Electronic Supplementary Informations

for

Solvent viscosity tuned highly selective NIR and ratiometric fluorescent sensing of Fe^{3+} by a symmetric chalcone analogue

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EXPERIMENTAL

1.1 Apparatus:

The IR Spectra for the receptors **1** was recorded on JASCO-FTIR Spectrophotometer while ^{1}H NMR and ^{13}C NMR spectra for the same were recorded on a JEOL AL 300 FT NMR Spectrometer. Mass spectrometric analysis was carried out on a MDS Sciex API 2000 LCMS/Brukar Compass data analysis spectrometer. Electronic spectra were recorded at room temperature (298 K) on a UV-1700 pharmaspec spectrophotometer with quartz cuvette (path length=1 cm). Emission spectra were recorded on JY HORIBA Fluorescence spectrophotometer.

1.2 Materials:

All reagents for synthesis were purchased from Sigma-Aldrich and were used without further purification.

1.3 General Methods:

All titration experiments were carried at room temperature. All the cations were used as their chloride. The ^{1}H NMR spectra were recorded by using tetramethylsilane (TMS) as an internal reference standard.. .

1.4. Theoretical studies:

All DFT calculations were carried out with the Gaussian 03 program. The structures of receptor **1** in the absence and presence of anions were fully optimized in gaseous phase using B3LYP functional with the 6-31g** basis set. To visualize the optimized structures Gauss View software was used.

