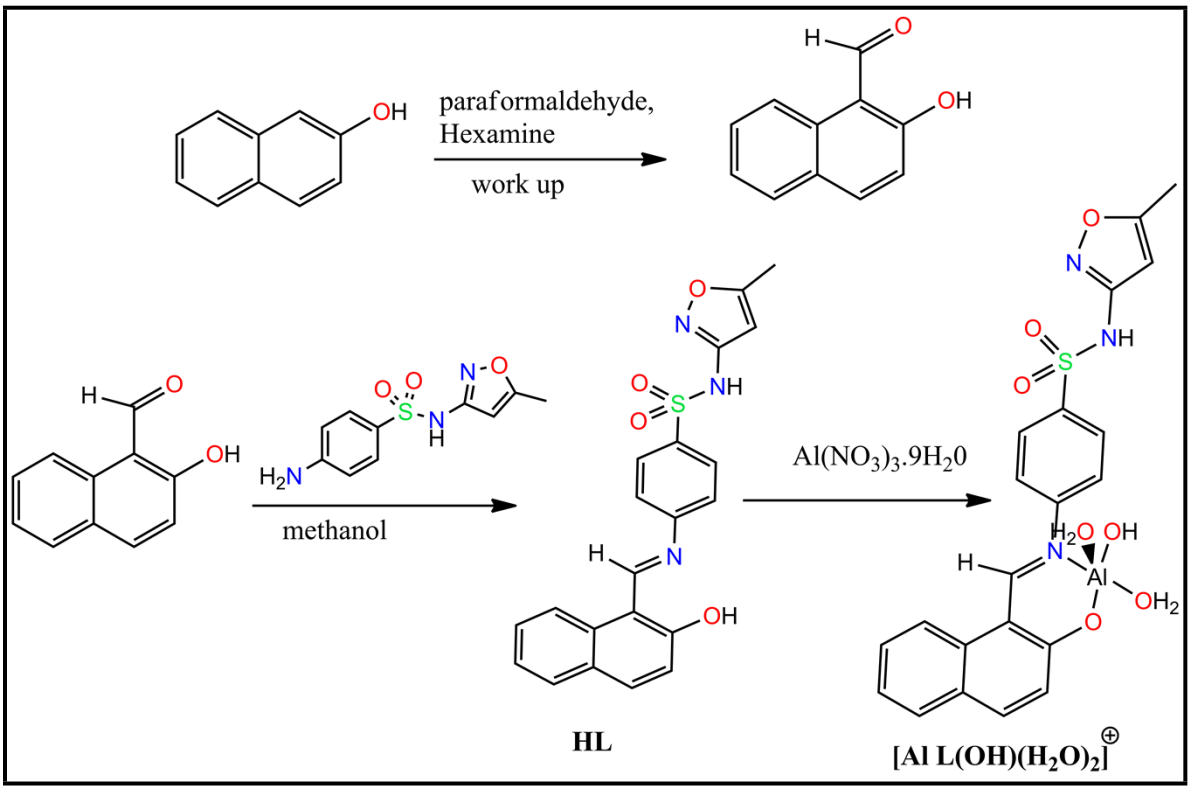
Electronic Supplementary Material (ESI) for RSC Advances.

Fluorescence sensing and intracellular imaging of Al^{3+} ions by using naphthalene based sulfonamide chemosensor : structure, computation and biological studies

Sudipa Mondal[a], Anup Kumar Bhanja[a], Durba Ojha[b], Tapan Kumar Mondal[a] , Debprasad Chattopadhyay[b] and Chittaranjan Sinha[a*]



