

## 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 $\beta$ (25-35) can intercalate into the lipid bilayers and affect the dynamics of bilayers. PFG NMR experiments were conducted for samples A $\beta$ (25-35), bicelle(DMPC/DHPC) and A $\beta$ (25-35) inside bicelle. We calculated the diffusion coefficient for A $\beta$ (25-35), bicelle(DMPC/DHPC) and A $\beta$ (25-35) inside bicelle. A linear diffusion pattern was observed for A $\beta$ (25-35) as well as bicelle alone samples. But when we incorporated A $\beta$ (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 $\beta$ (25-35) in bicelle.