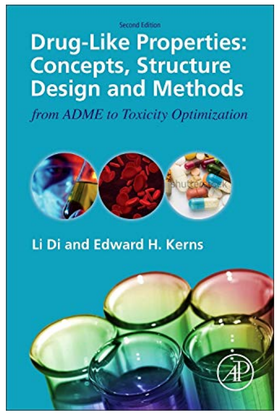

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Drug-like Properties: Concepts, Structure Design and Methods-Li Di 2010-07-26 Of the thousands of novel compounds that a drug discovery project team invents and that bind to the therapeutic target, typically only a fraction of these have sufficient 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

Drug-like Properties-Edward Harvel Kerns 2008 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

Drug-Like Properties-Li Di 2015-12-17 Of the thousands of novel compounds that a drug discovery project team invents and that bind to the therapeutic target, only a fraction have sufficient ADME (absorption, distribution, metabolism, elimination) properties, and acceptable toxicology properties, to become a drug product that will successfully complete human Phase I clinical trials. Drug-Like Properties: Concepts, Structure Design and Methods from ADME to Toxicity Optimization, Second Edition, provides scientists and students the background and tools to understand, discover, and develop optimal clinical candidates. This valuable resource explores physiochemical properties, including solubility and permeability, before exploring how compounds are absorbed, distributed, and metabolized safely and stably. Review chapters provide context and underscore the importance of key concepts such as pharmacokinetics, toxicity, the blood-brain barrier, diagnosing drug limitations, prodrugs, and formulation. Building on those foundations, this thoroughly updated revision covers a wide variety of current methods for the screening (high throughput), diagnosis (medium throughput) and in-depth (low throughput) analysis of drug properties for process and product improvement. From conducting key assays for interpretation and structural analysis, the reader learns to implement modification methods and improve each ADME property. Through valuable case studies, structure-property relationship descriptions, and structure modification strategies, Drug-Like Properties, Second Edition, offers tools and methods for ADME/Tox scientists through all aspects of drug research, discovery, design, development, and optimization. Provides a comprehensive and valuable working handbook for scientists and students in medicinal chemistry Includes expanded coverage of pharmacokinetics fundamentals and effects Contains updates throughout, including the authors' recent work in the importance of solubility in drug development; new and currently used property methods, with a reduction of seldom-used methods; and exploration of computational modeling methods

Drug Metabolism and Pharmacokinetics Quick Guide-Siamak Cyrus Khojasteh 2011-04-07 Drug Metabolism and Pharmacokinetics Quick Guide covers a number of aspects of drug assessment at drug discovery and development stages, topics such as pharmacokinetics, absorption, metabolism, enzyme kinetics, drug transporters, drug interactions, drug-like properties, assays and in silico calculations. It covers key concepts, with useful tables on physiological parameters (eg. blood flow to organs in x-species, expression and localization of enzymes and transporters), chemical structure, nomenclature, and moieties leading to bioactivation (with examples). Overall it includes a number of key topics useful at the drug discovery stage, which would serve as a quick reference with several examples from the literature to illustrate the concept.

Introduction to Biological and Small Molecule Drug Research and Development-C. Robin Ganellin 2013-05-07 Introduction to Biological and Small Molecule Drug Research and Development provides, for the first time, an introduction to the science behind successful pharmaceutical research and development programs. The book explains basic principles, then compares and contrasts approaches to both biopharmaceuticals (proteins) and small molecule drugs, presenting an overview of the business and management issues of these approaches. The latter part of the book provides carefully selected real-life case studies illustrating how the theory presented in the first part of the book is actually put into practice. Studies include Herceptin/T-DM1, erythropoietin (Epogen/Eprex/NeoRecormon), anti-HIV protease inhibitor Darunavir, and more. Introduction to Biological and Small Molecule Drug Research and Development is intended for late-stage undergraduates or postgraduates studying chemistry (at the biology interface), biochemistry, medicine, pharmacy, medicine, or allied subjects. The book is also useful in a wide variety of science degree courses, in post-graduate taught material (Masters and PhD), and as basic background reading for scientists in the pharmaceutical industry. For the first time, the fundamental scientific principles of biopharmaceuticals and small molecule chemotherapeutics are discussed side-by-side at a basic level Edited by three senior scientists with over 100 years of experience in drug research who have compiled the best scientific comparison of small molecule and biopharmaceuticals approaches to new drugs Illustrated with key examples of important drugs that exemplify the basic principles of pharmaceutical drug research and development