Scheme S1: Syenthesis of **HL** and its Al complex**.**

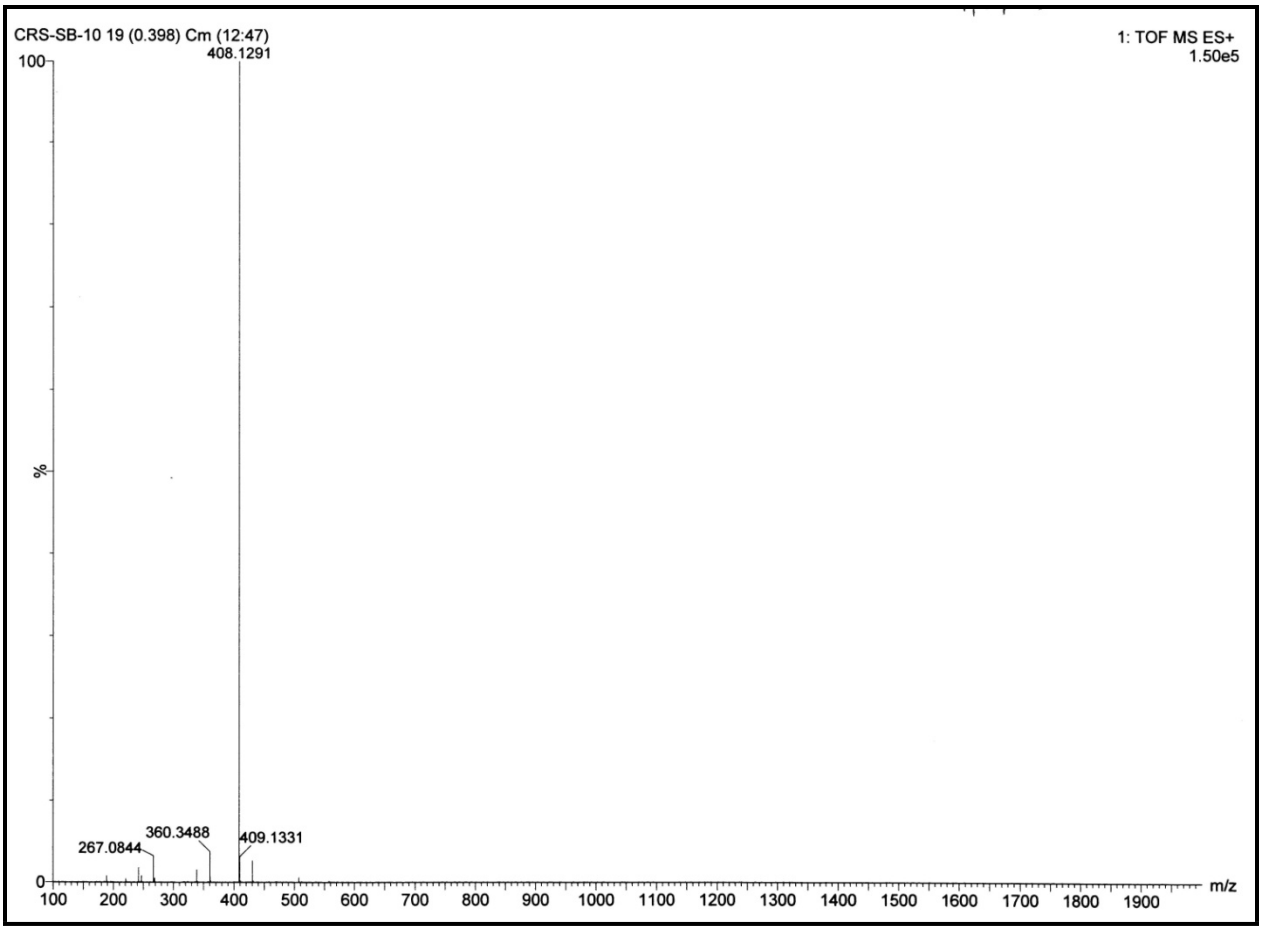


Fig. S1. MS spectrum of **HL**.

