Supplementary Information

CONTENTS:

Table S1: Comparison of a few aspects of some recently published Al^{3+} sensors.

Sl. No.	**Probe**	Method for Al^{3+} detection	Interfering Ions	Excitation(nm)/ Emission(nm)	Limit of detection (LOD)	Cell imaging	Refs.
1.	2-Hydroxybenzene-1-carbohydrazide-1-(benzo[1,3]-oxazino[2,3- a]phthalazin-4-one)	CHEF	None	330/406	8.8×10^{-9} M	Yes	**14a**
2.	2-((naphthalen-6-yl)methylthio)ethanol	CHEF	None	350/449	1.0×10^{-8} M	Yes	**14e**
3.	(Coumarin-Triazolyl-Bipyridyl) Click Fluoroionophore	CHEF	None	320/443	1.0×10^{-7} M	No	**14i**
4.	2-hydroxy-((2-phenyl-2H-1,2,3-triazol-4-yl)methylene)benzohydrazide	CHEF	None	358/442	1.2×10^{-8} M	No	**14j**
5.	(1-((E)-(2-(2-(phenylthio)ethylthio)phenylimino)methyl)naphthalen-2-ol (L_2)	CHEF	None	360/455	5.0×10^{-8} M	Yes	**14k**
6.	Rhodamine-Based Fluorescent Probe	CHEF/FRET	None	460/585	5.0×10^{-9} M	Yes	**14l**
7.	Rhodamine Schiff base (**L**)	CHEF	None	525/590	60.37×10^{-9} M	Yes	**14m**
8.	(Z)-N-benzylidenenaphthalen-1-amine	CHEF	None	310/430	5.0×10^{-5} M	Yes	**14n**
9.	(E)-N'-((E)-3-(4-(dimethylamino)phenyl)allylidene)picolinohydrazide (**L_1**)	CHEF	Cd^{2+}	410/505	8.7×10^{-6} M	Yes	**14o**
10.	spirobenzopyran-quinoline (SBPQ)	CHEF	Fe^{3+},Cr^{3+}	460/675	3.24×10^{-8} M	Yes	**14p**
11.	(E)-6,6'-((1E,1'E)-(propane-1,3-diylbis(azanylylidene))bis(methanylylidene))bis(2-methoxy-4-((E)-phenyldiazenyl)phenol)	CHEF	None	388/478	**6.93×10^{-9} M**	NO	This work

Table S. Data of lifetime of $\mathbf{H_2L}$ and $\mathbf{H_2L}$+ Al^{3+}

	τ_f (ns) (average)	χ^2	Φ_f
$\mathbf{H_2L}$	1.324	1.072185	0.00939
$\mathbf{H_2L}$+ Al^{3+}	2.058	1.128573	0.2133

Table S3.Energy (eV) of selected M.O.s of **H_2L** and $[Al(L)]^+$.

M.O.s	**H_2L**	$[Al(L)]^+$
	Energy(eV)	
LUMO+5	0.05	-0.78
LUMO+4	0.01	-0.78
LUMO+3	-1.12	-1.04
LUMO+2	-1.36	-1.86
LUMO+1	-1.92	-2.41
LUMO	-1.97	-2.62
HOMO	-5.35	-6.59
HOMO-1	-5.46	-6.62

HOMO-2	-5.93	-7
HOMO-3	-5.98	-7.21
HOMO-4	-6.24	-7.33
HOMO-5	-6.35	-7.34

Table S4. Mulliken atomic charge distribution of **[Al(L)]$^{+}$** complex**.**

Complex 1
Mulliken atomic charges:
1 O -0.404536
2 O -0.435455
3 O -0.478657
4 O -0.483326
5 N -0.229747
6 N -0.251442
7 N -0.329038
8 N -0.323436
9 N -0.267103
10 N -0.272469
11 C 0.326391
12 C -0.400138
13 C -0.095726
14 H 0.154695
15 C 0.216592
16 C -0.164443
17 H 0.156349
18 C 0.354697
19 C -0.224421
20 H 0.181811
21 H 0.202674
22 H 0.180897
23 C 0.233869
24 C -0.109529
25 H 0.114254
26 C -0.097171
27 H 0.128830
28 C -0.092996
29 H 0.126952

30	C	-0.109485
31	H	0.125098
32	C	-0.108678
33	H	0.094019
34	C	-0.072738
35	H	0.203269
36	C	-0.167410
37	H	0.203223
38	H	0.205489
39	C	-0.337972
40	H	0.203710
41	H	0.196424
42	C	-0.146297
43	H	0.167064
44	H	0.215603
45	C	-0.129332
46	H	0.183245
47	C	-0.187025
48	C	0.295823
49	C	0.341025
50	C	-0.229563
51	H	0.173201
52	H	0.201479
53	H	0.187836
54	C	-0.176619
55	H	0.143779
56	C	0.234311
57	C	-0.140111
58	H	0.144796
59	C	0.226672
60	C	-0.113613
61	H	0.119777
62	C	-0.096821

63	H	0.129015
64	C	-0.089331
65	H	0.129357
66	C	-0.105230
67	H	0.129645
68	C	-0.118527
69	H	0.129170
70	Al	1.227343

Sum of Mulliken atomic charges = 1.00000

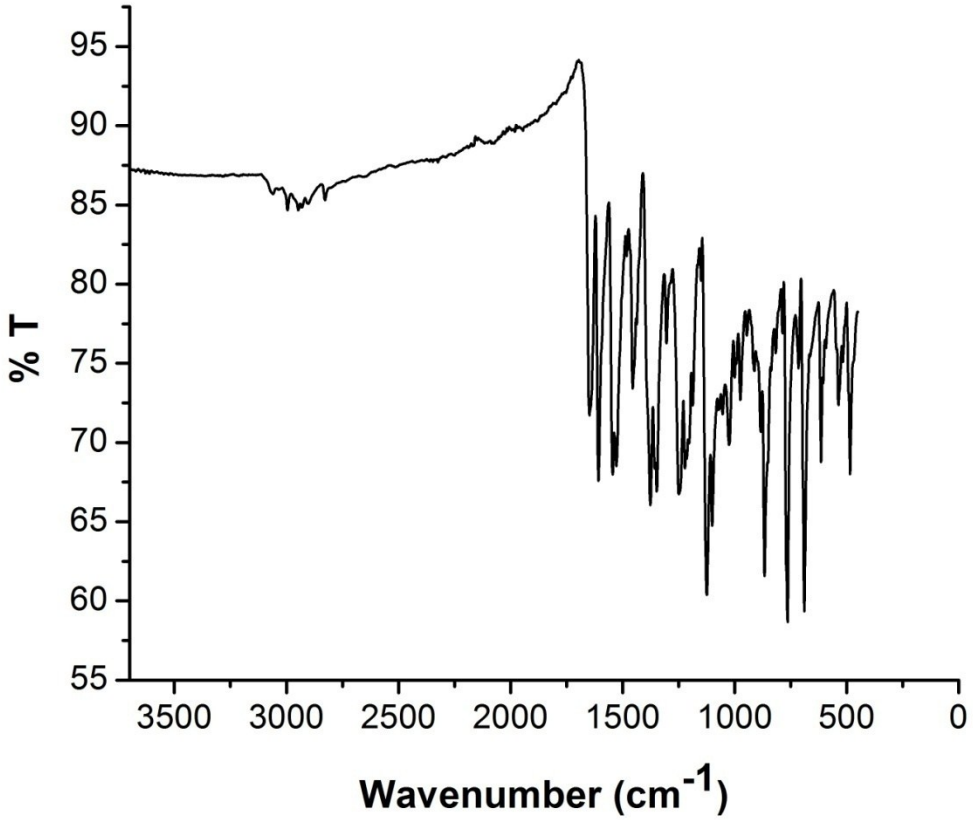


Figure S1. FT-IR spectrum of **H_2L**.

