Computational Approaches In Cheminformatics And Bioinformatics

Computational Approaches in Cheminformatics and Bioinformatics Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences Cheminformatics and Bioinformatics at the Interface with Systems Biology Cheminformatics and its Applications *Handbook of Chemoinformatics Algorithms* Advances in Bioinformatics Chemoinformatics Approaches to Virtual Screening *Big Data Analytics in Chemoinformatics and Bioinformatics* Encyclopedia of Bioinformatics and Computational Biology Chemoinformatics Bioinformatics and Drug Discovery Practical Chemoinformatics Chemoinformatics and Advanced Machine Learning Perspectives: Complex Computational Methods and Collaborative Techniques Tutorials in Chemoinformatics *Clustering in Bioinformatics and Drug Discovery* Chemoinformatics and Computational Chemical Biology *Molecular Informatics: Confronting Complexity* Computational Drug Design Machine Learning in Bioinformatics Translational Bioinformatics in Healthcare and Medicine *An Introduction to Chemoinformatics* Bioinformatics and Drug Discovery Advanced AI Techniques and Applications in Bioinformatics Chemoinformatics Handbook of Data Structures and Applications *Handbook of Chemoinformatics Algorithms* Alternative Toxicological Methods In Silico Drug Design Emerging Trends in Computational Biology, Bioinformatics, and Systems Biology Handbook of Chemoinformatics Computational Approaches Agriculture Bioinformatics Applied Chemoinformatics Chemoinformatics in Drug Discovery MacHine-Learning Based Sequence Analysis, Bioinformatics and Nanopore Transduction Detection *Chemometrics and Chemoinformatics* Dictionary of Natural Products *Structural Bioinformatics: Applications in Preclinical Drug Discovery Process* Bioinformatics--from Genomes to Drugs: Applications

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Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences Sep 27 2022 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

Practical Chemoinformatics Oct 16 2021 Chemoinformatics is equipped to impact our life in a big way mainly in the fields of chemical, medical and material sciences. This book is a product of several years of experience and passion for the subject written in a simple lucid style to attract the interest of the student community who wish to master chemoinformatics as a career. The topics chosen cover the entire spectrum of chemoinformatics activities (methods, data and tools). The algorithms, open source databases, tutorials supporting theory using standard datasets, guidelines, questions and do it yourself exercises will make it valuable to the academic research community. At the same time every chapter devotes a section on development of new software tools relevant for the growing pharmaceutical, fine chemicals and life sciences industry. The book is intended to assist beginners to hone their skills and also constitute an interesting reading for the experts.

Tutorials in Chemoinformatics Aug 14 2021 30 tutorials and more than 100 exercises in chemoinformatics, supported by online software and data sets Chemoinformatics is widely used in both academic and industrial chemical and biochemical research worldwide. Yet, until this unique guide, there were no books offering practical exercises in chemoinformatics methods. Tutorials in Chemoinformatics contains more than 100 exercises in 30 tutorials exploring key topics and methods in the field. It takes an applied approach to the subject with a strong emphasis on problem-solving and computational methodologies. Each tutorial is self-contained and contains exercises for students to work through using a variety of software packages. The majority of the tutorials are divided into three sections devoted to theoretical background, algorithm description and software applications, respectively, with the latter section providing step-by-step software instructions. Throughout, three types of software tools are used: in-house programs developed by the authors, open-source programs and commercial programs which are available for free or at a modest cost to academics. The in-house software and data sets are available on a dedicated companion website. Key topics and methods covered in Tutorials in Chemoinformatics include: Data curation and standardization Development and use of chemical databases Structure encoding by molecular descriptors, text strings and binary fingerprints The design of diverse and focused libraries Chemical data analysis and visualization Structure-property/activity modeling (QSAR/QSPR) Ensemble modeling approaches, including bagging, boosting, stacking and random subspaces 3D pharmacophores modeling and pharmacological profiling using shape analysis Protein-ligand docking Implementation of algorithms in a high-level programming language Tutorials in Chemoinformatics is an ideal supplementary text for advanced undergraduate and graduate courses in chemoinformatics, bioinformatics, computational chemistry, computational biology, medicinal chemistry and biochemistry. It is also a valuable working resource for medicinal chemists, academic researchers and industrial chemists looking to enhance their chemoinformatics skills.

