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DNA Interaction Studies of a Water-Soluble Cu(II) Complex Derived from Diethanolamine and Dipicolinic Acid Ligands: Spectroscopic and Molecular Docking Investigations

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ABSTRACT

A copper(II) complex containing diethanolamine and dipicolinic acid ligands, [Cu(DEA)(PDCA)], was synthesized and characterized. The binding interaction of this complex with CT-DNA was investigated using various methods such as UV-vis spectroscopy, fluorescence and molecular binding study s and at physiological PH. Based on UV-vis and fluorescence spectroscopy, it can be concluded that [Cu(DEA)(PYDC)] interacts with CT-DNA via groove binding mode. The thermodynamic parameters obtained from the Van't Hoff equation are $\Delta H > 0$ and $\Delta S > 0$, indicating that the reaction is further entropically proceeds. Also, at different temperatures, the corresponding numbers of binding sites (n) and the binding constant (Kf) were calculated.

Keywords: Native Calf Thymus; Groove Binding; DNA Interaction; Diethanolamine; Dipicolinic Acid; Molecular Docking Simulation

Abbreviations: DNA: Deoxyribonucleic Acid; CT-DNA: Native Calf Thymus; DEA: Diethanolamine; PDCA: Pyridine-2,6-Dicarboxylic Acid; UV-Vis: UV-Visible; A: Adenine; G: Guanine; T: Thymine; C: Cytosine

Introduction

Inorganic elements are important in biological processes and have also been used in medicines for many centuries and metal ions among them are the necessary components in all aspects of the chemistry of living organisms [1]. Among them, element copper is an important for plant growth and human health and animal [2]. Copper is involved in many metabolic functions and act as a vital cofactor is enzymes, including (cytochrome oxidase, tyrosinase, elastase, ascorbic acide oxidase, ceruloplasmin, dopamine-B-hydroxylase, lysyl oxidase and superoxide dismutase) [3]. However, excessive use of copper can lead to health problems such as nerve inflammation and\or anemia, and brain, kidney or liver damage [4]. Numerous Pathological changes happen accompanied with changes in trace metals as the cancer expansion and development. Several reports have shown that trace metals concentrations in both serum and tumor tissue is significantly increased or decreased [5]. The most related trace metal is copper. Copper is mostly stored in the liver and main source of Cu in humans is dietary supplementation [6]. The role of Cu in the past two decades has been extensively investigated in both the growth of tumors and etiology [7]. Cu(II) complexes are significant because they illustrate interesting biological properties such as enzyme, DNA and protein interactions. Also,

Cu(II) complexes showed significantly stronger biological activity than did free ligands, related to the synergistic effect between the ligand and central Cu(II) ion [8,9]. The pharmacological activity has also been found to be highly dependent on the nature of the metal ion and the donor sequence of the ligands as different ligands exhibit different biological properties [10]. Coordinating complexes that have medicinal uses, dipicolinic acid (PDCA) and its derivatives are introduced as ligands in it [11]. Recently in Pharmacological researches dipicolinic acids has been considered and its reason is their amphophilic nature and low toxicity [12]. Also, Ethanolamines (Ea's) are a class of organic molecules including amine and alcohol groups. Ethanolamines (Ea,s) readily form coordination compounds with almost all metal ions as versatile ligands and also act as N and O donor ligands [13]. The biological assay of complexes achieved from the coordination of a ß-amino alcohol ligand to some transition metal ions confirms their anticancer activity [14].

Metal complexes bind with DNA trough covalent interaction or non-covalent interactions including hydrophobic, and hydrogen bonding interactions along the major or minor groove of the DNA helix, groove binding through van der Waals, π-π* stacking with the DNA nucleobases, and external/ electrostatic interaction with the phosphate groups of DNA [15]. These interactions can cause inhibition of the cancer cell division, DNA damage, and ultimately lead in cell death [16]. Therefore, our understanding of the mechanism of anticancer drug treatment is increase by studying the interactions of metal complexes with DNA and protein [17,18]. Generally, The main intracellular target of anticancer drugs is DNA. DNA is composed of a deoxyribose sugar, four bases containing nitrogen, and phosphate group. The bases consist of the pyrimidines, cytosine and thymine and the purines, adenine and guanine; an additional base, uracil, replaces thymine in RNA. DNA is double stranded, and the two strands bind to one another through hydrogen bonds between the bases on each strand. The composition of DNA is equal quantities of adenine and thymine and equal quantities of guanine and cytosine, because, in general, adenine binds to thymine and guanine binds to cytosine. There are two hydrogen bonds between adenine (A) and thymine (T) and three hydrogen bonds between cytosine (C) and guanine (G) [19,20].

