Electronic Supporting Information (ESI)

1. EXPERIMENTAL

Materials

All the experimental procedures are done under aerobic condition. High-purity PBS, 2-Hydroxy-1-napthaldehyde, Salisaldehyde, Diethyl acetelenedicarboxylate, Triphenylphophine, Hydrazine and DMSO were purchased from Sigma–Aldrich (India) (Technical grade). NaOCl and $Y(NO_3)_3.6H_2O$ was purchased from Merck (India). The solvents used were of spectroscopic grade. Other chemicals were of analytical reagent grade and used without further purification unless specified otherwise. Mili-Q Milipore 18.2 $M\Omega cm^{-1}$ water was used whenever required.

Physical measurements

Physical measurements have been carried out using below mention instruments. A Shimadzu Multi Spec 2450 spectrophotometer was used for recording UV-Vis spectra. FTIR spectra were recorded on a Shimadzu FTIR (model IR Prestige 21 CE) spectrophotometer. High resolution mass spectra are measured using Xevo G2S/Q-Toff. micro™ spectrometer. ^{1}HNMR spectra are recorded in DMSO-d_6 and $CDCl_3$ usingw a Bruker Advance 400 (400 MHz) instrument. The steady state emission and excitation spectra were recorded with a Hitachi F-4500 spectrofluorimeter. Elemental analysis was performed on a Perkin Elmer 2400 CHN analyzer. A Systronics digital pH meter (model 335) was used for pH measurement. FluoroCube-01-NL spectrometer using a Laser-diode (Model: DD-450L-8666, typical FWHM ~ 170 ps, λ_{ex} = 336 nm) was used for Time-resolved fluorescence lifetime measurements.

2. Spectroscopic characterization

A. Ligand A2 (8-Hydrazonomethyl-2-oxo-2H-chromene-4-carboxylic acid methyl ester)

A2 has molecular formula $C_{12}H_{10}N_2O_4$ (MW, 246.22). Anal. found (%): C, 58.54; H, 4.09 and N, 11.38; Cal(%),C, 57.97; H, 4.03 and N, 11.13. ESI-MS (*m/z*): $[M+H]^+$, 247.07; [Figure S1a]. FTIR (KBr, Cm^{-1}): 3500.75, *ν*(N–H, stretch); 3075.34, *ν*(C–H, Aromatic); 3046.76, *ν*(C–H, sp^2); 2923.65, *ν*(C–H, sp^3); 1736.37, *ν*(C=O, stretch); 1673.76, *ν*(C=N, stretch); 1583.87, *ν*(C=C, stretch); 1434.95, *ν*(C–O, stretch).[Figure S1b] ^{1}H NMR ($CDCl_3$, 500 MHz, *J*, Hz, δ ppm,

reference peak 7.26 ppm) [Figure S1c and S1d]: 10.473 (1H, s, =CH); 4.132 (3H, s, -CH_3); 1.905 (2H, s, -NH_2); and 7.162-8.002 (4H, m, Aromatic protons).

B. Ligand A3 (8-[(2-Hydroxy-naphthalen-1-ylmethylene)-hydrazonomethyl]-2-oxo-2H-chromene-4-carboxylic acid methyl ester)

A3 has molecular formula $C_{23}H_{16}N_2O_5$ (MW, 400.38). Anal. found (%): C, 69.00; H, 4.03 and N, 7.00; Cal(%),C, 68.89; H, 4.02 and N, 6.94. ESI-MS (*m/z*): $[M+H]^+$, 401.27; $[M+Na]^+$, 422.13 [Figure S2a]. FTIR (KBr, Cm^{-1}): 3521.43-3646.76, *v*(O–H, stretch); 2970.65, *v*(C–H, Aromatic); 2789.86, *v*(C–H, sp^3); 1694.34, *v*(C=O, stretch); 1638.76, *v*(C=N, stretch); 1520.45, *v*(C=C, stretch); 1395.67, *v*(C–O, stretch)[Figure S2b]. ^1H NMR (DMSO-d_6, 500 MHz, *J*, Hz, δ ppm, reference peak 2.50 ppm) [Figure S2c and S2d]: 13.158 (1H, s, -OH); 10.830 (1H, s, =CH); 10.320 (1H, s, =CH); 3.532 (3H, s, -CH_3) and 7.139-8.372 (10H, m, Aromatic protons).

C. Ligand A3-OCl^- Adduct (Ad1)

Molecular formula: $C_{23}H_{20}N_2O_6Cl$. Anal. Found (%): C, 61.14; H, 3.57 and N, 6.20; Cal(%),C, 61.03; H, 3.56 and N, 6.17. ESI-MS (*m/z*): [**Ad1**+H] $^+$, 452.35, [**Ad1**+Na] $^+$, 474.25 [Figure S3a]. FTIR (KBr, Cm^{-1}): 3451.86, *v*(O–H, broad); 3066.43, *v*(C–H, Aromatic); 3066.43, *v*(C–H, Aromatic); 2907.14, *v*(C–H, sp^3); 1742.76, *v*(C=O, stretch); 1638.76, *v*(C=N, stretch); 1544.54, *v*(C=C, stretch) and 1391.34, *v*(C–O, stretch) [Figure S3b]

D. Ligand A3-Y^{3+} Adduct (Ad2)

Molecular formula: $C_{23}H_{19}N_4O_{13}Y$. Anal. Found (%): C, 42.63; H, 2.96; N, 8.62 and O, 32.07; Calculated (%), C, 42.61; H, 2.95 N, 8.64 and O, 32.08. ESI-MS (*m/z*): [**Ad2**+H] $^+$, 649.35 [Figure S4a] FTIR (KBr, Cm^{-1}): 3095.8, *v*(C–H, Aromatic); 2843.5, *v*(C–H, sp^3); 1739.2, *v*(C=O, stretch); 1748.3, *v*(C=O, stretch); 1570.9, *v*(C=C, stretch); 1445.5, *v*(C-H, bend.) and 1282.6, *v*(C–O, stretch) [Figure S4b]

3. General method of UV-*Vis* and fluorescence titration

For absorption and emission titration cell used having path length is 1 cm. Stock solutions of ligand, **OCl^-** and **Y^{3+}** are prepared in DMSO-water (1:7, v/v). Their working solutions are prepared from respective stock solutions via appropriate dilution. Fluorescence measurements are performed using 2.5 nm × 2.5 nm slit and 5 nm × 2.5 nm widths, where the excitation wavelength is (365nm and 440nm). All spectra are recorded at room temperature.

4. Job's plot from fluorescence experiment

The sets of solutions containing ligand(**A3**) and analyte($\mathbf{OCl^-}$) are prepared, that the concentration of ligand and analyte in total remain constant (5 μM) in all the sets. The mole fraction (X) of $\mathbf{OCl^-}$ is varied from 0.1 to 0.9. The emission intensity (at 484nm, λex 365nm) is plotted as a function of mole fraction of $\mathbf{OCl^-}$. Ligand forms **1:1** (mole ratio) adduct, this is also confirmed from their mass spectra. Similar method is applied for $\mathbf{Y^{3+}}$.

5. Determination of Binding constant:

The binding constants between ligand (**A3**) and $\mathbf{OCl^-}$ ions is determined through using a modified Benesi-Hildebrand equation[1]: $\mathbf{(F_{max}–F_0)/ (F_x–F_0) = 1+ (1/K) (1/[C]^n)}$ where, F_{max}, F_0 and F_x are emission intensities for ligand (**A3**) in presence of $\mathbf{OCl^-}$ ions at saturation, in absence of $\mathbf{OCl^-}$ ions and at any intermediate $\mathbf{OCl^-}$ ion concentrations, respectively. A plot of $(F_{max}–F_0)/(F_x–F_0)$ vs. $[C]^{-1}$ (here, n = 1.0) gives the binding constants (**K**) from the slope while [C] is molar concentration of analyte. Similar method is applied in case of $\mathbf{Y^{3+}}$ interaction with **Ad1**.

6. Calculation of detection limit

The detection limit (**DL**) is determined from the following equation[2]:

$$DL = \frac{3\sigma}{S}$$

σ is the standard deviation of the blank solution, **S** is the slope of the calibration curve.

For the determination of standard deviation the emission intensity of **A3** without any analyte was measured by 10 times[3].

7. Determination of quantum yield

The fluorescence quantum yields are determined using anthracene as reference having ϕ_R, 0.2 in MeOH[4]. The sample and the reference dye are excited at same wavelength (λex, 365 nm, in water-DMSO medium), maintaining nearly equal absorbance (0.1) and emission intensities. The area of the emission spectra are measured and the quantum yields are calculated following the equation[5], $\phi_S / \phi_R = [A_S/A_R] \times [(Abs)_R/(Abs)_S] \times [\eta_S^2/\eta_R^2]$, where ϕ_S and ϕ_R are fluorescence quantum yields of the sample and reference respectively, A_S and A_R are area under the

fluorescence spectra of the sample and the reference respectively, $(Abs)_S$ and $(Abs)_R$ are the corresponding optical densities of the sample and the reference solution at the wavelength of excitation; η_S and η_R are the refractive indices of the sample and reference, respectively[6].

