Kinase Drug Discovery Modern Approaches

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Designing Multi-target Drugs - J. Richard Morphy 2012
This is the first book to pull together studies and reviews from cutting edge authors who work in the emerging and exciting field of multi-targeted drug discovery.
Anti-Inflammatory Drug Discovery - Jeremy I. Levin 2012
A comprehensive review of recent medicinal chemistry approaches to a variety of important therapeutic targets and a key reference for those interested in the prosecution of modern drug discovery programs directed at anti-inflammatory mechanisms of action.
Peripheral T-cell Lymphomas - Pier Paolo Piccaluga 2019-08-07
In this book the reader will find a collection of chapters written by different research teams describing different aspects of peripheral T-cell lymphoma pathobiology, classification, and treatment. This work is mainly addressed to researchers already working in this area, but it is also accessible to anyone with a scientific background who desires to have an updated overview of the recent progress in this domain. It will also be valuable to scientists and physicians who have become newly involved in this field. Each chapter is self-contained and can be read independently of the others. This book intends to provide highlights of the current research as well as the current gold standards for diagnosis and treatment of these diseases, showing the recent advances in the personalized approach to T-cell derived lymphomas.
Kinase Inhibitors - Bernhard Kuster 2011-10-06
Protein and lipid kinases are often the master regulators of cell signaling in eukaryotic systems. The human genome codes for more than 500 of these enzymes and their misregulation has been shown to be involved in the onset and progression of many diseases including cancer and inflammation. Therefore, small molecule kinase inhibitors have become important research tools for the elucidation of the many biological roles of kinases and their mechanisms of action. Kinase inhibitors thus also contribute significantly to the drug pipelines of the pharmaceutical and biotechnology industries and to the growing need to treat cancer and inflammation. In Kinase Inhibitors: Methods and Protocols, experts in kinase biology, drug discovery, and clinical research present a series of exemplary methods that can be used to address the many challenges facing scientists in the discovery and development of kinase inhibitors both for research and clinical use. Written in the highly successful Methods in Molecular BiologyTM series format, chapters contain introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible laboratory protocols, and notes on troubleshooting and avoiding known pitfalls. Authoritative and accessible, Kinase Inhibitors: Methods and Protocols aims to provide scientists with modern and relevant methods to accelerate or strengthen their research and drug discovery programs through the utilization of these vital regulators.
Kinase Drug Discovery - Richard A Ward 2018-10-31
Kinase inhibition remains an area of significant

interest, and growing importance, across academia and the pharmaceutical industry. There are now many marketed drugs that target kinases and a significant number of compounds are currently in various stages of clinical development. This book is a forward-looking analysis of a number of key areas for kinase inhibition in the coming years and builds on the first volume. This includes topics such as screening approaches to target kinases along with different modes of inhibition such as allosteric and covalent. Novel approaches such as macrocyclisation are considered along with how the properties of kinase inhibitors have evolved, including the potential for brain penetration. Recent areas of great importance also covered include cutting edge molecular modelling approaches and the importance of kinase mutations. The evolving biology of kinases has also resulted in increased interest in the immuno-oncology area and also pseudokinases as a target family. As with the first volume the book finishes with a forward looking view of how research against this fascinating target class may evolve.

Tyrosine Kinases as Druggable Targets in Cancer - Huan Ren 2019-09-25

Protein tyrosine kinase (PTK) deregulation contributes to growth of cancer and many other diseases. The development of small-molecule tyrosine kinase inhibitors (TKIs) that target the deregulated PTKs, such as epidermal growth factor receptor (EGFR) in non-small-cell lung cancer (NSCLC) and Bcr-ABL in chronic myeloid leukemia (CML), has revolutionized disease management. In this book, we examine a few aspects of PTKs and cancer, considering efficacy, predictive markers to therapeutic response, limitations, and future directions in TKI treatment. In this rapidly evolving field, overcoming therapeutic resistance is most challenging, and multi-targeting directs the next-generation TKIs and combination therapy as ongoing strategies in cancer treatment.

