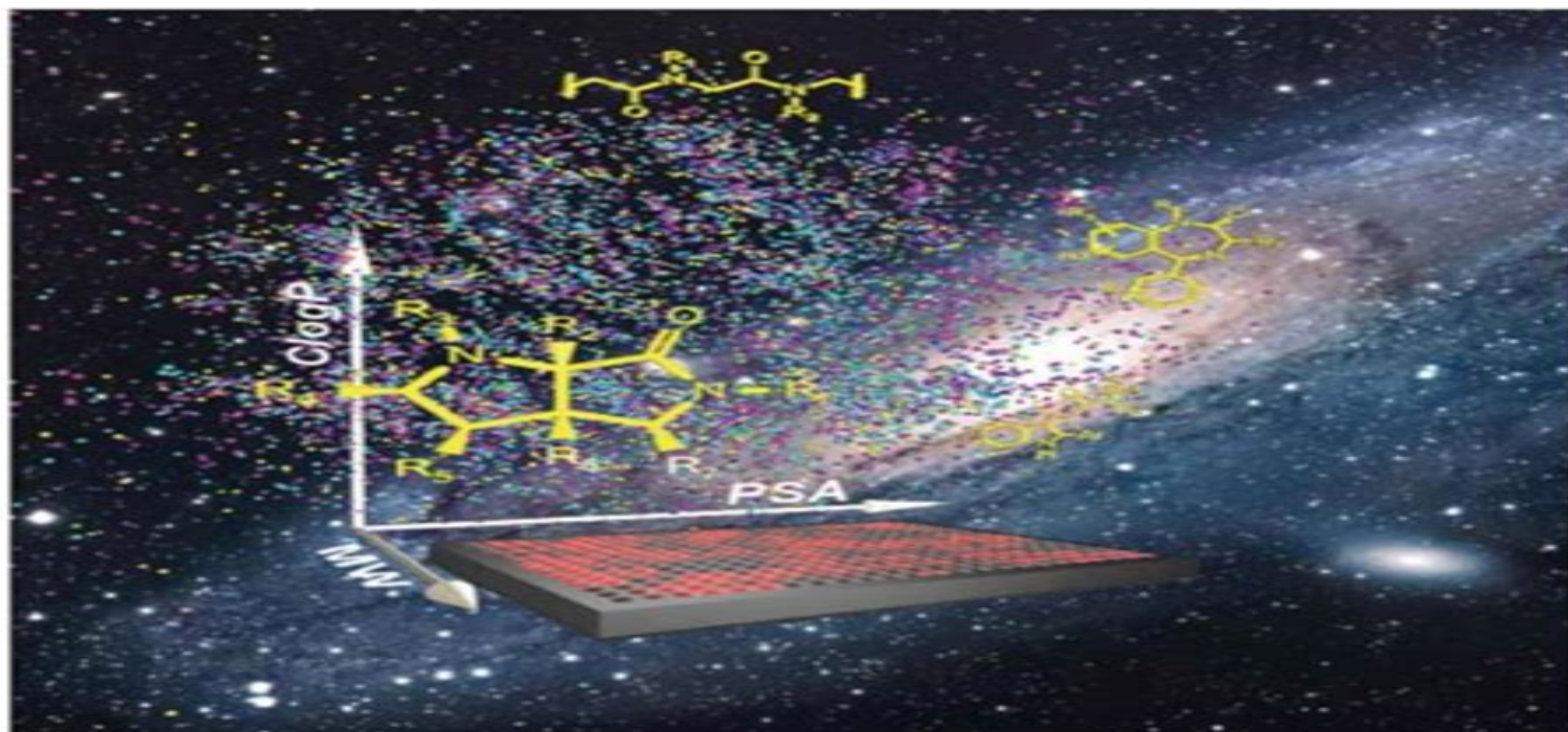


RSC Biomolecular Sciences

Edited by Paul A Bartlett and Michael Entzeroth

Exploiting Chemical Diversity for Drug Discovery



RSC Publishing

Exploiting Chemical Diversity For Drug Discovery Rsc Rsc Biomolecular Sciences

Jens Kurreck



Exploiting Chemical Diversity For Drug Discovery Rsc Rsc Biomolecular Sciences:

