Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Supramolecular Architecture, Photophysical and Biological Properties of Ruthenium(II) Polypyridyl Complexes

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Table S1. Crystal data and structure refinement parameters for complexes **2**.

Chemical formula	$C_{36}H_{22}N_8RuS{\cdot}2(Cl){\cdot}10(H_2O)$
Formula weight ($g{\cdot}mol^{-1}$)	950.81
Temperature (K)	100
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.0785(12) Å α = 76.422(2)°
	b = 11.9068(13) Å β = 75.205(2)°
	c = 16.6733(18) Å γ = 79.014(2)°
Volume ($Å^3$)	2047.0(4)
Z	2
F(000)	976
Density (Mg/m^3)	1.543
Absorption coefficient (mm^{-1})	0.630
Crystal size (mm)	0.16×0.12×0.08
θ range (°)	1.29 to 25.00
Range of *h*, *k*, *l*	−13,13/ −14,14/ −19,19
Refinement on	F^2
Reflections collected	19774
Unique reflections [R_{int}]	7189 [0.0670]
Goodness-of-fit on F2	1.11
R_1 [I>2σ(I)]	0.0786
wR_2 (all data)	0.1863

$w = 1/[\sigma^2(F_0^2) + (AP)^2 + BP]$; where $P = [2F_C^2 + Max(F_0^2, 0)]/3$

Table S2. Selected bond lengths [Å] and angles [°] for complex **2**.

Bond lengths			
Ru-N(1)	2.060 (5)	Ru-N(4)	2.062 (5)
Ru-N(2)	2.066 (5)	Ru-N(5)	2.053 (5)
Ru-N(3)	2.054 (5)	Ru-N(6)	2.071 (5)
Bond angles			
N(1)-Ru-N(2)	79.80 (2)	N(3)-Ru-N(2)	89.70(2)
N(3)-Ru-N(1)	93.80 (2)	N(3)-Ru-N(4)	79.80(2)
N(4)-Ru-N(1)	171.9 (2)	N(5)-Ru-N(3)	95.42(2)
N(5)-Ru-N(1)	93.47 (2)	N(3)-Ru-N(6)	172.9(2)
N(1)-Ru-N(6)	91.81 (2)	N(5)-Ru-N(4)	92.20(2)
N(4)-Ru-N(2)	95.10 (2)	N(4)-Ru-N(6)	94.90(2)
N(5)-Ru-N(2)	171.8 (2)	N(5)-Ru-N(6)	79.95(2)
N(2)-Ru-N(6)	95.52 (2)		

