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Structural Bioinformatics: Applications in Preclinical Drug Discovery Process C. Gopi Mohan 2019-01-10 This book reviews the advances and challenges of structure-based drug design in the preclinical drug discovery process, addressing various diseases, including malaria, tuberculosis and cancer. Written by internationally recognized researchers, this edited book discusses how the application of the various in-silico techniques, such as molecular docking, virtual screening, pharmacophore modeling, molecular dynamics simulations, and residue interaction networks offers insights into pharmacologically active novel molecular entities. It presents a clear concept of the molecular mechanism of different drug targets and explores methods to help understand drug resistance. In addition, it includes chapters dedicated to natural-product- derived medicines, combinatorial drug discovery, the CryoEM technique for structure-based drug design and big data in drug discovery. The book offers an invaluable resource for graduate and postgraduate students, as well as for researchers in academic and industrial laboratories working in the areas of chemoinformatics, medicinal and pharmaceutical chemistry and pharmacoinformatics.

Fragment-Based Drug Discovery Steven Howard 2015-07-03 Fragment-based drug discovery is a rapidly evolving area of research, which has recently seen new applications in areas such as epigenetics, GPCRs and the identification of novel allosteric binding pockets. The first fragment-derived drug was recently approved for the treatment of melanoma. It is hoped that this approval is just the beginning of the many drugs yet to be discovered using this fascinating technique. This book is written from a Chemist's perspective and comprehensively assesses the impact of fragment-based drug discovery on a wide variety of areas of medicinal chemistry. It will prove to be an invaluable resource for medicinal chemists working in academia and industry, as well as anyone interested in novel drug discovery techniques.

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

Drug Discovery and Development - E-Book Raymond G Hill 2012-07-20 The modern pharmacopeia has enormous power to alleviate disease, and owes its existence almost entirely to the work of the pharmaceutical industry. This book provides an introduction to the way the industry goes about the discovery and development of new drugs. The first part gives a brief historical account from its origins in the mediaeval apothecaries' trade, and discusses the changing understanding of what we mean by disease, and what therapy aims to achieve, as well as summarising case histories of the discovery and development of some important drugs. The second part focuses on the science and technology involved in the discovery process: the stages by which a promising new chemical entity is identified, from the starting point of a medical need and an idea for addressing it. A chapter on biopharmaceuticals, whose discovery and development tend to follow routes somewhat different from synthetic compounds, is included here, as well as accounts of patent issues that arise in the discovery phase, and a chapter on research management in this environment. The third section of the book deals with drug development: the work that has to be undertaken to turn the drug candidate that emerges from the discovery process into a product on the market. The definitive introduction to how a pharmaceutical company goes about its business of discovering and developing drugs. The second edition has a new editor: Professor Raymond Hill ● non-executive director of Addex Pharmaceuticals, Covagen and of Orexo AB ● Visiting Industrial Professor of Pharmacology in the University of Bristol ● Visiting Professor in the School of Medical and Health Sciences at the University of Surrey ● Visiting Professor in Physiology and Pharmacology at the University of Strathclyde ● President and Chair of the Council of the British Pharmacological Society ● member of the Nuffield Council on Bioethics and the Advisory Council on Misuse of Drugs. New to this edition: Completely rewritten chapter on The Role of Medicinal Chemistry in the Drug Discovery Process. New topic - DMPK Optimization Strategy in drug discovery. New chapter on Scaffolds: Small globular proteins as antibody substitutes. Totally updated chapters on Intellectual Property and Marketing 50 new illustrations in full colour Features Accessible, general guide to pharmaceutical research and development. Examines the interfaces between cost and social benefit, quality control and mass production, regulatory bodies, patent management, and all interdisciplinary intersections essential to effective drug development. Written by a strong team of scientists with long experience in the pharmaceutical industry. Solid overview of all the steps from lab bench to market in an easy-to-understand way which will be accessible to non-specialists. From customer reviews of the previous edition: '... it will have everything you need to know on this module. Deeply referenced and, thus, deeply reliable. Highly Commended in the medicine category of the BMA 2006 medical book competition Winner of the Royal Society of Medicine Library Prize for Medical Book of the Year

