Electronic Supplementary Material (ESI) for RSC Advances

Supplementary Information (SI)

Interaction of soft donor sites with a hard metal ion: Crystallographically characterized blue emitting fluorescent probe for Al(III) with cell staining studies

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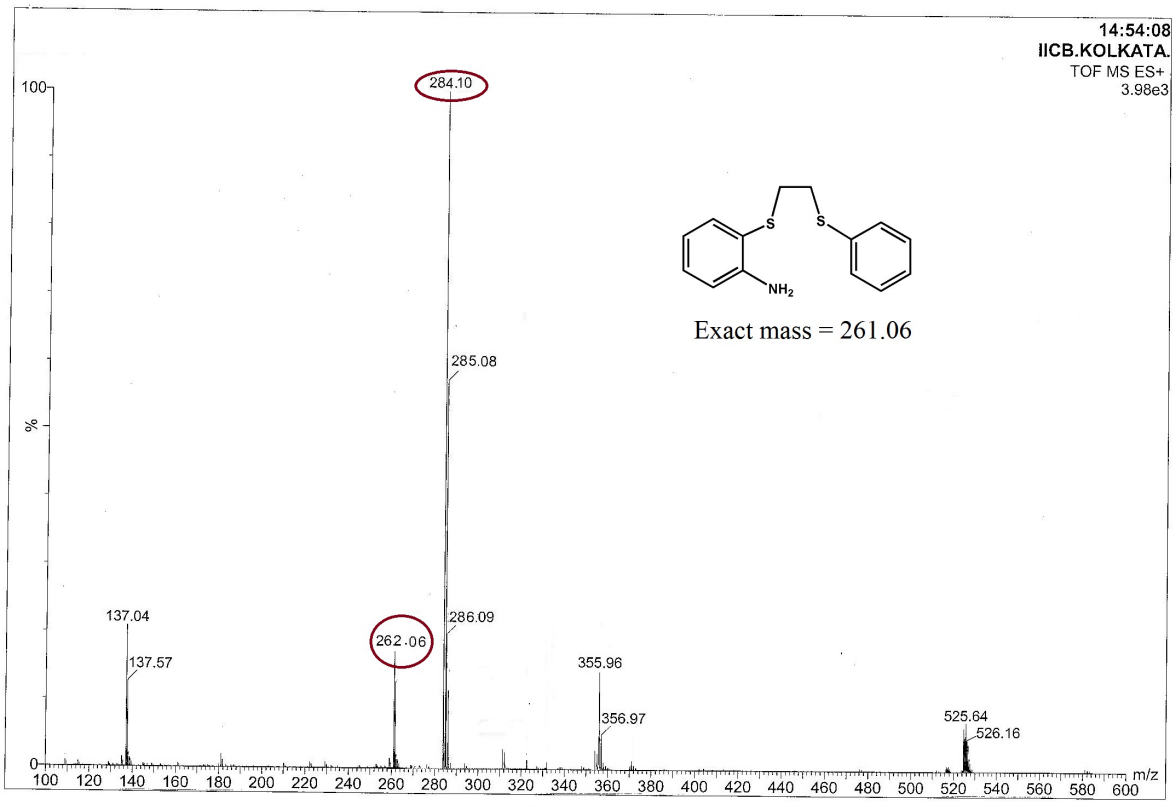


