

MOLECULAR DYNAMICS SIMULATION OF GLYCOLIPIDS BILAYER

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Membrane components are not uniformly (randomly) distributed in the membrane plane, they are associated into clusters or domains of different composition and size [Schroeder, F. *et al.* **Proc. Soc. Exp. Biol. Med.** 196 (1991) 235]. Biologically the most important example are rafts, lipid domains present in the outer cellular membrane composed of saturated sphingolipids, glycolipids, and Cholesterol. Rafts are involved in numerous cellular processes such as intercellular signaling, cell recognition, phagocytosis, apoptosis, and cellular transport [Simons, K. and Ikonen, E. **Nature** 387 (1997) 569]. In order to understand the atomic level mechanisms leading to raft formation, series of molecular dynamics simulations of lipid bilayers composed of glycolipids were performed. Glycolipids are vital component of lipid rafts. The simulations were performed using GROMACS software. Lipid bilayers used in these studies are composed of 128 molecules of di-palmitoyl glycerolo-glucose and shale of water (3600 water molecules). Due to lack of glycolipid simulations described in literature, four different bilayers using different combination of force fields were tested. For alkyl chains all and united atom OPLS or united atom modified OPLS parameters were used, for water, TIP3P or SPC parameters were used, and for glucose headgroup extended OPLS parameters for carbohydrates were used. Comparative analysis of all models and their verification against experimental results allow as to select the best simulation protocol.

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