Figure S1: ^{1}HNMR spectrum of receptor 1

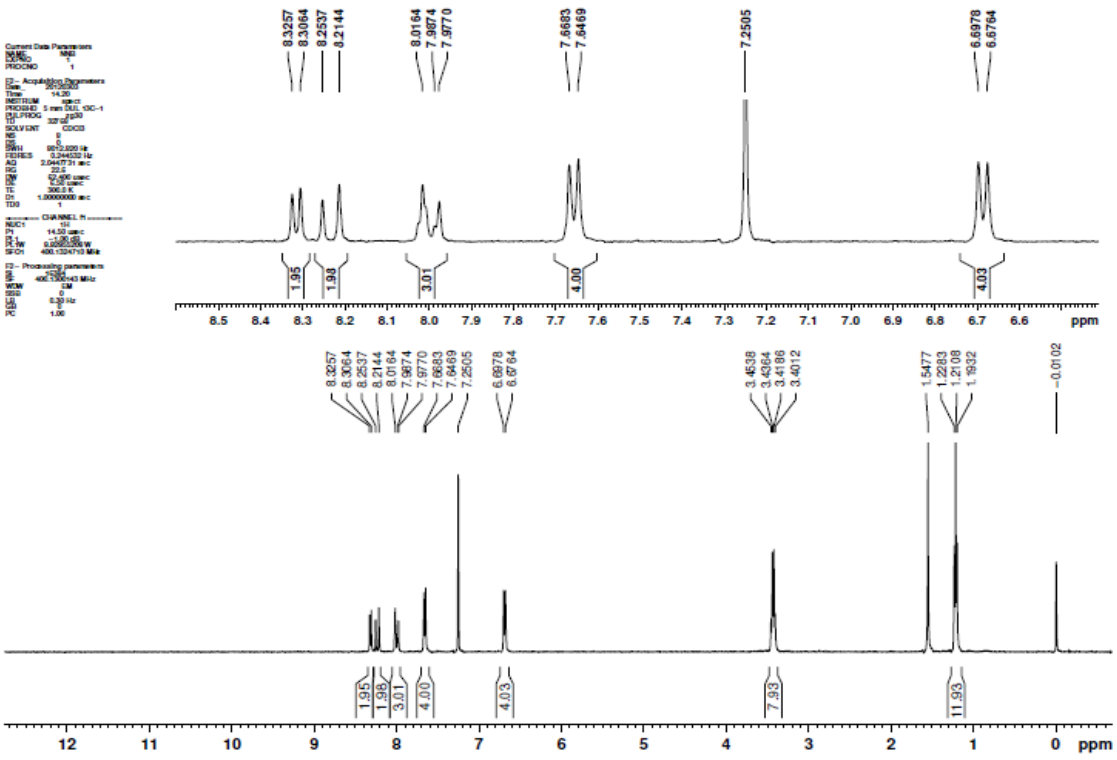


Figure S2: ^{13}C NMR spectrum of receptor 1

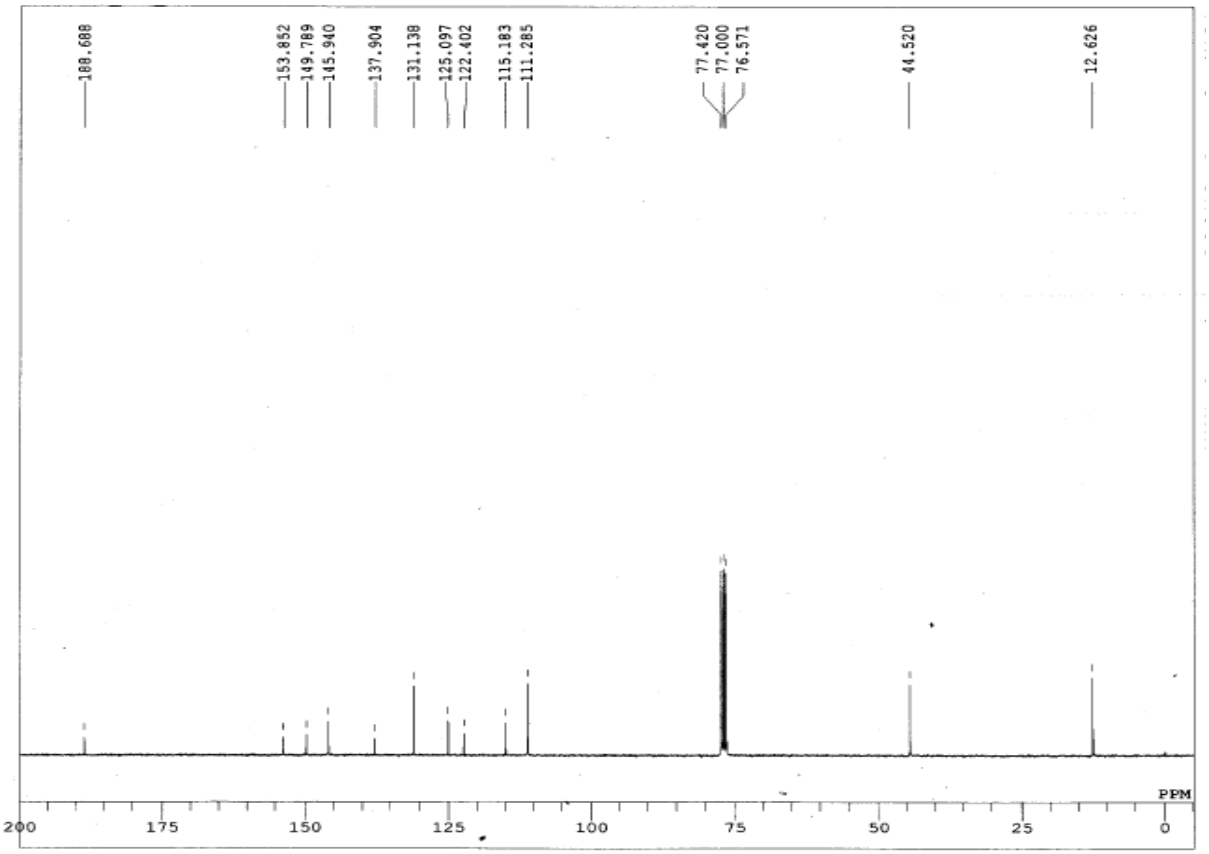


Figure S3: IR spectrum of receptor 1

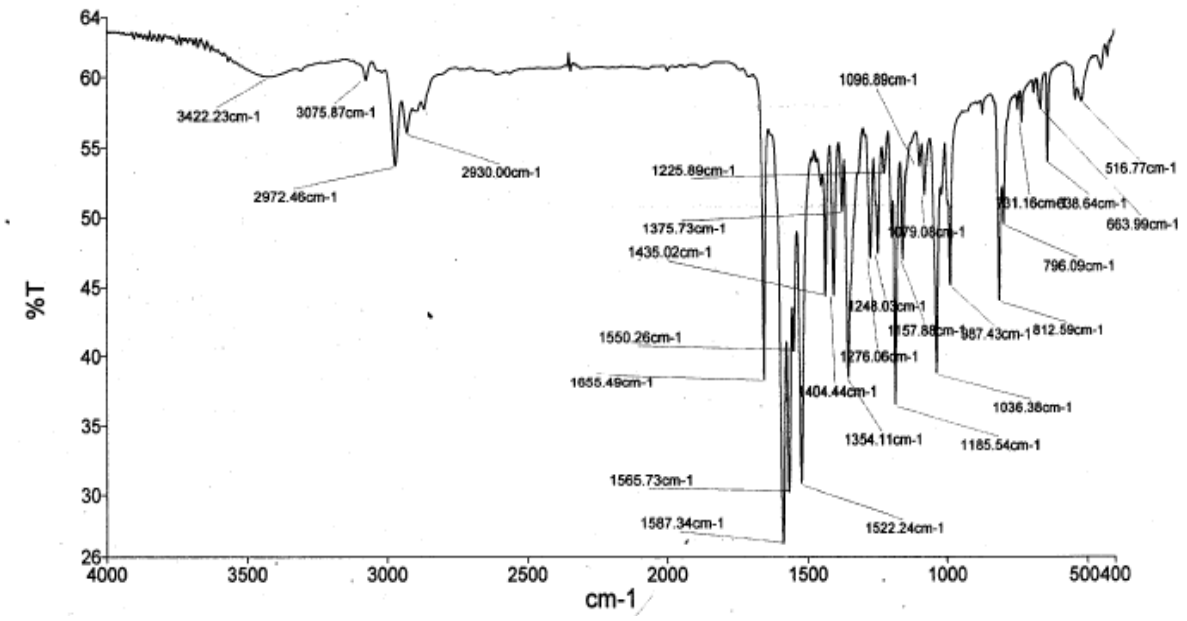
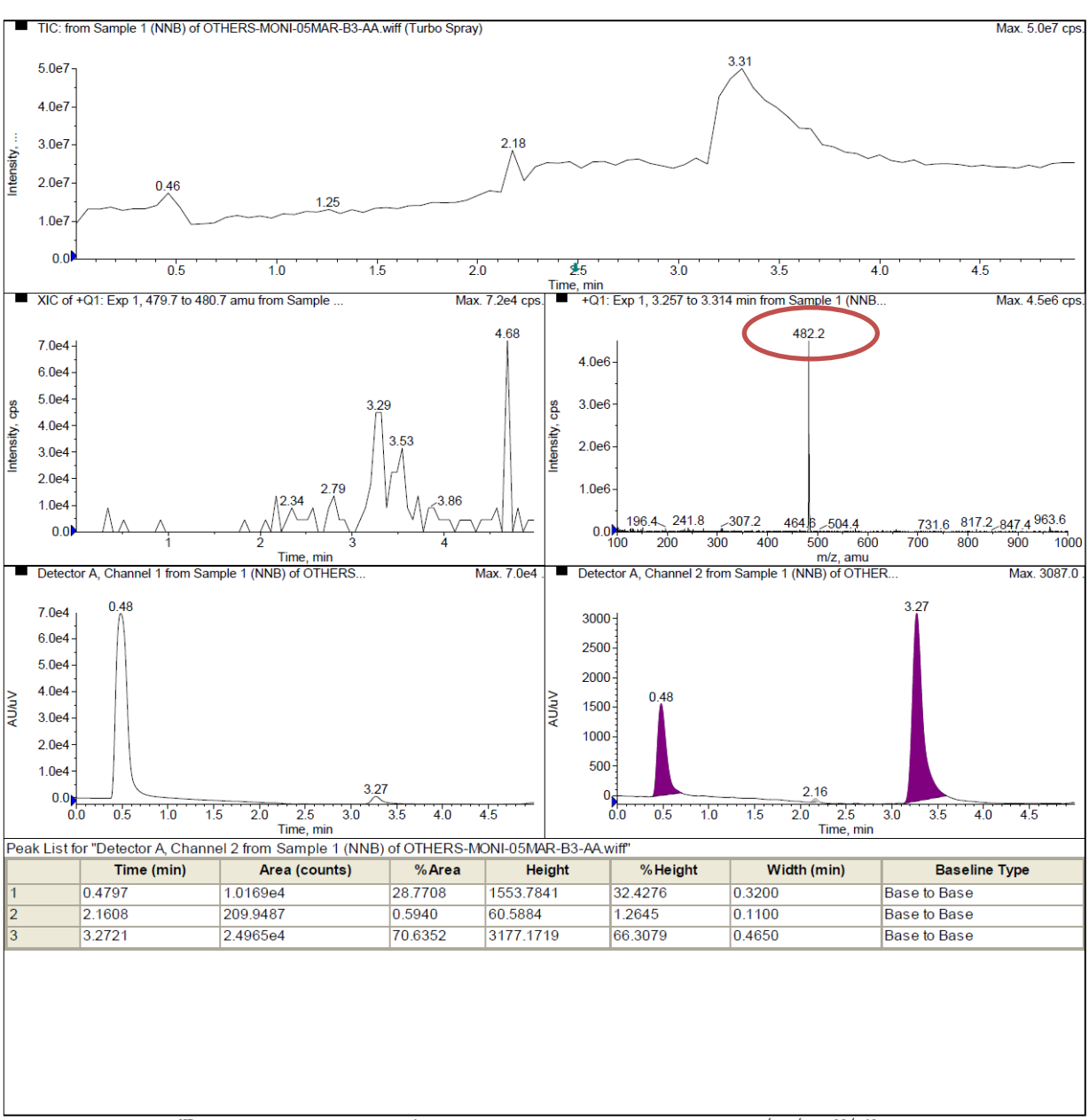


Figure S4: Mass spectrum of receptor 1



Peak List for "Detector A, Channel 2 from Sample 1 (NNB) of OTHERS-MONI-05MAR-B3-AA.wiff"

	Time (min)	Area (counts)	%Area	Height	%Height	Width (min)	Baseline Type
1	0.4797	1.0169e4	28.7708	1553.7841	32.4276	0.3200	Base to Base
2	2.1608	209.9487	0.5940	60.5884	1.2645	0.1100	Base to Base
3	3.2721	2.4965e4	70.6352	3177.1719	66.3079	0.4650	Base to Base

LCMS MONITORING SAMPLE-NP ACN:NH4OAc TCGLS/ARD/LCMS08/K42

Channel 1 at wavelength 220 nm,
Channel 2 at wavelength 260 nm

Column: ZORBAX EXTEND C18(50x4.6mm),5µ

Analyzed by

Figure S5: Absorbance of receptor 1 in different solvent at 1×10^{-5} M concentration

