

## Supplementary Data:

### Selective Sensing and Efficient Capture of $\text{Hg}^{2+}$ from Aqueous Medium with a Pyrene based Amphiphilic Receptor

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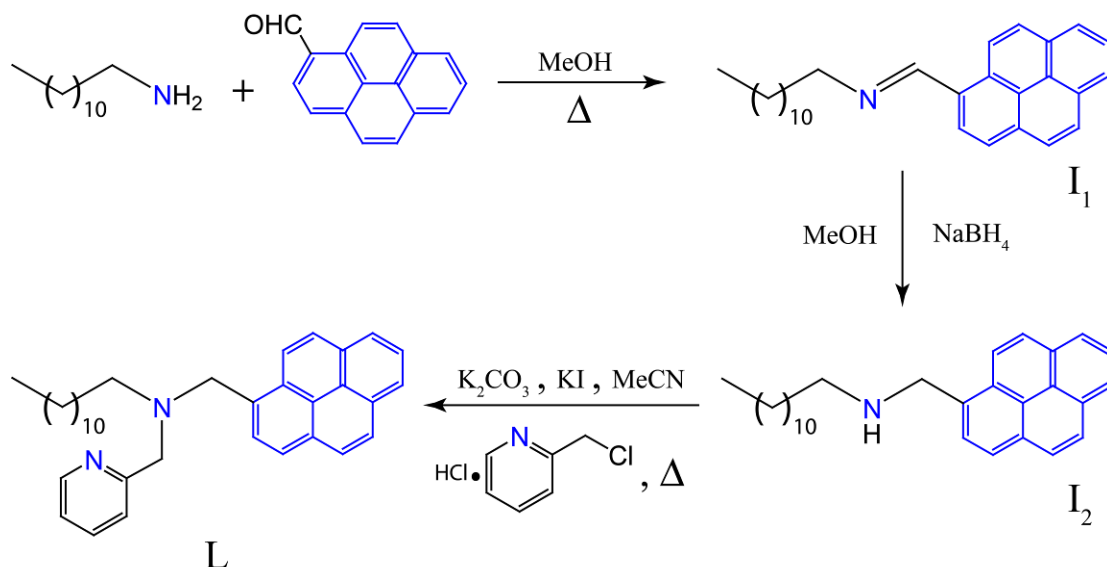
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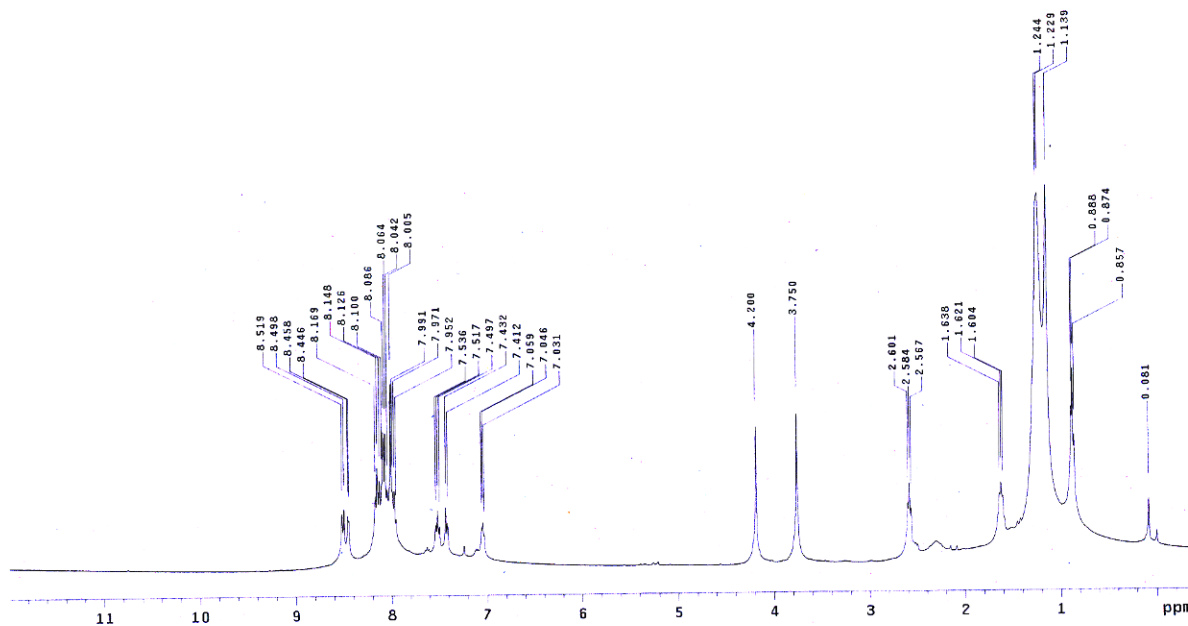
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#### Synthetic procedure of ligand L:

Synthetic pathways of fluorogenic molecule **L** is summarized in Scheme S1. The reaction of 1-pyrenealdehyde with 1.1 equiv of dodecyl amine affords the desired Schiff base in 70 % yield. Reduction of the Schiff base with  $\text{NaBH}_4$  in methanol leads to *N*-pyrenyl-*N'*-dodecyl amine. Refluxing *N*-pyrenyl-*N'*-dodecyl amine with 1-chloromethyl(pyridine hydrochloride) in the presence of  $\text{K}_2\text{CO}_3$  in  $\text{CH}_3\text{CN}$  for 48 hours produced reference material **L**.



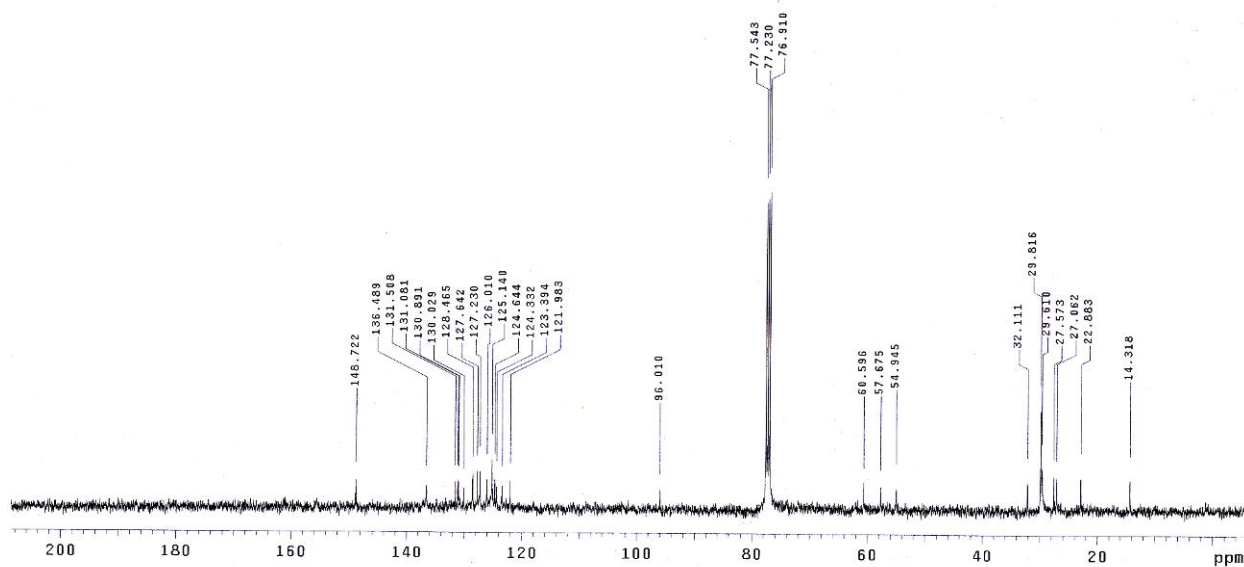
**Scheme S1:** Synthetic scheme of the ligand **L**.



