Electronic Supplementary Informations

A Zn^{2+} responsive highly sensitive fluorescent probe and 1D coordination polymer based on a coumarin platform

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CONTENTS

Experimental section:

1.1 Apparatus: The IR Spectra for the receptor **1** and Zn^{2+} complex were recorded on JASCO-FTIR Spectrophotometer while ^{1}H NMR spectra were recorded on JEOL AL 300 FT NMR Spectrometer. Mass spectrometric analysis was carried out on a MDS Sciex API 2000 LCMS 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 Varian Cary Eclipse Fluorescence spectrophotometer and JY HORIBA Fluorescencespectrophotometer.

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/nitrate salts. The ^{1}H NMR spectra were recorded by using tetramethylsilane (TMS) as an internal reference standard.

1.4. X-ray diffraction studies: Single crystal X-ray diffraction measurements were carried out on an Oxford Diffraction Xcalibur system with a Ruby CCD detector. All the determinations of unit cell and intensity data were performed with graphite-mono-chromated Mo-Kα radiation (λ= 0.71073 A°). Data for the ligand and metal complex were collected at room temperature. The structures were solved by direct methods, using Fourier techniques, and refined by full-matrix least-squares on F2 using the SHELXTL-97 program package. Crystal data and details of the structure determination for ligand and complex are summarized in Table 1. CCDC **873620 and 873621** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/cgi-bin/catreq.cgi.

Table S1: Crystal data and details of the structure determination of receptor1and receptor 1 with Zn^{2+}

Identification code	**RECEPTOR 1**	**1+Zn^{2+} COMPLEX**
CCDC No.	**873620**	**873621**
Empirical formula	C21 H22 N4 O3	C21 H21 N5 O6 Zn
Formula weight	378.43	504.80
Temperature	293(2) K	293(2)
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Orthorhombic
space group	P 21	P 21 21 21
Unit cell dimensions	a = 6.3154(4) Å alpha = 90° b = 12.2970(7) Å beta = 97.703(7) c = 12.3905(9) Å gamma = 90°	a = 12.3149(17) Å alpha = 90° b = 12.7297(7) Å beta = 90° c = 14.0515(11) Å gamma = 90°
Volume	953.57(11) $Å^3$	2202.8(4) $Å^3$
Z	2	4
Density (calculated)	1.318 mg/m^{-3}	1.522 mg/m^{-3}
Absorption coefficient	0.090 mm^{-1}	1.164 mm^{-1}
F(000)	400	1040
Crystal size	0.40 x 0.20 x 0.20 mm	0.32 x 0.24 x 0.22 mm
Crystal color and habit	Red and Rectangular	Red and Rectangular
Diffractometer	'Xcalibur, Eos	'Xcalibur, Eos
Theta range for data collection	3.26 to 28.90 deg.	3.20 to 32.50 deg
Limiting indices	-8<=h<=8,-15<=k<=9,-6<=l<=11	-17<=h<=5, -19<=k<=18, -21<=l<=
Reflections collected / unique	4028 / 3058 [R(int)= 0.0199]	9340 / 6068 [R(int) = 0.0621]
Completeness to theta = 25.00	99.9 %	99.8 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission		1.00000 and 0.86938
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	3058 / 1 / 256	6068 / 0 / 301
Goodness-of-fit on F^2	1.028	0.894
Final R indices [I>2sigma(I)]	R1 = 0.0546, wR2 = 0.1123	R1 = 0.0566, wR2 = 0.0626
R indices (all data)	R1 = 0.0937, wR2 = 0.1340	R1 = 0.1218, wR2 = 0.0816
Absolute structure parameter	2.8(18)	0.001(15)
Largest diff. peak and hole	0.270 and -0.239 e. $Å^{-3}$	0.630 and -0.566 e. $Å^{-3}$