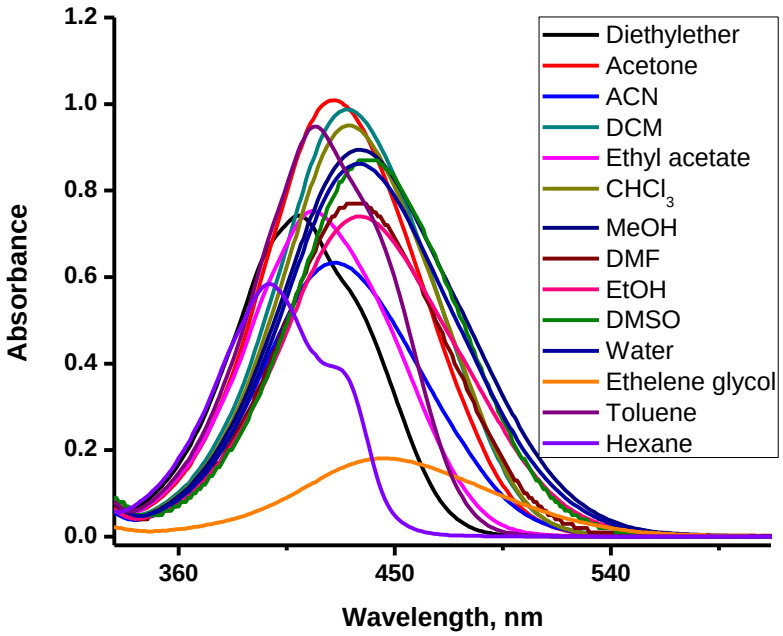


Table 1: UV-visible absorption band of receptor 1 in various solvents and corresponding absorbance

S. No	Solvent	Wavelength, nm	Absorbance
1.	ACN	423 nm	0.64
2.	$CHCl_3$	430 nm	0.94
3.	CH_2Cl_2	430 nm	0.98
4.	Diethyl ether	409 nm	0.74
5.	MeOH	435 nm	0.89
6.	EtOH	436 nm	0.73
7.	Acetone	424 nm	1.04
8.	DMF	434 nm	0.76
9.	DMSO	439 nm	0.87
10.	Water	435 nm	0.86
11.	Ethyl acetate	415 nm	0.75
12.	Ethylene glycol	445 nm	0.18
13.	Hexane	397, 426 nm	0.58, 0.38
12.	Toluene	410 nm	0.85

Figure S6: Colour changes of receptor 1 upon respective additions of Cu^{2+}, from left to right; receptor 1, 1+10 equiv. Cu^{2+} and 1+5 equiv. of Cu^{2+}

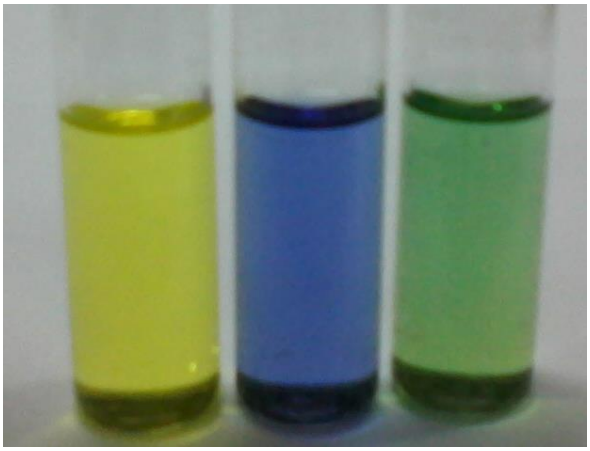
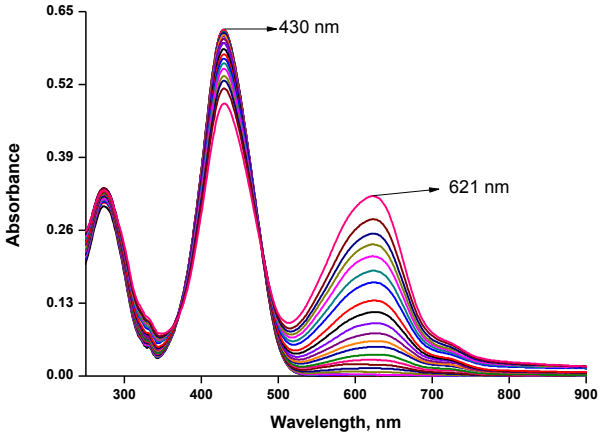


Figure S7: Family of absorbance spectra of receptor 1 upon concomitant additions of Fe^{2+} ion and its corresponding color changes



