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Theoretical Study of A and B Anomers of Dodecanoyl Xylopyranose Stability using DFT Method

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ABSTRACT

The development of theoretical tools is closely linked to the development of information technology, which make it possible to group together and analyze an increasing number informational. The determination by calculating the structure of a molecule has developed considerably and has made it possible to better understand the theory of molecular structure. It involves the use of theoretical calculation methods. Molecular modelling is an application of theoretical and computational methods to solve problems involving molecular structure and chemical reactivity [1]. The GAUSSIAN program has made it possible to bring quantum chemistry into the laboratories of chemistry, biochemistry, biotechnology and physics and pharmacology [2]. The main of our work is to study the reactivity of the two anomers of synthetized biosurfactants by investigating the molecular structure using Gaussian 9.

Keywords: Anomers, Gaussian 9, biosurfactant, molecular modelling

1 Introduction

Enzymatic synthesis of non-ionic surfactants from renewable sources in organic media allows for a more simplified and environmentally friendly production process than the traditional chemical route. This process represents a new challenge in biotechnology. Nonionic surfactants composed of a hydrophilic carbohydrate moiety and fatty acids as lipophilic moiety are of great importance, they represent an eco-friendly alternative to conventional surfactants with a wide range of applications. Due to their sustainable character and low toxicity, these biosurfactants are key ingredients in many types of consumer goods, for instance, formulated products in pharmaceutics, cosmetics, and personal care [3]. The α- and β-anomers of dodecanoyl xylopyranose were easily separated and characterized through analytical methods. To complete this study, molecular modeling was performed on two anomers to understand the forces involved in the stability of the compounds.

2 Experimental

In this work we have used Gaussian 9 to optimize molecular structures of the two anomers by using DFT/B3LYP method with 3.21 G and 6-31G basis-set. The most stable optimized geometric structure obtained by 6.31 G basis-set were investigated.

3 Results and discussion

We conducted a comparative study of two anomers alpha and beta of dodecanoyl xylopyranose using the Gaussian09 program based on functional theory density (DFT) with correlation and exchange function B3LYP and base-set (6-31G and 3.31G) . The geometric parameters calculated by molecular modeling on the Gaussian software using the DFT method and the functional B3LYP with the two basis showed that the best basis is 6.31 G Molecular symmetry can be used to predict many molecular properties such as its dipole. Accordingly, to the results of mediums of bond presented in TABLES 1. The most optimized structural parameters (bond length, bond angle) is calculated by B3LYP with 6-31G basis set.

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Table1:. *Medium bond of compound α and β obtained by basis-set 3.21G and 6.31G*

Medium bond	Xy-12 (β) (3.21G)	Xy-12 (α) (3.21G)	Xy-12 (β) (6.31G)	(Xy-12α)(6.31G)
	1,25864909	1,26073273	1,25254182	1,25269273

To determine their reactivity, we have used basis-set 6.31G. For this reason, we have calculated the energy gap, the results show that alpha anomer is more reactive than beta anomer (TABLE 2)

Table2: *Calculated energy values for compounds*

Anomère	HOMO	LUMO	Energy gap (ev)
Xy-12(α)	-0,25801	0,00493	0,26294
Xy-12(β)	-0,25548	0,00767	0,26315

4 Conclusion

The compound Xy-12(α) is the softest so more reactive than the Xy-12(β) because it have lowest gap .

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