8. Time resolved emission spectra measurements

Fluorescence lifetime was measured by the method of time correlated single photon counting (TCSPC) technique.The sample was excited using a picosecond diode laser and the fluorescence signal was recorded keeping the emission polariser at the magic angle (54.70) with respect to the excitation polariser to eliminate the loss of signal for the contribution of anisotropy decay and fluorescence decays were deconvoluted using DAS6 software.[7] The relative contributions (α_n) to the fluorescence decay of the multi exponential decay were obtained using the following relation.[8-9]

$$a_n = \frac{B_n}{\sum_{i=1}^{n} B_i}$$

B_i is the pre-exponential factor of a single exponential decay. The average lifetime of the compound was calculated using the following relation:

$$\langle \tau \rangle = \frac{\sum_{i=1}^{n} a_i t_i^2}{\sum_{i=1}^{n} a_i t_i}$$

Reference

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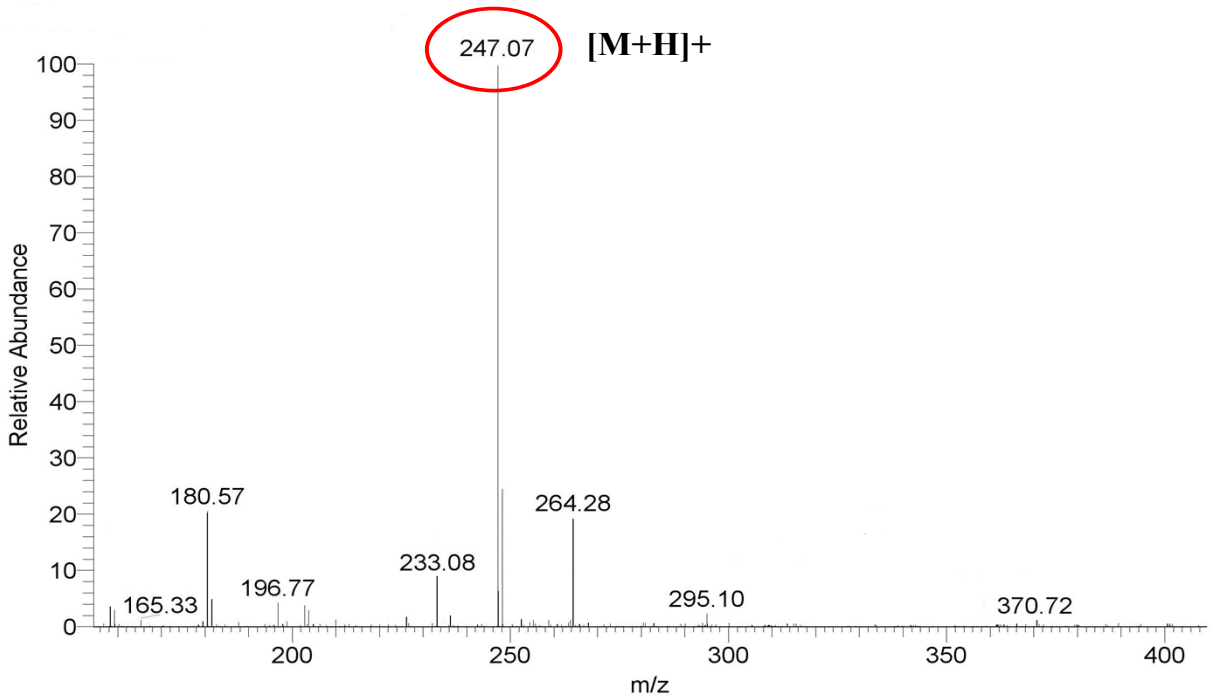