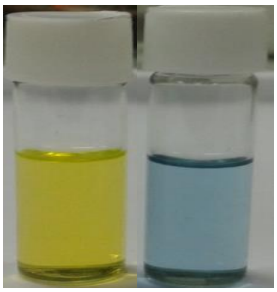


FIGURE S8: Job's Plot of Fe^{3+} with receptor 1 showing 1:1 stoichiometry

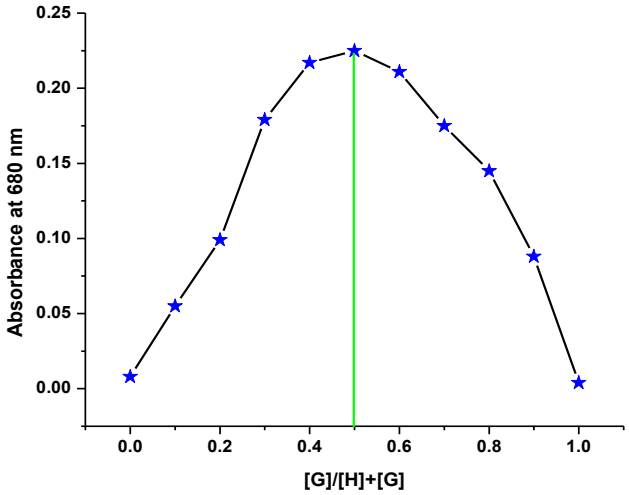


Figure S9: Job's Plot of Cu^{2+} with receptor 1 showing 1:2 stoichiometries

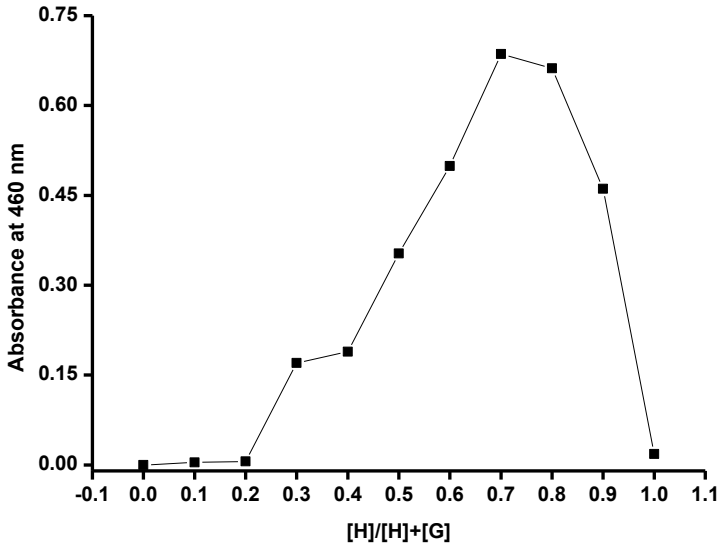


Figure S10: Mass spectrum of 1+Fe^{3+} complex

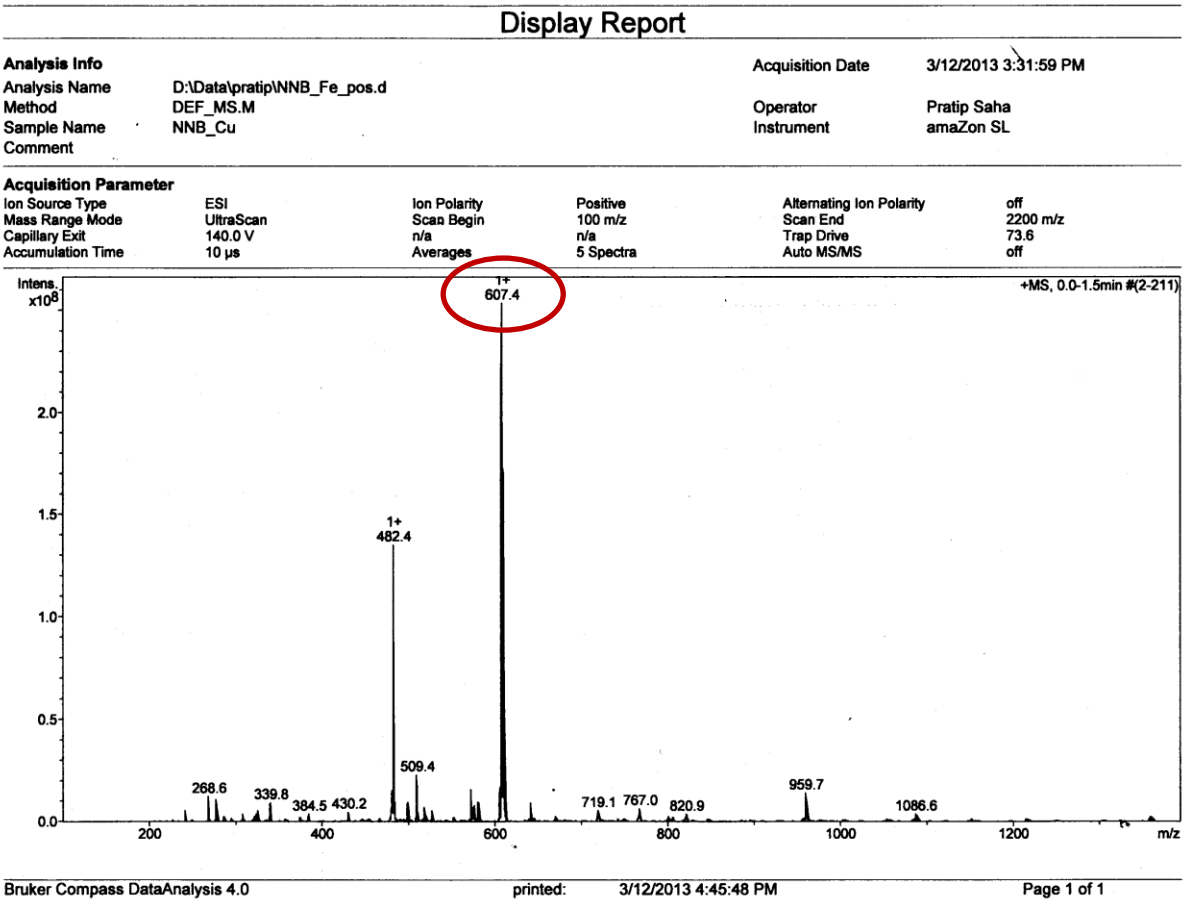


Figure S11: Mass spectrum of 1+Cu^{2+} complex

