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Molecular Dynamics Simulation of protein unfolding on lipid nanodomains LIMING QIU, MARK VAUGHN, KWAN CHENG, Texas Tech University — Beta amyloid (beta-40), a short peptide associated with Alzheimer disease, can exist in the alpha-helix, beta-sheet or global conformation depending on its environment. The role of self-assembling lipid nanodomains on the conformational transition of this peptide was examined using Coarse-grained MD simulations. A stable cholesterol superlattice consisting of phosphatidylcholine and cholesterol was constructed to mimic the neuronal membrane. The unfolding kinetics of beta-40 on this superlattice surface as compared with that in solution was determined. Our results suggest a critical role of the nanostructure of lipid surface on protein unfolding at a biologically relevant time scale of hundreds of nanoseconds.

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