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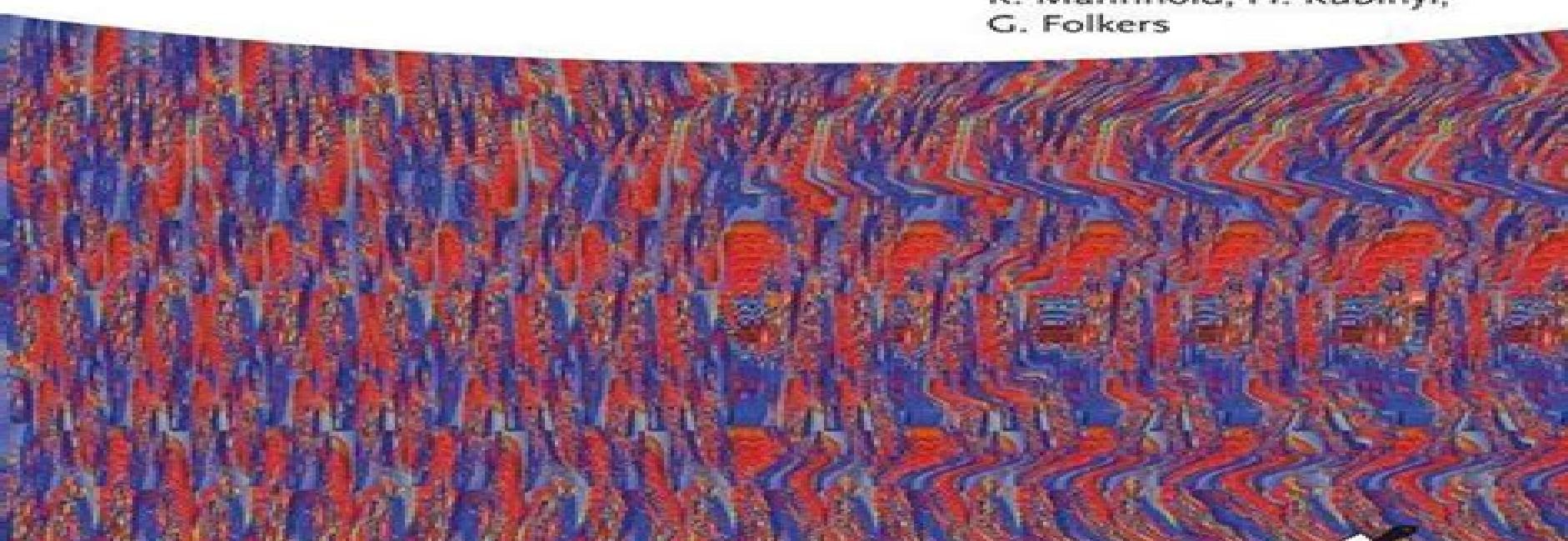
Rémy D. Hoffmann, Arnaud Gohier, Pavel Pospisil

Data Mining in Drug Discovery

Volume 57

Series Editors:

R. Mannhold, H. Kubinyi,
G. Folkers



Methods and Principles in Medicinal Chemistry



Data Mining In Drug Discovery Volume 57

György Keserü, David C. Swinney



Data Mining In Drug Discovery Volume 57:

Data Mining in Drug Discovery Rémy D. Hoffmann, Arnaud Gohier, Pavel Pospisil, 2013-09-25 Written for drug developers rather than computer scientists this monograph adopts a systematic approach to mining scientific data sources covering all key steps in rational drug discovery from compound screening to lead compound selection and personalized medicine Clearly divided into four sections the first part discusses the different data sources available both commercial and non commercial while the next section looks at the role and value of data mining in drug discovery The third part compares the most common applications and strategies for polypharmacology where data mining can substantially enhance the research effort The final section of the book is devoted to systems biology approaches for compound testing Throughout the book industrial and academic drug discovery strategies are addressed with contributors coming from both areas enabling an informed decision on when and which data mining tools to use for one's own drug discovery project **In vivo Models for Drug Discovery**

