Abstract Submitted
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Exploring the Membrane Association Behavior of Beta-Amyloid Protein Using Multiscale MD Simulations[1] YIYI CAO, Trinity University, SARA CHENG, University of Texas at Austin, CAMPBELL COMPTON, HOA NGUYEN, K. CHENG, Trinity University — Interactions of beta-amyloid (A-beta) protein with lipid membranes have been linked to Alzheimer's disease (AD). At present, the mechanisms of A-beta/lipid interactions remain unclear. Using a multiscale molecular dynamics (MD) simulation technique, we have investigated the membrane-association behavior of A-beta in a lipid bilayer. The protein was initially in a gamma or alpha state and associated with the membrane surface. The protein in the gamma state was mostly in random coil. However, the protein in the alpha state comprised of alpha-helix and random coil structures and with the hydrophobic lipid insertion domain embedded in the lipid hydrocarbon region. Using a coarse-grained (CG) MD simulation, the gamma state detached from while the alpha state remained attached to the membrane. Applying a reverse mapping (CG to atomistic) procedure and a subsequent atomistic simulation, the alpha state still remained attached to the membrane. We propose that the association of the lipid insertion domain with the hydrocarbon region of the membrane is important to stabilize the membrane association behavior of A-beta. This membrane associate behavior might play a key role in the self-aggregation of A-beta on the 2D membrane surface that eventually lead to AD.

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