Supporting Information

Crystal Engineering with a Purine Rare Tautomer: Structures and Luminescence Properties

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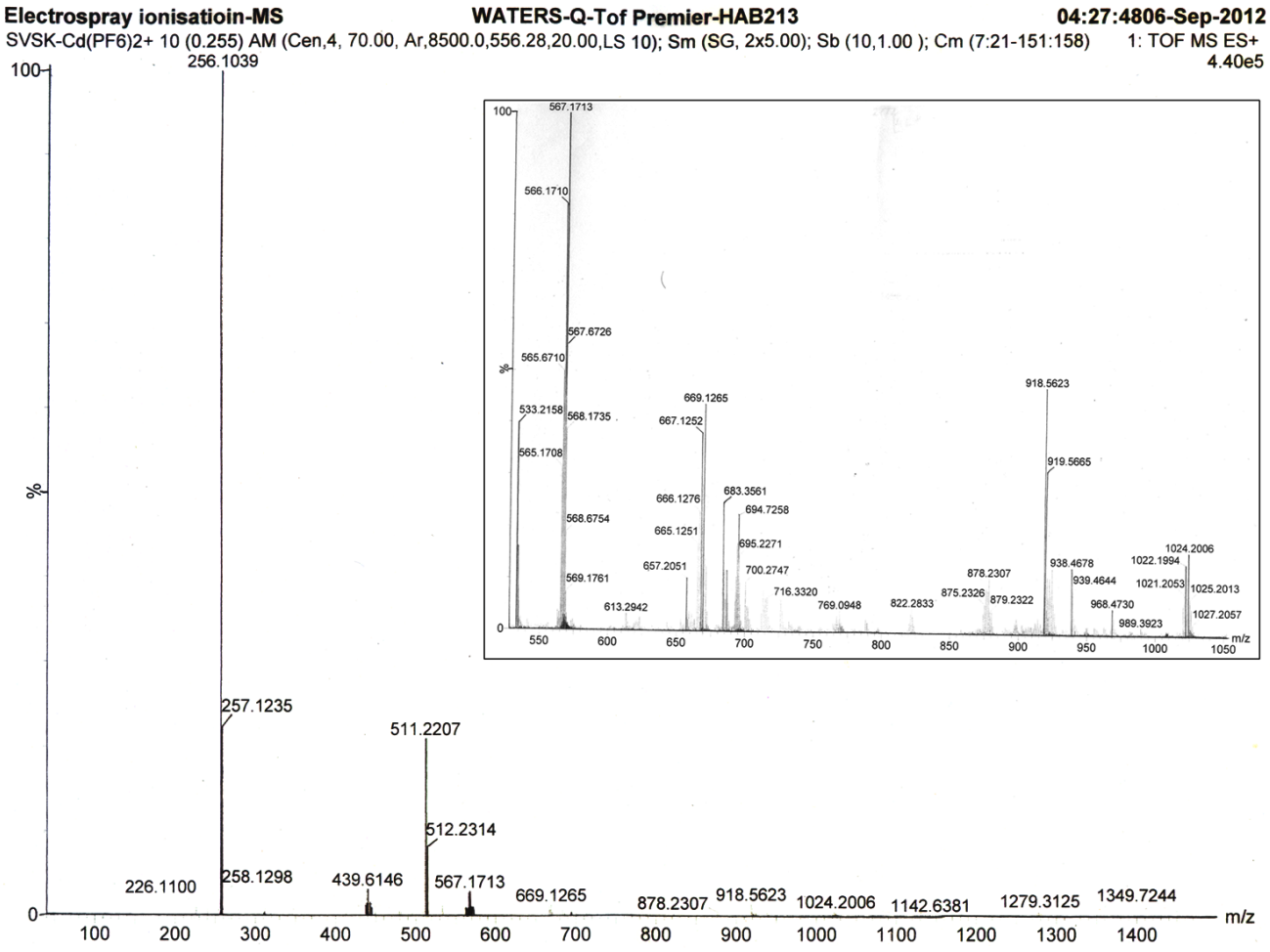
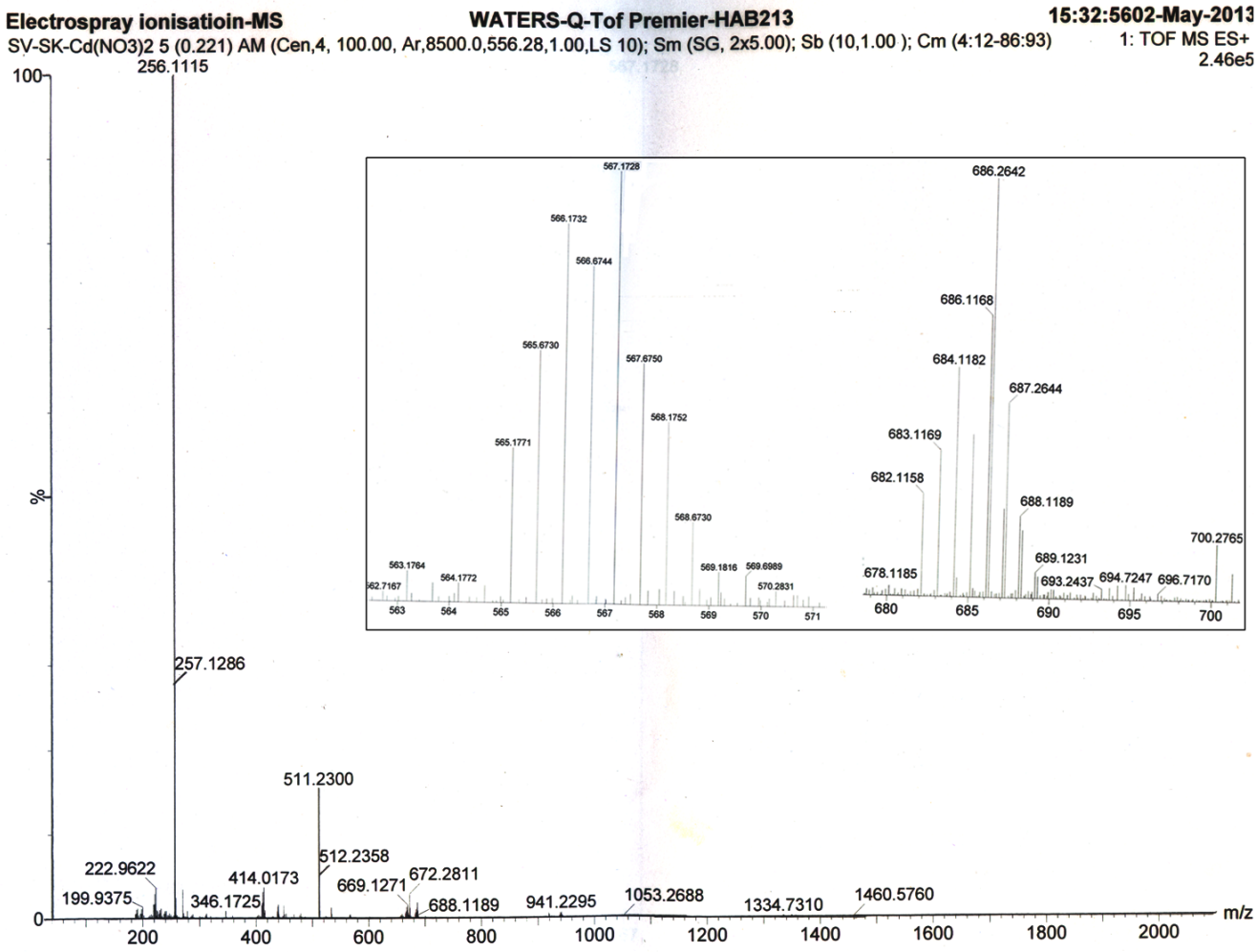
General Experimental Information.

