Supporting Information

For

A napthelene-pyrazol conjugate: Al(III) ion selective blue shifting chemosensor applicable as biomarker in aqueous solution

Manjira Mukherjee,[a] Siddhartha Pal,[a] Somenath Lohar,[a] Buddhadeb Sen,[a] Supriti Sen,[a] Samya Banerjee,[b] Snehasis Banerjee[c] and Pabitra Chattopadhyay[a]*

[a]*Department of Chemistry, Burdwan University, Golapbag, Burdwan-713104, West Bengal, India, E-mail: pabitracc@yahoo.com*

[b]*Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, 560012, India*

[c] *Govt. college of Engineering and Leather Technology, Salt Lake Sector-III, Kolkata 9*

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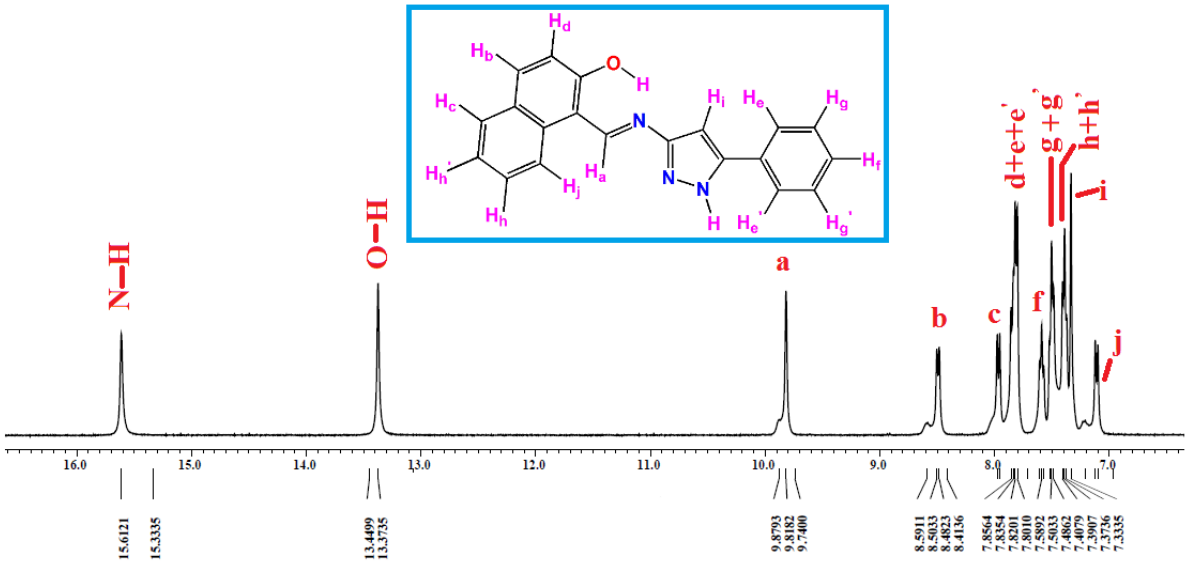

