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Simulation of Interaction Energy and Thermodynamic Investigations of Hemoglobin Docking with Nanomaterial in Heroin Addiction Case

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Abstract
The study analyzed the thermodynamic parameters of Gibbs free energy, enthalpy, and entropy using the B3LYP function with basis set 6 – 311G(d,p) and density functional theory in the Gaussian 16 software program. The results showed that the Gibbs free energy of oxygen is spontaneous, which facilitating the docking process with deoxyhemoglobin. The change in Gibbs free energy of oxyhemoglobin is (0.566 eV) and this value is used as a standard to compare all other results. The Gibbs free energy of deoxyhemoglobin is greater than both Gibbs energies of the heroin and nano cinnamon, and all entropy values are positive, indicating that all compounds release heat. The total energy is more stable than the total amount of oxygen, and the binding energy is unstable for all substances. The study also found that heroin and nano cinnamon do not directly affect deoxyhemoglobin, but rather affect it gradually due to non-spontaneous reactions. Nano cinnamon works well as a treatment to get rid of the negative effects of heroin on the body.

Keyword: Heroin • docking • hemoglobin • nanomaterial • density functional theory.

Introduction

The human body is a complex system made up of many organs that are organized from a variety of tissues to perform specific functions. These tissues consist of a group of many identical cells. The cell is the basic form of living matter capable of sustaining life. The human body contains many different types of cells, the most important of which are blood cells, which are divided into three basic categories: white blood cells, red blood cells, and platelets [1, 2].

Red blood cells (RBC) react to foreign bodies and intruding elements because they are very sensitive and have powerful defense systems. Stress-induced RBC death differs from unintentional hemolysis or typical cellular senescence, and it works by removing damaged RBCs and causing the subsequent release of hemoglobin into the bloodstream. There are many pressures that may cause erythrocytosis, which leads to a change in its function, which is characterized by cell shrinkage and bleeding from the cell membrane [3, 4].

It can be started by looking at the idea of hemoglobin. Hemoglobin (HB) is a transport protein for many substances in human blood, the most important of which is oxygen transport, which plays an important role in maintaining aerobic metabolism by transporting it from respiratory exchange surfaces (such as lungs, gills, or skin) [5].

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Hemoglobin consists of four chains of amino acids (the basic structure of peptide proteins). A heme fragment consisting of an organic protoporphyrin ring and a central iron ion in the ferrous state (Fe^{+2}) is present in each globin subunit. Each piece of heme contains an iron molecule (Fe^{+2}), which carries oxygen. Iron becomes "ferrous" (Fe^{+3}) during the oxidation of hemoglobin to form methemoglobin (MetHB), which is unable to interact with oxygen throughout the body [6].

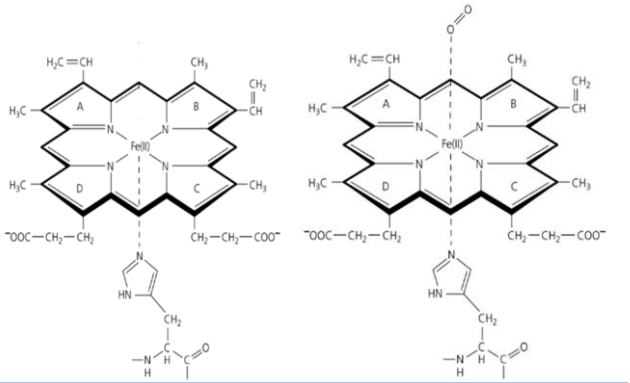

Figure 1. The structure of hemoglobin without oxygen and the represents the structure of hemoglobin with oxygen [6].

Heroin, a potent opioid derived from morphine is a highly addictive drug with severe health risks and consequences [7]. Upon entering the brain, heroin is metabolized back into morphine, binding to opioid receptors and inducing euphoria and pain relief. Chronic heroin use can lead to physical and psychological dependence, intense cravings, and withdrawal symptoms upon cessation [8]. Overdosing on heroin is a grave concern due to its ability to depress the central nervous system and suppress breathing, potentially resulting in coma, brain damage, or death. Intravenous heroin use poses additional health risks like infections, heart problems, and collapsed veins [9]. **Figure 2** illustrates the chemical structure of heroin [10].

