Supporting Information

Active Bromoaniline–Aldehyde Conjugate Systems and Their Complexes as Versatile Sensors of Multiple Cations with Logic Formulation and Efficient DNA/HSA Binding Efficacy: Combined Experimental and Theoretical Approach

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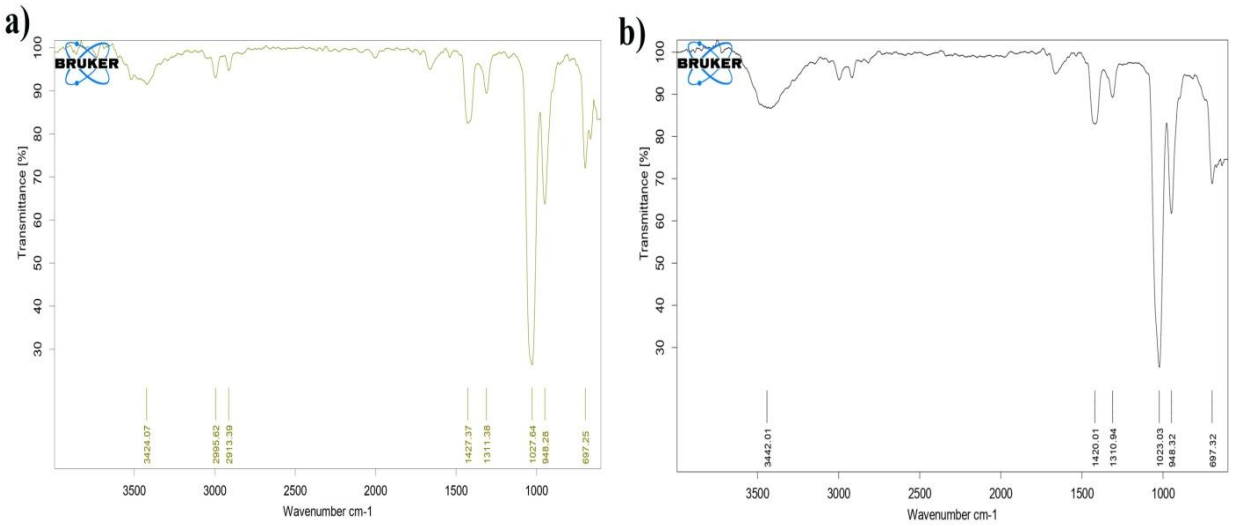

Figure S1. IR spectrum of complex (a) **1** and (b) **2**.

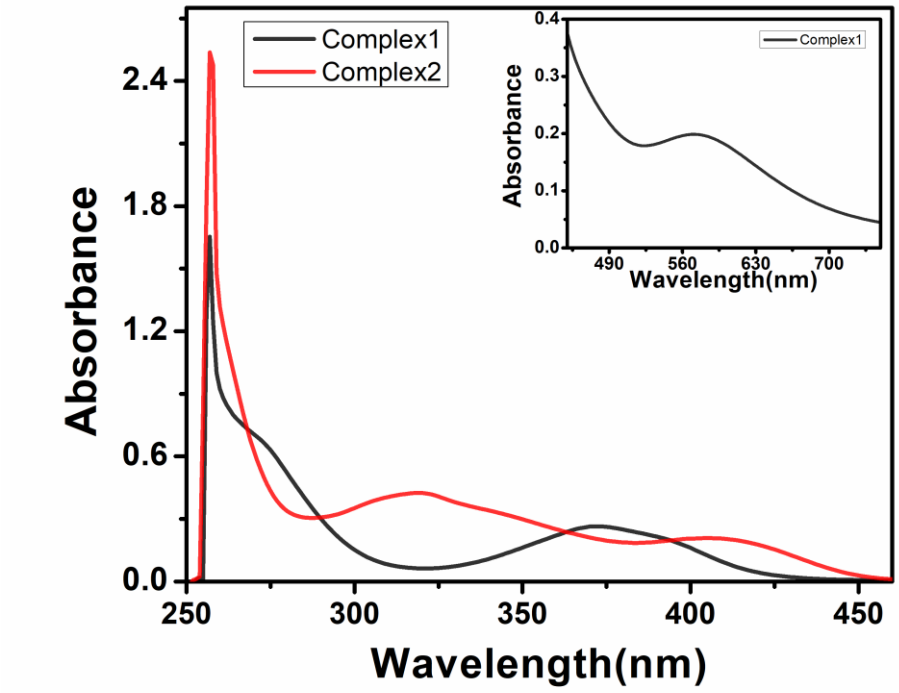

Figure S2. UV spectrum of complex **1** and **2**.

