

## *Supporting Information*

### **For**

### **A quinazoline derivative as quick-response red-shifted reporter for nanomolar Al<sup>3+</sup> ions and applicable to living cell staining**

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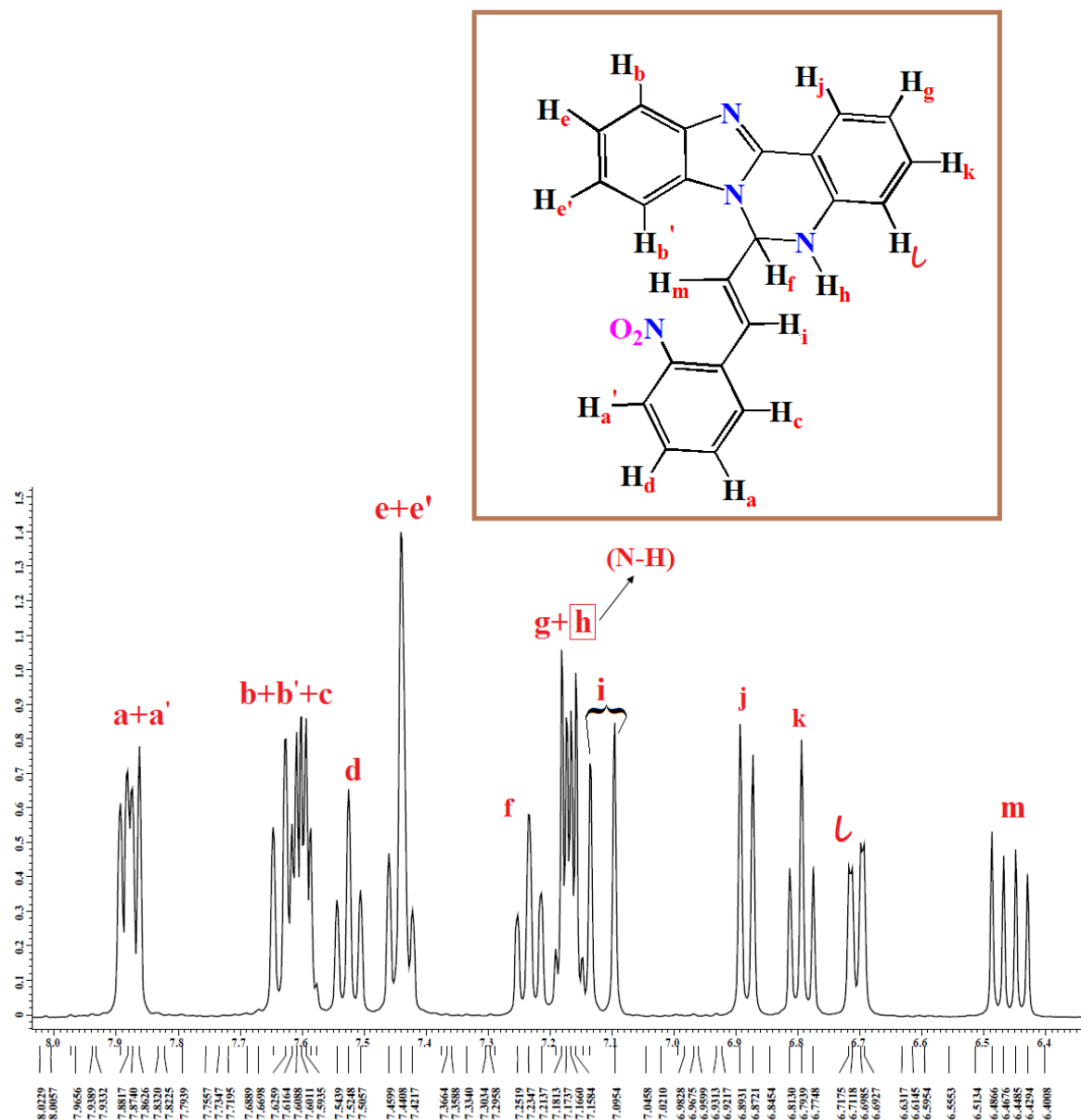
1. **Fig. S1** <sup>1</sup>H NMR spectrum of **L** in DMSO-d<sub>6</sub>
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15. **Fig. S14**  $^1\text{H}$ NMR titration of **L**

16. **Fig. S15** Fluorescence response to pH of **L** (10  $\mu\text{M}$ ) in absence and in presence of  $\text{Al}^{3+}$  (one equivalent) at different pH in 100 mM HEPES buffer (DMSO/ water: 1/9) at 27  $^\circ\text{C}$ .

