

SUPPORTING INFORMATION

A novel chemosensor based on rhodamine and azobenzene moieties for selective detection of Al³⁺ ion

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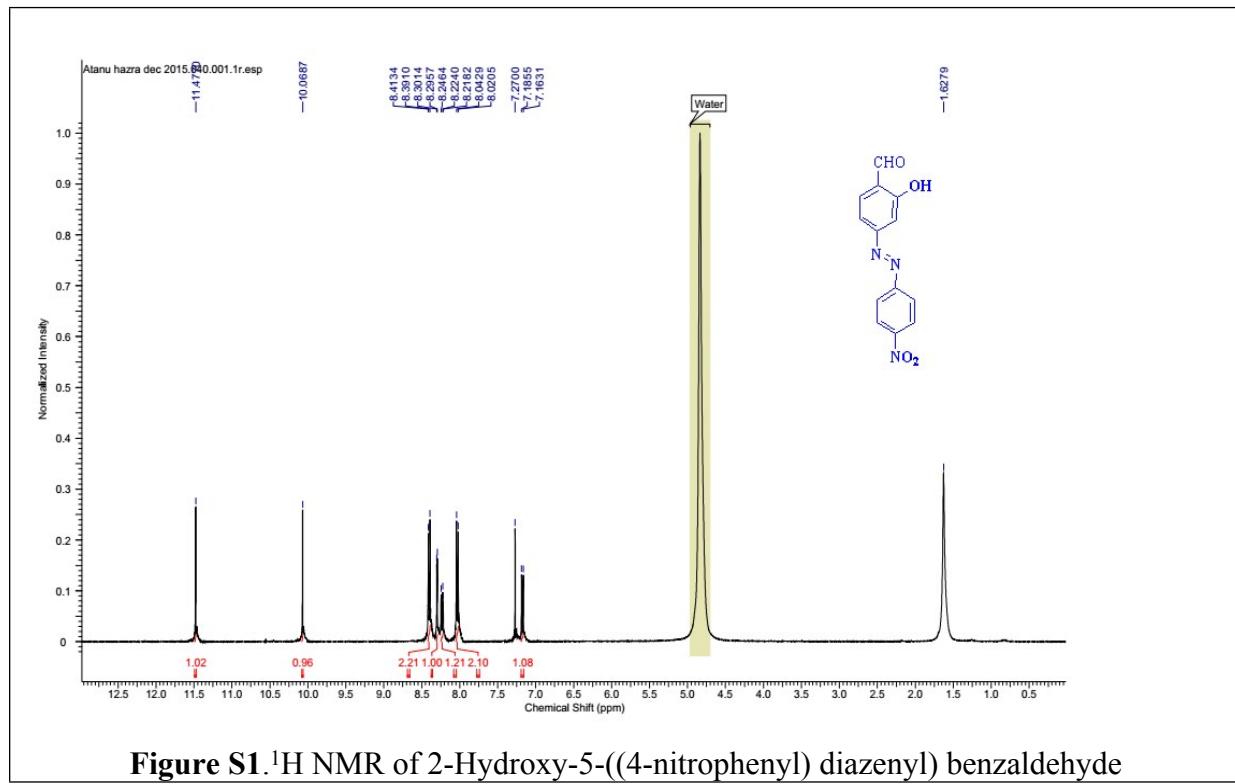
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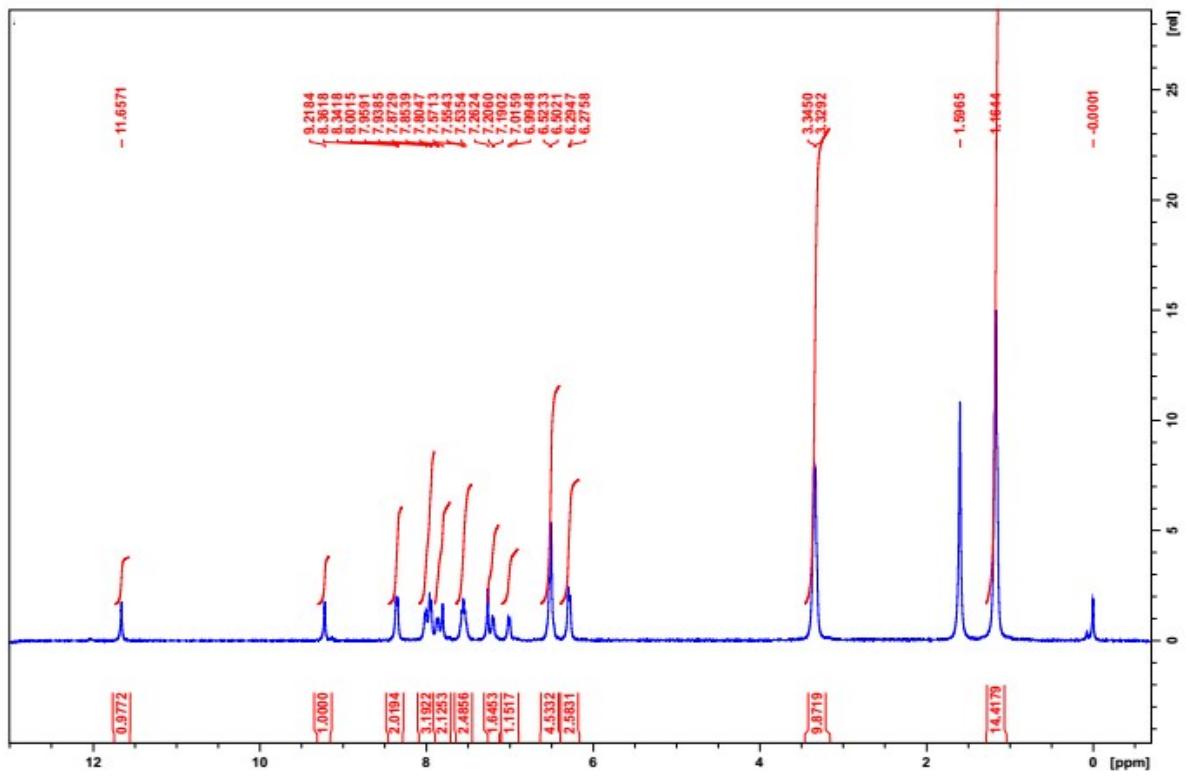