**Figure S2:**  $^1\text{H}$  NMR of **L** in  $\text{CDCl}_3$  solution.

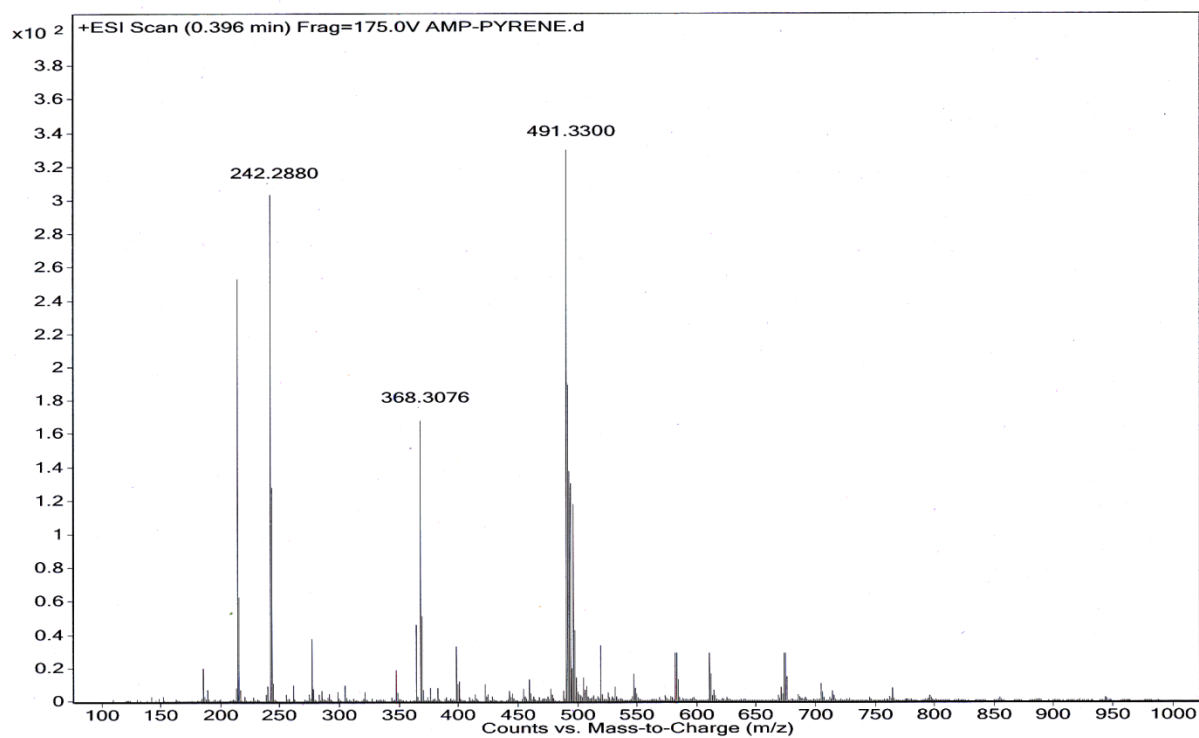
$^1\text{H}$ NMR ( $\text{CDCl}_3$ ):  $\delta$  0.874 (t, 3H,  $J=0.017$ );  $\delta$  1.229 (broad multiplet, 18H);  $\delta$  1.621 (q, 2H,  $J=0.017$ );  $\delta$  2.584 (t, 2H,  $J=0.017$ );  $\delta$  3.750 (s, 2H);  $\delta$  4.200 (s, 2H);  $\delta$  7.046 (t, 1H,  $J=0.014$ );  $\delta$  7.422 (d, 1H,  $J=0.02$ );  $\delta$  7.517 (t, 1H,  $J=0.02$ );  $\delta$  7.942–8.169 (m, 7H);  $\delta$  8.452 (d, 1H,  $J=0.027$ );  $\delta$  8.508 (d, 2H,  $J=0.012$ ).

**Elem. Anal.:**  $\text{C}_{35}\text{H}_{42}\text{N}_2$  (490.72): calcd. C 85.66, H 8.63, N 5.71; found C 85.68, H 8.66, N 5.65.

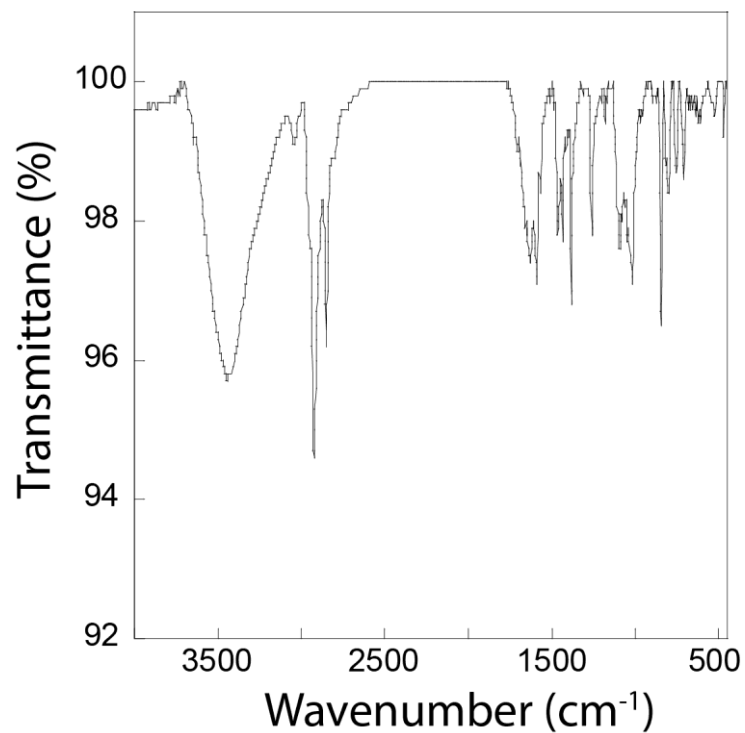


**Figure S3:**  $^{13}\text{C}$  NMR of **L** in  $\text{CDCl}_3$  solution.

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz). 148.722 ppm, 136.489 ppm, 139.508 ppm, 131.081 ppm, 130.891 ppm, 130.029 ppm, 128.465 ppm, 127.642 ppm, 127.230 ppm, 126.010 ppm, 125.140 ppm, 124.644 ppm, 124.332 ppm, 123.394 ppm, 121.983 ppm, 96.010 ppm, 60.596 ppm, 57.675 ppm, 54.945 ppm, 32.111 ppm, 29.816 ppm, 29.610 ppm, 27.573 ppm, 27.062 ppm, 22.883 ppm, 14.318 ppm.