Pharmacokinetics and Metabolism in Drug Design-Dennis A. Smith 2006-05-01 In this new edition of a bestseller, all the contents have been updated and new material has been added, especially in the areas of toxicity testing and high throughput analysis. The authors, all of them employed at Pfizer in the discovery and development of new active substances, discuss the significant parameters and processes important for the absorption, distribution and retention of drug compounds in the body, plus the potential problems created by their transformation into toxic byproducts. They cover everything from the fundamental principles right up to the impact of pharmacokinetic parameters on the discovery of new drugs. While aimed at all those dealing professionally with the development and application of pharmaceutical substances, the readily comprehensible style makes this book equally suitable for students of pharmacy and related subjects.

Drug Design Strategies-David J. Livingstone 2011-11 Shows how different parts of the drug discovery process have developed, with particular emphasis on quantitative aspects and possible future progress.

Early Drug Development-Mitchell N. Cayen 2011-02-25 The focus of early drug development has been the submission of an Investigational New Drug application to regulatory agencies. Early Drug Development: Strategies and Routes to First-in-Human Trials guides drug development organizations in preparing and submitting an Investigational New Drug (IND) application. By explaining the nuts and bolts of preclinical development activities and their interplay in effectively identifying successful clinical candidates, the book helps pharmaceutical scientists determine what types of discovery and preclinical research studies are needed in order to support a submission to regulatory agencies.

Handbook of Essential Pharmacokinetics, Pharmacodynamics and Drug Metabolism for Industrial Scientists-Younggil Kwon 2007-05-08 In the pharmaceutical industry, the incorporation of the disciplines of pharma- kinetics, pharmacodynamics, and drug metabolism (PK/PD/DM) into various drug development processes has been recognized to be extremely important for approp- ate compound selection and optimization. During discovery phases, the identifi- tion of the critical PK/PD/DM issues of new compounds plays an essential role in understanding their pharmacological profiles and structure-activity relationships. Owing to recent progress in analytical chemistry, a large number of compounds can be screened for their PK/PD/DM properties within a relatively short period of time. During development phases as well, the toxicology and clinical study designs and trials of a compound should be based on a thorough understanding of its PK/PD/DM properties. During my time as an industrial scientist, I realized that a reference work designed for practical industrial applications of PK/PD/DM could be a very valuable tool for researchers not only in the pharmacokinetics and drug metabolism departments, but also for other discovery and development groups in pharmaceutical companies. This book is designed specifically for industrial scientists, laboratory assistants, and managers who are involved in PK/PD/DM-related areas. It consists of thirteen chapters, each of which deals with a particular PK/PD/DM issue and its industrial applications. Chapters 3 and 12 in particular address recent topics on higher throughput in vivo exposure screening and the prediction of pharmacokinetics in humans, respectively. Chapter 8 covers essential information on drug metabolism for industrial scientists.

Discovering and Developing Molecules with Optimal Drug-Like Properties-Allen C Templeton 2014-10-31 This authoritative volume provides a contemporary view on the latest research in molecules with optimal drug-like properties. It is a valuable source to access current best practices as well as new research techniques and strategies. Written by leading scientists in their fields, the text consists of fourteen chapters with an underlying theme of early collaborative opportunities between pharmaceutical and discovery sciences. The book explores the practical realities of performing physical pharmaceutical and biopharmaceutical research in the context of drug discovery with short timelines and low compound availability. Chapters cover strategies and tactics to enable discovery as well as predictive approaches to establish, understand and communicate risks in early development. It also examines the detection, characterization, and assessment of risks on the solid state properties of advanced discovery and early development candidates, highlighting the link between solid state properties and critical development parameters such as solubility and stability. Final chapters center on techniques to improve molecular solubilization and prevent precipitation, with particularly emphasis on linking physiochemical properties of molecules to formulation selection in preclinical and clinical settings.

Optimizing the "Drug-Like" Properties of Leads in Drug Discovery-Ronald Borchardt 2007-12-31 This book arises from a workshop organized by the American Association of Pharmaceutical Scientists entitled "Optimizing the Drug-Like Properties of Leads in Drug Discovery," which took place in Parsippany, NJ in September 2004. The workshop focused on the optimization of the drug-like properties of leads in drug discovery. The volume outlines strategies and methodologies designed to guide pharmaceutical and biotechnology companies through the drug discovery and development process.

