Supporting Information

Highly selective and sensitive turn-on chemosensor for Al(III) ion at the nanomolar level in aqueous media and living organism

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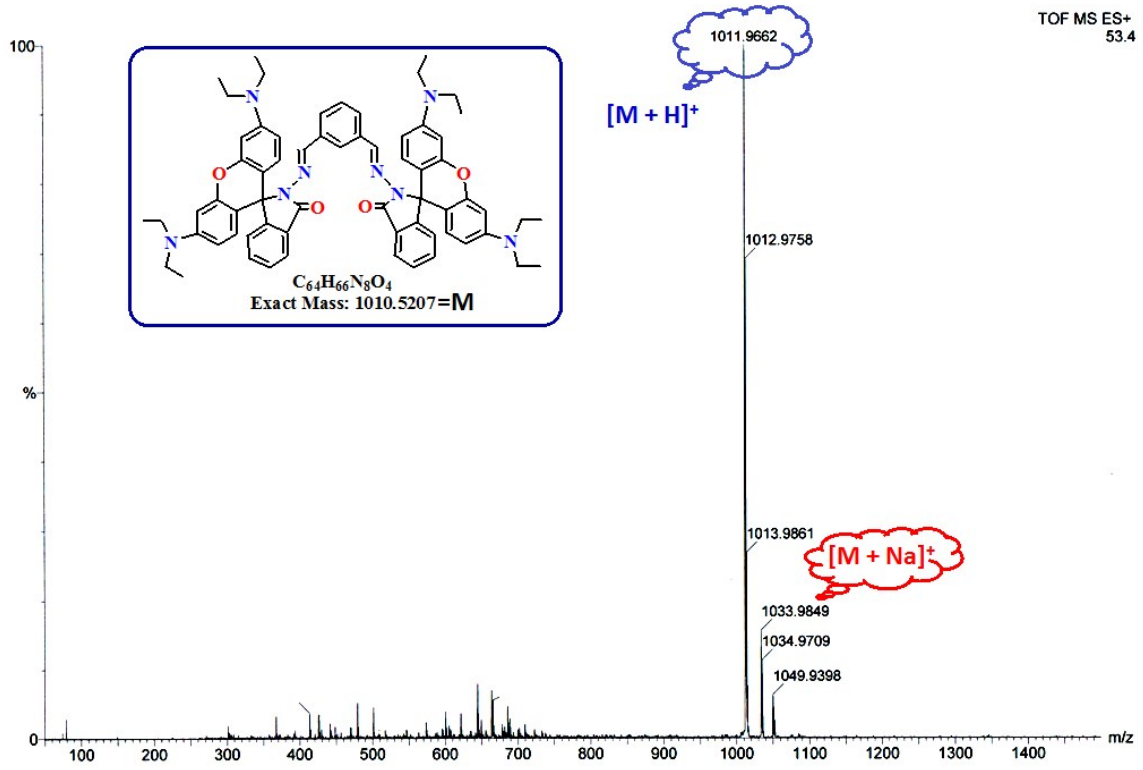

