Electronic Supporting Information (ESI) for

Nanomolar Zn(II) Sensing and Subsequent PPi Detection in Physiological Medium and Live Cells with A Benzothiazole Functionalized Chemosensor

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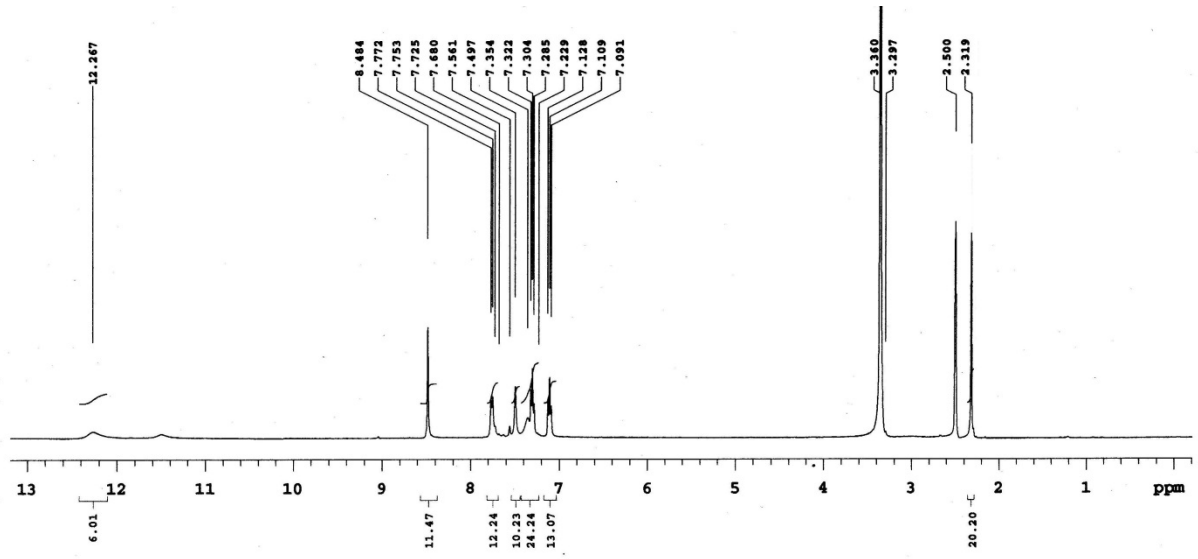


Figure S1. ^{1}H NMR of $\mathbf{L_1}$ in DMSO-d_6 solution at room temperature.

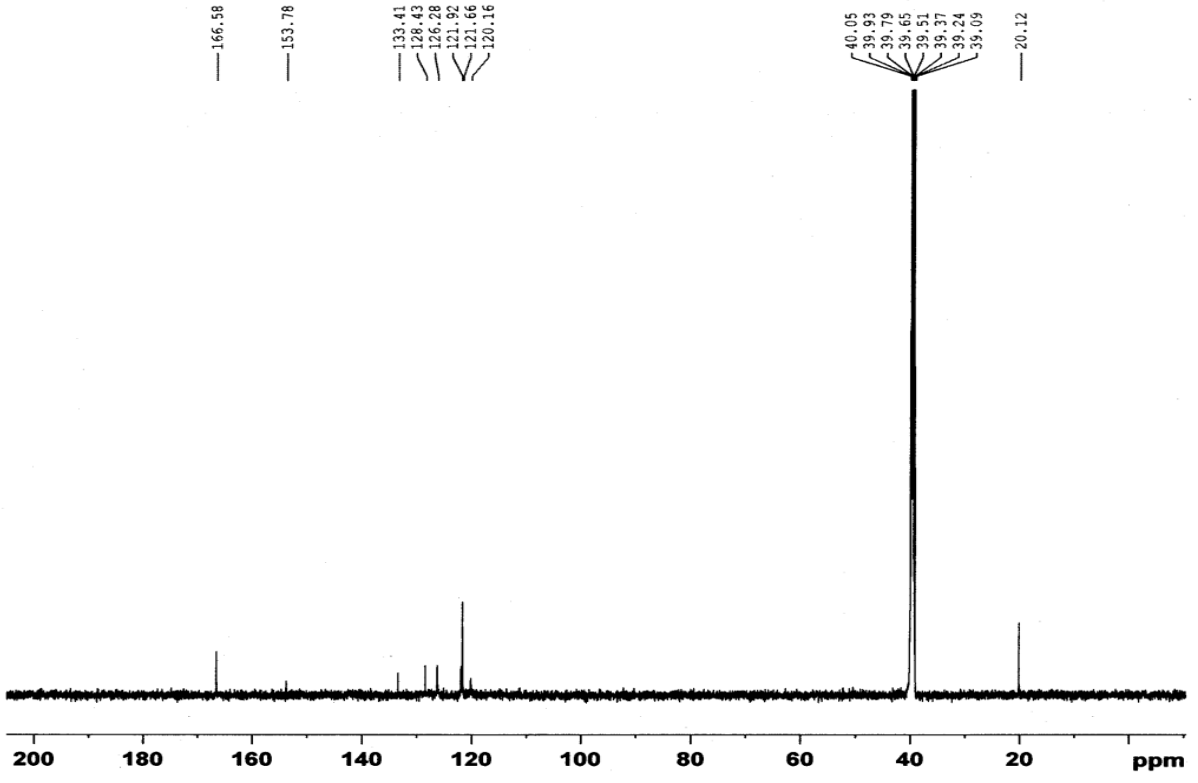


Figure S2. ^{13}C NMR of $\mathbf{L_1}$ in DMSO-d_6 solution at room temperature.