Figure S1a QTOF mass spectrum of **A2**

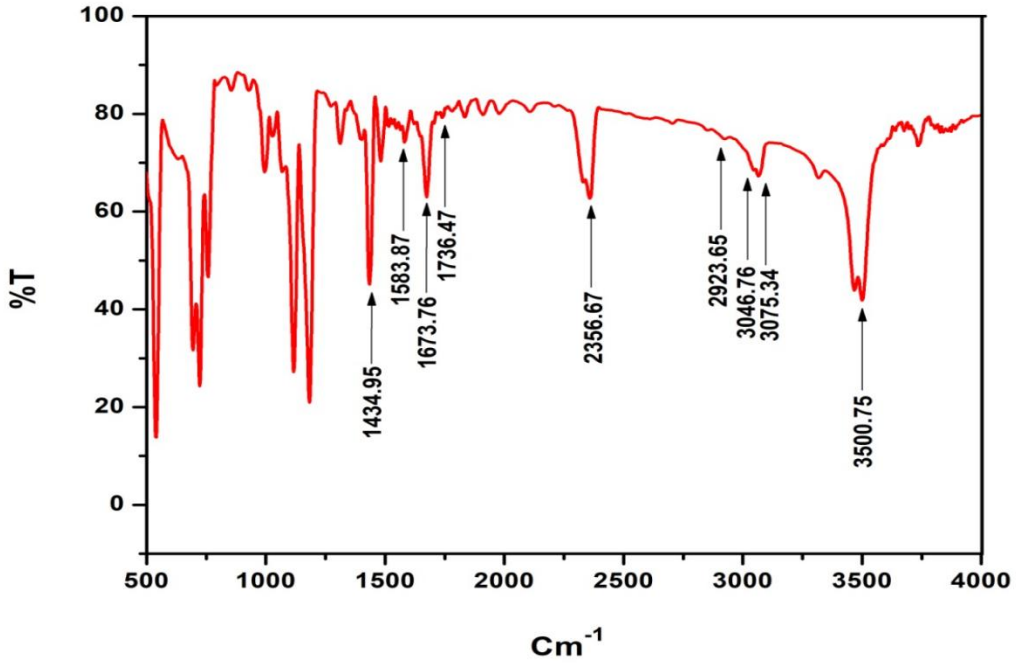

Figure S1b FTIR spectrum of **A2**

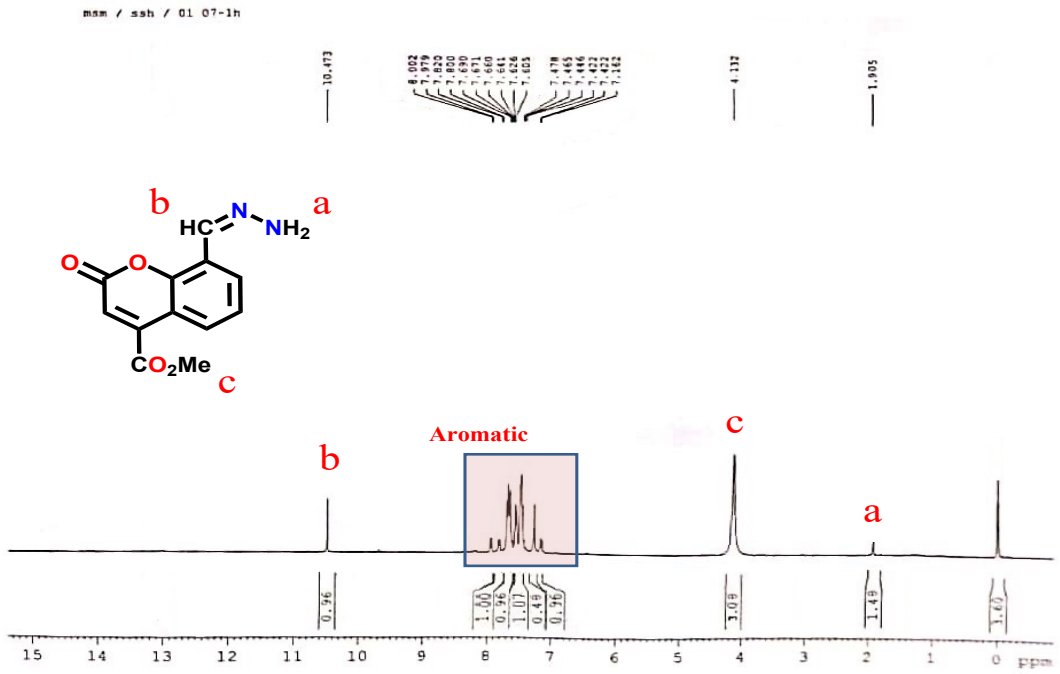

Figure S1c ^{1}H NMR spectrum of **A2** in $CDCl_3$

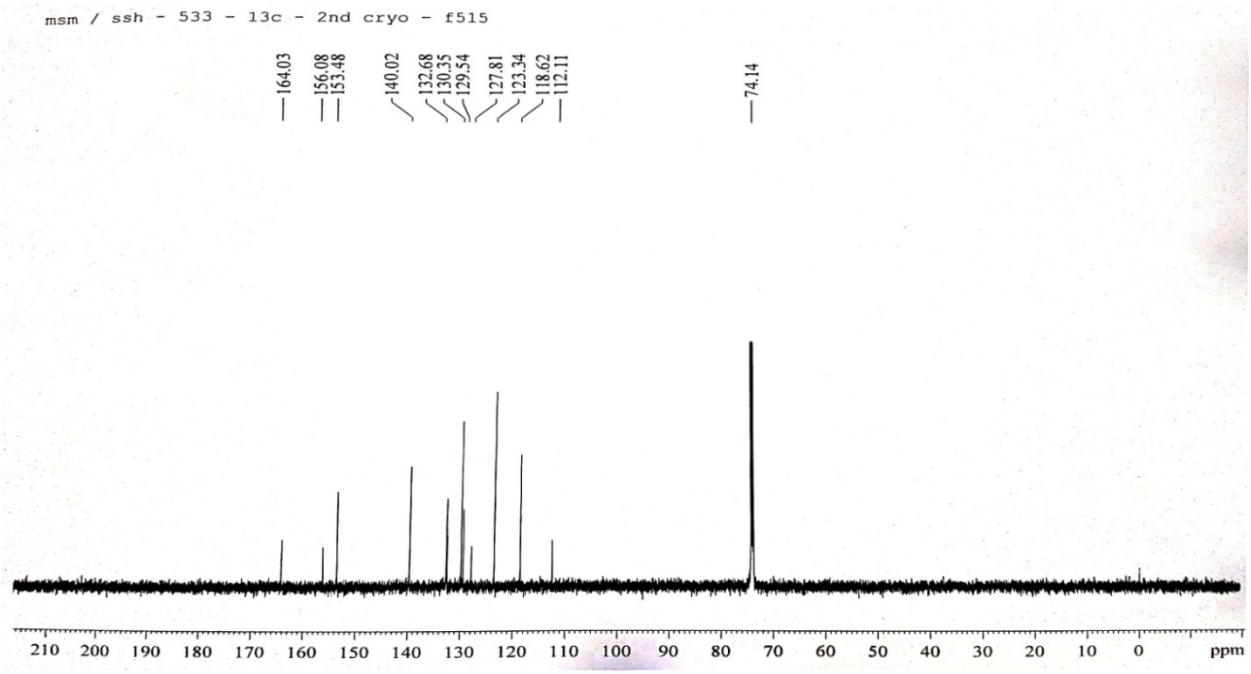

Figure S1d ^{13}C NMR spectrum of **A2** in $CDCl_3$

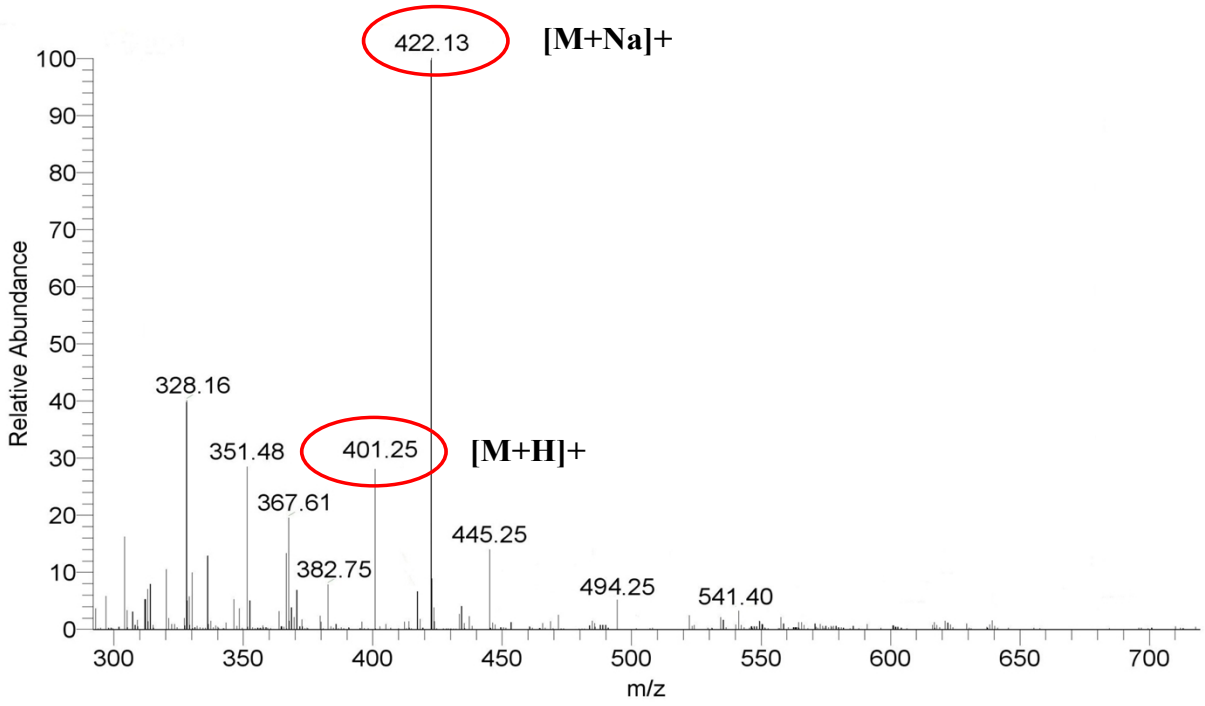

Figure S2a QTOF mass spectrum of **A3**

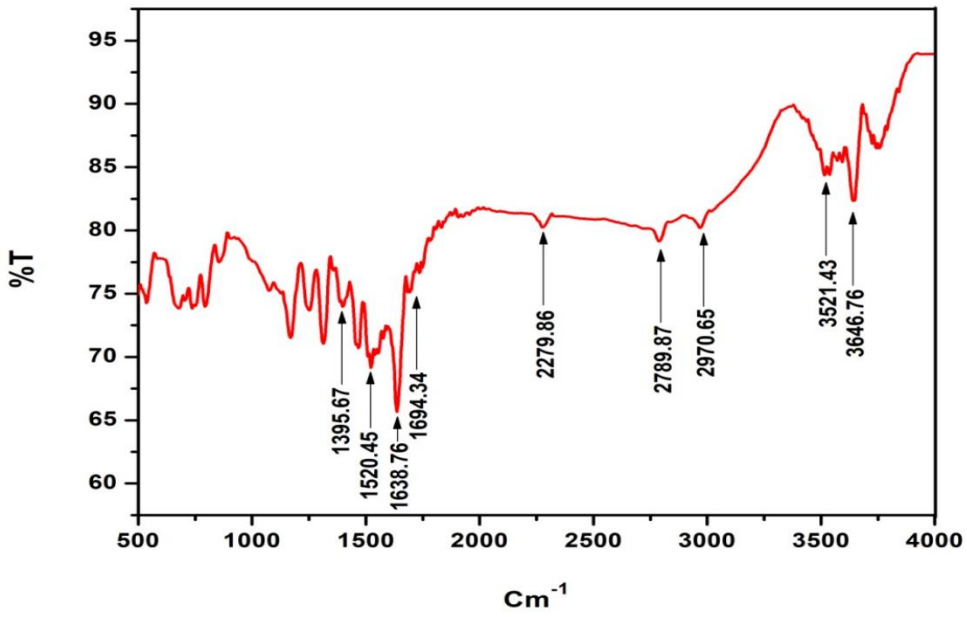

Figure S2b FTIR spectrum of **A3**

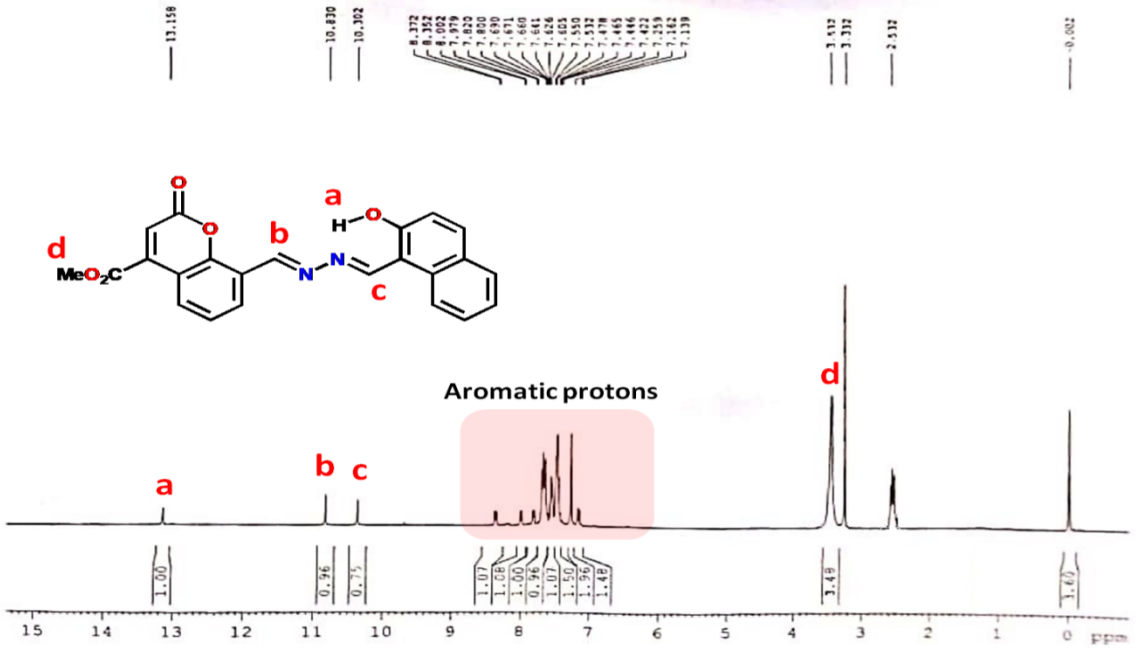

Figure S2c ^{1}H NMR spectrum of **A3** in DMDO-d_6

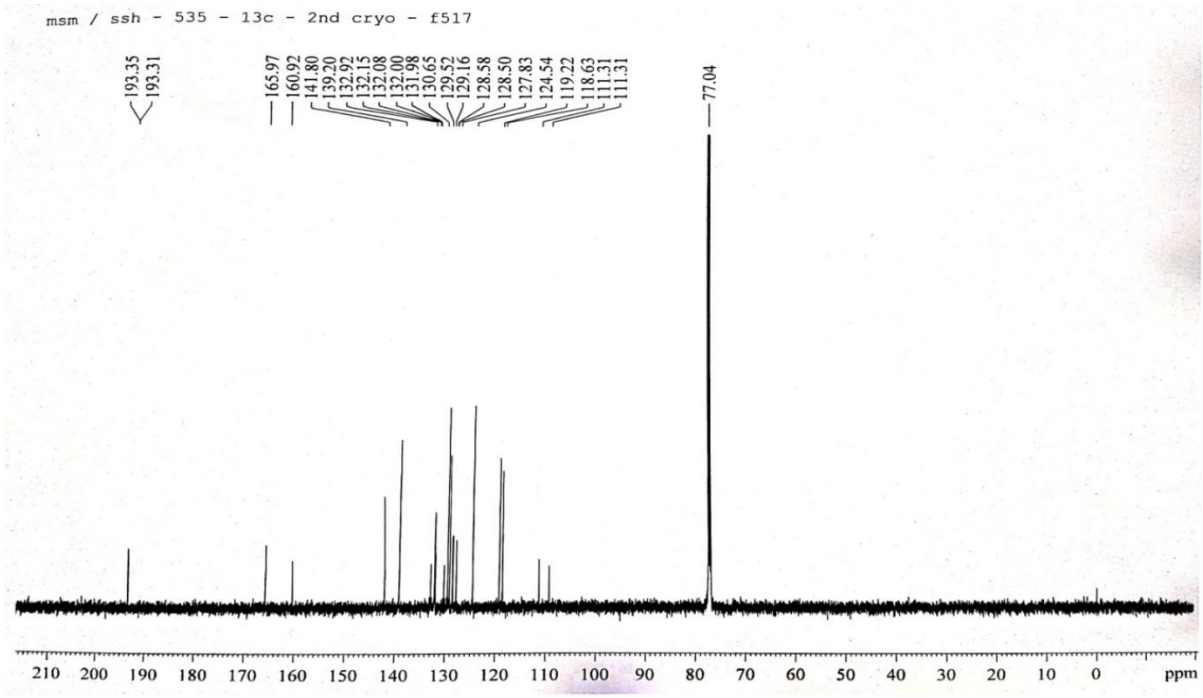

