Computer Modelling of Glucoside System with Water

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Abstract—**Lauryl glucoside is a surfactant that exhibits self-assembly. Lauryl glucoside has relatively simple molecular structure of 12 carbons chains makes it easier to be simulated with molecular dynamics (MD) simulation. From previous study, it was found that the amount of water molecules plays an important role in the stability of intermolecular interaction between glucoside and water molecules. In this research, MD simulation was applied to discover the interaction of glucoside system in water by using COMPASS force field. The objective of this research is to study the stability effect of different number of water molecules on glucoside. The simulation was performed by using Material Studio (MS) software at 2 ns simulation time. From the trajectory output files, the Radial Distribution Function (RDF) were analysed. By using MD simulation, various possible hydrogen bonds can be determined and the interactions between lauryl glucoside and water molecules can be investigated. Thus, the simulation lead to a discussion of the effects of interaction between a single lauryl glucoside molecule and different number of water molecules, and the stability on the interaction between lauryl glucoside-water system. These finding also analysed the difference of simulation between lauryl glucoside and stearyl glucoside.**

Keywords— Glucoside, Molecular modelling, Hydrogen bonds, Intermolecular interaction.

I. INTRODUCTION

Throughout various science researches, the development in research of organic chemistry has extensively increased the pace of scientific discovery. Current interest considering the eccentric properties of glycosides for sustainable development [1]. Lauryl glucoside is a form of alkyl polyglucoside with 12 carbons chains [2]. Alkyl polyglucosides is a sugar-based surfactant, widely used in the industry such as cosmetic and detergent [3]. The use of organic material in the form of renewable raw material allows for the sustainable development in applied research. Furthermore, hydrogen bonds are essential for the self-assembly of glycolipids compared to other intermolecular interactions due to the presence of OH groups on the sugar head group [4]. Hydrogen bonding interactions have been interesting to researcher due to its importance in various properties and reactivity of molecules [5]. Water can be used as a solvent in hydrogen bonding interactions as it is known as active participants in biochemical processes [6]. Water also has a different solubility, which able to determine the stability in the interaction between water molecule and glucoside.

Glucosides are commonly used as a surfactant due to its amphiphilic properties. There are various of experimental work in determining the interaction between glucoside and solvent but none are able to describe the interaction at molecular level of solvent effect on lauryl glucoside. Thus, molecular dynamics (MD) simulation technique has been applied as a modernize alternative to resolve the problem. The molecular dynamics simulation provides adequate information to study the relationship between the structures of the molecules. Furthermore, MD simulation can identify the most stable hydrogen bond interactions between molecule and solvent [7]. Eventually, the stability of the interaction is depending on the number of water molecules. Lauryl glucoside is a natural surfactant which is widely used in cleansing applications. It can easily interact with water molecules that contain hydrogen bond since it is water soluble. In this research, various number of water molecules are chosen to be studied for the intermolecular interaction of glucoside in order to obtain the most stable hydrogen bond.

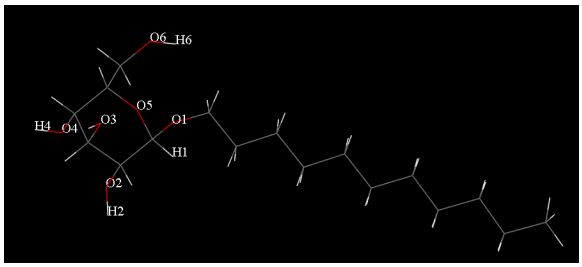
For this research, lauryl glucoside is chosen to interact with water as a solvent to determine the intermolecular and intramolecular interaction at molecular level. The selection of glucoside was based on its properties as a water-soluble molecule with 12 carbons chains. This molecule also has the ability to self-assemble. This study is fixed at 1 atm for all simulation systems. The simulation was carried out by the software from Accelrys known as Materials Studio 7.0 (MS). The interaction is simulated by considering one molecule of lauryl glucoside and various numbers of water molecules. The force field used are COMPASS force field to discover the structural, conformational, vibrational and thermophysical properties of molecules under fixed conditions of pressure. The results are analysed from Radial Distribution Function (RDF).

