Synthesis, X-ray Structure of a New Zinc(II) Coordination Polymer : Interaction With DNA, Double Stranded RNA and Elucidation of the Molecular Aspects of the Binding to Bovine Serum Albumin.

Swapan K. Jana,†,§ Saikat K. Seth,⊥ Horst Puschmann,‡ Maidul Hossain,*,†, § and Sudipta Dalai,*, †,§

† Department of Chemistry and Chemical Technology, Vidyasagar University, Midnapore 721 102, West Bengal, India.

⊥ Department of Physics, M. G. Mahavidyalaya, Bhupatinagar, Purba Medinipur, West Bengal-721425, India.

‡ Department of Chemistry, Durham University, Durham DH1 3LE, UK

■ AUTHOR INFORMATION

Corresponding Authors

*(M.H.) E-mail: hossainm@ mail.vidyasagar.ac.in/maidulhossain@yahoo.com

*(S.D.) E-mail: sudipta@mail.vidyasagar.ac.in / icsdalai@gmail.com

Author Contributions

§ These authors made equal contributions.

Supplementary Information

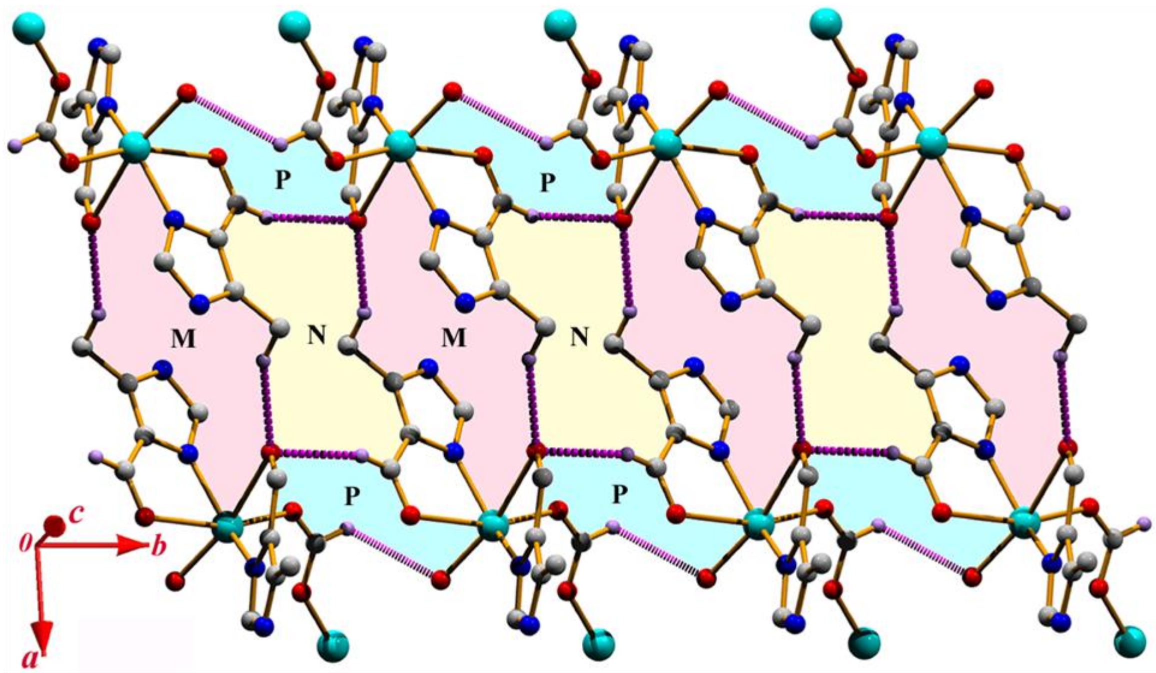

Fig. S1 Formation of ring motifs and propagation of 1D network along (0 1 0) direction.

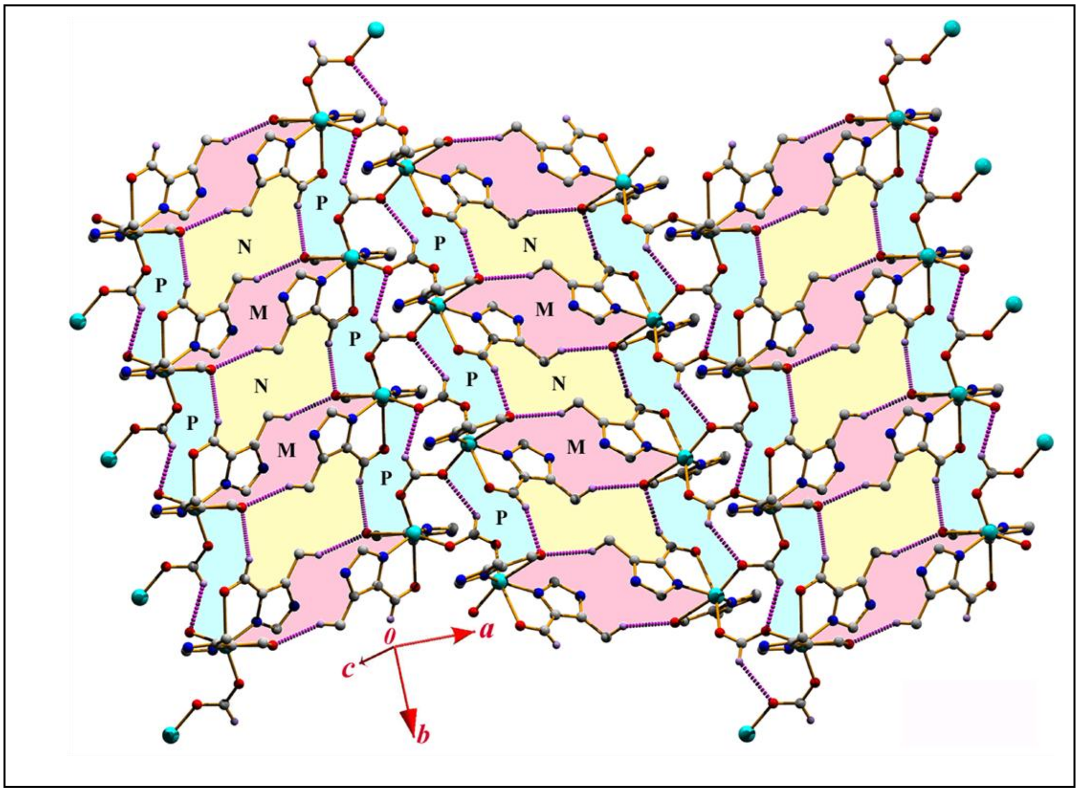

Fig. S2 Generation of 2D supramolecular layer network through weak C–H···O hydrogen bonds and multiple ring motifs are acting as building blocks.

