Supporting Information

A New '*Turn-on*' PET-CHEF based fluorescent sensor for Al^{3+} and CN^- ions: Applications in real samples

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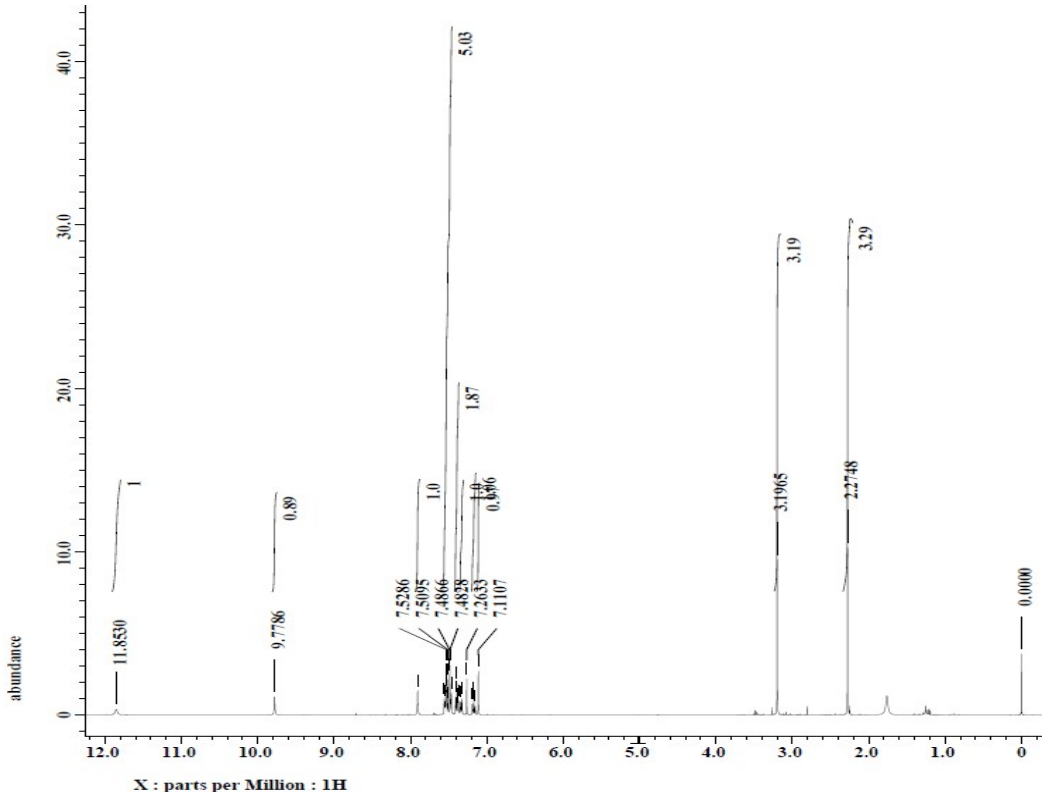


