Bioinformatics And Drug Discovery

Covering topics from individual molecules to systemic diseases, from basic concepts to advanced technologies, Pharmacogenomics in Drug Discovery and Development , Second Edition provides a practical, state-of-the-art and integrative view of the application of pharmacogenomics in drug discovery and development. A wide range of theoretical and experimental approaches are introduced to meet the problem-solving objectives for understanding the complexity in health and diseases, from laboratory tests to computational analysis. The development of pharmacogenomics represents the evolution of biomedicine from treating the disease itself to treating the malfunction of an individual person, the “root” of diseases. With the change of focus from disease-centered to human-centric medicine, pharmacogenomics brings hope for the transformation from simple disease treatment to accurate prediction and effective prevention. Written in the successful Methods in Molecular Biology series format, chapters include introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible protocols, and notes on troubleshooting and avoiding known pitfalls. Authoritative and easily accessible, Pharmacogenomics in Drug Discovery and Development, Second Edition seeks to serve both professionals and novices with comprehensive resources and a holistic view for the translation of pharmacogenomics into better preventive and personalized medical care.

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 in Healthcare and Medicine offers an overview of main principles of bioinformatics, biological databases, clinical informatics, health informatics, viroinformatics and real-case applications of translational bioinformatics in healthcare. Written by experts from both technology and clinical sides, the content brings together essential knowledge to make the best of recent advancements of the field. The book discusses topics such as next generation sequence analysis, genomics in clinical care, IoT applications, blockchain technology, patient centered interoperability of EHR, health data mining, and translational bioinformatics methods for drug discovery and drug repurposing. In addition, it discusses the role of bioinformatics in cancer research and viroinformatics approaches to counter viral diseases through informatics. This is a valuable resource for bioinformaticians, clinicians, healthcare professionals, graduate students and several members of biomedical field who are interested in learning more about how bioinformatics can impact in their research and practice. Covers recent advancements in translational bioinformatics and its healthcare applications Discusses integrative and multidisciplinary approaches to U-healthcare systems development and management Bridges the gap among various knowledge domains in the field, integrating both technological and clinical knowledge into practical content

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.

Cheminformatics has emerged as an applied branch of Chemistry that involves multidisciplinary knowledge, connecting related fields such as chemistry, computer science, biology, pharmacology, physics, and mathematical statistics.The book is organized in two sections, including multiple aspects related to advances in the development of informatic tools and their specific use in compound structure databases with various applications in life sciences, mainly in medicinal chemistry, for identification and development of new therapeutically active molecules. The book covers aspects related to genomic analysis, semantic similarity, chemometrics, pattern recognition techniques, chemical reactivity prediction, drug-likeness assessment, bioavailability, biological target recognition, machine-based drug discovery and design. Results from various computational tools and methods are discussed in the context of new compound design and development, sharing promising opportunities, and perspectives.

Bioinformatics and Drug DiscoveryHumana Press

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. Bioinformatics can be loosely defined as the collection, classification, storage, and analysis of biochemical and biological information using computers and mathematical algorithms. Bioinformatics represents a marriage of biology, medicine, computer science, physics, and mathematics, fields of study that have historically existed as mutually exclusive disciplines. Edited by Gavin Gordon, Bioinformatics in Cancer and Cancer Therapy, the focus of this book is to provide a historical and technical perspective on the analytical techniques, methodologies, and platforms used in bioinformatics experiments, to show how a bioinformatics approach has been used to characterize various cancer-related processes, and to demonstrate how a bioinformatics approach is being used to bridge basic science and the clinical arena to positively impact patient care and management.

