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Research Article

Computational Quantum Mechanical Investigation and Targeted of the Boron Nitride Nanotubes as a Nanocarrier for Nortriptyline Drug Delivery: a DFT Analysis

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A B S T R A C T

In this research, structural investigation and targeted drug delivery of nortriptyline by boron nitride nanotubes using quantum mechanical calculations were studied. The transfer of the targeted drug to the targeted organ is done using a series of quantum mechanics calculations, and this method is one of the most useful and important new drug delivery methods in the pharmaceutical and nanotechnology industries. The initial structures were optimized at the 6-31g (d,p) level of theory in Gaussian 09 software and the density functional theory (DFT) method to investigate the structure of nortriptyline. Moreover, the desired structure and its connection with boron nitride nanotubes with zigzag and armchair structures with the scales (8,0), (6,6), (5,5), and (5,0) for the targeted connection of the drug to the nervous systems and brain neurons were investigated. Based on the simulation findings, the results demonstrate that boron nitride nanotubes can interact with nortriptyline and the estimated recovery times vary considerably among the investigated structures, suggesting that drug-release behavior should be considered alongside adsorption strength. Therefore, boron nitride nanotubes may be regarded as potential candidates as nortriptyline and other drugs nanocarriers.

K E Y W O R D S

Nortriptyline drug, Boron nitride nanotubes, Density functional theory (DFT), Drug delivery, Quantum mechanics.

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Introduction

Nortriptyline is a tricyclic substituted by a 3-(methylamino) propylidene group at position 5 with a chemical formula $C_{19}H_{21}N$ (Fig. 1) which widely treats depression, nerve-related disorders, and nerve pains. Depression and bedwetting in children (nocturnal enuresis) are occasionally treated by Nortriptyline. Moreover, it treats for smoking cessation after varenicline and bupropion as a third option [1–3]. Furthermore, bipolar disorders and other conditions such as pain and tingling in the hands and feet, chronic pain and insomnia, and pain caused by MS [3], are treated by Tricyclic Antidepressants (TCAs).

Nortriptyline, an antidepressant, is used not only for treating depression but also for conditions like bipolar disorder, chronic pain, and insomnia. Research suggests that, in addition to its antidepressant effects, nortriptyline may slow down the progression of Parkinson's disease by inhibiting the formation of a specific brain protein linked to the condition. According to the researchers, depression and its disorders are common in Parkinson's patients for this reason, studies have proven that antidepressant medicines prevent the development of this disease and slow down its progress to some extent [4, 5]. One of the main causes of depression is the decrease in the level of activity of chemical carriers of nerve messages in the brain, which is the exact target of the drug nortriptyline. So, by increasing the effectiveness of the nortriptyline with the help of nanotubes, especially boron nitride nanotubes, with this plan to connect to chemical carriers in a targeted way and by increasing the excitement of nerve messengers in the brain, it creates mental energy and motivation [6, 7].

Recently, density functional theory (DFT) is a quantum-mechanical atomistic simulation method to compute a wide variety of properties of almost any kind of atomic system: molecules, crystals, and surfaces, the field of medicine has benefited a lot from this technology, and one of its popular examples is the introduction of various types of nanoparticles as drug delivery systems and drug release systems in general. In this study, we use modern drug delivery, one of the most suitable methods in the field of targeted drug delivery to the desired organ and molecule, and nanotubes and quantum mechanical calculations to investigate this process of targeted drug delivery [8]. By precisely delivering medication to specific targets at predetermined times, this new system offers superior efficacy and safety compared to traditional, systemic drug administration [9].

Nanocarriers have been extensively studied over the past decades and are designed to improve clinical efficiency while reducing the toxicity associated with traditional intravenous administration methods. Moreover, they have shown promising results in drug delivery [10]. Nanotube-based drug delivery systems have received considerable attention due to their salient features, such as their high surface area-to-volume ratio for encapsulating different drugs and their ability to penetrate cells, tissues, and bacteria due to their open ends. Therefore, it is important to understand drug-nanotube interactions to evaluate drug encapsulation behavior in nanotubes [11]. Drug encapsulation inside the nanostructure is challenging because not only does it need to carry the drug without any chemical modification, but it is also necessary for releasing the drug near the cancer cells [12]. Various nanocarriers have been approached for targeted delivery with promising results over the past few decades, including polymeric nanoparticles, mesoporous silica nanoparticles, iron oxide nanoparticles, gold

nanoparticles, copper oxide nanoparticles, and carbon nanotubes [13- 20].

