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Molecular Docking for Computer-Aided Drug Design

Fundamentals, Techniques, Resources and Applications

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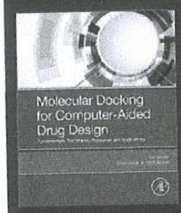

Edited by:
Mohane S. Coumar

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Book description

Molecular Docking for Computer-Aided Drug Design: Fundamentals, Techniques, Resources and Applications offers in-depth coverage on the use of molecular docking for drug design. The ... read full description

About the book

Description

Molecular Docking for Computer-Aided Drug Design: Fundamentals, Techniques, Resources and Applications offers in-depth coverage on the use of molecular docking for drug design. The book is divided into three main sections that cover basic techniques, tools, web servers and applications. It is an essential reference for students and researchers involved in drug design and discovery.

Key Features

- Covers the latest information and state-of-the-art trends in structure-based drug design methodologies
- Includes case studies that complement learning
- Consolidates fundamental concepts and current practice of molecular docking into one convenient resource

Details

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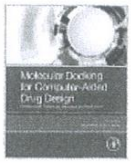

2021, Pages 119-140

Chapter 6 - 3D Structural Determination of Macromolecules Using X-ray Crystallography Methods

Mutharasappan Nachiappan, Ravi Guru Raj Rao, Mariadasse Richard, Dhamodharan Prabhu, Sundarraj Rajamanikandan, Jeyaraj Pandian Chitra, Jeyaraman Jeyakanthan

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Abstract

Several structure determination techniques such as X-ray diffraction (XRD), nuclear magnetic resonance (NMR), cryogenic electron microscopy (cryo-EM), small angle X-ray scattering (SAXS), and X-ray free electron laser (XFEL) are widely used to decode the structural information of biological macromolecules and its complexes, among which NMR, cryo-EM, SAXS, and XFEL are categorized by solution state and can only analyze the relative stereochemistry of the macromolecule, while single-crystal XRD is the ultimate method to determine the most accurate high-resolution atomic crystalline structure. The main bottle neck of X-ray crystallography is to determine the phase problem which