Fig. S1

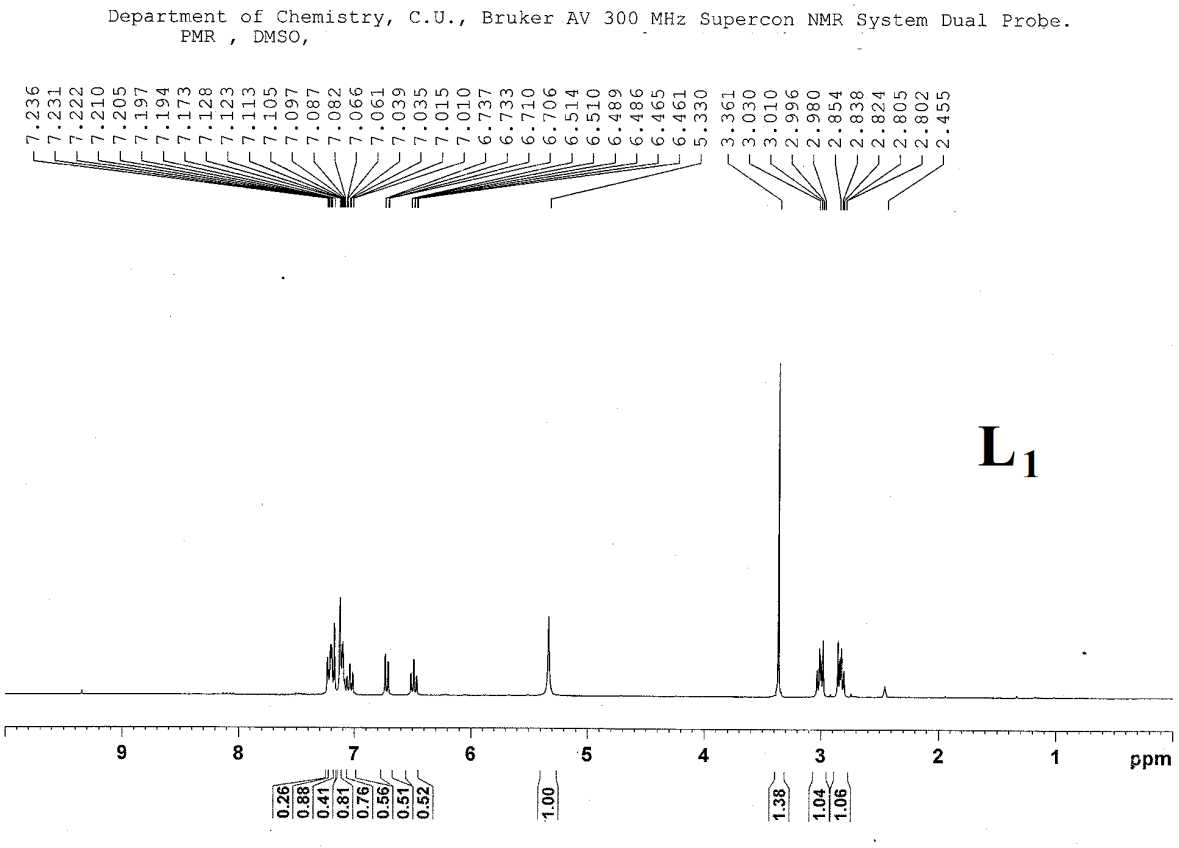


Fig. S2

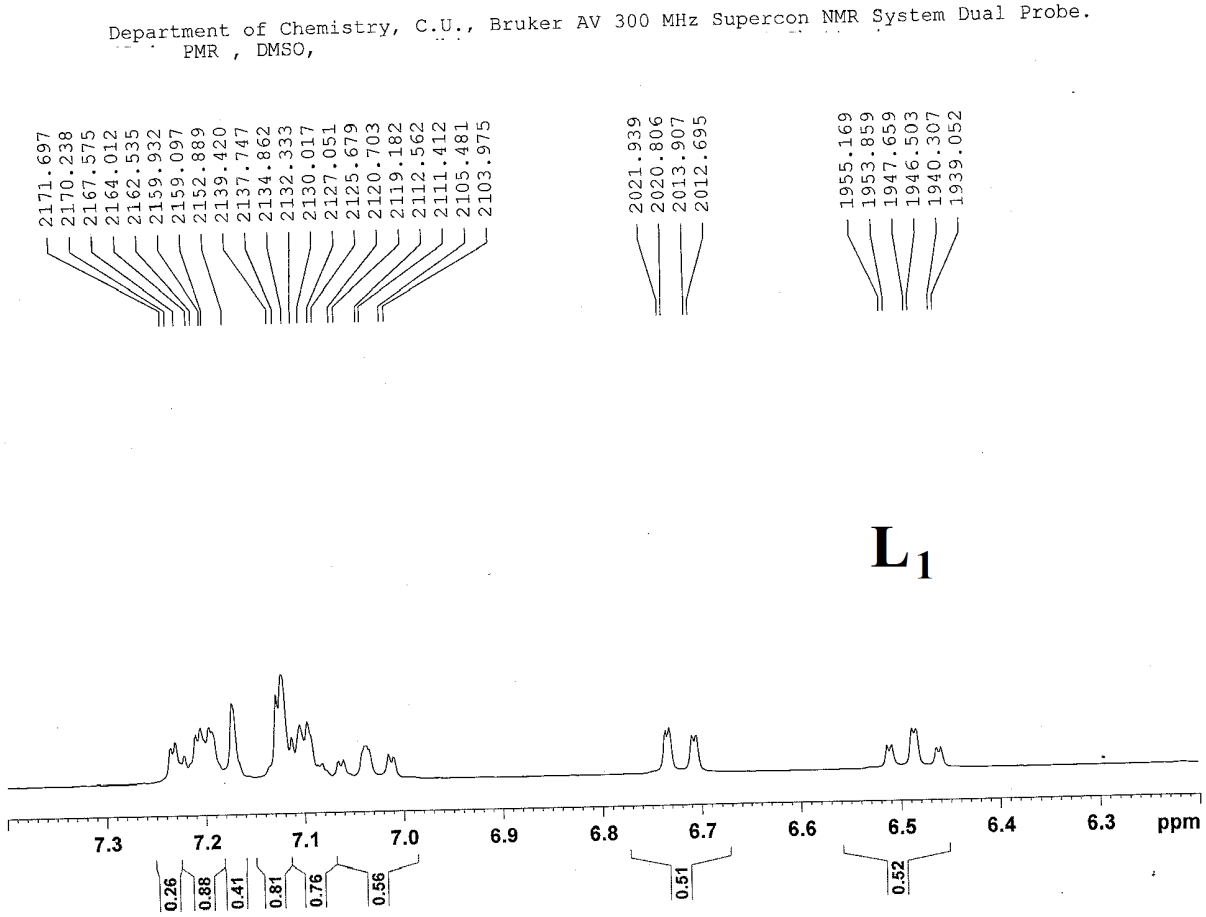


