

Edited by Jeremy I Levin



Macrocycles In Drug Discovery Rsc Drug Discovery

David C. Blakemore, Paul M. Doyle, Yvette M. Fobian

Macrocycles In Drug Discovery Rsc Drug Discovery:

Macrocycles in Drug Discovery Jeremy I Levin,2015 This series provides a comprehensive resource for postgraduate students and for scientists in academia or industry wanting to learn topics outside their own areas of expertise

Macrocycles in Drug Discovery Jeremy Levin, 2014-10-03 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 Drug Discovery for Leishmaniasis Carmen Gil,2017-11-02 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 Allosterism in Drug Discovery Dario Doller, 2016-11-24 Although the concept of allosterism has been known for over half a century its application in drug discovery has exploded in recent years The emergence of novel technologies that enable molecular level ligand receptor interactions to be studied in studied in unprecedented detail has driven this trend This book written by the leaders in this young research area describes the latest developments in allosterism for drug discovery Bringing together research in a diverse range of scientific disciplines Allosterism in Drug Discovery is a key reference for academics and industrialists interested in understanding allosteric interactions The book provides an in depth review of research using small molecules as chemical probes and drug candidates that interact allosterically with proteins of relevance to life sciences and human disease Knowledge of these interactions can then be applied in the discovery of the novel therapeutics of the future This book will be useful for people working in all disciplines associated with drug discovery in academia or industry as well as postgraduate students who may be working in the design of allosteric modulators Green Chemistry Strategies for Drug Discovery Emily A. Peterson, Julie B Manley, 2015-06-11 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 development of a drug candidate Written by experts who have pioneered green chemistry efforts within their own institutions this book provides a practical guide for both academic and industrial labs wanting to know where to start with introducing greener approaches for greatest 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 Emerging techniques for performing greener drug discovery chemistry are addressed as well as cutting edge topics like biologics discovery and continuous processing Moreover important surrounding issues such as intellectual property are included This book serves 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 down their science **Epigenetics for Drug Discovery** Nessa Carey, 2015-11-20 Epigenetics is one of the fastest moving fields in drug discovery with almost every large pharmaceutical company and a substantial number of biotechnology companies targeting epigenetic processes to treat diseases ranging from cancer to Huntington's disease and from inflammation to sickle cell anaemia. The book is structured in three main sections. The first section introduces epigenetics and explain its importance at both a phenomenological and molecular level The second section goes on to review how each of the big breakthroughs in drug discovery in this field have developed with a strong emphasis on case histories The final section highlights the ongoing challenges in creating safe and efficacious epigenetic drugs Written and edited by experts within the field from both industry and academia this book provides an invaluable guide to this developing field for medicinal chemists working in academia and in the pharmaceutical industry Synthetic Methods in <u>Drug Discovery</u> David C. Blakemore, Paul M. Doyle, Yvette M. Fobian, 2016 The number of available synthetic methods can be overwhelming In order to create novel motifs and templates which confer new and potentially valuable drug like properties it is important to know which synthetic methodologies will give the best results Similarly which methodologies are used to progress potential drug candidates from leads through the development process What are the current industrial research problems and how can they be resolved in an industrial setting This book highlights key methods that have real impact in drug discovery and facilitate delivery of drug molecules Synthetic Methods in Drug Discovery Volume 1 focuses on the hugely important area of transition metal mediated methods used in industry Current methods of importance such as the Suzuki Miyaura coupling Buchwald Hartwig couplings and CH activation are discussed In addition exciting emerging areas such as decarboxylative coupling and the uses of iron and nickel in coupling reactions are also covered This book provides both academic and industrial perspectives on some key reactions giving the reader an excellent overview of the techniques used in modern synthesis Reaction types are conveniently framed in the context of their value to industry and the challenges and limitations of methodologies are discussed with relevant illustrative examples Edited and authored by leading scientists from both academia and industry this book will be a valuable reference for all chemists involved in drug discovery as well as postgraduate students in medicinal chemistry **Drug Transporters** Glynis Nicholls, Kuresh Youdim, 2016-08-16 Understanding and quantifying the effects of membrane transporters within the human body is essential for modulating drug safety and drug efficacy In this first volume on Drug Transporters the current knowledge and techniques in the transporter sciences and their relations to drug metabolism and pharmacokinetics are comprehensively reviewed The second volume of the book is specifically dedicated to emerging science and technologies highlighting potential areas for future advances within the drug transporter field The topics covered in both volumes ensure that all relevant aspects of transporters are described across the drug development process from in silico models and preclinical tools through to the potential impact of transporters in the clinic Contributions are included from expert leaders in the field at the bench industrial scientists renowned academics and international regulators Case studies and emerging developments are highlighted together with the merits and limitations of the available methods and tools and extensive references to reviews on specific in depth topics are also included for those wishing to pursue their knowledge further As such this text serves as an essential handbook of information for postgraduate students academics industrial scientists and regulators who wish to understand the role of transporters in absorption distribution metabolism and excretion processes In addition it is also a useful reference tool on the models and calculations necessary to predict their effect on human pharmacokinetics and pharmacodynamics Drug Transporters Volume 2 Dr Glynis Nicholls ,Dr Kuresh Youdim, 2016 Understanding and quantifying the effects of membrane transporters within the human body is essential for modulating drug safety and drug efficacy. The first volume comprehensively reviewed current knowledge and techniques in the transporter sciences and their relations to drug metabolism and pharmacokinetics In this second volume on Drug Transporters emphasis is placed on emerging sciences and technologies highlighting potential areas for future advances within the drug transporter field The topics covered in both volumes ensure that all relevant aspects of transporters are described across the drug development process from in silico models and preclinical tools through to the potential impact of transporters in the clinic Contributions are included from expert leaders in the field at the bench industrial scientists renowned academics and international regulators Case studies and emerging developments are highlighted together with the merits and limitations of the available methods and tools and extensive references to reviews on specific in depth topics are also included for those wishing to pursue their knowledge further As such this text serves as an essential handbook of information for postgraduate students academics industrial scientists and regulators who wish to understand the role of transporters in absorption distribution metabolism and excretion processes In addition it is also a useful reference tool on the models and calculations necessary to predict their effect on

