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Mechanism of physicochemical interactions of four Aβ42 peptids onto GM1 ganglioside-containing lipid membrane

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The physicochemical interaction of amyloid β (Aβ)-peptide with cell membrane and the subsequent aggregation of Aβ have been reported to be involved in dozens of neurodegeneration diseases including Alzheimer's disease. In this work, molecular dynamics (MD) simulation for four Aβ42s was performed to investigate the behaviors of Aβ42s on GM1-ganglioside-containing lipid membrane. The initial atom coordinate of Aβ42 were extracted from one of the conformations which had been determined by solution nuclear magnetic resonance (NMR) spectroscopy (PDB accession code: 1Z0Q). A computational model for mixed membrane was composed of 48 monosialotetrahexosylganglioside (GM1), 96 sphingomyelin (SM) and 96βcholesterol (CHL). A 1000ns simulation was executed with NAMD 2.9 programs to analyze the probability of the Aβ binding to the mixed lipid membrane. The hydrogen bond occupancy was calculated using visual molecular dynamics (VMD). Our MD simulation showed that Aβ42s were tightly bounds to GM1-contaning lipid membrane and hardly detached from the membrane during the simulation. The molecular principal axis was almost parallel to the membrane surface through the simulation. The secondary structures of four Aβ42s through MD simulations were examined, which indicated that the most frequent structure was helixβbut the residues 29~42 was strand form due to high hydrophobicity. Since, The h-bound interaction between Aβs was initially observed in C-terminal hydrophobic region and finally extended to the N-terminal that established close contact with the membrane. The complex of Aβs with the membrane was efficient to increase hydrophobicity at this area and plays a critical role in the oligomerization.

Biography

Majid Vahed has completed his MS from Azad University and Doctoral studies from Chiba University School of Medicine. He is a Researcher and his research work focuses on "Molecular dynamic simulation of Alzheimer's disease". He has published more than two papers in international journals and has one patent.

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