Figure S2. Proton NMR of chemosensor (L)

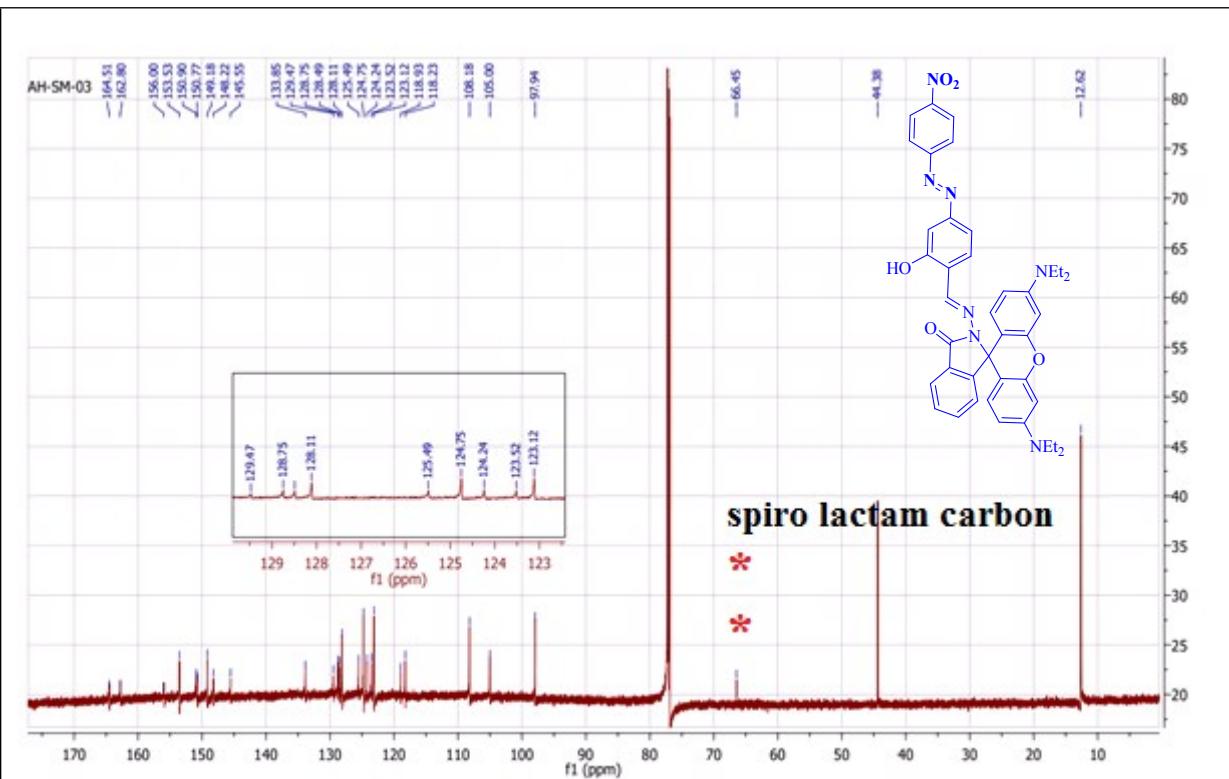


Figure S3. ¹³C NMR of chemosensor (L)

