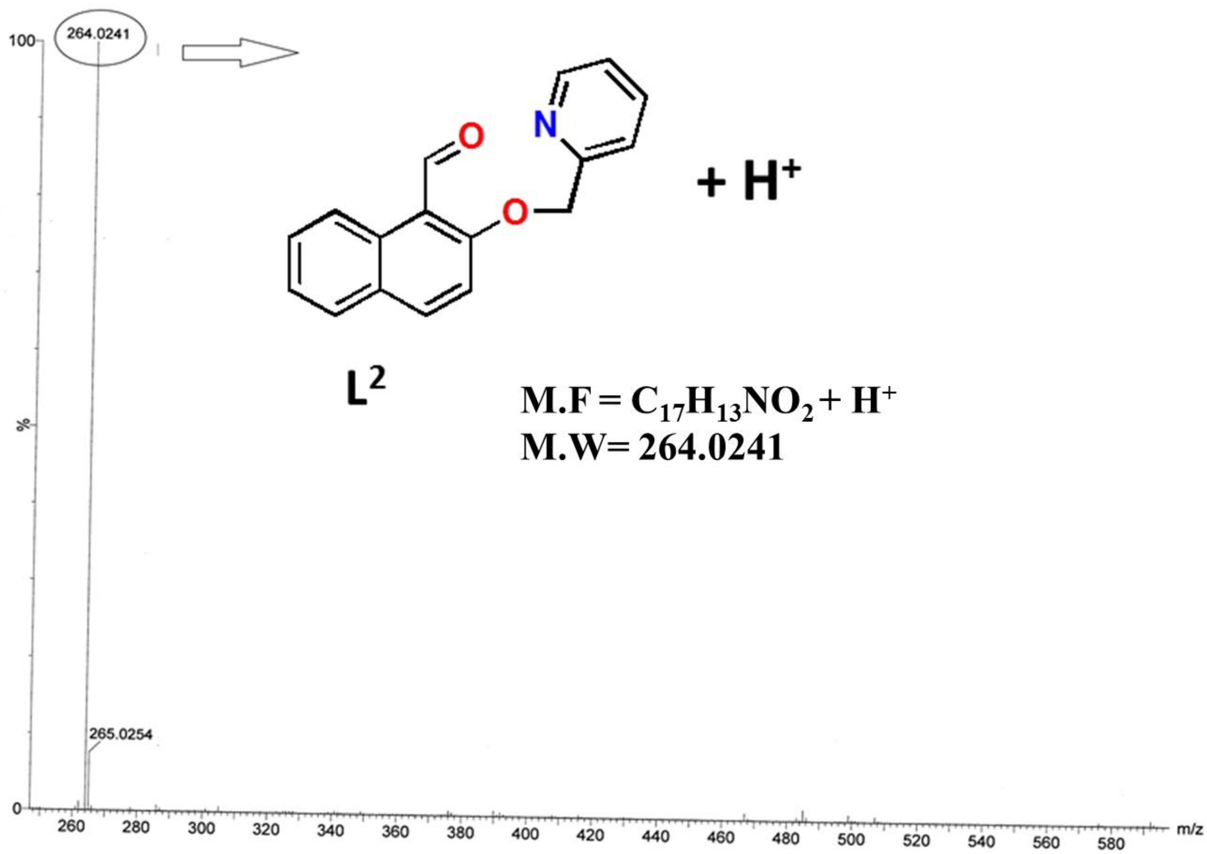


Fig. S2. Mass spectrum of **H_2L^3** in MeOH.