This research is conducted in order to obtain the objective which is to study the effect of different number of water molecules as solvent in glucoside using molecular dynamics simulation. The significance for this study is to understand the molecular interaction as well as the stability of glucoside and water molecule at 2 ns. The simulation also done for stearyl glucoside with water to study the differences between lauryl glucoside-water system and stearyl glucoside-water system. Stearyl glucoside is a less water-soluble glucoside, thus give a better understanding of the effect of water solvent towards different type of glucoside.

II. METHODOLOGY

A. Material structures

The molecular structure of lauryl glucoside and water were first drawn using the built-in tool in Material Studio software. The structure of the molecule is set with numbering and labelling intended for molecular recognition. This is done due to the ability of lauryl glucoside to form hydrogen bonding during the interaction with water molecule. Figure 1 shows the partial numbering and labelling of atom in the molecules.



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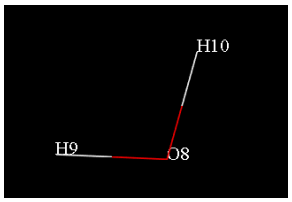

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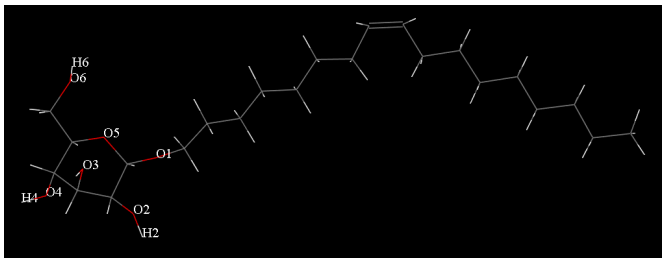

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Figure 2.1: The partial numbering and labelling of (a) lauryl glucoside (b) water (c) stearyl glucoside

B. Construction of Amorphous Cell of System

An interaction between lauryl glucoside and the water molecules was simulated by using software from Accelrys known as Materials Studio 7.0 (MS). The amorphous cell box was constructed by using Amorphous Cell module at 200K. The number and density of the molecules present in the cell was taken into consideration during configuration of the amorphous cell model. In this simulation, lauryl glucoside is referred as C12, stearyl glucoside as C18 and water as W. Table 2.1 shows the information of constructed systems.

System	Number of molecules	Cell Volume ($Å^3$)	Density (g/cm^3)
C12-W	1-1	1217.1	0.5
	1-2	1276.9	
	1-4	1396.6	
C18-W	1-1	1496.8	0.5
	1-2	1556.4	
	1-4	1676.2	

C. Geometry Optimization

The energy of the system is analyzed in the geometry optimization module to obtain the stability of geometry molecules. Calculation of atomic charges is done by using forcefield assigned for geometry optimization and molecular dynamic simulations. The total energy was calculated by using COMPASS force field and atom based for both electrostatic and van der Waals summation method. Later, the lowest energy of glucoside is chosen for dynamic simulation.

D. Molecular Dynamics Simulation

The potential functional groups linked with the water molecule throughout the interaction were analyzed by the dynamic simulation. In this system, the pressure is kept constant at 1 atm by using COMPASS forcefield with Ewald summation method for electrostatic interaction with 1fs timestep. Initially, the system was simulated by NVE (constant volume-constant energy) at 100K for 20 ps simulation time. Then, simulation was run by NPT (constant pressure-constant temperature) type of ensemble included Nose thermostat and Berendsen thermostat for 2 ns simulation time. The step size used in the simulation is 100 steps. The trajectory output was analyzed using Radial Distribution Function for the simulation between the chosen functional groups. Then, the step is repeated to analyze the interaction between stearyl glucoside with 1, 2 and 4 number of water molecules.

III. RESULTS AND DISCUSSION

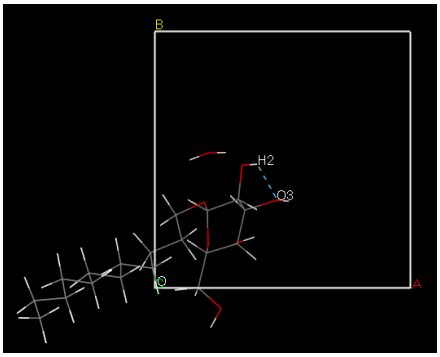
A. Construction of systems

Lauryl glucoside-water system and stearyl glucoside-water system are constructed to study the possible interactions by using different types of glucoside. The cell box constructions involve polymorphism. Usage of different number of water molecules can give different effects of interactions. There are three major steps of the molecular modelling simulation, which is amorphous cell construction, geometry optimization and molecular dynamics. The intramolecular and intermolecular interactions of systems are interpreted by Radial Distribution Function (RDF). The hydrogen bond is created when water molecules interact with the glucoside where the proton donor attached covalently to a highly electronegative atom as depicted in Figure 3.1 (blue dashed-line) [8].

