

## Multi-responsive thiosemicarbazone-based probe for detection and discrimination of group 12 metal ions and its application in logic gate

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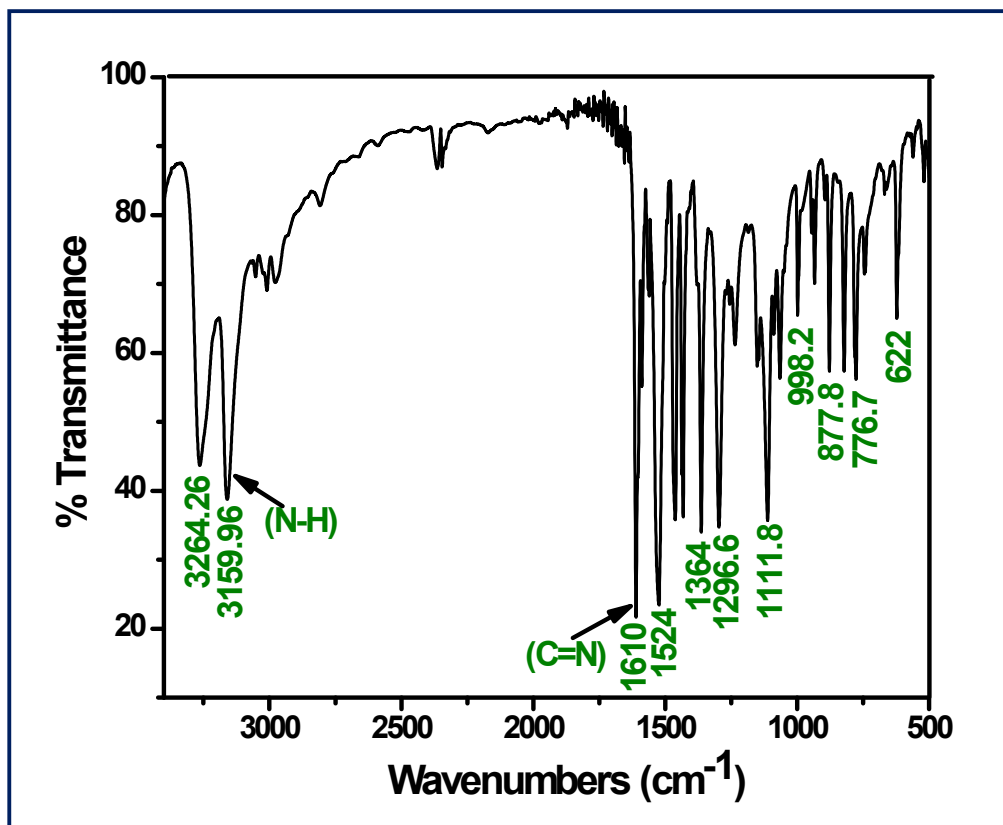
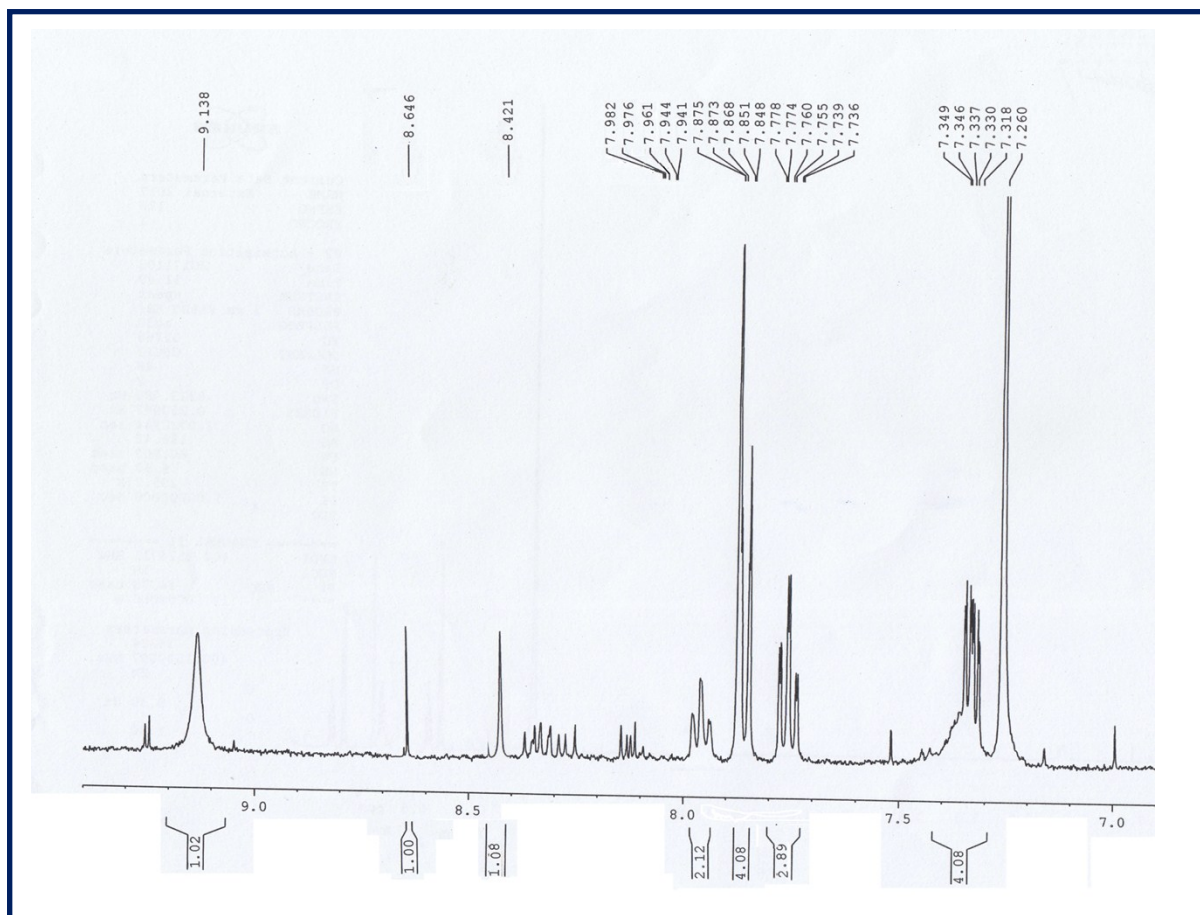
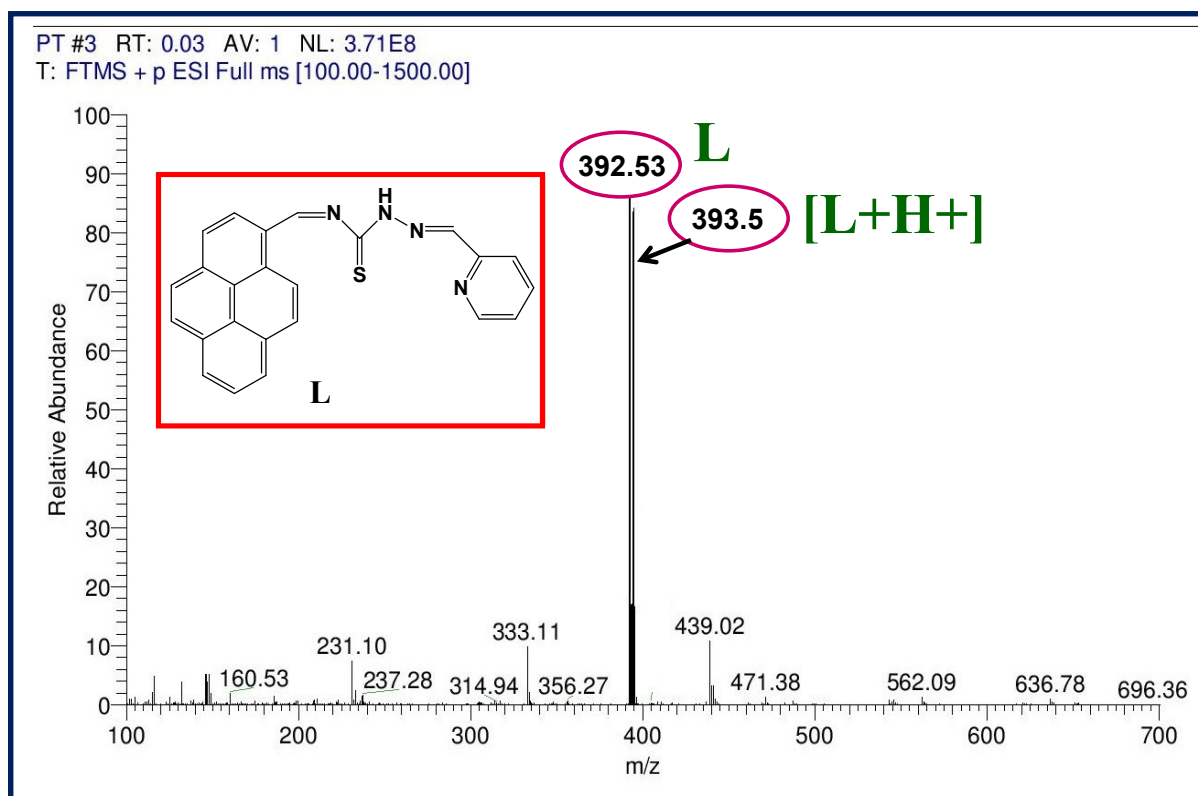


Fig. S1. FTIR spectrum of L.