Table S1. Selected bond length and bond angle table of Complex **1** and **2.**

Bond length (Å)			
Complex 1		**Complex 2**	
Cu1-O1	1.888(4)	Zn1-O1	1.899(3)
Cu1-N1	2.011(3)	Zn1-N1	2.022(3)
Bond angle (°)			
Complex 1		**Complex 2**	
O1-Cu1-N1	90.83(14)	O1-Zn1-N1	96.60(11)
O1-Cu1-N1a	89.17(14)	N1-Zn1-N1a	122.03(11)
N1-Cu1-N1a	180	O1-Zn1-O1a	119.60(12)
O1-Cu1-O1a	180.	O1-Zn1-N1a	111.87(11)

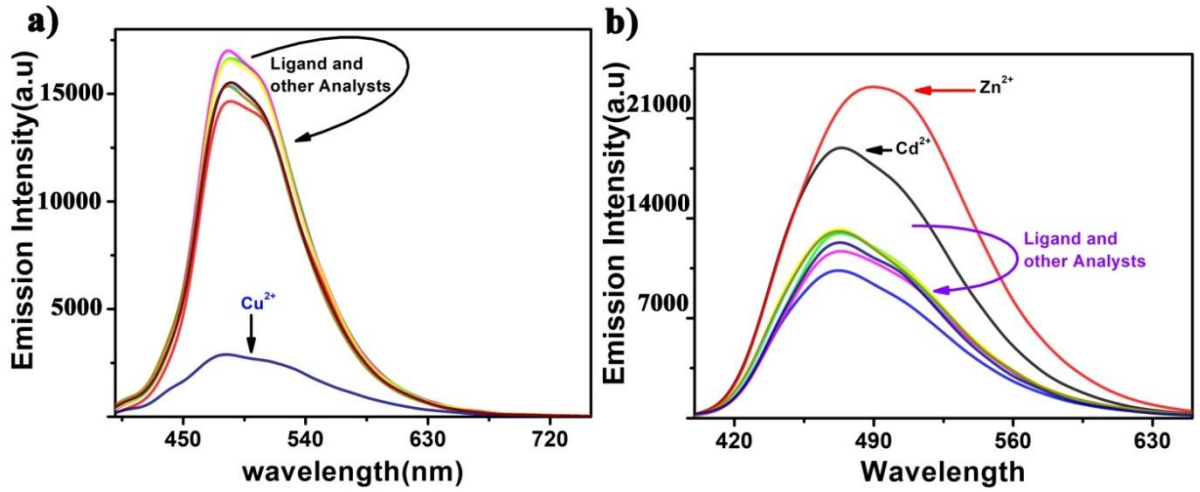

Figure S3. Change of fluorescence intensity after addition of deferent analytes (60 μM) to a fixed concentration of ligand (a) $\mathbf{HL_1}$ and (b) $\mathbf{HL_2}$ (40 μM) DMSO/H_2O