The double helix structure of DNA contains a minor groove and major groove. The grooves are important in the attachment of DNA binding proteins involved in replication and trascription. The minor and major groove differ significantly in hydration, position of hydrogen bonding sites, size, electrostatic potential and shape [21]. The most well-know forms of DNA are A-DNA, B-DNA and Z-DNA. Segments of DNA that cells have methylated for regulatory purposes may adopt the Z geometry, in which the strands turn about the helical axis the opposite way to A-DNA and B-DNA. A-DNA is made up of deoxyribonucleotides, a right-handed double helix that resembles the B-DNA form. Overall, A-DNA is wider than the more commonly found B-DNA. B-DNA is the most common form of DNA that exists under physiological condition and is a right-handed double helix. The different puckering of their ribose units causes many of the structural differences between B-DNA and A-DNA. Z-DNA has a very different structural compared with A-DNA and B-DNA and is a left-handed double helix [22,23].

Experimental

Materials

All starting chemicals and solvents (Merck, Aldrich) were used as received without further purification. Calf thymus DNA (CT-DNA) and Hoechst 33258 was purchased from Sigma Co. Methylene blue (MB), dimethyl sulfoxide (DMSO), Na2 HPO4 and NaH2 PO4, Tris-HCl were purchased form Merck. We prepared all solutions using doubly distilled deionized water. All solvents and present materials were used as without purification.

Apparatus

The UV-Vis absorbance spectra were recorded using an Agilent 8453 spectrophotometer with a 1 cm quartz cell. Fluorescence measurements were done using a JASCO spectrofluorometer model FP-2600 with a quartz cuvette of 1,00 cm path length.

Synthesis of Complex [Cu(DEA)(PDCA)]

The synthesis of the Cu(II) complex was performed according to previously published method [24].

Molecular Docking Simulation

The docking calculation has been conducted by the open-source AutoDock Vina (version 1.1.2) with MGL tools 1.5.6. The known crystal structure of HSA (PDB ID: 1A06) was obtained from the Protein Data Bank. Receptor (HSA) and ligand (Cu(II) complex) files were provided using AutoDock Tools. The selected HSA model was enclosed in a box with the number of points in x, y and z dimensions of 34, 26 and 28 and center grid box of 17.847, -17.623 and 16.698 with a grid spacing of 1.00 Å. Lamarckian genetic algorithm was employed to perform docking calculations. All other parameters were default settings. Visualization of the docked pose has been carried out by using BIOVIA Discovery Studio Visualizer 2021 and LigPlot+.

Sample Preparation

To prepare stock solution from ct-DNA, it must be dissolved in Tris-HCl buffer solution (M: 0.05, PH: 7.4) and this solution must be kept in a dark place for 24 hours at 4 C0 to be completely dissolved. The purity of the ct-DNA solution is estimated by calculating the absorbance ratio at 260 and 280 nm is 1.8. Using uv spectrophotometry at 260 nm and an extinction coefficient (εp) of 6600 $m^{-1}cm^{-1}$, it was determined that the concentration of CT-DNA solution in the monomer unit was expressed. To prepare the phosphate

buffer solution, we use $N_aH_2PO_4$ and Na_2HPO_4 salts and dissolve it in double distilled water and set the PH to 7.4. By dissolving the specified amount of complex powder in 2 mL of phosphate buffer, stock solution of Cu(II) complex (1×10^{-2}) was prepared.

Experimental Procedures

UV-Vis Absorption Measurements: Absorption titration experiments were performed by keeping the concentration of DNA constant (5×10^{-5} M) while varying the complex Cu(II) concentration 1.5 to 6×10^{-4} M. Absorbance values were recorded after each successive addition of DNA solution, followed by an equilibration period.