**Figure S4:** Mass spectra of **L** (Mass spectrum obtained in positive mode).



**Figure S5:** FTIR spectra of intermediate **L**.

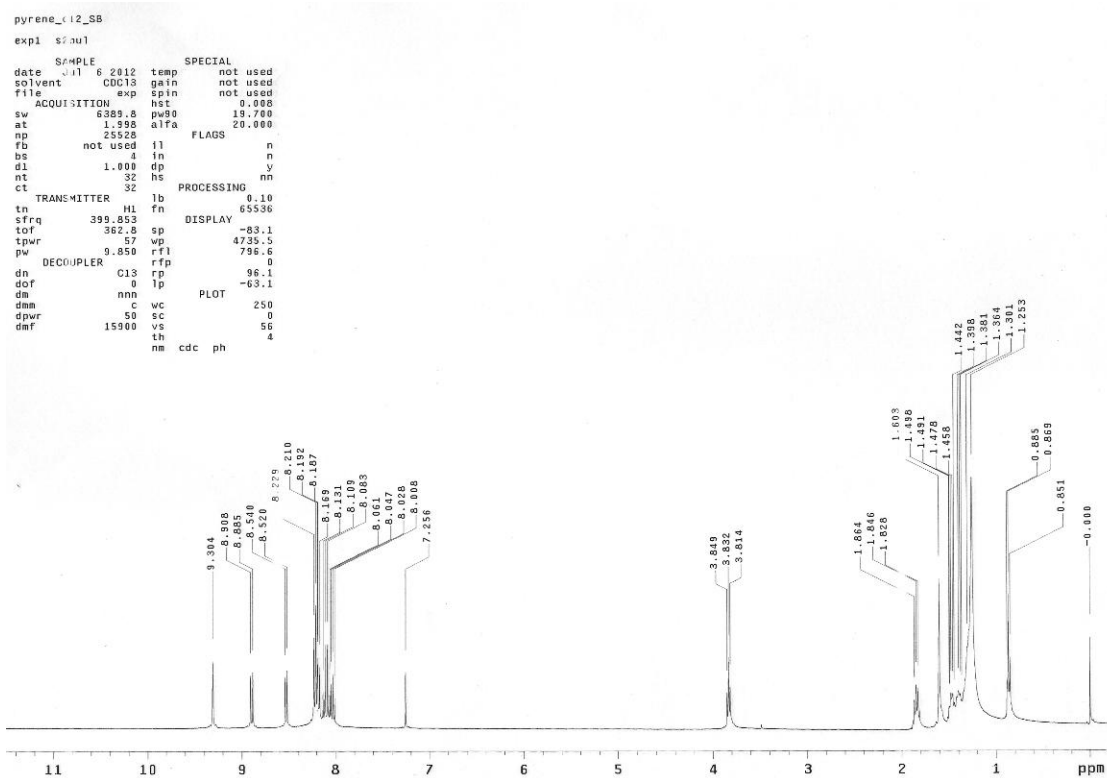
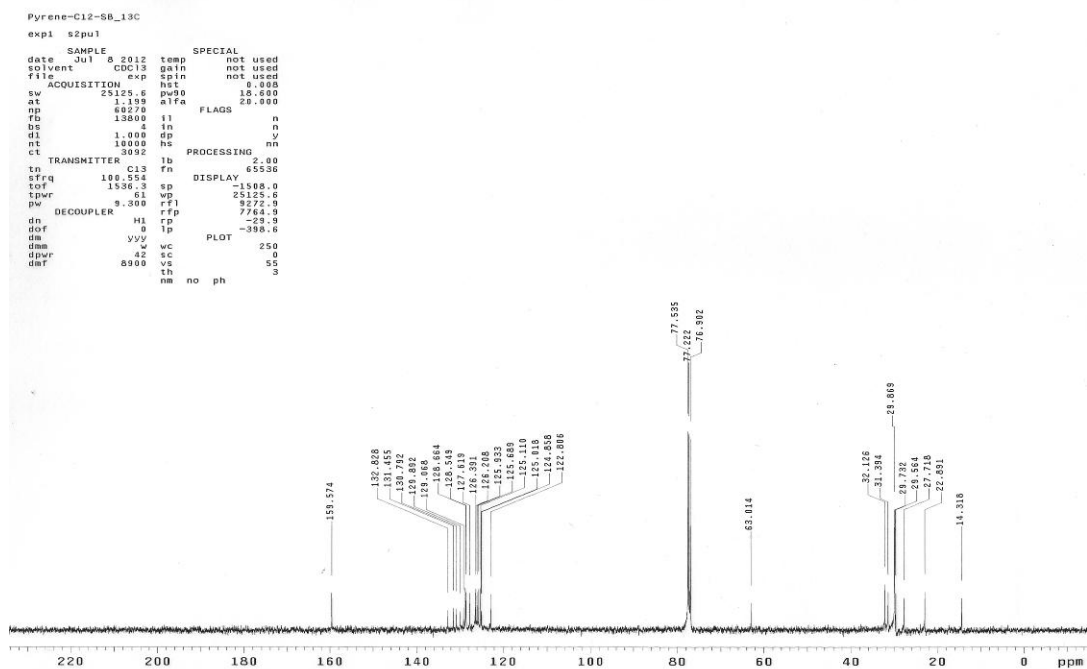
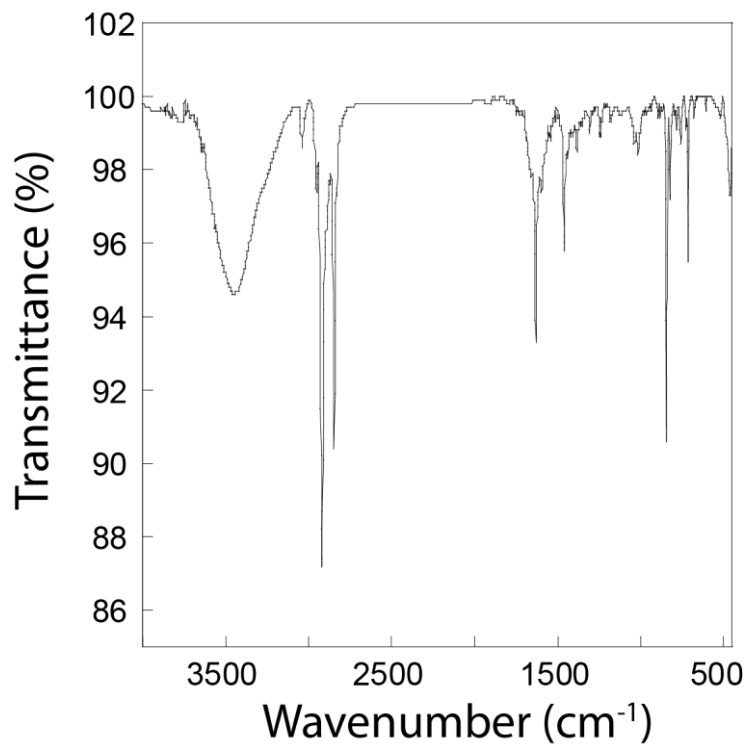


Figure S6:  $^1\text{H}$  NMR spectra of intermediate  $\text{I}_1$  in  $\text{CDCl}_3$ .



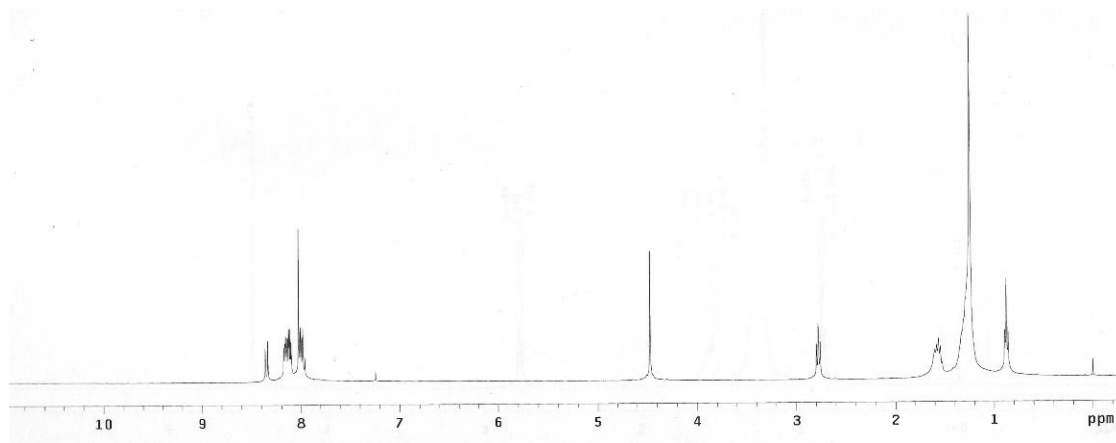
**Figure S7:**  $^{13}\text{C}$  NMR spectra of intermediate **I**<sub>1</sub> in  $\text{CDCl}_3$ .



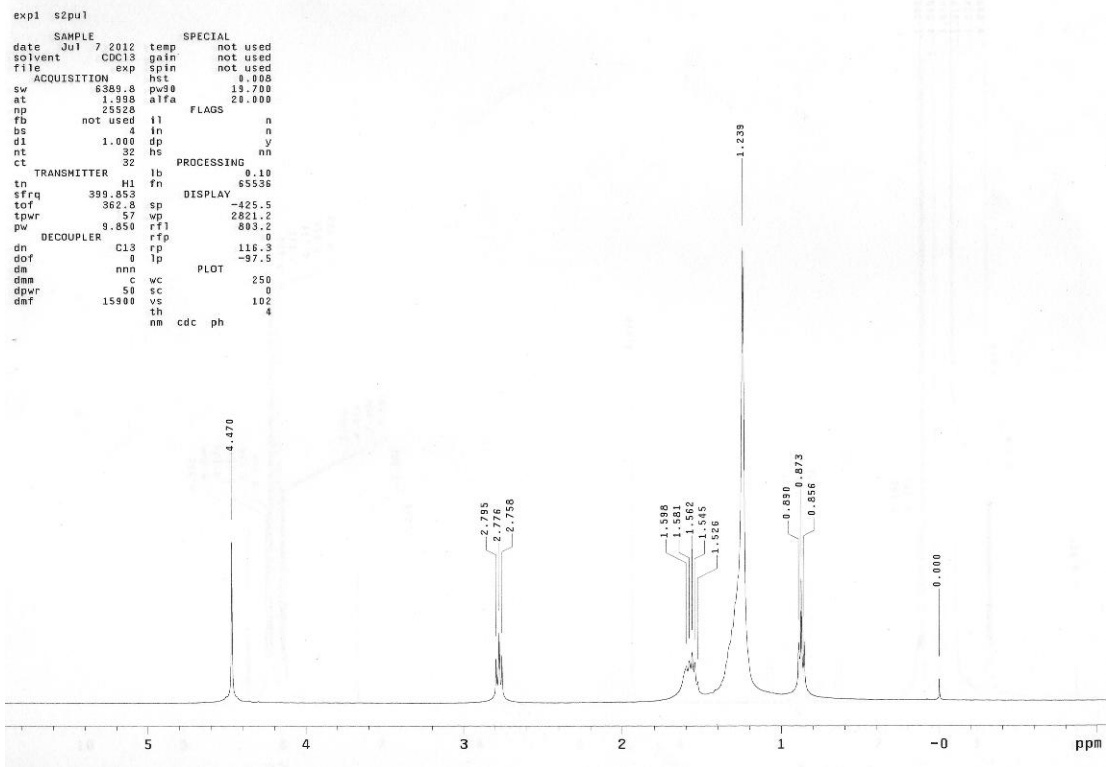
**Figure S8:** FTIR spectra of intermediate **I**<sub>1</sub>.

**Mass of I<sub>1</sub>:**  $m/z$  calcd. for [**I**<sub>1</sub>+H] is 398.2848 found 398.2844 (mass spectrum obtained in positive mode).