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

Metabolism, Pharmacokinetics and Toxicity of Functional Groups-Dennis A Smith 2010-04-09 Until now, the area of drug metabolism and pharmacokinetics has been lacking in texts written for the Medicinal Chemist. This outstanding book, aimed at postgraduate medicinal chemists and those working in industry, fills this gap in the literature. Written by medicinal chemists and ADMET scientists with a combined experience of around 300 years, this aid to discovering drugs addresses the absorption, distribution, metabolism, excretion and toxicity (ADMET) issues associated with drugs. The book starts by describing drug targets and their structural motifs before moving on to explain ADMET for the medicinal chemist. It is the functional groups which most profoundly influence the drug molecules of which they form a part. They characterise the pharmacology, are essential to the activity, and alter the ADMET characteristics of each drug. Their effects follow a pattern, thus allowing medicinal chemists to predict and overcome potential challenges. For this reason, the Editors have taken the unique approach of dividing the remainder of the book into chapters which each focus on a different functional group. They describe drugs containing the functional group under consideration, explain why the group is there, and outline its physicochemical properties before going on to detail the ADMET issues. Where possible, prodrugs and bioisosteres, which may give alternative ADMET outcomes, are described. The chapters cross refer where similar matters are covered but individual chapters can be used in a stand alone manner. The book ends with a discussion of future targets and chemistry needs.

Medicinal Chemistry for Practitioners-Jie Jack Li 2020-06-29 Presenting both a panoramic introduction to the essential disciplines of drug discovery for novice medicinal chemists as well as a useful reference for veteran drug hunters, this book summarizes the state-of-the-art of medicinal chemistry. It covers key drug targets including enzymes, receptors, and ion channels, and hit and lead discovery. The book hen surveys a drug's pharmacokinetics and toxicity, with a solid chapter covering fundamental bioisosteres as a guide to structure-activity relationship investigations.

Privileged Scaffolds in Medicinal Chemistry-Stefan Bräse 2015-11-20 One strategy to expedite the discovery of new drugs, a process that is somewhat slow and serendipitous, is the identification and use of privileged scaffolds. This book covers the history of the discovery and use of privileged scaffolds and addresses the various classes of these important molecular fragments. The first of the benzodiazepines, a class of drugs that is powerful for treating anxiety, may not have been discovered had it not been for a chance experiment on the contents of a discarded flask found during a lab clean-up. Some years later, scientists discovered that benzodiazepine derivatives were also effective in treating other diseases. This class of molecules was the first to be described as privileged in the sense that it is especially effective at altering the course of disease. Other privileged molecular structures have since been discovered, and since these compounds are so effective at interacting with numerous classes of proteins, they may be an effective starting point to look for new drugs against the supposedly "undruggable" proteins. Following introductory chapters presenting an overview, a historical perspective and the theoretical background and findings, main chapters describe the structure of privileged structures in turn and discuss major drug classes associated with them and their syntheses. This book provides comprehensive coverage of the subject through chapters contributed by expert authors from both academia and industry and will be an excellent reference source for medicinal chemists of a range of disciplines and experiences.

The Practice of Medicinal Chemistry-Camille Georges Wermuth 2015-07-01 The Practice of Medicinal Chemistry, Fourth Edition provides a practical and comprehensive overview of the daily issues facing pharmaceutical researchers and chemists. In addition to its thorough treatment of basic medicinal chemistry principles, this updated edition has been revised to provide new and expanded coverage of the latest technologies and approaches in drug discovery. With topics like high content screening, scoring, docking, binding free energy calculations, polypharmacology, QSAR, chemical collections and databases, and much more, this book is the go-to reference for all academic and pharmaceutical researchers who need a complete understanding of medicinal chemistry and its application to drug discovery and development. Includes updated and expanded material on systems biology, chemogenomics, computer-aided drug design, and other important recent advances in the field Incorporates extensive color figures, case studies, and practical examples to help users gain a further understanding of key concepts Provides high-quality content in a comprehensive manner, including contributions from international chapter authors to illustrate the global nature of medicinal chemistry and drug development research An image bank is available for instructors at www.textbooks.elsevier.com