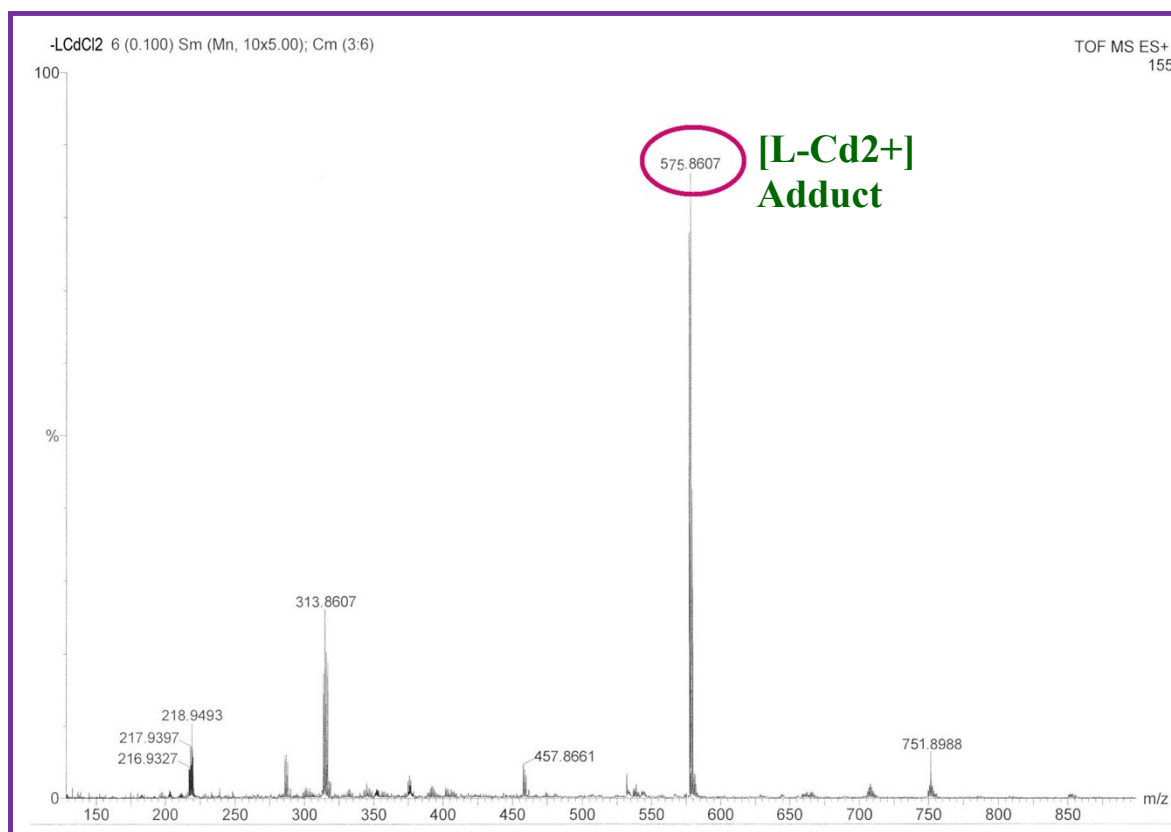
**Fig. S2.** <sup>1</sup>H NMR spectrum of L.



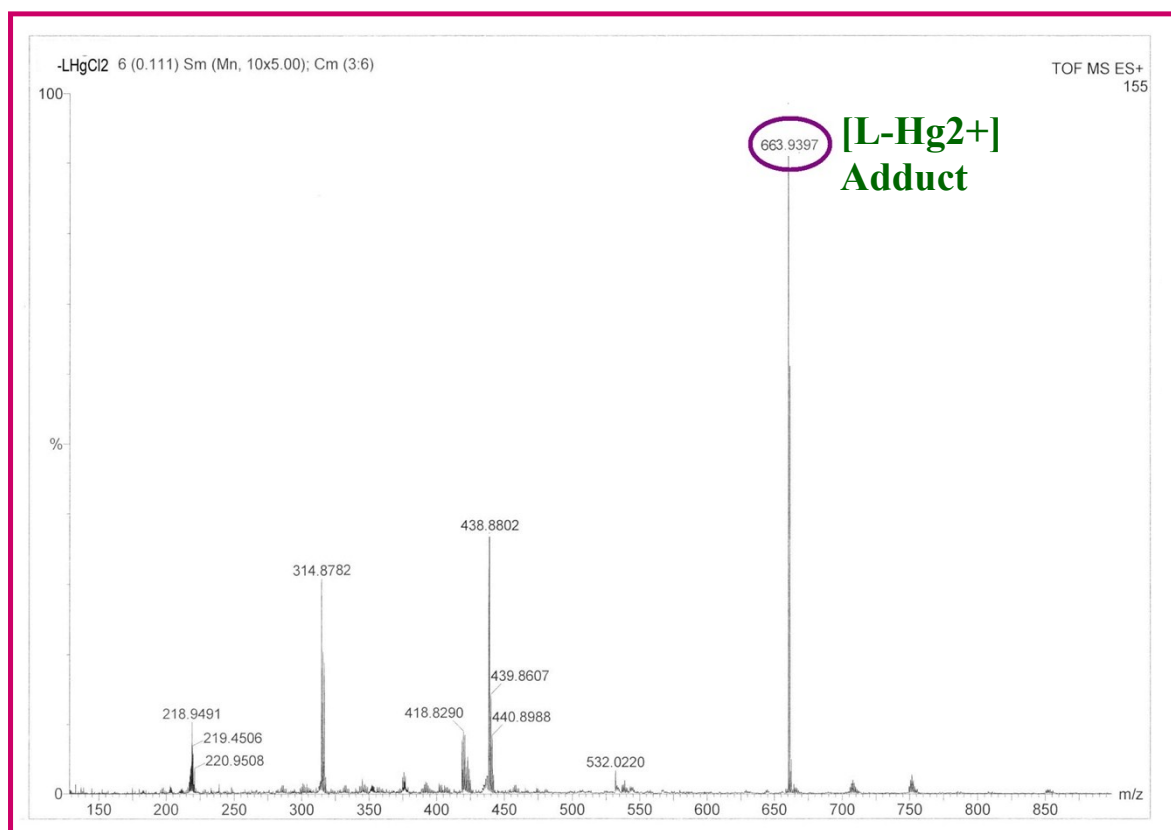
**Fig. S3.** Mass spectrum of **L**.



**Fig. S4.** Mass spectrum of  $[\text{L-Zn}^{2+}]$  adduct.



**Fig. S5.** Mass spectrum of [L-Cd<sup>2+</sup>] adduct.



**Fig. S6.** Mass spectrum of [L-Hg<sup>2+</sup>] adduct.

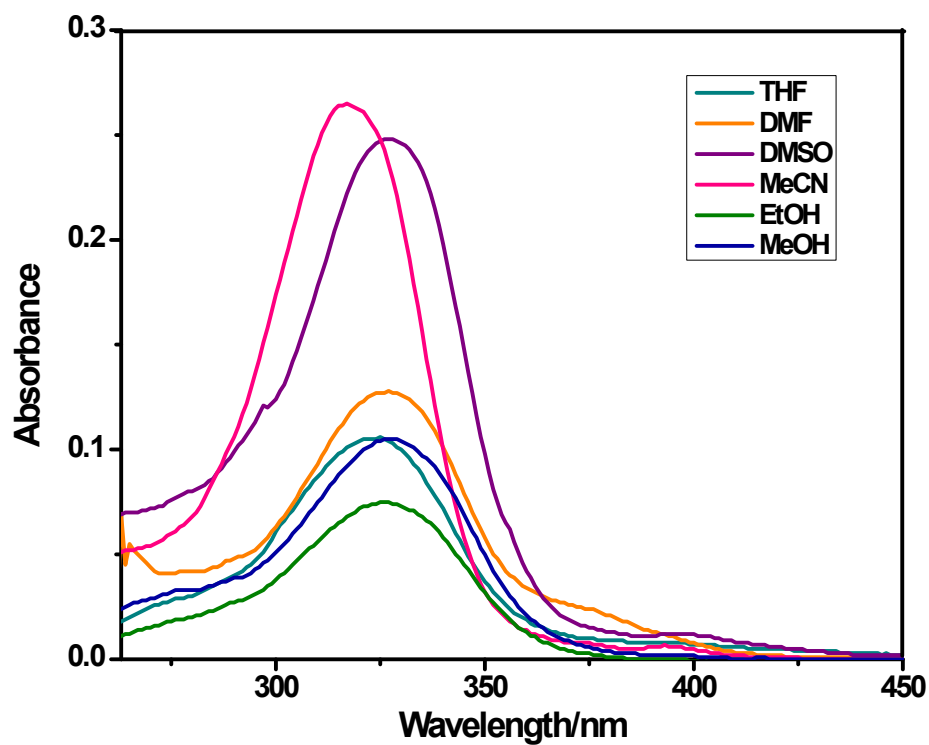


Fig. S7. UV-Vis absorption spectra of L (5  $\mu\text{M}$ ) in different solvents.