Fluorescence Measurements: In this thesis, two fluorescence probes are methylene blue (intercalator) and Hoechst 33258 (groove binder), are used to determine the type of binding mode of the Cu(II) complex to CT-DNA. Competitive interaction was performed between Hoechst 33258 and the complex with CT-DNA as follows: fixed amounts of the DNA and Hoechst 33258 (6.7×10^{-4} and 5×10^{-6} M, respectively) were titrated in the wavelength range of 360-550 nm by addition successive amounts of the Cu(II) complex solution. Also the binding mode of complex with CT-DNA was investigated using methylene blue (MB) (5×10^{-6}). Then the effect of complex on the emission intensity was measured by adding the complex to the fixed of the MB and CT- DNA. Emission was observed between 640 and 730nm and samples were excited at 630 nm. All fluorescence emission measurements were performed at room temperature and 0.05 M Tris-HCl buffer (PH 7.4).

Results and Discussion

Synthesis of Cu(II) Complex

Cu(II) complex with diethanolamine (DEA) and dipicolinic acid (PDCA) ligand [Cu(DEA)(PDCA)](Figure 1), were pre-synthesized [24] and given to us for further study.

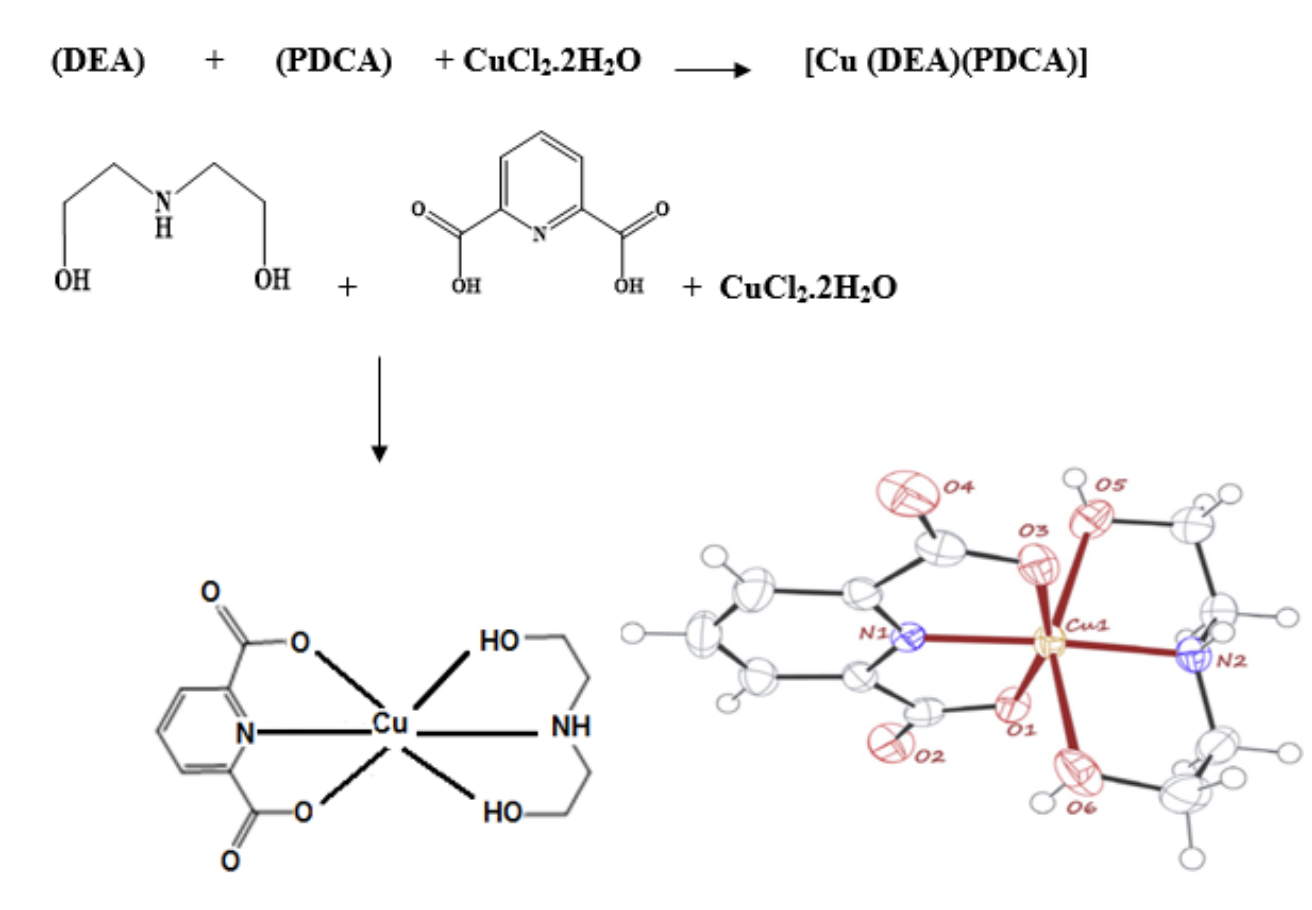

Figure 1: Chemical procedure for the synthesis of the [Cu(DEA)(PDCA)]complex.

UV-Vis Absorption Spectroscopy

UV-Vis absorption measurement is one of the most effective ways for investigating the binding mode of metal complexes to DNA [25]. In general, when a small molecule interacts with DNA and forms a new complex, we can observe considerable changes in the absorbance and peak position [26]. In general, hypochromism