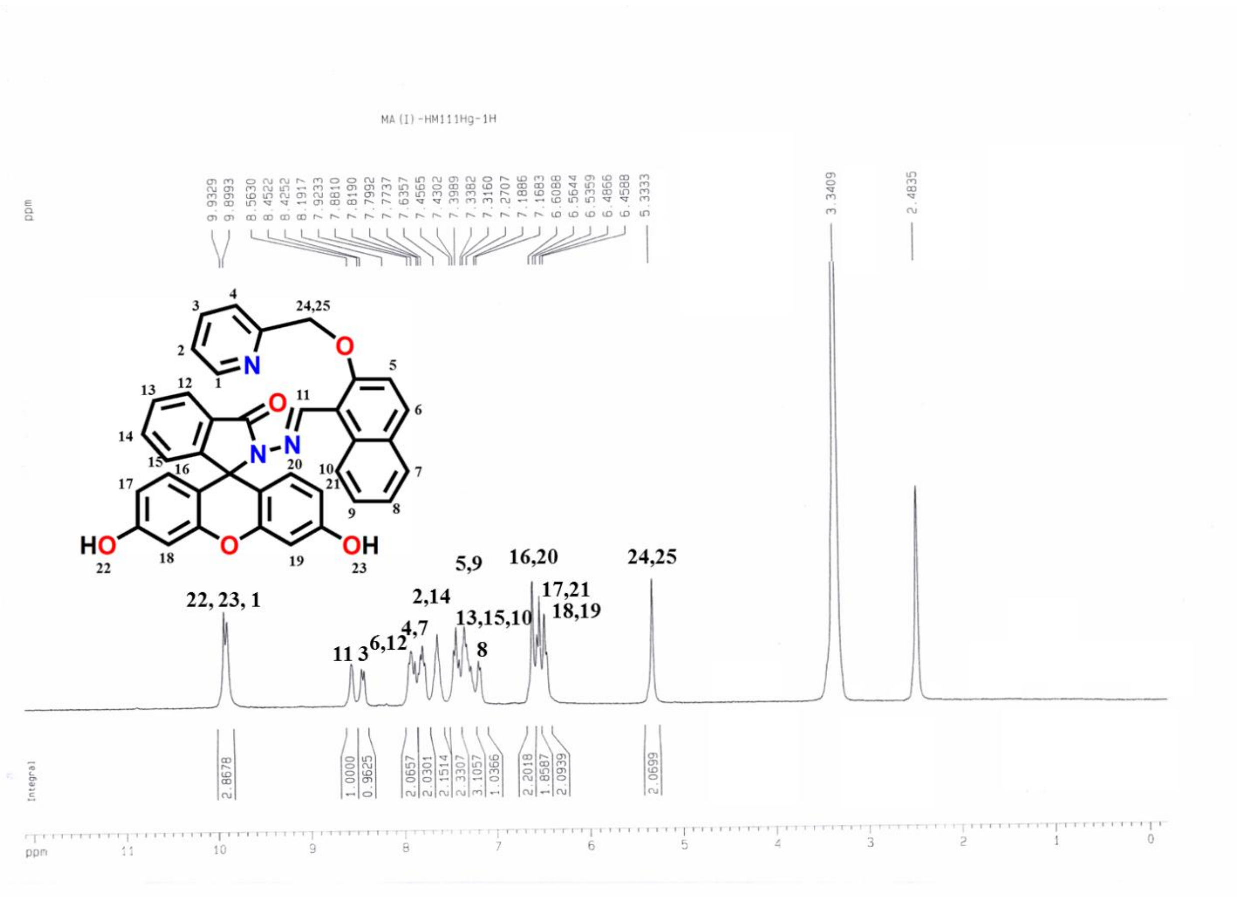


Fig.S3. ^{1}H-NMR spectrum of **H_2L^3**

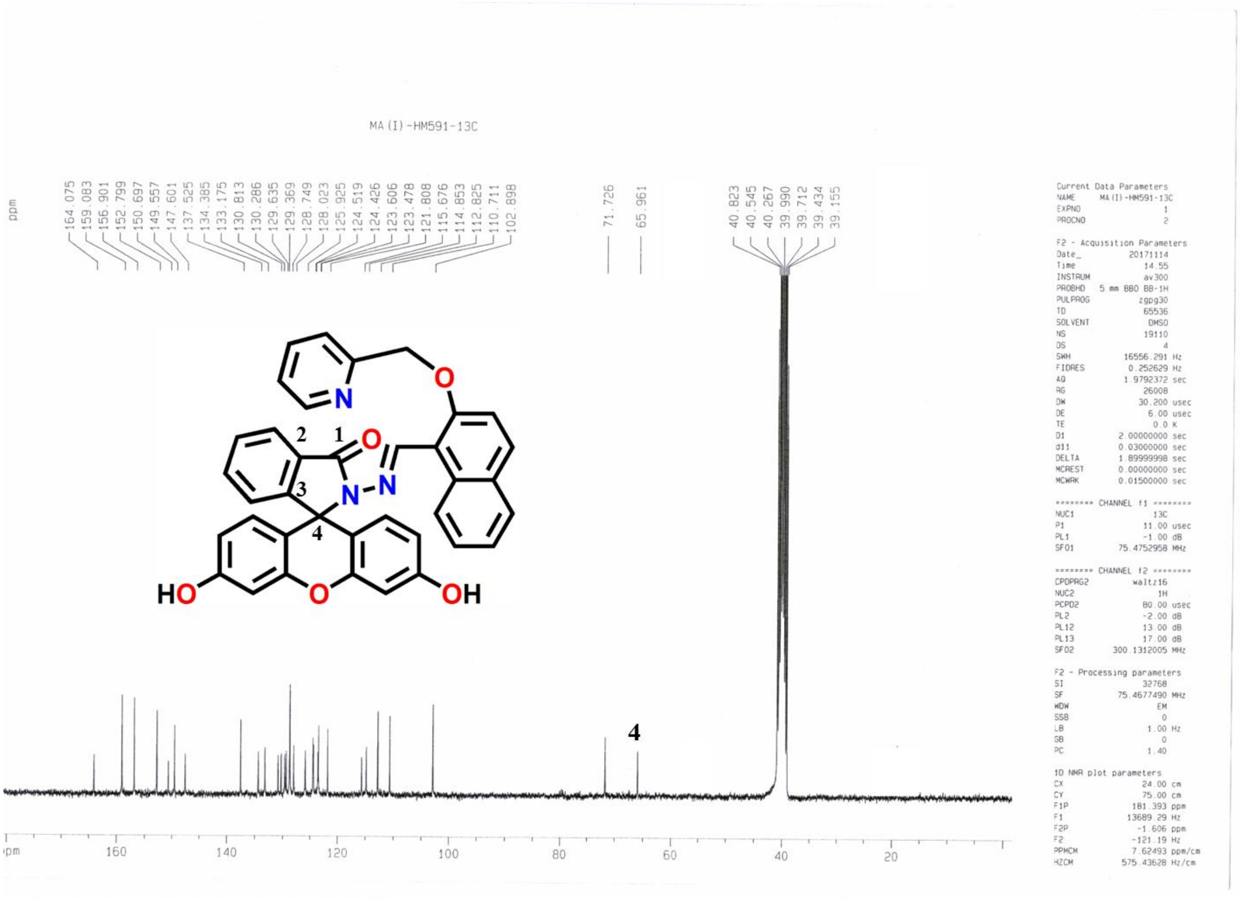


Fig. S4. ^{13}C-NMR spectrum of **H_2L^3** in DMSO-d_6.

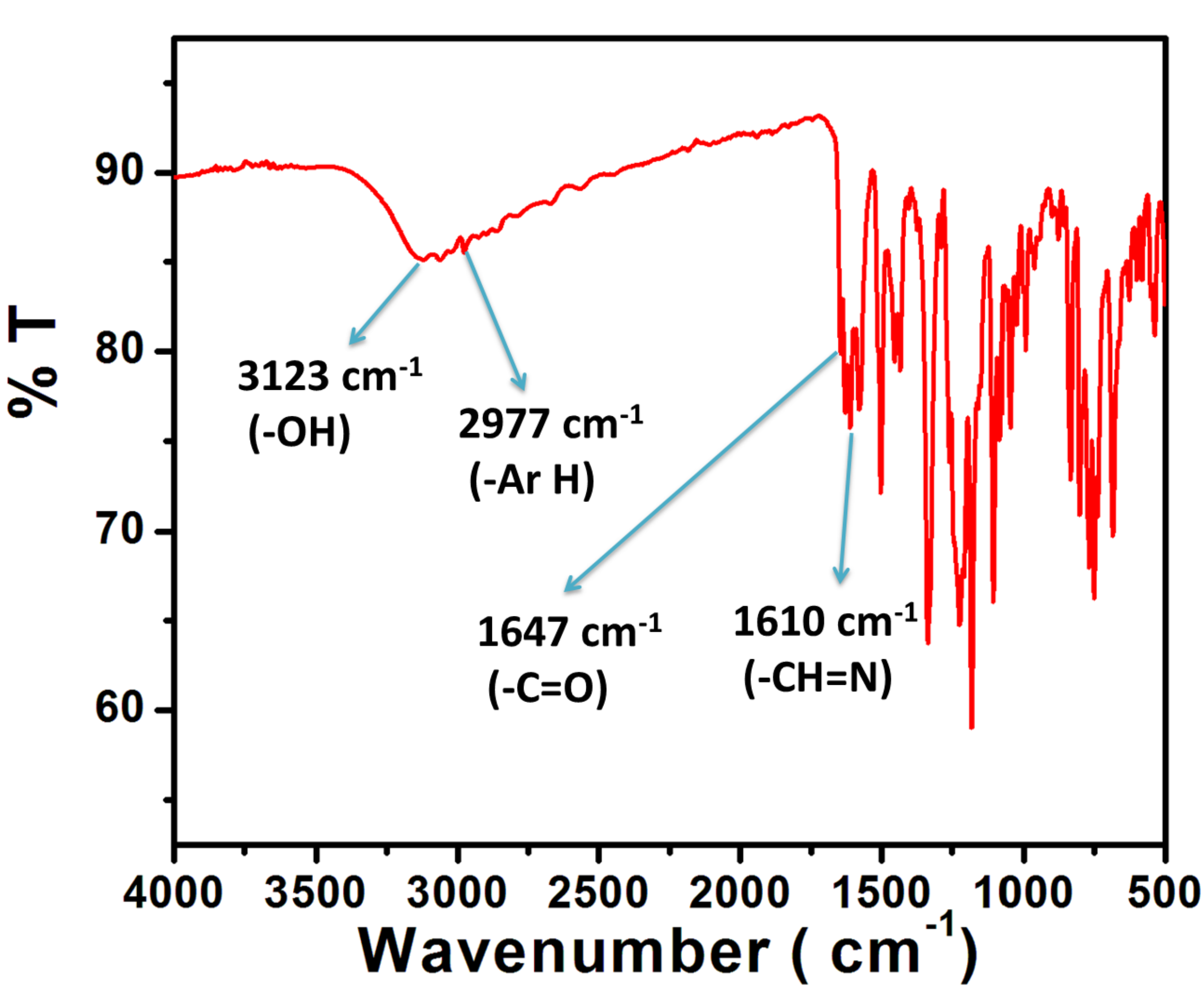


Fig. S5. IR spectrum of $\mathbf{H_2L^3}$.

