Bioinformatics And Drug Discovery

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Therapeutic Protein Targets For Drug Discovery And Clinical Evaluation: Bio-crystallography And Drug Design - D Velmurugan 2022-10-04
The book reviews the recent research advances and their outcomes in the areas of structural biology, bioinformatics, phytochemistry and drug discovery. Chapters in the book cover multidisciplinary research to understand the molecular mechanisms involved in protein-protein/ligand interactions. It employs an integrative approach to identify the therapeutic targets for HIV, and cancer, pathogen and viral infection pathways and the identification of their potential drug candidates. The book also provides examples of computational molecular dynamics simulations to understand the conformational changes in the molecules. Some chapters are focused on exploring potent bioactive compounds from natural sources.This book can serve as a single source that covers several interdisciplinary research fields which will be beneficial to Researchers and students in postgraduate studies.
Bioinformatics Tools for Pharmaceutical Drug Product Development - Vivek Chavda 2023-02-09
BIOINFORMATICS TOOLS FOR Pharmaceutical DRUG PRODUCT DLEVELOPMENT A timely book that details bioinformatics tools, artificial intelligence, machine learning, computational methods, protein interactions, peptide-based drug design, and omics technologies, for drug development in the pharmaceutical and medical sciences industries. The book contains 17 chapters categorized into 3 sections. The first section presents the latest information on bioinformatics tools, artificial intelligence, machine learning, computational methods, protein interactions, peptide-based drug design, and omics technologies. The following 2 sections include bioinformatics tools for the pharmaceutical sector and the healthcare sector. Bioinformatics brings a new era in research to accelerate drug target and vaccine design development, improving validation approaches as well as facilitating and identifying side effects and predicting drug resistance. As such, this will aid in more successful drug candidates from discovery to clinical trials to the market, and most importantly make it a more cost-effective process overall. Readers will find in this book: Applications of bioinformatics tools for pharmaceutical drug product development like process development, pre-clinical development, clinical development, commercialization of the product, etc.; The ever-expanding application of this novel technology and discusses some of the unique challenges associated with such an approach; The broad and deep background, as well as updates, on recent advances in both medicine and AI/ML that enable the application of these cutting-edge bioinformatics tools. Audience The book will be used by researchers and scientists in academia and industry including drug developers, computational biochemists, bioinformaticians, immunologists, pharmaceutical and medical sciences, as well as those in artificial intelligence and machine learning.
BIOINFORMATICS, FIFTH EDITION - RASTOGI, S.C. 2022-04-05
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.
Bioinformatics - Thomas Lengauer 2002
V.1: Basic technologies: From Genomes to drugs with bioinformatics (Thomas Lengauer); Sequence analysis (Martin Vingron); Structure, properties and computer identification of eukaryotic genes (Victor Solovyev). Analyzing regulatory regions in genomes (Thomas Werner). Homology modeling in biology and medicine (Roland L. Dunbrack, Jr.). Protein structure prediction (Ralf Zimmer and Thomas Lengauer). Protein-ligand docking in drug design (Matthias Rarey). Modellimg protein-protein and protein-DNA docking (Michael J. E. Sternberg and Gidon Moont). v.2: Applications: Integrating and accessing molecular biology resources (David P. Hansen and Thure Etzold). Bioinformatics support of genome sequencing projects (Xiaoqiu Huang). Analysis of sequence variations (Christopher S. Carlson, Mark J. Rieder and Deborah A. Nickerson). Proteome analysis (Pierre-Alain Binz, Elisabeth Gasteiger, Jean-Charles Sanchez, Amos Bairoch, Denis F. Hochstrasser, Ron D. Appel). Target finding in genomes and proteomes (Stephanie Fuhrman Liang, Xiling Wen and Roland Somogyi). Screening of drug databases (Martin Stahl, Matthias Rarey and Gerhard Klebe). Future trends (Thomas Lengauer).
Bioinformatics Approaches to Biomarker and Drug Discovery in Aging and Disease - Kristen Fortney 2012

Bioinformatics and Computational Biology in Drug Discovery and Development - William T. Loging 2016-03-17
A comprehensive overview of the use of computational biology approaches in the drug discovery and development process.
Bioinformatics and Drug Discovery - Richard S. Larson 2012
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 Biology 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.

