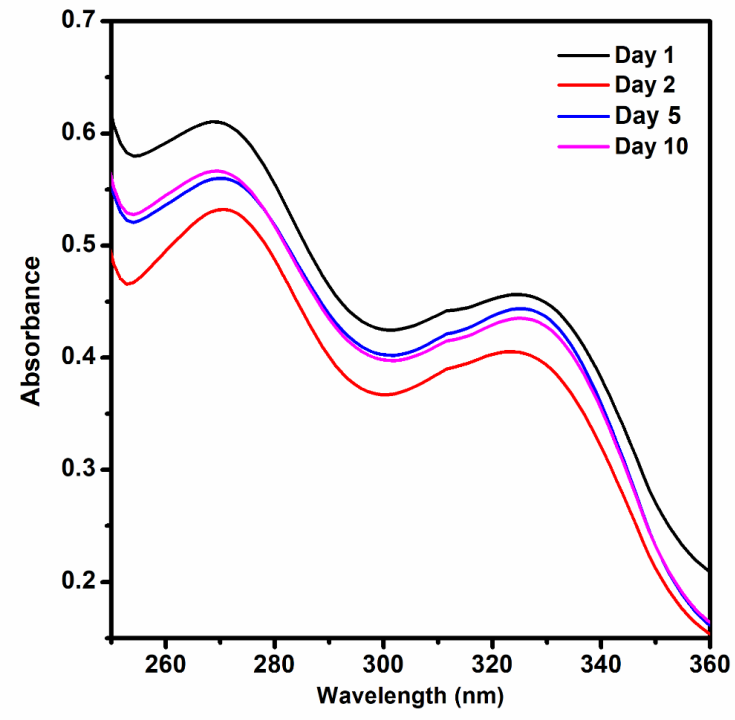


Figure S1 Electronic absorption spectra of the complex in HEPES buffer for different times (Day 1, Day 2, Day 5 and Day 10)

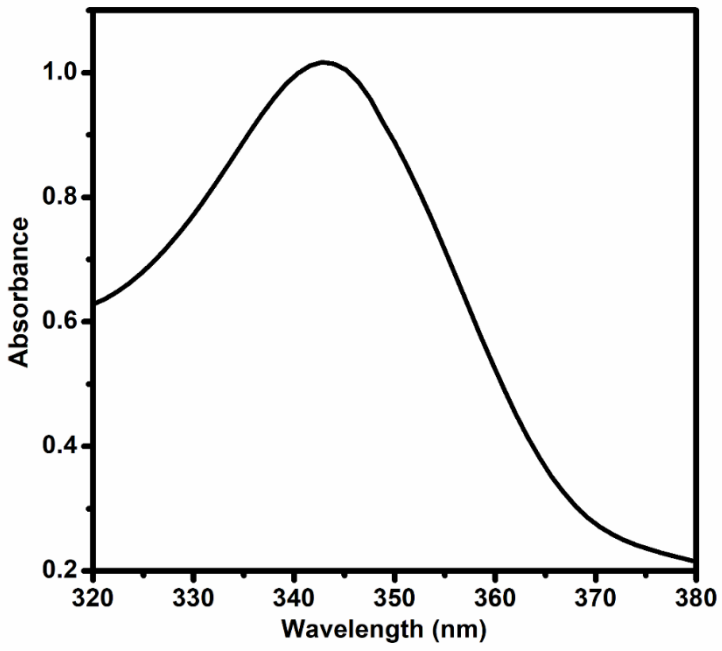
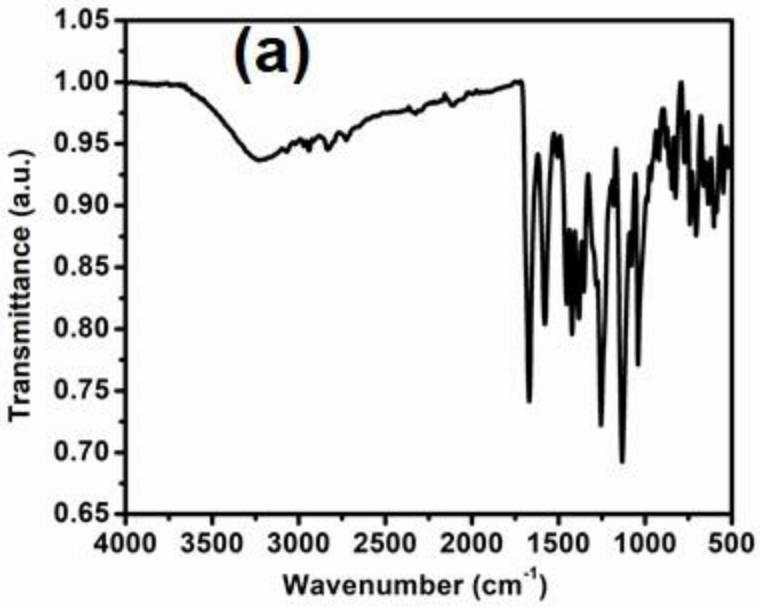
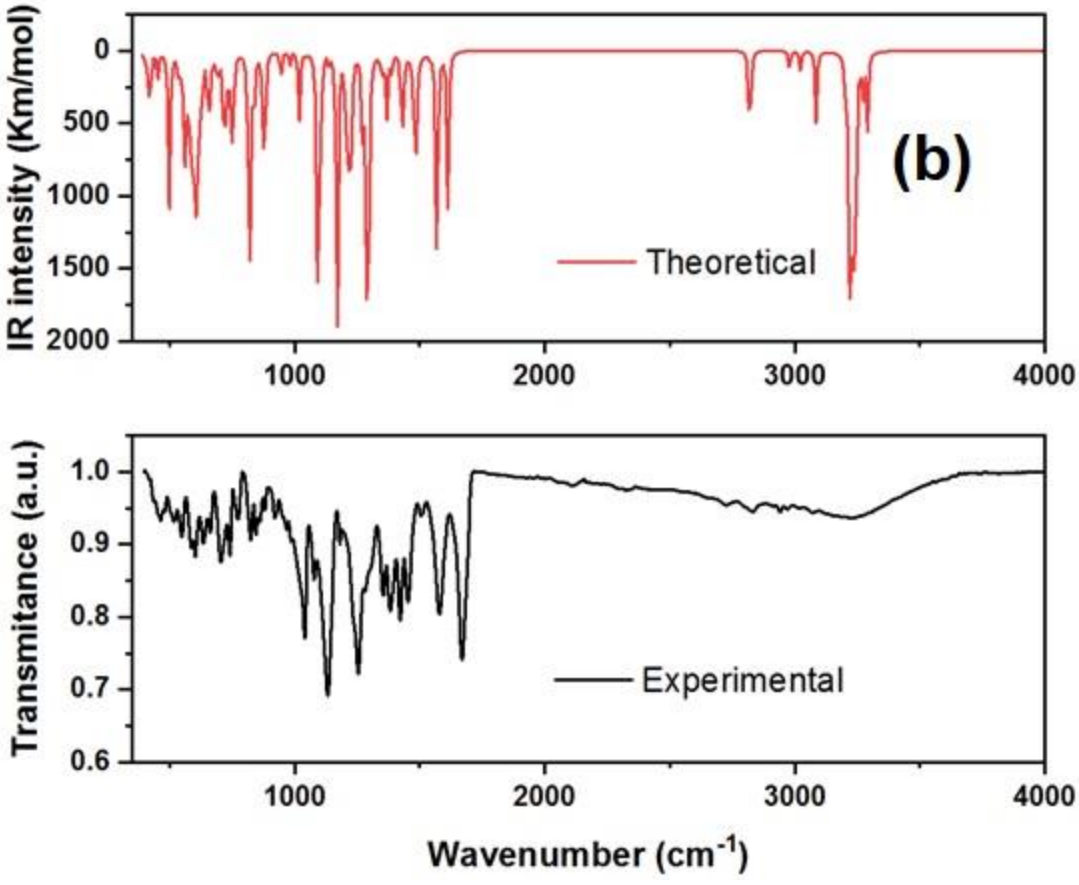