B. Molecular Dynamics Simulation

Graph of all systems after dynamic simulation shows the similar linear trend at 2ns which indicates that the periodic molecules moves at the similar frequency and rate. Table 4.1 shows the total energy obtained for dynamic simulation of the system. Negative total energy obtained for all systems are significant. This indicates that the more negative the energy value, the more energy is being released. Higher negative energy value is required to obtain stronger and better stability of the interaction [7]. Figure 3.1 shows the hydrogen bond interactions obtained in C12-W1, C12-W2, C12-W4 and C18-W1 systems whereas no interaction occurs for C18-W2 and C18-W4 systems

System	Number of molecules	Total energy (kcal/mol)
C12-W	1-1	-9.661
	1-2	-26.67
	1-4	-43.83
C18-W	1-1	-32.34
	1-2	-44.68
	1-4	-54.21



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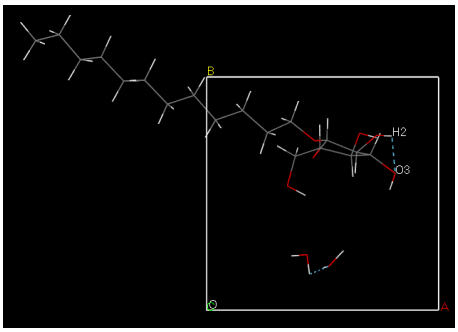

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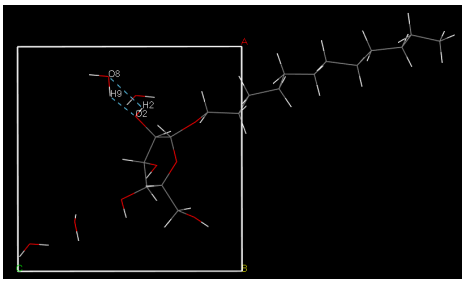

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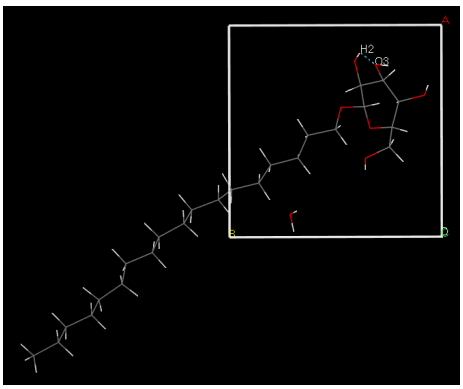

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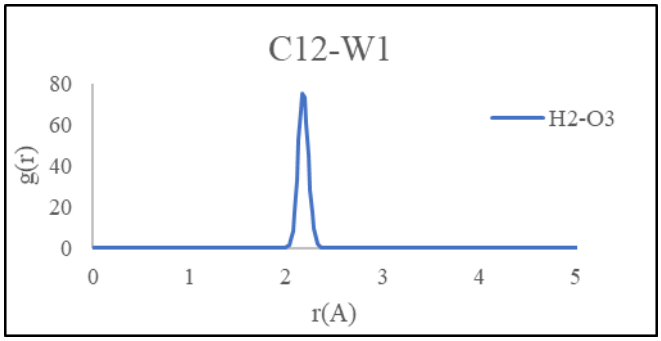
Figure 3.1 : Hydrogen bond interactions of a) C12-W1 b) C12-W2 c) C12-W4 d) C18-W1

C. *RDF Analysis*

Figure 3.2 shows the RDF analysis of interaction for all systems. For C12-W1 and C18-W1, both systems have one intramolecular hydrogen bond at the same atom position H2-O3, as shown in Figure 3.1(a)(d). This shows that both systems have the same long-range electrostatic interaction from the hydroxyl group [8]. Higher peak (g(r)) and shorter distance (r) indicates stronger hydrogen bond interactions. Based on Figure 3.2(a)(d), the peak of C12-W1 system is at 2.17 Å whereas for C18-W1 system is 3.69 Å. From the RDF analysis, C12-W1 has shorter radius and higher peak which describe the system has stronger hydrogen bonding interaction. The elongation of the alkyl chain results in the reduction of hydrogen bonding interaction [10].



