Supplementary Information

Photophysical aspects of BODIPY-Coumarin conjugated sensor and detection of Al^{3+} in MCF-7 cell

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Fig. S1: ^{1}H-NMR spectra of compound 3($CDCl_3$, 400 MHz)

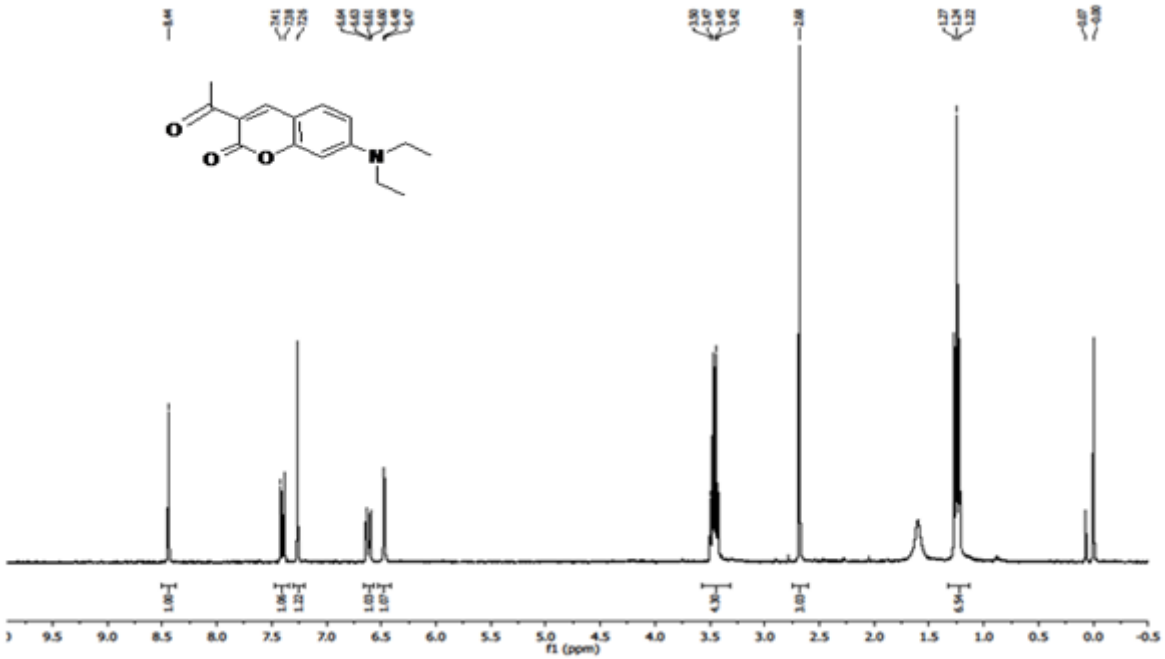


Fig.S2:^{1}H-NMR spectra of ($CDCl_3$, 400 MHz) compound 2

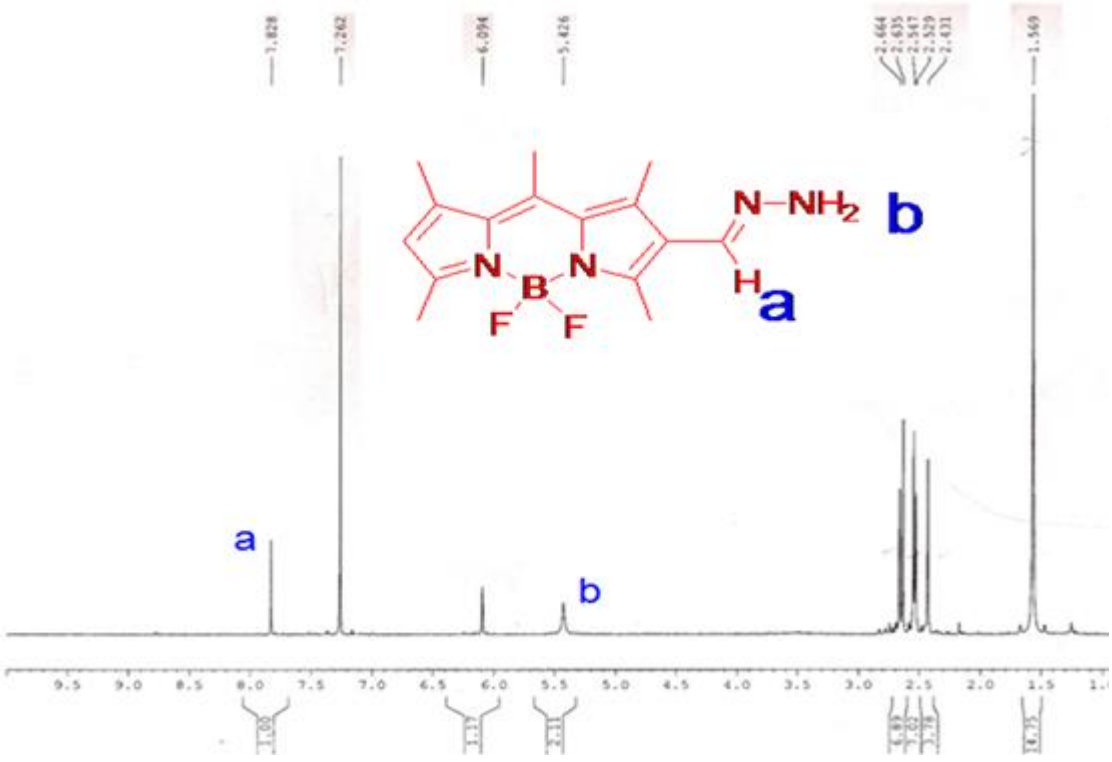


Fig. S3: ^{1}H-NMR spectra of R1 ($CDCl_3$, 400 MHz)

