Bioinformatics And Drug Discovery

MORROW FRANKLIN

A Revolution in Drug Discovery Birkhäuser
This book offers a detailed overview of translational bioinformatics together with real-case applications. Translational bioinformatics integrates the areas of basic bioinformatics, clinical informatics, statistical genetics and informatics in order to further our understanding of the molecular basis of diseases. By analyzing voluminous amounts of molecular and clinical data, it also provides clinical information, which can then be applied. Filling the gap between clinic research and informatics, the book is a valuable resource for human geneticists, clinicians, health educators and policy makers, as well as graduate students majoring in biology, biostatistics, and bioinformatics.
A Guide for Computational and Medicinal Chemists PHI Learning Pvt. Ltd.
This book provides up-to-date information on bioinformatics tools for the discovery and development of new drug molecules. It discusses a range of computational applications, including three-dimensional modeling of protein structures, protein-ligand docking, and molecular dynamics simulation of protein-ligand complexes for identifying desirable drug candidates. It also explores computational approaches for identifying potential drug targets and for pharmacophore modeling. Moreover, it presents structure- and ligand-based drug design tools to optimize known drugs and guide the design of new molecules. The book also describes methods for identifying small-molecule binding pockets in proteins, and summarizes the databases used to explore the essential properties of drugs, drug-like small molecules and their targets. In addition, the book highlights various tools to predict the absorption, distribution, metabolism, excretion (ADME) and toxicity (T) of potential drug candidates. Lastly, it reviews in silico tools that can facilitate vaccine design and discusses their limitations.
BIOINFORMATICS, FIFTH EDITION Academic Press
Ebola epidemics have had immediate and lasting impact in Africa and beyond, with its high case fatality and societal disruption. Its rapid spread, coupled with the limited knowledge, serves as a recipe for disaster and panic in the community. Health workers are particularly at risk, paying heavily with their lives. Sharing knowledge from various experts in basic sciences that support vaccine and drug development, as well as improving community surveillance and case management, enriches our understanding of this highly fatal and contagious disease. In a world that is fast becoming a global village, communicable diseases from low-resource setting are gradually becoming a global health threat. This book seeks to discuss emerging advances in the Ebola control.
Computational Drug Discovery Bioinformatics and Drug Discovery
With a DVD of color figures, Clustering in Bioinformatics and Drug Discovery provides an expert guide on extracting the most pertinent information from pharmaceutical and biomedical data. It offers a concise overview of common and recent clustering methods used in bioinformatics and drug discovery.Setting the stage for subsequent material, the firs
Bioinformatics and Drug Discovery Elsevier

A comprehensive overview of the use of computational biology approaches in the drug discovery and development process.
Computational Approaches Cambridge University Press
Shows how different parts of the drug discovery process have developed, with particular emphasis on quantitative aspects and possible future progress.
Applications for Complex Diseases Academic Press
Bioinformatics and Drug DiscoveryHumana Press
Drug Discovery Process & Methods Humana
This book is a collection of original research articles in the field of computer-aided drug design. It reports the use of current and validated computational approaches applied to drug discovery as well as the development of new computational tools to identify new and more potent drugs.
Introduction to Pharmaceutical Bioinformatics Springer
Recent advances in drug discovery have been rapid. The second edition of Bioinformatics and Drug Discovery has been completely updated to include topics that range from new technologies in target identification, genomic analysis, cheminformatics, protein analysis, and network or pathway analysis. Each chapter provides an extended introduction that describes the theory and application of the technology. In the second part of each chapter, detailed procedures related to the use of these technologies and software have been incorporated. Written in the highly successful Methods in Molecular BiologyTM series format, the chapters include the kind of detailed description and implementation advice that is crucial for getting optimal results in the laboratory. Thorough and intuitive, Bioinformatics and Drug Discovery, Second Edition seeks to aid scientists in the further study of the rapidly expanding field of drug discovery.
