Supporting Information

A two-in-one dual channel chemosensor for Fe^{3+} and $Cu^{2+}$with nanomolar detection mimicking IMPLICATION logic gate

Anil Kuwar*[a], Rahul Patil[a], Amanpreet Singh[b], Suban K. Sahoo[c], Jaromir Marek[d], Narinder Singh*[b],

[a]School of Chemical Sciences, North Maharashtra University, Jalgaon-425001 (MS), India.

[b]Department of Chemistry, Indian Institute of Technology, Ropar, Rupanagar, (Punjab), India.

[c]Department of Applied Chemistry, SV National Institute of Technology, Surat-395007 (Gujrat), India.

[d]Central European Institute of Technology, Masaryk University, Kamenice 562500 Brno, Czech Republic.

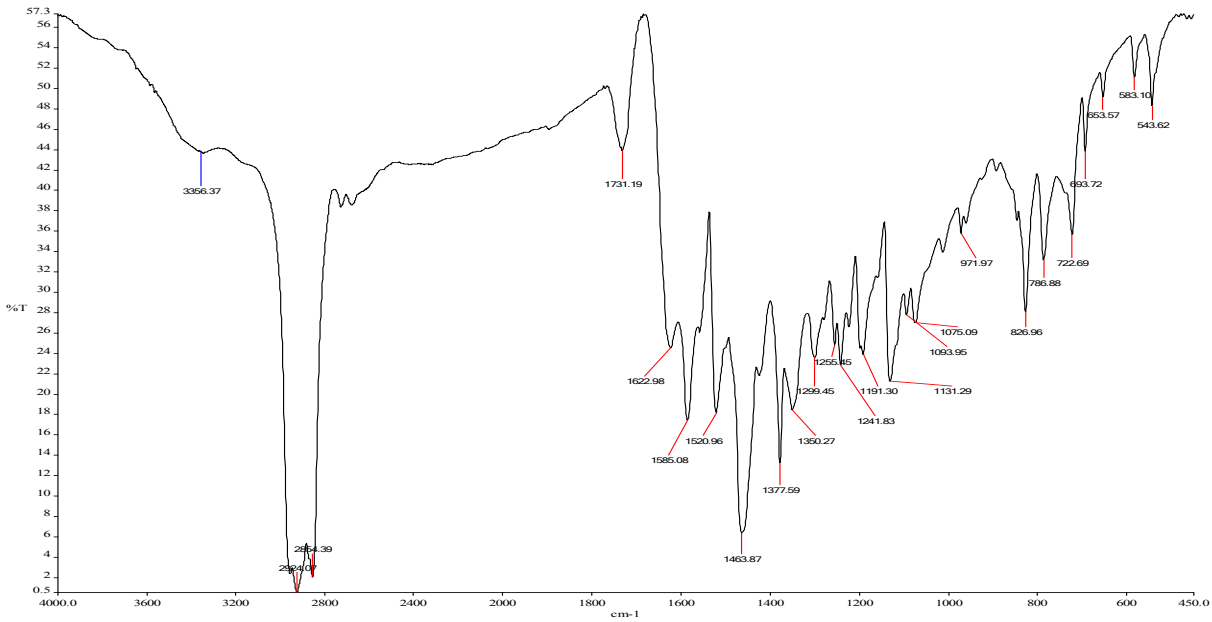

Figure S1: IR Spectra of receptor **1**