Over the past few decades, there has been a burgeoning interest in boron, its compounds, and boron-based materials within the scientific and technological communities. This heightened attention stems from their exceptional potential applications across a wide spectrum of fields, spanning from materials science to biomedical research, owing to their remarkable characteristics. These extraordinary properties make including biotechnology, medicine (drug delivery systems and technologies, bio imaging systems, and radiation therapy), radiation-shielding materials, capping agents, and mechanical strength, among others. It will offer insights into the medical, applications of boron-containing materials, such boron nitride nanotubes as a nanocarriers. Notably, to the best of our knowledge, there were no reported targeted drug delivery of nortriptyline by boron nitride nanotubes using quantum mechanics calculations and DFT calculations.

The boron nitride nanotubes (BNNTs) were first discovered in 1995 [21], they are similar in structure to the CNTs. Compared with CNTs, BNNTs are constructed by boron and nitrogen atoms. The ionic characteristic of bonds between B and N atoms makes them especially chemically stable and resistant to oxidation [22, 23]. Boron-nitride nanotubes (BNNTs) offer a promising alternative to carbon nanotubes for drug delivery applications due to their superior biocompatibility. Unlike carbon nanotubes, theoretical studies indicate that BNNTs possess a wide bandgap of about 5.5 eV, rendering them electrically insulating [24-26]. Moreover, rather than the nonionic and hydrophobic characteristics of CNTs, BNNTs are easy to functionalize with molecules to improve their dispersion and solubility in water due to the ionic characteristics of B-N bonds [27, 28]. This property contributes to their reduced toxicity profile. Given the established role of nanocarriers in enhancing drug delivery outcomes, BNNTs emerge as a potential platform for improving therapeutic efficacy and reducing adverse effects.

This study employed quantum mechanical calculations to explore the structural properties of nortriptyline and its potential delivery using boron nitride nanotubes (BNNTs) as a targeted carrier. Furthermore, with an increase in the nanotube radius, the drug adsorption energy also increases. This increase is attributed to the fact that nanotubes with larger radii provide a larger surface area for interaction with drugs. The cohesive energy results indicated that the absorbed structures are stable; their findings indicated that the BN nanotubes could serve as a suitable biomedical carrier for delivering the drugs.

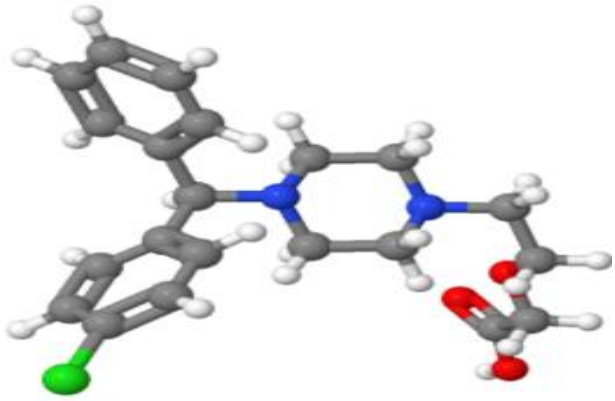

Figure 1. The chemical structure of Nortriptyline drug.

2. Theoretical section

2.1. Computational details

Recently, theoretical methods based on density functional theory (DFT) have emerged as an alternative to traditional ab initio methods for the study structure and reaction of chemical systems [29]. In this work, all calculations, including geometric optimization, energy, and charge transfer, were performed in the framework of density functional theory (DFT) at the 6-31g (d,p) / M062X level using Gaussian 09 [30, 31].

M062X is a function that incorporates the van der Waals scattering effects, which are very important in the physical adsorption of drugs on nanotubes. In other words, two types of interactions are involved in the drug absorption process on the nanocarrier. It should be noted that the adsorption energies reported in this study were calculated without applying the counterpoise correction for basis set superposition error (BSSE). Although the counterpoise method can improve the accuracy of calculated interaction energies, its application to the relatively large drug–nanotube complexes investigated in this work would require substantial additional computational resources and time. Therefore, this correction was not performed within the scope of the present study. Accordingly, the reported adsorption energies should be interpreted as uncorrected theoretical values, and the resulting trends in adsorption strength should be considered with this methodological limitation in mind.

