Electronic Supplementary Information (ESI) for New Journal of Chemistry

A highly selective and biocompatible chemosensor for sensitive detection of zinc(II)

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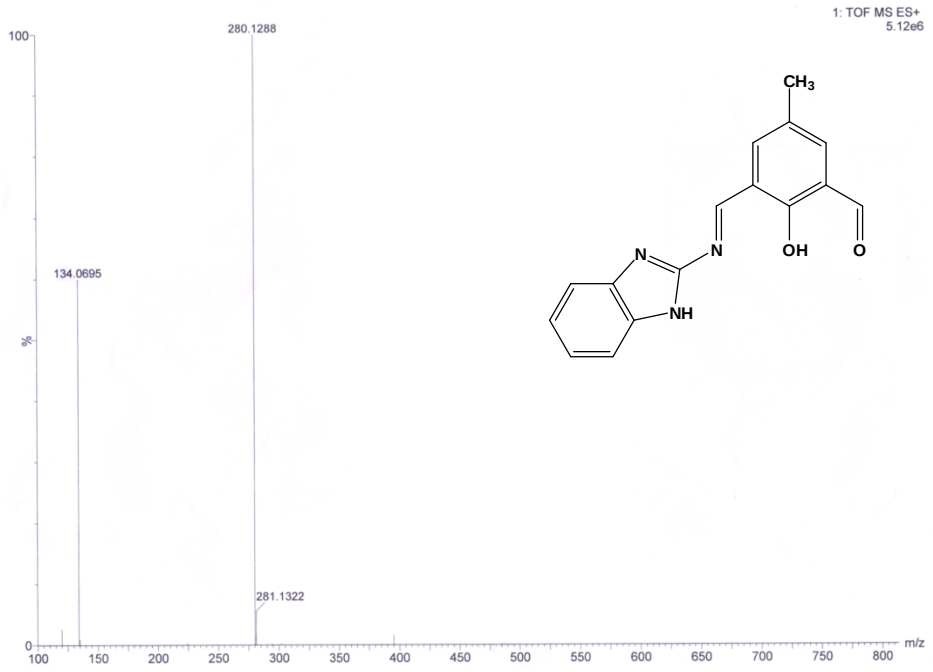

