Supporting Information

A novel chemosensor with visible light excitability for sensing Zn^{2+} in physiological medium and in HeLa cells

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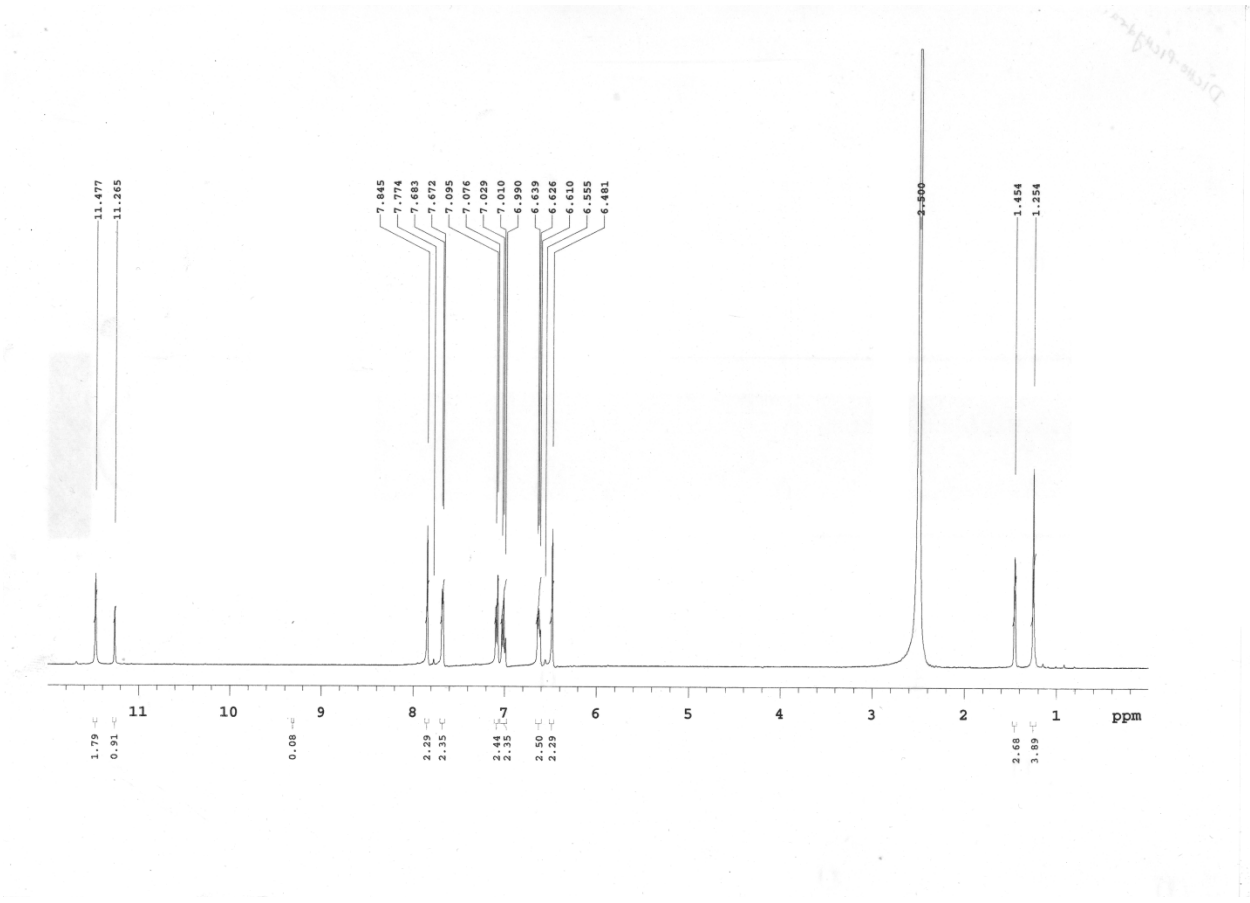


Fig. S1: ^{1}H- NMR spectra of $\mathbf{L_1}$ in DMSO-d_6.

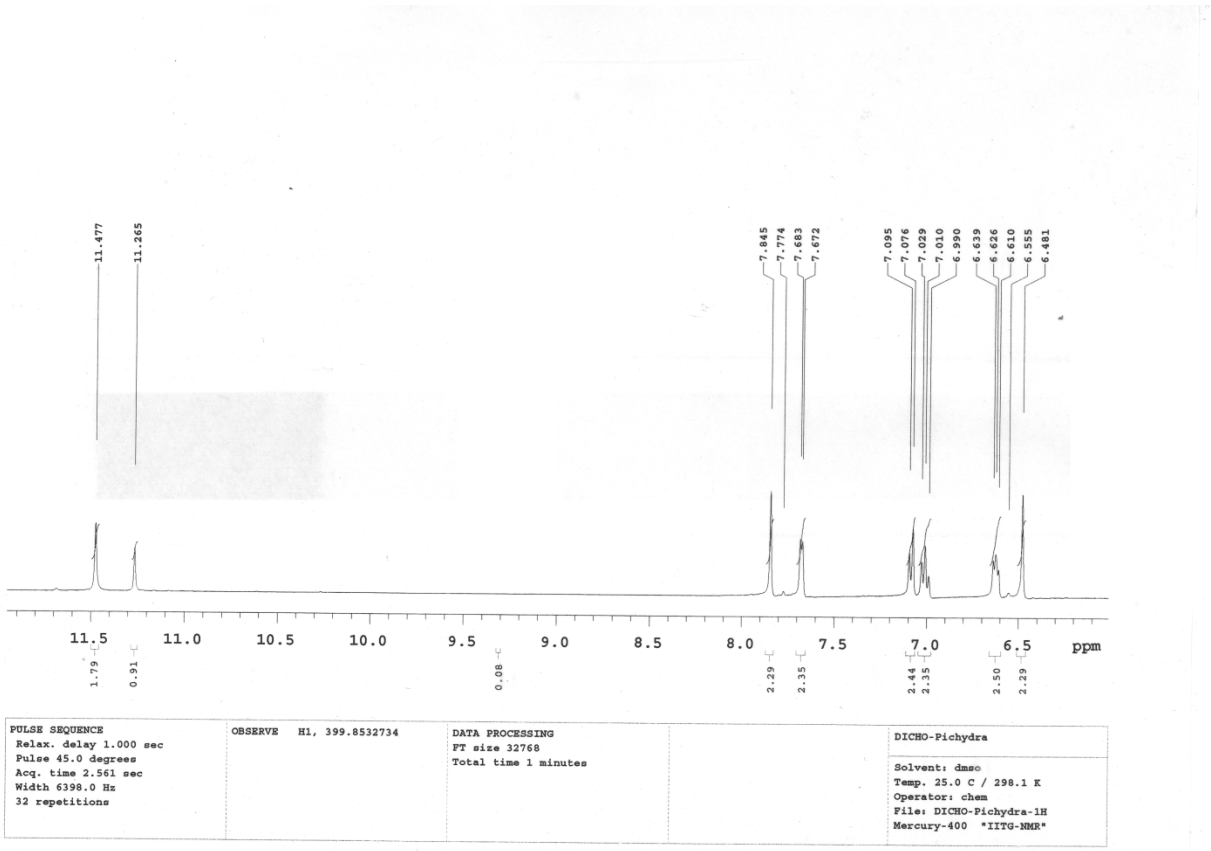


Fig. S2: Expanded ^{1}H- NMR spectra of $\mathbf{L_1}$ in DMSO-d_6.