High resolution (ESI^+ mode) mass spectra were obtained on WATERS HAB 213 machine, Department of Chemistry, IIT Kanpur. Absorbance spectra were recorded on Varian Cary 100 BIO with 10 mm quartz cell at 25±0.1°C. Emission spectra were recorded on Varian Luminescence Cary eclipsed with 10 mm quartz cell at 25±0.1°C. Photoluminescence spectra were recorded on Horiba FluoroLog 3 with 10 mm quartz cell at 25±0.1°C.

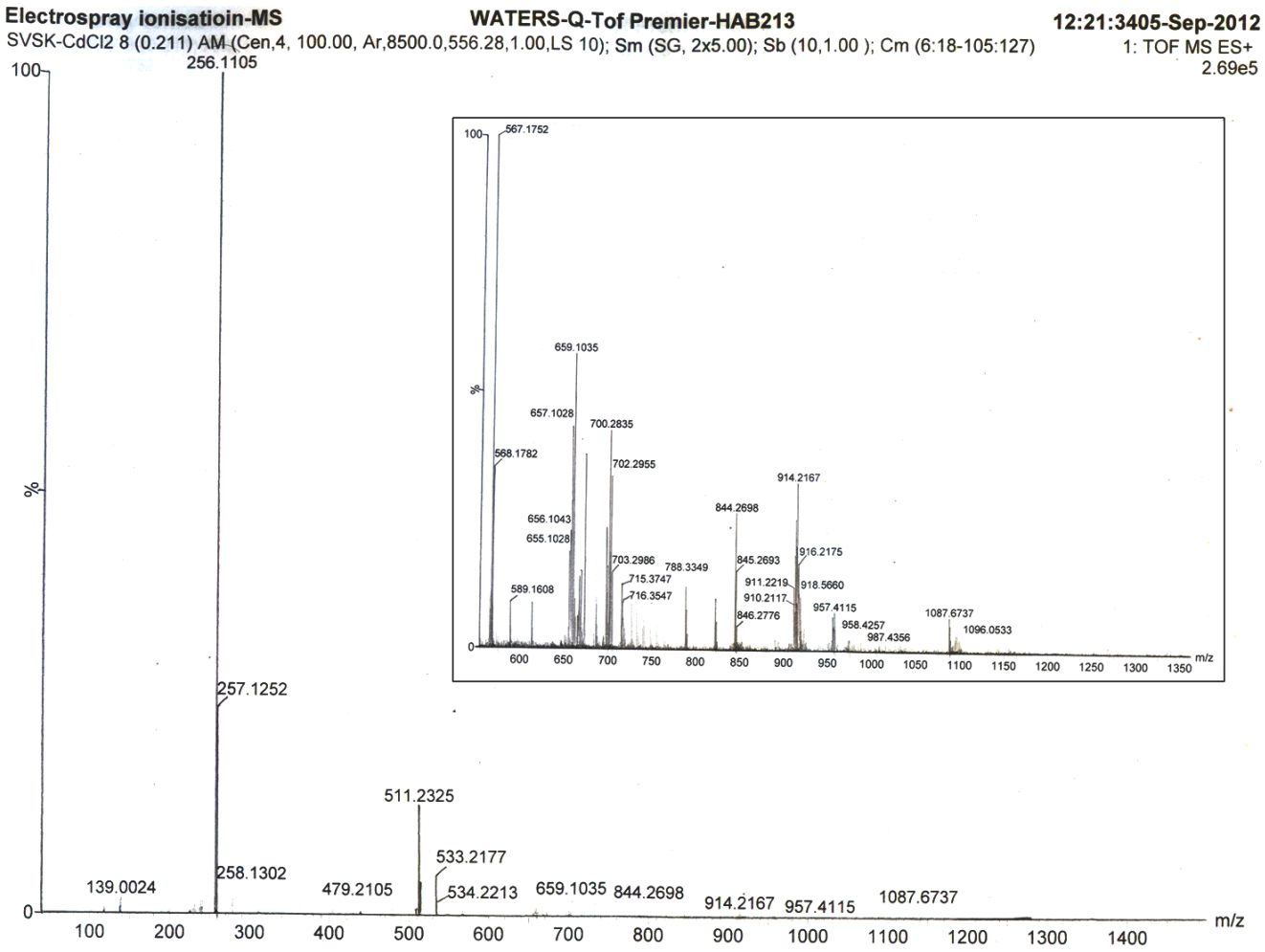
HRMS of Complex 1:



HRMS of complex 2:



HRMS of complex 3:



HRMS of complex 4:

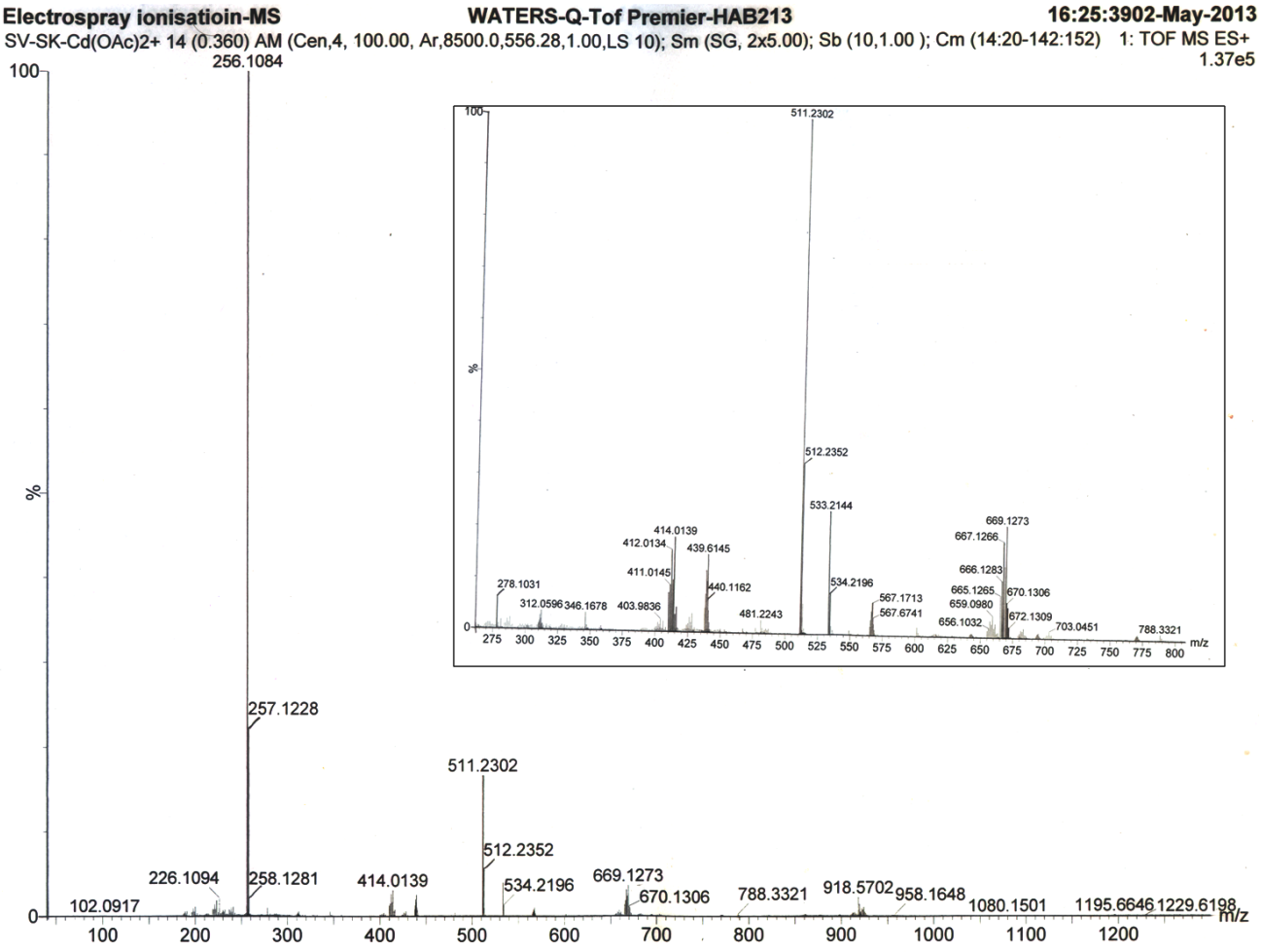


Table S1: Selected Bond Lengths (Å) and Bond Angles (°) for complexes **1-4**

Complex 1

Bond Lengths (Å)	
Cd–N(7A)	2.21
Cd–N(7B)	2.24
Cd–N(7C)	2.19
Cd–N(7D)	2.19
Bond Angles (°)	
N7(A)–Cd–N7(B)	107.52
N7(A)–Cd–N7(D)	103.64
N7(C)–Cd–N7(D)	111.77
N7(C)–Cd–N7(B)	110.68