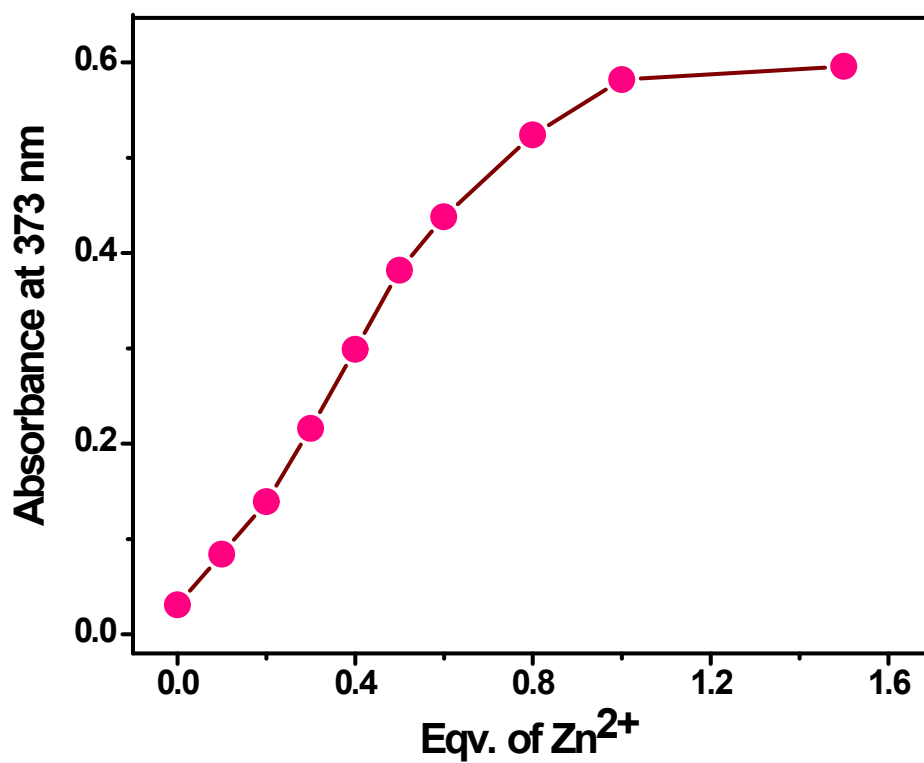


Fig. S8. Changes of absorbance at  $\lambda_{\text{max}} = 373 \text{ nm}$  as a function of equivalents of  $\text{Zn}^{2+}$ .

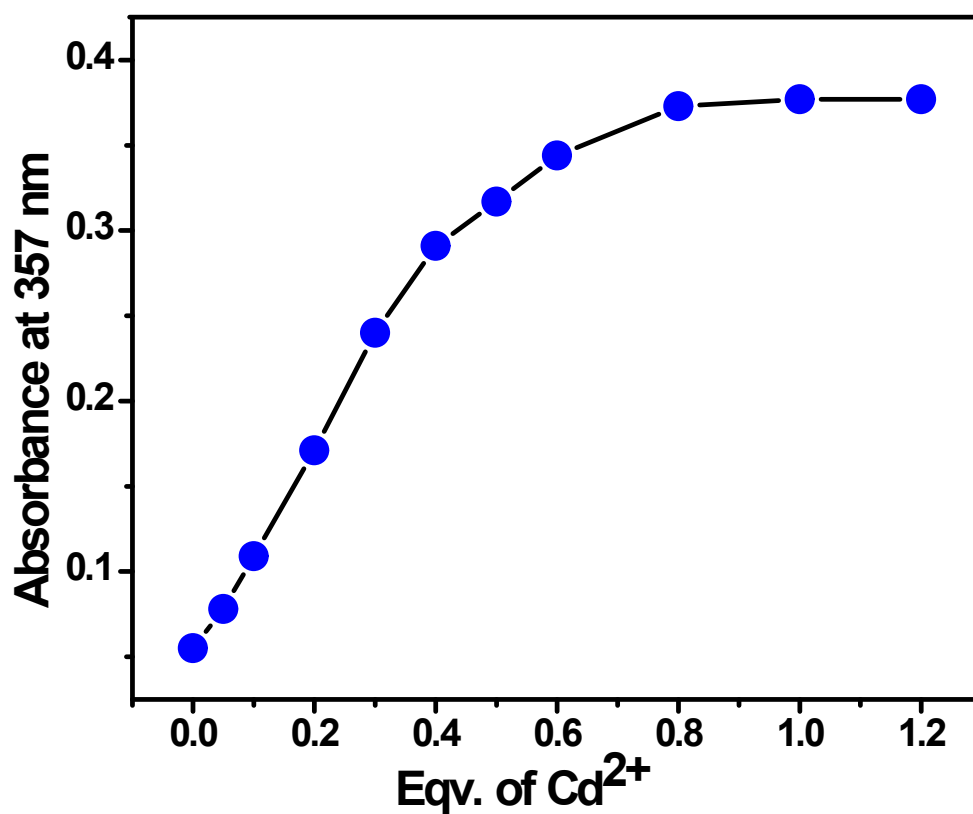


Fig. S9. Changes of absorbance at  $\lambda_{\text{max}} = 357$  nm as a function of equivalents of Cd<sup>2+</sup>.

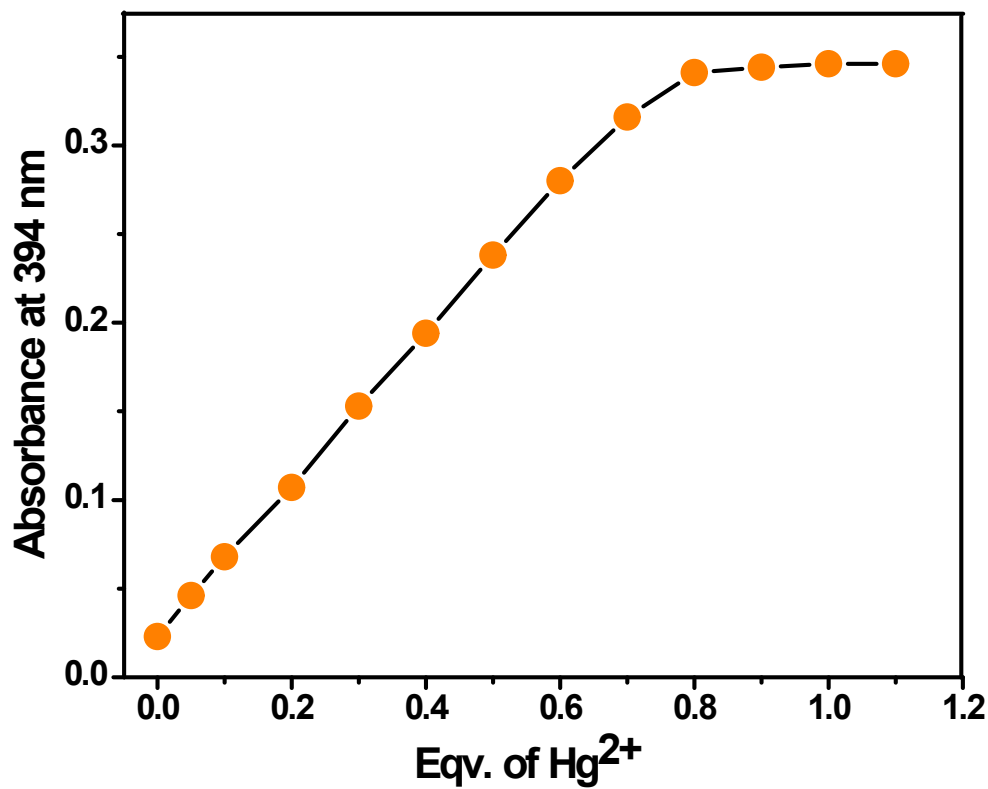


Fig. S10. Changes of absorbance at  $\lambda_{\text{max}} = 394$  nm as a function of equivalents of Hg<sup>2+</sup>.