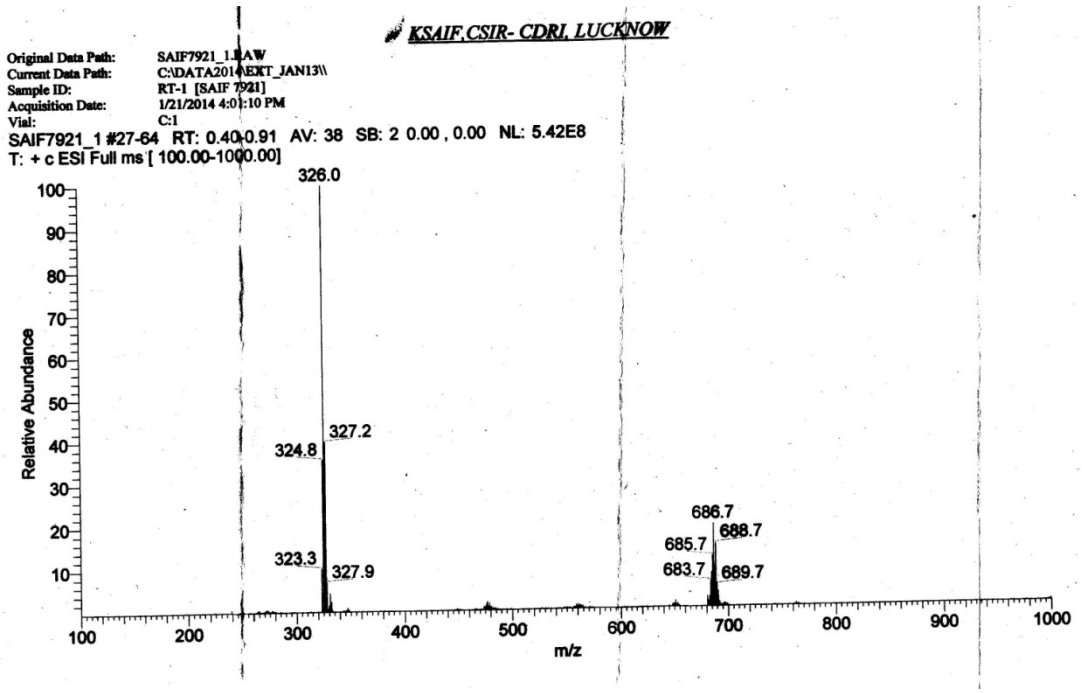
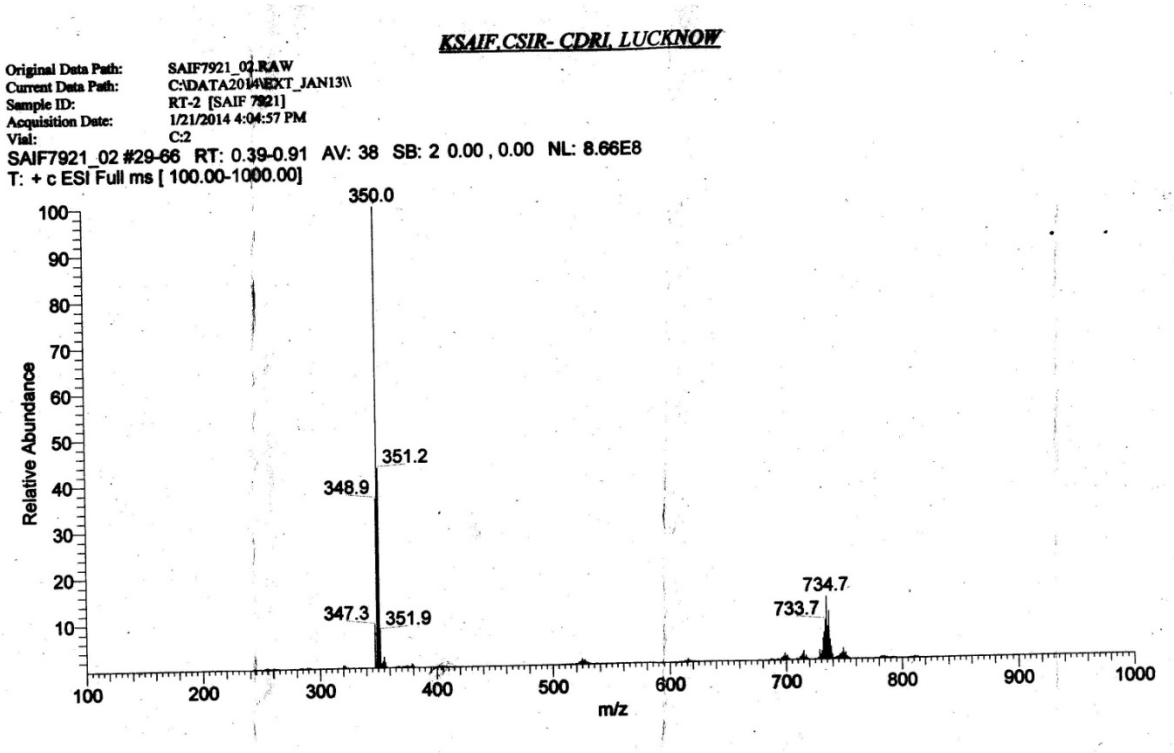


Figure S1. ESI-MS (Positive mode) Spectrum of complex **1**.



Figgure S2. ESI-MS (Positive mode) Spectrum of complex **2**.

