Supporting Information

For

A new turn-on benzimidazole based greenish-yellow fluorescent sensor for Zn^{2+} ion at biological pH applicable in cell imaging.

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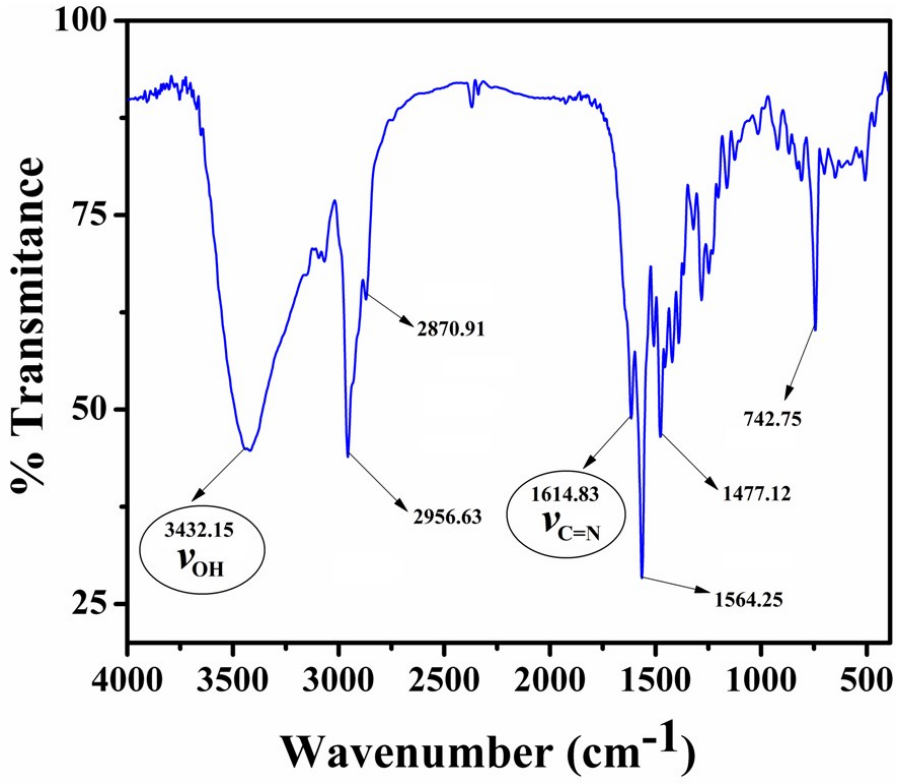