MacHine-Learning Based Sequence Analysis, Bioinformatics and Nanopore Transduction Detection Oct 24 2019 This is intended to be a simple and accessible book on machine learning methods and their application in computational genomics and nanopore transduction detection. This book has arisen from eight years of teaching one-semester courses on various machine-learning, cheminformatics, and bioinformatics topics. The book begins with a description of ad hoc signal acquisition methods and how to orient on signal processing problems with the standard tools from information theory and signal analysis. A general stochastic sequential analysis (SSA) signal processing architecture is then described that implements Hidden Markov Model (HMM) methods. Methods are then shown for classification and clustering using generalized Support Vector Machines, for use with the SSA Protocol, or independent of that approach. Optimization metaheuristics are used for tuning over algorithmic parameters throughout. Hardware implementations and short code examples of the various methods are also described.

Bioinformatics and Drug Discovery Dec 06 2020 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.

Chemoinformatics and Advanced Machine Learning Perspectives: Complex Computational Methods and Collaborative Techniques Sep 15 2021 "This book is a timely compendium of key elements that are crucial for the study of machine learning in chemoinformatics, giving an overview of current research in machine learning and their applications to chemoinformatics tasks"--Provided by publisher.

Alternative Toxicological Methods Jul 01 2020 Bringing together the recent and relevant contributions of over 125 scientists from industry, government, and academia in North America and Western Europe, Alternative Toxicological Methods explores the development and validation of replacement, reduction, and refinement alternatives (the 3Rs) to animal testing. Internationally recognized scientist

Molecular Informatics: Confronting Complexity May 11 2021 The Beilstein Institute organizes and sponsors scientific meetings, workshops and seminars, with the aim of catalysing advances in chemical science by facilitating the interdisciplinary exchange and communication of ideas amongst the participants. This workshop " Molecular Informatics: Confronting Complexity" addressed some of the new challenges that face scientists in the post-genome era, in particular, the integration of two, until recently, disparate sciences - chemistry and biology. The underlying theme of the workshop was to gain insight into the behaviour of biological and molecular systems through the application of molecular informatics. The flood of data being generated as a result of research into genomics and proteomics is often overwhelming. Well publicised successes tend to draw the focus away from some of the significant issues relating to a better understanding of molecular systems which are still far from clear. Whereas the development of predictive models based on analogy has been very successful in chemistry and cheminformatics, the non-linear nature of biomolecular systems, often with multiple pathways, restricts similar transference within bioinformatics. However, without a critical analysis, taking into account the assumptions and limitations of hypotheses and predictive models, advances in molecular informatics will not assume significance. Before this can be effectively carried out, more effort needs to be made in bridging the gap between chemists, dealing with the structure and properties of molecules, and biologists, working with complex molecular and cell physiological systems. Participants, as well as, speakers were confronted with the following complex challenges from cheminformatics and bioinformatics: knowledge discovery and data mining, rational drug design, prediction of small molecule bioavailability (ADME Tox) properties, protein structure and function determination, new methods of drug-target modelling, cellular metabolism and metabolic pathways, and the use of high-throughput methods (biochips, x-ray crystallography) for acquiring gene expression and protein structure, as well as, binding information.

Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences Aug 26 2022 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

Handbook of Data Structures and Applications Sep 03 2020 The Handbook of Data Structures and Applications was first published over a decade ago. This second edition aims to update the first by focusing on areas of research in data structures that have seen significant progress. While the discipline of data structures has not matured as rapidly as other areas of computer science, the book aims to update those areas that have seen advances. Retaining the seven-part structure of the first edition, the handbook begins with a review of introductory material, followed by a discussion of well-known classes of data structures, Priority Queues, Dictionary Structures, and Multidimensional structures. The editors next analyze miscellaneous data structures, which are well-known structures that elude easy classification. The book then addresses mechanisms and tools that were developed to facilitate the use of data structures in real programs. It concludes with an examination of the applications of data structures. Four new chapters have been added on Bloom Filters, Binary Decision Diagrams, Data Structures for Cheminformatics, and Data Structures for Big Data Stores, and updates have been made to other chapters that appeared in the first edition. The Handbook is invaluable for suggesting new ideas for research in data structures, and for revealing application contexts in which they can be deployed. Practitioners devising algorithms will gain insight into organizing data, allowing them to solve algorithmic problems more efficiently.

Chemoinformatics Dec 18 2021 This essential guide to the knowledge and tools in the field includes everything from the basic concepts to modern methods, while also forming a bridge to bioinformatics. The textbook offers a very clear and didactical structure, starting from the basics and the theory, before going on to provide an overview of the methods. Learning is now even easier thanks to exercises at the end of each section or chapter. Software tools are explained in detail, so that the students not only learn the necessary theoretical background, but also how to use the different software packages available. The wide range of applications is presented in the corresponding book Applied Chemoinformatics - Achievements and Future Opportunities (ISBN 9783527342013). For Master and PhD students in chemistry,

biochemistry and computer science, as well as providing an excellent introduction for other newcomers to the field.

Computational Drug Design Apr 10 2021 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.

Handbook of Chemoinformatics Algorithms Aug 02 2020 Unlike in the related area of bioinformatics, few books currently exist that document the techniques, tools, and algorithms of chemoinformatics. Bringing together worldwide experts in the field, the Handbook of Chemoinformatics Algorithms provides an overview of the most common chemoinformatics algorithms in a single source. After a historical perspective of the applications of algorithms and graph theory to chemical problems, the book presents algorithms for two-dimensional chemical structures and three-dimensional representations of molecules. It then focuses on molecular descriptors, virtual screening methods, and quantitative structure–activity relationship (QSAR) models, before introducing algorithms to enumerate and sample chemical structures. The book also covers computer-aided molecular design, reaction network generation, and open source software and database technologies. The remaining chapters describe techniques developed in the context of bioinformatics and computational biology and their potential applications to chemical problems. This handbook presents a selection of algorithms relevant in practice, making the book useful to those working in the field. It offers an up-to-date account of many algorithmic aspects of chemoinformatics.

Translational Bioinformatics in Healthcare and Medicine Feb 08 2021 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

Computational Approaches in Cheminformatics and Bioinformatics Oct 28 2022 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.

Structural Bioinformatics: Applications in Preclinical Drug Discovery Process Jul 21 2019 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.

Handbook of Chemoinformatics Mar 29 2020 "The new discipline of chemoinformatics covers the application of computer-assisted methods to chemical problems such as information storage and retrieval, the prediction of physical, chemical or biological properties of compounds, spectra simulation, structure elucidation, reaction modeling, synthesis planning and drug design. ... this four-volume Handbook contains in-depth contributions from top authors from around the world, with the content organized into chapters dealing with the representation of molecular structures and reactions, data types and databases/data sources, search methods, methods for data analysis as well as applications"--Back cover.

Big Data Analytics in Chemoinformatics and Bioinformatics Feb 20 2022 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

