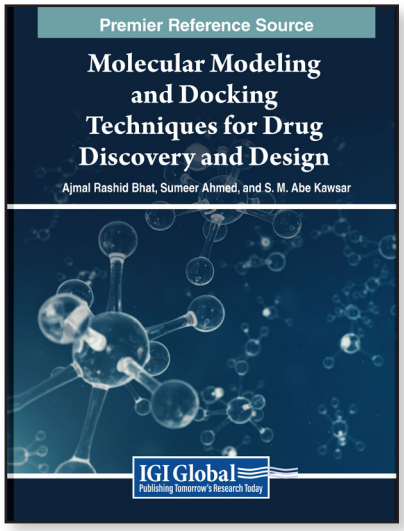
Molecular Modeling and Docking Techniques for Drug Discovery and Design



Part of the Advances in Medical Technologies and Clinical Practice Book Series

Ajmal Rashid Bhat (RTM Nagpur University, India), Sumeer Ahmed (The New College (Autonomous), University of Madras, India) and S. M. Abe Kawsar (University of Chittagong, Bangladesh)

Description:

In the realm of pharmaceutical research, the challenge of efficiently discovering and designing new drugs to combat diseases is ever-present. Traditional approaches to drug discovery often rely on time-consuming and costly experimental methods, leading to lengthy development timelines and high failure rates. This problem is exacerbated by the complexity of molecular interactions and the vast chemical space to explore. As a result, there is a pressing need for innovative solutions that can streamline the drug discovery process and improve its success rate.

Molecular Modeling and Docking Techniques for Drug Discovery and Design addresses this critical challenge by offering a comprehensive guide to advanced computational methods in pharmaceutical research. Edited by leading experts in the field, the book provides insights into molecular modeling, docking, and other computational approaches that can significantly accelerate the drug discovery process. By leveraging computational tools and software, researchers can simulate molecular interactions, predict drug efficacy, and optimize chemical structures with greater speed and accuracy than traditional experimental methods.

With its emphasis on practical applications and real-world case studies, this book equips researchers, educators, and students with the knowledge and tools needed to overcome the challenges of modern drug discovery. By integrating computational techniques into their research workflows, pharmaceutical scientists can enhance their ability to identify promising drug candidates, ultimately leading to the development of more effective treatments for a wide range of diseases. **Molecular Modeling and Docking Techniques for Drug Discovery and Design** serves as a valuable resource for anyone seeking to harness the power of computational chemistry to revolutionize the field of pharmaceutical research.

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Topics Covered:

- Biopharmaceutics and Drug Disposition
- Chemo-Informatics and Molecular Descriptors
- Computational Approaches of Design Discovery
- Computational Chemistry
- Computational Tools and Software
- Concept and Applications of POM Theory
- Development Of Computer-Aided Prediction Models
- DFT Approach for Drug Discovery and Design
- Dynamic Simulation Modeling (DMS) Approach in Pharmaceutical Engineering
- Efficiency In Medicinal Chemistry
- In Silico ADME Modeling Progress and Prospects
- Ligand-Based Drug Design
- Modern Approach to Drug Design
- Molecular Docking
- Pharmacophore Modeling

Subject: Medicine & Healthcare

Classification: Edited Reference

Readership Level: Advanced-Academic Level (Research Recommended)

Research Suitable for: Advanced Undergraduate Students; Graduate Students; Researchers; Academicians; Professionals; Practitioners

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