2.2. Quantum mechanics (QM) calculation method

Electrical interactions are investigated by the quantum mechanics method. Quantum mechanics relies on the Schrodinger equation to describe the molecule by considering the explicit behavior of its electronic structure [32].

In this research, we first draw the desired structures using Avogadro software, then, with specialized chemistry software such as Gaussian 09 software and a series of quantum mechanics calculations and DFT calculations by high-speed computers, we investigate the structure of the drug and its targeted delivery. In general, in this method, the chemical model is built first and is examined from all structural aspects. Using the mentioned software, we examine the built model and how to deliver it using a series of quantum mechanics calculations. Finally, these necessary quantities are extracted from the Gaussian output, arranged in tables and graphs, and then used to interpret and compare the results of the desired nanotubes-drug complex [33, 34].

3. Results and discussion

3.1. The van der Waals energy

By considering the M062X function, the contribution of van der Waals effects is practically included in the calculations. First, zigzag and armature boron nitride nanotubes with chiral indices (6,6) (5,0) (5,5) (6,0) (8,0) and a length of 10 angstroms were made using (vdW) software. The structure of the drug was designed by Gauss View software (Gauss View 6.0). Before carrying out the absorption process, the optimization of the drug and the carriers was done separately to reach the lowest energy and the most stable configuration. Drugs and optimized nanotubes with the same orientation are combined using Gauss View software, and after the optimization of the drug, the carrier complex is done [31, 35].

3.2. Investigation of absorption energy

The adsorption energy of a system for a drug shows its adsorption power, which has a direct relationship with the size of the structure of the adsorbent and the drug. Here, the absorption energy of the nortriptyline drug is given in (Table 1).

$$E_{ad} = E_{complex} - (E_{BN} + E_{drug}) \quad (1)$$

where E_{drug}, E_{BN}, $E_{complex}$, and E_{ad} are, respectively, the absorption energy, the energy of the drug-nanotube system, the energy of the nanotube in the state without drug absorption, and the energy of the drug alone (not absorbed).

Table 1. Total energies of different drugs and nanotubes.

Structure	Total energy (eV)
Nortriptyline drug	-791.1
BN (5,0)	-2396.47
BN (5,5)	-3199.72
BN (6,0)	-2876.03
BN (6,6)	-3839.88
BN (8,0)	-3835.07

As the absorption energies show, the comparison of armchair (n, 0) and zigzag (n, n) nanotubes shows that the zigzag state has a higher absorption energy than the armchair state. In other words, the order can be written as BN (6,6) > BN (6,0) > BN (5,0). On the other hand, the absorption energy for the desired drug increases with the increase in the radius of the nanotube.

The order of absorption energy based on increasing radius for two armchair and zigzag states can be written separately as follows:

For armchair mode: BN (8,0) > BN (6,0) > BN (5,0)

For zigzag mode: BN (5,5) > BN (6,6)

As it is known, for zigzag structures, unlike armchair structures, the absorption energy of the smaller nanotube, BN (5,5), is greater than BN (6,6) for the drug in question, and this is an exception, as shown in (Table. 2).

Table 2. Absorption energies of nortriptyline on different boron nitride nanotubes.

Nanotubes	Nortriptyline drug absorption energy (eV)
BN (5,0)	-0.653
BN (5,5)	-1.589
BN (6,0)	-1.197
BN (6,6)	-1.306
BN (8,0)	-1.279

For a better understanding of the effect of increasing the radius on absorption energy, see BN (8,0), BN (6,6), and BN (6,0) as examples of radius change and absorption energy. One of them is an armchair and the other one is a zigzag. The figure below shows the comparison of the radii of these three nanotubes. As we can see, BN (8,0) has a radius between BN (6,0) and BN (6,6), which is the same as the energy order of the corresponding absorptions. In other words, the size of the radius of the nanotube is more effective than its chirality in terms of absorption power. It can be concluded that, firstly, as the radius of the nanotube increases, the absorption is better regardless of whether it is armchair or zigzag. Secondly, it seems that by increasing the size of the nanotube, more drug molecules can be absorbed on the carrier [35, 36].

