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Study of Target Recognition of MAA-based Molecularly Imprinted Polymer (MIP) Using Density Functional Theory (DFT) Computation on the Interaction of Methacrylic Acid (MAA)-D-Glucose

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Abstract Methacrylic Acid (MAA) based Molecularly Imprinted Polymer (MIP) is potentially used as an active material for biosensor. MIP is prepared to contain cavities that are leaved by template molecules. In the next time, target molecules that have a similar physical structure and properties with that of target molecules, can be trapped in the cavities. The main mechanism of the target recognition is the similarity of the space structure of the cavities and target molecules, but the molecular interaction between MAA and target molecules is also important. In this study, the interaction between two MAA molecules and one D-Glucose molecule is investigated using the Density Functional Theory (DFT). In the calculation, the Gaussian 09 with B3LYP and 631+G(d) basis sets is used to calculate all the electronic properties. The presence of the interaction was observed through the changes of the distances between specified atoms of the two molecules. The result is in line with the previous experimental study on potentiometric measurement of MAA-based MIP sensor for D-glucose as target molecule.

Keywords: *D-glucose, template, MAA-based molecularly imprinted polymer, DFT*

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1. Introduction

Molecularly Imprinted Polymers (MIPs) which have been attracted many researchers around the world, have specific characteristic structure cavities as with template molecules. The studies on the application of MIPs cover many research areas such as biosensors [1,2], solid-phase extraction [3,4], chromatography [5], and drug delivery [6]. In the preparation of MIPs, molecularly imprinting polymerization, the imprinting process takes place during the polymerization process, after which the template molecules were then removed from the polymer network. This results in cavities that are similar to the template molecules. [7,8,9,10].

Since the cavities in a MIP can be filled with molecules having the same or similar space structure to that of cavities, the MIP can be used as active sensor materials. In the target recognition process, i.e. MAA-based MIP, beside the similarity of space structure of cavities and target molecules, the molecular interaction between MAA and target molecules also plays an important role. Target recognition of MAA-based MIP with D-glucose as target molecule has been studied through Potentiometric measurement [11]. The result shows that the MIP is potentially used as active sensor material. The interaction between MAA and D-glucose as target molecules has been examined computationally using Density Functional Theory (DFT) for one MAA molecule and one D-glucose molecule [12]. In fact, there should be more than one MAA molecule and one D-glucose is involved in the target recognition. In this study the interaction between two MAA molecules and one D-glucose molecule has been examined using Density Functional Theory (DFT).

The synthesis route of MAA-based MIP using D-glucose as template molecules has been discussed [13]. The polymerization was carried out at 60°C for 21 h. Unreacted monomers were removed using several solvent (acetonitrile, methanol, acetic acid, and aquabidest). The cavities were formed after the template was removed. Next, the cavities can recognize the target molecules, i.e. D-glucose.

2. Computational Method

The iteration process in DFT computation is shown by Figure 1. The DFT was applied at ground state (temperature 0K). Initially, the position of each atom of each molecule was defined. After a series of iteration computation process through Effective Potential calculation, solving the Kohn-Sham Equations and evaluate the electron density and total energy, the final position was defined.