human pharmacokinetics and pharmacodynamics Successful Drug Discovery, Volume 2 János Fischer, Wayne E. Childers, 2017-06-06 Retaining the successful approach found in the previous volume in this series the inventors and primary developers of drugs that successfully made it to market tell the story of the drug s discovery and development and relate the often twisted route from the first candidate molecule to the final marketed drug 11 selected case studies describe recently introduced drugs that have not been previously covered in textbooks or general references. These range across six different therapeutic fields and provide a representative cross section of the current drug development efforts Backed by copious data and chemical information the insight and experience of the contributors makes this one of the most useful training manuals that a junior medicinal chemist can hope to find and has won the support and endorsement of IUPAC for Schizophrenia Tatiana Lipina, John Roder, 2015-04-28 Since the pioneering pharmacotherapy for treatment of schizophrenia in the 1950s by antipsychotics only a few major innovations have been made pointing to a general stagnation in the field of pharmacology of schizophrenia Drug Discovery for Schizophrenia covers new insights in the field of schizophrenia with an aim to advance the understanding of scientists and clinicians in this area and to fuel drug discovery The book outlines a change in the way schizophrenia is treated by moving away from focusing only on treating symptoms in patients Innovative drugs emerge from deeper comprehension of the pathological processes that emerge earlier in life hence providing strategies for preventative therapy to alter the course of this mental disorder Amongst other current topics the book covers new findings in genetics and epigenetics progress in animal models for schizophrenia and the usage of induced pluripotent stem cells The combination of these important areas benefit psychiatric neuroscience filling the gaps in the knowledge of neurobiology of schizophrenia and providing novel perspectives for future drug development Peptide-based Drug Discovery Ved Srivastava, 2017-06-22 With potentially high specificity and low toxicity biologicals offer promising alternatives to small molecule drugs Peptide therapeutics have again become the focus of innovative drug development efforts backed up by a resurgence of venture funds and small biotechnology companies What does it take to develop a peptide based medicine What are the key challenges and how are they overcome What are emerging therapeutics for peptide modalities This book answers these questions with a holistic story from molecules to medicine combining the themes of design synthesis and clinical applications of peptide based therapeutics and biomarkers Chapters are written and edited by leaders in the field from industry and academia and they cover the pharmacokinetics of peptide therapeutics attributes necessary for commercially successful metabolic peptides medicinal chemistry strategies for the design of peptidase resistant peptide analogues disease classes for which peptide therapeutic are most relevant and regulatory issues and guidelines The critical themes covered provide essential background information on what it takes to develop peptide based medicine from a chemistry perspective and views on the future of peptide drugs This book will be a valuable resource not only as a reference book for the researcher engaged in academic and pharmaceutical setting from basic research to manufacturing and from