17. **Fig. S16** Fluorescence image of MCF-7 cell

18. **Fig. S17** Cytotoxic effect of **L**



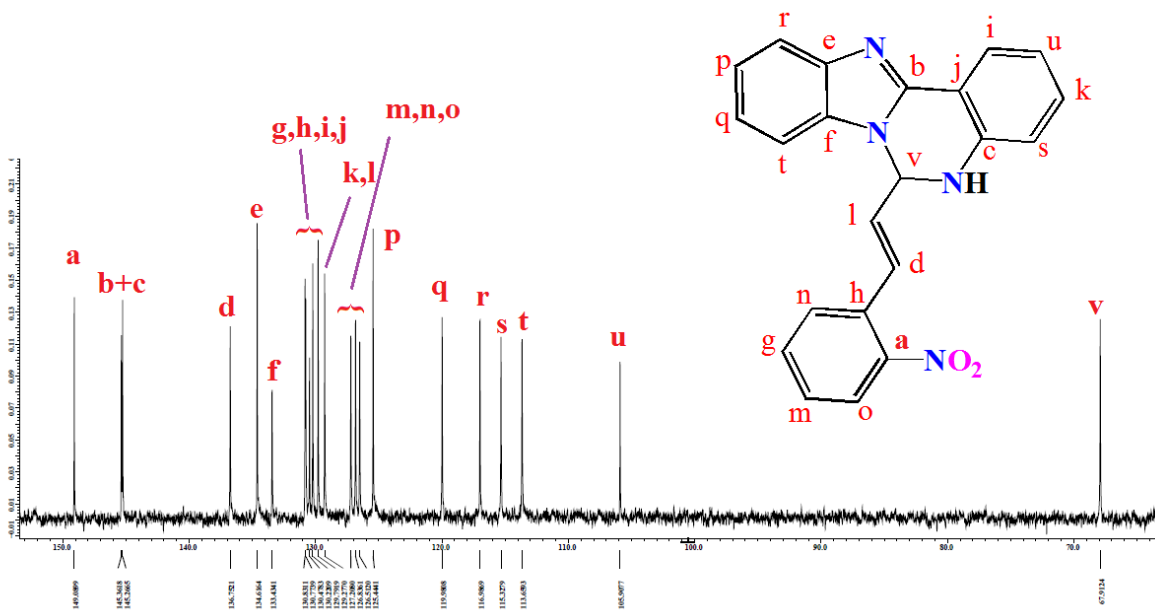


Fig. S2 <sup>13</sup>C NMR spectrum of L in DMSO-d<sub>6</sub>

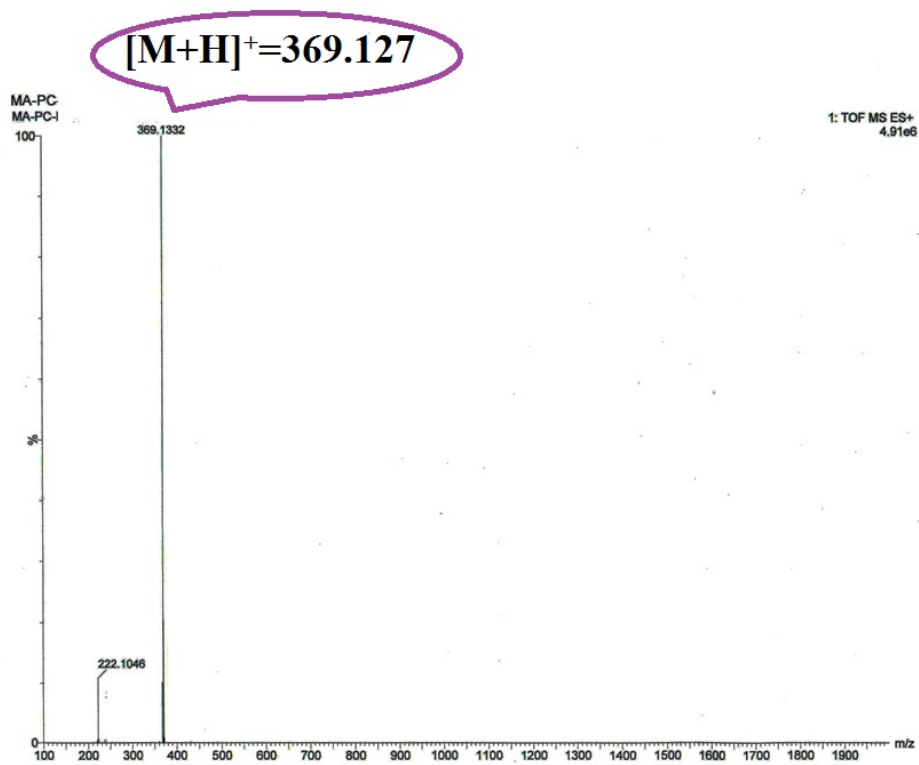


Fig.S3 Mass spectrum of L