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

Chemoinformatics Approaches to Virtual Screening-Alexandre Varnek 2008 Chemoinformatics is broadly a scientific discipline encompassing the design, creation, organization, management, retrieval, analysis, dissemination, visualization and use of chemical information. It is distinct from other computational molecular modeling approaches in that it uses unique representations of chemical structures in the form of multiple chemical descriptors; has its own metrics for defining similarity and diversity of chemical compound libraries; and applies a wide array of statistical, data mining and machine learning techniques to very large collections of chemical compounds in order to establish robust relationships between chemical structure and its physical or biological properties. Chemoinformatics addresses a broad range of problems in chemistry and biology; however, the most commonly known applications of chemoinformatics approaches have been arguably in the area of drug discovery where chemoinformatics tools have played a central role in the analysis and interpretation of structure-property data collected by the means of modern high throughput screening. Early stages in modern drug discovery often involved screening small molecules for their effects on a selected protein target or a model of a biological pathway. In the past fifteen years, innovative technologies that enable rapid synthesis and high throughput screening of large libraries of compounds have been adopted in almost all major pharmaceutical and biotech companies. As a result, there has been a huge increase in the number of compounds available on a routine basis to quickly screen for novel drug candidates against new targets/pathways. In contrast, such technologies have rarely become available to the academic research community, thus limiting its ability to conduct large scale chemical genetics or chemical genomics research. However, the landscape of publicly available experimental data collection methods for chemoinformatics has changed dramatically in very recent years. The term "virtual screening" is commonly associated with methodologies that rely on the explicit knowledge of three-dimensional structure of the target protein to identify potential bioactive compounds. Traditional docking protocols and scoring functions rely on explicitly defined three dimensional coordinates and standard definitions of atom types of both receptors and ligands. Albeit reasonably accurate in many cases, conventional structure based virtual screening approaches are relatively computationally inefficient, which has precluded them from screening really large compound collections. Significant progress has been achieved over many years of research in developing many structure based virtual screening approaches. This book is the first monograph that summarizes innovative applications of efficient chemoinformatics approaches towards the goal of screening large chemical libraries. The focus on virtual screening expands chemoinformatics beyond its traditional boundaries as a synthetic and data-analytical area of research towards its recognition as a predictive and decision support scientific discipline. The approaches discussed by the contributors to the monograph rely on chemoinformatics concepts such as: -representation of molecules using multiple descriptors of chemical structures -advanced chemical similarity calculations in multidimensional descriptor spaces -the use of advanced machine learning and data mining approaches for building quantitative and predictive structure activity models -the use of chemoinformatics methodologies for the analysis of drug-likeness and property prediction -the emerging trend on combining chemoinformatics and bioinformatics concepts in structure based drug discovery The chapters of the book are organized in a logical flow that a typical chemoinformatics project would follow - from structure representation and comparison to data analysis and model building to applications of structure-property relationship models for hit identification and chemical library design. It opens with the overview of modern methods of compounds library design, followed by a chapter devoted to molecular similarity analysis. Four sections describe virtual screening based on the using of molecular fragments, 2D pharmacophores and 3D pharmacophores. Application of fuzzy pharmacophores for libraries design is the subject of the next chapter followed by a chapter dealing with QSAR studies based on local molecular parameters. Probabilistic approaches based on 2D descriptors in assessment of biological activities are also described with an overview of the modern methods and software for ADME prediction. The book ends with a chapter describing the new approach of coding the receptor binding sites and their respective ligands in multidimensional chemical descriptor space that affords an interesting and efficient alternative to traditional docking and screening techniques. Ligand-based approaches, which are in the focus of this work, are more computationally efficient compared to structure-based virtual screening and there are very few books related to modern developments in this field. The focus on extending the experiences accumulated in traditional areas of chemoinformatics research such as Quantitative Structure Activity Relationships (QSAR) or chemical similarity searching towards virtual screening make the theme of this monograph essential reading for researchers in the area of computer-aided drug discovery. However, due to its generic data-analytical focus there will be a growing application of chemoinformatics approaches in multiple areas of chemical and biological research such as synthesis planning, nanotechnology, proteomics, physical and analytical chemistry and chemical genomics.

Pharmacology for Chemists-Joseph Cannon 1999 Pharmacology has traditionally been a part of the educational experience of medicinal chemists, but this has not been the case for graduate students in organic and most other areas of chemistry. This practical book provides an ideal guide. Assuming no background in physiology and pharmacology, it covers the aspects of pharmacology most important and useful to organic (and other) chemists engaged in drug discovery. The book is based upon a popular three-day American Chemical Society short course, "Pharmacology for Chemists," which the author has taught for twenty years, and the book retains the lively and accessible presentation of the course while including more detailed discussions, references, and definitions. Any chemist who is considering research on drugs will find this volume an invaluable tool.