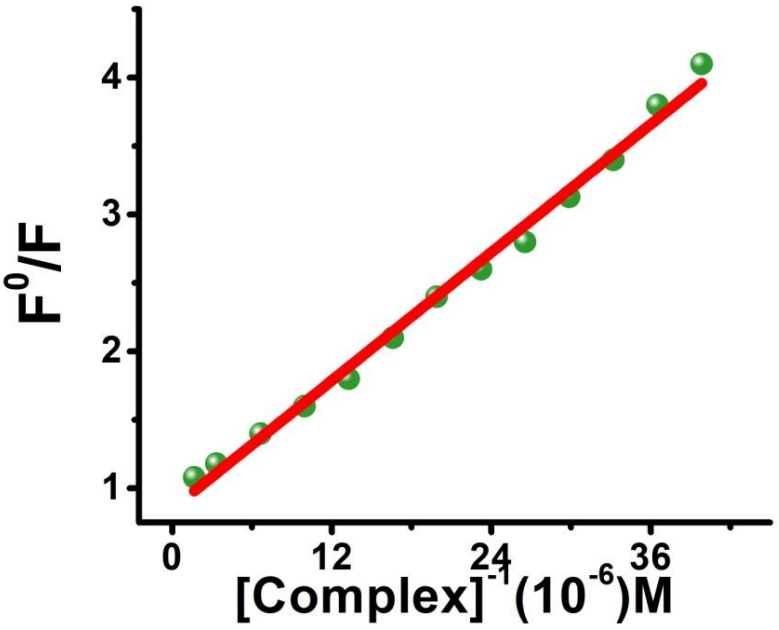

Figure S4. Stern-Volmer graph for determination of quenching constant of $\mathbf{HL_1}$ after addition of Cu^{2+} ion.

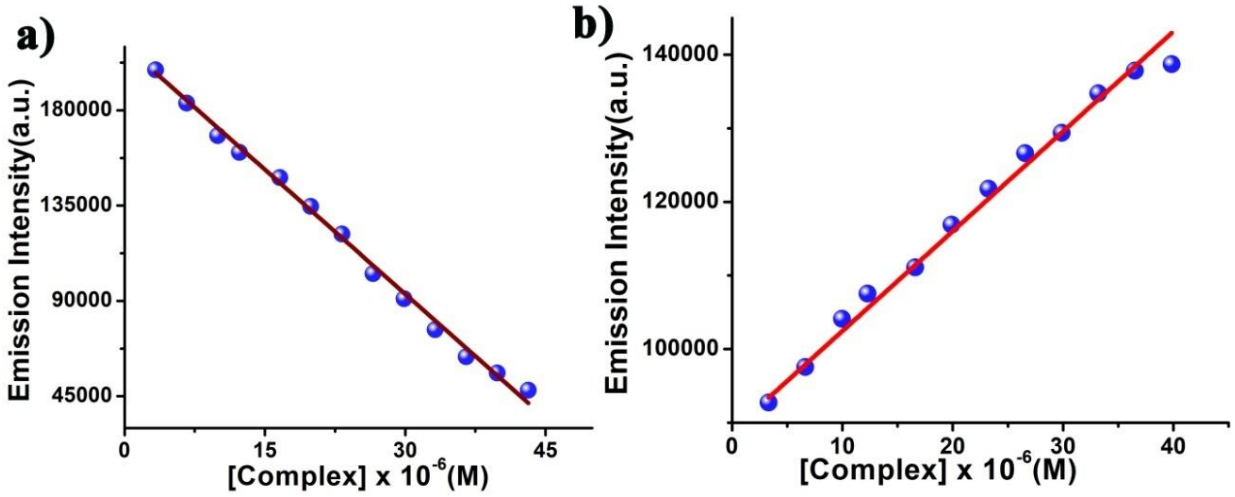

Figure S5. Change of Fluorescence emission intensity of (a) $\mathbf{HL_1}$ as a function of Cu^{2+} ion and (b) $\mathbf{HL_2}$ as a function of Zn^{2+} ion for detection limit calculation.