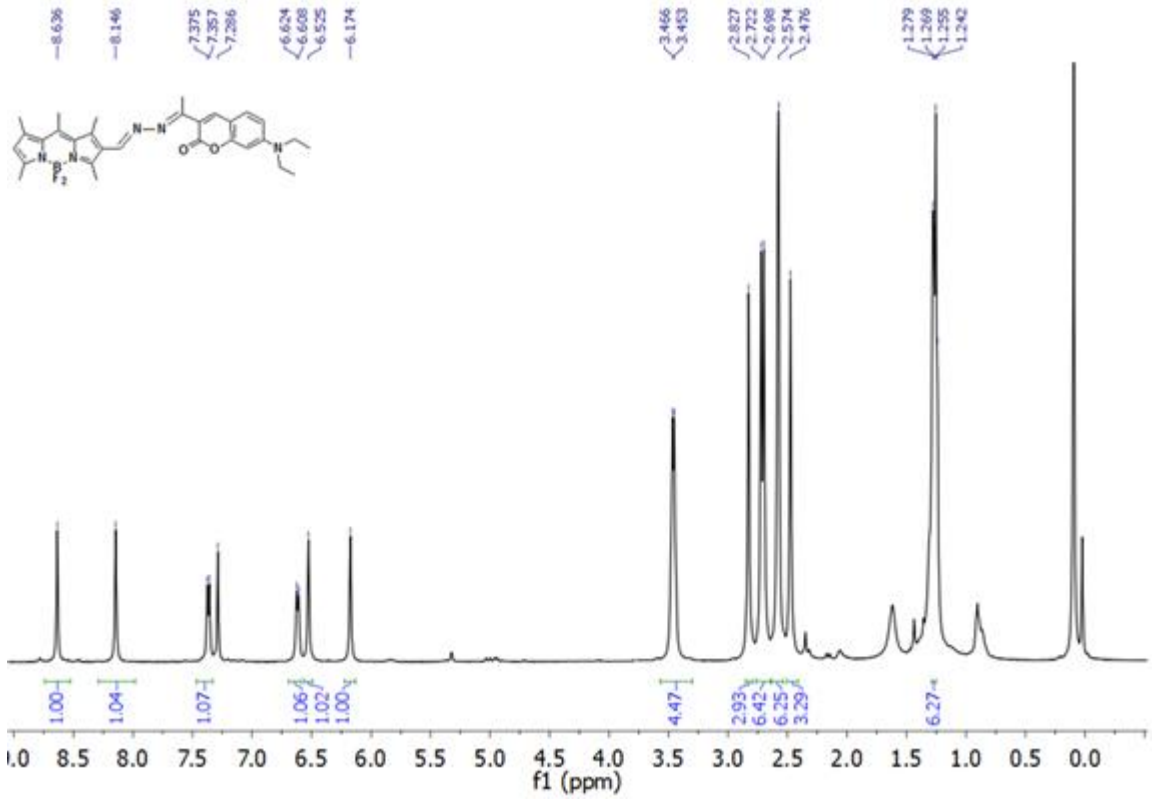


Fig.S4: ^{1}H-NMR spectra of R1:Al^{3+} ($CDCl_3$, 500 MHz)