Complex 2

Bond Lengths (Å)	
Cd–N(7)	2.412
Cd–N(7′)	2.409
Cd–O(1W)	2.252
Bond Angles (°)	
N(7)–Cd–N(7′)	92.836

Complex 3

Bond Lengths (Å)	
Cd–N(7)	2.378
Cd–N(7′)	2.389
Cd–Cl_t	2.530
Cd–Cl_b	2.356
Cd–$Cl_{b'}$	2.455
Bond Angles (°)	
Cd1–Cl_b–Cd2	74.23
Cl_b–Cd–$Cl_{b'}$	105.76
N7–Cd–N7′	177.92

Complex 4

Bond Lengths (Å)	
Cd–N(7)	2.403
Cd–N(7′)	2.387
Cd–O(1W)	2.240
Cd–O(2)	2.330
Cd–O(3)	2.585
Cd–O(4)	2.328
Cd–O(5)	2.458

Bond Angles (°)	
O2–Cd–O3	52.89
O4–Cd–O5	54.45
N7–Cd–N7′	178.38

Table S2: Hydrogen bonding Table for complexes **1-4**[#]

D-H...A	Symmetryof A	D-H	H...A	D-A	∠D—H...A
Complex 1					
N(1A)—H(1A)...N(3B)	-1+x,y,-1+z	0.86	2.11	2.891	150
N(1B)—H(1B)...N(3C)	x,y,1+z	0.86	2.06	2.860	155
N(1C)—H(1C)...N(3D)	x,-1+y,-1+z	0.86	2.12	2.907	153
N(1D)—H(1D)...N(3A)	1+x,1+y,1+z	0.86	2.05	2.842	152
Complex 2					
N(1)—H(1)...O(5)	x,y,-1+z	0.86	2.33	2.987	134
N(1')—H(1')...O(6)	1+x,y,z	0.86	1.95	2.753	155
O(1W)—H(1W)...N(6')		0.83	1.89	2.715	170
O(1W)—H(2W)...N(6)	2-x,-y,-z	0.83	1.92	2.736	168
O(6)—H(6)...O(3)		0.82	1.94	2.757	177
Complex 3					
N(1)—H(1)...Cl(2)	1-x,1-y,1-z	0.86	2.40	3.220	159
C(2)—H(2)…N(3')	1+x,1+y,z	0.93	2.59	3.490	164
Complex 4					
N(1)—H(1)...O(5)	1-x,1-y,1-z	0.86	1.97	2.753	151
N(1')—H(1')...O(2)	2-x,2-y,1-z	0.86	2.00	2.764	148
C(2)—H(2)…N(3)	-x,1-y,1-z	0.93	2.50	3.287	143

[#] Where D is donor and A is acceptor, the bond lengths are in Å and angles are in deg.