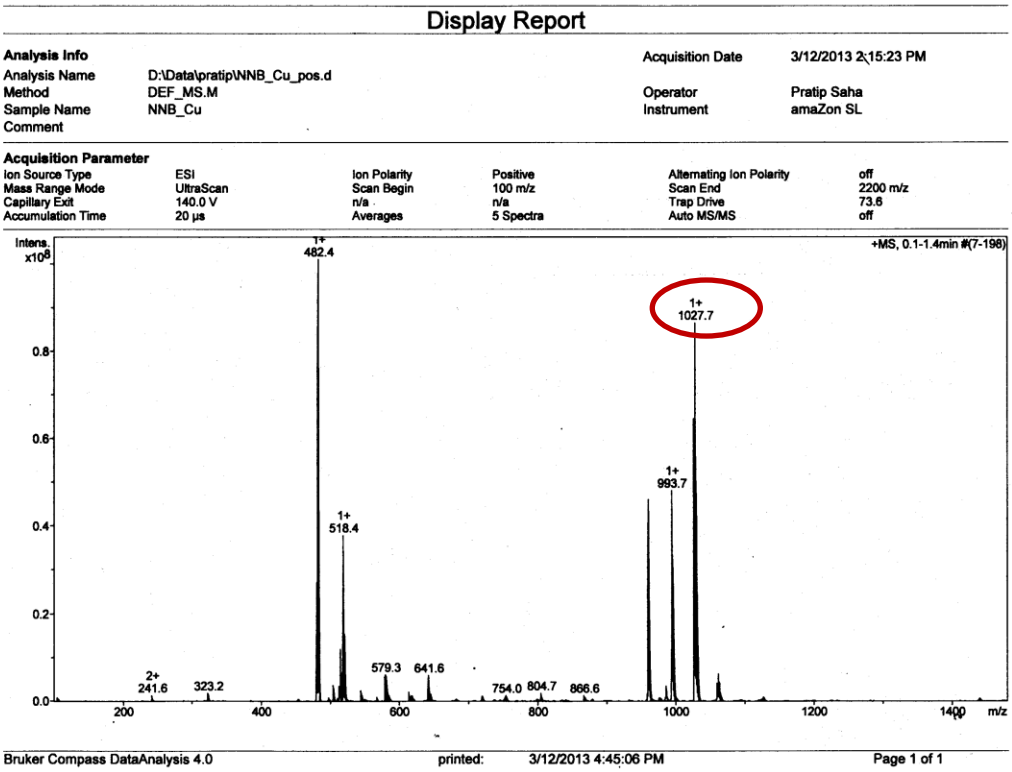


Figure S12: (a) Colour changes of receptor 1 upon addition of 5 equivalent various metal ions,

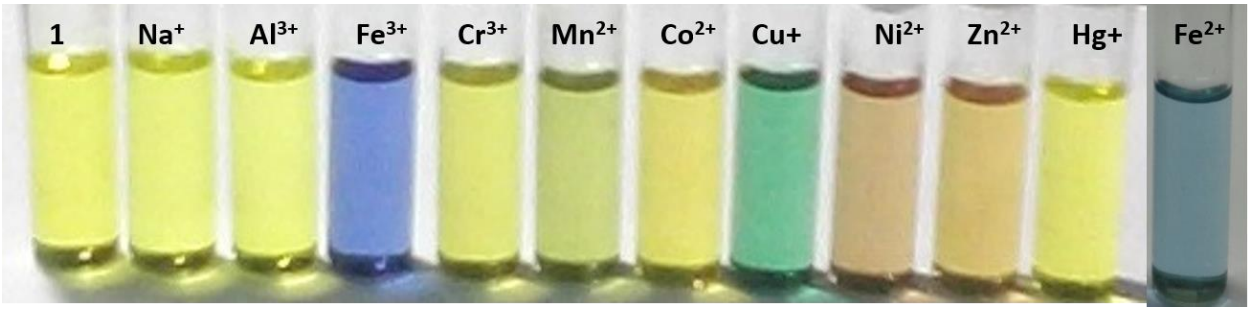


Figure S12: (b) Effect of various metal ions on the colour of 1+Fe^{3+} complex, from left to right; receptor 1, Fe^{3+}, Cr^{3+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Cd^{2+}, Hg^{2+} and Al^{3+}