Demystifies Biomedical and Biological Big Data Analyses Big Data Analysis for Bioinformatics and Biomedical Discoveries provides a practical guide to the nuts and bolts of Big Data, enabling you to quickly and effectively harness the power of Big Data to make groundbreaking biological discoveries, carry out translational medical research, and implement personalized genomic medicine. Contributing to the NIH Big Data to Knowledge (BD2K) initiative, the book enhances your computational and quantitative skills so that you can exploit the Big Data being generated in the current omics era. The book explores many significant topics of Big Data analyses in an easily understandable format. It describes popular tools and software for Big Data analyses and explains next-generation DNA sequencing data analyses. It also discusses comprehensive Big Data analyses of several major areas, including the integration of omics data, pharmacogenomics, electronic health record data, and drug discovery. Accessible to biologists, biomedical scientists, bioinformaticians, and computer data analysts, the book keeps complex mathematical deductions and jargon to a minimum. Each chapter includes a theoretical introduction, example applications, data analysis principles, step-by-step tutorials, and authoritative references.

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

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.

This collection of 25 research papers comprised of 22 original articles and 3 reviews is brought together from international leaders in bioinformatics and biostatistics. The collection highlights recent computational advances that improve the ability to analyze highly complex data sets to identify factors critical to cancer biology. Novel deep learning algorithms represent an emerging and highly valuable approach for collecting, characterizing and predicting clinical outcomes data. The collection highlights several of these approaches that are likely to become the foundation of research and clinical practice in the future. In fact, many of these technologies reveal new insights about basic cancer mechanisms by integrating data sets and structures that were previously immiscible. Accordingly, the series presented here bring forward a wide range of artificial intelligence approaches and statistical methods that can be applied to imaging and genomics data sets to identify previously unrecognized features that are critical for cancer. Our hope is that these articles will serve as a foundation for future research as the field of cancer biology transitions to integrating electronic health record, imaging, genomics and other complex datasets in order to develop new strategies that improve the overall health of individual patients.

This book offers a unique balance between a basic introductory knowledge of bioinformatics and a detailed study of algorithmic techniques. Bioinformatics and RNA: A Practice-Based Approach is a complete guide on the fundamental concepts, applications, algorithms, protocols, new trends, challenges, and research results in the area of bioinformatics and RNA. The book offers a broad introduction to the explosively growing new discipline of bioinformatics. It covers theoretical topics along with computational algorithms. It explores RNA bioinformatics, which contribute to therapeutics and drug discovery. Implementation of algorithms in a DotNet Framework with code and complete insight on the state-of-the-art and recent advancements are presented in detail. The book targets both novice readers as well as practitioners in the field. FEATURES Offers a broad introduction to the explosively growing new discipline of bioinformatics Covers theoretical topics and computational algorithms Explores RNA bioinformatics to unleash the potential from therapeutics to drug discovery Discusses implementation of algorithms in DotNet Frameworks with code Presents insights into the state of the art and recent advancements in bioinformatics The book is useful to undergraduate students with engineering, science, mathematics, or biology backgrounds. Researchers will be equally interested.

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.

In the fiercely competitive pharmaceutical marketplace, your organization cannot afford to spend excess dollars developing drugs that will fail to get FDA approval or have profoundly poor characteristics. Biochips as Pathways to Drug Discovery takes a comprehensive look at how the industry faces these challenges, using new technologies such as biochips to reduce the cost of drug discovery and improve drug safety. The book explores the tools and skills required at each step of the discovery process when using biochips to determine biological outcomes. The authors provide an in-depth review of the clinical and pharmacogenomic relevance of biochips, ChIP-chip assays, and high-throughput approaches. They discuss how biochips are used to develop biomarkers in the drug discovery process, primarily for gene expression profiling and Single Nucleotide Polymorphism (SNP) analysis. The book includes coverage of experimental theory, quality control, clinical laboratory sampling considerations, database concepts, industrial laboratory design, and the analysis of the resultant large data sets. It discusses the application of biochips to the study of malaria, toxicogenomics, and SNPs, as well as intellectual property and market overviews. The book concludes with a comprehensive overview of how these chips are employed from early target discovery through preclinical toxicology and on through to pharmacogenomic and proof of concept studies in humans. Written in an easily accessible style, the breadth of coverage introduces the subject to those new to the field, while the depth of coverage forms a foundation for future work. The book gives you the knowledge required to leverage the technology into bona fide discoveries. Daniel E. Levy, editor of the Drug Discovery Series, is the founder of DEL BioPharma, a consulting service for drug discovery programs. He also maintains a blog that explores organic chemistry.