Computation in BioInformatics - S. Balamurugan 2021-10-19

COMPUTATION IN BIOINFORMATICS Bioinformatics is a platform between the biology and information technology and this book provides readers with an understanding of the use of bioinformatics tools in new drug design. The discovery of new solutions to pandemics is facilitated through the use of promising bioinformatics techniques and integrated approaches. This book covers a broad spectrum of the bioinformatics field, starting with the basic principles, concepts, and application areas. Also covered is the role of bioinformatics in drug design and discovery, including aspects of molecular modeling. Some of the chapters provide detailed information on bioinformatics related topics, such as silicon design, protein modeling, DNA microarray analysis, DNA-RNA barcoding, and gene sequencing, all of which are currently needed in the industry. Also included are specialized topics, such as bioinformatics in cancer detection, genomics, and proteomics. Moreover, a few chapters explain highly advanced topics, like machine learning and covalent approaches to drug design and discovery, all of which are significant in pharma and biotech research and development. Audience Researchers and engineers in computation biology, information technology, bioinformatics, drug design, biotechnology, pharmaceutical sciences.

Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences - Navneet Sharma 2021-05-21

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

Bioinformatics Techniques for Drug Discovery - Aman Chandra Kaushik 2018-04-25

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.

Recent Advances in Computer Aided Drug Designing - Ashutosh Mani 2021

"We are extremely happy to introduce our new book, Recent Advances in Computer Aided Drug Designing. While interacting with many researchers in the field of biotechnology and allied sciences, we felt that there was need for a book that could easily bridge the gap between in silico methods applied in structural bioinformatics for drug designing and wet lab workers. Today, when computational skills in biology and biomedical research are in high demand, this book presents updated content for methods and tools applicable in modern computer-aided drug designing. Researchers are pouring knowledge into databases that are publicly available and laboratories across the globe are accessing this information for analysis and further investigation. There is a battery of data scientists involved in development and maintenance of online databases. Alongside them, there is another class of programmers and scientists involved in development of software tools for analysis of this data. Modern tools based on machine learning are available to provide accuracy and efficiency with speedy analysis of biological and biomedical data. In many cases, analysis of readily available biological data helps to decide future directions for laboratory work. Indications obtained from such analytics save time and resources which could be very crucial in general. Publicly available protein three-dimensional structure and drug databank libraries have facilitated the drug discovery process. Millions of drugs can be screened in a few hours by using virtual screening tools. Molecular viewing tools can be used to visualize macromolecules and their interactions with drugs. Findings from such studies are being used to validate results directly in laboratories. Efforts have been made to cover all areas relevant for computer-aided drug designing to allow this book to serve as a standard reference book and meet the requirements of graduate students and researchers working in drug design and structural bioinformatics. Some chapters are dedicated to basic concepts in computer-aided drug discovery while other chapters present applications of the available tools in the field. Contents from exemplary method-based chapters are easy to follow and will help new researchers in applying contemporary tools for their studies. The book will also stimulate programmers and data scientists interested in developing tools for structural bioinformatics applications to develop new and improved versions of software. Chapters presenting the basic concepts of methods involved in drug design will help new learners in the field to meet the challenges of designing novel therapeutics by using computational tools. Cross-disciplinary research is in trend nowadays and such investigations involving experts of their respective fields are highly promising and fruitful. Drug discovery requires experts from health sciences and medical sciences, molecular biologists, bioinformaticians, biotechnologists, biochemists, statisticians, biophysicists and clinicians. For a complete piece of translated product such as a drug, inputs from specialist researchers are needed. Modern rational drug discovery approaches are truly inter-disciplinary fields which require a systems biology approach for successful ventures. This book covers all steps of drug design, from drug target identification to intermediate steps to successful clinical trials, making it truly essential for modern researchers in the drug discovery and structural bioinformatics fields"--