Figure S2d ^{13}C NMR spectrum of **A3** in $CDCl_3$

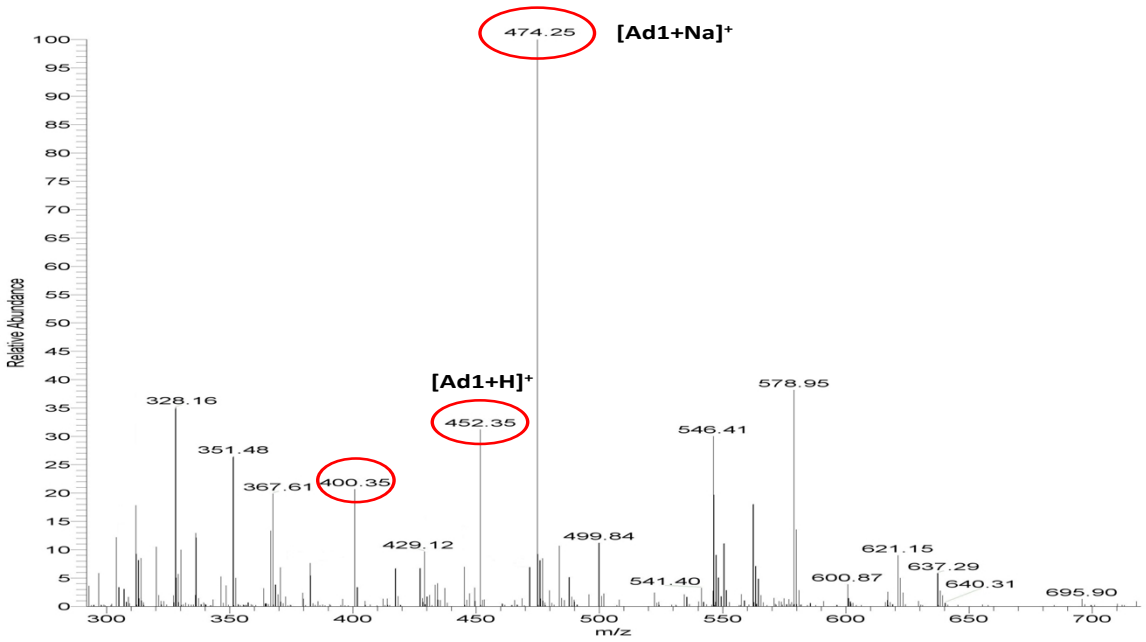

Figure S3a QTOF mass spectrum of **Ad1**

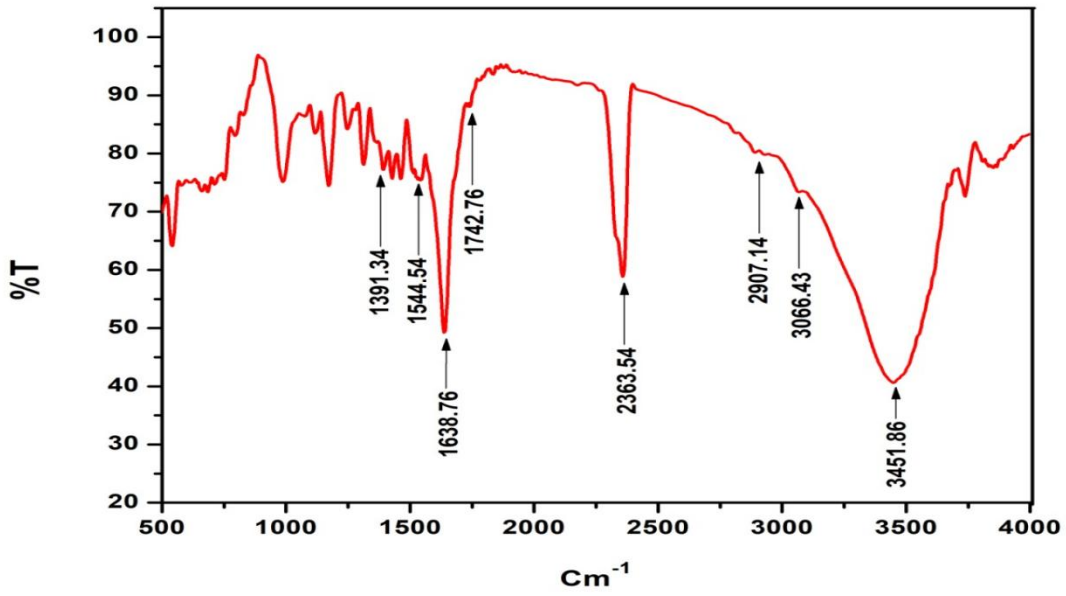

Figure S3b FTIR spectrum of **Ad1**

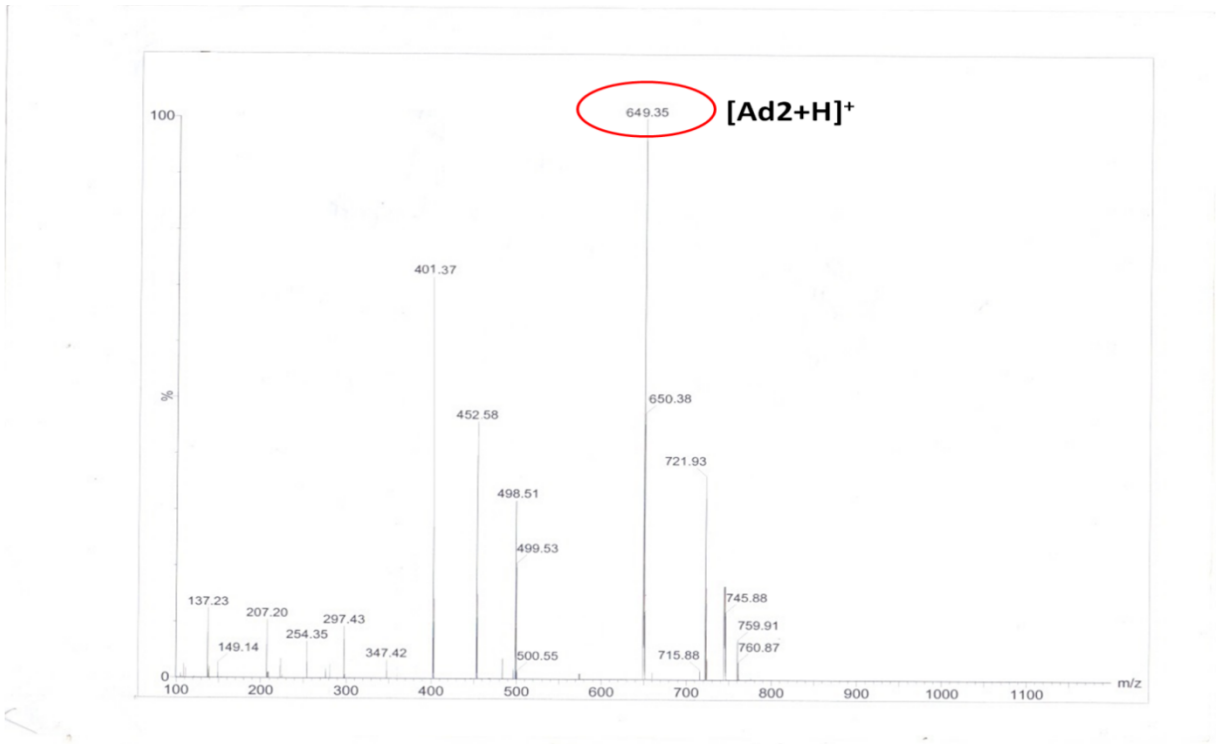

Figure S4a QTOF mass spectrum of **Ad2**

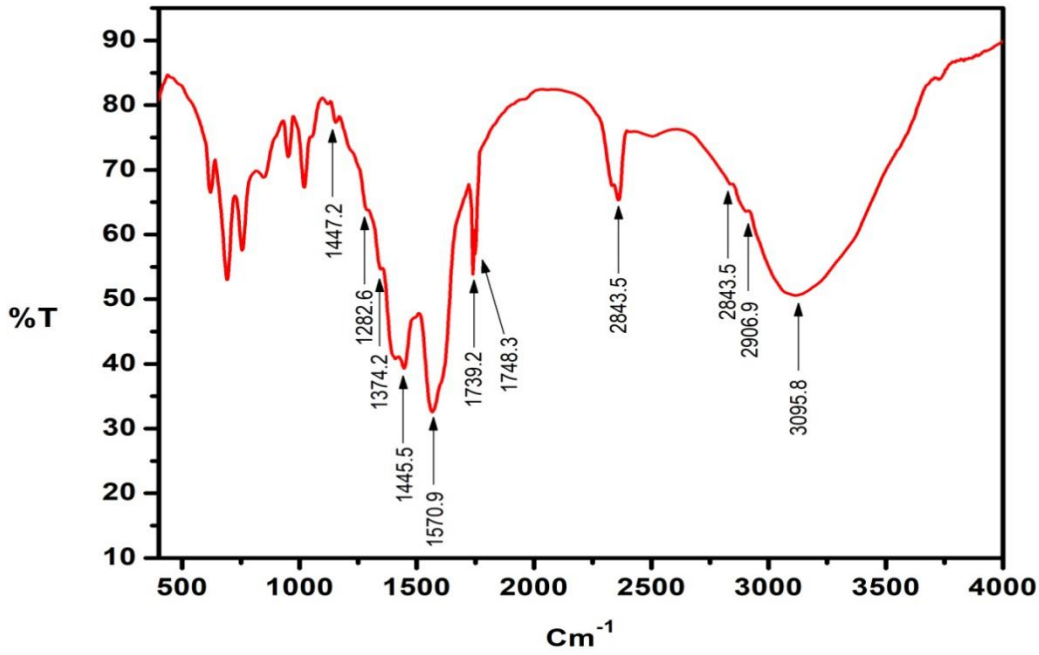

Figure S4b FTIR spectrum of **Ad2**

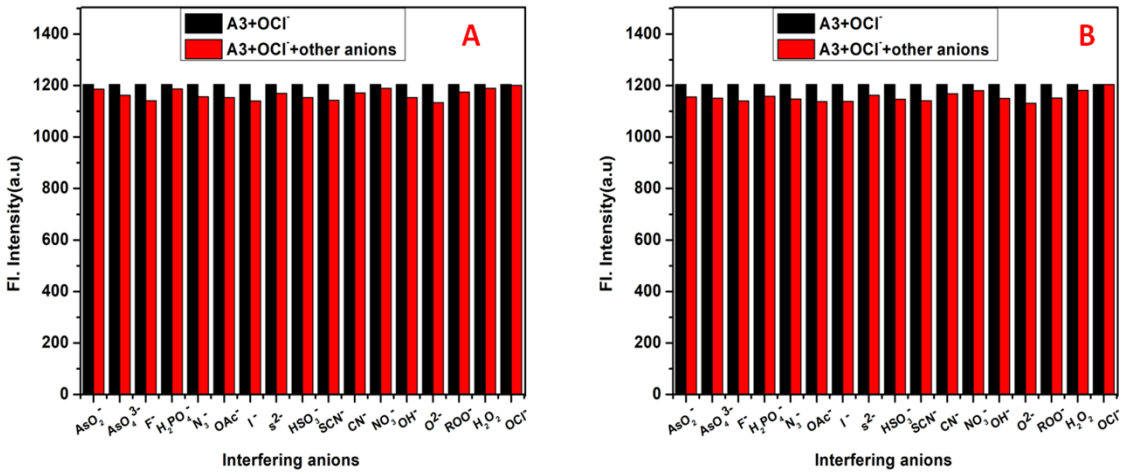

Figure S5 Interference studies for fluorescence detection of Y^{3+} (1500 μ M) using **A3** (20 μ M) with different ions (A) 1000μM each and (B)1500 μM each (λ_{ex} = 365 nm, λ_{em} = 484 nm).

