

## Supporting Information

# NIR Sensing of Zn(II) and Subsequent Dihydrogen Phosphate Detection by a Benzothiazole Functionalized Ninhydrin Based Receptor

Abhijit Gogoi and Gopal Das

Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati 781039, India.

Fax: + 91 361 2582349; Tel: +91 3612582313; E-mail: [gdas@iitg.ernet.in](mailto:gdas@iitg.ernet.in)

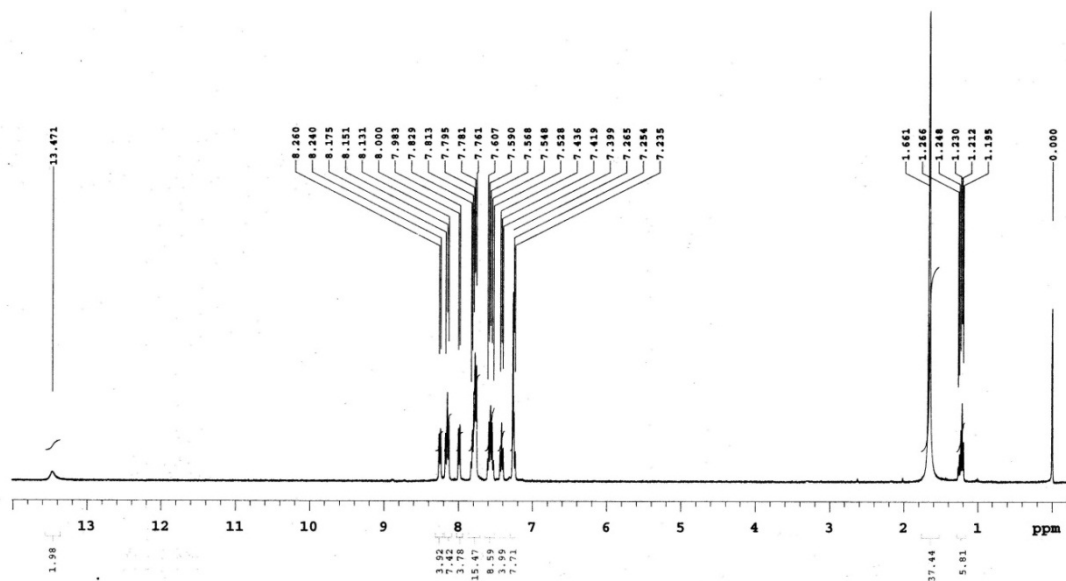


Figure S1.  $^1\text{H}$  NMR of  $\text{L}_1$  in  $\text{CDCl}_3$  solution at room temperature.

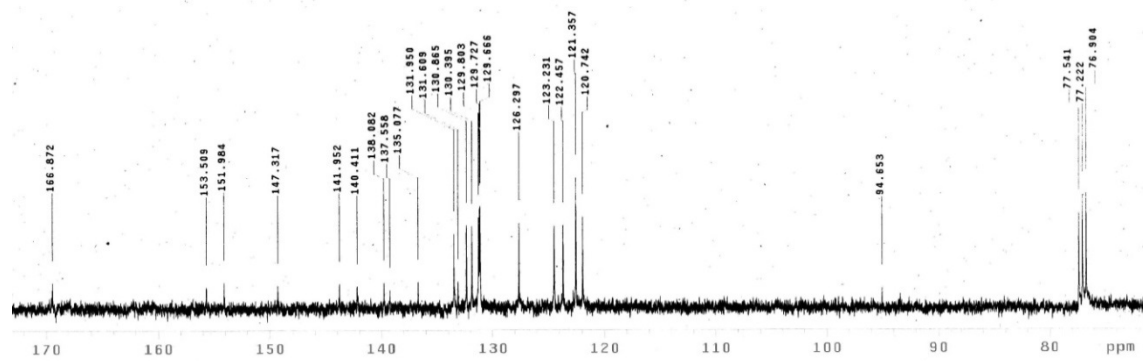


Figure S2.  $^{13}\text{C}$  NMR of  $\text{L}_1$  in  $\text{CDCl}_3$  solution at room temperature.