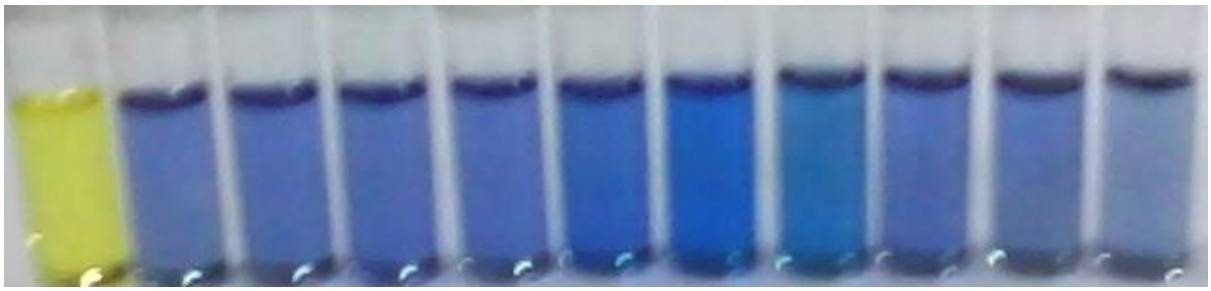


Figure S12: (c) Effect of various metal ions on the UV-visible spectra of 1+Fe^{3+} complex, from left to right; receptor 1, Fe^{3+}, Cr^{3+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Cd^{2+}, Hg^{2+} and Al^{3+}

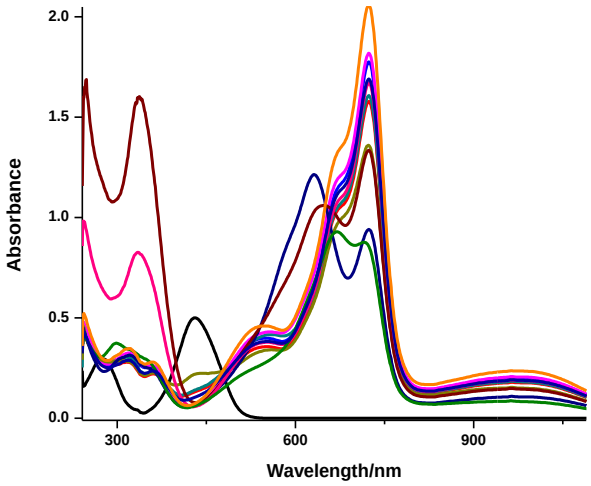


Figure S13: Non-linear fit plot of receptor 1with Fe^{3+}

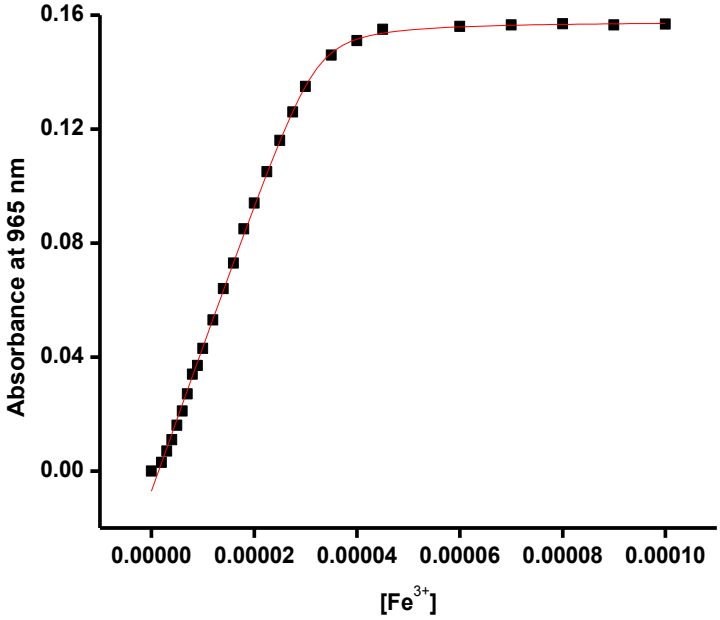


Figure S14: Determination of detection limit and calibration curves of receptor with Fe^{3+}