and hyperchromism are two spectral features of the interaction of small molecules with DNA that are related to the double helical structure of DNA. Hypochromism is due to the contraction of DNA in the helix axis due to outside binding (e.g. groove binding and electrostatic interactions). However, the damage, breakage of the secondary structure of DNA is attributed to the hyperchromism effect. The absorption spectra of CT-DNA with increasing amounts of Cu(II) complex are given in (Figure 2). As increasing concentration of Cu(II) complex, the UV-Vis absorption intensity of CT-DNA was influenced, resulting in hypochromicity. Intrinsic binding constant (k_b) was calculated using the Eq. (3.1) to further investigate the intensity of the interaction between the Cu(II) complex and CT-DNA [27]:

$$1/(A-A_0)=1(A_\infty-A_0)+1/K_b(A-A_0).1/[complex] \quad (3.1)$$

The binding constant (k_b) is computed from the intercept ratio to the slope of the linear double reciprocal plot of 1/(A-A0) versus 1/[complex] (Figure 3), A0 is the initial free DNA absorbance at 260 nm, and A is the noted absorbance at different concentration of Cu(II) complex. The obtained value of the intrinsic binding constant for the complex is 1.5×10^3, which is specified binding mode between DNA and the Cu(II) complex was groove-binder compared with groove-binding drugs such as 2-imidazolidinethione and levetiracetam (Kb = 1.4×10^3 and $(4.9 \pm 0.2) \times 10^3\ M^{-1}$ respectively [28,29].

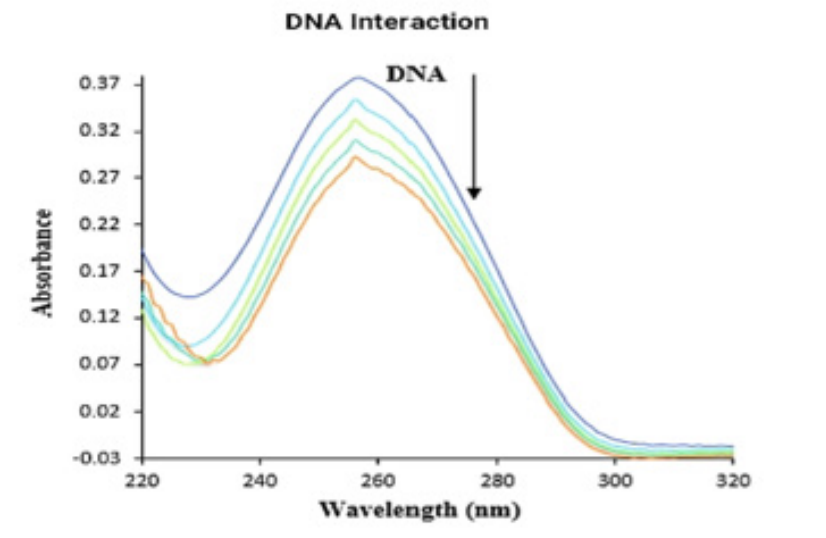

Figure 2: UV-Vis spectra of CT-DNA with increasing amounts of Cu(II) complex at T=298, pH= 7.4.