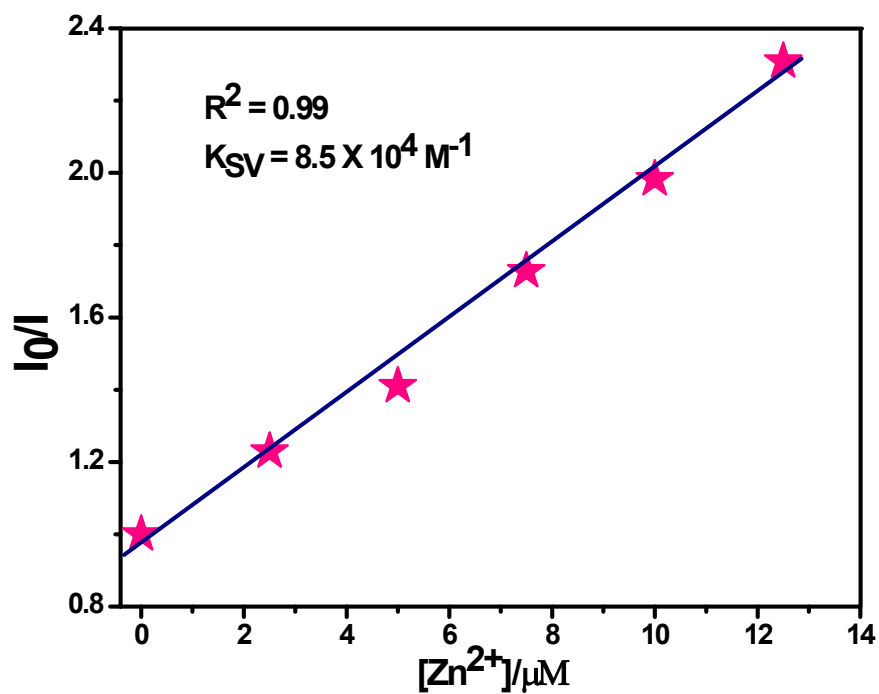


Fig. S11. Stern–Volmer plot for **L** as a function of  $Zn^{2+}$  concentration.

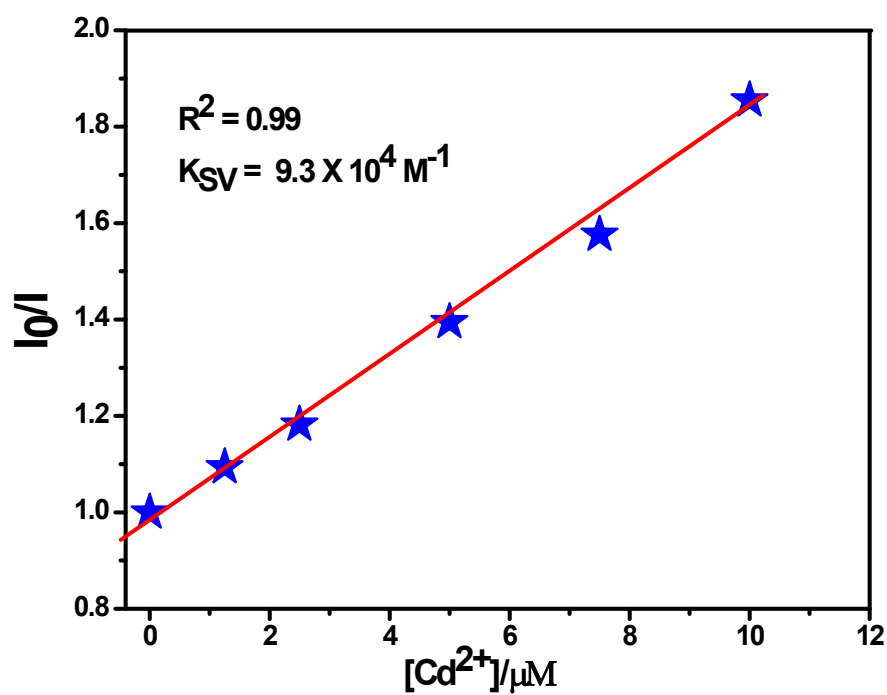


Fig. S12. Stern–Volmer plot for **L** as a function of  $Cd^{2+}$  concentration.



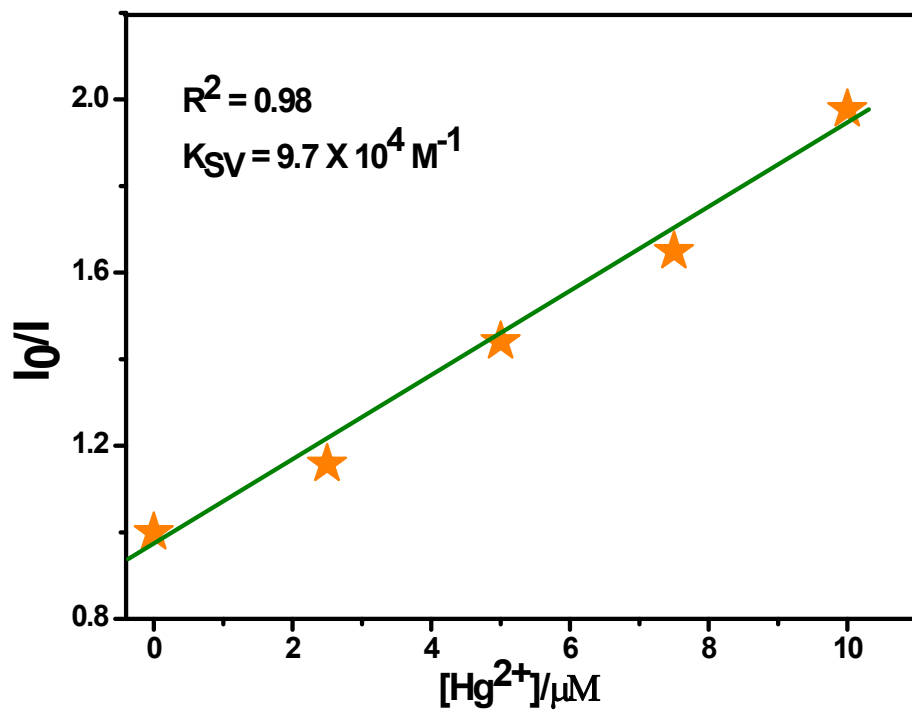


Fig. S13. Stern–Volmer plot for **L** as a function of  $\text{Hg}^{2+}$  concentration.