Fig. S1 ESI-MS of the probe (**L**) in acetonitrile

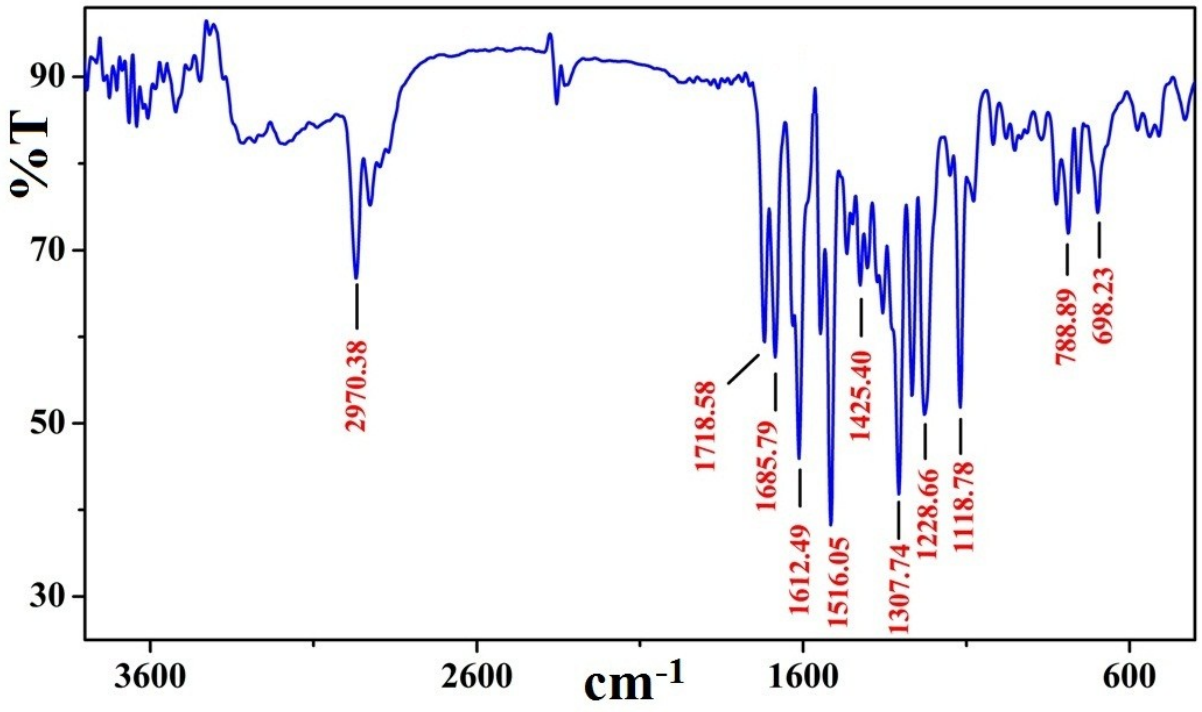

Fig. S2 FTIR spectrum of **L**

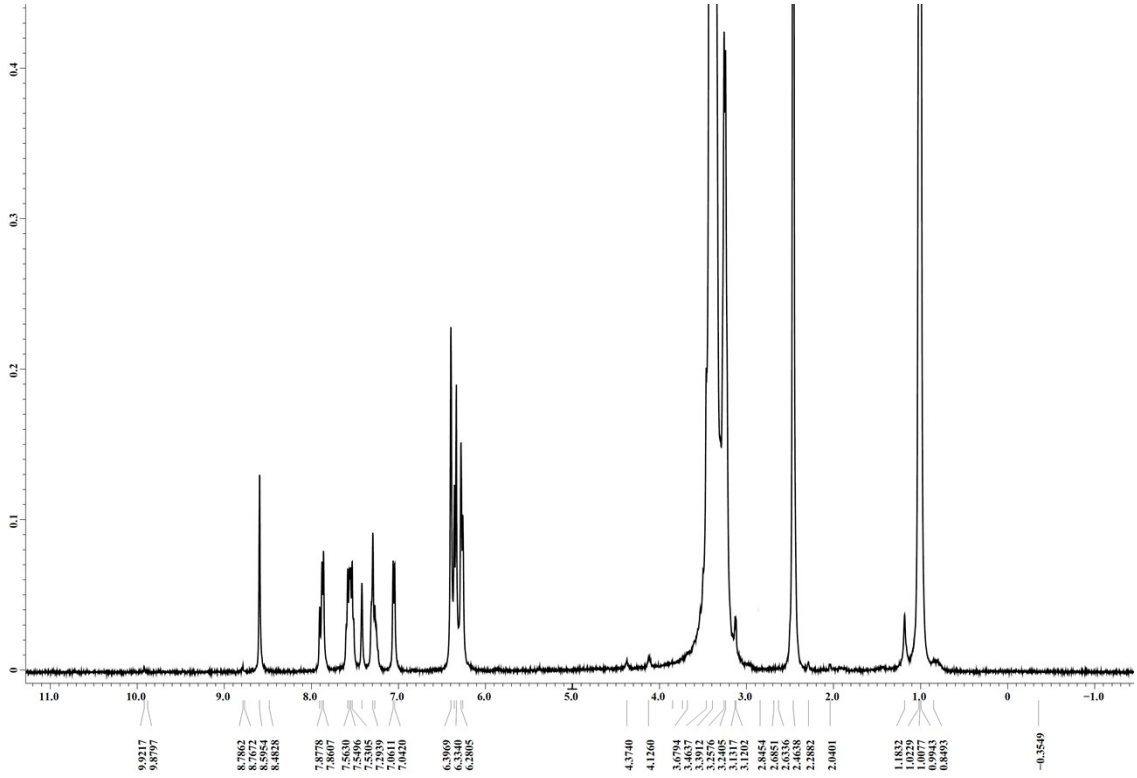