Figure S1: IR spectrum of receptor 1

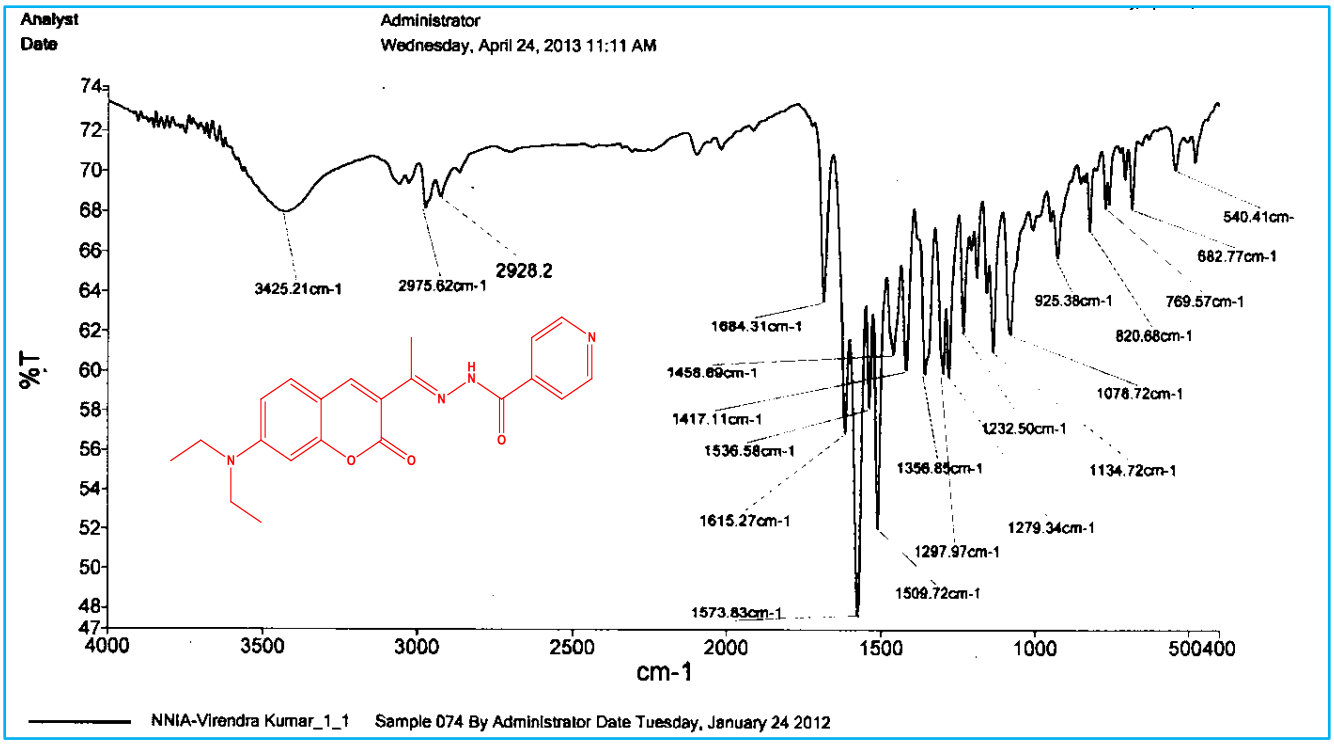


Figure S2: ^{1}H