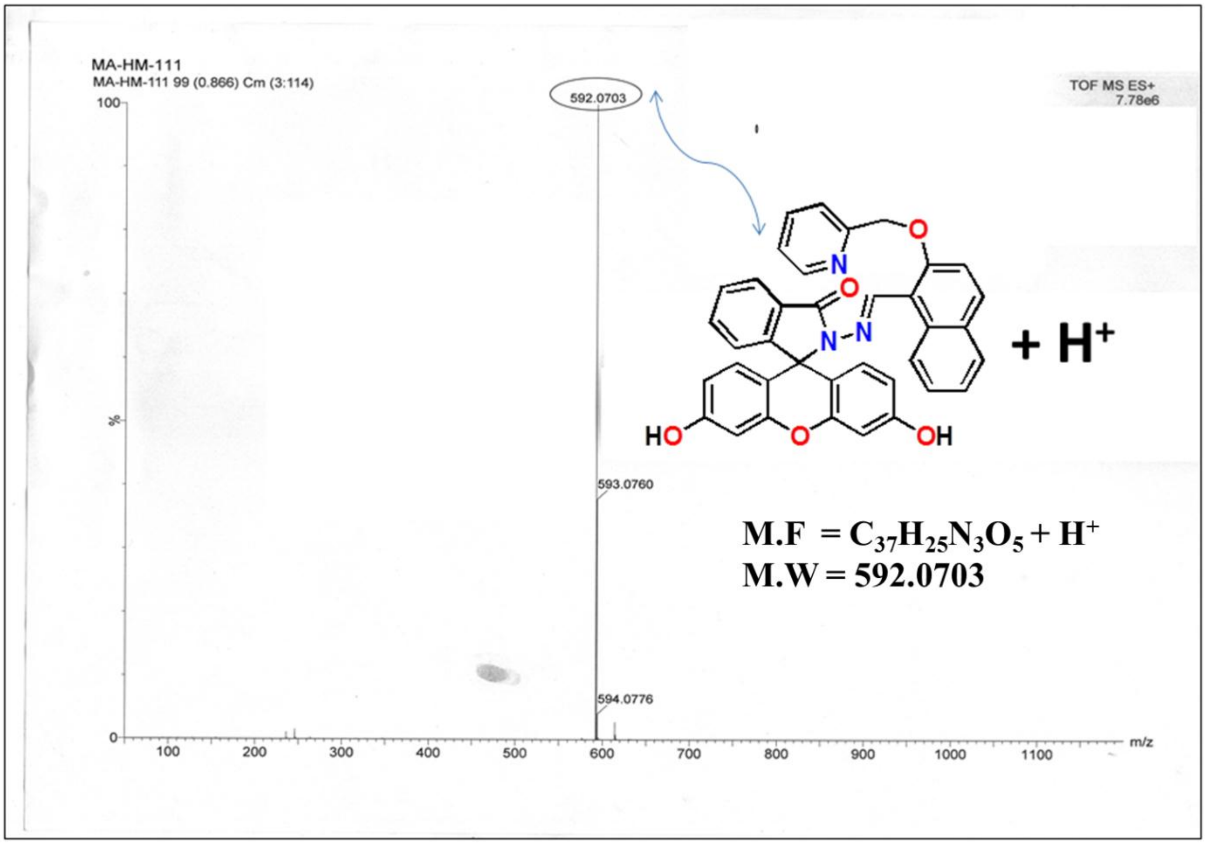


Fig. S6. Mass spectrum of $\mathbf{H_2L^3}$ in MeOH.