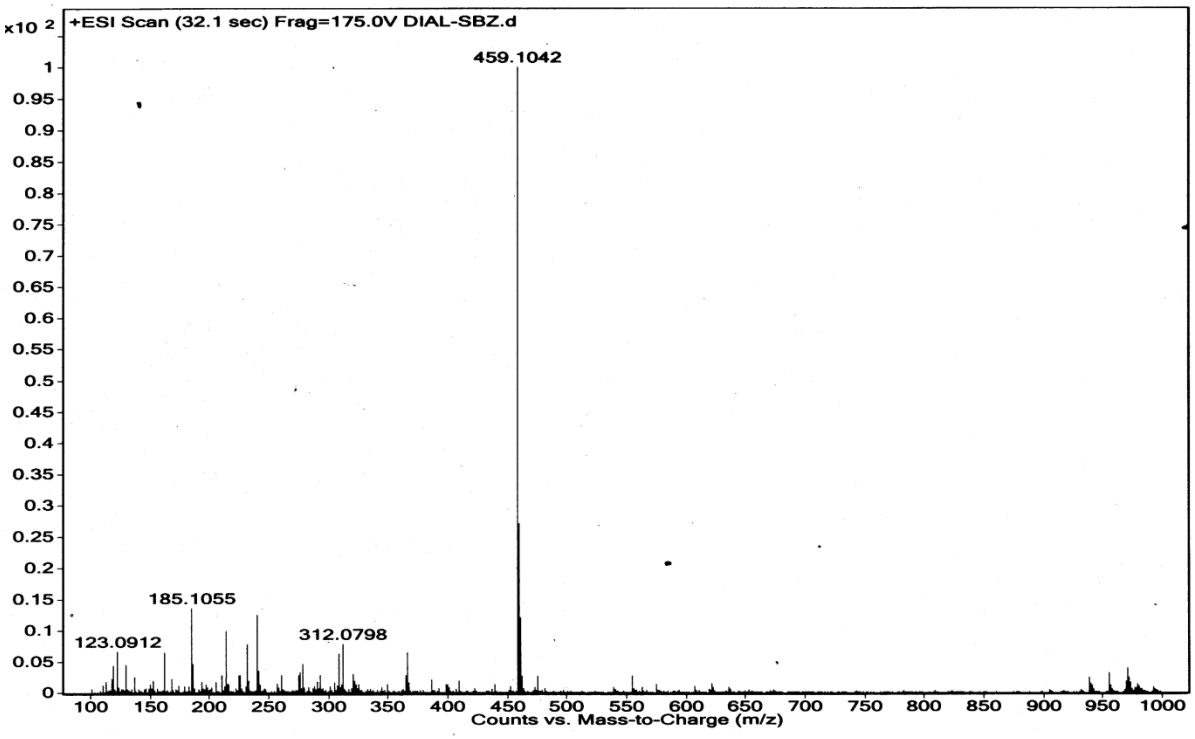


Figure S3. ESI-MS Mass Spectrum of $\mathbf{L_1}$ in positive mode.

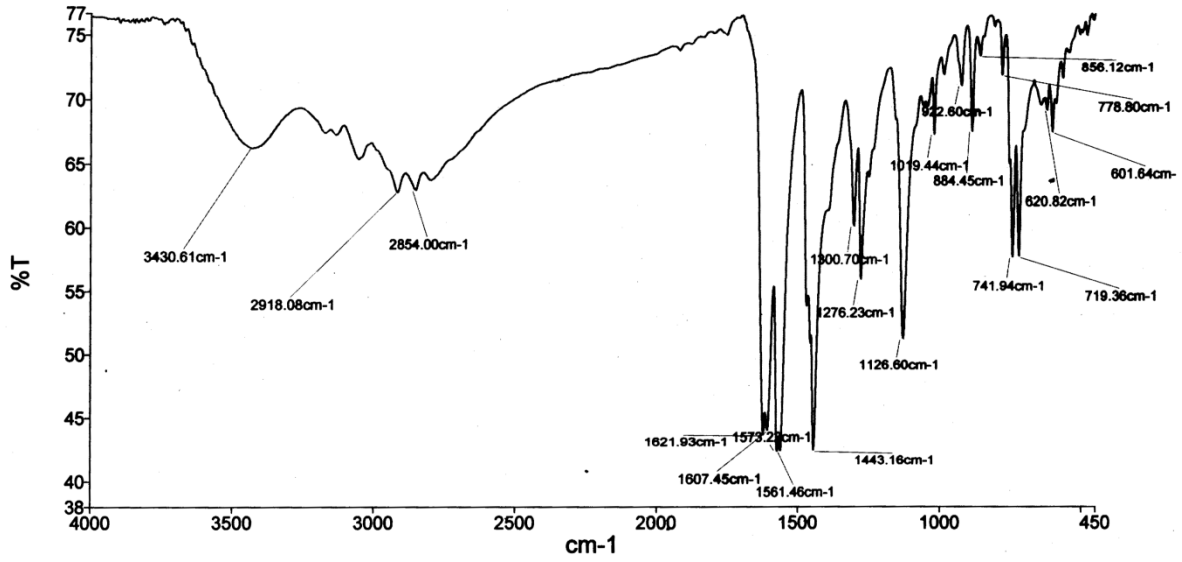


Figure S4. IR spectrum of $\mathbf{L_1}$ recorded on KBr disc.

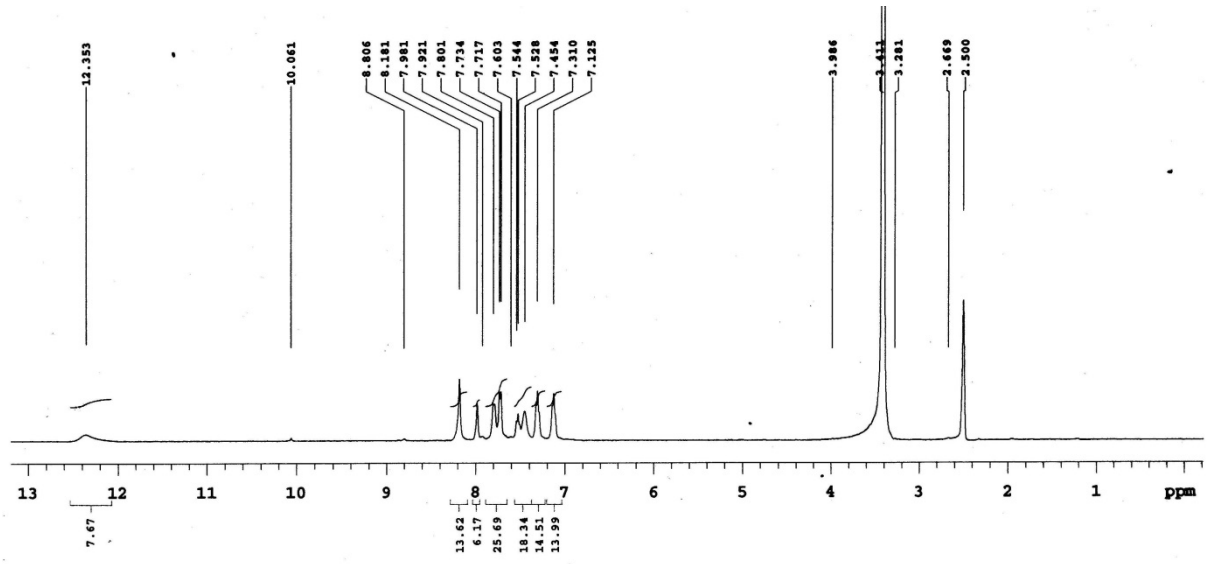


Figure S5. ^{1}H NMR of $\mathbf{L_2}$ in DMSO-d_6 solution at room temperature.