Translational Bioinformatics and Its Application Humana Press
The application of bioinformatics approaches in drug design involves an interdisciplinary array of sophisticated techniques and software tools to elucidate hidden or complex biological data. This work reviews the latest bioinformatics approaches used for drug discovery. The text covers ligand-based and structure-based approaches for computer-aided drug design, 3D pharmacophore modeling, molecular dynamics simulation, the thermodynamics of ligand−receptor and ligand−enzyme association, thermodynamic characterization and optimization, and techniques for computational genomics and proteomics.
Computational Drug Discovery and Design Academic Press
Designed as a comprehensive text for students and professionals pursuing careers in the fields of bioinformatics, molecular biology, pharmacy and drug research, the Fifth Edition continues to offer a fascinating and authoritative treatment of the entire spectrum of bioinformatics, covering a wide range of high-throughput technologies. The content can be used for four core courses: bioinformatics fundamentals, genomics, proteomics and drug discovery and design. The Fifth Edition takes a completely new pedagogical approach and the book is divided into eight distinct Units for the ease of learning: Bioinformatics Fundamentals, Sequence Alignment, Phylogenetic Analysis, Genomics, Protein Structure and Function, Drug Discovery Methods, Drug Design and Development and Integrative Topics. Accordingly, all the chapters are revised and updated in the new edition, besides introduction of seven new chapters and another seven completely re-written chapters. As a student-friendly text, it embodies several pedagogical features such as detailed examples, numerous tables, a large number of diagrams, flow charts and web resources. The book in its present edition should prove an invaluable asset to the students and researchers in the fields of bioinformatics, biotechnology, computer-aided drug design, information technology, medical diagnostics, molecular biology and pharmaceutical sciences. NEW TO THE FIFTH EDITION • Re-written chapters — Biological database search and data retrieval, Pair-wise alignment of sequences, PSSMs and Hidden Markov Models, Gene Mapping, Gene Prediction, Protein Structure Overview and Protein Structure Prediction. • Inclusion of new chapters—Scoring Matrices, Gene Sequencing, Regulatory Elements Prediction, Comparative Genomics, Protein Structure Databases, Protein Function Prediction and Potential Drug Targets. KEY FEATURES • Covers the field of bioinformatics in a complete and integrated approach – moving from the fundamentals to theory and practical applications. • State-of-the-art technologies for gene identification, molecular modeling and monitoring of cellular processes. • Data mining, data curation and analysis, classification, interpretation and efficient structure determination of genomes and proteomes. • Companion website provides useful resources for the teachers as well as for the students. So, visit Learning Centre https:// www.phindia.com/bioinformatics_mendiratta_rastogi to have access of Lecture notes, solutions manual, MCQs, problems set for practice, glossary of important terms, etc. TARGET AUDIENCE • UG and PG Students of Bioinformatics, Biotechnology, Molecular Biology and Pharmacy.
Proteomics and Protein-Protein Interactions John Wiley & Sons
Structural Bioinformatics was the first major effort to showthe application of the principles and basic knowledge of the largerfield of bioinformatics to questions focusing on macromolecularstructure, such as the prediction of protein structure and howproteins carry out cellular functions, and how the application ofbioinformatics to these life science issues can improve healthcareby accelerating drug discovery and development. Designed primarilyas a reference, the first edition nevertheless saw widespread useas a textbook in graduate and undergraduate university coursesdealing with the theories and associated algorithms, resources, andtools used in the analysis, prediction, and theoreticalunderpinnings of DNA, RNA, and proteins. This new edition contains not only thorough updates of theadvances in structural bioinformatics since publication of thefirst edition, but also features eleven new chapters dealing withfrontier areas of high scientific impact, including: sampling andsearch techniques; use of mass spectrometry; genome functionalannotation; and much more. Offering detailed coverage for practitioners while remainingaccessible to the novice, Structural Bioinformatics, SecondEdition is a valuable resource and an excellent textbook for arange of readers in the bioinformatics and advanced biologyfields. Praise for the previous edition: "This book is a gold mine of fundamental and practicalinformation in an area not previously well represented in bookform." —Biochemistry and Molecular Education "... destined to become a classic reference work for workers atall levels in structural bioinformatics...recommended with greatenthusiasm for educators, researchers, and graduatestudents." —BAMBED "...a useful and timely summary of a rapidly expandingfield." —Nature Structural Biology "...a terrific job in this timely creation of a compilation ofarticles that appropriately addresses this issue." —Briefings in Bioinformatics

Computation in BioInformatics CRC Press