ADME and Translational Pharmacokinetics / Pharmacodynamics of Therapeutic Proteins-Honghui Zhou 2015-10-26 With an emphasis on the fundamental and practical aspects of ADME for therapeutic proteins, this book helps readers strategize, plan and implement translational research for biologic drugs. • Details cutting-edge ADME (absorption, distribution, metabolism and excretion) and PKPD (pharmacokinetic / pharmacodynamics) modeling for biologic drugs • Combines theoretical with practical aspects of ADME in biologic drug discovery and development and compares innovator biologics with biosimilar biologics and small molecules with biologics, giving a lessons-learned perspective • Includes case studies about leveraging ADME to improve biologics drug development for monoclonal antibodies, fusion proteins, pegylated proteins, ADCs, bispecifics, and vaccines • Presents regulatory expectations and industry perspectives for developing biologic drugs in USA, EU, and Japan • Provides mechanistic insight into biodistribution and target-driven pharmacokinetics in important sites of action such as tumors and the brain

Basic Principles of Drug Discovery and Development-Benjamin Blass 2015-04-24 Basic Principles of Drug Discovery and Development presents the multifaceted process of identifying a new drug in the modern era, providing comprehensive explanations of enabling technologies such as high throughput screening, structure based drug design, molecular modeling, pharmaceutical profiling, and translational medicine, all areas that have become critical steps in the successful development of marketable therapeutics. The text introduces the fundamental principles of drug discovery and development, also discussing important drug targets by class, in vitro screening methods, medicinal chemistry strategies in drug design, principles in pharmacokinetics and pharmacodynamics, animal models of disease states, clinical trial basics, and selected business aspects of the drug discovery process. It is designed to enable new scientists to rapidly understand the key fundamentals of drug discovery, including pharmacokinetics, toxicology, and intellectual property." Provides a clear explanation of how the pharmaceutical industry works Explains the complete drug discovery process, from obtaining a lead, to testing the bioactivity, to producing the drug, and protecting the intellectual propertyIdeal for anyone interested in learning about the drug discovery process and those contemplating careers in the industry Explains the transition process from academia or other industries

A Pharmacology Primer-Terry Kenakin 2010-07-26 The Second Edition will continue this tradition of better preparing researchers in the basics of pharmacology. In addition, new human interest material including historical facts in pharmacology will be added. A new section on therapeutics will help readers identify with diseases and drug treatments. Over 30 new figures and tables More human interest information to provide readers with historical facts on pharmacology research New section on therapeutics to help identify diseaes and drug treatments New section on new biological concepts relevant to pharmacological research (i.e., systems biology) New study sections organized with ASPET and other international pharmacology organizations New coverage of pharmacokinetics and drug disposition

Phytochemicals as Lead Compounds for New Drug Discovery-Chukwuebuka Egbuna 2019-09-07 Phytochemicals as Lead Compounds for New Drug Discovery presents complete coverage of the recent advances in the discovery of phytochemicals from medicinal plants as models to the development of new drugs and chemical entities. Functional bioactive compounds of plant origin have been an invaluable source for many human therapeutic drugs and have played a major role in the treatment of diseases around the world. These compounds possess enormous structural and chemical diversity and have led to many important discoveries. This book presents fundament concepts and factors affecting the choice for plant-based products, as well as recent advances in computer-aided drug discovery and FDA drug candidacy acceptance criteria. It also details the various bioactive lead compounds and molecular targets for a range of life-threatening diseases including cancer, diabetes, and neurodegenerative diseases. Written by a global team of experts, Phytochemicals as Lead Compounds for New Drug Discovery is an ideal resource for drug developers, phytochemists, plant biochemists, food and medicinal chemists, nutritionists and toxicologists, chemical ecologists, taxonomists, analytical chemists, and other researchers in those fields. It will also be very valuable to professors, students, and researchers in this domain. Presents fundamental concepts and factors affecting choice for plant-based products Details the FDA drug candidacy acceptance criteria, including bottlenecks and way forward Highlights recent advances in computational-based drug discovery Focuses on the discovery of new drugs and potential druggable targets for the treatment of chronic diseases of world importance

Molecular Design-Gisbert Schneider 2008-02-26 This first introductory-level textbook on the design of small molecules is written with the first-time user in mind. Aimed at students and scientists alike, it uses computer-based methods to design and analyze such small molecules as drugs, enzyme inhibitors, probes and markers for biomolecules. Both authors have extensive practical experience of modeling and design and share their knowledge of what can and cannot be done with computer-assisted design. Divided into four sections, the book begins with a look at molecular objects and design objectives, including molecular geometry, properties, recognition and dynamics. Two further sections deal with virtual synthesis and screening, while the final section covers navigation in chemical space. The result is a textbook that takes the modeler one step further, to the de novo design of functional molecules. With its study questions at the end of each learning unit, this is equally suitable for teaching and self-learning.