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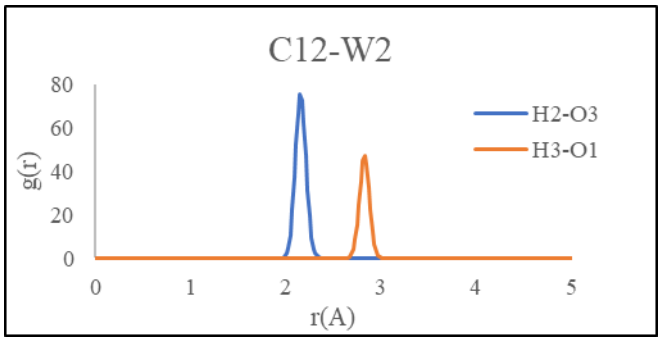

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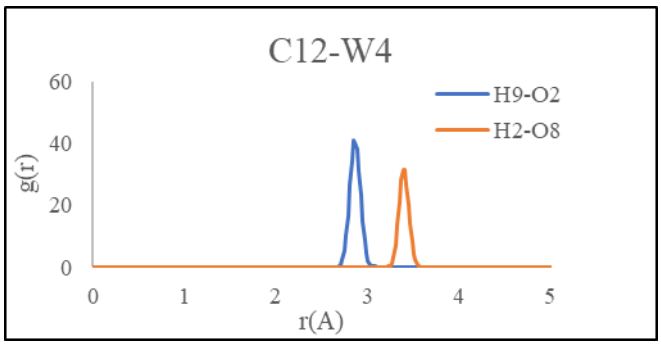

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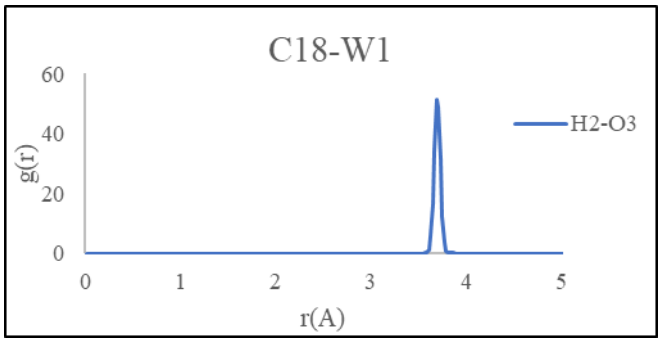

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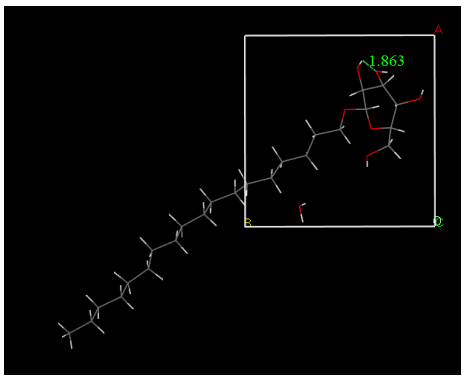
Figure 3.2 : RDF analysis for a) C12-W1 b) C12-W2 c) C12-W4 d) C18-W1

For C12-W2, the intramolecular interaction occurs at the same condition as C12-W1 which has peak at 2.15 Å depicted in Figure 3.2(b). However, the water molecules of C12-W2 possess intermolecular interaction at atom position H3-O1. This system occurs between water and water at distance 2.83 Å which involves the non-bonded van der Waals force. It shows that the water itself has stronger intermolecular forces of polar bond. The system of C12-W4 consists of higher number of water molecules which have higher tendency for possible hydrogen bond intermolecular interaction. Based on Figure 3.1(c), C12-W4 system possesses two

intermolecular hydrogen bonds with 1 water molecule at position H9-O2 and H2-O8 that explain anomalous stability of self-assemble molecules [8]. No intramolecular interaction occurs for C12-W4 system. The intermolecular interactions occur between H from water molecule attached to O of glucoside molecule and vice versa. C12-W4 system provide 4 potential binding sites, but not all four water molecules able to interact with the glucoside. It shows that C12 glucoside can only form hydrogen bond interactions with 1 water molecule. The RDF analysis of C12-W4 from Figure 3.2(c) shows that intermolecular interaction between H9-O2 is more stable than H2-O8 because of its higher peak and shortest distance. The distance for H9-O2 is 2.85 Å whereas for H2-O8 is 3.39 Å.