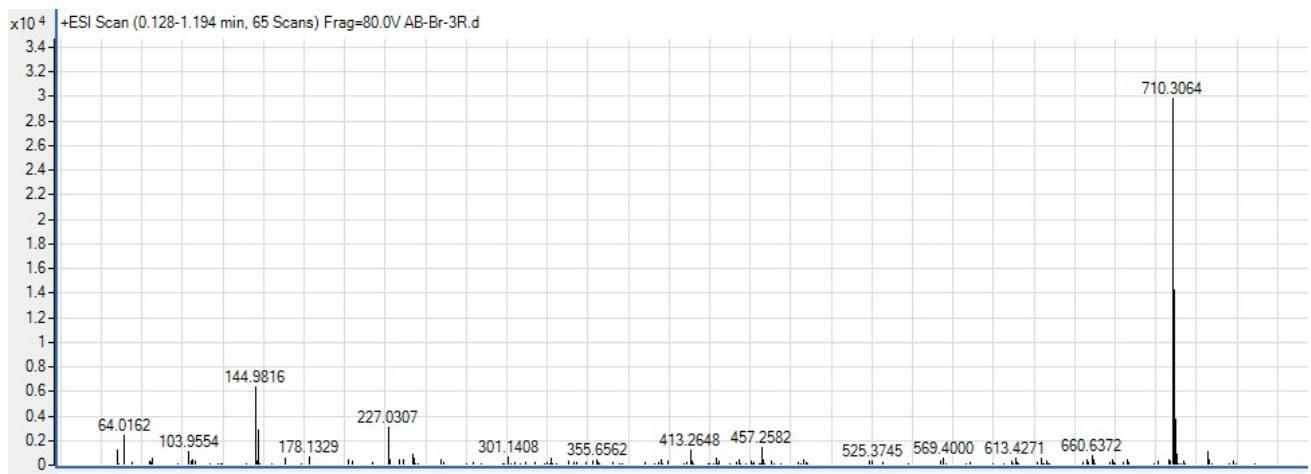


Figure S4. Mass of the chemosensor (L)