Exploiting Chemical Diversity for Drug Discovery Paul Allan Bartlett, Michael Entzeroth, 2006 This book examines the many aspects of the drug discovery process and presents the current state of the art and a clear overview of approaches to lead identification

Natural Product Chemistry for Drug Discovery Antony D. Buss, Mark S. Butler, 2010 This text provides a comprehensive summary of where natural product chemistry is today in drug discovery It covers emerging technologies and case studies and is a source of up to date information on the topical subject of natural products

Structural Biology of Membrane Proteins Reinhard K. Grishammer, Susan K. Buchanan, 2006 The book provides up to date reference source for researchers Introductory sections to each topic are followed by detailed discussions for the experienced biochemist

Molecular Simulations and Biomembranes Mark S. P. Sansom, Philip Charles Biggin, 2010 The need for information in the understanding of membrane systems has been caused by three things an increase in computer power methodological developments and the recent expansion in the number of researchers working on it worldwide However there has been no up to date book that covers the application of simulation methods to membrane systems directly and this book fills an important void in the market It provides a much needed update on the current methods and applications as well as highlighting recent advances in the way computer simulation can be applied to the field of membranes and membrane proteins The objectives are to show how simulation methods can provide an important contribution to the understanding of these systems The scope of the book is such that it covers simulation of membranes and membrane proteins but also covers the more recent methodological developments such as coarse grained molecular dynamics and multiscale approaches in systems biology Applications embrace a range of biological processes including ion channel and transport proteins The book is wide ranging with broad coverage and a strong coupling to experimental results wherever possible including colour illustrations to highlight particular aspects of molecular structure With an internationally respected list of authors its publication is timely and it will prove indispensable to a large scientific readership

Protein-Nucleic Acid Interactions Phoebe A. Rice, Carl C. Correll, 2008-05-22 The structural biology of protein nucleic acid interactions is in some ways a mature field and in others in its infancy High resolution structures of protein DNA complexes have been studied since the mid 1980s and a vast array of such structures has now been determined but surprising and novel structures still appear quite frequently High resolution structures of protein RNA complexes were relatively rare until the last decade Propelled by advances in technology as well as the realization of RNA's importance to biology the number of example structures has ballooned in recent years New insights are now being gained from comparative studies only recently made possible due to the size of the database as well as from careful biochemical and biophysical studies As a result of the explosion of research in this area it is no longer possible to write a comprehensive review Instead current review articles tend to focus on particular subtopics of interest This makes it difficult for newcomers to the field to attain a solid understanding of the basics One goal

of this book is therefore to provide in depth discussions of the fundamental principles of protein nucleic acid interactions as well as to illustrate those fundamentals with up to date and fascinating examples for those who already possess some familiarity with the field The book also aims to bridge the gap between the DNA and the RNA views of nucleic acid protein recognition which are often treated as separate fields However this is a false dichotomy because protein DNA and protein RNA interactions share many general principles This book therefore includes relevant examples from both sides and frames discussions of the fundamentals in terms that are relevant to both The monograph approaches the study of protein nucleic acid interactions in two distinctive ways First DNA protein and RNA protein interactions are presented together Second the first half of the book develops the principles of protein nucleic acid recognition whereas the second half applies these to more specialized topics Both halves are illustrated with important real life examples The first half of the book develops fundamental principles necessary to understand function An introductory chapter by the editors reviews the basics of nucleic acid structure Jen Jacobsen and Jacobsen discuss how solvent interactions play an important role in recognition illustrated with extensive thermodynamic data on restriction enzymes Marmorstein and Hong introduce the zoology of the DNA binding domains found in transcription factors and describe the combinatorial recognition strategies used by many multiprotein eukaryotic complexes Two chapters discuss indirect readout of DNA sequence in detail Berman and Lawson explain the basic principles and illustrate them with in depth studies of CAP while in their chapter on DNA bending and compaction Johnson Stella and Heiss highlight the intrinsic connections between DNA bending and indirect readout Horvath lays out the fundamentals of protein recognition of single stranded DNA and single stranded RNA and describes how they apply in a detailed analysis of telomere end binding proteins Nucleic acids adopt more complex structures Lilley describes the conformational properties of helical junctions and how proteins recognize and cleave them Because RNA readily folds due to the stabilizing role of its 2 hydroxyl groups Li discusses how proteins recognize different RNA folds which include duplex RNA With the fundamentals laid out discussion turns to more specialized examples taken from important aspects of nucleic acid metabolism Schroeder discusses how proteins chaperone RNA by rearranging its structure into a functional form Berger and Dong discuss how topoisomerases alter the topology of DNA and relieve the superhelical tension introduced by other processes such as replication and transcription Dyda and Hickman show how DNA transposases mediate genetic mobility and Van Duyne discusses how site specific recombinases cut and paste DNA Horton presents a comprehensive review of the structural families and chemical mechanisms of DNA nucleases whereas Li in her discussion of RNA protein recognition also covers RNA nucleases Lastly Ferr D Amar shows how proteins recognize and modify RNA transcripts at specific sites The book also emphasises the impact of structural biology on understanding how proteins interact with nucleic acids and it is intended for advanced students and established scientists wishing to broaden their horizons