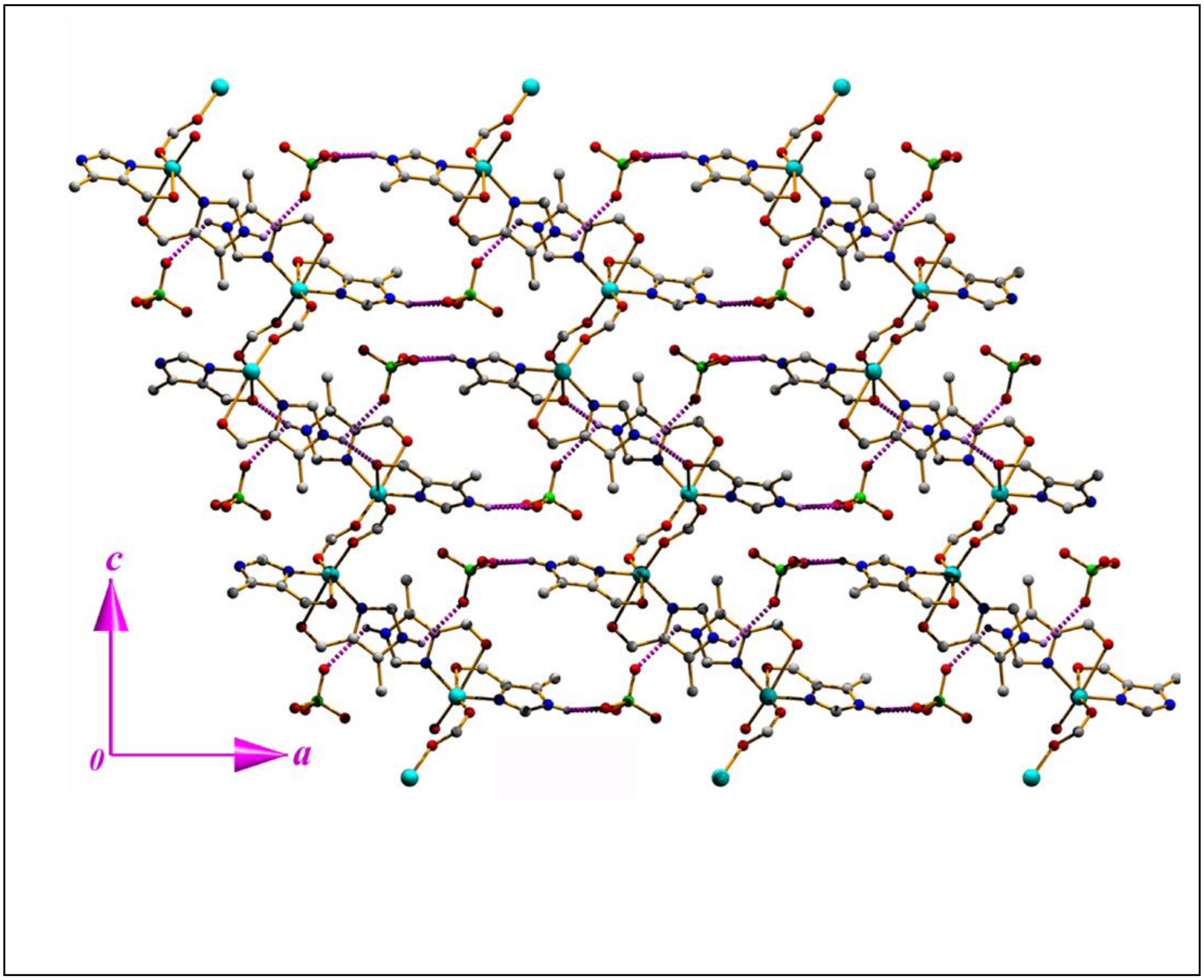

Fig. S3 Formation of another 2D supramolecular network through N–H···O hydrogen bonds.

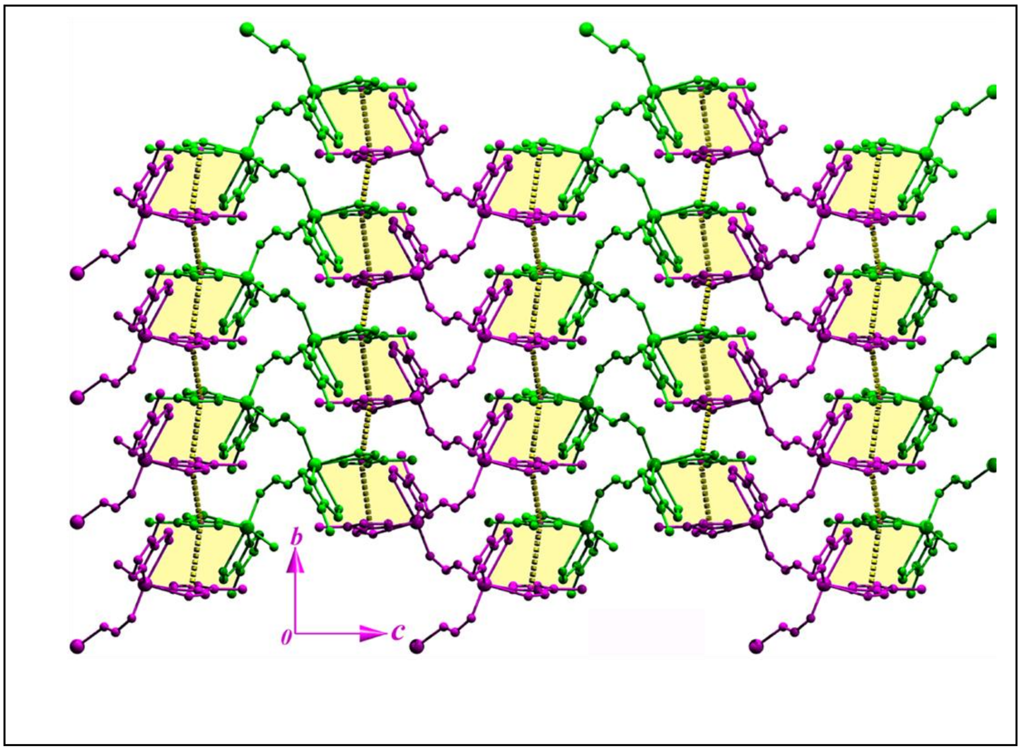

Fig.S4 Perspective view of the unique multi π-stacked layer assembly.