Figure S2 Electronic absorption spectrum of the ligand


(a)
Transmittance (a.u.)
1.05
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
4000 3500 3000 2500 2000 1500 1000 500
Wavenumber (cm-1)


IR intensity (Km/mol)
0
500
1000
1500
2000
(b)
Theoretical
1000 2000 3000 4000
Transmitance (a.u.)
1.0
0.9
0.8
0.7
0.6
Experimental
1000 2000 3000 4000
Wavenumber (cm-1)

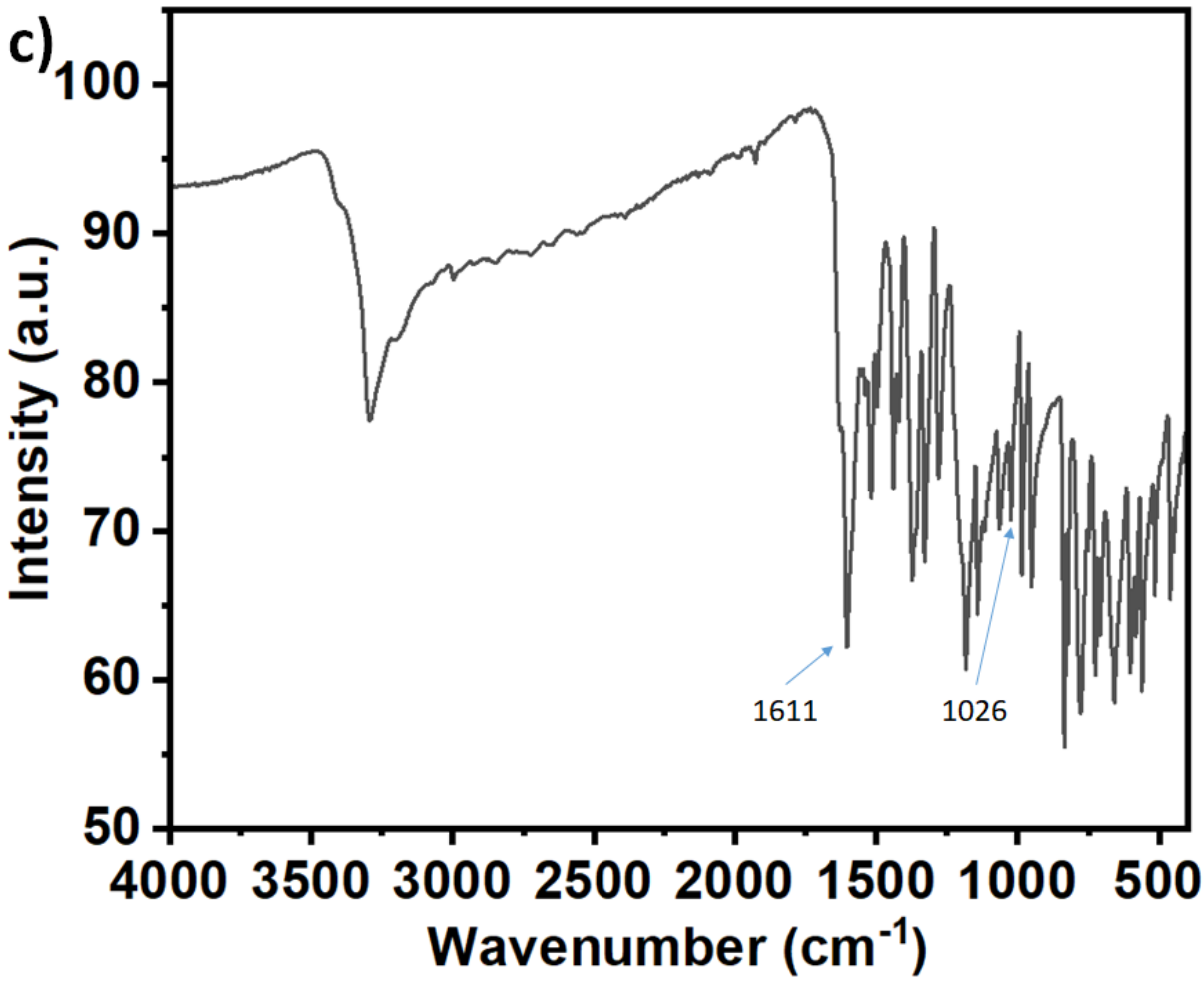


Figure S3 (a) FTIR spectrum of the complex (b) The experimental and DFT-simulated IR spectroscopy of the complex (c) FTIR spectrum of the ligand

