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Computational studies of protein fibrils and their interactions with micelles

CRISTIANO DIAS, New Jersey Inst of Tech

The aggregation of proteins into amyloid-like fibrils is a ubiquitous process that arises for many amino acid sequences given the right template and conditions. While some naturally occurring fibrils contribute to the survival of living organisms, e.g., silk fibrils that are used by spiders to capture their prey, amyloid fibrils are responsible for plaque formation in tissues which is a hallmark of Alzheimer's disease. Thus, a detailed understanding of how proteins aggregate forming fibrils has important implications in biology and medicine. Here, I will present a toy model to show that mature fibrils exist in equilibrium with dissolved proteins in a solution. The existence of equilibrium enables thermodynamic quantities to be determined from temperature dependent studies. I will then present results from all-atom molecular dynamics simulations in which thermodynamic quantities related to the dissociation of a protein from a fibril have been computed. This study is enabling an understanding of the molecular mechanisms accounting for the stability of amyloid fibrils. Thermodynamic quantities are also being incorporated into a coarse-grained model of fibril growth. If time permits, I will discuss how this model is being used to study micelle deformation by amyloid fibrils.