ADME Processes in Pharmaceutical Sciences-Alan Talevi 2018-11-30 Absorption, Distribution, Metabolism and Excretion (ADME) processes and their relationship with the design of dosage forms and the success of pharmacotherapy form the basis of this upper level undergraduate/graduate textbook. As an introduction oriented to pharmacy students, it is also written for scientist from different fields outside of pharmaceutics. (e.g. material scientist, material engineers, medicinal chemists) who might be working in a positions in pharmaceutical companies or whose work might benefit from basic training in the ADME concepts and some biological background. Pedagogical features such as objectives, keywords, discussion questions, summaries and case studies add valuable teaching tools. This book will provide not only general knowledge on ADME processes but also an updated insight on some hot topics such as drug transporters, multi-drug resistance related to pharmacokinetic phenomena, last generation pharmaceutical carriers (nanopharmaceuticals), in vitro and in vivo bioequivalence studies, biopharmaceuticals, pharmacogenomics, drug-drug and food-drug interactions, and in silico and in vitro prediction of ADME properties. In comparison with other similar textbooks, around half of the volume would be focused on the relationship between expanding scientific fields and ADME processes. Each of these burgeoning fields has a separate chapter in the second part of the volume, and was written with leading experts on the correspondent topic, including scientists and academics from USA and UK (Duquesne University School of Pharmacy, Indiana University School of Medicine, University of Utah College of Pharmacy, University of Maryland, University of Bath). Additionally, each of the initial chapters dealing with the generalities of drug absorption, distribution, metabolism and excretion would include relevant, classic examples related to each topic with appropriate illustrations (e.g. importance of active absorption of levodopa, implications in levodopa administration, drug drug interactions and food drug interactions emerging from the active

uptake; intoxication with paracetamol as a result of glutathione depletion, CYP induction and its relationship with acute liver failure caused by paracetamol, etc). ADME Processes and Pharmaceutical Sciences is written as a core textbook for ADME processes, pharmacy, pharmacokinetics, drug delivery, biopharmaceutics, drug disposition, drug design and medicinal chemistry courses.

An Introduction to Medicinal Chemistry-Graham L. Patrick 2013-01-10 This volume provides an introduction to medicinal chemistry. It covers basic principles and background, and describes the general tactics and strategies involved in developing an effective drug.

Fundamentals of Medicinal Chemistry-Gareth Thomas 2004-04-20 Provides a concise introduction to the chemistry of therapeutically active compounds, written in a readable and accessible style. The title begins by reviewing the structures and nomenclature of the more common classes of naturally occurring compounds found in biological organisms. An overview of medicinal chemistry is followed by chapters covering the discovery and design of drugs, pharmacokinetics and drug metabolism, The book concludes with a chapter on organic synthesis, followed by a brief look at drug development from the research stage through to marketing the final product. The text assumes little in the way of prior biological knowledge. relevant biology is included through biological topics, examples and the Appendices. Incorporates summary sections, examples, applications and problems Each chapter contains an additional summary section and solutions to the questions are provided at the end of the text Invaluable for undergraduates studying within the chemical, pharmaceutical and life sciences.

Medicinal Chemistry-Erland Stevens 2014 Emphasizing applications of chemistry while reinforcing theory – especially in the areas of organic and physical chemistry – this new text prepares readers for career success in the pharmaceutical, medical, and biotech industries. Medicinal Chemistry: The Modern Drug Discovery Process delivers a comprehensive introduction to medicinal chemistry at an appropriate level of detail for a diverse range of readers. By highlighting the concepts and skills related to drug discovery, Stevens deepens readers' understanding of the knowledge and techniques necessary for their careers.

