MOLECULAR DYNAMICS SIMULATIONS OF HYDRATED UNSATURATED PHOSPHATIDYLCHOLINE BILAYERS

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Molecular dynamics (MD) simulations were carried out for hydrated bilayers of 1,2-stearoyl-*sn*-glycero-3-phosphatidylcholine (PC), 1-stearoyl-2-oleoyl-*sn*-glycero-3-PC, 1-stearoyl-2-linoleoyl-*sn*-glycero-3-PC, 1-stearoyl-2-linolenoyl-*sn*-glycero-3-PC, 1-stearoyl-2-arachidonoyl-*sn*-glycero-3-PC, and 1-stearoyl-2-docosahexaenoyl-*sn*-glycero-3-PC. The simulation boxes of the bilayers consisted of 96 PC molecules and 2304 water molecules (48 lipid molecules per layer and 24 H_2O molecules per lipid). The structure of lipid molecules (the two hydrocarbon tails, the glycerol section, the head group of PC) were treated in accordance with their real chemical structure, all hydrogen atoms were included explicitly in the calculations. The C-H and C-C bond order parameter $-S_{CH}$, S_{CC} profiles of the hydrocarbon tails, the bond orientation distribution functions and the root-mean-square values of the positional fluctuations of the lipid chain carbons, mass density and charge density profiles along the bilayer normal (Z) for different atoms and groups of atoms were calculated. Simulation results are compared to the available experimental data and to other computer investigations of these lipid molecules. The mass density profiles of the bilayer systems have two peaks (the locations of the phosphate groups) and a minimum (or plateau) near the center of the bilayers. The minimum of polyunsaturated bilayer is deeper than that for monounsaturated one. The distribution of the N is wider than that of the P. The distribution of the head group and glycerol unit overlap weakly. Some of the carbon atom distributions are polymodal: the mass density picture is rather complex. The mass density distributions of the glycerol backbone carbons are the narrowest in the PC molecule. The charge distributions for the various parts of the PC molecule have similar characteristics for the six bilayer systems. A region with negative charge (due to the phosphate) is bracketed by regions of positive charge (due to the choline group). The order-parameter characteristics of lipid hydrocarbon chains in the "liquid" region of the bilayer (somewhat remote from the membrane-water interface) are qualitatively similar to those of single unperturbed hydrocarbon chains: the behavior of the acyl chains in this region is dominated by the intramolecular short-range interactions. The long-range interactions of the segments of the lipids in this region of the bilayer and the interactions with atoms of the bilayer-water interface may be considered as a disturbance: the intermolecular interactions are largely used to orient the lipid molecules in the direction of the membrane normal. A close relationship between the investigated characteristics and the structure of the chains is elucidated: the number of the chain carbons, the number of cis double bonds and their position in the chain determine principally the calculated properties. Some aspects of the physical properties of unsaturated lipids and their biological significance are discussed.

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