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Research Article

Keywords: Molecular mechanics, · Hydroxyapatite, · Cucurbit[n]urils, · Bambus[6]uril, · Composite biomaterials, Molecular modeling

Posted Date: October 21st, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-11153724/v1>

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Additional Declarations: No competing interests reported.

Assessment of Interaction and Deformation Energies of Cucurbit[n]urils (where $n = 6, 7, 8$) and Bambus[6]uril with a Hydroxyapatite Surface in Composite Biomaterials using Molecular Mechanics

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Abstract

Context:

The development of composite biomaterials based on hydroxyapatite (HA) and macrocyclic compounds like cucurbit[n]urils (CB[n]) and bambus[6]uril (Bu[6]) is a promising strategy for creating functional surfaces in targeted drug delivery and regenerative medicine. However, the molecular-level interactions governing the stability and structure of these composites remain insufficiently understood. This study aimed to computationally evaluate the thermodynamic favorability and structural implications of the adsorption of CB[n] ($n = 6, 7, 8$) and Bu[6] onto the hydroxyapatite (0001) surface. Molecular mechanics simulations revealed that all macrocycles form stable complexes with HA, with CB[8] and perpendicular Bu[6] exhibiting the strongest binding energies of -16.73 and -15.07 kcal/mol, respectively. A key finding is the trade-off between binding strength and structural deformation; while CB[8] shows the strongest adhesion, it also incurs the highest deformation energy. In contrast, the parallel orientation of Bu[6] offers an optimal balance with substantial interaction energy (-13.81 kcal/mol) and minimal deformation (0.11 kcal/mol), highlighting its potential for stable surface functionalization where preserving the macrocycle's architecture is crucial.

Methods:

The calculations were performed using molecular mechanics methods with the MM+ force field as implemented in the HyperChem 7 software package. The hydroxyapatite (0001) surface model was obtained from the CCDC database. The interaction and deformation energies were calculated for two principal orientations (perpendicular and parallel) of each macrocycle relative to the HA surface. The interaction energy ($E_{interaction}$) () was defined as the difference between the adsorption energy (E_{ads}) and the deformation energy (E_{deform}), the latter being the energy difference between the macrocycle in its adsorbed state and its optimized geometry in isolation. The simulations were conducted in vacuo, without explicit solvent molecules.

Keywords: Molecular mechanics, · Hydroxyapatite, · Cucurbit[n]urils, · Bambus[6]uril, · Composite biomaterials, Molecular modeling

Introduction

In recent years, there has been active development of composite materials aimed for use in targeted medicine, including targeted drug delivery and regenerative therapy [1-3]. The modern strategy for creating functional biomaterials seeks to

combine biocompatibility, mechanical strength, and the ability for targeted interaction with biomolecules. Particular attention is paid to the development of composite materials comprising organic and inorganic components capable of selective binding and release of biologically active substances. However, the approaches used do not yield unambiguous results regarding the formation process of these composite materials. Thus, studying such materials using molecular mechanics methods becomes highly relevant, as it allows for modeling interactions at the atomic level and predicting component behavior under biological conditions.

Molecular modeling holds a significant place in modern materials science for investigating and substantiating the processes of sorption and interaction between components of a composite material [4]. Theoretical approaches are especially valuable when obtaining experimental data is challenging or economically unfeasible [5]. Typical modeling tasks include studying the structure of molecules, associates, or solid-phase fragments, as well as analyzing the mechanisms of chemical reactions at the molecular level. Quantum mechanics methods provide deep insight into molecular structure and reactions [6]. At the same time, molecular mechanics, based on a phenomenological description of potential energy, utilizes parameters that are often easier to compute using quantum chemical methods rather than to fit from experimental data [7].

However, empirical models are incapable of adequately describing chemical reactions, as they do not account for changes in electronic structure [8]. A significant advancement is the development of hybrid QM/MM methods, which combine the accuracy of the quantum mechanical part with the computational efficiency of the classical part [9]. QM/MM methods are widely used for modeling interaction processes in biomolecules, condensed phases, and biomaterials [10-13], including those formed on porous inorganic substrates, such as hydroxyapatite.