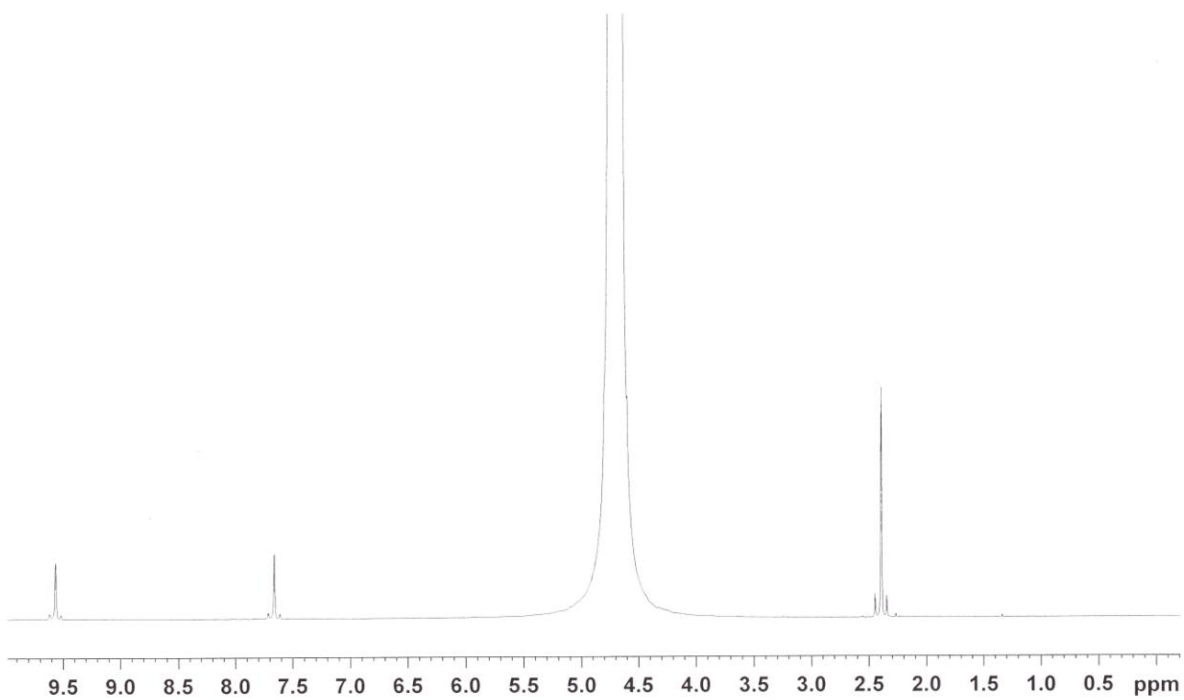

Fig.S5 ^{1}H NMR spectra in D2O of the free ligand (4-Me-5-CHOIm) .

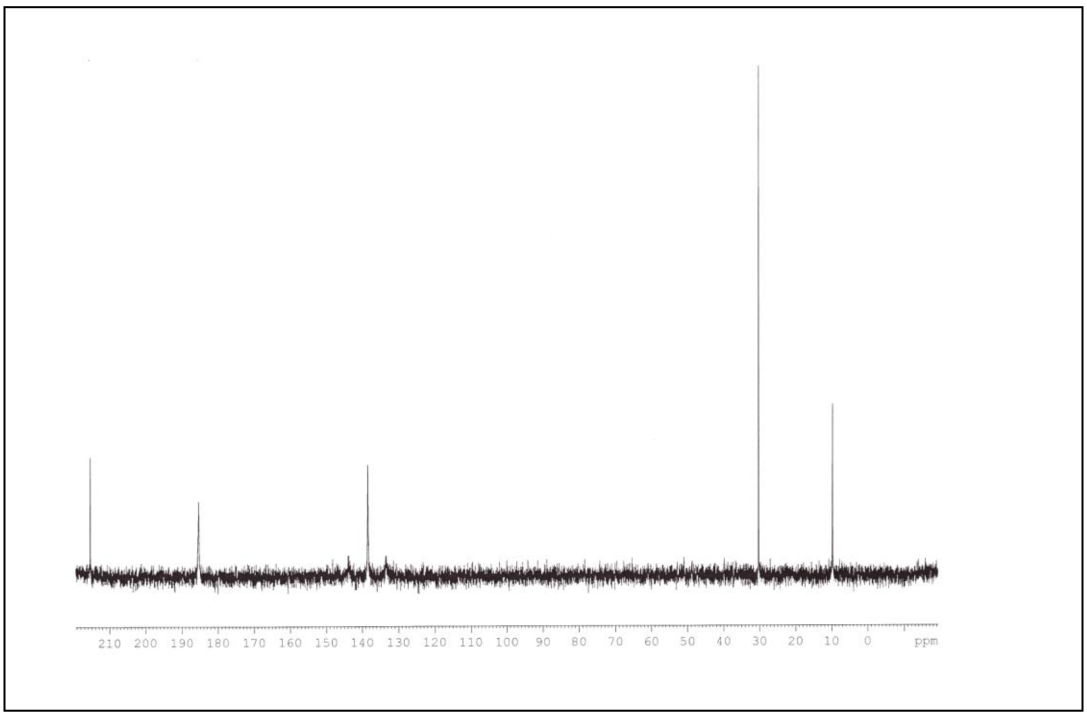

Fig.S6 ^{13}C NMR spectra in D2O of the free ligand (4-Me-5-CHOIm) .