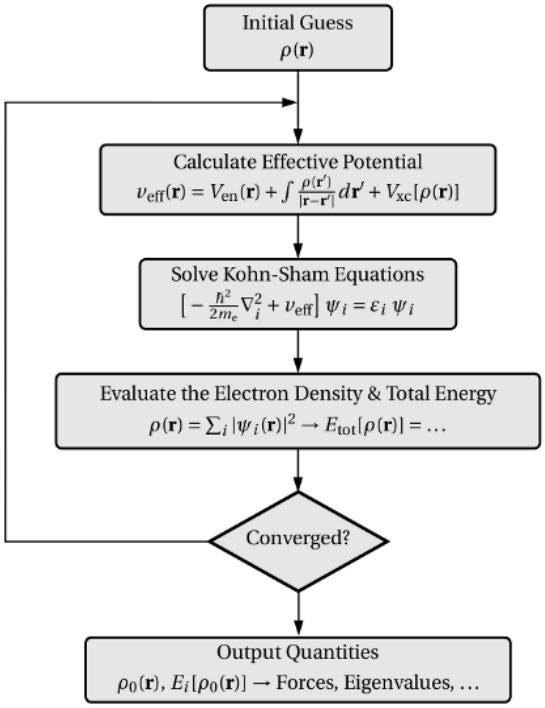

Figure 1. The iteration scheme in the DFT calculation

A molecule structure of MAA (Figure 2a) consists of 12 atoms while a molecule structure of D-Glucose (Figure 2b) consists of 22 atoms. The optimization calculation has been done by completely relaxing all atoms without any symmetry constraint. The optimized structure of one MAA molecule and one D-glucose molecule is shown in Figure 2.

Next, the initial arrangement of two MAA molecules and one D-glucose molecule is shown by Figure 3. Notice the distance between two closely spaced specific atoms of the two different molecules.

To calculate all the electronic properties, the DFT method was carried out using the Gaussian 09 Program. The molecular properties of M and D-Glucose molecules, was calculated using the B3LYP/6-311+G(d) basis set.

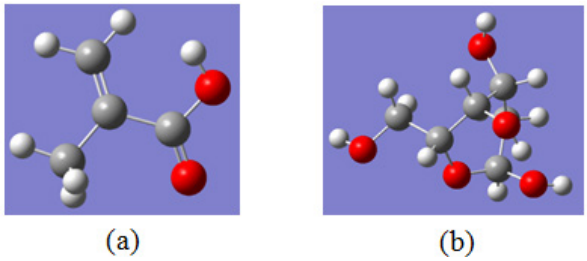

Figure 2. The structure of (a) MAA molecule and (b) D-glucose molecule after optimization using Basis set (6-311+G(d))

3. Results and Discussion

After the computation process, it was found that the final arrangement has different configuration with the initial one. Figure 4 shows the new arrangement after the computation process. The interaction between the MAA and D-Glucose molecules is represented by the changes in the distance between marked atoms: O_8-H_{15}, O_2-H_{10} and O_6-H_{19} as follow:

After the computation, there are three distances decrease (O_2-H_{10}, O_6-H_{19} and C_4-C_{11}) and one distance increases (O_8-H_{15}). As the changes were dominated by decreases in the distance of atoms of two different molecules, thus in overall, the changes show that the three molecules get closer. This indicates the presence of attractive physical interaction between the molecules.

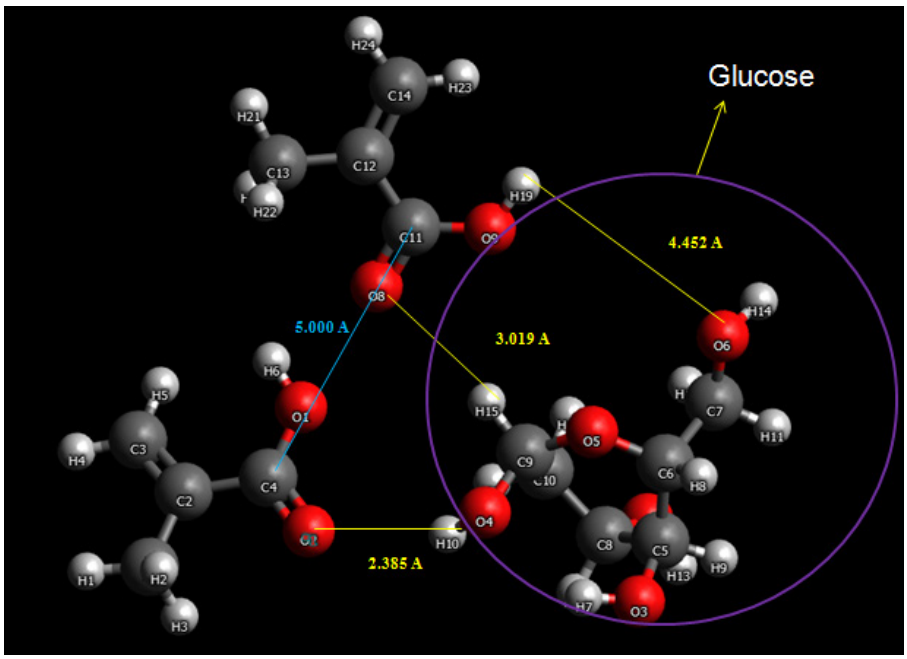

Figure 3. The initial configuration of two MAA molecules and one D-glucose molecule