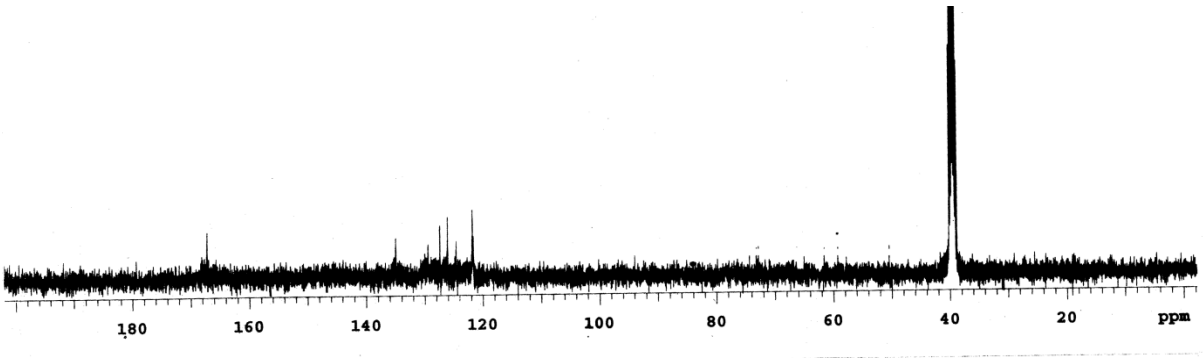


Figure S6. ^{13}C NMR of $\mathbf{L_2}$ in DMSO-d_6 solution at room temperature

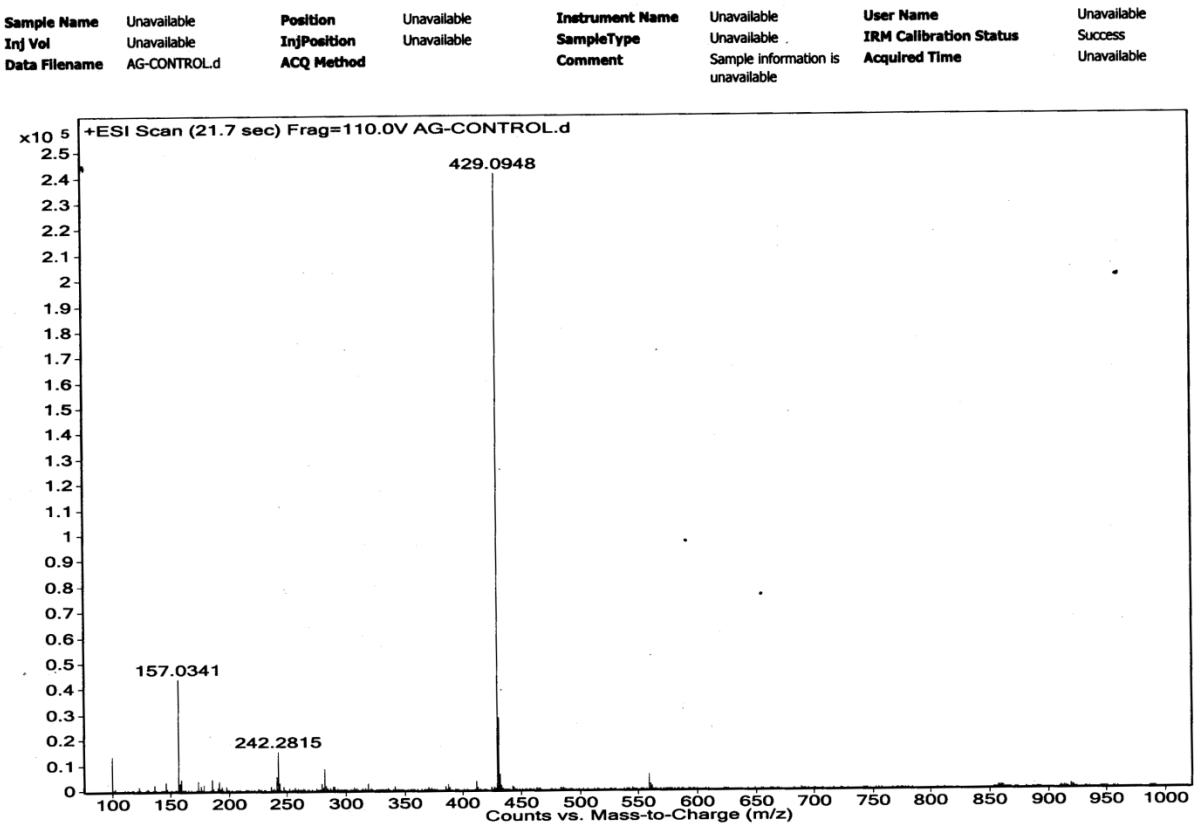


Figure S7. ESI-MS Mass Spectrum of $\mathbf{L_2}$ in positive mode.

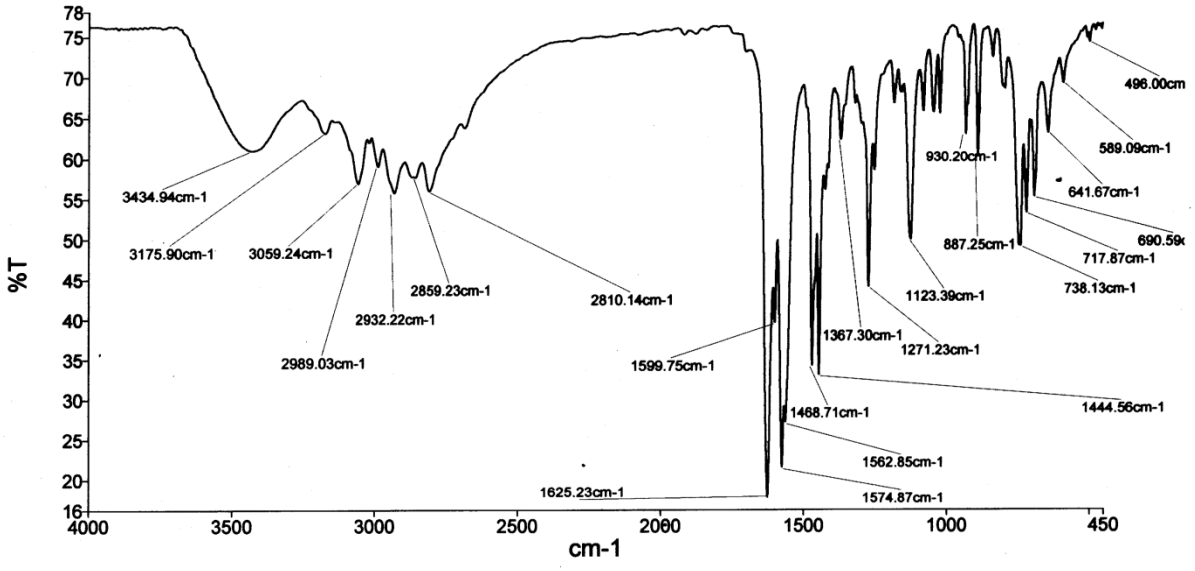


Figure S8. IR spectrum of $\mathbf{L_2}$ recorded on KBr disc.