PXRD Patterns

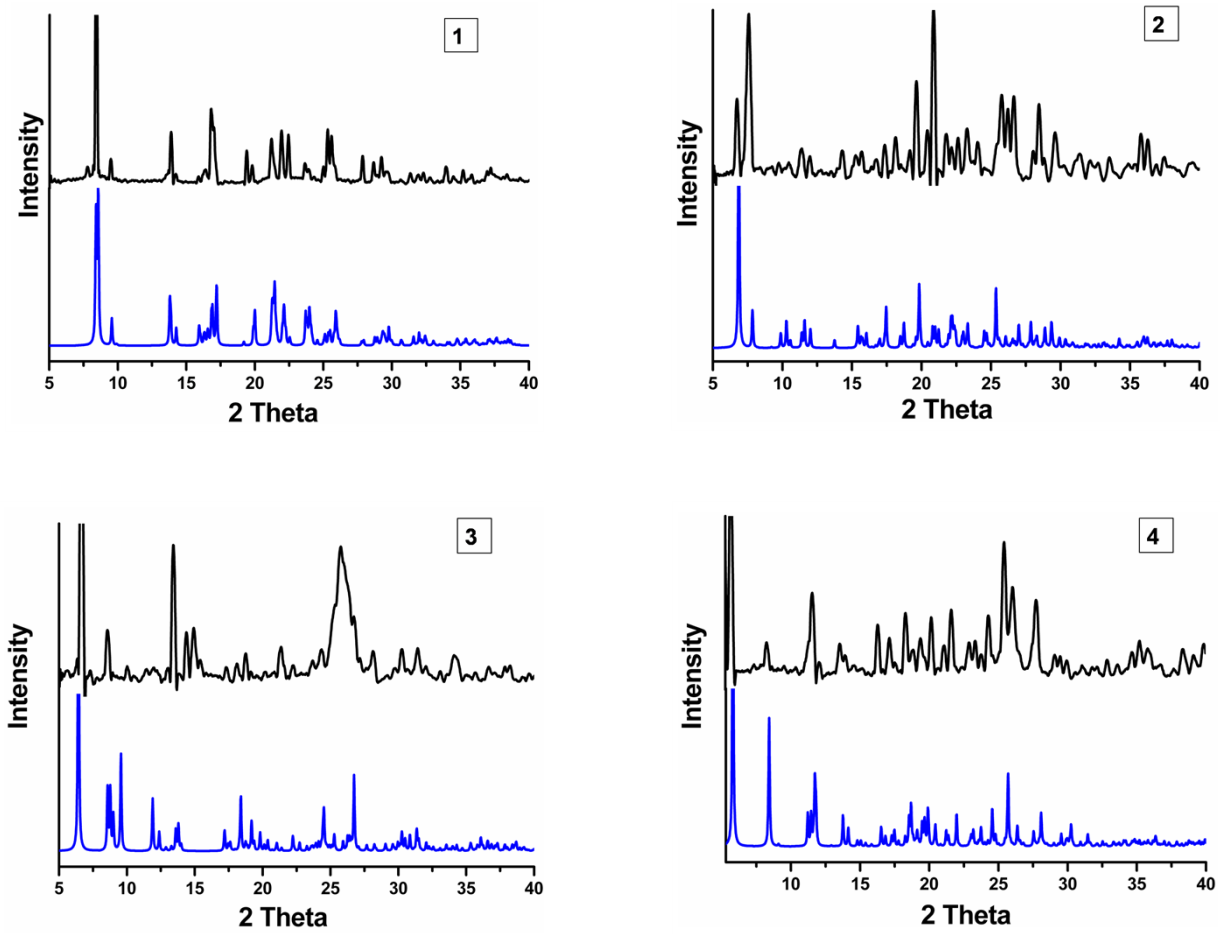


Figure S1. The simulated (blue) and experimental (black) PXRD patterns for four complexes **1**-**4**.

TGA Curve

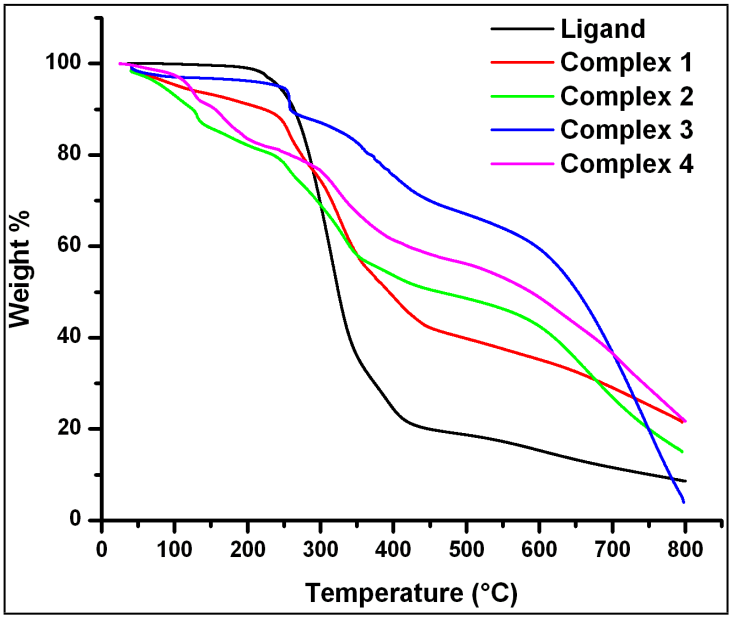


Figure S2. The TGA curves for ligand, **L** and complexes **1**-**4**.