Fig. s1: Mass spectrum of HL^1 in methanol

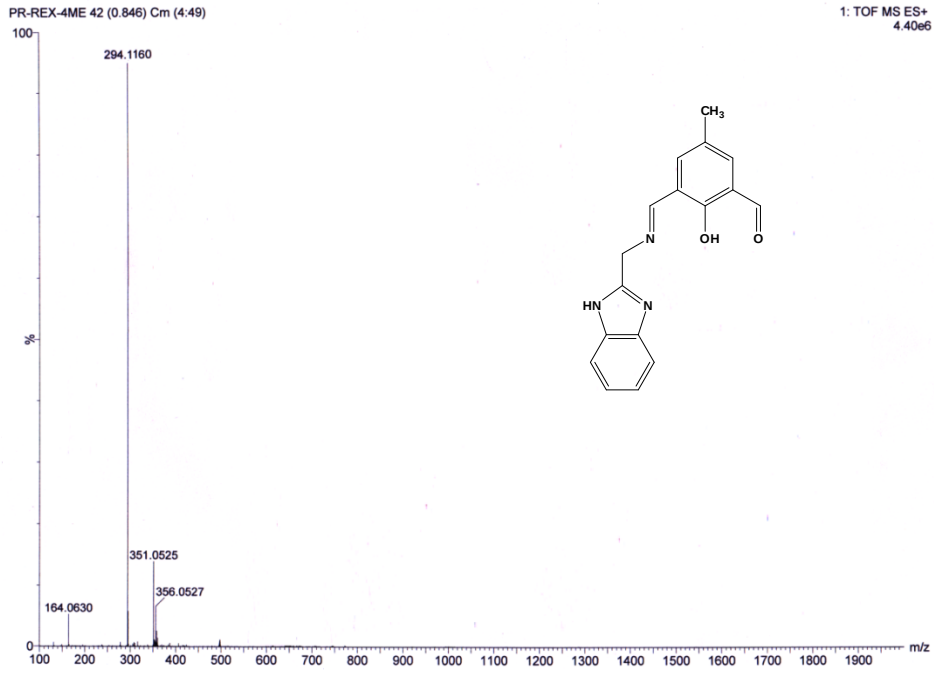

Fig. s2: Mass spectrum of HL^2 in methanol

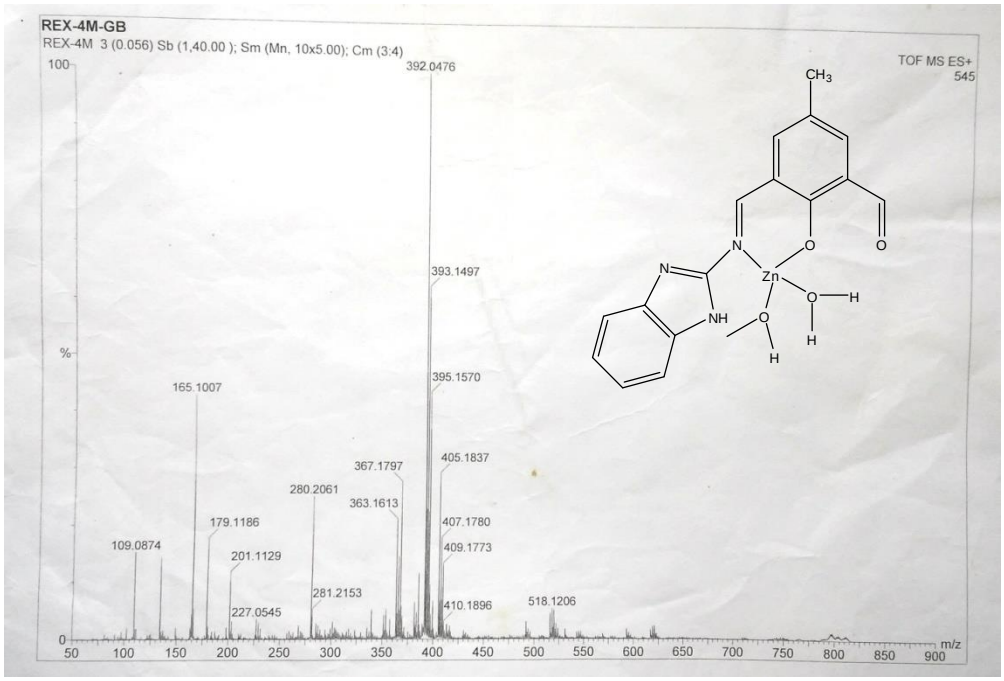

Fig. s3: Mass spectrum of HL^1 with Zn^{2+} in 1:1 ratio (Complex 1) in methanol

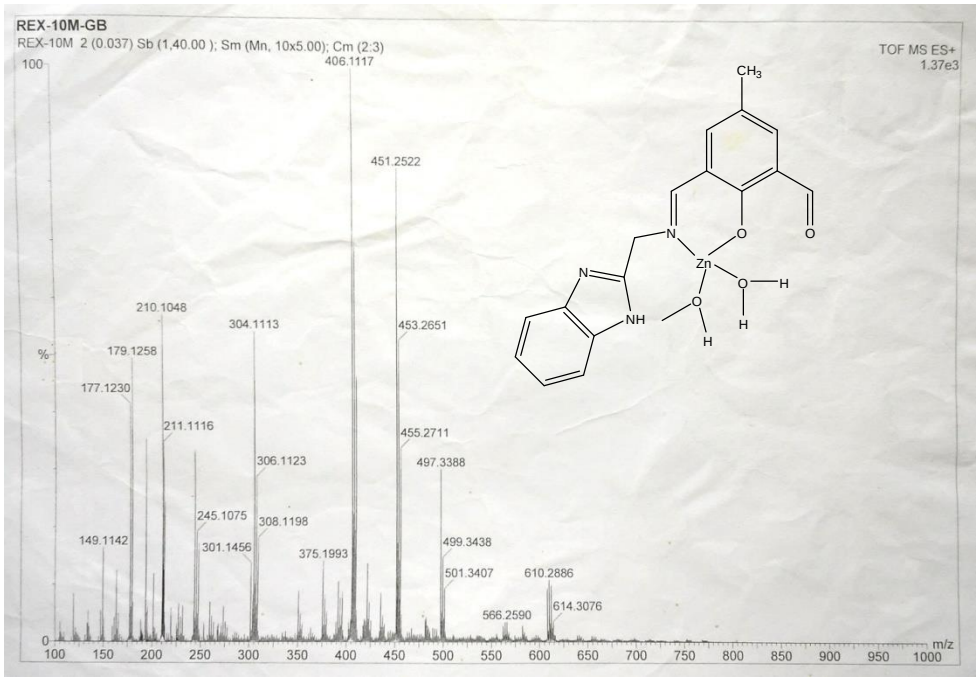

Fig. s4: Mass spectrum of HL^2 with Zn^{2+} in 1:1 ratio (Complex 2) in methanol

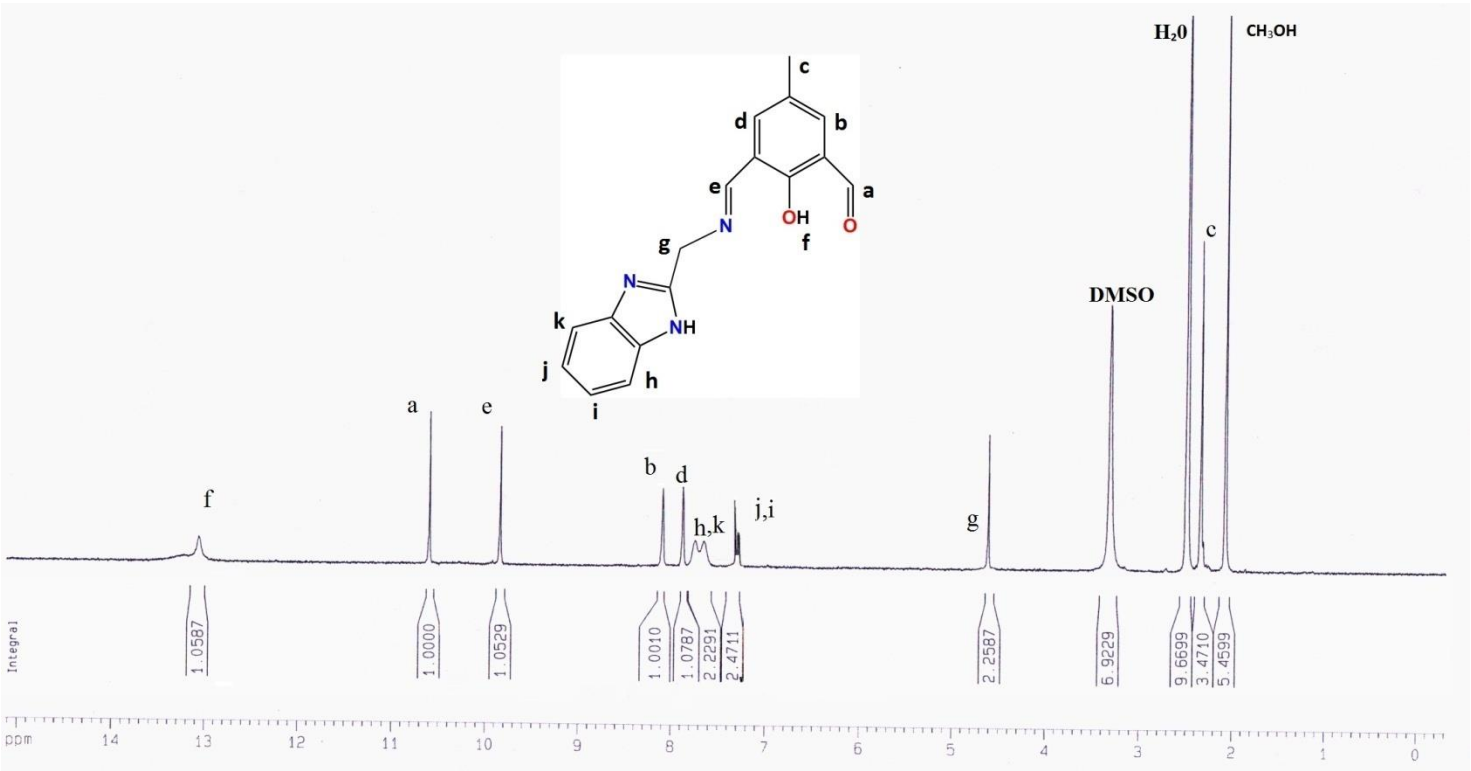

Fig. s5: ^{1}H NMR spectrum of HL^{2} in DMSO-d_6.

