

Coarse-grained molecular dynamics simulation of DPPC membrane self-assembly in the presence of amyloid beta 25-35 peptides

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At the present time there is a hypothesis about the key role of amyloid beta peptide in the onset of Alzheimer's disease. It is considered that its interaction with cell membranes causes a disruption of their permeability and integrity, which may trigger further neurodegenerative processes. The experimental study showed that the peptide takes part in the morphological changes of the phospholipid membrane during its transition through the main lipid phase transition temperature. However, this study does not allow us to look into the processes and resulting structures at the atomic level, as a result of which theoretical studies were carried out.

In order to describe the assembly process of phospholipid membranes in the presence of amyloid beta peptides, the interaction of A β (25-35) with zwitterionic DPPC phospholipids was simulated using the coarse-grained molecular dynamics method in the GROMACS 2019.3 software package. It was found that at a temperature below the phase transition temperature of the lipid, the system assembled into bicelle-like structures with peptides on the rim, while at a temperature above the phase transition temperature, it assembled into a system of small vesicles with peptides embedded in the lipid bilayer. The results obtained are in good agreement with earlier experimental results and complement the picture of what is happening in phospholipid membranes.

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