STRUCTURAL/FUNCTIONAL ADAPTATION OF PROTEINS TO MEMBRANE ENVIRONMENT

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Apart from the barrier role, cell membranes fulfill the equally important task of providing an effective accommodation of numerous external agents, including membrane proteins (MPs). Molecular mechanisms of such processes have been poorly studied, but recently it has been shown that the most important property of lipid bilayers is their dynamic heterogeneous character, which critically depends on their local structural features (up to ~ 1 nm), hydrophobic and electrical properties, and so on. Moreover, when analyzing membranes, it is necessary to take into account the parameters of their dynamic behavior at times from 10 ps. The totality of these factors represents the so-called. "membrane response", i.e. active reaction of the water-lipid medium to interacting external molecules. Thus, the study of protein-membrane systems is possible only if mutual influence (adaptation) of partners at the molecular level is taken into account. One of the most informative methods for solving such problems is atomistic computer modeling. A computational approach to the analysis of the structural and dynamic parameters of model membranes has been developed. It is established that local changes in the membrane environment play an important role in the binding of peptides and MPs, causing specific clustering of lipids and initiating the formation of defects in the membrane. It is shown for the first time that lipids make a significant contribution to the free energy of spontaneous dimerization of MPs. Thus, MPs and their water-lipid environment equally determine the nature of the biological behavior of cell membranes, mutually strongly affecting each other and responding to external influences in a self-consistent manner.