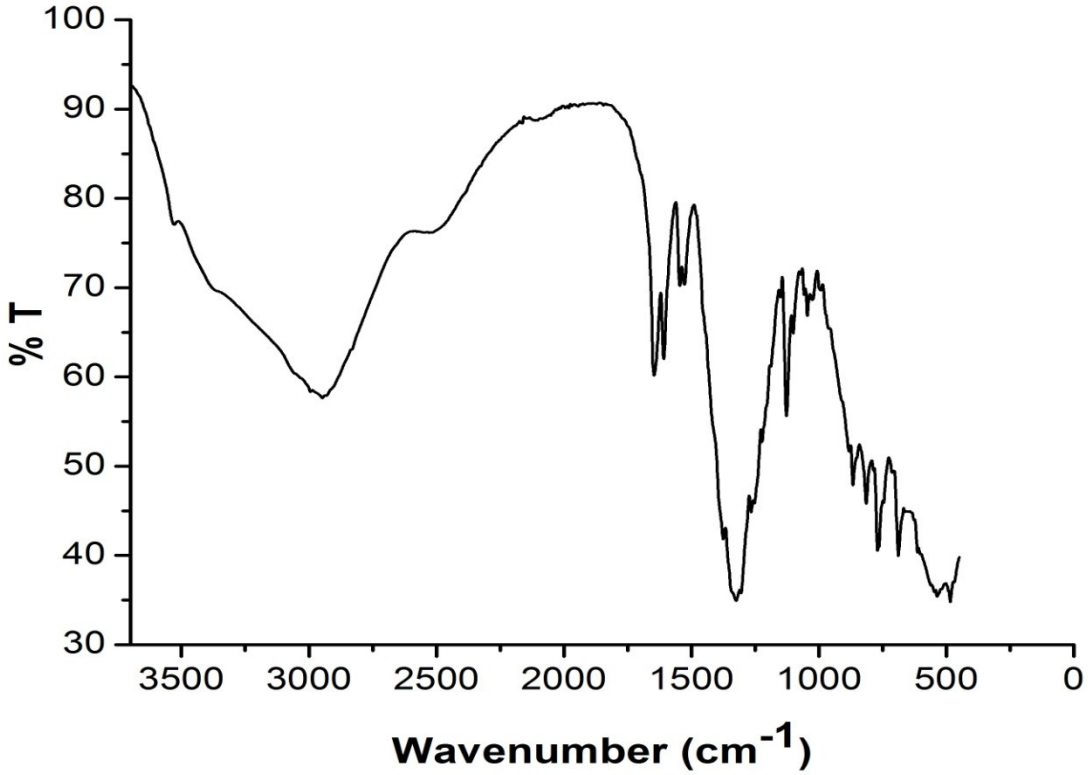
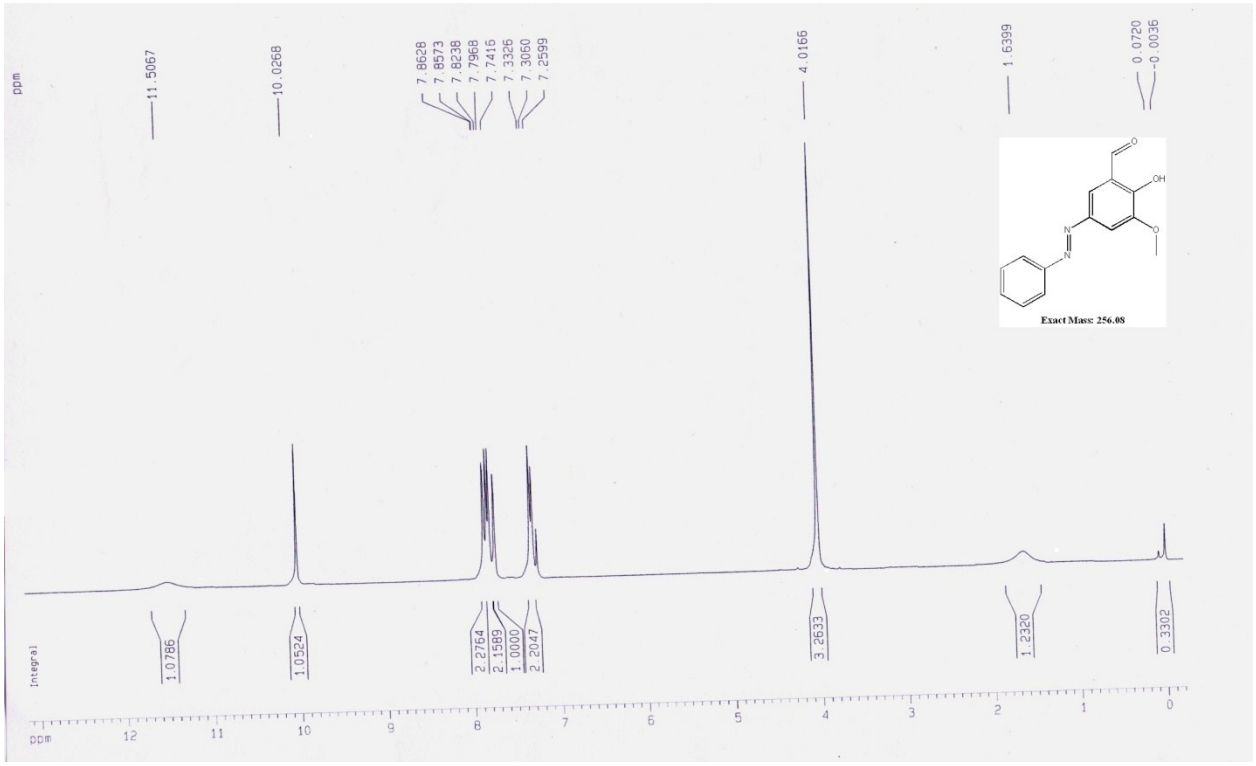
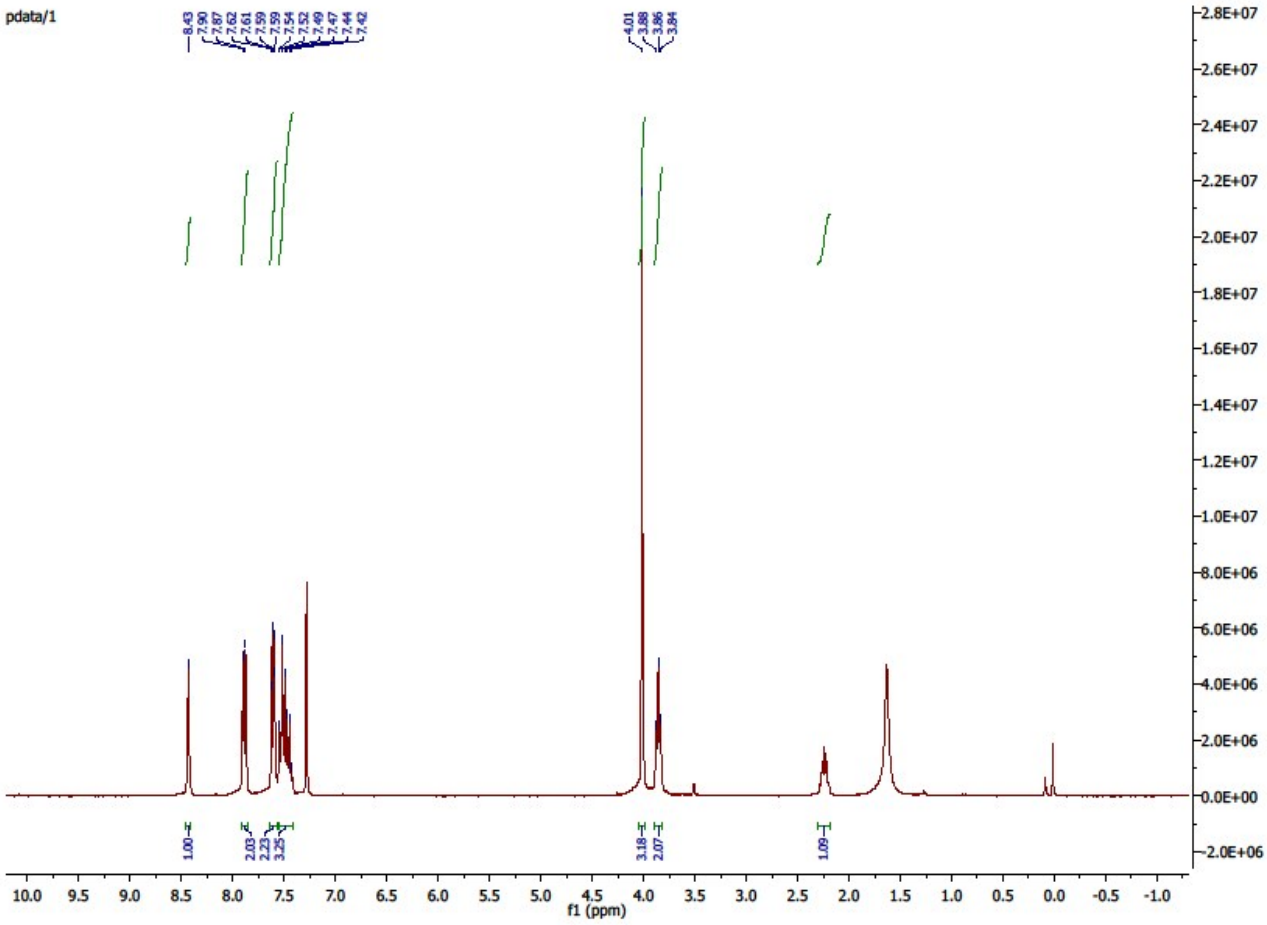