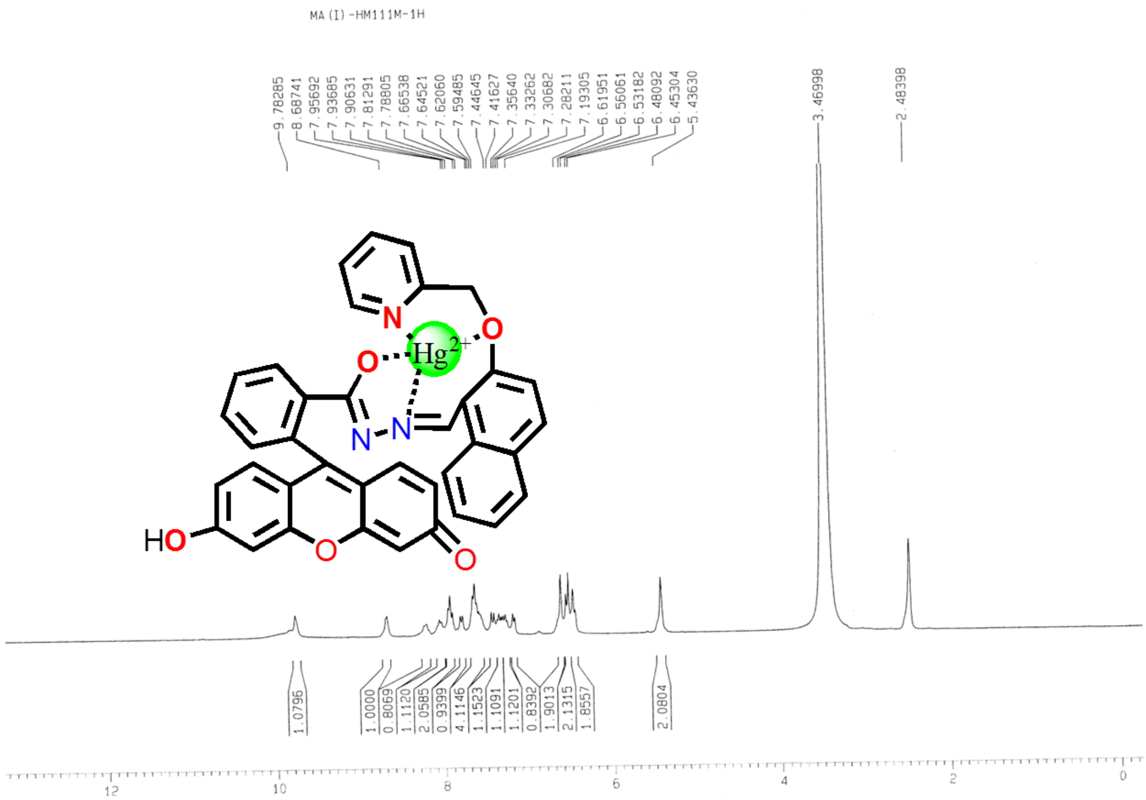


Fig. S7. ^{1}H-NMR spectrum of $\mathbf{H_2L^3\text{-}Hg^{2+}}$ Complex

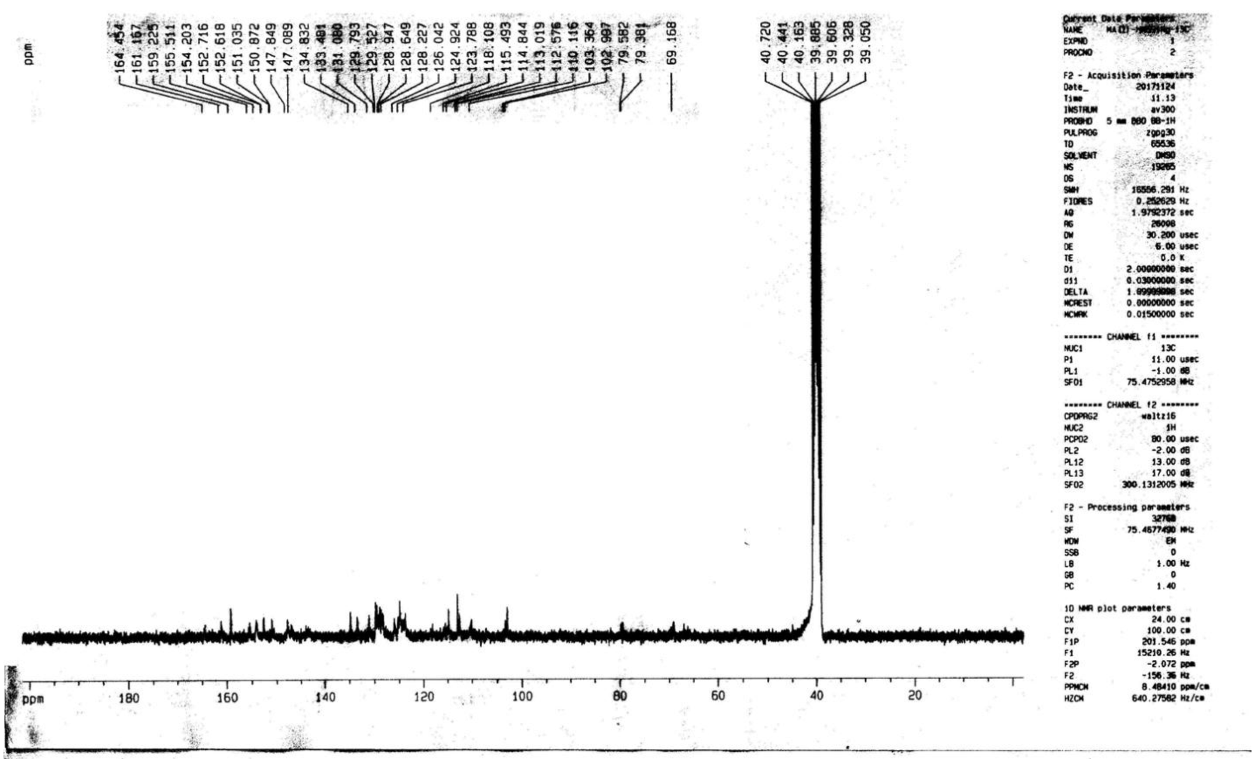


Fig.S8. ^{13}C-NMR spectrum of **H_2L^3-Hg^{2+}** Complex in DMSO-d_6.

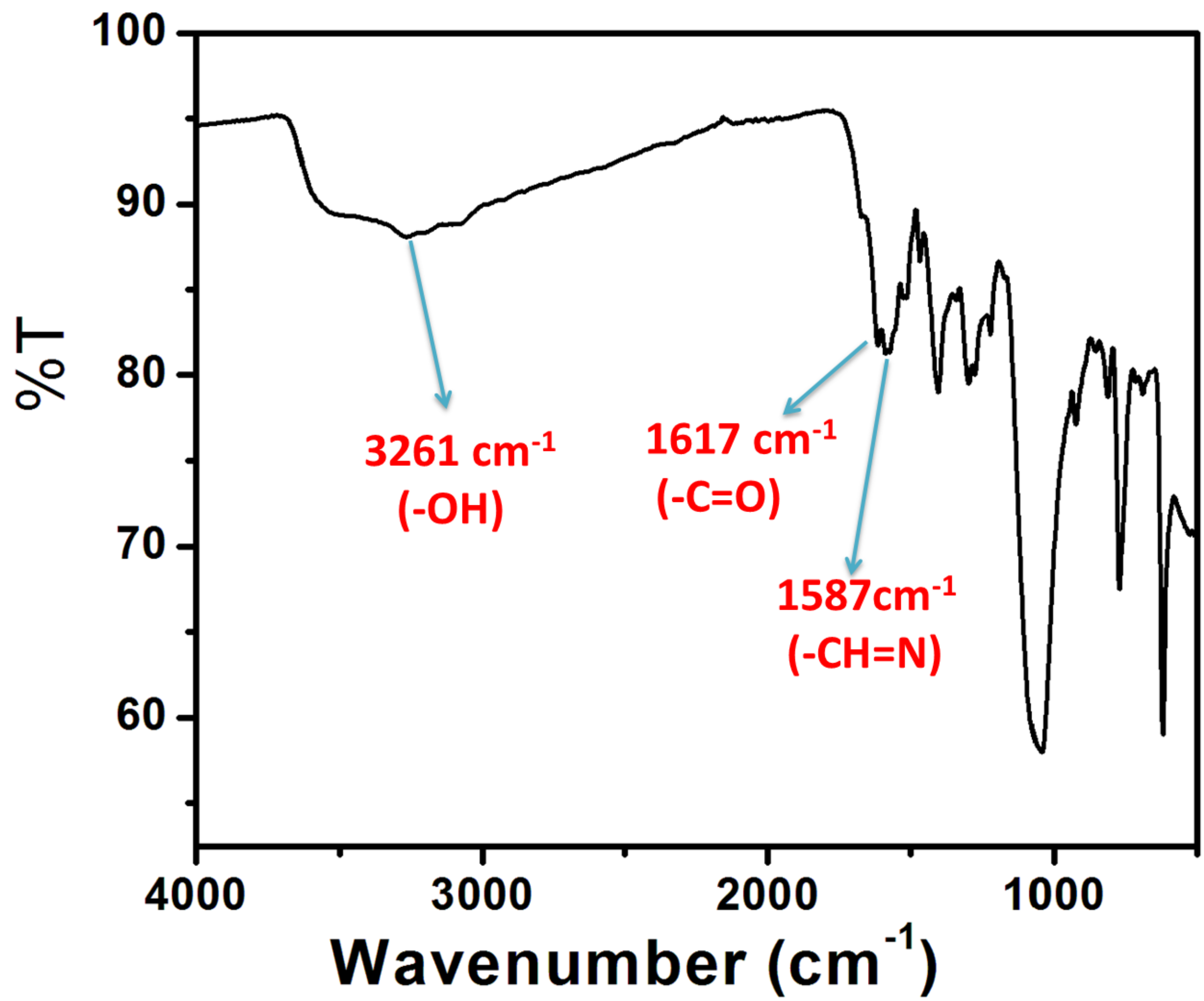


Fig. S9. IR spectrum of $\mathbf{H_2L^3}$-$\mathbf{Hg^{2+}}$ Complex.