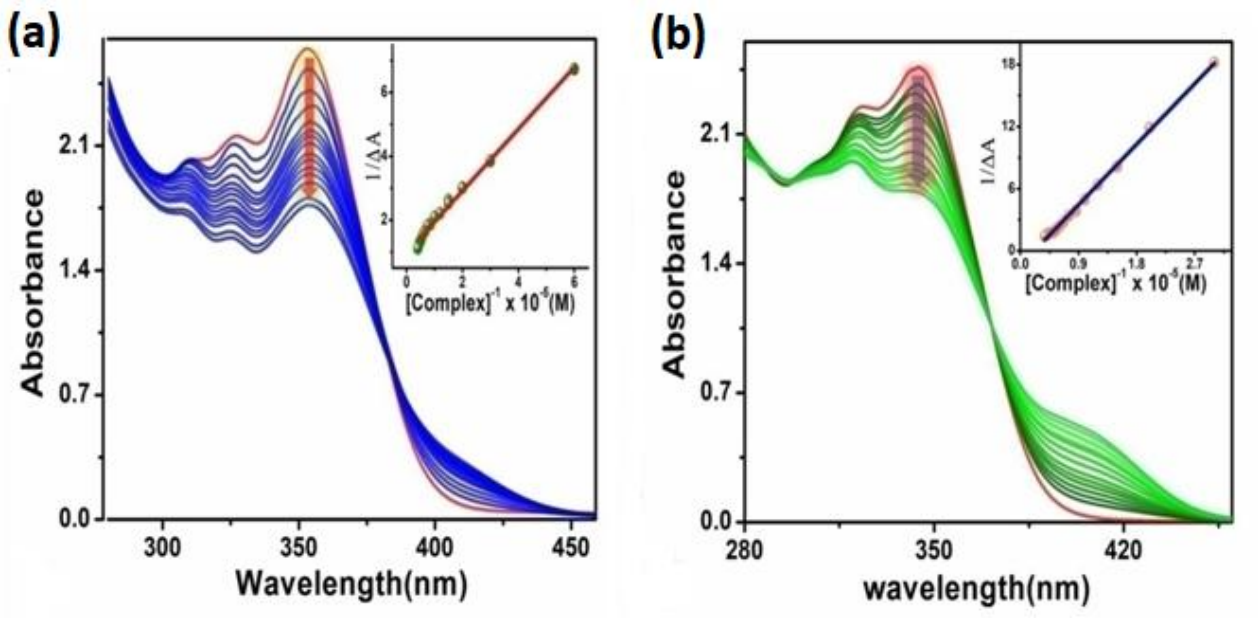

Figure S6. UV spectral titration of (a) $\mathbf{HL_1}$ with Cu^{2+} and (b) $\mathbf{HL_2}$ with Zn^{2+} ion solution respectively.

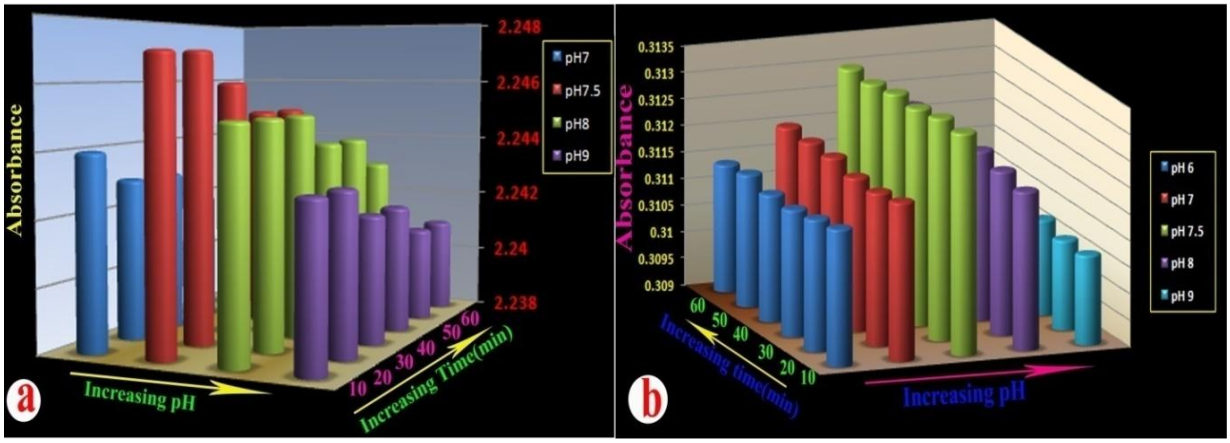

Figure S7. Stability in DMSO/H_2O (9:1) HEPES buffer medium at different pH and the stability in DMSO/water (9:1) solvent at a fixed pH value (7.4) by means of time–scan experiment of (a) $\mathbf{HL_1}$ and (b) $\mathbf{HL_2}$