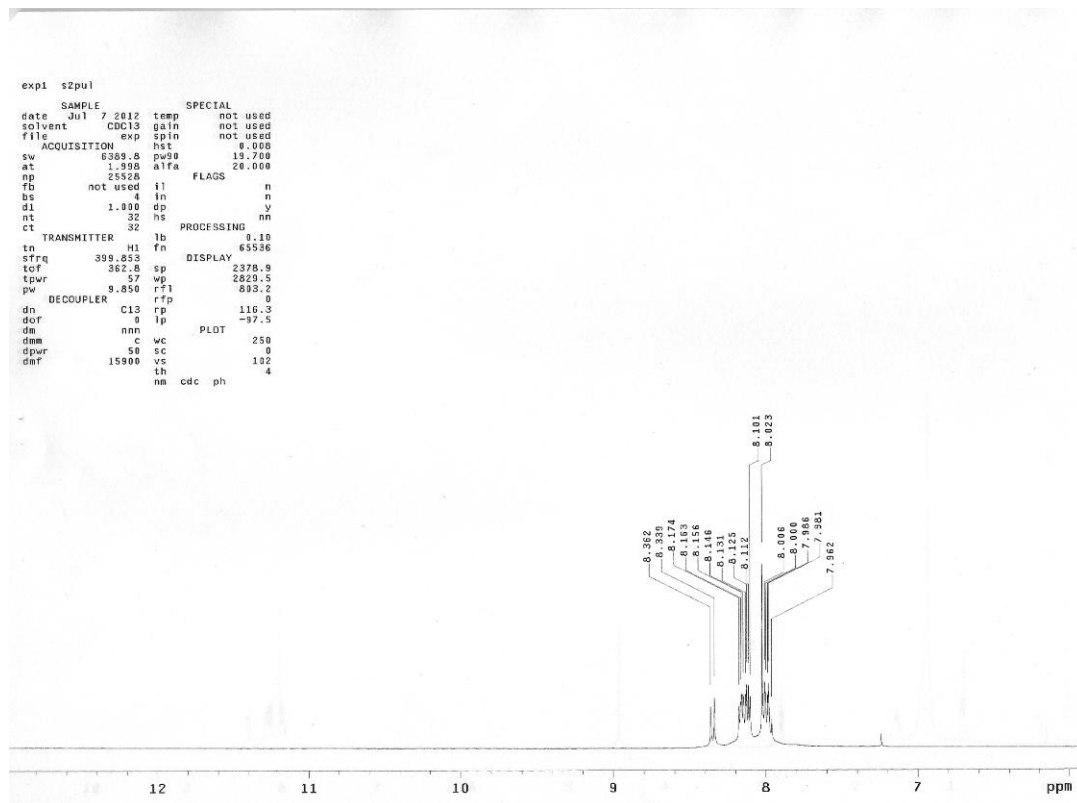
**Elem. Anal.:**  $\text{C}_{29}\text{H}_{35}\text{N}$  (397.59): calcd. C 87.60, H 8.87, N 3.52; found C 87.65, H 8.85, N 3.49.



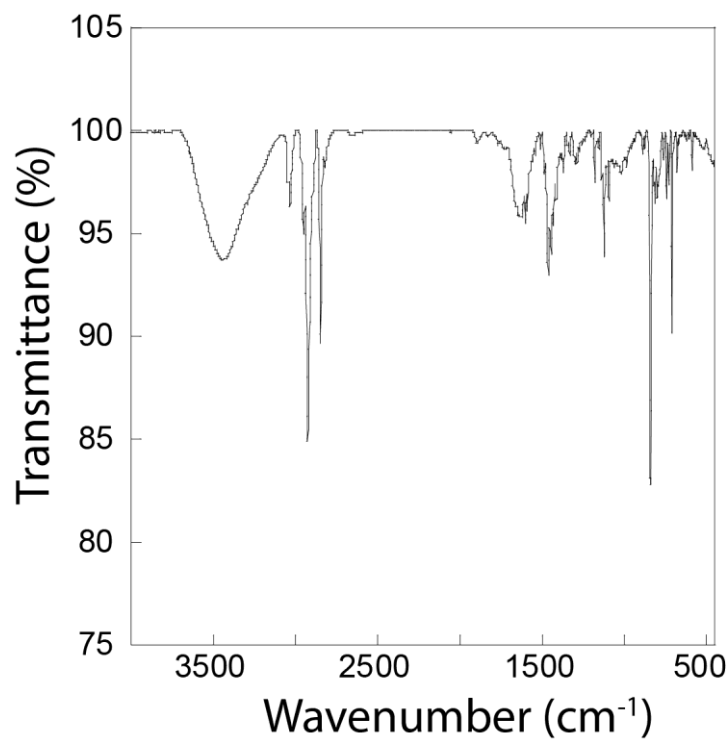
**Figure S9:**  $^1\text{H}$  NMR spectra of intermediate **I**<sub>2</sub> in  $\text{CDCl}_3$ .



**Figure S10:**  $^1\text{H}$  NMR spectra (extended aliphatic region) of intermediate **I<sub>2</sub>** in  $\text{CDCl}_3$ .



**Figure S11:**  $^1\text{H}$  NMR spectra (extended aromatic region) of intermediate **I<sub>2</sub>** in  $\text{CDCl}_3$ .

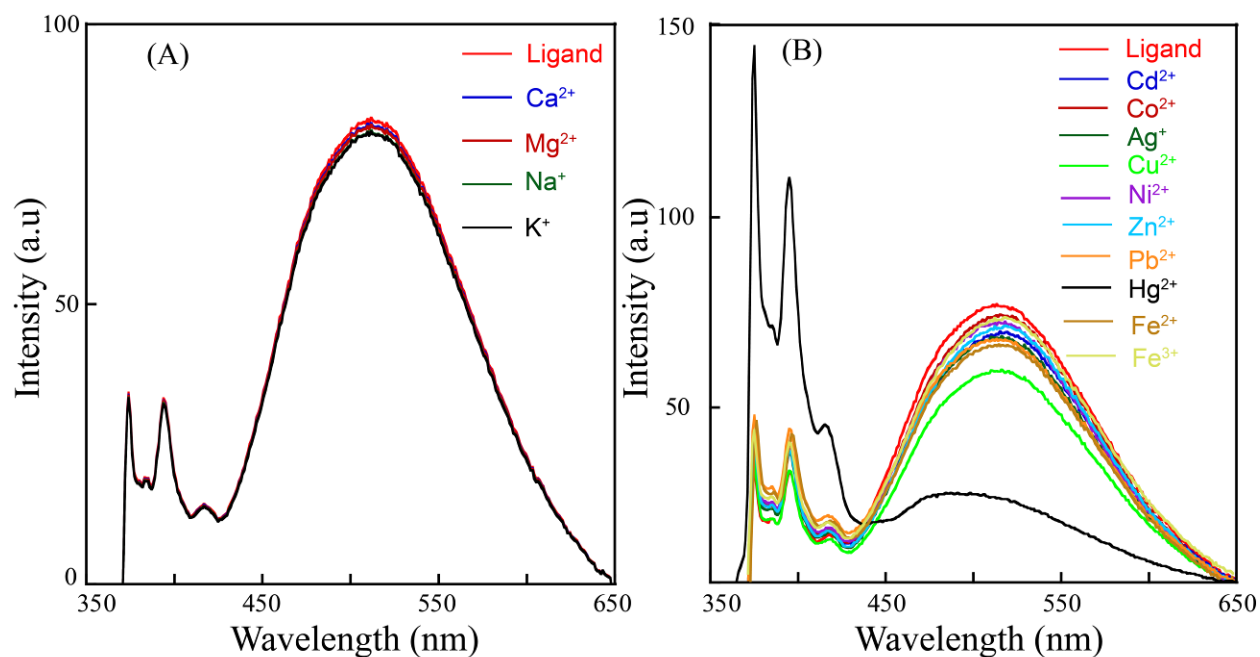


**Figure S12:** FTIR spectra of intermediate **I<sub>2</sub>**.

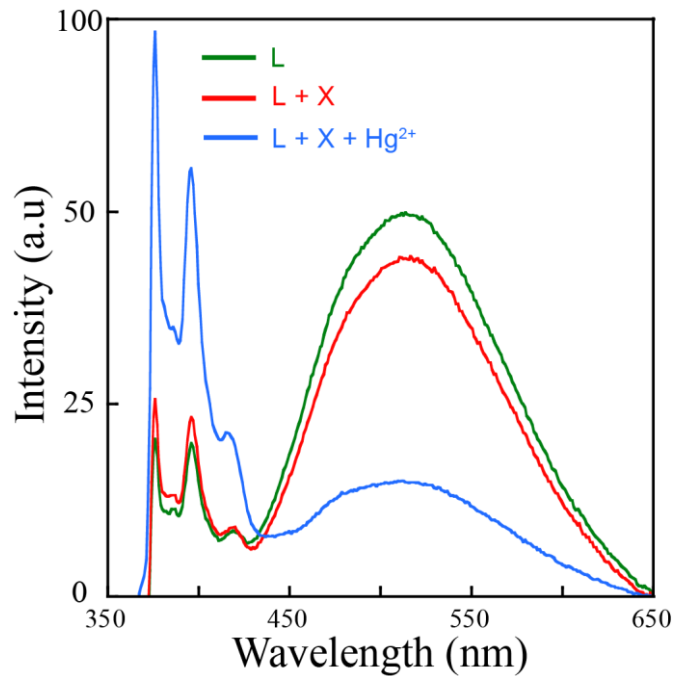
**Mass of I<sub>2</sub>:**  $m/z$  calcd. for  $[\text{I}_2+\text{H}]$  is 400.3004 found 400.3004 (mass spectrum obtained in positive mode).