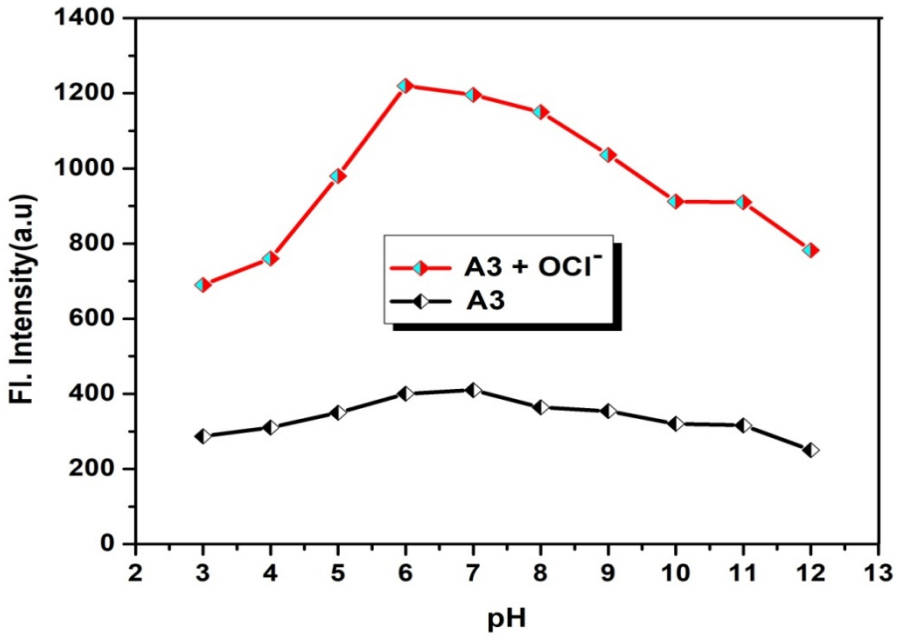

Figure S6 Effect of pH on the emission intensities of compound **A3,** (λ_{ex} = 365 nm λ_{em} = 484 nm) in presence and absence of **OCl⁻**

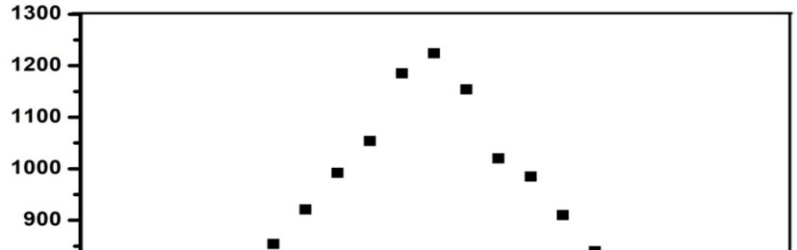

Figure S7 Job's plot for stoichiometry determination of [**A3-OCl$^-$**] complex, ($\boldsymbol{\lambda_{ex}}$ = 365 nm, $\boldsymbol{\lambda_{em}}$ = 484 nm.).

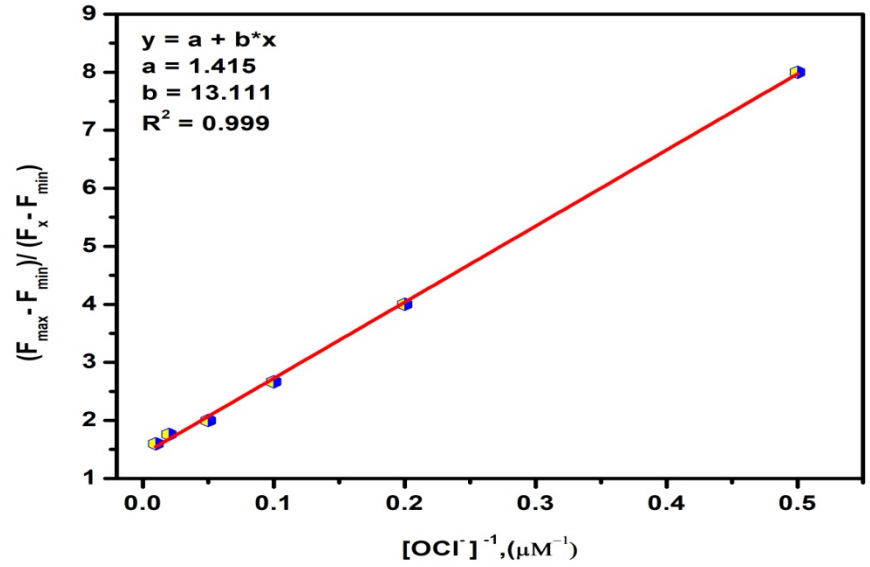

Figure S8 Benesi−Hildebrand plot for determination of association constant of compound **A3** with **OCl$^-$**(linier portion only), $\boldsymbol{\lambda_{ex}}$ = 365 nm, $\boldsymbol{\lambda_{em}}$ = 484 nm.