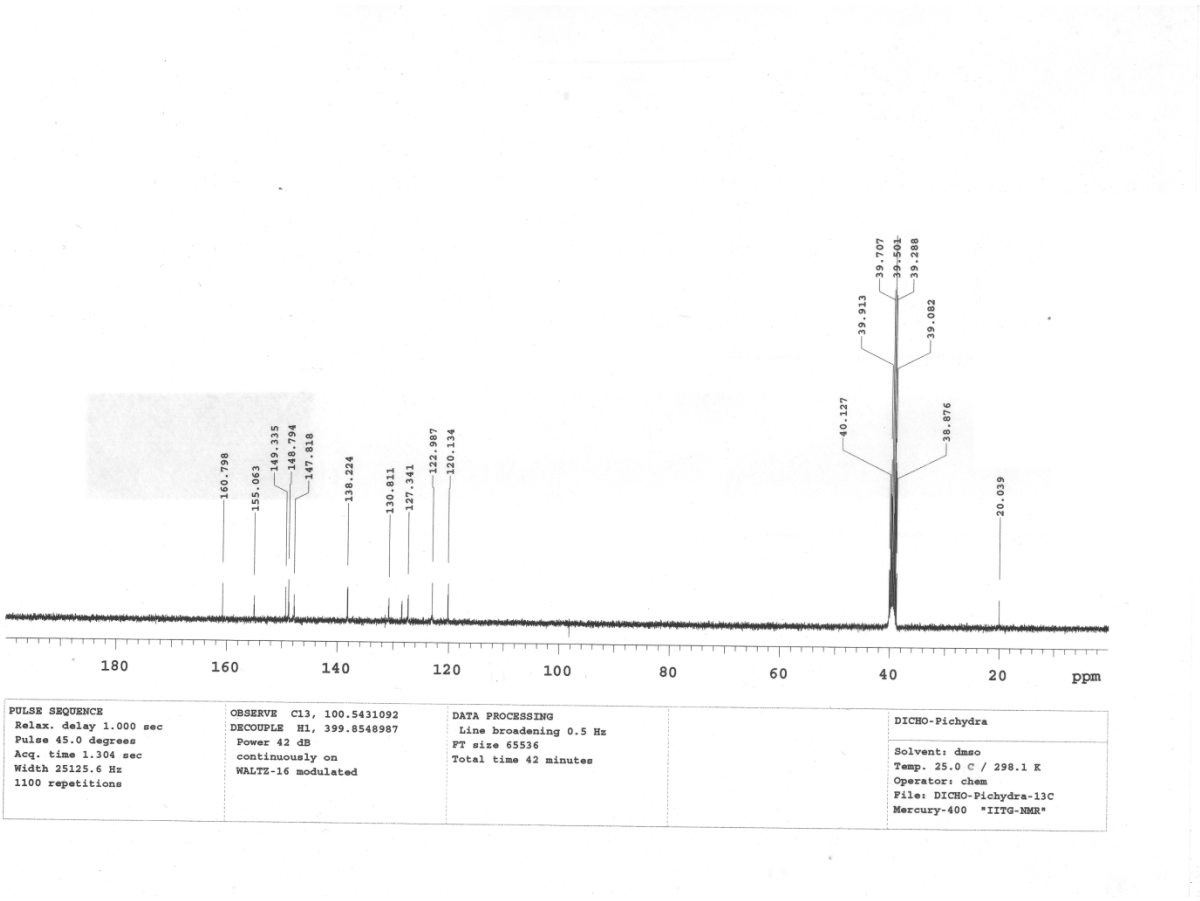


Fig. S3: ^{13}C- NMR spectra of $\mathbf{L_1}$ in DMSO-d_6.