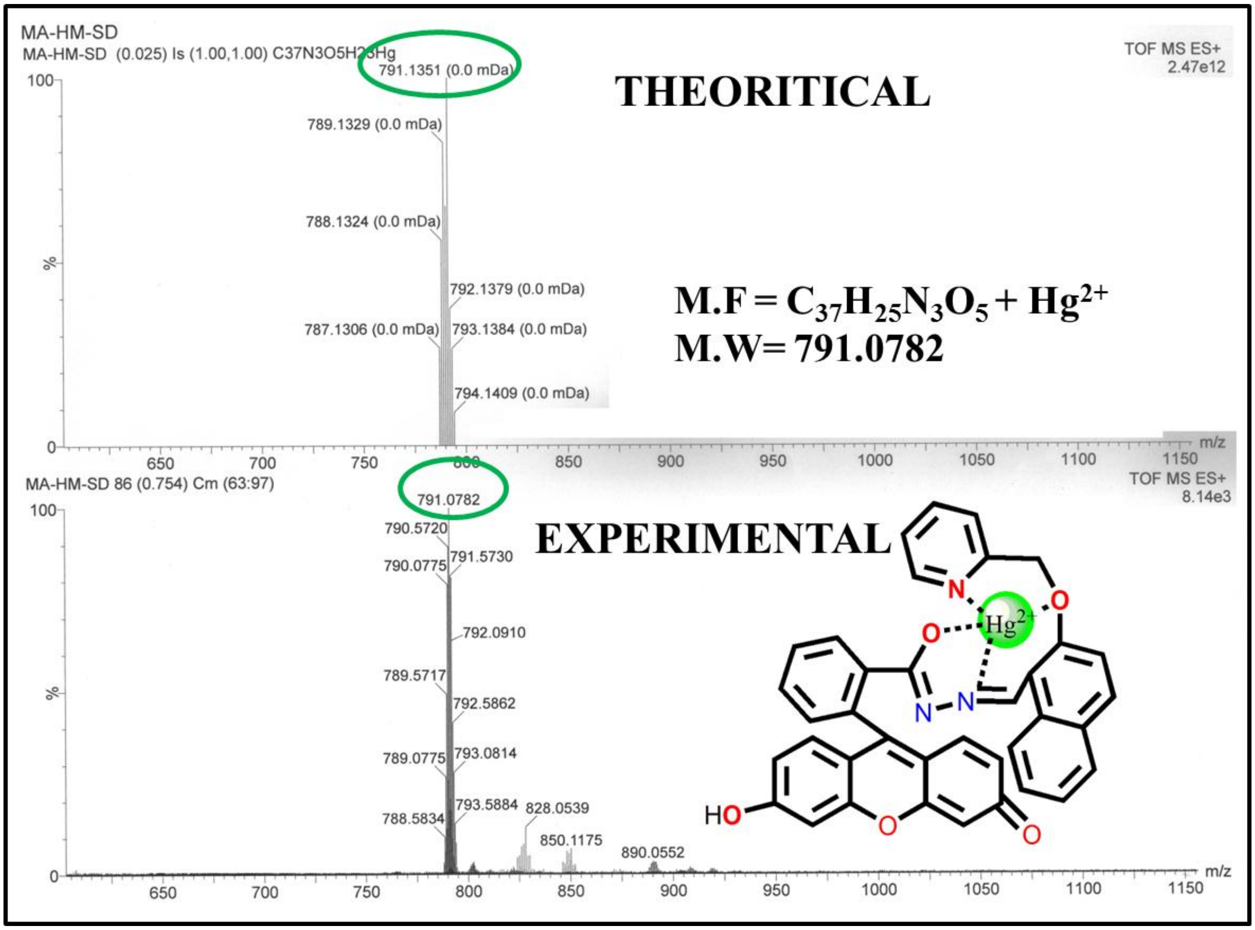


Fig. S10. Mass spectrum of H_2L^3-Hg^{2+} Complex in MeOH.

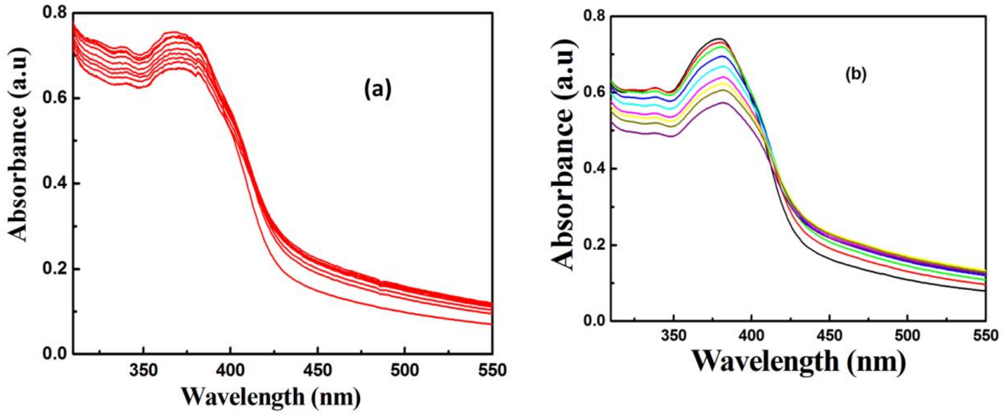


Fig.S11. (a) Absorption titration of H_2L^3 with gradual addition of Hg^{2+} solution (b) Absorption titration of H_2L^3 with gradual addition of water.

JOB's Plot

This method is based on the measurementof a series of solutions in which molar concentrations of two reactants varybut their sum remains constant. The fluorescence intensity of each solution was measuredat a suitable wavelength and plotted against the mole fraction of one reactant. Amaximum in fluorescence intensity appeared at themole ratio corresponding to the combiningratio of the reactants.The composition of the complex was determined by JOB's method and found to be (1:1) with respect to ligand for Hg^{2+}.