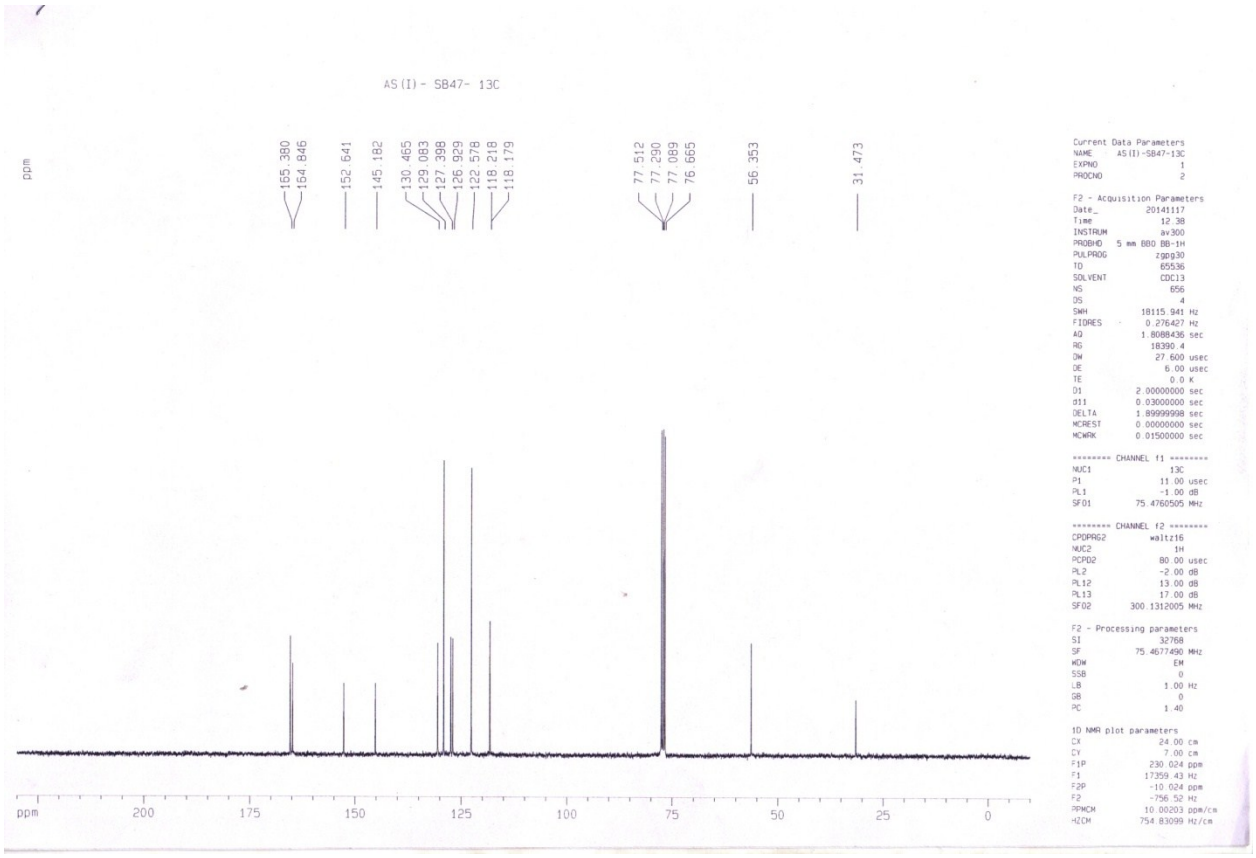
Figure S2. FT-IR spectrum of **H_2L**with $Al(NO_3)_3$ salt in 1:1 ratio.



