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Data Mining in Drug Discovery
Structural and Dynamic Aspects of Protein Function and Allostery
Handbook of Computational Chemistry
Oncology: Breakthroughs in Research and Practice
Statistical Modelling of Molecular Descriptors in QSAR/QSPR
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The Advances in Semen Evaluation
Preclinical Development Handbook
Translational Bioinformatics and Its Application
Artificial Intelligence: Concepts, Methodologies, Tools, and Applications
Materiomics
Pharmacological Actions of Drugs in the Brain: Exploring the Intricacies and Potential Therapeutic Applications
Comprehensive Biophysics
Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment
Drugs from Nature: Targets, Assay Systems and Leads
Redox Chemistry and Biology of Thiols
Virtual Drug Design
9789815223026

Drug Design Strategies
In Silico Methods for Drug Design and Discovery
Nanomedicine, Volume I
Introduction to Biological and Small Molecule Drug Research and Development
Oral Bioavailability and Drug Delivery
Computational Intelligence and Predictive Analysis for Medical Science
Classification as a Tool for Research
Structural Bioinformatics: Applications in Preclinical Drug Discovery Process

PERKINS MILLS

Chemoinformatics: Theory, Practice, & Products MDPI

Redox Chemistry and Biology of Thiols offers an applied, comprehensive overview of redox chemistry and biology of thiol-dependent processes. Running from basic biology and chemistry of redox phenomena to research methods and highlighting recently identified roles of thiols across cellular and bodily systems, this book draws upon a range of disciplines to illuminate new research directions, new applications of thiol studies, and clinical translation. Sections cover thiol oxidizing species, thiol reactivity and modifications, thioredoxin, glutaredoxin, glutathione, peroxidases,

thiol repair enzymes, thiol oxidative signaling, disulfide bond formation, thiol-based redox biosensors, cysteine and hydrogen sulfide metabolism, iron-sulfur cluster biogenesis, thiols in chloroplasts, blood thiols, sugar and polyamine thiols in pathogenic organisms, redox medicine (therapeutic applications of thiols and drug development), as well as methods and bioinformatics tools. - Runs from basic thiol biology and chemistry to applications and clinical translation - Provides methods and protocols that will power new research across biomedicine, cell biology, plant biology, drug development, and protein folding and modulation - Includes chapter contributions from international leaders in the field

Peptide Therapeutics

Frontiers Media SA

This book explains how peptide-based drug design works, what steps are needed to develop a peptide-based therapeutic, and challenges in synthesis as well as regulatory issues. It covers the design concept of peptide therapeutics from fundamental principles using structural biology and computational approaches. The chapters are arranged in a linear fashion. A fresh graduate or a scientist who works on small molecules can use this to follow the design and development of peptide therapeutics to use as understanding the basic concepts. Each chapter is written by

experts from academia as well as industry. Rather than covering extensive literature, the book provides concepts of design, synthesis, delivery, as well as regulatory affairs and manufacturing of peptides in a systematic way with examples in each case. The book can be used as a reference for a pharmaceutical or biomedical scientist or graduate student who wants to pursue their career in peptide therapeutics. Some chapters will be written as a combination of basic principles and protocol so that scientists can adopt these methods to their research work. The examples provided can be used to perform peptide formulation considerations for the designed peptides. The book has nine chapters, and each chapter can be read as an independent unit on a particular concept.

Pseudokinases Royal Society of Chemistry

Advancements in cancer diagnosis and treatment have extended the lives of many patients facing numerous types of cancer over the years. Research on best practices, new drug development, early identification, and treatment continues to advance with the ultimate goal of uncovering a cure for cancer in all its forms. Oncology: Breakthroughs in Research and Practice features international perspectives on cancer identification, treatment, and management methodologies in addition to patient considerations and outlooks for the future. This collection of

emerging research provides valuable insight for researchers, graduate-level students, and professionals in the medical field.

An Updated View on an Emerging Target: Selected Papers from the 8th International Conference on Protein Kinase CK2 Springer Science & Business Media

Molecular nanotechnology has been defined as the three-dimensional positional control of molecular structure to create materials and devices to molecular precision. The human body is comprised of molecules, hence the availability of molecular nanotechnology will permit dramatic progress in human medical services. More than just an extension of "molecular medicine," nanomedicine will employ molecular machine systems to address medical problems, and will use molecular knowledge to maintain and improve human health at the molecular scale. Nanomedicine will have extraordinary and far-reaching implications for the medical profession, for the definition of disease, for the diagnosis and treatment of medical conditions including aging, for our very personal relationships with our own bodies and ultimately for the improvement and extension of natural human biological structure and function. This book will be published in three volumes over the course of several years. Readers wishing to keep up-to-

date with the latest developments may visit the nanomedicine website maintained by the Foresight Institute (http://foresight.org/Nanomedicine/index.html).