Fig. S3

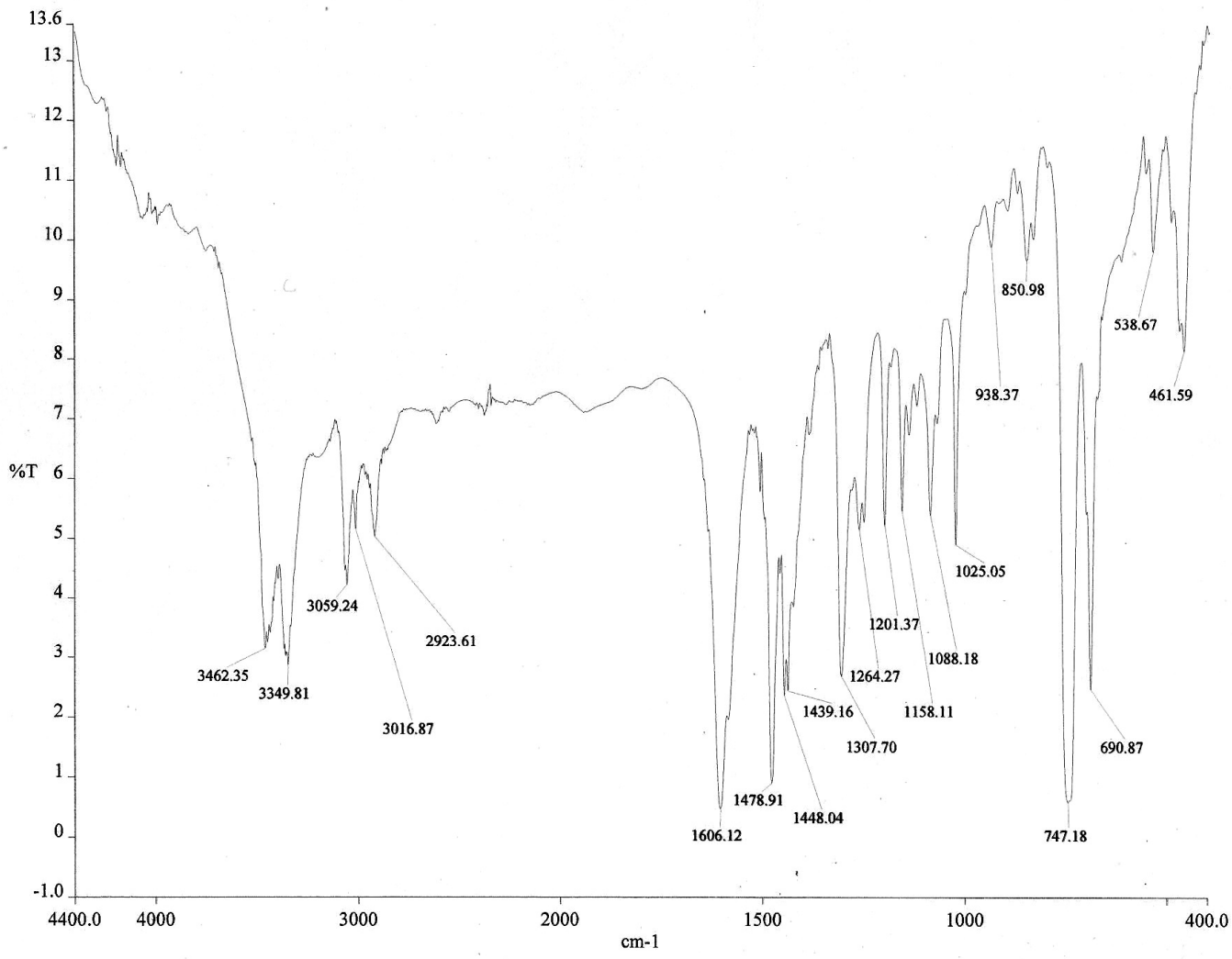


Fig. S4