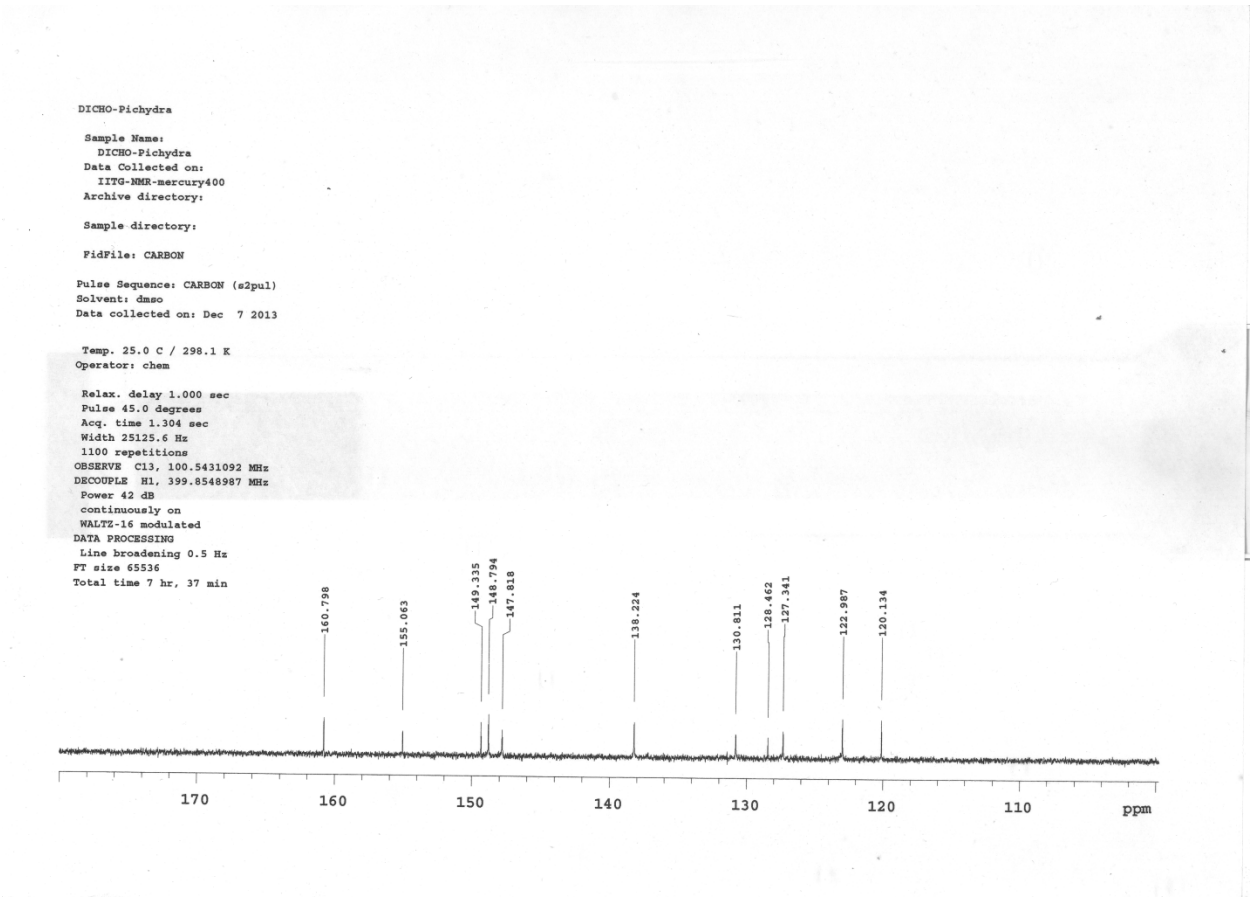


Fig. S4: Expanded ^{13}C- NMR spectra of $\mathbf{L_1}$ in DMSO-d_6.

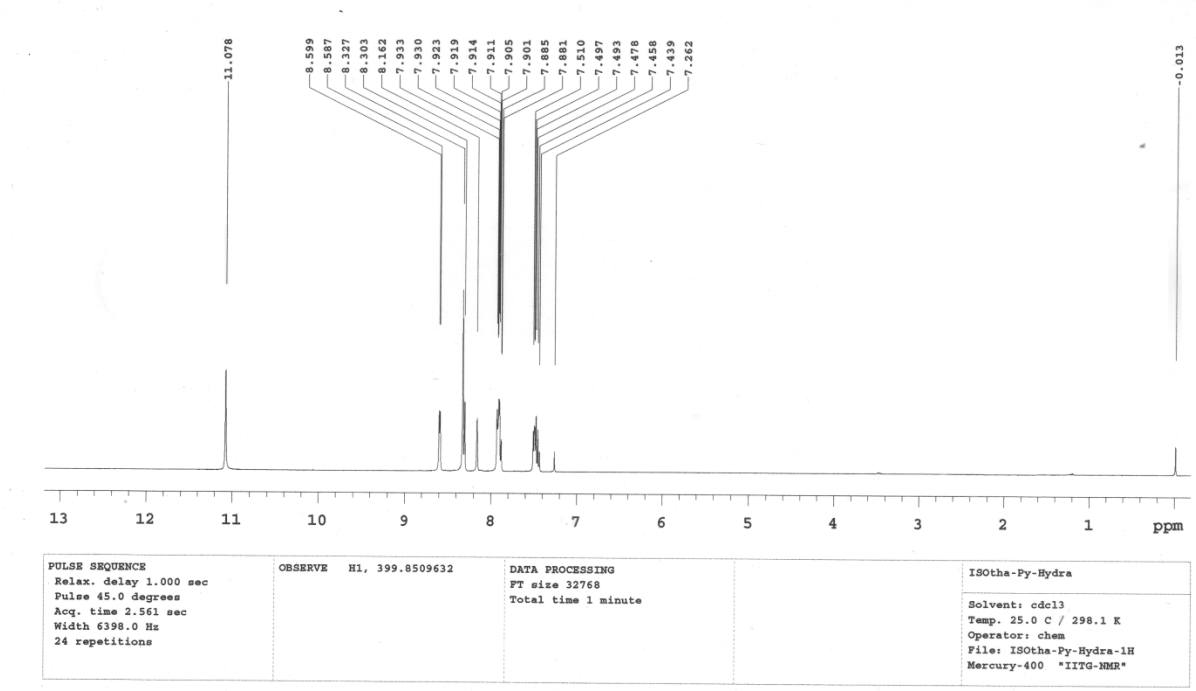


Fig. S5: ^{1}H- NMR spectra of $\mathbf{L_2}$ in $CDCl_3$.