Figure S1: ^{1}H NMR spectrum of probe **1**

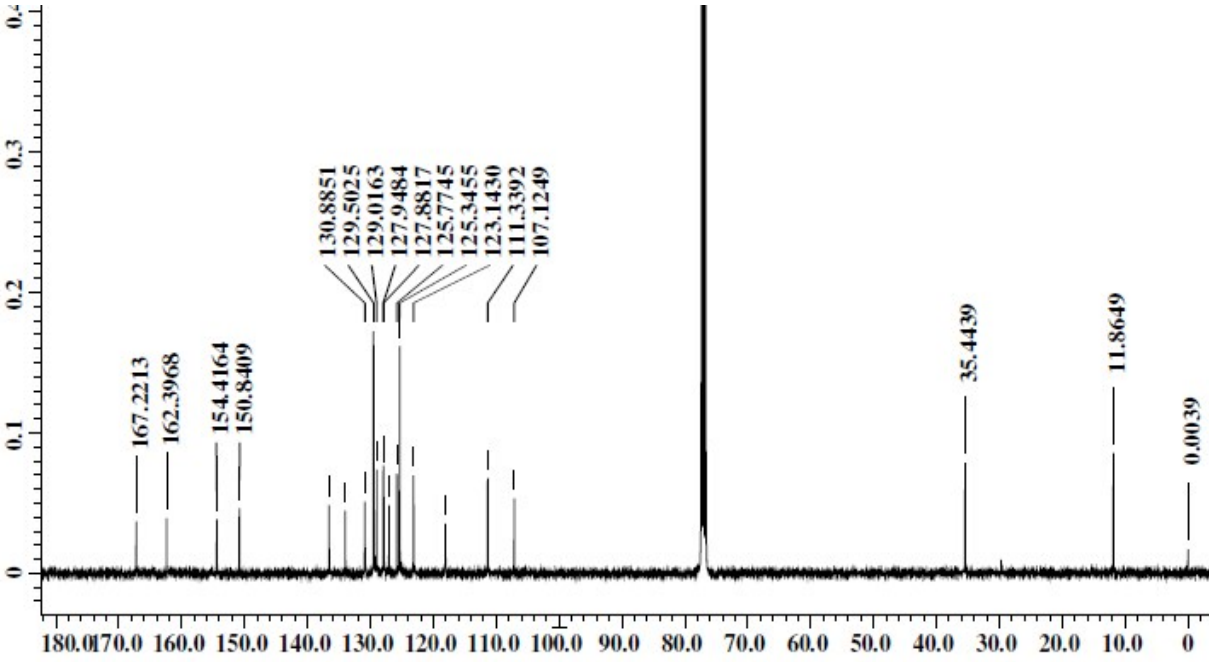


Figure S2: ^{13}C NMR spectrum of probe **1**

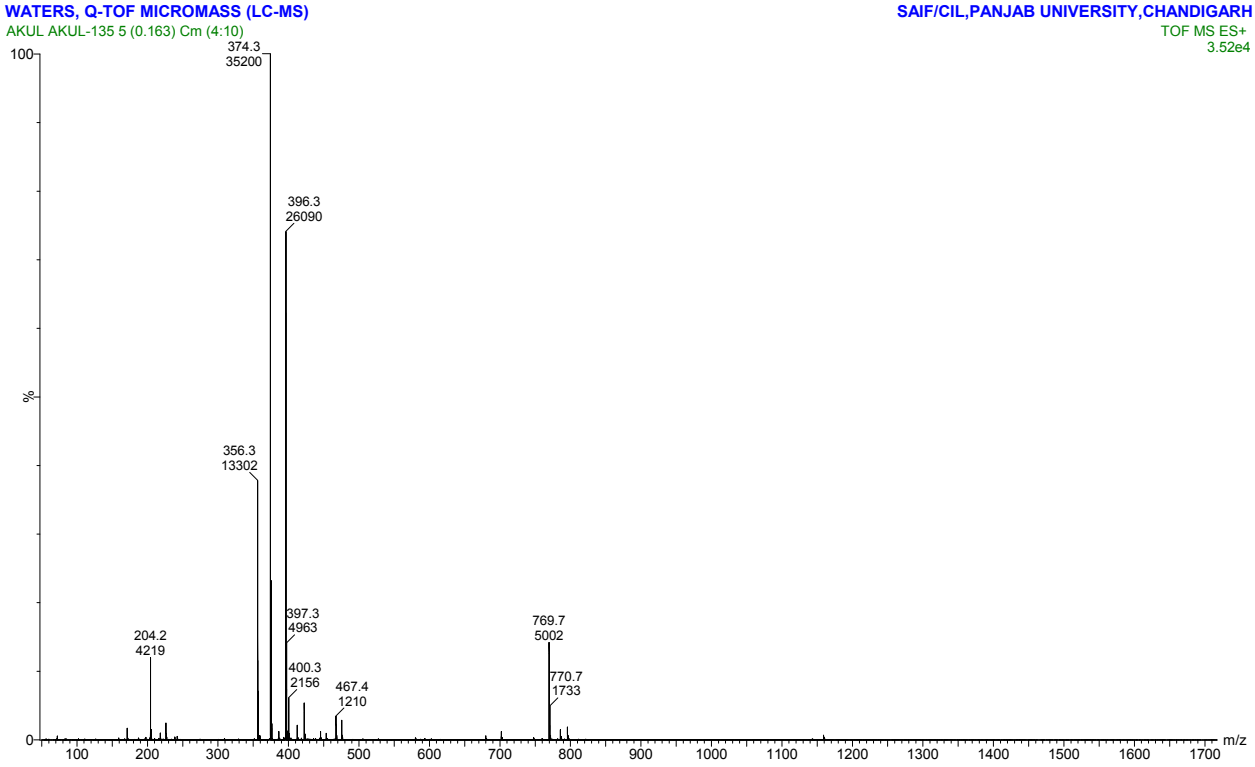


Figure S3: Mass spectrum of probe **1**

Calculations of binding constant

Binding constant was calculated according to the Benesi-Hildebrand equation. K_a was calculated following the equation stated below.

$$1/(A\text{-}A_o) = 1/\{K(A_{max} - A_o)\,[M^{x+}]^n\} + 1/[A_{max}\text{-}A_o]$$

Here A_o is the absorbance of receptor in the absence of guest, A is the absorbance recorded in the presence of added guest, A_{max} is absorbance in presence of added $[M^{x+}]_{max}$ and K is the association constant. The association constant (K) could be determined from the slope of the straight line of the plot of 1/(A-Ao) against $1/[M^{x+}]$ and is found to be 1.78 X $10^3 M^{-1}$ in case of case aluminium ions in methanol.

