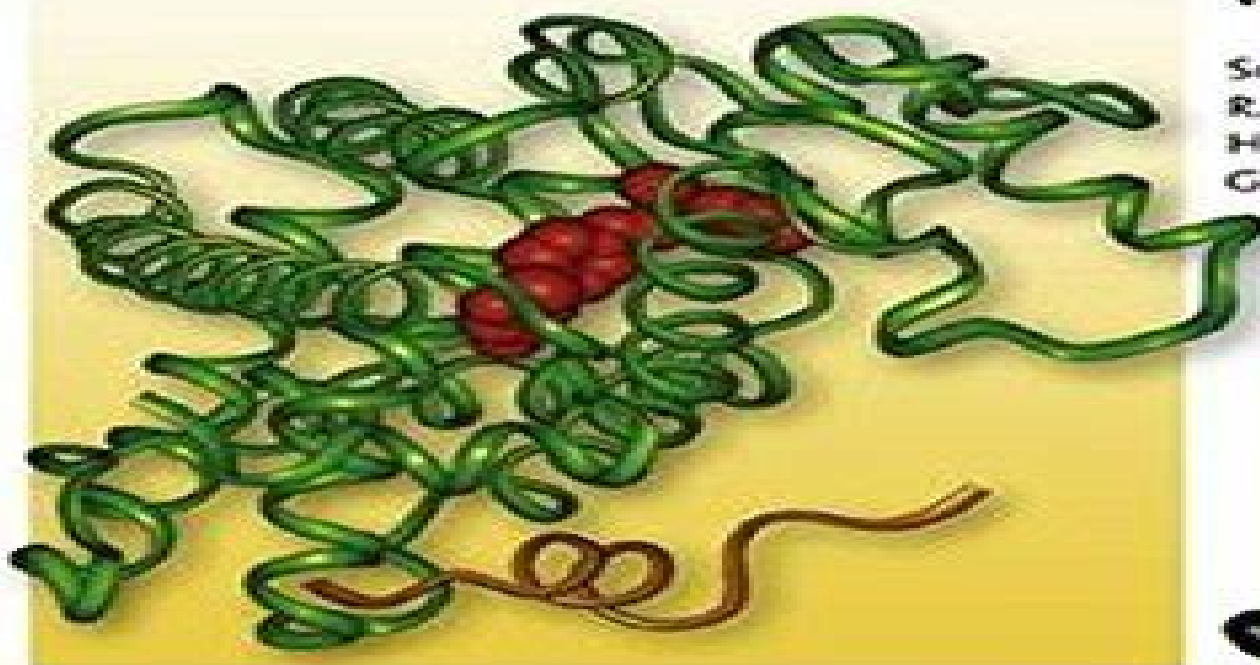


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R. E. Babine and S. S. Abdel-Meguid

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Protein Crystallography in Drug Discovery



Volume 20

Series Editors:
R. Mannhold,
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G. Folkers



Protein Crystallography In Drug Discovery Volume 20 Methods And Principles In Medicinal Chemistry

**Michael Hamacher, Katrin Marcus, Kai
Stühler, Andre van Hall, Bettina
Warscheid, Helmut E. Meyer**

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Protein Crystallography in Drug Discovery Robert E. Babine, Sherin S. Abdel-Meguid, 2008-07-15 The rational structure based approach has become standard in present day drug design As a consequence the availability of high resolution structures of target proteins is more often than not the basis for an entire drug development program Protein structures suited for rational drug design are almost exclusively derived from crystallographic studies and drug developers are relying heavily on the power of this method Here researchers from leading pharmaceutical companies present valuable first hand information much of it published for the first time They discuss strategies to derive high resolution structures for such important target protein classes as kinases or proteases as well as selected examples of successful protein crystallographic studies A special section on recent methodological developments such as for high throughput crystallography and microcrystallization is also included A valuable companion for crystallographers involved in protein structure determination as well as drug developers pursuing the structure based approach for use in their daily work

Chemogenomics in Drug Discovery Hugo Kubinyi, Gerhard Müller, 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

Proteomics in Drug Research Michael Hamacher, Katrin Marcus, Kai Stühler, Andre van Hall, Bettina Warscheid, Helmut E. Meyer, 2006-08-21 From skillful handling of the wide range of technologies to successful applications in drug discovery this handbook has all the information professional proteomics users need Edited by experts working at one of the hot spots in European proteomic research the numerous contributions by experts from the pharmaceutical industry and public proteomics consortia to provide the necessary perspective on current trends and developments in this exciting field Following an introductory chapter the book moves on to proteomic technologies such as protein biochips protein protein interactions and proteome analysis in situ The section on applications includes bioinformatics Alzheimer s disease neuroproteomics plasma and T cell proteomics differential phosphoproteome analysis and biomarkers as well as pharmacogenomics Invaluable reading for medicinal and pharmaceutical chemists gene technologists molecular biologists and those working in the pharmaceutical industry