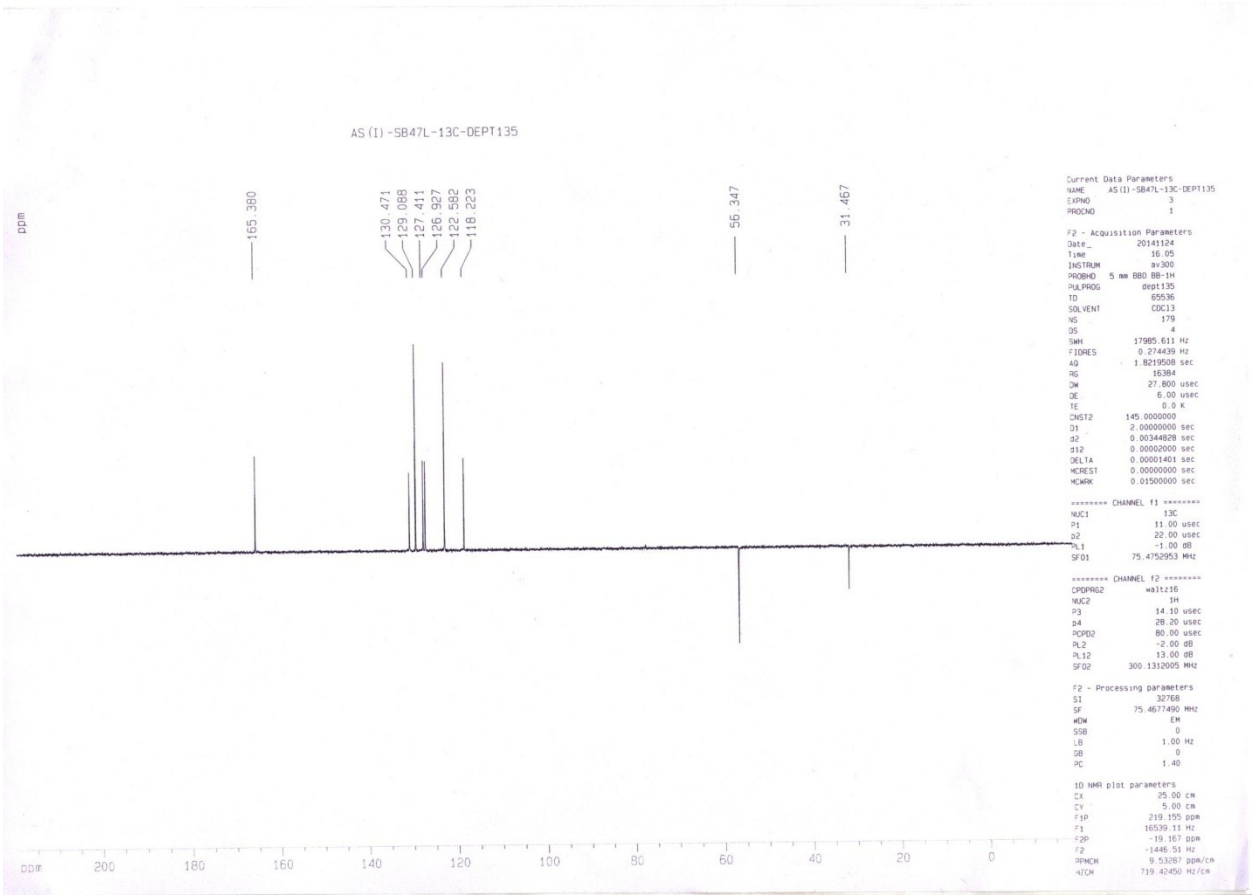
FigureS3. ^{1}H NMR(d$_6$-DMSO, 300 MHz) spectrum of **azo aldehyde.**



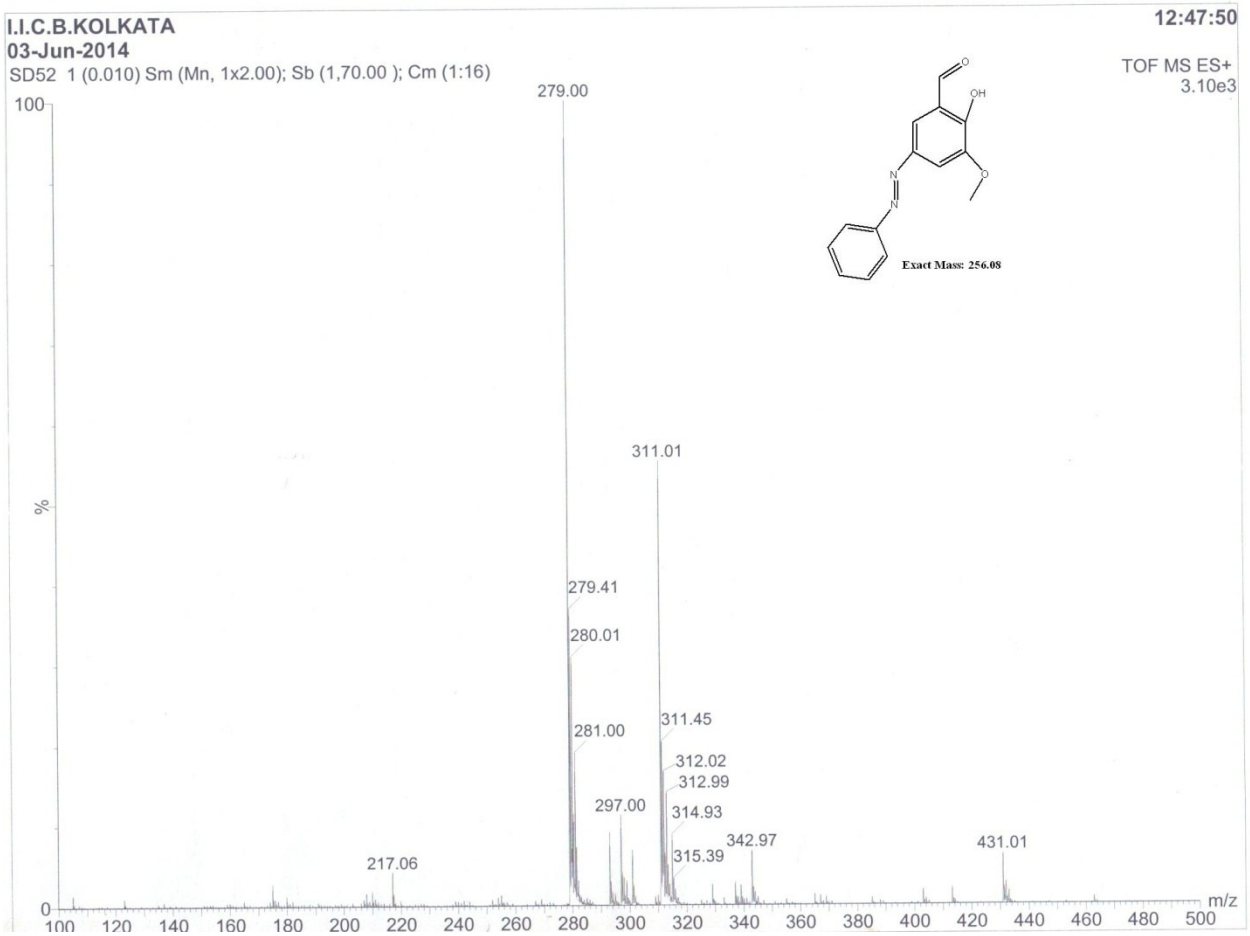
FigureS4. ^{1}HNMR($CDCl_3$, 300 MHz) spectrum of **H_2L.**