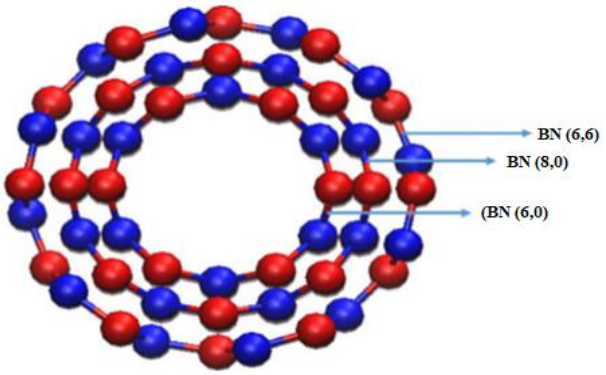

Figure 2. Comparison of changes in the radius of three different types of zigzag and armchair nanotubes.

3.3. Investigation of the cohesive energy

The stability of the formed complexes is one of the parameters that must be evaluated. The cohesive energy is a measure of the stability of the studied systems. As this parameter becomes more negative, stability and complexity increase, and the more we go towards positive values, the system's stability decreases. In this research, the cohesive energy for different pharmaceutical systems was calculated using the following equation:

$$E_{cohesive}=\frac{E_{Complex}-(nE_B+mE_N+lE_H+iE_C)}{n+m+l+i} \quad (2)$$

where E_C, E_H, E_N, E_B, and E_{comlex} are the total energy of the absorbed system, the energy of a single boron atom, the energy of a single nitrogen atom, the energy of a single hydrogen atom, and the energy of a single carbon atom, respectively. The values of m, n, and i show the number of atoms of each species in the system. The calculated values of cohesive energies are listed in (Table. 3) [34-36].

Table 3. Cohesive energies of the investigated boron nitride nanotubes.

Nanotubes	Cohesive energy (eV)
BN (5,0)	-10.518
BN (5,5)	-10.471
BN (6,0)	-10.803
BN (6,6)	-10.586
BN (8,0)	-10.991

All adsorbent systems demonstrated stability and potential as suitable carriers. However, while stability is crucial, the adsorption energy must also exhibit a favorable negative value for optimal performance.

3.4. Investigation of Charge Transfer

Charge transfer plays an important role in the interaction between an adsorbate and an adsorbent and contributes to the electrostatic component of their interaction. In this study, the charge redistribution associated with the adsorption of nortriptyline on boron nitride nanotubes (BNNTs) was investigated by comparing the net charge of the drug in its isolated state with that in the adsorbed configurations.

Table 4. Atomic charges of nortriptyline in the isolated state.

Atom	No	Charge
C	1	-0.05678
C	2	-0.02486
C	3	-0.05095
C	4	-0.48484
C	5	-0.02162
C	6	-0.49208
H	7	0.26241
H	8	0.26021
H	9	0.25778
H	10	0.26115
C	11	-0.25332
C	12	-0.23041
C	13	-0.24019
C	14	-0.24595

H	15	0.25216
H	16	0.25492
H	17	0.24760
H	18	0.25187
C	19	-0.22475
C	20	-0.25121
C	21	-0.24438
C	22	-0.23492
H	23	0.25146
H	24	0.25136
H	25	0.25076
H	26	0.24412
C	27	-0.04603
C	28	-0.18958
H	29	0.24367
C	30	-0.52742
H	31	0.26149
H	32	0.25292
C	33	-0.26421
H	34	0.20786
H	35	0.24043
N	36	-0.73738
H	37	0.40144
C	38	-0.50149
H	39	0.23894
H	40	0.23089
H	41	0.20801
Total	*	0.00000

As presented in Table 4, the total net charge of the isolated nortriptyline molecule is zero. The net charges of nortriptyline after adsorption on the different BNNT structures are presented in Table 5.

Table. 5 shows the total load of the desired drug in the state after absorption in different nanotubes. These amounts indicate the charge transfer from the drug to the nanotubes. In other words, in the process of drug absorption and on nanotubes, the drug acts as an electron donor and the nanotube acts as an electron acceptor.

Table 5. Net charges of nortriptyline after adsorption on different boron nitride nanotubes.

