

Electronic Supplementary Information

Rhodamine-based molecular clips for highly selective recognition of Al^{3+} ions: synthesis, crystal structure and spectroscopic properties

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Fig. S1 ^1H NMR ($\text{DMSO}-d_6$, 500 MHz) spectrum of chemosensor **L**.

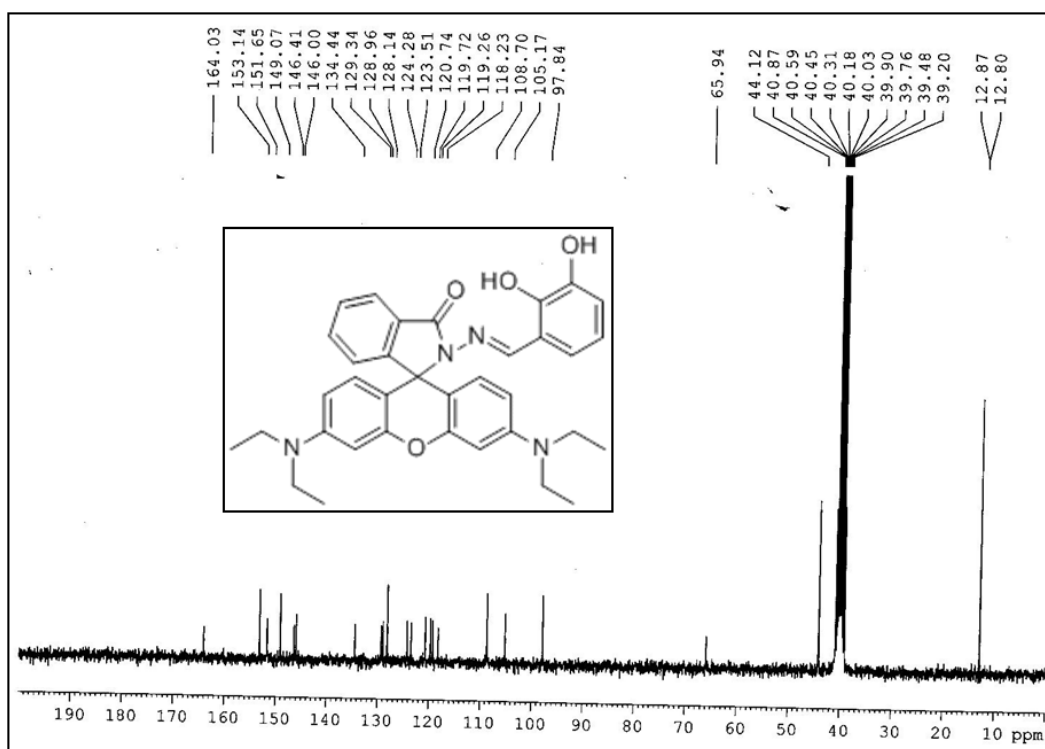


Fig. S2 ¹³C NMR (DMSO-*d*₆, 300 MHz) spectrum of chemosensor **L**.