Pocket Guide-Donald J. Birkett 2009-12-18 Presents a complex topic in a simple, easy-to-understand way Pocket Guide: Pharmacokinetics Made Easy is the latest update of the popular Pharmacokinetics Made Easy. It is suitable for a wide audience including medical practitioners, health professionals, and students. The individual chapters were initially published as a series of articles in Australian Prescriber to assist practitioners in drug dosing and therapy. The physiological approach herein adopted addresses clinical issues in drug therapy and makes them directly applicable to practice situations. Key Selling Features: - Self-assessment questions in each chapter - Glossary of symbols - Use of equations to explain physiological factors underlying important pharmacokinetics processes - Endorsed and co-published with Australian Prescriber - List of key points summarizing the content to improve accessibility and understanding

Advances in Peptide and Peptidomimetic Design Inspiring Basic Science and Drug Discovery-Henry I. Mosberg 2020-03-13 Advances in Peptide and Peptidomimetic Design Inspiring Basic Science and Drug Discovery is a book dedicated to Prof. Victor J. Hruby on the occasion of his 80th birthday. This book includes twenty contributions from authors representing diverse multidisciplinary fields of scientific expertise, and is focused on the extraordinary potential of peptides and peptidomimetics as a surging therapeutic modality and as tools for basic research and technology development.

Emerging Concepts in Analysis and Applications of Hydrogels-Sutapa Biswas Majee 2016-08-24 This book is an Up-to-date and authoritative account on physicochemical principles, pharmaceutical and biomedical applications of hydrogels. It consists of eight contributions from different authors highlighting properties and synthesis of hydrogels, their characterization by various instrumental methods of analysis, comprehensive review on stimuli-responsive hydrogels and their diverse applications, and a special section on self-healing hydrogels. Thus, this book will equip academia and industry with adequate basic and applied principles related to hydrogels.

A Framework to Guide Selection of Chemical Alternatives-National Research Council 2014-10-29 Historically, regulations governing chemical use have often focused on widely used chemicals and acute human health effects of exposure to them, as well as their potential to cause cancer and other adverse health effects. As scientific knowledge has expanded there has been an increased awareness of the mechanisms through which chemicals may exert harmful effects on human health, as well as their effects on other species and ecosystems. Identification of high-priority chemicals and other chemicals of concern has prompted a growing number of state and local governments, as well as major companies, to take steps beyond existing hazardous chemical federal legislation. Interest in approaches and policies that ensure that any new substances substituted for chemicals of concern are assessed as carefully and thoroughly as possible has also burgeoned. The overarching goal of these approaches is to avoid regrettable substitutions, which occur when a toxic chemical is replaced by another chemical that later proved unsuitable because of persistence, bioaccumulation, toxicity, or other concerns. Chemical alternative assessments are tools designed to facilitate consideration of these factors to assist stakeholders in identifying chemicals that may have the greatest likelihood of harm to human and ecological health, and to provide guidance on how the industry may develop and adopt safer alternatives. A Framework to Guide Selection of Chemical Alternatives develops and demonstrates a decision framework for evaluating potentially safer substitute chemicals as primarily determined by human health and ecological risks. This new framework is informed by previous efforts by regulatory agencies, academic institutions, and others to develop alternative assessment frameworks that could be operationalized. In addition to hazard assessments, the framework incorporates steps for life-cycle thinking - which considers possible impacts of a chemical at all stages including production, use, and disposal - as well as steps for performance and economic assessments. The report also highlights how modern information sources such as computational modeling can supplement traditional toxicology data in the assessment process. This new framework allows the evaluation of the full range of benefits and shortcomings of substitutes, and examination of tradeoffs between these risks and factors such as product functionality, product efficacy, process safety, and resource use. Through case studies, this report demonstrates how different users in contrasting decision contexts with diverse priorities can apply the framework. This report will be an essential resource to the chemical industry, environmentalists, ecologists, and state and local governments.

Toxicological Survey of African Medicinal Plants-Victor Kuete 2014-05-30 Toxicological Survey of African Medicinal Plants provides a detailed overview of toxicological studies relating to traditionally used medicinal plants in Africa, with special emphasis on the methodologies and tools used for data collection and interpretation. The book considers the physical parameters of these plants and their effect upon various areas of the body and human health, including chapters dedicated to genotoxicity, hepatotoxicity, nephrotoxicity, cardiotoxicity, neurotoxicity, and specific organs and systems. Following this discussion of the effects of medicinal plants is a critical review of the guidelines and methods in use for toxicological research as well as the state of toxicology studies in Africa. With up-to-date research provided by a team of experts, Toxicological Survey of African Medicinal Plants is an invaluable resource for researchers and students involved in pharmacology, toxicology, phytochemistry, medicine, pharmacognosy, and pharmaceutical biology. Offers a critical review of the methods used in toxicological survey of medicinal plants Provides up-to-date toxicological data on African medicinal plants and families Serves as a resource tool for students and scientists in the various areas of toxicology

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.

