

The Effects of Different Sugar Head Groups on the formation of Glycolipids N-Octyl- β -D-Glycoside Micelles: A Molecular Dynamics Simulation

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Abstract

Three glycolipids n-octyl- β -D- maltopyranoside (om), n-octyl- β -D-galactopyranoside (OGal) and n-octyl- β -D-glucopyranoside (OG) were investigated for their micellar properties using molecular dynamics (MD) simulation. The effects of sugar head groups due to C4-linked hydroxyl group were investigated. Micelles of OM gave totally different geometry and radius of gyration compared to those of OG and OGal. From the simulation with Amber force field for Saccharides (Ambers), we found that OM formed bigger spherical micelles with gyration radii ranging from 8.93 to 12.27 Å while those of OGal formed micelles with gyration radii ranging from 7.47 to 11.00Å. Meanwhile OG formed a cylindrical micelle with a radius of 12.24 Å. Some of these results are qualitatively comparable to those obtained by the scattering experiments (SANS and SAXS) for the structural analysis of octyl-glycopyranoside micelles. Our results do show that different sugar head groups can affect the Physical Properties of the micelles formed.