Nanotubes	Net charge on nortriptyline (|e|)
BN (5,0)	0.042
BN (5,5)	0.123
BN (6,0)	0.026
BN (6,6)	0.025
BN (8,0)	0.014

The positive net charges obtained for nortriptyline after adsorption indicate that electron density is transferred from the drug molecule to the BNNT surface. Therefore, nortriptyline acts as an electron donor, whereas the BNNTs act as electron acceptors. The calculated net charge transfer values are 0.042, 0.123, 0.026, 0.025, and 0.014 |e| for BN (5,0), BN (5,5), BN (6,0), BN (6,6), and BN (8,0), respectively. Among the investigated systems,

BN (5,5) exhibits the largest net charge transfer, whereas BN (8,0) shows the smallest value. The calculated net charge transfer values are 0.042, 0.123, 0.026, 0.025, and 0.014 |e| for BN (5,0), BN (5,5), BN (6,0), BN (6,6), and BN (8,0), respectively. Among the investigated systems, BN (5,5) exhibits the largest net charge transfer, whereas BN (8,0) shows the smallest value.

It should be noted that the reported values represent the net charge redistribution upon adsorption and describe the overall direction and magnitude of electron transfer between the drug and the nanotube. These values do not, by themselves, identify individual orbital-to-orbital donor-acceptor interactions or their corresponding stabilization energies. Nevertheless, the observed charge redistribution indicates an electronic contribution to the interaction between nortriptyline and BNNTs. The adsorption of nortriptyline on BNNTs also affects the distribution of partial atomic charges within the drug molecule compared with its isolated state. Owing to the large number of atoms in the drug molecule, the charge distribution is schematically illustrated for one of the investigated configurations before and after adsorption (Fig. 3). According to the color scale, the transition from red to green represents a decrease in negative charge and a shift toward positive charge. As illustrated in Fig. 3, the charge distribution around the nitrogen and hydrogen atoms changes after adsorption, reflecting the electronic redistribution associated with the interaction between the drug molecule and the nanotube surface.

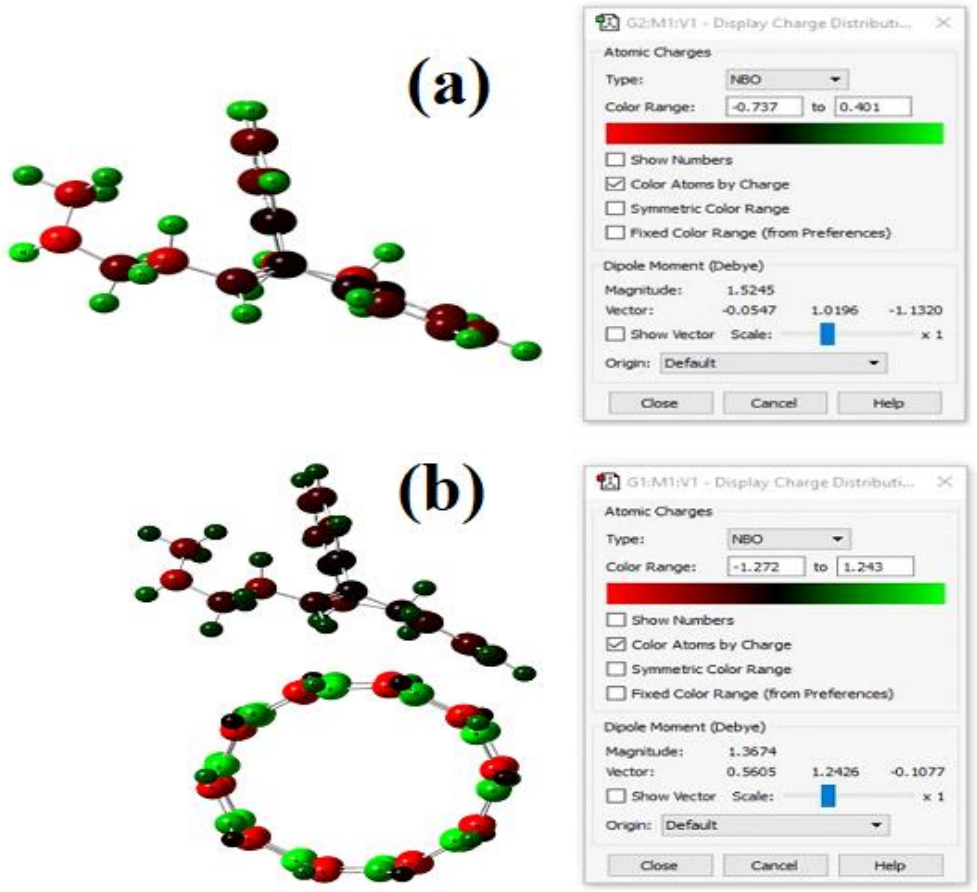

Figure 3. Charge distribution of the nortriptyline molecule in its isolated state (a) and after adsorption on a BNNT (b).