Protein Folding, Misfolding and Aggregation Victor Muñoz, 2008 Protein folding and aggregation is the process by which newly synthesized proteins fold

into the specific three dimensional structures defining their biologically active states It has always been a major focus of research in biochemistry and has often been seen as the unsolved second part of the genetic code In the last 10 years we have witnessed a quantum leap in the research in this exciting area Computational methods have improved to the extent of making possible to simulate the complete folding process of small proteins and the early stages of protein aggregation

Experimental methods h **Quantum Tunnelling in Enzyme-catalysed Reactions** Rudolf Konrad Allemann, Nigel S. Scrutton, 2009 In recent years there has been an explosion in knowledge and research associated with the field of enzyme catalysis and H tunneling Rich in its breath and depth this introduction to modern theories and methods of study is suitable for experienced researchers those new to the subject Edited by two leading experts and bringing together the foremost practitioners in the field this up to date account of a rapidly developing field sits at the interface between biology chemistry and physics It covers computational kinetic and structural analysis of tunnelling and the synergy in combining these methods with a major focus on H tunneling reactions in enzyme systems The book starts with a brief overview of proton and electron transfer history by Nobel Laureate Rudolph A Marcus The reader is then guided through chapters covering almost every aspect of reactions in enzyme catalysis ranging from descriptions of the relevant quantum theory and quantum classical theoretical methodology to the description of experimental results The theoretical interpretation of these large systems includes both quantum mechanical and statistical mechanical computations as well as simple more approximate models Most of the chapters focus on enzymatic catalysis of hydride proton and H transfer an example of the latter being proton coupled electron transfer There is also a chapter on electron transfer in proteins This is timely since the theoretical framework developed fifty years ago for treating electron transfers has now been adapted to H transfers and electron transfers in proteins Accessible in style this book is suitable for a wide audience but will be particularly useful to advanced level undergraduates postgraduates and early postdoctoral workers **Therapeutic Oligonucleotides** Jens Kurreck, 2008 This book provides a compelling overall update on current status of RNA interference RNA Polymerases as Molecular Motors Henri C. Buc, Terence Strick, 2009-04-16 This book focuses on two aspects of the transcription cycle the recognition of the promoter by the enzyme and the achievement of consecutive translocation steps during elongation of the RNA product

Nucleic Acid-metal Ion Interactions Nicholas V. Hud, 2009 Provides a perspective on nucleic acid metal ion interactions with an emphasis on experimental biophysical studies which will prove indispensable to biophysicists and molecular biologists **The British National Bibliography** Arthur James Wells, 2006 *Structure-based Drug Discovery* R. E. Hubbard, 2006 Structure based drug discovery is a collection of methods that exploits the ability to determine and analyse the three dimensional structure of biological molecules These methods have been adopted and enhanced to improve the speed and quality of discovery of new drug candidates After an introductory overview of the principles and application of structure based methods in drug discovery this book then describes the essential features of the various methods Chapters