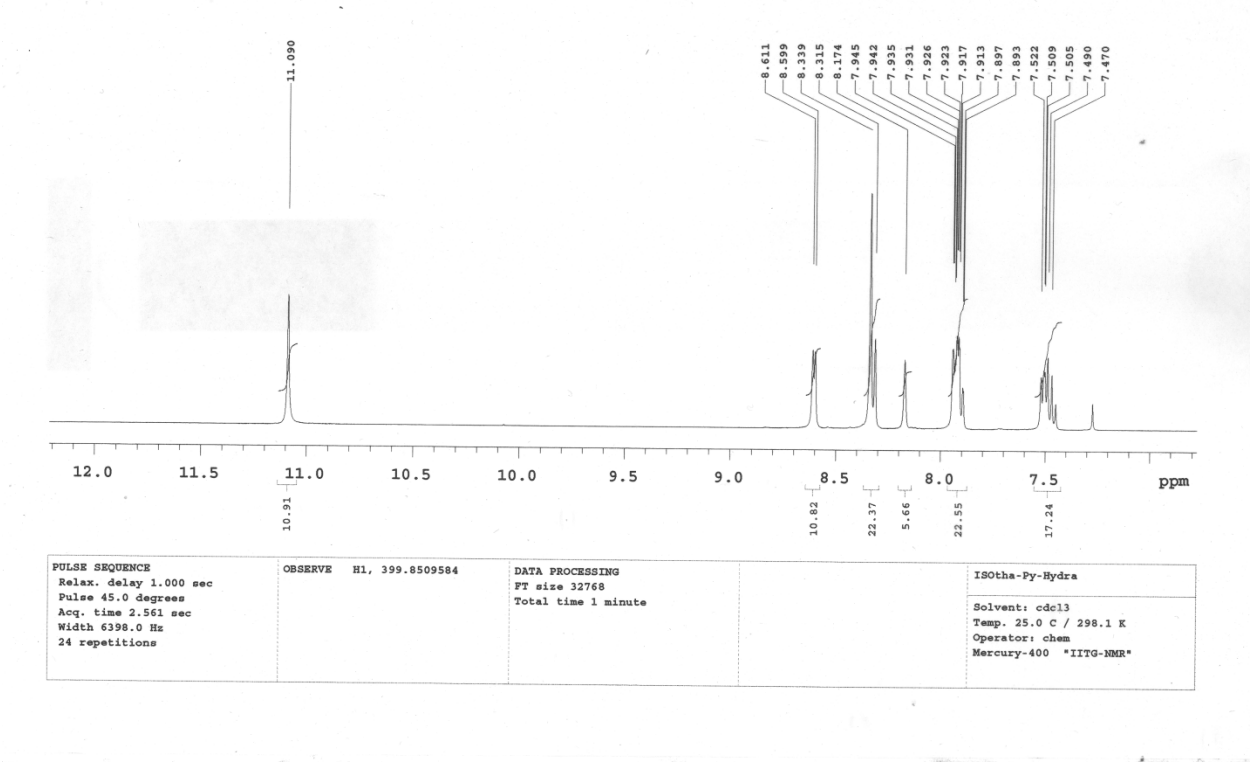


Fig. S6: Expanded ^{1}H- NMR spectra of $\mathbf{L_2}$ in $CDCl_3$.

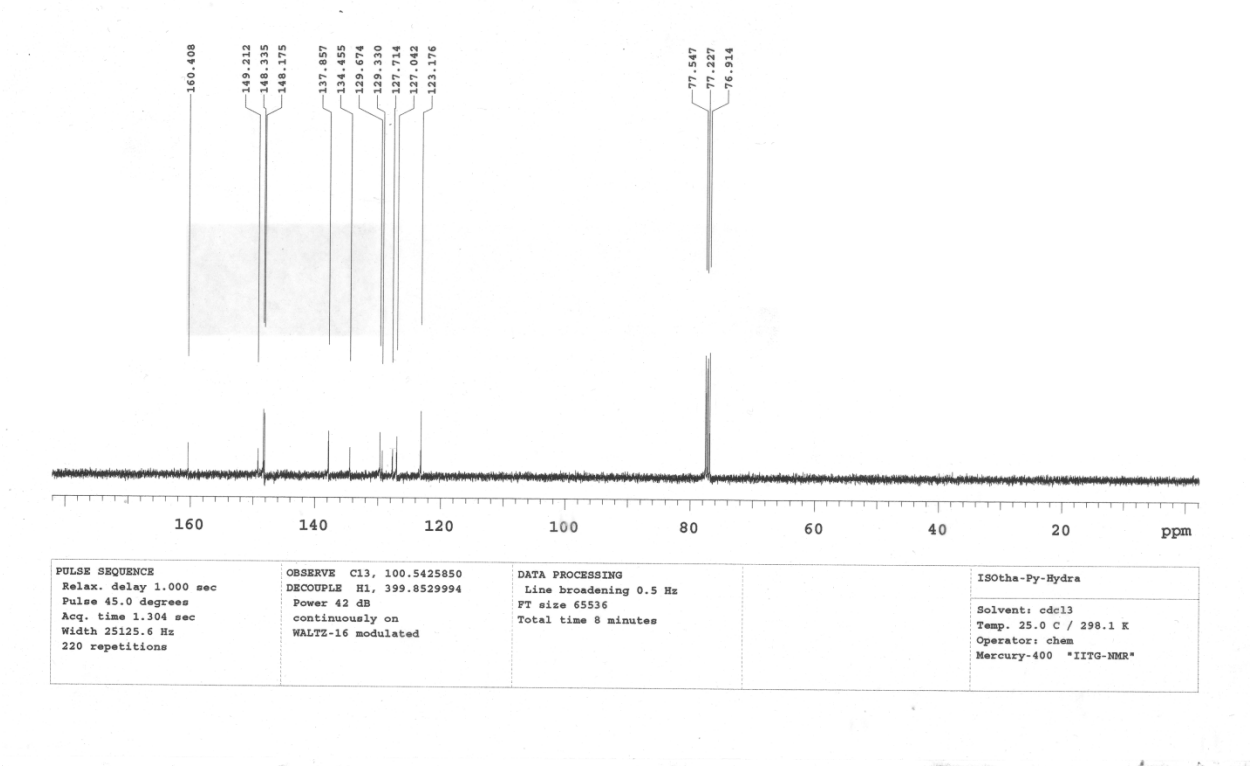


Fig. S7: ^{13}C- NMR spectra of $\mathbf{L_2}$ in $CDCl_3$.