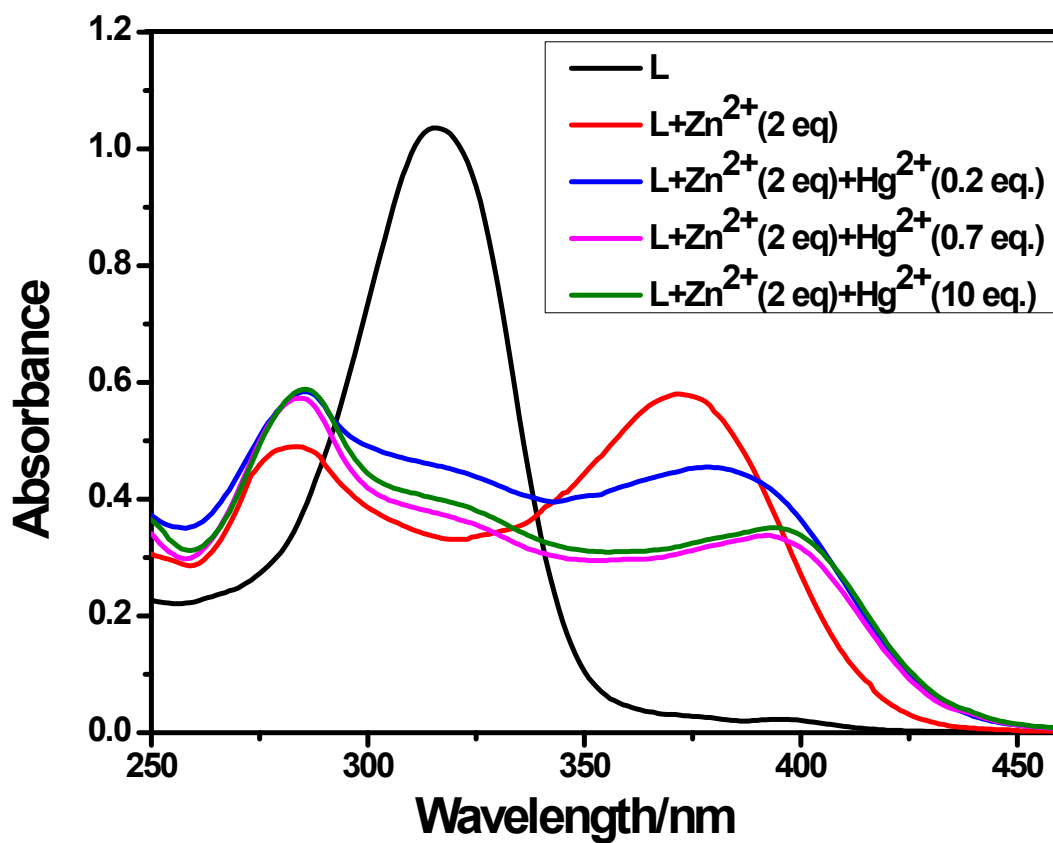
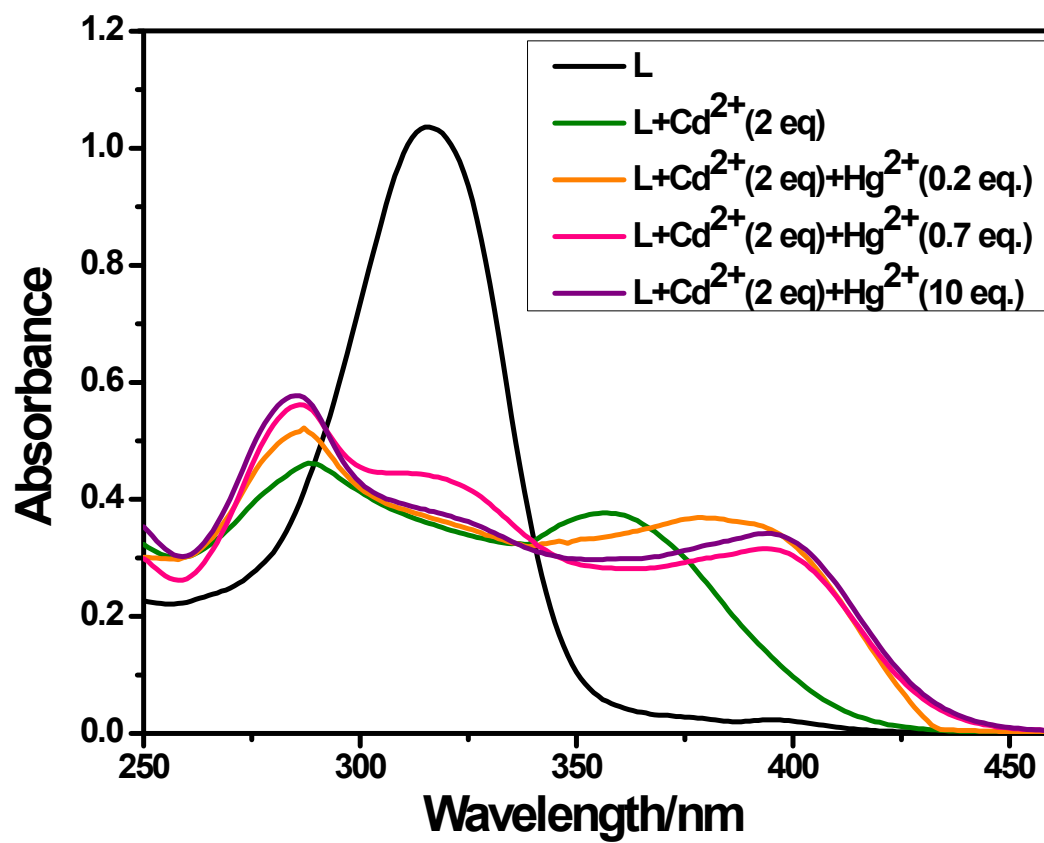
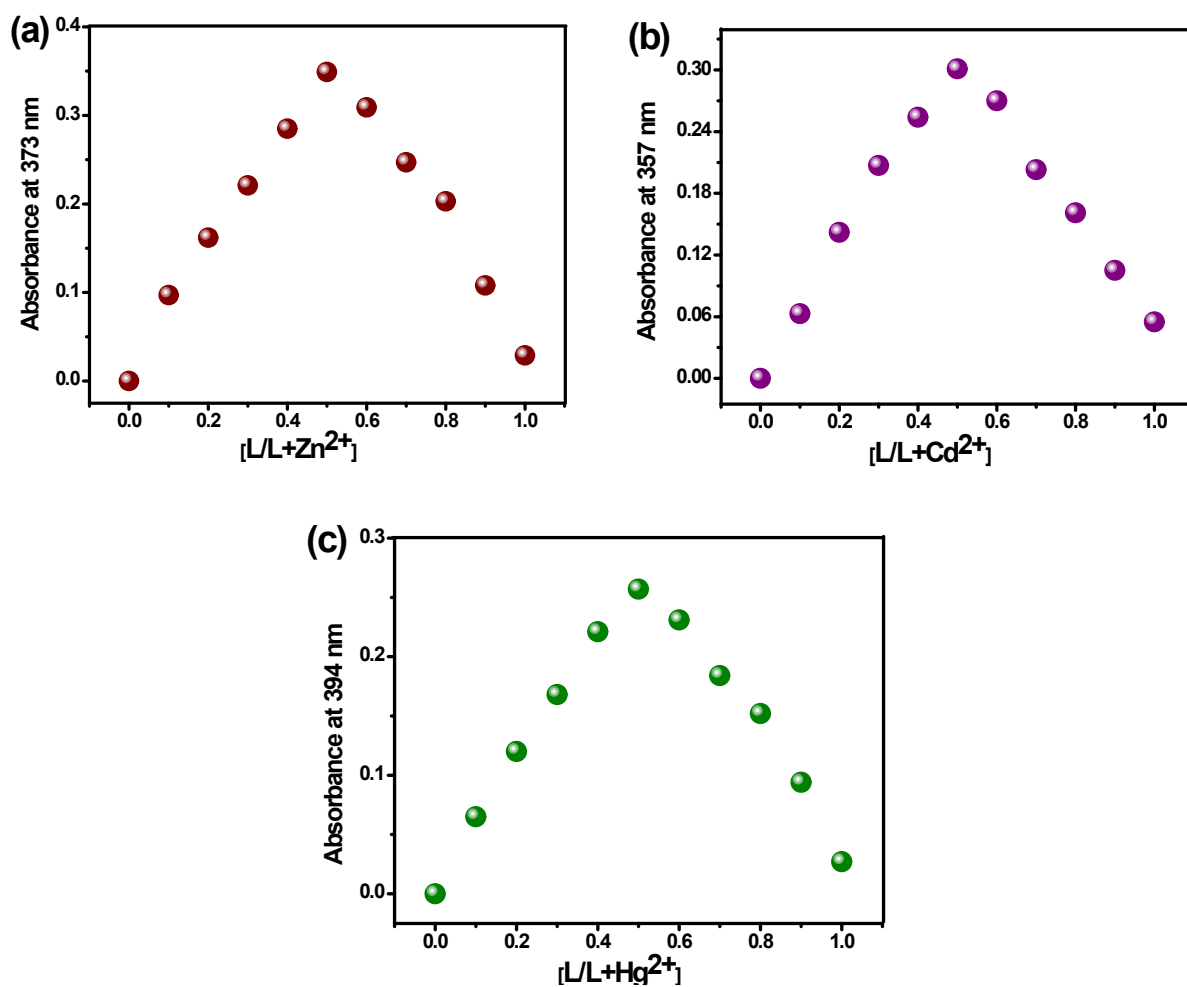


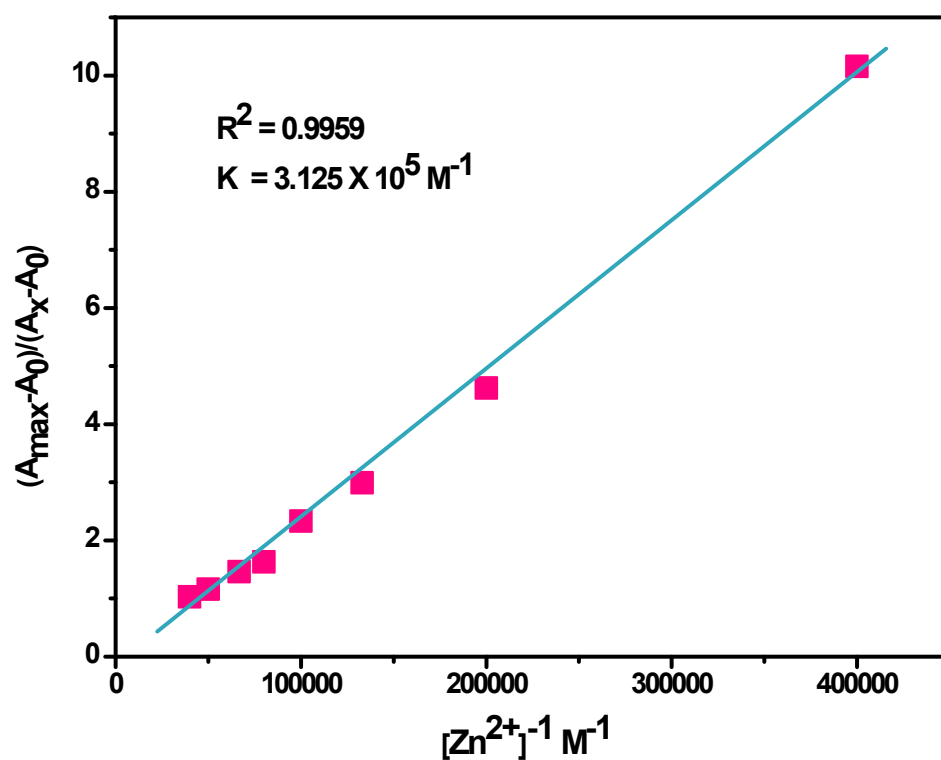
Fig. S14. Changes in the absorption spectra of  $[\text{L-Zn}^{2+}]$  adduct upon addition of  $\text{Hg}^{2+}$  in Tris buffered MeCN/ $\text{H}_2\text{O}$  (1:1, v/v, pH = 7) solution.



