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PDF文档

分子对接在基于结构药物设计中的应用

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分子对接是研究分子间(如配体和受体)相互作用, 并预测其结合模式和亲合力的一种理论模拟方法。近年来, 分子对接方法已成为计算机辅助药物研究领域的一项重要技术, 在数据库搜寻, 组合库设计及蛋白作用研究方面得到了广泛发展。

MOLECULAR DOCKING FOR IN STRUCTURE-BASED DRUG DESIGNING

Molecular docking serves as a method to simulate the interactions of two molecules (such as ligand and receptor) and to predict their binding mode and affinity. In recent years, molecular docking has emerged as an important technology in the field of computer-aided drug research, including database searching, combinatorial library design and protein-protein interaction investigation.

关键词

分子对接(Molecular docking); 基于结构药物设计(Structure-based drug design); 计算机辅助药物设计(Computer-aided drug design)