**Elem. Anal.:**  $\text{C}_{29}\text{H}_{37}\text{N}$  (399.61): calcd. C 87.16, H 9.33, N 3.51; found C 87.18, H 9.38, N 3.48.

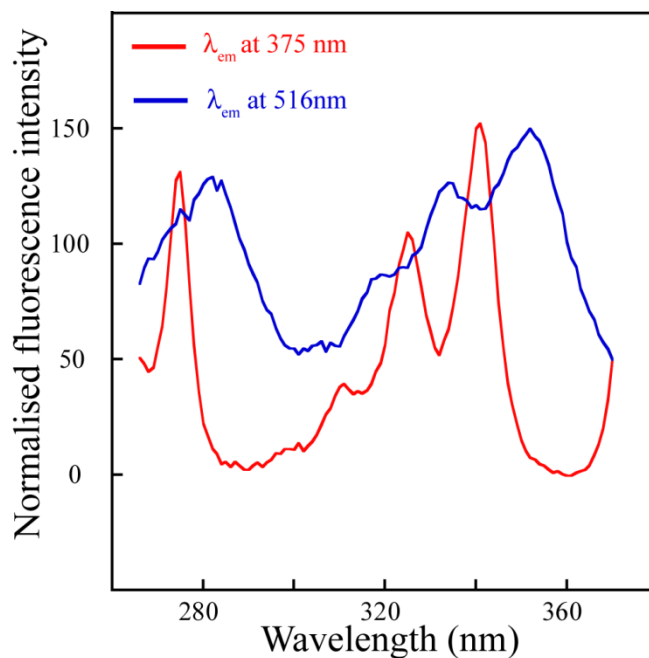




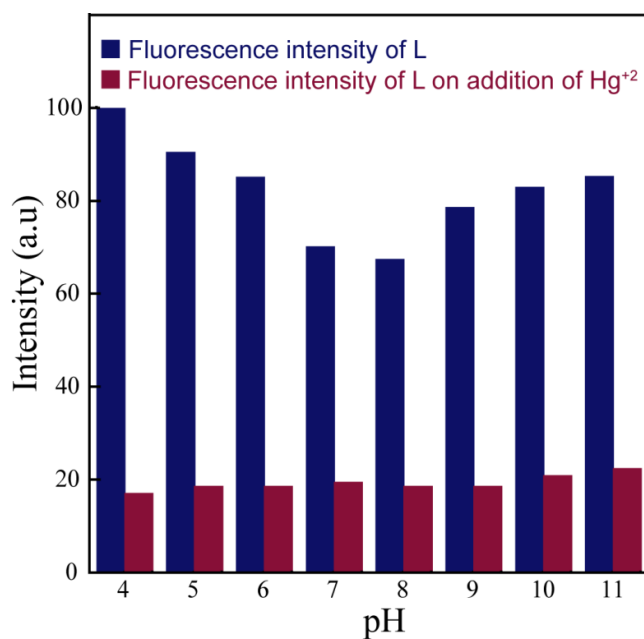
**Figure S13:** Emission spectra of **L** in water/DMSO (9.5:0.5, v/v) (10 μM) in presence of various metal ion in excess (50 μM).



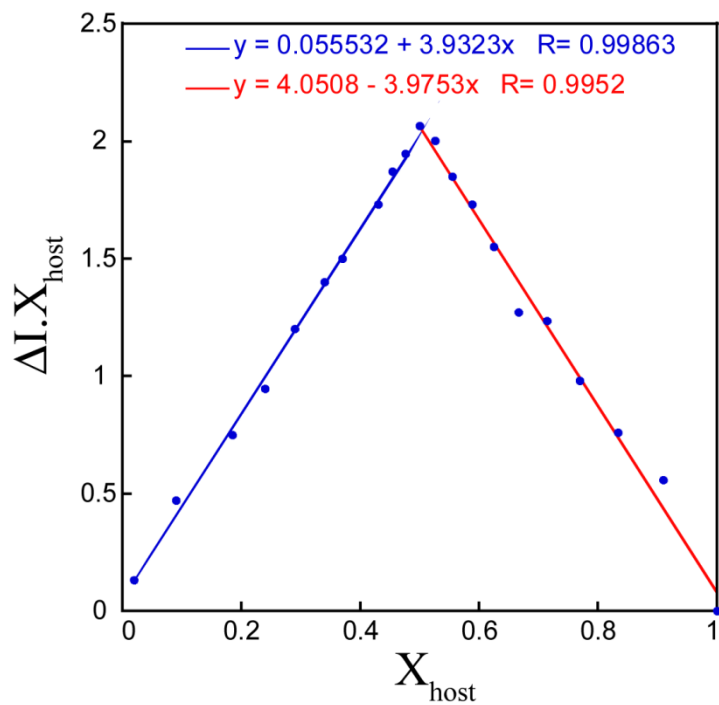
**Figure S14:** Emission spectra of **L** (10  $\mu\text{M}$ ) in the presence of the  $\text{Hg}^{2+}$  ion and miscellaneous anions (X) including chloride, sulphate, carbonate, hydrogencarbonate, fluoride (as their corresponding Sodium salt) respectively.



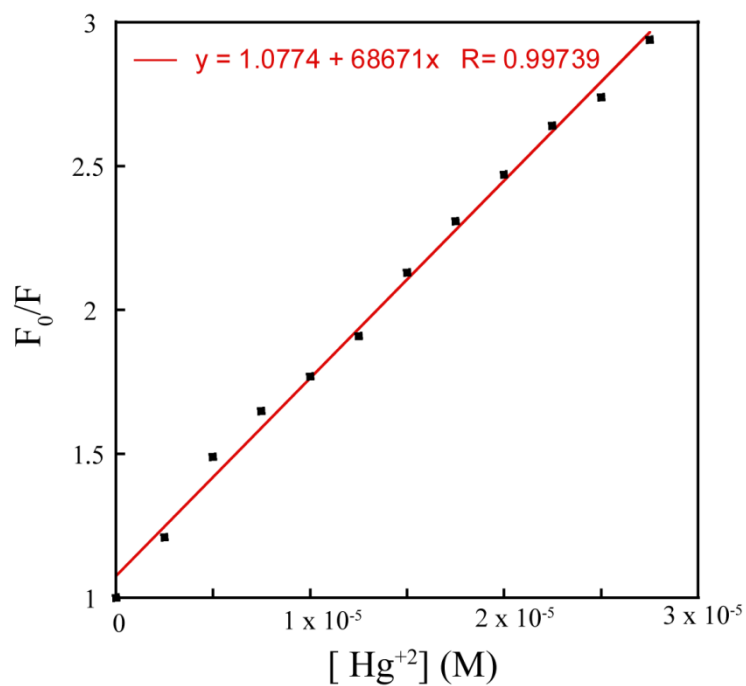
**Figure S15:** Excitation spectra (normalized) of **L** monitored at 376 (red line) and 516 (blue line).



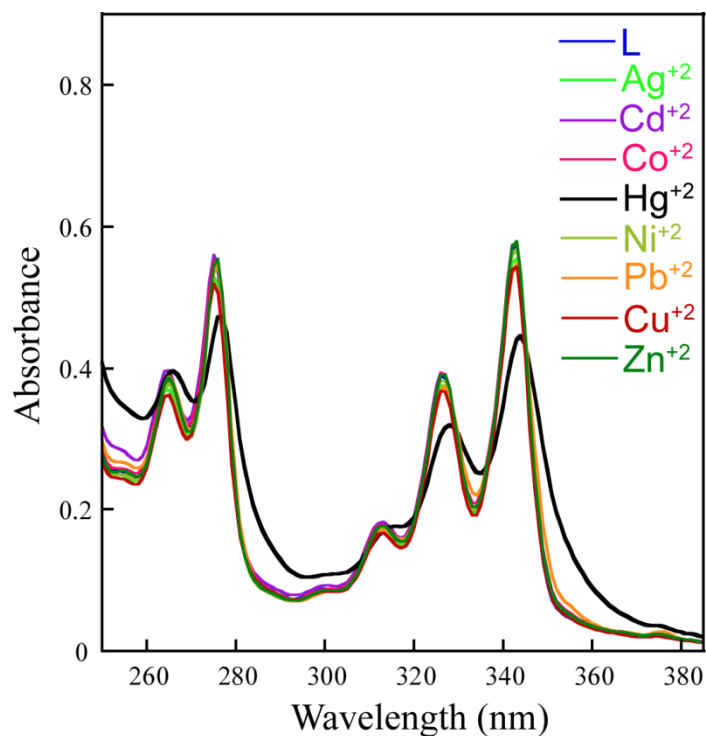
**Figure S16:** Change in fluorescence intensity of **L** (25  $\mu\text{M}$ ) on addition of one equivalent of  $\text{Hg}^{2+}$  at different pH.