The Organic Chemistry of Drug Design and Drug Action - Richard B. Silverman 2012-12-02

Standard medicinal chemistry courses and texts are organized by classes of drugs with an emphasis on descriptions of their biological and pharmacological effects. This book represents a new approach based on physical organic chemical principles and reaction mechanisms that allow the reader to extrapolate to many related classes of drug molecules. The Second Edition reflects the significant changes in the drug industry over the past decade, and includes chapter problems and other elements that make the book more useful for course instruction. New edition includes new chapter problems and exercises to help students learn, plus extensive references and illustrations Clearly presents an organic chemist's perspective of how drugs are designed and function, incorporating the extensive changes in the drug industry over the past ten years Well-respected author has published over 200 articles, earned 21 patents, and invented a drug that is under consideration for commercialization

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.

Textbook of Drug Design and Discovery, Third Edition - Tommy Liljefors 2002-07-25

Building on the success of the previous editions, Textbook of Drug Design and Discovery has been thoroughly revised and updated to provide a complete source of information on all facets of drug design and discovery for students of chemistry, pharmacy, pharmacology, biochemistry, and medicine. The book follows drug design from the initial lead identification through optimization and structure-activity relationship with reference to the final processes of clinical evaluation and registration. Chapters investigate the design of enzyme inhibitors and drugs for particular cellular targets such as ion channels and receptors, and also explore specific

classes of drug such as peptidomimetics, antivirals and anticancer agents. The use of gene technology in pharmaceutical research, computer modeling techniques, and combinatorial approaches are also included.

Structure-based Design of Drugs and Other Bioactive Molecules - Arun K. Ghosh 2014-08-11

Drug design is a complex, challenging and innovative research area. Structure-based molecular design has transformed the drug discovery approach in modern medicine. Traditionally, focus has been placed on computational, structural or synthetic methods only in isolation. This one-of-akind guide integrates all three skill sets for a complete picture of contemporary structure-based design. This practical approach provides the tools to develop a high-affinity ligand with drug-like properties for a given drug target for which a high-resolution structure exists. The authors use numerous examples of recently developed drugs to present "best practice" methods in structurebased drug design with both newcomers and practicing researchers in mind. By way of a carefully balanced mix of theoretical background and case studies from medicinal chemistry applications, readers will quickly and efficiently master the basic skills of successful drug design. This book is aimed at new and active medicinal chemists, biochemists, pharmacologists, natural product chemists and those working in drug discovery in the pharmaceutical industry. It is highly recommended as a desk reference to guide students in medicinal and chemical sciences as well as to aid researchers engaged in drug design today.

Privileged Scaffolds in Medicinal Chemistry - Stefan Bräse 2015-11-20

This book addresses the various classes of privileged scaffolds and covers the history of their discovery and use.

Designing Multi-Target Drugs - J. Richard Morphy 2012-03-28

Multi-target drug discovery (MTDD) is an emerging area of increasing interest to the drug discovery community. Drugs that modulate several targets have the potential for an improved balance of efficacy and safety compared to single targets agents. Although there are a number of marketed drugs that are thought to derive their therapeutic benefit by virtue of interacting with multiple targets, the majority of these were discovered accidentally. Written by world renowned experts, this is the first book to gather together knowledge and experiences of the rational discovery of multi-target drugs. It describes the current state of the art, the achievements and the challenges of the field and importantly the lessons learned by researchers to date and their application to future MTDD.

Protein Allostery in Drug Discovery - Jian Zhang 2019-11-09

The book focuses on protein allostery in drug discovery. Allosteric regulation, 'the second secret of life', fine-tunes virtually most biological processes and controls physiological activities. Allostery can both cause human diseases and contribute to development of new therapeutics. Allosteric drugs exhibit unparalleled advantages compared to conventional orthosteric drugs, rendering the development of allosteric modulators as an appealing strategy to improve selectivity and pharmacodynamic properties in drug leads. The Series delineates the immense significance of protein allostery—as demonstrated by recent advances in the repertoires of the concept, its mechanistic mechanisms, and networks, characteristics of allosteric proteins, modulators, and sites, development of computational and experimental methods to predict allosteric sites, small-molecule allosteric modulators of protein kinases and G-protein coupled receptors, engineering allostery, and the underlying role of allostery in precise medicine. Comprehensive understanding of protein allostery is expected to guide the rational design of allosteric drugs for the treatment of human diseases. The book would be useful for scientists and students in the field of protein science and Pharmacology etc.