Fig. S1 FTIR spectrum of **HL**

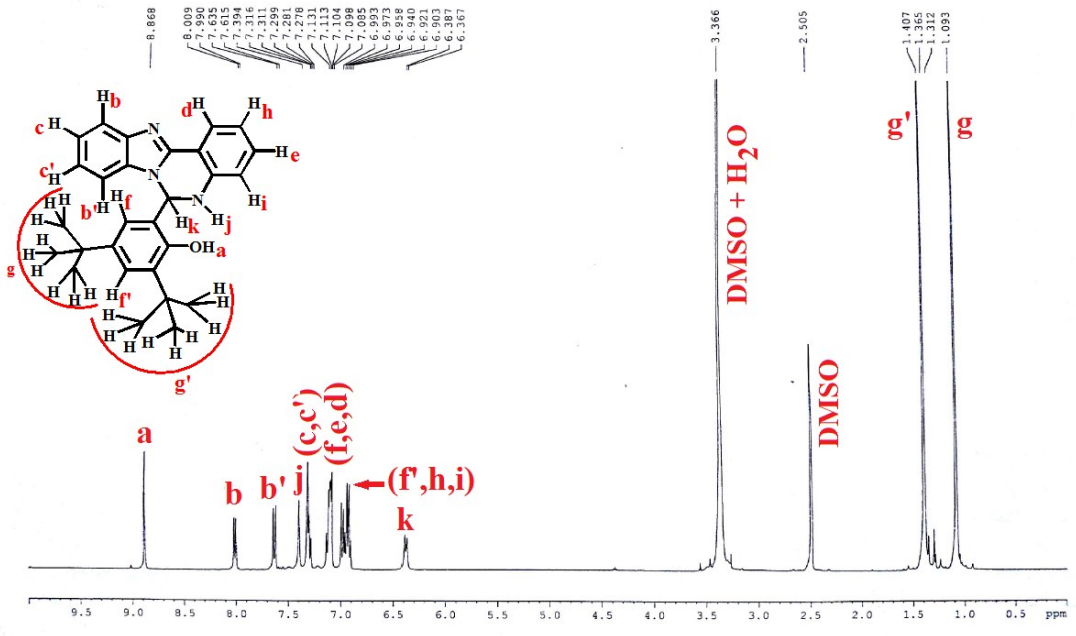

Fig. S2 [1]HNMR spectrum of **HL**

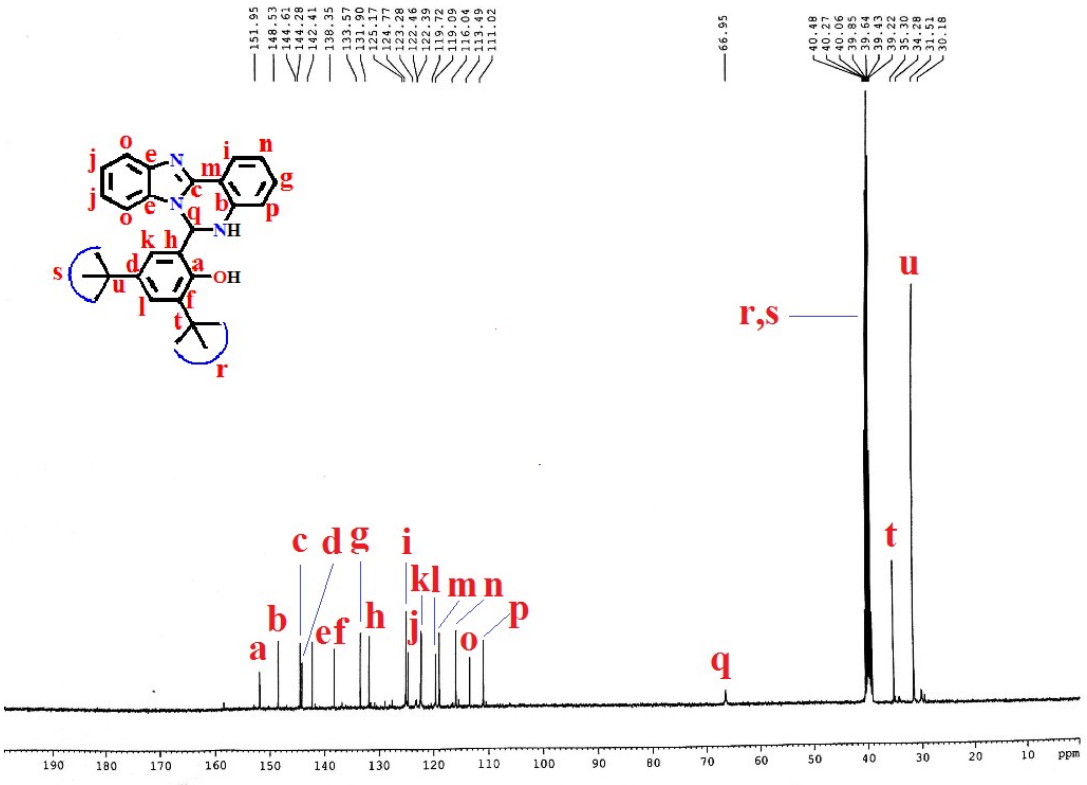

Fig. S3 [13]C NMR spectrum of **HL**

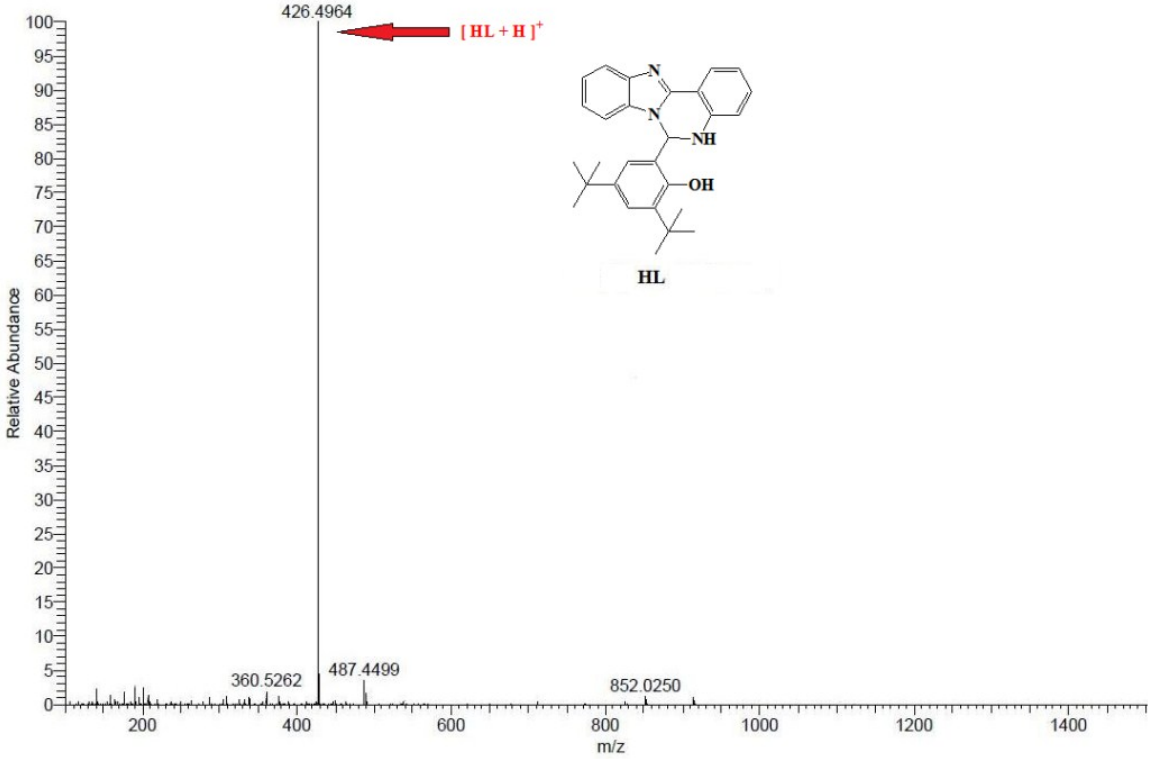

Fig. S4 ESI-Mass spectrum of **HL**

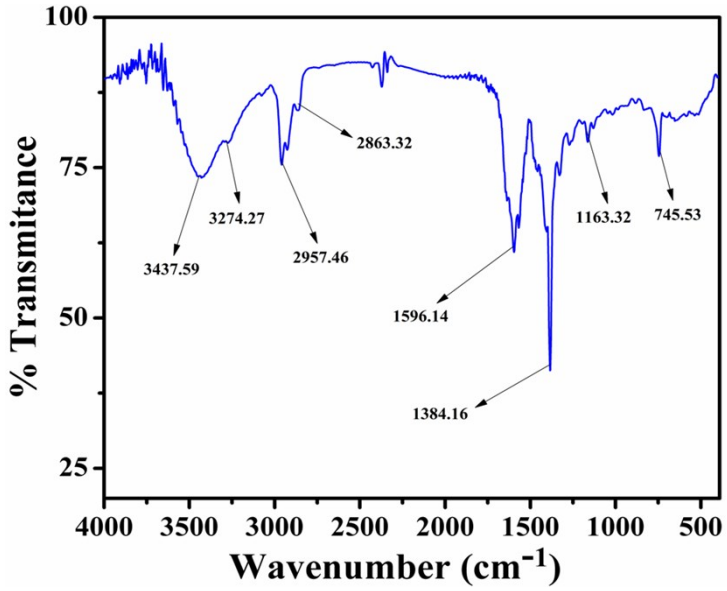

Fig. S5 FTIR spectrum of **[Zn(L^1)$_2$]** complex

