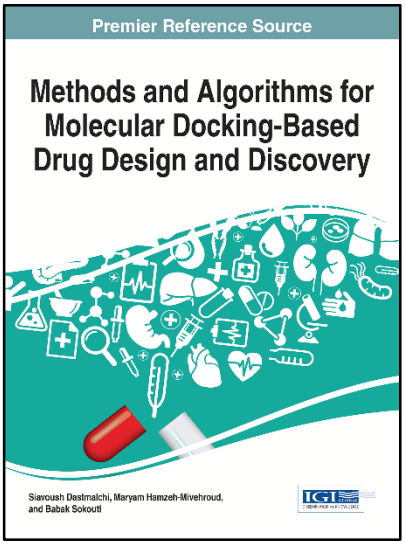
Methods and Algorithms for Molecular Docking-Based Drug Design and Discovery



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

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Description:

The role of technology in the medical field has resulted in significant developments within the pharmaceutical industry. Computational approaches have emerged as a crucial method in further advancing drug design and development.

Methods and Algorithms for Molecular Docking-Based Drug Design and Discovery presents emerging research on the application of computer-assisted design methods for drugs, emphasizing the benefits and improvements that molecular docking has caused within the pharmaceutical industry. Focuses on validation methods, search algorithms, and scoring functions.

Readers:

This book is a pivotal resource for professionals, researchers, students, and practitioners in the field of theoretical and computational chemistry.

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Topics Covered:

- Docking Methodologies
- Docking Search Algorithms
- Enzyme-Ligand Interactions
- Online Docking Resources
- Protein Structure Prediction
- Protein-Ligand Interactions
- Protein-Protein Docking

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Siavoush Dastmalchi graduated as Doctor of Pharmacy from Tabriz University of Medical Sciences (TUMS). Then he moved to Sydney where he received his PhD from the Faculty of Pharmacy at the University of Sydney in 2002. Since then he has worked as a full academic in the Medicinal Chemistry Department at the School of Pharmacy, TUMS, teaching medicinal chemistry, instrumental drug analysis and bioinformatics to graduate and postgraduate students. He is currently the Director of the Biotechnology Research Centre at TUMS where he leads his research team mainly with interests in molecular modelling, structural biology, and chemo-bioinformatics for their application to drug discovery.