Fig

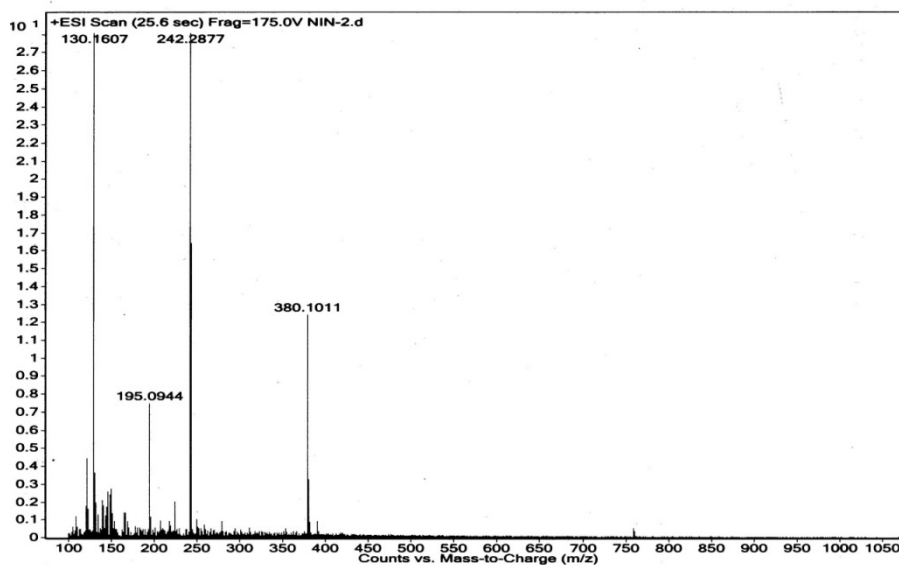


Figure S3. Mass Spectrum of L<sub>1</sub> in positive mode.

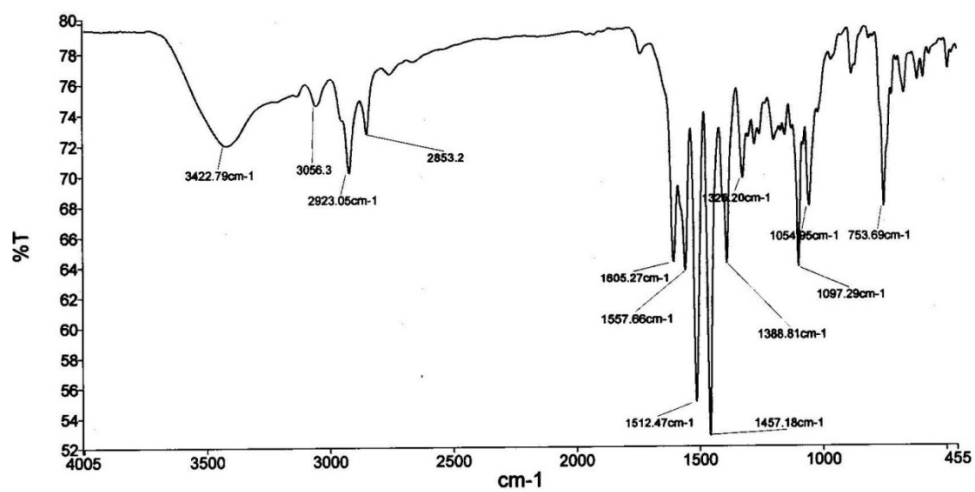


Figure S4. IR spectrum of L<sub>1</sub> recorded on KBr disc.

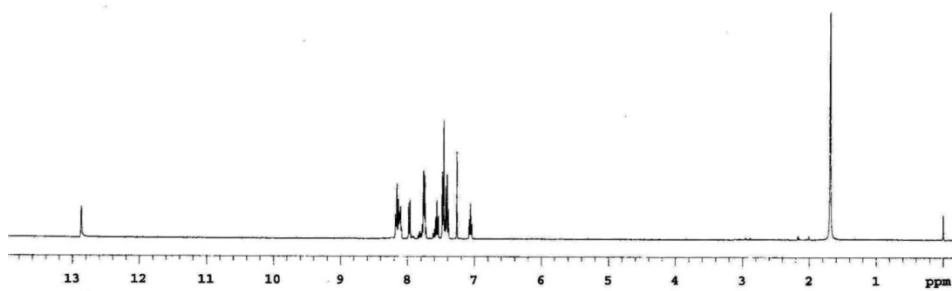


Figure S5. <sup>1</sup>H NMR of **L**<sub>2</sub> in CDCl<sub>3</sub> solution at room temperature.