A comprehensive overview of the use of computational biology approaches in the drug discovery and development process.

Chemoinformatics is broadly a scientific discipline encompassing the design, creation, organization, management, retrieval, analysis, dissemination, visualization and use of chemical information. It is distinct from other computational molecular modeling approaches in that it uses unique representations of chemical structures in the form of multiple chemical descriptors; has its own metrics for defining similarity and diversity of chemical compound libraries; and applies a wide array of statistical, data mining and machine learning techniques to very large collections of chemical compounds in order to establish robust relationships between chemical structure and its physical or biological properties. Chemoinformatics addresses a broad range of problems in chemistry and biology; however, the most commonly known applications of chemoinformatics approaches have been arguably in the area of drug discovery where chemoinformatics tools have played a central role in the analysis and interpretation of structure-property data collected by the means of modern high throughput screening. Early stages in modern drug discovery often involved screening small molecules for their effects on a selected protein target or a model of a biological pathway. In the past fifteen years, innovative technologies that enable rapid synthesis and high throughput screening of large libraries of compounds have been adopted in almost all major pharmaceutical and biotech companies. As a result, there has been a huge increase in the number of compounds available on a routine basis to quickly screen for novel drug candidates against new targets/pathways. In contrast, such technologies have rarely become available to the academic research community, thus limiting its ability to conduct large scale chemical genetics or chemical genomics research. However, the landscape of publicly available experimental data collection methods for chemoinformatics has changed dramatically in very recent years. The term "virtual screening" is commonly associated with methodologies that rely on the explicit knowledge of three-dimensional structure of the target protein to identify potential bioactive compounds. Traditional docking protocols and scoring functions rely on explicitly defined three dimensional coordinates and standard definitions of atom types of both receptors and ligands. Albeit reasonably accurate in many cases, conventional structure based virtual screening approaches are relatively computationally inefficient, which has precluded them from screening really large compound collections. Significant progress has been achieved over many years of research in developing many structure based virtual screening approaches. This book is the first monograph that summarizes innovative applications of efficient chemoinformatics approaches towards the goal of screening large chemical libraries. The focus on virtual screening expands chemoinformatics beyond its traditional boundaries as a synthetic and data-analytical area of research towards its recognition as a predictive and decision support scientific discipline. The approaches discussed by the contributors to the monograph rely on chemoinformatics concepts such as: -representation of molecules using multiple descriptors of chemical structures -advanced chemical similarity calculations in multidimensional descriptor spaces -the use of advanced machine learning and data mining approaches for building quantitative and predictive structure activity models -the use of chemoinformatics methodologies for the analysis of drug-likeness and property prediction -the emerging trend on combining chemoinformatics and bioinformatics concepts in structure based drug discovery The chapters of the book are organized in a logical flow that a typical chemoinformatics project would follow - from structure representation and comparison to data analysis and model building to applications of structure-property relationship models for hit identification and chemical library design. It opens with the overview of modern methods of compounds library design, followed by a chapter devoted to molecular similarity analysis. Four sections describe virtual screening based on the using of molecular fragments, 2D pharmacophores and 3D pharmacophores. Application of fuzzy pharmacophores for libraries design is the subject of the next chapter followed by a chapter dealing with QSAR studies based on local molecular parameters. Probabilistic approaches based on 2D descriptors in assessment of biological activities are also described with an overview of the modern methods and software for ADME prediction. The book ends with a chapter describing the new approach of coding the receptor binding sites and their respective ligands in multidimensional chemical descriptor space that affords an interesting and efficient alternative to traditional docking and screening techniques. Ligand-based approaches, which are in the focus of this work, are more computationally efficient compared to structure-based virtual screening and there are very few books related to modern developments in this field. The focus on extending the experiences accumulated in traditional areas of chemoinformatics research such as Quantitative Structure Activity Relationships (QSAR) or chemical similarity searching towards virtual screening make the theme of this monograph essential reading for researchers in

the area of computer-aided drug discovery. However, due to its generic data-analytical focus there will be a growing application of chemoinformatics approaches in multiple areas of chemical and biological research such as synthesis planning, nanotechnology, proteomics, physical and analytical chemistry and chemical genomics.