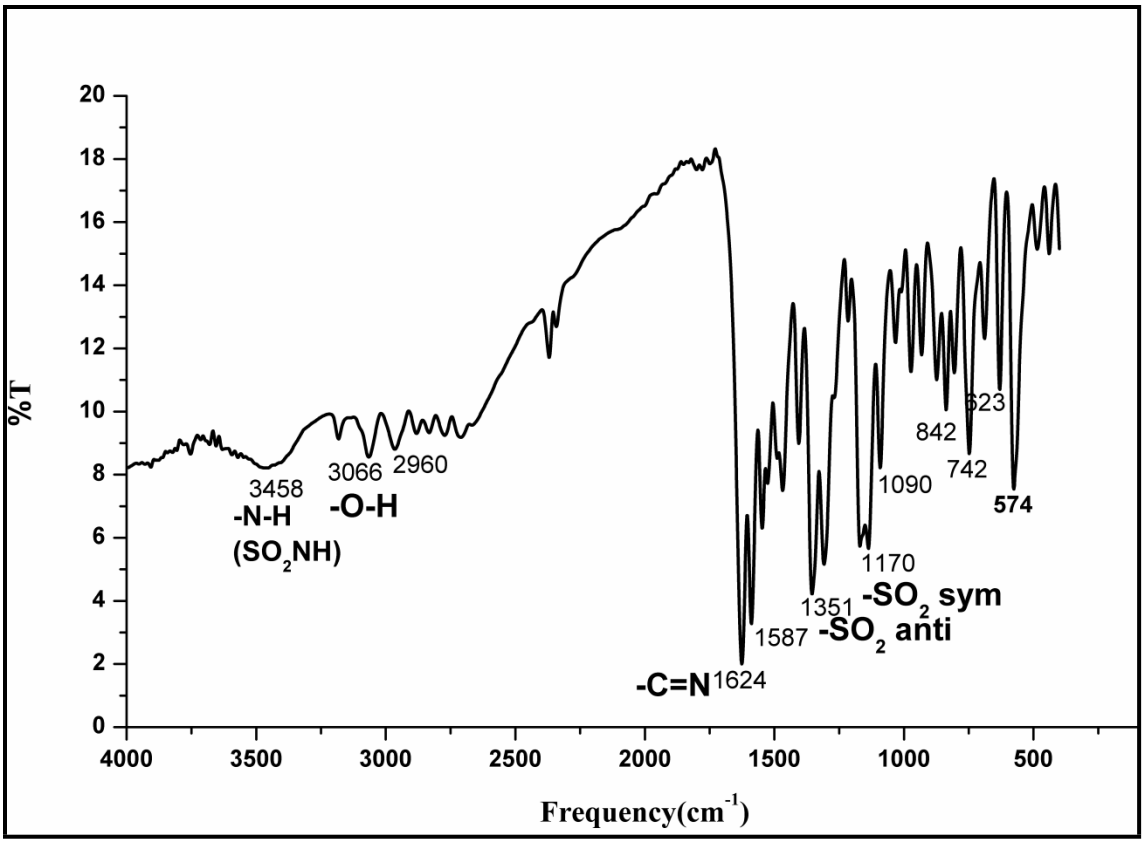


Fig. S2. IR spectrum of HL

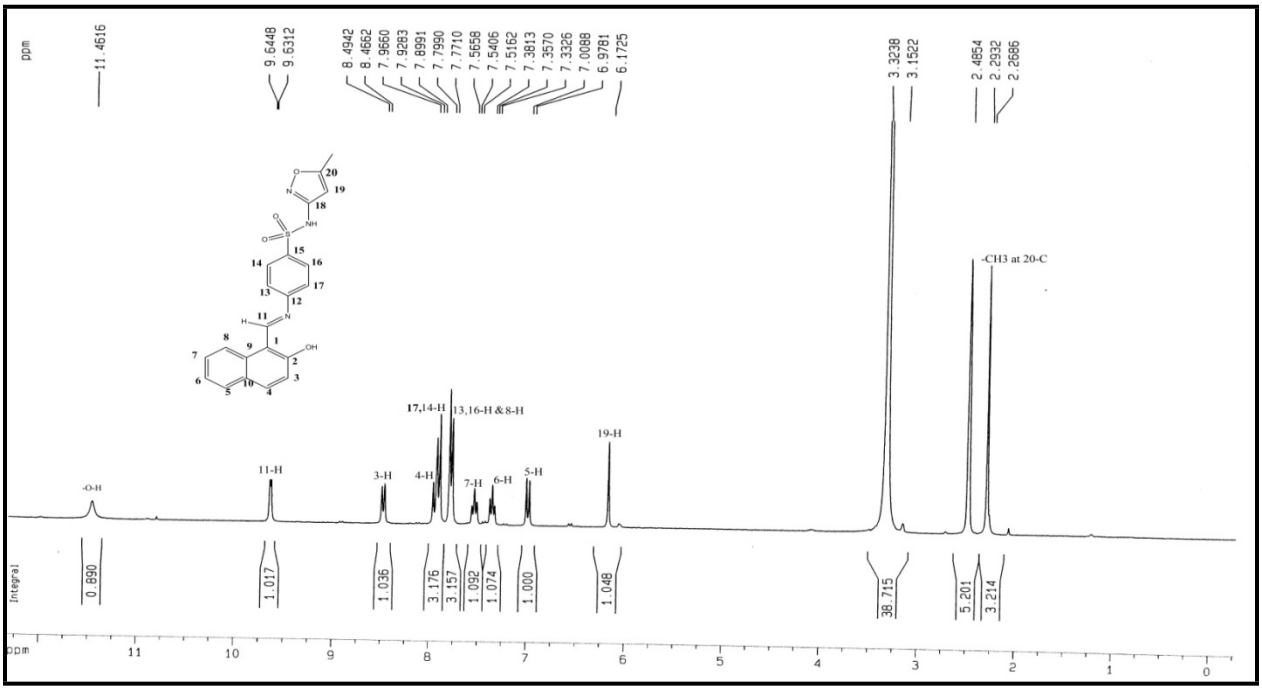


Fig. S3. ^{1}H NMR spectrum of HL in DMSO-d_6.

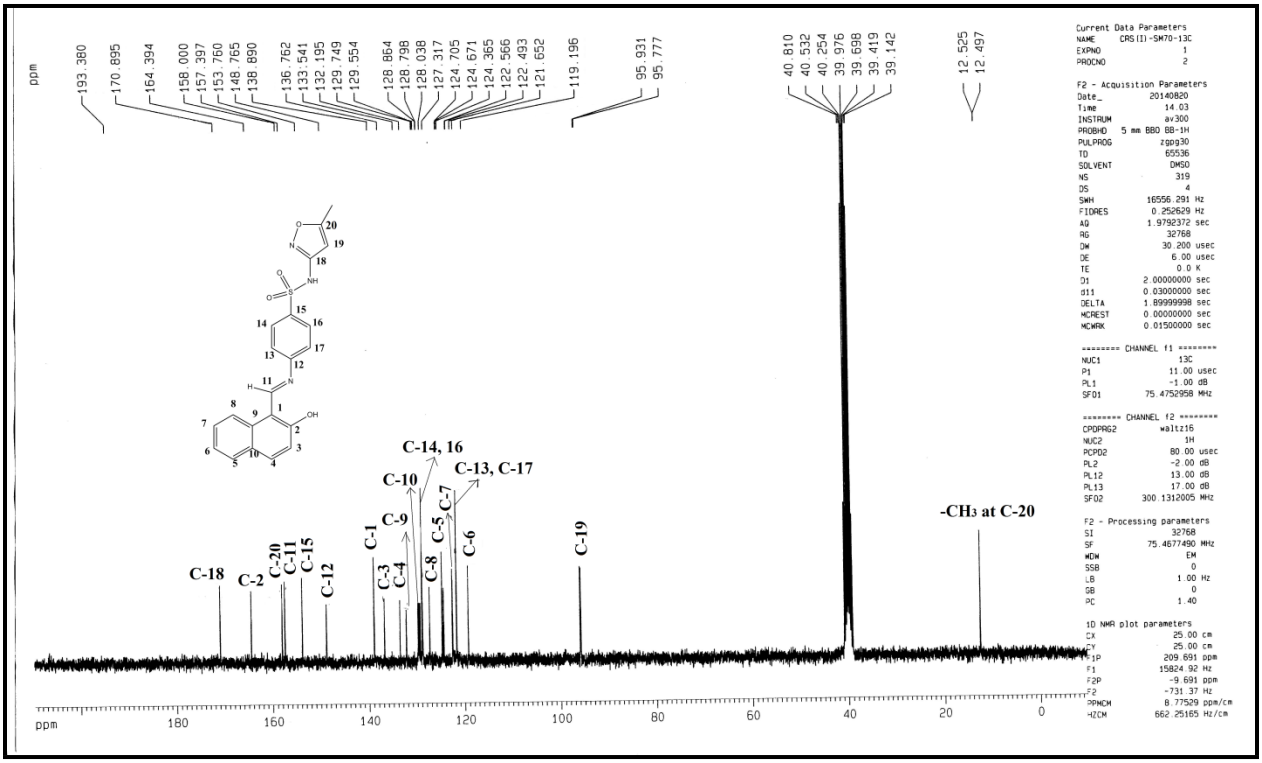


Fig. S4. ^{13}C NMR spectrum of HL in DMSO-d_6.

