Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers

Supporting Information

Nano Dispersion of 3D Cd(II) Co-ordination Polymer:

Synthetic Blood Plasma Anticoagulant

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Materials and instrumentation: All chemicals and reagents were purchased from Sigma Aldrich. The IR spectral studies were performed on Perkin Elmer FT-IR spectrometer using KBr pellets. Fluorescence studies were carried on Agilent Technologies cary eclipse fluorescence spectrophotometer. U.V studies were carried on SHIMADZU UV-2450 spectrophotometer using quartz cuvettes. Single crystal X-ray diffraction (SXRD) data was collected on dual core Agilent Technologies super nova CCD system. Powder X-ray diffraction (PXRD) data were collected on Rigaku SmartLab 9 KW rotating anode Powder X-ray Diffractometer at room temperature. The thermogravimetric analysis was carried out using The Mettler Toledo thermal analyzer in N_2 atmosphere at a heating rate of 10 °C/ min. TEM images collected on SEI TECNAI F20 HRTEM (high resolution transmission electron microscope). SEM images were taken on SEI 15KV SEM (scanning electron microscope) instrument.

X-ray crystallography details. Single crystal X-ray structural studies of **RAM 1** were performed on a CCD Agilent Technologies (Oxford Diffraction) SUPER NOVA diffractometer. Data were collected at 150(2) K using graphite-monochromoated Mo Kα radiation (λ_α = 0.71073 Å). The strategy for the Data collection was evaluated by using the CrysAlisPro CCD software. The data were collected by the standard 'phi-omega scan techniques, and were scaled and reduced using CrysAlisPro RED software. The structure was solved by direct methods using SHELXS-97 and refined by full matrix least-squares with SHELXL-97, refining on F^2.[1]

The positions of all the non-hydrogen atoms were obtained by direct methods and were refined anisotropically. The hydrogen atoms were placed in geometrically constrained positions and refined with isotropic temperature factors, generally 1.2U_{eq} of their parent atoms. The crystal and refinement data are summarized in **Table 1**, and selected bond distances and bond angles are shown in **Table 2**.

(1) Sheldrick, G. M. *Acta Crystallogr., Sect. A* **2008**, *A64,* 112-122. *Program for Crystal Structure Solution and Refinement;* University of Goettingen: Goettingen, Germany, 1997.

Experimental for synthesis of RAM 1

Synthesis of $\{[Cd(NDC)(QN)]\}_n$ (**RAM 1**): A mixture of 0.085 g (0.46 mmol) $CdCl_2$, 0.050 g (0.23 mmol) of 2,6-H_2NDC, 110 µl (0.92 mmol) of QN, and 4 ml of DMF was placed in Parr's acid digestion bomb and then heated in an oven at 125°C for 24 h. The mixture was allowed to cool at room temperature for 12 h to obtain cream colored crystals (0.057 g, yield 27.2%) which were washed with DMF (3×1 ml) and dried under vacuum at room temperature.

Table 1 Crystal data and structure refinement parameters for **RAM 1**

Empirical formula	$C_{21}H_{13}CdNO_4$
Formula weight	455.72
Temperature (K)	150(2)
Crystal size (mm)	0.23 x 0.18 x 0.13
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P -1
a(Å)	7.858(5)
b(Å)	10.508(5)
c(Å)	11.554(5)
α(°)	112.221(5)
β (°)	95.625(5)
γ (°)	105.097(5)
Z	2
Volume (Å^3)	831.8(8)
Density (Mg m^{-3})	1.819
Absorption coefficient (mm^{-1})	1.341
F(000)	452
θ range for data collection (°)	3.00 to 25.00 deg.
Limiting indices	-9<=h<=9, -12<=k<=12, -13<=l<=13
Reflections collected / unique	4423 / 4423
R(int)	0.0000
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8449 and 0.7478
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4423 / 0 / 244
Goodness-of-fit on F^2	1.070
Final R indices [$I>2s\sigma(I)$]	R1 = 0.0506, wR2 = 0.1341
R indices (all data)	R1 = 0.0539, wR2 = 0.1371
Largest diff. peak and hole (e.Å^{-3})	1.259 and -0.963

