

**UNIVERSITI TEKNOLOGI MARA**

**COMPUTER MODELLING OF GLUCOSIDE  
SYSTEM IN 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. A simulation using stearyl glucoside is to study the differences on the effects of interactions. The simulation shows that the system results in polymorphism and intramolecular hydrogen bonding dominates the interactions.

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# CHAPTER ONE

## INTRODUCTION

### 1.1 Research Background

Throughout various science researches, the development in research of organic chemistry has extensively increased the pace of scientific discovery. Glucoside is a form of glycosides from glucose (Pelley, 2012). Current interest considering the eccentric properties of glycosides for sustainable development (Cortes-Sanchez et.al, 2013).

Lauryl glucoside is a form of alkyl polyglucoside with twelve carbons length of alkyl chains (Fiume et.al, 2013). Alkyl polyglucosides is a sugar-based surfactant, widely used in the industry such as cosmetic and detergent (Hill et.al, 1999). There are industrial processes that require surfactants to control foaming, emulsion or even dispersion stability (Claesson et.al, 2006). It is produced from coconut oil and sugar makes it qualified as the perfectly safe ingredient with no adverse effects in cosmetic by safety assessment conducted in 2011 (Fiume et.al, 2013). The use of organic material in the form of renewable raw material allows for the sustainable development in applied research as well as providing researchers to elevate an understanding of the nature of glucoside and its interactions among the constituent molecules.

Furthermore, this amphiphile molecule consists of the hydrophilic and hydrophobic region, thus enables, self-assembles (Kotena et.al, 2012). As stated by Chong et.al, hydrogen bonds are essential for the self-assembly of glycolipids compared to other intermolecular interactions (Chong et.al, 2007). Hydrogen bonding interactions have been interesting to researcher due to its importance in various properties and reactivity of molecules (Kaur et.al, 2011). Therefore, hydrogen bonding interaction has often been studied using different type of molecules and different methods. Water can be used as a solvent in hydrogen bonding interactions. According to Ball, the water is known as active participants in biochemical processes (Ball, 2008). It is believed that water provides further understanding of the interaction between water and other molecules. Thus, water plays significant role as a solvent in the interaction of glucosides.