Electronic Supplementary Material (ESI) for Dalton Transactions.

Intracellular detection of hazardous Cd^{2+} through fluorescence imaging technique by a nontoxic coumarin based sensor

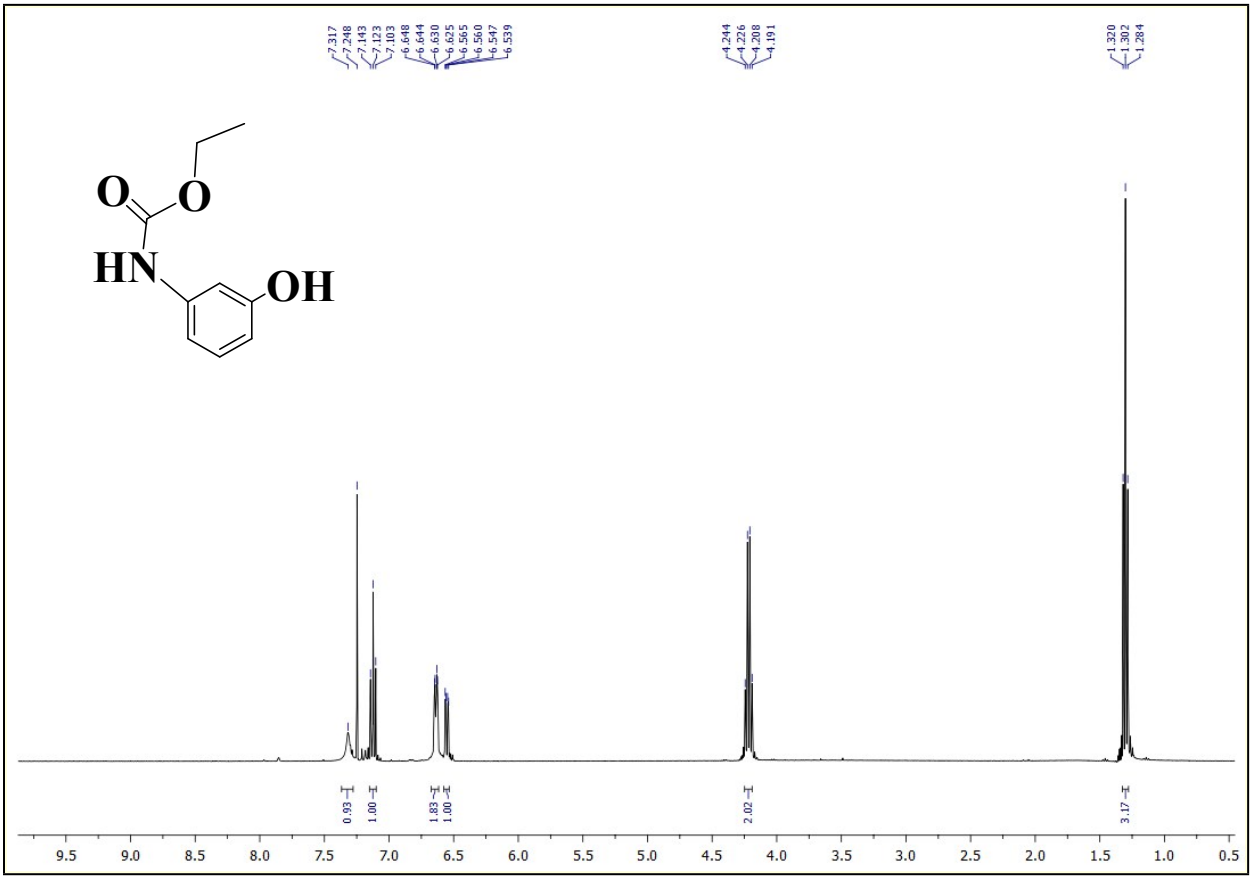
Chanda Kumari,[a] Dibyendu Sain,[a,b] Ashish Kumar,[a] Sushanta Debnath,[c] Partha Saha[c] and Swapan Dey*[a]

Table of content	Page No.