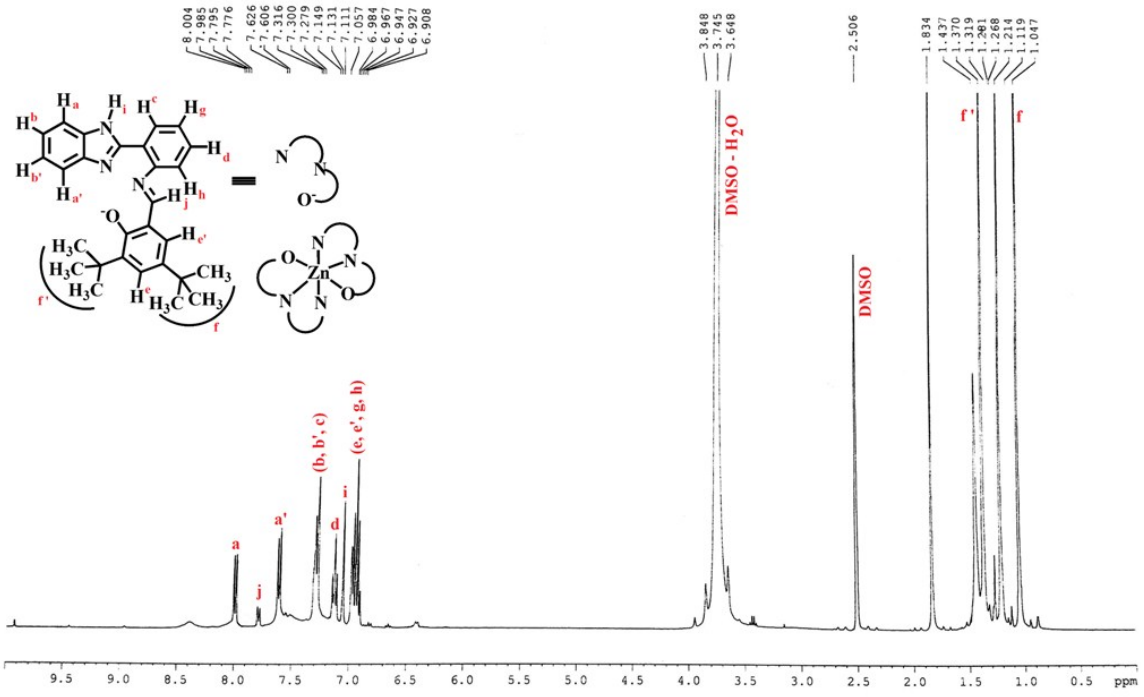

Fig. S6 ^{1}HNMR spectrum of **[Zn(L^{1})$_2$]** complex

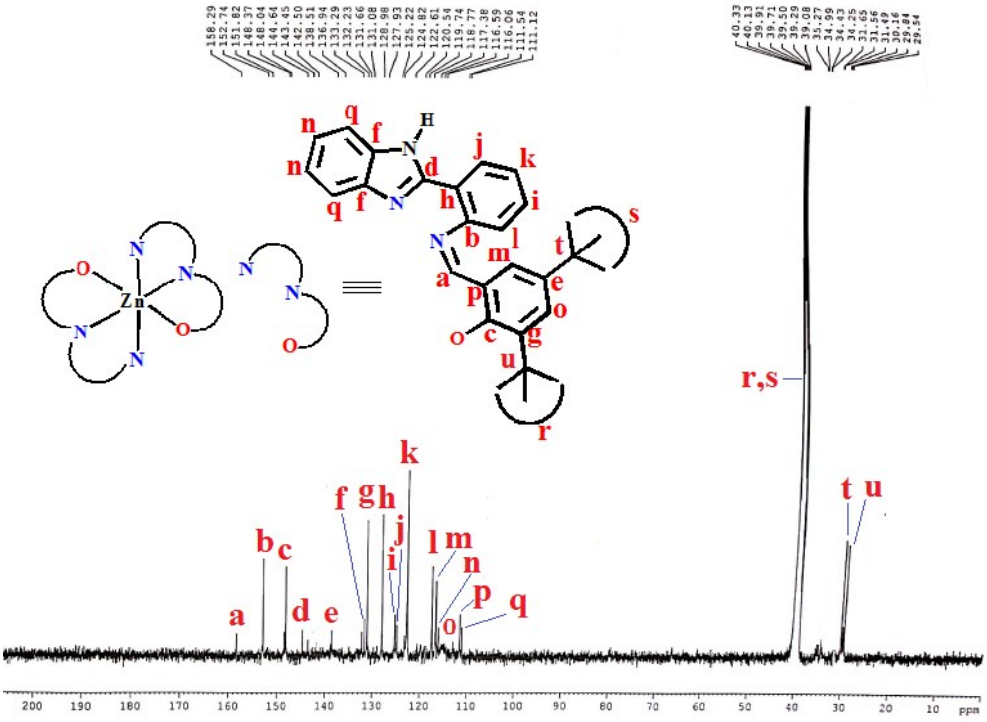

Fig. S7 ^{13}C NMR spectrum of **[Zn(L^{1})$_2$]** complex

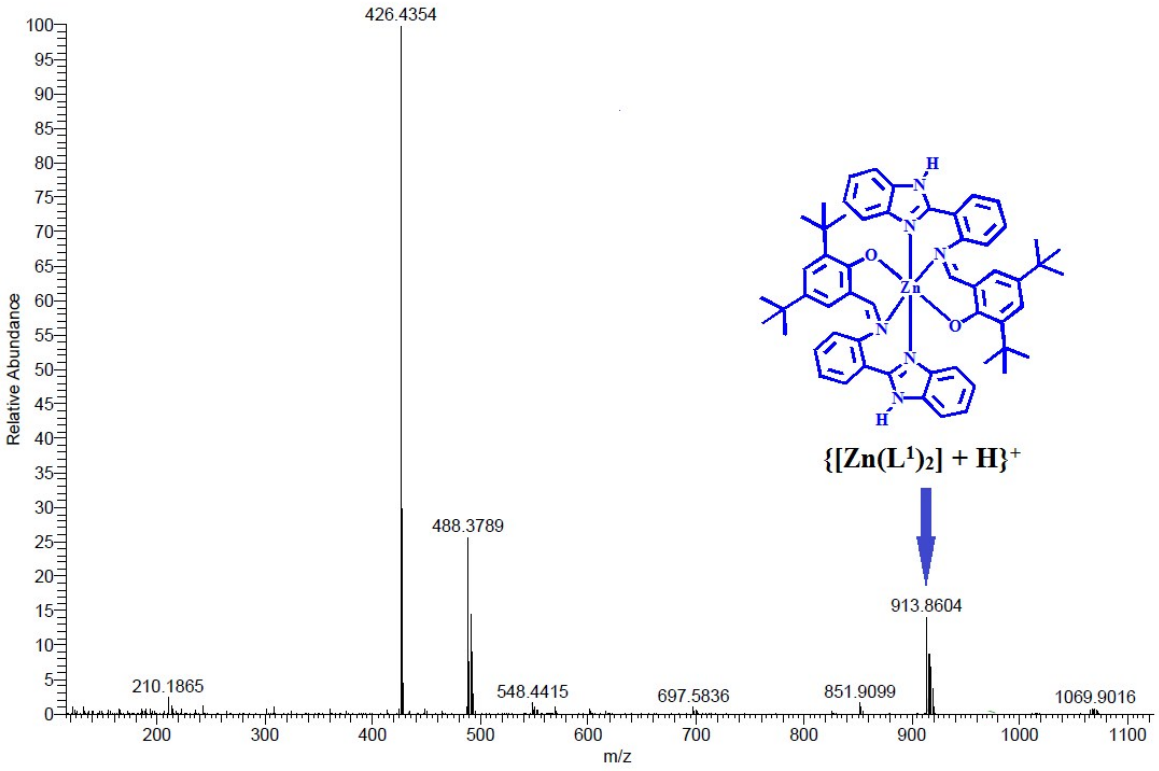

Fig. S8 ESI-Mass spectrum of **[Zn(L^1)$_2$]** complex

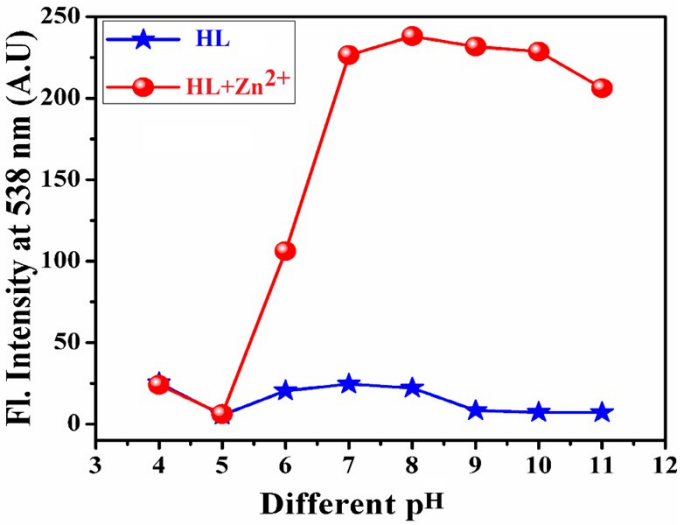