Table 2 Selected bond lengths (Å) and angles (°) for **RAM 1**

Cd(1)-O(1)	2.262(4)	Cd(1)-O(2)#1	2.551(4)
Cd(1)-N(1)	2.266(5)	Cd(1)-O(3)#2	2.588(4)
Cd(1)-O(4)	2.313(4)	Cd(1)-C(16)	2.664(5)
Cd(1)-O(3)	2.354(4)	Cd(1)-C(10)	2.745(5)
Cd(1)-O(2)	2.460(4)		
O(1)-Cd(1)-N(1)	100.04(18)	N(1)-Cd(1)-C(16)	139.35(19)
O(1)-Cd(1)-O(4)	98.78(15)	O(4)-Cd(1)-C(16)	27.76(15)
N(1)-Cd(1)-O(4)	159.52(18)	O(3)-Cd(1)-C(16)	28.42(15)
O(1)-Cd(1)-O(3)	132.10(15)	O(2)-Cd(1)-C(16)	80.25(15)
N(1)-Cd(1)-O(3)	114.41(17)	O(2)#1-Cd(1)-C(16)	119.69(14)
O(4)-Cd(1)-O(3)	56.09(13)	O(3)#2-Cd(1)-C(16)	88.82(14)
O(1)-Cd(1)-O(2)	129.93(14)	O(1)-Cd(1)-C(10)	26.99(16)
N(1)-Cd(1)-O(2)	83.78(17)	N(1)-Cd(1)-C(10)	96.16(18)
O(4)-Cd(1)-O(2)	77.96(14)	O(4)-Cd(1)-C(10)	96.95(15)
O(3)-Cd(1)-O(2)	87.65(15)	O(3)-Cd(1)-C(10)	148.66(15)
O(1)-Cd(1)-O(2)#1	54.04(14)	O(2)-Cd(1)-C(10)	103.08(15)
N(1)-Cd(1)-O(2)#1	91.82(16)	O(2)#1-Cd(1)-C(10)	27.06(15)
O(4)-Cd(1)-O(2)#1	92.72(13)	O(3)#2-Cd(1)-C(10)	108.10(14)
O(3)-Cd(1)-O(2)#1	147.56(13)	C(16)-Cd(1)-C(10)	123.77(16)
O(2)-Cd(1)-O(2)#1	76.05(14)	C(10)-O(1)-Cd(1)	98.4(3)
O(1)-Cd(1)-O(3)#2	81.76(13)	C(10)#1-O(2)-Cd(1)	170.4(3)
N(1)-Cd(1)-O(3)#2	85.21(15)	C(10)#1-O(2)-Cd(1)#1	85.1(3)
O(4)-Cd(1)-O(3)#2	105.47(13)	Cd(1)-O(2)-Cd(1)#1	103.95(14)
O(3)-Cd(1)-O(3)#2	69.71(14)	C(16)-O(3)-Cd(1)	89.5(3)
O(2)-Cd(1)-O(3)#2	147.84(12)	C(16)-O(3)-Cd(1)#2	126.9(4)
O(2)#1-Cd(1)-O(3)#2	134.50(12)	Cd(1)-O(3)-Cd(1)#2	110.29(14)
O(1)-Cd(1)-C(16)	118.83(17)	C(16)-O(4)-Cd(1)	92.1(3)