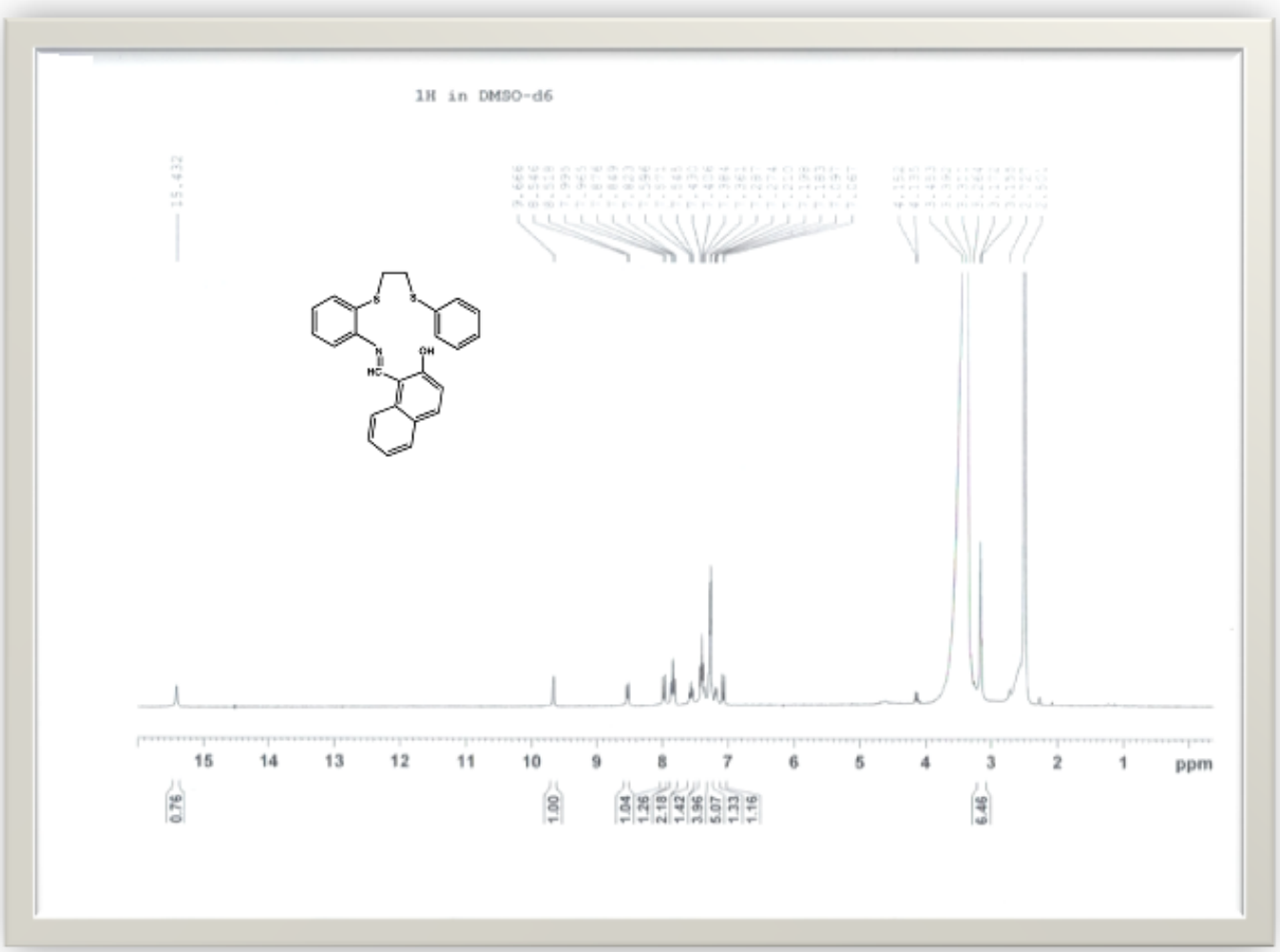
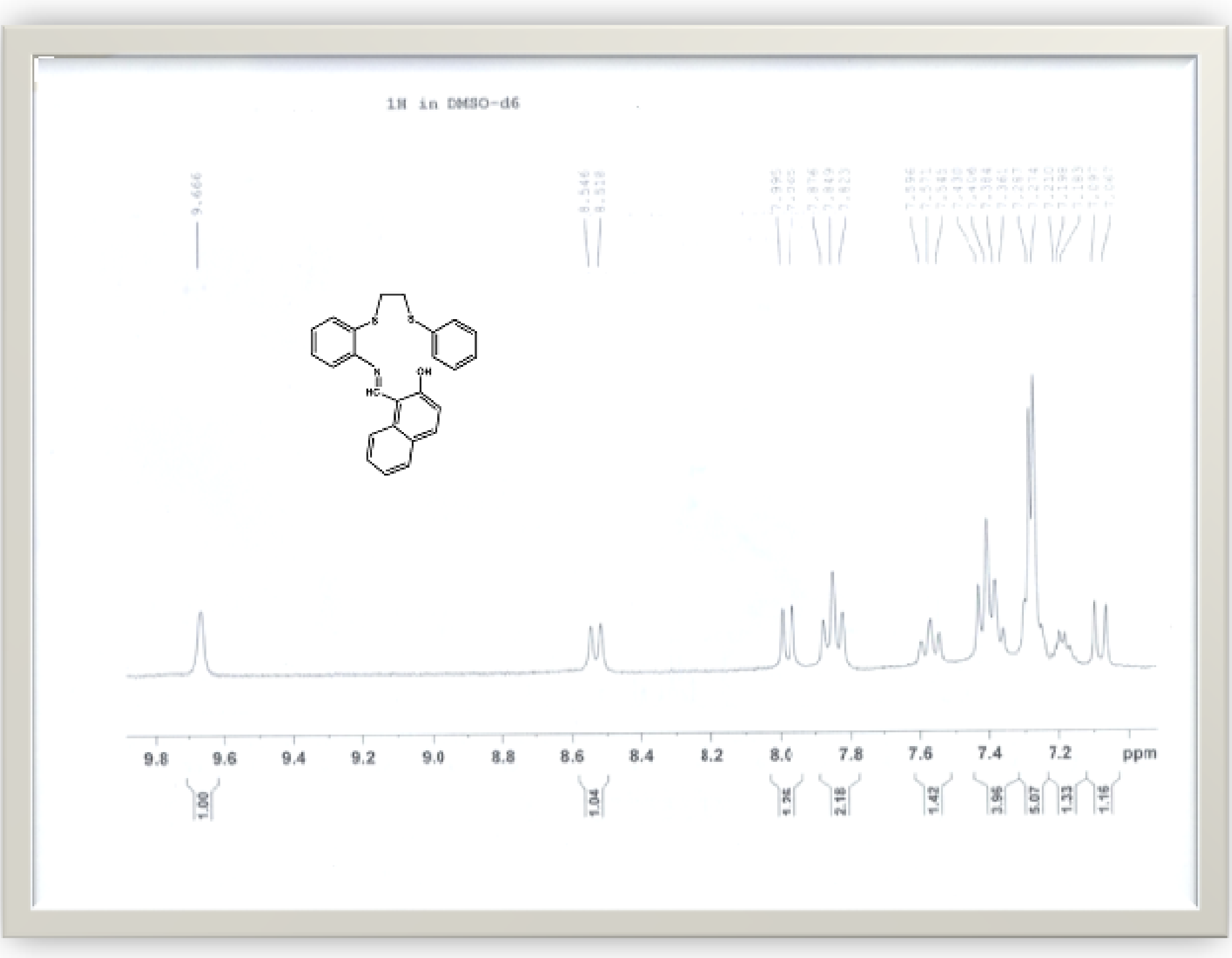