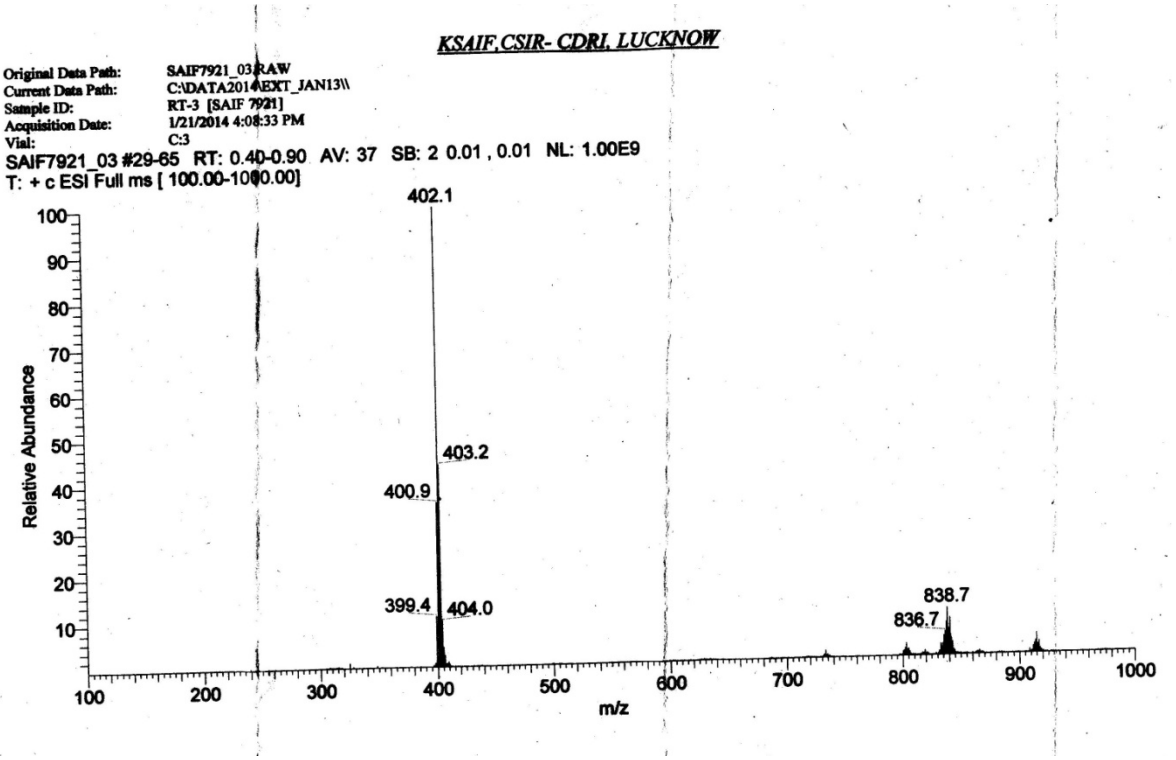


Figure S3. ESI-MS (Positive mode) Spectrum of complex **3**.