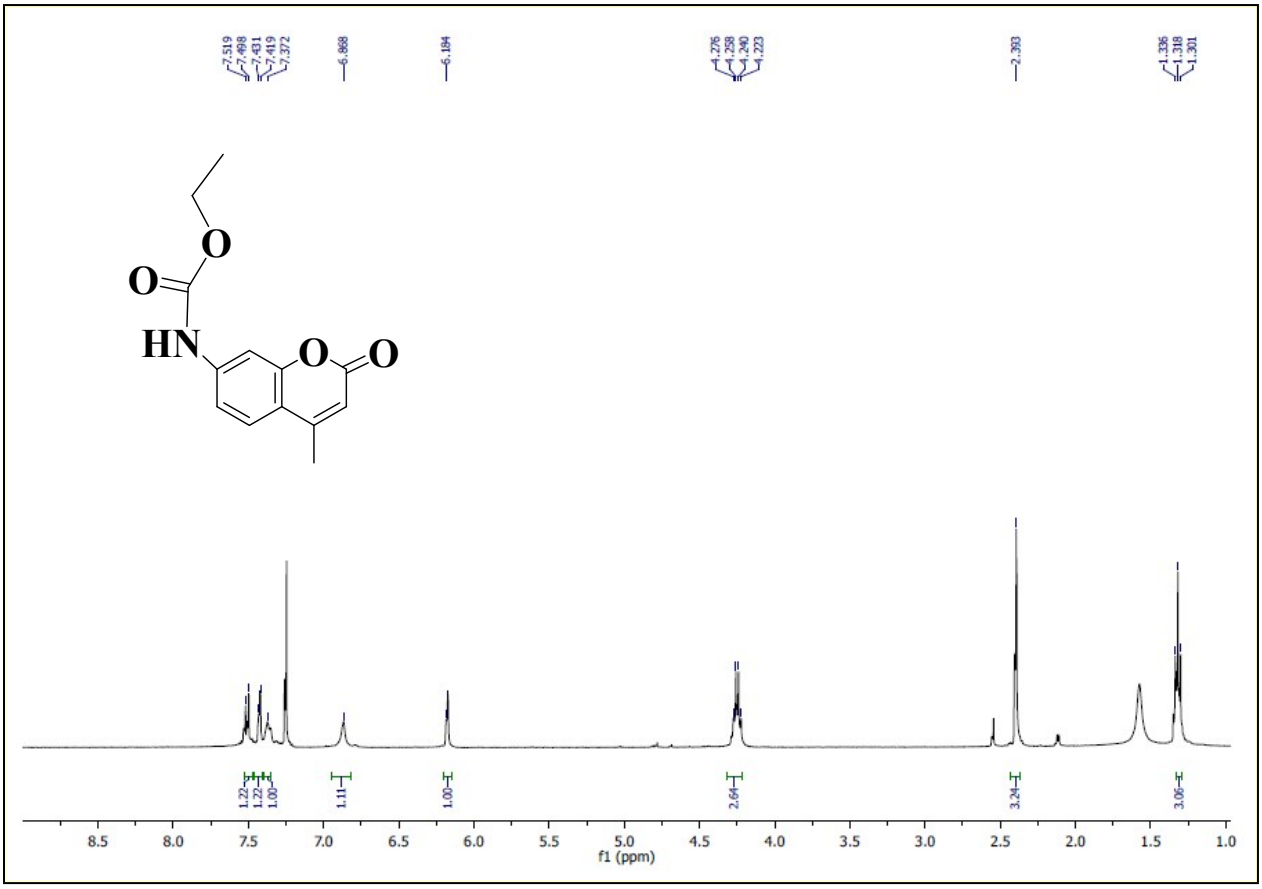
Table S1: ***Crystallographic data for*** **R1**

CCDC No	1524036
Empirical formula	$C_{38}H_{37}N_3O_4$
Formula weight	599.70
Temperature/K	296(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.6575(3)
b/Å	12.1006(4)
c/Å	15.5767(5)
α/°	108.837(2)
β/°	92.772(2)
γ/°	94.376(2)
Volume/Å^3	1712.65(10)
Z	2
ρ_{calc}g/cm^3	1.163
μ/mm^{-1}	0.076
F(000)	636.0
Crystal size/mm^3	? × ? × ?
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.574 to 56.624
Index ranges	$-12 \leq h \leq 12$, $-16 \leq k \leq 16$, $-20 \leq l \leq 20$
Reflections collected	31919
Independent reflections	8465 [R_{int} = 0.0336, R_{sigma} = 0.0343]
Data/restraints/parameters	8465/0/406
Goodness-of-fit on F^2	1.097
Final R indexes [I>=2σ (I)]	R_1 = 0.0650, wR_2 = 0.1848
Final R indexes [all data]	R_1 = 0.1040, wR_2 = 0.2055
Largest diff. peak/hole / e Å^{-3}	0.66/-0.28

