



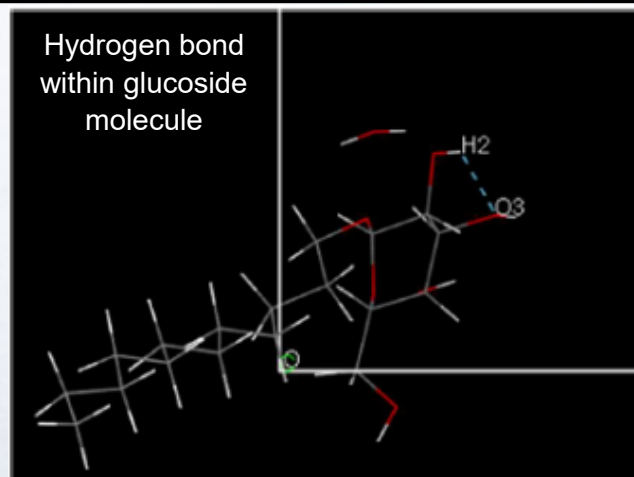
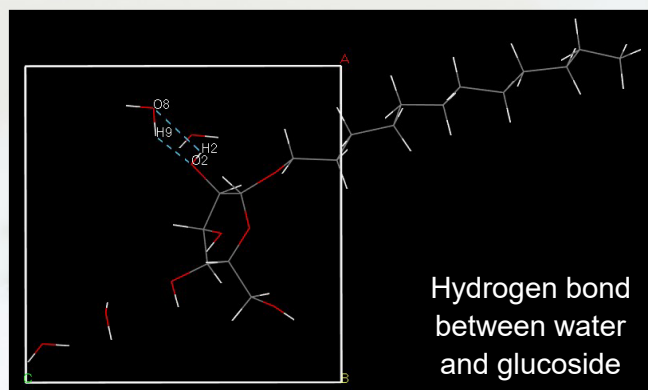
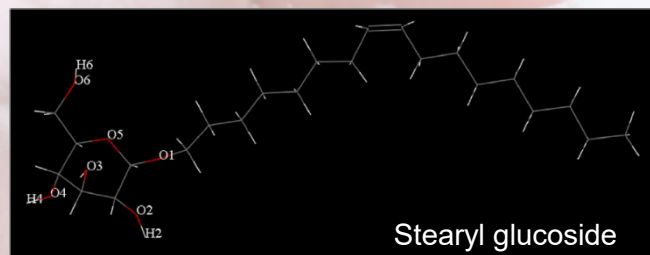
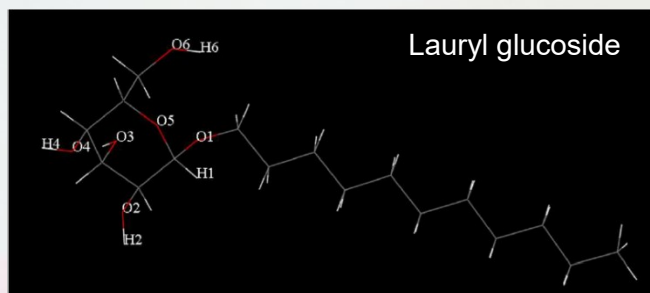
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Unveiling the Nature of Interactions between Sugar-based Surfactants and Water through Computer Modelling

by Nur Farina Mohamad Silan, Assoc. Prof. Dr. Nornizar Anuar & Dr. Nurul Fadhilah Kamalul Aripin



Alkyl poly glucosides, sugar-based surfactants widely used in the cosmetics and detergent industries, owe their functionality to their amphiphilic properties. The interaction between water and glucoside plays a crucial role in the stability of these surfactants. While previous experimental works have explored this interaction, they have not delved into the molecular-level details. This is where our study, utilizing the molecular dynamics (MD) simulation technique, makes a unique contribution. By providing detailed information on the relationship between the structures of the molecules, our study enhances the understanding of the molecular dynamics of glucosides.

In our recent study, we used molecular dynamics simulation to examine the interactions between water and two types of glucosides - lauryl glucoside (with a 12-carbon alkyl chain) and stearyl glucoside (with an 18-carbon

alkyl chain). Our findings revealed that a single water molecule establishes specific hydrogen bonds with both glucosides at the same atom position, H2-O3. However, the hydrogen bonding interaction was more pronounced in lauryl glucoside, suggesting a more robust interaction. By analysing the radial

distribution function (RDF), we observed that the elongation of the alkyl chain leads to a decline in hydrogen bonding. Furthermore, we found that water itself exhibits more vital intermolecular forces of polar bonds. The system with one molecule of lauryl glucoside and four water molecules exhibited the most favourable hydrogen-bonding interaction among the various systems we investigated.

This study provides valuable insights into the effect of water solubility on different types of glucosides. It could also help design better surfactants for various applications.

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