Chemoinformatics in Drug Discovery Tudor I. Oprea, 2006-03-06 This handbook provides the first ever inside view of today s integrated approach to rational drug design Chemoinformatics experts from large pharmaceutical companies as well as from chemoinformatics service providers and from academia demonstrate what can be achieved today by harnessing the power of computational methods for the drug discovery process With the user rather than the developer of chemoinformatics software in mind this book describes the successful application

of computational tools to real life problems and presents solution strategies to commonly encountered problems It shows how almost every step of the drug discovery pipeline can be optimized and accelerated by using chemoinformatics tools from the management of compound databases to targeted combinatorial synthesis virtual screening and efficient hit to lead transition An invaluable resource for drug developers and medicinal chemists in academia and industry

Computer Applications in Pharmaceutical Research and Development Sean Ekins, 2006-06-12 A unique holistic approach covering all functions and phases of pharmaceutical research and development While there are a number of texts dedicated to individual aspects of pharmaceutical research and development this unique contributed work takes a holistic and integrative approach to the use of computers in all phases of drug discovery development and marketing It explains how applications are used at various stages including bioinformatics data mining predicting human response to drugs and high throughput screening By providing a comprehensive view the book offers readers a unique framework and systems perspective from which they can devise strategies to thoroughly exploit the use of computers in their organizations during all phases of the discovery and development process Chapters are organized into the following sections Computers in pharmaceutical research and development a general overview Understanding diseases mining complex systems for knowledge Scientific information handling and enhancing productivity Computers in drug discovery Computers in preclinical development Computers in development decision making economics and market analysis Computers in clinical development Future applications and future development Each chapter is written by one or more leading experts in the field and carefully edited to ensure a consistent structure and approach throughout the book Figures are used extensively to illustrate complex concepts and multifaceted processes References are provided in each chapter to enable readers to continue investigating a particular topic in depth Finally tables of software resources are provided in many of the chapters This is essential reading for IT professionals and scientists in the pharmaceutical industry as well as researchers involved in informatics and ADMET drug discovery and technology development The book s cross functional all phases approach provides a unique opportunity for a holistic analysis and assessment of computer applications in pharmaceuticals

G Protein-Coupled Receptors as Drug Targets Roland Seifert, Thomas Wieland, 2006-05-12 With its particular emphasis on the constitutive activity of G protein coupled receptors GPCRs s this book comprehensively discusses an important biological process that has not yet been covered in such depth in any other existing books on GPCRs The international team of highly distinguished authors addresses in detail current models and concepts to introduce medicinal chemists physiologists pharmacologists and medical researchers into the advances in the understanding of GPCR activation and constitutive activity In addition the book provides an overview on methods of investigating constitutive GPCR activity The text is well illustrated by selected experimental data and schemes _The chapters are all cross referenced with each other and cover general mechanisms methodological approaches and cover selected important GPCR systems the consequences for drug action including side effects and rational drug

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Molecular Biology in Medicinal Chemistry Theodor Dingeramn,Dieter Steinhilber,Gerd Folkers,2006-03-06 This readily comprehensible book explains the identification of molecular targets via cellular assays reporter genes or transgenic models as well as surveying recent advances in the synthesis separation and analysis of drugs A special section is devoted to molecular genetics methods With its examination of these novel methods and generous practical advice this is essential reading for all pharmaceutical chemists molecular biologists and medical researchers using molecular methods to study drugs and their action

Macromolecular Crystallography Mark R. Sanderson,Jane V. Skelly,2007-08-23 Macromolecular crystallography is the study of macromolecules using X ray crystallographic techniques to determine their molecular structure This title synthesises contributions from a team of internationally recognized leaders offering chapters on conventional and high throughput methods

Molecular Interaction Fields Gabriele Cruciani,2006-05-12 This unique reference source edited by the world s most respected expert on molecular interaction field software covers all relevant principles of the GRID force field and its applications in medicinal chemistry Entire chapters on 3D QSAR pharmacophore searches docking studies metabolism predictions and protein selectivity studies among others offer a concise overview of this emerging field As an added bonus this handbook includes a CD ROM with the latest commercial versions of the GRID program and related software

Voltage-Gated Ion Channels as Drug Targets David J. Triggie,Murali Gopalakrishnan,David Rampe,Wei Zheng,2006-08-21 Edited by the most prominent person in the field and top researchers at US pharmaceutical companies this is a unique resource for drug developers and physiologists seeking a molecular level understanding of ion channel pharmacology After an introduction to the topic the authors evaluate the structure and function of ion channels as well as related drug interaction A section on assay technologies is followed by a section each on calcium sodium and potassium channels Further chapters cover genetic and acquired channelopathies before the book closes with a look at safety issues in ion channel drug development For medicinal and pharmaceutical chemists biochemists molecular biologists and those working in the pharmaceutical industry

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Introduction

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