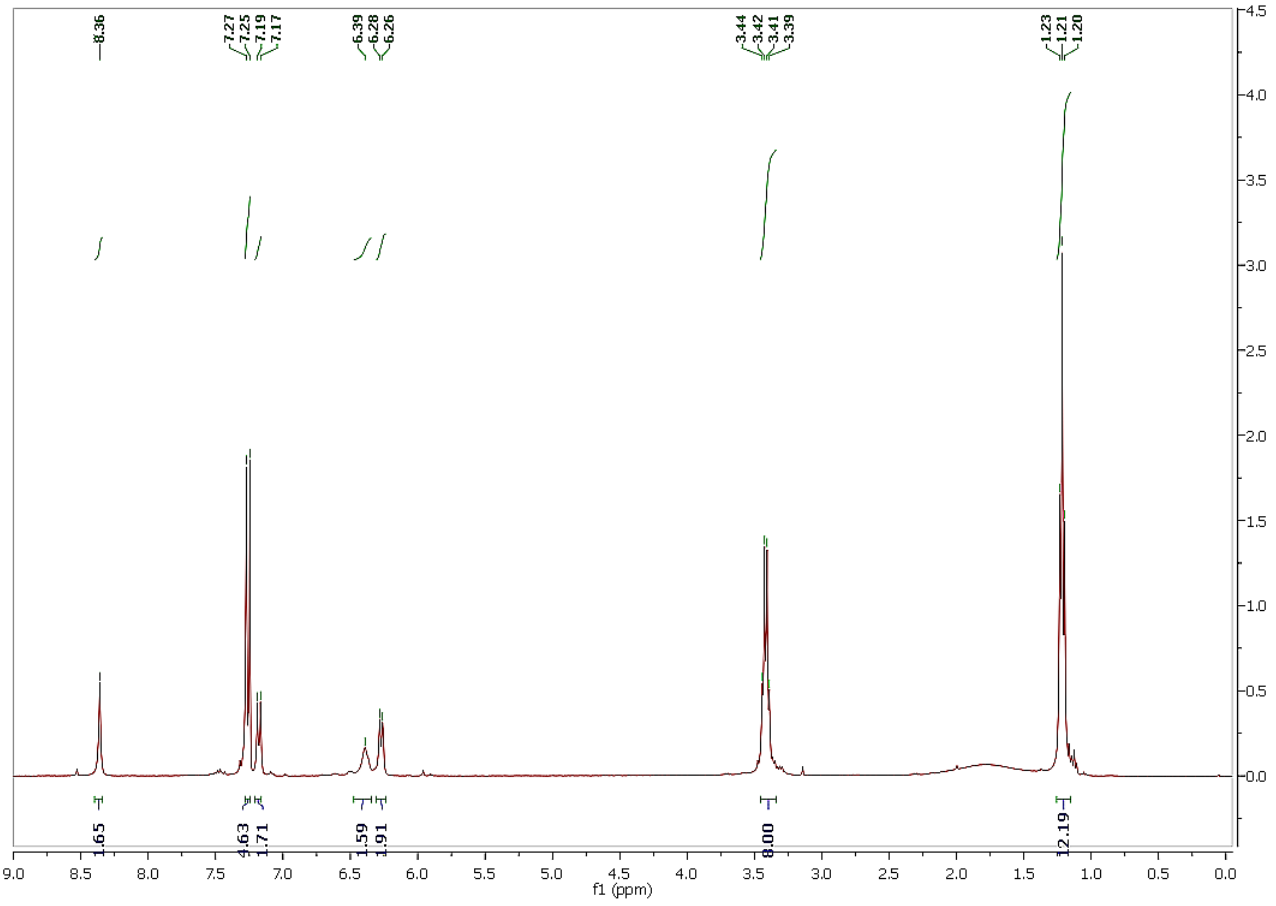

Figure S2: ^{1}H-NMR spectra of receptor **1**

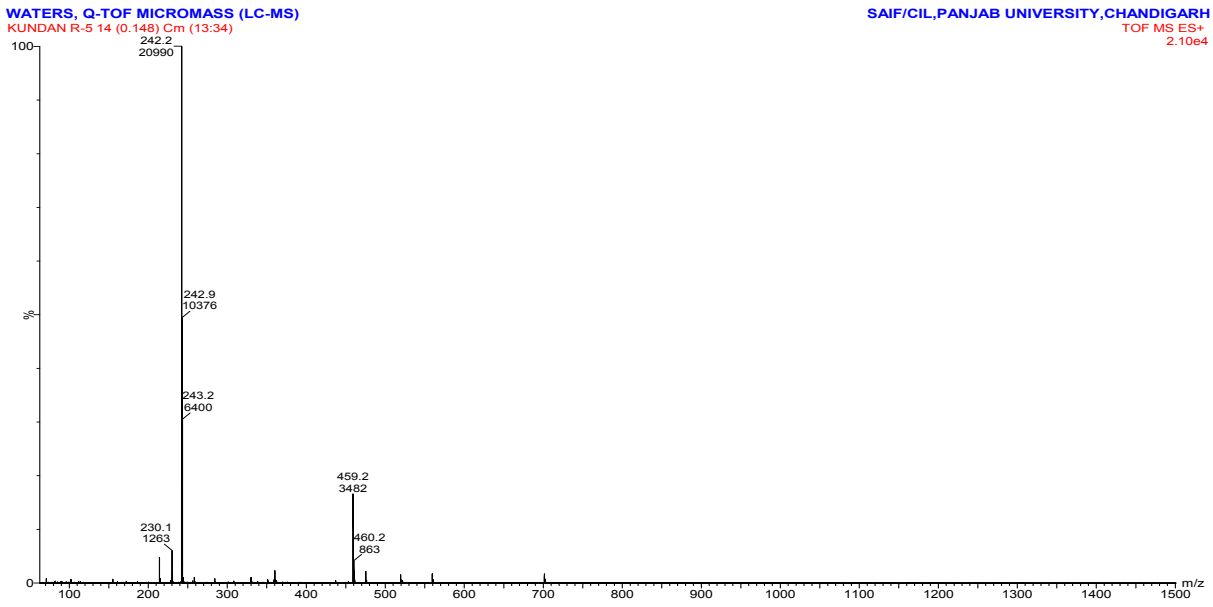

Figure S3- Mass spectra of receptor **1**

Table S1- Crystal data and structure refinement for receptor **1**

Identification code	**Receptor 1**	
Empirical formula	$C_{28}H_{34}N_4O_2$	
Formula weight	458.3	
Temperature	120 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P1 21/n 1	
Unit cell dimensions	a = 7.7300(15) Å	α= 79.75°.
	b = 11.040(2) Å	β= 87.94(3)°.
	c = 14.680(3) Å	γ = 89.29(3)°.
Volume	1231.19(4) $Å^3$	
Z	2	
Density (calculated)	1.134 Mg/m^3	
Absorption coefficient	0.07 mm^{-1}	
F(000)	450	
Theta range for data collection	4.06 to 75.66°.	