Fig. S1 ^{1}H NMR spectrum of **HL** in DMSO-d_6

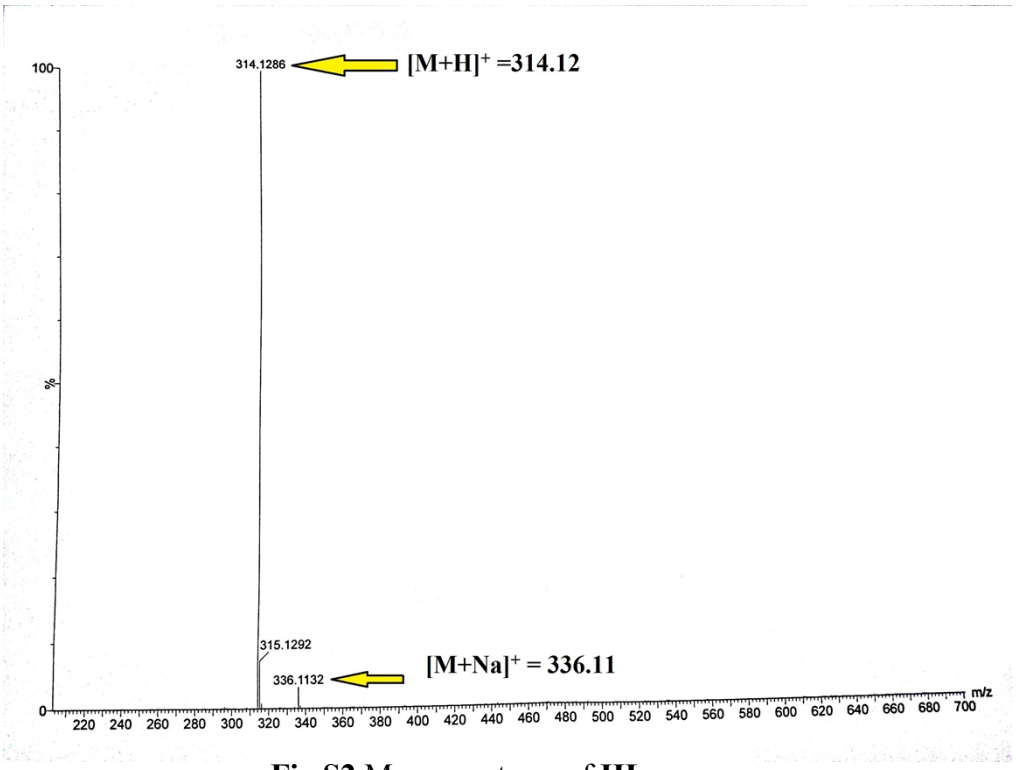

Fig.S2 Mass spectrum of **HL**

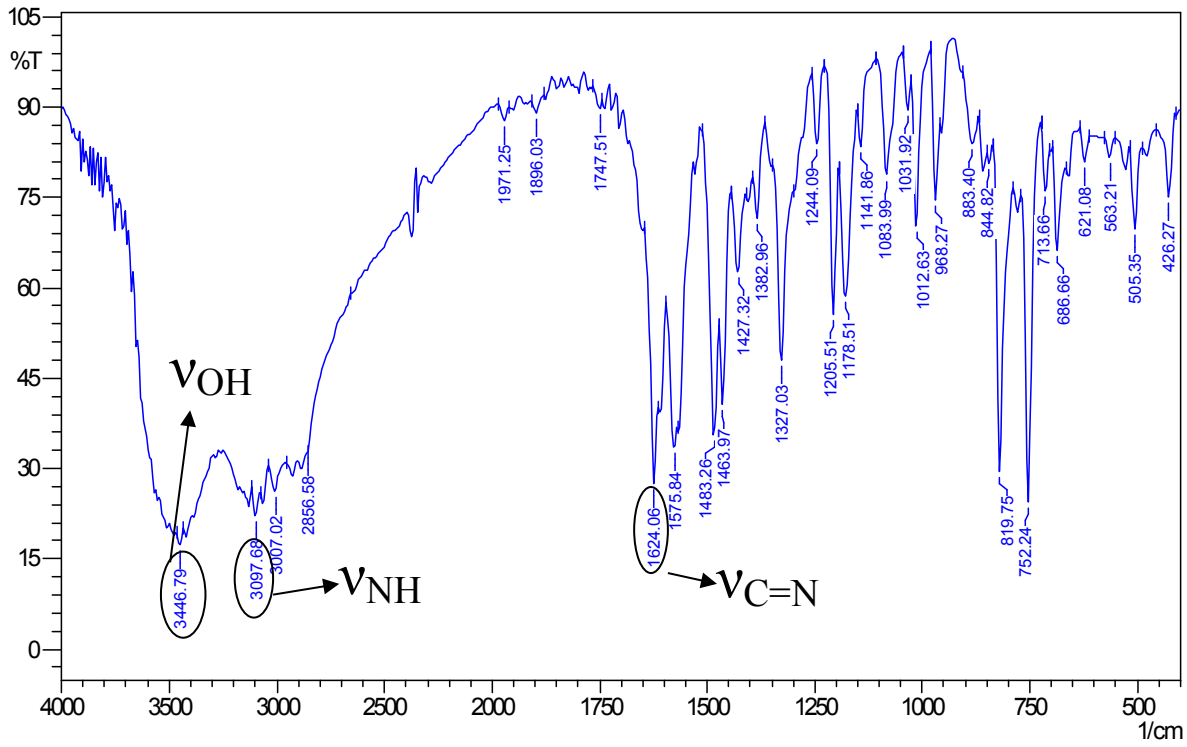

Fig. S3 IR spectrum of **HL**