**Figure S17:** Job's plot from fluorescence titration of L.  $X_{\text{host}}$  is the mole fraction of the host (L),  $\Delta I$  is the change in fluorescence intensity.



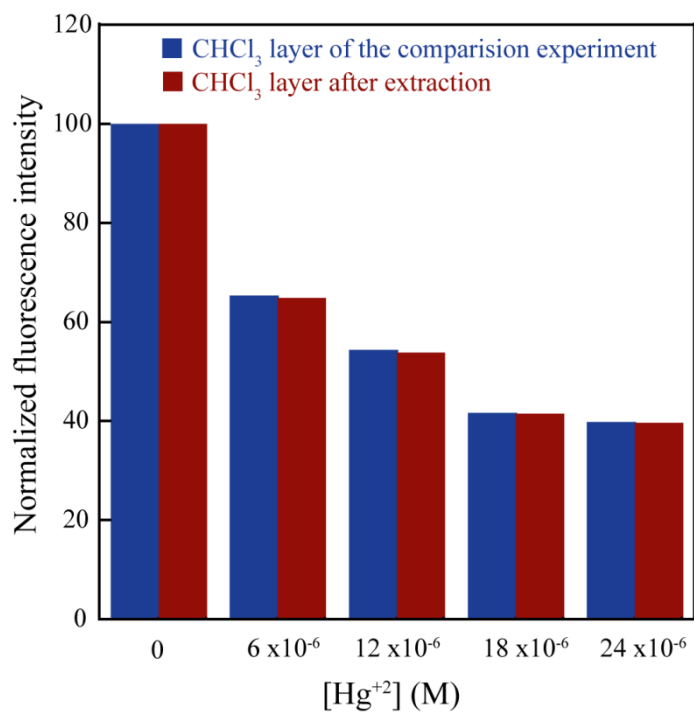
**Figure S18:** Stern-Volmer plot for calculation of  $K_{\text{SV}}$ .



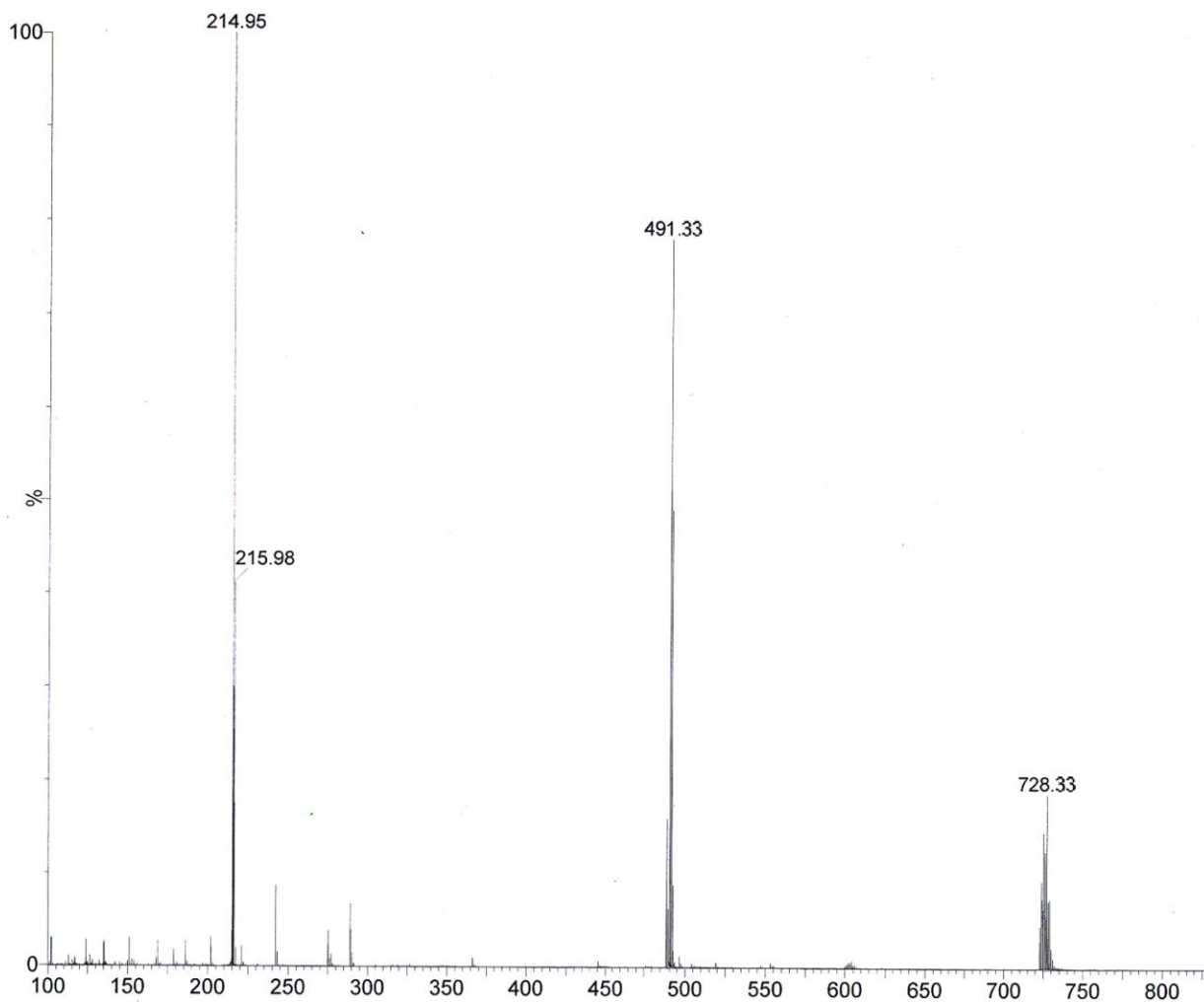
**Figure S19:** Absorption spectra of **L** in water/DMSO (9.5:0.5, v/v) (25  $\mu$ M) in presence of various metal ions (5 eqv.)

### **Measurement of Extraction efficiency of L:**

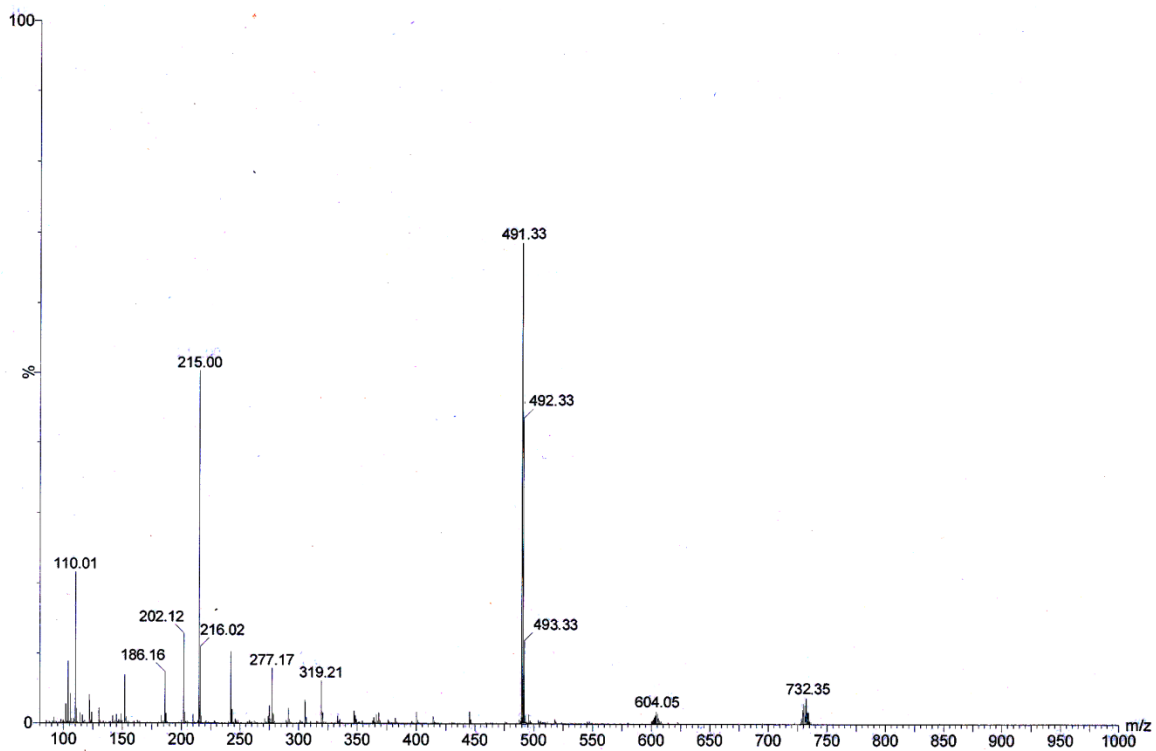
Known concentration of  $\text{Hg}(\text{NO}_3)_2$  dissolved in MeOH solution was treated with  $\text{CHCl}_3$  (15 ml) solution of **L** to record the electronic spectra, then identical concentration of the aqueous solution of  $\text{Hg}(\text{NO}_3)_2$  was extracted several times (three times) with the  $\text{CHCl}_3$  solution of **L**. All non-aqueous layer were collected together, final volume was adjusted to 15 ml and after that the emission spectra of the nonaqueous layer was recorded. emission at 516 nm was compared with the previous one to get the extraction efficiency, which was found to be above 99% in all the five different concentration of  $\text{Hg}^{2+}$  tried.



