In Silico Drug Discovery And Design Theory Methods Challenges And Applications

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Chemoinformatics for Drug Discovery - Jürgen Bajorath 2013-09-25 Chemoinformatics strategies to improve drug discoveryresults With contributions from leading researchers in academia and thepharmaceutical industry as well as experts from the softwareindustry, this book explains how chemoinformatics enhances drugdiscovery and pharmaceutical research efforts, describing whatworks and what doesn't. Strong emphasis is put on tested and provenpractical applications, with plenty of case studies detailing thedevelopment and implementation of chemoinformatics methods tosupport successful drug discovery efforts. Many of these casestudies depict groundbreaking collaborations between academia andthe pharmaceutical industry. Chemoinformatics for Drug Discovery is logicallyorganized, offering readers a solid base in methods and models andadvancing to drug discovery applications and the design ofchemoinformatics infrastructures. The book features 15 chapters,including: What are our models really telling us? A practical tutorial onavoiding common mistakes when building predictive models Exploration of structure-activity relationships and transfer ofkey elements in lead optimization Collaborations between academia and pharma Applications of chemoinformatics in pharmaceuticalresearch—experiences at large international pharmaceuticalcompanies Lessons learned from 30 years of developing successfulintegrated chemoinformatic systems Throughout the book, the authors present chemoinformaticsstrategies and methods that have been proven to work inpharmaceutical research, offering insights culled from their owninvestigations. Each chapter is extensively referenced withcitations to original research reports and reviews. Integrating chemistry, computer science, and drug discovery,Chemoinformatics for Drug Discovery encapsulates the fieldas it stands today and opens the door to further advances.

Biochips as Pathways to Drug Discovery - Gary Hardiman 2006-10-19

In the fiercely competitive pharmaceutical marketplace, your organization cannot afford to spend excess dollars developing drugs that will fail to get FDA approval or have profoundly poor characteristics. Biochips as Pathways to Drug Discovery takes a comprehensive look at how the industry faces these challenges, using new technologies such as biochips to reduce the cost of drug discovery and improve drug safety. The book explores the tools and skills required at each step of the discovery process when using biochips to determine biological outcomes. The authors provide an in-depth review of the clinical and pharmacogenomic relevance of biochips, ChIP-chip assays, and high-throughput approaches. They discuss how biochips are used to develop biomarkers in the drug discovery process, primarily for gene expression profiling and Single Nucleotide Polymorphism (SNP) analysis. The book includes coverage of experimental theory, quality control, clinical laboratory sampling considerations, database concepts, industrial laboratory design, and the analysis of the resultant large data sets. It discusses the application of biochips to the study of malaria, toxicogenomics, and SNPs, as well as intellectual property and market overviews. The book concludes with a comprehensive overview of how these chips are employed from early target discovery through preclinical toxicology and on through to pharmacogenomic and proof of concept studies in humans. Written in an easily accessible style, the breadth of coverage introduces the subject to those new to the field, while the depth of coverage forms a foundation for future work. The book gives you the knowledge required to leverage the technology into bona fide discoveries. Daniel E. Levy, editor of the Drug Discovery Series, is the founder of DEL BioPharma, a consulting service for drug discovery programs. He also maintains a blog that explores organic chemistry.

Applied Chemoinformatics - Thomas Engel 2018-06-05

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.

Drug-like Properties: Concepts, Structure Design and Methods - Li Di 2010-07-26

Of the thousands of novel compounds that a drug discovery project team invents and that bind to the therapeutic target, typically only a fraction of these have sufficient ADME/Tox properties to become a drug product. Understanding ADME/Tox is critical for all drug researchers, owing to its increasing importance in advancing high quality candidates to clinical studies and the processes of drug discovery. If the properties are weak, the candidate will have a high risk of failure or be less desirable as a drug product. This book is a tool and resource for scientists engaged in, or preparing for, the selection and optimization process. The authors describe how properties affect in vivo pharmacological activity and impact in vitro assays. Individual drug-like properties are discussed from a practical point of view, such as solubility, permeability and metabolic stability, with regard to fundamental understanding, applications of property data in drug discovery and examples of structural modifications that have achieved improved property performance. The authors also review various methods for the screening (high throughput), diagnosis (medium throughput) and in-depth (low throughput) analysis of drug properties. * Serves as an essential working handbook aimed at scientists and students in medicinal chemistry * Provides practical, step-by-step guidance on property fundamentals, effects, structure-property

relationships, and structure modification strategies * Discusses improvements in pharmacokinetics from a practical chemist's standpoint

Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment - Kunal Roy 2015-03-03

Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment describes the historical evolution of quantitative structure-activity relationship (QSAR) approaches and their fundamental principles. This book includes clear, introductory coverage of the statistical methods applied in QSAR and new QSAR techniques, such as HQSAR and G-QSAR. Containing real-world examples that illustrate important methodologies, this book identifies QSAR as a valuable tool for many different applications, including drug discovery, predictive toxicology and risk assessment. Written in a straightforward and engaging manner, this is the ideal resource for all those looking for general and practical knowledge of QSAR methods. Includes numerous practical examples related to QSAR methods and applications Follows the Organization for Economic Co-operation and Development principles for QSAR model development Discusses related techniques such as structure-based design and the combination of structure- and ligand-based design tools

Drug Selectivity - Norbert Handler 2018-02-27

The book "Drug Selectivity - An Evolving Concept in Medicinal Chemistry" provides a current overview and comprehensive compilation for medicinal chemists that discusses the effects of aiming for multiple targets on the entire drug development process. The result is a broad survey of current and future strategies for drug selectivity in medicinal chemistry with theoretical but also practical aspects. Different strategies are presented and evaluated, such as various design approaches, merged multiple ligands, discovery technologies and a broad range of successful examples of unselective drugs taken from all major disease areas. With its wide-ranging view of an emerging new paradigm in drug development, this handbook is of prime importance for every medicinal and pharmaceutical chemist.

Recent Advances of the Fragment Molecular Orbital Method - Yuji Mochizuki 2021-01-04

This book covers recent advances of the fragment molecular orbital (FMO) method, consisting of 5 parts and a total of 30 chapters written by FMO experts. The FMO method is a promising way to calculate large-scale molecular systems such as proteins in a quantum mechanical framework. The highly efficient parallelism deserves being considered the principal advantage of FMO calculations. Additionally, the FMO method can be employed as an analysis tool by using the inter-fragment (pairwise) interaction energies, among others, and this feature has been utilized well in biophysical and pharmaceutical chemistry. In recent years, the methodological developments of FMO have been remarkable, and both reliability and applicability have been enhanced, in particular, for non-bio problems. The current trend of the parallel computing facility is of the many-core type, and adaptation to modern computer environments has been explored as well. In this book, a historical review of FMO and comparison to other methods are provided in Part I (two chapters) and major FMO programs (GAMESS-US, ABINIT-MP, PAICS and OpenFMO) are described in Part II (four chapters). dedicated to pharmaceutical activities (twelve chapters). A variety of new applications with methodological breakthroughs are introduced in Part IV (six chapters). Finally, computer and information science-oriented topics including massively parallel computation and machine learning are addressed in Part V (six chapters). Many color figures and illustrations are included. Readers can refer to this book in its entirety as a practical textbook of the FMO method or read only the chapters of greatest interest to them.

In Silico Technologies in Drug Target Identification and Validation - Darryl Leon 2006-06-13

The pharmaceutical industry relies on numerous well-designed experiments involving high-throughput techniques and in silico approaches to analyze potential drug targets. These in silico methods are often predictive, yielding faster and less expensive analyses than traditional in vivo or in vitro procedures. In Silico Technologies in Drug Target Identification and Validation addresses the challenge of testing a

growing number of new potential targets and reviews currently available in silico approaches for identifying and validating these targets. The book emphasizes computational tools, public and commercial databases, mathematical methods, and software for interpreting complex experimental data. The book describes how these tools are used to visualize a target structure, identify binding sites, and predict behavior. World-renowned researchers cover many topics not typically found in most informatics books, including functional annotation, siRNA design, pathways, text mining, ontologies, systems biology, database management, data pipelining, and pharmacogenomics. Covering issues that range from prescreening target selection to genetic modeling and valuable data integration, In Silico Technologies in Drug Target Identification and Validation is a self-contained and practical guide to the various computational tools that can accelerate the identification and validation stages of drug target discovery and determine the biological functionality of potential targets more effectively. Daniel E. Levy, editor of the Drug Discovery Series, is the founder of DEL BioPharma, a consulting service for drug discovery programs. He also maintains a blog that explores organic chemistry.