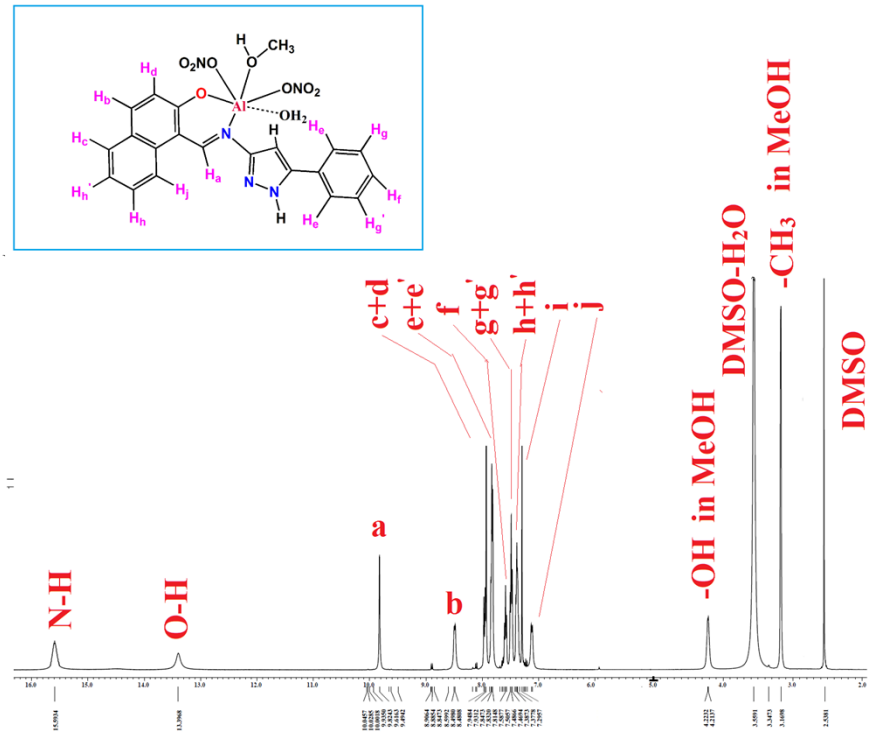

Fig. S4 ^{1}H NMR spectrum of Al(III) complex of **HL** in DMSO-d_6

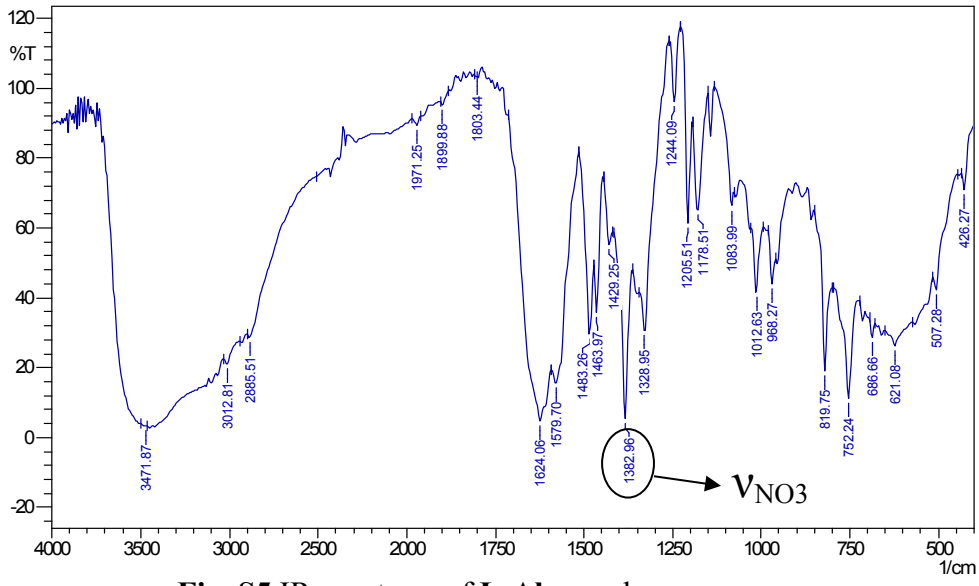

Fig. S5 IR spectrum of **L-Al** complex

