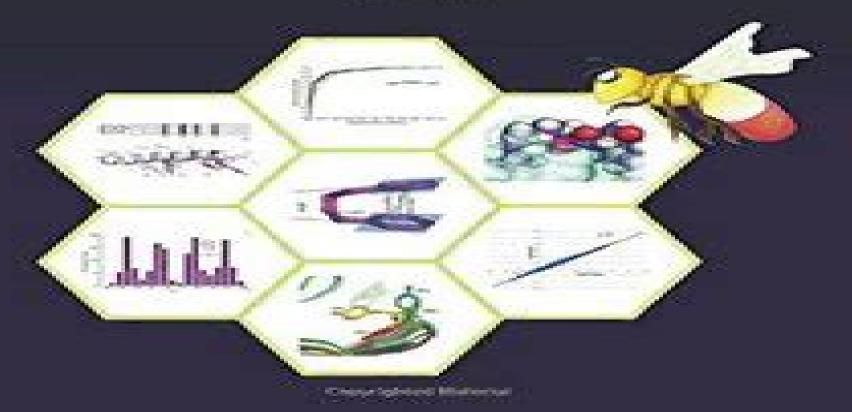
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Mithun Rudrapal

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A Practical Guide to Rational Drug Design Sun Hongmao, 2015-10-05 This book is not going to be an exhaustive survey covering all aspects of rational drug design Instead it is going to provide critical know how through real world examples Relevant case studies will be presented and analyzed to illustrate the following how to optimize a lead compound whether one has high or low levels of structural information how to derive hits from competitors active compounds or from natural ligands of the targets how to springboard from competitors SAR knowledge in lead optimization how to design a ligand to interfere with protein protein interactions by correctly examining the PPI interface how to circumvent IP blockage using data mining how to construct and fully utilize a knowledge based molecular descriptor system how to build a reliable QSAR model by focusing on data quality and proper selection of molecular descriptors and statistical approaches A Practical Guide to Rational Drug Design focuses on computational drug design with only basic coverage of biology and chemistry issues such as assay design target validation and synthetic routes Discusses various tactics applicable to daily drug design Readers can download the materials used in the book including structures scripts raw data protocols and codes making this book suitable resource for short courses or workshops Offers a unique viewpoint on drug discovery research due to the author's cross discipline education background Explores the author's rich experiences in both pharmaceutical and academic settings

Drug Design Gerhard Klebe, 2025-02-04 This English language textbook based on the successful German edition Wirkstoffdesign brings the subject of drug design back to the cutting edge of research The reader learns about new methods in genetic engineering and the expanded range of structural biological methods Especially in the last 10 years many complex target structures such as G protein coupled receptors or ion channels have been elucidated by using these methods The reader learns how these long sought complex structures with classical drugs look like and how the therapeutic effect is achieved This textbook is aimed at students of pharmacy chemistry and the life sciences but also at career changers and medicinal chemists in research and development departments of the pharmaceutical industry Conceptually it is very different from classical textbooks on pharmaceutical chemistry It focuses on the path to a new drug substance The selection of case studies is based on didactic aspects and attempts to give a broad overview of methods and strategies without forgetting to look back at the beginnings of this field of work Thus the arc spans from the history of drug research the mechanisms of action of drugs and the methods for lead structure search and optimisation to structure determination methods modelling molecular dynamics and QSAR methods to structure and computer aided design This textbook also discusses new methods and concepts such as epigenetics the PROTAC approach CRISPR Cas9 gene scissors structural predictions from sequence the use of artificial intelligence and new screening technologies from biophysics It presents successes in disrupting or enhancing protein protein interactions as a concept for drug therapy and discusses optimising drugs considering their thermodynamic as well as kinetic binding profiles Videos via app simply download the SN More Media app free of charge scan a link with the

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Computational Methods for Rational Drug Design Mithun Rudrapal,2025-02-05 Comprehensive resource covering computational tools and techniques for the development of cost effective drugs to combat diseases with specific disease examples Computational Methods for Rational Drug Design covers the tools and techniques of drug design with applications to the discovery of small molecule based therapeutics detailing methodologies and practical applications and addressing the

challenges of techniques like AI ML and drug design for unknown receptor structures Divided into 23 chapters the contributors address various cutting edge areas of therapeutic importance such as neurodegenerative disorders cancer multi drug resistant bacterial infections inflammatory diseases and viral infections Edited by a highly qualified academic with significant research contributions to the field Computational Methods for Rational Drug Design explores topics including Computer assisted methods and tools for structure and ligand based drug design virtual screening and lead discovery and ADMET and physicochemical assessments In silico and pharmacophore modeling fragment based design de novo drug design and scaffold hopping network based methods and drug discovery Rational design of natural products peptides enzyme inhibitors drugs for neurodegenerative disorders anti inflammatory therapeutics antibacterials for multi drug resistant infections and antiviral and anticancer therapeutics Protac and protide strategies in drug design intrinsically disordered proteins IDPs in drug discovery and lung cancer treatment through ALK receptor targeted drug metabolism and pharmacokinetics Helping readers seamlessly navigate the challenges of drug design Computational Methods for Rational Drug Design is an essential reference for pharmaceutical and medicinal chemists biochemists pharmacologists and phytochemists along with molecular modeling and computational drug discovery professionals Cheminformatics. OSAR and Machine Learning Applications for Novel Drug Development Kunal Roy, 2023-05-23 Cheminformatics QSAR and Machine Learning Applications for Novel Drug Development aims at showcasing different structure based ligand based and machine learning tools currently used in drug design It also highlights special topics of computational drug design together with the available tools and databases The integrated presentation of chemometrics cheminformatics and machine learning methods under is one of the strengths of the book The first part of the content is devoted to establishing the foundations of the area Here recent trends in computational modeling of drugs are presented Other topics present in this part include QSAR in medicinal chemistry structure based methods chemoinformatics and chemometric approaches and machine learning methods in drug design The second part focuses on methods and case studies including molecular descriptors molecular similarity structure based based screening homology modeling in protein structure predictions molecular docking stability of drug receptor interactions deep learning and support vector machine in drug design The third part of the book is dedicated to special topics including dedicated chapters on topics ranging from de design of green pharmaceuticals to computational toxicology The final part is dedicated to present the available tools and databases including QSAR databases free tools and databases in ligand and structure based drug design and machine learning resources for drug design The final chapters discuss different web servers used for identification of various drug candidates Presents chemometrics cheminformatics and machine learning methods under a single reference Showcases the different structure based ligand based and machine learning tools currently used in drug design Highlights special topics of computational drug design and available tools and databases **Computational Chemistry** David Young, 2004-04-07 A practical easily accessible guide for bench top

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