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Amyloid-β Fibrils Remodeling by an Organic Molecule: Insight from All-Atomic Molecular Dynamics Simulations

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Abstract : Alzheimer's disease (AD) is one of the most common forms of dementia, which is caused by misfolding and aggregation of amyloid beta (Aβ) peptides into amyloid-β fibrils (Aβ fibrils). To disrupt the remodeling of Aβ fibrils, a number of candidate molecules have been proposed. To study the molecular mechanisms of Aβ fibrils remodeling we performed a series of all-atom molecular dynamics simulations, a total time of 3μs, in explicit solvent. Several previously undiscovered candidate molecule-Aβ fibrils binding modes are unraveled; one of which shows the direct conformational change of the Aβ fibril by understanding the physicochemical factors responsible for binding and subsequent remodeling of Aβ fibrils by the candidate molecule, open avenues into structure-based drug design for AD can be opened.

Keywords : alzheimer's disease, amyloid, MD simulations, misfolded protein
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