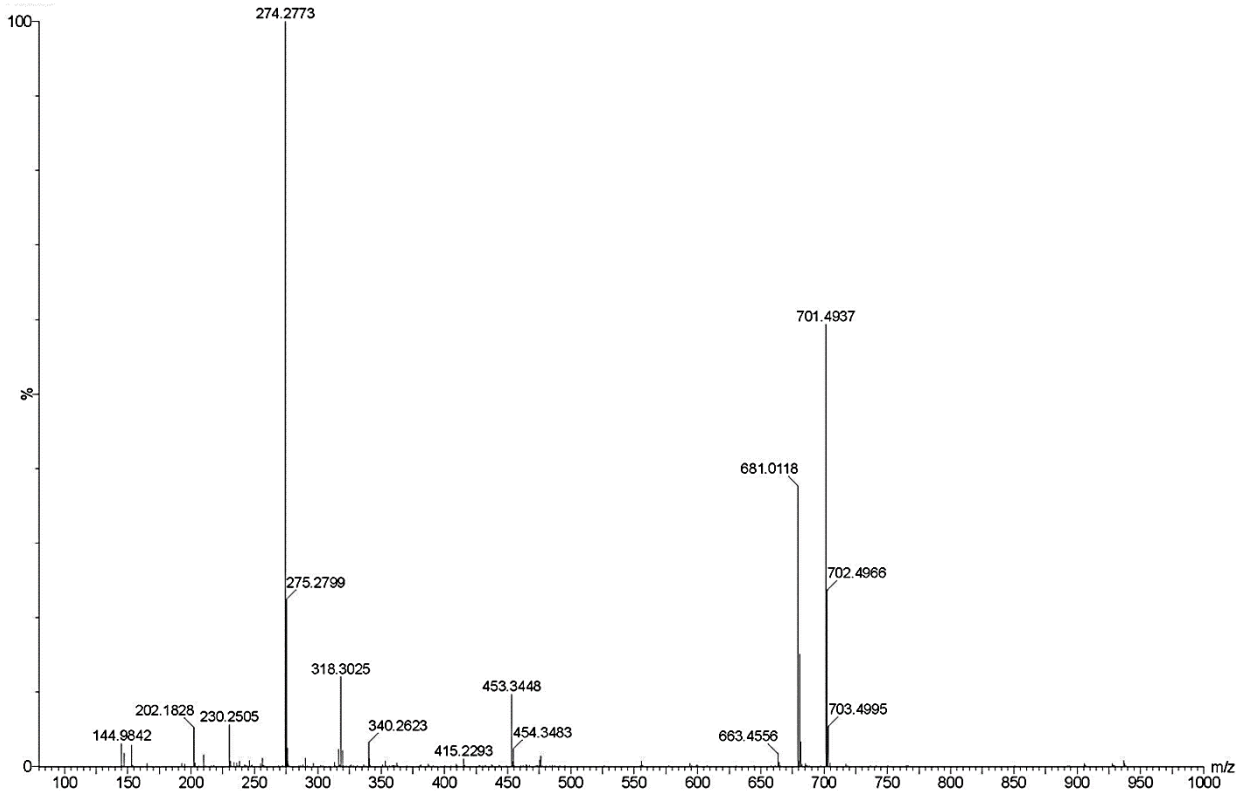


Figure S4 ESI-MS spectrum of the complex

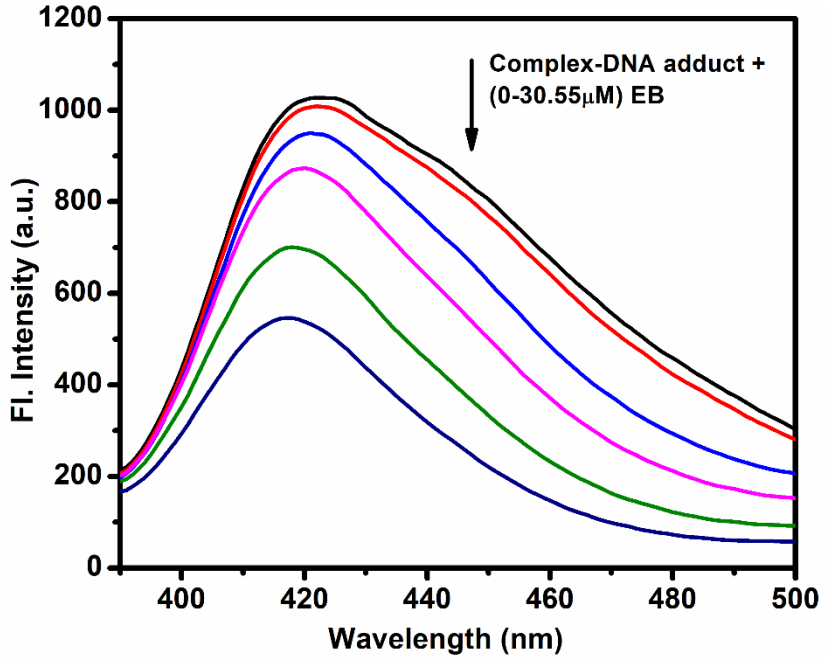


Figure S5 Fluorescence displacement assay of the complex by EB

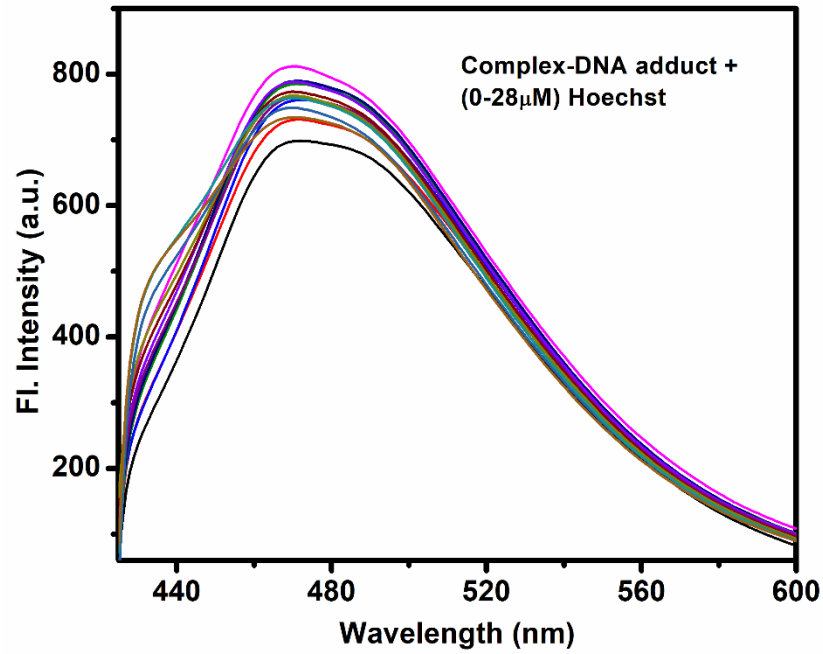


Figure S6 Fluorescence displacement assay of the complex by Hoechst

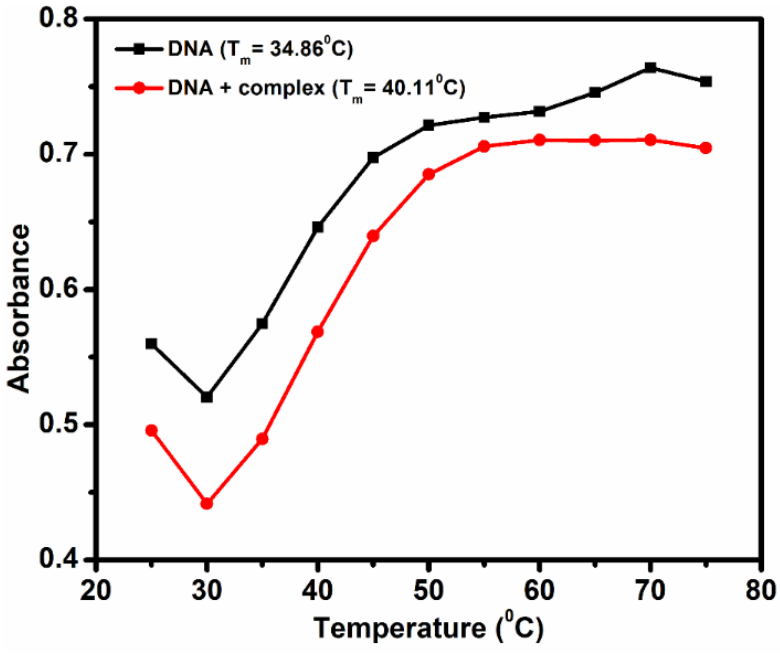


Figure S7 Melting temperature of CT-DNA with and without the complex