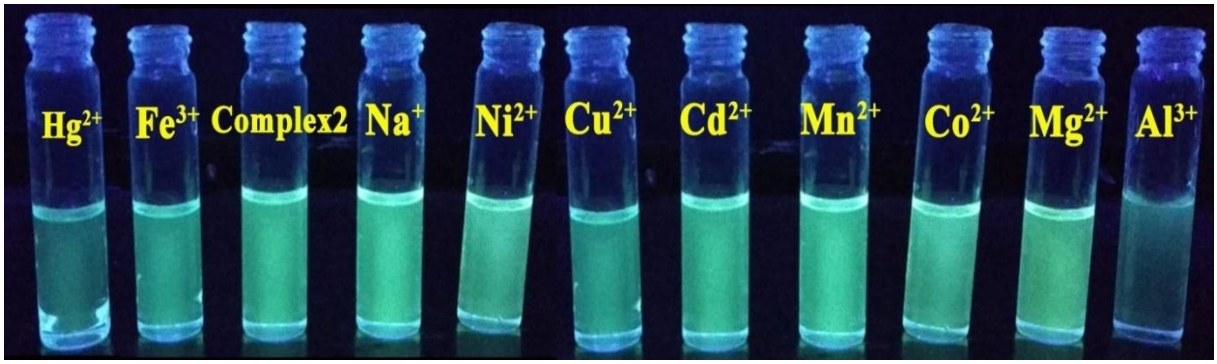

Figure S8 Naked eye colour changes after addition of Al^{3+} and Hg^{2+} to complex **2** in the presence of different cotions in 9:1 (DMSO/H_2O) HEPES buffer (pH = 7.4) solution.

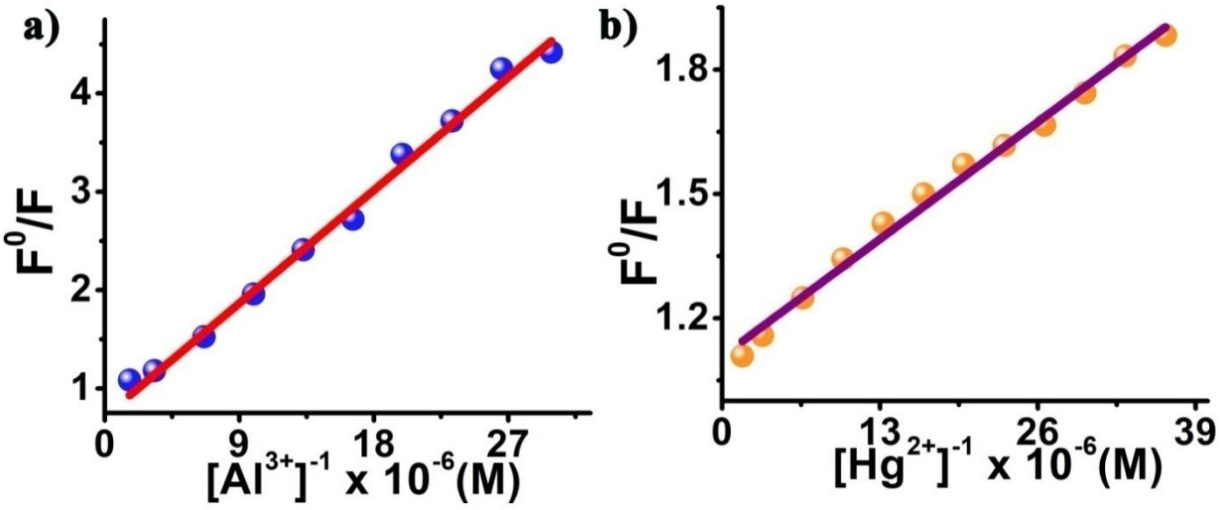

Figure S9. Stern-Volmer graph for detection of quenching constant of complex **2** after addition of (a) Al^{3+} ion and (b) Hg^{2+} ion.