Fig. S9 Fluorescence response of **HL** (16 μM) in absence and in presence of Zn^{2+} ions (0.5 equivalent) at different pH in 5 mM HEPES buffer (DMSO:water, 1/5,v/v) at 27 °C

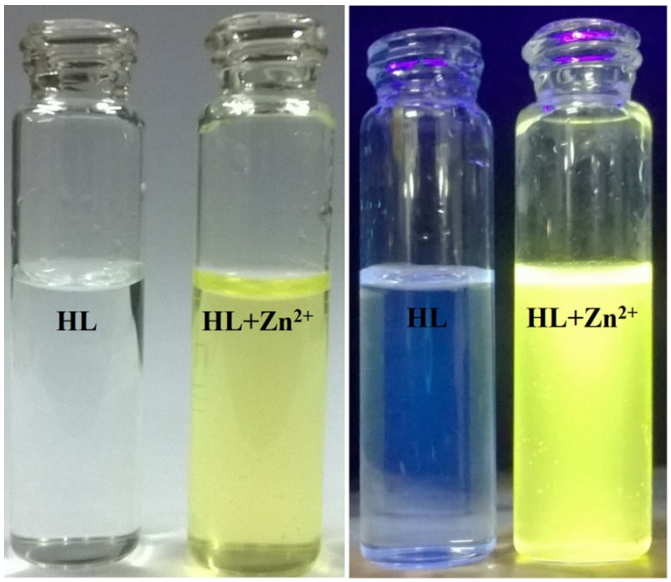

Fig. S10 Naked eye (left) and fluorescence (right) colour change of the probe (**HL**) in absence and presence of Zn^{2+} ions