NMR spectrum of receptor 1

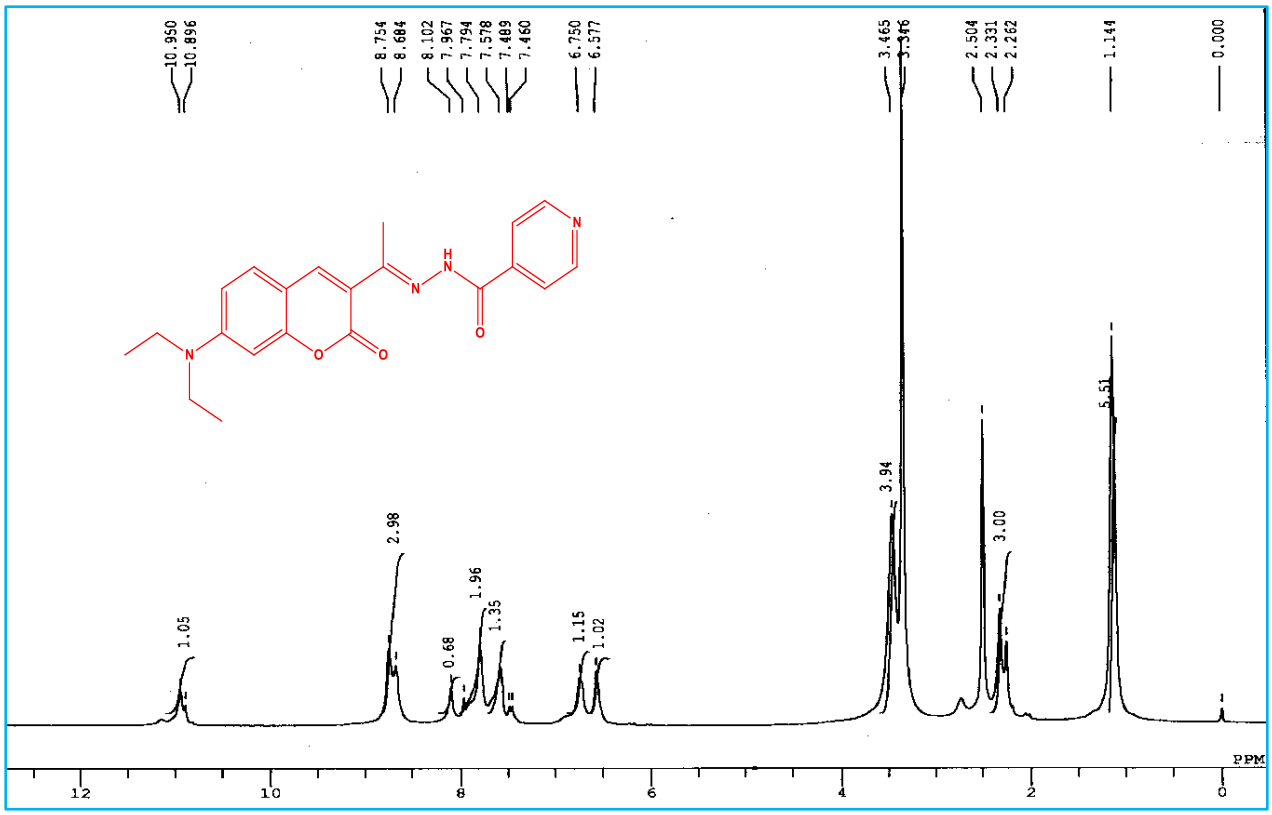


Figure S3: ^{13}C NMR spectrum