Fig. S5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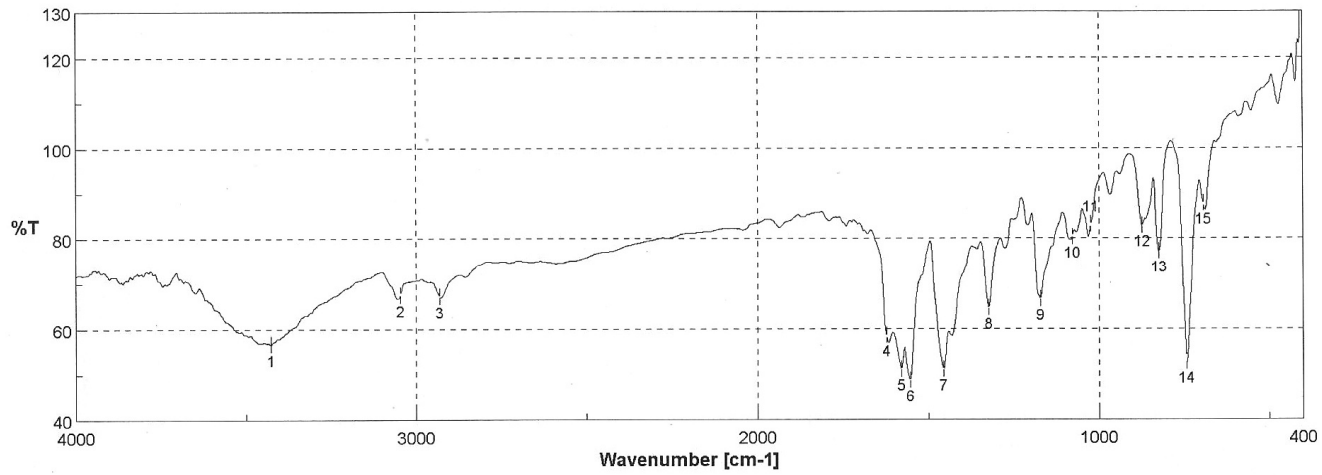
8.546
8.518
ppm
9.8
9.6
9.4
9.2
9.0
8.8
8.6
8.4
8.2
7.8
7.6
7.4
7.2
1.00
1.04
2.18
1.42
3.96
5.07
1.33
1.16

Fig. S6



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Zero Filling	ON	Apodization	Cosine
Gain	Auto (16)	Scanning Speed	Auto (2 mm/sec)
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Operator	ARNAB		
File Name	Memory#4		
Sample Name	NEDAIA		
Comment	Nil		

No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3426.89	56.7104	2	3046.98	67.5349	3	2930.31	67.2137	4	1622.8	58.6639	5	1579.41	51.2744
6	1553.38	48.8912	7	1455.03	51.2252	8	1321.96	64.6626	9	1170.58	66.5477	10	1077.05	80.4086
11	1023.05	83.2629	12	872.631	82.8645	13	822.491	77.174	14	741.496	52.8277	15	693.284	87.8685