Table 1. The distance between marked atoms: O_8-H_{15}, O_2-H_{10} and O_6-H_{19}

The distance of	Initial condition (A)	Final condition (A)	The distance change (A)	Molecules
O_8-H_{15}	3.090	4.365	1.275	MAA_1 - D-Glucose
O_2-H_{10}	2.385	1.848	-0.537	MAA_2 - D-Glucose
O_6-H_{19}	4.452	1.854	-2.598	MAA_1 - D-Glucose
C_4-C_{11}	5.000	4.079	-0.921	MAA_1-MAA_2

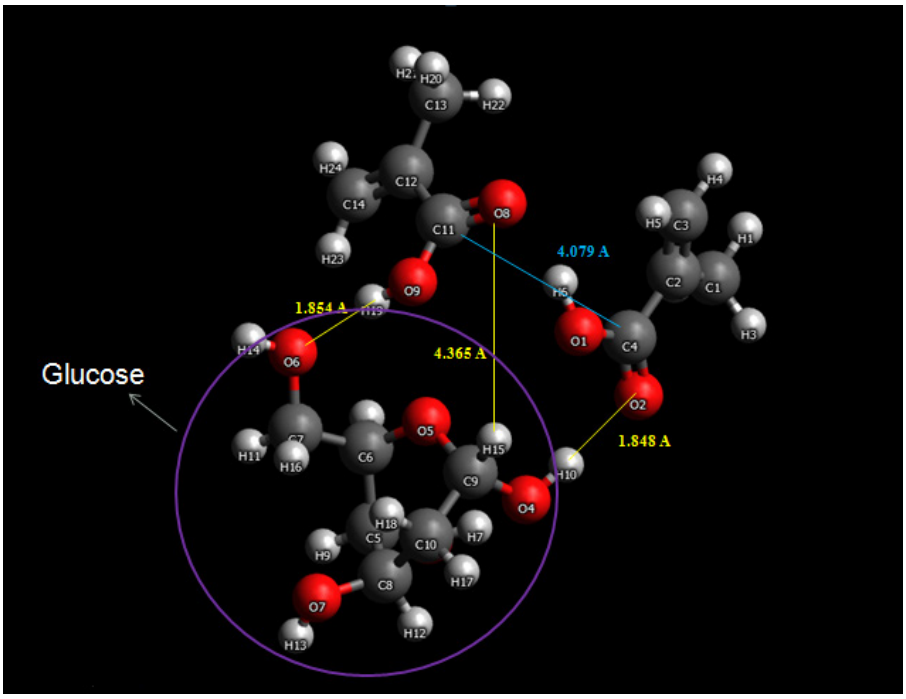

Figure 4. The configuration of two MAA molecules and one D-glucose molecule after the computation process

Previous DFT study on one MAA molecule and one D-Glucose molecule also shows similar result [12]. It means that the attractive physical interaction between MAA and D-glucose consistently occurs. This interaction supposes to contribute in the target (D-Glucose) recognition for MAA-based MIP. The previous experimental study on potentiometric measurement of MAA-based MIP sensor for D-glucose as target molecule has demonstrated this recognition [11].

3. Conclusion

From this study it can be concluded that there is an attractive physical interaction exist between two MAA molecules and one D-Glucose molecule. Thus, beside the similarity in space form of D-glucose and cavities in MAA-based MIP prepared using D-glucose as template molecules, the attractive physical interaction should contribute in the mechanism of target (D-Glucose) recognition. The target recognition is a basis for the MIP to be potentially used as active biosensor material.

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