UV-Visible Spectrum

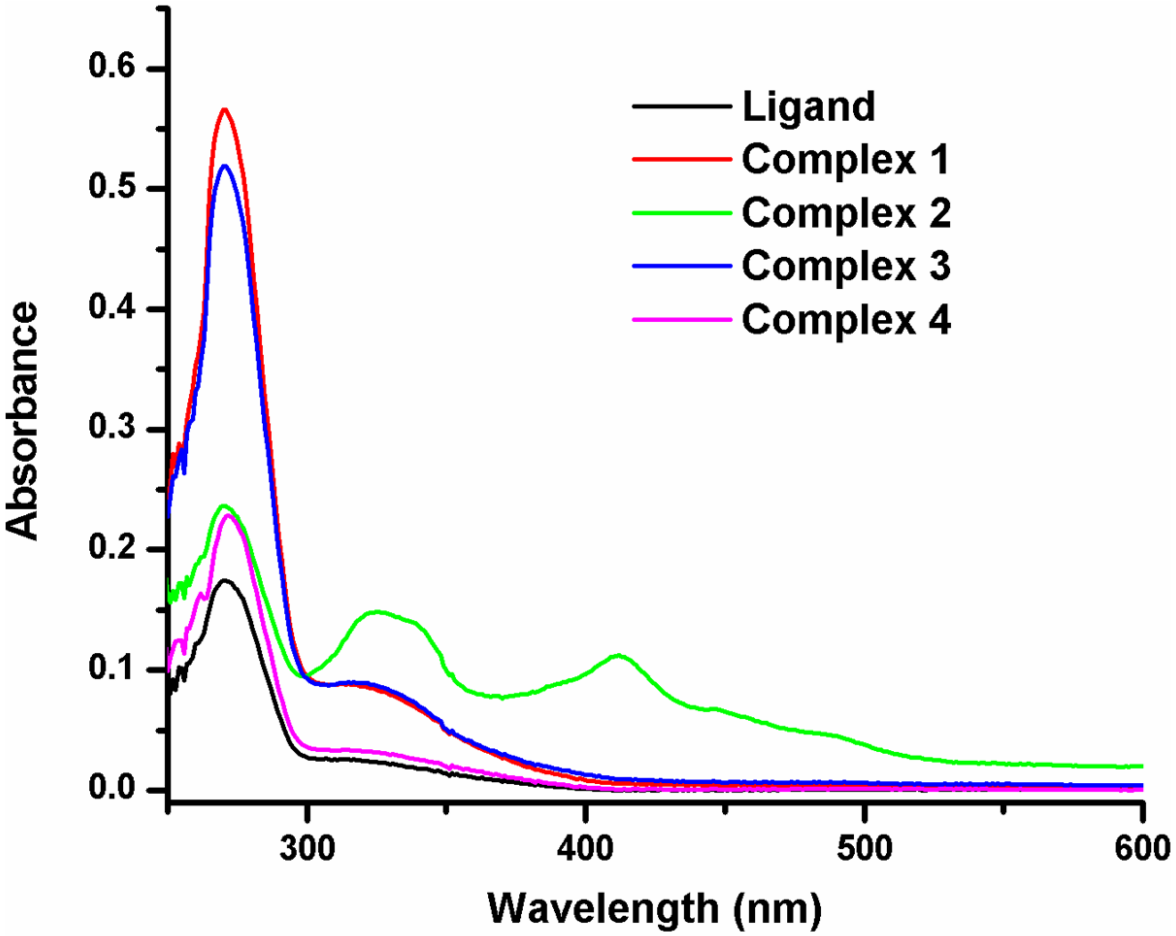


Figure S3: UV-Vis spectra of ligand, **L** and cadmium complexes, **1-4** were recorded in DMF at 10^{-5} M concentration.