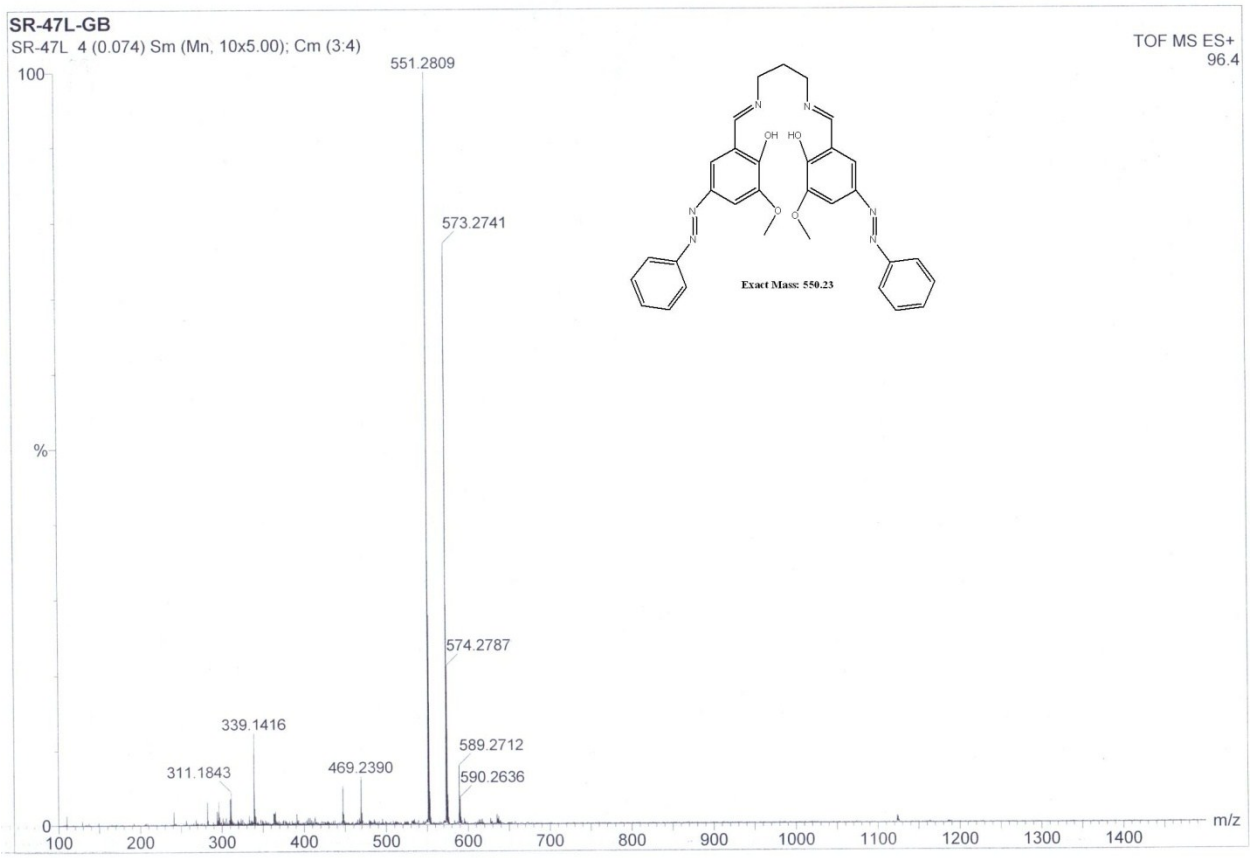
FigureS5. ^{13}CNMR(d$_6$-DMSO, 300 MHz) spectrum of **H_2L.**



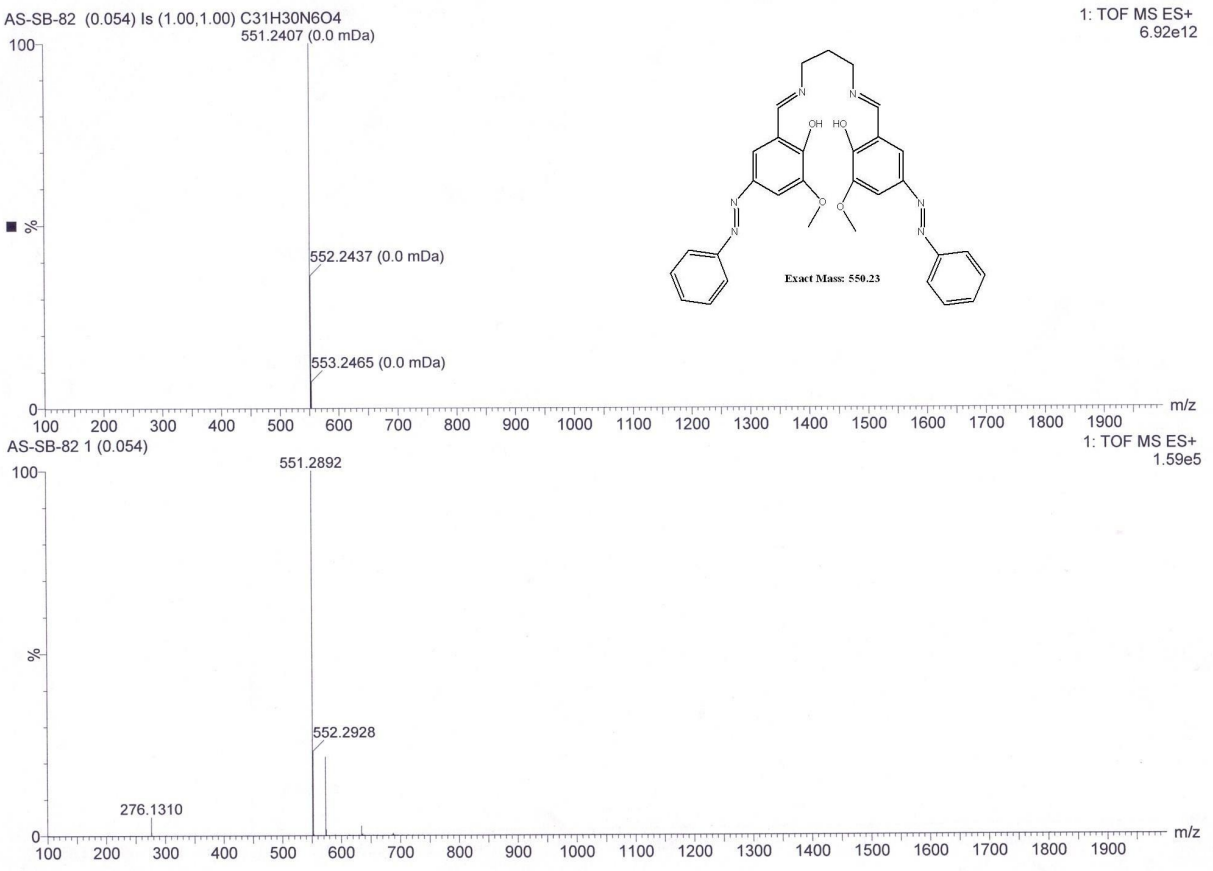
FigureS6. ^{13}CNMR-DEPT135(d$_6$-DMSO, 300 MHz) spectrum of **H_2L.**