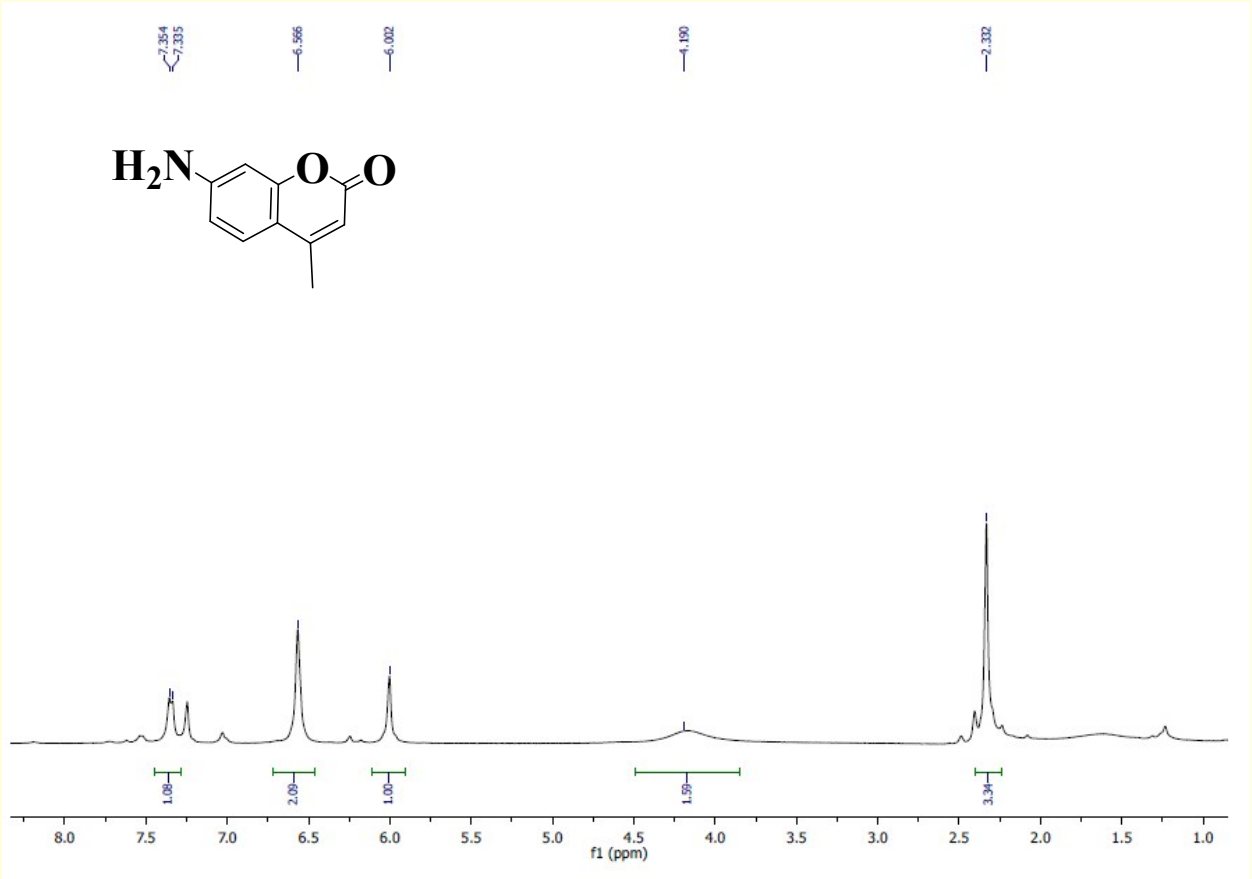
^{1}H-NMR (400 MHz, $CDCl_3$) spectra of compound 1