In Silico Drug Design - Kunal Roy 2019-02-12

In Silico Drug Design: Repurposing Techniques and Methodologies explores the application of computational tools that can be utilized for this approach. The book covers theoretical background and methodologies of chem-bioinformatic techniques and network modeling and discusses the various applied strategies to systematically retrieve, integrate and analyze datasets from diverse sources. Other topics include in silico drug design methods, computational workflows for drug repurposing, and network-based in silico screening for drug efficacy. With contributions from experts in the field and the inclusion of practical case studies, this book gives scientists, researchers and R&D professionals in the pharmaceutical industry valuable insights into drug design. Discusses the theoretical background and methodologies of useful techniques of cheminformatics and bioinformatics that can be applied for drug repurposing Offers case studies relating to the in silico modeling of FDA-approved drugs for the discovery of antifungal, anticancer, antiplatelet agents, and for drug therapies against diseases Covers tools and databases that can be utilized to facilitate in silico methods for drug repurposing

Frontiers in Computational Chemistry - Zaheer-ul-Haq 2015-02-06

Computational Chemistry is a very diverse field spanning from the development and application of linear free energy relationships (QSAR, QSPR), to electronic structure calculations, molecular dynamics simulations, and to solving coupled differential equations (e.g. drug metabolism). Frontiers in Computational Chemistry presents contemporary research on molecular modeling techniques used in drug discovery and the drug development process: computer aided molecular design, drug discovery and development, lead generation, lead optimization, database management, computer and molecular graphics, and the development of new computational methods or efficient algorithms for the simulation of chemical phenomena including analyses of biological activity. The first volume this eBook series brings together eight different articles detailing the application of computational methods towards drug design.

Bioinformatics and Drug Discovery - Richard S. Larson 2016-08-23

Recent advances in drug discovery have been rapid. The second edition of Bioinformatics and Drug Discovery has been completely updated to include topics that range from new technologies in target identification, genomic analysis, cheminformatics, protein analysis, and network or pathway analysis. Each chapter provides an extended introduction that describes the theory and application of the technology. In the second part of each chapter, detailed procedures related to the use of these technologies and software have been incorporated. Written in the highly successful Methods in Molecular BiologyTM series format, the chapters include the kind of detailed description and implementation advice that is crucial for getting optimal results in the laboratory. Thorough and intuitive, Bioinformatics and Drug Discovery, Second Edition seeks to aid scientists in the further study of the rapidly expanding field of drug discovery.

Concepts and Experimental Protocols of Modelling and Informatics in Drug Design - Om Silakari 2020-11-05

Concepts and Experimental Protocols of Modelling and Informatics in Drug Design discusses each experimental protocol utilized in the field of bioinformatics, focusing especially on computer modeling for drug development. It helps the user in understanding the field of computer-aided molecular modeling (CAMM) by presenting solved exercises and examples. The book discusses topics such as fundamentals of molecular modeling, QSAR model generation, protein databases and how to use them to select and analyze protein structure, and pharmacophore modeling for drug targets. Additionally, it discusses data retrieval system, molecular surfaces, and freeware and online servers. The book is a valuable source for graduate students and researchers on bioinformatics, molecular modeling, biotechnology and several members of biomedical field who need to understand more about computer-aided molecular modeling. Presents exercises with solutions to aid readers in validating their own protocol Brings a thorough interpretation of results of each exercise to help readers compare them to their own study Explains each parameter utilized in the algorithms to help readers understand and manipulate various features of molecules and target protein to design their study

Physico-chemical and Computational Approaches to Drug Discovery - Javier Luque 2012

This title covers a wide range of topics relevant to the development of drugs. It provides a comprehensive description of the major methodological strategies available for rational drug discovery.

In Silico Drug Discovery and Design - Claudio N. Cavasotto 2015-08-06

In Silico Drug Discovery and Design: Theory, Methods, Challenges, and Applications provides a comprehensive, unified, and in-depth overview of the current methodological strategies in computer-aided drug discovery and design. Its main aims are to introduce the theoretical framework and algorithms, discuss the range of validity, strengths and limita

In Silico Chemistry and Biology - Girish Kumar Gupta 2022-05-09

In Silico Chemistry and Biology: Current and Future Prospects provides a compact overview on recent advances in this highly dynamic branch of chemistry. Various methods of protein modelling and computer-assisted drug design are presented, including fragment- and ligand-based approaches. Many successful practical applications of these techniques are demonstrated. The authors also look to the future and describe the main challenges of the field.