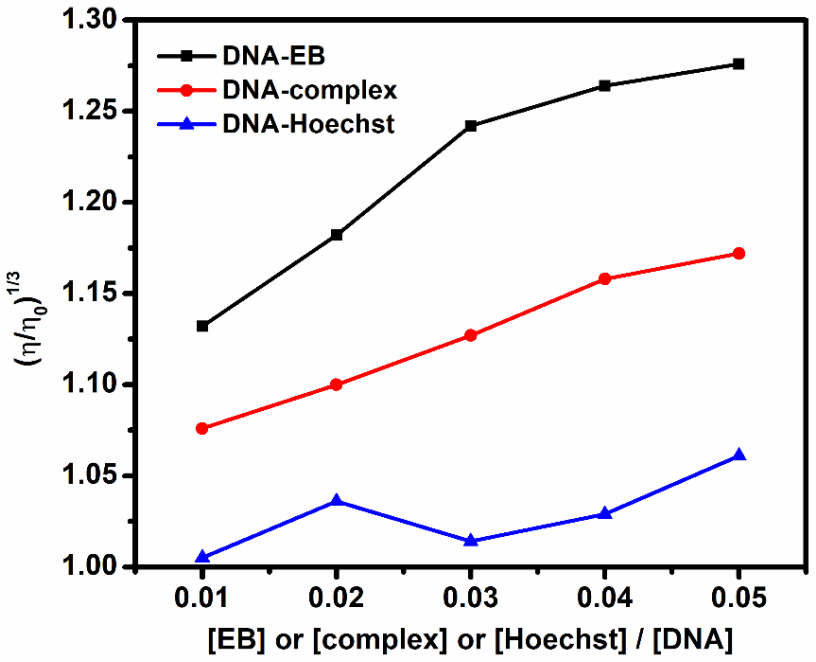


Figure S8 Relative viscosities of the CT-DNA-EB, CT-DNA-Hoechst and CT-DNA-complex solutions with increasing amounts of EB or complex or Hoechst (0.01–0.05 μM)

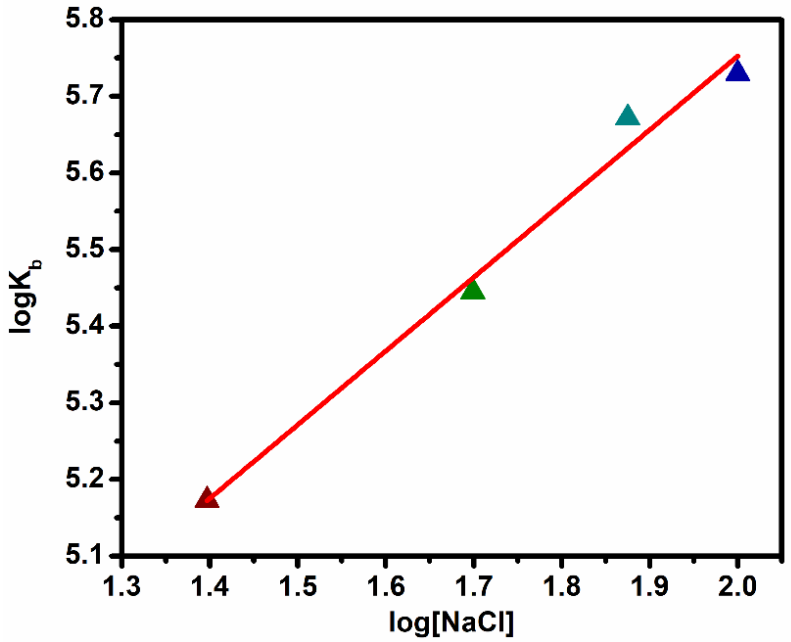


Figure S9 Plot of association constants (K_b) of complex and CT-DNA adduct against concentration of NaCl [25-100 µM]