Drug Design Strategies - David J. Livingstone 2011

Shows how different parts of the drug discovery process have developed, with particular emphasis on quantitative aspects and possible future progress.

Drug Discovery and Development - Vishwanath Gaitonde 2020-03-11

The process of drug discovery and development

is a complex multistage logistics project spanned over 10-15 years with an average budget exceeding 1 billion USD. Starting with target identification and synthesizing anywhere between 10k to 15k synthetic compounds to potentially obtain the final drug that reaches the market involves a complicated maze with multiple inter- and intra-operative fields. Topics described in this book emphasize the progresses in computational applications, pharmacokinetics advances, and molecular modeling developments. In addition the book also contains special topics describing target deorphaning in Mycobacterium tuberculosis, therapy treatment of some rare diseases, and developments in the pediatric drug discovery process.

Computational and Structural Approaches to Drug Discovery - Robert M. Stroud 2008

This insightful book represents the experience and understanding of the global experts in the field and spotlights both the structural and medicinal chemistry aspects of drug design. The need to 'encode' the physiological factors of pharmacology, a key area, is explored.

Target Discovery and Validation - Alleyn T. Plowright 2020-02-18

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.

Kinase Drug Discovery - Richard A. Ward 2018-11-06

Kinase inhibition remains an area of significant interest, and growing importance, across academia and the pharmaceutical industry. There are now many marketed drugs that target kinases and a significant number of compounds are currently in various stages of clinical development. This book is a forward-looking analysis of a number of key areas for kinase inhibition in the coming years and builds on the first volume. This includes topics such as screening approaches to target kinases along with different modes of inhibition such as allosteric and covalent. Novel approaches such as macrocyclisation are considered along with how the properties of kinase inhibitors have evolved, including the potential for brain penetration. Recent areas of great importance also covered include cutting edge molecular modelling approaches and the importance of kinase mutations. The evolving biology of kinases has also resulted in increased interest in the immuno-oncology area and also pseudokinases as a target family. As with the first volume the book finishes with a forward looking view of how research against this fascinating target class may evolve.

Phenotypic Drug Discovery - Angelique Augustin 2020-12-10

Phenotypic drug discovery has been highlighted in the past decade as an important strategy in the discovery of novel medical entities. This book aims to equip researchers with a thought-provoking guide to the application and development of contemporary phenotypic drug discovery for clinical success.

Fragment-based Approaches in Drug Discovery - Wolfgang Jahnke 2006-12-13

This first systematic summary of the impact of fragment-based approaches on the drug development process provides essential information that was previously unavailable. Adopting a practice-oriented approach, this represents a book by professionals for professionals, tailor-made for drug developers in the pharma and biotech sector who need to keep up-to-date on the latest technologies and strategies in pharmaceutical ligand design. The book is clearly divided into three sections on ligand design, spectroscopic techniques, and screening and drug discovery, backed by numerous case studies.

Artificial Intelligence in Oncology Drug Discovery and Development - John Cassidy 2020-09-09

There exists a profound conflict at the heart of oncology drug development. The efficiency of the drug development process is falling, leading to higher costs per approved drug, at the same time personalised medicine is limiting the target market of each new medicine. Even as the global economic burden of cancer increases, the current paradigm in drug development is unsustainable. In this book, we discuss the development of techniques in machine learning for improving the efficiency of oncology drug development and delivering cost-effective precision treatment. We consider how to structure data for drug repurposing and target identification, how to improve clinical trials and how patients may view artificial intelligence.