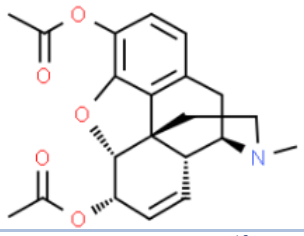

Figure 2. Chemical structure of Heroin [10].

As seen in **Figure 3**, nano cinnamon [11] is made from the inner bark of cinnamomum genus trees [12]. Cinnamaldehyde, a compound with the molecular formula C_9H_8O, is a key component in the distinct aroma and scent of nano cinnamon. More research is required to have a complete understanding; however, research indicates that nano cinnamon may help lower heroin addiction levels and boost dopamine sensitivity. cinnamaldehyde, coumarin, and cinnamomic acid are some of the chemical components that make up nano cinnamon [13]. The distinct aroma and scent of nano cinnamon are primarily due to cinnamon aldehyde. The anti-inflammatory characteristics and high antioxidant content of nano cinnamon may also play a role in its potential advantages for heroin addiction management. Nonetheless, the particular variety of cinnamon and the portion of the plant that is utilized can affect the chemical makeup of nano cinnamon as a whole. To properly comprehend how nano cinnamon affects heroin addiction management and its possible medical uses, more research is required [14].

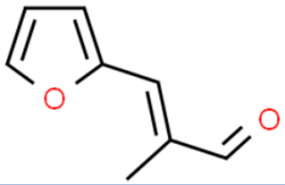

Figure 3. Chemical structure of nano cinnamon (C_9H_8O) [11].

Many studies have addressed the content of the axes of the current research path, as researcher XL Zeng and others studied the density functional theory studies on the molecular structures and thermodynamic properties of polychlorinated anthracenes[15], AL Bédé *et. al.* addressed the topic, theoretical study by density functional theory method of the thermodynamic properties of specific compounds[16], also E Boz and M. Stein was discussed computational approaches to calculate Gibbs free energies of binding, emphasizing the use of density functional theory and molecular dynamics simulations to predict ligand-receptor interactions accurately[17], M. Bursch *et. al.*, were introduced a work offers guidance on methodological and technical aspects of DFT calculations, including the selection of functionals and basis sets, to accurately compute thermodynamic properties [18]

The current study is a simulation based on the treatment of solid state, quantum mechanics, thermodynamics and aims to simulate how hemoglobin docking with the drug (nano cinnamon) as, which is used to treat heroin addiction and the simulate the effect of heroin as well as nano cinnamon on hemoglobin, applying computational methods that include the density functional theory at a level B3LYP with basis set 6-311G(d,p) to calculate the thermodynamic properties of the studied molecule using the Gaussian 16 and Gauss view 6.0.16 programs [19].

Theoretical Considerations

One of the most important aims of simulation physics is to depict the physical properties of interacting many-particle systems[20]. This can be done by deriving the properties of many-particle systems from the quantum mechanical laws[21]. Computational Chemistry methods: Various paradigms employ several approximations to output outcome of different levels of precision [22]. Yuliya Luzinova mention in his thesis at 2010, "there is a tradeoff between accuracy and computational time. There are two main kinds of models depending on the starting point of the theory: Classical methods are used Newton mechanics to model molecular systems [23] and quantum chemistry methods, which makes use of quantum mechanics to model the system. These methods use different kind of approximation to solve the Schrödinger equation [24, 25]. Computational researchers can used different applications, which can be classified by four broad methods [26]: molecular mechanics (MM), Semiempirical (SE) methods, *ab initio* methods, and (DFT) methods. The major focus is on density functional theory method to solve the Schrödinger equation [27].

The total energy of a molecular of the system was defined as the sum of the total electronic energy and the energy of inter nuclear repulsion. The geometry optimization is the operation through which the equilibrium positions of atomic nuclei are specified, within a given symmetry restriction. In most of the status, the geometry optimization is necessary since the accurate position of the atoms, which enter parametrically the electronic Hamilitonian are not recognize exactly. Thus, geometry optimizations, which include the calculation of forces in addition to the calculation of energies, are a main ingredient of most of the computation [28]**.** Density functional theory partition the total energy as [29]:

$$E = E_T + E_v + E_J + E_{XC} \quad \text{... (1)}$$

E_T: Electronic kinetic energy, E_v : Electronuclear interaction energy, E_J : Electron-electron repulsion energy, E_{XC} : exchange correlation term.