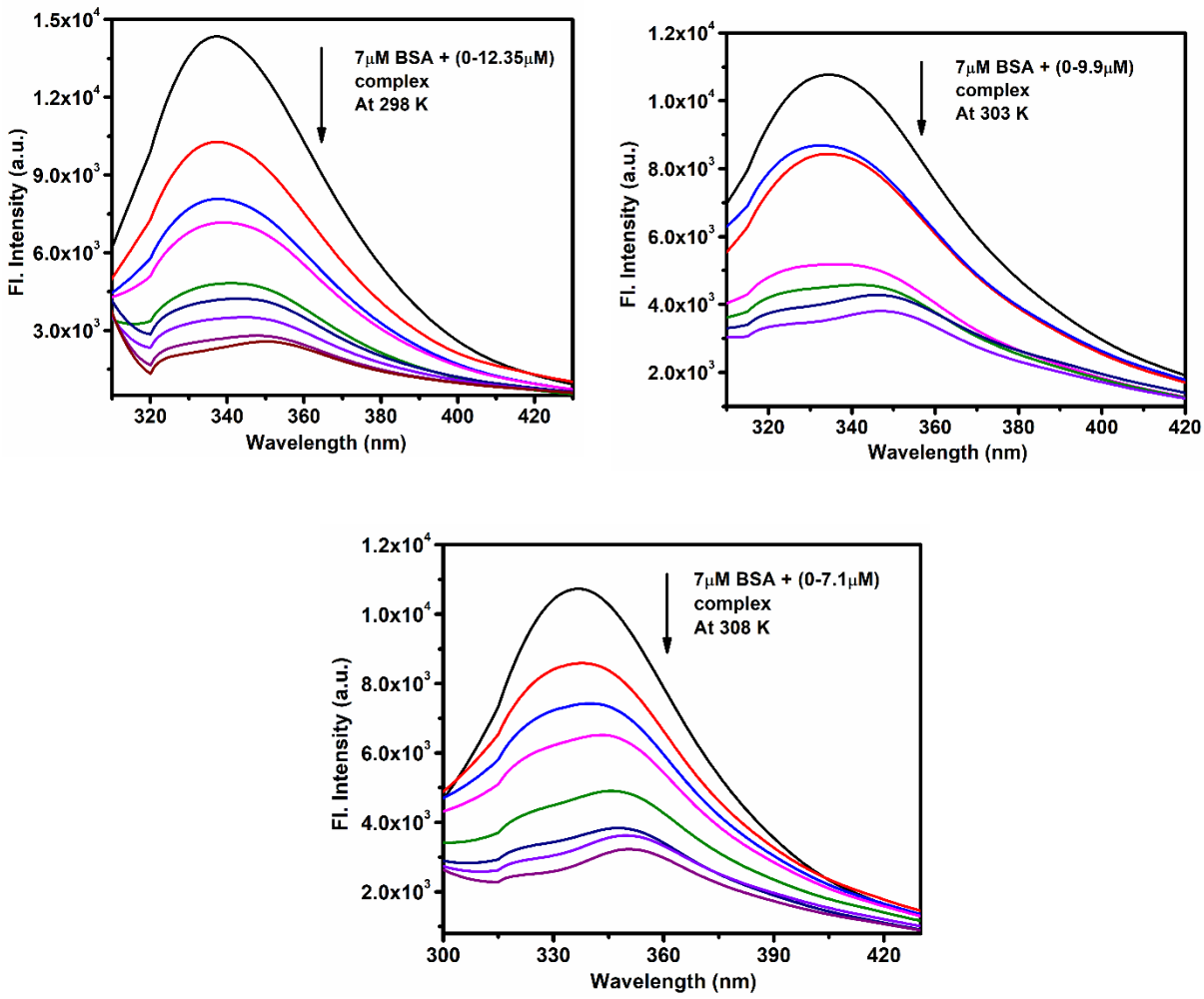


Figure S10 Effect of the addition of complex on the emission intensity of BSA at 298, 303 and 308 K