In Silico Methods for Drug Design and Discovery - Simone Brogi 2020-10-09

This eBook is a collection of articles from a Frontiers Research Topic. Frontiers Research Topics are very popular trademarks of the Frontiers Journals Series: they are collections of at least ten articles, all centered on a particular subject. With their unique mix of varied contributions from Original Research to Review Articles, Frontiers Research Topics unify the most influential researchers, the latest key findings and historical advances in a hot research area! Find out more on how to host your own Frontiers Research Topic or contribute to one as an author by contacting the Frontiers Editorial Office: frontiersin.org/about/contact.

Drug Discovery and Development - Ramarao Poduri 2021-02-15

This book describes the processes that are involved in the development of new drugs. The authors discuss the history, role of natural products and concept of receptor interactions with regard to the initial stages of drug discovery. In a single, highly readable volume, it outlines the basics of pharmacological screening, drug target identification, and genetics involved in early drug discovery. The final chapters introduce readers to stem therapeutics, pharmacokinetics, pharmacovigilance, and toxicological testing. Given its scope, the book will enable research scholars, professionals and young scientists to understand the key fundamentals of drug discovery, including stereochemistry, pharmacokinetics, clinical trials, statistics and toxicology.

In Silico Drug Discovery and Design - Claudio N. Cavasotto 2017-07

In Silico Drug Discovery and Design: Theory, Methods, Challenges, and Applications provides a comprehensive, unified, and in-depth overview of the current methodological strategies in computer-aided drug discovery and design. Its main aims are to introduce the theoretical framework and

algorithms, discuss the range of validity, strengths and limitations of each methodology, and present applications to real world problems in the drug discovery arena. Special emphasis has been given to the emerging and most pressing methodological challenges in in silico drug discovery and design. The book assumes a basic knowledge of physical principles and molecular modeling. Particular attention has been paid to outline the underlying physico-chemical foundation of the methods described, thus providing the necessary background to avoid a -black-box- approach. In each self-contained chapter, this is presented together with the latest developments and applications, and the challenges that lie ahead. Assembling a unique team of experts to weigh in on the most important issues influencing modern computational drug discovery and design, this book constitutes both a desktop reference to academic and industrial researchers in the field, and a textbook for students in the area of molecular modeling and drug discovery. Comprised of 18 chapters and divided into three parts, this book: Provides a comprehensive, unified, and in-depth overview of the current methodological strategies in computer-aided drug discovery and design Outlines the underlying physico-chemical foundation of the methods described Presents several applications of computational methods to real world problems in the drug design field Helps to avoid a -black-box- approach to in silico drug discovery Constitutes an actual textbook for students in the area of molecular modeling and drug discovery Gives the reader the adequate background to face the current challenges of the field In Silico Drug Discovery and Design: Theory, Methods, Challenges, and Applications describes the theoretical framework, methods, practical applications and case examples relevant to computer-aided drug lead discovery and design. This text will surely aid in understanding the underlying physical foundation of computational tools and their range of application, thus facilitating the interpretation of simulation results.

Frontiers in Computational Chemistry - Zaheer Ul-Haq 2017-02-22

Frontiers in Computational Chemistry presents contemporary research on molecular modeling techniques used in drug discovery and the drug development process: computer aided molecular design, drug discovery and development, lead generation, lead optimization, database management, computer and molecular graphics, and the development of new computational methods or efficient algorithms for the simulation of chemical phenomena including analyses of biological activity. The third volume of this series features four chapters covering in silico approaches to computer aided drug design, modeling of platinum and adjuvant anti-cancer drugs, allostery in proteins and studies on the theory of chemical space in electron systems.

De novo Molecular Design - Gisbert Schneider 2013-12-23

Systematically examining current methods and strategies, this ready reference covers a wide range of molecular structures, from organic-chemical drugs to peptides, Proteins and nucleic acids, in line with emerging new drug classes derived from biomacromolecules. A leader in the field and one of the pioneers of this young discipline has assembled here the most prominent experts from across the world to provide first-hand knowledge. While most of their methods and examples come from the area of pharmaceutical discovery and development, the approaches are equally applicable for chemical probes and diagnostics, pesticides, and any other molecule designed to interact with a biological system. Numerous images and screenshots illustrate the many examples and method descriptions. With its broad and balanced coverage, this will be the firststop resource not only for medicinal chemists, biochemists and biotechnologists, but equally for bioinformaticians and molecular designers for many years to come. From the content: * Reaction-driven de novo design * Adaptive methods in molecular design * Design of ligands against multitarget profiles * Free energy methods in ligand design * Fragment-based de novo design * Automated design of focused and target family-oriented compound libraries * Molecular de novo design by nature-inspired computing * 3D QSAR approaches to de novo drug design * Bioisosteres in de novo design * De novo design of peptides, proteins and nucleic acid structures, including RNA aptamers and many more.