Hydroxyapatite ($\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$, **HA**) is a primary micro- and nano-component of bone tissue that has proven to be a biocompatible and bioactive carrier in targeted drug delivery systems. It provides efficient binding of biomolecules, high loading capacity for bioactive substances, and controlled release dependent on the pH of the environment, which is particularly important in regenerative medicine and cancer therapy. Furthermore, **HA** is the most suitable ceramic material for artificial teeth or bones due to its excellent biocompatibility and biological activity [14]. These materials are inert towards living tissues and exhibit low toxicity. Their use is associated with a low probability of allergic reactions, inflammation, and mutagenic effects. Moreover, modified hydroxyapatites can accelerate the process of reparative osteogenesis at the implantation site and enhance the proliferation of osteoblasts [15].

For the fine-tuning of materials with tailored biological properties, the use of a class of macrocyclic compounds—cucurbit[n]urils and bambus[6]uril—is potentially promising. In this context, cucurbit[n]urils (**CB[n]**) and bambus[6]uril (**Bu[6]**) serve as elements for functionalizing surfaces and matrices due to their ability to form unique complexes with biological substrates for targeted drug delivery [16-18].

Cucurbit[n]urils (Fig. 1), represented by a series of macrocycles composed of glycoluril units linked by methylene bridges, possess high structural rigidity, the ability to form complexes with both ionized and neutral molecules, as well as chemical and thermal stability [19, 20]. Owing to these properties, they find applications in drug delivery systems, sensors, and tissue engineering scaffolds [21-23]. Depending on the number of monomeric units ($n = 5-8$ and higher), cucurbit[n]urils vary in their internal cavity diameter and, consequently, in their capability to form host-guest complexes with various biologically active molecules [24, 25].

Bambus[n]urils (Fig. 1), a class of macrocycles discovered in 2010, consist of single-chain N-substituted fragments within one of the imidazolinoine cycles of glycoluril and exhibit a unique ability for selective anion binding through multiple hydrogen bonds [26-28].

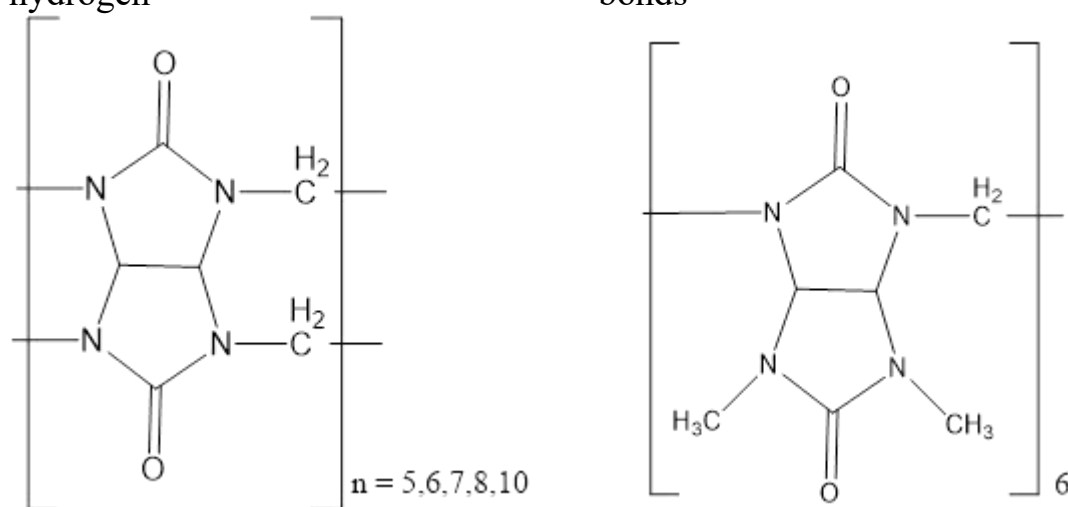


Figure 1 – Chemical structures of cucurbit[n]urils and bambus[6]uril

The integration of **CB[n]** and bambus[6]uril into the structure of composite biomaterials based on porous inorganic scaffolds leads to the emergence of new functional properties in the resulting composite materials. Previously, composite materials based on porous inorganic compounds with cucurbit[6,7,8]urils and bambus[6]uril have been synthesized and investigated [29-30].

Study [29] demonstrated that composite materials of **CB[6,7,8]** and hydroxyapatite (**HA**) showed high biocompatibility and low toxicity of the obtained biocomposite materials in in vitro tests. When investigating the effect of biocomposite samples on the expression of $\text{TNF-}\alpha$, $\text{IL-1}\beta$, and IL-6 , it was revealed that all studied samples from both donors did not lead to increased expression of these cytokines. At the same time, studies on composite materials based on bambus[6]uril have shown [31, 32] that bambus[6]uril is present as a conglomerate of molecular ensembles, which reduces protein adsorption from blood plasma and increases the hemocompatibility of these materials.