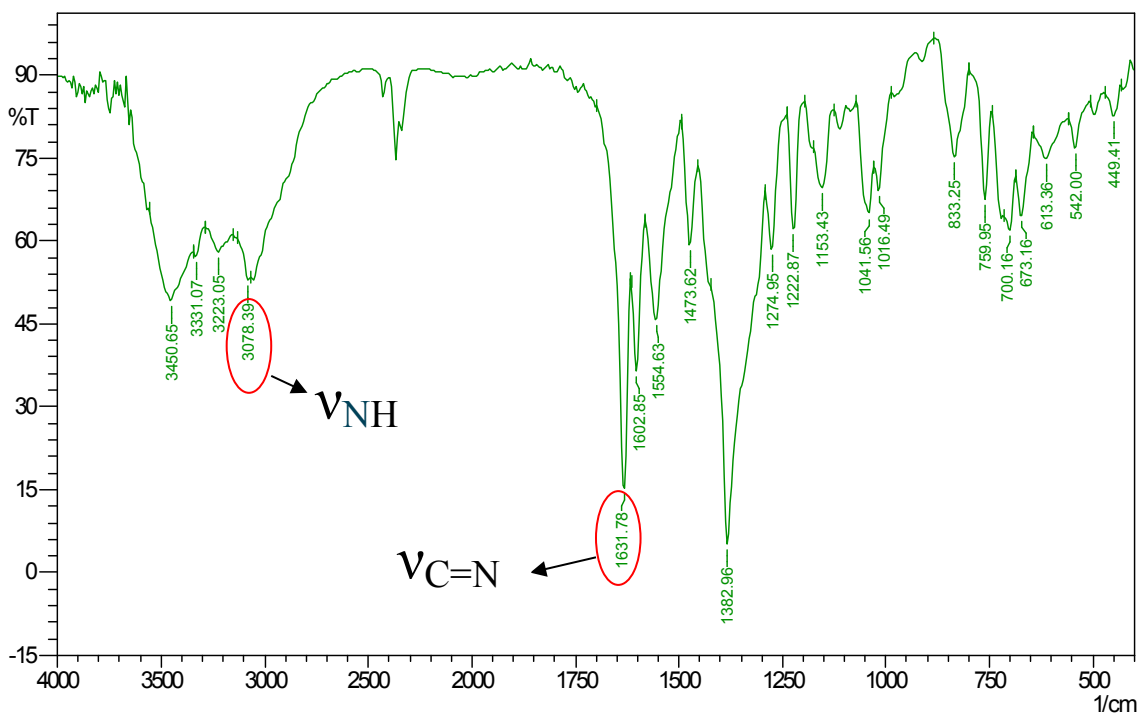


Fig. S4 IR spectrum of L

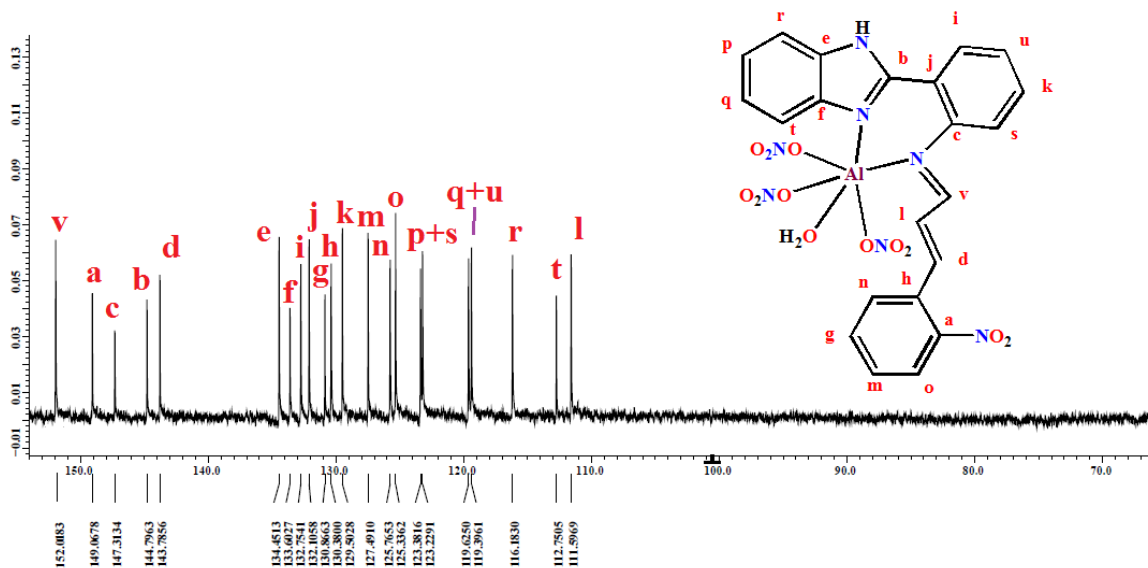


Fig. S5  $^{13}\text{C}$ NMR spectrum of aluminium(III) complex of L in  $\text{DMSO-d}_6$

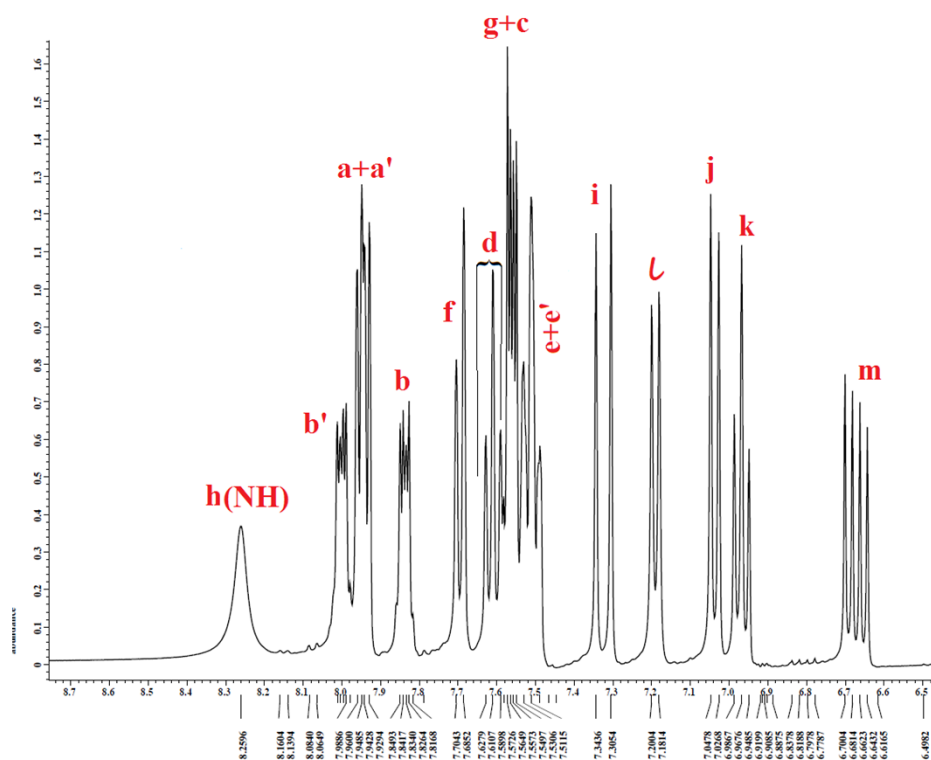
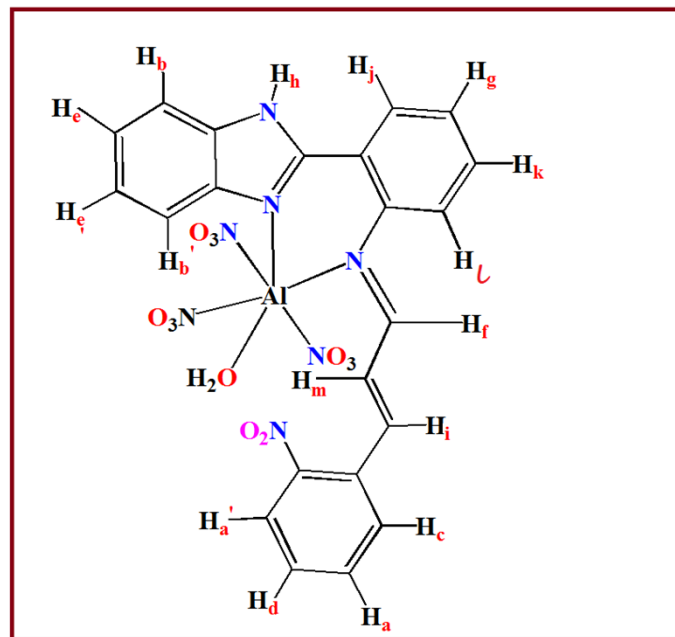