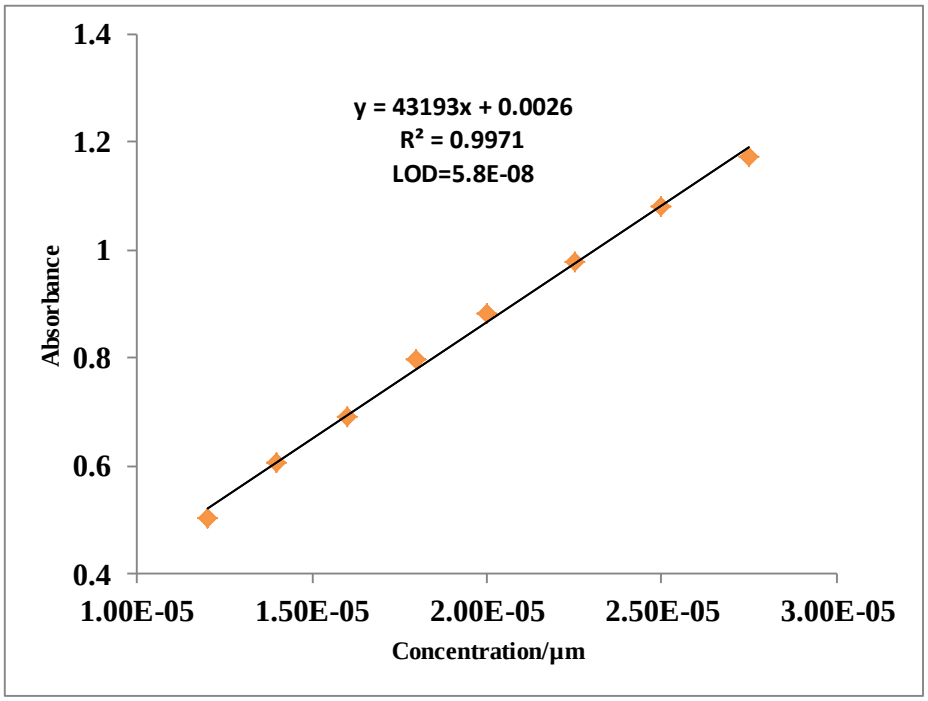


Figure S15: Emission responses of receptor 1 in different solvents:

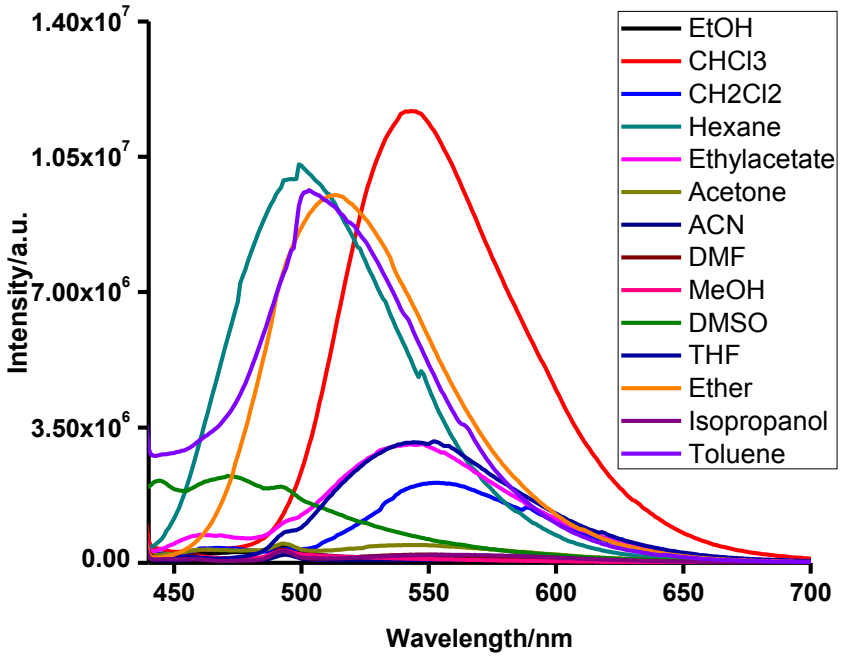


Figure S16: Non-linear fit plots of receptor 1 obtained from fluorescence titration data between receptor 1 and Fe^{3+}

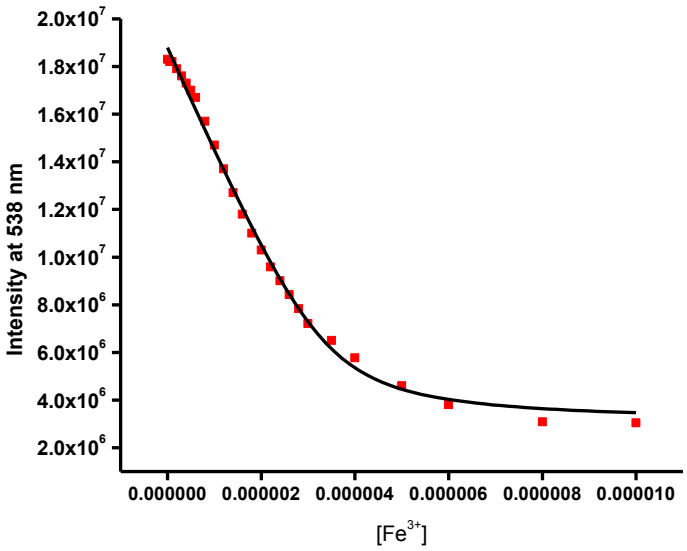


Figure S17: Determination detection limit and calibration curves of receptor 1 with Fe^{3+} through fluorescence data