Advanced AI Techniques and Applications in Bioinformatics Nov 05 2020 The advanced AI techniques are essential for resolving various problematic aspects emerging in the field of bioinformatics. This book covers the recent approaches in artificial intelligence and machine learning methods and their applications in Genome and Gene editing, cancer drug discovery classification, and the protein folding algorithms among others. Deep learning, which is widely used in image processing, is also applicable in bioinformatics as one of the most popular artificial intelligence approaches. The wide range of applications discussed in this book are an indispensable resource for computer scientists, engineers, biologists, mathematicians, physicians, and medical informaticists. Features: Focusses on the cross-disciplinary relation between computer science and biology and the role of machine learning methods in resolving complex problems in bioinformatics Provides a comprehensive and balanced blend of topics and applications using various advanced algorithms Presents cutting-edge research methodologies in the area of AI methods when applied to bioinformatics and innovative solutions Discusses the AI/ML techniques, their use, and their potential for use in common and future bioinformatics applications Includes recent achievements in AI and bioinformatics contributed by a global team of researchers

Agriculture Bioinformatics Jan 27 2020 Biotechnological tools supplement various conventional approaches in conservation, characterization and utilization for increasing production and productivity of agricultural and horticultural crops. The emerging field of bioinformatics is an integrated field arising from merging of biology and informatics. It is a conglomeration of various new frontiers of science like genomics, proteomics, metabolomics etc. The rich warehouse of proteome and genome information nearly doubling every year has significant implications and applications in various areas of science including agriculture, horticulture, forestry and food science. Cheminformatics is specialized to a range of problems in the field of chemistry. Chemical pesticide reduction is possible by adopting cheminformatics methods to identify naturally occurring chemical compounds in crops which act against pests. Bioinformatics has transformed the discipline of life science from a purely lab based science to an information science as well. The ICAR has recently launched a National Agricultural Bioinformatics Grid (NABG) to serve as a computational facility in developing national biodatabases and data warehouses. The present book Agriculture Bioinformatics is a compilation of 17 information packed s authored by working scientists in the respective discipline. In addition to the theoretical information, practical and applied aspects to boost productivity and quality of crops are given.

Clustering in Bioinformatics and Drug Discovery Jul 13 2021 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 Nov 17 2021 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.

Emerging Trends in Computational Biology, Bioinformatics, and Systems Biology Apr 29 2020 Emerging Trends in Computational Biology, Bioinformatics, and Systems Biology discusses the latest developments in all aspects of computational biology, bioinformatics, and systems biology and the application of data-analytics and algorithms, mathematical modeling, and simu- lation techniques. • Discusses the development and application of data-analytical and theoretical methods, mathematical modeling, and computational simulation techniques to the study of biological and behavioral systems, including applications in cancer research, computational intelligence and drug design, high-performance computing, and biology, as well as cloud and grid computing for the storage and access of big data sets. • Presents a systematic approach for storing, retrieving, organizing, and analyzing biological data using software tools with applications to general principles of DNA/RNA structure, bioinformatics and applications, genomes, protein structure, and modeling and classification, as well as microarray analysis. • Provides a systems biology perspective, including general guidelines and techniques for obtaining, integrating, and analyzing complex data sets from multiple experimental sources using computational tools and software. Topics covered include phenomics, genomics, epigenomics/epigenetics, metabolomics, cell cycle and checkpoint control, and systems biology and vaccination research. • Explains how to effectively harness the power of Big Data tools when data sets are so large and complex that it is difficult to process them using conventional database management systems or traditional data processing applications. Discusses the development and application of data-analytical and theoretical methods, mathematical modeling and computational simulation techniques to the study of biological and behavioral systems. Presents a systematic approach for storing, retrieving, organizing and analyzing biological data using software tools with applications. Provides a systems biology perspective including general guidelines and techniques for obtaining, integrating and analyzing complex data sets from multiple experimental sources using computational tools and software.

Cheminformatics and Bioinformatics at the Interface with Systems Biology Jul 25 2022 Addressing the fundamental aspects of the various computational tools for drug discovery, this book compiles recent bioinformatics and chemoinformatics approaches, and their integration with systems biology.

Handbook of Chemoinformatics Algorithms May 23 2022 Unlike in the related area of bioinformatics, few books currently exist that document the techniques, tools, and algorithms of chemoinformatics. Bringing together worldwide experts in the field, the Handbook of Chemoinformatics Algorithms provides an overview of the most common

chemoinformatics algorithms in a single source.After a historical persp

Computational Approaches Feb 26 2020 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.