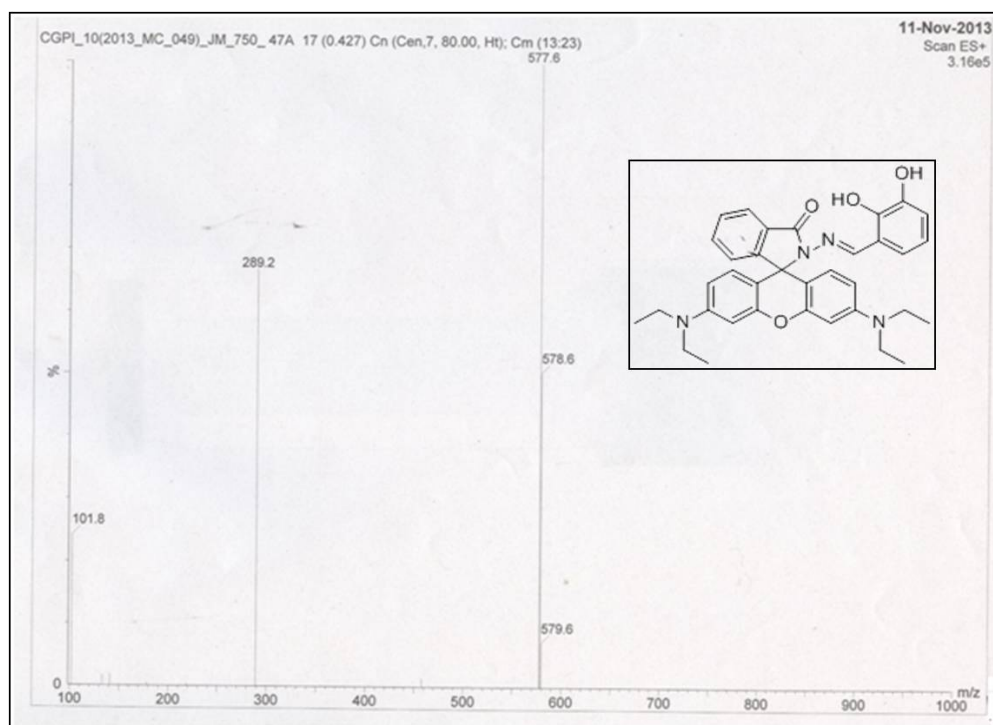


Fig. S3 ESI MS spectrum of chemosensor **L**.

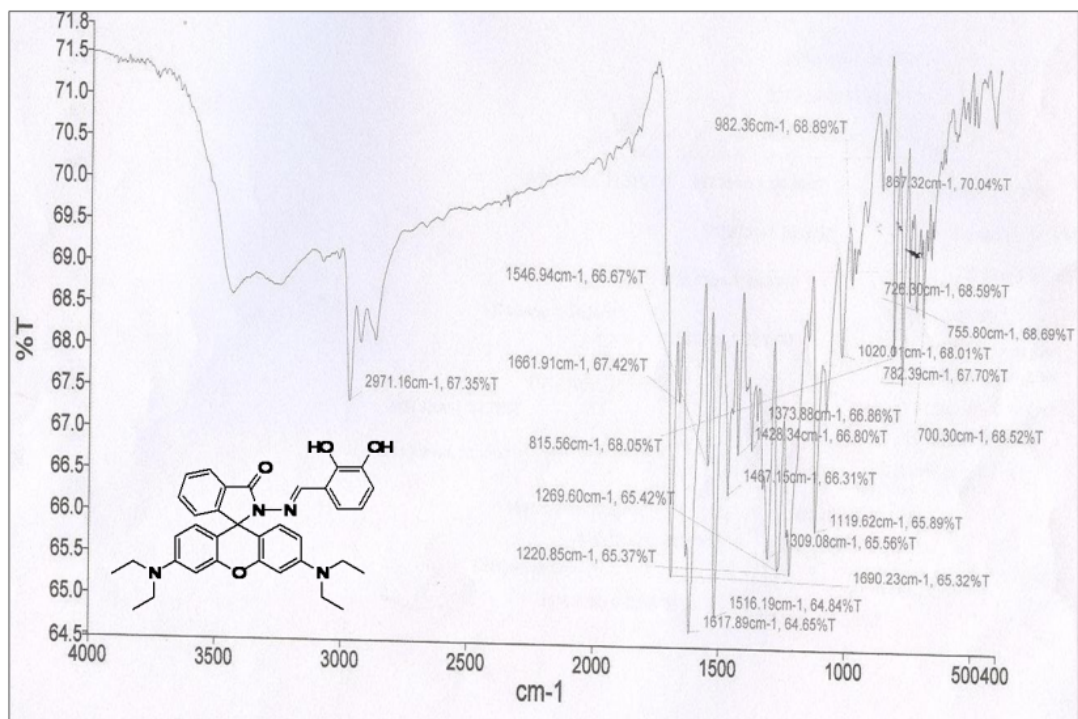


Fig. S4 FT- IR spectrum of chemosensor **L**.