#1 -x+2,-y+2,-z+1 #2 -x+1,-y+2,-z+1

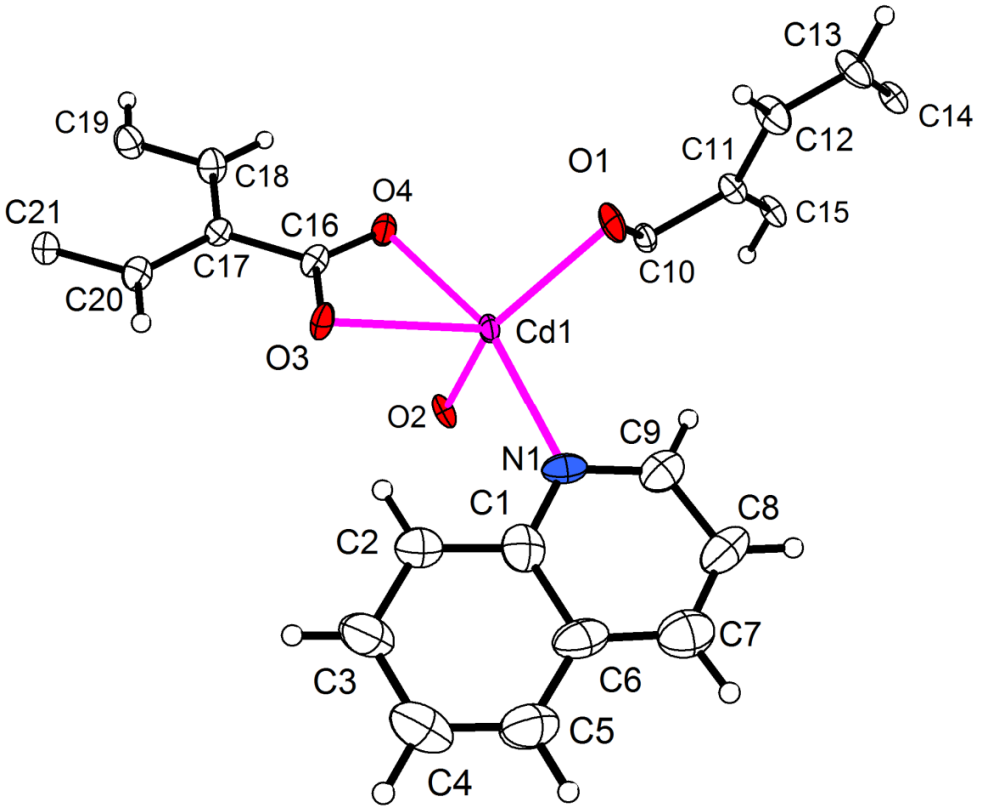

Fig . S1. Asymmetric unit

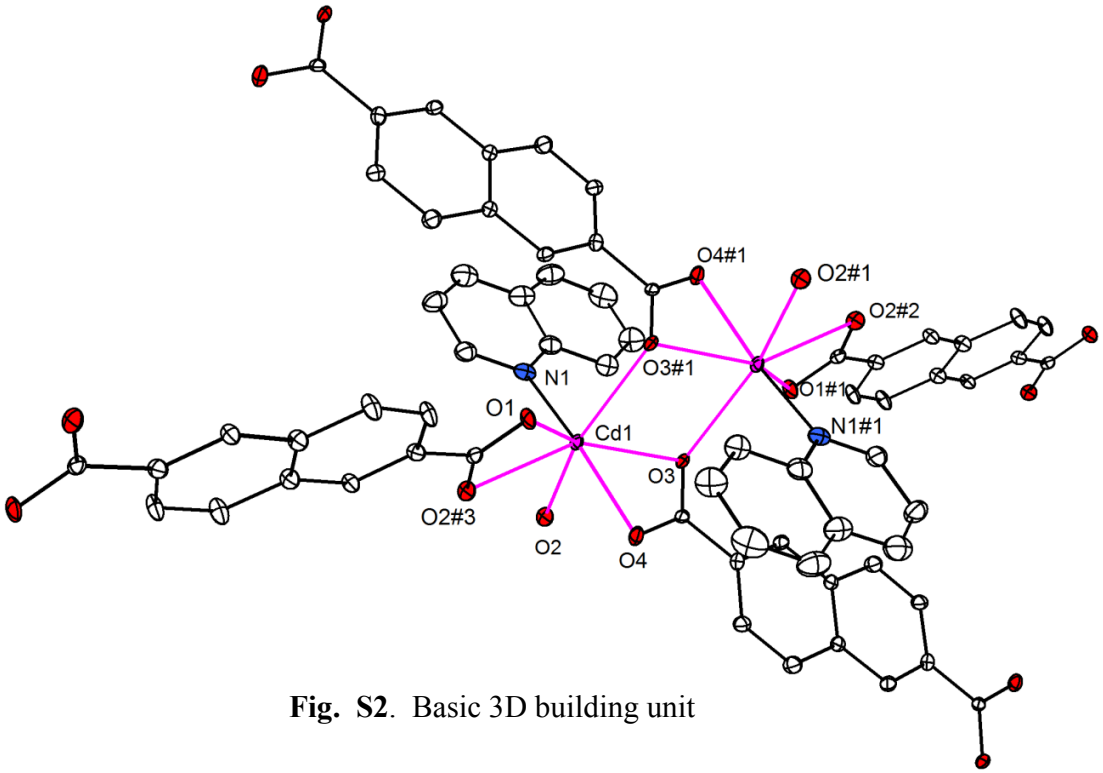

Fig. S2. Basic 3D building unit