Multi-Scale Approaches in Drug Discovery Alejandro Speck-Planche 2017-02-14 Drug discovery is an expensive, time-consuming process and the modern drug discovery community is constantly challenged not only with discovering novel bioactive agents to combat resistance from known diseases and fight against new ones, but to do so in a way that is economically effective. Advances in both experimental and theoretical/computational methods envisage that the greatest challenges in drug discovery can be most successfully addressed by using a multi-scale approach, drawing on the specialties of a whole host of different disciplines. Multi-Scale Approaches to Drug Discovery furnishes chemists with the detail they need to identify drug leads with the highest potential before isolating and synthesizing them to produce effective drugs with

greater swiftness than classical methods may allow. This significantly speeds up the search for more efficient therapeutic agents. After an introduction to multi-scale approaches outlining the need for and benefits of their use, the book goes on to explore a range of useful techniques and research areas, and their potential applications to this process. Profiling drug binding by thermodynamics, machine learning for predicting enzyme sub-classes, and multitasking models for computer-aided design and virtual compound screening are discussed, before the book goes on to review Alkaloid Menispermaceae leads, natural chemotherapeutic agents and methods for speeding up the design and virtual screening of therapeutic peptides. Flavonoids as multi-target compounds are then explored, before the book concludes with a review of Quasi-SMILES as a novel tool. Collecting together reviews and original research contributions written by leading experts in the field, Multi-Scale Approaches to Drug Discovery highlights cutting-edge approaches and practical examples of their implementation for those involved in the drug discovery process at many different levels. Using the combined knowledge of medicinal, computational, pharmaceutical and bio- chemists, it aims to support growth in the multi-scale approach to promote greater success in the development of new drugs. Offers practical guidance on ways to implement multiscale approaches for increased efficiency in drug discovery Draws on the experience of a highly skilled team of authors under the editorial guidance of one of the field's leading experts Includes cutting-edge techniques at the forefront of medicinal chemistry and drug discovery optimization

New Horizons in Predictive Drug Metabolism and Pharmacokinetics Alan G E Wilson 2015-11-20 Drug metabolism, pharmacokinetics and toxicokinetics as determinants of drug attrition and the safety of xenobiotics are critically important. This book presents a comprehensive treatise on the current issues and challenges facing drug metabolism and pharmacokinetics. Readers will find a thorough exploration of their predictive role in impacting drug discovery and development and in improving the success rate and safety assessment of pharmaceuticals and industrial or occupational chemicals. Chapters not only focus on the current state of art, with distinct examples, but on future needs and approaches likely to improve our prediction of potential human risk. Discussions of critical properties that are determinants of a compound’s metabolic and pharmacokinetic fate follow introductory chapters. The Drug Discovery process increasingly incorporates pharmacokinetics and drug metabolism screening and focus has shifted towards in silico, computational and systems biology approaches. Core chapters reflect this and the recent interest and need to assess the role of transporters, along with drug metabolizing enzymes, as potential determinants of pharmacokinetic behaviour, toxicity and drug-drug interactions. Lastly, chapters cover the issues and factors involved in translating pharmacokinetics from in silico to in vivo and from animal models to man, and postulate future directions and opportunities. Leading experts from academia, industry and regulatory bodies across the globe contribute their knowledge to this book, which scientists involved in many aspects of the drug discovery process, as well as regulators and postgraduate students, will find a useful resource.

