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Atomistic MD simulations reveal the protective role of cholesterol in dimeric beta-amyloid induced disruptions in neuronal membrane mimics LIMING QIU, CREIGHTON BUIE, SARA CHENG, GEORGE CHOU, MARK VAUGHN, Texas Tech University, K. CHENG, Trinity University — Interactions of oligomeric beta-amyloid peptides with neuronal membranes have been linked to the pathogenesis of Alzheimer's disease (AD). The molecular details of the interactions of different lipid components, particularly cholesterol (CHOL), of the membranes with the peptides are not clear. Using an atomistic MD simulations approach, the water permeability barrier, structural geometry and order parameters of binary phosphatidylcholine (PC) and PC/CHOL lipid bilayers were examined from various 200 ns-simulation replicates. Our results suggest that the longer length dimer (2 x 42 residues) perturbs the membrane more than the shorter one (2 x 40 residues). In addition, we discovered a significant protective role of cholesterol in protein-induced disruptions of the membranes. The use of a new Monte-Carlo method in characterizing the structures of the conformal annular lipids in close proximity with the proteins will be introduced. We propose that the neurotoxicity of beta-amyloid peptide may be associated with the nanodomain or raft-like structures of the neuronal membranes in-vivo in the development of AD.

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