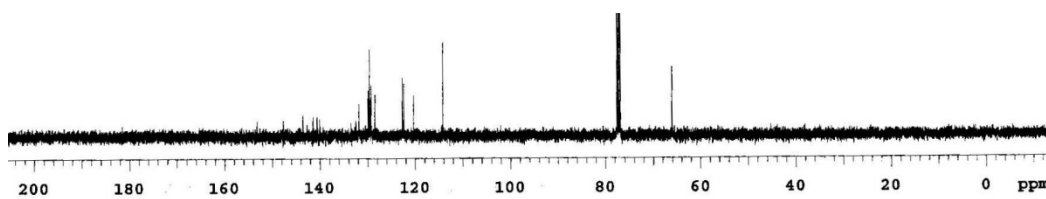


Figure S6. <sup>13</sup>C NMR of **L**<sub>2</sub> in CDCl<sub>3</sub> solution at room temperature

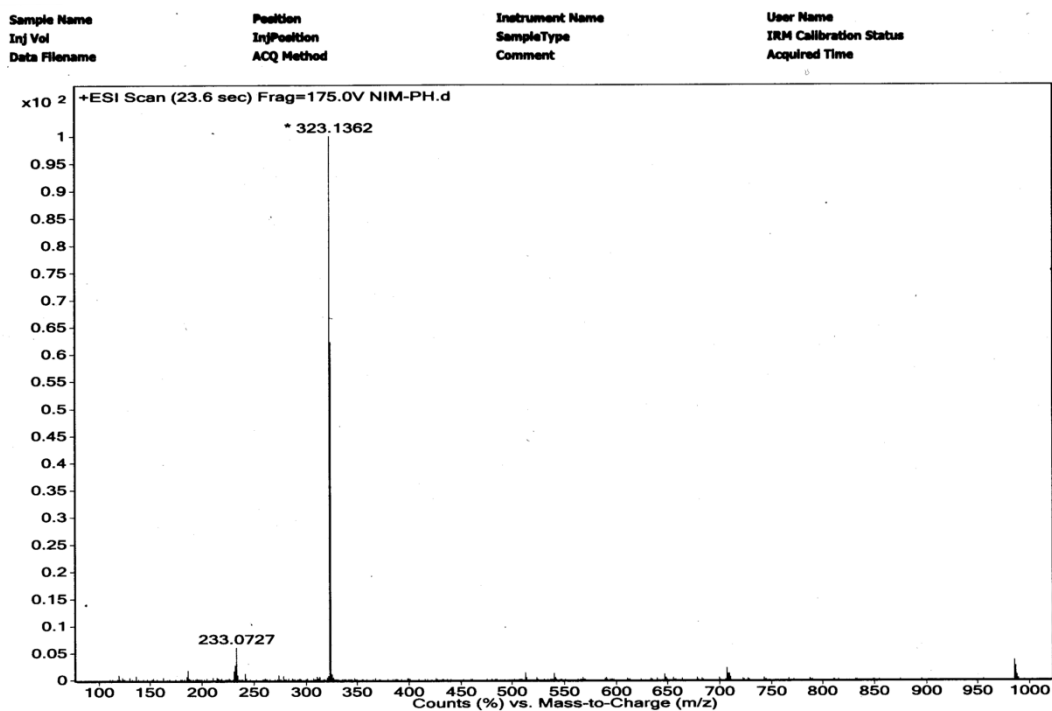


Figure S7. Mass Spectrum of  $L_2$  in positive mode.

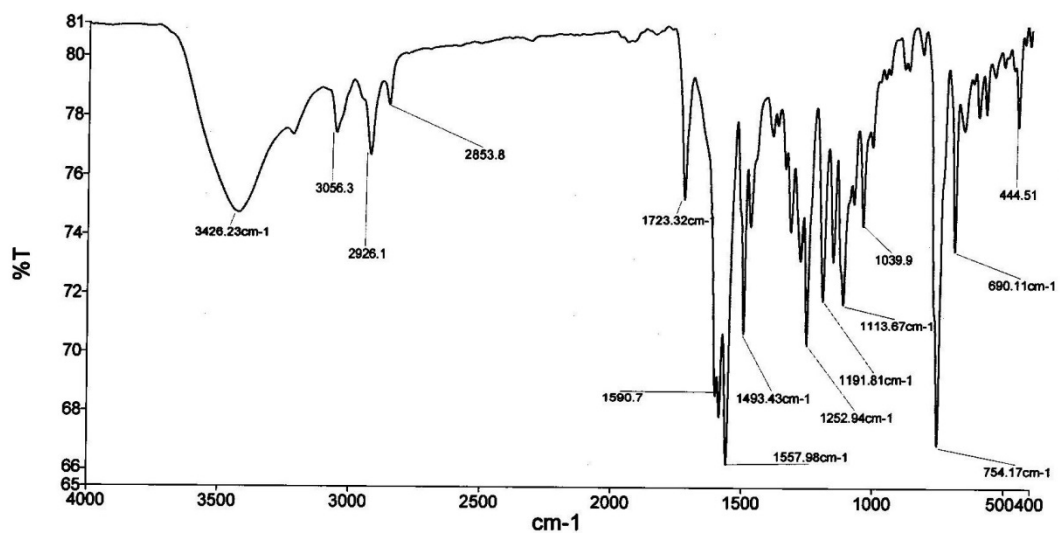


Figure S8. IR spectrum of  $L_2$  recorded on KBr disc.