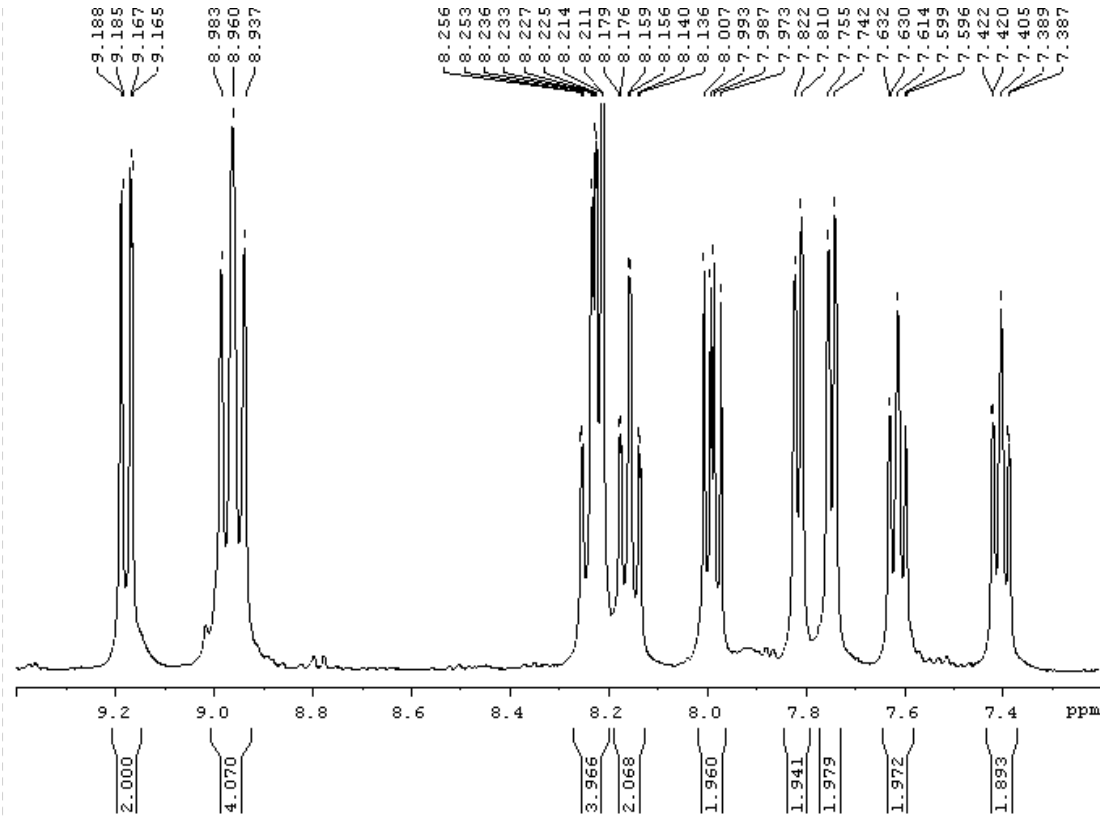


Figure S4. ^{1}H-NMR spectrum of complex **1** in DMSO-d_6 in the range 7.0-9.4 ppm.

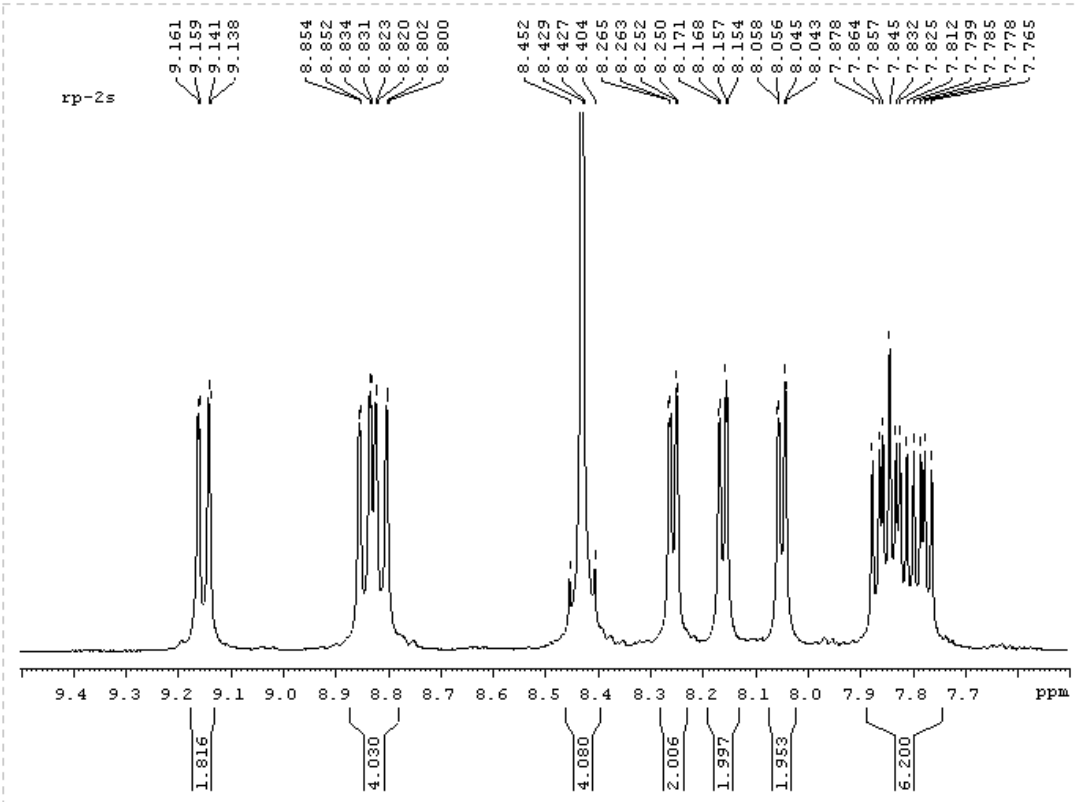


Figure S5. ^{1}H-NMR spectrum of complex **2** in DMSO-d_6 in the range 7.5-9.5 ppm.