José Miguel Vela, Rafael Maldonado, Michel Hamon, 2014-08-11 This one stop reference is the first to present the complete picture covering all relevant organisms from single cells to mammals as well as all major disease areas including neurological disorders cancer and infectious diseases Addressing the needs of the pharmaceutical industry this unique handbook adopts a broad perspective on the use of animals in the early part of the drug development process including regulatory rules and limitations as well as numerous examples from real life drug development projects After a general introduction to the topic the expert contributors from research driven pharmaceutical companies discuss the basic considerations of using animal models including ethical issues The main part of the book systematically surveys the most important disease areas for current drug development from cardiovascular to endocrine disorders and from infectious to neurological diseases For each area the availability of animal models for target validation hit finding and lead profiling is reviewed backed by numerous examples of both successes and failures among the use of animal models The whole is rounded off with a discussion of perspectives and challenges Key knowledge for drug researchers in industry as well as academia Lead Generation, 2

Volume Set Jörg Holenz, 2016-06-27 In this comprehensive two volume resource on the topic senior lead generation medicinal chemists present a coherent view of the current methods and strategies in industrial and academic lead generation This is the first book to combine both standard and innovative approaches in comparable breadth and depth including several recent successful lead generation case studies published here for the first time Beginning with a general discussion of the underlying principles and strategies individual lead generation approaches are described in detail highlighting their strengths and weaknesses along with all relevant bordering disciplines like e.g target identification and validation predictive methods molecular recognition or lead quality matrices Novel lead generation approaches for challenging targets like DNA encoded library screening or chemical biology approaches are treated here side by side with established methods as high throughput and affinity screening knowledge or fragment based lead generation and collaborative approaches Within the

entire book a very strong focus is given to highlight the application of the presented methods so that the reader will be able to learn from real life examples The final part of the book presents several lead generation case studies taken from different therapeutic fields including diabetes cardiovascular and respiratory diseases neuroscience infection and tropical diseases The result is a prime knowledge resource for medicinal chemists and for every scientist involved in lead generation

Antitargets and Drug Safety Laszlo Urban, Vinod Patel, Roy J. Vaz, 2015-06-08 With its focus on emerging concerns of kinase and GPCR mediated antitarget effects this vital reference for drug developers addresses one of the hot topics in drug safety now and in future Divided into three major parts the first section deals with novel technologies and includes the utility of adverse event reports to drug discovery the translational aspects of preclinical safety findings broader computational prediction of drug side effects and a description of the serotonergic system The main part of the book looks at some of the most common antitarget mediated side effects focusing on hepatotoxicity in drug safety cardiovascular toxicity and signaling effects via kinase and GPCR anti targets In the final section several case studies of recently developed drugs illustrate how to prevent anti target effects and how big pharma deals with them if they occur The more recent field of systems pharmacology has gained prominence and this is reflected in chapters dedicated to the utility in deciphering and modeling anti targets The final chapter is concerned with those compounds that inadvertently elicit CNS mediated adverse events including a pragmatic description of ways to mitigate these types of safety risks Written as a companion to the successful book on antitargets by Vaz and Klabunde this new volume focuses on recent progress and new classes methods and case studies that were not previously covered

Predictive Toxicology Friedlieb Pfannkuch, Laura Suter-Dick, 2015-01-20 Ein moderner integrierter Ansatz für die Sicherheitsprüfung in der Arzneimittelentwicklung Dieses Praktikerbuch behandelt In silico und In vitro Methoden sowie den Einsatz von Biomarkern mit denen bei kleinen Arzneistoffmolekülen und Biologika frühzeitig und zuverlässig Toxizitäts Screenings durchgeführt werden können