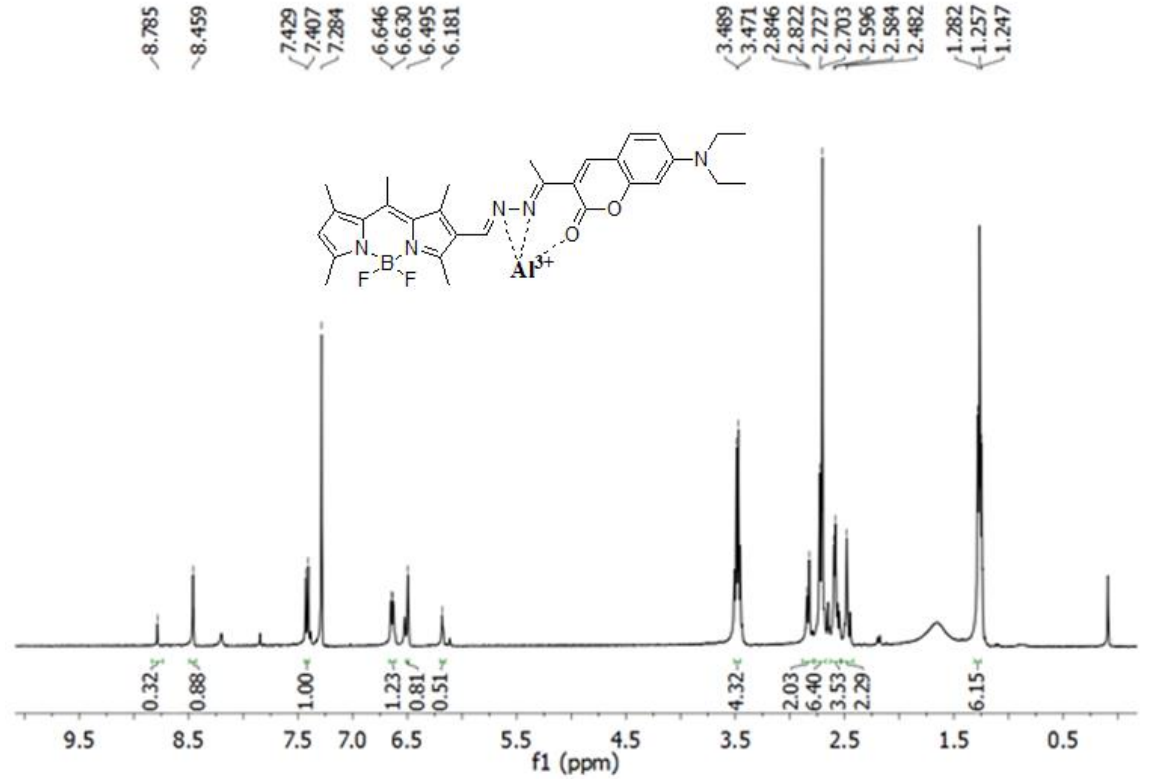


Fig. S5: ^{13}C NMR of compound 2

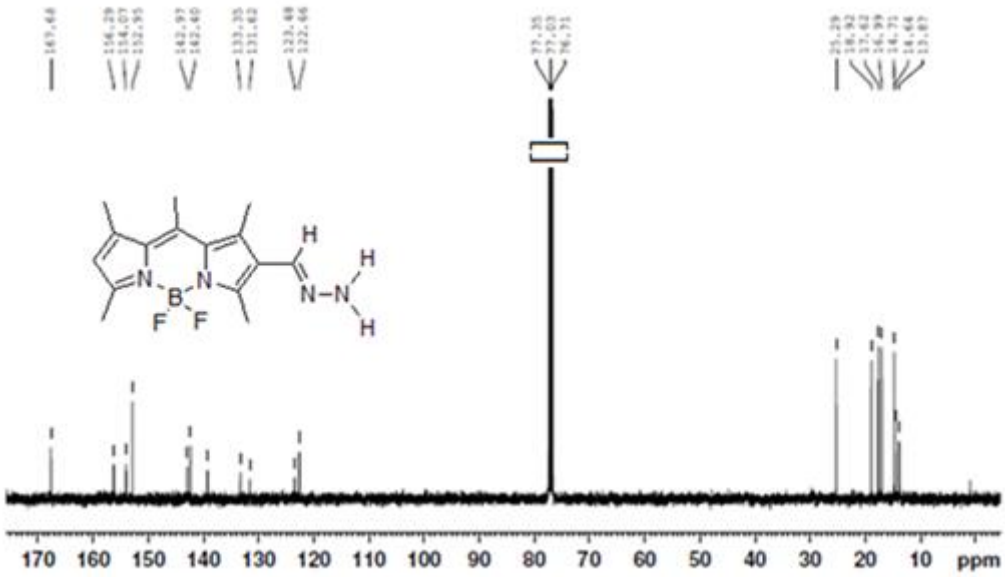


Fig. S6: ^{13}C NMR of compound 3

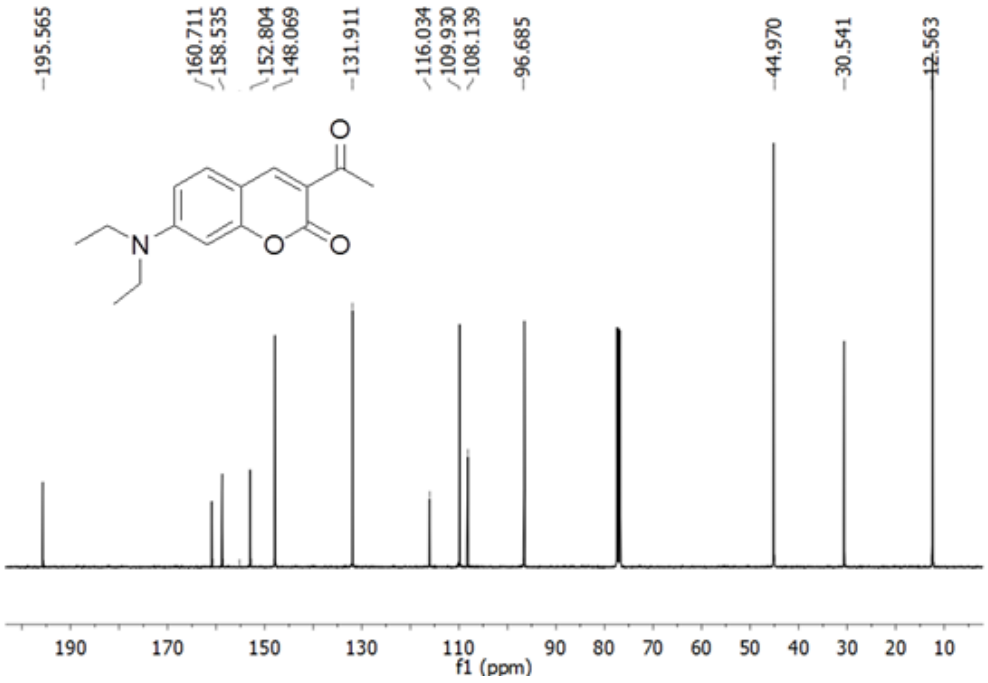


Fig. S7: ^{13}C NMR of R1

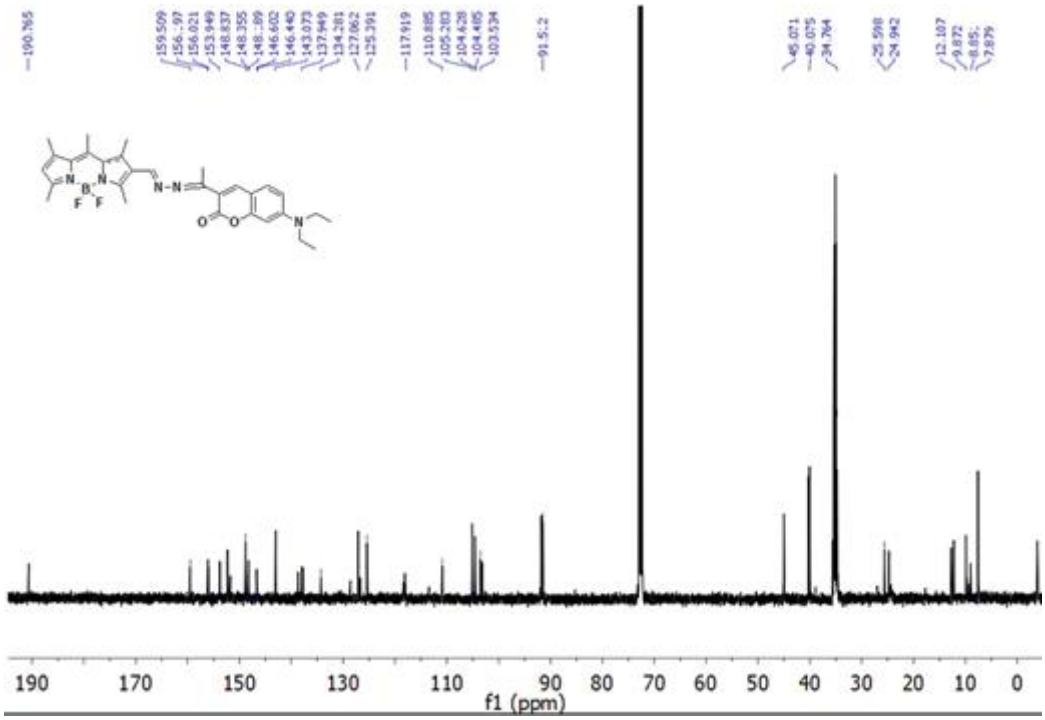