organic chemistry to biotechnology but also a valuable resource to graduate students to understand discovery and development process for peptide based medicine Fragment-Based Drug Discovery Steven Howard, Chris Abell, 2015-07-03 Fragment based drug discovery is a rapidly evolving area of research which has recently seen new applications in areas such as epigenetics GPCRs and the identification of novel allosteric binding pockets The first fragment derived drug was recently approved for the treatment of melanoma It is hoped that this approval is just the beginning of the many drugs yet to be discovered using this fascinating technique This book is written from a Chemist's perspective and comprehensively assesses the impact of fragment based drug discovery on a wide variety of areas of medicinal chemistry It will prove to be an invaluable resource for medicinal chemists working in academia and industry as well as anyone interested in novel drug discovery techniques Green Approaches in Medicinal Chemistry for Sustainable Drug Design Bimal Banik, 2024-05-31 Extensive experimentation and high failure rates are a well recognized downside to the drug discovery process with the resultant high levels of inefficiency and waste producing a negative environmental impact Sustainable and Green Approaches in Medicinal Chemistry 2e reveals how medicinal chemistry can play a direct role in addressing this issue After providing essential context to the growth of green chemistry in relation to drug discovery the book goes on to identify a broad range of practical techniques and useful insights revealing how medicinal chemistry techniques can be used to improve efficiency mitigate failure and increase the environmental benignity of the entire drug discovery process Drawing on the knowledge of a global team of experts Sustainable and Green Approaches in Medicinal Chemistry Second Edition encourages the growth of green medicinal chemistry and supports medicinal chemists drug discovery researchers pharmacologists and all those in related fields across both academia and industry in integrating these approaches into their own work This second volume of the second edition includes the development of nanoparticles and nanocomposites as well as the application of ultrasound and microwave induced methods studies solventless synthesis defines the role of steroids studies reactions in aqueous solution identifies enzyme mediated reactions investigates ionic liquids and deep eutectic solvents explores natural products investigates solid supports realizes the effects of salts focuses on combinatorial chemistry develops one pot methods analyzes multi component reactions investigates dipole moment values and examines computer assisted methods Highlights the need for adoption of sustainable and green chemistry pathways in drug development Reveals risk factors associated with the drug development process and the ways sustainable approaches can help address these Identifies novel and cost effective green medicinal chemistry approaches for improved efficiency and sustainability