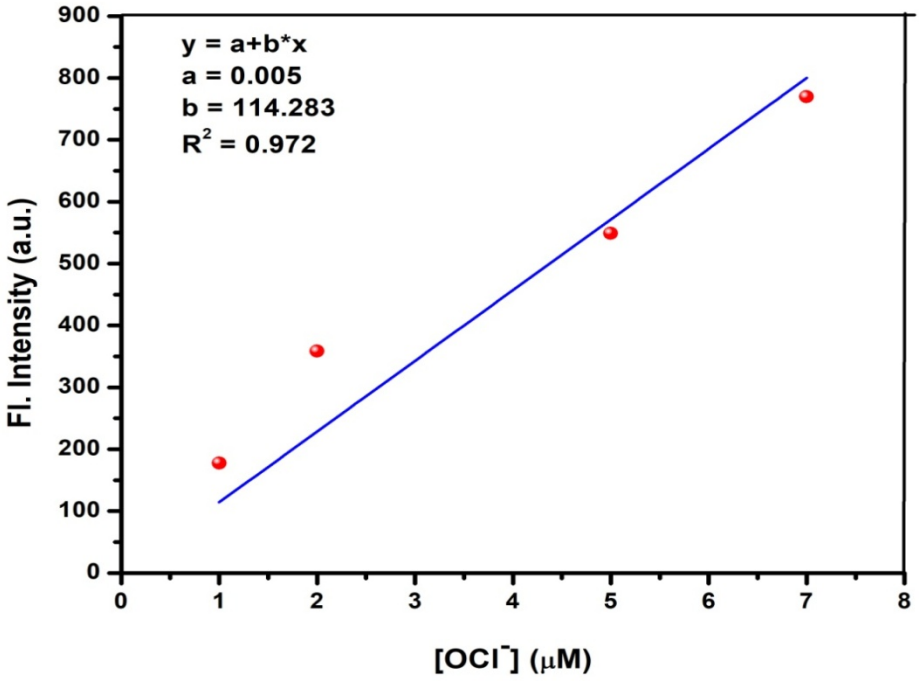

Figure S9 Determination of the detection limit based on change in the ratio (fluorescence intensity at λ_{ex} = 365nm, λ_{em} = 484 nm) of **A3** (5 μM) with **OCl$^-$**, linier portion of **Figure S6**

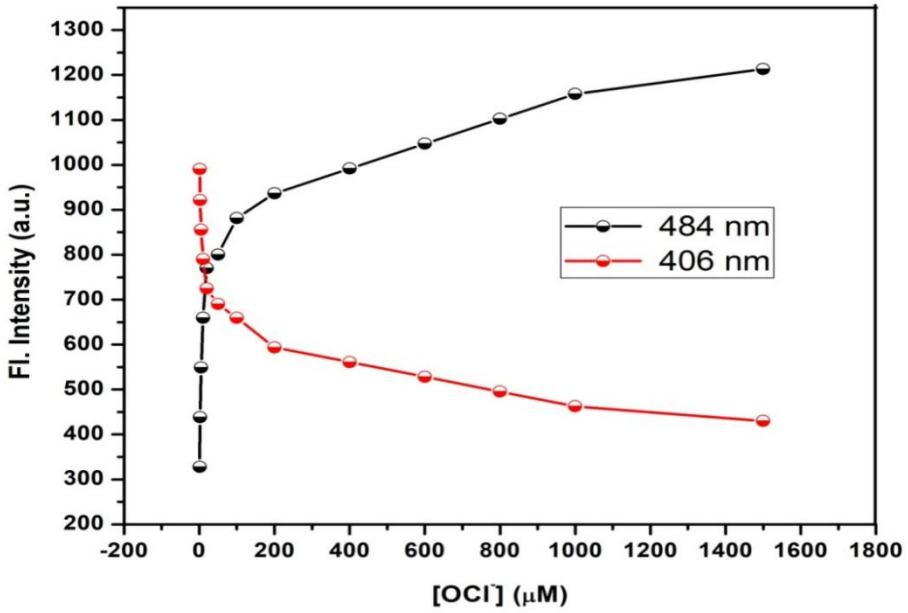

Figure S10 Plot of emission intensities of **A3** (5 μM, λ_{ex} = 365 nm, λ_{em} = 484 nm) as a function of externally added **OCl$^-$** (1.0-1500μM)

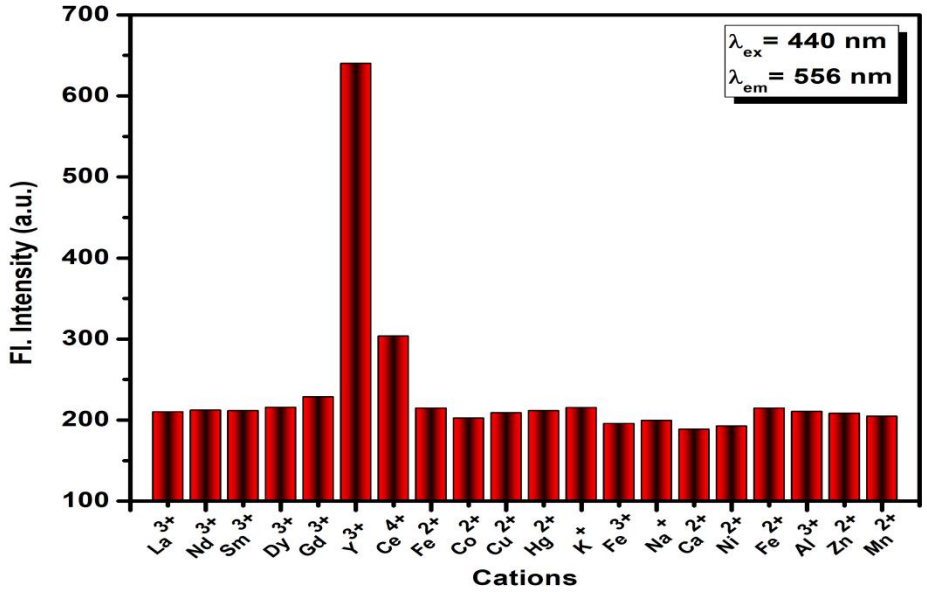

Figure S11 Selectivity plot of different cations with **Ad1**

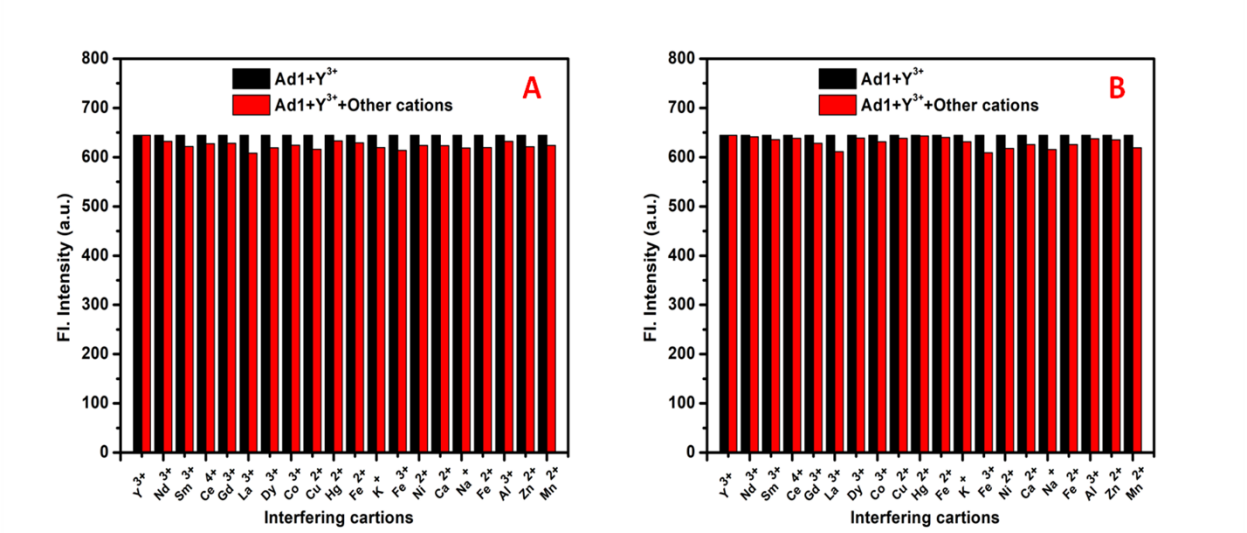

Figure S12 Interference studies for fluorescence detection of Y^{3+} (1500 μ M) using **Ad1** (20 μ M) with different ions (A) 1000μM each and (B)1500 μM each (**λ_{ex}** = 440 nm, **λ_{em}** = 556 nm) .