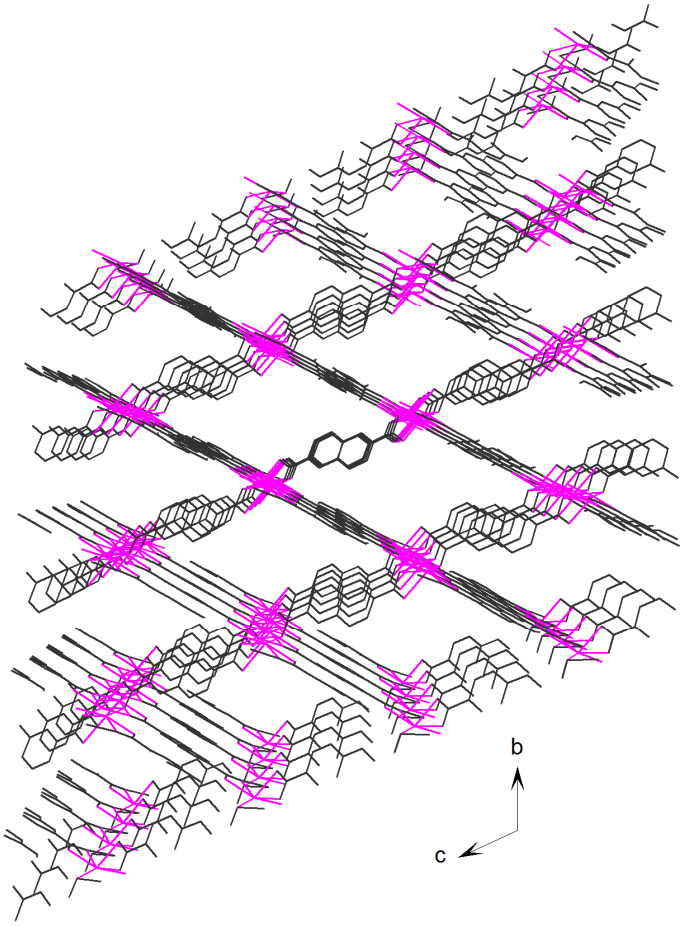

Fig. S3. 3D framework view along c axis. quinoline units have been omitted.

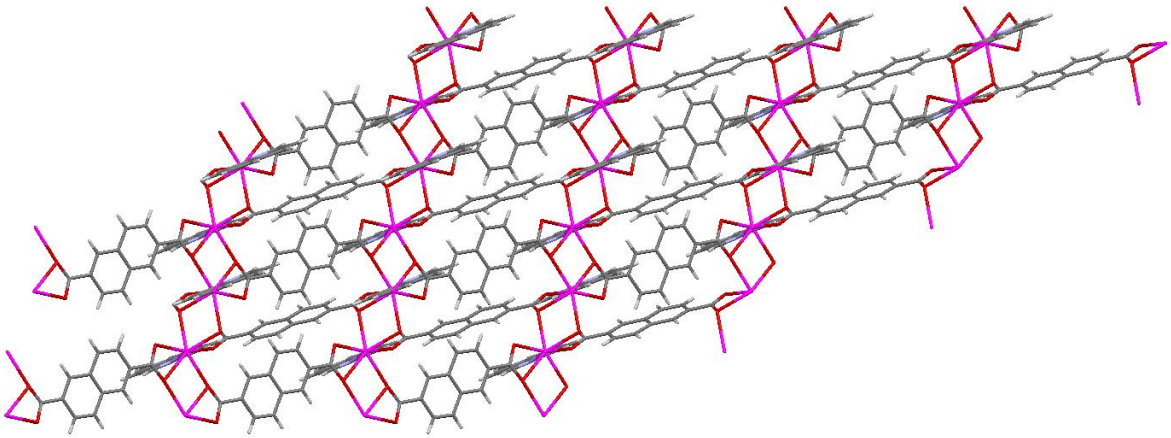

Fig. S4. View along b axis.