The binding energy defined as the amount of energy, which wanted pulling the system apart into a set of free atoms. The computation of the binding energy requires a value of the total energy for the solid and for the free atoms [30]. The electronic structure yields the energy of the system. Binding energy (E_B) can be calculated for a system as [31]:

$$E_B = [(N\,E_X + M\,E_Y) - E_{XY}]/(N + M) \quad \text{... (2)}$$

Where, E_{XY} stands for the total energy considered for XY docking atoms, E_X, E_Y energy of X and Y atoms respectively. N and M are the number of X and Y atoms present in the system structure respectively.

Generally, solids are stable structures; interactions hold atoms in a crystal together. The energy of the crystal is less than the energy of free atoms. Binding energy is highly significant characteristic because it conserves survival of arrangement and that considered for the bound strength of

solids. It is also basic quantity for the thermodynamics of materials [32].

Thermodynamic properties includes enthalpy, entropy, and Gibbs free energy serve as symbols for the components of thermodynamics in the equation below [33]:

$$\Delta G = \Delta H - \Delta ST \quad \ldots (3)$$

The rate at which the medication deoxyhemoglobin reacts with the drug can be found using the following equation [34]:

$$\frac{\partial[\text{Docking}]}{\text{dt}} = -\text{C}[\text{DHB}][\text{drug}]\text{K}(\text{T}) \quad \ldots (4)$$

Regarding response, hemoglobin interacts with the medication. The following provides the reaction rate [35]:

$$\text{K}(\text{T}) = \frac{\text{K}_\text{B}\text{T}}{\text{hc}} \text{e}^{-\frac{\Delta G}{\text{K}_\text{B}\text{T}}} \quad \ldots (5)$$

Where: K(T)) is the reaction rate constant, T is the room temperature, K_B is Boltzmann constant, c is the concentration, h is planks constant, ΔG is Gibbs free energy, ΔH is Enthalpy energy, ΔS is entropy energy, C[DHB][drug] is an experimental structure constant for the reactants.

Computational and Methodology

Gaussian utilizes a keyword system, keywords are brief and typically hidden instructions to the software that depict what the user wishes to do, the program user needs to know the program's keywords to implement the calculation with more exact, therefore the using of this program is not simple. Most of the keywords that needed in this work programmed into the different input windows as pull-down menus [36].

There are two types of quantum calculations (job type) that is carried out through the study. The first type is the "geometry optimization (OPT) calculations, with the minimum energy obtained for a given geometry. The second type of the calculations used in the study is Vibrational Frequencies (FREQ).

All the computations have performed using DFT implemented in the Gaussian 09.5 package running and visualized by Gauss View 6.0.16 program. The calculated properties of materials under study have computed by DFT applied the standard 6-311G (d,p) basis sets, calculations in DFT were carried out with the B3LYP hybrid functional. B3LYP (beck three-parameter hybrid functional combined with Lee-Yang-Parr correlation functional) is one of the often-employed hybrid functional used in theoretical studies of drugs as well as pathogenic materials[37].

Before it proceeds in calculations, it is necessary to find the geometry optimization of the structures for materials under study. The optimized structure for these materials has the minimum energy; which performed by finding the first derivative of the energy with respect to the distance between different atoms, known as the gradient.

Results and Discussion

The thermodynamic parameters of Gibbs free energy, enthalpy, and entropy were obtained through simulation utilizing the B3LYP function, DFT theory, and the chosen bassist 6-311G(d,p) in the Gaussian 16 software.

Figure 4 demonstrates the simulated optimization of the materials (O_2, DHB, nanocinnamon, and heroin) before the docking process. **Figure 5a-5c** demonstrates the stabilization of their charges, which enabled the weak Vander Waals bond to dock with DHB. This connection allows us to understand how these medications affect the blood and whether they are beneficial or harmful.

Subsequently, as illustrated in **Figure 5d**, another docking procedure was performed to ascertain the impact of nanocinnamon docking with heroin and whether or not it is useful in treating heroin usage. OHB is used to compare each of these compounds.