Fig. S8: LC-MS of compound 2 (m/z,%): calculated For $C_{23}H_{25}BF_2N_4$; 304.5, **found**: 303.5 [compound 2-H^+]

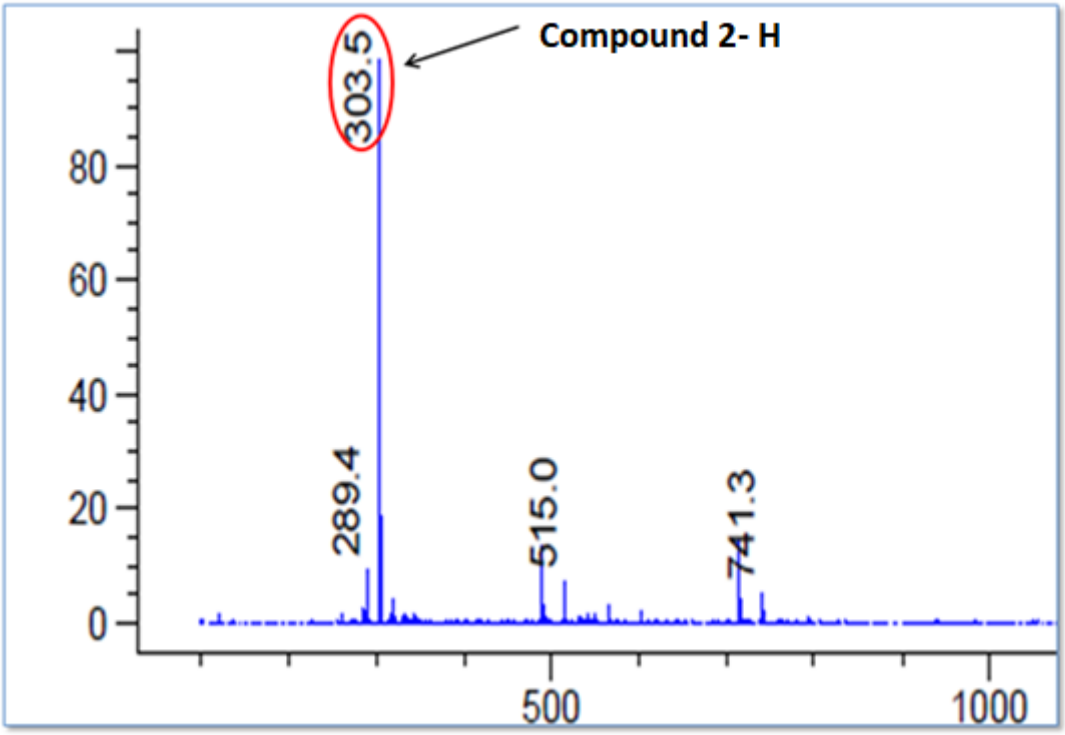


Fig. S9: ESI-MS of R1 (m/z,%): Calculated 545.2771**; found** 546.2871 **(**R1+H^+)