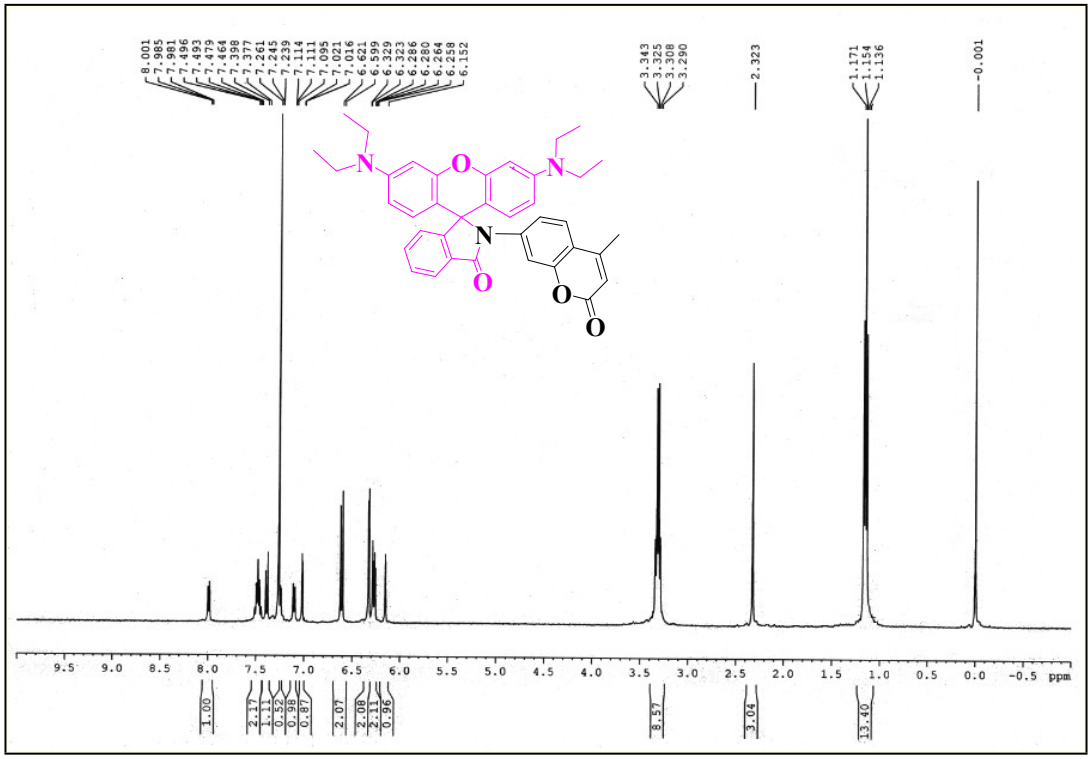
^{1}H-NMR (400 MHz, $CDCl_3$) spectra of compound 2



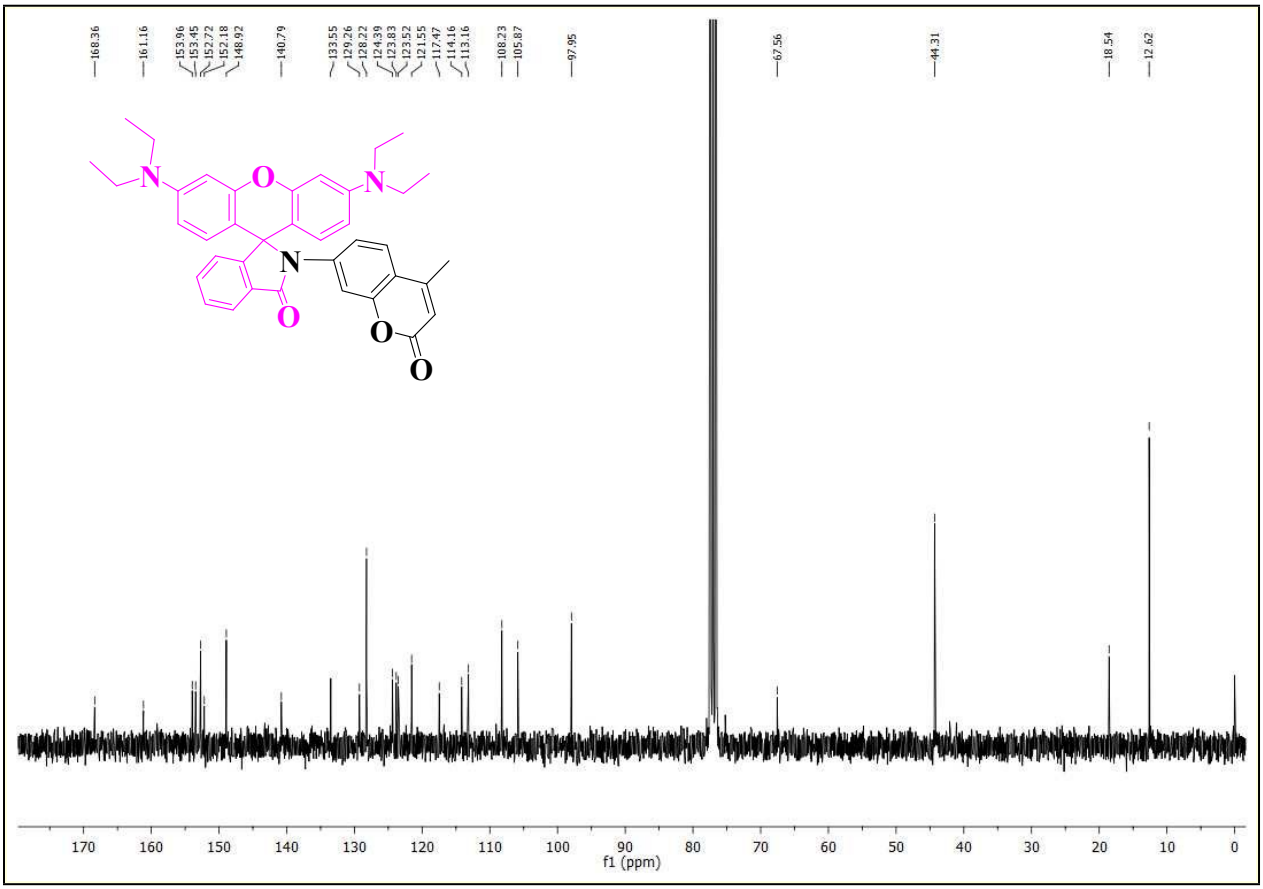
^{1}H-NMR (400 MHz, $CDCl_3$) spectra of compound 3