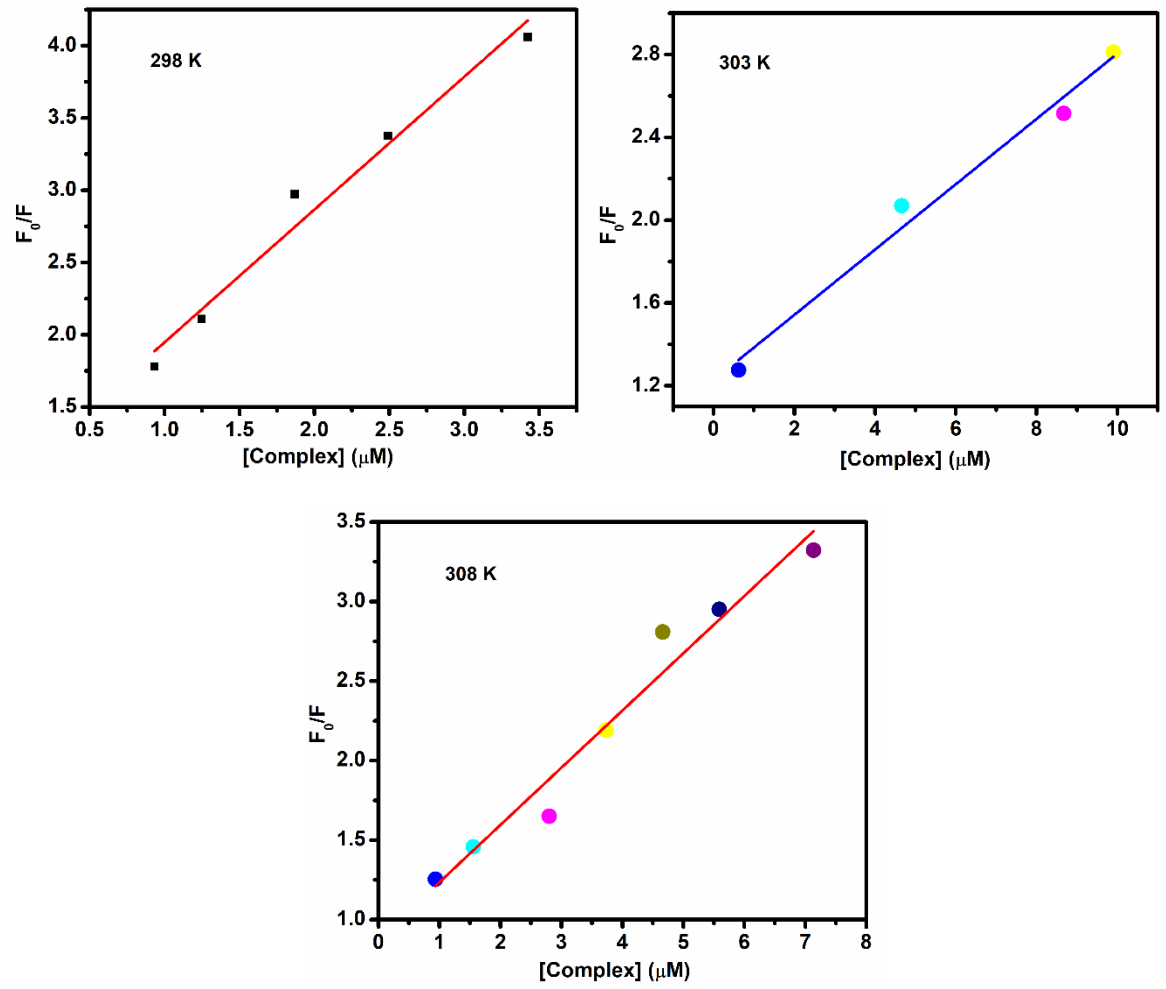


Figure S11 Stern volmer plots for fluorescence quenching of BSA at 298, 303 and 308 K

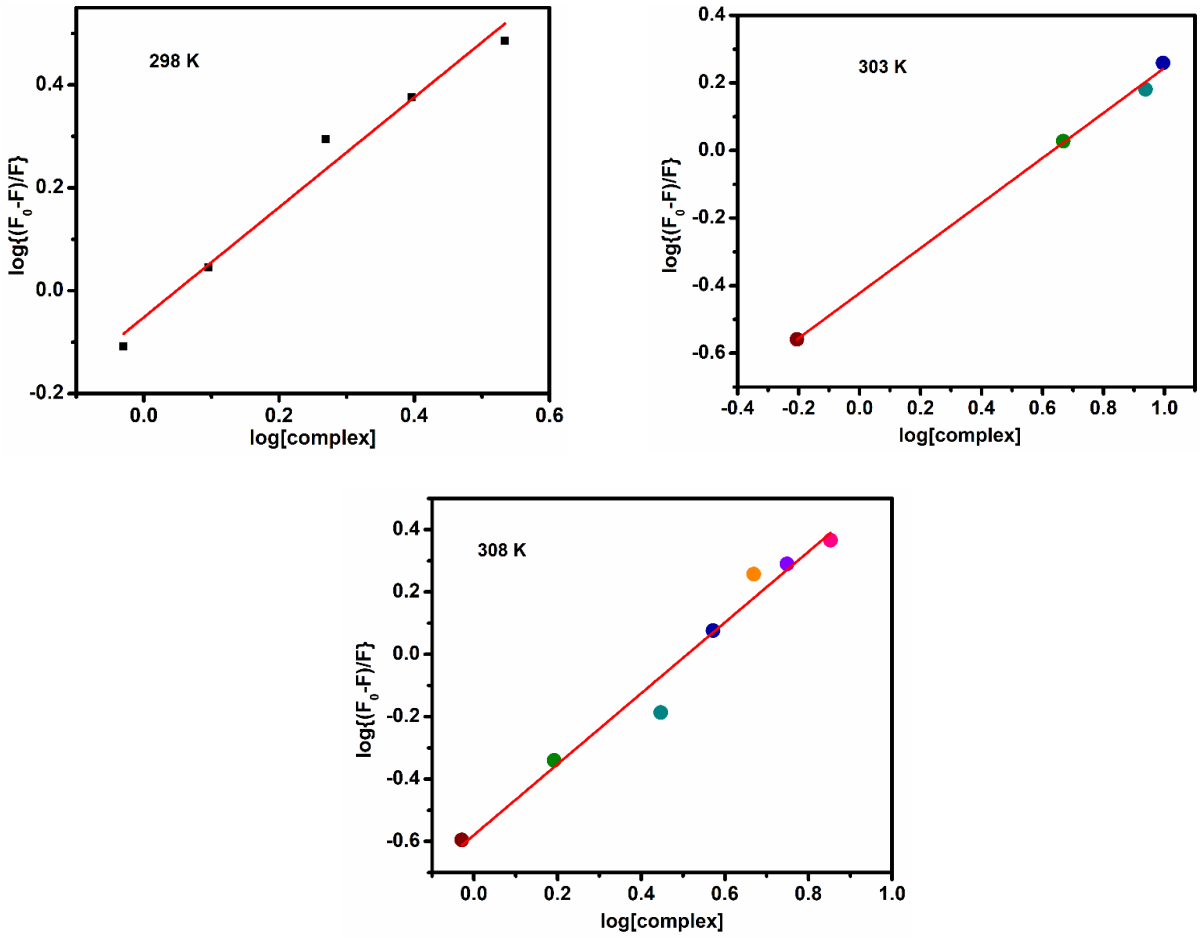


Figure S12 Plot of log ((F_0-F)/F) versus log [complex] at 298, 303 and 308 K for binding interaction of BSA with the complex