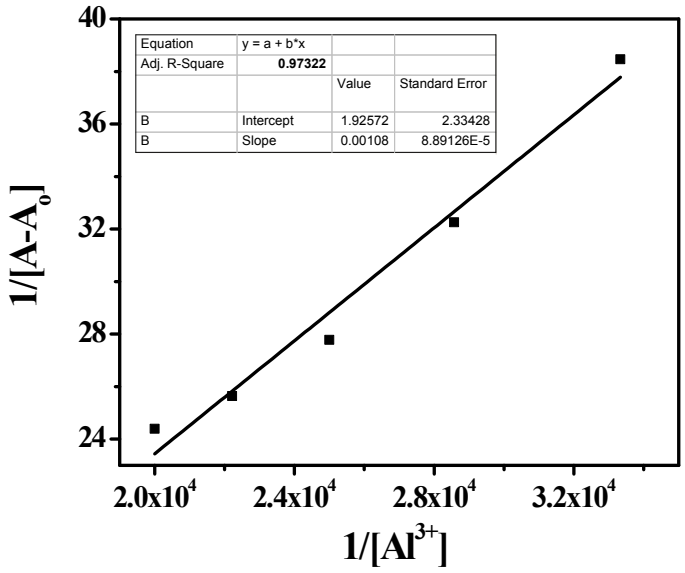


Figure S4: Benesi-Hildebrand plot from absorption titration data of receptor (20 μM) with Al^{3+}.

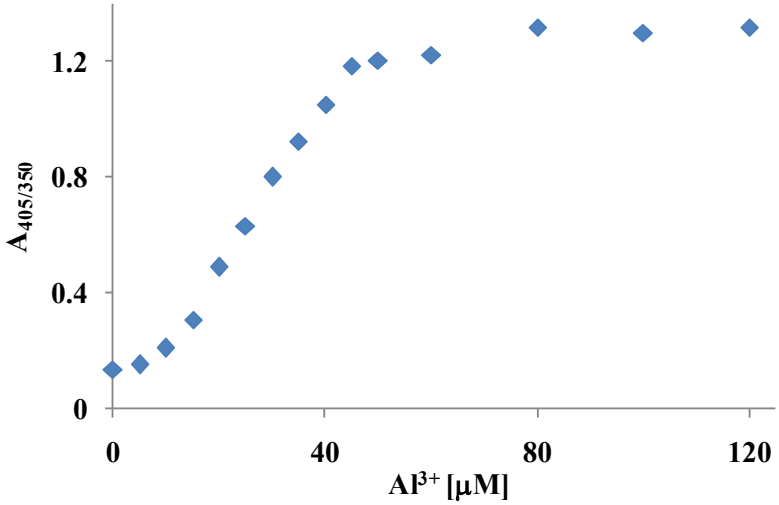


Figure S5. Plot of absorption intensity ratio between 405 and 350 nm (A_{405} / A_{350}) vs [Al^{3+}] ions of probe **1** (20 μM, CH_3OH)

By fluorescence method

The binding constant value of anions with receptor has been determined from the emission intensity data following the modified Benesi–Hildebrand equation,

1//ΔI = 1//ΔImax + (1/K[C]) (1//ΔI max)

Here ΔI = I-I_{min} and ΔI max = I_{max}-I_{min}, where I_{min}, I, and I_{max} are the emission intensities of receptor observed in the absence of anions, at an intermediate anion concentration, and at a concentration of complete saturation where K is the binding constant and [C] is the anion concentration respectively. From the plot of [1 / (Imin –I)] against [C]-1 for receptor, the value of K has been determined from the slope. The association constant (*Ka*) as determined by fluorescence titration method for the receptor with cyanide ions in methanol is found to be 5.2 X 10^3 M^{-1} (error < 10%).

The detection limit was calculated on the basis of emission studies. The fluorescence intensity of probe **1** (20 μM) was measured thrice and the standard deviation of blank measurements was calculated in order to determine the signal-to-noise ratio. The limit of detection was therefore calculated using the mathematical expression,

$$\text{Detection limit} = 3\sigma bi/m$$

where σbi is the standard deviation of blank measurements; m is the intensity slope v/s sample concentration.

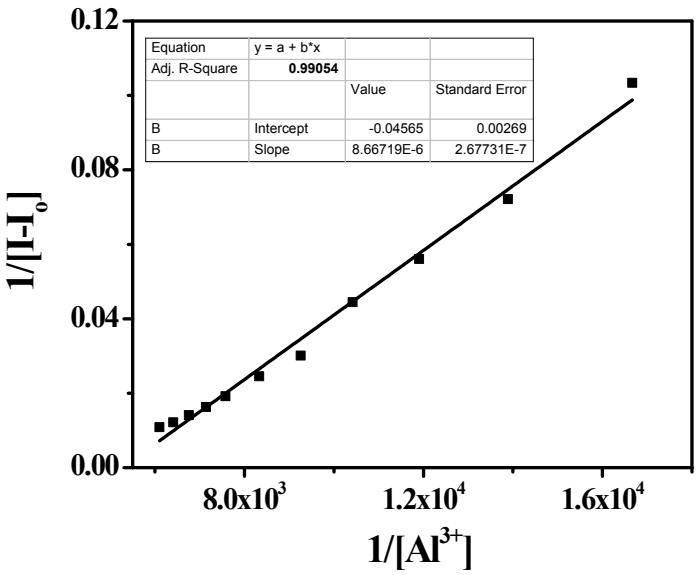


Figure S6: Benesi-Hildebrand plot from emission titration data of receptor (20 μM) with Al^{3+} in CH_3OH.