Index ranges	-9<=h<=8, -13<=k<=13, -17<=l<=17	
Reflections collected	13118	
Independent reflections	3622 [R(int) = 0.032]	
Completeness to theta = 67.50°	99.9 %	
Absorption correction	Analytical	
Max. and min. transmission	0.810 and 0.638	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3245 / 23 / 219	
Goodness-of-fit on F^2	1.14	
Final R indices [I>2sigma(I)]	R1 = 0.0387, wR2 = 0.0993	
R indices (all data)	R1 = 0.0414, wR2 = 0.1022	
Extinction coefficient	0.0015(5)	
Largest diff. peak and hole	0.34 and -0.32 $e.Å^{-3}$	

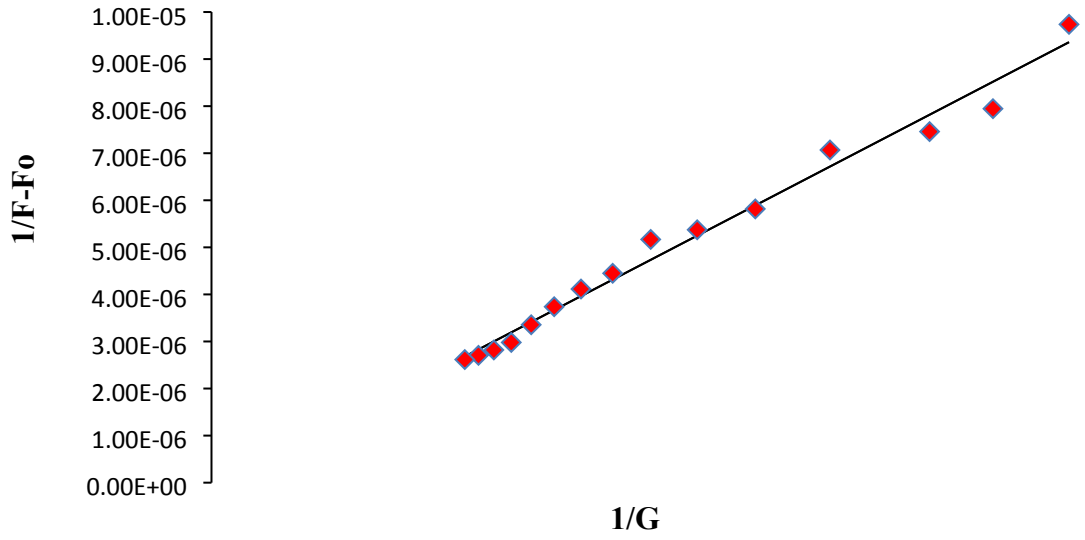

Figure S4 Benesi-Hildebrand Plot (adjusted equation: $1/F\text{-}F_0$=-1E-11x+1E-07 1/[G], R=0.984) and the K value for Fe^{3+} at 70000 M^{-1}.