3.5. Survey of interactions between different parts of nortriptyline and BN nanotubes

In general, two types of adsorptions occur in processes where there is an adsorbent and an adsorbed component: chemical adsorption, which is caused by the formation of covalent bonds between the adsorbent and adsorbed species and is irreversible. Physical adsorption, which involves van der Waals interactions, electrostatic interactions, or a combination of both, is generally reversible. However, reversibility does not necessarily imply rapid desorption, as the rate of drug release depends on the strength of adsorption and the conditions required for desorption. Therefore, the recovery-time estimates presented in Section 3.8 provide additional information about the potential desorption behavior of nortriptyline from the investigated BNNTs. The final forms of absorption in this research show that there is no chemical bond between the absorbent and absorbed species; in other words, the absorption of the drug has a physical nature, which is vital for drug delivery systems. Because the absorbed drug must have the ability to be absorbed so that it can have the required function in the body, as can be seen in the simulation snapshots. Fig. 4, shows the final configurations after nortriptyline adsorption on the surfaces of BN nanotubes [37, 38].

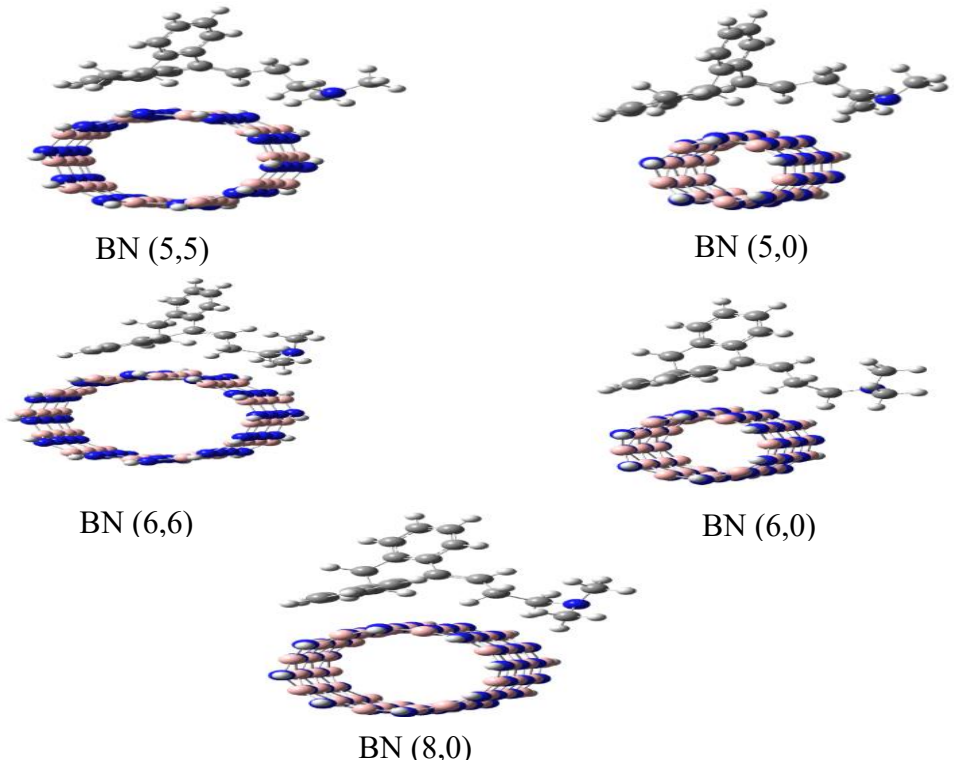

Figure 4. Schematic of the drug interaction and absorption with nanotubes in the framework of density functional (DFT) at the M062X/6-31g (d, p) level.

3.6. Bond Length Examination

The alteration in the bond length of the nearest bond to the absorbed molecule was investigated before and after absorption to evaluate structural changes. As observed, in the case of the BN (5,0) nanotube, the nearest B–N bond length remains unchanged at the reported precision after drug absorption. However, this does not indicate the absence of absorption, since a negative absorption energy of - 0.653 eV was calculated

for this system (Table 2). Rather, it indicates that the adsorption interaction is relatively weak and does not produce a measurable change in the nearest B–N bond length. For the other investigated systems, a slight increase in the nearest B–N bond length is observed after absorption, indicating minor structural changes associated with drug-nanotube interactions.