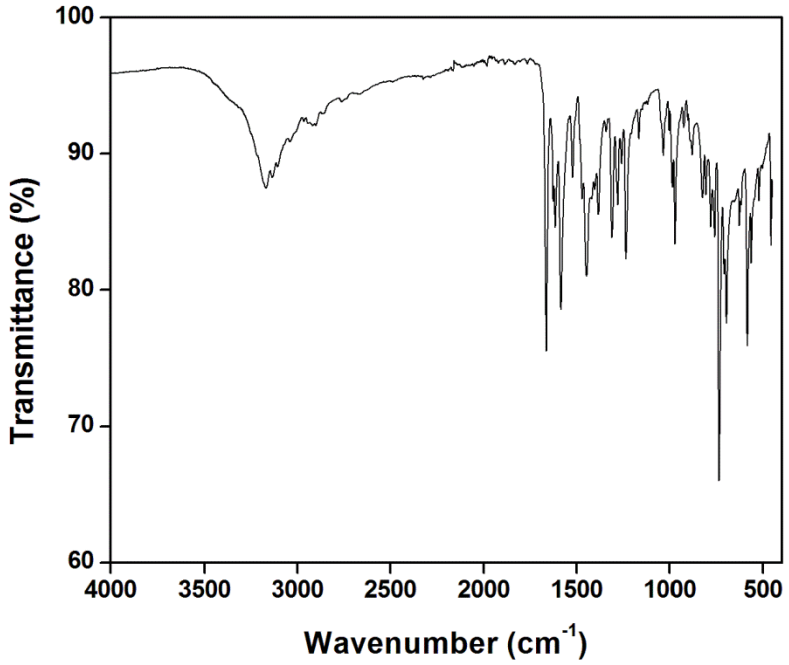

Fig. s6: FT-IR spectrum of HL^1

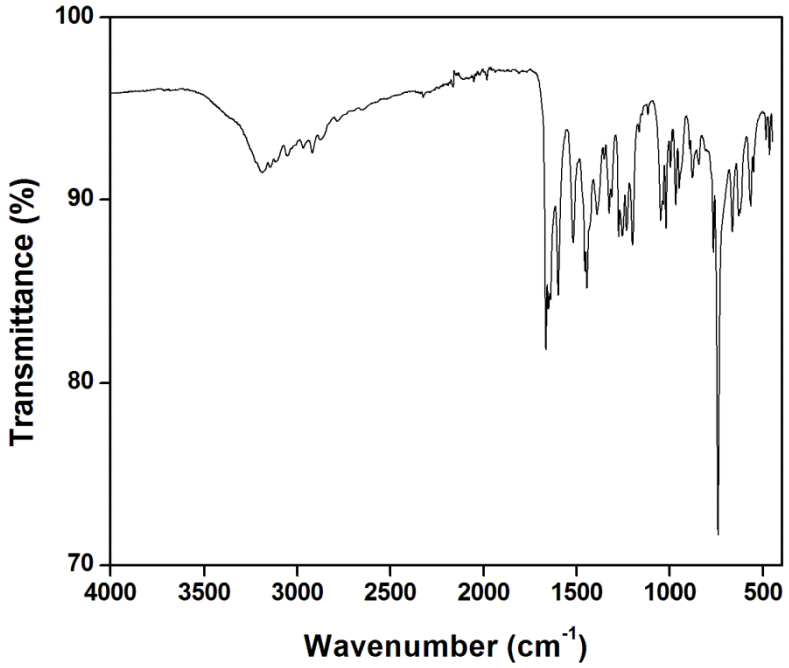

Fig. s7: FT-IR spectrum of HL^2

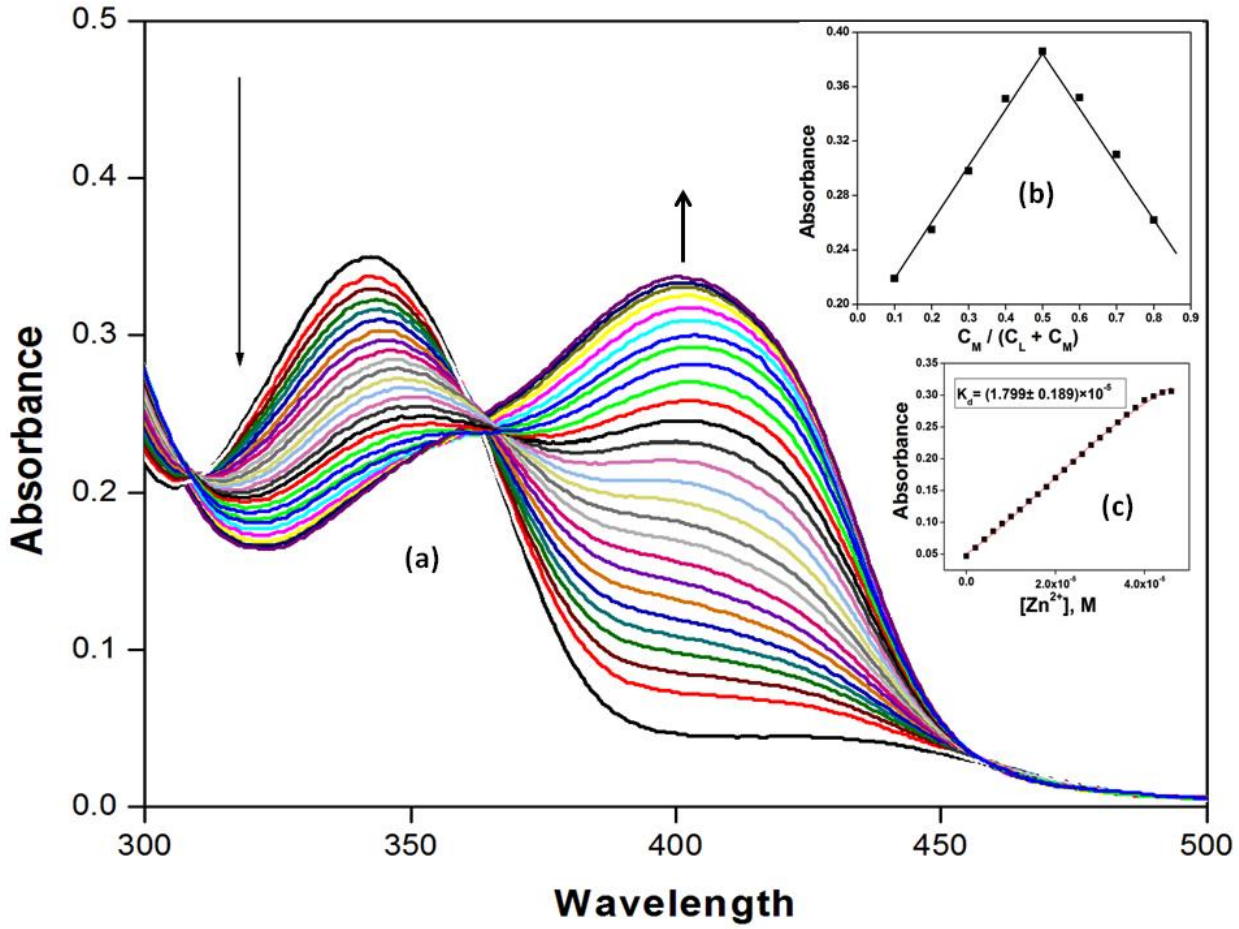

Fig. s8: (a) Absorption spectra of HL^2 (40 μM) with the gradual addition of Zn^{2+} ion (0-40 μM) in 10 mM HEPES buffer in water:methanol (1:9, *v/v*) (pH = 7.2) at room temperature; (b) Job's plot indicating 1:1 complex formation and (c) Plot of absorption at 398 nm *vs.* concentration of Zn^{2+}.