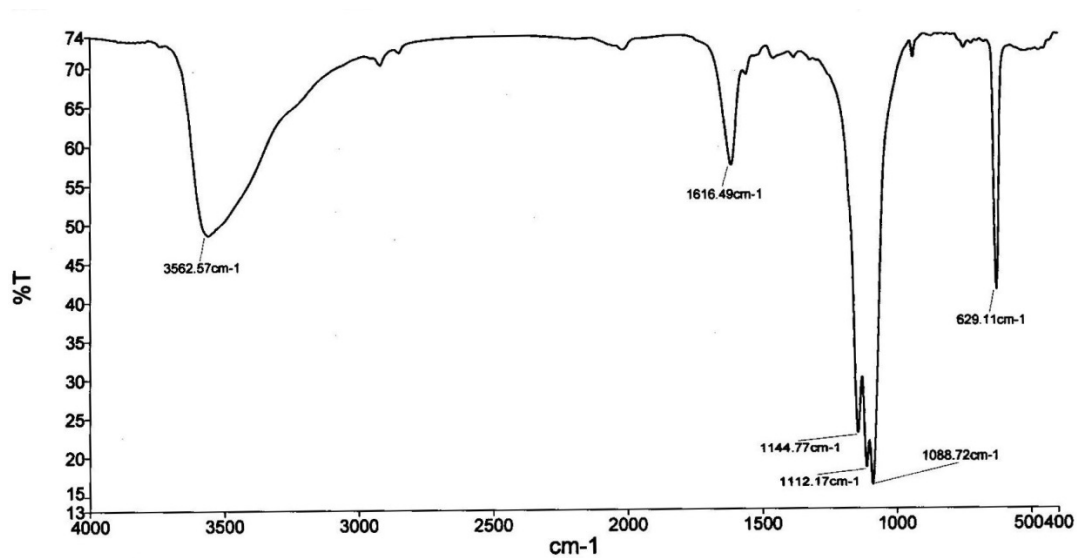


Figure S9. IR spectrum of L<sub>1</sub> zinc complex recorded on KBr disc.

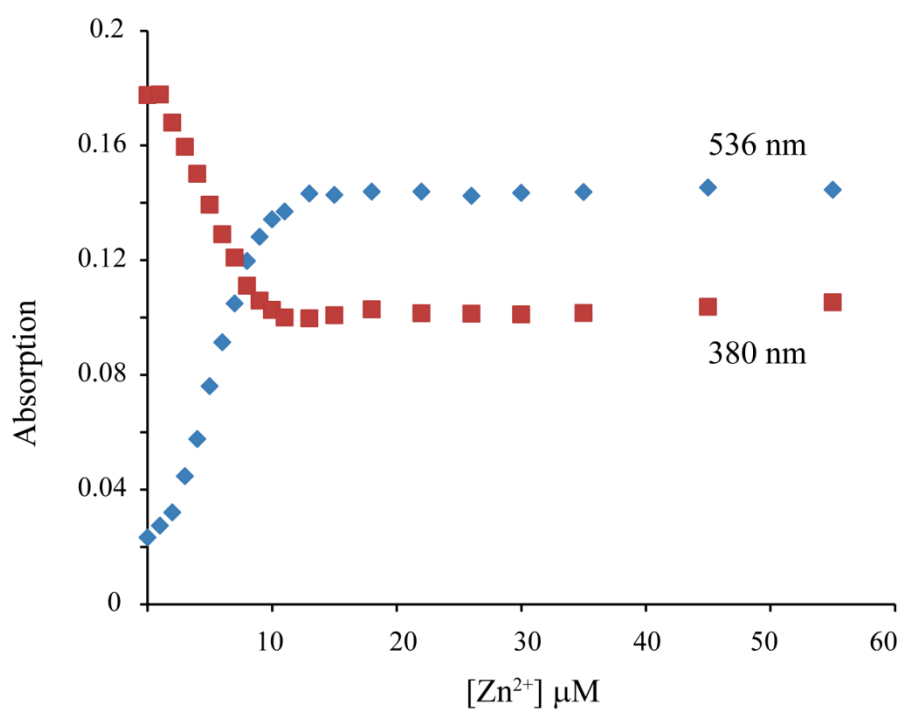


Figure S10. Changes of absorption intensities at 380 nm and 536 nm with the incremental addition of Zn<sup>2+</sup> ion to L<sub>1</sub>.