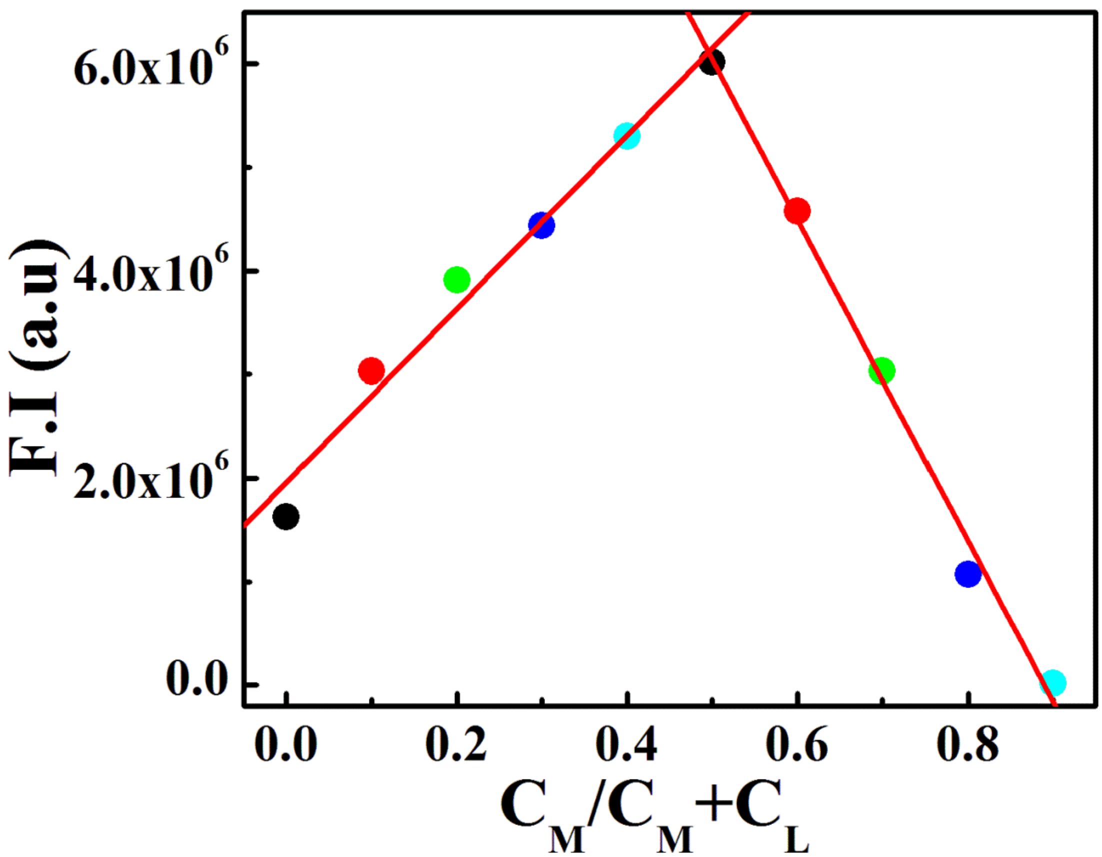


Fig. S12. JOB's plot for Hg^{2+}.

Calculation of LOD value

To determine the detection limit, fluorescence titration of $\mathbf{H_2L^3}$ with Hg^{2+} was carried out by adding aliquots of micromolar concentration of Hg^{2+}.

However, the detection limit (LOD) of Hg^{2+} have been calculated by 3σ method.

$$LOD = 3 \times S_d/S$$

whereS_d is the standard deviation of the intercept of the blank ($\mathbf{H_2L^3}$) obtained from a plot of FI vs. [$\mathbf{H_2L^3}$], and S is the slope obtained from linear part of the plot of FI vs.[Hg^{2+}].

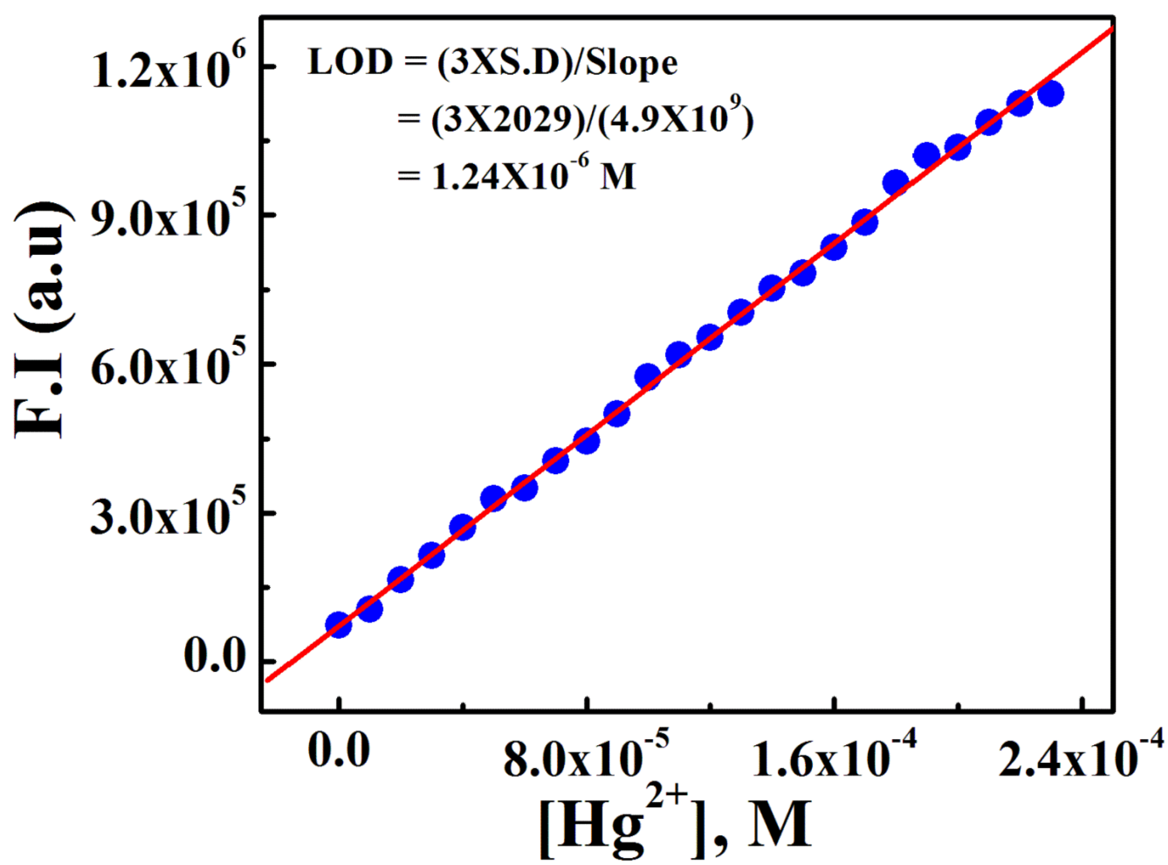


Fig.S13. LOD of Hg^{2+}

Calculation of Quantum Yield:

Fluorescence quantum yields (Φ) were estimated by integrating the area under the fluorescence curves using the equation,

$$\Phi_{sample} = (OD_{std} \times A_{sample})/(OD_{sample} \times A_{std}) \times \Phi_{std}$$

Where A_{sample} and A_{std} are the area under the fluorescence spectral curves and OD_{sample} and OD_{std} are the optical densities of the sample and standard, respectively at the excitation wavelength.

Fluorescein has been used as the standard with Φ_{std} = 0.5 in ethanol for measuring the quantum yields of **H_2L^3** and of **$[Hg(HL^3)]^+$** Complex.