FigureS7. Mass Spectrum of **Azo aldehyde.**



FigureS8. Mass Spectrum of **H_2L.**



FigureS9. Simulated Mass Spectrum of **H_2L.**

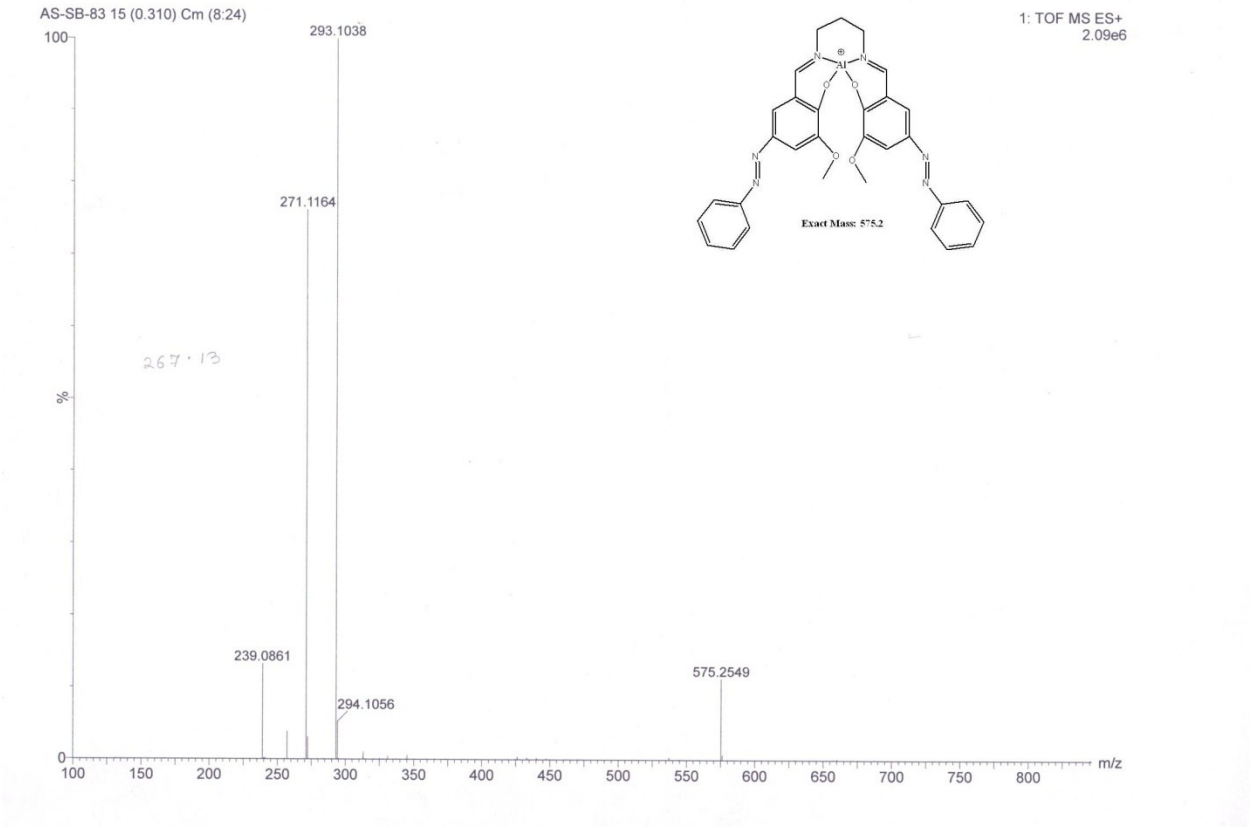


Figure S10. Mass Spectrum of $\mathbf{H_2L}$with $\mathbf{Al^{3+}}$system in 1:1 molar ratio in methanol.

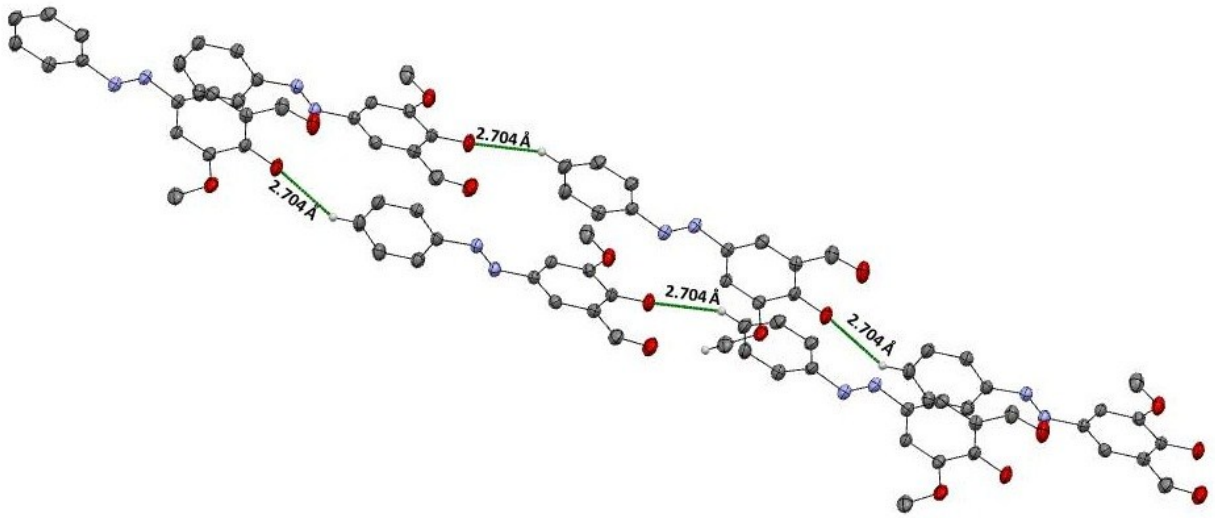


Figure S11. 2D supramolecular sheet of azoaldehyde showing H-bonding and edge to edge π- π interactions. Hydrogen atoms of least interest are omitted for clarity.

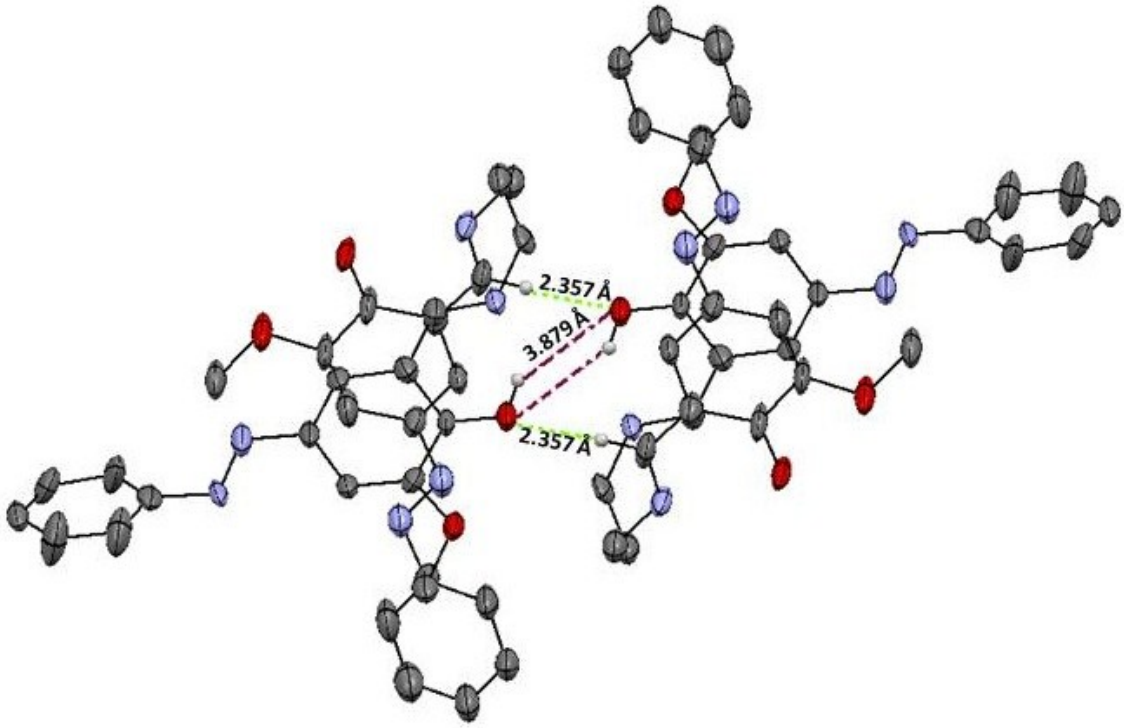


Figure S12. Dimerized form of **H_2L**. Hydrogen atoms of least interest are omitted for clarity.