Bioinformatics - Andrew Lyall 1998

Bioinformatics and the Effective Use of the Internet for Rapid Drug Discovery - Wendy Mori 1997-06-01

Structural Bioinformatics - Jenny Gu 2011-09-20

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

Innovations in Bioinformatics - 2007

R&D laboratories are facing increasing volumes of biological data. Bioinformatics-enabled data management has enabled companies to improve productivity by identifying new drug targets, and diagnostic, efficacy, and toxicity biomarkers.

Computer-Aided Drug Design - Dev Bukhsh Singh 2020-10-09

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.

Biosimulation in Drug Development - Martin Bertau 2007-11-28

This first comprehensive survey to cover all pharmaceutically relevant topics provides a comprehensive introduction to this novel and revolutionary tool, presenting both concepts and application examples of biosimulated cells, organs and organisms. Following an introduction to the role of biosimulation in drug development, the authors go on to discuss the simulation of cells and tissues, as well as simulating drug action and effect. A further section is devoted to simulating networks and populations, and the whole is rounded off by a look at the potential for biosimulation in industrial drug development and for regulatory decisions. Part of the authors are members of the BioSim Network of Excellence that encompasses more than 40 academic institutions, pharmaceutical companies and regulatory authorities dealing with drug development; other contributors come from industry, resulting in a cross-disciplinary expert reference.

Structural Bioinformatics: Applications in Preclinical Drug Discovery Process - C. Gopi Mohan 2019-01-10

This book reviews the advances and challenges of structure-based drug design in the preclinical drug discovery process, addressing various diseases, including malaria, tuberculosis and cancer. Written by internationally recognized researchers, this edited book discusses how the application of the various in-silico techniques, such as molecular docking, virtual screening, pharmacophore modeling, molecular dynamics simulations, and residue interaction networks offers insights into pharmacologically active novel molecular entities. It presents a clear concept of the molecular mechanism of different drug targets and explores methods to help understand drug resistance. In addition, it includes chapters dedicated to natural-product- derived medicines, combinatorial drug discovery, the CryoEM technique for structure-based drug design and big data in drug discovery. The book offers an invaluable resource for graduate and postgraduate students, as well as for researchers in academic and industrial laboratories working in the areas of chemoinformatics, medicinal and pharmaceutical chemistry and pharmacoinformatics.

Pharmaceutical Data Mining - Konstantin V. Balakin 2009-11-19

Leading experts illustrate how sophisticated computational data mining techniques can impact contemporary drug discovery and development In the era of post-genomic drug development, extracting and applying knowledge from chemical, biological, and clinical data is one of the greatest challenges facing the pharmaceutical industry. Pharmaceutical Data Mining brings together contributions from leading academic and industrial scientists, who address both the implementation of new data mining technologies and application issues in the industry. This accessible, comprehensive collection discusses important theoretical and practical aspects of pharmaceutical data mining, focusing on diverse approaches for drug discovery—including chemogenomics, toxicogenomics, and individual drug response prediction. The five main sections of this volume cover: A general overview of the discipline, from its foundations to contemporary industrial applications Chemoinformatics-based applications Bioinformatics-based applications Data mining methods in clinical development Data mining algorithms, technologies, and software tools, with emphasis on advanced algorithms and software that are currently used in the industry or represent promising approaches In one concentrated reference, Pharmaceutical Data Mining reveals the role and possibilities of these sophisticated techniques in contemporary drug discovery and development. It is ideal for graduate-level courses covering pharmaceutical science, computational chemistry, and bioinformatics. In addition, it provides insight to pharmaceutical scientists, principal investigators, principal scientists, research directors, and all scientists working in the field of drug discovery and development and associated industries.