Fig. S3 ^{1}H NMR of the probe (**L**) in DMSO-d_6

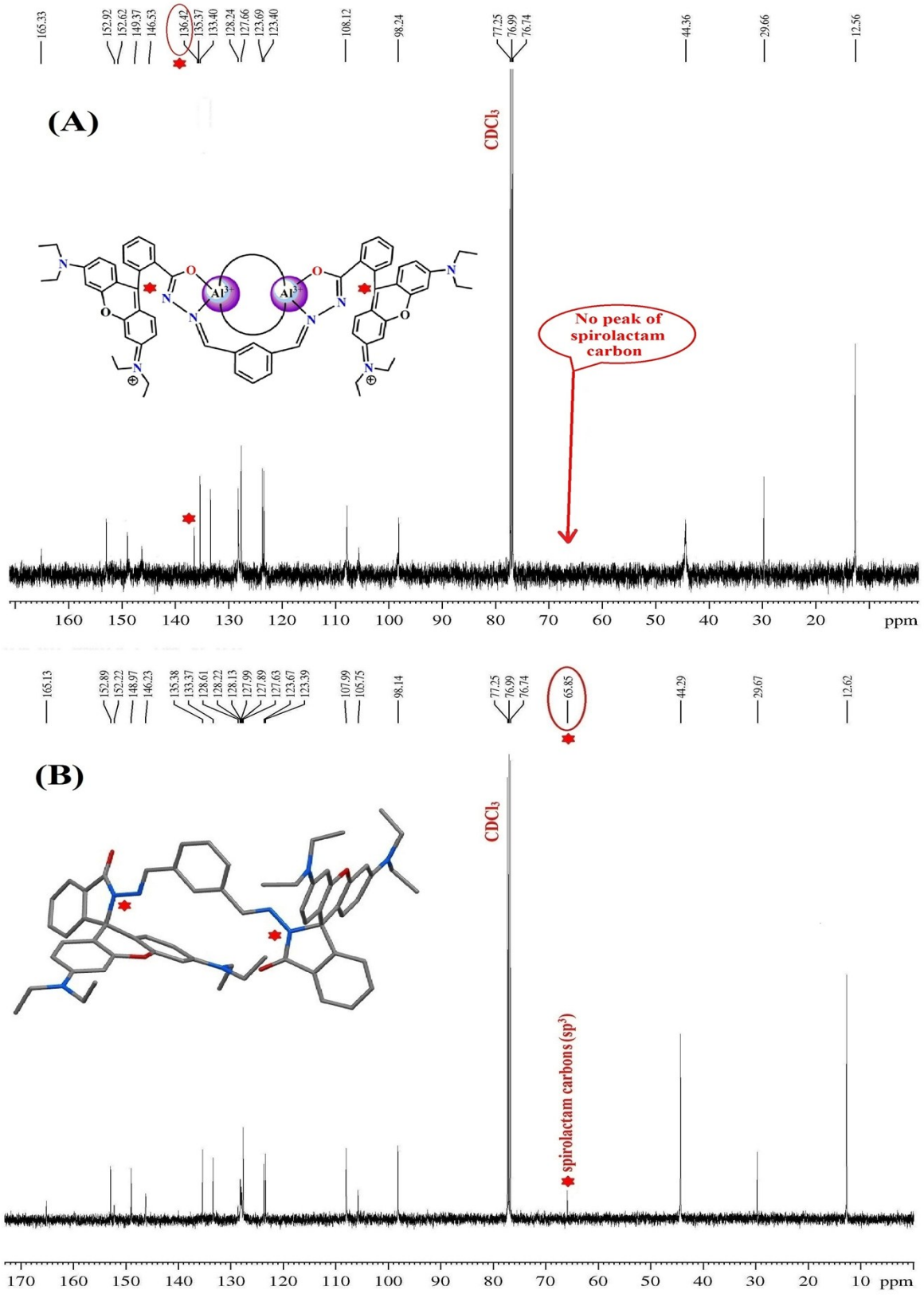

Fig. S4 Partial ^{13}CNMR titration with Al(III) ions. [(B) **L** and (A) **L :** Al(III) (1:2)]