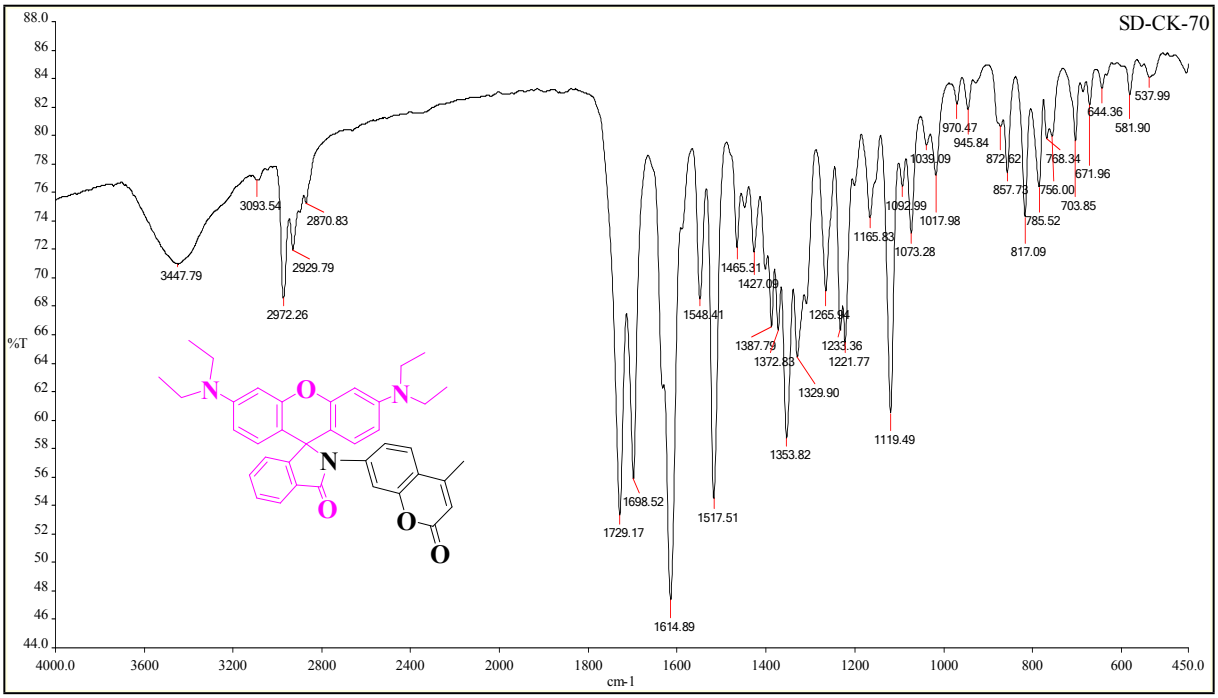
^{1}H-NMR (400 MHz, $CDCl_3$) spectra of R1