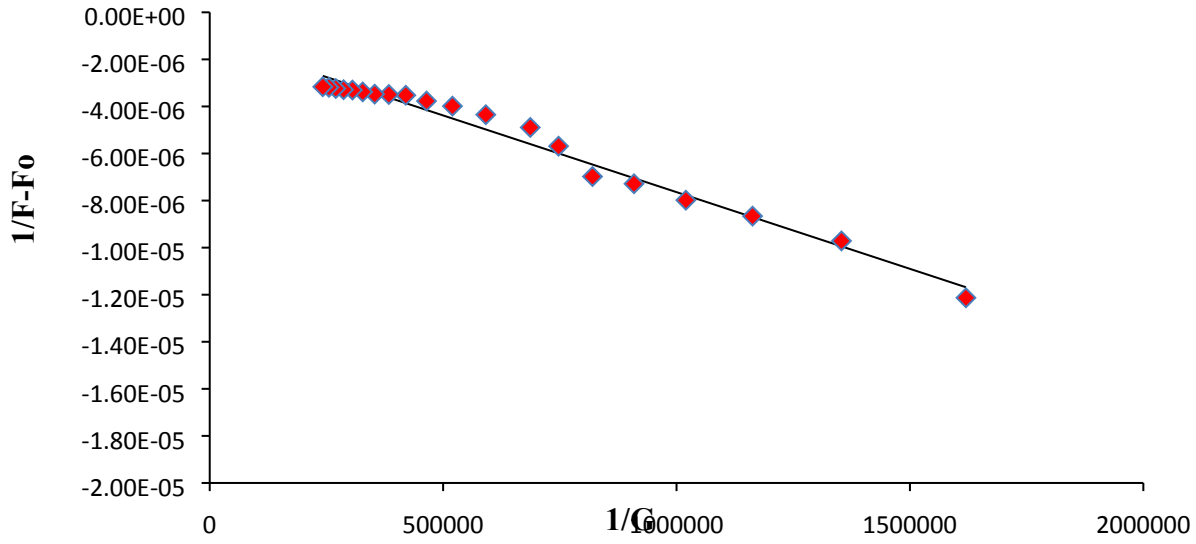

Figure S5 Benesi-Hildebrand Plot (adjusted equation: $1/F\text{-}F_0$=-7E-12x+1E-06 1/[G], R=0.978) and the K value for Cu^{2+} at 857143 M^{-1}.

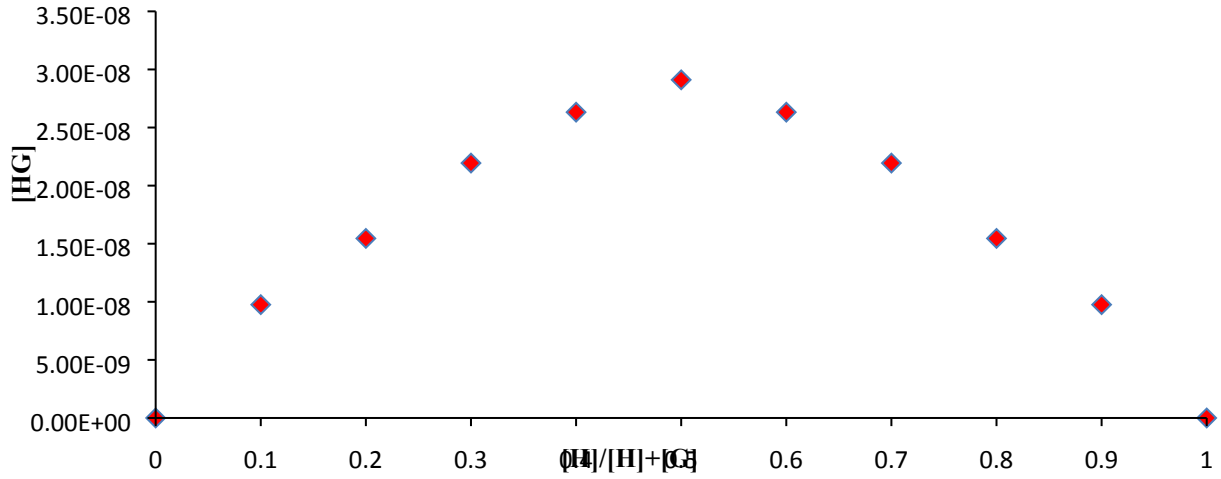

Figure S6 1:1 Stoichiometry of the host guest relationship realised from the Job's plot for receptor **1** with Fe^{3+}.

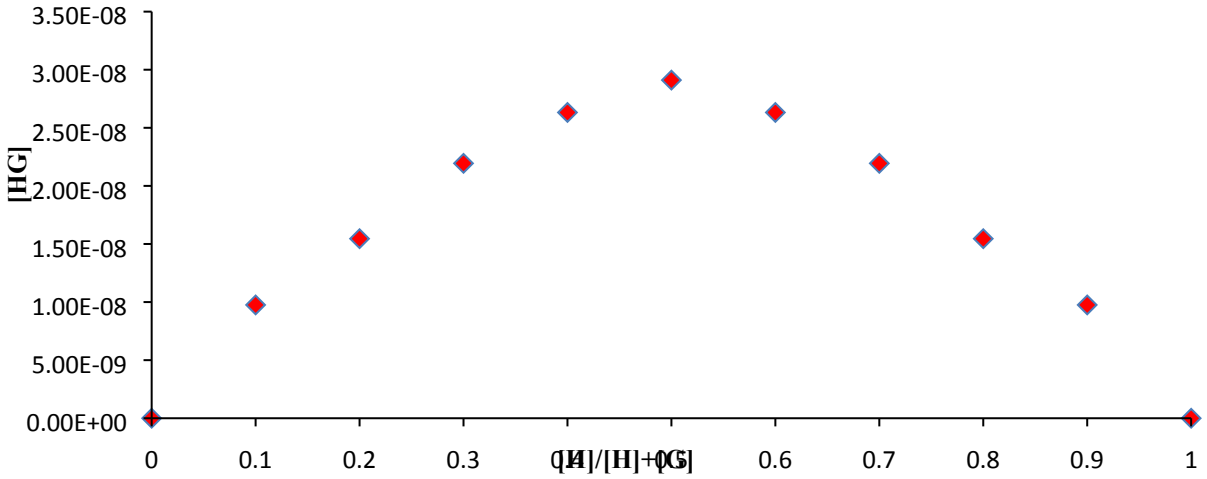

Figure S7 1:1 Stoichiometry of the host guest relationship realised from the Job's plot for receptor **1** with Cu^{2+}.