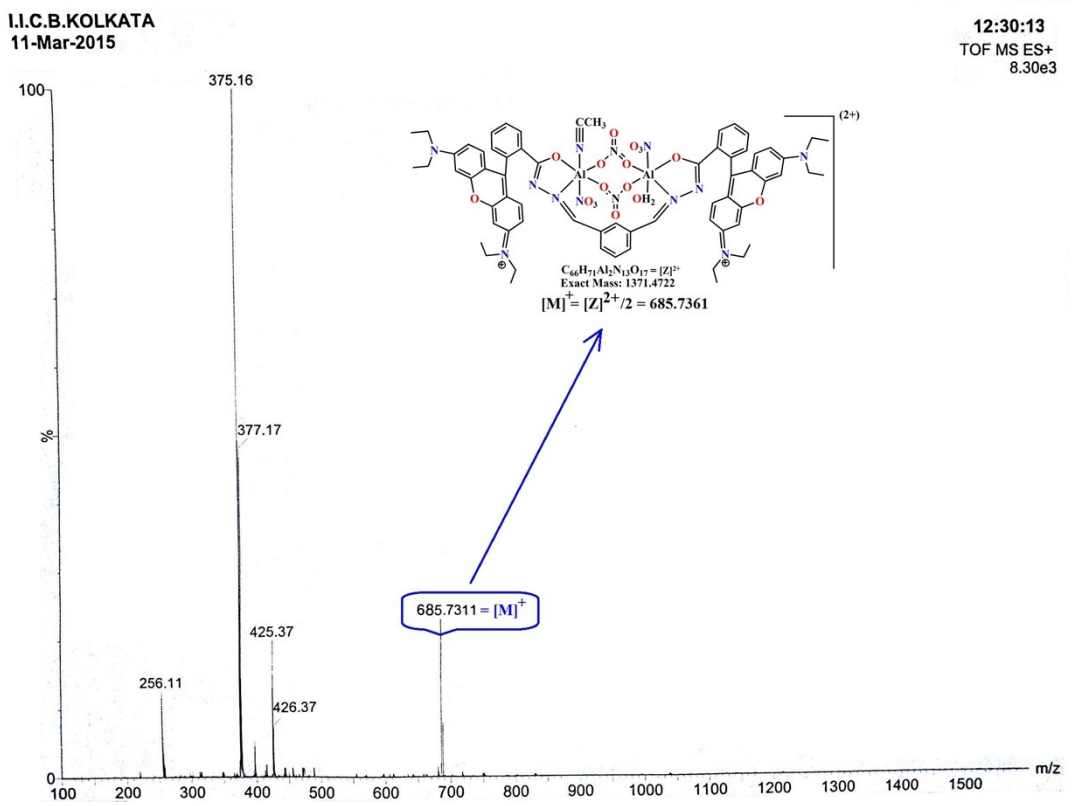

Fig. S5 ESI-MS of Al(III) complex by $Al(NO_3)_3$ salt in acetonitrile

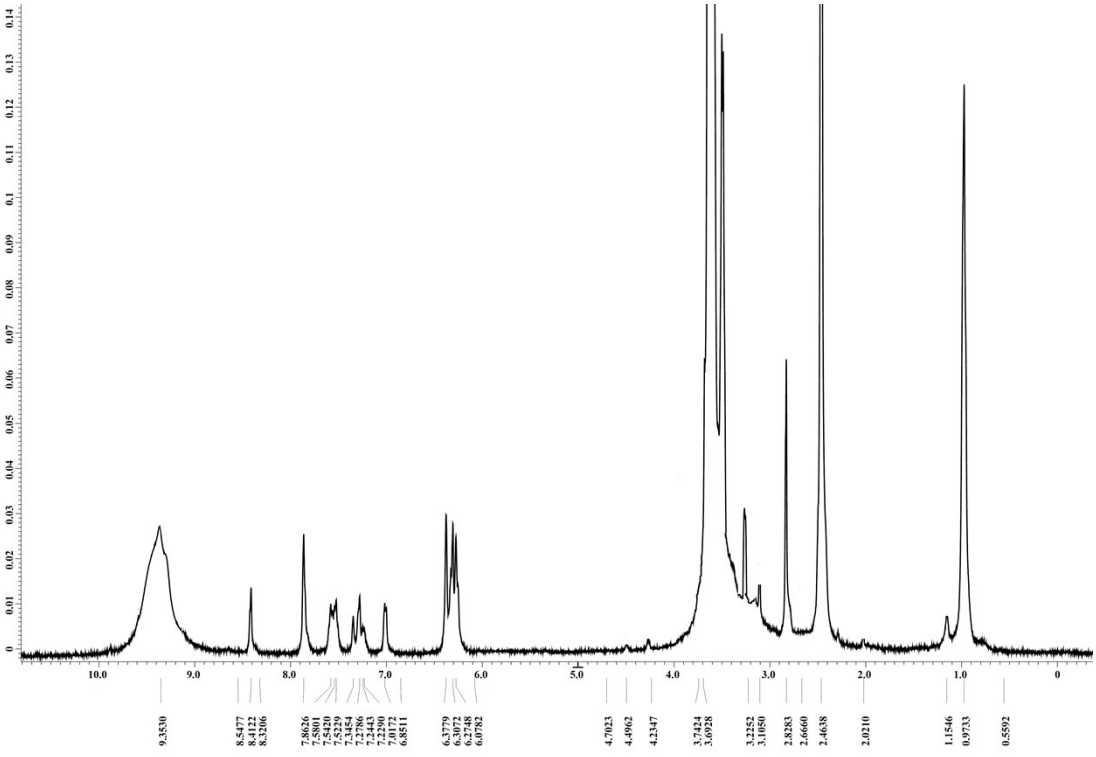

Fig. S6 ^{1}H NMR of the **L**-Al complex in DMSO-d_6

