Ab initio Protein Structure Prediction

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Abstract

Protein structure elucidation from amino acid sequence is listed among the top hundred outstanding problems in modern science, both at the conceptual and practical levels. Computational approaches promise to supplement the time consuming and expensive experimental approaches, at least partially. *Ab initio* structure prediction methods enable the discovery of novel folds and folding mechanisms, although their applicability is restricted to small proteins. In contrast, homology-based methods are computationally rapid and reliable when suitable experimental reference structures are available, but offer no possibility of exploring novel folds. This article describes the evolution of some successful *ab initio* and homology hybrid methodologies for protein tertiary structure prediction.

Keywords

Ab initio protein structure prediction; *de novo* protein modeling; free modeling of protein structures; physics-based protein structure prediction; energy based scoring functions; knowledge-based scoring functions; conformational sampling of protein structures; protein structure quality assessment