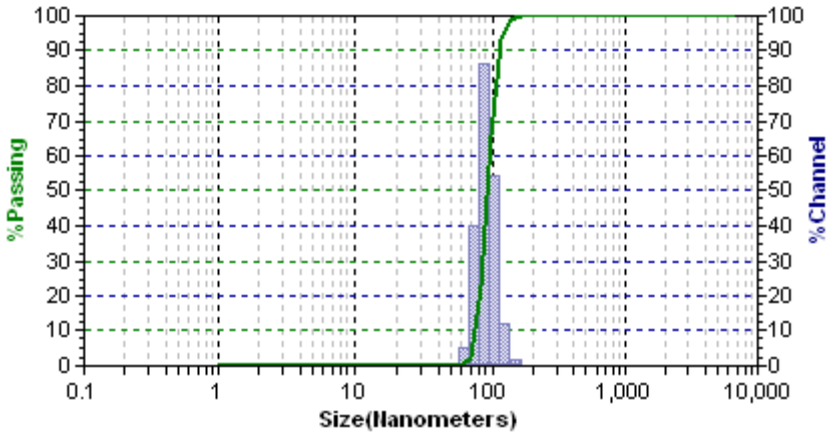

Figure S8. DLS histograms of R1 (showing average particle size = 89 nm) in CH_3CN/H_2O (1:99, v/v).

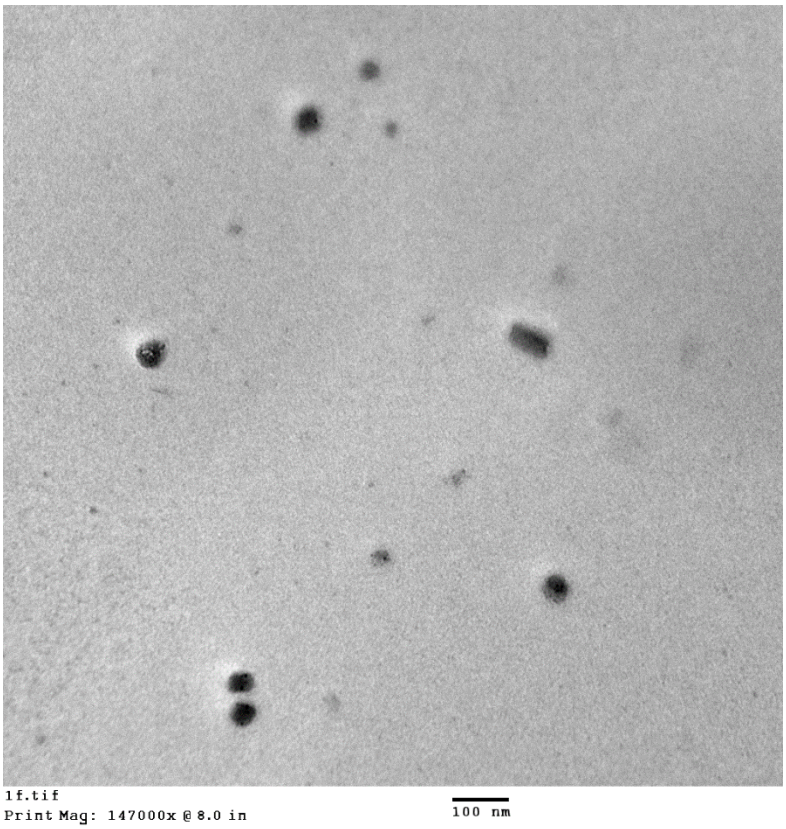

Figure S9. TEM image of R1 (showing average particle size = 80 nm)

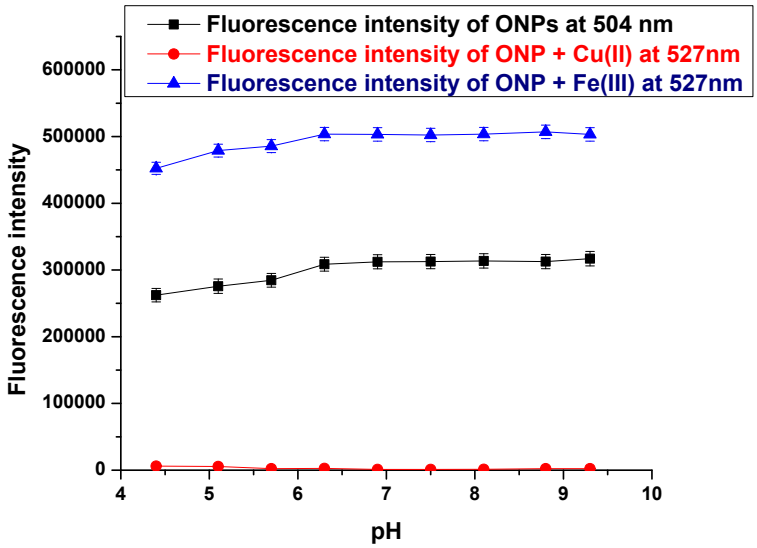

Figure S10. Effect of pH on emission profile of ONP and detection of Cu(II) and Fe(III) in aqueous medium.