Drug Design: Principles and Applications - Abhinav Grover 2017-08-09

This book offers an in-depth discussion of the latest strategies in the field of drug design and their applications in various disorders, in order to encourage readers to undertake their own projects.It also includes the contemporary application of drug-designing methodologies to inspire others to further expand the utility of this field in other diseases.It is intended for advanced undergraduate and graduate students, postdocs, researchers, lecturers and professors in bioinformatics, computational biology, medicine, pharmaceutics and other related fields.

Chemogenomics in Drug Discovery - Hugo Kubinyi 2006-03-06

Chemogenomics brings together the most powerful concepts in modern chemistry and biology, linking combinatorial chemistry with genomics and proteomics. This first reference devoted to the topic covers all stages of the early drug discovery process, from target selection to compound library and lead design. With the combined expertise of 20 research groups from academia and leading pharmaceutical companies, this is a must-have for every drug developer and medicinal chemist applying the powerful methods of chemogenomics to speed up the drug discovery process.

Biodiversity and Human Health - Francesca Grifo 1997-02

Biodiversity and Human Health brings together leading thinkers on the global environment and biomedicine to explore the human health consequences of the loss of biological diversity.

Kinase Drug Discovery - Richard A. Ward 2012

This is the first book to examine the future opportunities and challenges in the development of drugs which target kinases

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

An integrated overview of modern approaches to lead discovery Lead generation is increasingly seen as a distinct and success-determining phase of the drug discovery process. Over recent years, there have been major advances in the understanding of what constitutes a good lead compound and how to improve the chances of finding such a compound. Written by leading scientists and established opinion leaders from industry and academia, this book provides an authoritative overview of the field, as well as the theory, practice, and scope, of the principal Lead Generation Approaches in Drug Discovery, including: The evolution of the lead discovery process, key concepts, current challenges, and future directions Strategies and technologies driving the high-throughput screening (HTS) approach to lead discovery, including the shifting paradigms in the design of compound collections and best practice in the hit confirmation process Knowledge-based in silico or "virtual" screening Theory and practice of the fragment-based approach to lead discovery The opportunities and challenges presented by multi-target drug discovery (MTDD) De novo design of lead compounds and new approaches to estimating the synthetic accessibility of de

novo–designed molecules The impact of natural products on drug discovery, and potential of natural product–like compounds for exploring regions of biologically relevant chemical space Using early screening of hits and leads for metabolic, pharmacokinetic, and toxicological liabilities to reduce attrition during the later phases of drug discovery The utility of parallel synthesis and purification in lead discovery With each topic supported by numerous case studies, this is indispensable reading for researchers in industry and academia who wish to keep up to date with the latest strategies and approaches in drug discovery.

Protein Degradation - R. John Mayer 2005-04-15

The first volume in a new series dedicated to protein degradation, this book lays the foundations of targeted protein breakdown via the ubiquitin pathway. The outstanding importance of the ubiquitin pathway has been recognized with the 2004 Nobel Prize in Chemistry for Aaaron Chiechanover, Avram Hershko, and Irwin Rose. Aaron Ciechanover is one of the editors of this series, and Avram Hershko has contributed to the opening chapter of the present volume. Drawing on the the expertise of two Nobel prize winners, this handy reference compiles information on the initial steps of the ubiquitin pathway. Starting out with a broad view of protein degradation and its functions in cellular regulation, it then goes on to examine the molecular mechanisms of ubiquitin conjugation and recycling in detail. All currently known classes of ubiquitin protein ligases are treated here, including latest structural data on these enzymes. Further volumes in the series cover the function of the proteasome, and the roles of the ubiquitin pathway in regulating key cellular processes, as well as its pathophysiological disease states. Required reading for molecular biologists, cell biologists and physiologists with an interest in protein degradation.