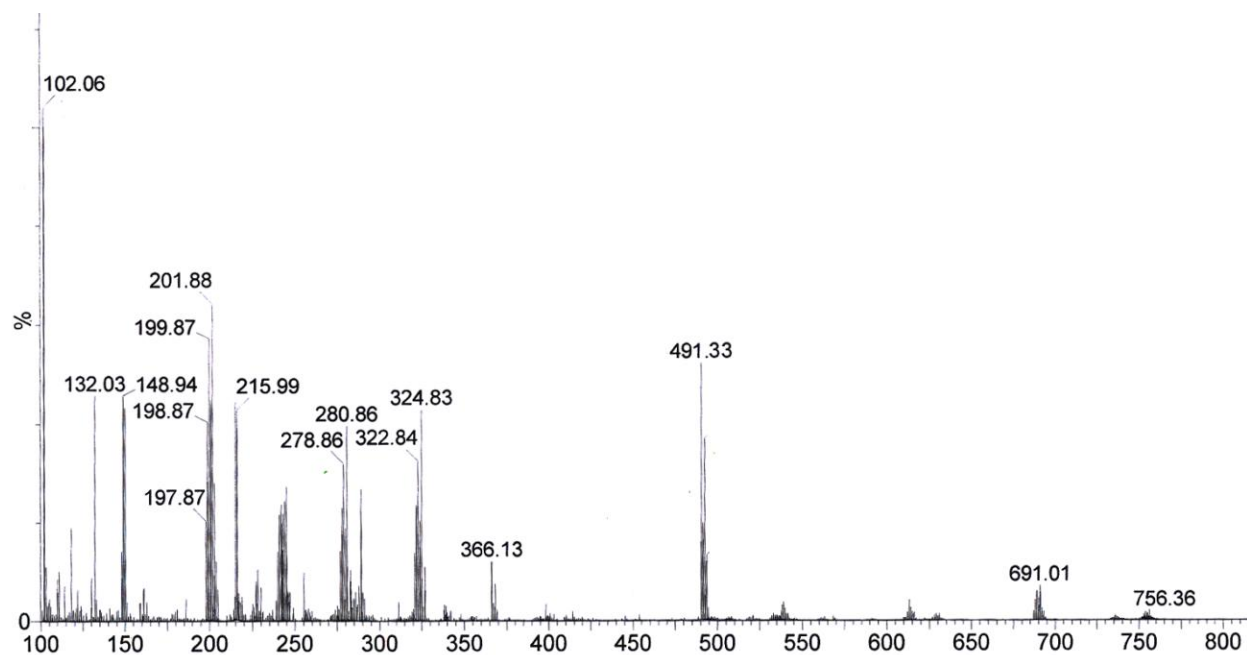
**Figure S20:** measurement of extraction efficiency.



**Figure S21** Mass spectra of the **L-Hg-2H<sub>2</sub>O (728.33)** complex, observed from the extracted **CHCl<sub>3</sub>** solution.

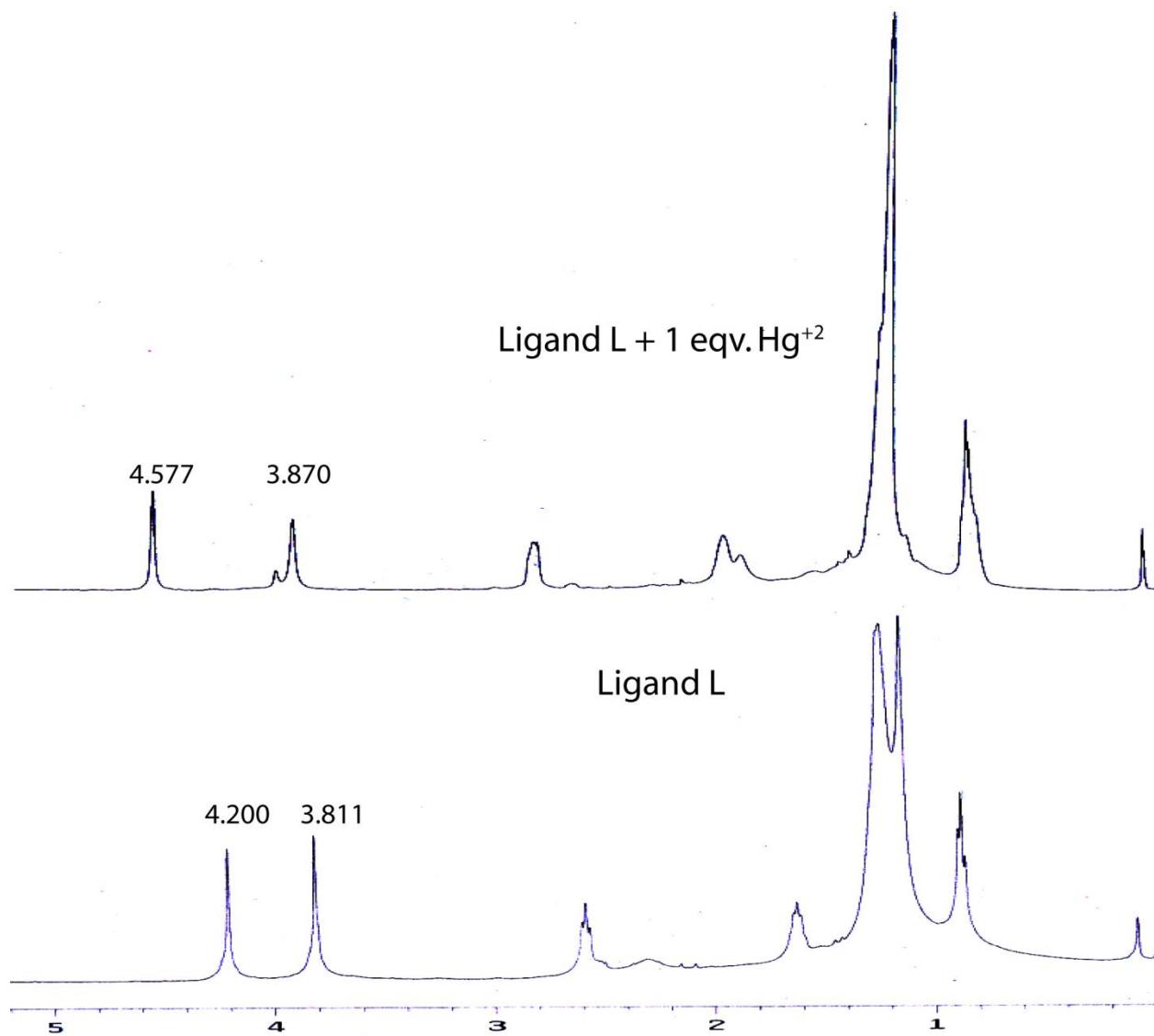


**Figure S22** Mass spectra of the L-Hg-2D<sub>2</sub>O (732.35) complex, observed from the extracted CDCl<sub>3</sub> solution of the <sup>1</sup>H NMR experiment.