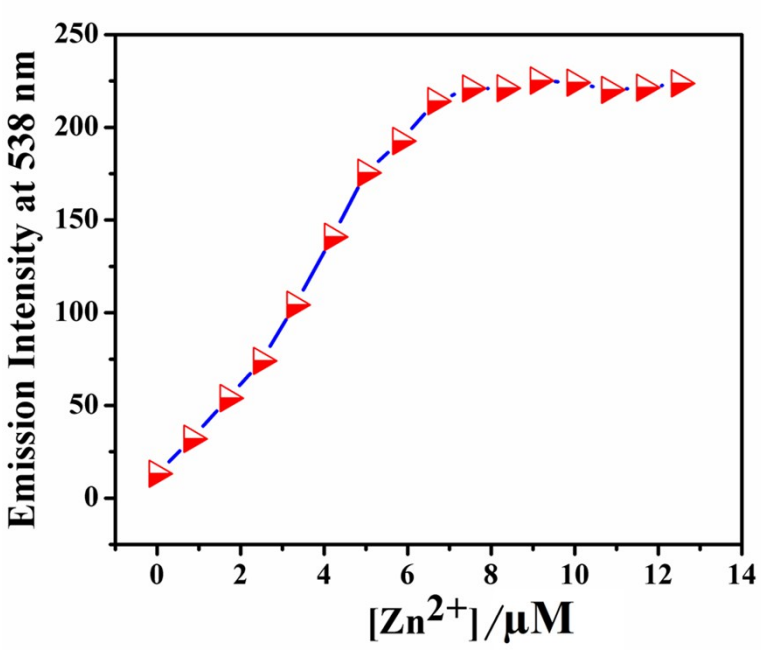

Fig. S11 The linear response curve of the emission of **HL** at 538 nm depending on Zn^{2+} ions concentration

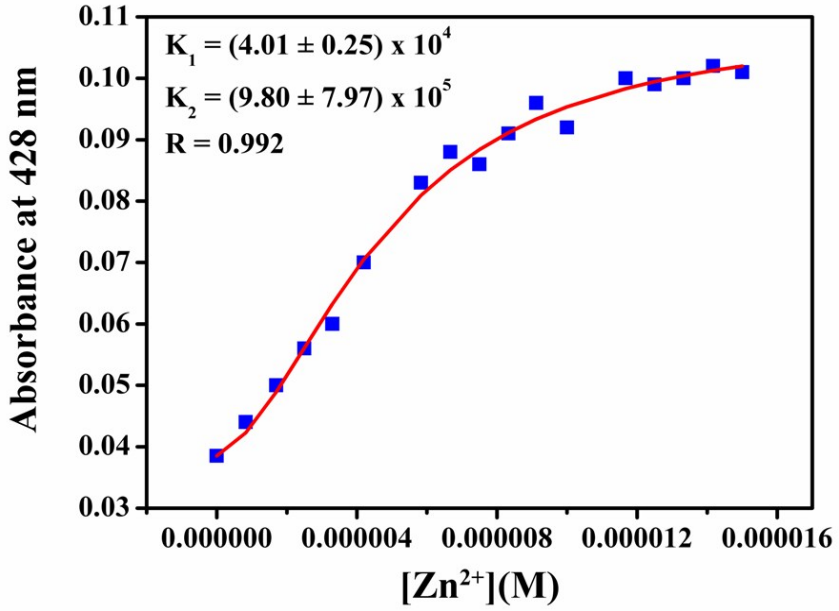

Fig. S12 Binding constant curve from non-linear fitting of UV-vis titration data

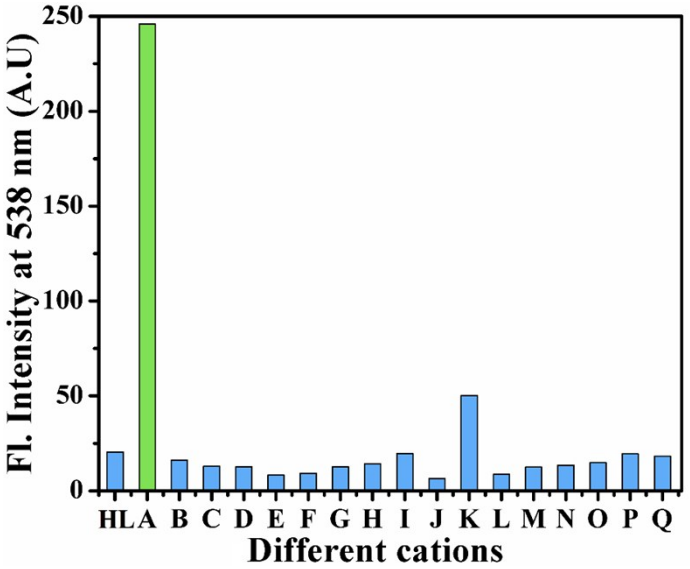

Fig. S13 Fluorescence intensity of **HL** in presence of different cations in 5 mM HEPES buffer (DMSO : water, 1 : 5, v/v, pH 7.4) at 27°C. **HL** + [(A) Zn^{2+}, (B) Na^{+}, (C) K^{+}, (D) Ca^{2+}, (E) Mg^{2+}, (F) Ba^{2+}, (G) Cr^{3+}, (H) Al^{3+}, (I) Mn^{2+}, (J) Fe^{2+}, (K) Co^{2+}, (L) Ni^{2+}, (M) Cu^{2+}, (N) Cd^{2+}, (O) Hg^{2+}, (P) Fe^{3+}, (Q) Pb^{2+}]