The high solubility of the hydrogen bonds formed where the glucoside molecule donates H atom while O atom in water is hydrogen acceptor. Furthermore, the interaction of C18-W2 and C18-W4 system did not show any hydrogen bonding interaction because of temperature dependence of glucoside [10]. The stearyl glucoside tends to have weak interaction at lower temperature since the RDF are analyzed at 50K. Figure 3.3 shows the partial labelling of difference in distance between molecule for C18-W1 and C18-W4 system. Hydrogen bond is created at distance of r < 2.5 Å while all of the distance acquired from C18-W2 and C18-W4 system is more than 2.5 Å as depicted in Figure 3.3. As can be seen, the hydrogen bonding created at C18-W1 system is due to relevant distance required which is 1.863 Å . The RDF analysis has shown the possibility of the hydrogen bonding interactions is in the following order: C12-W4 > C12-W2 > C12-W1 > C18-W1 > C18-W2 > C18-W4. The result of C12-W4 shows the fine hydrogen-bonding interaction at shortest distance and higher peak which explains the good affinity of the system.



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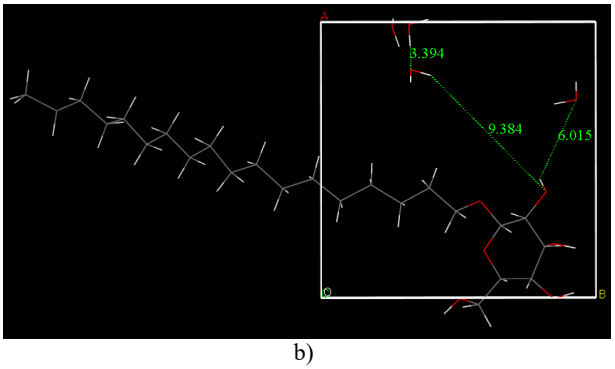

b)

Figure 3.3 : The distance of (a) C18-W1 (b) C18-W4 system

IV. Conclusion

Computer modelling simulation of molecular dynamic has shown the differences of molecular interaction of lauryl glucoside with water and stearyl glucoside with water. The analysis of the system describes that lauryl glucoside has higher solubility in water. Lauryl glucoside also possesses better intermolecular interaction based on its shorter distance and highest peak RDF analysis. Overall interaction explains that glucoside requires higher water molecules for better stability and good hydrogen bonding interaction. Thus, this simulation provides better understanding of glucoside system with water at molecular level.

Acknowledgment

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References

[1] J. Cortes-Sanchez (2013). Biological activity of glycolipids produced by microorganisms: new trends and possible therapeutic alternatives. Microbiol Res, 168(1), 22-32

[2] M.M. Fiume (2013). Safety assessment of decyl glucoside and other alkyl glucosides as used in cosmetics. Int J Toxicol, 32(5), 22S-48S.

[3] K. Hill (1999). Sugar-based surfactants for consumer products and technical applications. Lipid / Fett, 101(1), 25-3

[4] T.T. Chong (2007). Computer modelling and simulation of thermotropic and lyotropic alkyl glycoside bilayers. Liquid Crystals, 34(2), 267-281.

[5] D. Kaur (2011). Intermolecular hydrogen bonding interactions of furan, isoxazole and oxazole with water, 963(1), 71-75.

[6] P. Ball (2008). Water as an active constituent in cell biology. Chemical Reviews, 108(1), 74-108.

[7] N. Anuar (2017). Prediction of interaction of citric acid modified cellulose with water region using molecular modelling technique.

[8] Z.M. Kotena (2012). Hydrogen bonds in galactopyranoside and glucopyranoside: a density functional theory study. J Mol Model, 19(2), 589-599.

[9] X. Yu (2018). Experimental Assessment and Modeling of the Solubility of Malonic Acid in Different Solvents. Chemical Engineering & Technology, 41(6), 1098–1107.

[10] K.A. Ishak (2019). Effects of lipid packing and intermolecular hydrogen bond on thermotropic phase transition of stearyl glucoside. Journal of Molecular Liquids