of receptor 1

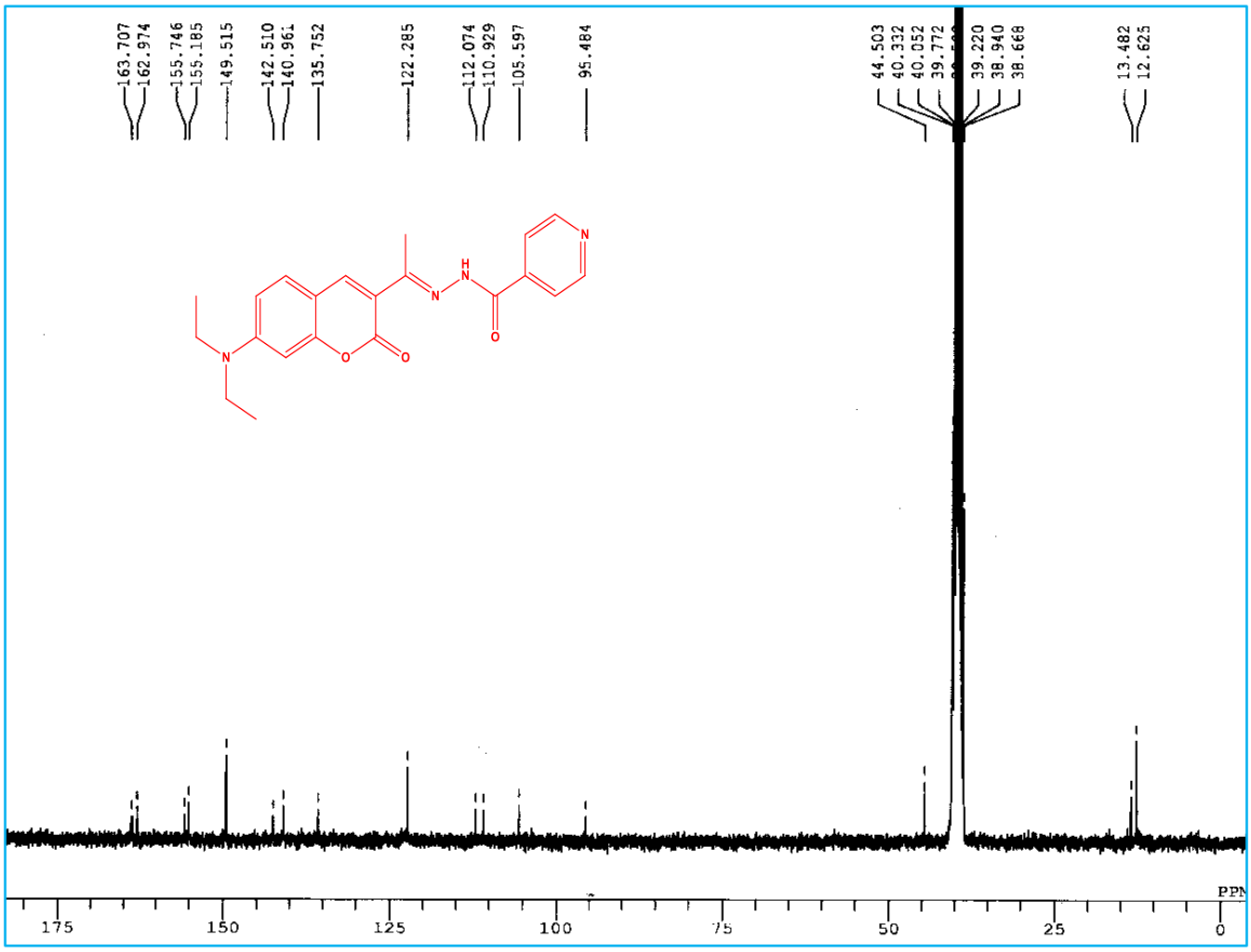
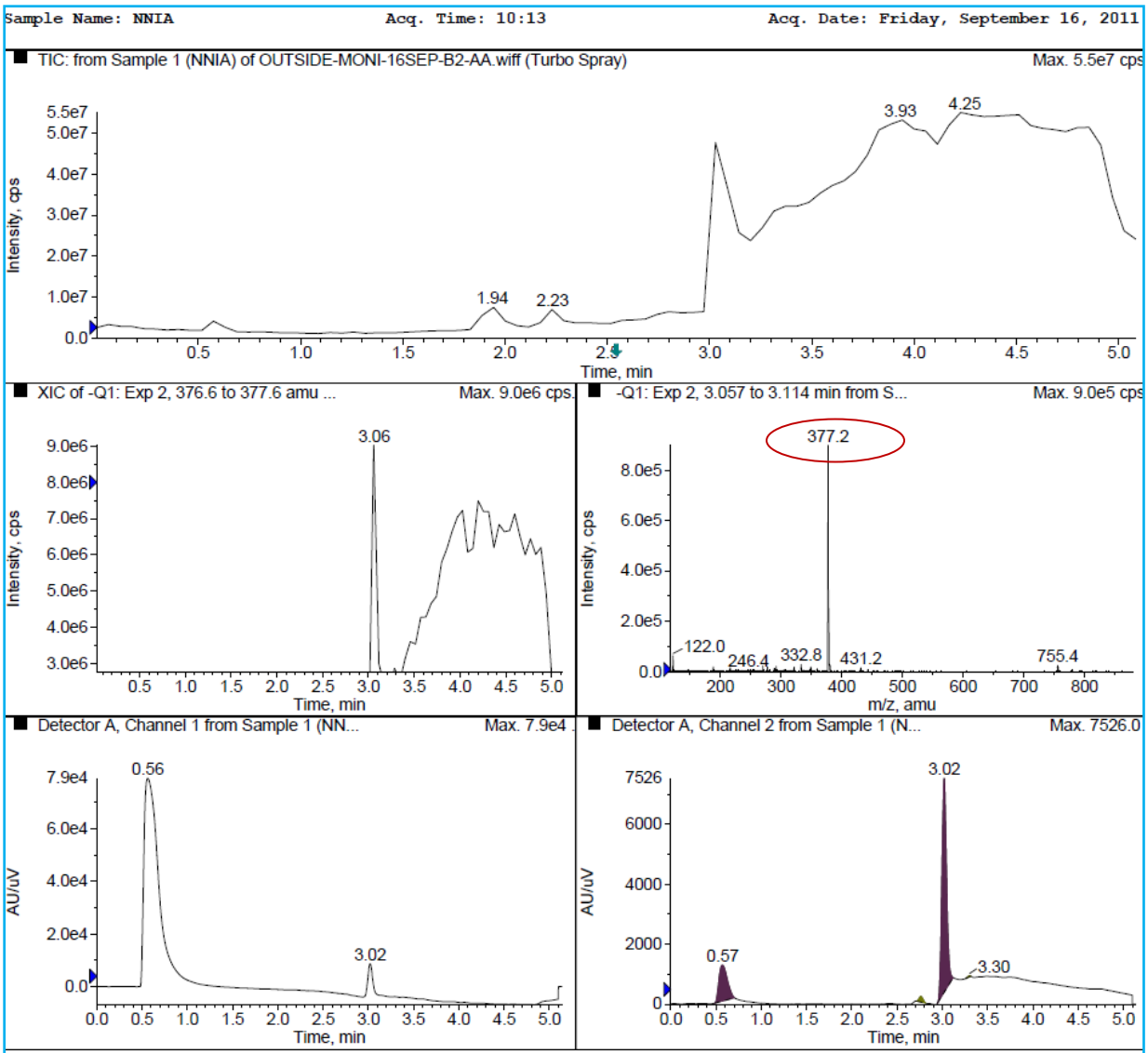