Table 6. Modifications in the nearest bond to the drug before and after absorption.

Nanotube	Before absorption (diameter (Å))	After absorption (diameter (Å))
BN (5,0)	1.439	1.439
BN (5,5)	1.450	1.453
BN (6,0)	1.441	1.443
BN (6,6)	1.439	1.443
BN (8,0)	1.448	1.452

As observed, in the case of the BN (5,0) nanotube, where no absorption was detected, no significant change in its bond was observed. On the other hand, for the other scenarios involving the target drug, after absorption, the carbon-nitrogen bond showed a minimal increase. This slight increase indicates the influence of the molecule's absorption on the nanotube and the stability of the nanotube after drug absorption.

3.7. Calculation of thermodynamic data for the nortriptyline drug

Thermodynamic quantities were achieved based on suitable functions by applying a minimum geometrical structure to the molecule. To confirm the stability of the boron nitride nanotubes (BNNTs) system, after geometry optimization of this nano-semiconductor, we performed DFT methods for energy calculations and thermodynamic data by using the 6-31g (d, p) basis set to consider the stability of the system at standard temperature (298.15 K) and pressure (1 atm.). Further, the thermodynamic parameters of the nortriptyline drug on boron nitride nanotubes, such as total energy ΔE (Kcal mol^{-1}), enthalpy ΔH (Kcal mol^{-1}), entropy ΔS (cal mol^{-1}. K^{-1}), and Gibbs free energy ΔG (Kcal mol^{-1}), have been computed after absorption using the following equations:

$$\Delta G^{\circ} = \Delta H^{\circ} - T\Delta S^{\circ} \qquad (3)$$

Table. 7 shows that the thermodynamic parameters of the adsorption of nortriptyline drug on boron nitride nanotubes are physical and the process is spontaneous. Drug release studies show that drug release is fast in the initial hours. Also, the thermodynamic results show that the drug absorption process on the nanocarrier is exothermic, and the Gibbs free energy values indicate the spontaneity of the absorption at low temperatures [39, 40].

Table 7. Thermodynamic data for the nortriptyline drug molecule were calculated using the DFT method with the 6-31 g (d, p) basis set.

Basic set				6-31g (d, p)			
Method	Dipole moment (Debye)	value of ΔE^{o} (Kcal mol^{-1})	value of ΔH^{o} (Kcal mol^{-1})	value of ΔG^{o} (Kcal mol^{-1})	Zero-point correction	value of ΔS^{o} (cal mol^{-1}. K^{-1})	E (Thermal)
M062X	1.3674	-496186.05	-495946.34	-495979.5	230.86	111.21	-495979.5

3.8. Estimation of Recovery Time

To further investigate the desorption behavior of nortriptyline from boron nitride nanotubes (BNNTs), the recovery time was estimated using an Arrhenius-type equation commonly employed in computational studies of drug–nanocarrier systems [23]:

$$\tau = \nu_0^{-1} \exp(-E_a d_s / kBT) \quad (4)$$

where τ is the estimated recovery time (s), ν_0 is the attempt frequency (10^{12} s^{-1}), $E_a d_s$ is the adsorption energy (eV), kB is the Boltzmann constant (8.6173×10^{-5} eV K^{-1}), and T is the absolute temperature (298.15 K). In this approach, the absolute magnitude of the adsorption energy is used as an approximation of the desorption activation energy. The estimated recovery times for nortriptyline desorption from the investigated BNNT structures are presented in Table 8. The results show considerable differences among the investigated systems. BN (5,0) exhibits the shortest estimated recovery time (1.09×10^{-1} s), whereas BN (5,5) shows the longest value (7.24×10^{14} s). The estimated recovery times for BN (6,0), BN (6,6), and BN (8,0) are 1.71×10^{8}, 1.19×10^{10}, and 4.16×10^{9} s, respectively. These results indicate that stronger drug–nanotube interactions are associated with considerably longer estimated desorption times. In particular, the relatively long recovery times predicted for BN (5,5), BN (6,0), BN (6,6), and BN (8,0) suggest strong drug retention and potentially slow thermal desorption under the assumed conditions. In contrast, the weaker adsorption interaction calculated for BN (5,0) is associated with a substantially shorter estimated recovery time. The estimation is based on the approximation of the desorption activation energy by the magnitude of the adsorption energy and does not account for solvent effects, pH, alternative desorption pathways, or other biological factors.

