Chapter 1 Drug Discovery And Development An Overview Of 54e89bb04dee2bf3687ace63fc53c

The Era of Artificial Intelligence, and Data Science in the Pharmaceutical Industry


Small molecules, 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 photometric 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 alkald-inspired small molecules. 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, libraries of small molecules are used for virtual screening 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, photometric screening and chemical genetics Presents the most advanced chemical characteristics of molecular libraries in terms of structure, structure diversity, properties, activity, profiling, 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 alkald-inspired small molecules This important book for scientists and nonscientists alike calls attention to a most urgent global problem: the rapidly accelerating loss of plant and animal species to increasing human population pressure and the demands of economic development. Based on a major conference sponsored by the Academy of Sciences of the Russian Federation, the School of Molecular Biology and the School of Molecular Biology: The Problem and Searching for Possible Solutions.Following significant advances in deep learning and related areas interest in artificial intelligence (AI) has rapidly grown. In particular, the application of AI in drug discovery provides an opportunity for challenges that previously have been difficult to solve, such as predicting properties, designing molecules and optimizing synthetic routes. Artificial Intelligence in Medicinal Chemistry and Machine Learning tools the reader to explore the challenges including designing new molecular structures, synthesis planning and simulation. Providing a wealth of knowledge from leading experts in the field this book is ideal for students, postgraduates and established researchers in both industry and academia. The Drug Discovery Handbook gives professionals a tool to facilitate drug discovery by bringing together, for the first time in one resource, a comprehensive and methods of techniques that need to be considered when developing new drugs. This comprehensive, practical guide provides a synopsis of the various techniques and methods in drug discovery, including: Genomics, proteomics, high-throughput screening, and systemsbiology. Summaries of how these techniques and methods are used todiscovernew central nervous system agents, antiviral agents, respiratory drugs, oncology drugs, and more Specific approaches to drug discovery, including problems that are encountered, solutions to these problems, and limitations of various methods and techniques The thorough coverage and practical, scientifically validated approach of Drug Discovery Handbook makes an invaluable aid in the discovery of new drugs. 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 techniques such as high throughput screening, structure-based drug design, molecular dynamics, 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 disciplines required for the multifaceted endeavor of drug discovery and development. It provides students, new industrial scientists, and academicians 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 The Era of Artificial Intelligence, Machine Learning and Data Science in the Pharmaceutical Industry examines the drug discovery process, assessing how new technologies have improved effectiveness. Artificial intelligence and machine learning are changing the landscape of disciplines and industries, including the pharmaceutical industry. In an environment where producing a single approved drug costs millions and takes many years of rigorous testing prior to its approval, reducing costs and time is of high interest. This book follows the journey that a drug company takes when producing a therapeutic, from the very beginning to ultimately benefiting a patient’s life. This comprehensive resource will be useful to those working in the pharmaceutical industry, but will also be of interest to anyone doing research in chemical biology, computational chemistry, medicinal chemistry, and drug development. Demonstrates how to reduce costs in drug discovery, highlights the key points of drug development, and its use in animal research Written by the industrial teams who are conducting the work, showcasing how the technology has improved and where it should be improved focuses on targets for medical applications of different disciplines, thus creating a complete guide The focus of early drug development has been the submission of an Investigational New Drug application to regulatory agencies, dose selection, 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. 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. Phytochemicals as Lead Compounds for New Drug Discovery is an ideal resource for drug developers, phytochemists, plant biologists, food and medicinal chemists, nutritionists and toxicologists, chemical ecologists, taxonomists, analytical chemists, and other researchers. It will also be of great value to students of this domain. Presenting fundamental concepts and factors affecting the 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 Phenotypic drug discovery has been highlighted in the past decade as a strategy in the search for new medicines. How many marketed drugs are derived from new medicine? From the most recent examples, what were the factors enabling target identification and validation? This book answers these questions by elaborating on fundamental capabilities required for phenotypic drug discovery and using case studies to illustrate approaches and key success factors. Written and edited by experienced practitioners from both industry and academia, this publication will equip researchers with a thought-provoking guide to the application and future of contemporary phenotypic drug discovery for clinical success.