Figure S4: Mass spectrum of receptor 1



Peak List for "Detector A, Channel 2 from Sample 1 (NNIA) of OUTSIDE-MONI-16SEP-B2-AA.wiff"

	Time (min)	Area (counts)	% Area	Height	% Height	Width (min)	Baseline Type
1	0.5708	7619.1322	22.6571	1193.1388	13.9760	0.2200	Base to Base
2	2.7625	540.2514	1.6066	185.9483	2.1781	0.0967	Base to Base
3	3.0202	2.5400e4	75.5338	7125.7618	83.4688	0.1733	Base to Base
4	3.3008	68.0923	0.2025	32.1828	0.3770	0.0533	Base to Base

Figure S5: UV-visible Spectrum of receptor **1** with Zn^{2+} and the color change of receptor 1 without and with Zn^{2+}

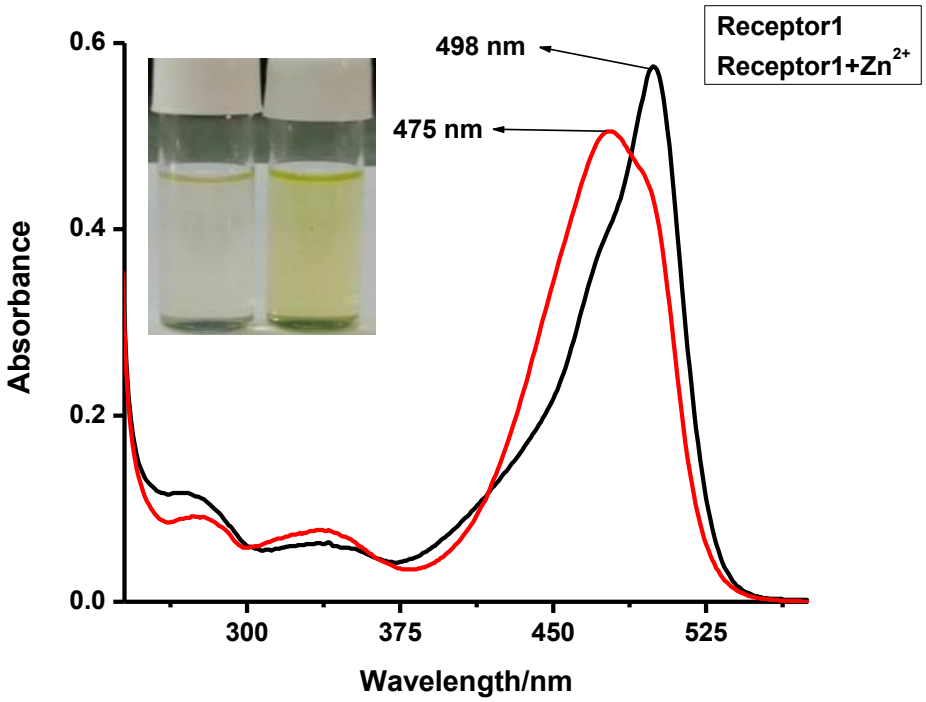


Figure S6: UV-visible Spectrum of receptor **1** with different metal ions at 10 µM in EtOH:H_2O (1:1, v/v)

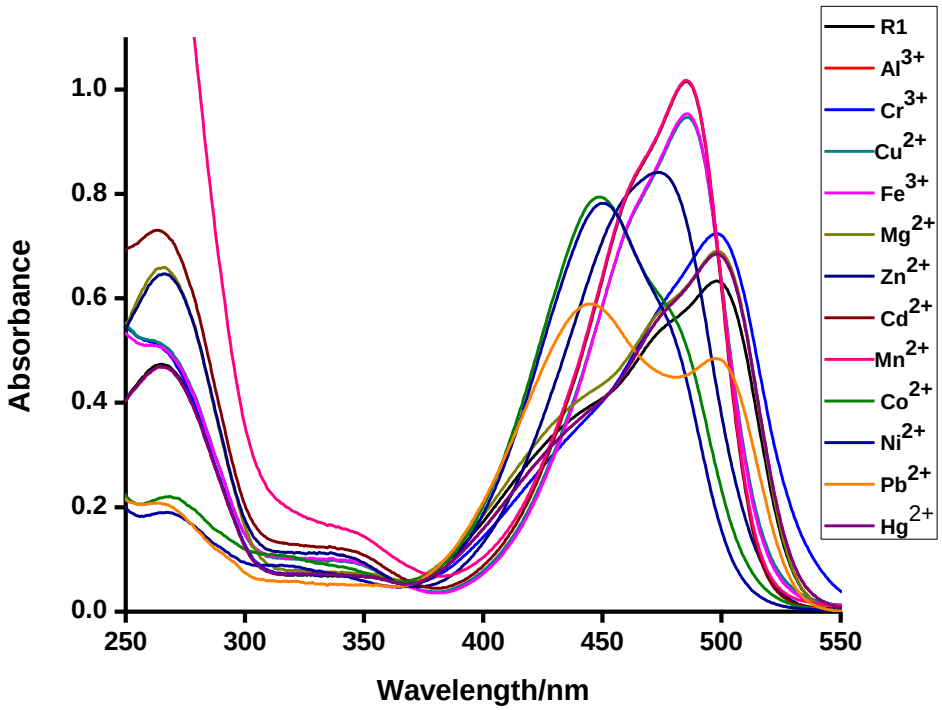


Figure S7: Fluorescence emission spectra of receptor **1** in the presence of various metal ions

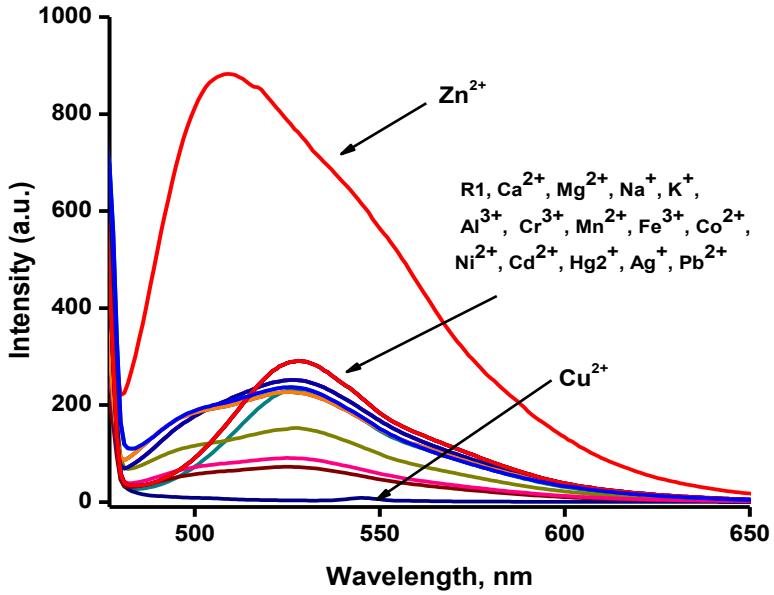


Figure S8: Fluorescence spectrum of receptor **1** in the presence of various counter anions of Zn^{2+}