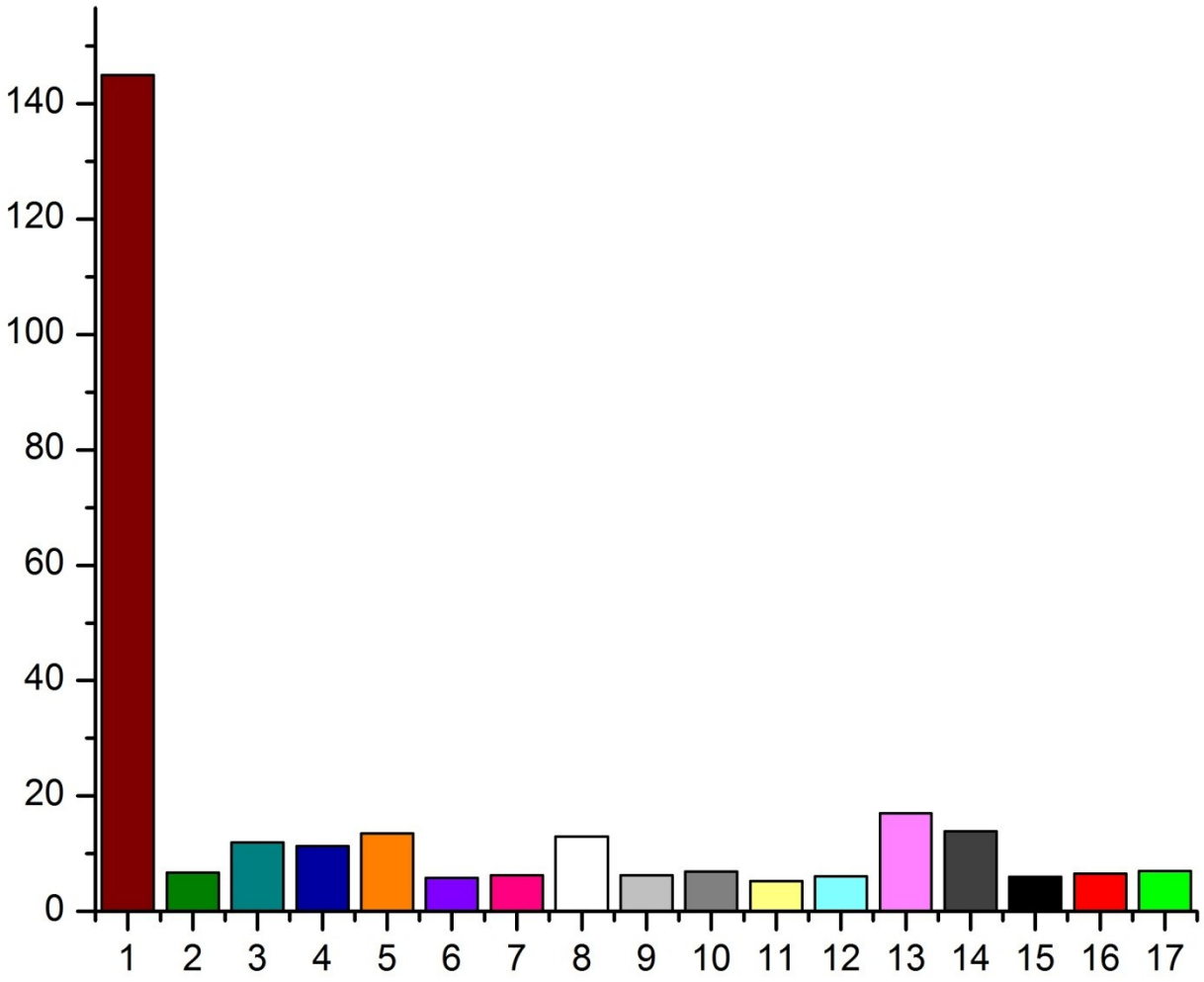


Figure S13. 1- $\mathbf{H_2L}$+Al^{3+}, 2- $\mathbf{H_2L}$, 3 – 17$\mathbf{H_2L}$ + Cations, Cations = 3-Ag^{+}, 4-Cd^{2+}, 5-Fe^{3+}, 6-Cu^{2+}, 7-Cr^{3+}, 8-K^{+}, 9-Hg^{2+}, 10-Ca^{2+}, 11-Fe^{2+}, 12-Mn^{2+}, 13-Zn^{2+}, 14-Sn^{2+}, 15-Ni^{2+}, 16-Na^{+},17-Co^{2+}.

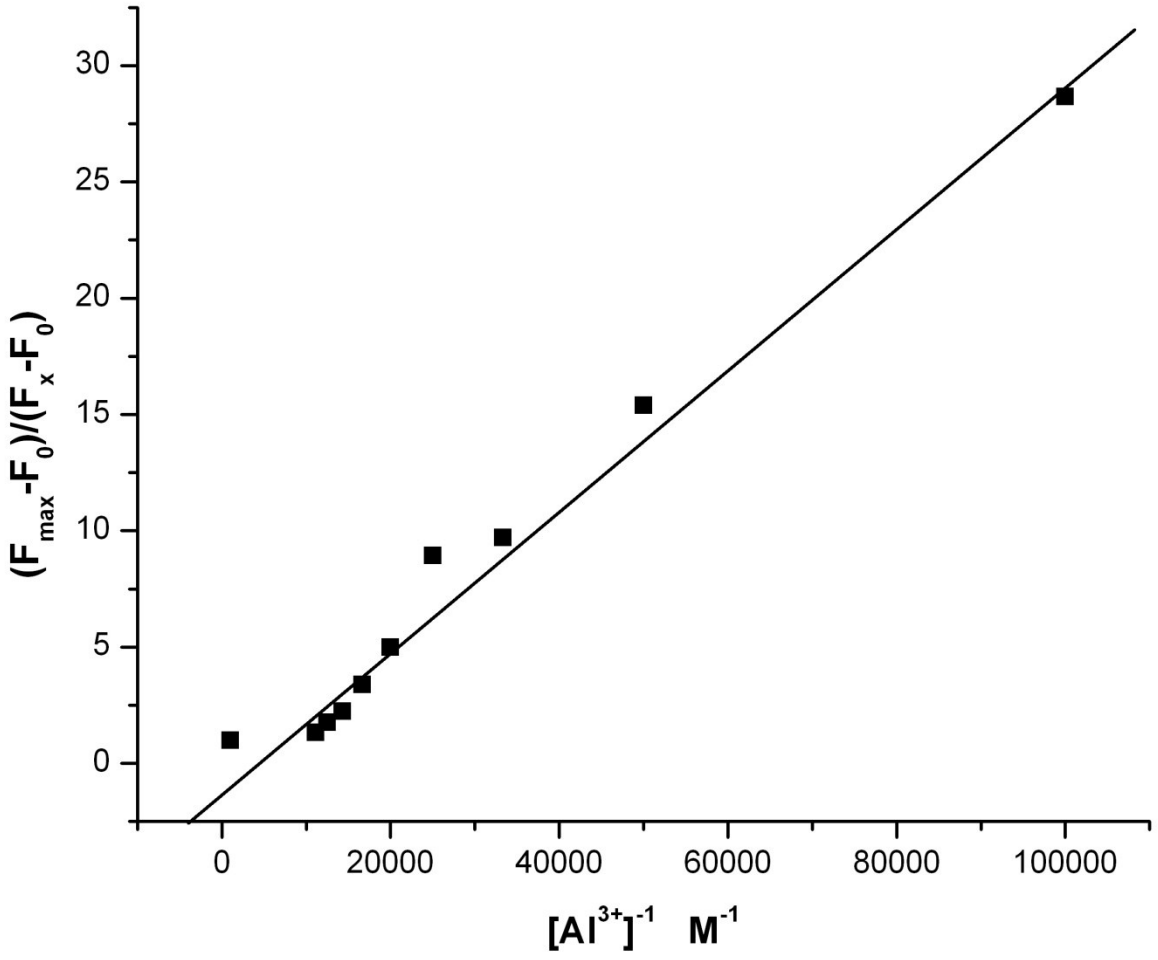
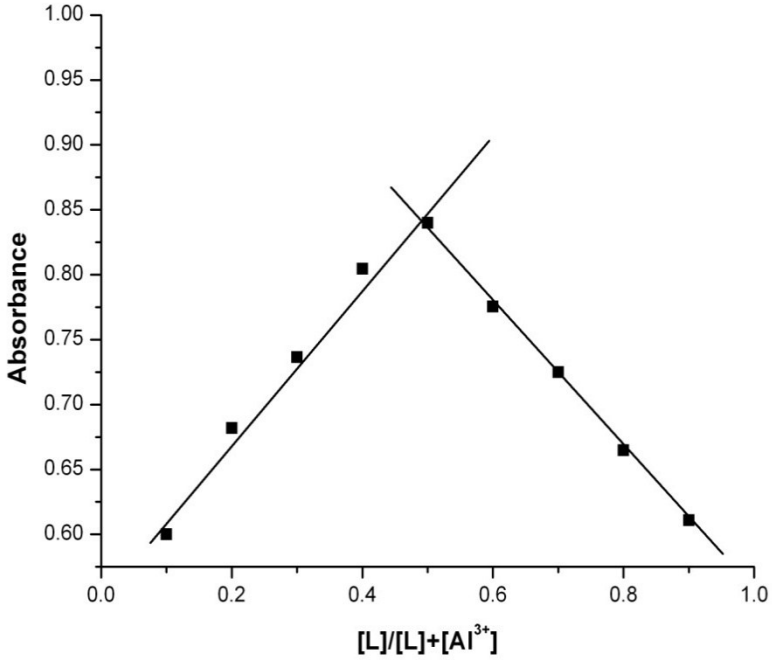
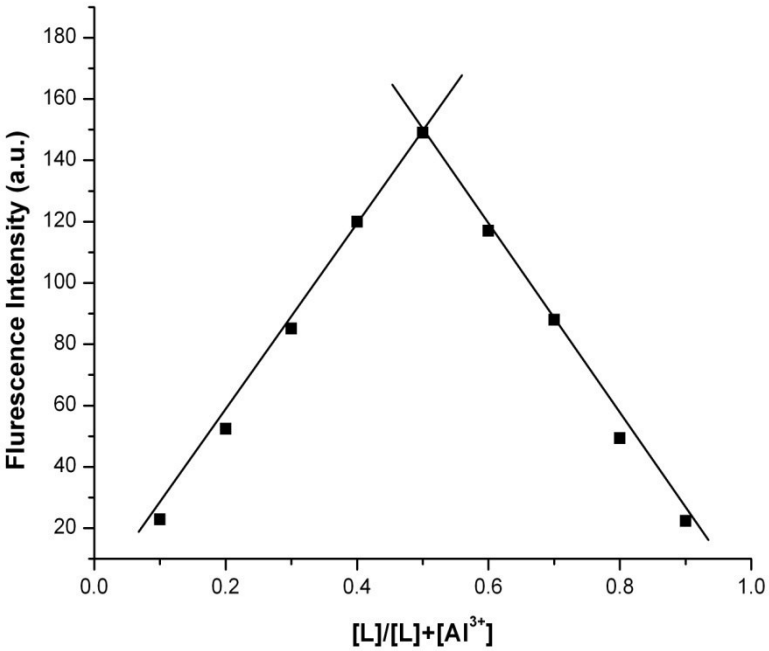