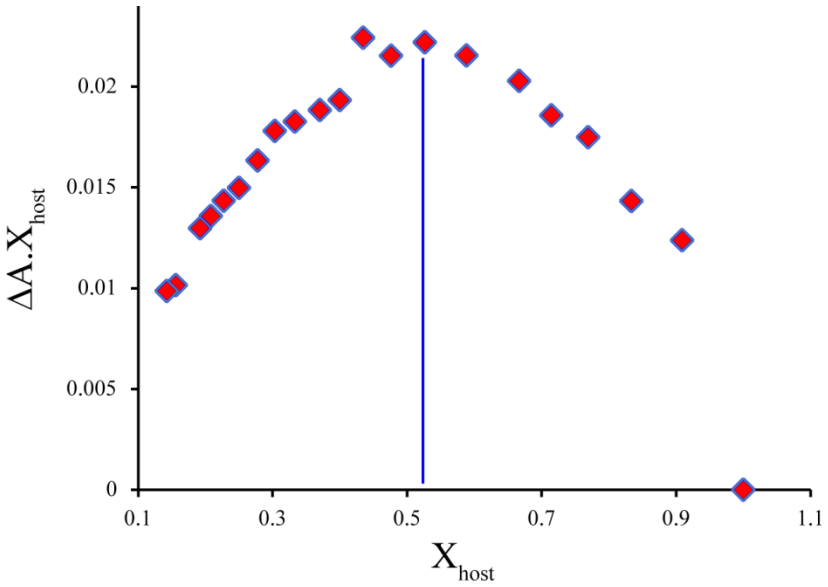


Figure S9. The Job's plot for determining the binding stoichiometry of $\mathbf{L_1}$ with Zn^{2+} (1:1 host-guest complex).

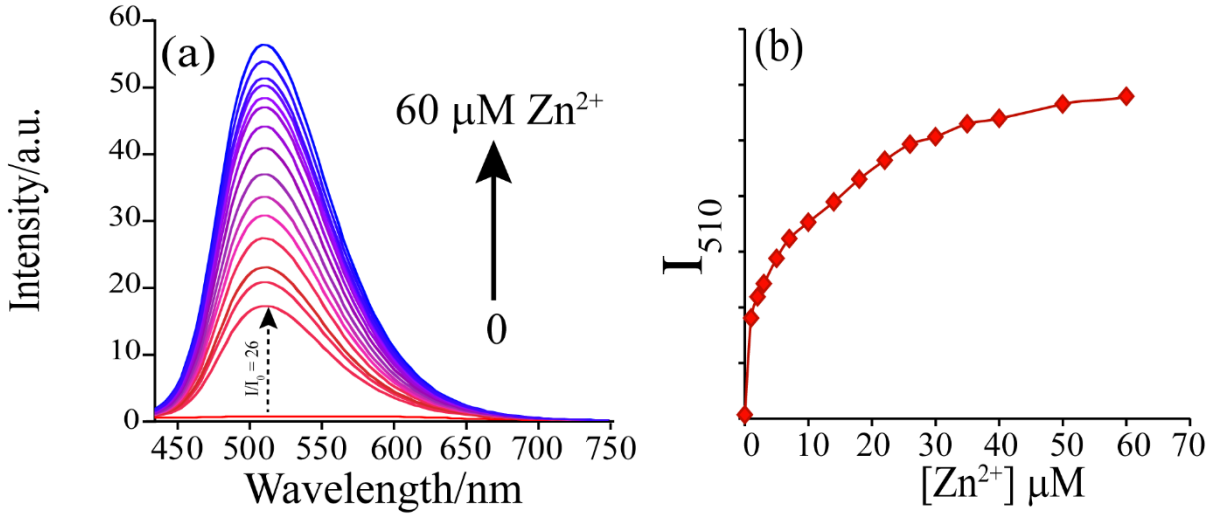


Figure S10. Fluorescence titration of $\mathbf{L_1}$ with varying Zn^{2+} concentration from 0 to 60 μM (λ_{ex} = 430 nm, slit = 3/3 nm) in buffered ethanol (1:1:: EtOH: 10 mM HEPES buffer, pH~7.2). (b) Fluorescence Intensity at 510 nm versus Zn^{2+} concentration (μM) plot.

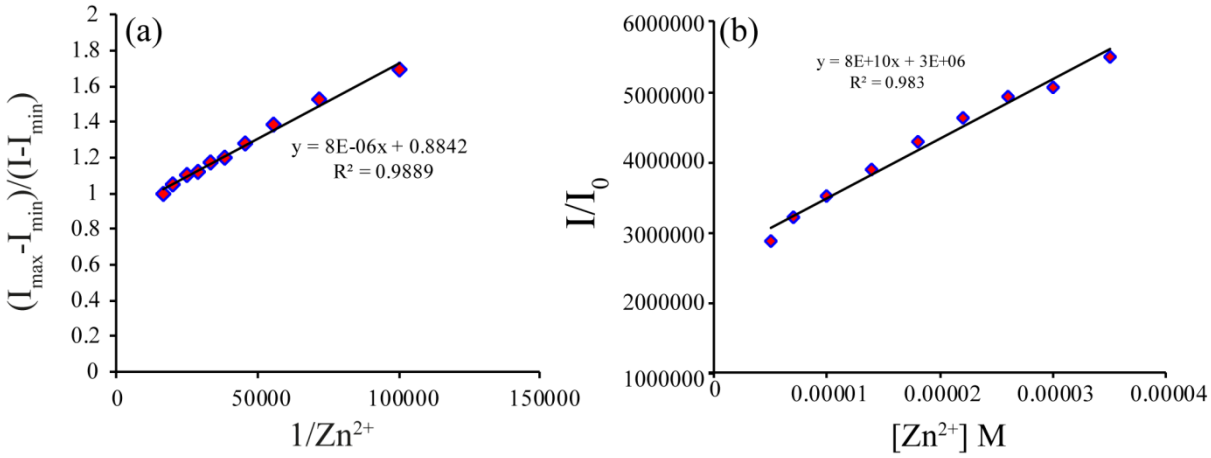


Figure S11. (a) The Bensei-Hildebrand plot to calculate the binding constant for Zn^{2+} ion in buffered ethanol solution. (b) Ratio of fluorescence emission intensity change at 510 nm versus Zn^{2+} concentrations for the LOD calculation.