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.

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

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.

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.

Designed as a text for students and professionals pursuing careers in the fields of molecular biology, pharmacy and bioinformatics, the fourth edition continues to offer a fascinating and authoritative treatment of the entire spectrum of bioinformatics, covering a wide range of high-throughput technologies. In this edition, four new chapters are included and two chapters are updated. As a student-friendly text, it embodies several pedagogic features such as detailed examples, chapter-end problems, numerous tables, a large number of diagrams, flow charts, a comprehensive glossary and an up-to-date bibliography. This book should prove an invaluable asset to students and researchers in the fields of bioinformatics, biotechnology, computer-aided drug design, information technology, medical diagnostics, molecular biology and pharmaceutical industry. NEW TO THE FOURTH EDITION: • Includes four new chapters—Introduction to Biological Databases, Introduction to Phylogenetic, Methods of Phylogenic analysis and RNA Predict. • Updates chapters on Information Search and Data Retrieval and Alignment of Multiple Sequences. • Incorporates Problem Sets containing more than 250 problems and Multiple Choice Questions so that students can test their knowledge and understanding. Key Features • State-of-the-art technologies for gene identification, molecular modeling and monitoring of cellular processes • Data mining, analysis, classification, interpretation and efficient structure determination of genomes and proteomes • Importance of cell cycle for discovering new drug targets and their ligands • Computer-aided drug design and ADME-Tox property prediction Companion website www.phindia.com/rastogi provides useful resources for the teachers as well as for the students.

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.

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

Shows how different parts of the drug discovery process have developed, with particular emphasis on quantitative aspects and possible future progress.

The modern pharmacopeia has enormous power to alleviate disease, and owes its existence almost entirely to the work of the pharmaceutical industry. This book provides an introduction to the way the industry goes about the discovery and development of new drugs. The first part gives a brief historical account from its origins in the mediaeval apothecaries' trade, and discusses the changing understanding of what we mean by disease, and what therapy aims to achieve, as well as summarising case histories of the discovery and development of some important drugs. The second part focuses on the science and technology involved in the discovery process: the stages by which a promising new chemical entity is identified, from the starting point of a medical need and an idea for addressing it. A chapter on biopharmaceuticals, whose discovery and development tend to follow routes somewhat different from synthetic compounds, is included here, as well as accounts of patent issues that arise in the discovery phase, and a chapter on research management in this environment. The third section of the book deals with drug development: the work that has to be undertaken to turn the drug candidate that emerges from the discovery process into a product on the market. The definitive introduction to how a pharmaceutical company goes about its business of discovering and developing drugs. The second edition has a new editor: Professor Raymond Hill ? non-executive director of Addex Pharmaceuticals, Covagen and of Orexo AB ? Visiting Industrial Professor of Pharmacology in the University of Bristol ? Visiting Professor in the School of Medical and Health Sciences at the University of Surrey ? Visiting Professor in Physiology and Pharmacology at the University of Strathclyde ? President and Chair of the Council of the British Pharmacological Society ? member of the Nuffield Council on Bioethics and the Advisory Council on Misuse of Drugs. New to this edition: Completely rewritten chapter on The Role of Medicinal Chemistry in the Drug Discovery Process. New topic - DMPK Optimization Strategy in drug discovery. New chapter on Scaffolds: Small globular proteins as antibody substitutes. Totally updated chapters on Intellectual Property and Marketing 50 new illustrations in full colour Features Accessible, general guide to pharmaceutical research and development. Examines the interfaces between cost and social benefit, quality control and mass production, regulatory bodies, patent management, and all interdisciplinary intersections essential to effective drug development. Written by a strong team of scientists with long experience in the pharmaceutical industry. Solid overview of all the steps from lab bench to market in an easy-to-understand way which will be accessible to non-specialists. From customer reviews of the previous edition: '... it will have everything you need to know on this module. Deeply referenced and, thus, deeply reliable. Highly Commended in the medicine category of the BMA 2006 medical book competition Winner of the Royal Society of Medicine Library Prize for Medical Book of the Year

The approaches in drug design are mainly comprised of these three multidisciplinary sciences. First, Bioinformatics has successfully gather biological data in form of biomolecular sequences, in order to construct knowledge on drug and vaccine design. It is of considerable importance for drug designers to comprehend the utilization of bioinformatics tools for resolving their research questions. Second, Nanotechnology has made possible the design and delivery of the nano-based drug. Third, Pharmaceutical Chemistry made it possible to investigate the adsorption, distribution, metabolism, and toxicology of the drug candidates in a fine-grained resolution.