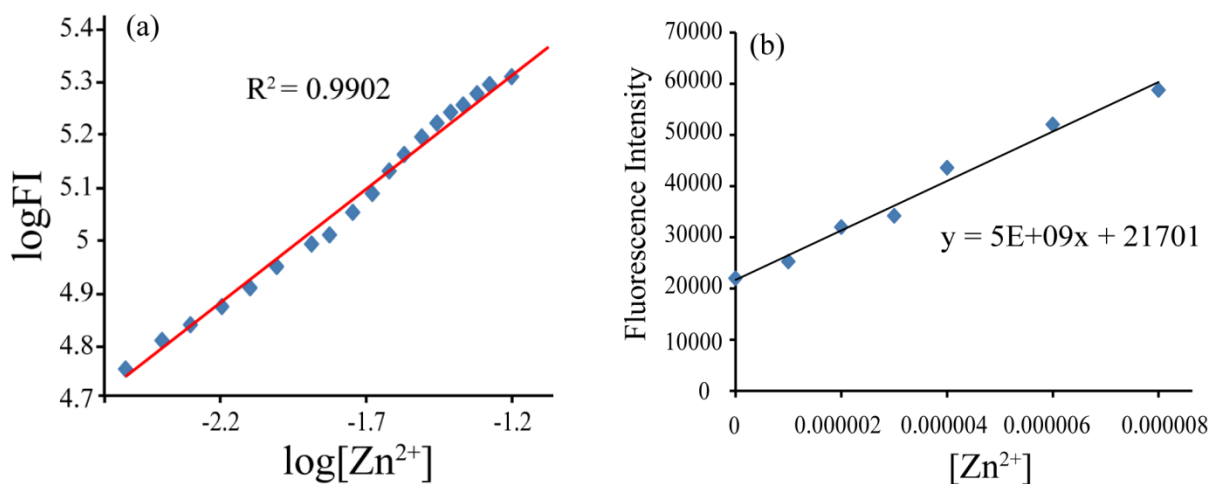


Figure S11. Plot of log FI (fluorescence intensity) versus log [Zn<sup>2+</sup>] in the range of 0–6 equiv. of Zn<sup>2+</sup>. (b) Plot of fluorescence intensity versus [Zn<sup>2+</sup>] for the detection limit calculation.

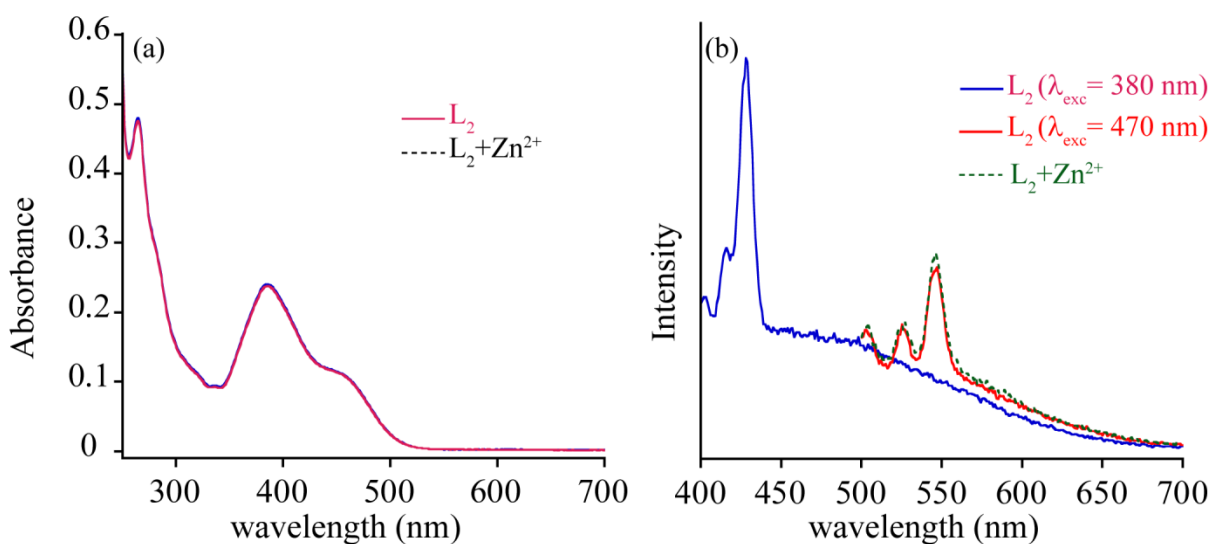


Figure S12. (a) Absorption spectra and (b) the corresponding fluorescence spectra of L<sub>2</sub> in the experimental medium.

