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Title: Molecular Dynamics Study on effects of Concentrations of GM1 ganglioside on physical properties of the phospholipid membranes

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A series of molecular dynamics (MD) simulations of fully hydrated DPPC bilayers containing GM1 gangliosides at several different concentrations (from 0 to 25 mol %) has been carried out to investigate the effect of GM1 on the structure and dynamics of the lipid membrane. Using the newly developed CHARMM force field for GM1 ganglioside, we carried out 100 ns-NPT-MD simulation of each GM1-DPPC membrane system. With increasing the GM1 concentration, the lipid membrane gradually becomes more rigid; the cross-sectional area per lipid was decreased, the order parameter of the hydrophobic tails was increased, and the lateral diffusion and the rotational relaxations of headgroups of GM1 and DPPC were slowed down. The structural analysis of GM1 molecules revealed that the oligosaccharide chain mostly extended toward aqueous solution and seldomly lay on the lipid bilayer plane. The structure and dynamics of water near the GM1/DPPC bilayer surface were also investigated. The orientational distribution of the water dipole with respect to the bilayer normal was calculated. At the low concentration of GM1 (e.g., 5