A Comprehensive Guide to Toxicology in Preclinical Drug Development is a resource for toxicologists in industry and regulatory settings, as well as directors working in contract resource organizations, who need a thorough understanding of the drug development process.

Incorporating real-life case studies and examples, the book is a practical guide that outlines day-to-day activities and experiences in preclinical toxicology. This multi-contributed reference provides a detailed picture of the complex and highly interrelated activities of preclinical toxicology in both small molecules and biologics. The book discusses discovery toxicology and the international guidelines for safety evaluation, and presents traditional and nontraditional toxicity models. Chapters cover development of vaccines, oncology drugs, botanicals, monoclonal antibodies, and more, as well as study development and personnel, the role of imaging in preclinical evaluation, and supporting materials for IND applications. By incorporating the latest research in this area and featuring practical scenarios, this reference enables actionable guidance by world-renowned authorities who are experts in their fields. Includes the latest research in preclinical drug testing and international guidelines Covers preclinical toxicology in small molecules and biologics in one single source 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 development of new medicines. In the first part, the book provides an overview of 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 somewhat different and more complex pathways, 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 President and Founder of the Publishing Industrial and Scientific Information Group of 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 Medicine in the Drug Discovery Process New Topologies Chapter 10: 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 areas of the drug market and all of the players in the field. This is a must-have for students and researchers. From 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 YearAn in-depth exploration of the applications of plant bioactive metabolites in drug research and development Highlighting the concepts of plant biotechnology and medicinal chemistry, Plant Bioactives and Drug Discovery: Principles, Practice, and Perspectives provides an in-depth overview of the ways in which plants can inform drug research and development. An edited volume featuring multidisciplinary international contributions from acclaimed scientists researching bioactive natural products, the book provides an incisive overview of one of the most important topics in pharmaceutical studies today. With coverage of strategic methods of natural compound isolation, structural manipulation, natural products in clinical trials, quality control, and more, and featuring case studies on medicinal plants, the book serves as a definitive guide to the field of plant biodiversity as it relates to medicine. In addition, chapters on using natural products as drugs that target specific disease areas, including neurological disorders, inflammation, infectious diseases, and cancer, illustrate the myriad possibilities for therapeutic applications. Wide ranging and comprehensive, Plant Bioactives and Drug Discovery also includes important information on marketing, regulations, intellectual property rights, and academic-industry collaboration as they relate to plant-based drug research, making it an essential resource for advanced students and academic and industry professionals working in both biochemical, pharmaceutical, and related fields. Discover how biomarkers can boost the success rate of drug development efforts As pharmaceutical companies struggle to improve the success rateand cost-effectiveness of the drug development process, biomarkers have emerged as a valuable tool. This book synthesizes and reviews the latest efforts to identify, develop, and integrate biomarkers into the drug development process. Filled with case studies, the book shows how biomarkers can improve drug development timelines, lower costs, facilitate better compound selection, reduce late-stage attrition, and open the door to personalized medicine. Biomarkers in Drug Development is divided into eight parts: Part One offers an overview of biomarkers and their role in drug development. Part Two highlights important technologies to help researchers identify new biomarkers. Part Three examines the characterization and validation process for both drugs and diagnostics, and provides practical advice on appropriate statistical methods to ensure that biomarkers fulfill their intended purpose. Parts Four through Six examine the application of biomarkers indiscovery, preclinical safety assessment, clinical trials, and translational medicine. Part Seven focuses on lessons learned and the practical aspects of implementing biomarkers in drug development programs. Part Eight explores future trends and issues, including data integration, personalized medicine, and ethical concerns. Each of the thirty-eight chapters was contributed by one or more leading experts, including scientists at major pharmaceutical firms, academic institutions, the U.S. Food and Drug Administration, or both. The inclusion of multi-disciplinary teams of pharmaceutical and clinical researchers the most up-to-date understanding of the strategies used for and applications of biomarkers in drug development. Molecular Evolutionary Models in Drug Discovery explores the application of evolutionary molecular models in drug discovery in which secondary metabolites play a fundamental role. Secondary metabolites are not produced in isolation, they are the result of the primary metabolism, metabolites that are produced in other organisms. The first volume of this two-volume series focuses on the discovery and on the development of a rational bioprospecting model for new medicines based on the evolution of secondary metabolism. These metabolites are part of biological systems and are the most reliable expression of the functioning of living beings. Examines the integration and application of evolutionary models in the pharmaceutical industry to create new drug development platforms Investigates the biotechnological prospecting of secondary metabolites and their potential use in the discovery of new drugs. Evaluates the ecosystem of living beings and how its molecular adaptation might improve the success of therapies. Pharmacognosy is a term derived from the Greek
words for drug (pharmakon) and knowledge (gnosis). It is a field of study within Chemistry focused on natural products isolated from different sources and their biological activities. Research on natural products began more than a hundred years ago and has continued up to now. Today, research groups are compiling new information on this field and will be of interest to scientists, researchers, and students.