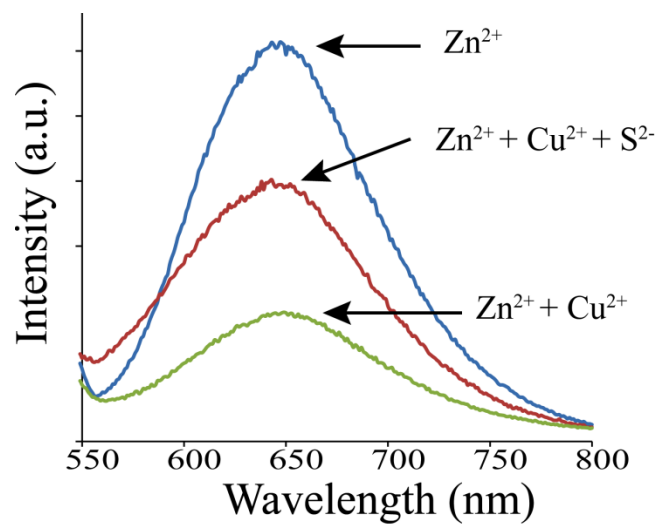


Figure S13. The fluorescence emission response of various ions to the ' $L_1$ - $Zn^{2+}$  ensembles'.

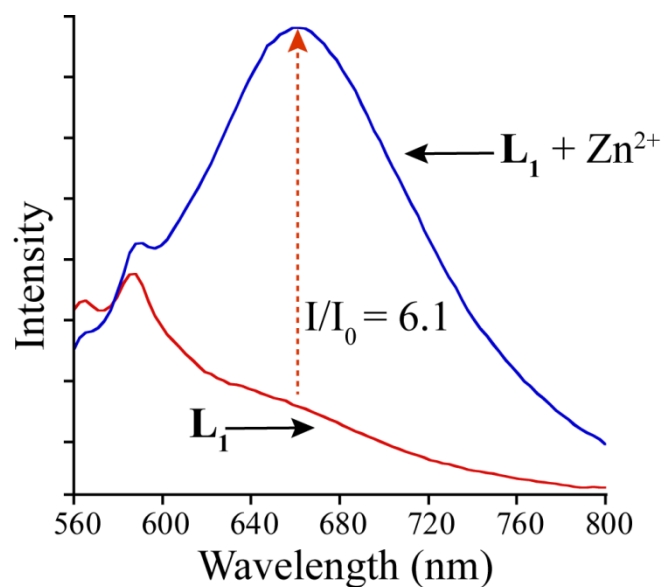


Figure S14. The fluorescence response of the receptor  $L_1$  towards  $Zn^{2+}$  ion in buffered acetonitrile (8:2 acetonitrile:water) at room temperature.



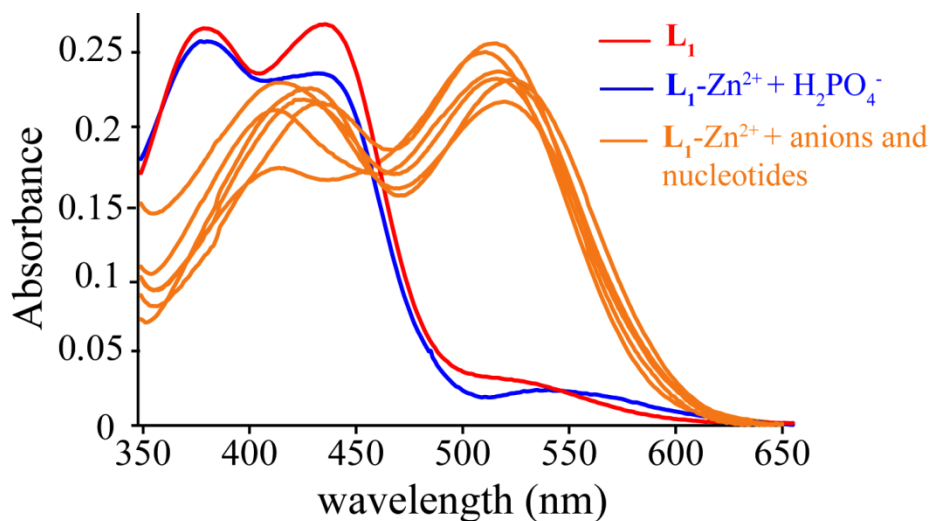


Figure S15. UV-Vis response of the anions and nucleotides towards ‘ $L_1$ -Zn ensemble’ in acetonitrile solution at room temperature.