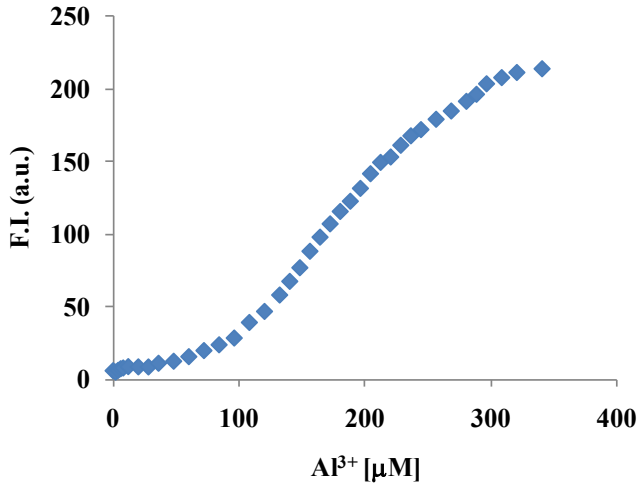


Figure S7. Plot of emission intensity at 505 nm (F_{505}) vs [Al^{3+}] ions of probe **1** (20 μM, CH_3OH)

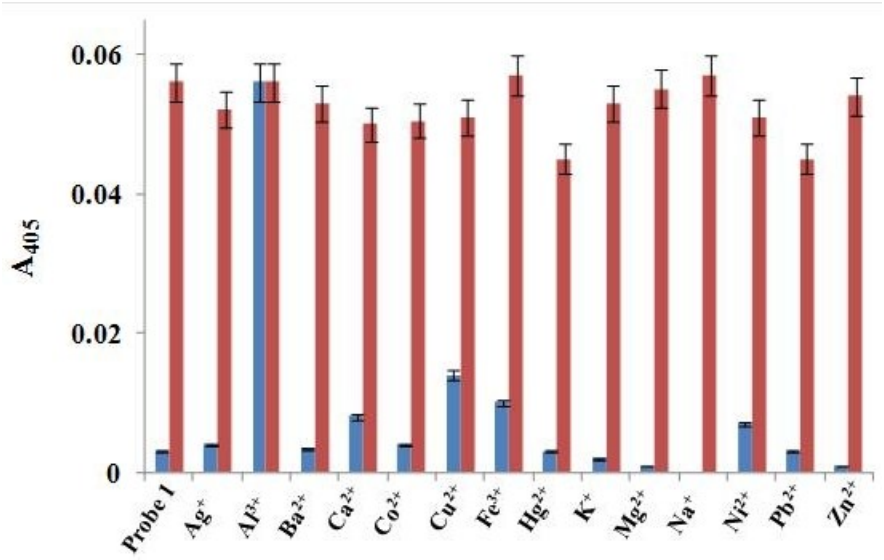


Figure S8. Blue bars represent selectivity of probe **1** (20 μM) upon addition of different metal ions in MeOH and red bars shows the competitive selectivity of probe **1** in the presence of Al^{3+}.

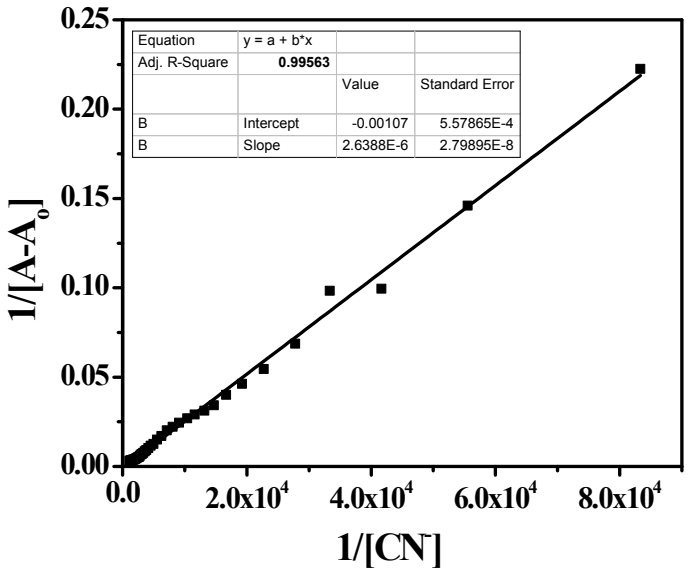


Figure S9: Benesi-Hildebrand plot from absorption titration data of receptor (20 μM) with CN^- in CH_3OH.