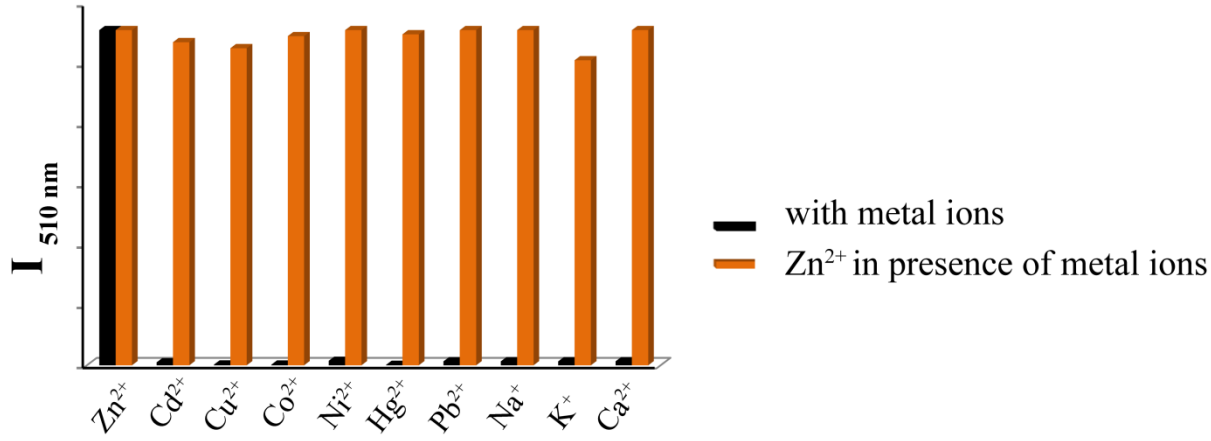


Figure S12. Bar plot presentation of $\mathbf{L_1}$ and Zn^{2+} in the presence of various other metal ions.

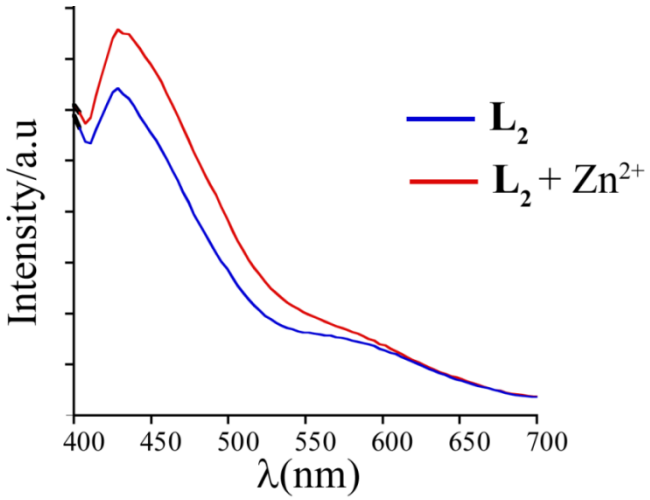


Figure S13. Fluorescence emission change after addition of Zn^{2+} to $\mathbf{L_2}$ under the same experimental condition.

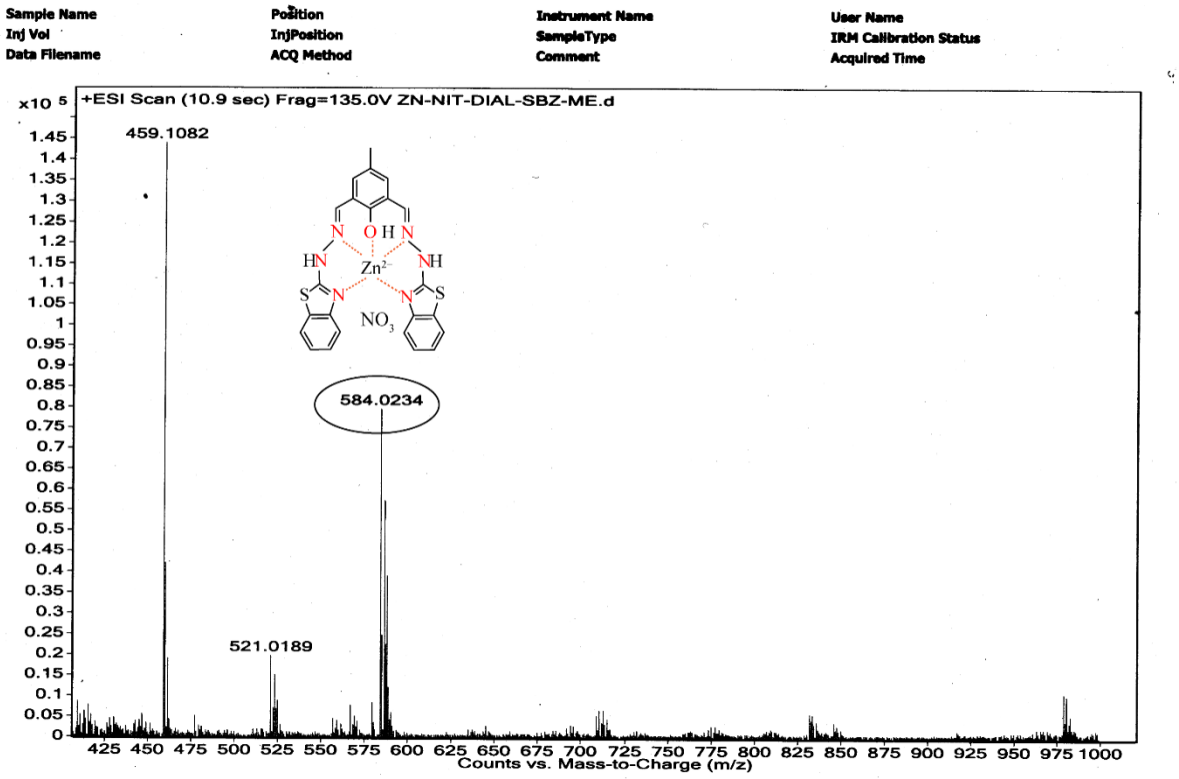


Figure S14. HRMS analysis of the solution of $\mathbf{L_1}$ with $Zn(NO_3)_2$.