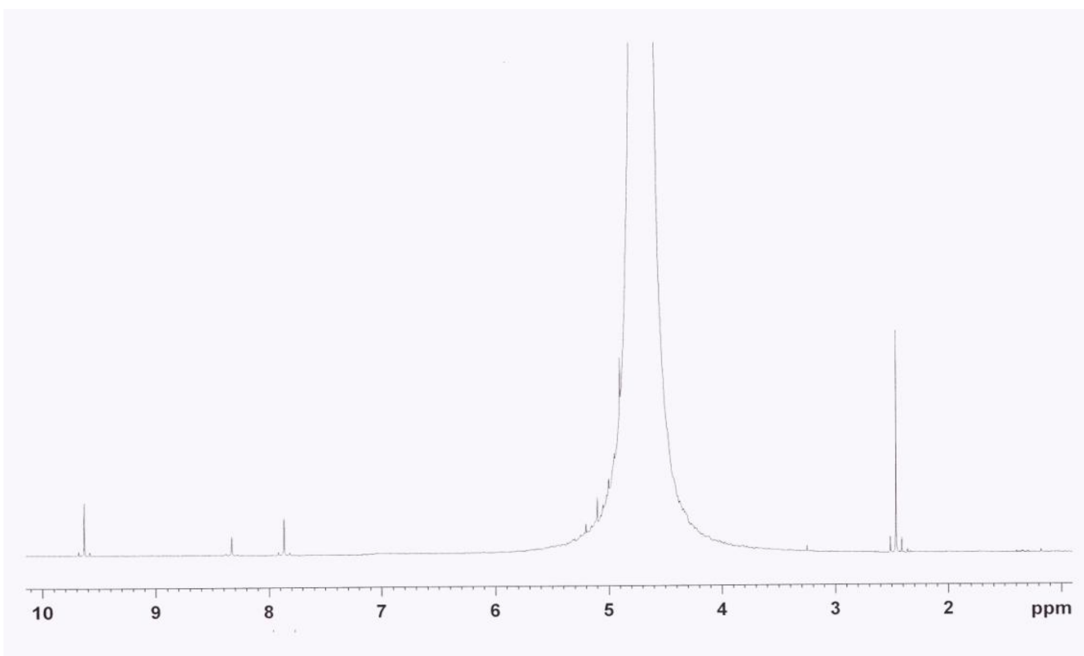

Fig.S7 ^{1}H NMR spectra in D2O of the complex $[Zn(4\text{-}Me\text{-}5\text{-}CHOIm)_2(HCOO)](ClO_4)$.

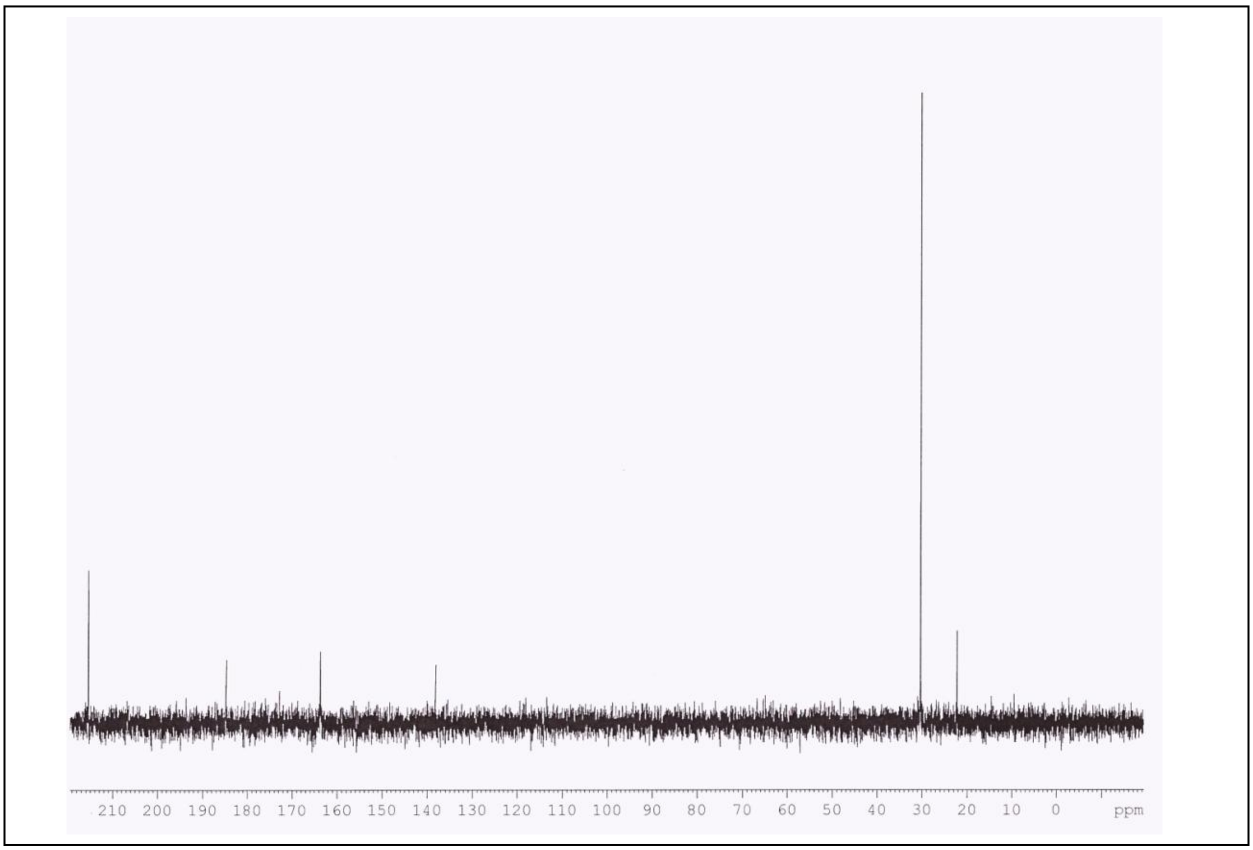

Fig.S8 ^{13}C NMR spectra in D2O of the complex $[Zn(4\text{-}Me\text{-}5\text{-}CHOIm)_2(HCOO)](ClO_4)$.