Defects in Regulation: How, Where and When The Immune System Can Go Wrong Frontiers Media SA

ORAL BIOAVAILABILITY AND DRUG DELIVERY

Improve the performance and viability of newly-developed and approved drugs with this crucial guide Bioavailability is the parameter which measures the rate and extent to which a drug reaches a user's circulatory system depending on the method of administration. For example, intravenous administration produces a bioavailability of 100%, since the drugs are injected directly into the circulatory system; in the case of oral administration, however, bioavailability can vary widely based on factors which, if not properly understood, can result in a failure in drug development, adverse effects, and other complications. The mechanics of oral bioavailability are therefore critical aspects of drug development. Oral Bioavailability and Drug Delivery provides a comprehensive coverage of this subject as well as its drug development applications. Beginning with basic terminology and fundamental concepts, it provides a thorough understanding of the challenges and barriers to oral bioavailability as well as the possibilities for

improving this parameter. The resulting book is an indispensable tool for drug development research. Oral Bioavailability and Drug Delivery readers will also find: Discussion questions in many chapters to facilitate comprehension Detailed discussion of topics including dissolution, absorption, metabolism, and more Real-world examples of methods in actions throughout Oral Bioavailability and Drug Delivery is ideal for pharmaceutical and biotechnology scientists working in drug discovery and development; researchers in chemistry, biology, pharmacology, immunology, neuroscience, and other related fields; and graduate courses in drug development and delivery. *Computational Intelligence Methods for Bioinformatics and Biostatistics* Springer Science & Business Media Chemoinformatics is equipped to impact our life in a big way mainly in the fields of chemical, medical and material sciences. This book is a product of several years of experience and passion for the subject written in a simple lucid style to attract the interest of the student community who wish to master chemoinformatics as a career. The topics chosen cover the entire spectrum of chemoinformatics activities (methods, data and tools). The algorithms, open source databases, tutorials supporting theory using standard datasets, guidelines, questions and

do it yourself exercises will make it valuable to the academic research community. At the same time every chapter devotes a section on development of new software tools relevant for the growing pharmaceutical, fine chemicals and life sciences industry. The book is intended to assist beginners to hone their skills and also constitute an interesting reading for the experts.

Analytical Techniques in Combinatorial Chemistry
Walter de Gruyter GmbH & Co KG

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.

Practical Chemoinformatics IGI Global

Edited by world-famous pioneers in chemoinformatics, this is a clearly structured and applications-oriented approach to the topic, providing up-to-date and focused information on the wide range of applications in this

exciting field. The authors explain methods and software tools, such that the reader will not only learn the basics but also how to use the different software packages available. Experts describe applications in such different fields as structure-spectra correlations, virtual screening, prediction of active sites, library design, the prediction of the properties of chemicals, the development of new cosmetics products, quality control in food, the design of new materials with improved properties, toxicity modeling, assessment of the risk of chemicals, and the control of chemical processes. The book is aimed at advanced students as well as lectures but also at scientists that want to learn how chemoinformatics could assist them in solving their daily scientific tasks. Together with the corresponding textbook Chemoinformatics - Basic Concepts and Methods (ISBN 9783527331093) on the fundamentals of chemoinformatics readers will have a comprehensive overview of the field.

Artificial Intelligence and Machine Learning in Drug Design and Development

Frontiers Media SA

Physical chemistry covers diverse topics, from biochemistry to materials properties to the development of quantum computers. Physical chemistry applies physics and math to problems that interest chemists, biologists, and engineers. Physical chemists use theoretical constructs and mathematical

computations to understand chemical properties and describe the behavior of molecular and condensed matter. Their work involves manipulations of data as well as materials. Physical chemistry entails extensive work with sophisticated instrumentation and equipment as well as state-of-the-art computers. This new volume presents a selection of articles on topics in the field.

Multiple Action-Based Design Approaches to Antibacterials John Wiley & Sons

The study of pharmacological actions of drugs in the brain is a field that constantly uncovers new insights into the mechanisms of action behind various substances. This proposal aims to explore into the intriguing topics of psychedelics, cannabinoids, classical and novel antidepressants, anxiolytic treatments, and substances commonly associated with neuropsychiatric disorders such as alcohol, ketamine, and opiates. The ultimate goal is to unravel their neurological impacts, shed light on potential therapeutic applications, and explore their relationship with brain disorders, while also investigating the influence of sex/gender on drug response. Biological differences between sexes can influence how medications are metabolized and processed in the body. Understanding these relationships and considering hormonal