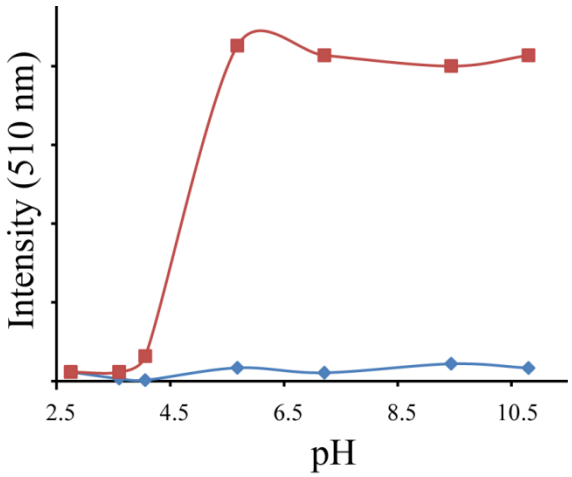


Figure S15. Effect of pH on emission behaviour of $\mathbf{L_1}$ and '$\mathbf{L_1}$-Zn^{2+} ensemble' (Blue line represents the change for $\mathbf{L_1}$, whereas the changes for '$\mathbf{L_1}$-Zn^{2+} ensemble' is represented by red line).

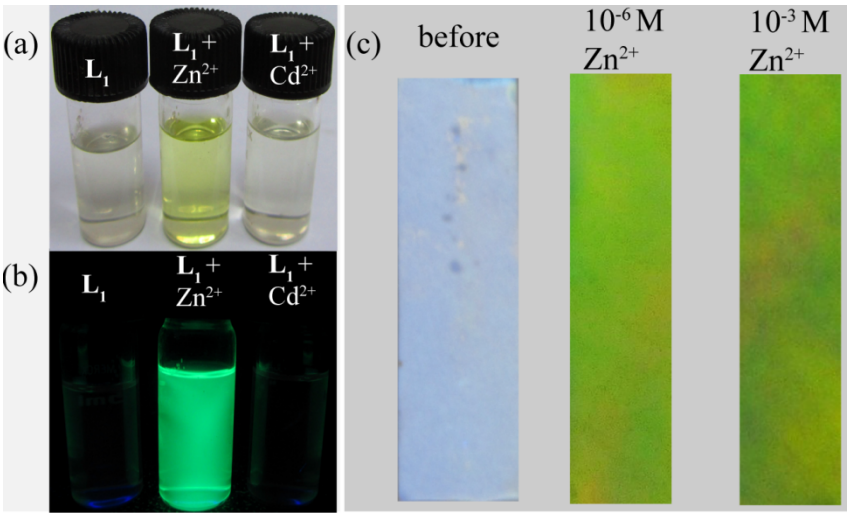


Figure S16. Change in colour after addition of Zn^{2+} and Cd^{2+} ions to $\mathbf{L_1}$ under normal light and (b) under the UV lamp. (c) The paper coated colour change experiment with different concentration of Zn^{2+} ion under the UV lamp (λ = 365 nm).

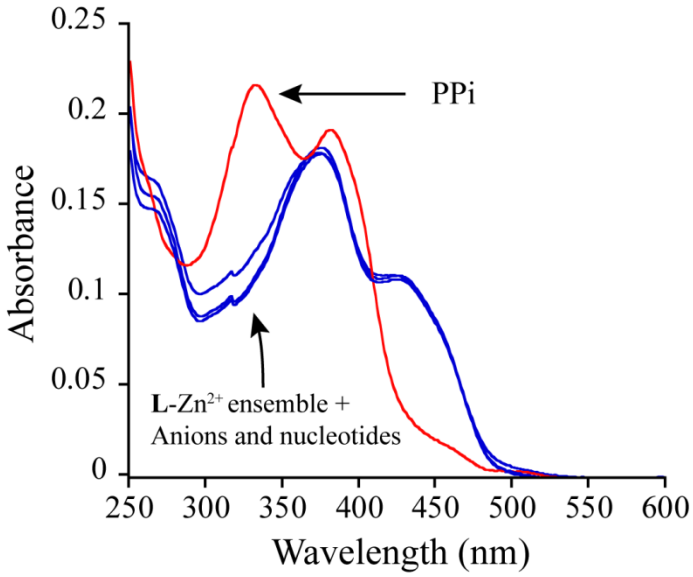


Figure S17. Change in UV-VIS absorption spectra of '$\mathbf{L_1}$-Zn^{2+}' ensemble with different anions in the buffered ethanol (1:1:: EtOH: 10 mM HEPES buffer, pH~7.2).

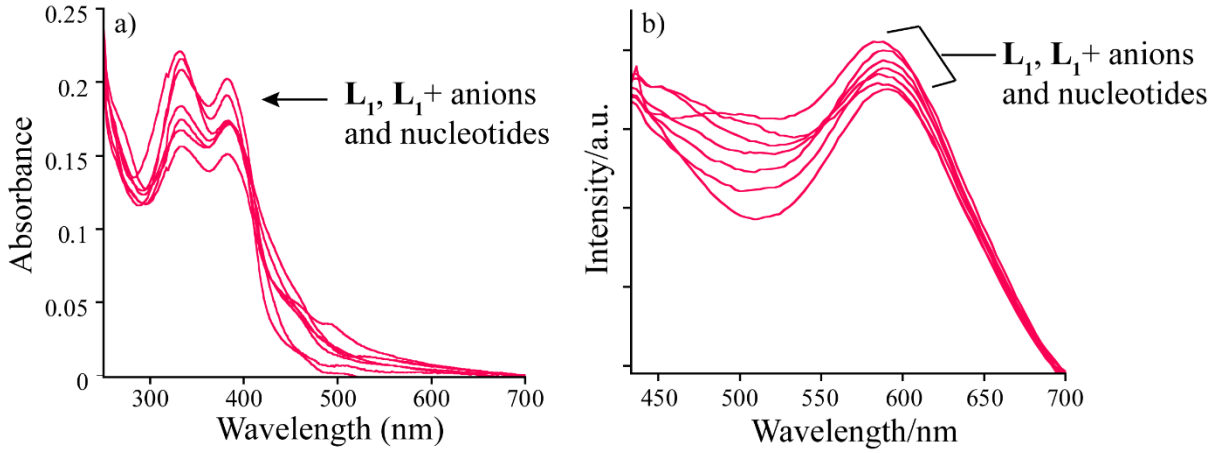


Figure S18. a) UV-Vis and b) fluorescence selectivity study of the naked probe $\mathbf{L_1}$ with anions and nucleotides in buffered ethanol (1:1 EtOH:10 mM HEPES buffer, pH~7.2).