Fig. S6  $^1\text{H}$  NMR spectrum of  $\text{Al}^{3+}$  complex of L in  $\text{DMSO-d}_6$

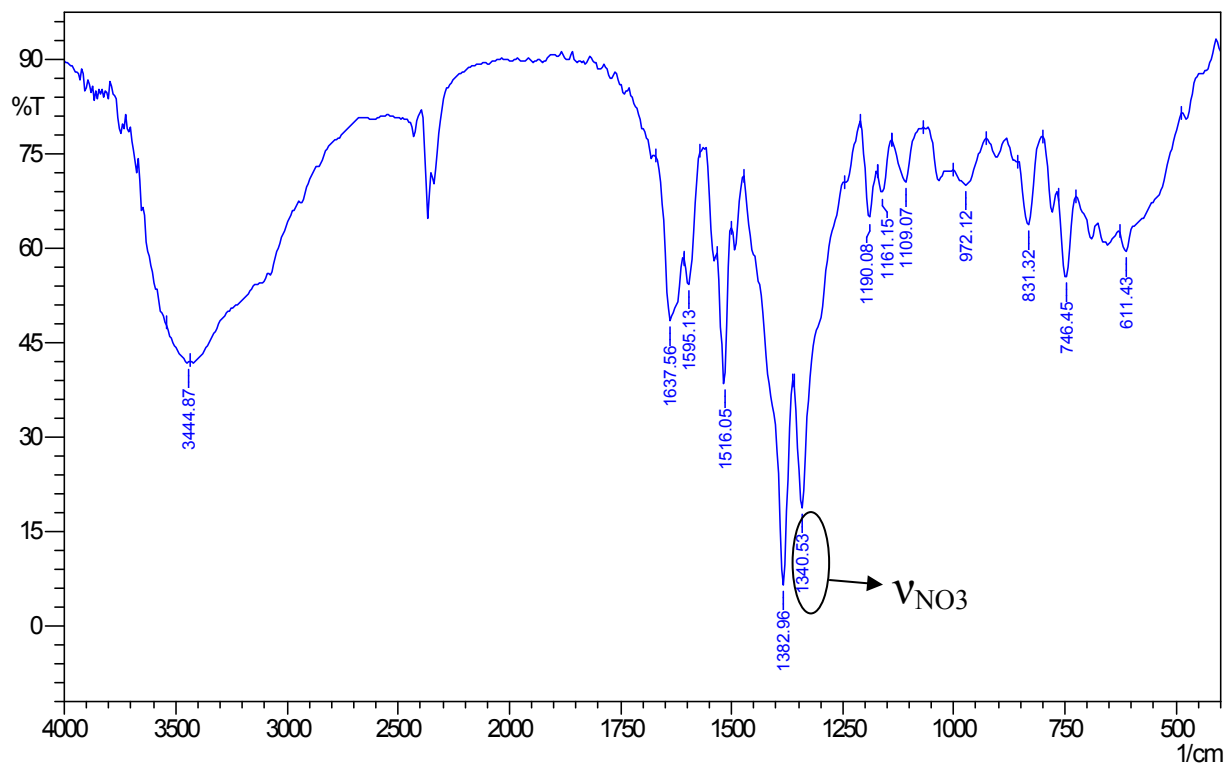