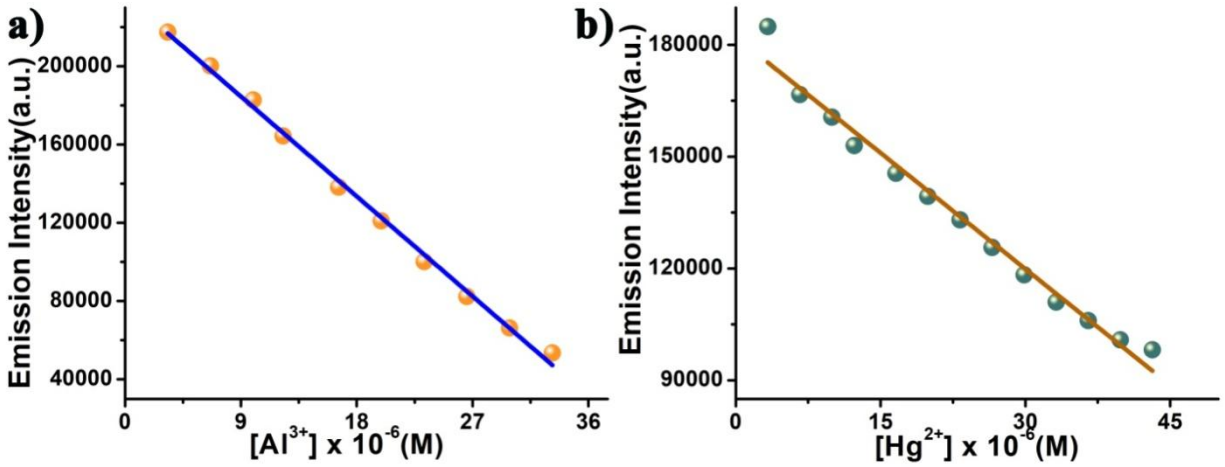

Figure S10. Change of fluorescence emission intensity of complex **2** as a function of (a) Al^{3+} ion and (b) Hg^{2+} ion for detection limit calculation.

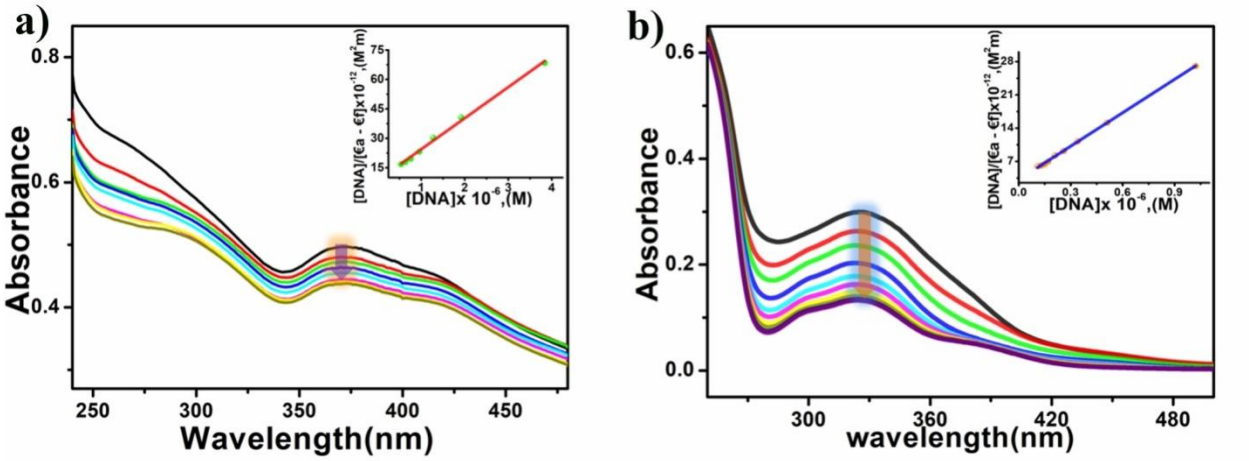

Figure 11. Absorption titration spectra of **(a)** complex **1 (b)** complex **2** in absence and presence of ct-DNA. Inset: best fitting graph for binding affinity calculation.