Antibiotic Drug Discovery Steven M. Firestine, Troy Lister, 2017-05-30 This book identifies and elaborates the most recent and compelling strategies for antibiotic drug discovery with a primary focus on new targets mechanisms and molecular entities Biophysical Techniques in Drug Discovery Angeles Canales, 2017-11-14 Biophysical techniques are used in many key stages of the drug discovery process including in screening for new receptor ligands in characterising drug

mechanisms and in validating data from biochemical and cellular assays This book provides an overview of the biophysical methods applied in drug discovery today including traditional techniques and newer developments Perspectives from academia and industry across a spectrum of techniques are brought together in a single volume Small and biotherapeutic approaches are covered and strengths and limitations of each technique are presented Case studies illustrate the application of each technique in real applied examples Finally the book covers recent developments in areas such as electron microscopy with discussions of their possible impact on future drug discovery This is a go to volume for biophysicists analytical chemists and medicinal chemists providing a broad overview of techniques of contemporary interest in drug discovery <u>Drugs</u> Glenn F. King, 2015-01-27 The pharmaceutical industry has become increasingly interested in biologics from animal venoms as a potential source for the rapeutic agents in recent years with a particularly emphasis on peptides To date six drugs derived from venom peptides or proteins have been approved by the FDA with nine further agents currently being investigated in clinical trials In addition to these drugs in approved or advanced stages of development many more peptides and proteins are being studied in varying stages of preclinical development This unique book provides an up to date and comprehensive account of the potential of peptides and proteins from animal venoms as possible therapeutics Topics covered include chemistry and structural biology of animal venoms proteomic and transcriptomic approaches to drug discovery bioassays high throughput screens and target identification and reptile scorpion spider and cone snail venoms as a platform for drug development Case studies are used to illustrate methods and successes and highlight issues surrounding administration and other important lessons that have been learnt from the development of approved therapeutics based on venoms. The first text to focus on this fascinating area and bridging an important gap this book provides the reader with essential and current knowledge on this fast developing area Venoms to Drugs will find wide readership with researchers working in academia and industry working in all medicinal and pharmaceutical areas Theranostics and Image Guided **Drug Delivery** Maya Thanou, 2018-01-02 Molecular imaging of drugs or drug carriers is a valuable tool that can provide important information on spatiotemporal distribution of drugs allowing improved drug distribution at target sites Chemically labelled drugs can be used to both diagnose and treat diseases This book introduces the topic of image guided drug delivery and covers the latest imaging techniques and developments in theranostics highlighting the interdisciplinary nature of this field as well as its translational ability These technologies and techniques hold potential for individualised safer therapies The book introduces the chemistry behind labelling drugs or drug carriers for imaging It then discusses current scientific progress in the discovery and development of theranostic agents as well as the latest advances in triggered drug delivery Novel imaging techniques that can be combined with the rapeutics are presented as well as results and findings from early clinical trials This text will provide postgraduates and researchers in various disciplines associated with drug discovery including chemistry device engineering oncology neurology cardiology imaging and nanoscience an overview of this

important field where several disciplines have been combined to improve treatments Readers will be introduced to techniques that can be translated to the clinic and be applied widely **Human-based Systems for Translational Research** Robert Coleman, 2014-12-08 This book provides a history and discussion of the use of human tissues as an alternative to animal based testing for assessing the efficacy and safety of new medicines Beginning by providing a historical background to animal based testing this text then describes in detail the issues relating to access to human cells and tissue and the rules and regulations governing their use The book illustrates what is currently possible in humanising medicines research and development and suggests more rational and reliable means of developing safe and effective drugs for the future than those on which we currently rely Early chapters establish the need to generate more data in human derived test systems and the need for resources such as tissue banks and standardised processes whilst highlighting the barriers that have prevented such developments so far Subsequent chapters explore the alternatives to current animal toxicology studies including stem cells and computational models with balanced views of the technical challenges and opportunities these offer In addition useful information on computational methods and pharmacokinetics are included This book is an essential read for anyone engaged in translational drug discovery who wishes to consolidate their understanding and broaden their awareness of the key issues involved in accessing primary human tissue and the advantages of doing so New Macrocycles and their Supramolecular Perspectives Carmine Gaeta, De-Xian Wang, 2020-03-25

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