Fig. S7 IR spectrum of aluminium(III) complex

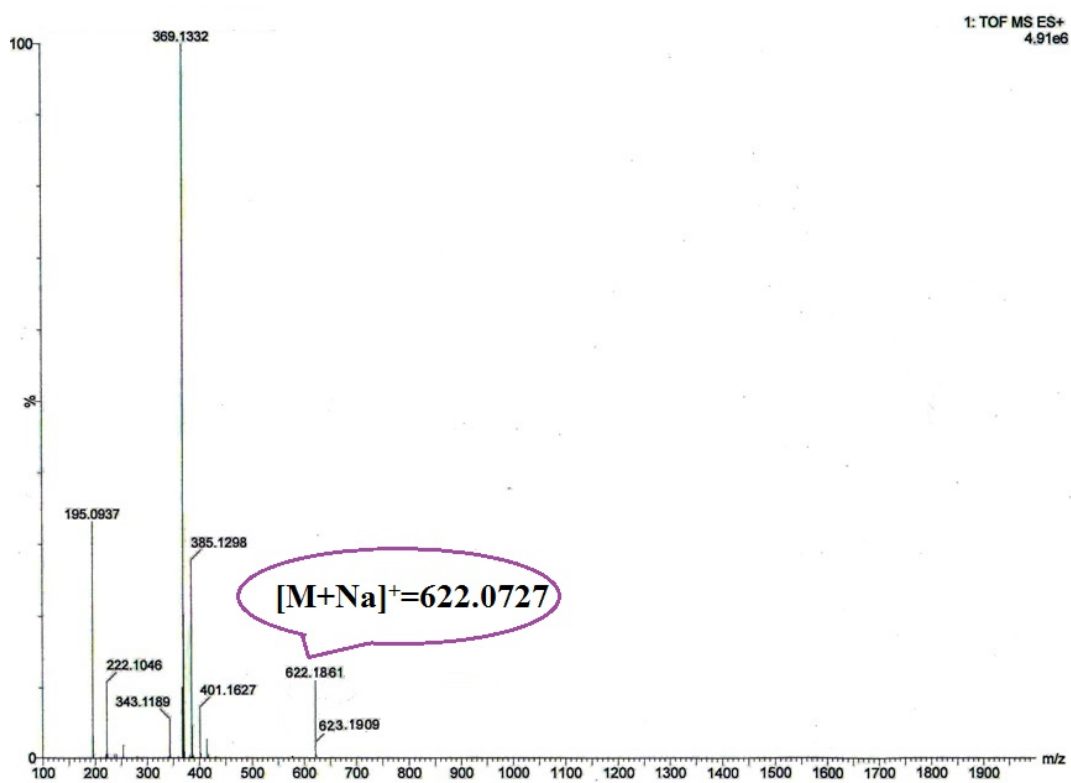
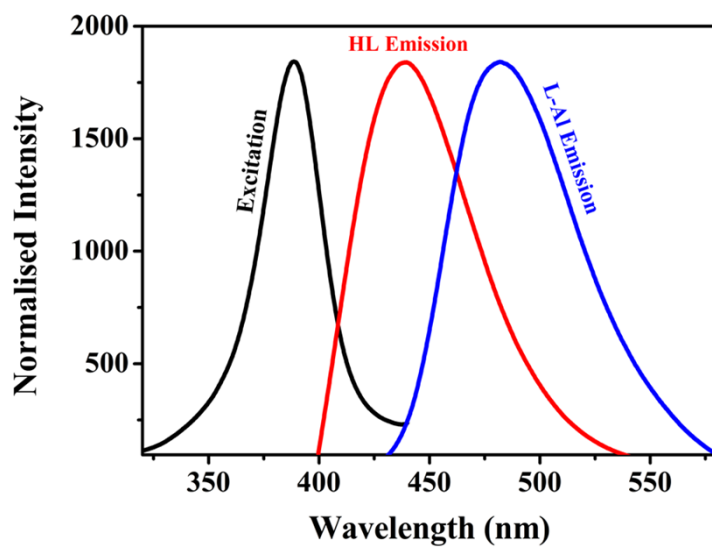
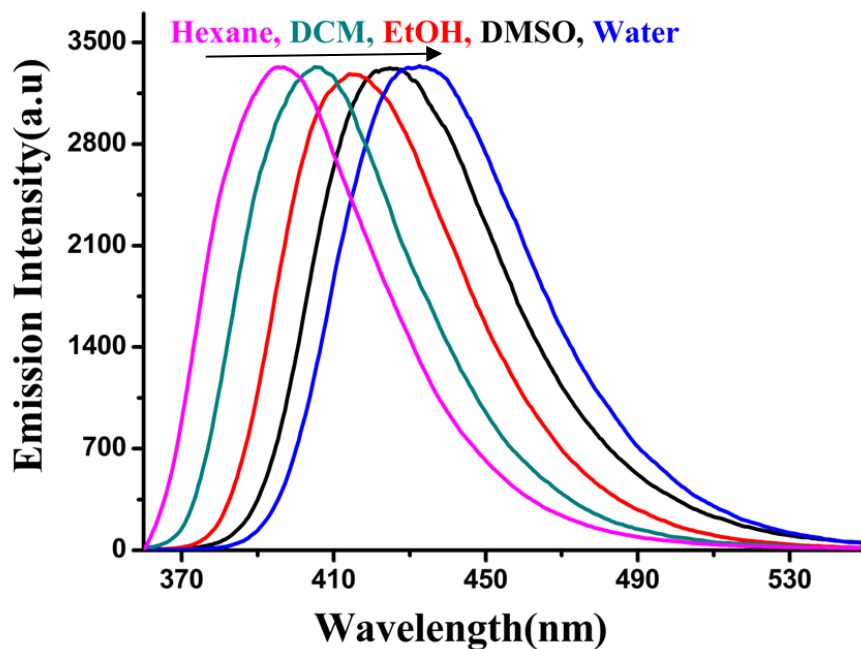