Fig. S7

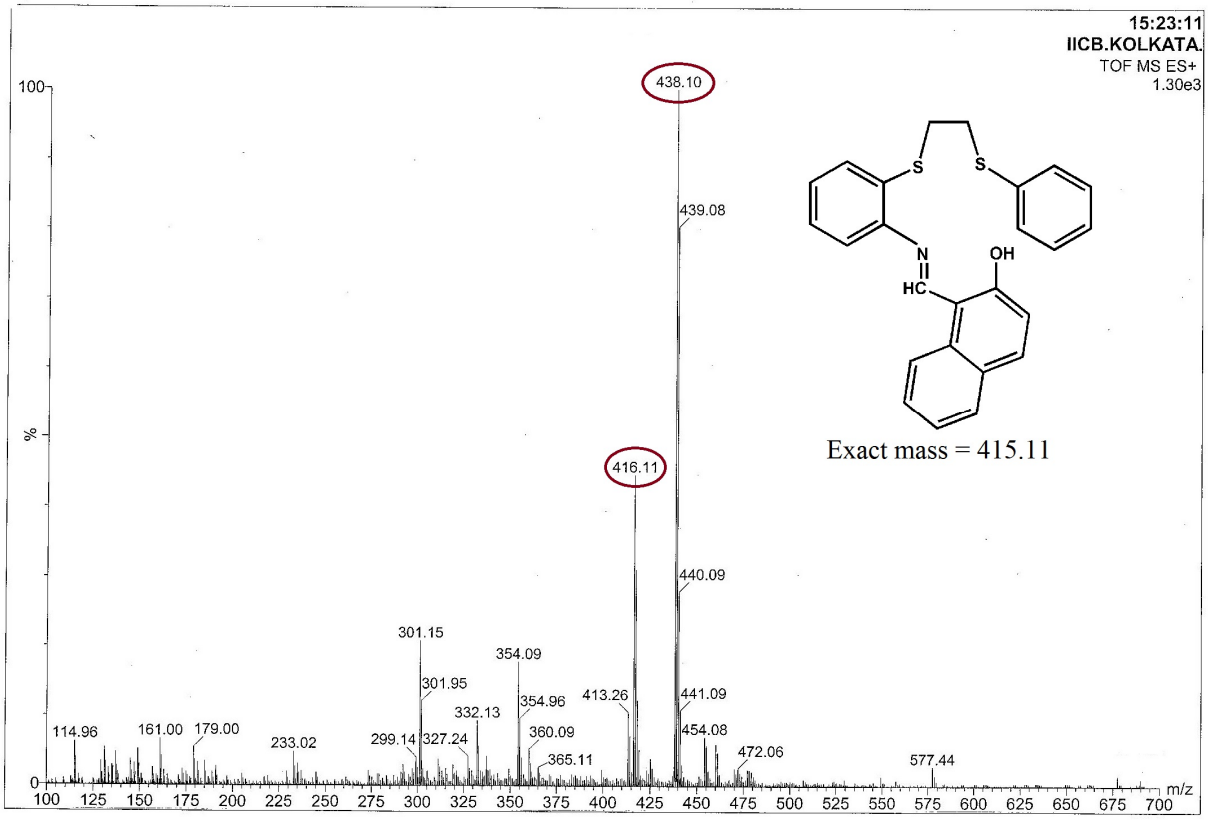

Fig. S8

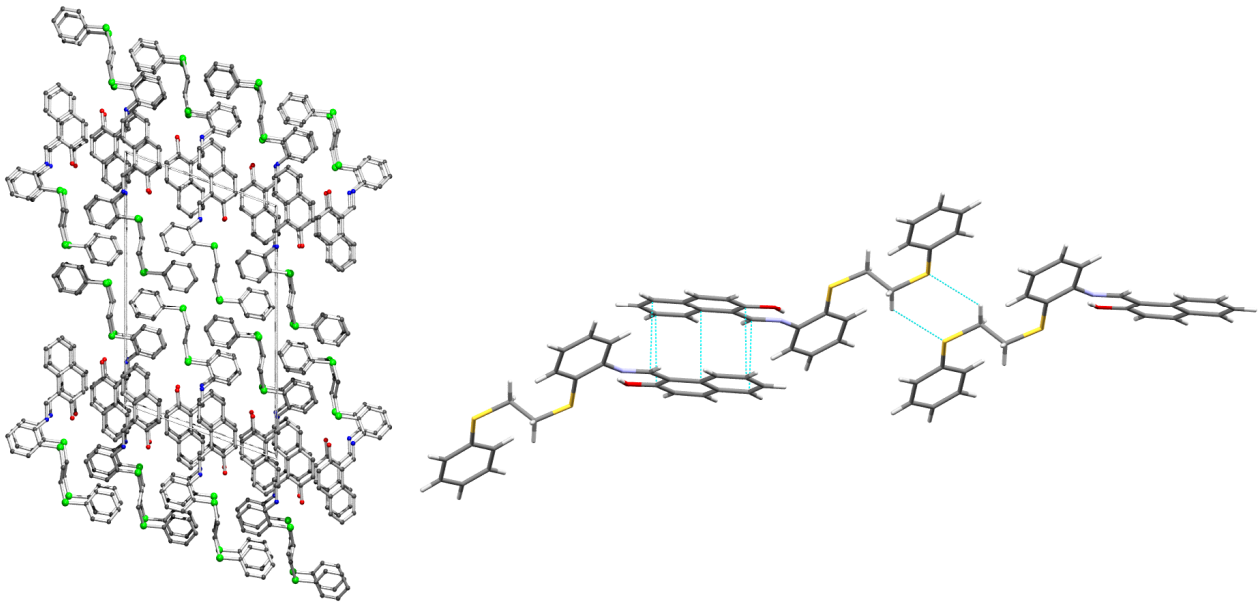

Fig. S9

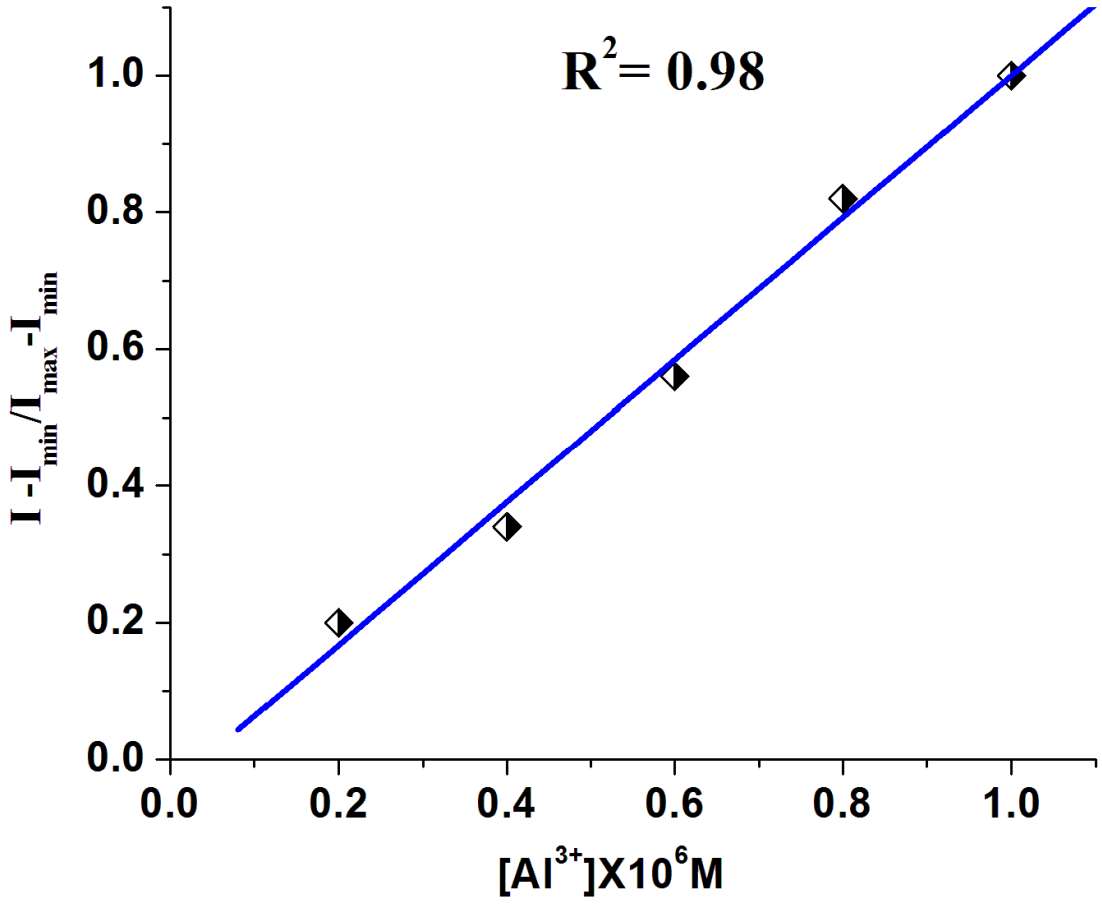

Fig. S10

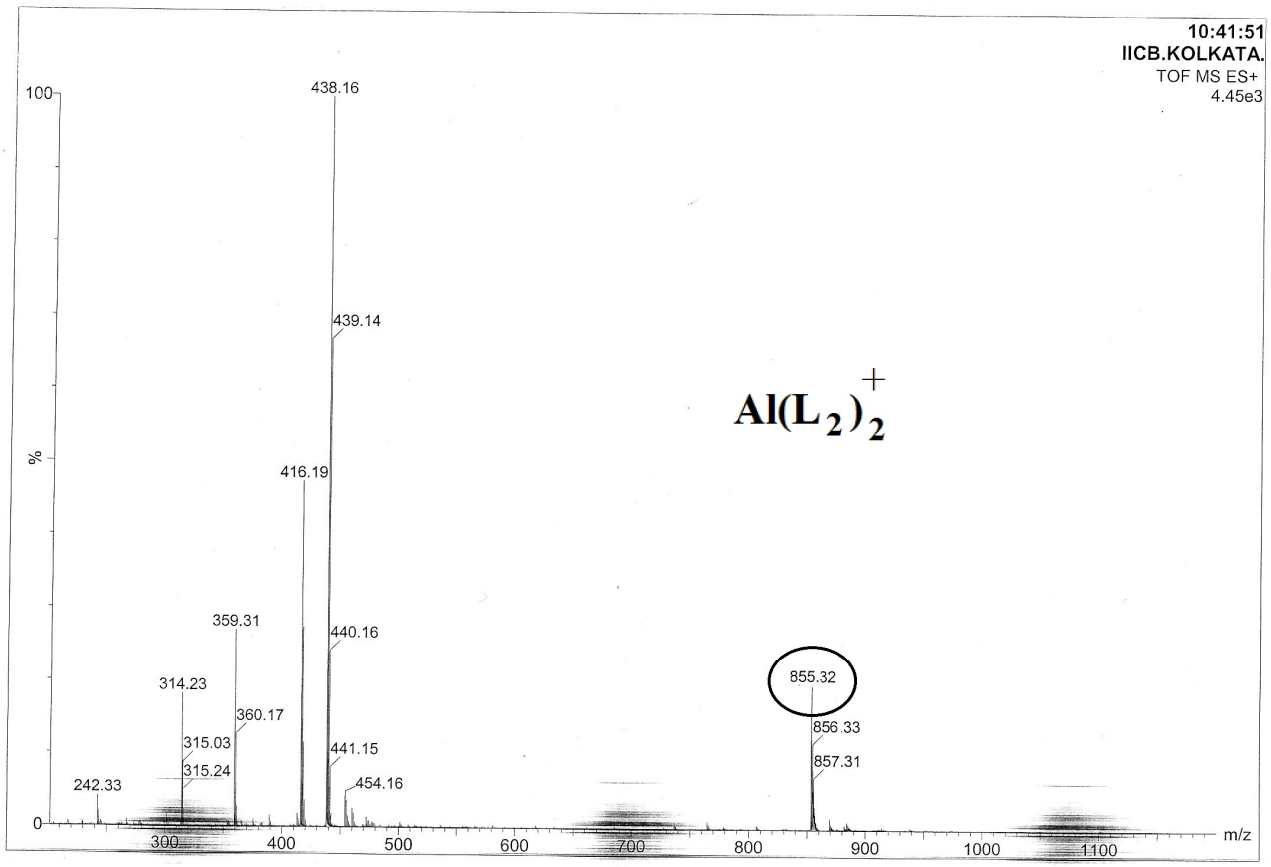

Fig. S11

2. Calculation of Quantum Yield

Fluorescence quantum yields (Φ) were estimated by integrating the area under the fluorescence curves using the equation,

$$\phi_{\text{sample}} = \frac{\text{OD}_{\text{standard}} \times A_{\text{sample}}}{\text{OD}_{\text{sample}} \times A_{\text{standard}}} \times \phi_{\text{standard}}$$

where A was the area under the fluorescence spectral curve and OD was optical density of the compound at the excitation wavelength[1]. Anthracene was used as quantum yield standard (quantum yield is 0.27 in ethanol)[2] for measuring the quantum yields of ligand and its Al^{3+} complex.

3. MTT cell toxicity assay of L_2[3-5]

For assaying toxicity of **L_2** in-vitro cell culture experiment, MTT assay has been performed. It is commonly known as cell viability and proliferation assay. MTT stands for (3-[4,5-dimethylthiazol-2-yl]-2, 5-diphenyltetrazolium bromide).

The assay depends on the reductive cleavage of the yellow tetrazolium salt, MTT, to a water soluble purple color formazan by metabolic active cells which can be measured by spectrophotometry at 570 nm.