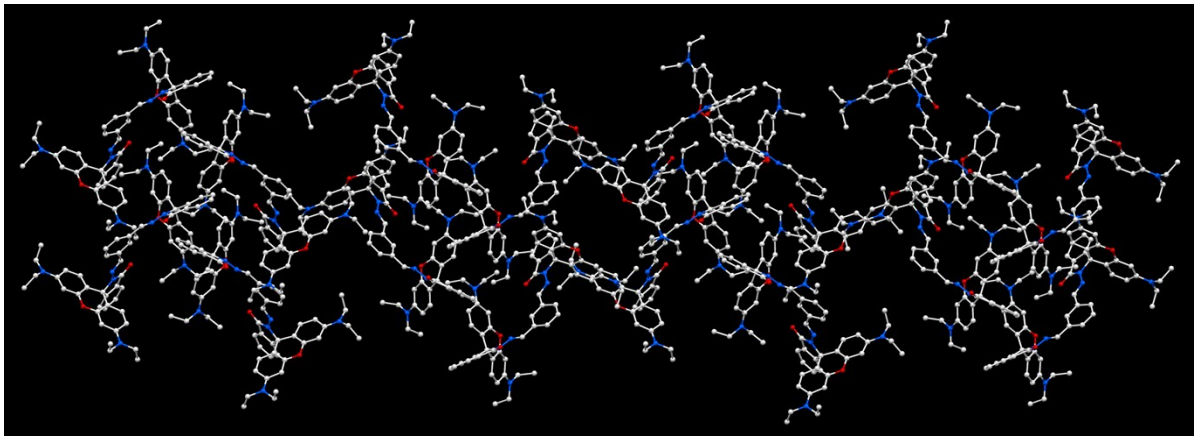

Fig. S7 Crystal packing arrangement of **L**

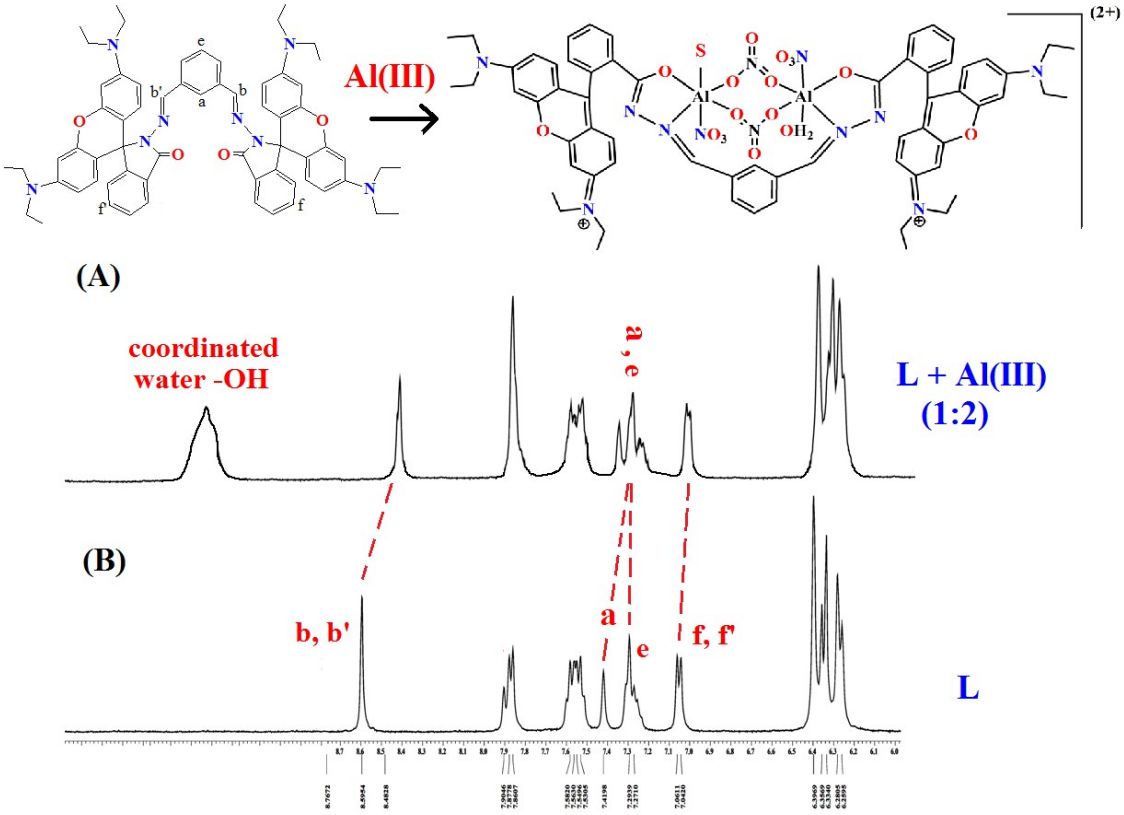

Fig. S8 Partial ^{1}H NMR titration with Al(III) ions. [(B) **L** and (A) **L :** Al(III) (1:2)]