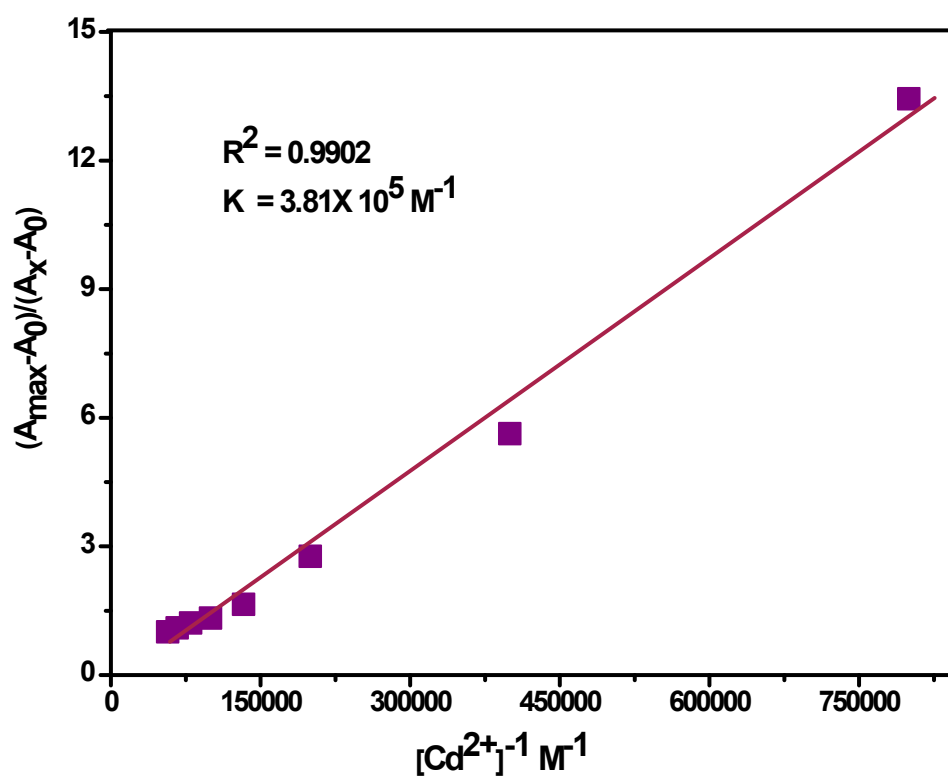
**Fig. S15.** Changes in the absorption spectra of [L-Cd<sup>2+</sup>] adduct upon addition of Hg<sup>2+</sup> in Tris buffered MeCN/H<sub>2</sub>O (1:1, v/v, pH = 7) solution.



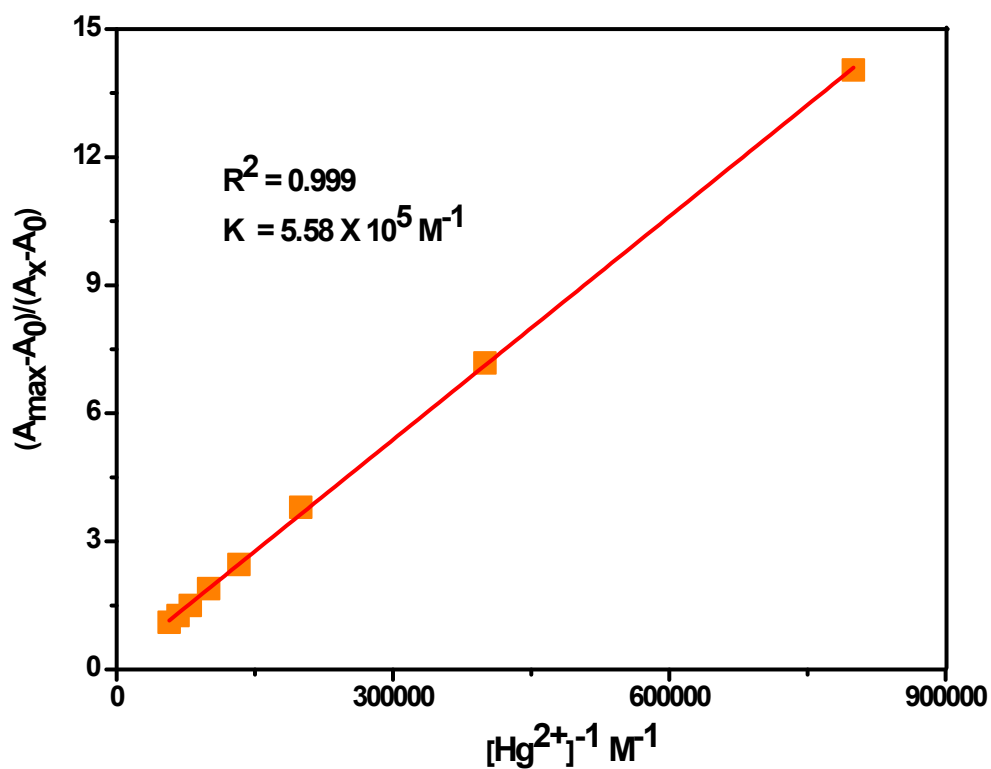
**Fig. S16.** Jobs plot for determining the stoichiometry of **L** and (a)  $\text{Zn}^{2+}$  adduct at  $\lambda_{\text{max}} = 373 \text{ nm}$ , (b)  $\text{Cd}^{2+}$  adduct at  $\lambda_{\text{max}} = 357 \text{ nm}$ , (c)  $\text{Hg}^{2+}$  adduct at  $\lambda_{\text{max}} = 394 \text{ nm}$  in Tris-HCl buffered (10 mM, pH=7) MeCN/ $\text{H}_2\text{O}$  (v/v = 1:1). Total concentration = 25  $\mu\text{M}$ .



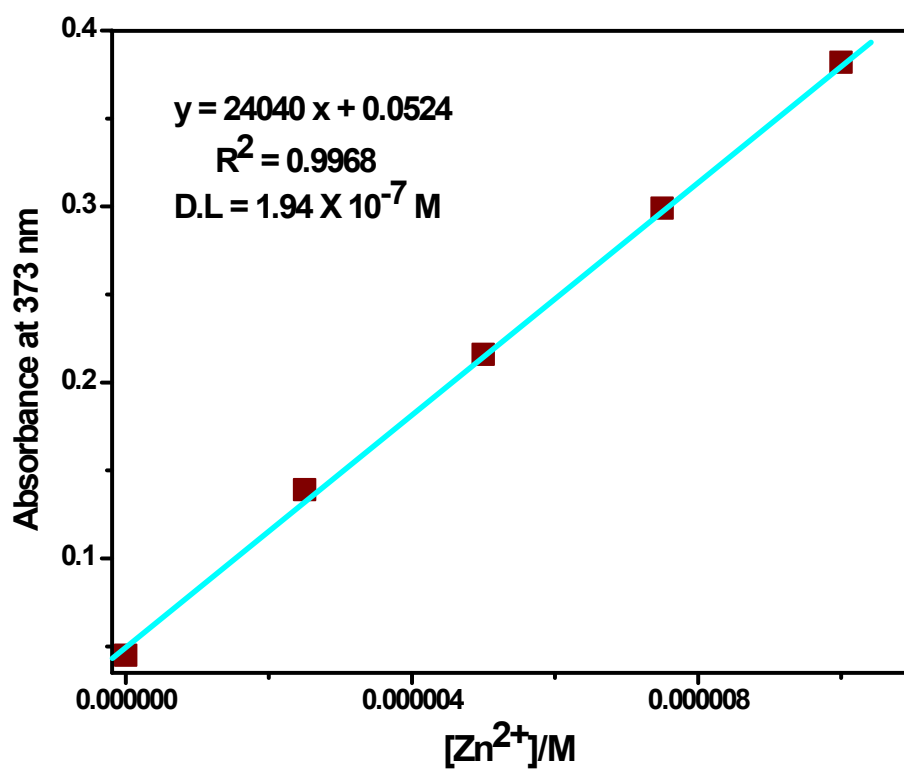
**Fig. S17.** Benesi-Hildebrand plot for determination of the binding constant of **L** with  $\text{Zn}^{2+}$  using the absorbance technique.



**Fig. S18.** Benesi-Hildebrand plot for determination of the binding constant of **L** with  $\text{Cd}^{2+}$  using the absorbance technique.



**Fig. S19.** Benesi-Hildebrand plot for determination of the binding constant of **L** with  $\text{Hg}^{2+}$  using the absorbance technique.