Structural Biology in Drug Discovery Jean-Paul Renaud 2020-01-09 With the most comprehensive and up-to-date overview of structure-based drug discovery covering both experimental and computational approaches, Structural Biology in Drug Discovery: Methods, Techniques, and Practices describes principles, methods, applications, and emerging paradigms of structural biology as a tool for more efficient drug development. Coverage includes successful examples, academic and industry insights, novel concepts, and advances in a

rapidly evolving field. The combined chapters, by authors writing from the frontlines of structural biology and drug discovery, give readers a valuable reference and resource that: Presents the benefits, limitations, and potentiality of major techniques in the field such as X-ray crystallography, NMR, neutron crystallography, cryo-EM, mass spectrometry and other biophysical techniques, and computational structural biology Includes detailed chapters on druggability, allostery, complementary use of thermodynamic and kinetic information, and powerful approaches such as structural chemogenomics and fragment-based drug design Emphasizes the need for the in-depth biophysical characterization of protein targets as well as of therapeutic proteins, and for a thorough quality assessment of experimental structures Illustrates advances in the field of established therapeutic targets like kinases, serine proteinases, GPCRs, and epigenetic proteins, and of more challenging ones like protein-protein interactions and intrinsically disordered proteins

Unsupervised Feature Extraction Applied to Bioinformatics Y-h. Taguchi 2019-08-23 This book proposes applications of tensor decomposition to unsupervised feature extraction and feature selection. The author posits that although supervised methods including deep learning have become popular, unsupervised methods have their own advantages. He argues that this is the case because unsupervised methods are easy to learn since tensor decomposition is a conventional linear methodology. This book starts from very basic linear algebra and reaches the cutting edge methodologies applied to difficult situations when there are many features (variables) while only small number of samples are available. The author includes advanced descriptions about tensor decomposition including Tucker decomposition using high order singular value decomposition as well as higher order orthogonal iteration, and train tenor decomposition. The author concludes by showing unsupervised methods and their application to a wide range of topics. Allows readers to analyze data sets with small samples and many features; Provides a fast algorithm, based upon linear algebra, to analyze big data; Includes several applications to multi-view data analyses, with a focus on bioinformatics.

Physico-Chemical and Computational Approaches to Drug Discovery Javier Luque 2012-03-31 Molecular modeling and simulation play a central role in academic and industrial research focused on physico-chemical properties and processes. The efforts carried out in this field have crystallized in a variety of models, simulation methods, and computational techniques that are examining the relationship between the structure, dynamics and functional role of biomolecules and their interactions. In particular, there has been a huge advance in the understanding of the molecular determinants that mediate the interaction between small compounds acting as ligands and their macromolecular targets. This book provides an updated description of the advances experienced in recent years in the field of molecular modeling and simulation of biomolecular recognition, with particular emphasis towards the development of efficient strategies in structure-based drug design.

In vivo Models for Drug Discovery José Miguel Vela 2014-08-11 This one-stop reference is the first to present the complete picture -- covering all relevant organisms, from single cells to mammals, as well as all major disease areas, including neurological disorders, cancer and infectious diseases. Addressing the needs of the pharmaceutical industry, this unique handbook adopts a broad perspective on the use of animals in the early part of the drug development process, including regulatory rules and limitations, as well as numerous examples from real-life drug development projects. After a general introduction to the topic, the expert

contributors from research-driven pharmaceutical companies discuss the basic considerations of using animal models, including ethical issues. The main part of the book systematically surveys the most important disease areas for current drug development, from cardiovascular to endocrine disorders, and from infectious to neurological diseases. For each area, the availability of animal models for target validation, hit finding and lead profiling is reviewed, backed by numerous examples of both successes and failures among the use of animal models. The whole is rounded off with a discussion of perspectives and challenges. Key knowledge for drug researchers in industry as well as academia.

Drug Discovery Toxicology Yvonne Will 2016-04-18 As a guide for pharmaceutical professionals to the issues and practices of drug discovery toxicology, this book integrates and reviews the strategy and application of tools and methods at each step of the drug discovery process. • Guides researchers as to what drug safety experiments are both practical and useful • Covers a variety of key topics – safety lead optimization, in vitro-in vivo translation, organ toxicology, ADME, animal models, biomarkers, and –omics tools • Describes what experiments are possible and useful and offers a view into the future, indicating key areas to watch for new predictive methods • Features contributions from firsthand industry experience, giving readers insight into the strategy and execution of predictive toxicology practices

Bioinformatics and Drug Discovery Richard S. Larson 2012 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 Biology 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.