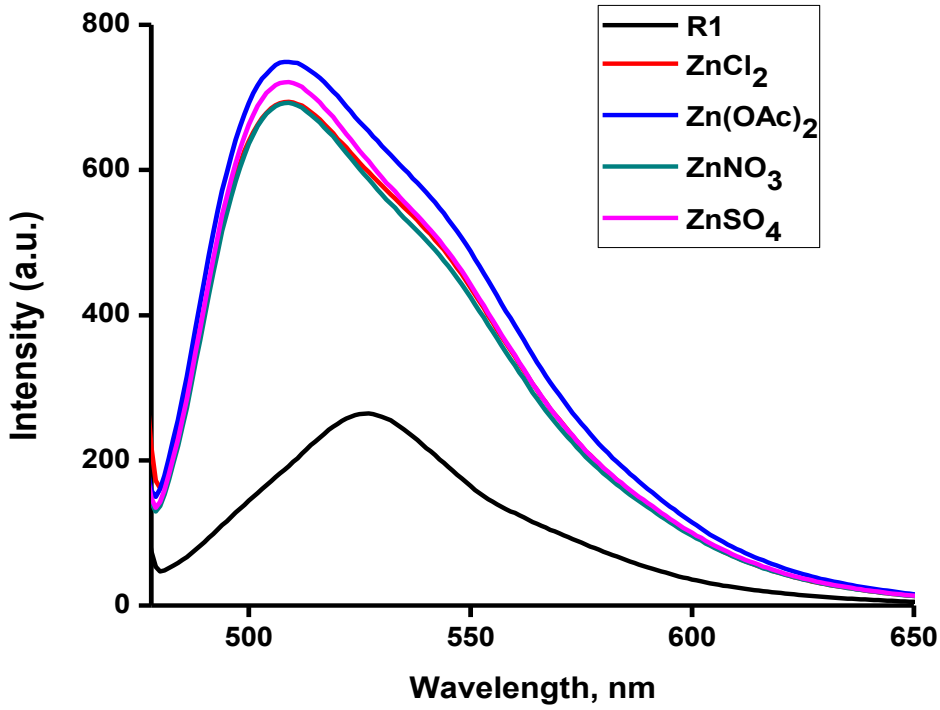


Figure S9: Job's Plot between receptor **1** and Zn^{2+} showing 1:1 binding stoichiometry