Antifungal Drug Discovery: New Theories and New Therapies - Chaminda Jayampath Seneviratne 2016-09-13

Fungal infections such as candidoses can range from superficial mucous membrane infection to life-threatening systemic mycoses. Candida infections are a significant clinical problem globally due to rapid rise in compromised host populations including HIV/AIDS, organ transplant recipients and patients on chemotherapy. In addition, sharp increase in aging populations which are susceptible to fungal infections is expected in next few decades. Antifungal drugs are relatively difficult to develop compared to the antibacterial drugs owing to the eukaryotic nature of the cells. Therefore, only a handful of antifungal agents are currently available to treat the myriad of fungal infections. Moreover, rising antifungal resistance and host-related adverse reactions have limited the antifungal arsenal against fungal pathogens. In this research topic, we tried to update the theoretical aspects pertaining to the antifungal drug discovery i.e. proposed novel mechanisms, new drug targets and pathways. In addition, invited authors explored the new antifungal drugs derived from natural and synthetic sources which are currently under development. Contributors were encouraged to bring new insight into the antifungal drug discovery. We hope the reader may arrive at a general consensus on the possible strategies to combat ever increasing ubiquitous fungal infection in this new century.

Next Generation Kinase Inhibitors - Paul Shapiro 2020-07-14

Protein kinases are fascinating enzymes that maintain the proper function of nearly every task performed by the cells of the human body. By extracting a phosphate from the energy molecule ATP and linking it to another protein, protein kinases alter the structure and ultimate function of other proteins. In this way, protein kinases help monitor the extracellular environment and integrate signaling cues that, for the most part, are beneficial for human health and survival. However, protein kinases are often dysregulated and responsible for the initiation and progression of many types of cancers, inflammatory disorders, and other diseases. Thus, decades of research have revealed much about how protein kinases are regulated and approaches to inhibit these enzymes to treat disease. However, nearly 30 years since the identification of the first clinically beneficial small molecule protein kinase inhibitor, there are only a few examples where these drugs provide sustained and durable patient responses. The goal of this book is to provide biomedical scientists, graduate, and professional degree students insight into different approaches using small molecules to block specific protein kinase functions that promote disease.

Density Functional Theory - Daniel Glossman-Mitnik 2022-05-18

Density Functional Theory (DFT) is a powerful technique for calculating and comprehending the molecular and electrical structure of atoms, molecules, clusters, and solids. Its use is based not only on the capacity to calculate the molecular characteristics of the species of interest but also on the provision of interesting concepts that aid in a better understanding of the chemical reactivity of the systems under study. This book presents examples of recent advances, new perspectives, and applications of DFT for the understanding of chemical reactivity through descriptors forming the basis of Conceptual DFT as well as the application of the theory and its related computational procedures in the determination of the molecular properties of different systems of academic, social, and industrial interest.

3D QSAR in Drug Design - Hugo Kubinyi 2006-04-11

Significant progress has been made in the study of three-dimensional quantitative structure-activity relationships (3D QSAR) since the first publication by Richard Cramer in 1988 and the first volume in the series. 3D QSAR in Drug Design. Theory, Methods and Applications, published in 1993. The aim of that early book was to contribute to the understanding and the further application of CoMFA and related approaches and to facilitate the appropriate use of these methods. Since then, hundreds of papers have appeared using the quickly developing techniques of both 3D QSAR and computational sciences to study a broad variety of biological problems. Again the editor(s) felt that the time had come to solicit reviews on published and new viewpoints to document the state of the art of 3D QSAR in its broadest definition and to provide visions of where new techniques will emerge or new appli- tions may be found. The intention is not only to highlight new ideas but also to show the shortcomings, inaccuracies, and abuses of the methods. We hope this

book will enable others to separate trivial from visionary approaches and me-too methodology from in- vative techniques. These concerns guided our choice of contributors. To our delight, our call for papers elicited a great many manuscripts.