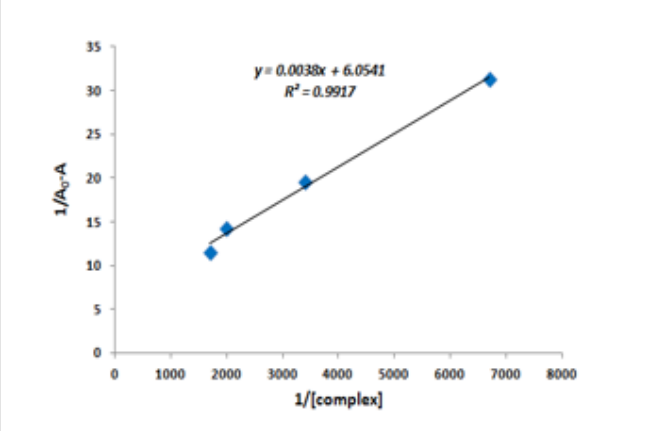

Figure 3: Plot $1/A_0$-A versus 1/[Complex].

Fluorescence Studies

Competitive Binding Studies with Hoechst 33258

In this study, a competitive binding experiment was performed to investigate the mode of complex binding to DNA. Hoechst is a well-known groove binder, which is often used as a fluorescence probe to investigate the mode of binding of Cu(II) complex to DNA. When the Cu(II) complex was added to a solution of Hoechst- CT-DNA, after an exchange of Cu(II) complex with some of the Hoechst molecules, the Hoechst molecules were released into solution and this phenomenon led to the fluorescence quenching (Figure 4) Therefore, it can be concluded that the Cu(II) complex competes with Hoechst when binding to CT-DNA, and since Hoechst 33258 binds to the minor groove of double-stranded DNA, it removes Hoechst from the duplex. These experimental results accurately showed that the Cu(II) complex binds to DNA via the groove binding mode [30,31]. The above experiment was performed at three different temperatures in order to establish the quenching mechanism.

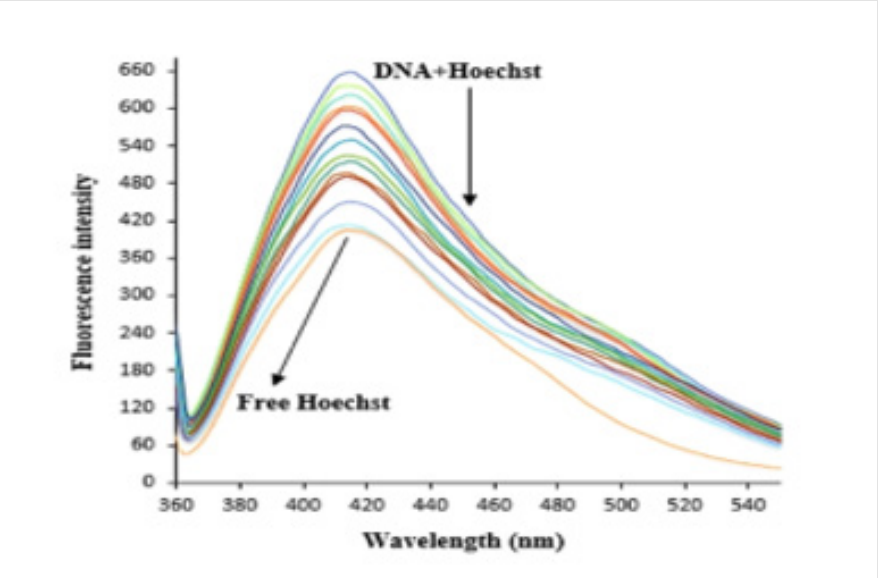

Figure 4: Fluorescence spectra of the competition between the Cu(II) complex and Hoechst, Hoechst=5×10-6 M, DNA=6.7×10^{-4} M, Complex=0 to1.12×10^{-3} M, T=310 K, pH=7.4.