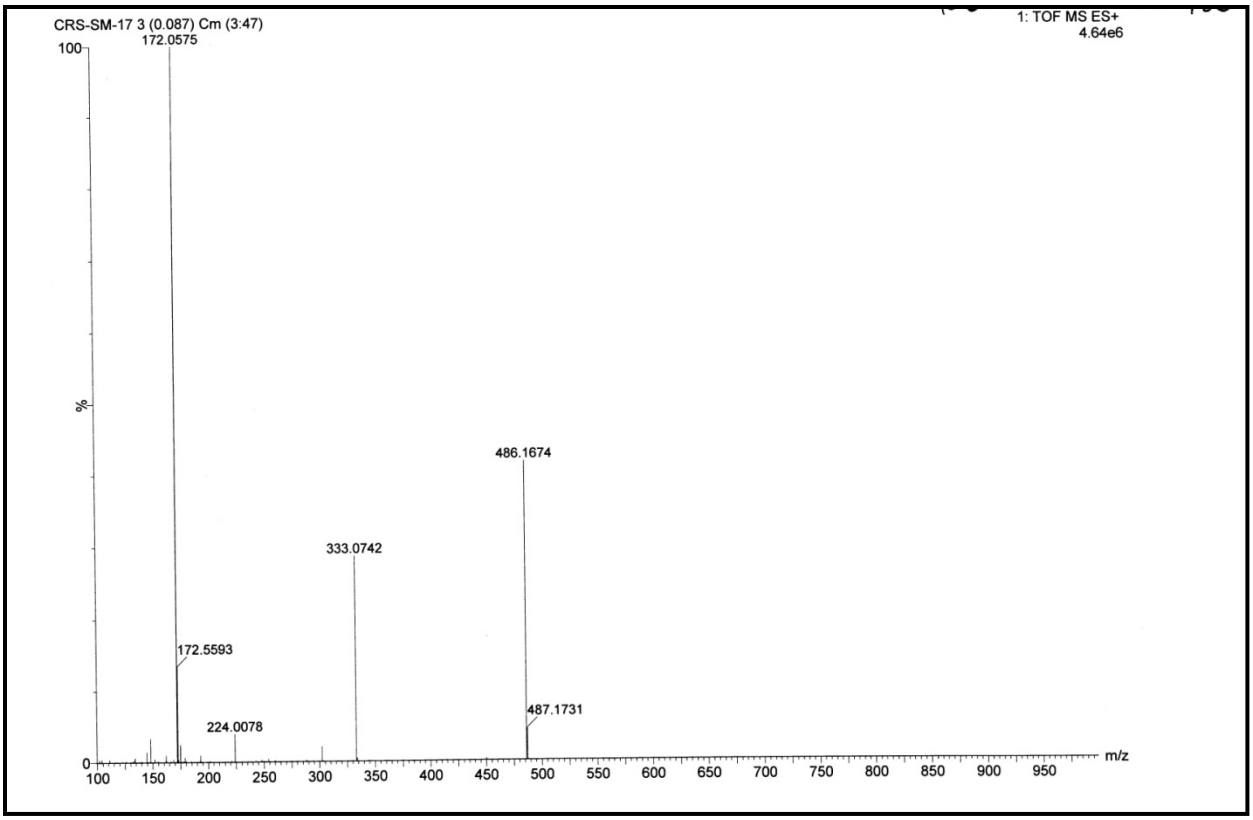


Fig. S5. MS spectrum of $[L\text{-}Al(OH)(H_2O)_2]^+$

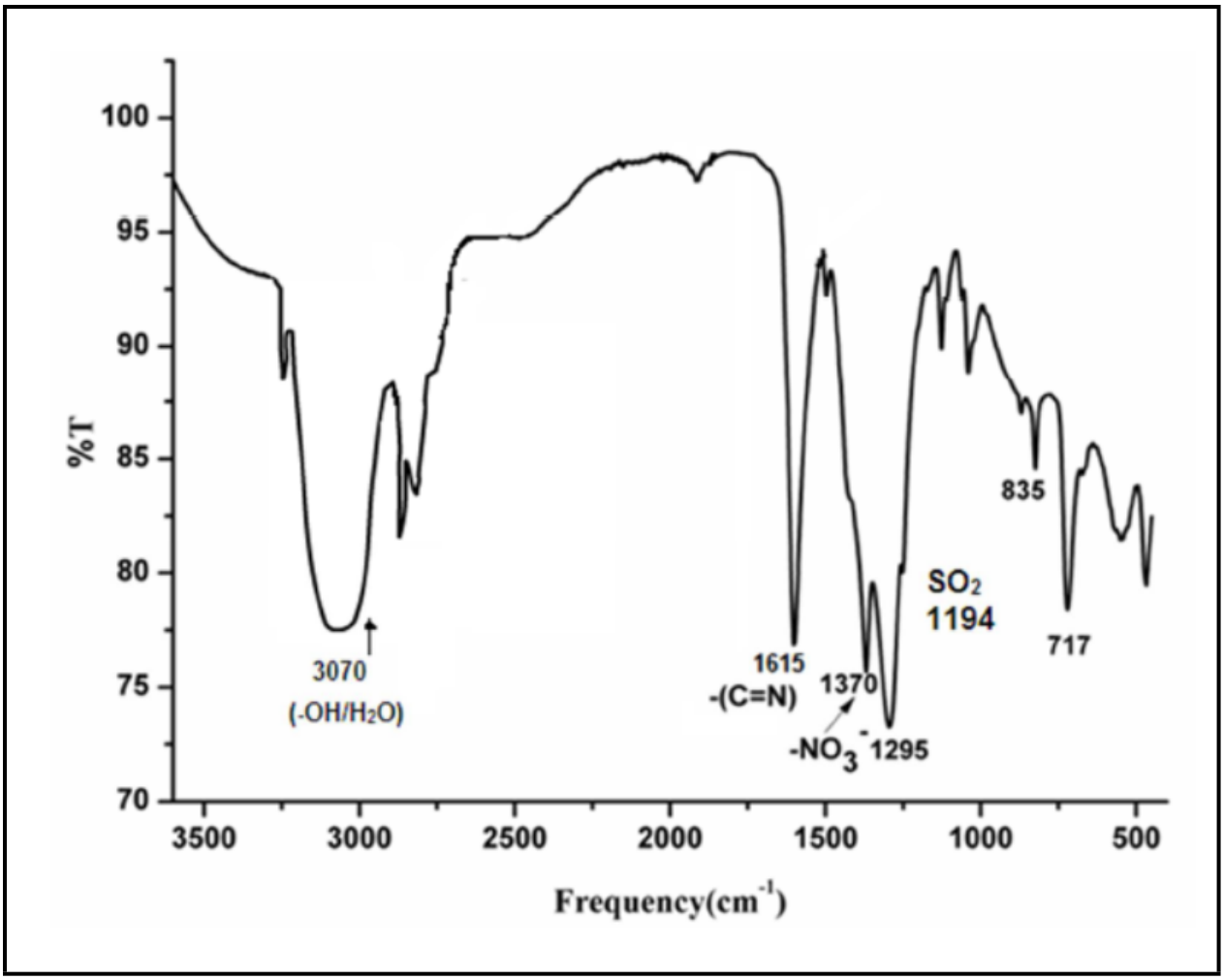


Fig. S6. IR spectrum of Al^{3+} complex of HL

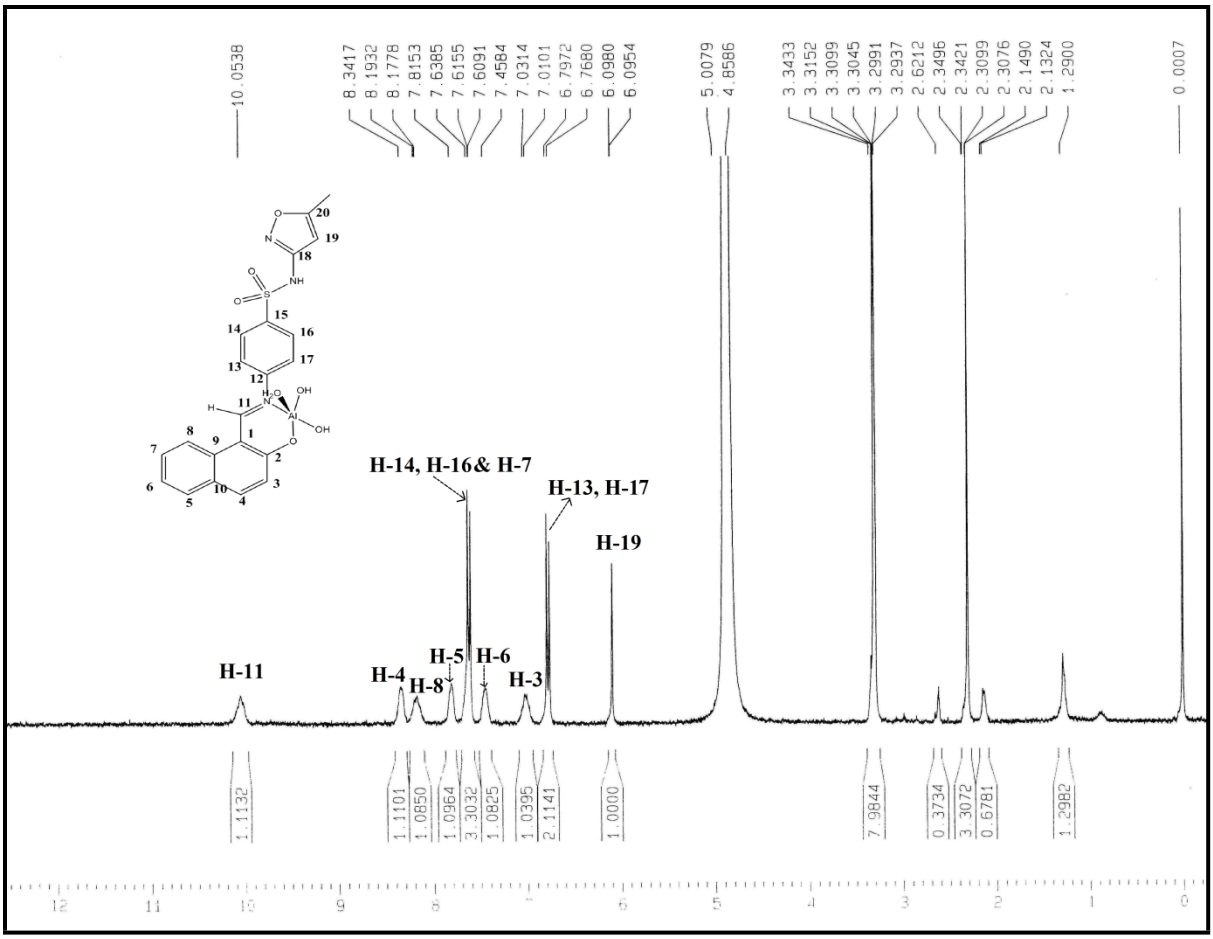


Fig. S7. ^{1}H NMR spectrum of $[L\text{-}Al(OH)(H_2O)_2]^+$ in CD_3OD**.**