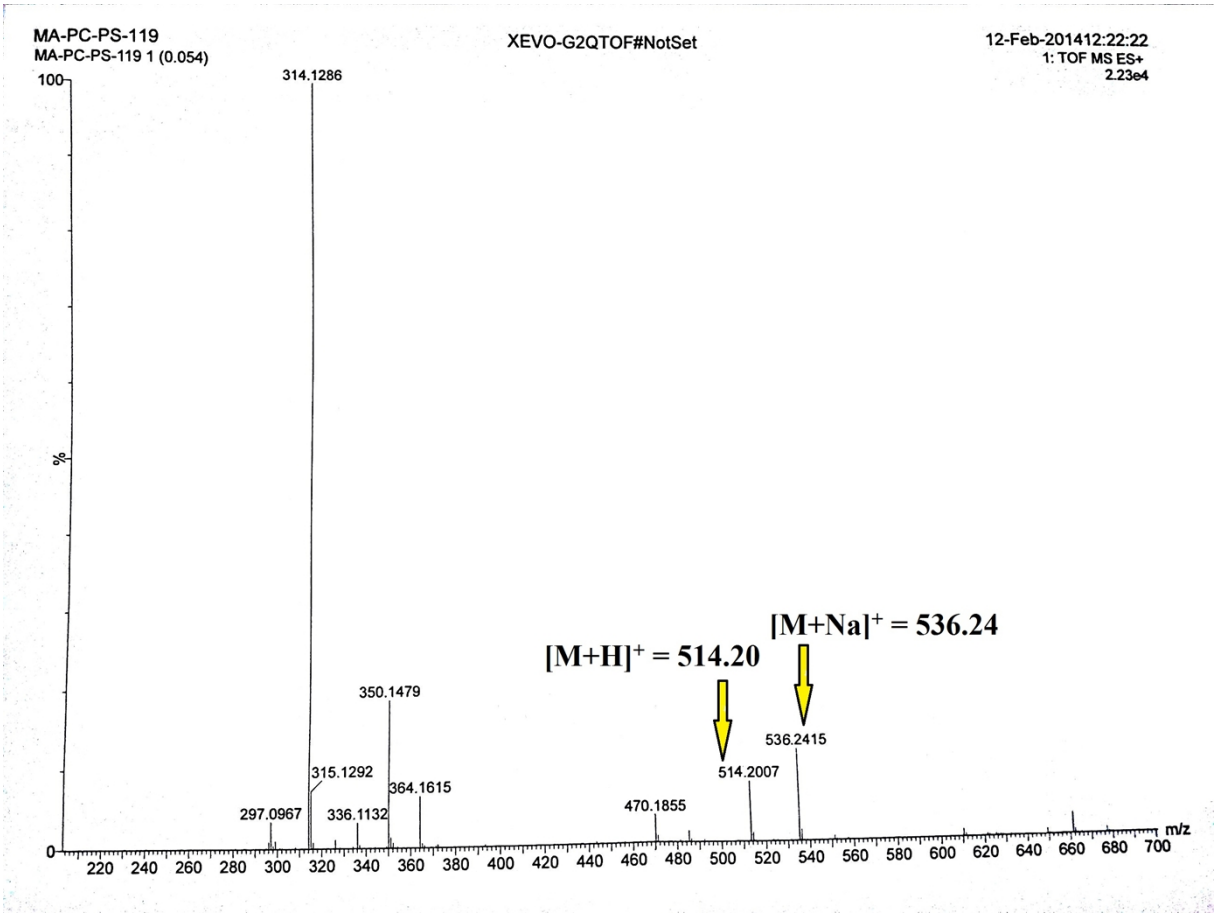

Fig.S6 Mass spectrum of **L-Al** complex

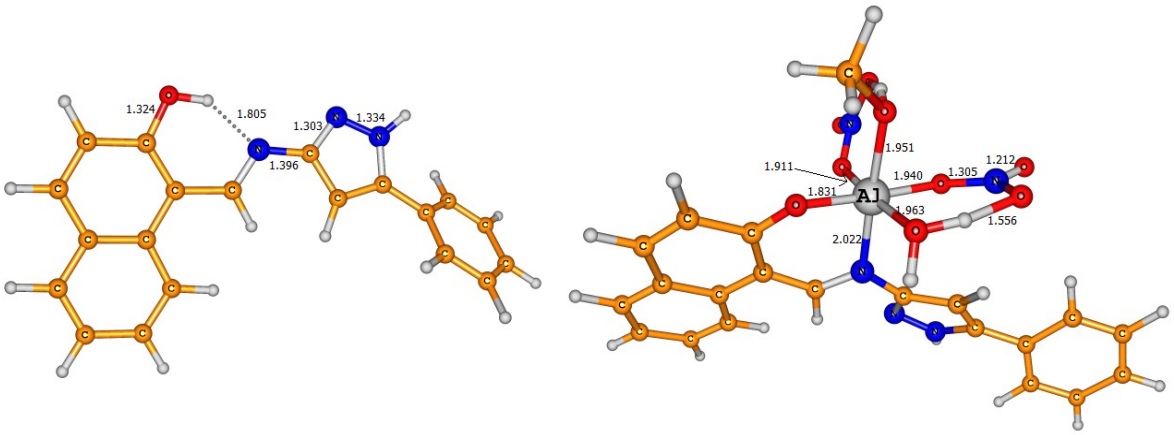

Fig.S7 Theoretically optimised structure of **HL** (left) and the **L-Al** complex (right)