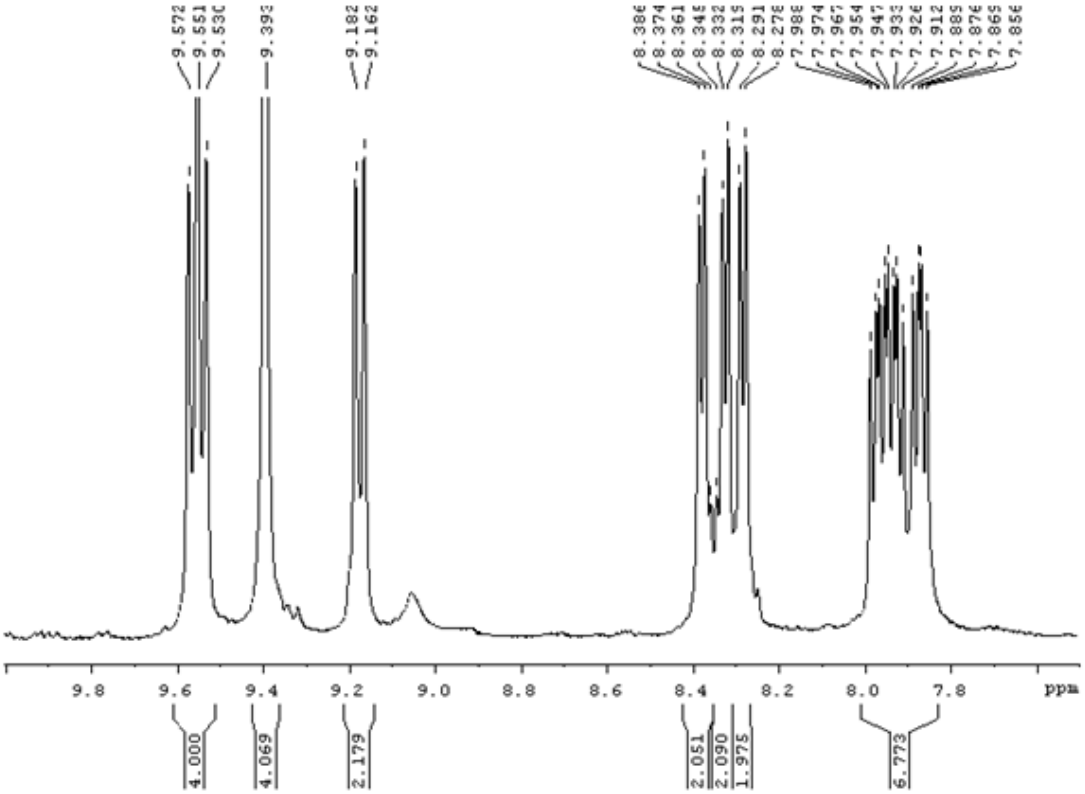


Figure S6. ^{1}H-NMR spectrum of complex **3** in DMSO-d_6 in the range 7.5-9.9 ppm.

