



生物信息学研究中心

Center of Bioinformatics

学术报告

题目： Simple models to uncover key factors for protein aggregation

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摘要：

Neurodegenerative diseases include Alzheimer's disease (AD), Huntington's disease (HD), etc. Such diseases are due to progressive loss of structure or function of neurons caused by protein aggregation. For example, AD is considered to be related to aggregation of A β 40 and A β 42 (protein with 42 amino acids). In this talk, I briefly review our recent discovery on key factors for protein aggregation. We have used a lattice model to study the aggregation rates of proteins and found that the probability for a protein sequence to appear in the conformation of the aggregated state can be used to determine the temperature at which proteins can aggregate most easily [1].

We have used molecular dynamics and simple models of polymer chains to study relaxation and aggregation of proteins under various conditions and found that when the bending-angle dependent and torsion-angle dependent interactions are zero or very small, then protein chains tend to aggregate at lower temperatures [2]. Such result is useful for understanding aggregation of A β 40 and A β 42. Our results [1,2] form good basis for further studies on protein aggregation.

[1] M. S. Li, N. T. Co, G. Reddy, C.-K. Hu, J. E. Straub, and D. Thirumalai, *Phys. Rev. Lett.* 105, 218101(2010).

[2] W.-J. Ma and C.-K. Hu, *J. Phys. Soc. Japan* 79, 024005, 024006, 054001, and 104002 (2010).