Emission Spectra

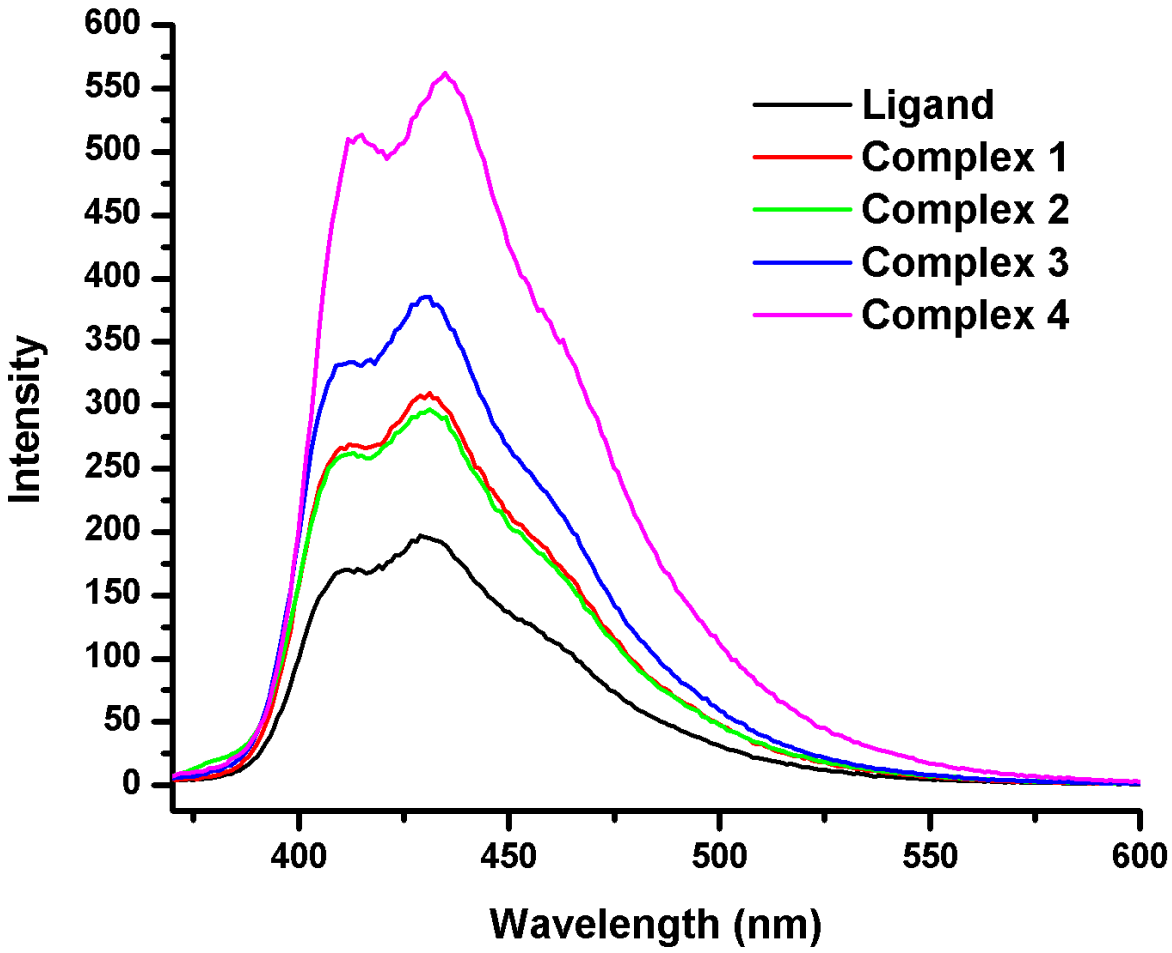


Figure S4. Emission spectra illustrating florescent intensities of ligand, **L** and cadmium complexes, **1-4** recorded in DMF at 10^{-5} M concentration.