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Conformation transition of betaA in solution and on surface of lipid bilayer LIMING QIU, ANDREW REAY, QING ZHU, MARK VAUGHN, KWAN CHENG — Beta amyloid (betaA) is a 39 to 43 residue peptide generated by a proteolytic cleavage of a large transmembrane amyloid precursor protein in neuronal membranes. The misfolding and self-aggregation of betaA, as well as its interactions with neuronal membranes, have been linked to the early onset of pathogenesis of Alzheimer disease. The secondary structure conformational transition of betaA from an alpha-helix to beta-sheet in some key regions of the peptide represents an important signature of the complex misfolding behavior of betaA. Using all-atom molecular dynamics simulations, the conformation changes of betaA in solution and on the surface of lipid bilayer containing nanodomains of cholesterol have been studied. Our results indicated that the appearance of beta-sheet structures depends strong on the initial structures of betaA and the arrangement of cholesterol molecules in the lipid bilayer.

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