Table 8. Estimated recovery times for nortriptyline desorption from different boron nitride nanotubes at 298.15 K.

Nanotube	Adsorption energy (eV)	Estimated recovery time (s)
BN (5,0)	-0.653	1.09×10^{-1}
BN (5,5)	-1.589	7.24×10^{14}
BN (6,0)	-1.197	1.71×10^{8}
BN (6,6)	-1.306	1.19×10^{10}
BN (8,0)	-1.279	4.16×10^{9}

4. Conclusions

This work studied the structural investigation and targeted drug delivery of nortriptyline by boron nitride nanotubes (BNNTs) using quantum mechanical calculations. The performed calculations revealed that, initially, the armchair structure has a higher absorption energy compared to the zigzag structure. Furthermore, with an increase in the nanotube radius, the drug absorption energy also increases. This increase is attributed to the fact that nanotubes with larger radii provide a larger surface area for interaction with drugs. The cohesive energy results indicated that the absorbed structures are stable, suggesting their potential as drug absorbers and carriers.

The calculated changes in the nearest B–N bond lengths indicate only minor structural perturbations upon drug absorption. The charge analysis indicates electron-density transfer from nortriptyline to the BNNT surface. The optimized configurations are consistent with predominantly physical adsorption, without apparent formation of covalent bonds. However, the estimated recovery times reveal substantial differences in the thermal desorption behavior of the investigated systems. BN (5,0) exhibits the shortest estimated recovery time (1.09×10^{-1} s), whereas the other four systems

show considerably longer estimated values. These results suggest strong drug retention and potentially slow thermal desorption from BN (5,5), BN (6,0), BN (6,6), and BN (8,0) under the assumed conditions. The findings of this research can serve as a valuable insight for both computational and experimental studies in this field.

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مقاله پژوهشی

بررسی محاسباتی مکانیک کوانتومی و به‌کارگیری هدفمند نانولوله‌های نیترید بورون به عنوان نانوحامل برای داورسانی نورتریپتیلین: تحلیلی مبتنی بر نظریه تابعی چگالی (DFT)

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چکیده

در این پژوهش، بررسی ساختاری و انتقال هدفمند داروی نورتریپتیلین توسط نانولوله‌های نیترید بورون با استفاده از محاسبات مکانیک کوانتومی مورد مطالعه قرار گرفت. انتقال داروی مورد نظر به اندام هدف از طریق محاسبات مکانیک کوانتومی انجام می‌شود و این روش یکی از کارآمدترین و مهم‌ترین رویکردهای نوین در حوزه داورسانی، به‌ویژه در صنایع داروسازی و فناوری نانو، به شمار می‌رود. ساختارهای اولیه با استفاده از روش نظریه تابعی چگالی (DFT) و در سطح نظری ۶-۳۱ g (d,p) با نرم‌افزار Gaussian 09 بهینه‌سازی شدند تا ساختار نورتریپتیلین مورد بررسی قرار گیرد. علاوه بر این، ساختار مطلوب و نحوه اتصال آن به نانولوله‌های نیترید بورون با پیکربندی‌های زیگزاگ و آرمیچر و ابعاد (۸,۰)، (۶,۶)، (۵,۵) و (۵,۰) به منظور اتصال هدفمند دارو به سیستم عصبی و نورون های مغزی مطالعه شد. بر اساس یافته‌های شبیه‌سازی، نتایج نشان می‌دهد که نانولوله‌های نیترید بورون می‌توانند با نورتریپتیلین برهمکنش داشته باشند و زمان‌های بازیابی تخمینی در بین ساختارهای مورد بررسی به طور قابل توجهی متفاوت است، که نشان می‌دهد رفتار رهایش دارو باید در کنار قدرت جذب در نظر گرفته شود. بنابراین، نانولوله‌های نیترید بورون ممکن است به عنوان کاندیداهای بالقوه به عنوان نانوحامل‌های نورتریپتیلین و سایر داروها در نظر گرفته شوند.

واژه‌های کلیدی

داروی نورتریپتیلین، نانولوله‌های نیترید بورون، نظریه تابعی چگالی (DFT)، داورسانی، مکانیک کوانتومی.

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