The rapidly evolving field of protein science has now come to realize the ubiquity and importance of protein-protein interactions. It had been known for some time that proteins may interact with each other to form functional complexes, but it was thought to be the property of only a handful of key proteins. However, with the advent of high throughput proteomics to monitor protein-protein interactions at an organism level, we can now safely state that protein-protein interactions are the norm and not the exception. Thus, protein function must be understood in the larger context of the various binding complexes that each protein may form with interacting partners at a given time in the life cycle of a cell. Proteins are now seen as forming sophisticated interaction networks subject to remarkable regulation. The study of these interaction networks and regulatory mechanism, which I would like to term "systems proteomics," is one of the thriving fields of proteomics. The bird-eye view that systems proteomics offers should not however mask the fact that proteins are each characterized by a unique set of physical and chemical properties. In other words, no protein looks and behaves like another. This complicates enormously the design of high-throughput proteomics methods. Unlike genes, which, by and large, display similar physico-chemical behaviors and thus can be easily used in a high throughput mode, proteins are not easily amenable to the same treatment. It is thus important to remind researchers active in the proteomics field the fundamental basis of protein chemistry. This book attempts to bridge the two extreme ends of protein science: on one end, systems proteomics, which describes, at a system level, the intricate connection network that proteins form in a cell, and on the other end, protein chemistry and biophysics, which describe the molecular properties of individual proteins and the structural and thermodynamic basis of their interactions within the network. Bridging the two ends of the spectrum is bioinformatics and computational chemistry. Large data sets created by systems proteomics need to be mined for meaningful information, methods need to be designed and implemented to improve experimental designs, extract signal over noise, and reject artifacts, and predictive methods need to be worked out and put to the test. Computational chemistry faces similar challenges. The prediction of binding thermodynamics of protein-protein interaction is still in its infancy. Proteins are large objects, and simplifying assumptions and shortcuts still need to be applied to make simulations manageable, and this despite exponential progress in computer technology. Finally, the study of proteins impacts directly on human health. It is an obvious statement to say that, for decades, enzymes, receptors, and key regulator proteins have been targeted for drug discovery. However, a recent and exciting development is the exploitation of our knowledge of protein-protein interaction for the design of new pharmaceuticals. This presents particular challenges because protein-protein interfaces are generally shallow and interactions are weak. However, progress is clearly being made and the book seeks to provide examples of successes in this area.
Springer Nature
Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences brings together two very important fields in pharmaceutical sciences that have been mostly seen as diverging from each other: chemoinformatics and bioinformatics. As developing drugs is an expensive and lengthy process, technology can improve the cost, efficiency and speed at which new drugs can be discovered and tested. This book presents some of the growing advancements of technology in the field of drug development and how the computational approaches explained here can reduce the financial and experimental burden of the drug discovery process. This book will be useful to pharmaceutical science researchers and students who need basic knowledge of computational techniques relevant to their projects. Bioscientists, bioinformaticians, computational scientists, and other stakeholders from industry and academia will also find this book helpful. Provides practical information on how to choose and use appropriate computational tools Presents the wide, intersecting fields of chemo-bio-informatics in an easily-accessible format Explores the fundamentals of the emerging field of chemoinformatics and bioinformatics
Structural Bioinformatics: Applications in Preclinical Drug Discovery Process Royal Society of Chemistry
Bioinformatics is a platform between the biology and information technology. The book covers a broad spectrum of the bioinformatics fields starting from the basic principles, concepts, and multidisciplinary application areas. It comprises a collection of chapters describing the role of bioinformatics in drug design and discovery including the molecular modeling aspects; chapters detailing topics such as silico design, protein modeling, DNA Microarray Analysis, DNA-RNA barcoding, gene sequencing; specialized topics such as bioinformatics in cancer detection, genomics, proteomics, machine learning, covalent approaches in drug design
Bioinformatics Biocuration Labs
This book presents the latest developments in bioinformatics, highlighting the importance of bioinformatics in genomics, transcriptomics, metabolism and cheminformatics analysis, as well as in drug discovery and development. It covers tools, data mining and analysis, protein analysis, computational vaccine, and drug design. Covering cheminformatics, computational evolutionary biology and the role of next-generation sequencing and neural network analysis, it also discusses the use of bioinformatics tools in the development of precision medicine. This book offers a valuable source of information for not only beginners in bioinformatics, but also for students, researchers, scientists, clinicians, practitioners, policymakers, and stakeholders who are interested in harnessing the potential of bioinformatics in many areas.