Thus, the present work aims to study the interactions of macrocyclic molecules—cucurbit[6,7,8]urils and bambus[6]uril—with the components of hydroxyapatite-based composite biomaterials using molecular mechanics. Understanding the nature of these interactions will advance the knowledge necessary

for the rational design of a new generation of biocompatible and functional materials.

Materials and Methods

Molecular Mechanics Method

To study the interaction process of macrocyclic compounds, the interaction energy of cucurbit[n]uril (where n=6,7,8) and bambus[6]uril molecules with sections (unit cell) of hydroxyapatite was calculated using the HyperChem 7 software with the MM+ force field, under the following assumptions:

The interaction between the molecules of cucurbit[n]urils (where n=6,7,8) and bambus[6]uril with the hydroxyapatite crystal surface does not lead to a change in the surface;

The absence of interaction between adsorbed molecules of cucurbit[n]urils (where n=6,7,8) and bambus[6]uril;

The calculation of interaction and deformation energies of the molecules was performed without considering the influence of the solvent;

The molecules of cucurbit[n]urils (where n=6,7,8) and bambus[6]uril were optimized separately and in isolation from the **HA** surface.

During the calculations, two orientation modes were considered – perpendicular (Perp.) and parallel (Par.) – for the cucurbit[n]uril (**CB[n]**) and bambus[6]uril (**Bu[6]**) molecules relative to the hydroxyapatite surface, as schematically shown in Fig. 2.

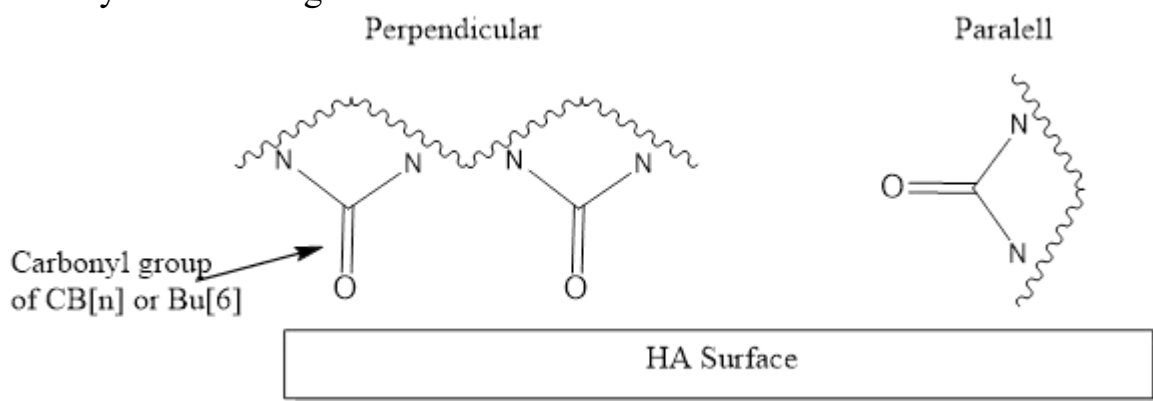


Figure 2 - Variants of the arrangement of the macrocycle in relation to the surface of hydroxyapatite

To elucidate the interaction process between cucurbit[n]uril (where n=6,7,8) or bambus[6]uril and the hydroxyapatite surface, the interaction energy was calculated using the formula:

$$E_{interaction} = E_{ads} - E_{deform},$$

where E_{deform} is the deformation energy of the **CB[n]** or **Bu[6]** molecule, and E_{ads} is the adsorption energy.

Subsequently, the deformation energy was calculated using the formula:

$$E_{deform} = E_{adsorbed_mol} - E_{optimized_mol}$$

where $E_{adsorbed_mol}$ is the energy of the **CB[n]** or **Bu[6]** molecule in the adsorbed state, and $E_{optimized_mol}$ is the energy of the optimized **CB[n]** or **Bu[6]** molecule (MM+).

Methods for Obtaining Composite Materials

An immersion coating method was used for deposition. To implement this, an HA pellet was immersed in aqueous solutions of **CB[6]**, **CB[7]**, and **CB[8]** for 45 minutes at a concentration of 1 mg/ml. The CB[6] and CB[8] solutions were dispersions, whereas CB[7] was completely soluble in water. The resulting samples were dried at room temperature to a constant mass over 24 hours [31, 32].