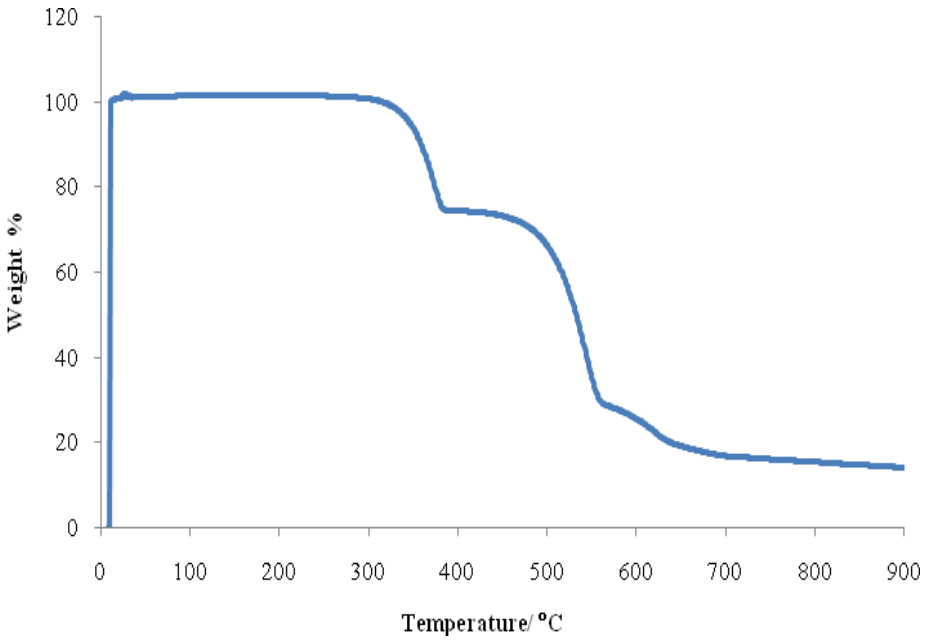

Fig. S5. Thermo gravimetric curve of **RAM 1** upto 1000 ^{0}C at heating rate of 10 ^{0}C/ min