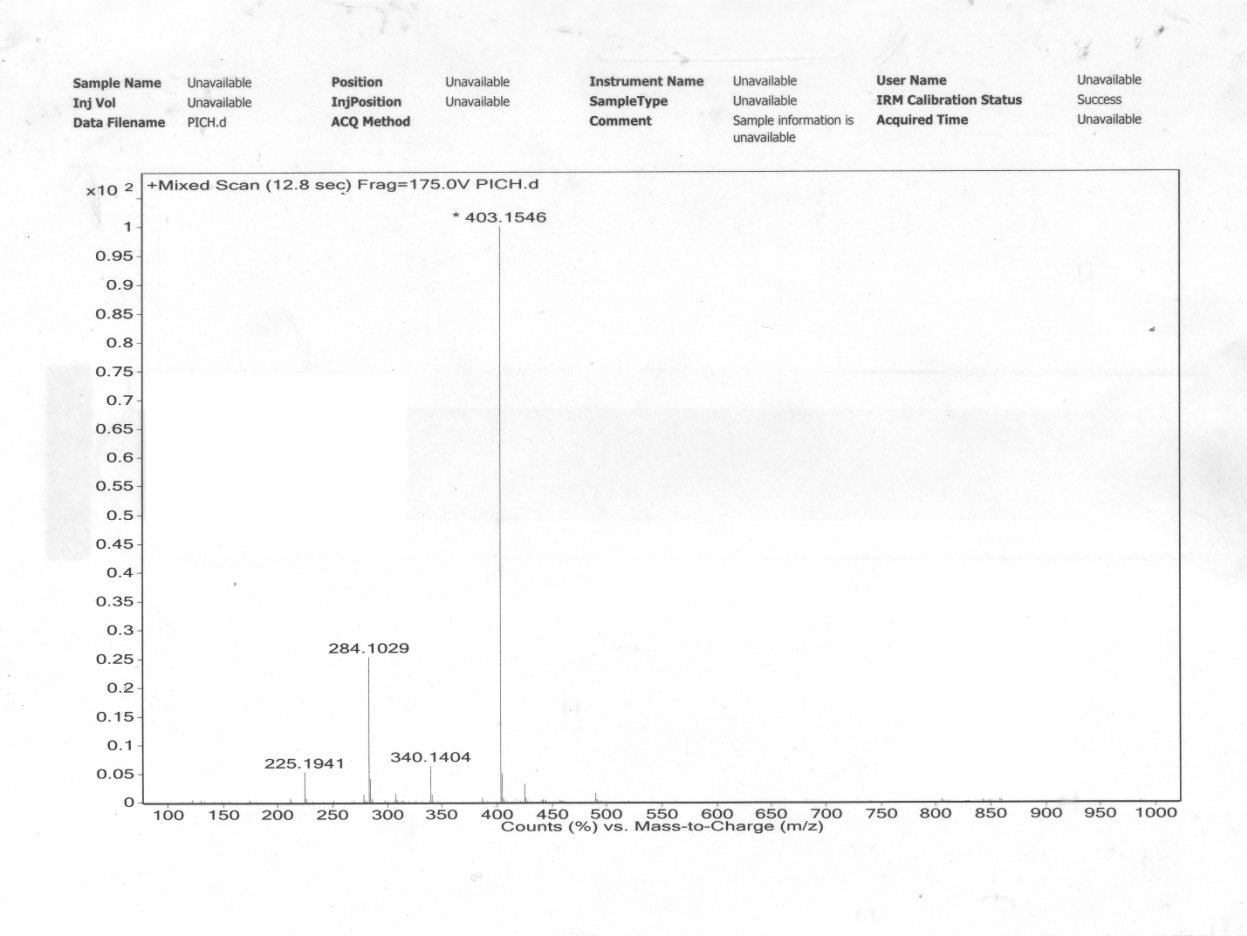


Fig. S8: Mass spectrum of $\mathbf{L_1}$ (positive mode), Expected *m/z* for $C_{21}H_{19}N_6O_3$ $(\mathbf{L_1}+H)^+$ = 403.1519, Found 403.1546.

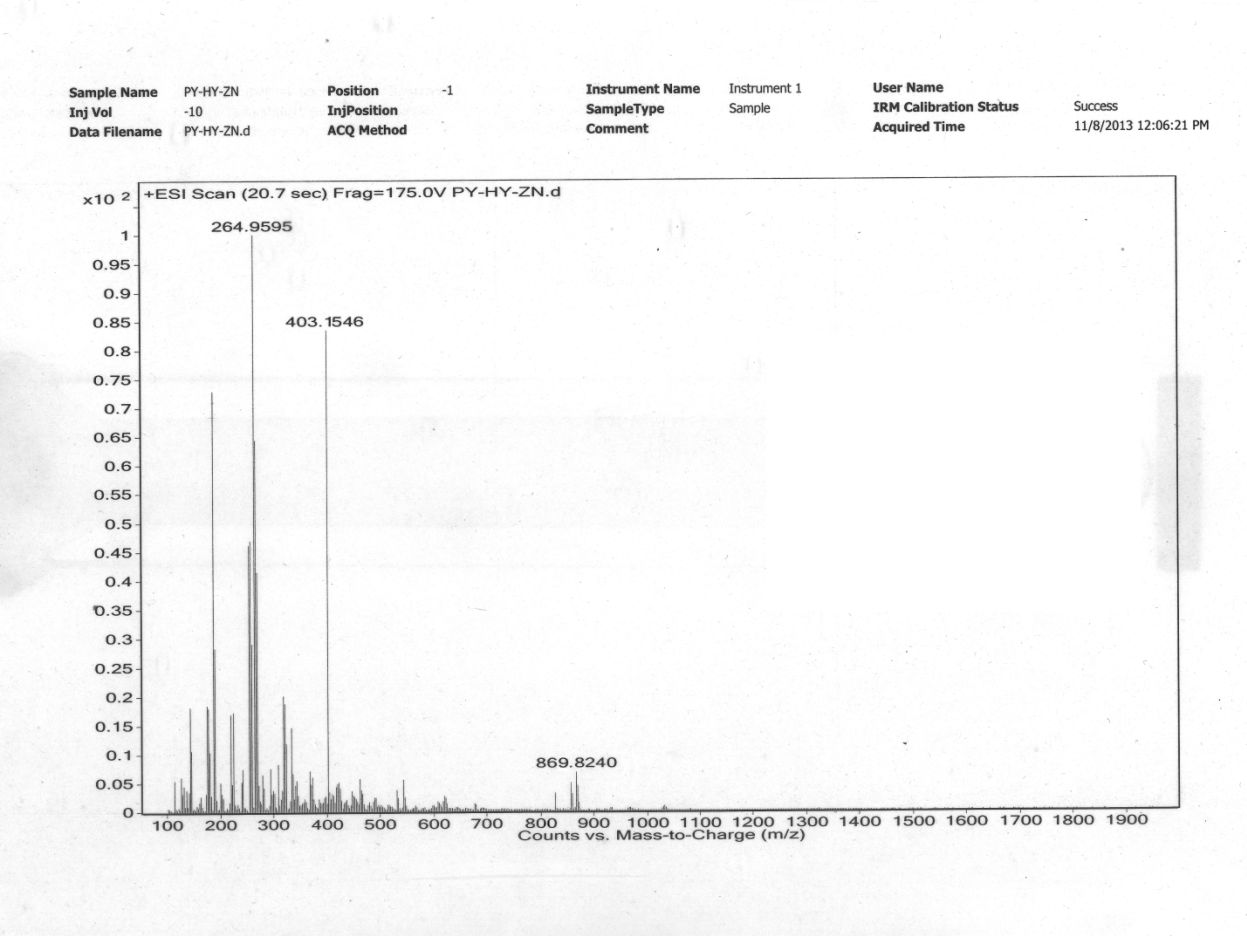


Fig. S9: Mass spectrum of zinc complex of $\mathbf{L_1}$ (positive mode). Expected *m/z* for $C_{23}H_{21}Cl_3N_7O_{15}Zn_2$ ($\mathbf{L_1}$+2Zn+3ClO_4+CH_3CN) = 869.8713, found 869.8240.