The incorporation of Green Chemistry is a relatively new phenomenon in the drug discovery discipline, since the scale that chemists operate on in drug discovery is smaller than those of process and manufacturing chemistry. The necessary metrics are more difficult to obtain in drug discovery due to the diversity of reactions conducted. However, pharmaceutical companies are realizing that incorporation of green chemistry techniques at earlier stages of drug development can speed the process and improve their green chemistry profile. This book provides a practical guide for both academic and industrial labs wanting to know where to start with introducing greener approaches for greater return on investment. The Editors have taken a comprehensive approach to the topic covering the entire drug discovery process from molecule conception, through synthesis, formulation and toxicology with specific examples and case studies where green chemistry strategies have been implemented. Current and greener drug development approaches are addressed as well as cutting-edge topics like biologics discovery. Moreover, important surrounding issues such as intellectual property are included. This book will serve as a practical guide for both academic and industrial chemists who work across the breadth of the drug discovery discipline. Ultimately, readers will learn how to incorporate green chemistry strategies into their everyday workflow without slowing drug Lead Candidates. The first volume in a new series, Pharmaceutical Leads from Medicinal Plants. The plant species described in this reference have been carefully selected based on pharmacological evidence and represent today’s most promising sources of natural products for the discovery of anti-cancer drugs. Containing references to primary source material, over a hundred botanical illustrations, a table of chemical structures and much more, this book is an essential starting point for cancer researchers and those interested in anti-cancer drug discovery helping you identify the best novel lead molecules for further anti-cancer drug development. Provides a compilation of hundreds of medicinal plants from Europe, Asia, North and South America and Africa that contain prominent lead candidates for anti-cancer drug discovery Contains primary source references and hundreds of the most relevant citations from the current literature for additional research Offers cancer researchers and pharmaceutical scientists valuable tools such as chemical structures and promising pharmacological data to help them select the novel lead compounds that will best aid drug discovery. A Comprehensive Guide to Toxicology. Second Edition, is a valuable reference designed to provide a complete understanding of all aspects of nonclinical toxicology in the development of small molecules and biologics. This updated edition has been reorganized and expanded to include important topics such as stem cells in nonclinical toxicology, inhalation and dermal toxicology, pitfalls in drug development, biomarkers in toxicology, and more. Thoroughly updated to reflect the latest scientific advancements covered in new and revised chapters, this second edition is an essential and comprehensive resource for all toxicologists involved in nonclinical testing in industry, academic, and regulatory settings. Provides unique content that is not always covered together in one comprehensive resource, including chapters on stem cells, liability, biomarkers, inhalation toxicology, biostatistics, and more. Updated with the latest international guidelines for nonclinical toxicology in both small and large molecules Incorporates examples in order to guide readers through the practical day-to-day work of nonclinical toxicology Drug Discovery Targeting Drug-Resistant Bacteria explores the status and possible future of developments in fighting drug-resistant bacteria. The book covers the majority of microbial diseases and the drugs targeting them. In addition, it discusses the potential targeting strategies and innovative approaches to address drug resistance. It brings together academic and industrial experts working on discovering and developing drugs targeting drug-resistant (DR) bacterial pathogens. New drugs active against drug-resistant pathogens are discovered using innovative new strategies being used to discover molecules acting via new modes of action. In addition, alternative therapies such as antibiotics and phages are included. Pharmaceutical scientists, microbiologists, medical professionals, pathologists, researchers in the field of drug discovery, infectious diseases and microbial drug discovery both in academia and in industrial settings will find this book helpful. Written by scientists with extensive industrial experience in drug discovery Provides a balanced view of the field, including its challenges and potential solutions Includes a special chapter on pathogens with the highest global impact and the potential to be used as weapons of war Drug Design and Discovery in Alzheimer’s Disease includes expert