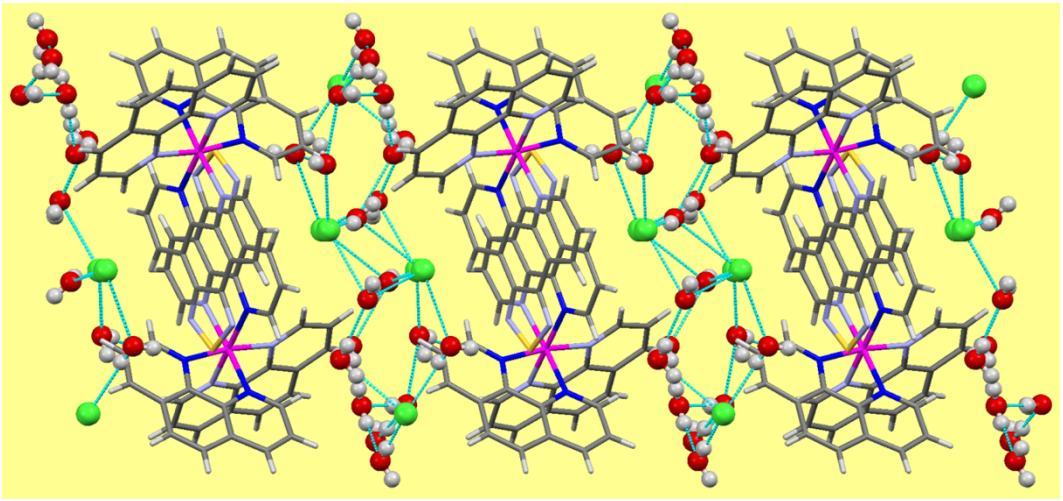


Figure S7.. Packing diagram showing water-chloride cluster formed by hydrogen bonding as seen along 'a' axis.

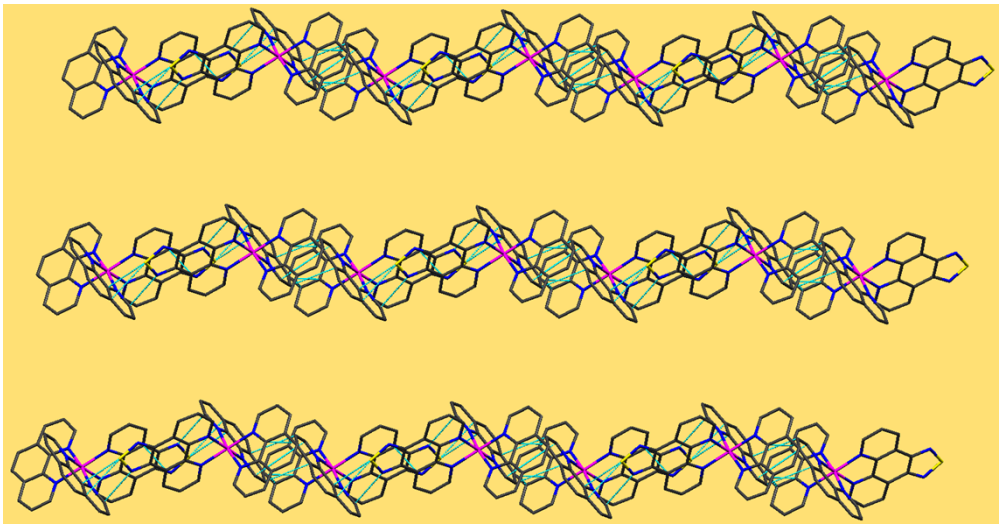


Figure S8. Crystal packing diagram chloride and water molecules have been omitted to show the cationic building block forming the channels.