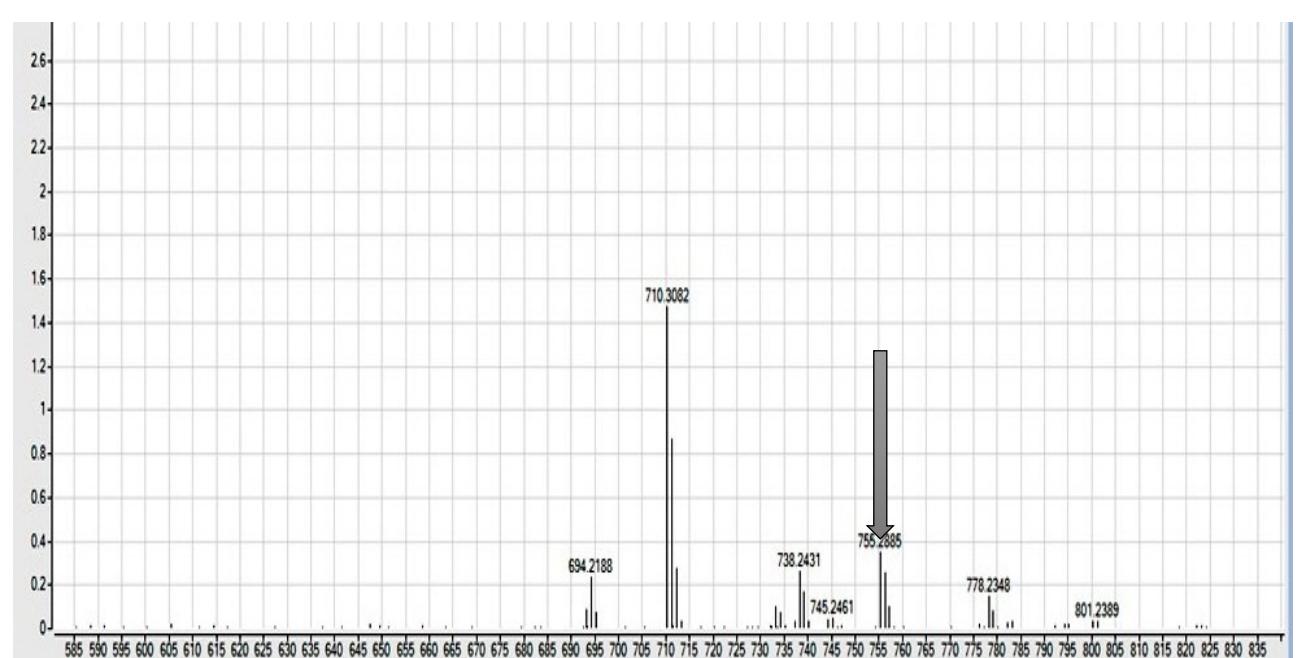


Figure S5. Mass spectrum of L-Al³⁺ complex

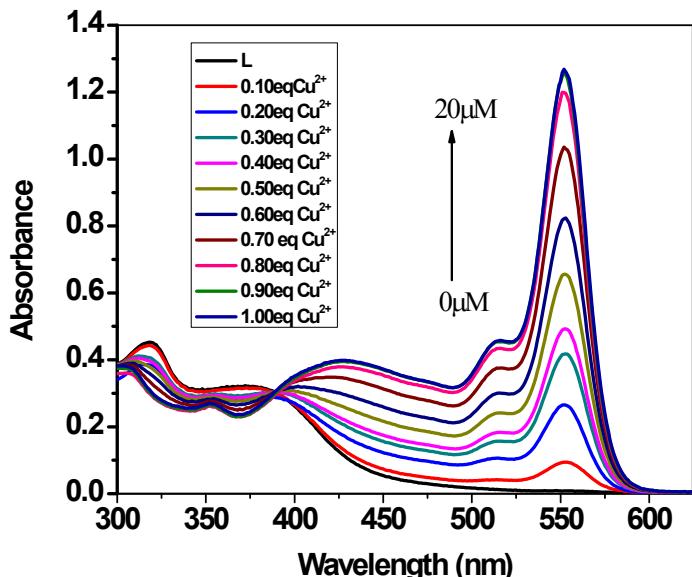


Figure S6. UV-Vis spectral changes of L (20 μM) upon addition of Cu^{2+} ions in a HEPES buffer [50 μM , $\text{C}_2\text{H}_5\text{OH}-\text{H}_2\text{O}$ (4:1, v/v, pH= 7.2)] at 25 $^{\circ}\text{C}$. $[\text{Cu}^{2+}] = 0\text{-}20 \mu\text{M}$

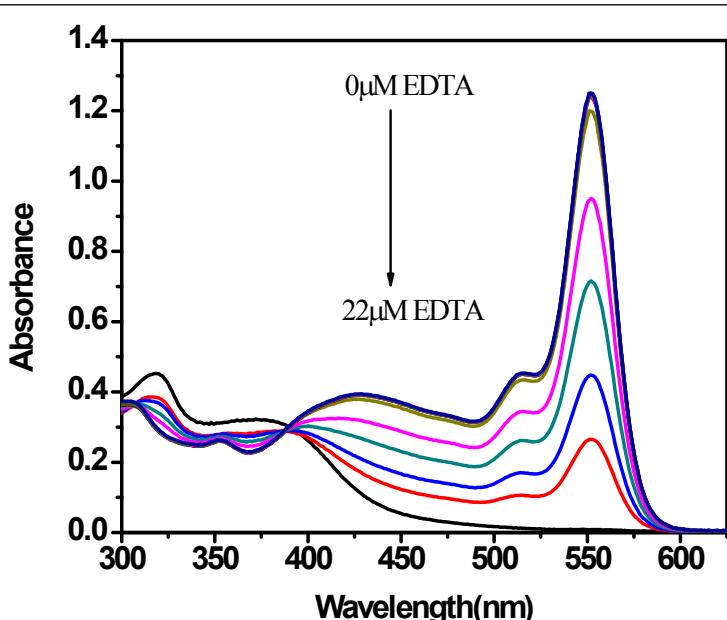


Figure S7. UV-Vis spectral changes of Cu^{2+} complex of L (20 μM) upon addition of EDTA in HEPES buffer [50 μM , $\text{C}_2\text{H}_5\text{OH}-\text{H}_2\text{O}$ (4:1, v/v, pH= 7.2)] at 25 $^{\circ}\text{C}$. EDTA added = 0-22 μM