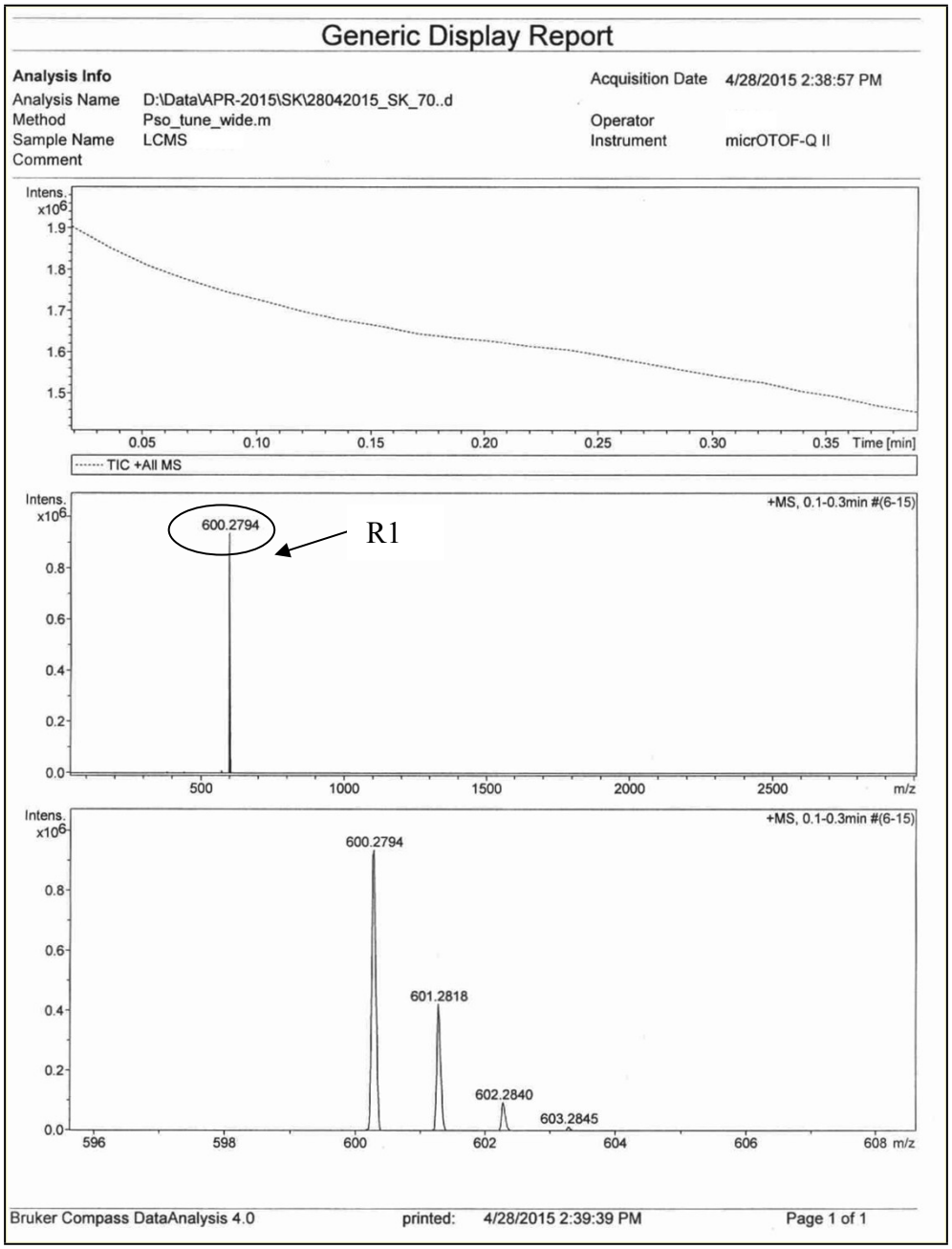
^{13}C-NMR (400 MHz, $CDCl_3$) spectrum of R1