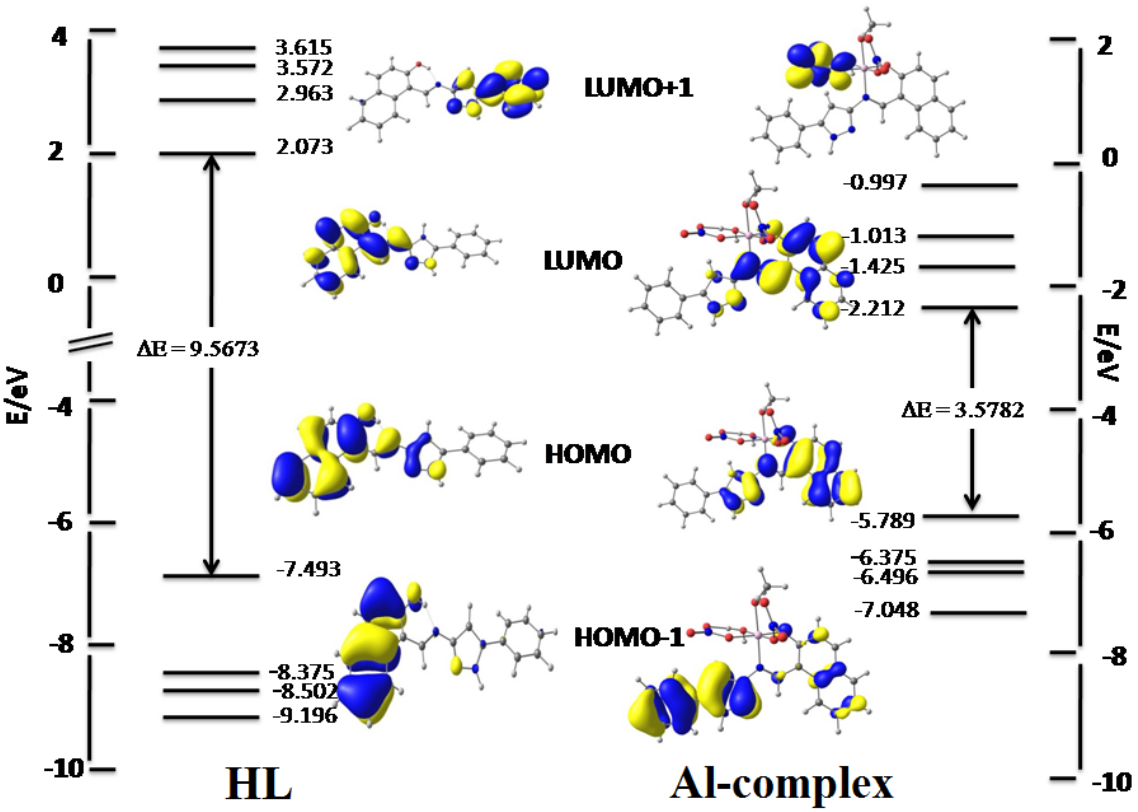

Fig.S8 Energy level diagram for the frontier p-MOs of **HL** (left) and **L-Al** complex (right).

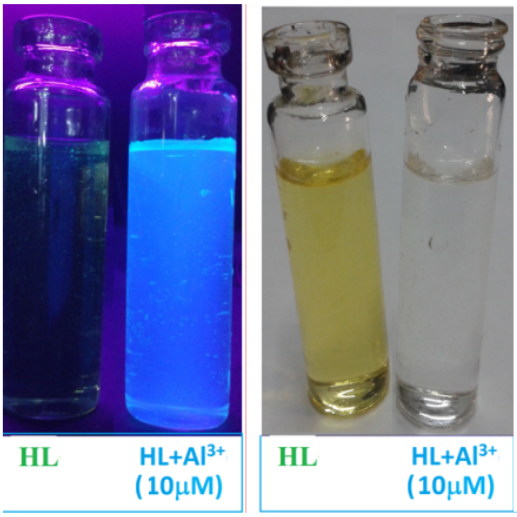

Fig.S9 Fluorescence (left) and naked eye (right) colour change of the probe in absence and presence of Al(III) ions

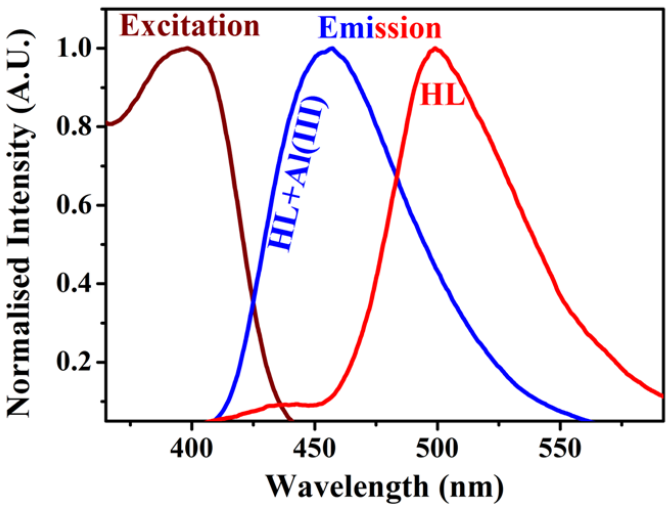

Fig.S10 Absorption and emission spectra of 10 μM of the probe in 100 mM HEPES buffer (DMSO/water 1:5, v/v) at 27°C