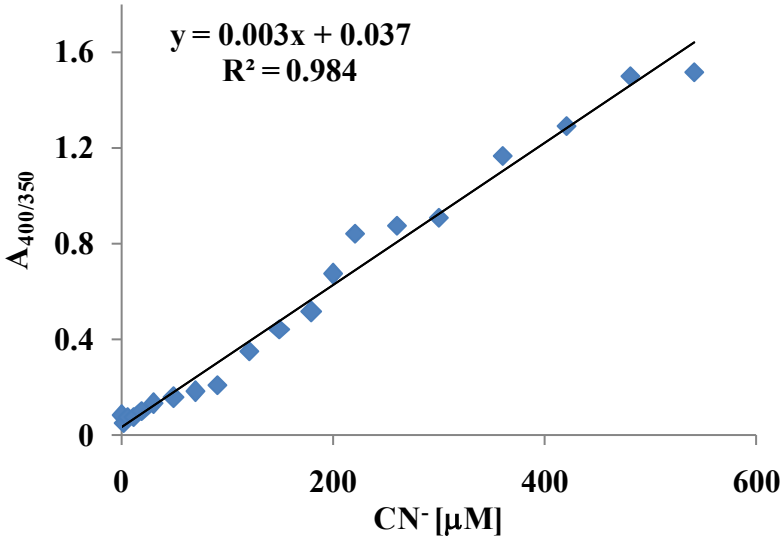


Figure S10. Plot of absorption intensity ratio between 400 and 350 nm (A_{400} / A_{350}) vs [CN^-] ions of probe **1** (20 μM, CH_3OH)

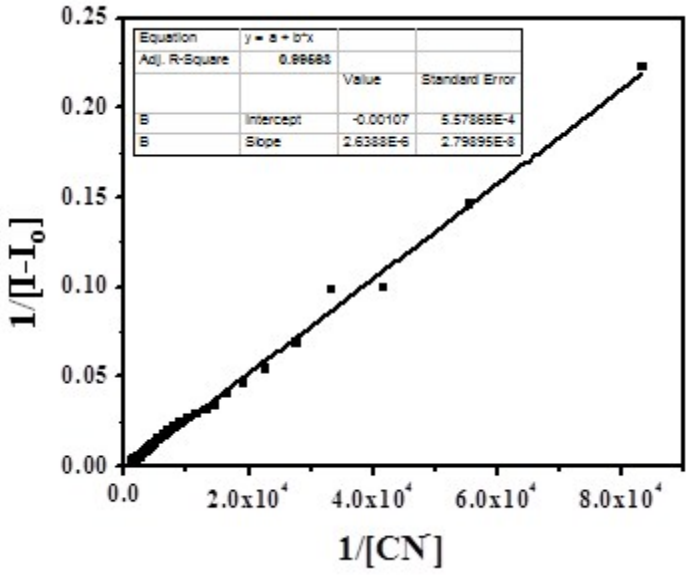


Figure S11: Benesi-Hildebrand plot from emission titration data of receptor (20 μM) with CN^- in CH_3OH.

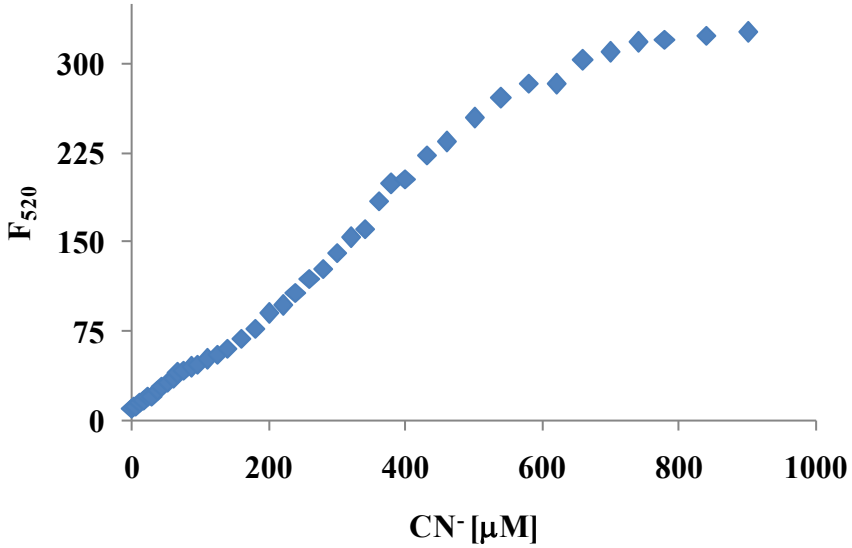


Figure S12. Plot of emission intensity at 520 nm (F_{520}) vs [CN^-] ions of probe **1** (20 μM, CH_3OH)