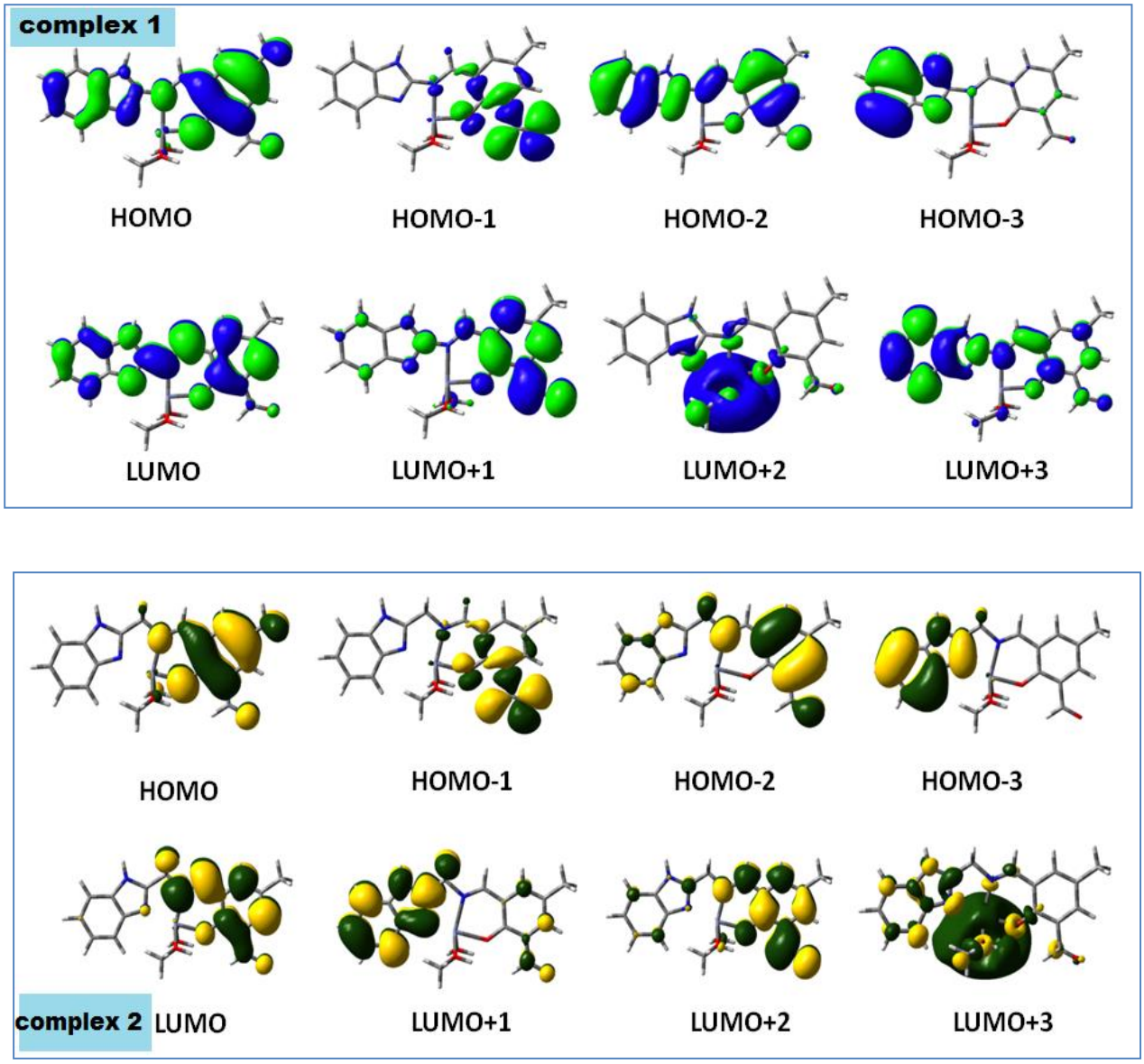

Fig. s9: Contour plots of some selected frontier molecular orbitals of complex 1 and complex 2 at their optimized S_0 geometry.

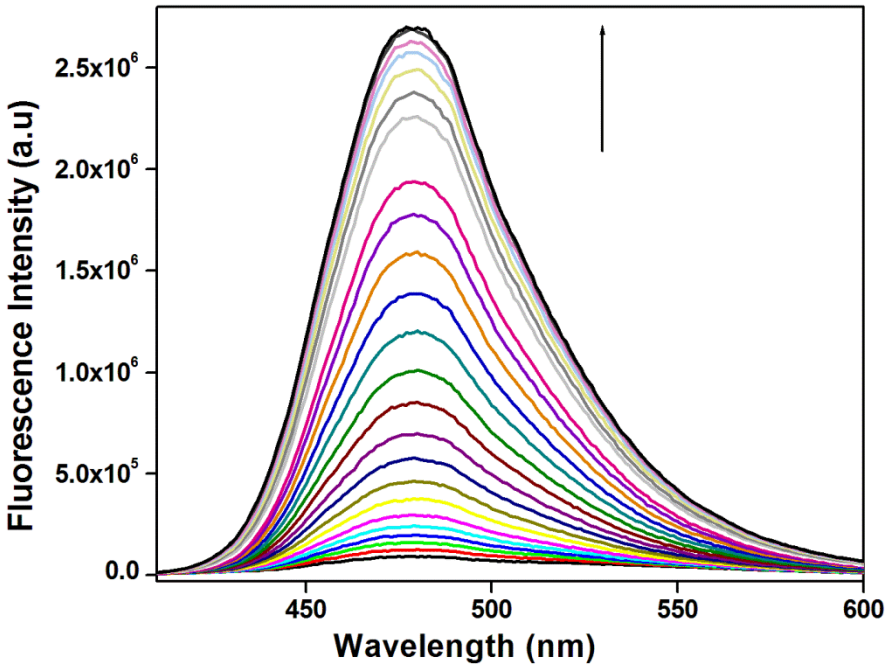

Fig. s10: Fluorescence intensity of HL^2 (40 μM) in the presence of 0, 4, 8, 12, 16, 20, 24, 28, 32, 36, 40 and 44 μM of Zn^{2+} ion in 10 mM HEPES buffer in water:methanol (1:9, *v/v*) (pH = 7.2) at room temperature (excitation: 398 nm)

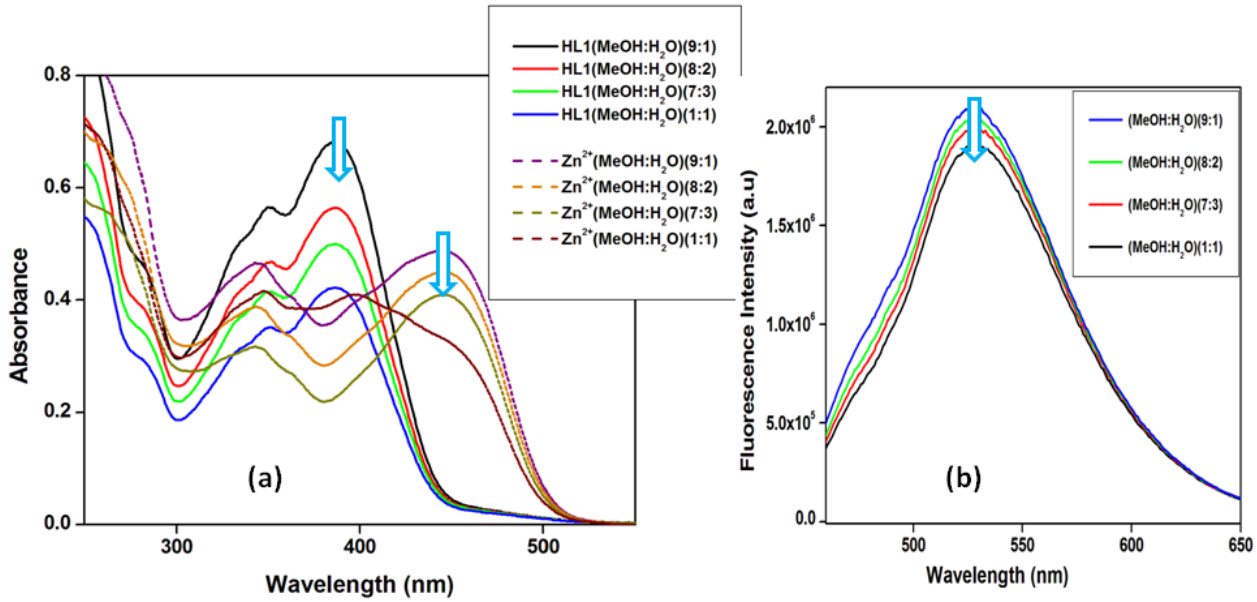

Fig. s11: UV-vis and fluorescence spectra of HL^1 in different water/methanol ratio.