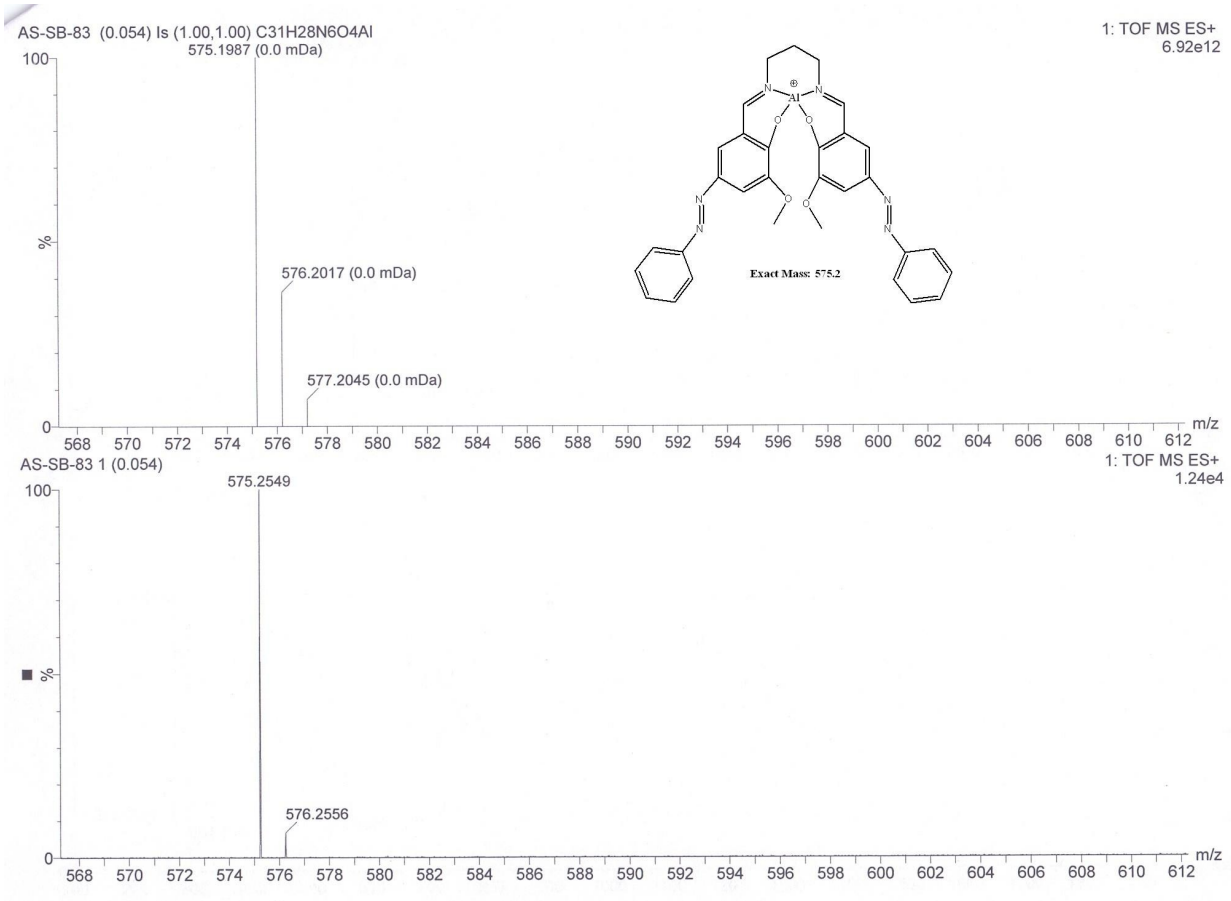
Figure S14. Benesi-Hildebrand equation : A plot of $\frac{F_{max} - F_0}{F_x - F_0}$ vs $(\frac{1}{[M]^1})$ .Symbols and solid lines represent the experimental and simulated profiles, respectively.



FigureS15. 1:1 binding stoichiometry shown by Job's plot. Symbols and solid lines represent the experimental and simulated profiles, respectively.



FigureS16. 1:1 binding stoichiometry shown by Job's plot Symbols and solid lines represent the experimental and simulated profiles, respectively.



FigureS17. Simulated Mass Spectrum of $\mathbf{H_2L}$with $\mathbf{Al^{3+}}$system in 1:1 molar ratio in methanol.