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Amyloid protein unfolding and insertion kinetics on neuronal membrane mimics[1] LIMING QIU, CREIGHTON BUIE, MARK VAUGHN, KWAN CHENG, Texas Tech University, BIOCOMPUTATION GROUP COLLABORATION — Atomistic details of beta-amyloid (Aβ) protein unfolding and lipid interaction kinetics mediated by the neuronal membrane surface are important for developing new therapeutic strategies to prevent and cure Alzheimer's disease. Using all-atom MD simulations, we explored the early unfolding and insertion kinetics of 40 and 42 residue long Aβ in binary lipid mixtures with and without cholesterol that mimic the cholesterol-depleted and cholesterol-enriched lipid nanodomains of neurons. The protein conformational transition kinetics was evaluated from the secondary structure profile versus simulation time plot. The extent of membrane disruption was examined by the calculated order parameters of lipid acyl chains and cholesterol fused rings as well as the density profiles of water and lipid headgroups at defined regions across the lipid bilayer from our simulations. Our results revealed that both the cholesterol content and the length of the protein affect the protein-insertion and membrane stability in our model lipid bilayer systems.

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