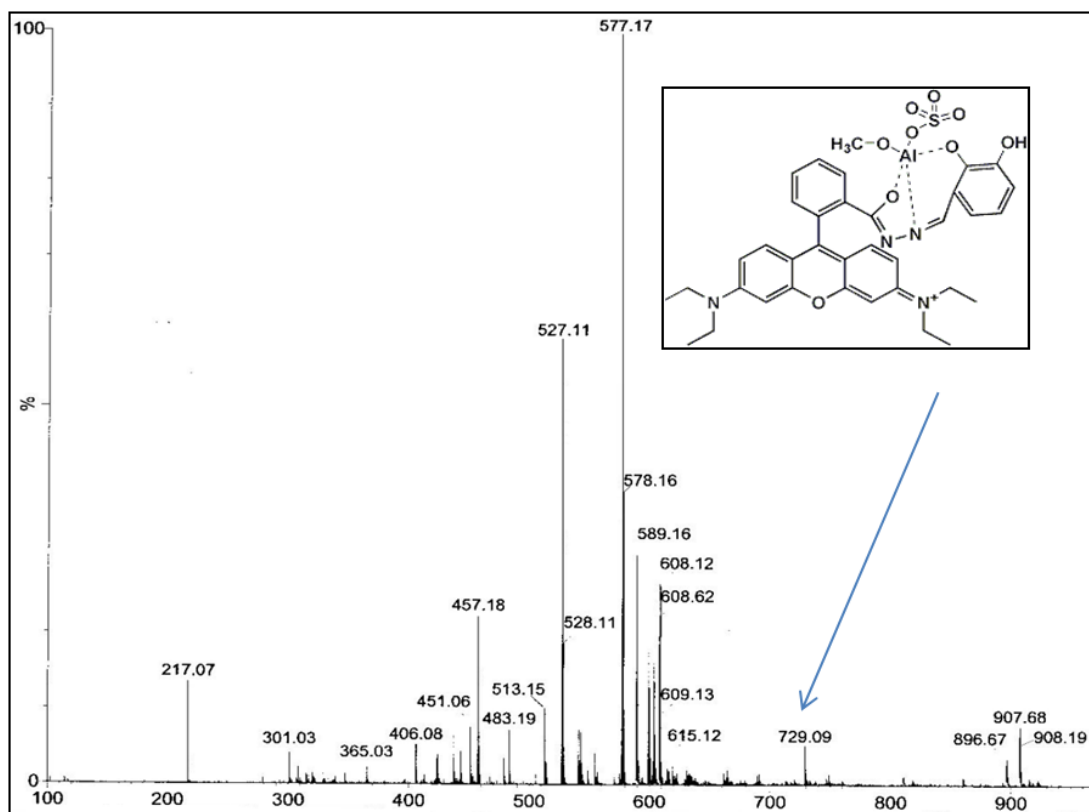


Fig. S5 TOF MS ES⁺ spectra of L-Al³⁺ complex. The peak at m/z = 729.09 was assigned to the derivative of L.Al(SO₄)(OMe).

