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Understanding the conformational dynamics of intrinsically disordered protein α-Synuclein in urea and Trimethylamine oxide (TMAO)

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Intracellular inclusion of aggregated and misfolded α-synuclein is the major cause of Parkinson's disease (PD) that leads to the degradation of dopaminergic neurons in the brain cells. α-synuclein aggregates are found in Lewy bodies which is the characteristics of PD. Understanding the mechanism of α-synuclein aggregation will facilitate the problem of dealing with neurodegenerative diseases in general and that of PD in particular. In our study, the mechanism of aggregates formation and behaviour of α-synuclein in presence of denaturing osmolyte 'urea' and protecting osmolyte 'TMAO' has been investigated through molecular dynamic (MD) simulation at various concentrations. Behaviour of α−synuclein in water at different temperature has also been investigated. Both of these osmolytes have contrasting effect on α−synuclein. Urea being a denaturing osmolyte, leads to extended conformation of protein by interacting more with α−synuclein through hydrogen bonds formation however; compact conformation has been adopted by protein in presence of TMAO. Along with the experimentally know region 61-95, some other regions of α−synuclein have also been identified which have the propensity to form an aggregates. Dynamics of water molecules has also been investigated and is correlated with the aggregation property of α-synuclein.

Biography

Ishrat Jahan is working as a postdoctoral fellow at Department of Chemistry, Indian Institute of Technology Delhi, India. Currently, working on understanding the aggregation behaviour of alpha-synuclein in silico and *in vitro*.

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