Scaffold Hopping in Medicinal Chemistry - Nathan Brown 2013-11-06

This first systematic treatment of the concept and practice of scaffold hopping shows the tricks of the trade and provides invaluable guidance for the reader's own projects. The first section serves as an introduction to the topic by describing the concept of scaffolds, their discovery, diversity and representation, and their importance for finding new chemical entities. The following part describes the most common tools and methods for scaffold hopping, whether topological, shape-based or structure-based. Methods such as CATS, Feature Trees, Feature Point Pharmacophores (FEPOPS), and SkelGen are discussed among many others. The final part contains three fully documented real-world examples of successful drug development projects by scaffold hopping that illustrate the benefits of the approach for medicinal chemistry. While most of the case studies are taken from medicinal chemistry, chemical and structural biologists will also benefit greatly from the insights presented here.

Drug Discovery for Leishmaniasis - Carmen Gil 2017-11-02

For human health, leishmaniasis is among the most important protozoan diseases, superseded only by malaria. Globally, 10 to 12 million people are infected with 1.5 million new cases every year. The development of cheaper new drugs is urgently needed for this neglected disease that is developing resistance to current treatments. Chemotherapy remains the only treatment option for the bulk of patients. However, this is largely unaffordable for most. In the past three years numerous advances in drug discovery have been made for treating this disease by exploiting diverging metabolic pathways between the Leishmania enzymes and their hosts, using nanotechnology to target the immune cell phagolysosomes where Leishmania resides. Drug Discovery for Leishmaniasis aims to provide a perspective of the current treatments and their challenges, blended with the emerging strategies and methodologies that will drive new target appraisals and drug developments, as well as addressing the molecular basis of resistance in Leishmania. Recent studies have shown that leishmaniasis affects some of the poorest people in the world, with 95% of fatal cases occurring in only 6 countries. With the WHO goal of eliminating this public health problem in the South-east Asia Region by 2020, this book will be important for anyone who is interested in neglected tropical diseases.

Updates on Cancer Treatment - Letícia Rangel 2015-10-28

In spite of advances in the cancer research field, cancer treatment still challenges researchers and clinicians, as proven by the still impressive and increasing number of worldwide cancer-related deaths. Updates on Cancer Treatment is an attempt to integrate into a book volume various aspects of cancer treatment, compiling comprehensive reviews written by an international team of experts in the field.

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

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

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

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

Cancer Drug Design and Discovery - Stephen Neidle 2011-04-28

The ultimate source of information on the design of new anticancer agents, emphasizing small molecules, this newest work covers recent notable successes resulting from the human genome and cancer genomics projects. These advances have provided information on targets involved in specific cancers that are leading to effective medicines for at least some of the common solid tumors. Unique sections explain the basic underlying principles of cancer drug development and provide a practical introduction to modern methods of drug design. Appealing to a broad audience, this is an excellent reference for translational researchers interested in cancer biology and medicine as well as students in pharmacy, pharmacology, or medicinal and biological chemistry and clinicians taking oncology options. * Covers both currently available drugs as well as those under development * Provides a clinical perspective on trials of new anticancer agents * Presents drug discovery examples through the use of case histories

Drug Discovery - Varaprasad Bobbarala PhD

2018-09-19
The book "Drug Discovery - Concepts to Market" is a collection of reviewed and relevant research chapters, offering a comprehensive overview of recent developments in the latest drug discovery trends that have been revolutionized with up-to-date technological developments. This book comprises single chapters authored by various researchers and edited by an expert active in the drug development research area. All chapters are independently complete but united under a common research study topic. This publication aims to provide a thorough overview of the latest research efforts in this field from international authors and open new possible research paths for further novel developments.

Structure-based Design of Drugs and Other Bioactive Molecules - Arun K. Ghosh 2014-07-16
Drug design is a complex, challenging and innovative research area. Structure-based molecular design has transformed the drug discovery approach in modern medicine. Traditionally, focus has been placed on computational, structural or synthetic methods only in isolation. This one-of-akind guide integrates all three skill sets for a complete picture of contemporary structure-based design. This practical approach provides the tools to develop a high-affinity ligand with drug-like properties for a given drug target for which a high-resolution structure exists. The authors use numerous examples of recently developed drugs to present "best practice" methods in structurebased drug design with both newcomers and practicing researchers in mind. By way of a carefully balanced mix of theoretical background and case studies from medicinal chemistry applications, readers will quickly and efficiently master the basic skills of successful drug design. This book is aimed at new and active medicinal chemists, biochemists, pharmacologists, natural product chemists and those working in drug discovery in the pharmaceutical industry. It is highly recommended as a desk reference to guide students in medicinal and chemical sciences as well as to aid researchers engaged in drug design today.