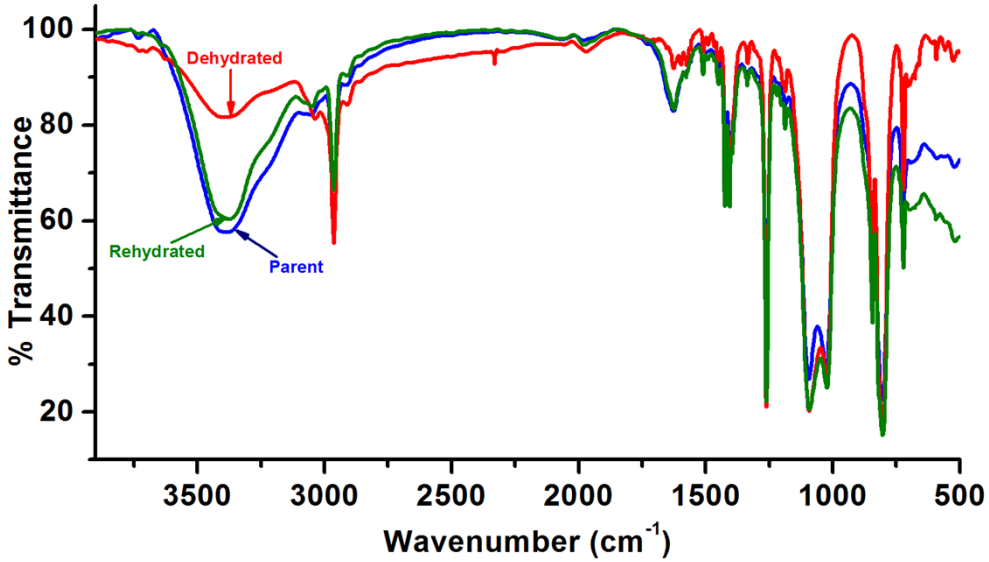
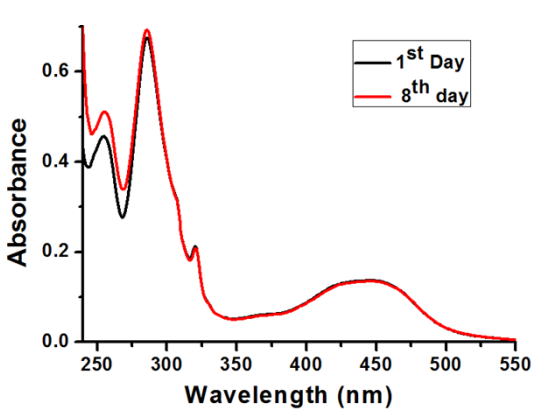
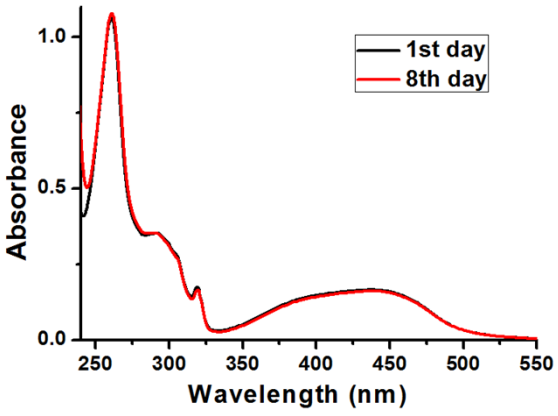


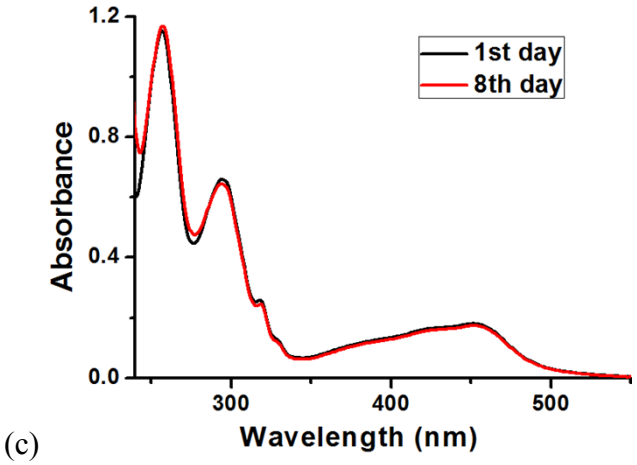
Figure S9. Comparative FT-IR spectra of parent, dehydrated and rehydrated sample of **2**



(a)

