

主编特约/综述

蛋白质-蛋白质分子对接方法中分子柔性处理与近天然结构筛选的研究

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摘要:

蛋白质-蛋白质分子对接方法是研究蛋白质分子间相互作用与识别的重要理论方法。该方法主要涉及复合物结合模式的构象搜索和近天然结构的筛选两个问题。在构象搜索中,分子柔性的处理是重点也是难点,围绕这一问题,近年来提出了许多新的方法。针对近天然结构的筛选问题,目前主要采用三种解决策略:结合位点信息的利用、相似结构的聚类 and 打分函数对结构的评价。本文围绕以上问题,就国内外研究进展和本研究小组的工作作详细的综述,并对进一步的研究方向进行了展望。

关键词: 蛋白质-蛋白质分子对接 分子柔性处理 结合位点信息 结构聚类 打分函数

The Study on Molecular Flexibility Treating and Near-Native Structure Screening in Protein-Protein Docking Approaches

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Abstract:

Molecular docking is an effective and important theoretical approach for prediction of inter-molecular interactions and recognition. This approach involves two main problems: how to search complex binding modes and how to screen out near-native structures. In conformation searching, it is very important but difficult to treat molecular flexibility. To solve this problem, many new methods have been proposed in recent years. Aiming at near-native structure screening, three kinds of strategies have been proposed: use of binding site information, clustering of similar structures, evaluating structures by scoring functions. In this article, combining recent studies of our group, we reviewed the progress on these two problems and gave a prospect for this field in the future.

Keywords: Protein-protein docking Molecular flexibility treating Binding site information Similar structure clustering Scoring function

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