Bioinformatics and Drug Discovery Springer
Exploring innovative routes of drug discovery in the postgenomic era, Microbial Genomics and Drug Discovery examines bioinformatic and genomic approaches for the identification, detection, selection, and validation of new antibacterial targets and vaccine candidates. The book discusses potential pathways for effective infection control, inhibition
Bioinformatics Techniques for Drug Discovery Vch Verlagsgesellschaft Mbh
This volume details methods and techniques for identification of drug targets, binding sites prediction, high-throughput virtual screening,and prediction of pharmacokinetic properties using computer based methodologies. Chapters guide readers through techniques of the available computational tools, developing prediction models for drug target prediction and de novo design of ligands, structure based drug designing, fragment-based drug designing, molecular docking, and scoring functions for assessing protein-ligand docking protocols. Written in the highly successful Methods in Molecular Biology series format, chapters include introductions to their respective topics, lists of the necessary materials, step-by-step, readily reproducible protocols, and tips on troubleshooting and avoiding known pitfalls. Authoritative and cutting-edge, Computational Drug

Discovery and Design aims to provide protocols for the use of bioinformatics tools in drug discovery and design.
Emerging Tools for Drug Discovery and Development CRC Press
A collection of readily reproducible bioinformatic methods to advance the drug discovery process from gene identification to protein modeling to the identification of specific drug candidates. The authors demonstrate these techniques, including microarray analysis, the analysis of genes as potential drug targets, virtual screening and in silico protein design, and cheminformatics, in a variety of practical situations. Because these technologies are still emergent, each chapter contains an extended introduction that explains the theory and application of the technology and techniques described.
METHODS AND APPLICATIONS - GENOMICS, PROTEOMICS AND DRUG DISCOVERY BoD – Books on Demand
Helps you choose the right computational tools and techniques to meet your drug design goals Computational Drug Design covers all of the major computational drug design techniques in use today, focusing on the process that pharmaceutical chemists employ to design a new drug molecule. The discussions of which computational tools to use and when and how to use them are all based on typical pharmaceutical industry drug design processes. Following an introduction, the book is divided into three parts: Part One, The Drug Design Process, sets forth a variety of design processes suitable for a number of different drug development scenarios and drug targets. The author demonstrates how computational techniques are typically used during the design process, helping readers choose the best computational tools to meet their goals. Part Two, Computational Tools and Techniques, offers a series of chapters, each one dedicated to a single computational technique. Readers discover the strengths and weaknesses of each technique. Moreover, the book tabulates comparative accuracy studies, giving readers an unbiased comparison of all the available techniques. Part Three, Related Topics, addresses new, emerging, and complementary technologies, including bioinformatics, simulations at the cellular and organ level, synthesis route prediction, proteomics, and prodrug approaches. The book's accompanying CD-ROM, a special feature, offers graphics of the molecular structures and dynamic reactions discussed in the book as well as demos from computational drug design software companies. Computational Drug Design is ideal for both students and professionals in drug design, helping them choose and take full advantage of the best computational tools available. Note: CD-ROM/DVD and other supplementary materials are not included as part of eBook file.