Dynamic and static quenching are two well-known processes of quenching mechanism. In general, due to the different dependence of dynamic and static quenching on the excited- state lifetime and temperature, they can be detected. We used the Stern-Volmer equation (Eq. 3.2) to investigate fluorescence quenching mechanism.

$$F_0/F = 1 + K_{sv}[Q] = 1 + K_q\tau^0[q] \quad (3.2)$$

Where F and F_0 indicate the fluorescence intensities in the presence and in the absence of quencher, respectively. Quenching rate constant of is Kq, quenching constant is Ksv, lifetime of the fluorophore in the absence of a quencher is τ_0 (τ_0=10^8) [32], concentration of quencher is [Q]. (Table 1) shows that the Ksv values increased with increasing temperature and this result indicates that the dynamic quenching is a possible quenching mechanism of CT-DNA by the Cu(II) complex [33]. According to literature τ0≈10-8s, so the bimolecular quenching constant (Kq) were calculated (Table 1) It is larger than the limiting diffusion rate constant of biomolecule (2.00×1010), which indicates the static quenching occurred. The binding constant (K_b) and the binding stoichiometry (n) for the complex formation between complex with DNA were measured using the (Eq. 3.3) and values obtained are shown in (Table 2) [34]:

Table 1: Quenching constants (Ksv) values using Stern-Volmer equation for Cu(II) complex interaction with CT-DNA at different temperature.

T(K)	Ksv(L mol^{-1})×103	Kq (L mol^{-1}) ×1011	R^2
288	4.96	4.96	0.9834
310	5.35	5.35	0.9959
315	5.5	5.5	0.997

Table 2: Binding constants (Kb) and number of binding sites (n) of the CT- DNA-complex Cu(II) system.

T(K)	Kb(L mol^{-1})	n	R^2
288	2.53×10^2	0.8834	0.9827
310	1.25×10^3	1.1313	0.997
315	1.49×10^3	1.159	0.997

$$\log\left(\frac{F_0 - F}{F}\right) = \log K_b + n\log[Q] \quad (3.3)$$

Here F and F0 are the fluorescence intensities of the fluorophore in the presence and in the absence of different concentration of [Q], respectively. (Table 2) shows that the calculated value of binding constant increases with enhancing the temperature. These results show that the binding between Cu(II) complex and CT-DNA becomes stronger after enhancing the temperature, and the Cu(II) complex-CT-DNA system become more stable [35].

Thermodynamic Parameters of DNA Binding

Electrostatic interactions, hydrogen bonds, hydrophobic bond interactions, and van der Waals forces are noncovalent interaction forces involved in the binding of drug molecules to biomolecules [36]. The model of interaction between drug and biomolecules can be inferred using from thermodynamic parameters values (enthalpy change ΔH and entropy change ΔS). When ΔH<0 and ΔS<0 refers to van der Waals forces and the hydrogen bonds, ΔH>0 and ΔS>0 indicates a hydrophobic interaction, ΔH≈0 and ΔS>0 is a dominant electrostatic force. In this section, the values of enthalpy change (ΔH) and entropy change (ΔS) were determined using the van't Hoff equations (Eq. 3.4):

$$\Delta G = -RT\ln K_b \quad (3.4)$$

The free energy change (ΔG) was calculated using the following equation (Eq.3.5) [37]

$$\Delta G = \Delta H - T\Delta S \quad (3.5)$$

(Table 3) shows the values of ΔS, ΔH and ΔG. In this experiment, hydrophobic interaction play main roles in the binding of Cu(II) complex to CT-DNA due to the ΔH>0 and ΔS>0 and the interaction process is spontaneous due to ΔG<0.

Table 3: Thermodynamics parameters of the interaction between the complex Cu(II) to DNA.

T(K)	ΔG(kJ mol^{-1})	ΔH(kJ mol^{-1})	ΔS(J mol^{-1} K^{-1})
288	-13.25	50.94	223
310	-18.39		
315	-19.14		

Competitive Binding Studies With Methylene Blue (MB)

Methylene blue is a well-known intercalator and is often used as a spectra probe to investigate the binding mode of metal complexes to DNA. After binding to CT-DNA, the fluorescence emission spectra of MB decreases due to intercalation [38]. When the Cu(II) complex is added, if it intercalates into the helix of CT-DNA, in which case it compete with methylene blue for the intercalation sites in DNA, and caused the fluorescence intensity of the CT-DNA-MB system to increases significantly. (Figure 5) shows that by increasing the concentration of the Cu(II) complex, there is no change in the fluorescence intensity of the MB-CT-DNA system. Therefore, these results indicate that after adding the complex, the MB molecules do not released from the DNA helix, indicating a non-intercalative mode of binding (Figure 6) [38].

