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Role of aromatic interaction in adhesion of amyloid beta peptides on glycolipid containing membrane

Vahed Majid[1], Hoshino Tyuji[1], Yoneda Tomoki[1], Neya Saburo[1], Mohammad Vahed[1] and **Matsuzaki Katsumi[2]**
[1]Chiba University, Japan
[2]Kyoto University, Japan

The CH−π and OH−π interaction of aromatic residues of amyloid beta (Aβ) with GM1 oligosaccharide is concluded to be effective to keep Aβ peptides attached to the membrane surface and play an important role to initial stages of Alzheimer's disease pathology. In this work, molecular dynamics (MD) simulations for Aβ42 were performed to investigate the behaviors of Aβ42 on GM1-ganglioside-containing lipid membrane. As far the computational model, 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/1IYT). A computational model for mixed membrane was composed of 48 monosialotetrahexosylganglioside (GM1), 96 sphingomyelin (SM), and 96 cholesterol (CHL). A 1000 ns 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) software. The results showed that binding affinity of Aβs were increases with GM1 in lipid membrane, suggesting the involvement of OH−π and CH-π interaction between the aromatic side chains of sugar carbohydrate moieties of GM1 with aromatic rings of Aβs. The aromatic rings of Phe4, Tyr10, Phe19, and Phe20 of Aβ was within distance that enabled CH−π and/or OH−π stacking interaction with to the GM1 head groups. In this seminar, I will discuss the cluster of GM1-ganglioside containing lipid membrane model and how effect to amyloid beta tightly connection with lipid membrane and subsequently, conformation transformation to toxicity folding shape, in recent study.

Biography

Vahed Majid has his expertise in Pharmaceutical and Neuroscience, especially in dementia. One of the major of his researches is focuses on Alzheimer's disease (AD). His laboratory designed a calculation model consisting of GM1-containing mixed lipid membrane, according to earlier study: He has identified a specific form of Aβ that was bound to monosialoganglioside GM1, a sugar lipid, in brains of patients who exhibited the early pathological changes associated with AD. Despite investigate of mechanism of AD, he studies chemical inhibitor to turn off the signal cell death and make agents to the early detection of early AD for development of a PET/SPECT amyloid imaging.

vahed.majid@chiba-u.jp

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