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Computer modelling and simulation of thermotropic and lyotropic alkyl glycoside bilayers
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Abstract
Simulations on bilayers have previously proven their ability to provide insights to membrane function, e.g. cell fusion. Most simulations are based on the major components of cell membranes, which are phospholipids and cholesterol. Membranes can be explained based on hydrophilic and hydrophobic interactions permeated through hydrogen bonding, van der Waals interactions and repulsion forces. Whereas especially phospholipids have gained significant attention in bio-related modelling and simulations, glycolipids, which constitute another major component of cell membranes, have not been likewise studied. Here we present the simulation of bilayers for the six most common and simple stereoisomeric glycolipids, namely the α- and β-octyl glycosides of glucose, galactose and mannose, in both thermotropic and lyotropic systems. All these compounds form thermotropic smectic A phases and can exhibit lyotropic lamellar assemblies. We have studied the hydrogen bonding and linked the results to the temperature stability of the corresponding liquid crystal phase. Besides a mesophase-stabilizing effect of hydrogen bonding in general, we found that thermal stability appears to be particularly affected by intralayer hydrogen bonding. The simulations also confirmed a significant difference in the density of the lipophilic region for α- and β-glycosides, which has previously been used to explain differences in clearing temperatures.

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