TEMPERATURE DEPENDENT AGGREGATION MECHANISM AND PATHWAY OF LYSOZYME: BY ALL ATOM AND COARSE GRAINED MOLECULAR DYNAMICS SIMULATION

Shahee Islam[1], Zarrin Shahzadi[1], and Chaitali Mukhopadhyay[1]

[1]University of Calcutta

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Abstract

Aggregation of protein causes various diseases including Alzheimer's disease, Parkinson's disease, and type II diabetes. It was found that aggregation of protein depends on many factors like temperature, pH, salt type, salt concentration, ionic strength, protein concentration, co solutes. Here we have tried to capture the aggregation mechanism and pathway of hen egg white lysozyme using molecular dynamics simulations at two different temperatures; 300K and 340K. Along with the all atom simulations to get the atomistic details of aggregation mechanism, we have used coarse grained simulation with MARTINI force field to monitor the aggregation for longer duration. Our results suggest that due to the aggregation, changes in the conformation of lysozyme are more at 340K than at 300K. The change in the conformation of the lysozyme at 300K is mainly due to aggregation where at 340K change in conformation of lysozyme is due to both aggregation and temperature. Also, a more compact aggregated system is formed at 340K.

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