عنوان مقاله:

Molecular Dynamic Simulation of α-synuclein Aggregation and Investigation of it,s Effective Factors

محل انتشار:

بیست و یکمین کنفرانس شیمی فیزیک انجمن شیمی ایران (سال: 1397)

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خلاصه مقاله:

Parkinson’s disease (PD) is the second most common neurodegenerative disorder, afflictingnearly 1% of the population over the age of 60 years. Aggregation of α-syn leading todopaminergic neuronal death has been recognized as one of the main pathogenic factors in theinitiation and progression of PD. Consequently, α-syn has been targeted for the development oftherapeutics for PD.Human α-syn is a natively unfolded 140-amino-acidresidue protein widely expressed inneurons, found predominantly in presynaptic terminals [1-3]. Structurally, α-synuclein features anN-terminal domain (residues 1–60), a central hydrophobic portion denoted as non-amyloid betacomponent (NAC, residues 61–95) and a C-terminal negatively charged region (residues 96–140). NAC domain, is required for alpha-synuclein to polymerize into amyloid filaments, whichare the major components of alpha-synuclein pathological inclusions.Here we present the mechanisms and kinetics of NAC domain of α-synuclein aggregationusing the molecular dynamics simulation method, as well as crucial factors affecting thisprocess.The results of the simulation studies were presented as structural data like hydrogenbonding, interacting residues and various distribution functions as well as energetics of theconsidered system. The interaction energies, and the contribution of lennard-Jones andelectrostatic interactions in intarction energy have been also analysed.

کلمات کلیدی:

Parkinson Disease, α-Synuclein, Aggregation, Molecular Dynamic Simulation