For coating Bu[6] onto the porous hydroxyapatite surface, a solution immersion method was also employed. To implement this methodological approach, a dispersed solution of Bu[6] in deionized water was prepared in an amount of 15 mg per 15 ml. Subsequently, the HA supports were immersed in the Bu[6] solution and maintained for 45 minutes. After this, the solution was decanted, and the composite samples were dried at room temperature to a constant mass [33].

At the first stage of the work, modeling of the interaction between optimized cucurbit[n]uril molecules (where $n = 6, 7, 8$) and the hydroxyapatite surface was carried out. The HA (0001) lattice from the open CCDC database was used as the model. Table 1 presents the results of molecular mechanics (MM+) calculations of the interaction energy and deformation energy for the interaction between cucurbit[n]urils of different dimensions (CB[6], CB[7], CB[8]) and the solid surface of hydroxyapatite (HA, (0001) plane).

Table 1 – Calculated interaction energies of crystal sections with different conformations of cucurbit[n]uril molecules (where $n=6,7,8$), kcal/mol

	Interaction Energy, kcal/mol					
	CB[6]		CB[7]		CB[8]	
Orientation	Perp.	Par.	Perp.	Par.	Perp.	Par.
HA (0001)	-12,83	-10,10	-15,02	-9,47	-16,73	-8,71

Interaction energy characterizes the thermodynamic favorability of interaction: the more negative the value, the stronger and more stable the complex. Deformation energy, on the contrary, reflects the energy cost associated with the change in geometry of the participating components (primarily the cucurbit[n]uril, where $n=6,7,8$) during the interaction. The lower the deformation energy value, the more natural and less energetically costly the binding process is.

Table 2 – Calculated deformation energies of crystal sections with different conformations of cucurbit[n]uril molecules, kcal/mol

	Deformation Energy, kcal/mol					
	CB[6]		CB[7]		CB[8]	
Orientation	Perp.	Par.	Perp.	Par.	Perp.	Par.
HA (0001)	0,75	0,22	0,40	0,31	0,99	0,66

According to the calculations, all cucurbit[n]urils (where $n=6,7,8$) demonstrate strong interaction with the hydroxyapatite surface. The interaction energy of CB[6] with HA has a magnitude of 12.83 kcal/mol. For CB[7], a similar trend is maintained: 10.10 kcal/mol in magnitude with **HA**. The most pronounced difference is observed for **CB[8]**, where the interaction energy with **HA** has a magnitude of 16.73 kcal/mol (Figs. 3-5).

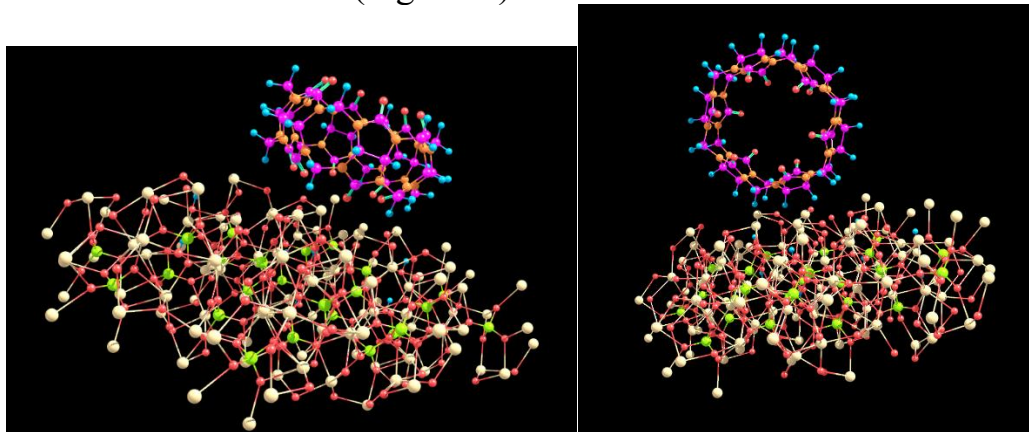


Figure 3 – Simulation of **CB[6]** interaction with the **HA** surface in perpendicular (left) and parallel (right) orientations

