

Simulating Proteins and their Polymerization through Evolution Techniques

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Abstract: Proteins are being very actively studied for the past several decades. However, there is no well established methodology that would lead to its native structure from the sequence information. This paper is an attempt to address this problem and to arrive at the protein structures through evolutionary and stochastic computing techniques like genetic algorithms and Monte Carlo methods. It is well known that, there are innumerable possible structures that proteins can assume but, they get directed to their native structures mainly based on the sequence. A number of methods have been developed to evolve the structures of poly peptides and small proteins. We could evolve structures of small proteins like villin head piece and crambin using genetic algorithms and its variations on parallel platforms with root mean square deviation of about 6 Angstroms. Recently, we developed a Monte Carlo based method of simulating polymerisation of proteins. A number of polymers like synthetic octa-alanine, poly collagen, vimentin were simulated. We find that, the structures simulated by this method give us insight in to the polymerisation process. Currently, studies are being made on the amyloid beta and other proteins that are responsible for the Alzheimer's disease. We would like to demonstrate the hypothesis that a misfolded protein polymerises faster than the native proteins leading to the disease. The main aim of our study is to know the cause of the disease and demonstrate a single framework of principles of simulations for both the proteins and their polymerisation.

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