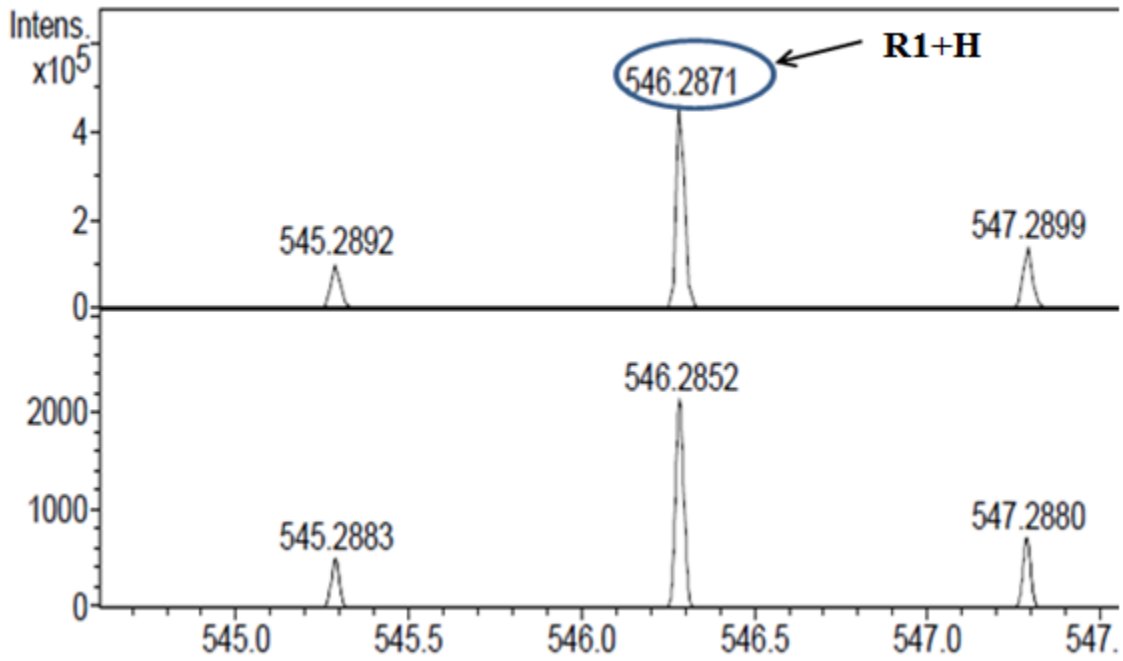


Fig. S10:LCMS-MS of R1:Al^{3+} (m/z,%): Calculated 572.2**; found** 590.3 **(**R1+Al^{3+}+H_2O)

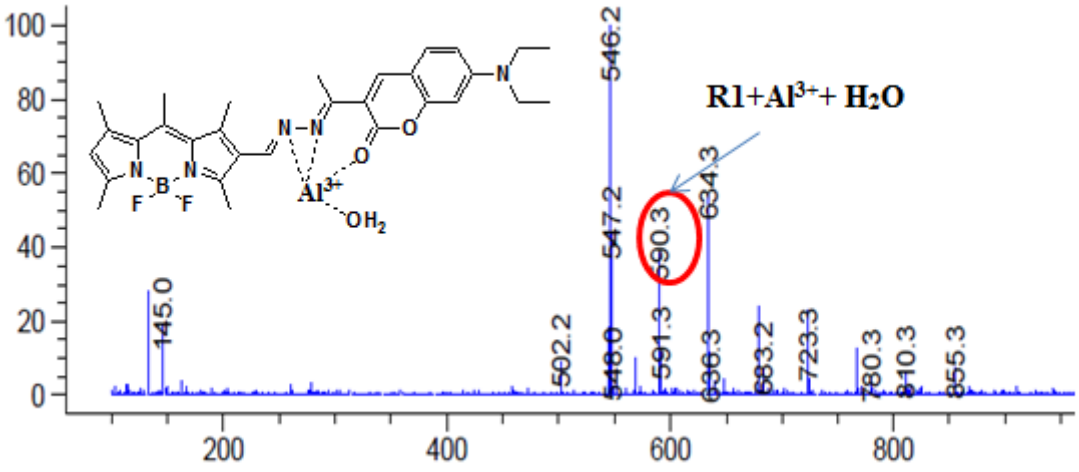


Fig. S11: FTIR spectra of R1:

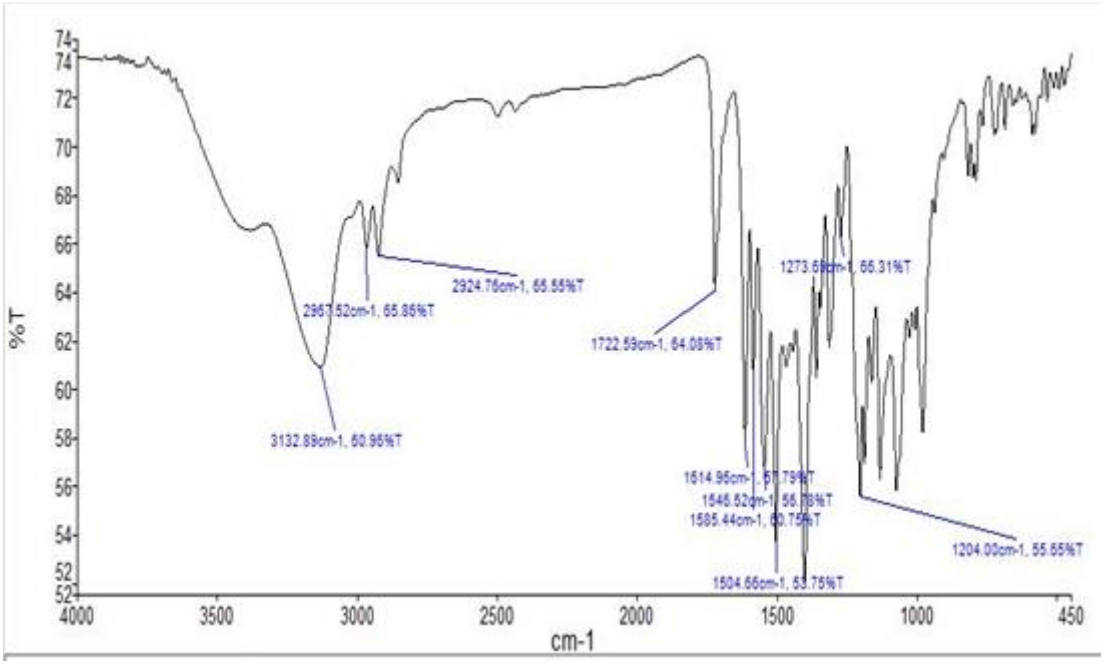
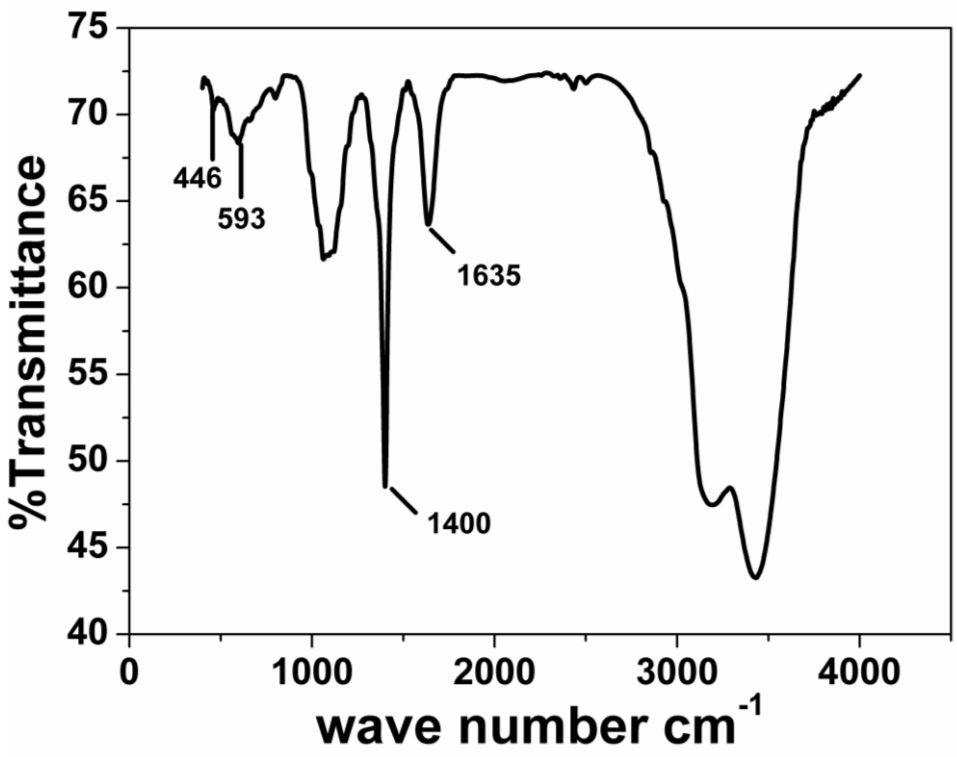


Fig. S12: FTIR spectra of R1:Al^{3+}



Binding Constant calculation (Fluorescence)

Binding constant (Ka) analysis was calculated by using Benesi-Hildebrand linear regression analysis subsequent equation (i).

$$1/(I - I_0) = 1/(I_\infty - I_0)K_a[G] + 1/(I_\infty - I_0)\ ) \qquad \ldots\ldots\ldots\ldots \text{ eqn. (i)}$$

$I = (I - I_0)$, $(1/\Delta I)$ = reciprocal of intensity difference, was plotted against the reciprocal of concentration of guest (1/[G]),association constant K_a = intercept/slope.

The binding constant (K_a) plot was calculated by plotting $1/\Delta I$ against1//[Al^{3+}]. The binding constant of complex R1:Al^{3+} were obtained $4.6x10^4$.