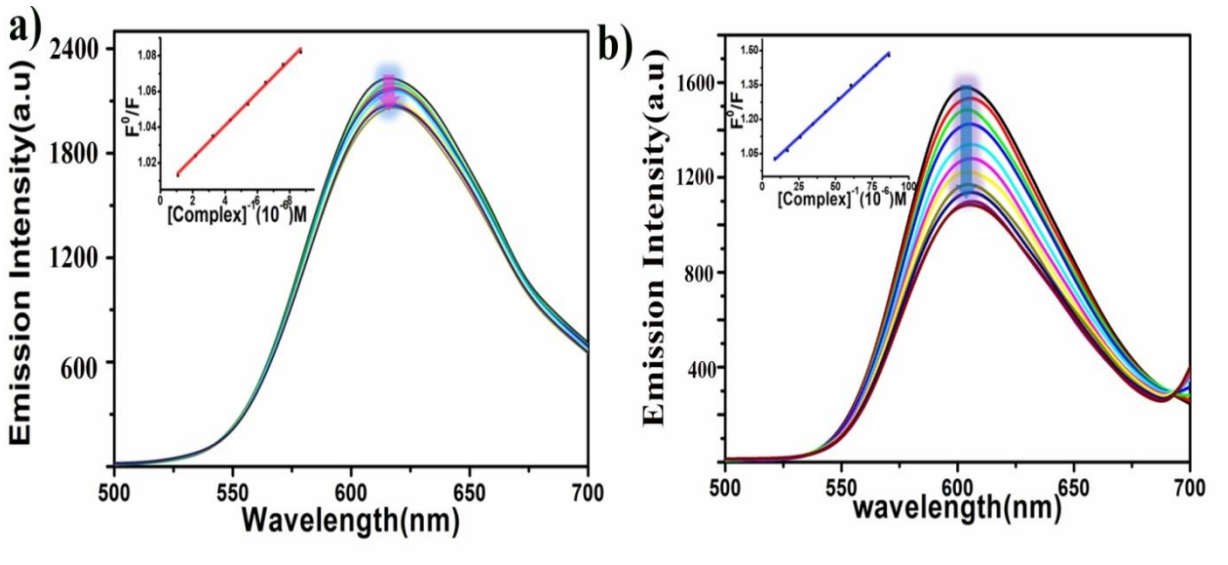

Figure S12. Change of Emission spectra of the ctDNA-EtBr complex with addition of increasing concentration of (**a)** Complex **1 (b)** Complex **2** and in inset the fractional fluorescence (F^0/F) plot of CT-DNA-EtBr as a function concentration of the complexes.

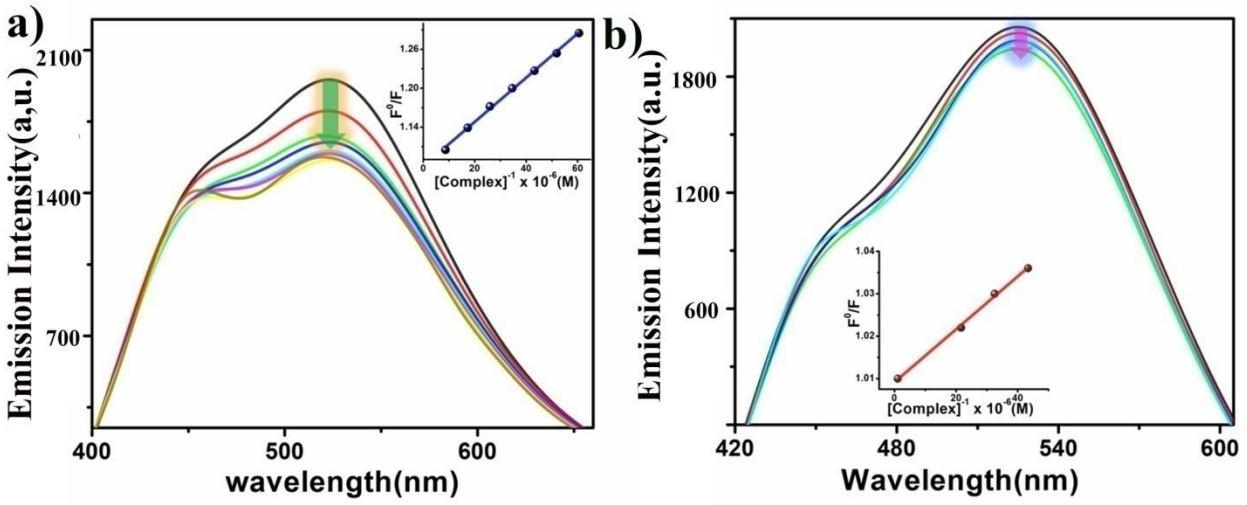

Figure S13. Change of Emission spectra of the ctDNA-DAPI complex with addition of increasing concentration of (**a)** Complex **1 (b)** Complex **2** and in inset the fractional fluorescence (F^0/F) plot of CT-DNA-DAPI as a function concentration of the complexes.

