Interactions of transmembrane peptides with lipid environment as probed by molecular dynamics simulations

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Annotation

Membrane proteins comprise about a quarter of all proteins in the cell and are prioritized targets of modern and developing therapeutic methods since they can transport signals and molecules through membrane. The role of lipid environment is not fully understood although the huge variety of mechanisms of membrane proteins functioning is already described. Neuraminidase is an enzyme which cleaves sialic acid residues from glycoproteins and glycolipids on the cell membrane surface. Dysfunction of neuraminidase is directly related to serious neurodegenerative genetic diseases, which currently have no effective methods of treatment.

This work is a complex study of a behavior of transmembrane domain of human neuraminidase-1 in the lipid environment using molecular dynamics (MD) method. In this work, three 500-ns MD trajectories of systems composed of α-helical peptide differently incorporated into the hydrated lipid bilayer. Several structural and dynamic features for each simulated trajectory were obtained, the behavior of α-helical transmembrane fragment was described and peptide-lipid interactions were analyzed.