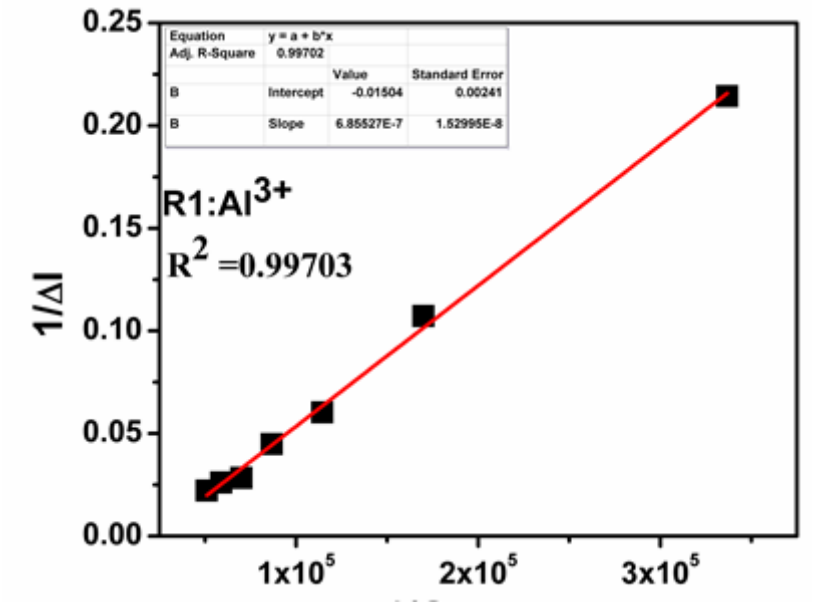


Fig. S13: Binding constant calculation was calculated using fluorescence spectra (a) plot with **R1:Al^{3+}**

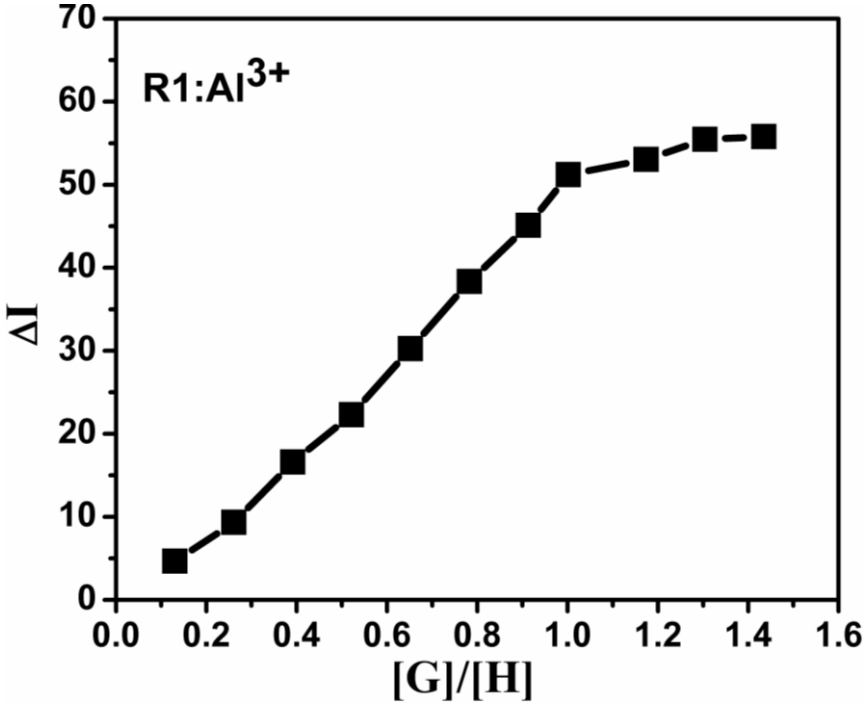


Fig.S14: Titration curve of **R1** with different concentration of metal ions using Fluorescence technique (a) **R1:Al^{3+}**

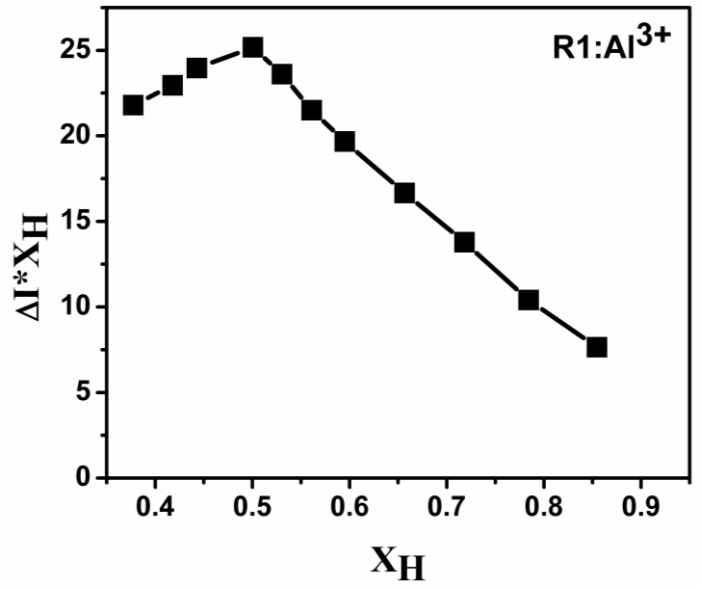


Fig.S15: Ratiometric analysis of complex using fluorescence technique by Job's plots in CH_3CN (a) **R1:Al^{3+}.**

Calculation of limit of detection (LOD):

The limit of detection of **R1:Al^{3+}**was calculated through fluorescence titration data. The limit of detection was calculated by using following equation.

$$LOD = K \times SD/S$$

Where, SD is the standard deviation of the receptor (**R1)** solution is 0.52, K= 2or 3 (we take 2 in this case) and S is the slop of the calibration curve.