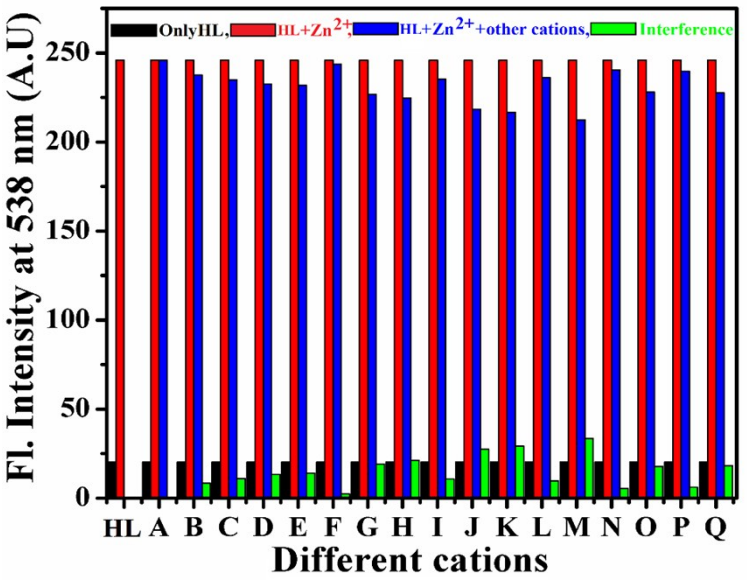

Fig. S14 Effect of different cations on the fluorescence intensity profile of **[Zn(L^1)$_2$]** in 5 mM HEPES buffer (DMSO : water, 1 : 5, v/v, pH 7.4) at 27°C. **HL** + [(A) Zn^{2+}, (B) Na^{+}, (C) K^{+}, (D) Ca^{2+}, (E) Mg^{2+}, (F) Ba^{2+}, (G) Cr^{3+}, (H) Al^{3+}, (I) Mn^{2+}, (J) Fe^{2+}, (K) Co^{2+}, (L) Ni^{2+}, (M) Cu^{2+}, (N) Cd^{2+}, (O) Hg^{2+}, (P) Fe^{3+}, (Q) Pb^{2+})]

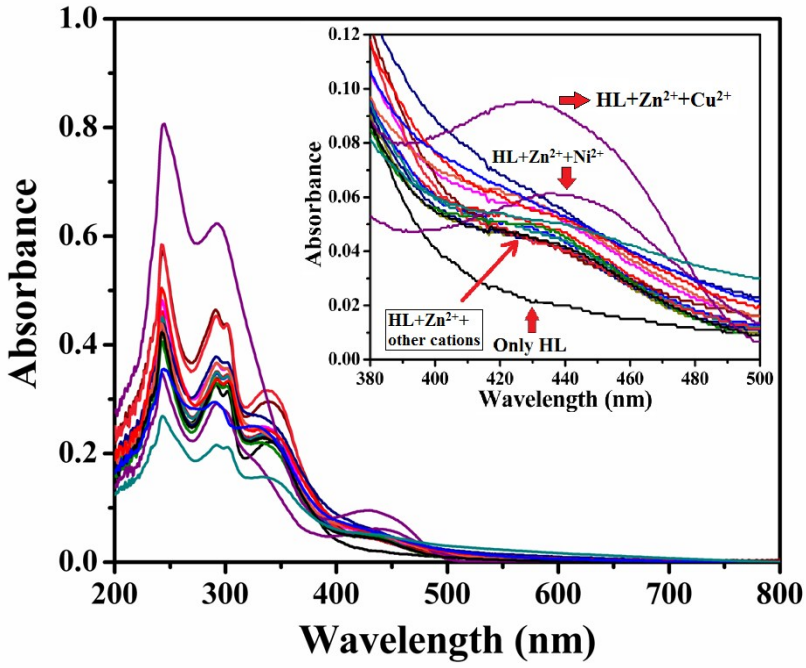

Fig. S15 Effect of different competitive cations on the absorbance property of **[Zn(L^1)$_2$]** in 5 mM HEPES buffer (DMSO : water, 1 : 5, v/v, pH 7.4) at 27°C. Different cations are [Na^{+}, K^{+}, Ca^{2+}, Mg^{2+}, Ba^{2+}, Cr^{3+}, Al^{3+}, Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Cd^{2+}, Hg^{2+}, Fe^{3+}, Pb^{2+}]

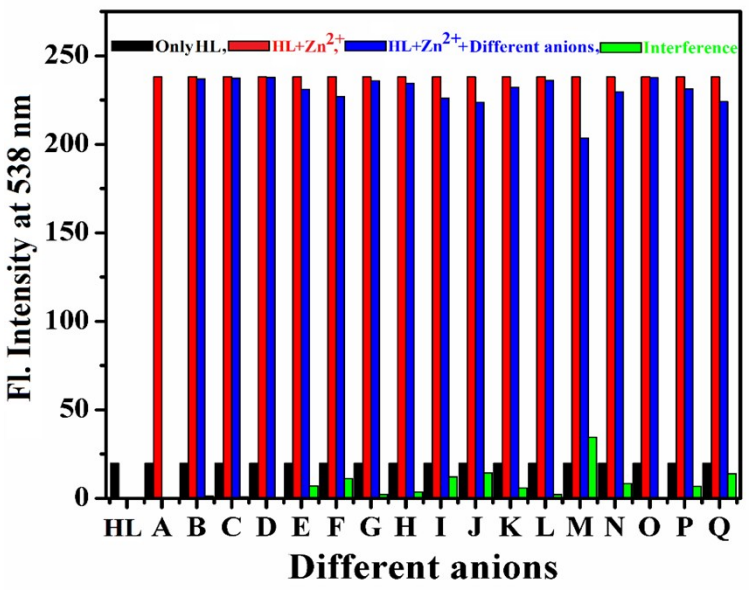

Fig. S16 Effect of different anions on the fluorescence intensity profile of **[Zn(L^1)$_2$]** in 5 mM HEPES buffer (DMSO : water, 1 : 5, v/v, pH 7.4) at 27°C. **HL**, **HL** + (A) Zn^{2+}, [**HL** + Zn^{2+} + (B) OAc^-, (C) S^{2-}, (D) CN^-, (E) MO_4^{2-}, (F) HSO_4^-, (G) SCN^-, (H) HPO_4^{2-}, (I) PO_4^{3-}, (J) ClO_4^-, (K) $HAsO_4^{2-}$, (L) $H_2AsO_4^-$, (M) $H_2PO_4^-$, (N) AsO_2^-, (O) N_3^-, (P) NO_3^-, (Q) F^-]