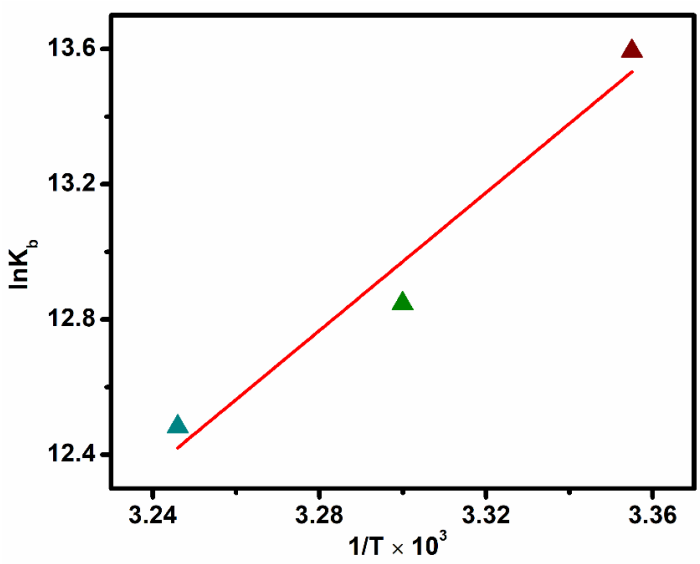


Figure S13 Plot of $\ln K_b$ versus 1/T for BSA binding with the complex

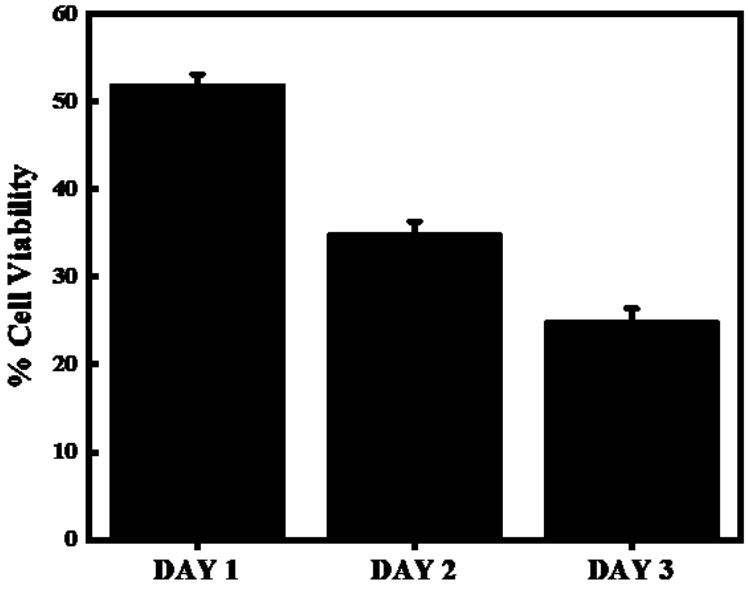


Figure S14 Day wise percentage of cell viability

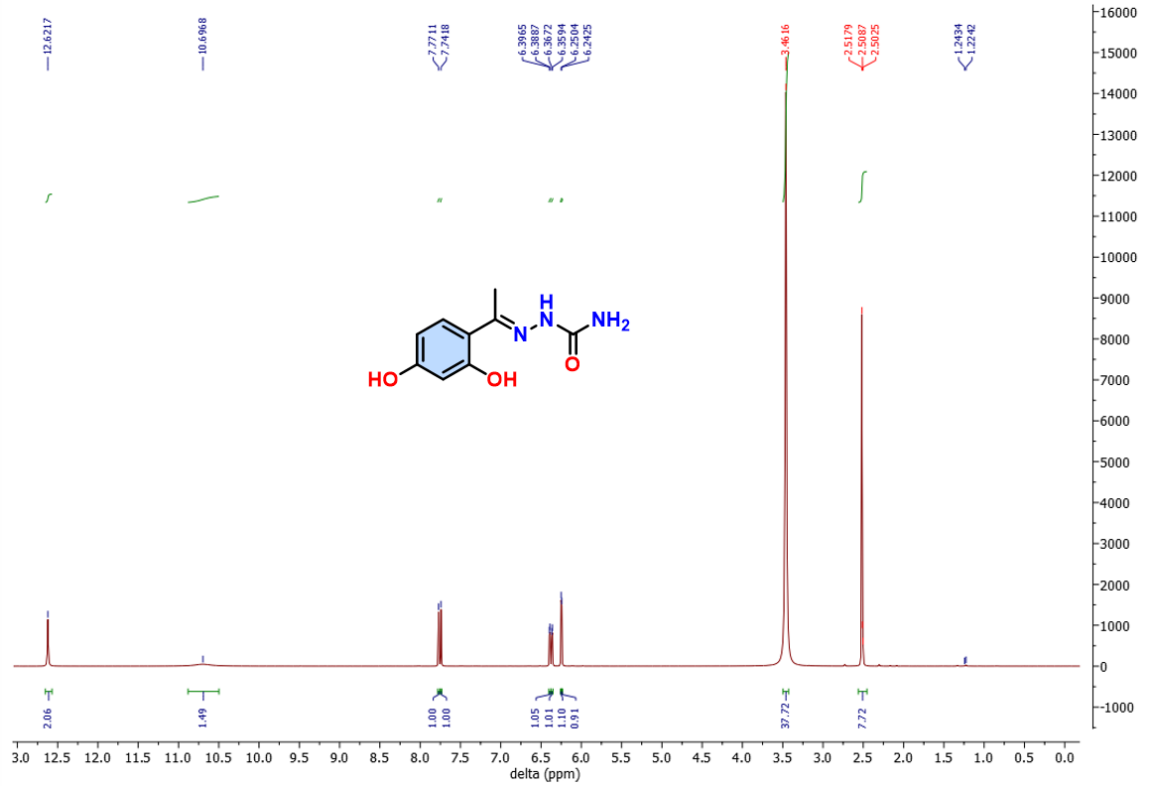


Figure S15 ^{1}H NMR of ligand

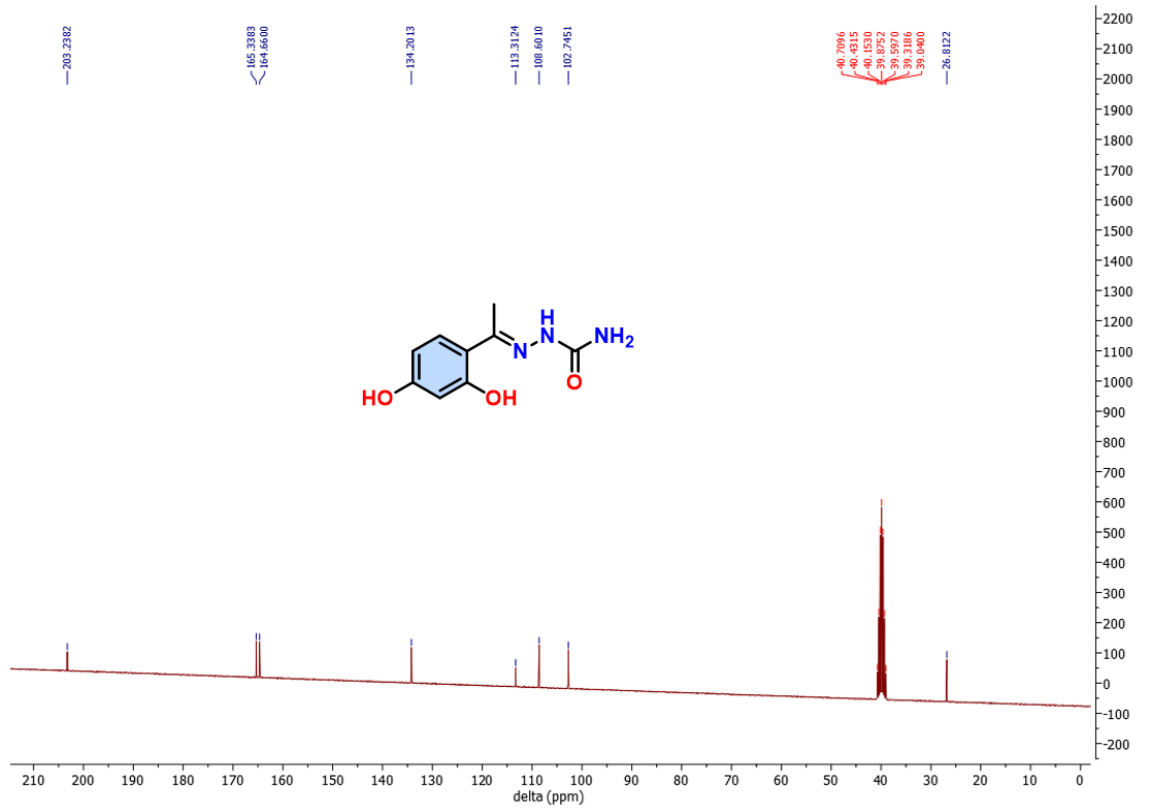


Figure S16 ^{13}C NMR of ligand

Table S1 Cu-O and Cu-N bond lengths in the complex

Atom	**Bond length (A^0)**
Cu1-O1	1.85220
Cu2-O2	1.85300
Cu1-O3	1.83012
Cu2-O3	1.83067
Cu1-O4	1.83067
Cu2-O4	1.83079
Cu1-N1	1.88809
Cu2-N2	1.88862
Cu1-N3	1.90974
Cu2-N4	1.91212

Table S2 Experimental and DFT-simulated IR spectroscopy data of the complex

Major indicative bands in FTIR	**Experimental value (cm^{-1})**	**DFT-simulated value (cm^{-1})**
ν(C=N)	1656	1611
ν(C−O)	1220-1227	1218-1228
ν(Cu−O)	477	470
ν(Cu−N)	444	442
N-H stretching	3250	3226
Aromatic C-H	3144	3096
Aliphatic C-H stretching	2810	2825

Table S3 Enhancement constants of DNA and complex interaction

Temperature (K)	K_E value
298	3×10^3
303	4×10^3
308	9×10^3

Table S4 Binding parameters of BSA and complex interaction

Temperature (K)	k_{sv}	k_b value	n	ΔG (kJ mol^{-1})
298	9.6×10^5	8.01×10^5	1.199	-33.68
303	1.577×10^5	3.8×10^5	0.92	-32.36
308	8.75×10^5	2.64×10^5	1.07	-31.96

DFT Study

