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Comparison and Analysis of 3,4 dihydrocylmandelic acid (DHMA) and noremetanephrine (NMN) on Amyloid-Beta 40 Monomer for treatment of Alzheimer's Disease using Molecular Dynamics Simulation WOOSUNG CHOI, Georgia Inst of Tech, SANG EUN JEE, Washington University in Saint Louis, SEUNG SOON JANG, Georgia Inst of Tech — Alzheimer's disease (AD) is type of degenerative dementia caused memory loss and behavior problem. Main reason of AD is Amyloid-Beta 40(Aβ) mostly composed of α -helix form misfolds to insoluble fibrils and soluble oilgomer. This insoluble fibrils aggregate with beta sheet structure and form the plaque which is caused nurotoxicity in brain. Both 3,4 dihydrocylmandelic acid (DHMA) and noremetanephrine (NMN) are the metabolite of norepinephrine in brain . Also these are inhibit the changing formation of fibrils and maintain the α –helix structure. In this computational modeling study, both NMN and DHMA molecules were modified and analyzed for specific effect on the Aβ-monomer using molecular dynamics simulation. Using molecular dynamic simulation, NMN and DHMA act as modulator on three Aβ-monomer batches and could observe the conformational changing of these Aβ-monomer under the physiologocal condition. This computational experiment is designed to compare and analyze both of chemicals for determining which chamecal would be more effective on the conformation of Aβ 40 monomer.

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