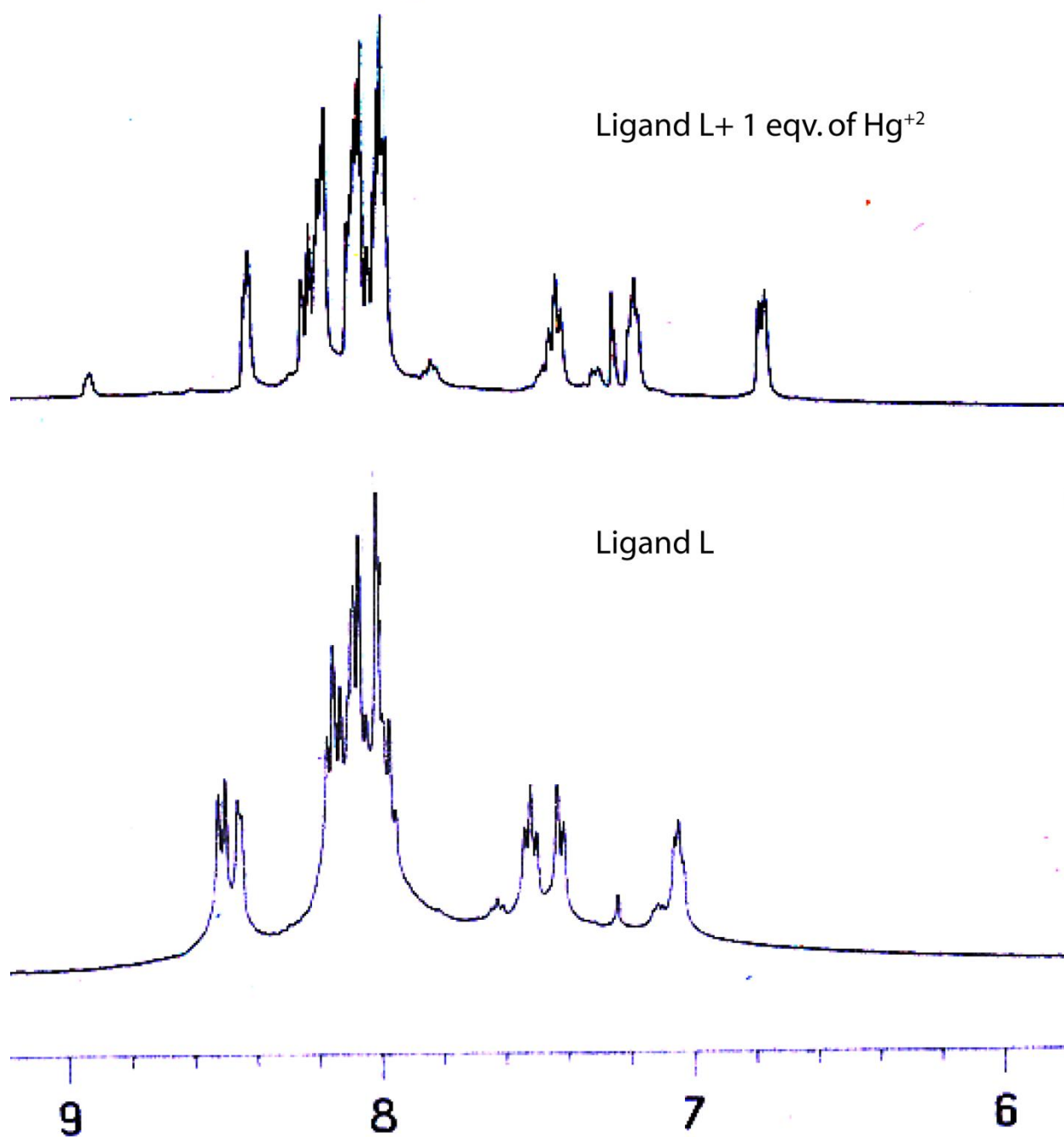


**Figure S23** Mass spectra of the L-Hg-2MeOH (756.36) complex, observed when the complexation is done in MeOH.

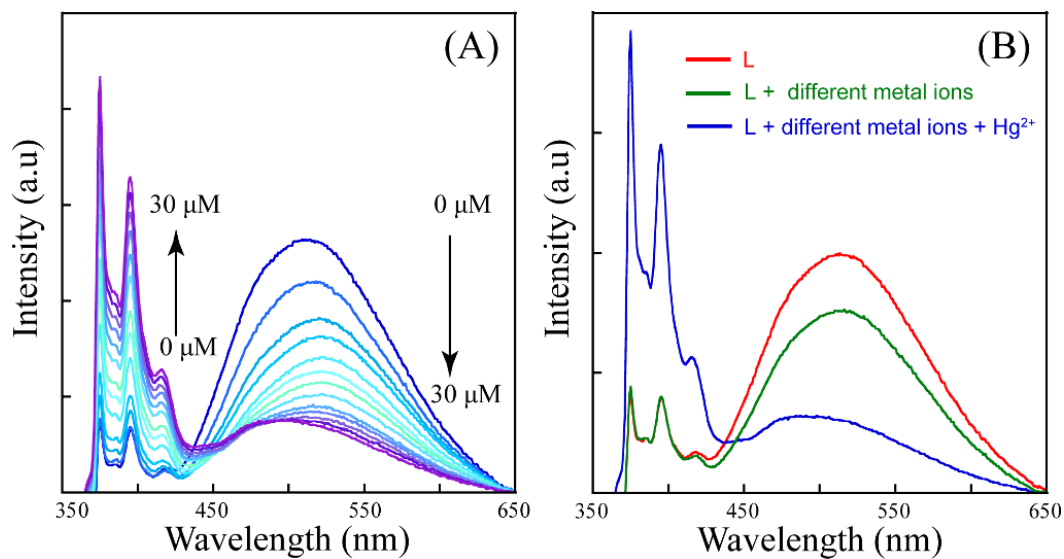




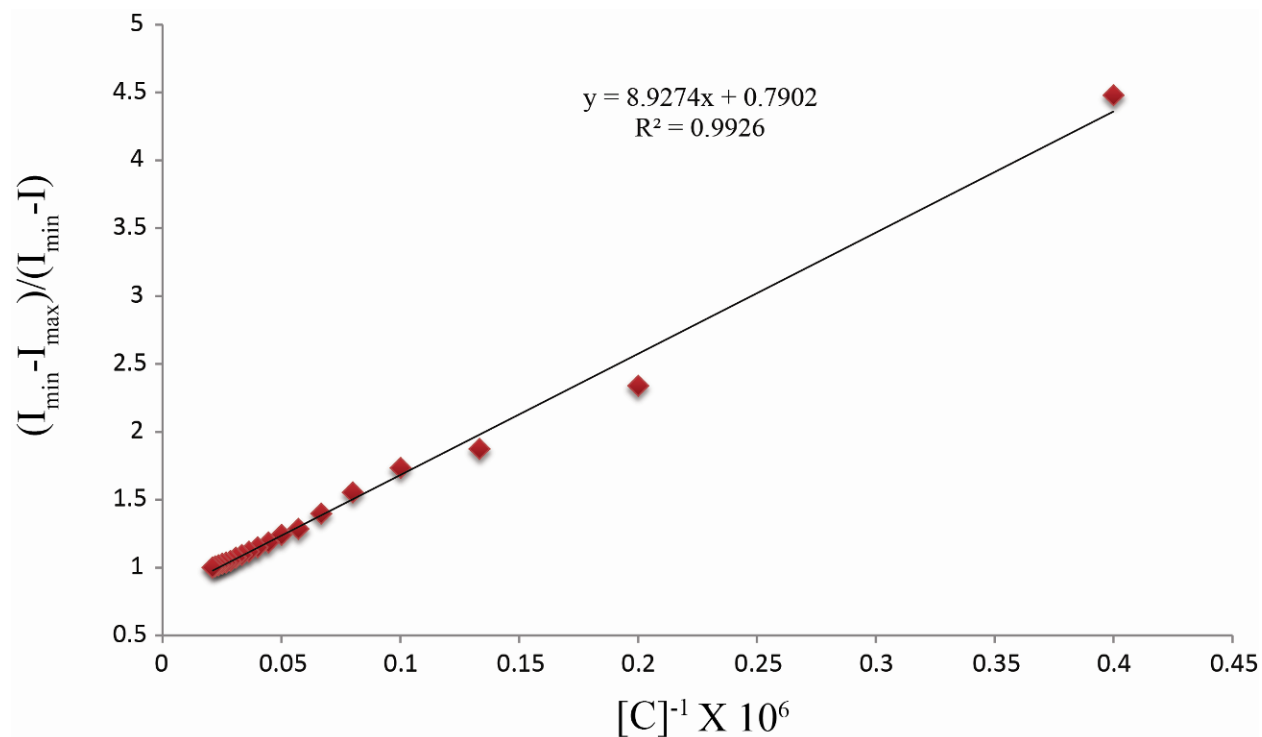
**Figure S24:** Shift in the aliphatic region of the <sup>1</sup>H NMR spectra of **L** (CDCl<sub>3</sub>) after addition of 1 equivalent of Hg(NO<sub>3</sub>)<sub>2</sub> salts ( in CD<sub>3</sub>OD).



**Figure S25:** Shift in the aromatic region of the  $^1\text{H}$  NMR spectra of **L** ( $\text{CDCl}_3$ ) after addition of 1 equivalent of  $\text{Hg}(\text{NO}_3)_2$  salts (in  $\text{CD}_3\text{OD}$ ).



**Figure S26:** (A) Emission spectra of **L** in water/DMSO (9.5:0.5, v/v) (25 μM) on gradual addition of Hg<sup>2+</sup> (0 to 30 μM as nitrate salt) (B) Emission spectra of **L** in water/DMSO (9.5:0.5, v/v) (25 μM) in the presence of the Hg<sup>2+</sup> ion and miscellaneous cations (25 μM each) including Co<sup>2+</sup>, Ni<sup>2+</sup>, Cu<sup>2+</sup>, Zn<sup>2+</sup>, Ag<sup>+</sup>, Cd<sup>2+</sup>, Pb<sup>2+</sup>, Ca<sup>2+</sup>, Mg<sup>2+</sup>, Na<sup>+</sup>, K<sup>+</sup> and Hg<sup>2+</sup> respectively.



**Figure S27:** Calculation of binding constant from Benesi-Hildebrand curve.