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Structural and Thermodynamic Properties of Amyloid-β Peptides: Impact of Fragment Size T. KITAHARA, O. WISE-SCIRA, O. COSKUNER — Alzheimer's disease is a progressive neurodegenerative disease whose physiological characteristics include the accumulation of amyloid-containing deposits in the brain and consequent synapse and neuron loss. Unfortunately, most widely used drugs for the treatment can palliate the outer symptoms but cannot cure the disease itself. Hence, developing a new drug that can cure it. Most recently, the "early aggregation and monomer" hypothesis has become popular and a few drugs have been developed based on this hypothesis. Detailed understanding of the amyloid-β peptide structure can better help us to determine more effective treatment strategies; indeed, the structure of Amyloid has been studied extensively employing experimental and theoretical tools. Nevertheless, those studies have employed different fragment sizes of Amyloid and characterized its conformational nature in different media. Thus, the structural properties might be different from each other and provide a reason for the existing debates in the literature. Here, we performed all-atom MD simulations and present the structural and thermodynamic properties of Aβ_{1-16}, Aβ_{1-28}, and Aβ_{1-42} in the gas phase and in aqueous solution. Our studies show that the overall structures, secondary structures, and the calculated thermodynamic properties change with increasing peptide size. In addition, we find that the structural properties of those peptides are different from each other in the gas phase and in aqueous solution.

Taizo Kitahara

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