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

Target Discovery and Validation Alleyn T. Plowright 2019-12-31 The modern drug developers? guide for making informed choices among the diverse target identification methods Target Discovery and Validation: Methods and Strategies for Drug Discovery offers a hands-on review of the modern technologies for drug target identification and validation. With contributions from noted industry and academic experts, the book addresses the most recent chemical, biological, and computational methods. Additionally, the book highlights techologies that are applicable to ?difficult? targets and drugs directed at multiple targets, including chemoproteomics, activity-based protein profiling, pathway mapping, genome-wide association studies, and array-based profiling. Throughout, the authors highlight a range of diverse approaches, and target validation studies reveal how these methods can support academic and drug discovery scientists in their target discovery and validation research. This resource: -Offers a guide to identifying and validating targets, a key enabling

technology without which no new drug development is possible -Presents the information needed for choosing the appropriate assay method from the ever-growing range of available options -Provides practical examples from recent drug development projects, e. g. in kinase inhibitor profiling Written for medicinal chemists, pharmaceutical professionals, biochemists, biotechnology professionals, and pharmaceutical chemists, Target Discovery and Validation explores the current methods for the identification and validation of drug targets in one comrpehensive volume. It also includes numerous practical examples.

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

Drug Repurposing Farid A. Badria 2020-12-02 Drug repurposing or drug repositioning is a new approach to presenting new indications for common commercial and clinically approved existing drugs. For example, chloroquine, an old antimalarial drug, showed promising results for treating COVID-19, interfering with MDR in several types of cancer, and chemosensitizing human leukemic cells.This book focuses on the hypothesis, risk/benefits, and economic impacts of drug repurposing on drug discovery in dermatology, infectious diseases, neurological disorders, cancer, and orphan diseases. It brings together up-to-date research to provide readers with an informative, illustrative, and easy-to-read book useful for students, clinicians, and the pharmaceutical industry.

In Silico Models for Drug Discovery Sandhya Kortagere 2013-04-09 Infectious diseases caused by viruses, parasites, bacteria, and fungi are the number one cause of death worldwide. Although new technologies have improved diagnosis of infectious diseases, the efficacy of all known current anti-infective agents is threatened by the spread of drug-resistant forms of the pathogens. Hence, there remains an urgent need to develop anti-infective agents that target drug-resistant pathogens. In Silico Models for Drug Discovery presents a comprehensive look at the role in silico models play in understanding infectious diseases and in developing novel therapeutics to treat them. Written by leading experts in the field, chapters cover topics such as techniques to derive novel antimicrobial targets, methods of interpreting polypharmacology-based drug target networks, and molecular dynamics techniques used to compute binding energies of drugs to their target proteins, to name a few. Written in the successful Methods in Molecular BiologyTM series or in review article format, chapters include introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible protocols, and notes on troubleshooting and avoiding known pitfalls. Authoritative and easily accessible, In Silico Models for Drug Discovery seeks to serve both professionals and novices involved in the study and treatment of infectious diseases.

Systems Biological Approaches in Infectious Diseases Helena I. Boshoff 2007-01-15 This book brings together the various fields of functional genomics and systems biology that provide information on metabolic function. There is special emphasis on the identification of drug targets. The book includes practical examples from the various "omic" sciences as well as theoretical examples of how integrated knowledge of these sciences can be applied to drug discovery. It is of interest to researchers in the pharmaceutical drug discovery environment.

Virtual Drug Design Daniela Schuster 2020-01-13 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.

In Silico Models for Drug Discovery Sandhya Kortagere 2013 Infectious diseases caused by viruses, parasites, bacteria, and fungi are the number one cause of death worldwide. Although new technologies have improved diagnosis of infectious diseases, the efficacy of all known current anti-infective agents is threatened by the spread of drug-resistant forms of the pathogens. Hence, there remains an urgent need to develop anti-infective agents that target drug-resistant pathogens. In Silico Models for Drug Discovery presents a comprehensive look at the role in silico models play in understanding infectious diseases and in developing novel therapeutics to treat them. Written by leading experts in the field, chapters cover topics such as techniques to derive novel antimicrobial targets, methods of interpreting polypharmacology-based drug target networks, and molecular dynamics techniques used to compute binding energies of drugs to their target proteins, to name a few. Written in the successful Methods in Molecular Biology series or in review article format, chapters include introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible protocols, and notes on troubleshooting and avoiding known pitfalls. Authoritative and easily accessible, In Silico Models for Drug Discovery seeks to serve both professionals and novices involved in the study and treatment of infectious diseases.