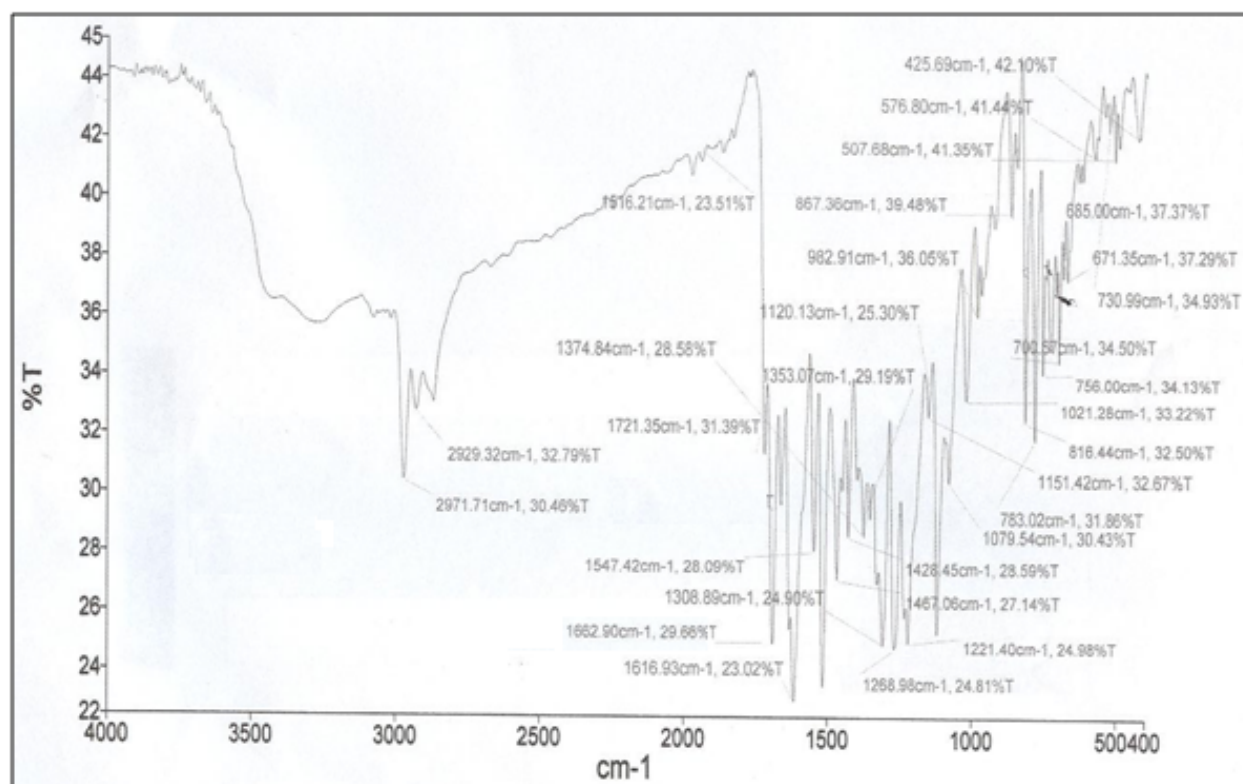


Fig. S6 FT IR (ν in cm^{-1} , KBr) Spectrum of **L** + Al^{3+} .

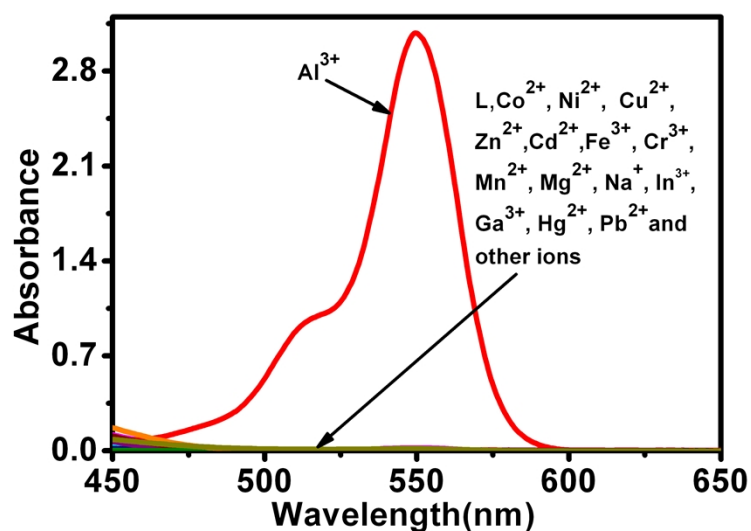


Fig. S7 UV-visible spectra of chemosensor **L** (10 μ M) with addition of different metal ions eg, Al^{3+} , Cr^{3+} , In^{3+} , Ga^{3+} , Na^+ , Mg^{2+} , Pb^{2+} , Hg^{2+} , Fe^{3+} , Cu^{2+} , Ni^{2+} , Co^{2+} , Mn^{2+} , Cd^{2+} and Zn^{2+} (100 μ M) in $\text{CH}_3\text{CN}/\text{H}_2\text{O}$ (8:2, v/v) using HEPES buffer, pH = 7.2 at 25 $^\circ\text{C}$.