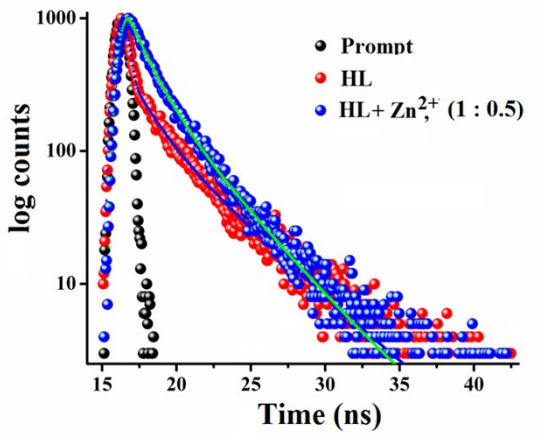

Fig. S17 Time resolved fluorescence decay of **HL** (16μM) in absence and presence of added Zn^{2+} ions in 5 mM HEPES buffer (DMSO : water, 1 : 5, v/v, pH 7.4) at 27 °C using a nano LED of 440 nm as the light source

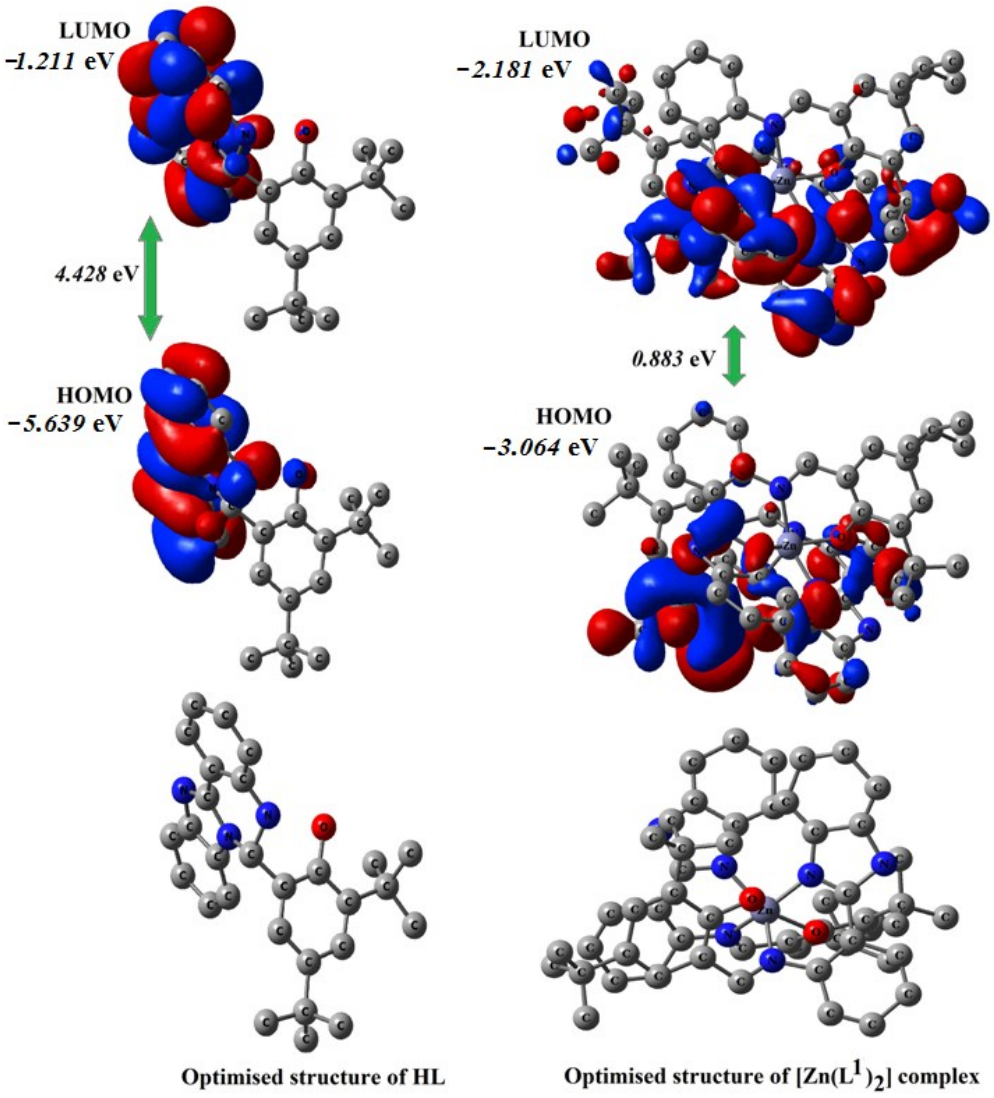

Fig. S18 (a) Computational study of probe **HL** and **[Zn(L^1)$_2$]** complex (H atoms are omitted for better clarity)