Medicinal Chemistry - Frank D. King 2002
This is an valuable introduction to medicinal chemistry for new graduates and PhDs. It will also serve to update more experienced scientists on the newer technologies in the field.

Polypharmacology in Drug Discovery - Jens-Uwe Peters 2012-03-13
An essential outline of the main facets of polypharmacology in drug discovery research Extending drug discovery opportunities beyond the "one drug, one target" philosophy, a polypharmacological approach to the treatment of complex diseases is emerging as a hot topic in both industry and academic research. Polypharmacology in Drug Discovery presents an overview of the various facets of polypharmacology and how it can be applied as an innovative concept for developing medicines for treating bacterial infections, epilepsy, cancer, psychiatric disorders, and more. Filled with a collection of instructive case studies that reinforce the material and illuminate the subject, this practical guide: Covers the two-sided nature of polypharmacology—its contribution to adverse drug reactions and its benefit in certain therapeutic drug classes Addresses the important topic of polypharmacology in drug discovery, a subject that has not been thoroughly covered outside of scattered journal articles Overviews state-of-the-art approaches and developments to help readers understand concepts and issues related to polypharmacology Fosters interdisciplinary drug discovery research by embracing computational, synthetic, in vitro and in vivo pharmacological and clinical aspects of polypharmacology A clear road map for helping readers successfully navigate around the problems involved with promiscuous ligands and targets, Polypharmacology in Drug Discovery provides real examples, in-depth explanations and discussions, and detailed reviews and opinions to spark inspiration for new drug discovery projects.

Modern Methods of Drug Discovery - Alexander Hillisch 2012-11-28
Research in the pharmaceutical industry today is in many respects quite different from what it used to be only fifteen years ago. There have been dramatic changes in approaches for identifying new chemical entities with a desired biological activity. While chemical modification of existing leads was the most important approach in the 1970s and 1980s, high-throughput screening and structure-based

design are now major players among a multitude of methods used in drug discov ery. Quite often, companies favor one of these relatively new approaches over the other, e.g., screening over rational design, or vice versa, but we believe that an intelligent and concerted use of several or all methods currently available to drug discovery will be more successful in the medium term. What has changed most significantly in the past few years is the time available for identifying new chemical entities. Because of the high costs of drug discovery projects, pressure for maximum success in the shortest possible time is higher than ever. In addition, the multidisciplinary character of the field is much more pronounced today than it used to be. As a consequence, researchers and project managers in the pharmaceutical industry should have a solid knowledge of the more important methods available to drug discovery, because it is the rapidly and intelligently combined use of these which will determine the success or failure of preclinical projects.

Immunotherapy – A Novel Facet of Modern Therapeutics - Sujata P. Sawarkar 2020-12-16

This book illustrates the significance and relevance of immunotherapy in modern-day therapeutics. Focusing on the application of immunotherapy in oncology, neurodegenerative and autoimmune diseases, it discusses the drug delivery systems, and pre-clinical and clinical methodologies for immunotherapy-based drugs. It also comprehensively reviews various aspects of immunotherapy, such as regulatory affairs, quality control, safety, and pharmacovigilance. Further, the book discusses the in vitro validation of therapeutic strategies prior to patient application and management of immunotherapy-related side effects and presents case studies demonstrating the design and development (pre-clinical to clinical) of immunotherapy for various diseases. It also describes various design considerations and the scale-up synthesis of immunotherapeutics and screening methods. Lastly, it explores the important aspect of cost-effectiveness and rational immunotherapy strategies.

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