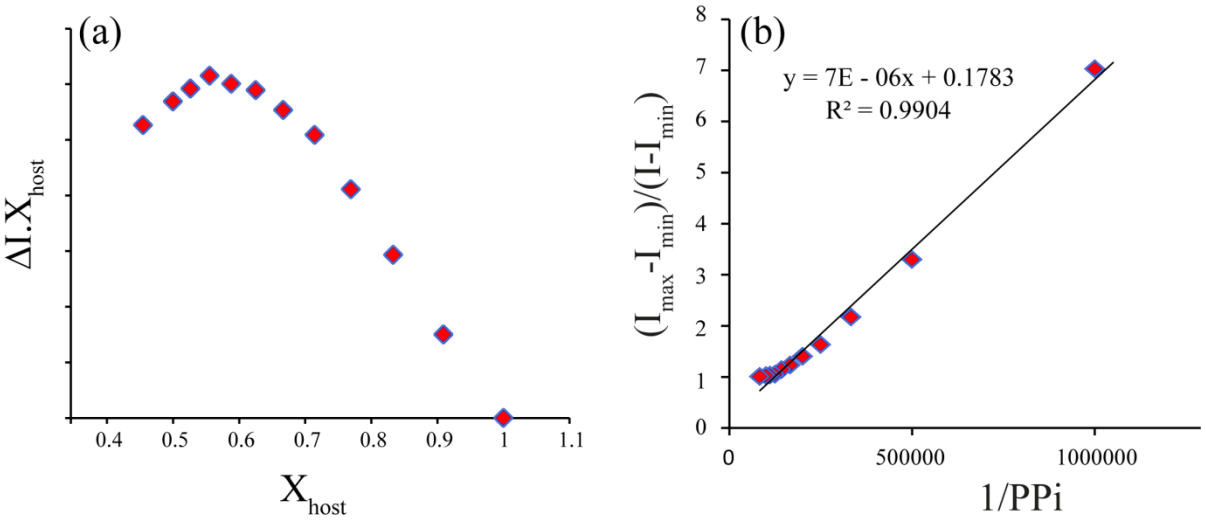


Figure S19. (a) Job's plot for determining the stoichiometry of '$\mathbf{L_1}$-Zn^{2+}' and PPi ion and (b) the corresponding Benesi−Hildebrand plot for binding constant determination.

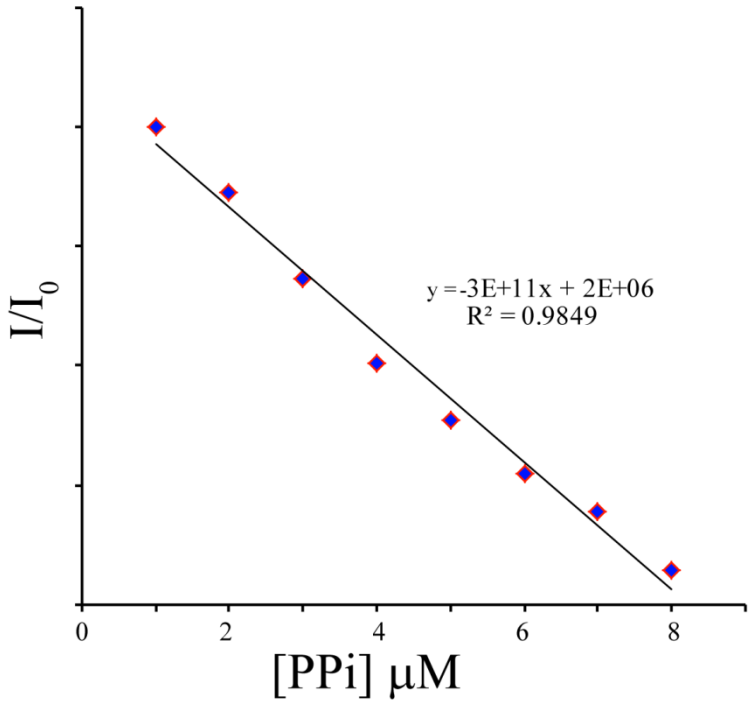


Figure S20. Ratio of fluorescence emission intensity change at 510 nm versus PPi concentrations for lowest detection limits (LOD) calculation.

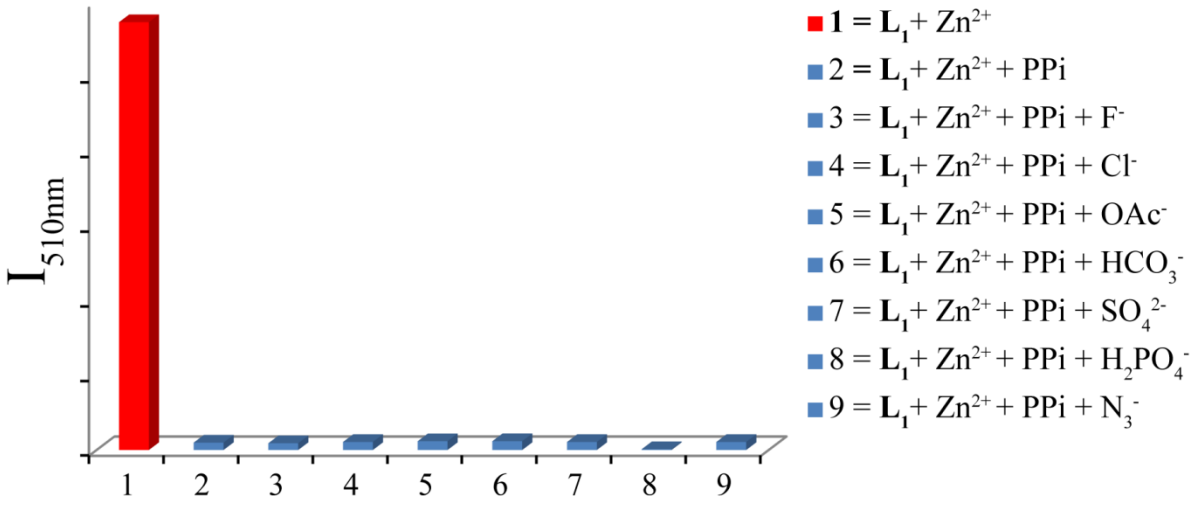


Figure S21. Competitive binding affinity of PPi towards the flourish '$\mathbf{L_1}$-Zn^{2+}' ensemble in presence of other anions (10 equivalents).