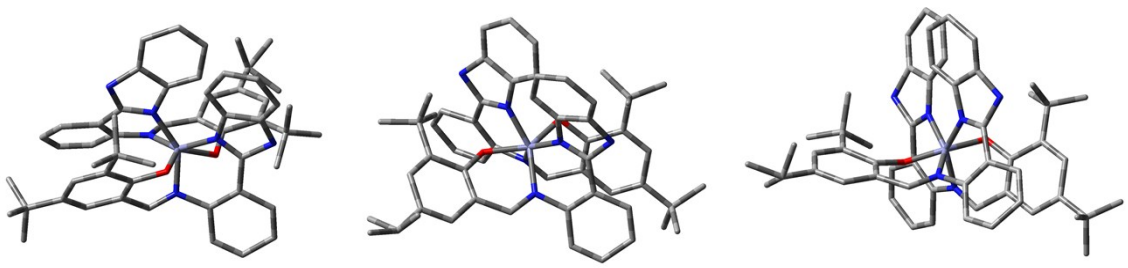

Fig. S18 (b) Optimized structure of **[Zn(L^1)$_2$]** complex in capstick style presenting with different planes of view (H atoms are omitted for better clarity)

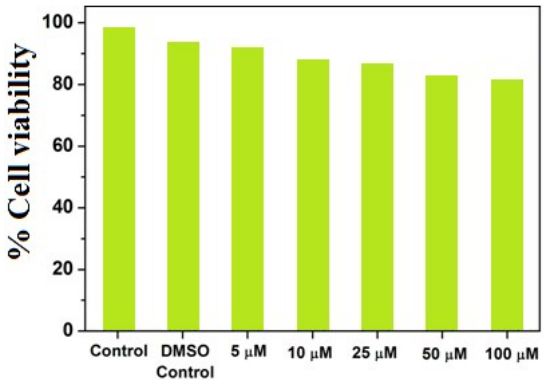

Fig. S19 Cytotoxic effect of **HL (**5, 10, 25, 50 and 100 μM**)** in *Candida sp*. cell incubated for 8 h in reaction buffer

Table S1 Selected bond distances (Å) and bond angles (°) for $C_{28}H_{32}N_3O.NO_3$

Bond length (Å)		**Bond angles (°)**	
O(1)-C16	1.380(4)	C(7)-N(1)-C(6)	109.4(3)
N(1)-C(7)	1.339(4)	C(13)-N(3)-C(14)	127.2(3)
N(1)-C(14)	1.480(4)	N(3)-C(13)-C(8)	121.4(3)
N(2)-C(7)	1.330(4)	N(3)-C(13)-C(12)	120.9(3)
N(3)- C(13)	1.352(4)	N(3)-C(14)-N1	108.3(3)
N(3)-C(14)	1.436(5)	N(1)-C(14)-C(15)	110.9(3)
C(15)-C(14)	1.510(5)	C(16)-C(15)-C(14)	122.3(3)
N(1)-C(6)	1.395(5)	N(2)-C(7)-N(1)	108.5(3)

Table S2 Life time details of **HL** and **[Zn(L^1)$_2$]** complex

	B_1	B_2	B_3	τ_1 (ns)	τ_2 (ns)	τ_3 (ns)	χ^2	τ_{av} (ns)	Φ	k_r	k_{nr}
HL	20.42	38.18	41.41	1.51	4.29	0.12	1.007	1.9959	0.0558	0.0279	0.4731
[Zn(L^1)$_2$]	50.75	49.25	-	1.37	3.53	-	1.019	2.4338	0.1895	0.0778	0.3330

Table S3 Comparison of the importance of this probe (**HL**) with the earlier reports

Sl No	Detection Limit	Medium	Reference
1.	0.53 nM	HEPES buffer (50mM, DMSO/water: 1:9 (v/v), pH=7.2);λ_{em} = 425 nm; blue fluorescence	37
2.	10.0 nM	EtOH : H_2O = 9:1 (HEPES buffer, pH 7.2); λ_{em} = 445 nm; blue fluorescence	51(a)
3	18.2 nM	Aqueous media, (10 mM HEPES buffer, pH 7.4); λ_{em} = 463 nm; blue fluorescence	51(b)
4	35.0 nM	DMSO/H_2O (50:50, v/v); λ_{em} = 470 nm; blue fluorescence	51(c)
5	39.9 nM	DMSO/H_2O (1:5, v/v), 5 mM HEPES buffer, pH = 7.4; λ_{em} = 538 nm; greenish-yellow fluorescence	*Present work*
6	40.0 nM	(H_2O/CH_3CN) 1:1, v/v, 0.1 M HEPES buffer, pH = 7.2); λ_{em} = 590 nm; redish fluorescence	32
7	48.9 nM	EtOH–H_2O (95:5 v/v); λ_{em} = 450 nm; blue fluorescence	51(d)
8.	80 nM	30% (v/v)ethanol/water, 10mM Tris–HCl at pH 7.03; λ_{em} = 460 nm; blue fluorescence	51(e)
9	286 nM	EtOH:H_2O (9:1, v/v); λ_{em} = 496 nm; green fluorescence	51(f)
10	600.0 nM	Aqueous media, (HEPES buffer 100 mM, pH 7.0); λ_{em} = 445 nm; blue fluorescence	51(g)
11	1120 nM	HEPES buffer (10 mM, EtOH/H_2O 3:1, pH 7.4); λ_{em} = 561 nm; yellow fluorescence	51(h)
12	3200 nM	Aqueous media, HEPES buffer solution at pH 7.4; λ_{em} = 506 nm; green fluorescence	51(i)
13	15,000 nM	HEPES-buffered CH_3CN/H_2O (1:1, v/v,pH = 7.0); λ_{em} = 425 nm; blue fluorescence	51(j)
14	15600 nM	1:9, v/v 0.01 M HEPES buffer, H_2O-CH_3CN, pH 7.4; λ_{em} = 460 nm; blue fluorescence	51(k)