Molecular Drug Properties-Raimund Mannhold 2008-06-25 This first systematic overview for more than a decade is tailor-made for the medicinal chemist. All the chapters are written by experienced drug developers and include practical examples from real drug candidates. Following an introduction to global drug properties and their impact on drug research, screening and combinatorial chemistry libraries, this handbook demonstrates the best and fastest way to estimate those properties most relevant for the efficiency and pharmacokinetic performance of a drug molecule: lipophilicity,solubility, electronic properties and conformation.

Forgotten Women: The Leaders-Zing Tsjeng 2018-03-08 'To say this series is "empowering" doesn't do it justice. Buy a copy for your daughters, sisters, mums, aunts and nieces - just make sure you buy a copy for your sons, brothers, dads, uncles and nephews, too.' - indy100 'Here's to no more forgotten women.' Evening Standard The women who shaped and were erased from our history. The Forgotten Women series will uncover the lost histories of the influential women who have refused over hundreds of years to accept the hand they've been dealt and, as a result, have formed, shaped and changed the course of our futures. The Leaders weaves together 48* unforgettable portraits of the true pioneers and leaders who made huge yet unacknowledged contributions to history, including: Grace O'Malley, the 16th century Irish pirate queen Sylvia Rivera, who spearheaded the modern transgender rights movement Agent 355, the unknown rebel spy who played a pivotal role in the American Revolution Noor Inayat Khan, who went undercover to spy for the French Resistance and became Nazi enemy no. 1 Amina of Zazzau, the formidable ancient Muslim warrior queen of Northern Nigeria Chapters including Rebels; Warriors; Rulers; Activists and Reformers shine a spotlight on the rebellious women who defied the odds, and the opposition, to change the world around them. *The number of Nobel-prize-winning women.

Spectroscopic Analyses-Eram Sharmin 2017-12-06 The book presents developments and applications of these methods, such as NMR, mass, and others, including their applications in pharmaceutical and biomedical analyses. The book is divided into two sections. The first section covers spectroscopic methods, their applications, and their significance as characterization tools; the second section is dedicated to the applications of spectrophotometric methods in pharmaceutical and biomedical analyses. This book would be useful for students, scholars, and scientists engaged in synthesis, analyses, and applications of materials/polymers.

Increasing Student Learning Through Multimedia Projects-Michael Simkins 2002-01-01 Addressed to K-12 teachers, discusses enhancing student achievement through project-based learning with multimedia and offers principles and guidelines to insure that multimedia projects address curriculum standards.

Teaching with Poverty in Mind-Eric Jensen 2010-06-16 In Teaching with Poverty in Mind: What Being Poor Does to Kids' Brains and What Schools Can Do About It, veteran educator and brain expert Eric Jensen takes an unflinching look at how poverty hurts children, families, and communities across the United States and demonstrates how schools can improve the academic achievement and life readiness of economically disadvantaged students. Jensen argues that although chronic exposure to poverty can result in detrimental changes to the brain, the brain's very ability to adapt from experience means that poor children can also experience emotional, social, and academic success. A brain that is susceptible to adverse environmental effects is equally susceptible to the positive effects of rich, balanced learning environments and caring relationships that build students' resilience, self-esteem, and character. Drawing from research, experience, and real school success stories, Teaching with Poverty in Mind reveals * What poverty is and how it affects students in school; * What drives change both at the macro level (within schools and districts) and at the micro level (inside a student's brain); * Effective strategies from those who have succeeded and ways to replicate those best practices at your own school; and * How to engage the resources necessary to make change happen. Too often, we talk about change while maintaining a culture of excuses. We can do better. Although no magic bullet can offset the grave challenges faced daily by disadvantaged children, this timely resource shines a spotlight on what matters most, providing an inspiring and practical guide for enriching the minds and lives of all your students.

Concepts, Compounds and the Alternatives of Antibacterials-Varaprasad Bobbarala 2015-12-09 This edition is intended to provide better understanding of antibacterial drugs and their mechanism, the role of a few metal drug complexes as antibacterials, cross-checking of a few compounds and biomaterials against drug-resistant bacterial strains as well as a few alternative approaches using medicinal plant based formulations in the control of antibiotic-resistant bacteria. The information in this book provides clues for upcoming trends in treating antibiotic resistance problems with which one can explore new approaches in the treatment of common infections with drug-resistant strains.