

“Dynamic molecular portraits” of biomembranes: a computational insight

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Motivation and Aim: To date, it has been reliably shown that the lipid bilayer/water interface can be thoroughly characterized by a sophisticated so-called “dynamic molecular portrait”. The latter reflects a combination of time-dependent surface distributions of various physicochemical properties, inherent in both model lipid bilayers and natural multi-component cell membranes. One of the most important features of biomembranes is their mosaicity, which is expressed in the constant presence of lateral inhomogeneities, the sizes and lifetimes of which vary in a wide range—from 1 to 10³ nm and from 0.1 ns to milliseconds. In addition to the relatively well-studied macroscopic domains (so-called “rafts”), the analysis of micro- and nanoclusters (or domains) that form an instantaneous picture of the distribution of structural, dynamic, hydrophobic, electrical, etc. properties at the membrane-water interface is attracting increasing interest. This is because such nanodomains (NDs) have been proven to be crucial for the proper membrane functioning in cells. Therefore, an understanding with atomistic details the phenomena associated with NDs is required.

Results: The present work describes the recent results of *in silico* studies of spontaneously formed NDs in lipid membranes. The main attention is paid to the methods of ND detection, characterization of their spatiotemporal parameters, the elucidation of the molecular mechanisms of their formation. Biological role of NDs in cell membranes is discussed. In particular, self-adaptation of “dynamic molecular portraits” of membrane peptides/proteins and lipids/water is considered in atomistic simulations.

Conclusion: Understanding such effects creates the basis for rational design of new prospective drugs, therapeutic approaches, and artificial membrane materials with specified properties.

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