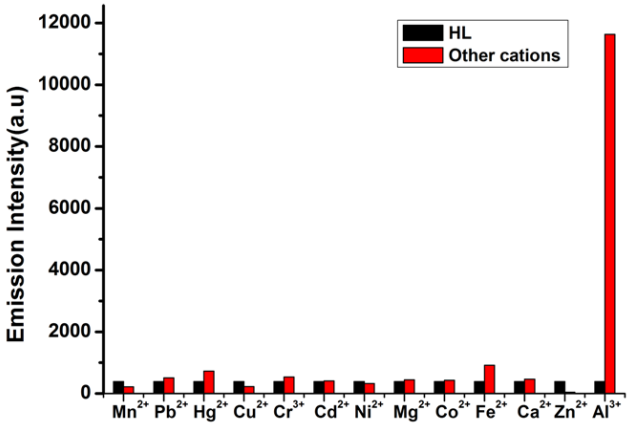

Fig. S11 Fluorescence intensity of **HL** in presence of different cations

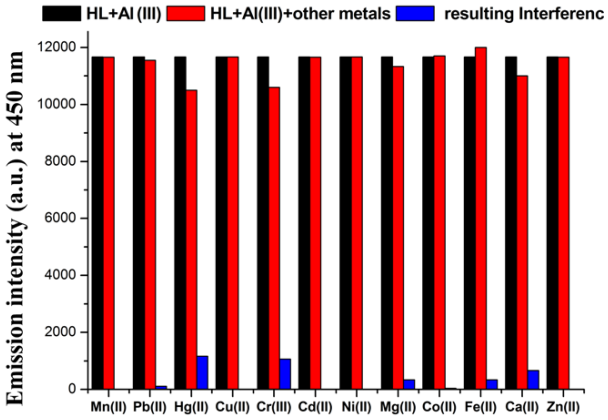

Fig. S12 Change of relative fluorescence intensity profile of **HL** in presence of different cations

	B_1	B_2	T_1 (ns)	T_2 (ns)	T_{av} (ns)	χ^2	ϕ	K_r	K_{nr}
Probe	**96.48**	**3.52**	**0.0277**	**0.911**	**0.033**	**1.05**	**0.1016**	**3.07878**	**27.224**
Probe + Al^{3+} (1:0.5)	**92.82**	**7.18**	**0.141**	**3.572**	**0.26**	**1.03**	**-**	**-**	**-**
Probe + Al^{3+} (1:1)	**89.11**	**10.89**	**0.553**	**5.61**	**0.61**	**1.02**	**0.329**	**0.5393**	**1.100044**

Table **S1** Life time details of **HL**

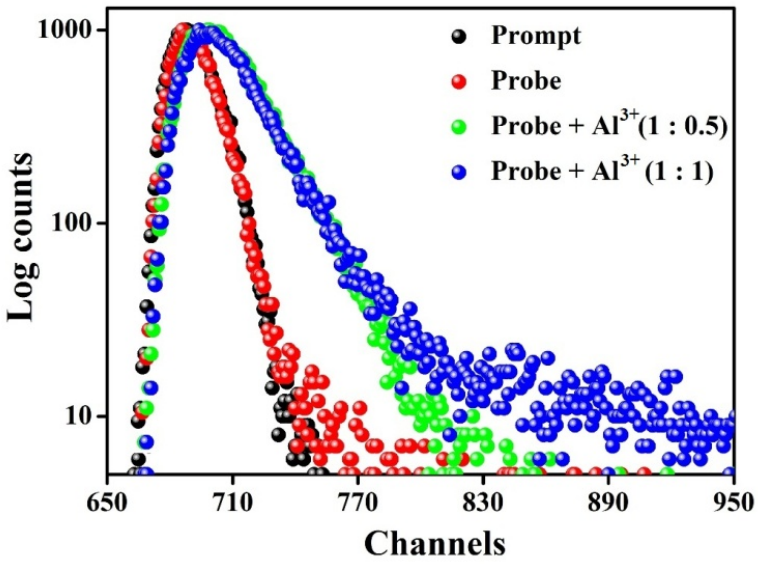

Fig. S13 Time-resolved fluorescence decay of **HL** (10 mM) in the absence and presence of added Al(III) ions (5 mM and 10 mM) (at λ_{ex} = 405 nm) in 100 mM HEPES buffer (DMSO/ water: 1/5, v/v) [λ_{em}: 450 nm].