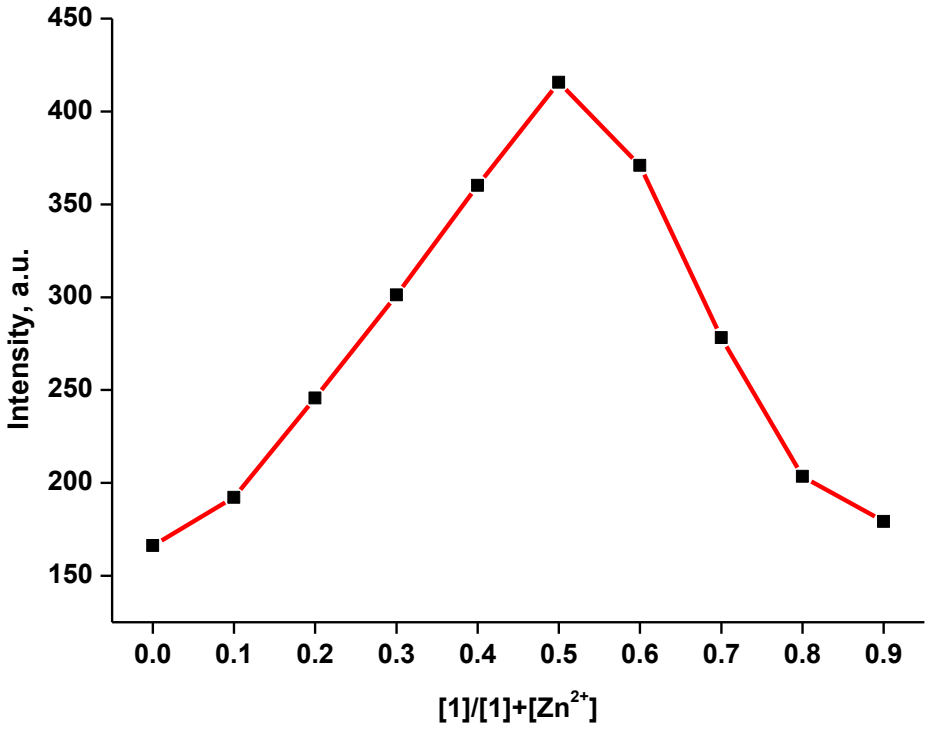


Figure S10: IR spectrum of receptor **1** with Zn^{2+}

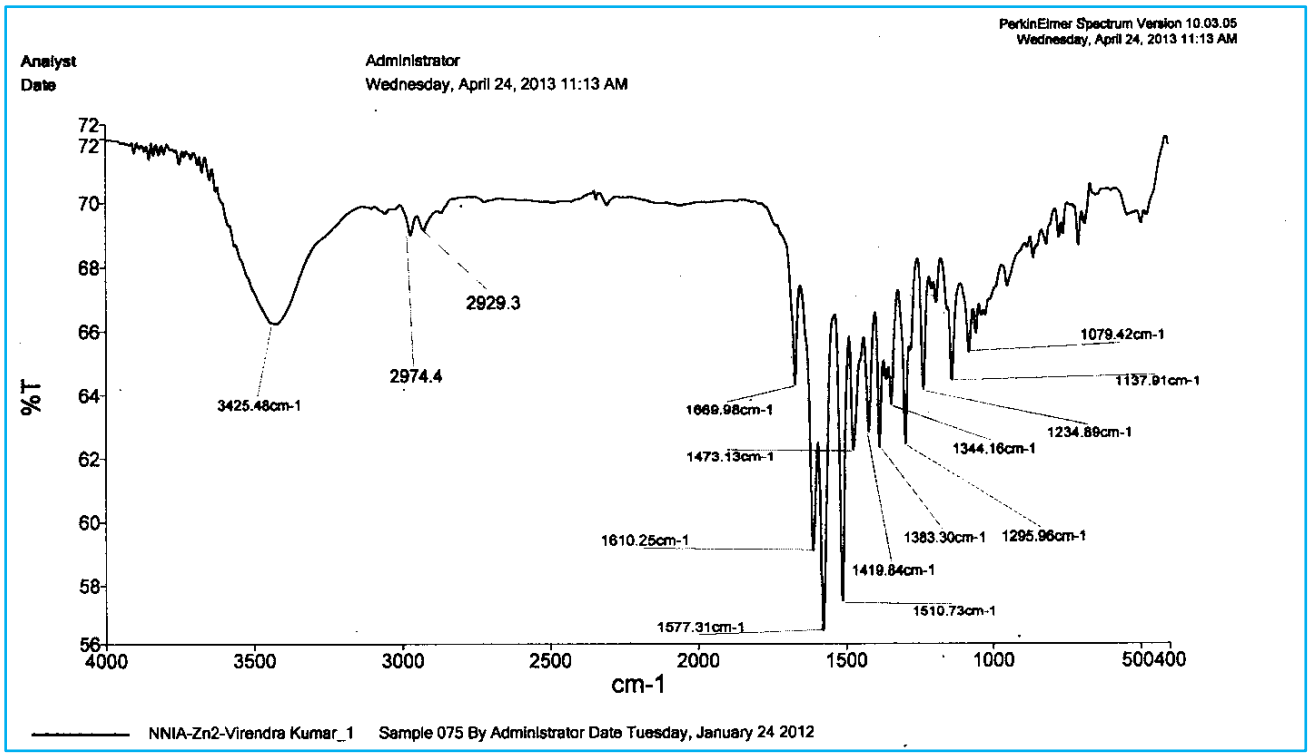
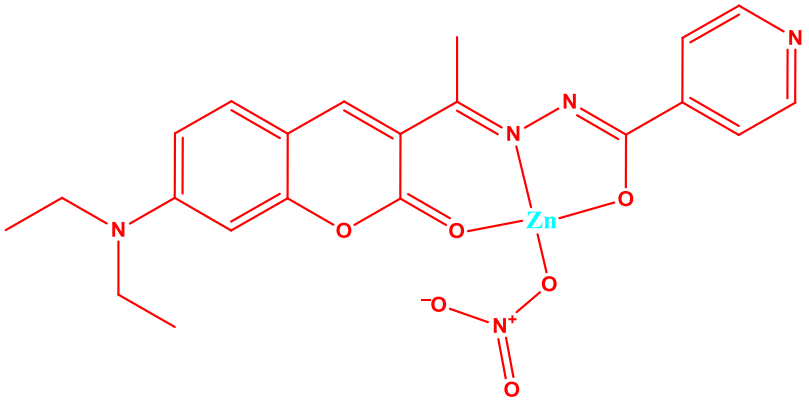