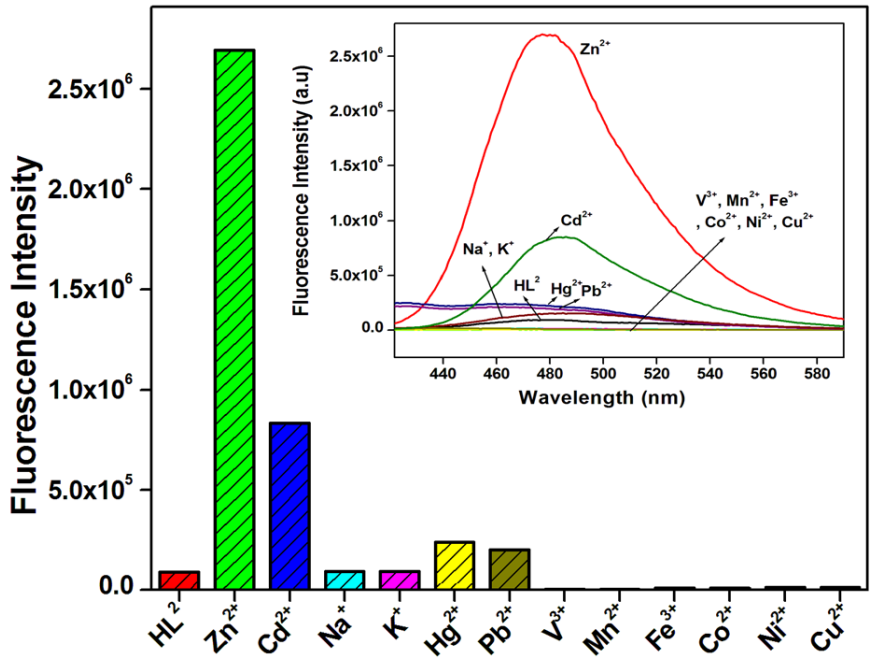

Fig. s12: Fluorescence intensity of HL^2 (40 μM) in the presence of different metal ions (200 μM) in 10 mM HEPES buffer in water:methanol (1:9, *v/v*) (pH = 7.2) at room temperature (excitation: 398 nm)

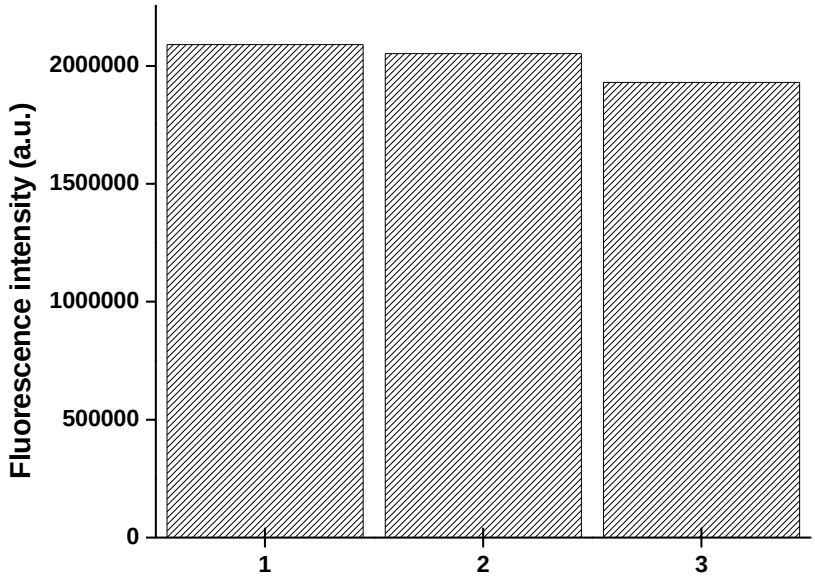

Fig. s13: Fluorescence intensity of HL^1 (40 μM) in the presence of (1) nitrate, (2) perchlorate and (3) chloride salt of Zn^{2+} (40 μM) in 10 mM HEPES buffer in water:methanol (1:9, *v/v*) (pH = 7.2) at room temperature (excitation: 445 nm)

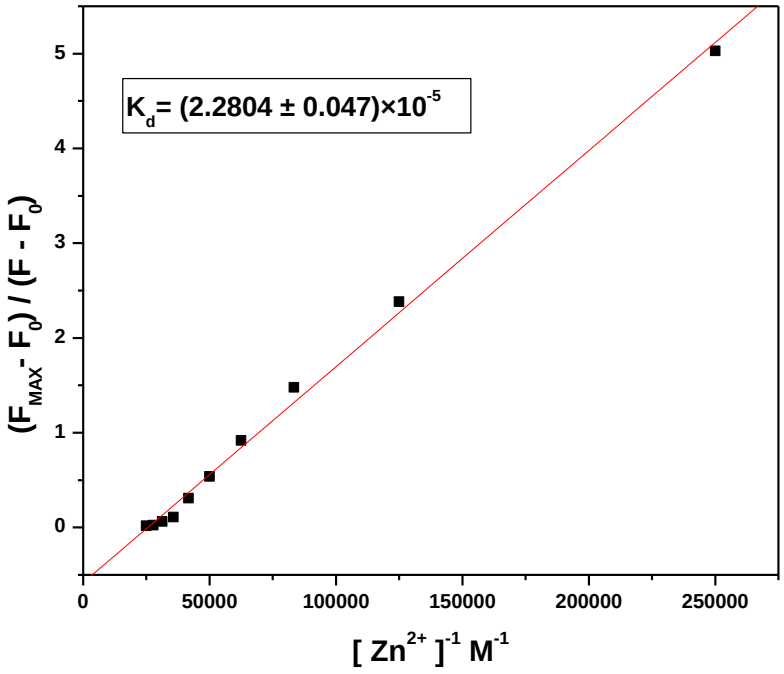

Fig. s14: A plot of $(F_{max}–F_0)/(F–F_0)$ *vs* 1/[Zn^{2+}] following Benesi-Hildebrand equation. The binding constant *K* was determined from the slop to be 4.38 (± 0.09) × 10^4 $M^{–1}$.

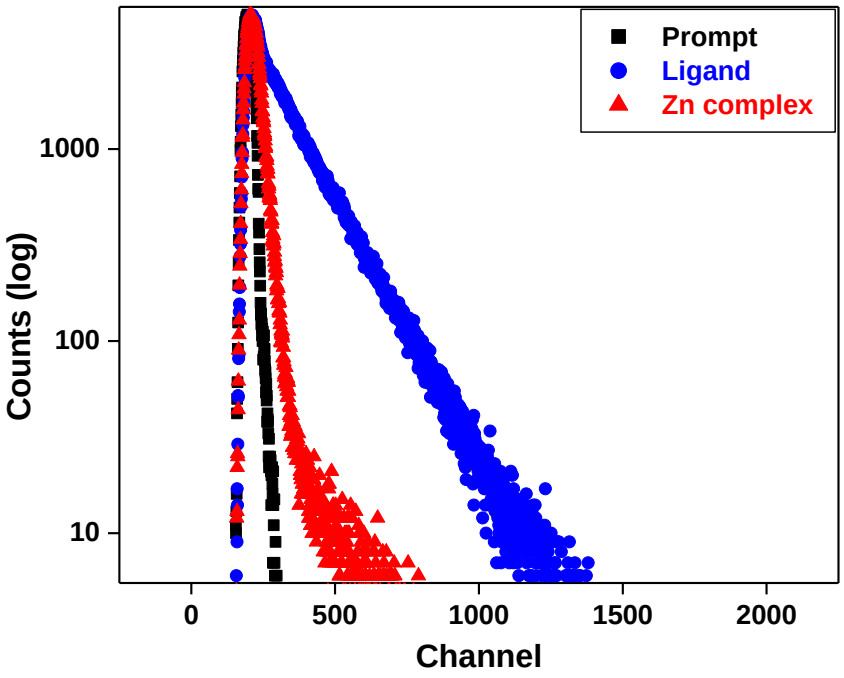

Fig. s15: Excited state fluorescence decay of HL^1 (red) and its zinc complex (blue)