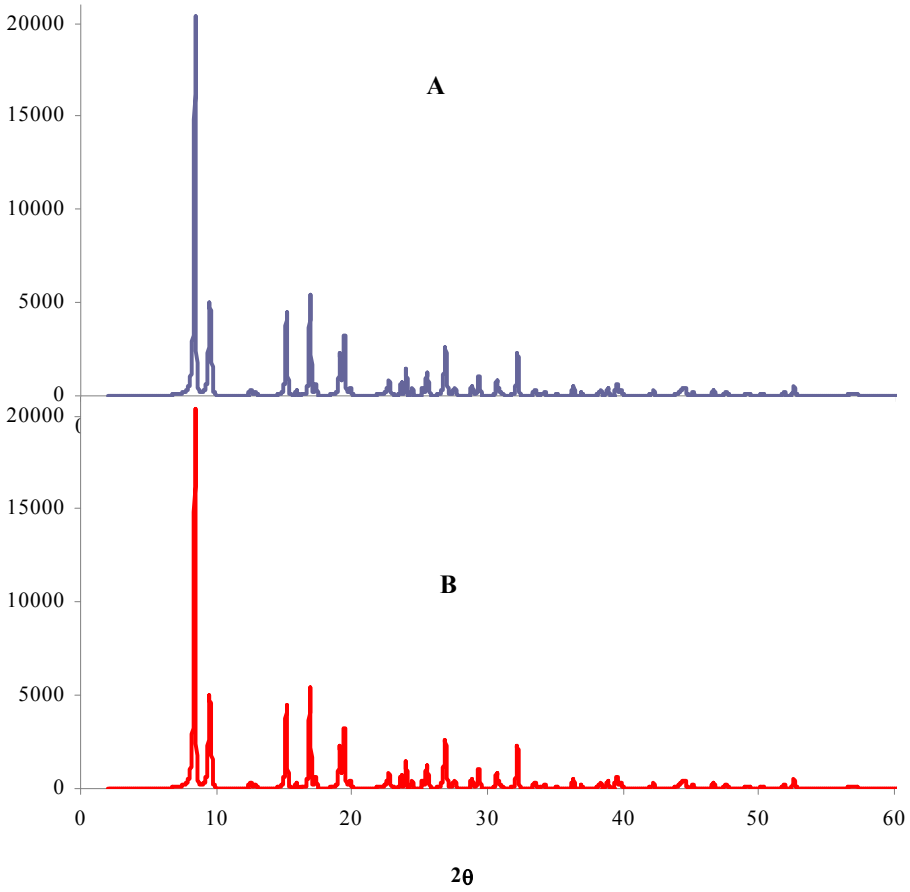

Fig. S6. (A) Powder X –ray diffraction of **RAM 1.** (B) Powder X-ray of **DRAM 1** at room temperature (The **DRAM 1** was ultra centrifuged and solid was collected which was used for the study).

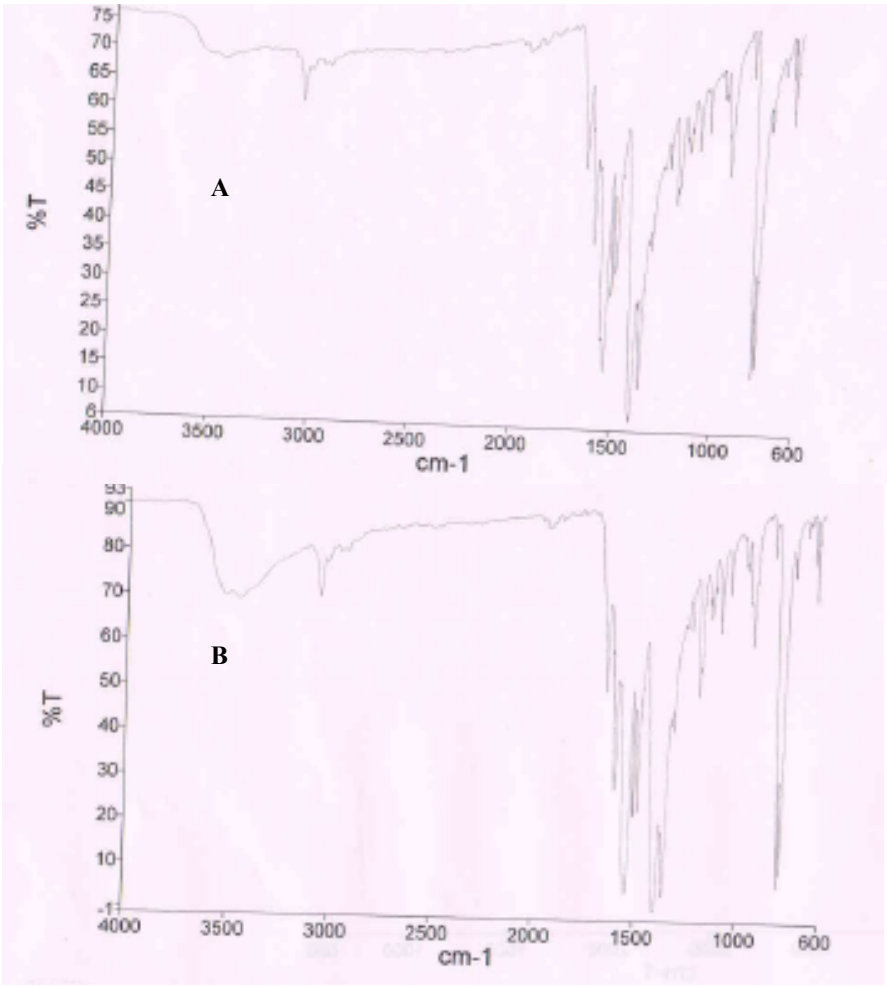

Fig. S7. (A) IR spectrum of **RAM 1**. (B) IR spectrum of **DRAM 1** using KBR pellets at room temperature (The **DRAM 1** was ultra centrifuged and solid was collected which was used for the study).