Bioinformatics and Drug Discovery - Richard S. Larson 2010-10-28

A collection of readily reproducible bioinformatic methods to advance the drug discovery process from gene identification to protein modeling to the identification of specific drug candidates. The authors demonstrate these techniques, including microarray analysis, the analysis of genes as potential drug targets, virtual screening and in silico protein design, and cheminformatics, in a variety of practical situations. Because these technologies are still emergent, each chapter contains an extended introduction that explains the theory and application of the technology and techniques described.

Small Molecule Drug Discovery - Andrea Trabocchi 2019-11-23

Small Molecule Drug Discovery: Methods, Molecules and Applications presents the methods used to identify bioactive small molecules, synthetic strategies and techniques to produce novel chemical entities and small molecule libraries, chemoinformatics to characterize and enumerate chemical libraries, and screening methods, including biophysical techniques, virtual screening and phenotypic screening. The second part of the book gives an overview of privileged cyclic small molecules and major classes of natural product-derived small molecules, including carbohydrate-derived compounds, peptides and peptidomimetics, and alkaloid-inspired compounds. The last section comprises an exciting collection of selected case studies on drug discovery enabled by small molecules in the fields of cancer research, CNS diseases and infectious diseases. The discovery of novel molecular entities capable of specific interactions represents a significant challenge in early drug discovery. Small molecules are low molecular weight organic compounds that include natural products and metabolites, as well as drugs and other xenobiotics. When the biological target is well defined and understood, the rational design of small molecule ligands is possible. Alternatively, small molecule libraries are being used for unbiased assays for complex diseases where a target is unknown or multiple factors contribute to a disease pathology. Outlines modern concepts and synthetic strategies underlying the building of small molecules and their chemical libraries useful for drug discovery Provides modern biophysical methods to screening small molecule libraries, including high-throughput screening, small molecule microarrays, phenotypic screening and chemical genetics Presents the most advanced chemoinformatics tools to characterize the structural features of small molecule libraries in terms of chemical diversity and complexity, also including the application of virtual screening approaches Gives an overview of structural features and classification of natural product-derived small molecules, including carbohydrate derivatives, peptides and peptidomimetics, and alkaloid-inspired small molecules

Computer-Aided Drug Design - Dev Bukhsh Singh 2020-10-09

This book provides up-to-date information on bioinformatics tools for the discovery and development of new drug molecules. It discusses a range of computational applications, including three-dimensional modeling of protein structures, protein-ligand docking, and molecular dynamics simulation of protein-ligand complexes for identifying desirable drug candidates. It also explores computational approaches for identifying potential drug targets and for pharmacophore modeling. Moreover, it presents structure- and ligand-based drug design tools to optimize known drugs and guide the design of new molecules. The book also describes methods for identifying small-molecule binding pockets in proteins, and summarizes the databases used to explore the essential properties of drugs, drug-like small molecules and their targets. In addition, the book highlights various tools to predict the absorption, distribution, metabolism, excretion (ADME) and toxicity (T) of potential drug candidates. Lastly, it reviews in silico tools that can facilitate vaccine design and discusses their limitations.

Computational Tools for Chemical Biology - Sonsoles Martín-Santamaría 2017-11-01

This book offers a fresh perspective on how computational tools can aid the chemical biology research community and drive new research.