Fig. S8. Bright yellow color of HL disappears in presence of Al^{3+} but persists in presence all other metals.

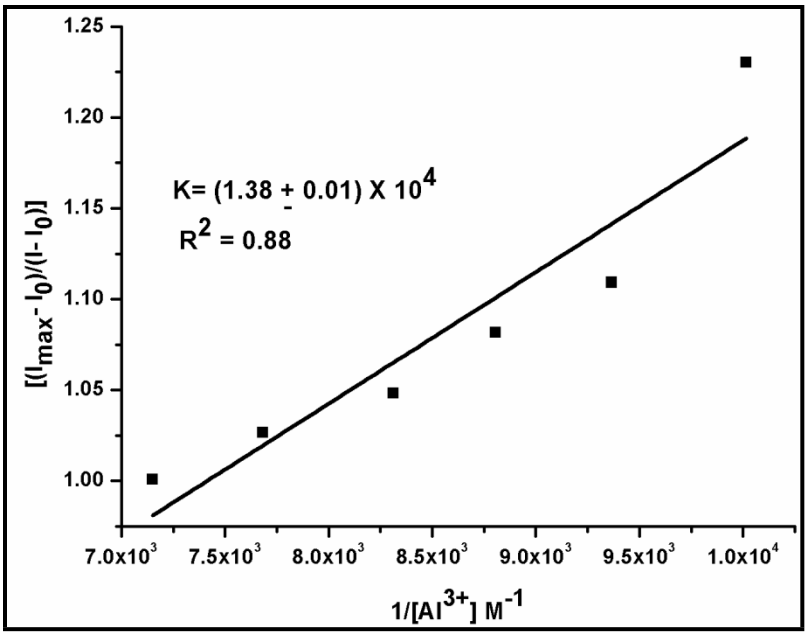


Fig. S9. Benesi-Hildebrand plot of HL vs Al^{3+} titration by UV-Vis absorption spectroscopy.