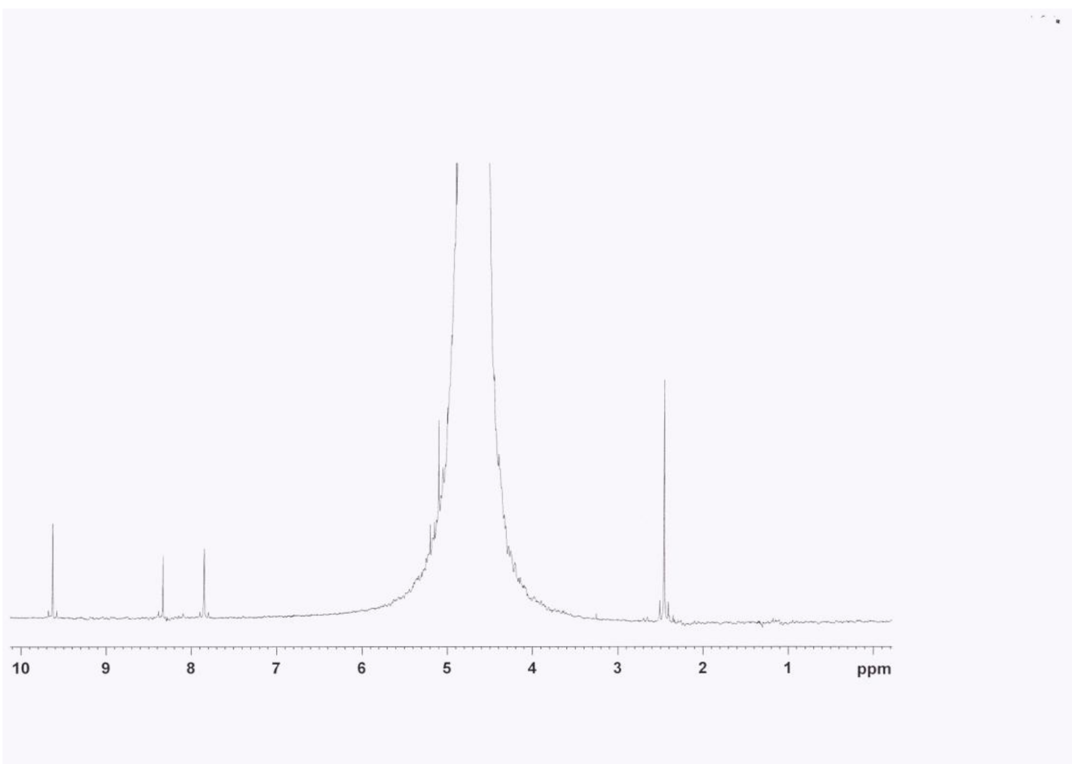

Fig.S9 ^{1}H NMR spectra in D2O of DNA + complex $[Zn(4\text{-}Me\text{-}5\text{-}CHOIm)_2(HCOO)](ClO_4)$..

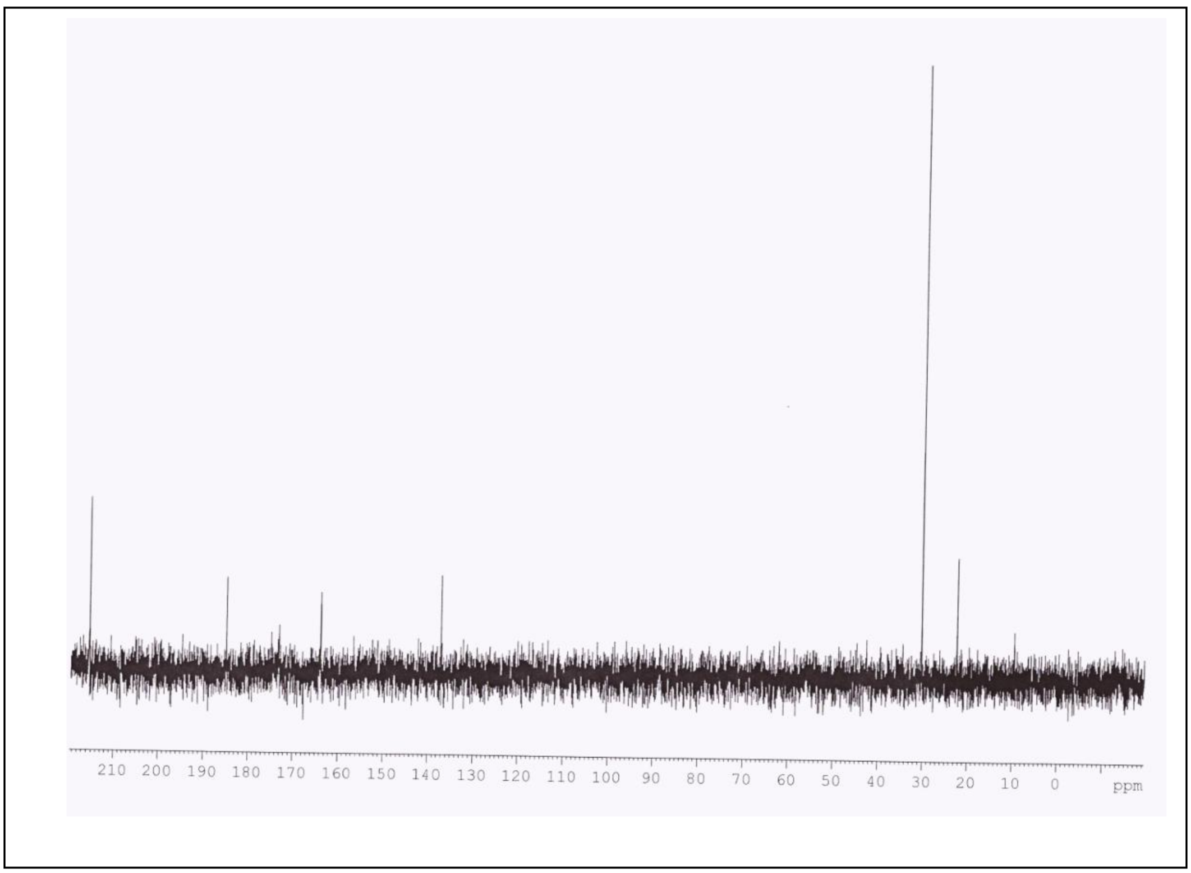

Fig.S10 ^{13}C NMR spectra in D2O of DNA + complex $[Zn(4\text{-}Me\text{-}5\text{-}CHOIm)_2(HCOO)](ClO_4)$.