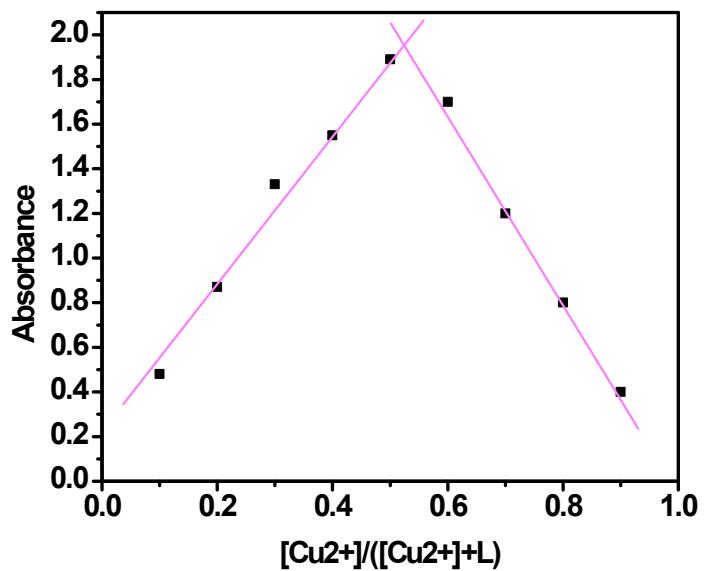


Figure S8. Job's plot from absorbance data of **L** and Cu^{2+} with a total solution volume of 2 ml in HEPES buffer [50 μ M, $C_2H_5OH-H_2O$ (4:1, v/v, pH= 7.2)] at 25 °C λ_{abs}^{max} = 550 nm.

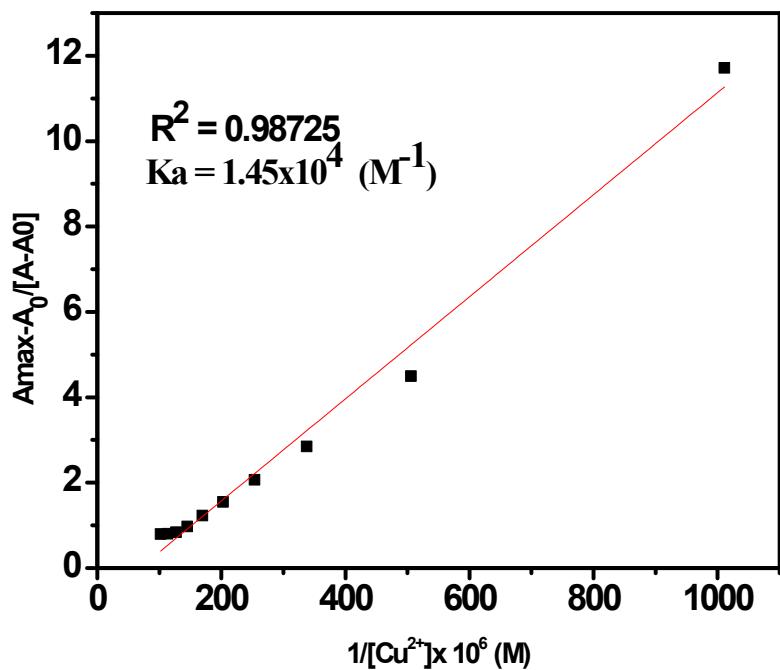


Figure S9. Benesi-Hildebrand plot of **L** (20 μ M) for Cu^{2+} determined by absorbance method in HEPES buffer [50 μ M, $C_2H_5OH-H_2O$ (4:1, v/v, pH= 7.2)] at 25 °C