Drug Metabolism Prediction Johannes Kirchmair, 2014-06-26 The first professional reference on this highly relevant topic for drug developers pharmacologists and toxicologists The authors provide more than a systematic overview of computational tools and knowledge bases for drug metabolism research and their underlying principles They aim to convey their expert knowledge distilled from many years of experience in the field In addition to the fundamentals computational approaches and their applications this volume provides expert accounts of the latest experimental methods for investigating drug metabolism in four dedicated chapters The authors discuss the most important caveats and common errors to consider when working with experimental data Collating the knowledge gained over the past decade this practice oriented guide presents methods not only used in drug development but also in the development and toxicological assessment of cosmetics functional foods agrochemicals and additives for consumer goods making it an invaluable reference in a variety of disciplines

Fragment-based Drug Discovery Daniel A. Erlanson, Wolfgang Jahnke, 2016-02-23 From its origins as a niche technique more than 15 years ago fragment based

approaches have become a major tool for drug and ligand discovery often yielding results where other methods have failed Written by the pioneers in the field this book provides a comprehensive overview of current methods and applications of fragment based discovery as well as an outlook on where the field is headed The first part discusses basic considerations of when to use fragment based methods how to select targets and how to build libraries in the chemical fragment space The second part describes established novel and emerging methods for fragment screening including empirical as well as computational approaches Special cases of fragment based screening e g for complex target systems and for covalent inhibitors are also discussed The third part presents several case studies from recent and on going drug discovery projects for a variety of target classes from kinases and phosphatases to targeting protein protein interaction and epigenetic targets

Thermodynamics and Kinetics of Drug Binding György Keserü, David C. Swinney, 2015-07-28 This practical reference for medicinal and pharmaceutical chemists combines the theoretical background with modern methods as well as applications from recent lead finding and optimization projects Divided into two parts on the thermodynamics and kinetics of drug receptor interaction the text provides the conceptual and methodological basis for characterizing binding mechanisms for drugs and other bioactive molecules It covers all currently used methods from experimental approaches such as ITC or SPR right up to the latest computational methods Case studies of real life lead or drug development projects are also included so readers can apply the methods learned to their own projects Finally the benefits of a thorough binding mode analysis for any drug development project are summarized in an outlook chapter written by the editors

Phosphodiesterases and Their Inhibitors Spiros Liras, Andrew S. Bell, 2014-03-03 Written by the pioneers of Viagra the first blockbuster PDE inhibitor drug Beginning with a review of the first wave of phosphodiesterase PDE inhibitors this book focuses on new and emerging PDE targets and their inhibitors Drug development options for all major human PDE families are discussed and cover diverse therapeutic fields such as neurological psychiatric cardiovascular metabolic pain and allergy respiratory diseases Finally emerging chemotherapeutic applications of PDE inhibitors against malaria and other tropical diseases are discussed

Medicinal Chemistry Approaches to Personalized Medicine Karen Lackey, Bruce Roth, 2013-11-22 Edited by two renowned medicinal chemists who have pioneered the development of personalized therapies in their respective fields this authoritative analysis of what is already possible is the first of its kind and the only one to focus on drug development issues Numerous case studies from the first generation of personalized drugs are presented highlighting the challenges and opportunities for pharmaceutical development While the majority of these examples are taken from the field of cancer treatment other key emerging areas such as neurosciences and inflammation are also covered With its careful balance of current and future approaches this handbook is a prime knowledge source for every drug developer and one that will remain up to date for some time to come From the content Discovery of Predictive Biomarkers for Anticancer Drugs Discovery and Development of Vemurafenib Targeting Basal Cell Carcinoma G Quadruplexes as Therapeutic Targets in Cancer From

Human Genetics to Drug Candidates An Industrial Perspective on LRRK2 Inhibition as a Treatment for Parkinson s Disease
Therapeutic Potential of Kinases in Asthma DNA Damage Repair Pathways and Synthetic Lethality Medicinal Chemistry in
the Context of the Human Genome and many more

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