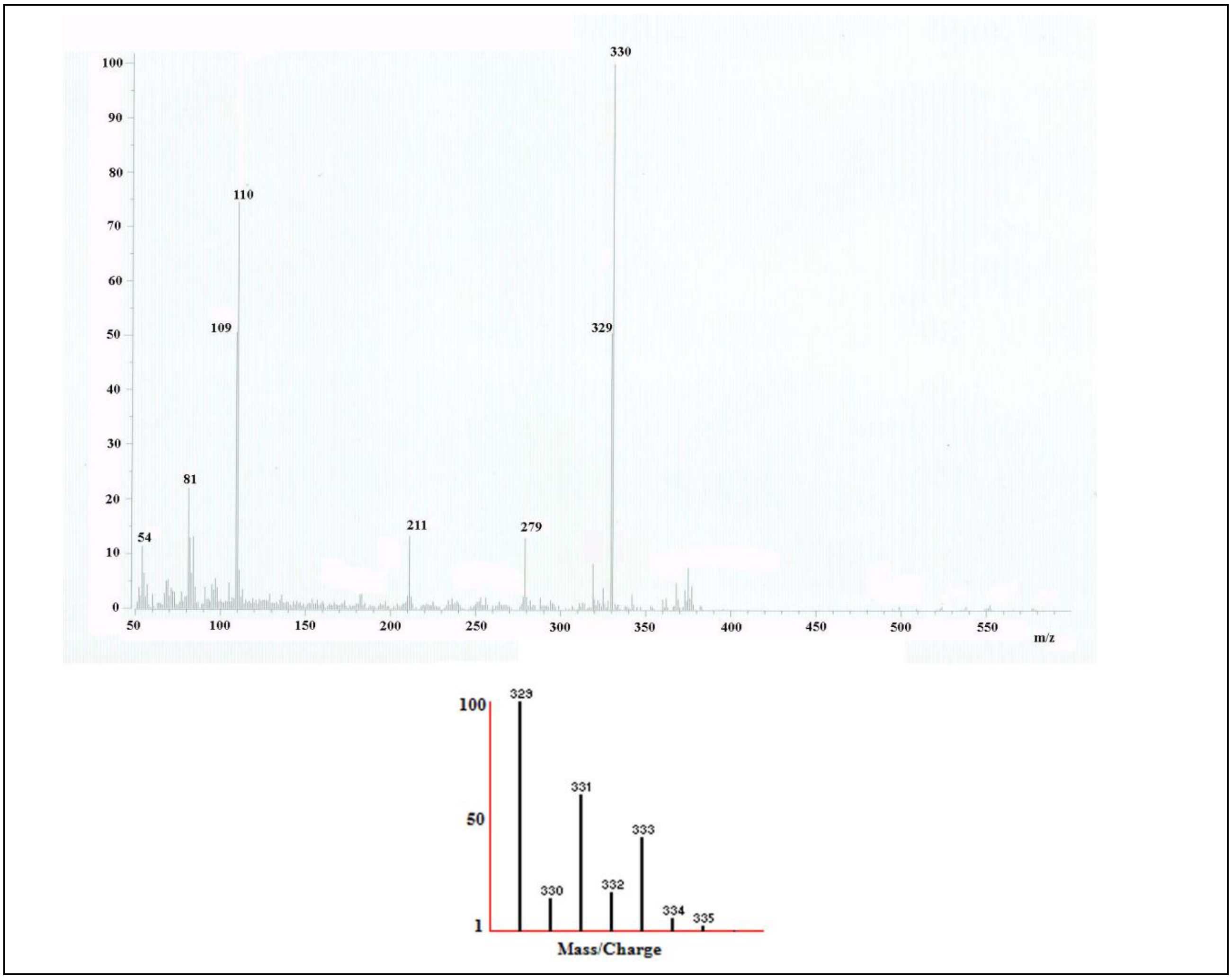

Fig.S11 m/z = 50 – 550 range of the ESI-MS spectrum of an aqueous solution of the complex and the simulated isotope distributions for $[Zn(4\text{-}Me\text{-}5\text{-}CHOIm)_2(HCOO)]^+$.

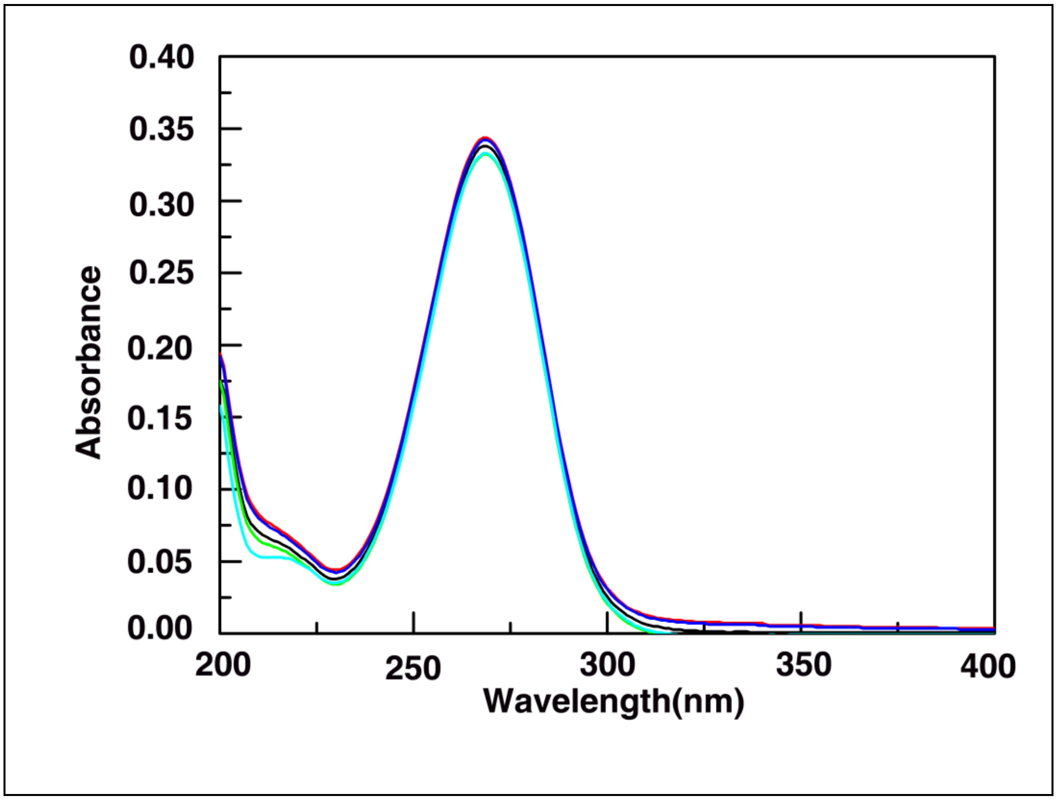

Fig.S12 Absorption spectral changes of 4-Me-5-CHOIm (5μM) treated with 0, 5, 10, 15 and 20μM (curves 1–5) of CT-DNA.