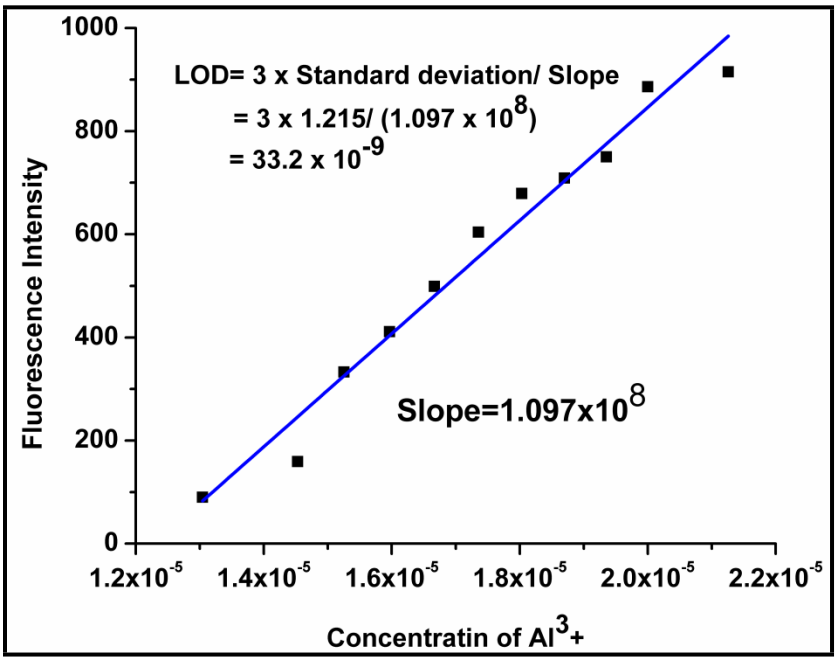


Fig. S10. Determination of LOD of Al^{3+} by HL at pH 7.4 (HEPES buffer) using 3σ method.

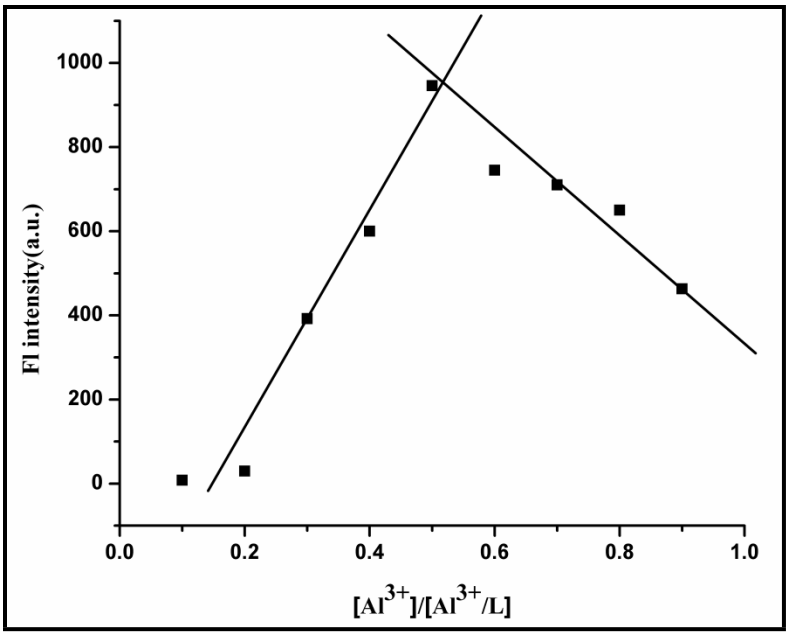


Fig. S11. Job's plot for the reaction between HL and Al^{3+} in methanol-water (1:5, v/v)

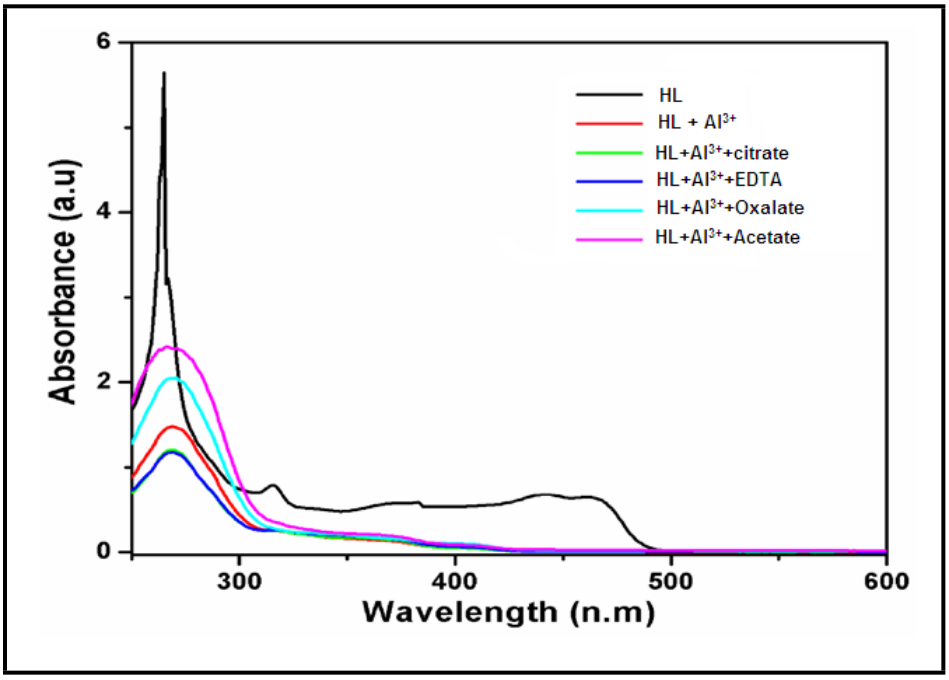


Fig.S12: Effect of chelating agents such as Na_2EDTA, oxalate, citrate, acetate on **L-Al^{2+}** stability by absorption technique

