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Data Mining in Drug Discovery

Volume 57

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Methods and Principles in Medicinal Chemistry



Data Mining In Drug Discovery Volume 57

Xiang Xie

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Drug Metabolism Prediction Johannes Kirchmair,2014-08-25 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

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

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 *Antitargets and Drug Safety* Laszlo Urban, Vinod Patel, Roy J. Vaz, 2015-02-23. 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.

The Journal of Biolaw & Business, 2003 *Proceedings of the IASTED International Conference, Artificial Intelligence and Soft Computing, July 27 to August 1 1997, Banff, Canada* M. H. Hamza, International Association of Science and Technology for Development, 1997

Text Mining for Biology and Biomedicine Sophia Ananiadou, 2006 Here's the first focused book that puts the full range of cutting edge biological text mining techniques and tools at your command. This comprehensive volume describes the methods of natural language processing NLP and their applications in the biological domain and spells out in detail the various lexical terminological and ontological resources now at your disposal and how best to utilize them.

Comprehensive Medicinal Chemistry II, Volume 4 John Bodenhan Taylor, D. J. Triggle, 2007 This e book comprises 8 volumes with all chapter sections available as PDF or HTML and includes bibliographical references and index.

Wiley Encyclopedia of Chemical Biology, Volume 1 Tadhg P. Begley, 2009 The first major reference at the interface of chemistry biology and medicine. Chemical biology is a rapidly developing field that uses the principles tools and language of chemistry to answer important questions in the life sciences. It has enabled researchers to gather critical information about the molecular biology of the cell and is the fundamental science of drug discovery playing a key role in the development of novel agents for the prevention diagnosis and treatment of disease. Now students and researchers across the range of disciplines that use chemical biology techniques have a single resource that encapsulates what is known in the field. It is an excellent place to begin any chemical biology investigation. Major topics addressed in the encyclopedia include Applications of chemical biology Biomolecules within the cell Chemical views of biology Chemistry of biological processes and systems Synthetic molecules as tools for chemical biology Technologies and

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Whispering the Techniques of Language: An Mental Quest through **Data Mining In Drug Discovery Volume 57**

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