In Silico Drug Design May 31 2020 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

Chemoinformatics and Computational Chemical Biology Jun 12 2021 Over the past years, the chem(o)informatics field has further evolved and new application areas have opened up, for example, in the broadly defined area of chemical biology. In Chemoinformatics and Computational Chemical Biology, leading investigators bring together a detailed series of reviews and methods including, among others, system-directed approaches using small molecules, the design of target-focused compound libraries, the study of molecular selectivity, and the systematic analysis of target-ligand interactions. Furthermore, the book delves into similarity methods, machine learning, probabilistic approaches, fragment-based methods, as well as topics that go beyond the current chemoinformatics spectrum, such as knowledge-based modeling of G protein-coupled receptor structures and computational design of siRNA libraries. As a volume in the highly successful Methods in Molecular BiologyTM series, this collection provides detailed descriptions and implementation advice that are exceedingly relevant for basic researchers and practitioners in this highly interdisciplinary research and development area. Cutting-edge and unambiguous, Chemoinformatics and Computational Chemical Biology serves as an ideal guide for experts and newcomers alike to this vital and dynamic field of study.

Chemoinformatics Approaches to Virtual Screening Mar 21 2022 "This book is the first monograph to summarize the innovative applications of efficient chemoinformatics approaches towards 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 monograph covers chemoinformatics approaches applicable to virtual screening of very large collections of chemical compounds to identify novel biologically active molecules. The discussed approaches rely on chemoinformatics concepts such as the representation of molecules using multiple descriptors of chemical structures, advanced chemical similarity calculations in multidimensional descriptor spaces, and machine learning and data mining approaches. Ligand-based approaches, which are in the focus of this work, are more computationally efficient compared to structure-based virtual screening."--BOOK JACKET.

An Introduction to Chemoinformatics Jan 07 2021 This book aims to provide an introduction to the major techniques of chemoinformatics. It is the first text written specifically for this field. The first part of the book deals with the representation of 2D and 3D molecular structures, the calculation of molecular descriptors and the construction of mathematical models. The second part describes other important topics including molecular similarity and diversity, the analysis of large data sets, virtual screening, and library design. Simple illustrative examples are used throughout to illustrate key concepts, supplemented with case studies from the literature.

Cheminformatics and its Applications Jun 24 2022 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.

Encyclopedia of Bioinformatics and Computational Biology Jan 19 2022 Encyclopedia of Bioinformatics and Computational Biology: ABC of Bioinformatics combines elements of computer science, information technology, mathematics, statistics and biotechnology, providing the methodology and in silico solutions to mine biological data and processes. The book covers Theory, Topics and Applications, with a special focus on Integrative –omics and Systems Biology. The theoretical, methodological underpinnings of BCB, including phylogeny are covered, as are more current areas of focus, such as translational bioinformatics, cheminformatics, and environmental informatics. Finally, Applications provide guidance for commonly asked questions. This major reference work spans basic and cutting-edge methodologies authored by leaders in the field, providing an invaluable resource for students, scientists, professionals in research institutes, and a broad swath of researchers in biotechnology and the biomedical and pharmaceutical industries. Brings together information from computer science, information technology, mathematics, statistics and biotechnology Written and reviewed by leading experts in the field, providing a unique and authoritative resource Focuses on the main theoretical and methodological concepts before expanding on specific topics and applications Includes interactive images, multimedia tools and crosslinking to further resources and databases

Chemometrics and Chemoinformatics Sep 22 2019 Chemometrics and Chemoinformatics will provide chemists and other scientists with the fundamental knowledge on chemometrics coupled with chemoinformatics.