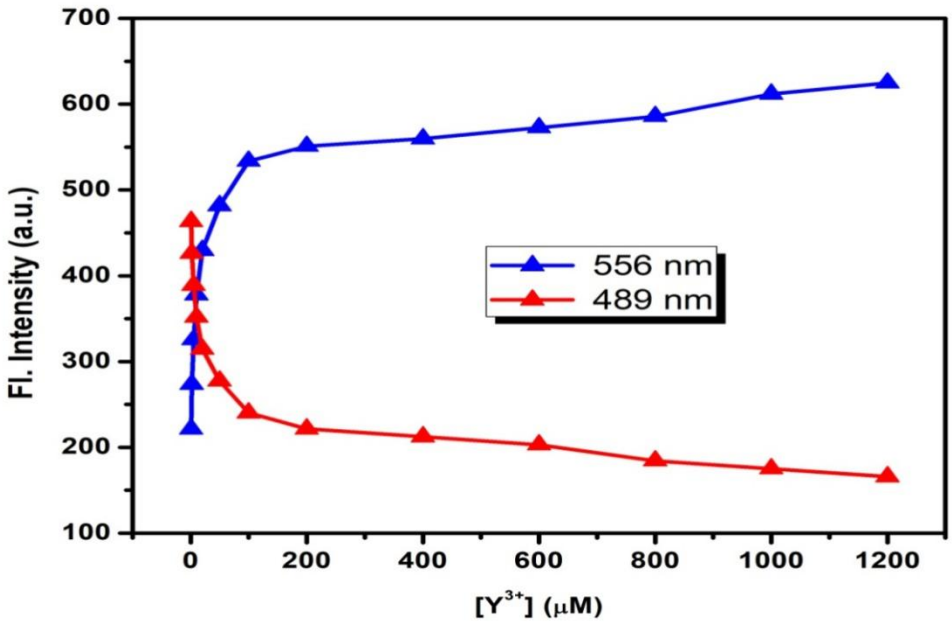

Figure S13 Plot of emission intensities of **Ad1** (5 μM, λ_{ex} = 440 nm, λ_{em} = 556 nm) as a function of externally added **Y^{3+}**(1.0-1200μM)

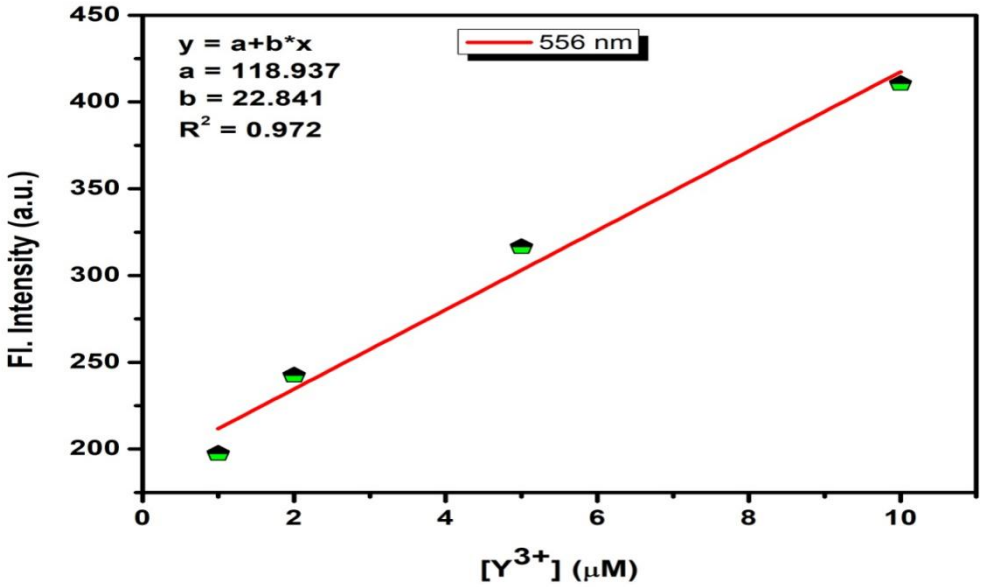

Figure S14 Determination of the detection limit based on change in the ratio (fluorescence intensity at λ_{ex} =440 nm, λ_{em} = 556nm) of **Ad1** (5 μM) with Y^{3+}, linier portion of **Figure S13**

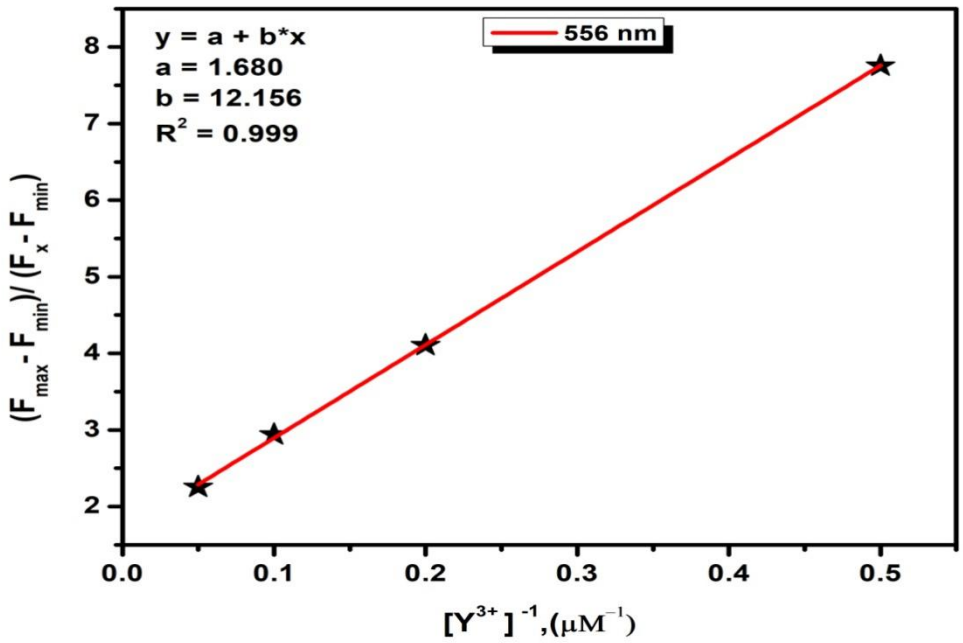

Figure S15 Benesi−Hildebrand plot for determination of association constant of compound **Ad1** with Y^{3+}(linier portion only), λ_{ex} = 440 nm, λ_{em} = 556 nm

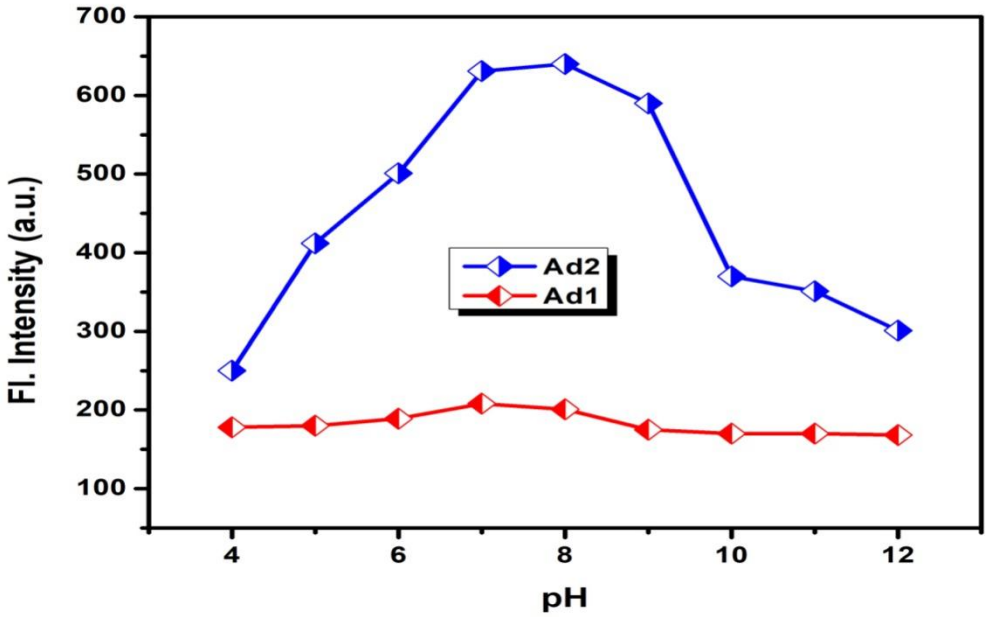

Figure S16 Effect of pH on the emission intensities of compound **Ad1,** (λ_{ex} = 440 nm λ_{em} = 556 nm) in presence and absence of Y^{3+}

