Atomistic simulation studies of the $\alpha/\beta$-glucoside and galactoside in anhydrous bilayers: effect of the anomeric and epimeric configurations

Abstract

Fully atomistic molecular dynamics simulation studies of thermotropic bilayers were performed using a set of glycosides namely n-octyl-$\beta$-D-glucopyranoside ($\beta$-C8Glc), n-octyl-$\alpha$-D-glucopyranoside ($\alpha$-C8Glc), n-octyl-$\beta$-D-galactopyranoside ($\beta$-C8Gal), and n-octyl-$\alpha$-D-galactopyranoside ($\alpha$-C8Gal) to investigate the stereochemical relationship of the epimeric/anomeric quartet linear glycolipids with the same octyl chain group. The results showed that, the anomeric stereochemistry or the axial/equatorial orientation of C1–O1 ($\alpha/\beta$) is an important factor controlling the area and $d$-spacing of glycolipid bilayer systems in the thermotropic phase. The head group tilt angle and the chain ordering properties are affected by the anomeric effect. In addition, the $L_C$ phase of $\beta$-C8Gal, is tilting less compared to those in the fluid $L_{\alpha}$. The stereochemistry of the C4-epimeric (axial/equatorial) and anomeric ($\alpha/\beta$) centers simultaneously influence the inter-molecular hydrogen bond. Thus, the trend in the values of the hydrogen bond for these glycosides is $\beta$-C8Gal > $\alpha$-C8Glc > $\beta$-C8Glc > $\alpha$-C8Gal. The four bilayer systems showed anomalous diffusion behavior with an observed trend for the diffusion coefficients; and this trend is $\beta$-C8Gal > $\beta$-C8Glc > $\alpha$-C8Gal > $\alpha$-C8Glc. The “bent” configuration of the $\alpha$-anomer results in an increase of the hydrophobic area, chain vibration and chain disorganization. Since thermal energy is dispensed more entropically for the chain region, the overall molecular diffusion decreases.


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