on X ray crystallography NMR spectroscopy and computational chemistry and molecular modelling describe how these particular techniques have been enhanced to support rational drug discovery with discussions on developments such as high throughput structure determination probing protein ligand interactions by NMR spectroscopy virtual screening and fragment based drug discovery The concluding chapters complement the overview of methods by presenting case histories to demonstrate the major impact that structure based methods have had on discovering drug molecules Written by international experts from industry and academia this comprehensive introduction to the methods and practice of structure based drug discovery not only illustrates leading edge science but also provides the scientific background for the non expert reader The book provides a balanced appraisal of what structure based methods can and cannot contribute to drug discovery It will appeal to industrial and academic researchers in pharmaceutical sciences medicinal chemistry and chemical biology as well as providing an insight into the field for recent graduates in the biomolecular sciences

Accounts in Drug Discovery Joel Charles Barrish, Joel Barrish, 2011 *Accounts in Drug Discovery* describes recent case studies in medicinal chemistry with a particular emphasis on how the inevitable problems that arise during any project can be surmounted or overcome The Editors cover a wide range of therapeutic areas and medicinal chemistry strategies including lead optimization starting from high throughput screening hits as well as rational structure based design The chapters include follow ons and next generation compounds that aim to improve upon first generation agents This volume surveys the range of challenges commonly faced by medicinal chemistry researchers including the optimization of metabolism and pharmacokinetics toxicology pharmaceutics and pharmacology including proof of concept in the clinic for novel biological targets The case studies include medicinal chemistry stories on recently approved and marketed drugs but also chronicle near misses i e exemplary compounds that may have proceeded well into the clinic but for various reasons did not result in a successful registration As the vast majority of projects fail prior to registration much can be learned from such narratives By sharing a wide range of drug discovery experiences and information across the community of medicinal chemists in both industry and academia the Editors believe that these accounts will provide insights into the art of medicinal chemistry as it is currently practiced and will help to serve the needs of active medicinal chemists

Synthetic Methods in Drug Discovery 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.

Green Chemistry Strategies for Drug Discovery Emily A. Peterson, Julie B. Manley, 2015-06-30

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. Edited 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. Currently employed as well as emerging techniques for performing greener drug discovery chemistry 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 down their science.

Fragment-Based Drug Discovery Steven Howard, Chris Abell, 2015-06-17

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.

Drug Discovery from Natural Products Olga Genilloud, Francisca Vicente, 2012-08-21

This book offers an integrated review of the most recent trends in natural products drug discovery and key lead candidates that are outstanding for their chemistry and biology as a starting point in novel drug development. The authors focus on different

trends that are and will continue to be impacting multiple stages of modern drug discovery from NPs that have not been included in other works. This is complemented with a series of case studies from leading experts from industry and academia on key molecules and derivatives that have been chosen for their novelty in chemistry, biology, and clinical applications. The book intends to reflect the current confluence of different disciplines in chemical biology and synthetic chemistry supported by a more profound knowledge of systems biology that ensures the concurrency and synergisms of expertise from different research fields that impact in the discovery of novel molecules. In the first section, the chapters reflect recent approaches to exploit the biosynthetic potential of microbial resources including genome mining, metagenomic, and epigenetic approaches as well as biosynthetic chemistry tools to respond to product supply and novel screening alternatives that have led to the discovery of novel chemistry. The second part reviews in the form of case studies some examples of bioactive molecules in the important therapeutic areas of anti-infectives, oncology, and antiparasitics.

Physico-chemical and Computational Approaches to Drug Discovery Javier Luque, Xavier Barril, 2012. This title covers a wide range of topics relevant to the development of drugs. It provides a comprehensive description of the major methodological strategies available for rational drug discovery.

Computational and Structural Approaches to Drug Discovery Robert M. Stroud, Janet Finer-Moore, 2008.

- 1 Facing the Wall in Computationally Based Approaches to Drug Discovery Janet S Finer Moore and Jeff Blaney and Robert M Stroud
- 2 The Changing Landscape in Drug Discovery Hugo Kubinyi
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- 17 A Link Means a Lot Disulfide Tethering in Structure Based Drug Design Jeanne A Hardy
- 18 The Impact of Protein Kinase Structures on Drug Discovery Chao Zhang and Sung Hou Kim

Privileged Scaffolds in Medicinal Chemistry Stefan

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

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