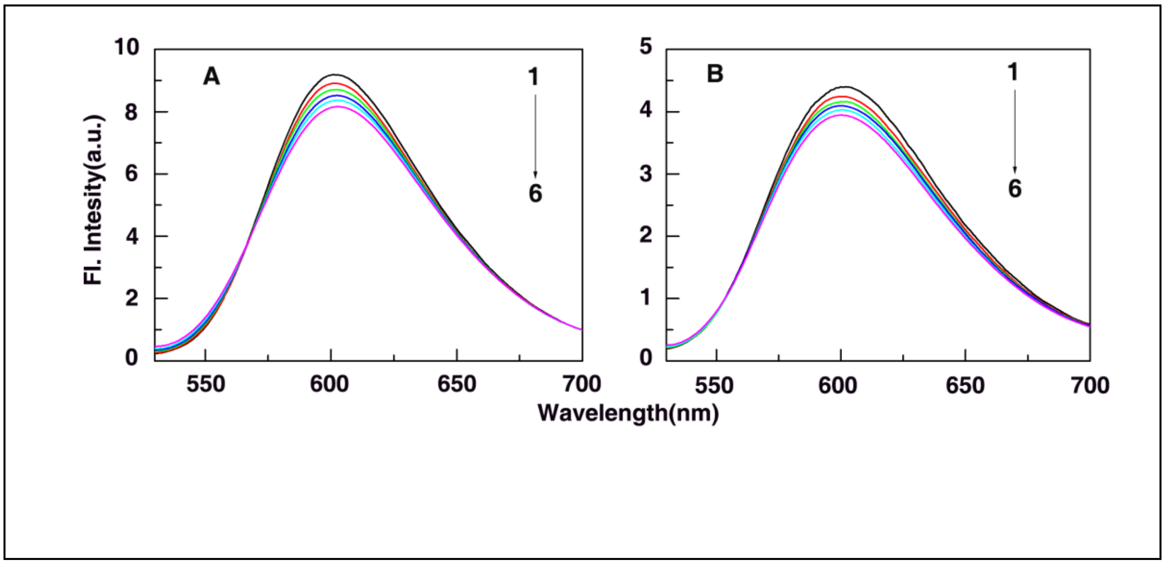

Fig. S13 Emission spectra of EtBr(5 μM) bound to the CT-DNA(15 μM) (A) and (B)RNA(PolyI.polyC)(15 μM) treated with increasing concentration of Zn complex. In panel (A,B) curves (1-6) denote 0, 10, 20,30, 40, and 50, μM of Zn complex.

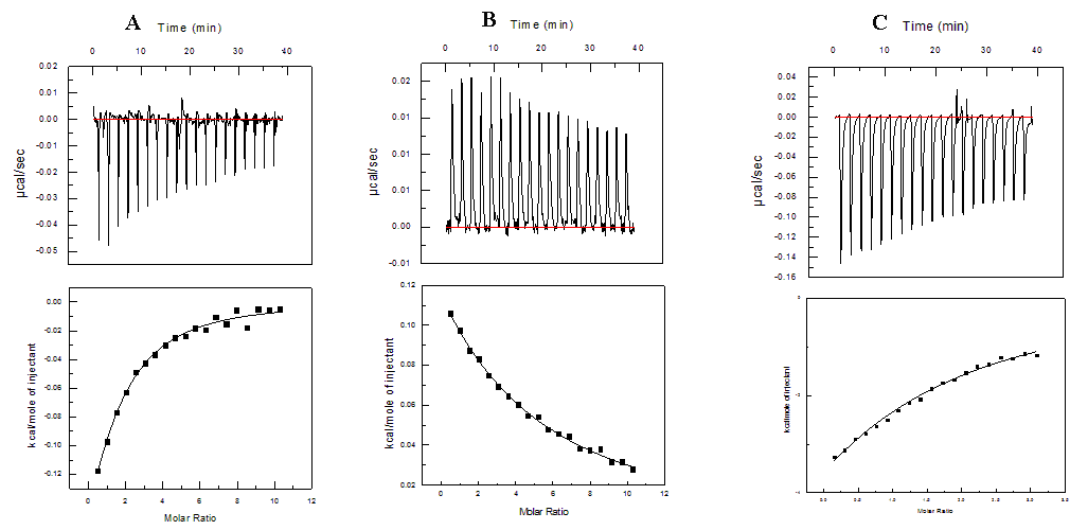

Fig. S14 ITC profiles for the binding of $Zn(ClO_4)_2$ to (A) CT-DNA, (B) RNA (PolyC.PolyI) and (C) BSA. Top panels present raw results for the sequential injection of (A) CT-DNA, (B) RNA (PolyC.PolyI) and (C) BSA in citrate-phosphate buffer, pH 7.01 at 25 ^{o}C .The bottom panels show the integrated heat results after correction of heat of dilution against the mole ratio. The data points were fitted to one site model and the solid lines represent the best-fit data.

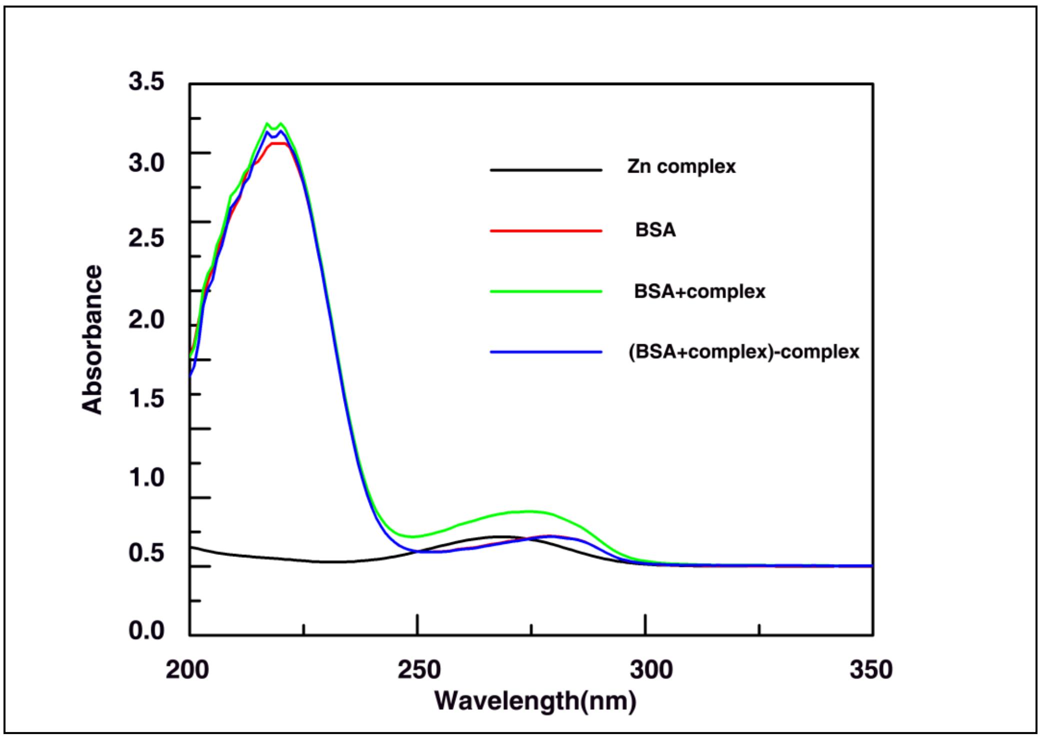

Fig. S15 UV/vis absorption spectra of BSA (5 μM, pH ~7.01) in the presence of Zn complex (5 μM).