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

Computer Applications in Pharmaceutical Research and Development Sean Ekins 2006-07-11 A unique, holistic approach covering all functions and phases of pharmaceutical research and development While there are a number of texts dedicated to individual aspects of pharmaceutical research and development, this unique contributed work takes a holistic and integrative approach to the use of computers in all phases of drug discovery, development, and marketing. It explains how applications are used at various stages, including bioinformatics, data mining, predicting human response to drugs, and high-throughput screening. By providing a comprehensive view, the book offers readers a unique framework and systems perspective from which they can devise strategies to thoroughly exploit the use of computers in their organizations during all phases of the discovery and development process. Chapters are organized into the following sections: * Computers in pharmaceutical research and development: a general overview * Understanding diseases: mining complex systems for knowledge * Scientific information handling and enhancing productivity * Computers in drug discovery * Computers in preclinical development * Computers in development decision making, economics, and market analysis * Computers in clinical development * Future applications and future development Each chapter is written by one or more leading experts in the field and carefully edited to ensure a consistent structure and approach throughout the book. Figures are used extensively to illustrate complex concepts and multifaceted processes. References are provided in each chapter to enable readers to continue investigating a particular topic in depth. Finally, tables of software resources are provided in many of the chapters. This is essential reading for IT professionals and scientists in the pharmaceutical industry as well as researchers involved in informatics and ADMET, drug discovery, and technology development. The book's cross-functional, all-phases approach provides a unique opportunity for a holistic analysis and assessment of computer applications in pharmaceutics.

Target Identification and Validation in Drug Discovery Jürgen Moll 2019-04-12 This second edition book explores breakthrough technologies in the field of drug target identification and validation. The volume emphasizes particularly revolutionary technologies, such as CRISPR-related screening, “big data,” and in silico approaches, as well as in vivo applications of CRISPR and best uses of animal models in drug development. Written for the highly successful Methods in Molecular Biology series, chapters include introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible laboratory protocols, and tips on troubleshooting and avoiding known pitfalls. Fully updated and authoritative, Target Identification and Validation in Drug Discovery: Methods and Protocols, Second Edition is an ideal guide for molecular and cellular biologists, pharmacologists, pathologists, bioinformaticians, clinical researchers, or investigators, as well as experts in other fields that need a quick overview of these state-of-the-art technologies.

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

Computational Approaches to Nuclear Receptors Pietro Cozzini 2012-11-30 Nuclear receptors (NR) are ligand-induced activated transcription factors that are involved in numerous biological processes. Since the 1990's when the first structures were determined by means of X ray diffraction, the number of NR structures has increased considerably. Moreover several 'omics' projects (genomics, pharmcogenomics and proteomics) have opened up great opportunities for the discovery of new targets, the characterization of abnormal protein patterns, the selection of "tailored" drugs and the evaluation of drug efficacy even with a lack of structural data. Furthermore, structure-based drug design, computational methods for in silico screening and nanobiotechnology- based tools are simplifying this time-consuming and money-intensive research of lead compounds and, possibly, new drugs. Biological interactions such as those that occur between a protein and ligand are concerted events where flexible molecules interact. Thus understanding flexibility of large molecules or biological complexes is of primary importance to help define the right model to approximate the reality for drug discovery, virtual screening, food safety analysis, etc. NRs are known as flexible targets, with many structural similarities, in particular for their Ligand Binding Domain: these similarities could be assumed to share behavioural qualities that belong to this class of compounds. Thus to supply a possible, complete and exhaustive answer to questions about the behaviour of NRs, their interactions with new potential drugs, endocrine disruptors such as animal and human food toxins, food additives or industry residuals, it is mandatory to approach the problem from a different point of view: a molecular modelling approach, steered synthesis, and in vitro and in vivo tests, etc. The aim of this book is to provide a state of the art review on investigations into Nuclear Receptors.