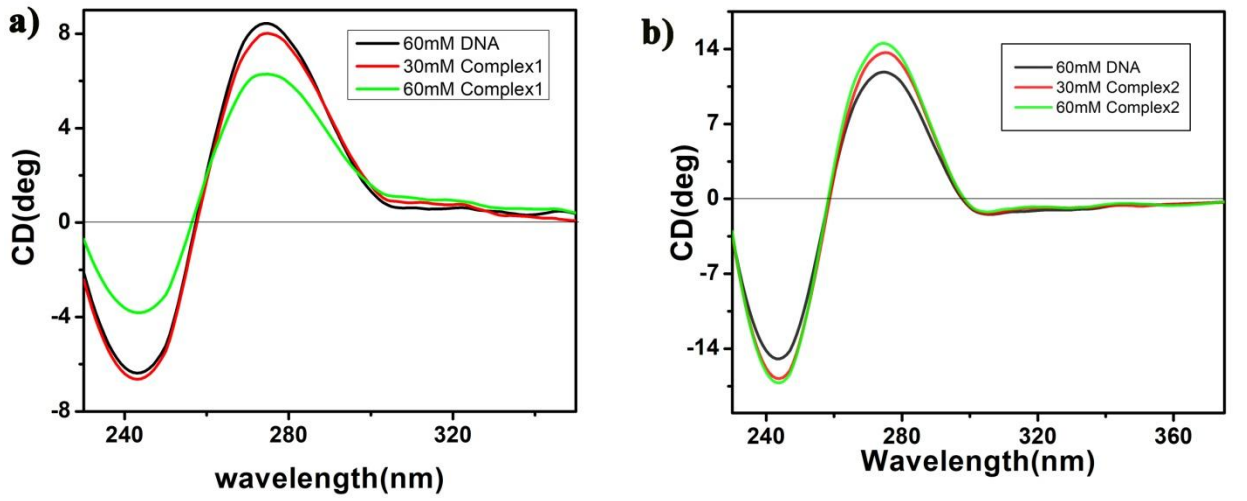

Figure S14. CD spectra of ctDNA in CP buffer in the presence and absence of (a) complex **1** and (b) **2**

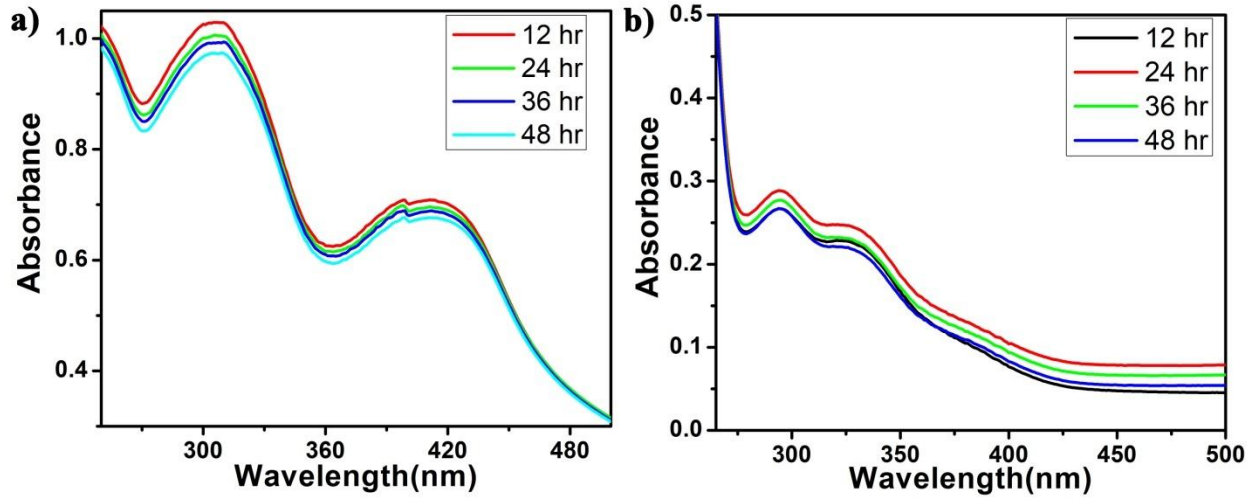

Figure S15. UV-Vis spectral analysis in tris buffer medium of (a) complex **1** and (b) **2.**

Table S2. Docked binding energy and other parameters of complex **1** and complex **2** with HSA and ctDNA.

HSA			
Complex	**Binding energy (kcal/mol)**	**Ligand Efficiency**	**Intermolecular Energy (kcal/mol)**
1	-8.96	-0.26	-9.55
2	-8.29	-0.25	-8.89
ctDNA			
Complex	**Binding energy (kcal/mol)**	**Ligand Efficiency**	**Intermolecular Energy (kcal/mol)**
1	-5.61	-0.22	-6.20
2	-5.96	-0.26	-6.55