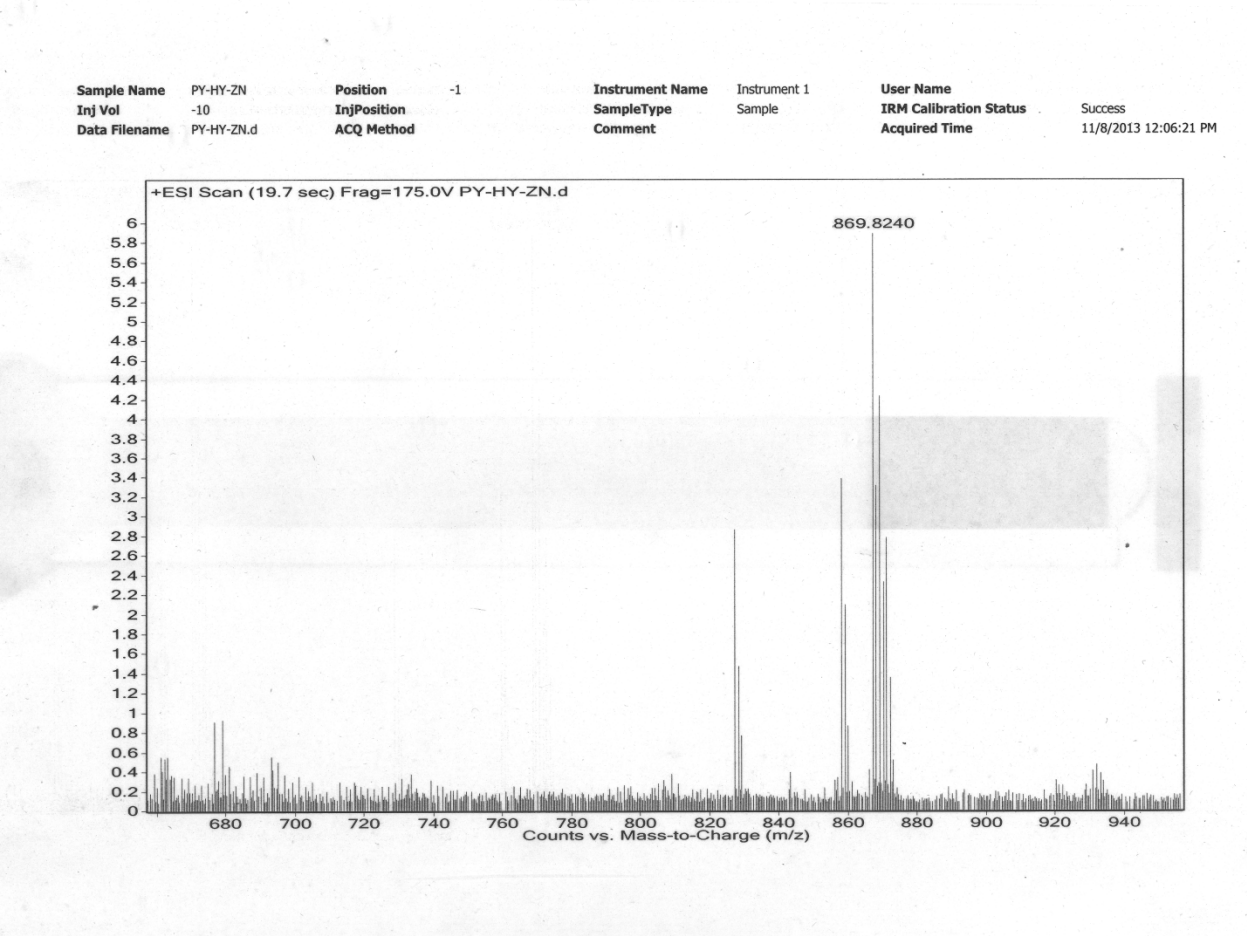


Fig. S10: Expanded mass spectrum of zinc complex of $\mathbf{L_1}$ (positive mode).

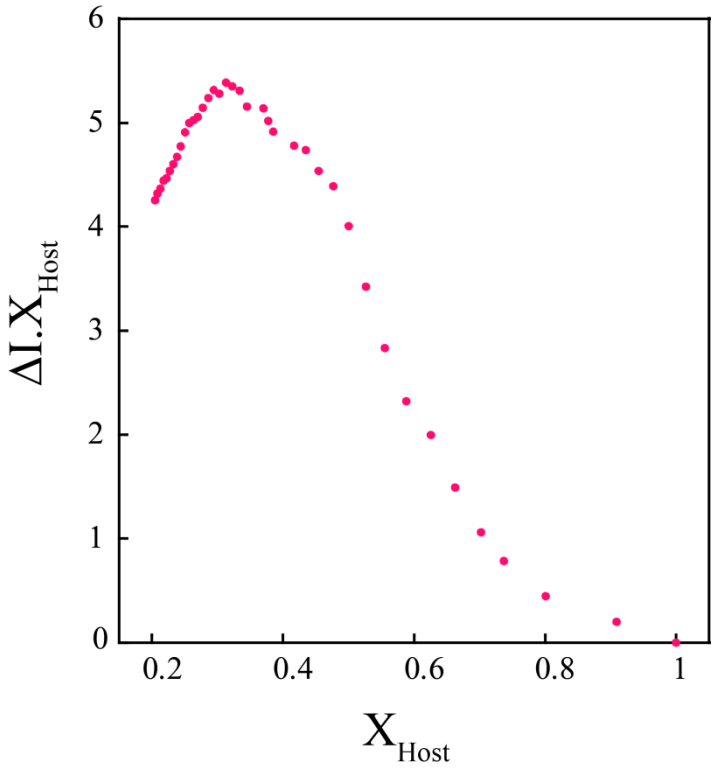


Fig. S11: Job's plot between $\mathbf{L_1}$ and Zn^{2+}.

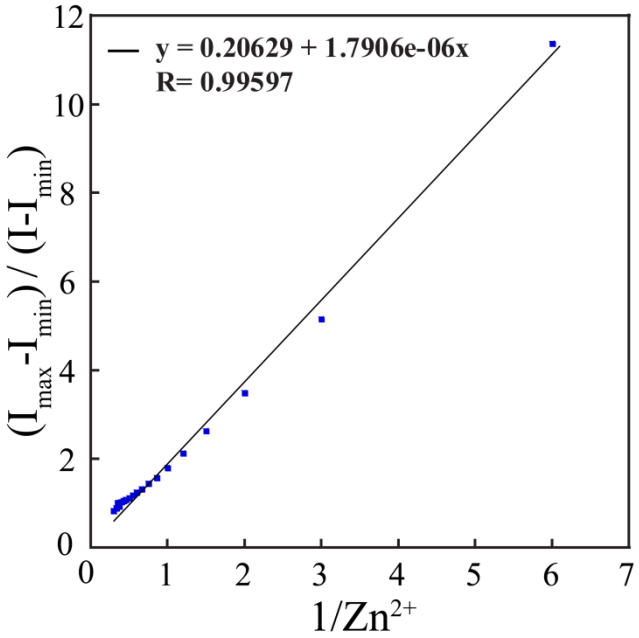


Fig. S12: Benesi–Hildebrand plot between $\mathbf{L_1}$ and Zn^{2+}.