Calculation of the detection limit(LOD) for HL^1:

The detection limit DL of HL^1 for Zn^{2+} was determined from 3σ method by following equation: DL = K* Sb1/S

Where K = 2 or 3 (we take 3 in this case); Sb1 is the standard deviation of the blank solution; S is the slope of the calibration curve obtained from Linear dynamic plot of F.I. *vs* $[Zn^{2+}]$.

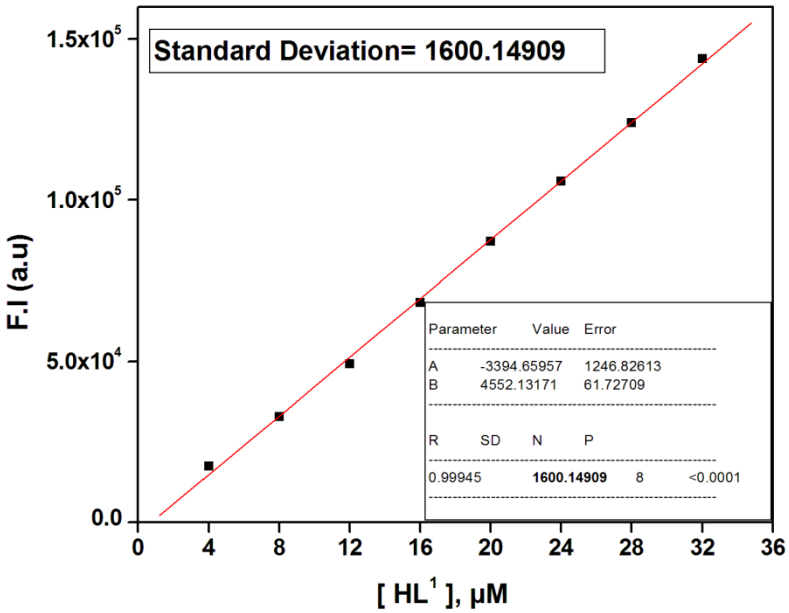

Fig. s16: Determination of Sb1 of the blank, HL^1 solution.

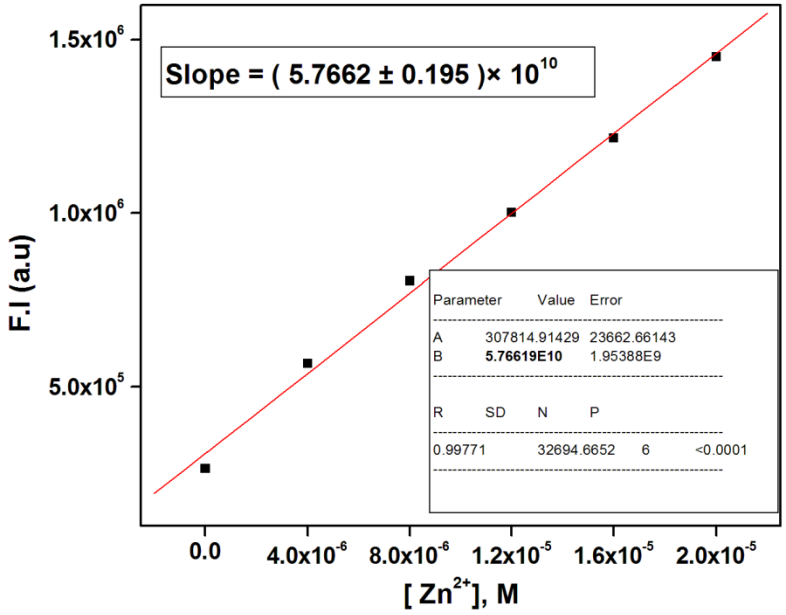

Fig. s17: Linear dynamic plot of F.I. (at 528 nm) *vs.* $[Zn^{2+}]$ for the determination of S (slope); HL^1 =40 µM

LOD (Zn^{2+}) = (3 × 1600.149)/5.76619 × 10^{10} = 0.832 nM

Calculation of the detection limit(LOD) for HL^2:

The detection limit (DL) of HL^2 for Zn^{2+} ion was determined from 3σ method by following equation: **DL = K* Sb1/S**

Where K = 2 or 3 (we take 3 in this case); Sb1 is the standard deviation of the blank solution; S is the slope of the calibration curve obtained from Linear dynamic plot of F.I. vs [Zn^{2+}].

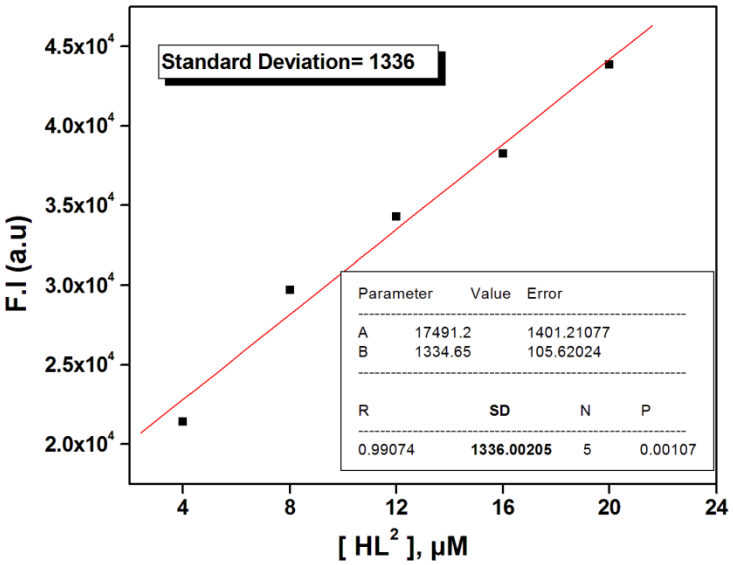

Fig. s18: Determination of Sb1 of the blank and HL^2 solution.