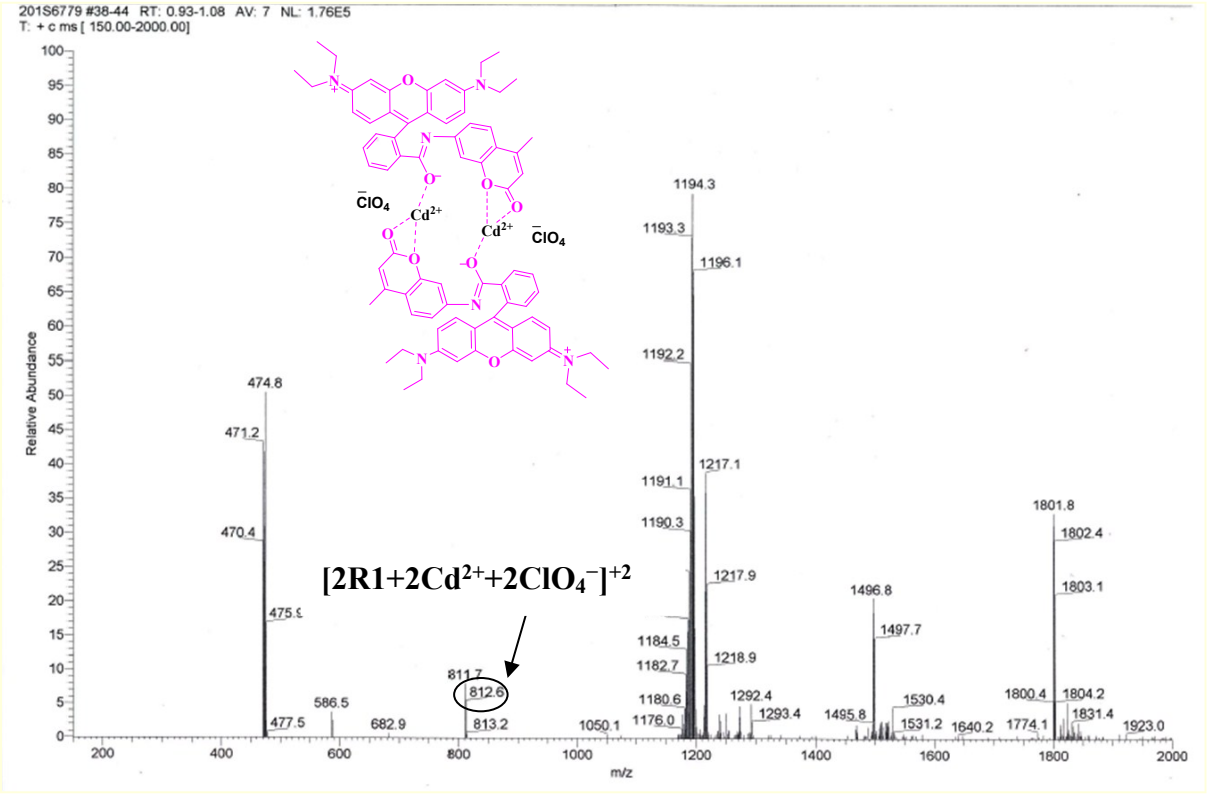
IR spectrum of R1



Mass spectrum of R1:



Mass spectrum of R1+ Cd^{2+}:



LOD of R1 with Cd^{2+}

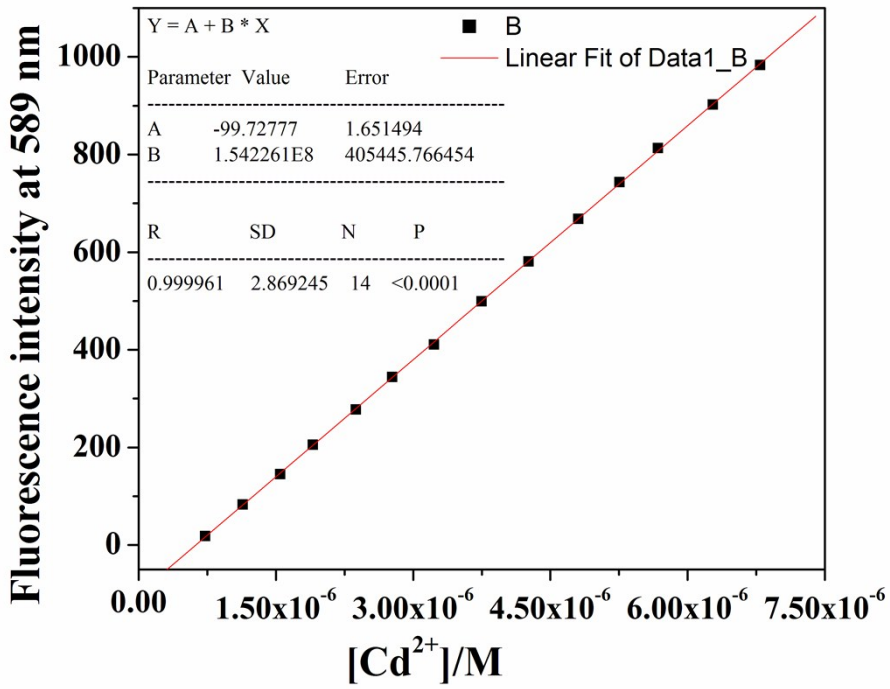
The detection limit of **R1** with **Cd^{2+}** was calculated on the basis of fluorescence titration data. To determine the standard deviation for the fluorescence intensity, the emission intensity of the individual receptors without any anion was measured by 10 times and the standard deviation of blank measurements was calculated.