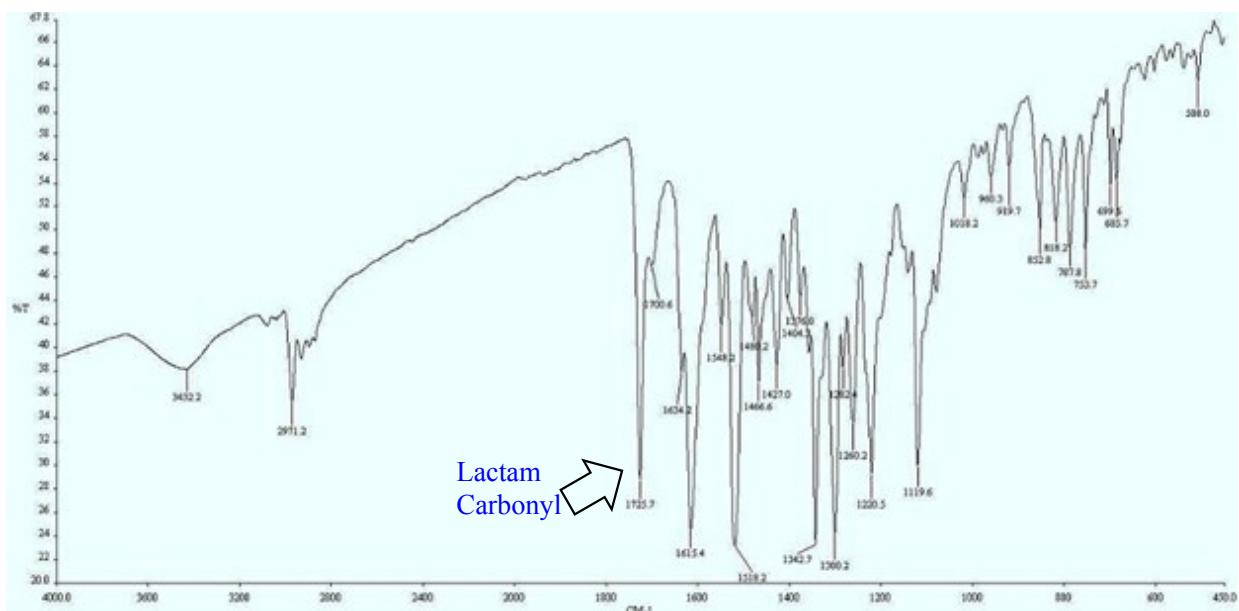


Figure S10. IR Spectrum of chemosensor (L)

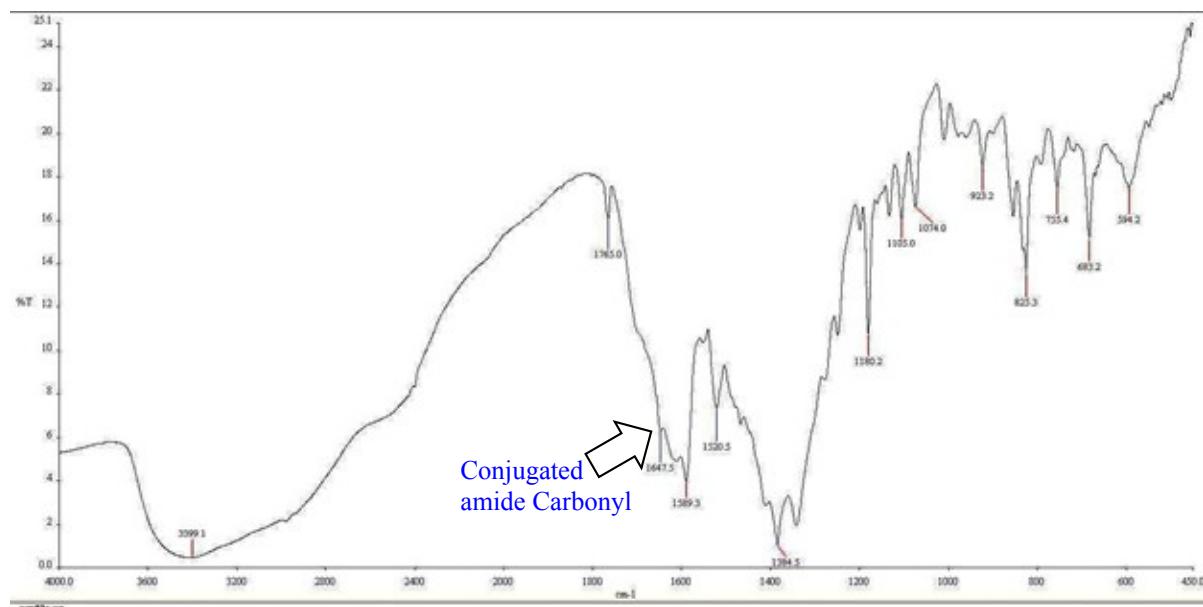


Figure S11. IR Spectrum of L-Al³⁺ complex

L + Al(III)

