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Multiscale MD Simulations of Folding Dynamics and Mobility of Beta-Amyloid Peptide on Lipid Bilayer Surfaces[1] SCOTT VAN TILBURG, KELVIN CHENG, Trinity University — Early interaction events of beta-amyloid peptides with the neuronal membranes play a key role in the pathogenesis of Alzheimer's disease. We have used multiscale Molecular Dynamics (MD) simulations to study the protein folding dynamics and lateral mobility of beta-amyloid protein on the cholesterol-enriched and -depleted lipid nano-domains. Several independent simulation replicates of all-atom and coarse-grained MD simulations of beta-amyloid on different lipid bilayer nano-domains have been generated. Using Define Secondary Structure of Proteins (DSSP) algorithm and mean-square-distance (MSD) analysis, the protein conformation and the lateral diffusion coefficients of protein, as well as the lipid and water, were calculated as a function of simulation time up to 200 nanoseconds for atomistic and 2 microseconds for coarse-grained simulations per replicate in different bilayer systems. Subtle differences in the conformation and mobility of the protein were observed in lipid bilayers with and without cholesterol. The structural dynamics information obtained from this work will provide useful insights into understanding the role of protein/lipid interactions in the membrane-associated aggregation of protein on neuronal membranes.

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