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Title: Diffusion Studies of Amyloid Beta Peptide in Bicelle

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Abstract: We studied the diffusion of amyloid beta peptide(25-35) inside bicelle using Pulse field gradient(PFG) Nuclear Magnetic Resonance(NMR) and molecular dynamics simulations. Amyloid beta peptide(A) is the main constituent of senile plaque in the Alzheimer's disease. The neurotoxic fragment A β (25-35) can intercalate into the lipid bilayers and affect the dynamics of bilayers. PFG NMR experiments were conducted for samples A β (25-35), bicelle(DMPC/DHPC) and A β (25-35) inside bicelle. We calculated the diffusion coefficient for A β (25-35), bicelle(DMPC/DHPC) and A β (25-35) inside bicelle. A linear diffusion pattern was observed for A β (25-35) as well as bicelle alone samples. But when we incorporated A β (25-35) into bicelle both systems were following anomalous diffusion. The NMR experiment results were validated by molecular dynamics simulations using the MD package Groningen Machine for Chemical Simulations(GROMACS). We did 2-dimensional homonuclear and heteronuclear NMR experiments for studying the structure of A β (25-35) in bicelle.

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