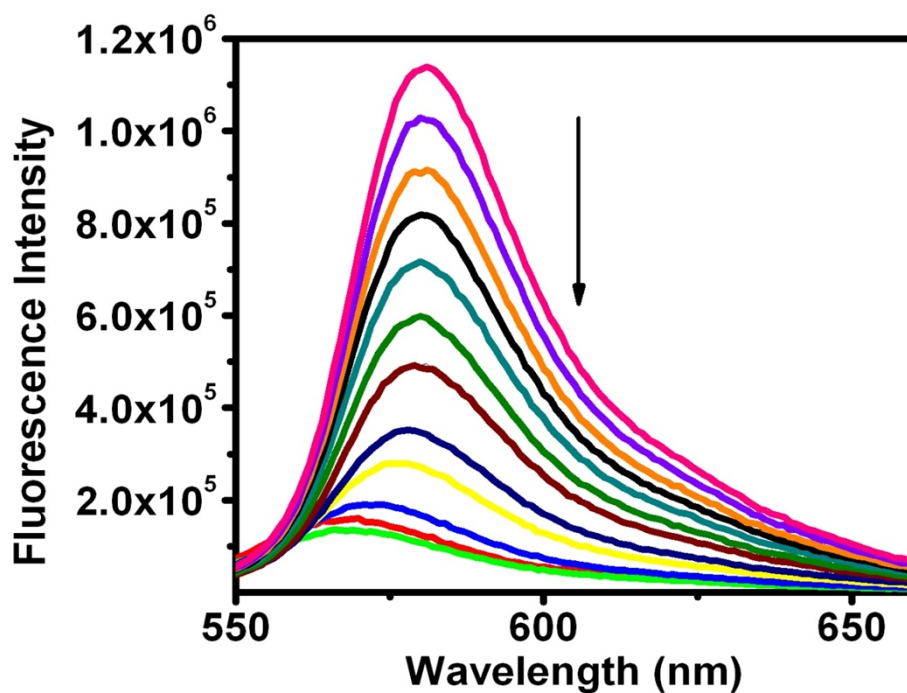


Fig. S8 Fluorescence titration of **L**-Al³⁺ complex with EDTA in CH₃CN/H₂O (8:2 v/v) using HEPES buffer, pH = 7.2 at 25^oC (λ_{ex} = 554 nm). Intensity gradually decreases upon gradual addition of EDTA (0-100 μ M) solution.

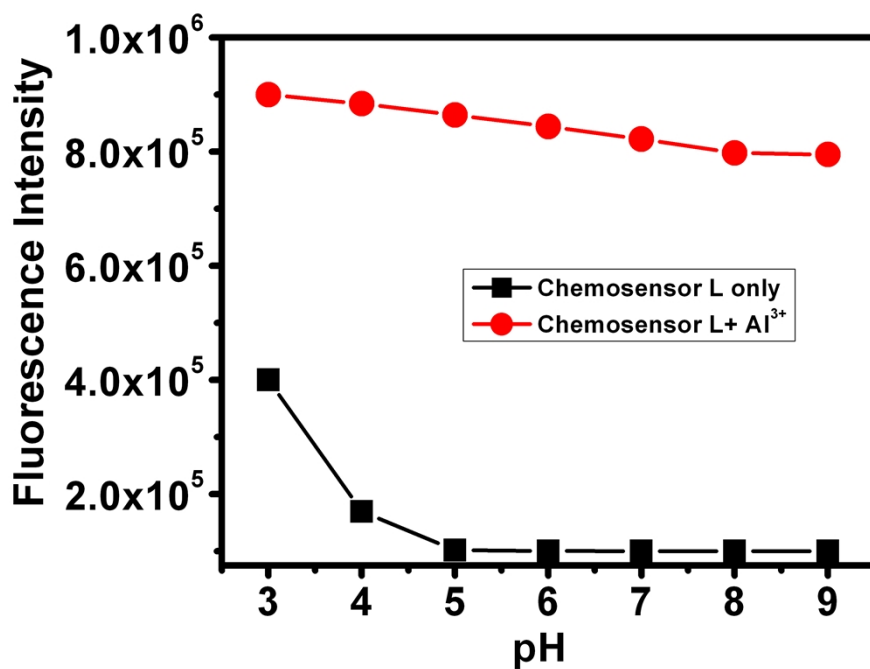


Fig. S9 Effects of pH on the fluorescence intensity of **L** in the absence and presence of Al³⁺ ion. **L** (10 μ M) in CH₃CN/H₂O (8:2, v/v) using HEPES buffer, pH = 7.2 at 25 ^oC. λ_{ex} / λ_{em} = 554 nm/ 581 nm.

Fluorescence lifetimes of free chemosensor L and Al³⁺ complex in aqueous-acetonitrile solvent

Table-S1

CH ₃ CN/H ₂ O	τ_1^a (ns)	τ_2^a (ns)	τ_3^a (ns)	α_1	α_2	α_3	χ^2	τ_{av} (ns)	Φ
L	1.20	4.38	0.49	0.155	0.045	0.80	1.08	2.66	0.02
L-Al³⁺	3.05	1.63	0.04	0.204	0.03	0.76	1.30	2.07	0.30

a: error in measurement $\pm 3\%$.