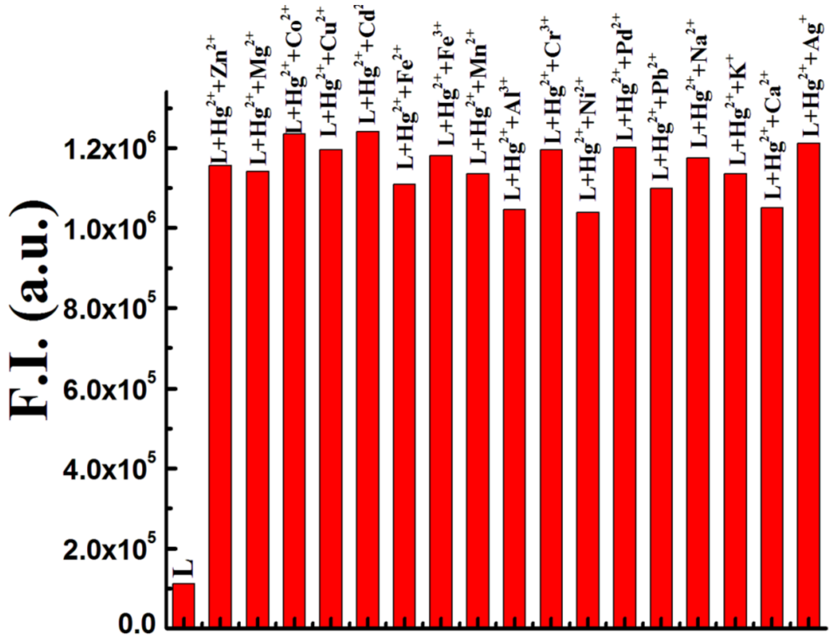


Fig.S14. Selectivity study of Hg^{2+} in presence of different cations

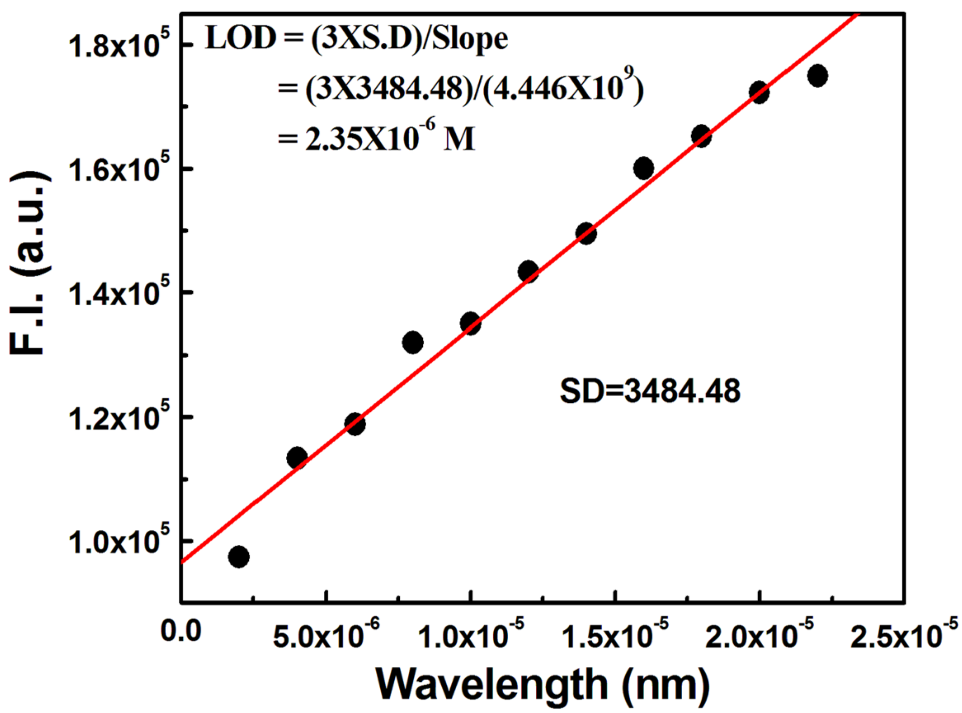


Fig.S15. LOD of S^{2-}

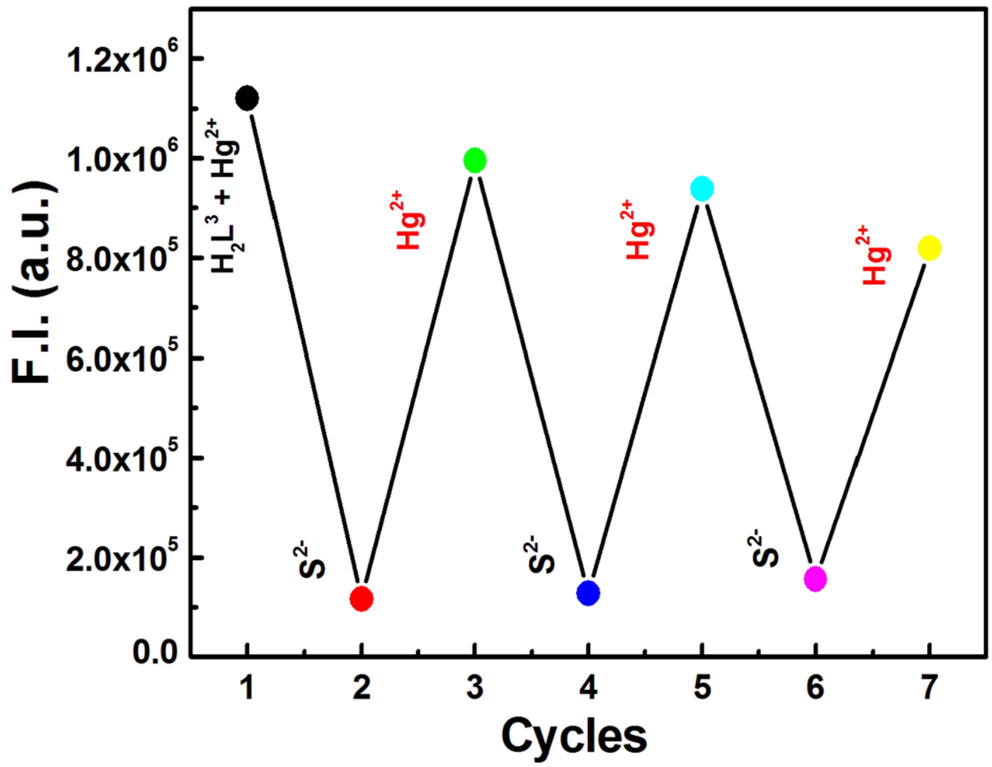


Fig.S16. Cascade fluorescence ON-OFF-ON response of $\mathbf{H_2L^3}$ with sequential addition of Hg^{2+} and S^{2-}.

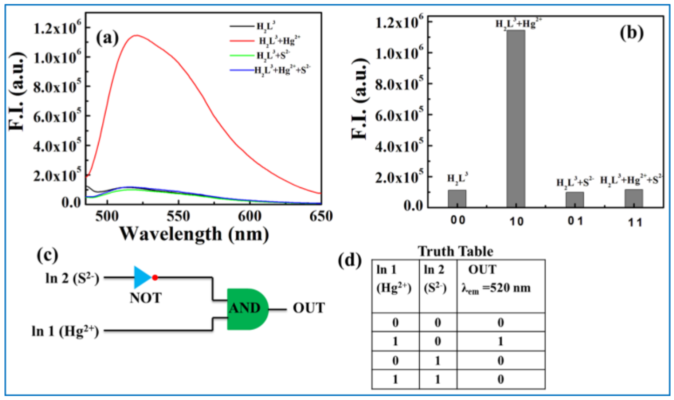


Fig.S17. (a) Output signals (λ_{em} = 520 nm) of the logic gate in the presence of different inputs with corresponding gray diagram (b). (c) a general representation of an INHIBIT logic gate. (d) corresponding truth table of the logic gate.