The predicted structure of the complex was investigated using the DFT method [1]. The functional B3LYP and basis set LanL2DZ for Cu, and 6-311G for C, H, N, and O were utilized to optimize the geometry of the molecule with the help of Gaussian 09W D1 revision [2]. The same basis set has been used for the frequency calculations. HOMO and LUMO were visualized using GaussView 5 software [3].

Molecular Docking

The molecular docking study was conducted using Auto Dock vina software. RCSB's website (https://www.rcsb.org/) provided structural coordinates for CT-DNA and BSA protein (PDB ID: 1BNA and 4F5S, respectively). For the calculation, a standard protocol was used. For this example, the grid box size was 26 × 26 × 26. We visualized the final results in Discovery studio client 2017 using the results derived from these calculations.

References:

1. Muthukkumar, M.; Bhuvaneswari, T.; Venkatesh, G.; Kamal, C.; Vennila, P.; Armaković, S.; Armaković, S.J.; Sheena Mary, Y.; Yohannan Panicker, C. Synthesis, characterization and computational studies of semicarbazide derivative. J. Mol. Liq. 2018, 272, 481–495, doi:10.1016/j.molliq.2018.09.123.

1.

2. 2009 Gaussian 09, Revision D.01; Gaussian, Inc.: Wallingford, CT, Gaussian 09, Revision D.01; Gaussian, Inc.: Wallingford, CT, 2009, (n.d.).

3. 2009. GaussView, Version 5; Gaussian, Inc.: Wallingford, CT, GaussView, Version 5; Gaussian, Inc.: Wallingford, CT, 2009, (n.d.).