reviews of recent developments in Alzheimer’s disease (AD) and neurodegenerative disease research. Originally published by Bentham as Frontiers in Drug Design and Discovery, Volume 16 and now distributed by Elsevier, this compilation of the sixteen articles, written by leading global researchers, focuses on the understanding of the disease at molecular level and innovative approaches towards drug discovery, development, and delivery. Beginning with an overview of AD pharmacotherapy and existing blockbuster drugs, the reviews cover the potential of both natural and synthetic small molecules; the role of cholinesterases in the on-set and progression of AD and their inhibition; the role of beta-site APP clearing enzyme-1 (BACE-1) in the production of A-amyloid proteins, one of the key reasons of the progression of AD; and other targets identified for AD drug discovery. Edited and written by leading experts in Alzheimer’s disease and other neurodegenerative disorders. The book provides a comprehensive and critical look at all stages of the condition Reviews recent advances in the field, including coverage of cholinesterases, BACE-1, and other drug development targets Molecular Advancements in Tropical Diseases Drug Discovery presents in-depth knowledge relating to the detection of infection, epidemiology, drugs against various tropical diseases, new target sites for drug discovery and multidrug resistance issues using bioinformatics approaches. The authors provide efficient guidelines so that researchers can pursue these topics in a rational manner and with a solid foundation on existing facts and prospective research ideas. Updates knowledge about tropical diseases with recent advancements in the field Provides an overview of new research covering detection, infection, epidemiology and risk factors of the most common tropical diseases using bioinformatics tools Encompasses a detailed description of developments in drug discovery, new drugs and their molecular mechanisms of action Provides unique insider insight into the current drug development process, and what it takes to achieve success. In this fourth volume in the series, inventors and primary developers of drugs that made it to the market continue telling the story of the drugs’ discovery and development, and discuss the sometimes twisted route from the first drug candidate molecule to the final marketed one. Beginning with a general section addressing overarching topics for drug discovery, the book offers seven chapters that feature selected case studies describing recently introduced drugs or drug classes. These include small molecule drugs as well as biopharmaceuticals and range across different therapeutic fields. Together, they provide a representative cross-section of the present-day drug development effort. Successful Drug Discovery: Volume 4 covers trends in peptide-based drug discovery and the physicochemical properties of recently approved oral drugs. The section on drug class studies looks at antibody-drug conjugates and the discovery, evolution, and therapeutic potential of dopamine partial agonists. Featured case studies examine the discovery of Etelcalcetide for the treatment of secondary hyperparathyroidism in patients with chronic kidney disease; the development of Venetoclax; and more. - Focuses on recently introduced drugs that have not been featured in any textbooks or general references, including Ocrelizumab, a new generation of anti-CD-20 mAb for the treatment of multiple sclerosis, and Venetoclax, a selective antagonist of BCL-2 - Features personal experiences of successful drug developers from industry and academia -Endorsed and supported by the International Union of Pure and Applied Chemistry (IUPAC) Successful Drug Discovery. Volume 4 provides a fascinating and informative look into the process of drug discovery and would be a great resource for developers and those in the pharmaceutical industry, organic and pharmaceutical chemists, and lecturers in pharmacy. “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 Overview state-of-the-art approaches and developments to help readers understand contemporary methods and the process of drug development.”-Provided by publisher. Starting 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 approaches and analytics developments. In addition the book also contains a chapter on target deorphaning in Mycobacterium tuberculosis, therapy treatment of some rare diseases, and developments in the pediatric drug discovery process. The Drug Discovery and Clinical Research bandwagon has been joined by scientists and researchers from all fields including basic sciences, medical sciences, biophysicists, biotechnologists, statisticians, regulatory officials and many more. The joint effort and contribution from all is translating into the fast development of this multi-faceted field. At the same time, it has become challenging for all stakeholders to keep abreast with the explosion in information. The race for the finish-line leaves very little time for the researchers to