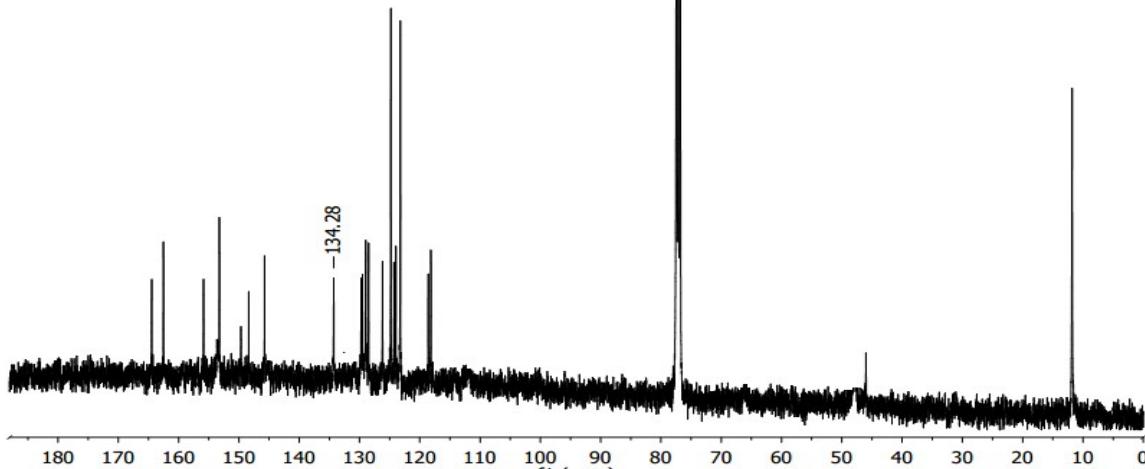


Figure S12: ^{13}C NMR of ligand + Al^{3+}

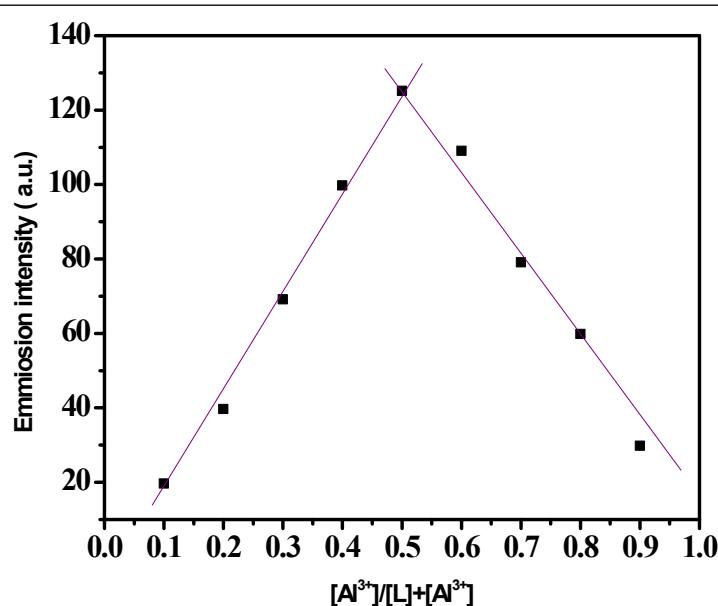


Figure S13. Job's plot of Fluorescence intensity at 554 nm of L and Al^{3+} with a total concentration of 20 μM cations in HEPES buffer [50 μM , $\text{C}_2\text{H}_5\text{OH-H}_2\text{O}$ (4:1, v/v, pH=7.2)] at 25 °C