In today's data driven biology, programming knowledge is essential in turning ideas into testable hypothesis. Based on the author's extensive experience, Python for Bioinformatics, Second Edition helps biologists get to grips with the basics of software development. Requiring no prior knowledge of programming-related concepts, the book focuses on the easy-to-use, yet powerful, Python computer language. This new edition is updated throughout to Python 3 and is designed not just to help scientists master the basics, but to do more in less time and in a reproducible way. New developments added in this edition include NoSQL databases, the Anaconda Python distribution, graphical libraries like Bokeh, and the use of Github for collaborative development.

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.

In Silico Drug Design: Repurposing Techniques and Methodologies explores the application of computational tools that can be utilized for this approach. The book covers theoretical background and methodologies of chem-bioinformatic techniques and network modeling and discusses the various applied strategies to systematically retrieve, integrate and analyze datasets from diverse sources. Other topics include in silico drug design methods, computational workflows for drug repurposing, and network-based in silico screening for drug efficacy. With contributions from experts in the field and the inclusion of practical case studies, this book gives scientists, researchers and R&D professionals in the pharmaceutical industry valuable insights into drug design. Discusses the theoretical background and methodologies of useful techniques of cheminformatics and bioinformatics that can be applied for drug repurposing Offers case studies relating to the in silico modeling of FDA-approved drugs for the discovery of antifungal, anticancer, antiplatelet agents, and for drug therapies against diseases Covers tools and databases that can be utilized to facilitate in silico methods for drug repurposing

Translational Biotechnology: A Journey from Laboratory to Clinics presents an integrative and multidisciplinary approach to biotechnology to help readers bridge the gaps between fundamental and functional research. The book provides state-of-the-art and integrative views of translational biotechnology by covering topics from basic concepts to novel methodologies. Topics discussed include biotechnology-based therapeutics, pathway and target discovery, biological therapeutic modalities, translational bioinformatics, and system and synthetic biology. Additional sections cover drug discovery, precision medicine and the socioeconomic impact of translational biotechnology. This book is valuable for bioinformaticians, biotechnologists, and members of the biomedical field who are interested in learning more about this promising field. Explains biotechnology in a different light by using an application-oriented approach Discusses practical approaches in the development of precision medicine tools, systems and dynamical medicine approaches Promotes research in the field of biotechnology that is translational in nature, cost-effective and readily available to the community

Following significant advances in deep learning and related areas interest in artificial intelligence (AI) has rapidly grown. In particular, the application of AI in drug discovery provides an opportunity to tackle challenges that previously have been difficult to solve, such as predicting properties, designing molecules and optimising synthetic routes. Artificial Intelligence in Drug Discovery aims to introduce the reader to AI and machine learning tools and techniques, and to outline specific challenges including designing new molecular structures, synthesis planning and simulation. Providing a wealth of information from leading experts in the field this book is ideal for students, postgraduates and established researchers in both industry and academia.

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.

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

Molecular Advancements in Tropical Diseases Drug Discovery presents in-depth knowledge relating to the detection of infection, epidemiology, drugs against various tropical diseases, new target sites for drug discovery and multidrug resistance issues using bioinformatics tools and approaches. The book's chapters are written by experts in their respective fields so that each disease is covered in a rational manner and with a solid foundation on existing facts and prospective research ideas. Updates knowledge about tropical diseases with recent advancements in the field Presents an overview of new research covering detection, infection, epidemiology and risk factors of the most common tropical diseases using bioinformatics tools Encompasses a detailed description of developments in drug discovery, new drugs and their molecular mechanisms of action

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.

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