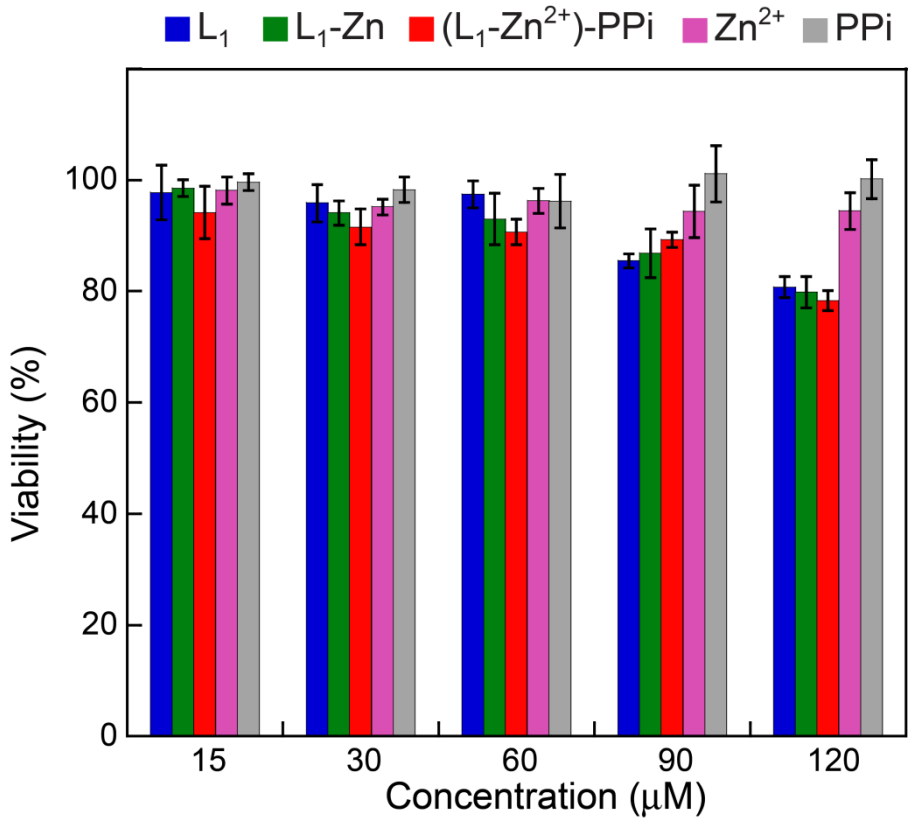


Figure S22. MTT based cytotoxicity assay for $\mathbf{L_1}$ and $\mathbf{L_1}$-zinc complex.

Table S1. Comparison of metal sensing aptitude of some reported dipodal Schiff base type chemosensor.

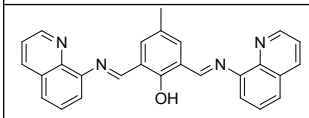
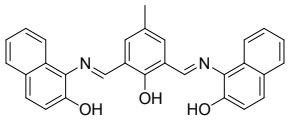
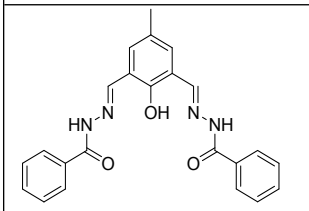
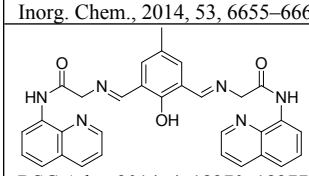
References	**Experimental Medium**	**Sensed Metal ion with LOD**	***In vivo* application**	**Anion Sensing with LOD**	***In vivo* application**
 Anal. Chem, 2013, 85, 8369	Methanolic HEPES Buffer (3:2), pH 7.4	Zn^{2+} sensor LOD for Zn^{2+} **56 ppb**	Zn^{2+} imaging	PPi sensing, LOD for PPi **2 ppb**	PCR
 Sensors and Actuators B 2013, 188, 1132– 1140	CH_3CN/aqueous HEPES buffer (1:4, v/v)	Zn^{2+} sensor LOD for Cu^{2+} **3 ppb**	Cu^{2+} imaging	No anion sensing	-------
 Inorg. Chem., 2014, 53, 6655–6664	CH_3CN/ buffer (2:8, v/v)	Zn^{2+} and Cu^{2+} sensing LOD not discussed	Zn^{2+} and Cu^{2+} images in HELa cells	PPi sensing, LOD for PPi **123 ppb**	No imaging Crystals of Zn and Cu
 RSC Adv., 2014, 4, 18270–18277	CH_3CH_2OH–Tris–HCl buffer solution (50 mM Tris, 50 : 50, v/v, pH 7.2)	Zn^{2+} sensor LOD for Zn^{2+} **0.1μM**	No imaging	S^{2-} sensing, LOD for S^{2-} **10^{6-} M**	No imaging Crystals of Zn and Cu

Table S2. Comparison of some latest reported Zn^{2+} chemosensors with the present work.

Sl No.	References	Lowest Detection limit of Zn^{2+}	Solvent system
1	Present work	25 ppb	7:3, v/v, MeOH, HEPES buffer, pH 7.2
2	Barun Kumar Datta, Sandipan Mukherjee, Chirantan Kar, Aiyagari Ramesh, and Gopal Das; Org. Biomol. Chem., 2014,12, 4975-4982	56 ppm	MeOH: aqueous HEPES buffer (1 mM, pH 7.4; 3:2 v/v)
3	Sharanjeet Kaur, Vandana Bhalla and Manoj Kumar; Chem. Commun., 2014,50, 9725-9728	110 nm	(8:2, v/v H_2O:THF)
4	Zhengping Dong, Xuanduong Le, Panpan Zhou, Chunxu Dong and Jiantai Ma; RSC Adv., 2014, 4, 18270	0.1μM	CH_3CH_2OH–Tris–HCl buffer solution (50 mM Tris, 50 : 50, v/v, pH 7.2)
4	Manoj Kumar, Naresh Kumar and Vandana Bhalla ; Chem. Commun., 2013,49, 877-879	20×10^{-8} mol L^{-1}	H_2O : CH_3CN (2 : 8, v/v) HEPES buffer, pH=7.0
5	Jie Guan, Peng Zhang, Tai-bao Wei, Qi Lin, Hong Yao and You-ming Zhang; RSC Adv., 2014, 4, 35797	0.13μM	DMSO–H_2O (8 : 2, v/v, containing 0.01 M HEPES, pH 7.24
6	Zhipeng Liu, Changli Zhang, Yuncong Chen, Fang Qian, Yang Bai, Weijiang He and Zijian Guo; Chem. Commun., 2014, 50, 1253-1255	0.5 nM	HEPES buffer (50 mM, 0.1 M KNO_3, pH 7.2,
7	Vijay Luxami, Kamaldeep Paula and In Howa Jeong; Dalton Trans., 2013, 42, 3783	-------	CH_3CN–H_2O::1 : 1) (HEPES buffer, pH = 7.0)
8	Junfeng Wang, Bin Liu, Xiumin Liu, Matthew J. Panzner, Chrys Wesdemiotisa and Yi Pang; Dalton Trans., 2014,43, 14142-14146	-------	EtOH