Fig. S13: Visual color change upon the addition of Zn^{2+} to $\mathbf{L_1}$ solution.

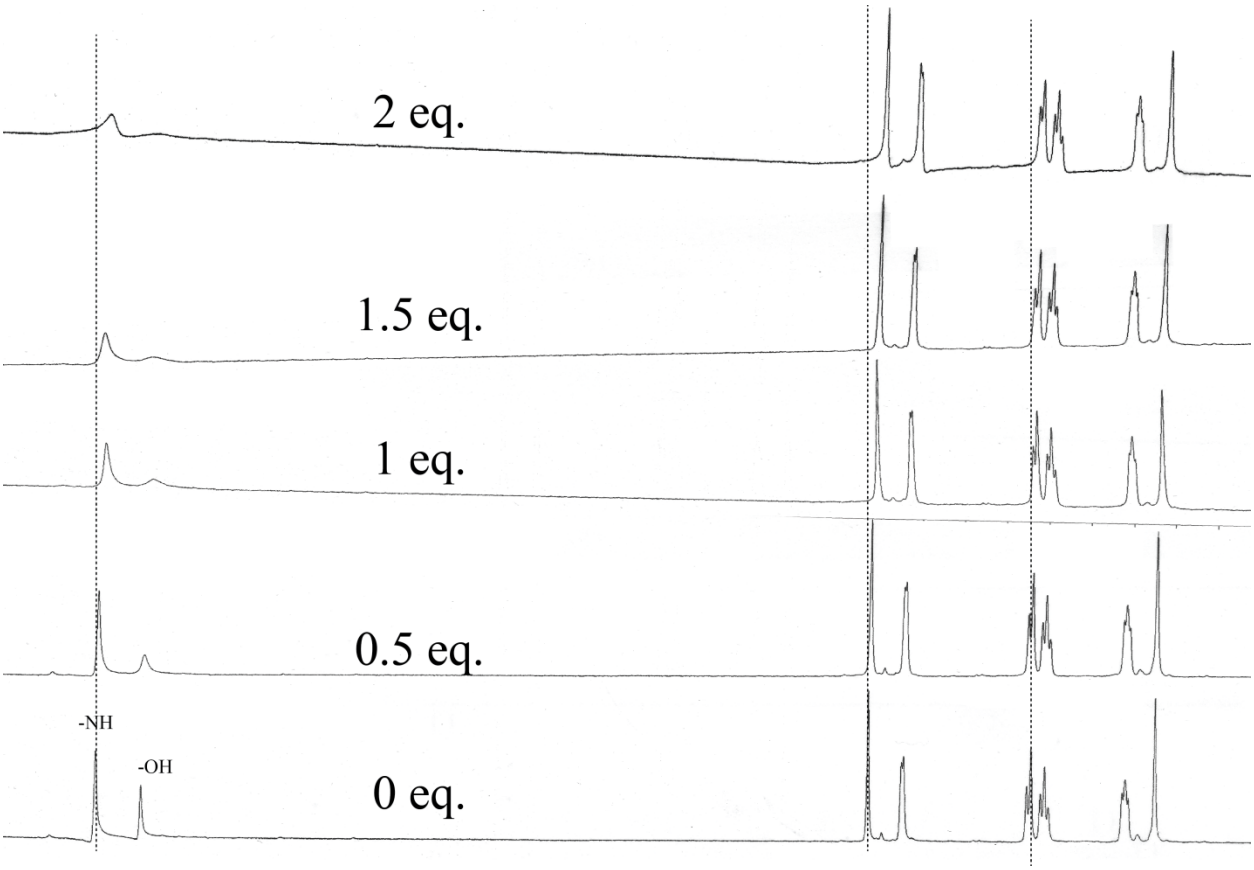


Fig. S14: ^{1}H-NMR titration of $\mathbf{L_1}$ with Zn^{2+} in DMSO-d_6.

Cytotoxicity assay for L_1 and L_1-Zn complex

A standard MTT assay was performed to determine the cytotoxic effect of **L_1** and **L_1**–Zn complex on HeLa cells. MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) solution was procured from Sigma-Aldrich, USA. Initially HeLa cells were grown in 25 cm^2 tissue culture flask in Dulbecco's modified Eagle medium (DMEM) supplemented with 10% (v/v) fetal bovine serum (FBS), penicillin (100g/mL) and streptomycin (100µg/mL) at 37◦C in a CO_2 incubator. Prior to MTT assay, cells were seeded onto 96-well tissue culture plates (approximately 10^4 cells per well) and incubated with various concentrations of compound **L_1** and **L_1**–Zn complex (5.0µM, 12.5µM, 15µM, 25µM and 50µM) made in DMEM for a period of 24h. HeLa cells treated with DMSO or $Zn(ClO_4)_2$ alone were also included in parallel sets. Following 24 h incubation, the growth media was carefully aspirated and fresh DMEM containing MTT solution was added to the cells and incubated for 3–4 h at 37◦C. Subsequently, the MTT solution was removed and the insoluble colored formazan product was solubilized in DMSO and its absorbance was measured in a microtitre plate reader (Infinite M200, TECAN, Switzerland) at 550 nm. MTT assay for every sample was performed in six sets. Data analysis and calculation of standard deviation was performed with Microsoft Excel 2010 (Microsoft Corporation, USA).

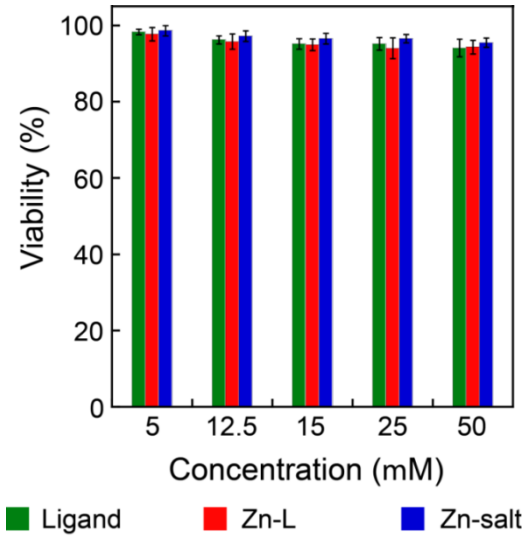


Fig. S15: MTT assay to determine the cytotoxic effect of compound **L_1** and **L_1**–Zn complex on HeLa cells.

