MOLECULAR DYNAMICS SIMULATIONS OF UNSATURATED DIACYLGLYCEROLIPID MONOLAYERS

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Molecular dynamics (MD) simulations were performed for six model monolayers of diacylglycerolipids (DG) with different number of *cis* double C=C bonds of the *sn*-2 hydrocarbon chains: 18:0, 18:1ω9, 18:2ω6, 18:3ω3, 20:4ω6 or 22:6ω3; the *sn*-1 18:0 chain was the constituent of all the DG molecules. The simulation systems consisted of 48 identical lipid molecules arranged in a rectangular box, with periodic boundary conditions in the surface plane (X, Y directions). The tails of the lipid molecules were treated in accordance with their real chemical structure and the molecule head groups were approximated by united atoms. All the atoms in the monolayer systems were treated classically. The simulation parameters have provided a liquid crystalline phase of the monolayers. The simulations were carried out under two different conditions: (i) the surface area per molecule A = const, (ii) the pressure of the systems P = const. The temperature T and the number of atoms N were always fixed. Several monolayers were investigated under different temperatures. The "velocity Verlet" algorithm was used for integration of Newton's equations of motion, the simulation time step was 1 fs. The time of each computation was 1000 ps.

A number of various properties including structural parameters, the C-C and C-H bond order parameters of the hydrocarbon chains (S_{CC} and S_{CH}), the bond-vector orientation distribution functions, and the mass density profiles for all the atoms and groups of atoms along the monolayer normals were calculated. The effect of the degree of unsaturation of the *sn*-2 hydrocarbon chains of the five DG monolayers compared to the fully saturated one as well as the temperature influence on the lipid properties have been investigated.

The $-S_{CH}$ profiles of *sn*-1 chains of all the monolayers are qualitatively similar to those obtained in experimental studies: there is a plateau region for the several CH_2-groups next to the head group, then the $-S_{CH}$ values drop towards zero. For all the unsaturated chains the dips in the values are observed near the locations of C=C bonds. The S_{CC} values of double bonds are higher than those calculated for adjacent single bonds. Both the bond order profile results and the results of the treatment of the bond orientation distributions can explain the high flexibility of unsaturated chains and allow to understand the mechanism of increasing the membrane fluidity with the increase of the degree of unsaturation of lipids. It is shown that temperature sensitivity of the DG properties is greatly dependent on the number of C=C bonds in the *sn*-2 chain. Hydrocarbon chains of highly unsaturated lipids are characterized by higher mobility and lower temperature sensitivity. These properties explain the role of polyunsaturated lipids in the temperature adaptations of biological membranes.

The results of this MD simulation are in a good (qualitative) agreement with the available experimental data and other computer simulations of similar systems.

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