factors is crucial for optimizing treatment outcomes and tailoring medication regimens to individual needs.
Chemical Genomics John Wiley & Sons
This book covers intentional design aspects for combinations of drugs, single-molecule hybrids with potential or actual multiple actions, pro-drugs which could yield multiple activity outcomes, and future possibilities. The approach of the book is interdisciplinary, and it provides greater understanding of the complex interplay of factors involved in the medicinal chemistry design and laboratory development of multiply active antibacterials. The scope of the book appeals to readers who are researching in the field of antibacterials using the approach of medicinal chemistry design and drug development.
Computational Methods for Rational Drug Design Frontiers Media SA
In the current drug research environment in academia and industry, cheminformatics and virtual screening methods are well established and integrated tools. Computational tools are used to predict a compound's 3D structure, the 3D structure and function of a pharmacological target, ligand-target interactions, binding energies, and other factors essential for a successful drug. This includes molecular properties such as solubility, logP value, susceptibility to metabolism, cell

permeation, blood brain barrier permeation, interaction with drug transporters and potential off-target effects. Given that approximately 40 million unique compounds are readily available for purchase, such computational modeling and filtering tools are essential to support the drug discovery and development process. The aim of all these calculations is to focus experimental efforts on the most promising candidates and exclude problematic compounds early in the project. In this Research Topic on virtual activity predictions, we cover several aspects of this research area such as historical perspectives, data sources, ligand treatment, virtual screening methods, hit list handling and filtering.

Physical Chemistry
Springer Science & Business Media
This complete, yet concise, guide introduces you to the rapidly developing field of high throughput screening of biomaterials: materiomics. Bringing together the key concepts and methodologies used to determine biomaterial properties, you will understand the adaptation and application of materomics in areas such as rapid prototyping, lithography and combinatorial chemistry. Each chapter is written by internationally renowned experts, and includes tutorial paragraphs on topics such as biomaterial-banking, imaging, assay development, translational aspects, and informatics. Case studies

of state-of-the-art experiments provide illustrative examples, whilst lists of key publications allow you to easily read up on the most relevant background material. Whether you are a professional scientist in industry, a student or a researcher, this book is not to be missed if you are interested in the latest developments in biomaterials research.

Phase II Conjugation Enzymes and Transport Systems Cambridge University Press

The book is a comprehensive guide that explores the use of artificial intelligence and machine learning in drug discovery and development covering a range of topics, including the use of molecular modeling, docking, identifying targets, selecting compounds, and optimizing drugs. The intersection of Artificial Intelligence (AI) and Machine Learning (ML) within the field of drug design and development represents a pivotal moment in the history of healthcare and pharmaceuticals. The remarkable synergy between cutting-edge technology and the life sciences has ushered in a new era of possibilities, offering unprecedented opportunities, formidable challenges, and a tantalizing glimpse into the future of medicine. AI can be applied to all the key areas of the pharmaceutical industry, such as drug discovery and development, drug repurposing, and improving productivity within a short period. Contemporary methods

have shown promising results in facilitating the discovery of drugs to target different diseases. Moreover, AI helps in predicting the efficacy and safety of molecules and gives researchers a much broader chemical pallet for the selection of the best molecules for drug testing and delivery. In this context, drug repurposing is another important topic where AI can have a substantial impact. With the vast amount of clinical and pharmaceutical data available to date, AI algorithms find suitable drugs that can be repurposed for alternative use in medicine. This book is a comprehensive exploration of this dynamic and rapidly evolving field. In an era where precision and efficiency are paramount in drug discovery, AI and ML have emerged as transformative tools, reshaping the way we identify, design, and develop pharmaceuticals. This book is a testament to the profound impact these technologies have had and will continue to have on the pharmaceutical industry, healthcare, and ultimately, patient well-being. The editors of this volume have assembled a distinguished group of experts, researchers, and thought leaders from both the AI, ML, and pharmaceutical domains. Their collective knowledge and insights illuminate the multifaceted landscape of AI and ML in drug design and development, offering a roadmap for navigating its complexities and harnessing its potential. In each section, readers will

find a rich tapestry of knowledge, case studies, and expert opinions, providing a 360-degree view of AI and ML's role in drug design and development. Whether you are a researcher, scientist, industry professional, policymaker, or simply curious about the future of medicine, this book offers 19 state-of-the-art chapters providing valuable insights and a compass to navigate the exciting journey ahead. Audience The book is a valuable resource for a wide range of professionals in the pharmaceutical and allied industries including researchers, scientists, engineers, and laboratory workers in the field of drug discovery and development, who want to learn about the latest techniques in machine learning and AI, as well as information technology professionals who are interested in the application of machine learning and artificial intelligence in drug development.

