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Poster 2

Structural Study of Neuropeptides in Trifluoroethanol-Water Mixture Using NMR Spectroscopy and Molecular Dynamics Simulation

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The three-dimensional structures of neuropeptides, β amyloid peptide fragment 25-35(Aβ25-35), neuromedin B(NMB), and substance P(SP) in trifluoroethanol(TFE)-water mixture solvent were determined by NMR spectroscopy. All the peptides adopt similar α-helical conformation in their C-terminal regions. In order to examine the influence of the solvent, molecular dynamics(MD) simulations were carried out in water and in a solvent containing 50%(v/v) TFE under periodic boundary conditions. In both cases, restrained-minimized average structure of Aβ25-35 in 50% TFE solution obtained from NMR data was used as the initial structure. These results will increase the understanding about the mechanism of peptide folding or unfolding process according to the solvent environment.