update themselves and keep tabs on the latest developments in the industry. To meet these challenges, this book entitled Drug Discovery and Clinical Research has been compiled. All chapters have been written by stalwarts of the field who have their finger on the pulse of the industry. This book is to provide a platform to discuss actively within the drug discovery and development community. The first chapter dealt here starting from drug discovery and development, clinical development, bioethics, medical devices, pharmacovigilance, data management, safety monitoring, patient recruitment, etc. are topics for full-blooded book in themselves, an effort has been made via this book to provide a bird’s eye view to readers and help them to keep abreast with the latest development despite constraints of time. It is hoped that the book will contribute to the growth of readers, which should translate into drug discovery and clinical research industry’s growth. The book is intended for scientists, practitioners, researchers, and students for scientific advancement in drug discovery research. The book demonstrates that various expertise are essential for drug discovery including synthetic or natural drugs, clinical pharmacology, receptor identification, drug metabolism, pharmacodynamic, and pharmacokinetic research. The following 5 sections cover diverse chapter topics in drug discovery: Natural Products as Sources of Leading Molecules in Drug Discovery; Oncology and Drug Discovery; Receptors Involvement in the Development of Oral Drug Delivery Systems; Drug Discovery and Development; and the Global Drug Development Industry. The book is designed for different therapeutic areas such as cardiovascular disease, infection, inflammation, cancer, metabolic syndrome, and allergies.

Some of today's most important and life-saving medications Drugs and Therapeutics: An Integrated Approach reflects on the current changes in this field, giving context to the current shift and using supported by real world case studies throughoutNatural products are a constant source of potentially active compounds for the treatment of rare or "orphan" diseases. The modern pharmacopeia has enormous power to alleviate disease, and owes its existence almost entirely to the pharmaceutical discoveries about the way the industrial world approaches the 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 an active molecule, through the identification of the molecule, and discovery and development tend to follow routes somewhat different from those of 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.Natural Products and Drug Discovery: An Integrated Approach is a fully illustrated volume which brings together, from theories to laboratory techniques, the principles of natural product drug discovery. Supported by real world case studies throughoutNatural products are a constant source of potentially active compounds for the treatment of various disorders. The Middle East and tropical regions are believed to have the richest supplies of natural products in the world. Plant derived secondary metabolites have been used by humans to treat acute infectious, health disorders and chronic illness for thousands of years. Only in the last 100 years have they been replaced by synthetic drugs. Natural products have always been of key importance to drug discovery, but as modern techniques and technologies have allowed researchers to identify, extract and synthesise their active compounds in new ways, they are once again coming to the forefront of drug discovery.

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projects. This book reviews macrocycles in drug discovery, both those of natural origin and semi-synthetic derivatives of natural products, and those designed and synthesized based on principles of medicinal chemistry. The medicinal chemistry of macrocyclic natural products is interesting in itself, but lessons learned from these compounds, in terms of the relationship between structure and desirable physicochemical properties, are now informing the design of fully synthetic macrocyclic drug candidates against a variety of targets including kinases, ATPases, proteases, GPCRs and others. Furthermore, as more non-classical drug targets, such as protein-protein interactions, are pursued in the pharmaceutical industry, macrocyclic molecules are generating increasing interest as they offer a way to provide drug-protein interactions that cover a larger surface area than traditional small molecules. A variety of macrocycles have become important drugs or have been identified as leads to marketed drugs. This text will discuss these compounds, their pharmacology and synthesis, in the context of their broad chemotype as compounds composed of large rings. Providing a wide reaching review of this important area in a single volume, this book will be of interest to biochemists, pharmaceutical scientists and medicinal chemists working in industry or academia. 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.

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