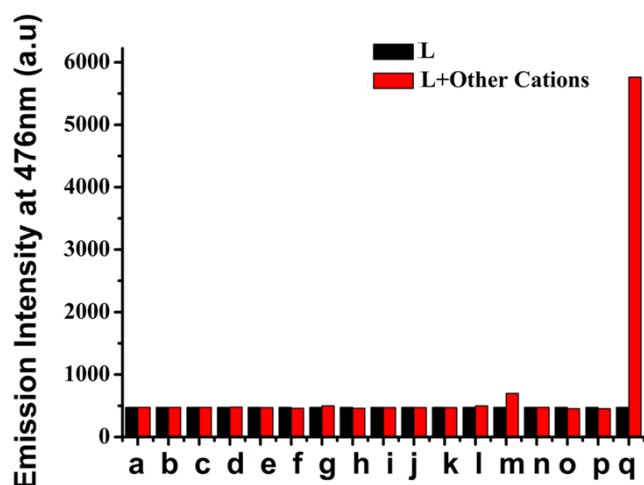
Fig.S8 Mass spectrum of aluminium(III) complex



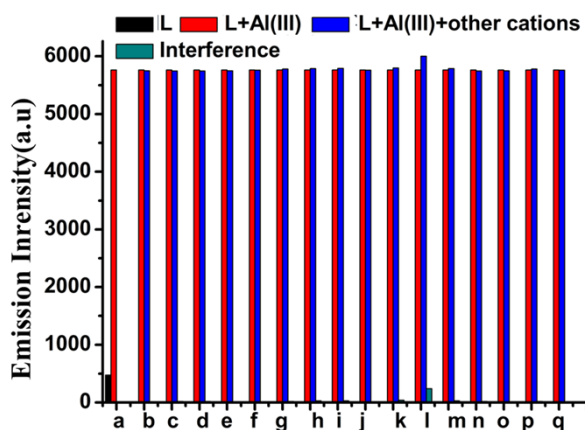
**Fig.S9** Absorption and emission spectra of 10  $\mu\text{M}$  of the probe in 100 mM HEPES buffer (DMSO/water 1:9, v/v) at 27°C



**Fig. S10** Emission spectra of L at different solvent



**Fig. S11** Fluorescence intensity of L in presence of different cations in HEPES buffer (100 mM, pH 7.4; DMSO/water: 1/9, v/v) at 25 °C, (a) Na<sup>+</sup>, (b) K<sup>+</sup>, (c) Mn<sup>2+</sup>, (d) Pb<sup>2+</sup>, (e) Hg<sup>2+</sup>, (f) Cu<sup>2+</sup>, (g) Cr<sup>3+</sup>, (h) Cd<sup>2+</sup>, (i) Ni<sup>2+</sup>, (j) Mg<sup>2+</sup>, (k) Co<sup>2+</sup>, (l) Fe<sup>2+</sup>, (m) Fe<sup>3+</sup>, (n) Ca<sup>2+</sup>, (o) Zn<sup>2+</sup>, (p) Ag<sup>+</sup>, (q) Al<sup>3+</sup>

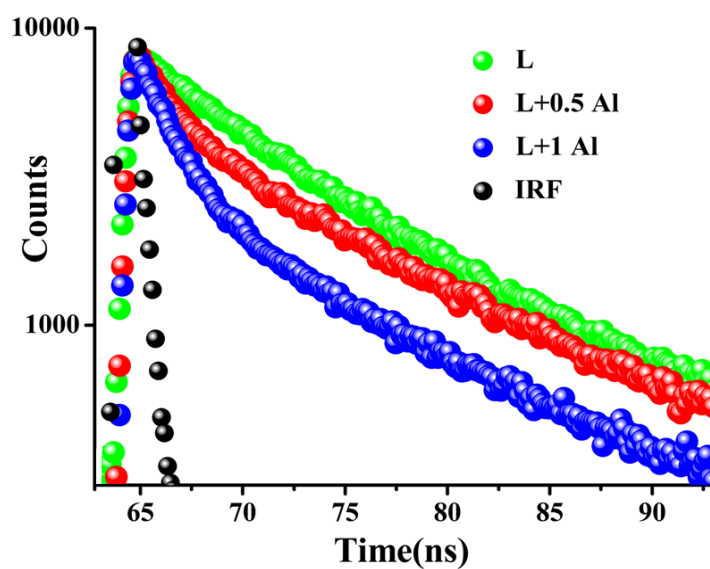


**Fig. S12** Change of relative fluorescence intensity profile of L in presence of different cations in HEPES buffer (100 mM, pH 7.4; DMSO/water: 1/9, v/v) at 25 °C, (a) L, (b) Mn<sup>2+</sup>, (c) Pb<sup>2+</sup>, (d) Hg<sup>2+</sup>, (e) Cu<sup>2+</sup>, (f) Cr<sup>3+</sup>, (g) Cd<sup>2+</sup>, (h) Ni<sup>2+</sup>, (i) Mg<sup>2+</sup>, (j) Co<sup>2+</sup>, (k) Fe<sup>2+</sup>, (l) Fe<sup>3+</sup>, (m) Ca<sup>2+</sup>, (n) Zn<sup>2+</sup>, (o) Ag<sup>+</sup>, (p) Na<sup>+</sup>, (q) K<sup>+</sup>



Table S1 Life time details of L

	$B_1$	$B_2$	$T_1$ (ns)	$T_2$ (ns)	$T_{av}$ (ns)	$\chi^2$	$\phi$	$K_r$	$K_{nr}$	$K_r/K_{nr}$
<b>L</b>	85	15	9	2	7.93	0.99	0.069	0.0087	0.1174	0.074
<b>L + Al<sup>3+</sup> (1:0.5)</b>	49	51	11	1.65	6.23	1.07	-	-	-	-
<b>L + Al<sup>3+</sup> (1:1)</b>	27	73	11.22	1.64	4.22	0.99	0.708	0.1677	0.069	2.26



**Fig. S13** Time-resolved fluorescence decay of L (10 mM) in the absence and presence of added Al<sup>3+</sup> ions (5 mM ,10 mM and 15 mM) (at  $\lambda_{ex} = 380$  nm) in 100 mM HEPES buffer (DMSO/ water: 1/9, v/v) [ $\lambda_{em}$ : 476 nm].