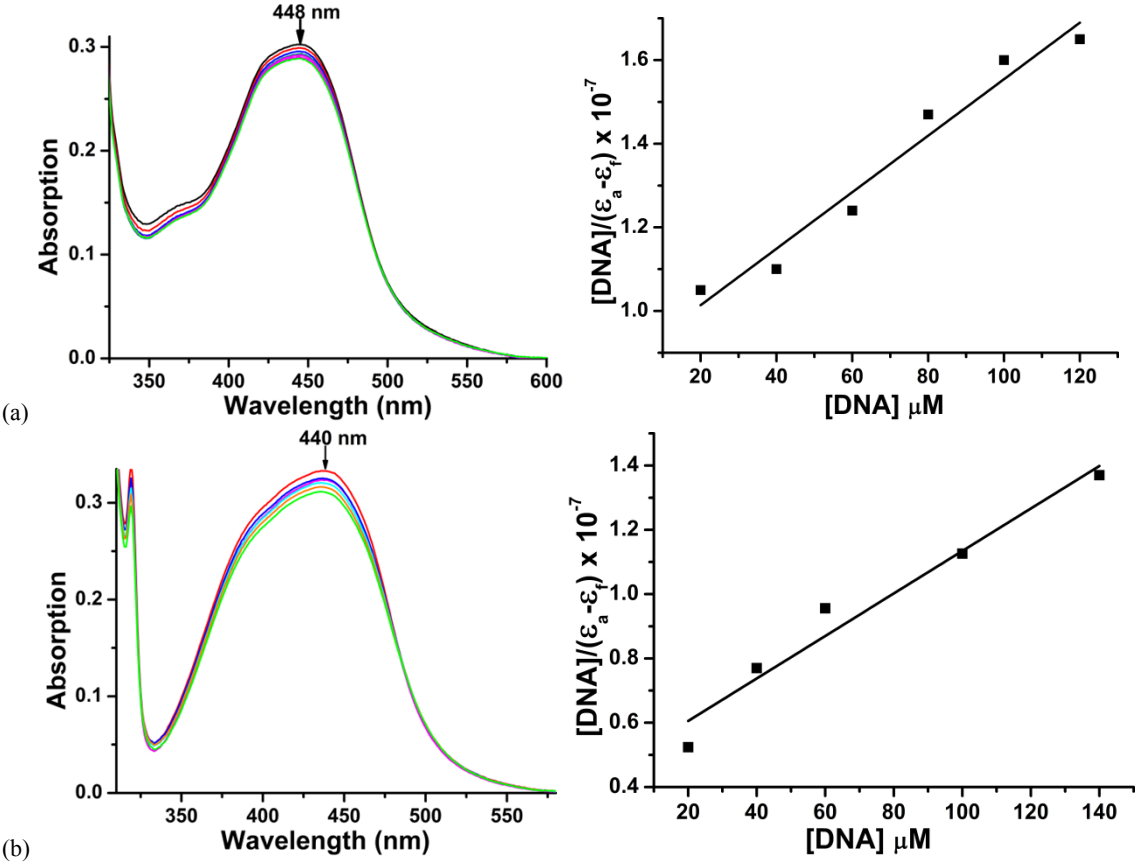


(b)



(c)

Figure S10. Comparative absorption spectra of complexes (10 μM) in water immediately after dissolving and after 8th day of dissolving.



(a)

(b)

Figure S11. Changes in the electronic absorption spectra of (a) complex **1** (20 μM) (left), fitting of the absorbance data used to obtain the binding constant (right), (b) complex **2** (20 μM) (left), fitting of the absorbance data used to obtain the binding constant (right), with increasing concentrations (0–140 μM) of CT-DNA (phosphate buffer, pH 7.2).

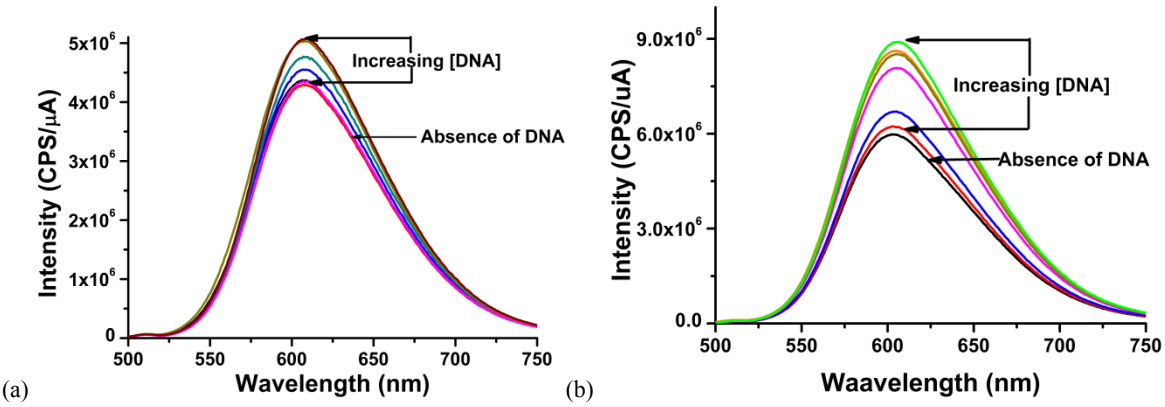


Figure S12. Emission spectra of complexes (a) **1**, (b) **2**, 10 μM in phosphate buffer, pH 7.2, at 298 K with increasing [CT-DNA]/[Ru] ratio 0-20; [complex] = 10μM , [DNA] =0-200 μM.