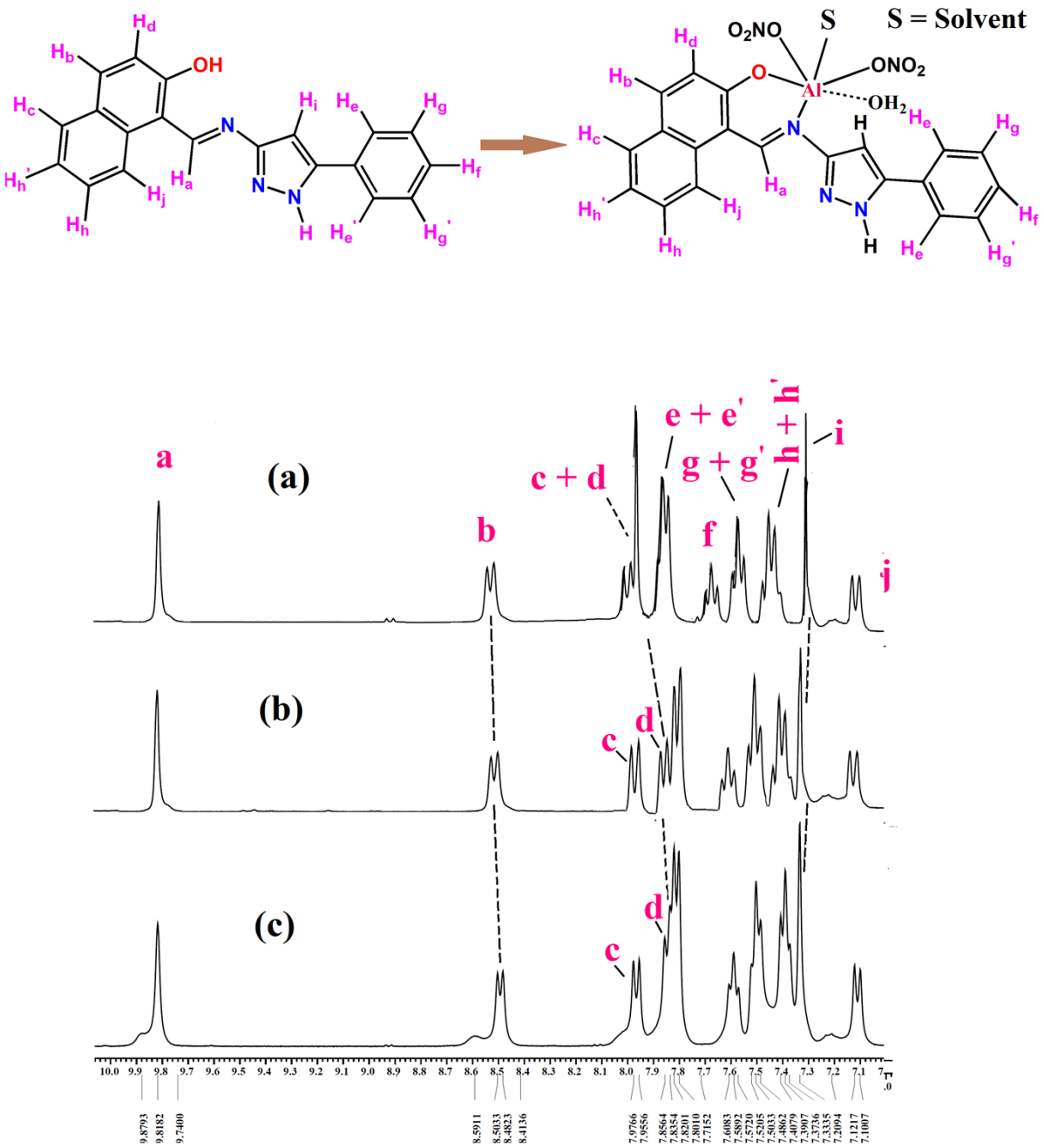

Fig. S14 [1]HNMR titration of **HL**(Expansion of aromatic region) in DMSO-d6 (a) <10 µM (b) 10 µM (c) 0 µM Al(III)

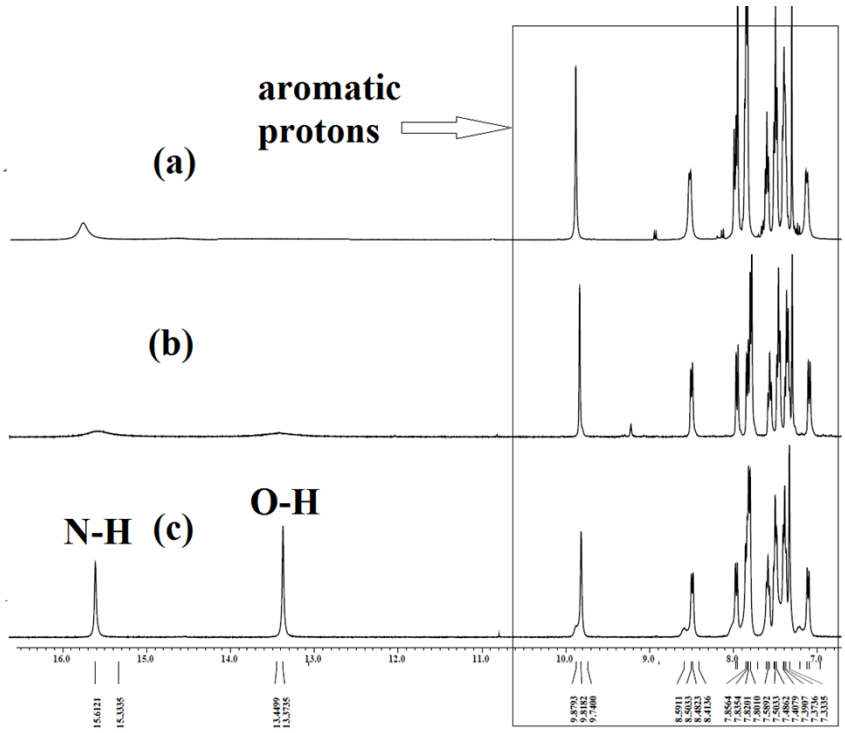

Fig. S15 ^{1}HNMR titration of **HL** in DMSO-d_6 (a) <10 µM (b) 10 µM (c) 0 µM Al(III) ions