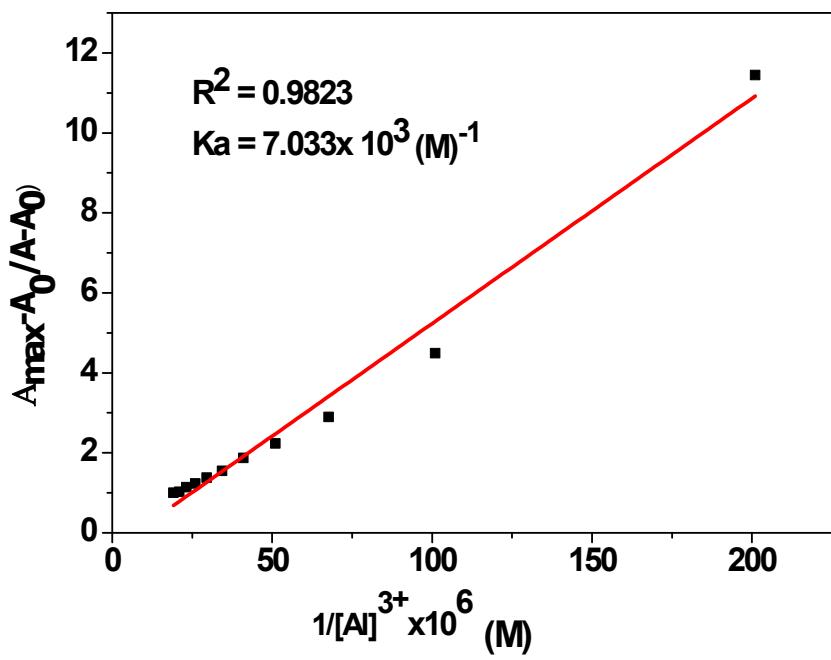


Figure S14. Benesi-Hildebrand plot of L (40 μM) for Al^{3+} determined by absorbance method in HEPES buffer [50 μM , $\text{C}_2\text{H}_5\text{OH}-\text{H}_2\text{O}$ (4:1, v/v, pH= 7.2)] at 25 °C

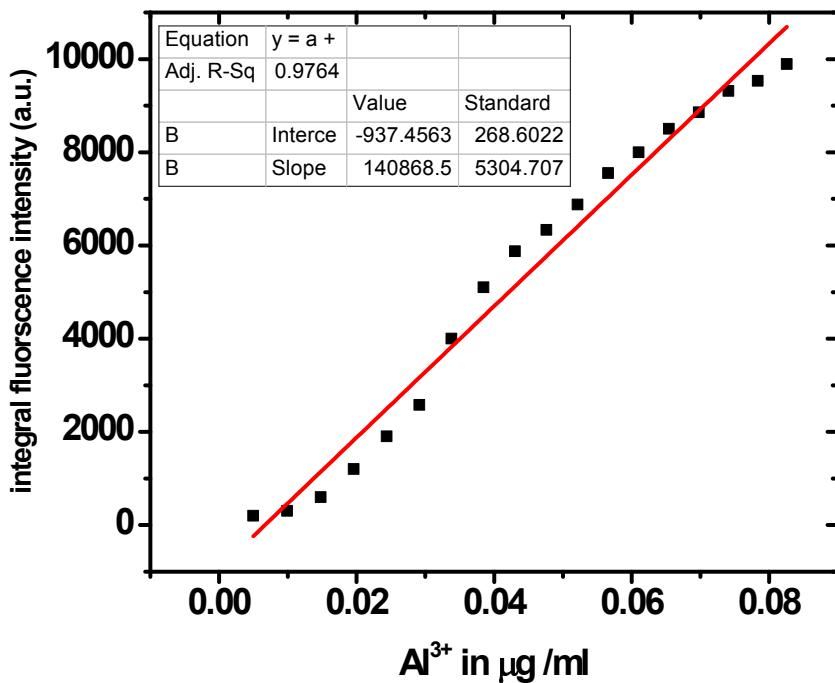


Figure S15. The limit of detection (LOD) and limit of quantification (LOQ) were calculated using $3\sigma/S$ and $10\sigma/S$ methods, respectively. σ = the standard deviation of y-intercept of regression line, S = the slope of the calibration curve

Table S1 The comparison of this probe with some other fluorescent probes for Al³⁺

Probe	λ_{em} (nm)	LOD (μM)	Total metal ions	Stokes shift (nm)	Solvent (V/V)	Detection method
Ref. [1]	582	3.98	19	20	CH ₃ CN/H ₂ O (95:5)	CHEF , Fluorescence quenching
Ref. [2]	582	0.196	21	22	EtOH-H ₂ O (1:1)	---
Ref. [3]	550	0.183	17	16	CH ₃ CN/H ₂ O (9:1)	CHEF,PET FRET
Ref. [4]	556	3.26	17	17	H ₂ O-EtOH (4:1)	CHEF
Ref. [5]	560	38.9	12	40	EtOH	FRET
Ref. [6]	558	4.17	16	28	DMF	CHEF
Ref. [7]	555	0.34	12	26	MeOH-H ₂ O (1:1)	CHEF
Ref. [8]	490	0.42	18	25	CH ₃ CN-H ₂ O(50:50)	ICT,CHEF
Ref. [9]	513	2.40	13	139	DMSO	ESIPT
Ref. [10]	503	1.04	17	57	EtOH-H ₂ O (9:1)	--
Ref. [11]	538	0.29	13	58	DMSO	ICT
Ref. [12]	450	1.54	20	45	CH ₃ CN-HEPES buffer	ICT
Our work	582	0.11	17	28	EtOH-H₂O (4:1)	CHEF, PET

References

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