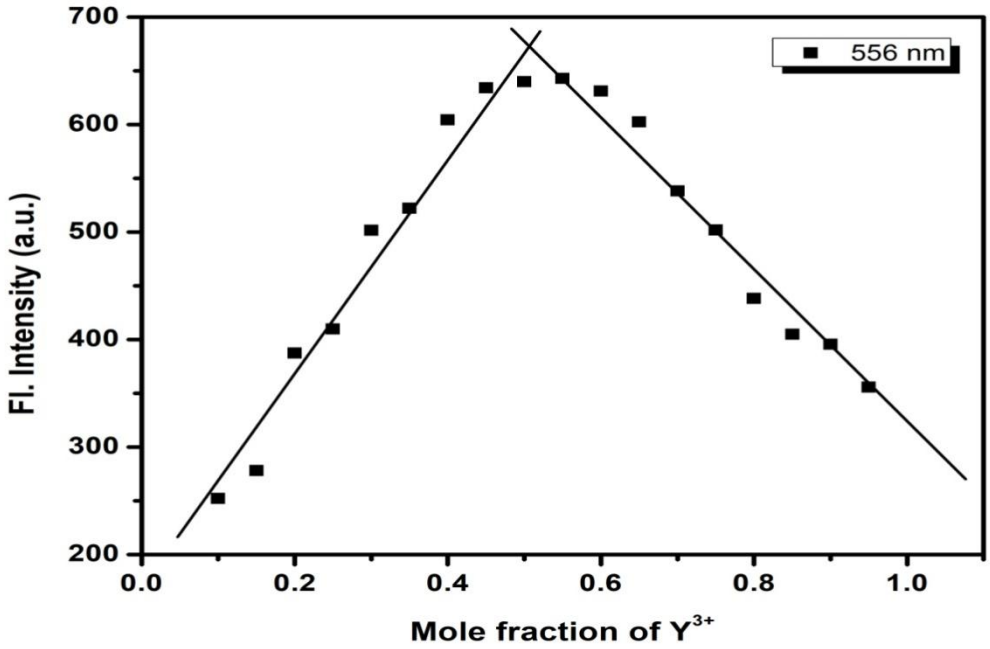

Figure S17 Job's plot for stoichiometry determination of **Ad2,** (λ_{ex} = 440 nm, λ_{em} = 556 nm.).

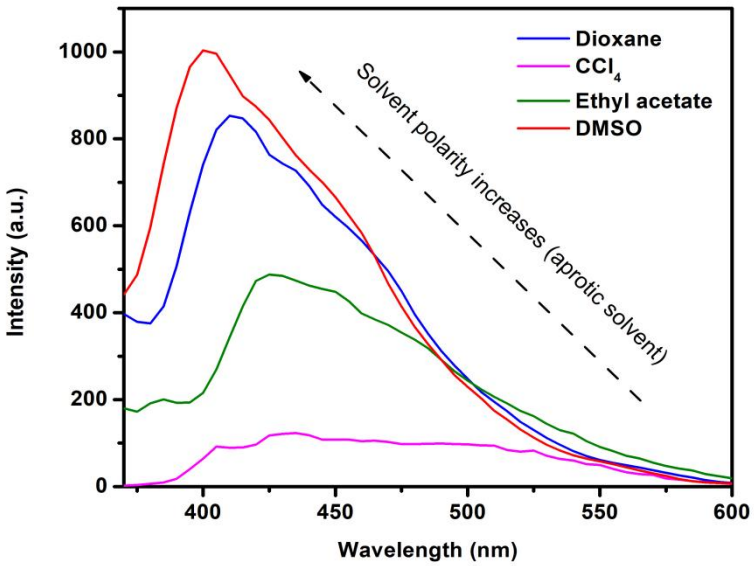

Figure S18 Polarity dependent emission of **A3** in different aprotic solvent (excitation 365 nm).

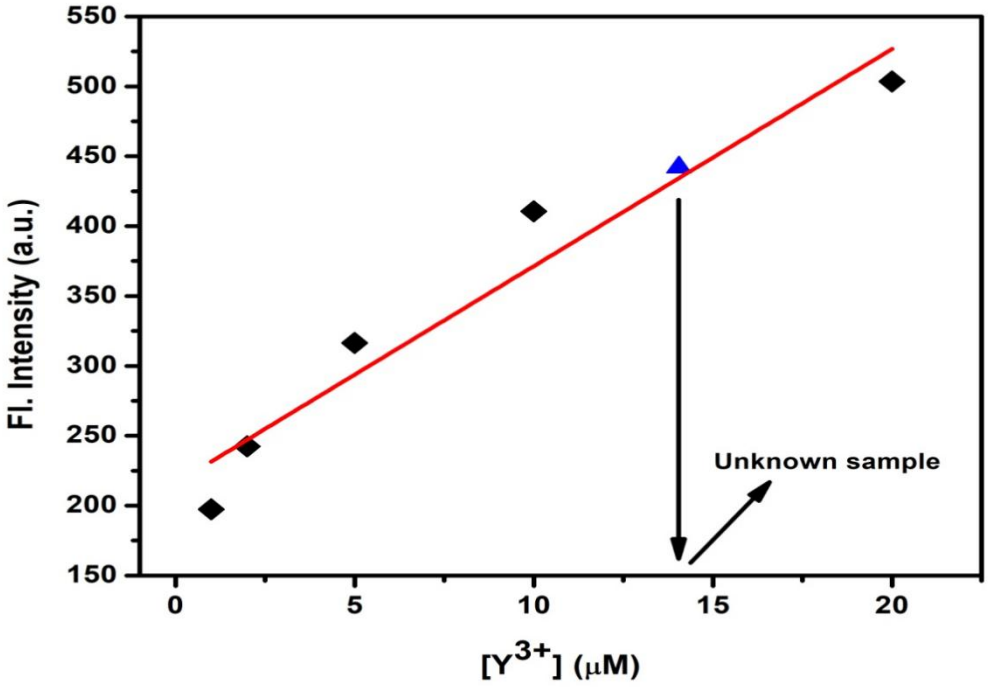

Figure S19 Calibration graph to determine unknown concentration of Y^{3+}

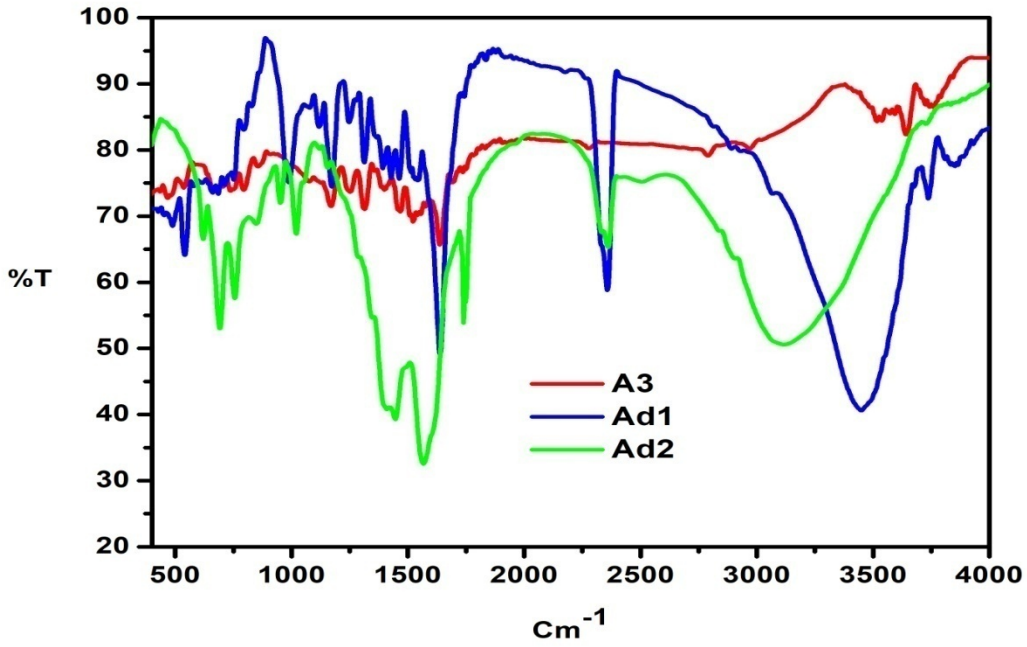

Figure S19 FTIR data comparison between **A3**, **Ad1** and **Ad2**

Table S1 ^{1}H NMR data comparison for interaction of OCl^- and Y^{3+} with A3 respectively

Proton type	**A3** (ppm)	**Ad1** (A3 + 1 eqV OCl^-) (ppm)	**Ad2** (Ad1+ 1 eqV Y^{3+}) (ppm)	Remarks
a (phenolic OH)	13.158	14.014	Almost disappear	Shifted downfield
b (imine)	10.830	10.836	10.886	Shifted downfield
c (imine)	10.302	10.314	10.384	Shifted downfield

Table S2 Results from TD-DFT calculations of A3

Compound	**Electronic Transitions**	**Energy[a] (eV)**	**Wavelength (nm)**	**f[b]**	**Transitions involved**
A3	**$S_0 \rightarrow S_1$**	**1.7539 eV**	**706.92 nm**	**f=0.0001**	**HOMO→LUMO HOMO→LUMO+1**
	$S_0 \rightarrow S_2$	**2.0829 eV**	**595.25 nm**	**f=0.0009**	**HOMO→LUMO HOMO→LUMO+1**
	$S_0 \rightarrow S_3$	**2.2881 eV**	**541.87 nm**	**f=0.0061**	**HOMO-1→LUMO-1**

Ad1	**$S_0 \rightarrow S_1$**	**0.5017 eV**	**2471.36 nm**	**f=0.0019**	**HOMO-1→LUMO-1**
	$S_0 \rightarrow S_2$	**1.0388 eV**	**1193.49 nm**	**f=0.0007**	**HOMO-1→LUMO-1**
	$S_0 \rightarrow S_3$	**1.4283 eV**	**868.03 nm**	**f=0.1045**	**HOMO→LUMO HOMO→LUMO+1 HOMO-1→LUMO**