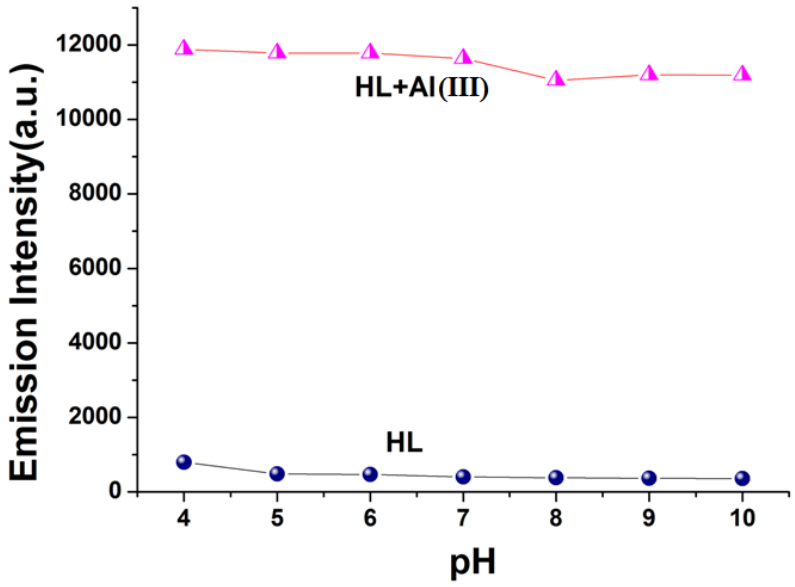

Fig. S16 Fluorescence response to pH of **HL** (10 µM) in absence and in presence of Al(III) (one equivalent) at different pH in 100 mM HEPES buffer (DMSO/ water: 1/5) at 25 °C.

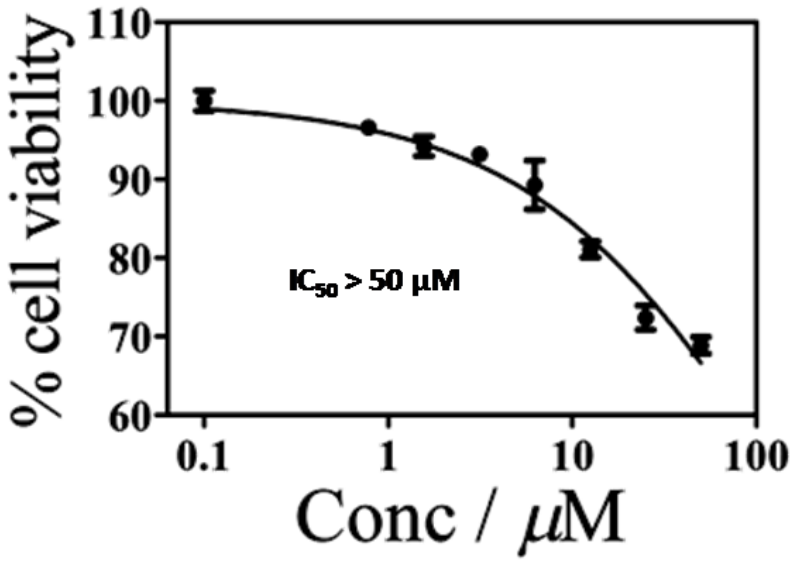

Fig. S17 Cytotoxic effect of **HL**

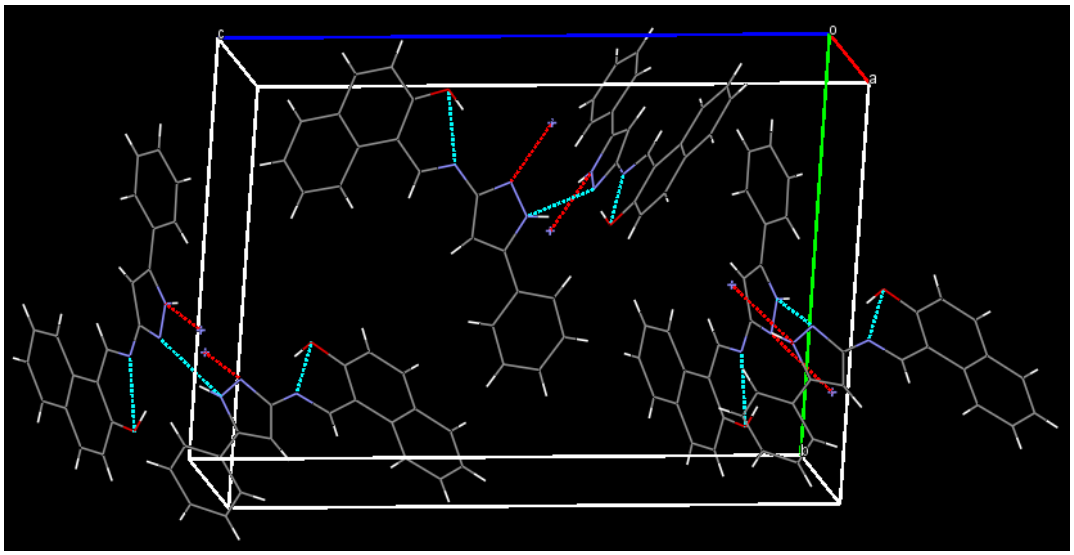

Fig. S18 Crystal Packing of **HL**