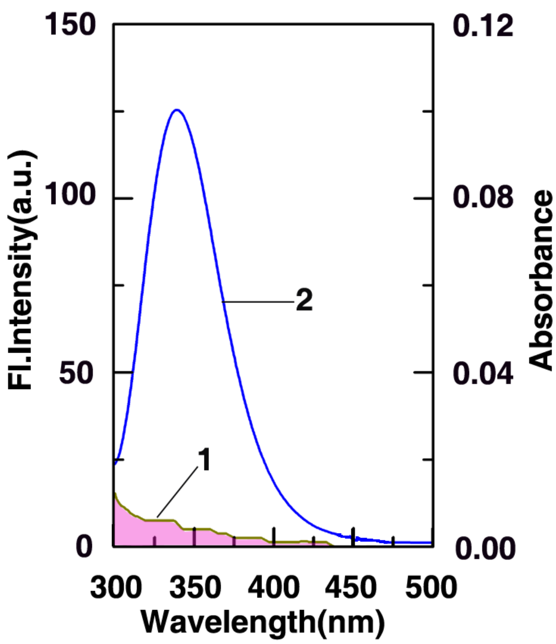

Fig. S16 Overlap (shaded portion) of the BSA fluorescence spectra (donor) and absorption spectra (acceptor) of Zn complex In panel curve 1 represent absorption spectra of complex and curve 2 represent the fluorescence spectrum of BSA at pH 7.01. The excitation of BSA was done at 295 nm. The ratio of the concentration of [BSA]:[complex] = 1:1.

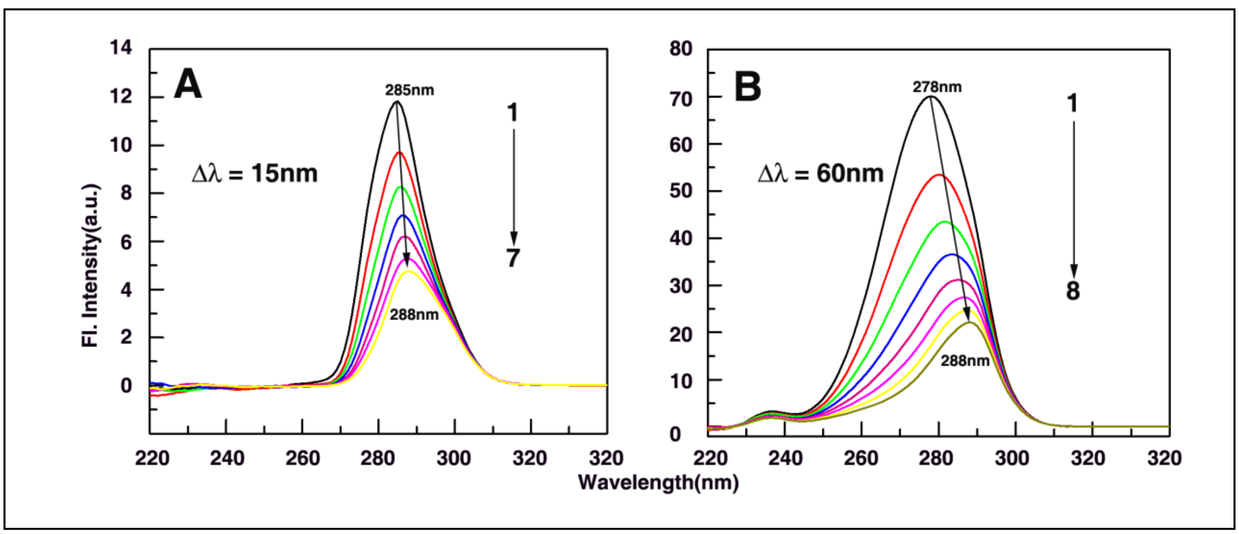

Fig.S17 Synchronous fluorescence (Δλ = 15 and 60 nm) spectra of BSA in the presence of different concentrations of (A, B) [BSA] = 5 μM. In panel (A), curves 1−7 denote 0 to 48 μM range of Zncomplex and in panel (B), curves 1−8 denote 0 to 56μM of Zn complex.

Table S1 Data derived from three-dimensional fluorescence from the interaction of BSA and BSA-Zn complex system.

System	Fluorescence Peak 1		Fluorescence Peak 2	
	Peak position ($\lambda_{ex}/\lambda_{em}$/Intensity) (nm/nm/F)	Stokes shift $\Delta\lambda$ (nm)	Peak position ($\lambda_{ex}/\lambda_{em}$/Intensity) (nm/nm/F)	Stokes shift $\Delta\lambda$ (nm)
BSA	280/340/748.4	60	230/340/298.9	110
BSA-Zn complex	290/340/310.3	50	230/340/245.8	110

Table S2 ITC derived thermodynamic parameters for the binding of $Zn(ClO_4)_2$ to CT-DNA, RNA and BSA in CP buffer of 10mM [Na^+], pH 7.01 [a]

	Temperature (K)	Binding constant (K_b) M^{-1}	Stoichiometry (N)	ΔG (kca/mol)	ΔH (kca/mol)	$T\Delta S$ (kca/mol)
CT-DNA	298.15	(2.4 ± 0.19) x10^4	0. 95±0.05	-7.17±1.90	-0.50±0.02	5.57
RNA(polyI.polyC)	298.15	(4.06 ± 0.11) x 10^3	0.98±0.04	-7.44 ± 0.03	1.46 ± 0.02	6.38
BSA	298.15	(4.26 ± 0.11) x10^4	0.99±0.05	-6.34 ± 0.20	-7.62± 0.40	-1.28

[a] Average from two determinations each. All ITC profiles fit to a model of single binding sites.