Materials

1. PBS- Phosphate buffer saline,
2. MTT (5 mg/ml in PBS) - filtered and kept in dark.
3. Freshly prepared isopropanol solution (DMSO: isopropanol, 1:1, v/v).
4. Stock solution of Al^{3+} salt.
5. Stock solution of **L_2.**

Procedure:

1.5 mL exponentially growing broth culture of *Candida albicans* (IMTECH No. 3018) grown in yeast extract glucose broth medium (pH 6.0, incubation temperature, 37 ^{0}C) was centrifuged at 3000 rpm for 10 minutes and the pellet was washed twice with normal saline and finally suspended in normal saline at cell density of ~ 10^8 cell/ml. Following five experimental sets (each set composed of three tubes) were prepared as below:

i) Set I- To each tube 2 ml *Candida* cell suspension + 0.2 mL normal saline were taken. This set was considered as negative control.

ii) Set II- To each tube 2 mL *Candida* cell suspension + 0.2 mL Tetrazolium salt solution. This set was considered as positive control.

iii) Set III- To each tube 2 mL *Candida* cell suspension + 0.2 mL Tetrazolium salt solution + 0.2 mL Al^{3+} salt solution from a stock of 1mg/mL,

iv) Set IV- Set V- To each tube 2 mL *Candida* cell suspension + 0.2 mL Tetrazolium salt solution + 0.2 mL $\mathbf{L_2}$ solution (from a 1mg/mL stock solution)

v) Set V- To each tube 2 mL *Candida* cell suspension + 0.2 mL Tetrazolium salt solution + 0.2 mL Al^{3+} salt solution from a stock of 1mg/mL + 0.2 mL $\mathbf{L_2}$ solution (from a 1mg/mL stock solution)

All sets were incubated for 4 h in dark at 37^0 C. After incubation 2 mL of freshly prepared isopropanol solution (DMSO: isopropanol, 1:1, v/v) was added to each tube of all the five experimental sets. Contents were mixed well and incubated for another 1 h in dark at 37^0 C. After incubation, absorbance (O.D.) of all the solutions for each set was measured at 570 nm.

MTT assay on *Candida* cells indicates that either $\mathbf{L_2}$ or Al^{3+} salt has almost no adverse effect when present independently. However combination of them has little effect on viability of cells.

1. E. Austin, M. Gouterman, *Bioinorg. Chem.*, 1978, **9**, 281.
2. W. H. Melhuish, *J. Phys. Chem.*, 1961, **65**, 229.
3. T. F. Slater et al. *Biochim. Biophys. Acta,* 1963, **77**, 383.
4. M. V. Berridge, P. M. Herst, A. S. Tan, *Biotech. Annual Review*, 2005, **11**, 127.
5. T. Mosmann, . *J. Immunolog. Methods* 1983, **65**, 55.