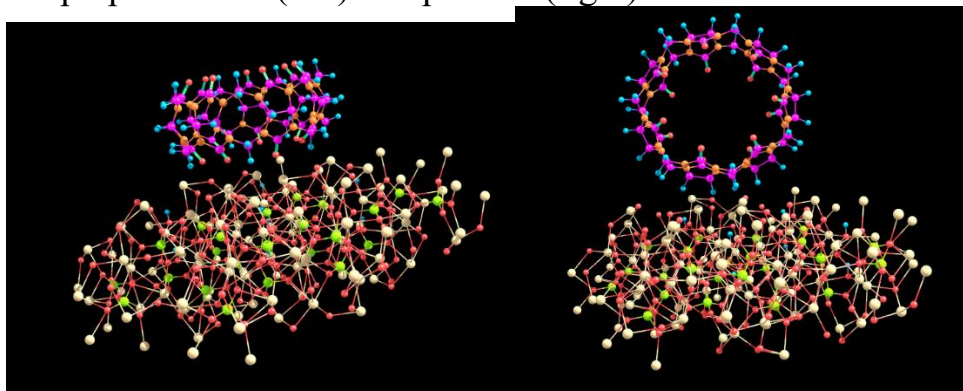


Figure 4 – Simulation of **CB[7]** interaction with the **HA** surface in perpendicular (left) and parallel (right) orientations

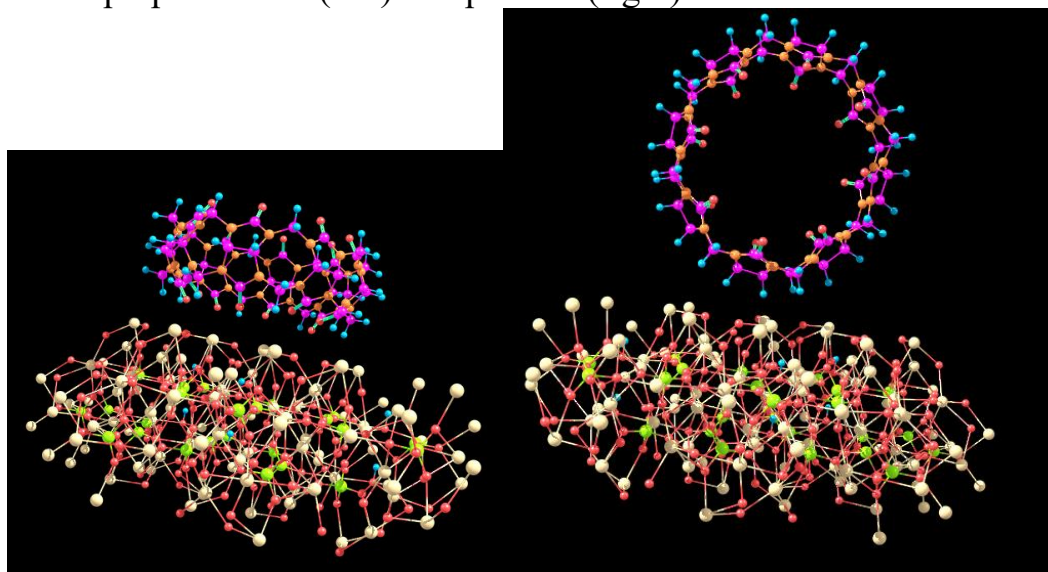


Figure 5 – Simulation of **CB[8]** interaction with the **HA** surface in perpendicular (left) and parallel (right) orientations

Such differences may be attributed to the variation in the sizes of **CB[n]** and the number of carbonyl groups participating in the interaction through ion-dipole, hydrogen bonding, or π -interactions. This is particularly pronounced in the case of **CB[8]**, which possesses the largest size among the considered macrocycles, potentially facilitating more extensive contact with the **HA** surface.

Analysis of the obtained deformation energies reveals that for all cucurbit[n]urils (where $n=6,7,8$), with the exception of **CB[8]**, the deformation energy values do not exceed 1 kcal/mol. This indicates that the structure of these macrocycles is almost undistorted upon binding to the surface. The highest deformation energy is observed for the **CB[8]** complex with **HA** and amounts to 0.99 kcal/mol, which may indicate significant rearrangement of the molecule or the surface during the interaction process.

In general, it can be concluded that **CB[8]** demonstrates the highest capacity for interaction with the material's surface (Tables 1 and 2). However, the high deformation energy in the case of the **CB[8]**-**HA** complex may necessitate additional analysis of the stability of such a complex under real conditions. The moderate interaction energies and minimal deformations of **CB[6]** and **CB[7]** make them potentially more preferable candidates for stable surface modification, especially in biomedical applications where excessive deformation may be undesirable.

Similar to the **CB[n]** systems, calculations of the bambus[6]uril molecule's interaction were performed; the results are presented in Table 3. For each system, two possible orientation variants of bambus[6]uril relative to the surface were considered: perpendicular and parallel. The provided values include the interaction energy in kcal/mol (Table 3), reflecting the thermodynamic stability of the complexes, as well as the deformation energy, characterizing the degree of structural distortion during the formation of the interfacial interaction.