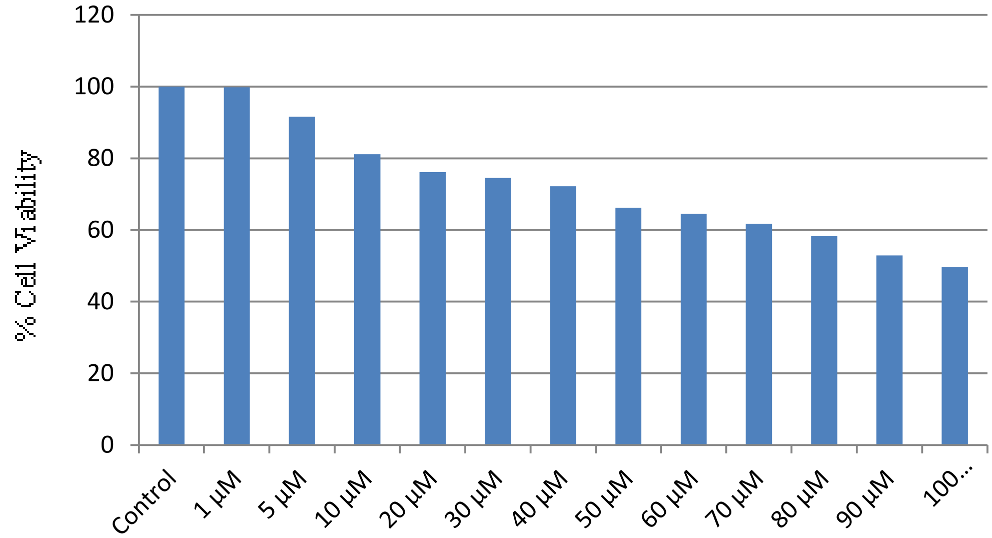
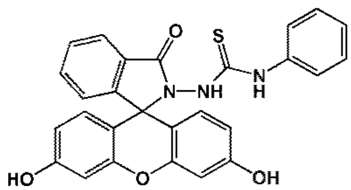
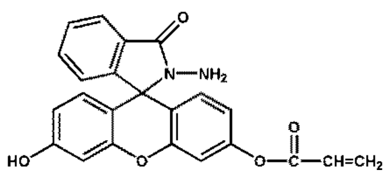
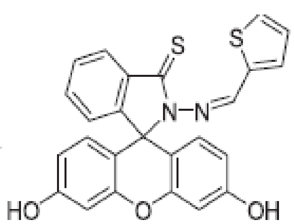
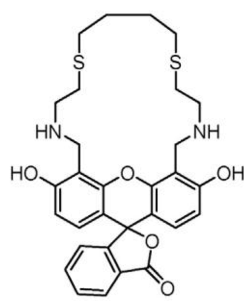
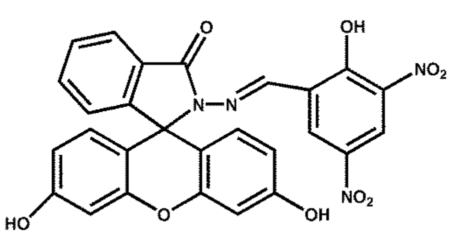
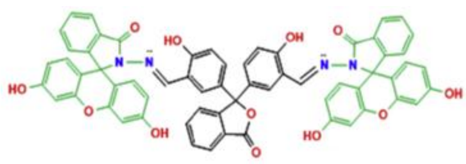
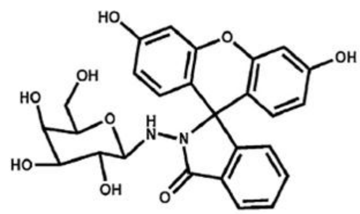
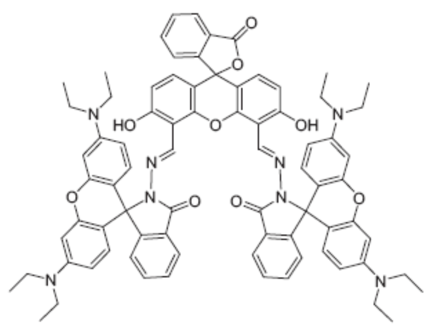
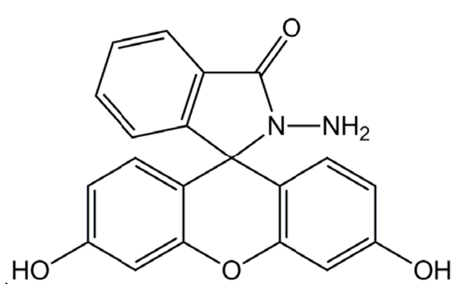
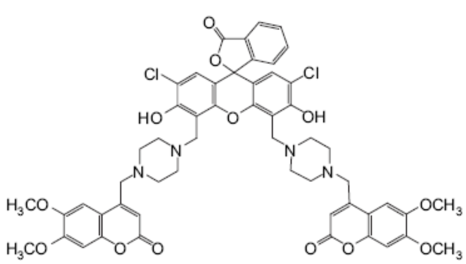
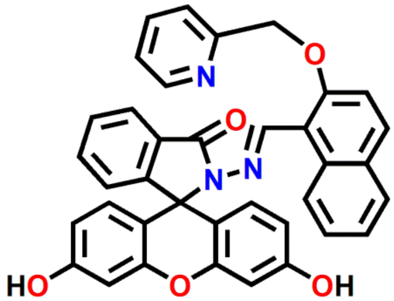


Fig.S18. Percent (%) cell viability of HepG2 cells treated with different concentrations (1-100 µM) of $\mathbf{H_2L^3}$ for 24 hours determined by MTT assay.

Table S1. Comparison of few aspects of some recently published fluorescent chemosensors for Hg^{2+} ion

Probe		Working System	Biological Study	Reversibility	Logic Gate	Quantum Yield	Ref
	Turn On	Methanol–water (30/70, v/v)	-	-	-	-	74
	Turn On	aqueous	Done	-	-	-	75
	Turn Off	EtOH/HEPES (1:1, v/v,)	Done	Done	-	-	76
	Turn Off	95:5 Tris–HCl buffer:MeOH	-	-	-	0.56	77
	Turn On	aqueous HEPES buffer: MeOH (8 : 2 v/v)	-	Done	Done	0.095	78

	Turn On	EtOH-H2O (v/v, 8/2).	-	Done	-	0.258	79
	Turn On	H_2O:CH_3CN (70:30,v/v)	-	-	-	-	80
	Turn On	DCM	-	Done	-	0.19	81
	Turn On	Ethanol /HEPES (v/v = 1:1)	-	-	-	-	82
	Turn On	aqueous 1% DMSO	-	-	-	-	83

 H_2L^3	Turn On	Semi aqueous	Done	Done	Done	0.1122	