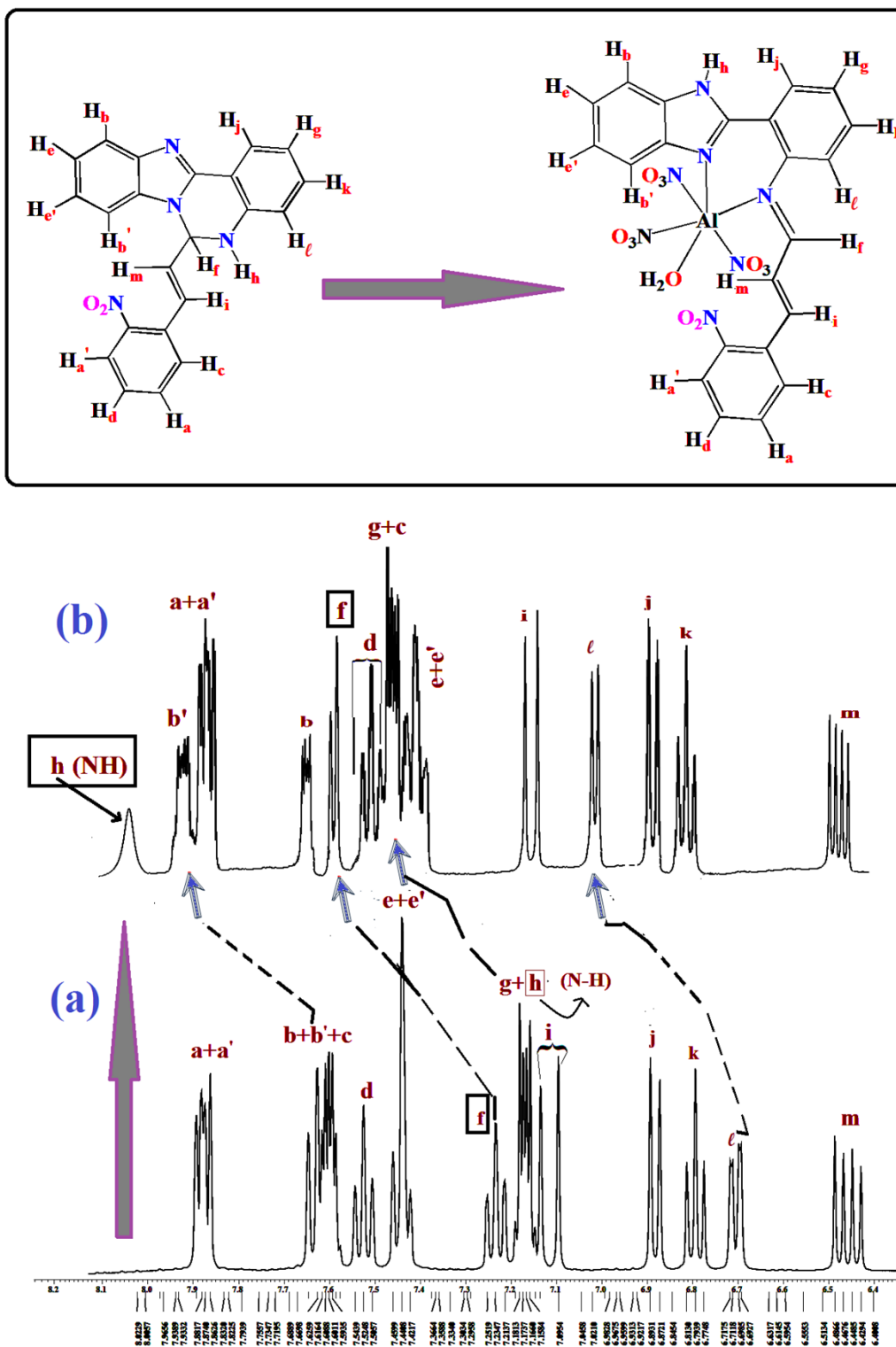
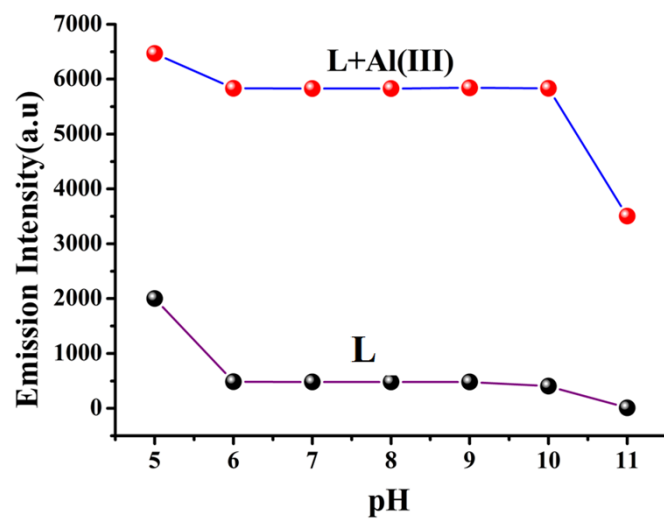