**Fig. S20.** The detection limit of **L** for  $\text{Zn}^{2+}$  by absorbance technique.

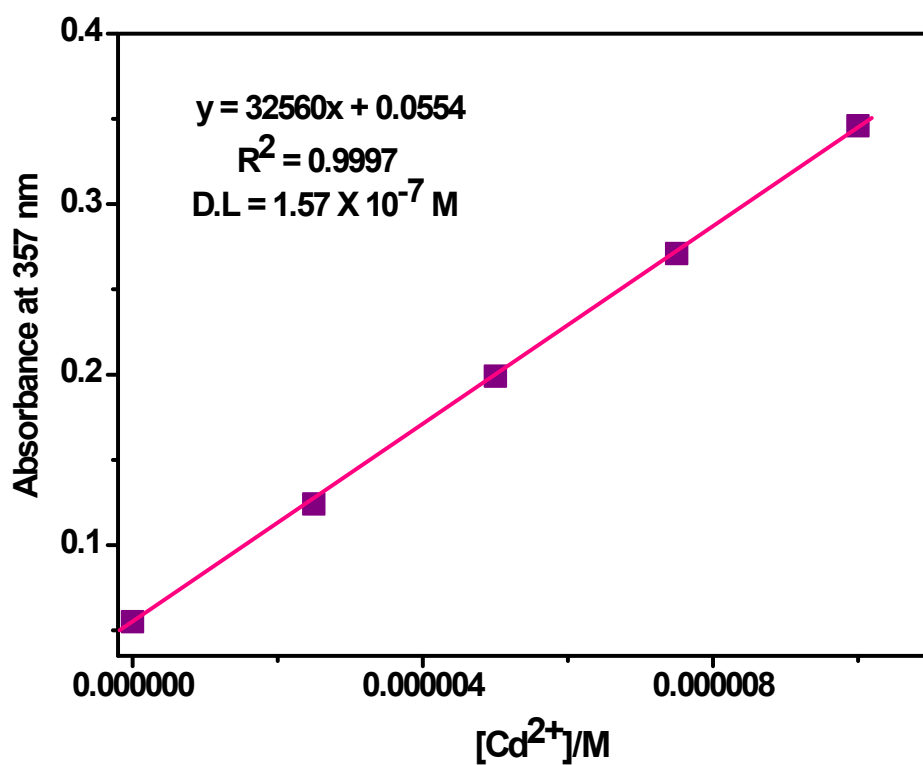


Fig. S21. The detection limit of L for  $\text{Cd}^{2+}$  by absorbance technique.

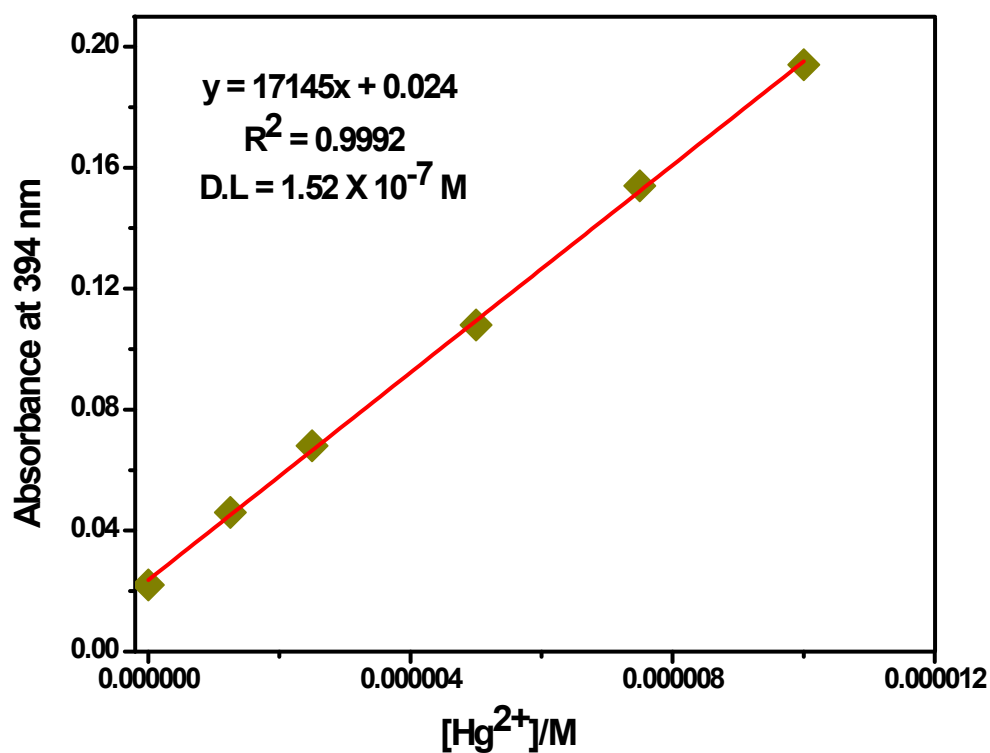
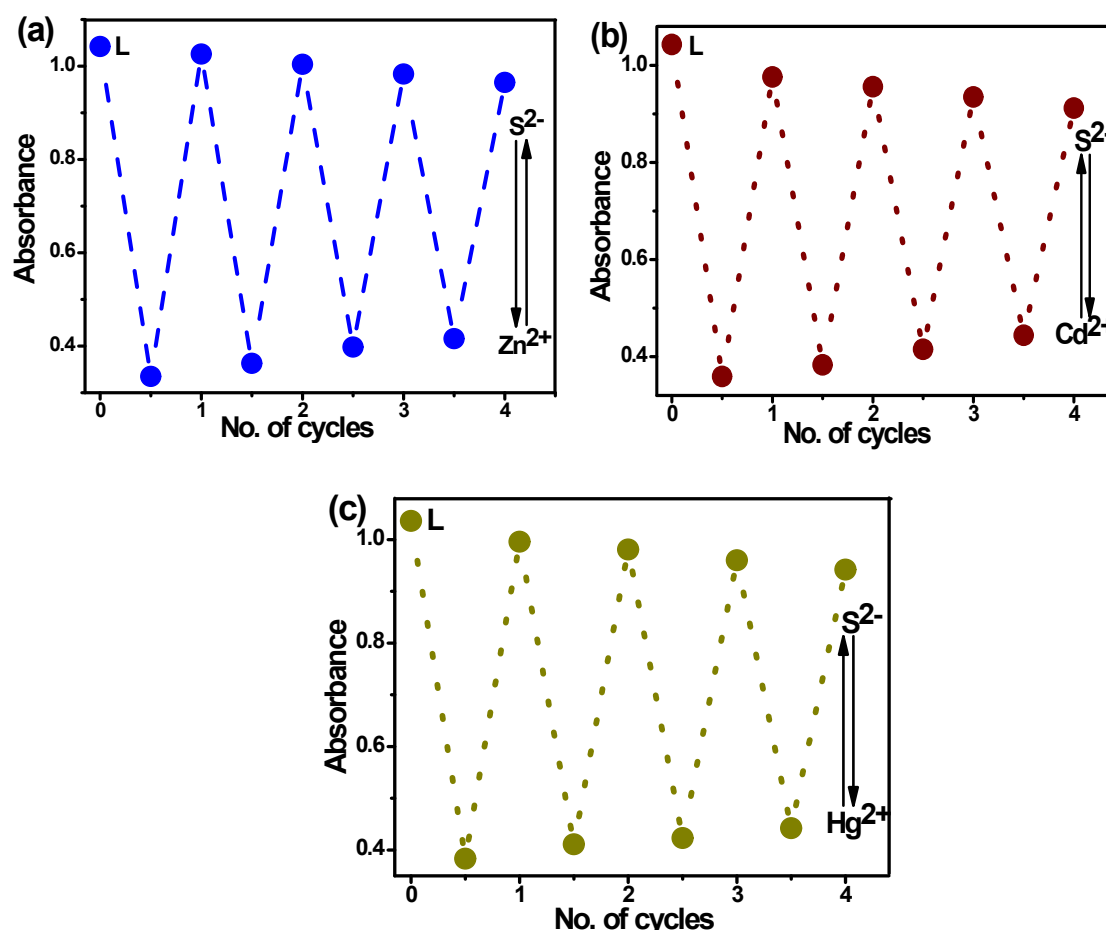
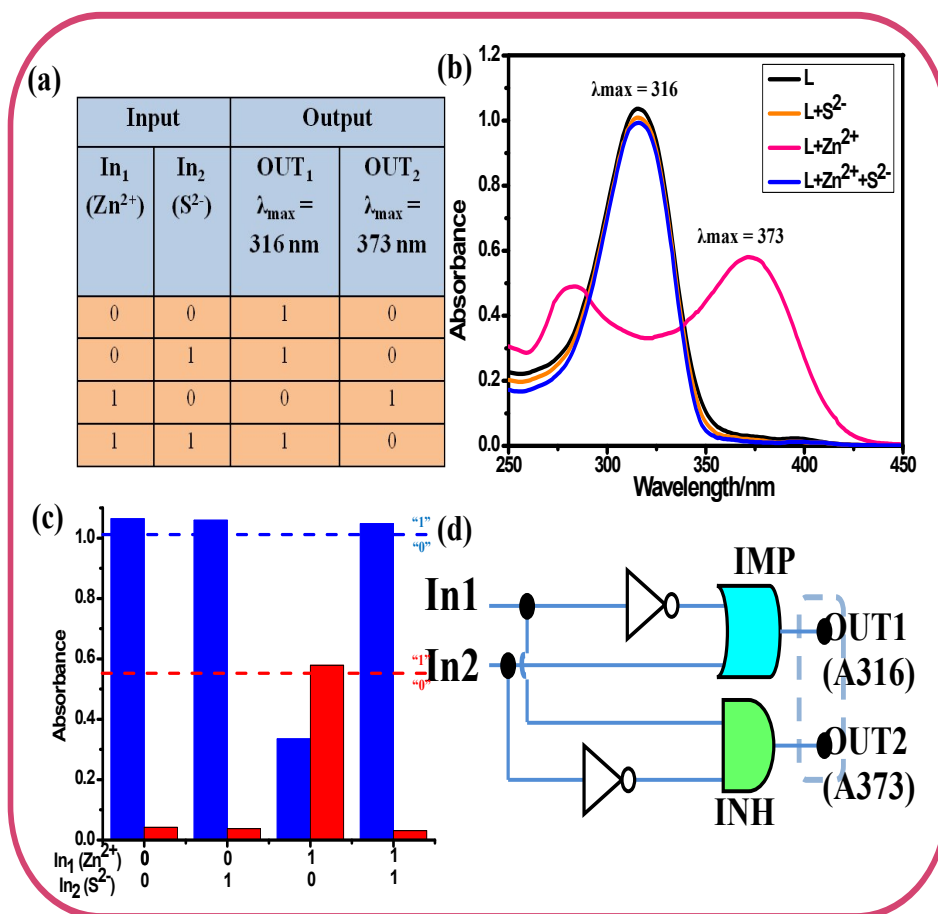


Fig. S22. The detection limit of L for  $\text{Hg}^{2+}$  by absorbance technique.

