UNIVERSITI TEKNOLOGI MARA

DETERMINATION OF MOLECULAR INTERACTIONS OF GALACTOSIDES SOLUTION WITH WATER USING COMPUTER MODELLING

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ABSTRACT

Galactosides as carbohydrate receptors play an important roles in biological recognition events. A galactoside is a glycoside that yields galactose on hydrolysis. Examination of the extent and pattern of hydrogen bonding between water and sugar molecule hydroxyl group resulting that galactose and glucose derivatives were substantially better hydrogen bond donors. The hydrophilic region is mainly dominate by the non-bonded van der Waals force, whilst in the hydrophilic region, the long range of electrostatic interaction from hydroxyl group plays a critical role. Molecular dynamics (MD) simulation of interaction between lauryl galactoside and water were assessed by using Accelrys Material Studio 7.0. Hence, the aim of this work is to identify the most stable hydrogen bond between lauryl galactoside and water by using computational technique. The viscoelastic properties by expansion in the amorphous region was shown in the molecular dynamic. By varying the number of water molecules with lauryl galactoside, the interaction between water molecules was observed. The simulations results show that for water with 4 molecules, the interaction between water molecules and lauryl galactoside is better at higher water molecules.

TABLE OF CONTENT

CHAPTER ONE
INTRODUCTION

1.1 Research Background

Nowadays, galactosides have been widely used in pharmaceuticals production and food production industry. A galactoside is a glucosides containing galactose. By an organic moiety, the H of the OH group on carbon-1 of galactose is being replaced. Galactosides are classified into two category which includes ∝ - galactosides and β – galactosides which depends on the glycosidic bond of the galactose molecule. In this project, computer modelling is been used to determine the intermolecular interactions between the galactosides. Since galactosides have been a focus on bio-surfactant from the pharmaceuticals productions, the solubility of water with galactosides are being measured in this project.

Glycosides are named for the sugar that provides the hemiacetal group. Hence, the resultant molecule is a glucoside if the glucose provides the hemiacetal group whilst if galactose provides the hemiacetal group, the result is a galactoside (Bhavagan, 2002). The nature of these molecules captivate many industries such as food and pharmaceuticals and have been used widely as emulsifiers to stabilize suspended food mixtures (Zahrabatoul et al., 2012).

It is crucial to consider the high hydroxyl (OH) content of carbohydrates when describing the interactions of the molecules which make with solvent and protein. Radial distribution function or also being referred as pair correlation function. It is used to measure of the probability of atoms present in a spherical shell with a distance, r from central atom. By integrating radial distribution function, the number of particle surrounding a central atom or coordination number can be determined.

In this study, the interactions between lauryl galactoside and water molecules was observed with varying the number of water molecules by using a molecular modelling technique. This study was carried out with the intention to determine their specific interactions.