Molecular Docking

Based on the competitive fluorescence studies, the Cu(II) complex is able to release the Hoechst molecules from DNA minor groove at A-T rich region. To confirm the experimental results, molecular docking simulation was performed with DNA dodecamer model (PDB ID: 1BNA). From the docking analysis, the best conformer with the lowest binding energy was picked from the 19 unique conformations among 500 runs (Figure 1). The selected docking pose showed that the Cu(II) complex can bind to DNA model with high affinity (-7.3 kcal/mol, Table 4). From (Figure 5), it is clear that the Cu(II) complex was located in DNA minor groove. Dock results also show the presence of hydrophobic forces in the interaction (Figure 5). Also two hydrogen bonds were formed between the Cu(II) complex with dG4 and dG22 at distances 3.12 and 3.15 Å, respectively.

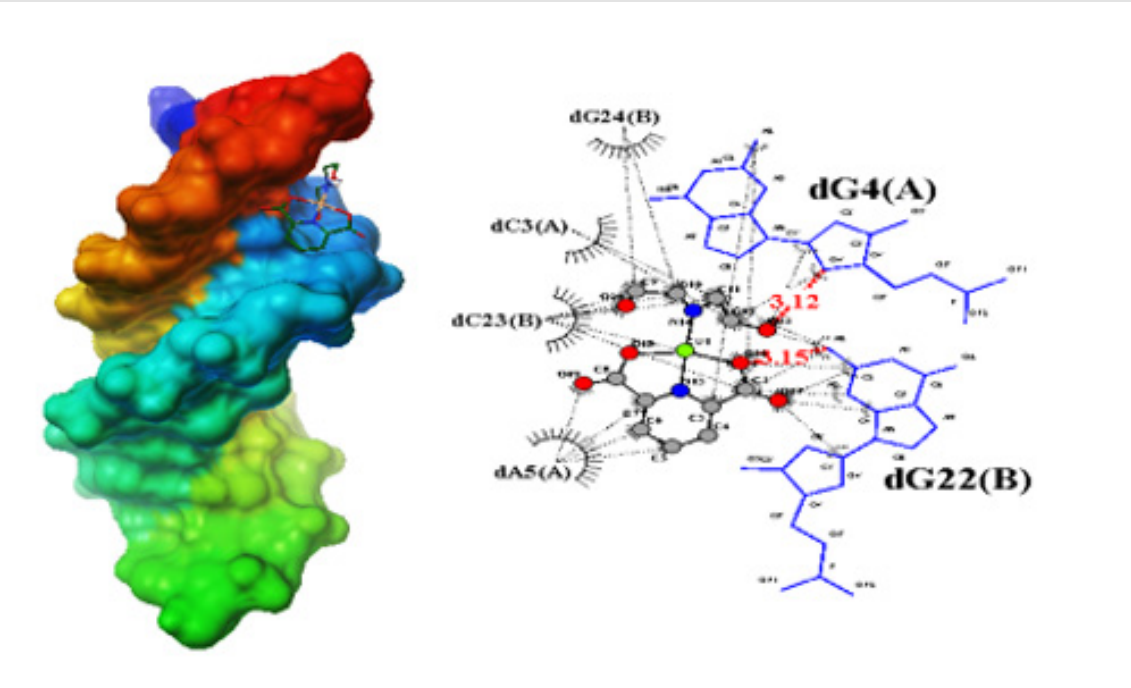

Figure 5: Molecular modeling of the interaction between the Cu(II) complex and DNA dodecamer (left), the involvement of hydrophobic and hydrogen bonds in the interaction of the Cu(II) complex with DNA model.