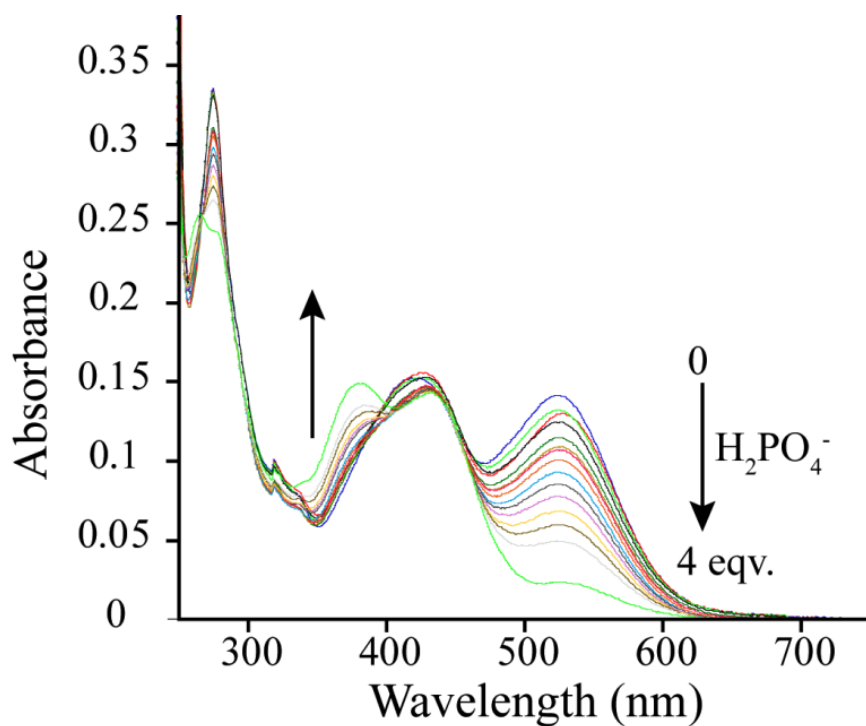


Figure S16. The absorption titration spectra of the ‘ $L_1$ -Zn $^{2+}$  ensemble’ with increasing concentration of potassium salt of  $H_2PO_4^-$  anion in acetonitrile solution.