A Systems Engineering Approach for Genetic Pathway Analysis and Towards In-silico Drug Development Rishi Raj Gupta 2006

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

Chemoinformatics in Drug Discovery Tudor I. Oprea 2006-03-06 This handbook provides the first-ever inside view of today's integrated approach to rational drug design. Chemoinformatics experts from large pharmaceutical companies, as well as from chemoinformatics service providers and from academia demonstrate what can be achieved today by harnessing the power of computational methods for the drug discovery process.

With the user rather than the developer of chemoinformatics software in mind, this book describes the successful application of computational tools to real-life problems and presents solution strategies to commonly encountered problems. It shows how almost every step of the drug discovery pipeline can be optimized and accelerated by using chemoinformatics tools -- from the management of compound databases to targeted combinatorial synthesis, virtual screening and efficient hit-to-lead transition. An invaluable resource for drug developers and medicinal chemists in academia and industry.

Frontiers in Computational Chemistry: Volume 1 Zaheer Ul-Haq 2015-12-14 Frontiers in Computational Chemistry, originally published by Bentham and now distributed by Elsevier, presents the latest research findings and methods in the diverse field of computational chemistry, focusing on molecular modeling techniques used in drug discovery and the drug development process. This includes 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. In Volume 1, the leading researchers in the field have collected eight different perspectives in the application of computational methods towards drug design to provide an up-to-date rendering of the current field. This volume covers a variety of topics from G protein-coupled receptors, to the use of cheminformatics and bioinformatics, computational tools such as Molecular Mechanics Poisson-Boltzmann Surface Area, protein-protein interactions, the use of computational methods on large biological data sets, various computational methods used to identify pharmaceutically relevant targets, and more. Brings together a wide range of research into a single collection to help researchers keep up with new methods Uniquely focuses on computational chemistry approaches that can accelerate drug design Makes a solid connection between experiment and computation and the novel application of computational methods in the fields of biology, chemistry, biochemistry, physics, and biophysics, with particular focus on the integration of computational methods with experimental data

Poisonous Plants and Phytochemicals in Drug Discovery Andrew G. Mtewa 2020-12-04 Focusing on phytochemicals and their potential for drug discovery, this book offers a comprehensive resource on poisonous plants and their applications in chemistry and in pharmacology. Provides a comprehensive resource on phytotoxins, covering historical perspectives, modern applications, and their potential in drug discovery - Covers the mechanisms, benefits, risks and management protocols of phytotoxins in a scientific laboratory and the usefulness in drug discovery - Written and edited by leading researchers in phytochemistry, medicinal chemistry, analytical chemistry, toxicology, and more - Presents chapters in a carefully designed, clear order, making it an ideal resource for the academic researcher or the industry professional at any stage in their career Provides a comprehensive resource on phytotoxins, covering historical perspectives, modern applications, and their potential in drug discovery Covers the mechanisms, benefits, risks and management protocols of phytotoxins in a scientific laboratory and the usefulness in drug discovery Presents chapters in a carefully designed, clear order, making it an ideal resource for the academic researcher or the industry professional at any stage in their career

Virtual ADMET Assessment in Target Selection and Maturation B. Testa 2006-12-19 Today, biologists and

medicinal chemists realize that there is a strong relationship between pharmacodynamic (what the drug does to the organism) and pharmacokinetic (what the organism does to the drug) effects. A significant contributing factor to the evolution in drug discovery was the methodological and technological revolution with the advent of combinatorial chemistry, high-throughput screening and profiling, and in silico prediction of target-based activity and ADMET (absorption, distribution, metabolism, excretion and toxicity) properties. High-throughput screening and in silico methods have accelerated the process towards drugability of new chemical structures. Another component of the revolution in drug discovery is the replacement of the disease (indication)-based approach by a target-based approach. A better understanding of pathophysiology of diseases and the underlying biological processes of diseases combined with explosive development of genomics and proteomics have been instrumental in the birth of this new paradigm. This volume summarizes discussions of these three aspects of modern drug discovery, i.e. priority for targets, early ADMET assessment, and in silico screening. We trust that readers from academia as well as from industry will benefit from these studies.