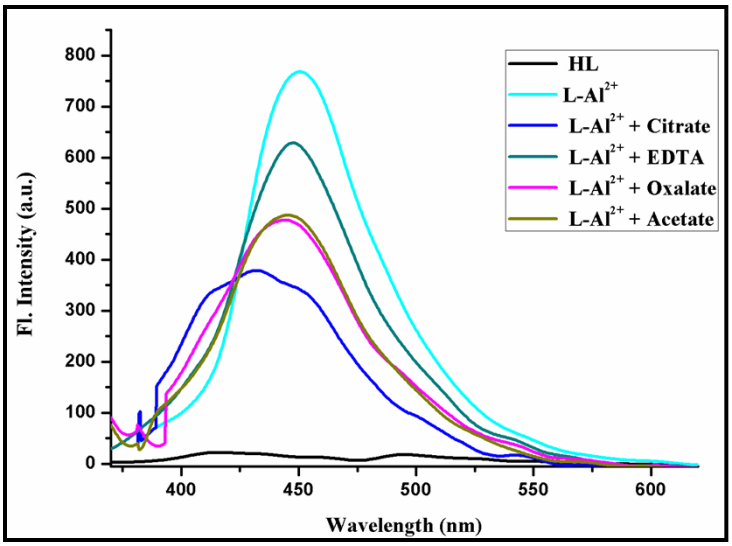


Fig.S13: Effect of chelating agents such as Na_2EDTA, oxalate, citrate, acetate on **L-Al^{2+}** stability by fluorescence technique

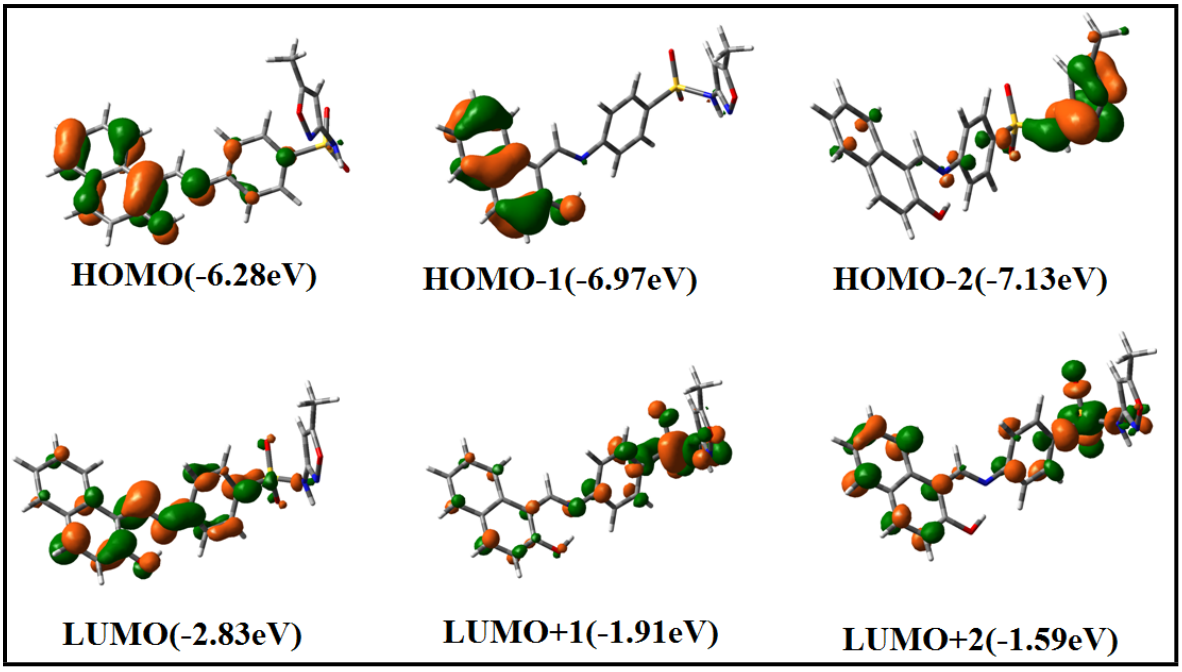


Fig. S14. Energy of some selected frontier molecular orbitals of HL.