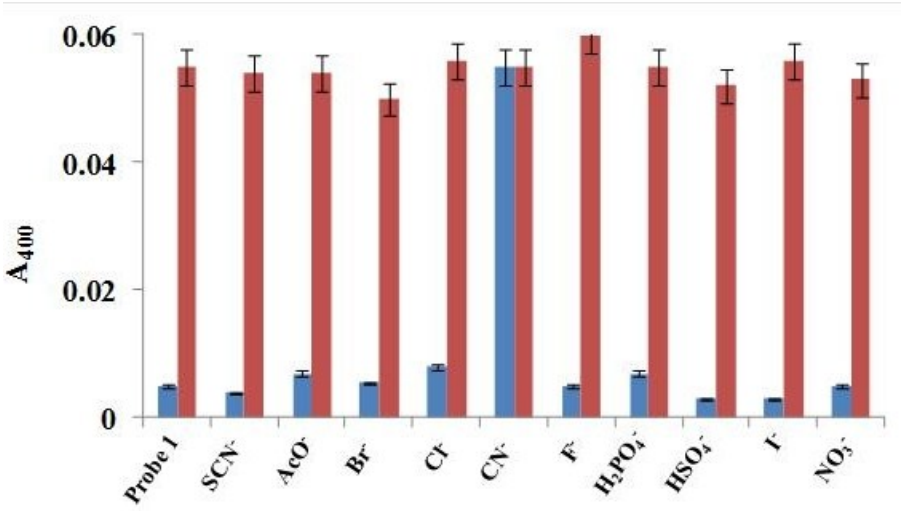
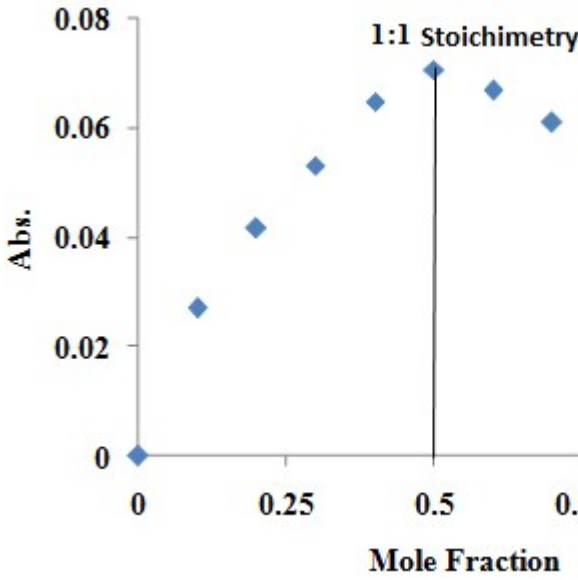


Figure S13. Blue bars represent selectivity of probe **1** (20 μM) upon addition of different anions in CH_3OH and red bars shows the competitive selectivity of probe **1** in the presence of CN^- .



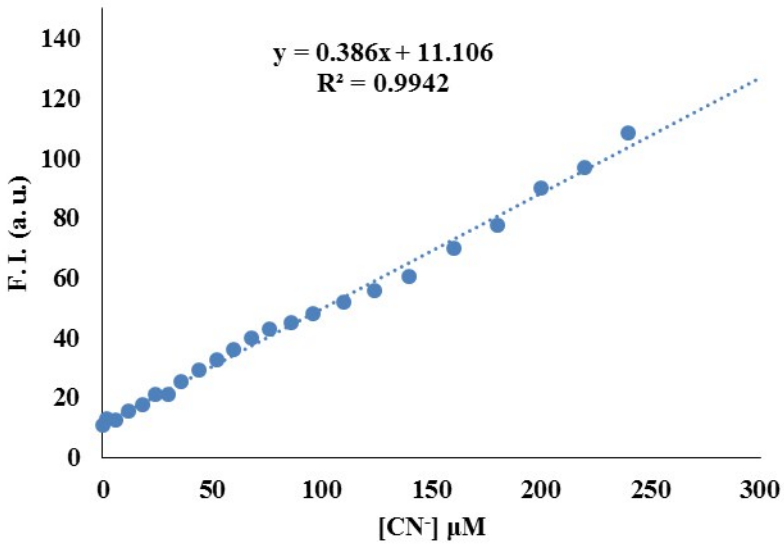


Figure S14: Job's plot diagram of probe **1** with Al^{3+} in CH_3OH.

Figure S15: linear dependence of emission for probe **1** with concentration of CN^- ions from 2-240 μM.