Molecular Modelling and Drug Design K Anand Solomon 2019-06-05 Molecular modelling is the scientific art of simulating chemicalor biological systems, so that computational methods can beapplied to understand the process concerned. Models usingcomputers are generated using mathematical equations and areevolved based on experimental information that is taken intoconsideration during model building. This book is anintroduction to the field of molecular modelling and drug designin which biological molecules effective in treating diseases arediscovered using in silico methods.

Molecular Dynamics and Machine Learning in Drug Discovery Sergio Decherchi 2021-06-08 Dr. Sergio Decherchi and Dr. Andrea Cavalli are co-founders of BiKi Technologies s.r.l. - a company that commercializes a Molecular Dynamics-based software suite for drug discovery. All other Topic Editors declare no competing interests with regards to the Research Topic subject.

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.

Molecular Modeling in Drug Design Rebecca Wade 2019-03-26 Since the first attempts at structure-based drug design about four decades ago, molecular modelling techniques for drug design have developed enormously, along with the increasing computational power and structural and biological information of active compounds and potential target molecules. Nowadays, molecular modeling can be considered to be an integral component of the modern drug discovery and development toolbox. Nevertheless, there are still many methodological challenges to be overcome in the application of molecular modeling approaches to drug discovery. The eight original research and five review articles collected in this book provide a snapshot of the state-of-the-art of molecular modeling in drug design, illustrating recent advances and critically discussing important challenges. The topics covered include virtual screening and pharmacophore modelling, chemoinformatic applications of artificial intelligence and machine learning, molecular dynamics simulation and enhanced sampling to investigate contributions of molecular flexibility to drug–receptor interactions, the modeling of drug–receptor solvation, hydrogen bonding and polarization, and drug design against protein–protein interfaces and membrane protein receptors.

Structure-Based Drug Design Pandi Veerapandian 2018-03-29 Introducing the most recent advances in crystallography, nuclear magnetic resonance, molecular modeling techniques, and computational combinatorial chemistry, this unique, interdisciplinary reference explains the application of three-dimensional structural information in the design of pharmaceutical drugs. Furnishing authoritative analyses by world-renowned experts, Structure-Based Drug Design discusses protein structure-based design in optimizing HIV protease inhibitors and details the biochemical, genetic, and clinical data on HIV-1 reverse transcriptase presents recent results on the high-resolution three-dimensional structure of the catalytic core domain of HIV-1 integrase as a foundation for divergent combination therapy focuses on structure-based design strategies for uncovering receptor antagonists to treat inflammatory diseases demonstrates a systematic approach to the design of inhibitory compounds in cancer treatment reviews current knowledge on the Interleukin-1 (IL-1) system and progress in the development of IL-1 modulators describes the influence of structure-based methods in designing capsid-binding inhibitors for relief of the common cold and much more!

In Silico Modeling and Its Applications on Biomolecules Reaz Uddin 2011-04 The book provides a general introduction to advanced computational techniques applied in various stages of drug discovery. In particular, it focuses on molecular modeling, ligand- and structure-based drug design methods, and data mining in chemical informatics. Application side of this book deals with the development of the first structure-based three-dimensional quantitative structure-activity relationship (3D-QSAR) model of butyrylcholinesterase - a putative drug target for the treatment of Alzheimer's disease. The other part is comprised of detailed work conducted on 5-HT2C agonists. It describes pharmacophore modeling and 3D-QSAR studies. Comparative Molecular Field Analysis coupled with a genetic algorithm (CoMFA-GA) was carried out for aligned ligands. The last part describes the drug target MTB-Thymidine monophosphate kinase (TMPKMtub). The molecular modeling analyses resulted in identification of a cluster of water molecules that mediate key interactions between bound

ligands and backbone atoms of the enzyme residues.