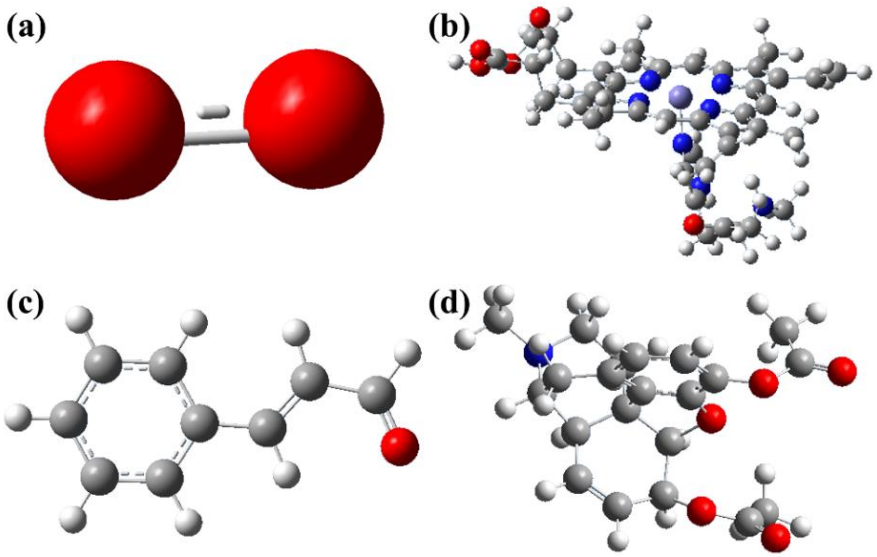

Figure 4. The simulated optimization chemical structures of (a) the oxygen molecule, (b) the DHB molecule, (c) the nanocinnamon molecule, and (d) the heroin molecule.

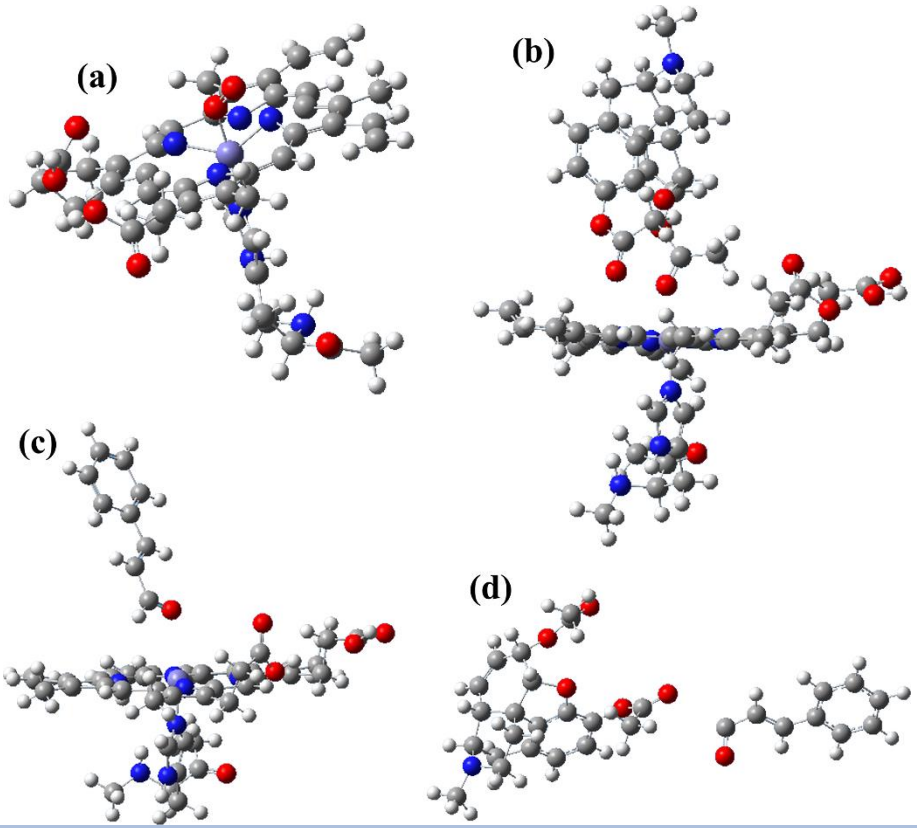

Figure 5. The stabilization chemical structures of (a) the OHB molecule., (b) docking of DHB with heroin, (c) docking of DHB with nanocinnamon, and (d) docking of heroin with nanocinnamon.