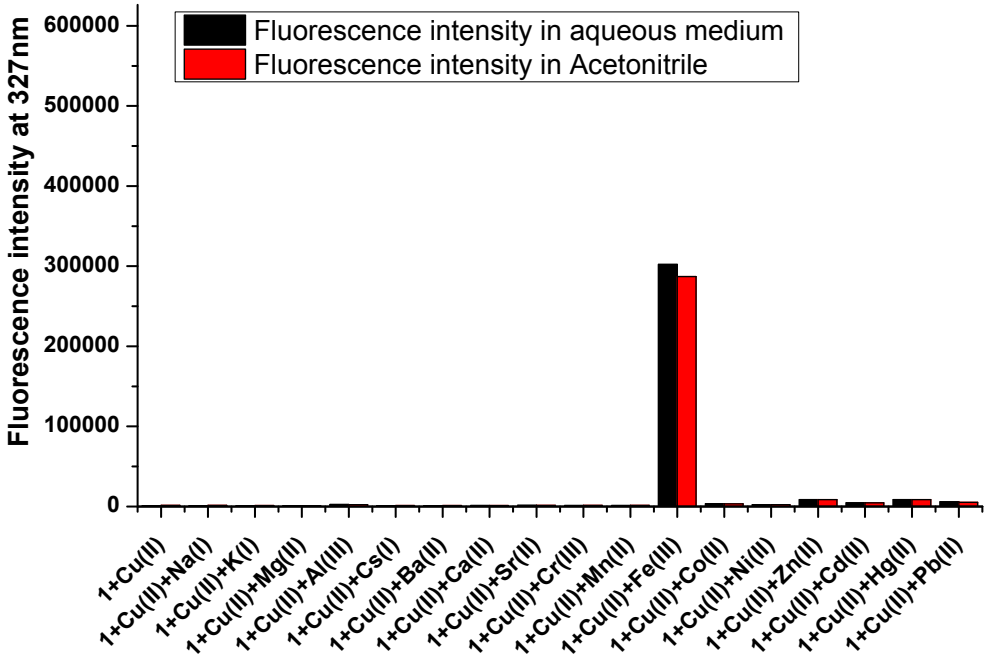

Figure S11. Competitive binding of Cu^{2+} with Receptor 1 in presence of 50 μM of Cu^{2+} and 50 μM of other competing cations.

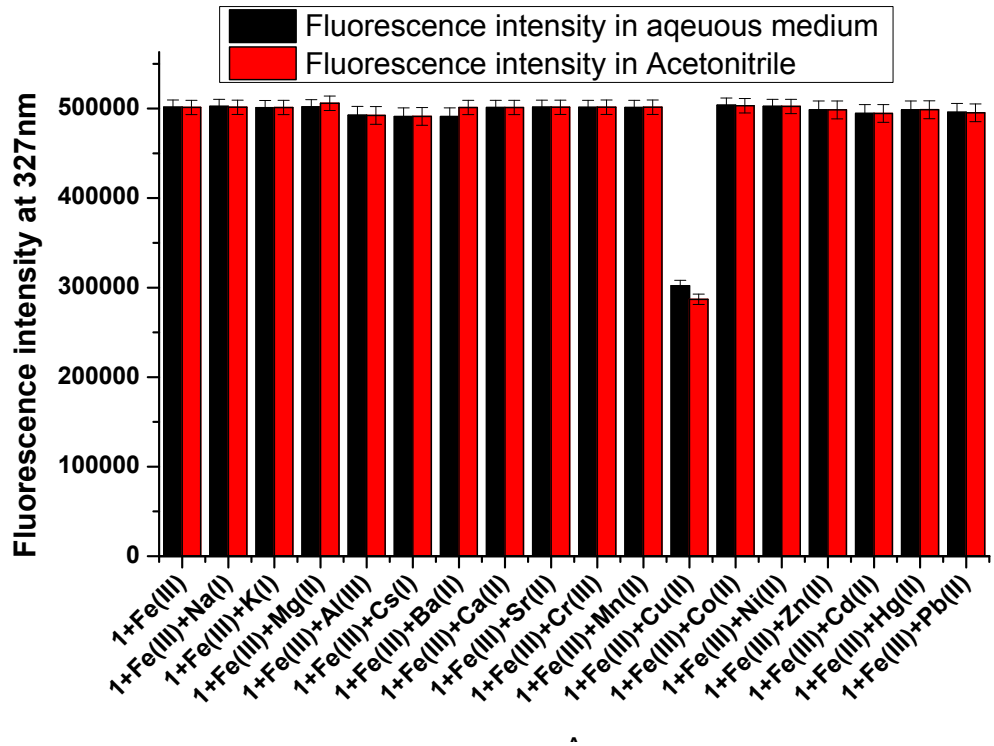

Figure S12. Competitive binding of Fe^{3+} with Receptor 1 in presence of 50 μM of Fe^{3+} and 50 μM of other competing cations.