The limit of detection (LOD) of the receptors for sensing **Cd^{2+}** was determined from the following equation:

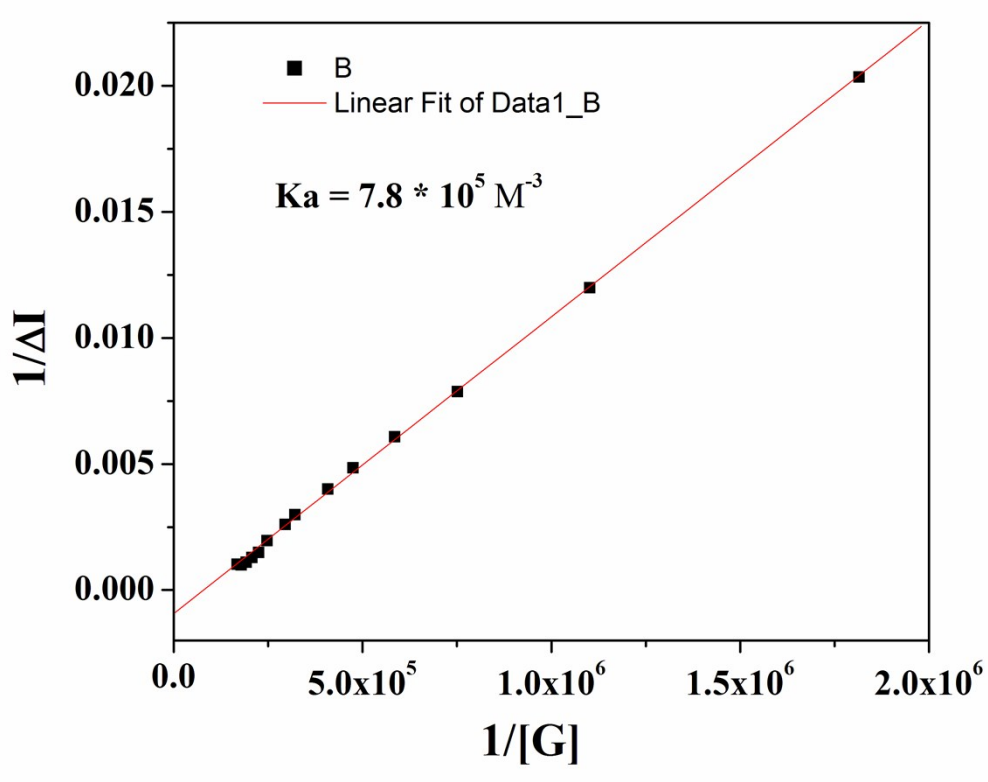
LOD = K × SD/S

Where K = 2 or 3 (we take 3 in this case); SD is the standard deviation of the blank receptor (**R1**) solution; S is the slope of the calibration curve.

From the linear fit graph we get slope 1.54×10^{8}, and SD value is 0.52. Thus using the above formula we get the Limit of Detection = 1.01×10^{-8} M i.e. **R1** can detect **Cd^{2+}** up to this very lower concentration by fluorescence techniques.



Association constant calculation by Fluorescence titration method



Association constant calculation by Fluorescence titration method of **R1** with $\mathbf{Cd^{2+}}$ using linear regression analysis.

Quantum yield calculation:

Fluorescence quantum yields (Φ) were calculated using Equation given below (1) (Wu, D.; Huang, W.; Duan, C.; Lin, Z.; Meng, Q. *Inorg. Chem.* **2007**, *46*, 1538) using Rhodamine B (Φ_f = 0.49 in ethanol) as standards.

$$\Phi_u = \Phi_s \times \frac{I_u}{I_s} \times \frac{A_s}{A_u} \times \left(\frac{\eta_u}{\eta_s}\right)^2$$

Where Φ_u and Φ_s are the fluorescence quantum yields of the sample and standard, I_u and I_s are the integrated emission intensities of the sample and standard, A_u and A_s are the absorbance of the sample and standard at the excitation wavelength (560 nm), and η_u and η_s are the refractive indices of the sample and standard solutions, respectively.