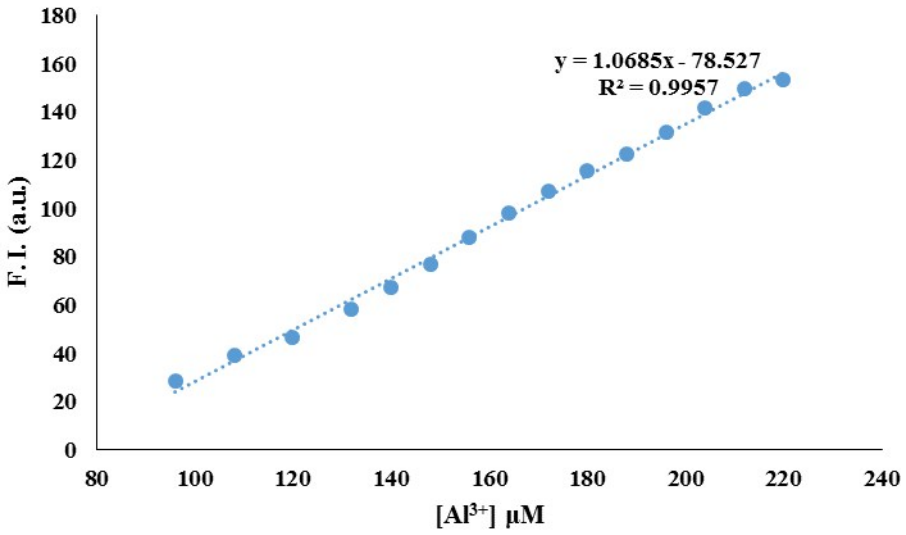
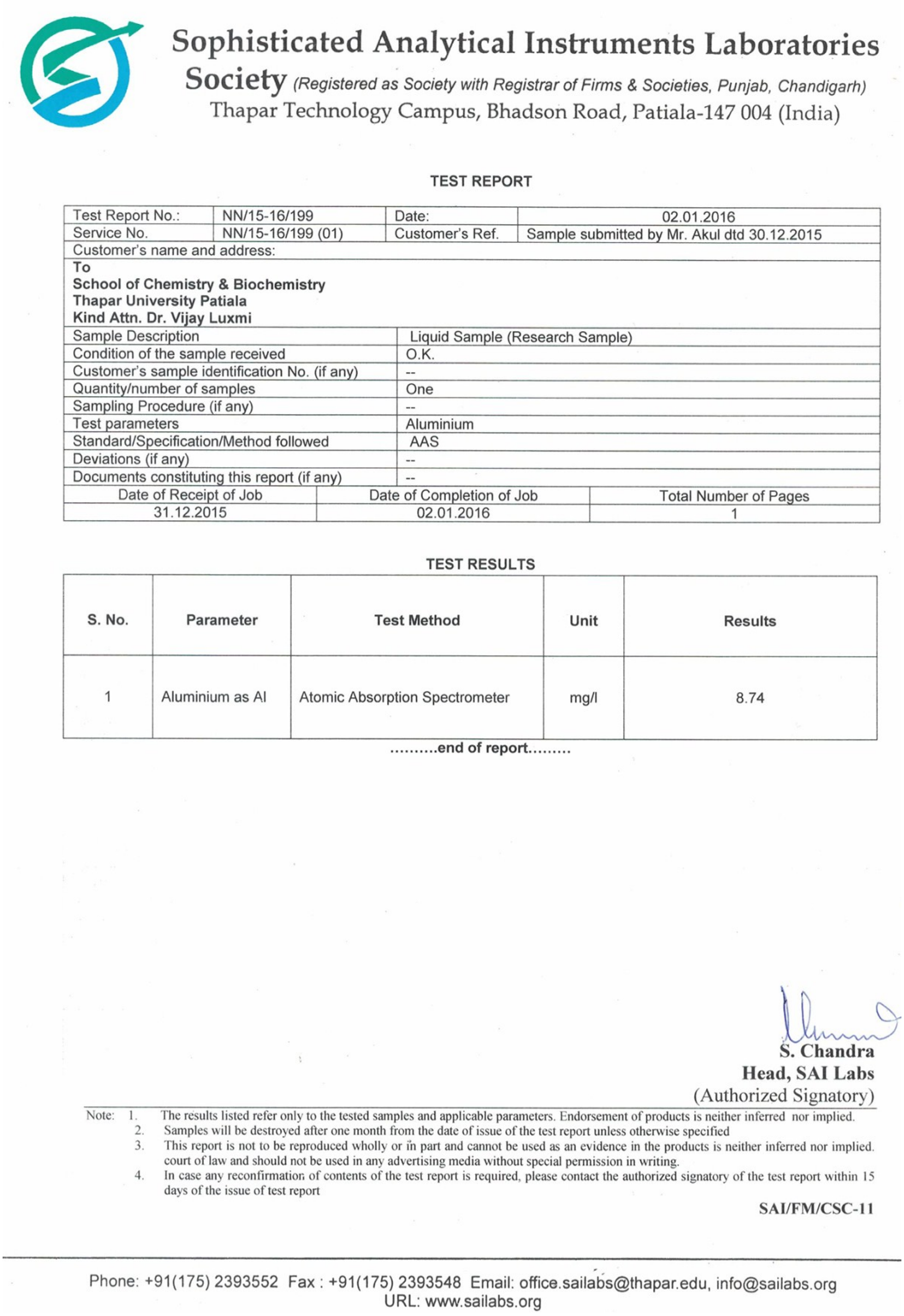