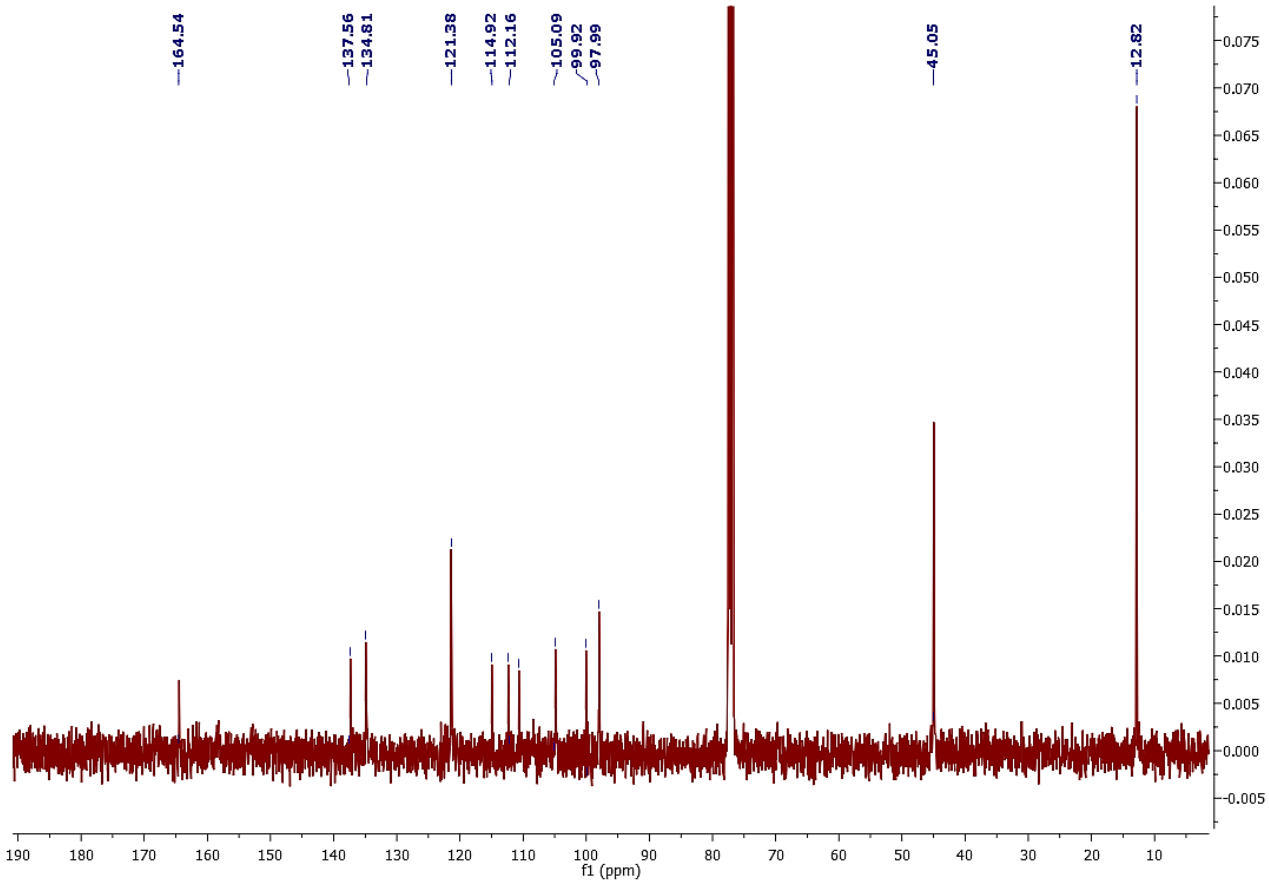

Figure S13: ^{13}C NMR spectra of receptor 1.