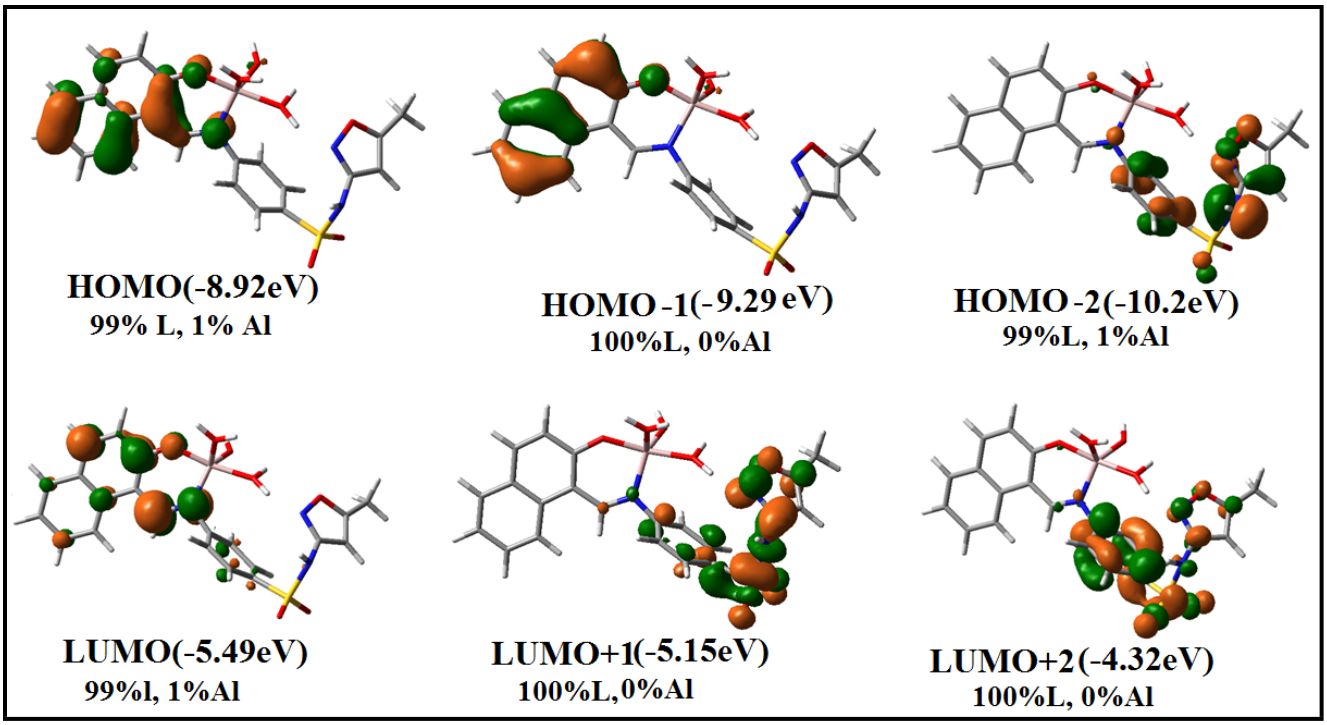


Fig. S1. Energy of some selected frontier molecular orbitals of $[L\text{-}Al(OH)(H_2O)_2]^+$

Table S1. Hydrogen Bonds (Å, °) for HL

D–H----A	D–H	H----A	D----A	∠D–H---A	Su=ymmetry
N2 -- H1N2 .. O4	0.79(4)	2.03(4)	2.791(5)	164(3)	-x,-y,-z
O4 -- H1O4 .. N3	0.90(5)	1.71(6)	2.538(3)	152(8)	
C3 -- H3 .. O3	0.9300	2.5200	3.012(5)	113.00	
C10 -- H10 .. O3	0.9300	2.5500	2.925(4)	104.00	
C10 -- H10 .. O3	0.9300	2.5100	3.372(5)	155.00	-x,-y,1-z

Table S2. Life time data of L and L-Al^{2+} complex

Compounds	τ1	τ2	τav	K_r	K_{nr}
L	$2.35x10^{-9}$	$5.07x10^{-11}$	$5.15x10^{-11}$	$11.06X10^{16}$	$19.28x10^{18}$
$L+Al^{3+}$	$8.68x10^{-10}$	$2.41x10^{-9}$	$9.0x10^{-10}$	$15.2x10^{16}$	$95.76x10^{16}$

Table S3. Selected geometrical parameter (calculated) of L-Al^{2+} in the ground state

Bond length(Å)			
Al(1)-N(3)	1.946	Al(1)-O(6)	1.746
Al(1)-O(4)	1.790	Al(1)-O(7)	1.984
Al(1)-O(5)	2.046	N(3)-C(11)	1.333
Bond angle(º)			
N(3)-Al(1)-O(4)	92.02	O(5)-Al(1)-O(6)	80.74
N(3)-Al(1)-O(5)	97.48	O(5)-Al(1)-O(4)	160.98
N(3)-Al(1)-O(7)	116.92	O(6)-Al(1)-O(7)	116.28
N(3)-Al(1)-O(6)	126.10	O(6)-Al(1)-O(4)	107.09
O(5)-Al(1)-O(7)	78.32	O(4)-Al(1)-O(7)	82.68

Table S4. Change in bond length (calculated) in (Al-L^{2+}) compared to free ligand (HL)

Bond length(Å)		
	Free ligand(L)	Complex (Al^{3+}-L)
C(8)-N(3)	1.408	1.437
C(11)-N(3)	1.316	1.333
C(11)-C(12)	1.435	1.409
C(12)-C(13)	1.420	1.427
C(13)-C(14)	1.419	1.420
C(13)-O(4)	1.352	1.370

Table S5. Calculated transitions and their assignment for ligand (HL) and Al^{3+}-complex

Ligand /Complex	Experimental [λ_{exp}(nm)]	Theoretical [λ_{theo} (nm)]	Electronic Transition	Character
Ligand	442	410	$S_0 \rightarrow S_1$[HOMO→LUMO(99%)]	ILCT
Ligand	370	343	$S_0 \rightarrow S_3$[HOMO-1→ LUMO(93%)]	ILCT
Ligand	314	277	$S_0 \rightarrow S_{11}$[HOMO-5→LUMO(35%), HOMO-3→LUMO+1(33%)]	ILCT
Ligand	259	242	$S_0 \rightarrow S_{20}$ [HOMO-7→LUMO+1(35%), HOMO-7→LUMO+1(24%), HOMO-2→LUMO+2(20%)]	ILCT
Complex	370	380	$S_0 \rightarrow S_1$[HOMO→LUMO(98%)]	ILCT
Complex	315	285	$S_0 \rightarrow S_4$[HOMO-2→LUMO(85%)]	ILCT
Complex	267	250	$S_0 \rightarrow S_{13}$[HOMO-2→LUMO+1(48%), HOMO-1→LUMO+2(31%)]	ILCT

Table S6. ADMET (Absorption, Distribution, Metabolism, Excretion, Toxicity) prediction data

Compd	Molecular Weight	ADMET Solubility (aqueous)	ADMET solubility level	ADMET absorption level≠	ADMET Log P	Molecular polar surface area	No of H-bond acceptor	No. of H- bond donor	Lipniski's filter	Drug likeness inference	Ames Prediction
HL	407.4	-5.166	2	0 (good)	3.719	0.295	5	2	yes	yes	non-mutagen

Table S7. Antimicrobial results (MIC) by agar dilution method

Compounds	MIC in µg/ml						
	Gram positive		Gram negative				
HL	*S.Aureus*ATCC21737	*Enterococcus facelis*ATCC 29212	*E.Coli*	*S.Typhi*MTCC734	*Sh dysenteriae* 5168	*Sh. flexneri*7130	*K. pneumonia* ATCC 714
	64	nd†	nd†	32	64	nd	64

†nd: not detected

Table S8. Docking score of HL with DHPS protein (downloaded from PDB)

Compound	CDOCKER energy	CDOCKER interaction energy	Protein energy (Kcal/mol)	Complex energy (Kcal/mol)	Binding energy (Kcal/mol)
DHPS@HL	-13.94	-40.6	-22,831	-22859	-53.7