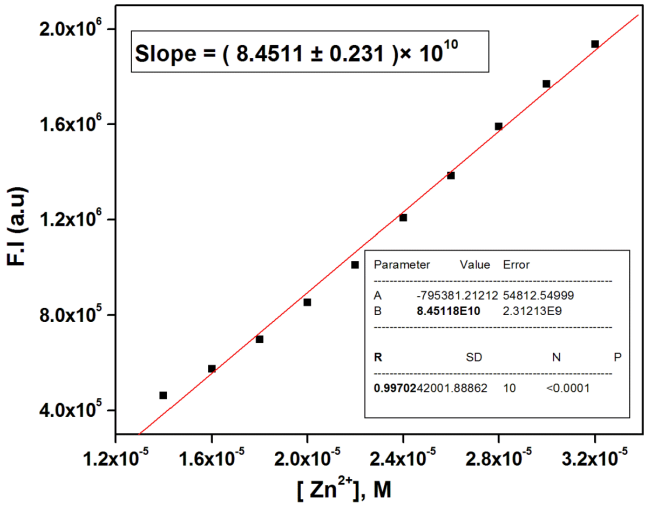

Fig. s19: Linear dynamic plot of FI (at 480 nm) *vs.* [Zn^{2+}] for the determination of S (slope); HL^2 =40 µM

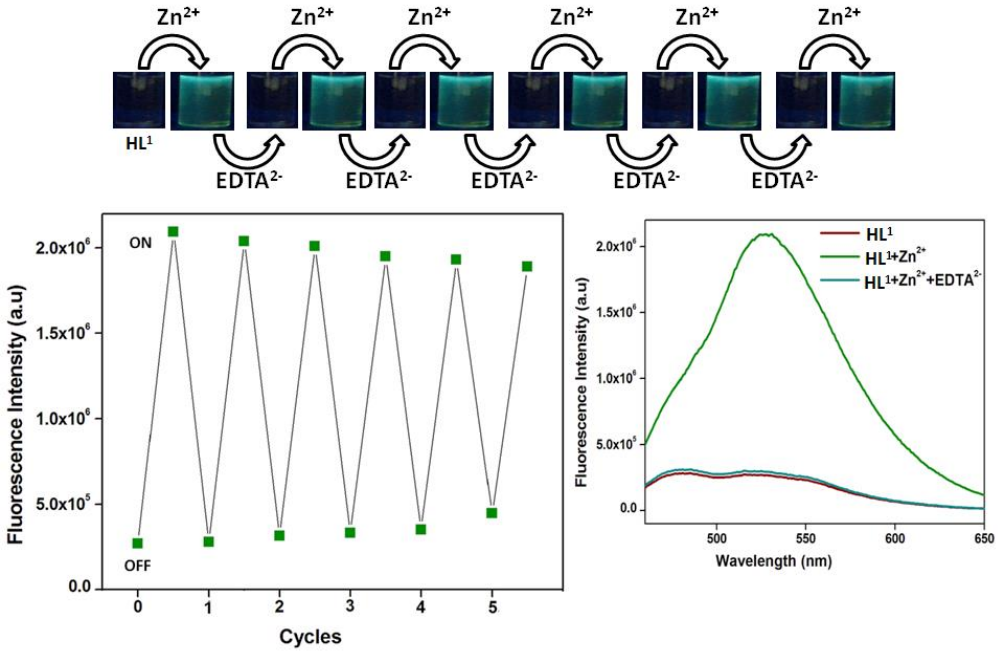

Fig. s20: Fluorescence reversibility of HL^1 in the presence of one eqv. of EDTA and one eqv. of Zn^{2+}.

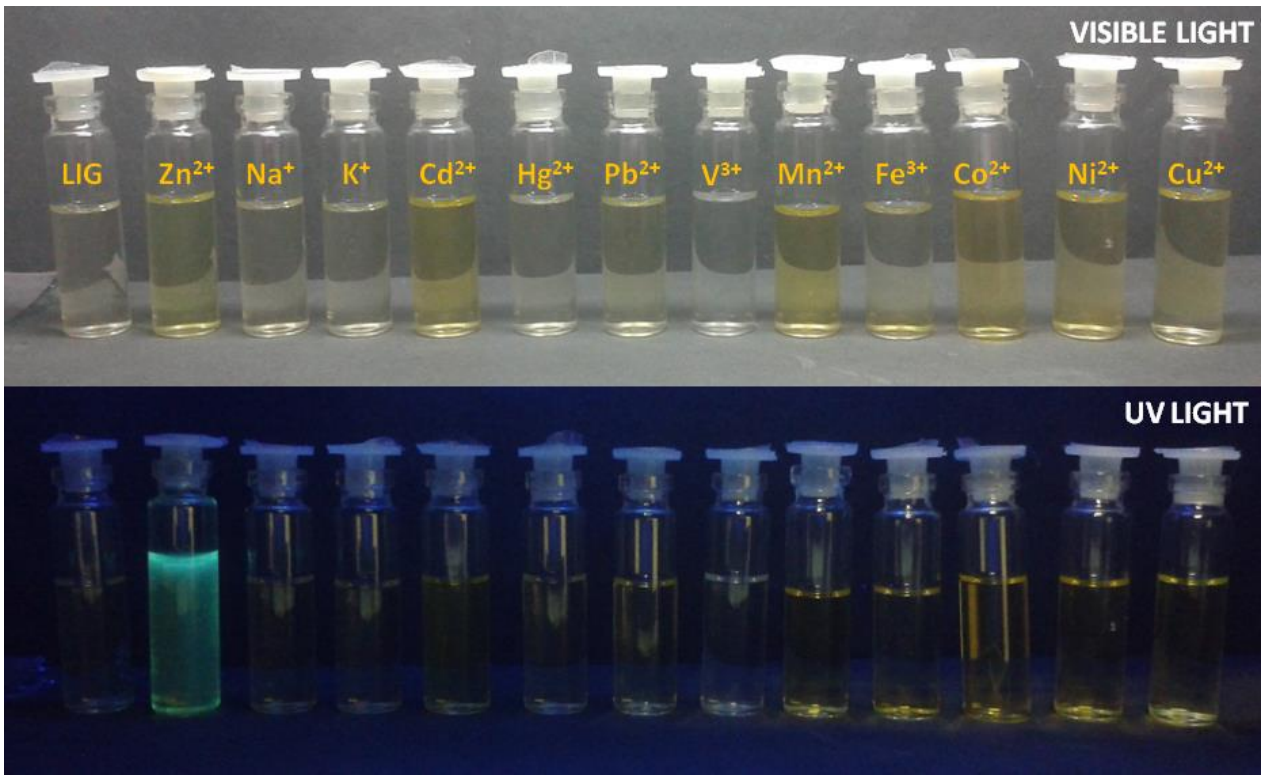

Fig. s21: Image of change in color of HL^1 in the presence of different metal ions in visible light and under UV radiation in 10 mM HEPES buffer in water:methanol (1:9, *v/v*) (pH = 7.2).