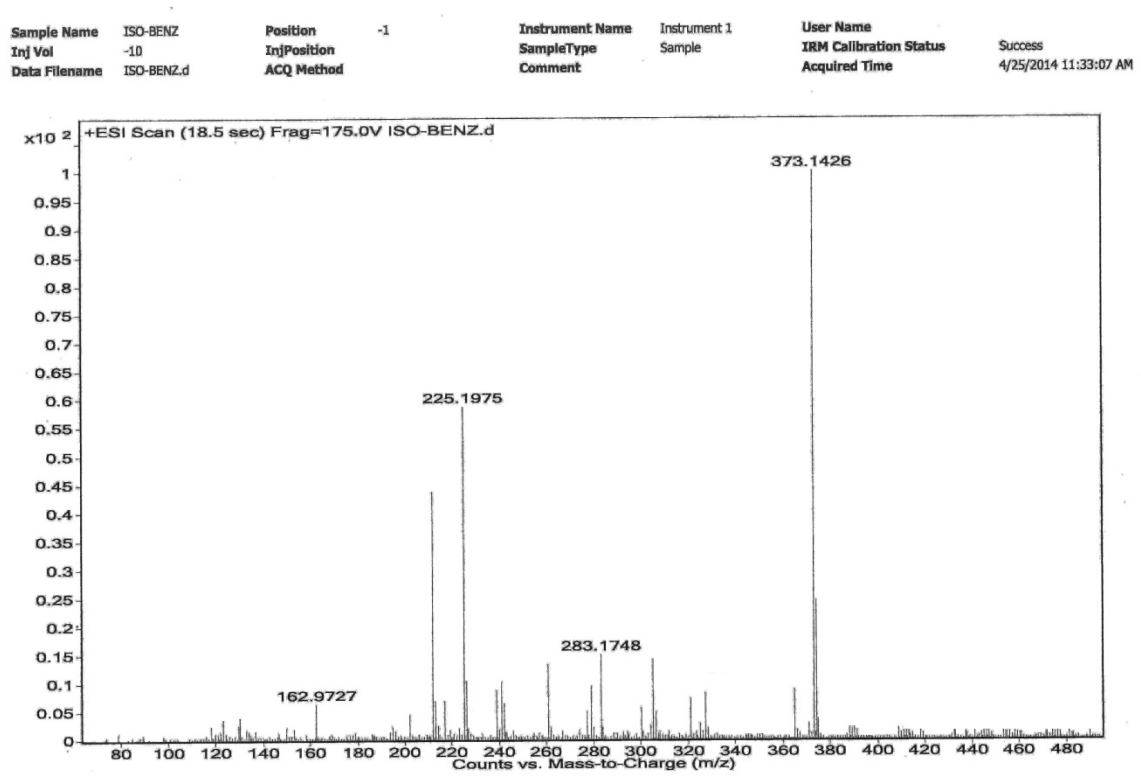


Fig. S16: Mass spectrum of $\mathbf{L_2}$ (positive mode), Expected *m/z* for $C_{20}H_{17}N_6O_2$ $(\mathbf{L_2}+H)^+$ = 373.1413, Found 373.1426.

Table S1. Selected orbitals and their energies for $\mathbf{L_1}$ at B3LYP/6-31G(d,p).

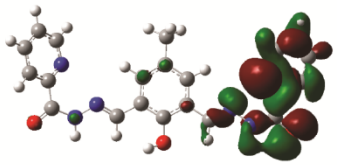
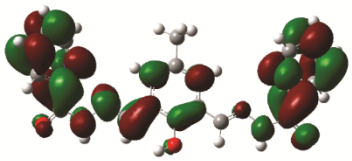
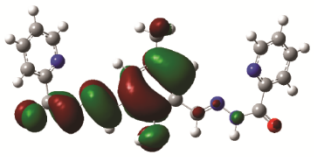
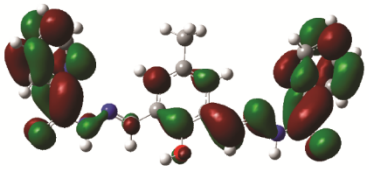
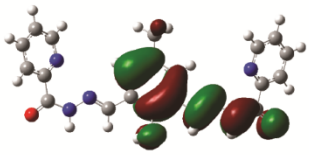
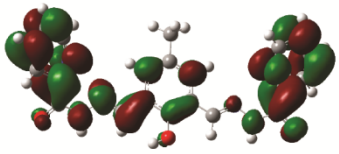
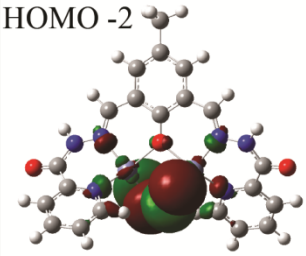
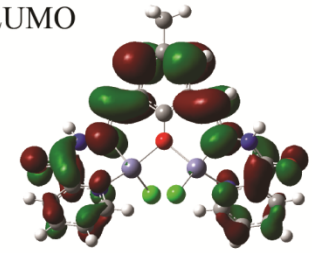
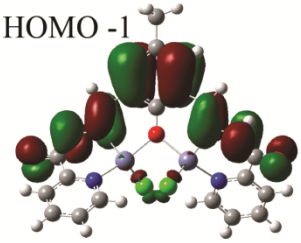
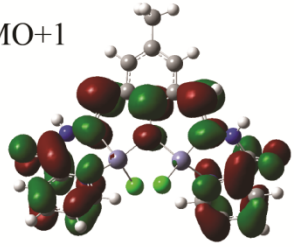
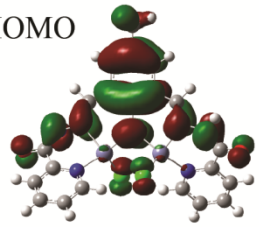
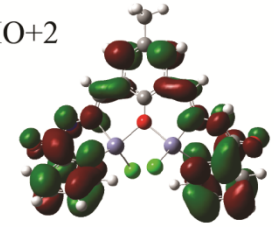
Occupied Orbitals	Energy (eV)	Vacant Orbitals	Energy (eV)
HOMO -2 	-6.6684	LUMO 	-1.7665
HOMO -1 	-5.9307	LUMO+1 	-1.4209
HOMO 	-5.7751	LUMO+2 	-1.1535

Table S2. Selected orbitals and their energies for $\mathbf{L_1}$-Zn^{2+} complex at B3LYP/6-31G(d,p).

Occupied Orbitals	Energy (eV)	Vacant Orbitals	Energy (eV)
HOMO -2 	-9.9906	LUMO 	-5.3925
HOMO -1 	-9.5457	LUMO+1 	-5.1796
HOMO 	-9.0872	LUMO+2 	-4.7617

Reference:

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian 03, Revision E.01, Gaussian, Inc., Wallingford CT, 2004.