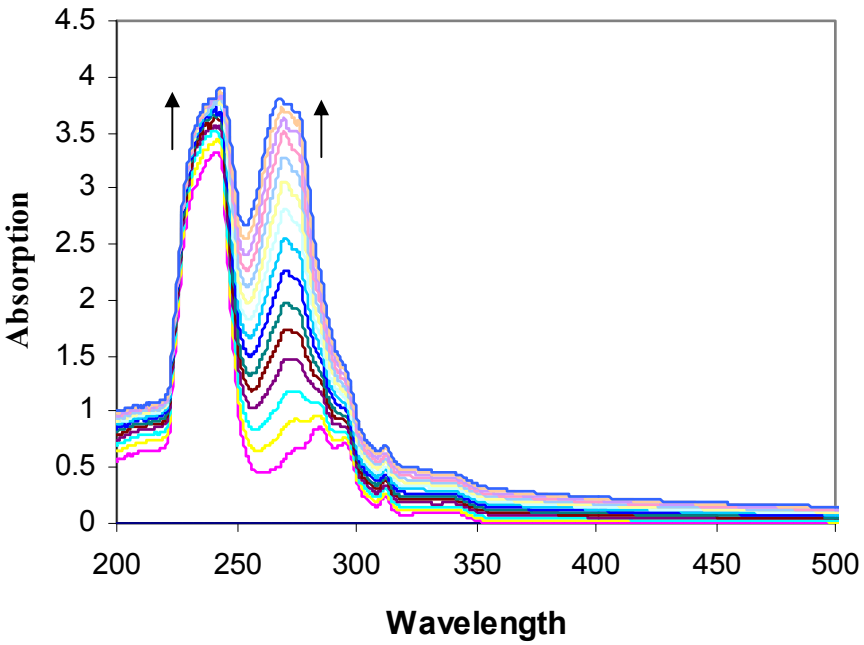

Fig. S8. UV-vis absorption spectra of **DRAM 1** on addition of **TP** (225 µl) in H_2O; pH = 7.4 buffered with HEPES.

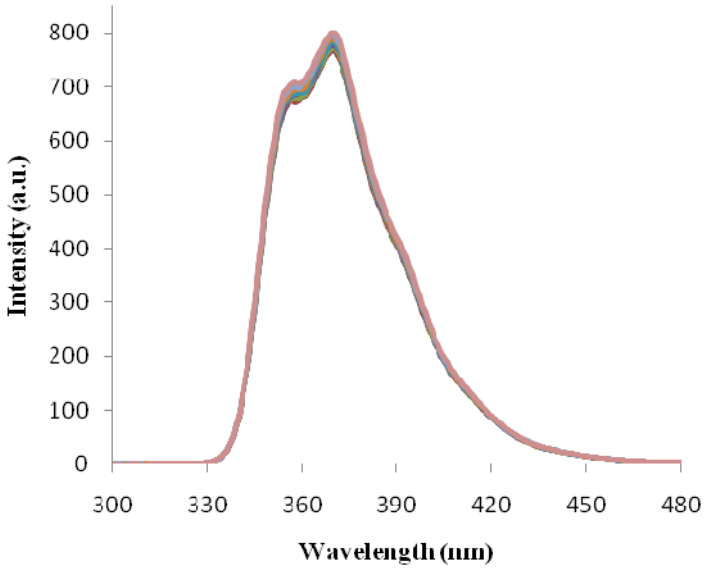

Fig S9: Fluorescence emission of **DRAM 1** on addition of 750 µL (2 mg in 1 ml) of HSA, λ_{ex} = 243 nm.