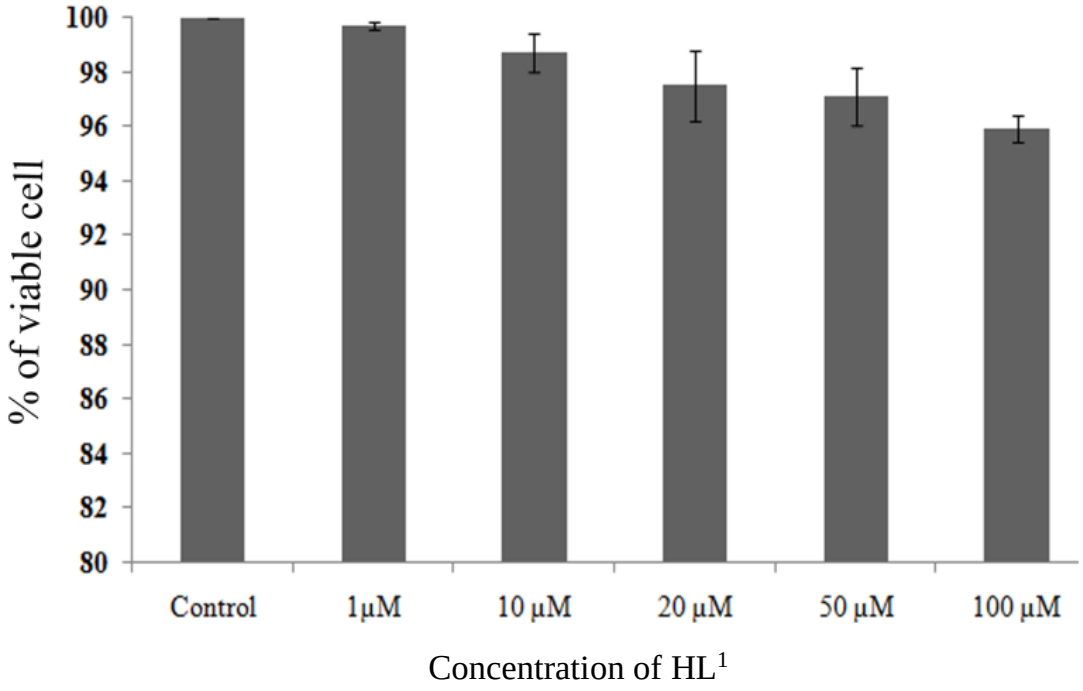

Fig. s22: % cell viability of A549 cells treated with different concentrations (1 µM-100 µM) of HL^1 for 6 h determined by MTT assay. Results are expressed as mean ± S.D. of three independent experiments.

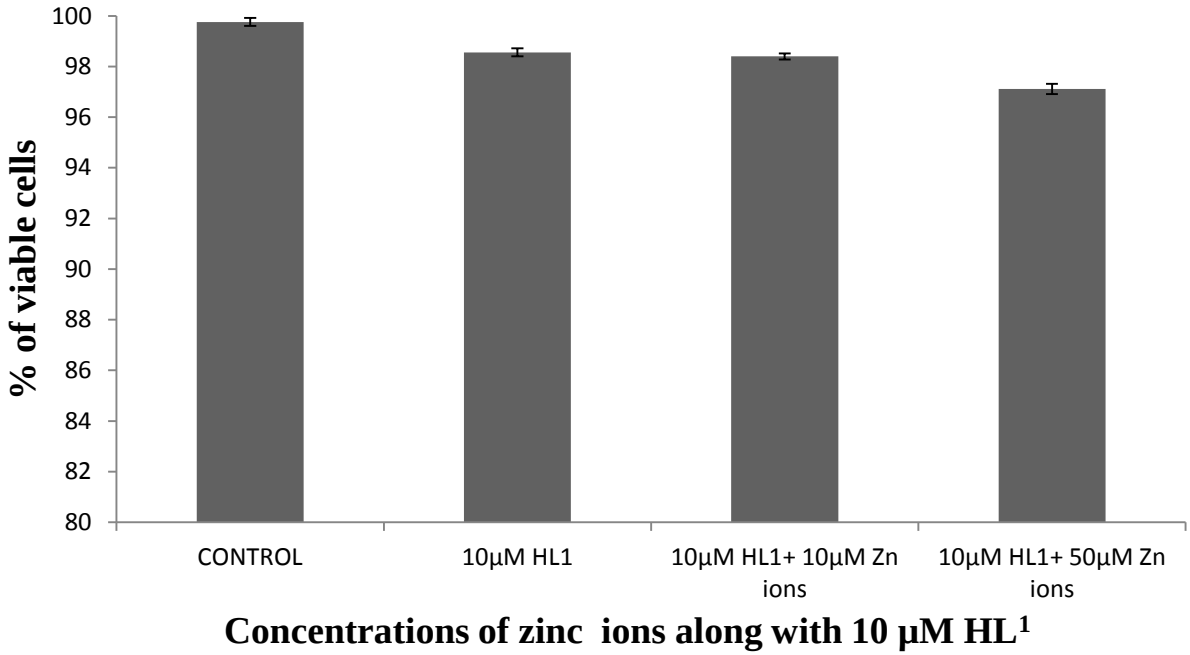

Fig. s23: % cell viability of A549 cells treated with fixed concentration (10 µM) of HL^1 along with different concentrations of zinc ions (10µM and 50 µM) for 6 h determined by MTT assay. Results are expressed as mean ± S.D. of three independent experiments.

Table s1: Selected optimized geometrical parameters for Complex 1 and Complex 2 in the ground state (S_0) calculated at B3LYP Levels.

Complex 1			
Bond Distance (Å)		Bond Angles (°)	
C27−O24	1.476	N10−Zn22−O24	125.7
C3−O21	1.326	N10−Zn22−O21	85.95
C8−N10	1.312	N10−Zn22−O23	124.37
H28−O24	0.975	O23−Zn22−O21	88.52
N10−Zn22	2.086	O24−Zn22−O21	93.60
O24−Zn22	2.043	O23−Zn22−N10	109.87
O23−Zn22	2.055		
O21−Zn22	2.001		
Complex 2			
Bond Distance (Å)		Bond Angles (°)	
C28−O25	1.467	C28−O25	1.467
C8−N10	1.312	C8−N10	1.312
C3−O22	1.333	C3−O22	1.333
H29−O25	0.978	H29−O25	0.978
N10−Zn23	2.091	N10−Zn23	2.091
O24−Zn23	2.082	O24−Zn23	2.082
O22−Zn23	2.028	O22−Zn23	2.028
O25−Zn23	2.074	O25−Zn23	2.074

Table s2: Main calculated optical transition for Complexes 1 and 2 with vertical excitation energies (E_{cal}), oscillator strengths (f_{cal}) of the lowest few excited singlets obtained from TDDFT/B3LYP/CPCM method in methanol.

	Excitation (eV)	**Electronic transition State**	**excitation (nm)**	**Osc. strength (f)**	**Key transitions**	**CI**
Complex 1	2.8055	S_0-S_1	442	0.5670	(82%)HOMO →LUMO	0.6436
	3.2554	S_0-S_2	382	0.4672	(03%)HOMO →LUMO+1	0.1183
					(86%)HOMO-1 →LUMO	0.6543
	3.5772	S_0-S_3	347	0.3208	(11%)HOMO-2 →LUMO	0.2394
					(77%)HOMO-1 →LUMO+2	0.6221
	5.0305	S_0-S_{12}	247	0.0810	(05%)HOMO-2 →LUMO+4	0.1518
					(02%)HOMO-1 →LUMO+4	0.1012
					(83%)HOMO →LUMO+2	0.6451
Complex 2	3.2444	S_0-S_1	398	0.2246	(03%)HOMO-1 →LUMO+1	0.1192
					(85%)HOMO →LUMO	0.6516
	3.852	S_0-S_2	346	0.0072	(10%)HOMO-3 →LUMO	0.2185
					(02%)HOMO-3 →LUMO+1	0.1038
					(63%)HOMO-2 →LUMO	0.5606
					(14%)HOMO-2 →LUMO+1	0.2665
	4.523	S_0-S_8	274	0.0032	(65%)HOMO-5 →LUMO	0.5705
					(03%)HOMO-5 →LUMO+1	0.1314
					(03%)HOMO-3 →LUMO+1	0.1363
					(25%)HOMO-2 →LUMO+1	0.3553