Figure S11: ^{1}H NMR spectrum of receptor **1**+ Zn^{2+}



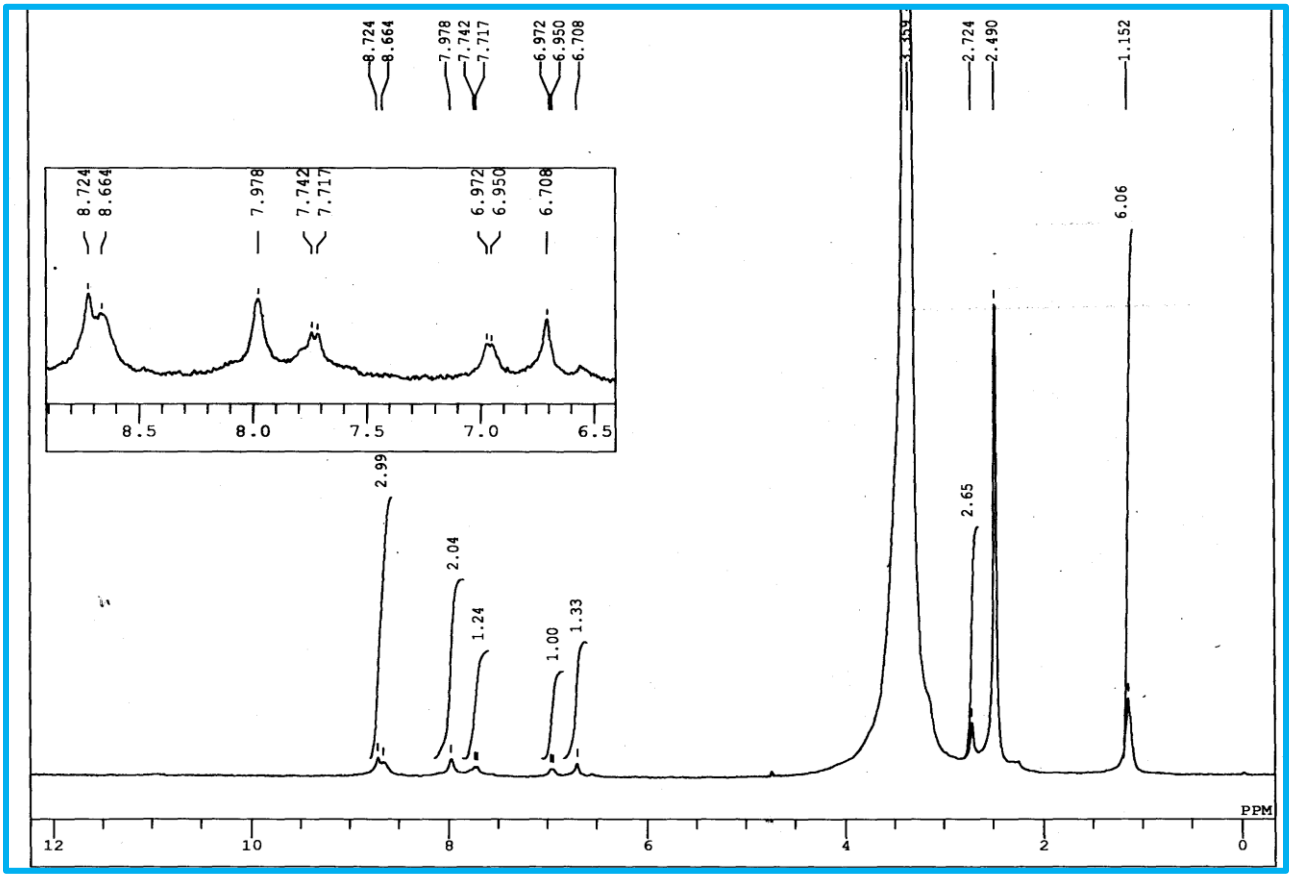


Figure S12: Nonlinear fit plot of receptor **1** with Zn^{2+}

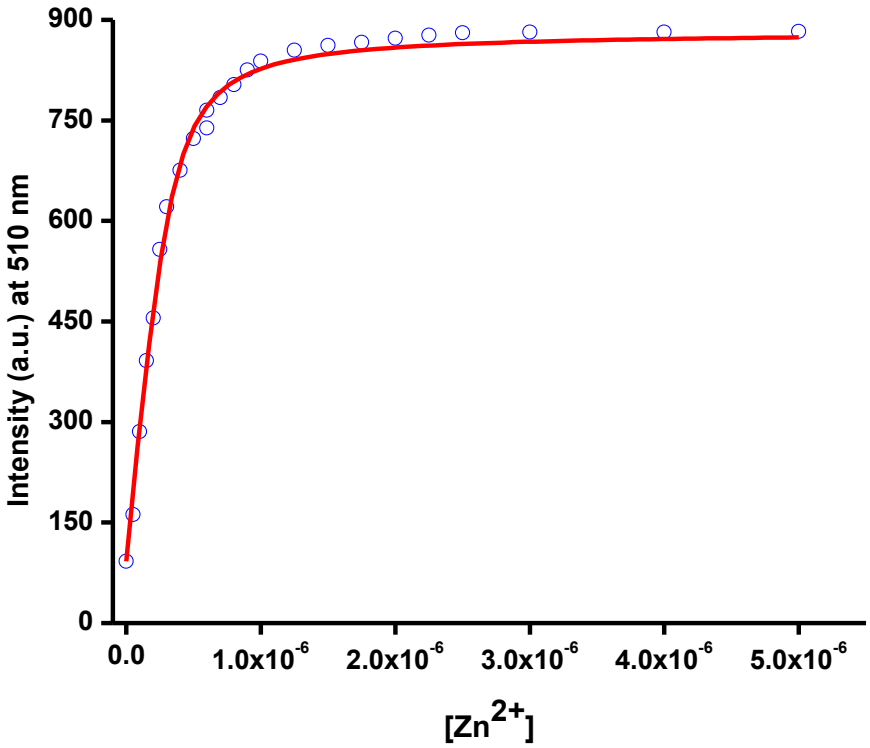


Figure S13: Detection limit and calibration curves of receptor **1** with Zn^{2+} with a linearity range of 1.5×10^{-7} to 4.5×10^{-7} M