In Silico Medicinal Chemistry - Nathan Brown 2015-11-02
Exploring the methodologies and applications ofcomputational tools in drug design, this book is a practical introduction to chemoinformatics, molecular modelling and computational chemistry for researchers.
Drug Design and Discovery - Seetharama D. Satyanarayanajois 2011-02-17
Research in the pharmaceutical sciences and medicinal chemistry has taken an important new direction in the past two decades with a focus on large molecules, especially peptides and proteins, as well as DNA therapeutics. In Drug Design and Discovery: Methods and Protocols, leading experts provide an in-depth view of key protocols that are commonly used in drug discovery laboratories. Covering both classic and cutting-edge techniques, this volume explores computational docking, quantitative structure-activity relationship (QSAR), peptide synthesis, labeling of peptides and proteins with fluorescent labels, DNA-microarray, zebrafish model for drug screening, and other analytical screening and biological assays that are routinely used during the drug discovery process. Written in the highly successful Methods in Molecular BiologyTM series format, chapters include introductions to their respective topics, lists of the necessary materials, step-by-step, readily reproducible laboratory protocols, and tips on troubleshooting and avoiding known pitfalls. Thorough and accessible, Drug Design and Discovery: Methods and Protocols serve as a vital laboratory reference for pharmaceutical chemists, medicinal chemists, and pharmacologists as well as for molecular biologists.
Innovations and Implementations of Computer Aided Drug Discovery Strategies in Rational Drug Design - Sanjeev Kumar Singh 2021-02-02
This book presents various computer-aided drug discovery methods for the design and development of ligand and structure-based drug molecules. A wide variety of computational approaches are now being used in various stages of drug discovery and development, as well as in clinical studies. Yet, despite the rapid advances in computer software and hardware, combined with the exponential growth in the available biological information, there are many challenges that still need to be addressed, as this book shows. In turn, it shares valuable insights into receptor-ligand interactions in connection with various biological functions and human diseases. The book discusses a wide range of phylogenetic methods and highlights the applications of Molecular Dynamics Simulation in the drug discovery process. It also explores the application of quantum mechanics in order to provide better accuracy when calculating protein-ligand binding interactions and predicting binding affinities. In closing, the book provides illustrative descriptions of major challenges associated with computer-aided drug discovery for the development of therapeutic drugs. Given its scope, it offers a valuable asset for life sciences researchers, medicinal chemists and bioinformaticians looking for the latest information on computer-aided methodologies for drug development, together with their applications in drug discovery.
Chirality in Drug Design and Development - Indra K. Reddy 2004-03-15
Covering every essential element in the development of chiral products, this reference provides a solid overview of the formulation, biopharmaceutical characteristics, and regulatory issues impacting the production of these pharmaceuticals. It supports researchers as they evaluate the pharmacodynamic, pharmacokinetic, and toxicological characteristics of specific enantiomers and chiral drug compounds and addresses in one convenient reference all the major challenges pertaining to drug chirality that have been neglected in the literature. Chirality in Drug Design and Development collects the latest studies from an interdisciplinary team of experts on chiral drug design.
Computational Toxicology - Sean Ekins 2018-01-08
A key resource for toxicologists across a broad spectrum of fields, this book offers a comprehensive analysis of molecular modelling approaches and strategies applied to risk assessment for pharmaceutical and environmental chemicals. • Provides a perspective of what is currently achievable with computational toxicology and a view to future developments • Helps readers overcome questions of data sources,

curation, treatment, and how to model / interpret critical endpoints that support 21st century hazard assessment • Assembles cutting-edge concepts and leading authors into a unique and powerful single-source reference • Includes in-depth looks at QSAR models, physicochemical drug properties, structure-based drug targeting, chemical mixture assessments, and environmental modeling • Features coverage about consumer product safety assessment and chemical defense along with chapters on open source toxicology and big data

Drug Metabolism in Drug Design and Development - Donglu Zhang 2007-11-16

The essentials of drug metabolism vital to developing new therapeutic entities Information on the metabolism and disposition of candidate drugs is a critical part of all aspects of the drug discovery and development process. Drug metabolism, as practiced in the pharmaceutical industry today, is a complex, multidisciplinary field that requires knowledge of sophisticated analytical technologies and expertise in mechanistic and kinetic enzymology, organic reaction mechanism, pharmacokinetic analysis, animal physiology, basic chemical toxicology, preclinical pharmacology, and molecular biology. With chapters contributed by experts in their specific areas, this reference covers: * Basic concepts of drug metabolism * The role of drug metabolism in the pharmaceutical industry * Analytical techniques in drug metabolism * Common experimental approaches and protocols Drug Metabolism in Drug Design and Development emphasizes practical considerations such as the data needed, the experiments and analytical methods typically employed, and the interpretation and application of data. Chapters highlight facts, common protocols, detailed experimental designs, applications, and limitations of techniques. This is a comprehensive, hands-on reference for drug metabolism researchers as well as other professionals involved in pre-clinical drug discovery and development.

Natural Products as Enzyme Inhibitors - Vijay L. Maheshwari 2022

This book provides an overview of the latest developments and future challenges in enzyme inhibitor research. It discusses the general enzyme inhibitory principles and mechanisms in enzyme activity regulation and application of enzyme inhibitors in different areas and sectors. The major areas of applications of enzyme inhibitors covered in this book are human health management, agriculture, food processing and research, which leads to drug discovery or enzyme activity mechanisms. The book also identifies the gaps in the existing knowledge and opens up new research ideas in this important area. Currently, most enzyme inhibitors are reported to inhibit various classes of enzymes. These enzyme inhibitors are the focus of the scientific community because they may answer an increasing array of questions in the research area of biological sciences, including biochemistry, medicine, physiology, pharmacy, agriculture, ecology etc. It also serves as a useful tool in the study of enzyme structures and reaction mechanisms and in the development of technologies in agriculture, food processing, and health management. Chapters in this book cover topics such as plant-derived inhibitors of serine proteases, pancreatic lipase (PL) inhibitors from indigenous medicinal plants, amylase inhibitors and their applications in agriculture and food processing industries and advances in silico techniques used in the study of enzyme inhibitors. The book will serve as a valuable resource for students and researchers in Life Sciences, agriculture, medicine, food processing, and allied industries.