Drug Transporters Glynis Nicholls 2015-12-31 Understanding and quantifying the effects of membrane transporters within the human body is essential for modulating drug safety and drug efficacy. In this first volume on Drug Transporters, the current knowledge and techniques in the transporter sciences and their relations to drug metabolism and pharmacokinetics are comprehensively reviewed. The second volume of the book is specifically dedicated to emerging science and technologies, highlighting potential areas for future advances within the drug transporter field. The topics covered in both volumes ensure that all relevant aspects of transporters are described across the drug development process, from in silico models and preclinical tools through to the potential impact of transporters in the clinic. Contributions are included from expert leaders in the field, at-the-bench industrial scientists, renowned academics and international regulators. Case studies and emerging developments are highlighted, together with the merits and limitations of the available methods and tools, and extensive references to reviews on specific in-depth topics are also included for those wishing to pursue their knowledge further. As such, this text serves as an essential handbook of information for postgraduate students, academics, industrial scientists and regulators who wish to understand the role of transporters in absorption, distribution, metabolism, and excretion processes. In addition, it is also a useful reference tool on the models and calculations necessary to predict their effect on human pharmacokinetics and pharmacodynamics.

Basic Principles of Drug Discovery and Development Benjamin E. Blass 2021-03-30 Basic Principles of Drug Discovery and Development presents the multifaceted process of identifying a new drug in the modern era, which requires a multidisciplinary team approach with input from medicinal chemists, biologists, pharmacologists, drug metabolism experts, toxicologists, clinicians, and a host of experts from numerous additional fields. Enabling technologies such as high throughput screening, structure-based drug design, molecular modeling, pharmaceutical profiling, and translational medicine are critical to the successful development of marketable therapeutics. Given the wide range of disciplines and techniques that are required for cutting edge drug discovery and development, a scientist must master their own fields as well as have a fundamental understanding of their collaborator's fields. This book bridges the knowledge gaps that invariably lead to communication issues in a new scientist's early career, providing a fundamental understanding of the various techniques and disciplines required for the multifaceted endeavor of drug research and development. It provides students, new industrial scientists, and academics with a basic understanding of the drug discovery and development process. The fully updated text provides an excellent overview of the process and includes chapters on important drug targets by class, in vitro screening methods, medicinal chemistry strategies in drug design, principles of in vivo pharmacokinetics and pharmacodynamics, animal models of disease states, clinical trial basics, and selected business aspects of the drug discovery process. Provides a clear explanation of how the pharmaceutical industry works, as well as the complete drug discovery and development process, from obtaining a lead, to testing the bioactivity, to producing the drug, and protecting the intellectual property Includes a new chapter on the discovery and development of biologics (antibodies proteins, antibody/receptor complexes, antibody drug conjugates), a growing and important area of the pharmaceutical industry landscape Features a new section on formulations, including a discussion of IV formulations suitable for human clinical

trials, as well as the application of nanotechnology and the use of transdermal patch technology for drug delivery Updated chapter with new case studies includes additional modern examples of drug discovery through high through-put screening, fragment-based drug design, and computational chemistry

Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences Navneet Sharma 2021-05-21 Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences brings together two very important fields in pharmaceutical sciences that have been mostly seen as diverging from each other: chemoinformatics and bioinformatics. As developing drugs is an expensive and lengthy process, technology can improve the cost, efficiency and speed at which new drugs can be discovered and tested. This book presents some of the growing advancements of technology in the field of drug development and how the computational approaches explained here can reduce the financial and experimental burden of the drug discovery process. This book will be useful to pharmaceutical science researchers and students who need basic knowledge of computational techniques relevant to their projects. Bioscientists, bioinformaticians, computational scientists, and other stakeholders from industry and academia will also find this book helpful. Provides practical information on how to choose and use appropriate computational tools Presents the wide, intersecting fields of chemo-bio-informatics in an easily-accessible format Explores the fundamentals of the emerging field of chemoinformatics and bioinformatics