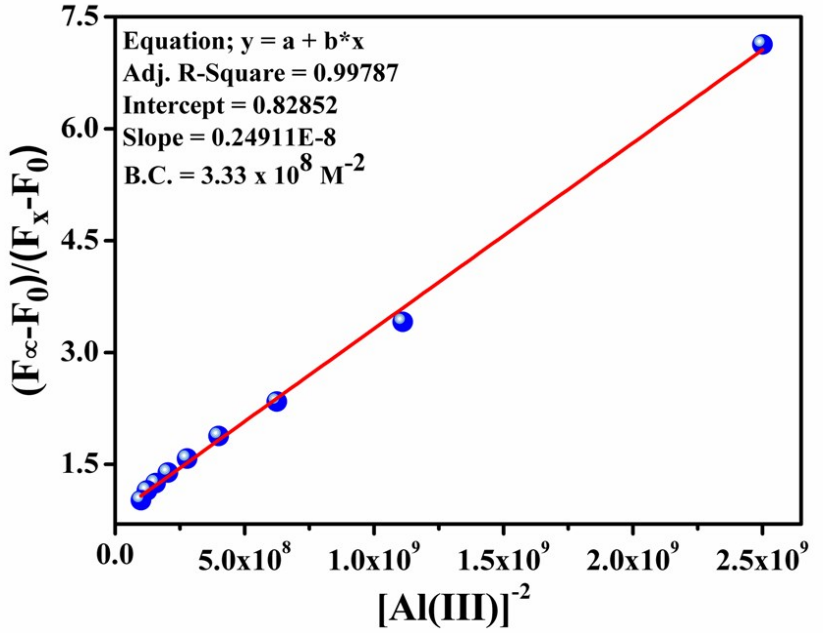

Fig. S9 Binding constant (K) value $3.33 \times 10^8\ M^{-2}$ determined from the interactions of **L** with Al(III) ions in HEPES buffer (1 mM, pH 7.4; acetonitrile/water: 1/3, v/v) at 25 °C

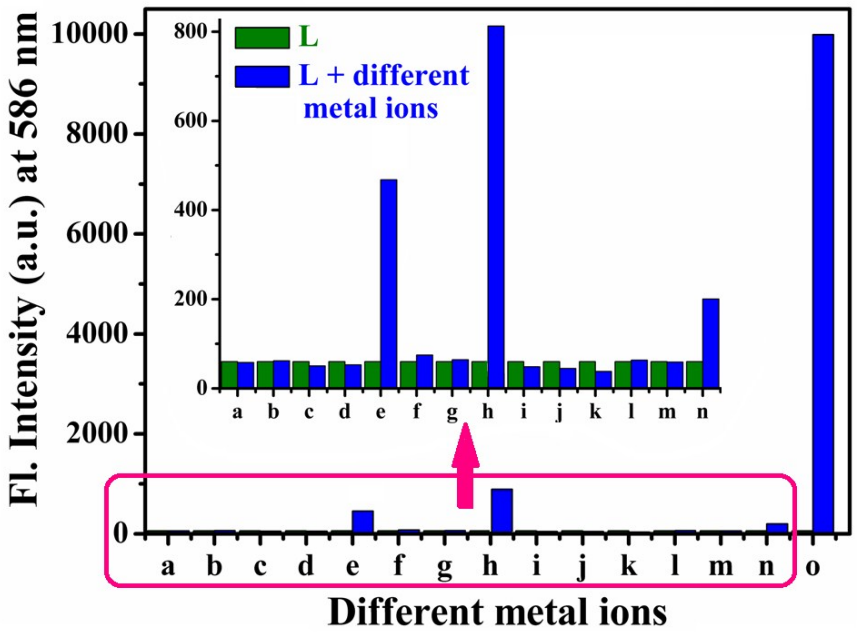

Fig. S10 Fluorescence intensity assay of **L** in presence of different metal ions in HEPES buffer (1 mM, pH 7.4; acetonitrile/water: 1/3, v/v) at 25 °C (λ_{ex} = 555 nm), (a) Na^+, (b) K^+, (c) Ca^{2+}, (d) Mg^{2+}, (e) Cu^{2+}, (f) Cr^{3+}, (g) Mn^{2+}, (h) Fe^{3+}, (i) Co^{2+}, (j) Ni^{2+}, (k) Pb^{2+}, (l) Zn^{2+}, (m) Cd^{2+}, (n) Hg^{2+} and (o) Al^{3+}