Structural Bioinformatics Tools for Drug Design - Jaroslav Koča 2017-01-24

The book describes the individual steps necessary for biomacromolecular fragments analysis, as well as a list of essential software tools. For each step, it also shows corresponding web-based tools in detail and provides practical examples of their use. All tools and databases mentioned in the examples are available free of charge, platform-independent, web-based, user-friendly and do not require a prior IT background to be fully used.

Bioinformatics And Drug Discovery - Larson 2007-12-01

Drug Discovery and Design - Sneha H. Galande 2014-04-30

The drug development process from the target identification to the final product being marketed, is a time and money consuming process with the total Research and Development (RD) costs reported as being up to 800 million dollars and an average of 10 years. So, Drug Discovery and Design by bioinformatics assists and makes the entire process faster. This book aims to discuss various computational techniques and its application related with drug discovery and design.

Clustering in Bioinformatics and Drug Discovery - John David MacCuish 2010-11-15

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

Proteomics and Protein-Protein Interactions - Gabriel Waksman 2005-12-21

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.

Modern Methods of Drug Discovery - Alexander Hillisch 2012-11-28

Research in the pharmaceutical industry today is in many respects quite different from what it used to be only fifteen years ago. There have been dramatic changes in approaches for identifying new chemical entities with a desired biological activity. While chemical modification of existing leads was the most important approach in the 1970s and 1980s, high-throughput screening and structure-based design are now major players among a multitude of methods used in drug discov ery. Quite often, companies favor one of these relatively new approaches over the other, e.g., screening over rational design, or vice versa, but we believe that an intelligent and concerted use of several or all methods currently available to drug discovery will be more successful in the medium term. What has changed most significantly in the past few years is the time available for identifying new chemical entities. Because of the high costs of drug discovery projects, pressure for maximum success in the shortest possible time is higher than ever. In addition, the multidisciplinary character of the field is much more pronounced today than it used to be. As a consequence, researchers and project managers in the pharmaceutical industry should have a solid knowledge of the more important methods available to drug discovery, because it is the rapidly and intelligently combined use of these which will determine the success or failure of preclinical projects.

Computational Approaches in Cheminformatics and Bioinformatics - Rajarshi Guha 2011-11-30

A breakthrough guide employing knowledge that unites cheminformatics and bioinformatics as innovation for the future Bridging the gap between cheminformatics and bioinformatics for the first time, Computational Approaches in Cheminformatics and Bioinformatics provides insight on how to blend these two sciences for progressive research benefits. It describes the development and evolution of these fields, how chemical information may be used for biological relations and vice versa, the implications of these new connections, and foreseeable developments in the future. Using algorithms and domains as workflow tools, this revolutionary text drives bioinformaticians to consider chemical structure, and similarly, encourages cheminformaticians to consider large biological systems such as protein targets and networks. Computational Approaches in Cheminformatics and Bioinformatics covers: Data sources available for modelling and prediction purposes Developments of conventional Quantitative Structure-Activity Relationships (QSAR) Computational tools for manipulating chemical and biological data Novel ways of probing the interactions between small molecules and proteins Also including insight from public (NIH), academic, and industrial sources (Novartis, Pfizer), this book offers expert knowledge to aid scientists through industry and academic study. The invaluable applications for drug discovery, cellular and molecular biology, enzymology, and metabolism make Computational Approaches in Cheminformatics and Bioinformatics the essential guidebook for evolving drug discovery research and alleviating the issue of chemical control and manipulation of various systems.

Computation in BioInformatics - Anand T. Krishnan 2021-10-05

COMPUTATION IN BIOINFORMATICS Bioinformatics is a platform between the biology and information technology and this book provides readers with an understanding of the use of bioinformatics tools in new drug design. The discovery of new solutions to pandemics is facilitated through the use of promising bioinformatics techniques and integrated approaches. This book covers a broad spectrum of the bioinformatics field, starting with the basic principles, concepts, and application areas. Also covered is the role of bioinformatics in drug design and discovery, including aspects of molecular modeling. Some of the chapters provide detailed information on bioinformatics related topics, such as silicon design, protein modeling, DNA microarray analysis, DNA-RNA barcoding, and gene sequencing, all of which are currently needed in the industry. Also included are specialized topics, such as bioinformatics in cancer detection, genomics, and proteomics. Moreover, a few chapters explain highly advanced topics, like machine learning and covalent approaches to drug design and discovery, all of which are significant in pharma and biotech research and development. Audience Researchers and engineers in computation biology, information technology, bioinformatics, drug design, biotechnology, pharmaceutical sciences.