Figure S16: linear dependence of emission for probe **1** with concentration of Al^{3+} ions from 95-220 μM for Al^{3+} ions



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TEST REPORT

Test Report No.:	NN/15-16/199	Date:	02.01.2016
Service No.	NN/15-16/199 (01)	Customer's Ref.	Sample submitted by Mr. Akul dtd 30.12.2015
Customer's name and address:			
To **School of Chemistry & Biochemistry** **Thapar University Patiala** **Kind Attn. Dr. Vijay Luxmi**			
Sample Description		Liquid Sample (Research Sample)	
Condition of the sample received		O.K.	
Customer's sample identification No. (if any)		--	
Quantity/number of samples		One	
Sampling Procedure (if any)		--	
Test parameters		Aluminium	
Standard/Specification/Method followed		AAS	
Deviations (if any)		--	
Documents constituting this report (if any)		--	

Date of Receipt of Job	Date of Completion of Job	Total Number of Pages
31.12.2015	02.01.2016	1

TEST RESULTS

S. No.	Parameter	Test Method	Unit	Results
1	Aluminium as Al	Atomic Absorption Spectrometer	mg/l	8.74

.....end of report.....

S. Chandra
Head, SAI Labs
(Authorized Signatory)

Note: 1. The results listed refer only to the tested samples and applicable parameters. Endorsement of products is neither inferred nor implied.
2. Samples will be destroyed after one month from the date of issue of the test report unless otherwise specified
3. This report is not to be reproduced wholly or in part and cannot be used as an evidence in the products is neither inferred nor implied. court of law and should not be used in any advertising media without special permission in writing.
4. In case any reconfirmation of contents of the test report is required, please contact the authorized signatory of the test report within 15 days of the issue of test report

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Figure S17: Al^{3+} detection by the standard method.

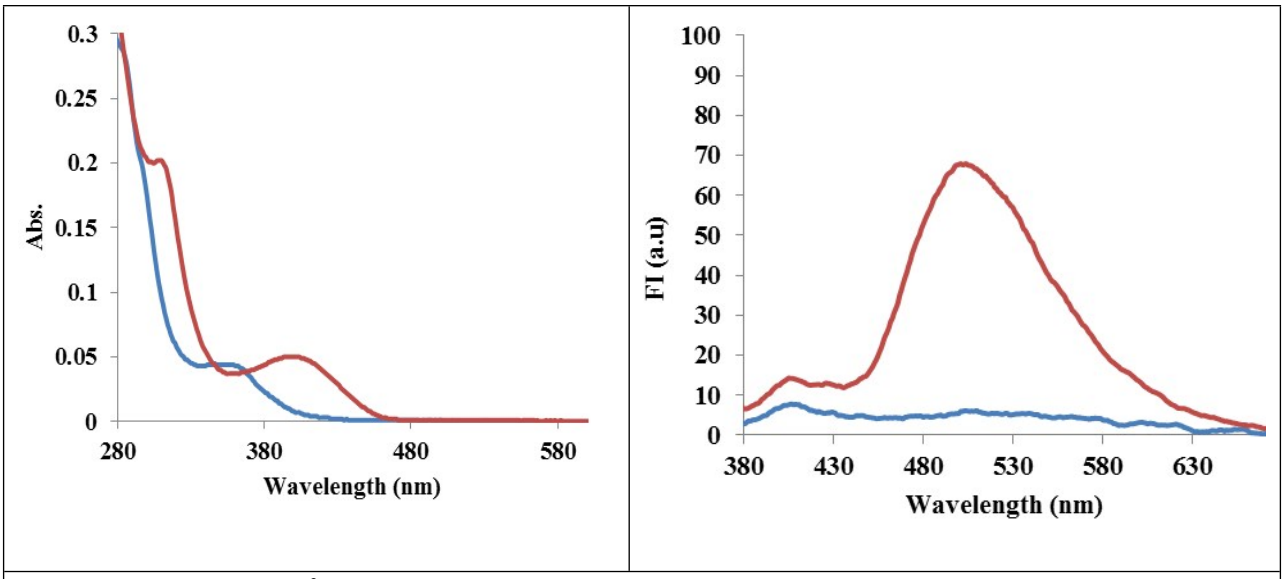

Figure S18: Effect of Al^{3+} ions on absorption and emission spectrum of probe **1** (20 μM, H_2O).