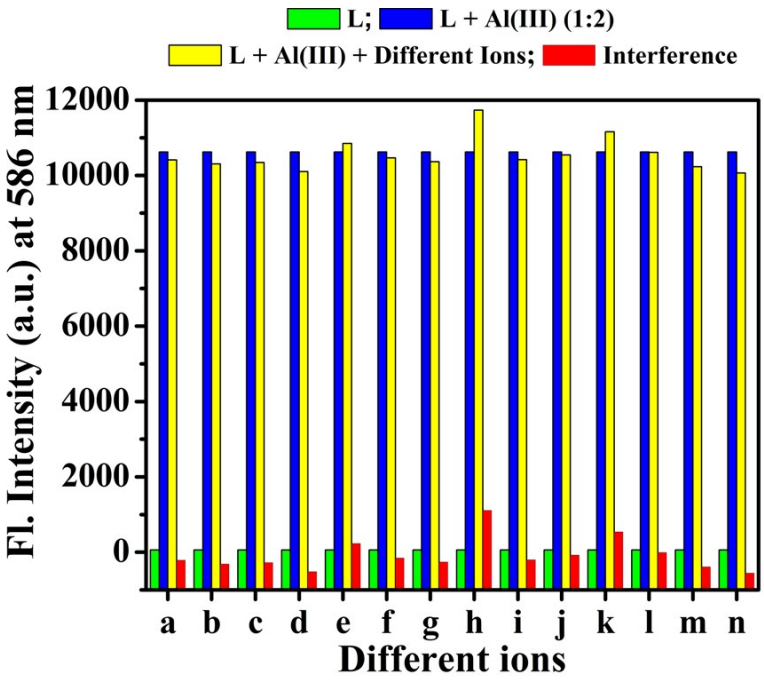

Fig. S11 Change of relative fluorescence intensity profile of **L** in HEPES buffer (1 mM, pH 7.4; acetonitrile/water: 1/3, v/v) at 25 °C (λ_{ex} = 555 nm). (a) Na^{+}, (b) K^{+}, (c) Ca^{2+}, (d) Mg^{2+}, (e) Hg^{2+}, (f) Cr^{3+}, (g) Mn^{2+}, (h) Fe^{3+}, (i) Co^{2+}, (j) Ni^{2+}, (k) Cu^{2+}, (l) Zn^{2+}, (m) Cd^{2+}, and (n) Pb^{2+}

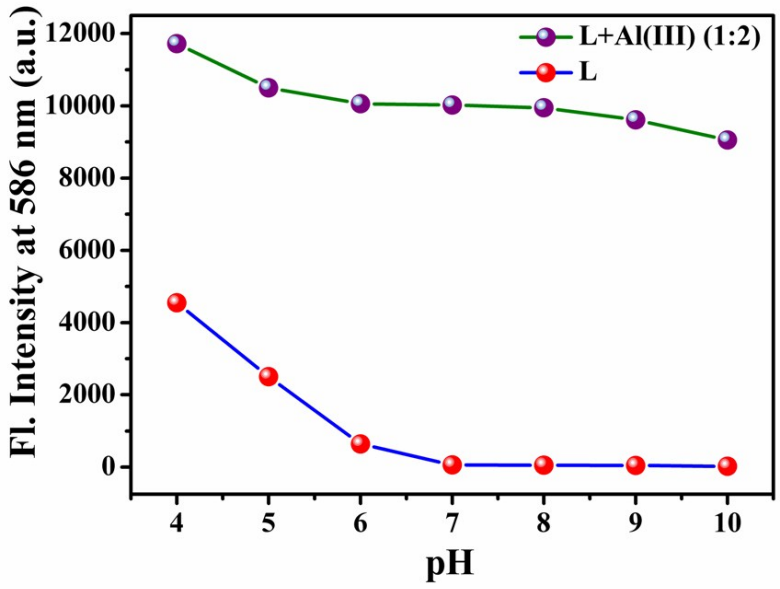

Fig. S12 pH Effect of **L** in absence and in presence of Al(III) ions

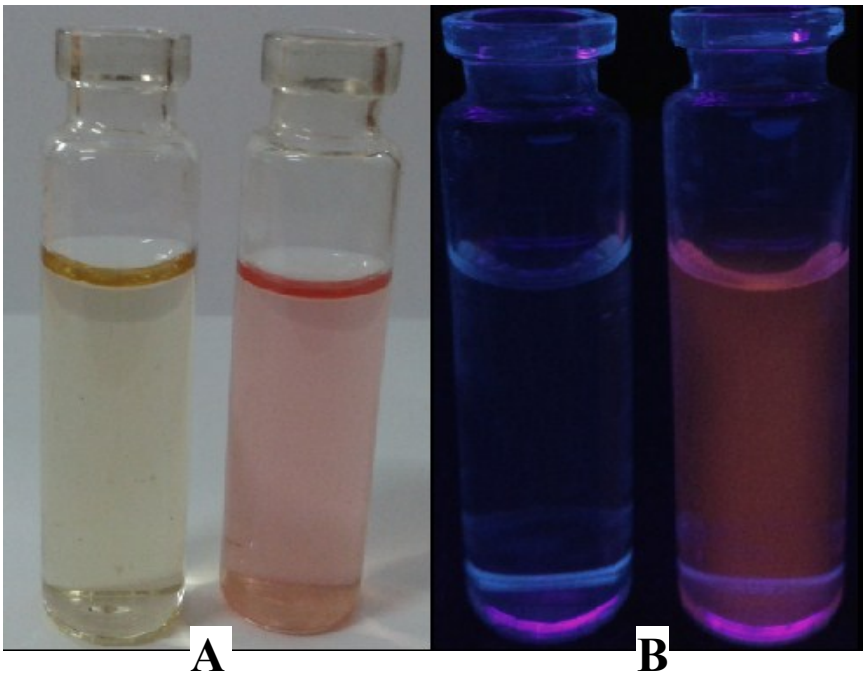

Fig. S13 (A) Represents the visual and (B) fluorescence color change without (left) and with (right) addition of **L** (50 µL) for the qualitative detection of aluminum in tea leaves