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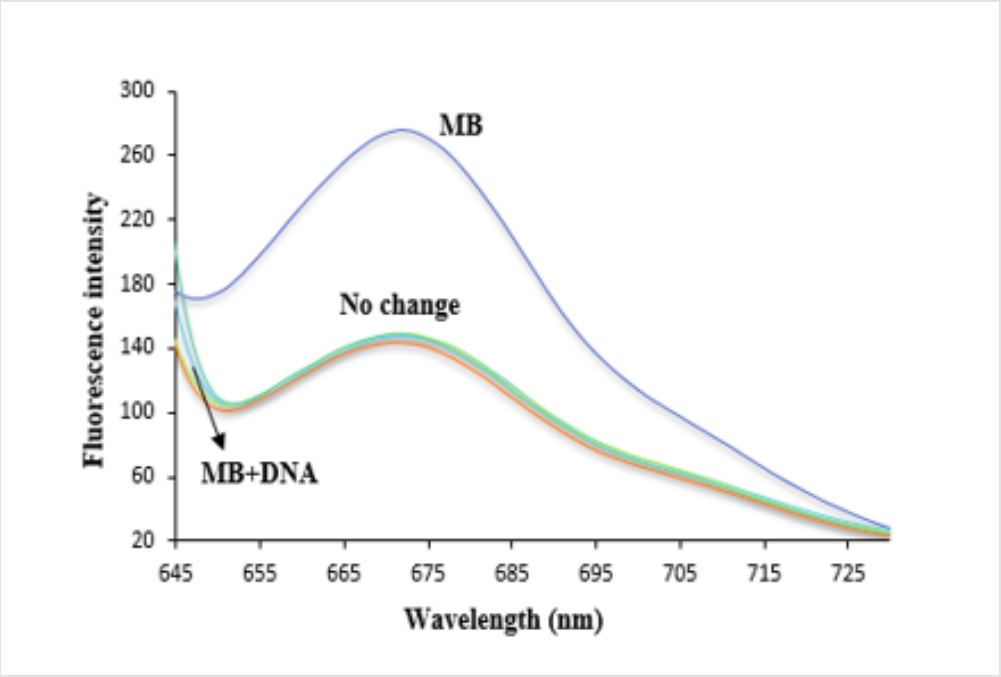

Figure 6: Fluorescence spectra of the competition between the Cu(II) complex and MB-CT-DNA, MB= 5×10^{-5} M, DNA=1.6×10^{-3} M, complex= 0 to 2.68 $\times10^{-4}$ M,T=310 K, pH=7.4.

Table 4: Docking results of DNA and the Cu(II) complex by using the AutoDock vina program generated different ligand conformers using Lamarkian Genetic Algorithm.

Mode	Binding Affinity (kcal/mol)	Dist. From Rmsd 1.b.	Best Mode Rmsd u.b.
1	-7.3	0	0
2	-7.1	0.503	3.914
3	-7.1	3.171	6.12
4	-6.9	3.951	5.982
5	-6.9	2.752	5.463
6	-6.6	1.579	5.164
7	-6.6	2.014	2.282
8	-6.6	12.174	13.742
9	-6.4	13.063	14.425
10	-6.4	26.601	28.184
11	-6.4	11.545	13.127
12	-6.4	28.32	29.741
13	-6.4	26.699	28.292
14	-6.3	2.599	3.679
15	-6.3	2.142	4.122
16	-6.2	13.889	15.654
17	-6.1	3.002	4.904
18	-6.1	13.091	14.414
19	-6.1	13.803	15.457

Conclusion

In this experiment, we investigated binding of CT-DNA with an Cu(II) complex containing diethanolamine and dipicolinic acid ligands using multi-spectroscopic methods and molecular docking. Experimental results showed that the interaction mode between the Cu(II) complex and CT-DNA is the groove binding mode. Therefore, the mean binding constant (K_b = 1.5×10^3) is similar to the groove binding. The reduction in CT-DNA-Hoechst fluorescence band due to the addition of the Cu(II) complex indicates the groove binding mode with CT-DNA. However, due to the addition of the Cu(II) complex, there is no change in the fluorescence intensity of the methylene blue (MB) molecule. Hydrophobic forces play major role in the interaction of the Cu(II) complex- DNA due to the positive values of ΔH and ΔS as well as the spontaneous reaction process due to the negative values of ΔG. Therefore, useful information on the binding mechanism to DNA is obtained through the binding mode of Cu(II) complex with DNA that has been studied in this article and has many applications in the design of anticancer drugs.

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