Table 3 – Calculated interaction and deformation energies of **HA** crystal sections with different conformations of bambus[6]uril molecules, kcal/mol

Orientation	Interaction Energy, kcal/mol		Deformation Energy, kcal/mol	
	Perp.	Par.	Perp.	Par.
HA (0001)	-15,07	-13,81	1,26	0,11

Analysis of the interaction energy reveals that in the perpendicular orientation, the interaction energy of bambus[6]uril with **HA** has a magnitude of 15.07 kcal/mol, while in the parallel orientation it is 13.81 kcal/mol, indicating a moderately stable interaction. The difference between the two orientations is insignificant, which may suggest isotropic interaction on this specific crystallographic plane of **HA** or geometric adaptation of Bu[6] on the surface (Fig. 6).

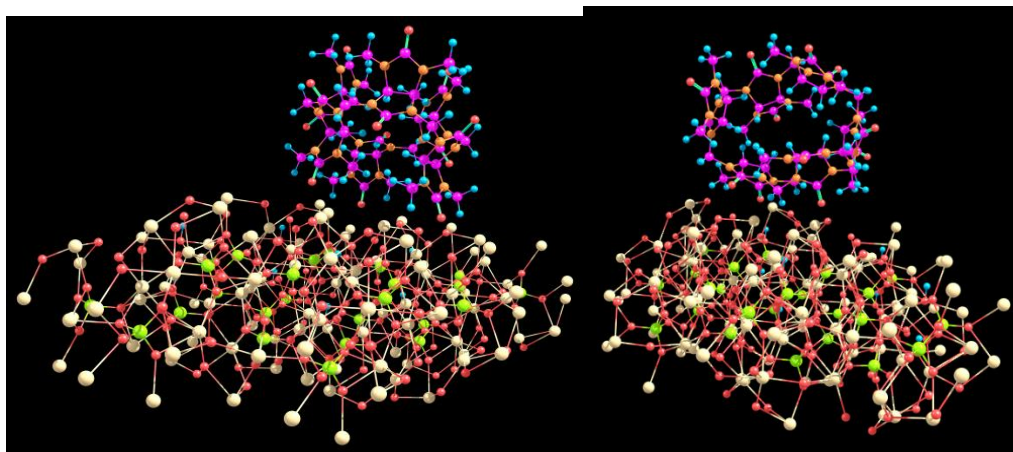


Figure 6 – Simulation of **Bu[6]** interaction with the **HA** surface in perpendicular (left) and parallel (right) orientations

However, high interaction energy values can be accompanied by significant structural rearrangements of the system, as evidenced by the deformation energy data. For **HA**, the energy costs for deformation are minimal: 1.26 kcal/mol for the perpendicular orientation and only 0.11 kcal/mol for the parallel orientation. This indicates high geometric compatibility between bambus[6]uril and the hydroxyapatite surface, particularly when the molecule is parallelly oriented, which may be important for preserving the macrocycle's functionality within coatings or composites.

Conclusion

The molecular mechanics calculations performed using the MM+ method allowed for a comparison of the interaction features of macrocycles—cucurbit[n]urils (where $n=6,7,8$) (**CB[6]**, **CB[7]**, **CB[8]**) and bambus[6]uril—with the hydroxyapatite (**HA**) surface. All macrocycles demonstrate significant interaction with the **HA** surface. Particularly strong binding is observed for **CB[8]** and bambus[6]uril in the perpendicular orientation, where the minimum interaction energies are achieved: -16.73 and -15.07 kcal/mol, respectively. This is likely due to the larger number of carbonyl groups in **CB[8]** and the higher charge of the extra-chain carbonyl groups in **Bu[6]**, stabilized by the electron-donating effect of the methyl groups.

Nevertheless, such interactions are accompanied by higher deformation energy values, especially for larger macrocycles, which may indicate significant structural changes upon adsorption. In this context, **HA** proves to be a soft surface, resulting in lower energy costs for deformation, particularly in the case of the parallel orientation of bambus[6]uril (only 0.11 kcal/mol).

Thus, when selecting a "macrocycle-surface" combination for creating composite or functional materials, it is necessary to consider the balance between the interaction strength and the preservation of the macrocycle's structure. Hydroxyapatite provides mild conditions for the stable retention of macrocycles with minimal distortion of their architecture.

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