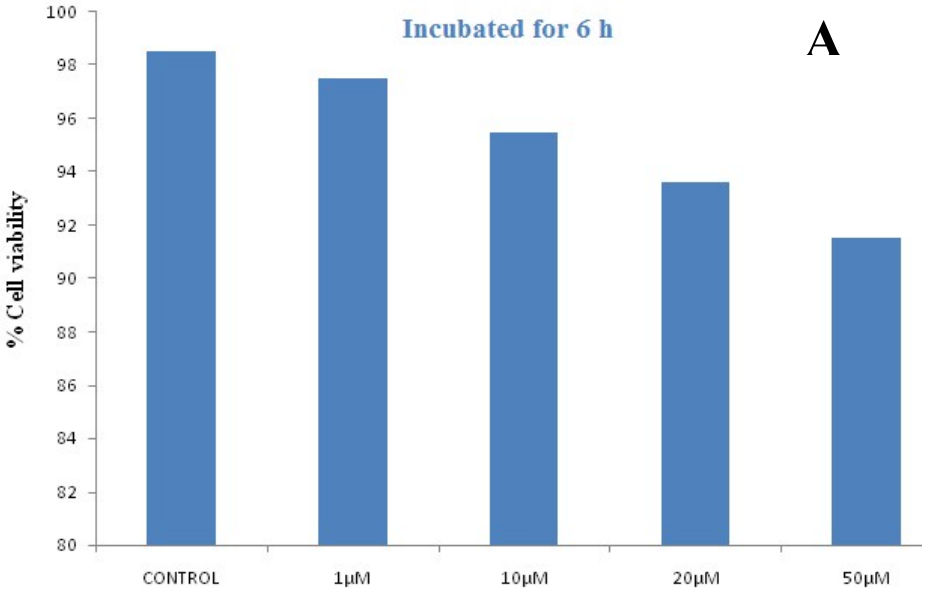

Fig. S14 (A) represents % cell viability of A549 cells treated with different concentrations (1 µM-50 µM) of **L** for 6 hrs determined by MTT assay. Results are expressed as mean of three independent experiments.

Table S1 Crystal data and details of refinements for **L**

L	
Empirical Formula	$C_{64}\,H_{66}\,N_8\,O_4$
Formula Weight	1011.24
Crystal system	orthorhombic
Space group	Fdd2
a (Å)	20.2211(17)
b (Å)	95.380(9)
c (Å)	12.5142(10)
α	90°
β	90°
γ	90°
Volume (Å^3)	24136(4)
Temperature (K)	296(2)
Z	16
ρ_{calc} (g/cm^3)	1.113
μ (mm^{-1})	0.071
F(000)	8608
θ range (deg)	1.926-25.677
Reflections collected / unique	11411/7333
R indices (all data)	0.0677
Goodness-of-fit on F^2	1.064

Table S2A Selected bond distances (Å) for **L**

L	
N1 - C5	1.379(7)
N1 - C2	1.449(8)
N1 - C3	1.468(9)
N2 - C15	1.371(7)
N2 - C19	1.452(8)
N2 - C20	1.473(8)
N3 - N4	1.383(6)
N3 - C28	1.393(7)
N3 - C11	1.515(7)
N4 - C29	1.276(7)
N5 - C48	1.390(8)
N5 - C52	1.435(10)
N5 - C53	1.461(9)
N6 - C58	1.392(9)
N6 - C63	1.430(13)
N6 - C62	1.462(11)

Table S2B Selected bond angles (°) for **L**

L	
C5 - N1 - C2	121.3(5)
C5 - N1 - C3	122.0(5)
C2 - N1 - C3	116.6(5)
C15 - N2 - C19	122.7(5)
C15 - N2 - C20	122.9(5)
C19 - N2 - C20	114.5(5)
N4 - N3 - C28	127.2(4)
N4 - N3 - C11	114.2(4)
C28 - N3 - C11	112.5(4)
C29 - N4 - N3	119.5(5)
C48 - N5 - C52	121.5(6)
C48 - N5 - C53	120.1(6)
C52 - N5 - C53	118.4(6)

Table S3 Life time detail of **L** at 586 nm (Nano-LED of 550 nm as the light source)

	B_1	B_2	T_1(ns)	T_2(ns)	T_{av}(ns)	χ^2	φ	K_r	K_{nr}
L	39.49	60.51	0.042	1.005	0.625	1.047	0.084	0.134	1.466
L + Al(III) (1:2)	12.06	87.94	0.575	1.274	1.189	1.005	0.75	0.631	0.20