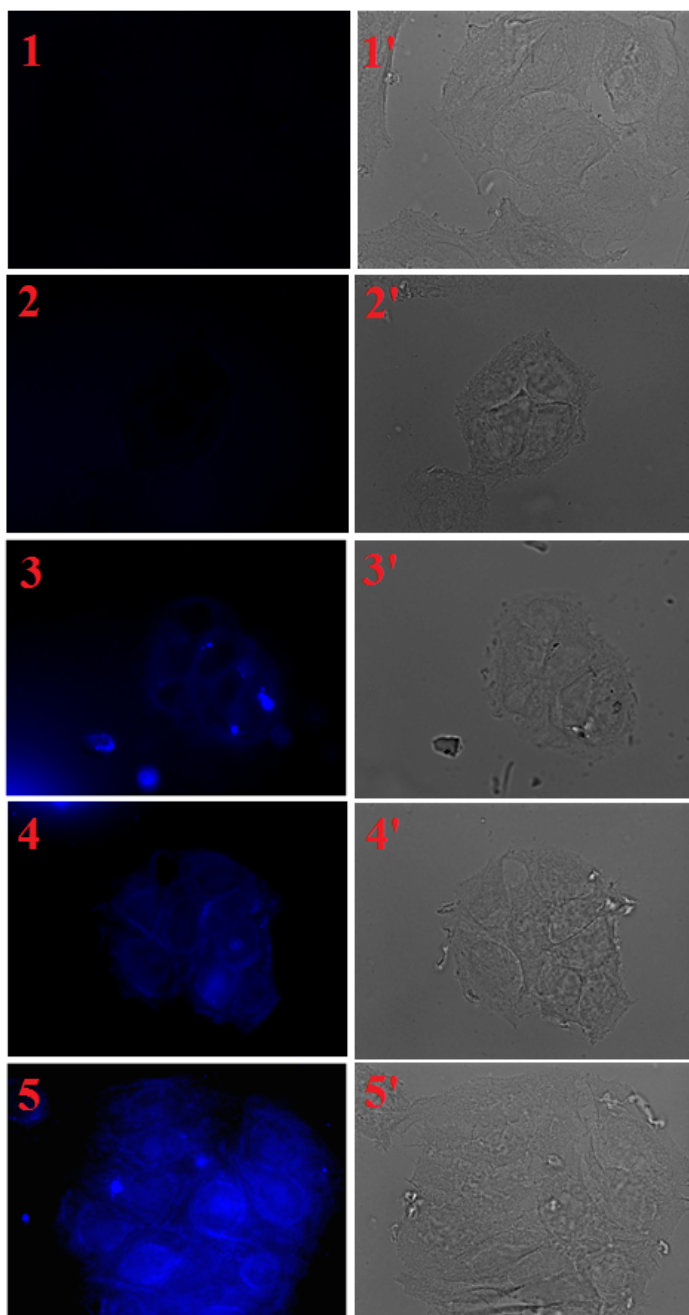
Fig. S14  $^1\text{H}$ NMR titration of **L** in  $\text{DMSO-d}_6$  (a)  $0 \mu\text{M}$  (b)  $10 \mu\text{M}$   $\text{Al}^{3+}$  ions



**Fig. S15** Fluorescence response to pH of **L** (10  $\mu$ M) in absence and in presence of  $\text{Al}^{3+}$  (one equivalent) at different pH in 100 mM HEPES buffer (DMSO/ water: 1/9) at 27  $^{\circ}\text{C}$ .

## Fluorescence Image

## Phase contrast



**Fig. S16** Fluorescence image of MCF-7 cell (1) Control (2) Cells were incubated with  $0 \mu\text{M Al}^{3+}$  (3) cells incubated with  $2 \mu\text{M Al}^{3+}$  (4)  $5 \mu\text{M Al}^{3+}$  and (5)  $10 \mu\text{M Al}^{3+}$ . All the samples were excited at 380 nm with emission 476 nm by using a [10 X] objective.

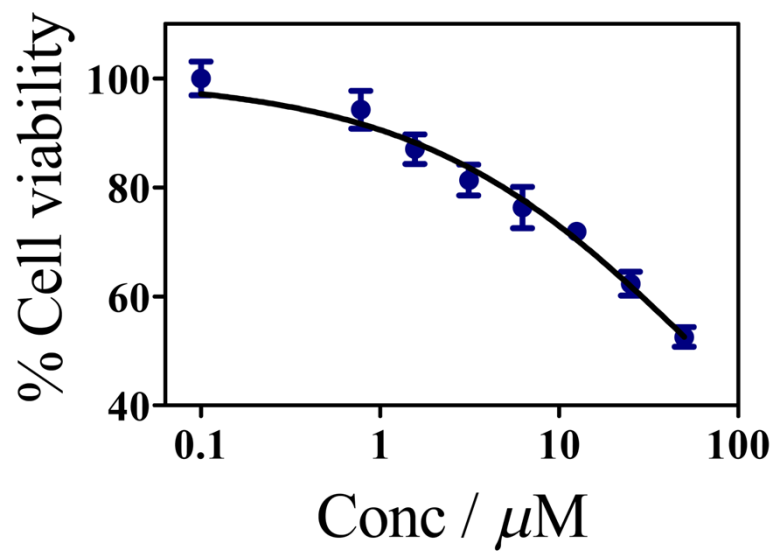


Fig. S17 Cytotoxic effect of L ( $\text{IC}_{50} > 50 \mu\text{M}$ )