Chemoinformatics in Drug Discovery Nov 24 2019 This handbook provides the first-ever inside view of today's integrated approach to rational drug design. Chemoinformatics experts from large pharmaceutical companies, as well as from chemoinformatics service providers and from academia demonstrate what can be achieved today by harnessing the power of computational methods for the drug discovery process. With the user rather than the developer of chemoinformatics software in mind, this book describes the successful application of computational tools to real-life problems and presents solution strategies to commonly encountered problems. It shows how almost every step of the drug discovery pipeline can be optimized and accelerated by using chemoinformatics tools -- from the management of compound databases to targeted combinatorial synthesis, virtual screening and efficient hit-to-lead transition. An invaluable resource for drug developers and medicinal chemists in academia and industry.

Bioinformatics--from Genomes to Drugs: Applications Jun 19 2019

Chemoinformatics Oct 04 2020 This first work to be devoted entirely to this increasingly important field, the "Textbook" provides both an in-depth and comprehensive overview of this exciting new area. Edited by Johann Gasteiger and Thomas Engel, the book provides an introduction to the representation of molecular structures and reactions, data types and databases/data sources, search methods, methods for data analysis as well as such applications as structure elucidation, reaction simulation, synthesis planning and drug design. A "hands-on" approach with step-by-step tutorials and detailed descriptions of software tools and Internet resources allows easy access for newcomers, advanced users and lecturers alike. For a more detailed presentation, users are referred to the "Handbook of Chemoinformatics", which will be published separately. Johann Gasteiger is the recipient of the 1991 Gmelin-Beilstein Medal of the German Chemical Society for Achievements in Computer Chemistry, and the Herman Skolnik Award of the Division of Chemical Information of the American Chemical Society (ACS) in 1997. Thomas Engel joined the research group headed by Johann Gasteiger at the University of Erlangen-Nuremberg and is a specialist in chemoinformatics.

Advances in Bioinformatics Apr 22 2022 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.

Applied Chemoinformatics Dec 26 2019 Edited by world-famous pioneers in chemoinformatics, this is a clearly structured and applications-oriented approach to the topic, providing up-to-date and focused information on the wide range of applications in this exciting field. The authors explain methods and software tools, such that the reader will not only learn the basics but also how to use the different software packages available. Experts describe applications in such different fields as structure-spectra correlations, virtual screening, prediction of active sites, library design, the prediction of the properties of chemicals, the development of new cosmetics products, quality control in food, the design of new materials with improved properties, toxicity modeling, assessment of the risk of chemicals, and the control of chemical processes. The book is aimed at advanced students as well as lectures but also at scientists that want to learn how chemoinformatics could assist them in solving their daily scientific tasks. Together with the corresponding textbook Chemoinformatics - Basic Concepts and Methods (ISBN 9783527331093) on the fundamentals of chemoinformatics readers will have a comprehensive overview of the field.

Machine Learning in Bioinformatics Mar 09 2021 An introduction to machine learning methods and their applications to problems in bioinformatics Machine learning techniques are increasingly being used to address problems in computational biology and bioinformatics. Novel computational techniques to analyze high throughput data in the form of sequences, gene and protein expressions, pathways, and images are becoming vital for understanding diseases and future drug discovery. Machine learning techniques such as Markov models, support vector machines, neural networks, and graphical models have been successful in analyzing life science data because of their capabilities in handling randomness and uncertainty of data noise and in generalization. From an internationally recognized panel of prominent researchers in the field, Machine Learning in Bioinformatics compiles recent approaches in machine learning methods and their applications in addressing contemporary problems in bioinformatics. Coverage includes: feature selection for genomic and proteomic data mining; comparing variable selection methods in gene selection and classification of microarray data; fuzzy gene mining; sequence-based prediction of residue-level properties in proteins; probabilistic methods for long-range features in biosequences; and much more. Machine Learning in Bioinformatics is an indispensable resource for computer scientists, engineers, biologists, mathematicians, researchers, clinicians, physicians, and medical informaticists. It is also a valuable reference text for computer science, engineering, and biology courses at the upper undergraduate and graduate levels.

Dictionary of Natural Products Aug 22 2019