For **R1**:Al^{3+} We obtained slop value = 2.5 x10^{6} respectively from linear fit graph. By using above formula we get the value of limit of detection of **R1**: $Al^{3+}$is 4.1x10^{-7}M.

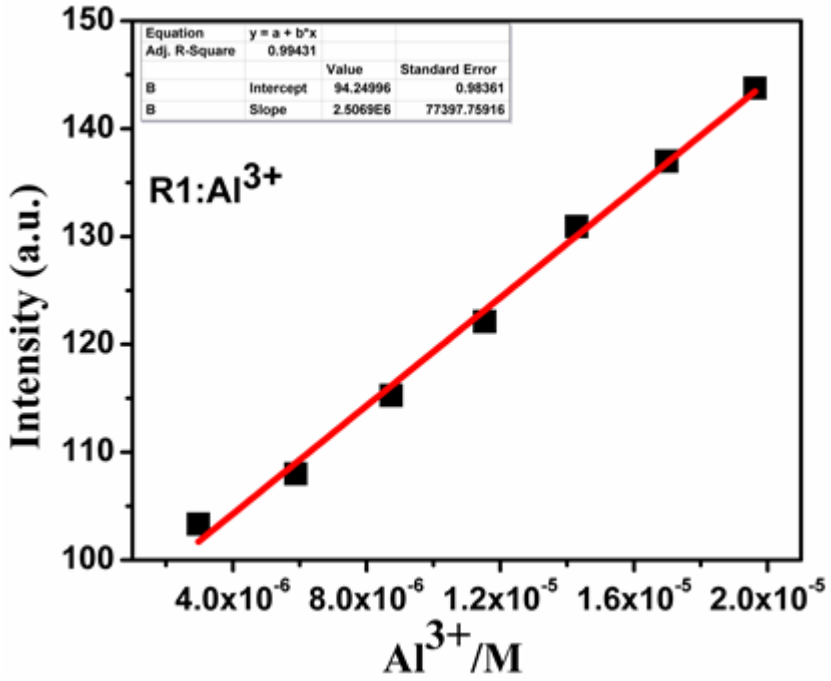


Fig.S16: LOD of **R1** towards **R1: Al^{3+}.**

pH studies

pH titration experiment was carried out in the presence and absence of metal ions for investigating practical application of sensor. **R1** was stable in between 6-13 pH range and maximum peak intensity was found at pH 1 due to protonation of **R1**. The intensity of **R1** was almost decreased at basic condition. In the presence of **Al^{3+}** ion the maximum fluorescence intensity was appeared at pH range at 7 and complex **R1: Al^{3+}** produced pink fluorescent. So, **R1** was applicable in biological environment for detecting of **Al^{3+}** ion.

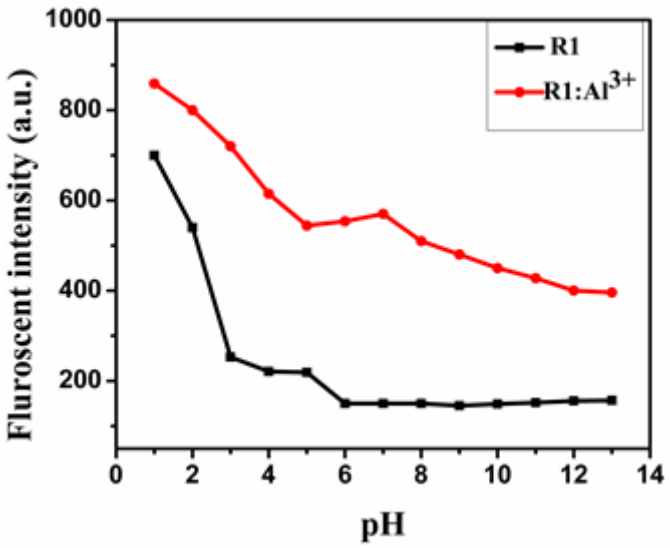
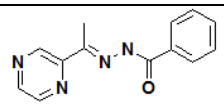
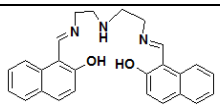
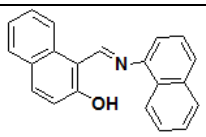
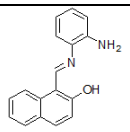
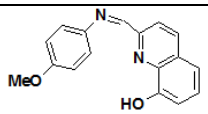
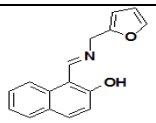
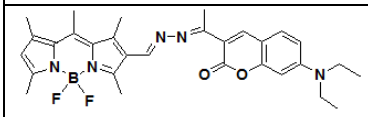


Fig. S17: pH titration curve in the presence and absence of metal ions (a) **R1** at 598 nm.

Table for comparing chemosensor for **Al^{3+}** ion.

Sensors	Detection of limit (μM)	Ref
	0.1	1
	0.1-0.3	2
	1	3
	0.1	4
	0.1	5

	0.6	6
	0.4	Present work

References

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