The reactants' enthalpy, entropy, and Gibbs free energy are displayed in **Table 1** before the docking procedure. This table shows that the oxygen Gibbs free energy has a favorable index and a spontaneous reaction, which help in the docking process with DHB, and that is agreement with reference [38]. Furthermore, it can be observed that DHB's Gibbs free energy is larger than the sum of its two Gibbs energies, which compatible with [39]. Additionally, it can be seen that all of the entropy numbers are positive and that all of the enthalpy values are positive, indicating that all of these compounds release heat [40]. Thus, from the study, it can be concluded that the products' energy is higher than the reactants' energy. it can be also observed that the total energy is more stable than the total amount of oxygen. For all materials, the binding energy is unstable.

Table 1. Comparison of binding energies of materials before docking under standard conditions with Gibbs energy and its components (enthalpy and entropy).

Energies (eV)	Oxygen	DHB	Heroin	Nanocinnamon
G	-0.414	19.525	9.701	2.947
H	0.190	23.485	11.8895	4.148
ST	0.602	3.945	2.188	1.201
E_T	-150.302	-3651.661	-1244.550	-423.115
E_B	4.572	106.239	158.786	6.068

The DHB docking process with oxygen, heroin, and nanocinnamon is displayed in **Tables 2**. It also docks heroin and nanocinnamon together. From this table, it can be seen that the Gibbs free energy for heroin docking with DHB is higher than the Gibbs free energy for nanocinnamon docking. The Gibbs free energy for the heroin docking mechanism is (30.248 eV), while for the oxygen docking mechanism, it is (22.965 eV). These energies are not spontaneous; rather, they are all weakly coupled.

Table 2. The Gibbs energy and its components (enthalpy and entropy) are compared with the binding, interaction, and adsorption energies of substances that dock with DHB under normal conditions.

Energies (eV)	Docking heroin with DHB	Docking nanocinnamon with DHB	Docking heroin with nanocinnamon	Oxy HB
G	30.248	22.965	13.361	19.677
H	35.6218	26.571	15.991	23.739
ST	5.373	3.605	2.630	4.047
ΔG	1.021	0.492	-9.111	0.566
ΔH	0.246	-1.063	-11.642	0.063
ΔST	-0.774	-1.555	-2.530	-0.501
E_T	-4894.591	-4074.167	-1667.345	-3802.026
E_B	6.896	-28.231	-3667.323	-96482.933

According to research, the reaction generates heat, and the products' release is greater than the reactants' energy [41-43]. The change in the Gibbs free energy OHB is (0.566 eV), as indicated in Table 2, and this value is used as a benchmark for comparing all other results. It can be concluded that while heroin and nanocinnamon do not directly influence DHB, heroin gradually affects DHB significantly, which is consistent with previous works [44, 45]. This is because the docking of heroin and nanocinnamon with DHB demonstrates non-spontaneous interactions. Additionally, it can be seen that the Gibbs free energy has reached (-9.111 eV) with a very strong connection and spontaneous response during the heroin and nanocinnamon docking process. This

suggests that nanocinnamon works well as a remedy to get rid of heroin's negative effects on the body. Additionally, it demonstrated that the total energy is more stable during the heroin docking process with nanocinnamon. It can be also observed that all binding energies are stable the only exception being the unstable heroin docking process with DHB and that all energies between the adsorption energies are stable, heat-emitting, and more stable during the heroin docking process with nano cinnamon [46].

Conclusions

The study examines the interaction between DHB, oxygen, heroin, and nanocinnamon. The oxygen Gibbs free energy has a favorable index and spontaneous reaction, facilitating the docking process. DHB's Gibbs free energy is larger than its two Gibbs energies, and all entropy numbers are positive, indicating that all compounds release heat. The total energy is more stable than the total amount of oxygen. The heroin docking with DHB is higher than the nanocinnamon docking, indicating a weakly coupled reaction. The study concludes that heroin gradually affects DHB significantly due to non-spontaneous interactions. Nanocinnamon works well as a remedy to eliminate heroin's negative effects on the body. All binding energies are stable, except for the unstable heroin docking process with DHB.

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Declaration of Competing Interests

The authors affirm that the publication of this paper is not impacted by any conflicts of interest.

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