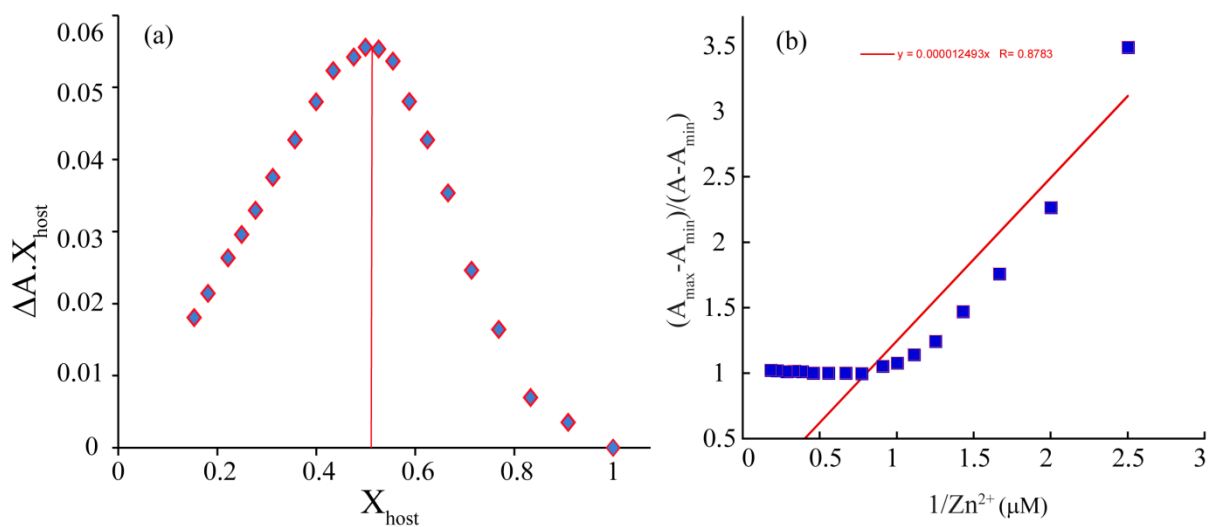


Figure S17. (a) Job's plot of  $\text{Zn}^{2+}$  titration with  $\text{L}_1$  ( the absorption intensity was calculated from  $\lambda = 536 \text{ nm}$ ) and (b) the corresponding Bensei-Hildebrand plot.

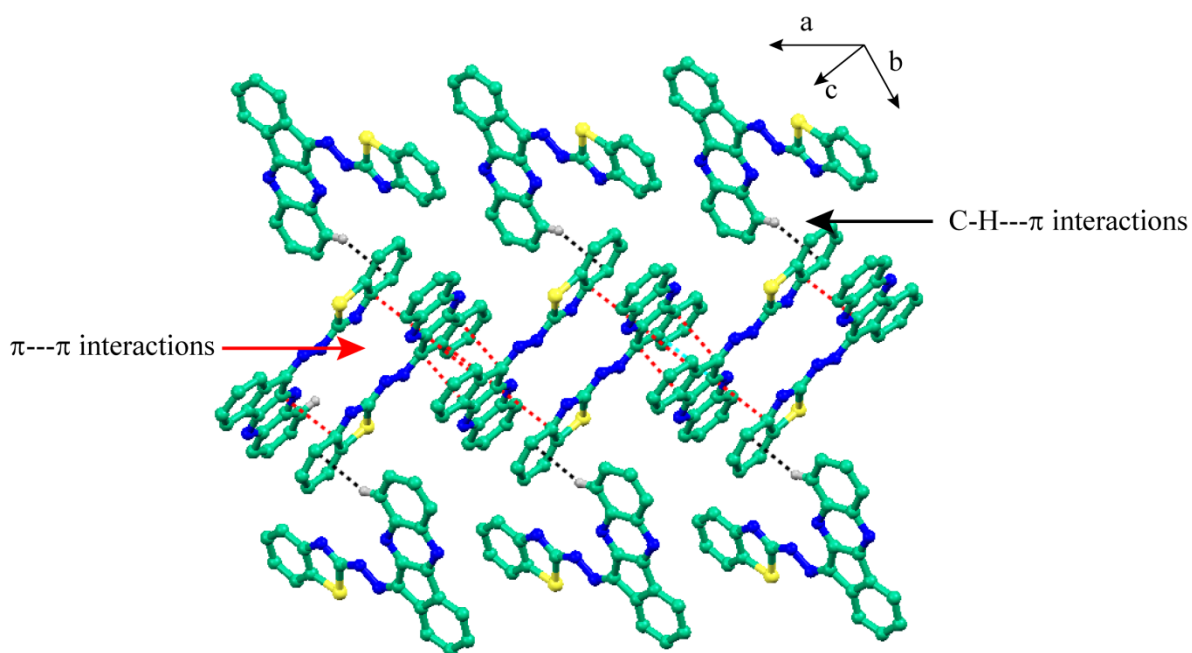


Figure S18. Crystal packing diagram of  $\text{L}_1$  with different  $\pi\text{---}\pi$  and  $\text{C-H}\text{---}\pi$  interactions.

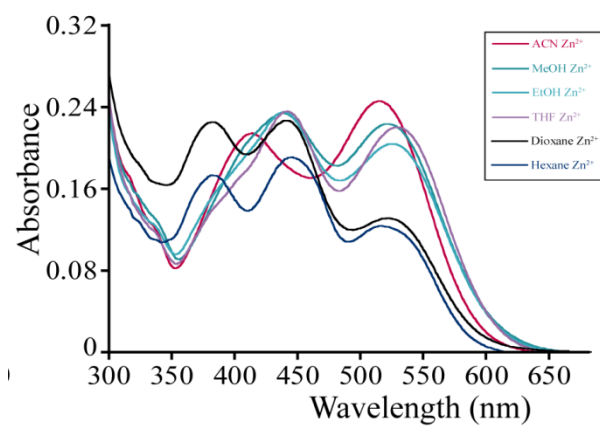


Figure S19. Changes in absorption spectral patterns of the ' $L_1-Zn^{2+}$  ensembles' in various solvents.