Computational Drug Discovery - Prof Mohammed 2015-09-05

This book has originated from Practical class on Genomics & Proteomics that are offered to students of Computational Biology, Bangalore University of Bangalore. The idea to write a book on Computational Biology was born during the preparations of these practical where I realized that it is extremely difficult to achieve an overview of the area of Drug Discovery and to follow the progress of this field. This is the first book in 2015 and was written in English .Computational Biology is a major topic in modern medical, Life science and pharmacological research and is of central importance in the computational biology science. Accordingly, The enormous increase in data on Drug Designing has led me to leave out the practical on Computational Biology and. This topic has since evolved into a huge research area of its own that could not be considered adequately within this book. My knowledge of Drug Designing practical has exploded in the past 5 years, Bioinformatics could be treated here with the same thoroughness. It is the aim of the present book to describe the Bioinformatics practical approach for life science students.

Essentials of Bioinformatics, Volume II - Noor Ahmad Shaik 2019-10-18

Bioinformatics is an integrative field of computer science, genetics, genomics, proteomics, and statistics, which has undoubtedly revolutionized the study of biology and medicine in past decades. It mainly assists in modeling, predicting and interpreting large multidimensional biological data by utilizing advanced computational methods. Despite its enormous potential, bioinformatics is not widely integrated into the academic curriculum as most life science students and researchers are still not equipped with the necessary knowledge to take advantage of this powerful tool. Hence, the primary purpose of our book is to supplement this unmet need by providing an easily accessible platform for students and researchers starting their career in life sciences. This book aims to avoid sophisticated computational algorithms and programming. Instead, it focuses on simple DIY analysis and interpretation of biological data with personal computers. Our belief is that once the beginners acquire these basic skillsets, they will be able to handle most of the bioinformatics tools for their research work and to better understand their experimental outcomes. Our second title of this volume set In Silico Life Sciences: Medicine provides hands-on experience in analyzing high throughput molecular data for the diagnosis, prognosis, and treatment of monogenic or polygenic human diseases. The key concepts in this volume include risk factor assessment, genetic tests and result interpretation, personalized medicine, and drug discovery. This volume is expected to train readers in both single and multi-dimensional biological analysis using open data sets, and provides a unique learning experience through clinical scenarios and case studies.

Advances in Bioinformatics - Vijai Singh 2021-07-31

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.

Computational Drug Discovery and Design - Umesh B. Jagtap 2018

Computational Approaches - Anna Maria Almerico 2022-01-03

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.

Bioinformatics and Drug Discovery - Richard S. Larson 2010-12-09

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.

Clustering in Bioinformatics and Drug Discovery - JOHN DAVID. MACCUISH MACCUISH (NORAH E.) 2019-07-02

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 first three chapters of the book introduce statistical learning theory, exploratory data analysis, clustering algorithms, different types of data, graph theory, and various clustering forms. In the following chapters on partitional, cluster sampling, and hierarchical algorithms, the book provides readers with enough detail to obtain a basic understanding of cluster analysis for bioinformatics and drug discovery. The remaining chapters cover more advanced methods, such as hybrid and parallel algorithms, as well as details related to specific types of data, including asymmetry, ambiguity, validation measures, and visualization. This book explores the application of cluster analysis in the areas of bioinformatics and cheminformatics as they relate to drug discovery. Clarifying the use and misuse of clustering methods, it helps readers understand the relative merits of these methods and evaluate results so that useful hypotheses can be developed and tested.