Data Mining in Drug Discovery John Wiley & Sons

This volume presents the necessary tools for developing methods and analyzing results in the drug discovery process, and supports documenting and managing the process in a combinatorial setting. It describes the chromatographic and spectroscopic techniques used to generate chemical and molecular diversity in new compounds, focusing on applications

Structural and Dynamic Aspects of Protein

Function and Allostery
Springer
This book is a printed edition of the Special Issue "An Updated View on an Emerging Target: Selected Papers from the 8th International Conference on Protein Kinase CK2" that was published in Pharmaceuticals
Handbook of Computational Chemistry
John Wiley & Sons
Clustering and Classification, Data Analysis, Data Handling and Business Intelligence are research areas at the intersection of statistics, mathematics, computer science and artificial intelligence. They cover general methods and techniques that can be applied to a vast set of applications such as in business and economics, marketing and finance, engineering, linguistics, archaeology, musicology, biology and medical science. This volume contains the revised versions of selected papers presented during the 11th Biennial IFCS Conference and 33rd Annual Conference of the German Classification Society (Gesellschaft für Klassifikation - GfKl). The conference was organized in cooperation with the International Federation of Classification Societies (IFCS), and was hosted by Dresden University of Technology, Germany, in March 2009.
Oncology: Breakthroughs in Research and Practice
Frontiers Media SA
Biophysics is a rapidly-evolving interdisciplinary science that applies theories and methods of the physical sciences to questions of biology.

Biophysics encompasses many disciplines, including physics, chemistry, mathematics, biology, biochemistry, medicine, pharmacology, physiology, and neuroscience, and it is essential that scientists working in these varied fields are able to understand each other's research. Comprehensive Biophysics, Nine Volume Set will help bridge that communication gap. Written by a team of researchers at the forefront of their respective fields, under the guidance of Chief Editor Edward Egelman, Comprehensive Biophysics, Nine Volume Set provides definitive introductions to a broad array of topics, uniting different areas of biophysics research - from the physical techniques for studying macromolecular structure to protein folding, muscle and molecular motors, cell biophysics, bioenergetics and more. The result is this comprehensive scientific resource - a valuable tool both for helping researchers come to grips quickly with material from related biophysics fields outside their areas of expertise, and for reinforcing their existing knowledge. Biophysical research today encompasses many areas of biology. These studies do not necessarily share a unique identifying factor. This work unites the different areas of research and allows users, regardless of their background, to navigate through the most essential concepts with ease, saving them time and vastly improving their

understanding The field of biophysics counts several journals that are directly and indirectly concerned with the field. There is no reference work that encompasses the entire field and unites the different areas of research through deep foundational reviews. Comprehensive Biophysics fills this vacuum, being a definitive work on biophysics. It will help users apply context to the diverse journal literature offering, and aid them in identifying areas for further research Chief Editor Edward Egelman (E-I-C, Biophysical Journal) has assembled an impressive, world-class team of Volume Editors and Contributing Authors. Each chapter has been painstakingly reviewed and checked for consistent high quality. The result is an authoritative overview which ties the literature together and provides the user with a reliable background information and citation resource

Statistical Modelling of Molecular Descriptors in QSAR/QSPR CRC Press

This volume on conjugation enzymes and transporters serves to bring together current methods and concepts in an interesting, important and rapidly developing field of cell and systems biology. Phase II Conjugation Enzymes and Transport Systems focuses on the so-called Phase II enzymes of drug metabolism (xenobiotics), which has important ramifications for endogenous metabolism and nutrition. Also included are aspects on Phase III, transport

systems. This volume of Methods in Enzymology presents current knowledge and methodology on glucuronidation, sulfation, acetylation, and transport systems in this field of research. Together with the volumes on Quinones and Quinone Enzymes (volumes 378 and 382), and on Glutathione Transferases and gamma-Glutamyl Transpeptidases (volume 401), the state of knowledge on proteomics and metabolomics of many pathways of (waste) product elimination, enzyme protein induction and gene regulation and feedback control is provided. This volume will help stimulate future investigations and speed the advance of knowledge in systems biology. A laboratory standard for more than 40 years Over 400 volumes strong Also available on ScienceDirect

Applied Chemoinformatics

Springer

This book offers a detailed overview of translational bioinformatics together with real-case applications. Translational bioinformatics integrates the areas of basic bioinformatics, clinical informatics, statistical genetics and informatics in order to further our understanding of the molecular basis of diseases. By analyzing voluminous amounts of molecular and clinical data, it also provides clinical information, which can then be applied. Filling the gap between clinic research and informatics, the book is a valuable resource for human geneticists, clinicians, health

educators and policy makers, as well as graduate students majoring in biology, biostatistics, and bioinformatics.