Pandemic Outbreaks in the 21st Century - Buddolla Viswanath 2021-08-24

In the past two decades, several pandemics have ravaged the globe, giving us several lessons on infectious disease epidemiology, the importance of initial detection and characterization of outbreak viruses, the importance of viral epidemic prevention steps, and the importance of modern vaccines. Pandemic Outbreaks in the Twenty-First Century: Epidemiology, Pathogenesis, Prevention, and Treatment summarizes the improvements in the 21st century to overcome / prevent / treat global pandemic with future prospective. Divided into 9 chapters, the book begins with an in-depth introduction to the lessons learned from the first pandemic of the 21st century. It describes the history, present and future in terms of detection, prevention and treatment. Followed by chapters on

the outbreak, treatment strategies and clinical management of several infectious diseases like MERS, SARD and COVID 19, Pandemic Outbreaks in the Twenty-First Century: Epidemiology, Pathogenesis, Prevention, and Treatment, presents chapters on immunotherapies and vaccine technologies to combat pandemic outbreak and challenges. The book finishes with a chapter on the current knowledge and technology to control pandemic outbreaks. All are presented in a practical short format, making this volume a valuable resource for very broad academic audience. Provides insight to the lessons learned from past pandemics Gives recommendations, future direction in terms of detection, prevention and treatment of pandemics Guides readers through the status and recent developments of vaccines to overcome or prevent pandemics Shows how to enhance the host innate immunity in infectious diseases Includes a chapter on immunotherapies to combat pandemic outbreaks

Drug Discovery and Evaluation: Safety and Pharmacokinetic Assays - H. Gerhard Vogel 2013-02-27

-A landmark in the continuously changing world of drugs -Essential reading for scientists and managers in the pharmaceutical industry involved in drug finding, drug development and decision making in the development process -Of use for government institutions and committees working on official guidelines for drug evaluation worldwide

Progress in the Chemistry of Organic Natural Products 110 - A. Douglas Kinghorn 2019-10-16

The book summarizes important aspects of cheminformatics that are relevant for natural product research. It highlights cheminformatics tools that help to match natural products with their respective biological targets or off-targets, and discusses the potential and limitations of this approach.

Lead Generation Approaches in Drug Discovery - Zoran Rankovic 2010-04-07

An integrated overview of modern approaches to lead discovery Lead generation is increasingly seen as a distinct and success-determining phase of the drug discovery process. Over recent years, there have been major advances in the understanding of what constitutes a good lead compound and how to improve the chances of finding such a compound. Written by leading scientists and established opinion leaders from industry and academia, this book provides an authoritative overview of the field, as well as the theory, practice, and scope, of the principal Lead Generation Approaches in Drug Discovery, including: The evolution of the lead discovery process, key concepts, current challenges, and future directions Strategies and technologies driving the high-throughput screening (HTS) approach to lead discovery, including the shifting paradigms in the design of compound collections and best practice in the hit confirmation process Knowledge-based in silico or "virtual" screening Theory and practice of the fragment-based approach to lead discovery The opportunities and challenges presented by multi-target drug discovery (MTDD) De novo design of lead compounds and new approaches to estimating the synthetic accessibility of de novo–designed molecules The impact of natural products on drug discovery, and potential of natural product–like compounds for exploring regions of biologically relevant chemical space Using early screening of hits and leads for metabolic, pharmacokinetic, and toxicological liabilities to reduce attrition during the later phases of drug discovery The utility of parallel synthesis and purification in lead discovery With each topic supported by numerous case studies, this is indispensable reading for researchers in industry and academia who wish to keep up to date with the latest strategies and approaches in drug discovery.

In-Silico Lead Discovery - Maria A. Miteva 2011

Computer-aided drug design and in silico screening have contributed to the discovery of several compounds that have either reached the market or entered clinical trials. In silico Lead Discovery is a compilation of the efforts of several experts on bioinf