## Absorbance at $\lambda_{\max} = 316 \text{ nm}$

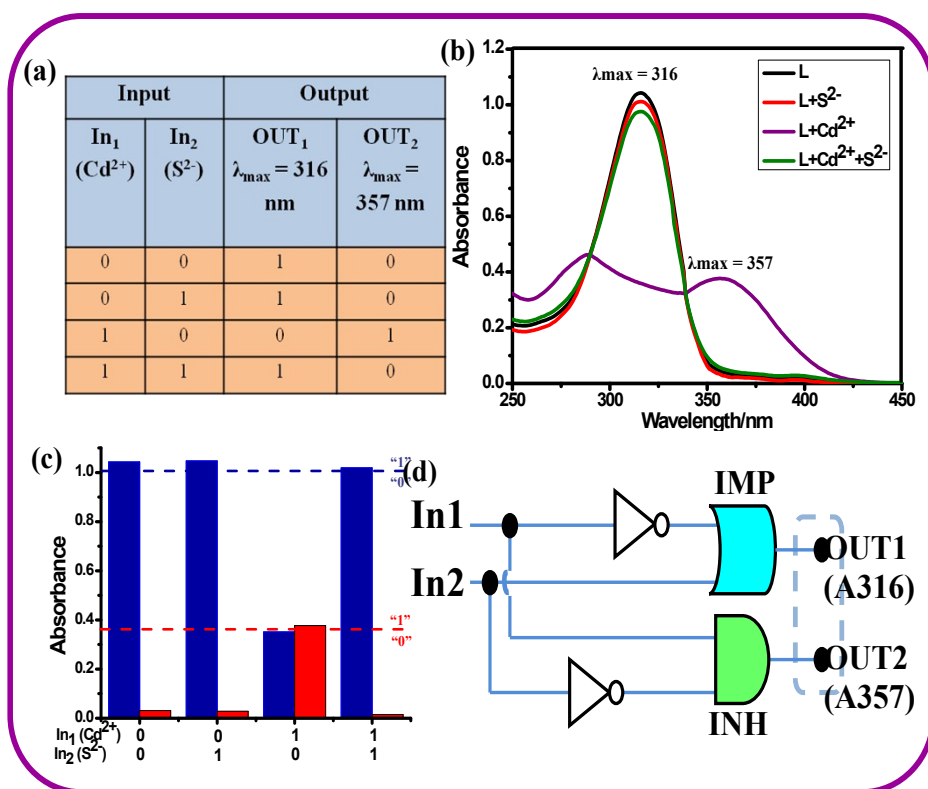


**Fig. S23.** Representative bar chart diagram for showing the change of absorbance at  $\lambda_{\max} = 316 \text{ nm}$  by adding various anions (100  $\mu\text{M}$ ) to solution of [L-Zn<sup>2+</sup>] (blue bars), [L-Cd<sup>2+</sup>] (red bars) and [L-Hg<sup>2+</sup>] (green bars) complexes. 1 = Cl<sup>-</sup>, 2 = F<sup>-</sup>, 3 = SO<sub>4</sub><sup>2-</sup>, 4 = OAc<sup>-</sup>, 5 = NO<sub>3</sub><sup>-</sup>, 6 = Br<sup>-</sup>, 7 = S<sup>2-</sup>. Sensing-recovery cycles for L (25  $\mu\text{M}$ ) at  $\lambda_{\max} = 316 \text{ nm}$  upon addition of (a) Zn<sup>2+</sup> (25  $\mu\text{M}$ ), (b) Cd<sup>2+</sup> (25  $\mu\text{M}$ ) and (c) Hg<sup>2+</sup> (25  $\mu\text{M}$ ) and subsequent regeneration by S<sup>2-</sup> (50  $\mu\text{M}$ ). Dotted lines serve guide to eyes.



**Fig. S24.** (a) Truth table of the logic gate, (b) Output signals of the logic gate in presence of different inputs, (c) corresponding bar diagram of absorbance outputs of **L** at  $\lambda_{\text{max}} = 316 \text{ nm}$  (OUT<sub>1</sub>, blue bars) and  $\lambda_{\text{max}} = 373 \text{ nm}$  (OUT<sub>2</sub>, red bars) in presence of two chemical inputs: In<sub>1</sub> (Zn<sup>2+</sup>) and In<sub>2</sub> (S<sup>2-</sup>) and (d) the corresponding logic circuit.





**Fig. S25.** (a) Truth table of the logic gate, (b) Output signals of the logic gate in presence of different inputs, (c) corresponding bar diagram of absorbance outputs of **L** at  $\lambda_{\text{max}} = 316$  nm (OUT<sub>1</sub>, blue bars) and  $\lambda_{\text{max}} = 357$  nm (OUT<sub>2</sub>, red bars) in presence of two chemical inputs: In<sub>1</sub> (Cd<sup>2+</sup>) and In<sub>2</sub> (S<sup>2-</sup>) and (d) the corresponding logic circuit.

**Table S1.** Data from theoretical TDDFT studies of **L**

| Compound | Electronic Transitions         | Energy (eV) | Wavelength (nm) | f <sup>b</sup> | Transitions involved                                                  |
|----------|--------------------------------|-------------|-----------------|----------------|-----------------------------------------------------------------------|
| <b>L</b> | S <sub>0</sub> -S <sub>1</sub> | 0.6569 eV   | 387.31 nm       | 0.0361         | HOMO→LUMO<br>HOMO→LUMO+1                                              |
|          | S <sub>0</sub> -S <sub>2</sub> | 1.3969 eV   | 317.58 nm       | 0.0126         | HOMO→LUMO+2<br>HOMO→LUMO+3                                            |
|          | S <sub>0</sub> -S <sub>3</sub> | 1.6689 eV   | 262.90 nm       | 0.0020         | HOMO-2→LUMO<br>HOMO-1→LUMO<br>HOMO→LUMO<br>HOMO→LUMO+1<br>HOMO-1→LUMO |

**Table S2.** Data from theoretical TDDFT studies of complexes

| Compound                      | Electronic Transitions         | Energy (eV) | Wavelength (nm) | f <sup>b</sup> | Transitions involved                                                        |
|-------------------------------|--------------------------------|-------------|-----------------|----------------|-----------------------------------------------------------------------------|
| (L-Zn <sup>2+</sup> ) complex | S <sub>0</sub> -S <sub>1</sub> | 0.7156 eV   | 422.53 nm       | 0.0676         | HOMO→LUMO<br>HOMO→LUMO+1                                                    |
|                               | S <sub>0</sub> -S <sub>2</sub> | 1.2632 eV   | 381.48 nm       | 0.0032         | HOMO-1→LUMO                                                                 |
|                               | S <sub>0</sub> -S <sub>3</sub> | 1.2949 eV   | 269.49 nm       | 0.0011         | HOMO-1→LUMO                                                                 |
| (L-Cd <sup>2+</sup> ) complex | S <sub>0</sub> -S <sub>1</sub> | 0.3450 eV   | 406.09 nm       | 0.0050         | HOMO→LUMO<br>HOMO→LUMO+1                                                    |
|                               | S <sub>0</sub> -S <sub>2</sub> | 0.4097 eV   | 369.75 nm       | 0.0577         | HOMO→LUMO<br>HOMO→LUMO+1                                                    |
|                               | S <sub>0</sub> -S <sub>3</sub> | 1.6215 eV   | 264.63 nm       | 0.0398         | HOMO-1→LUMO<br>HOMO→LUMO+2<br>HOMO-1→LUMO<br>HOMO-1→LUMO+1<br>HOMO-1→LUMO+2 |
| (L-Hg <sup>2+</sup> ) complex | S <sub>0</sub> -S <sub>1</sub> | 0.3673 eV   | 475.81 nm       | 0.0472         | HOMO→LUMO<br>HOMO→LUMO+2                                                    |
|                               | S <sub>0</sub> -S <sub>2</sub> | 1.4707 eV   | 413.00 nm       | 0.0031         | HOMO→LUMO+1<br>HOMO-1→LUMO<br>HOMO-1→LUMO+2                                 |
|                               | S <sub>0</sub> -S <sub>3</sub> | 1.5599 eV   | 292.80 nm       | 0.0225         | HOMO→LUMO+1<br>HOMO→LUMO+2                                                  |