Big Data Analytics in Chemoinformatics and Bioinformatics - Subhash C. Basak 2022-12-09

Big Data Analytics in Chemoinformatics and Bioinformatics: With Applications to Computer-Aided Drug Design, Cancer Biology, Emerging Pathogens and Computational Toxicology provides an up-to-date presentation of big data analytics methods and their applications in diverse fields. The proper management of big data for decision-making in scientific and social issues is of paramount importance. This book gives researchers the tools they need to solve big data problems in these fields. It begins with a section on general topics that all readers will find useful and continues with specific sections covering a range of interdisciplinary applications. Here, an international team of leading experts review their respective fields and present their latest research findings, with case studies used throughout to analyze and present key information. Brings together the current knowledge on the most important aspects of big data, including analysis using deep learning and fuzzy logic, transparency and data protection, disparate data analytics, and scalability of the big data domain Covers many applications of big data analysis in diverse fields such as chemistry, chemoinformatics, bioinformatics, computer-assisted drug/vaccine design, characterization of emerging pathogens, and environmental protection Highlights the considerable benefits offered by big data analytics to science, in biomedical fields and in industry

Understanding and Exploiting Bioinformatics for Drug Discovery and Development - Paolo Zanella 1997

The Bioinformatic Age - Pamela Bassett 2001-04-01

Bioinformatics Methods And Applications: Genomics Proteomics And Drug Discovery 3Rd Ed. - S. C. Rastogi 2008

Quick Guideline for Computational Drug Design (Revised Edition) - Sheikh Arslan Sehgal 2021-09-16

Bioinformatics allows researchers to answer biological questions with advanced computational methods which involves the application of statistics and mathematical modeling. Structural bioinformatics enables the prediction and analysis of 3D structures of macromolecules while Computer Aided Drug Designing (CADD) assists scientists to design effective active molecules against diseases. However, the concepts in structural bioinformatics and CADD can be complex to understand for students and educated laymen. This quick guideline is intended as a basic manual for beginner students and instructors involved in bioinformatics and computational chemistry courses. Readers will learn the basics of structural bioinformatics, primary and secondary analysis and prediction, structural visualization, structural analysis and molecular docking. The book provides the reader an easy to read summary of the tools and techniques in structural bioinformatics as well as their limitations. In this revised edition, the authors have updated information in a number of chapters with a specific focus on the section on protein structure visualization and evaluation. Additional information on protein-ligand interaction studies has also been provided in this new edition. Therefore, the book is a useful handbook for aspiring scholars who wish to learn the basic concepts in computational analysis of biomolecules.

Bioinformatics - Thomas Lengauer 2002

V.1: Basic technologies: From Genomes to drugs with bioinformatics (Thomas Lengauer); Sequence analysis (Martin Vingron); Structure, properties and computer identification of eukaryotic genes (Victor Solovyev). Analyzing regulatory regions in genomes (Thomas Werner). Homology modeling in biology and medicine (Roland L. Dunbrack, Jr.). Protein structure prediction (Ralf Zimmer and Thomas Lengauer). Protein-ligand docking in drug design (Matthias Rarey). Modellimg protein-protein and protein-DNA docking (Michael J. E. Sternberg and Gidon Moont). v.2: Applications: Integrating and accessing molecular biology resources (David P. Hansen and Thure Etzold). Bioinformatics support of genome sequencing projects (Xiaoqiu Huang). Analysis of sequence variations (Christopher S. Carlson, Mark J. Rieder and Deborah A. Nickerson). Proteome analysis (Pierre-Alain Binz, Elisabeth Gasteiger, Jean-Charles Sanchez, Amos Bairoch, Denis F. Hochstrasser, Ron D. Appel). Target finding in genomes and proteomes (Stephanie Fuhrman Liang, Xiling Wen and Roland Somogyi). Screening of drug databases (Martin Stahl, Matthias Rarey and Gerhard Klebe). Future trends (Thomas Lengauer).