生物物理学报 2011, 27(3) 187-194 DOI: ISSN: 1000-6737 CN: 11-1992/Q

综述

用计算机折叠蛋白质：我们走了多远？

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摘要：

蛋白质折叠是现代科学最具挑战性的难题之一。Anfinsen的先驱性工作已经过去数十年了，我们对蛋白质折叠的机理仍不甚了然。但值得庆幸的是，科学工作者们在解析几个模型蛋白质的折叠机理上已经取得了明显的进展。这篇综述将主要回顾在蛋白质折叠的计算研究方面的进展。受益于计算机技术的迅猛发展，在1998年首次实现了一个微秒的全原子水平的蛋白质折叠，从2000年开始，folding@home将全球分布式计算技术应用于蛋白质折叠。在经历了数十年艰苦的努力之后，天然蛋白质亚埃精度的折叠终于在2007年成功实现。近年来，一种全新的概念开始出现，人们越来越多地用网络来解释蛋白质折叠的机理。随着分子力场的不断完善，分子模拟将会在解析蛋白质折叠的机理上起到越来越重要的作用。

关键词： 蛋白质折叠 分子动力学 折叠路径 折叠地形 折叠网络

Protein Folding by Computer: How Far Have We Gone?

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Abstract:

Protein folding is one of the most challenging problems in modern science. Several decades after Anfinsen's pioneering work, the mechanism governing protein folding remains elusive. Nevertheless, significant progress has been made toward decoding the folding of a few model systems. This review will focus on the progress in computational protein folding. Benefiting from the fast development of computer technology, one microsecond of protein folding with all-atom model was reached in 1998, and world-wide distributed computing was adopted by folding@home in 2000. After decades of struggle, protein folding with sub-angstrom resolution was finally reached in 2007. Recently, a new concept has emerged where protein folding is depicted as a network. With the continuous improvement of force fields, molecular simulation will play a more important role in the understanding of protein folding.

Keywords: Protein folding Molecular dynamics Pathway Landscape Network

收稿日期 2010-11-04 **修回日期** 2010-11-06 **网络版发布日期**

DOI:

基金项目:

NIH (GM79383, GM67168)，国家自然科学基金项目(30870474)，留学回国人员基金项目

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