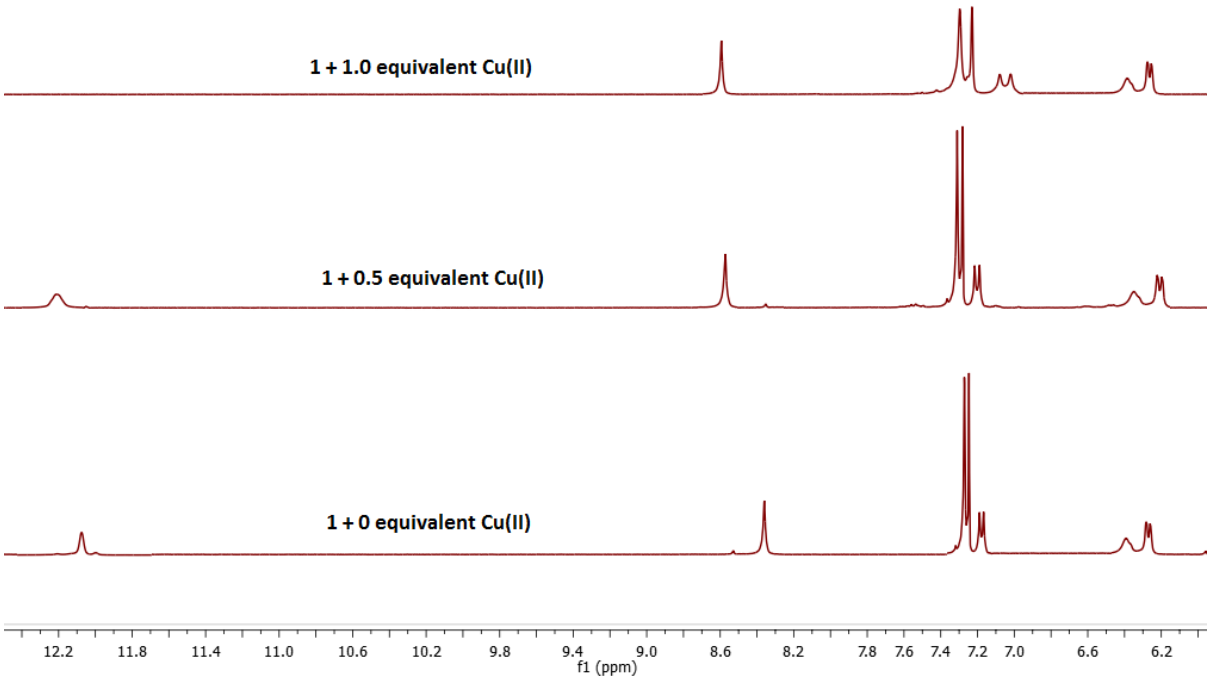

Figure S14. NMR spectra of 1 upon addition of different equivalent of Cu(II) ion**.**

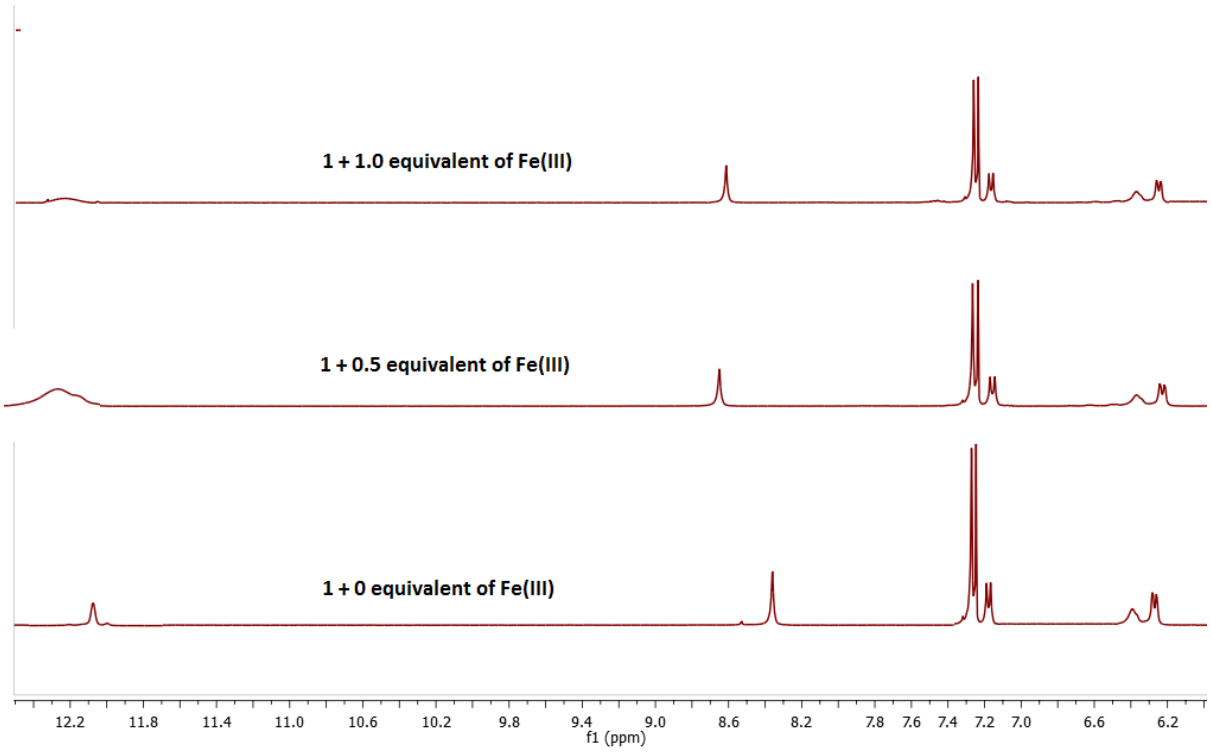

Figure S15. NMR spectra of 1 upon addition of different equivalent of Fe (III) ion.