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Bioinformatics And Computational Biology In Drug Discovery And Development

**Tiratha Raj Singh, Hemraj Saini, Moacyr
Comar Junior**



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

Computational Approaches in Drug Discovery, Development and Systems Pharmacology Rupesh Kumar Gautam, Mohammad Amjad Kamal, Pooja Mittal, 2023-02-15 Computational Approaches in Drug Discovery Development and Systems Pharmacology provides detailed information on the use of computers in advancing pharmacology Drug discovery and development is an expensive and time consuming practice and computer assisted drug design CADD approaches are increasing in popularity in the pharmaceutical industry to accelerate the process With the help of CADD scientists can focus on the most capable compounds so that they can minimize the synthetic and biological testing pains This book examines success stories of CADD in drug discovery drug development and role of CADD in system pharmacology additionally including a focus on the role of artificial intelligence AI and deep machine learning in pharmacology Computational Approaches in Drug Discovery Development and Systems Pharmacology will be useful to researchers and academics working in the area of CADD pharmacology and Bioinformatics Explains computer use in pharmacology using real life case studies Provides information about biological activities using computer technology thus allowing for the possible reduction of the number of animals used for research Describes the role of AI in pharmacology and applications of CADD in various diseases

Computational Biology in Drug Discovery and Repurposing Rajani Sharma, A. V. Senthil Kumar, Kunal Kumar, 2024-08-16 This new book takes an in depth look at the emerging and prospective field of computational biology and bioinformatics which possesses the ability to analyze large accumulated biological data collected from sequence analysis of proteins and genes and cell population with an aim to make new predictions pertaining to drug discovery and new biology The book explains the basic methodology associated with a bioinformatics and computational approach in drug designing It then goes on to cover the implementation of computational programming bioinformatics pharmacophore modeling biotechnological techniques and pharmaceutical chemistry in designing drugs The major advantage of intervention of computer language or programming is to cut down the number of steps and costs in the field of drug designing reducing the repeating steps and saving time in screening the potent component for drug or vaccine designing The book describes algorithms used for drug designing and the use of machine learning and AI in drug delivery and disease diagnosis which are valuable in clinical decision making The implementation of robotics in different diseases like stroke cancer COVID 19 etc is also addressed Topics include machine learning AI databases in drug design molecular docking bioinformatics tools target based drug design and immunoinformatics chemoinformatics and nanoinformatics in drug design Drug repurposing in drug design in general as well as for specific diseases including cancer Alzheimer s disease tuberculosis COVID 19 etc is also addressed in depth *Bioinformatics and Computational Biology* Tiratha Raj Singh, Hemraj Saini, Moacyr Comar Junior, 2023-12-11

Designed as a reference text 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

Systems Biology in Drug Discovery and Development Qing Yan,2010-09-21 Due to the failing one drug fits all model it has become increasingly necessary to develop personalized medicine that treats whole systems and brings the right drug to the right patient with the right dosages In Systems Biology in Drug Discovery and Development Methods and Protocols leading experts provide a practical state of the art and holistic view of the translation of systems biology into better drug discovery and personalized medical practice While the first part of the book describes cutting edge technologies and methods in the field the second part illustrates how the technologies can be applied in science for disease understanding and therapeutic discovery As a volume in the highly successful Methods in Molecular Biology™ series this collection provides the kind of detailed description and implementation advice that is crucial for getting optimal results Authoritative and up to date Systems Biology in Drug Discovery and Development Methods and Protocols covers topics from fundamental concepts to advanced technologies in order to best serve biomedical students and professionals at all levels who are interested in vital integrative studies in molecular biology genetics bioinformatics bioengineering biochemistry physiology pathology microbiology immunology pharmacology toxicology drug discovery and clinical medicine Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences Navneet Sharma,Himanshu Ojha,Pawan Raghav,Ramesh K. Goyal,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,Ajay Kumar,Shiv Bharadwaj,Ravi Chaudhary,Shakti Sahi,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 Neuroreceptor Endocytosis and Signaling in Health and Disease Indra Mani,2025-04-26 This book covers a wide range of neuroreceptor topics including receptor endocytosis and signaling and the role of neuroreceptors in health and disease conditions It focuses on various important nervous system receptors and their biomedical applications especially receptor signaling The book provides a look into the current developments of various neuroreceptors responsible for pathophysiological conditions It is a valuable cutting edge in depth reference on neuroreceptors featuring clearly written chapters from major contributors in the field The central aim is to aid future investigators researchers students and stakeholders to perform their research with greater ease This book provides an excellent basis from which scientific knowledge can grow widen and accelerate receptor biology tools toward biomedical applications **Phytochemicals as Lead Compounds for New Drug Discovery** Chukwuebuka Egbuna,Shashank

Kumar,Jonathan C. Ifemeje,Shahira M. Ezzat,Saravanan Kaliyaperumal,2019-09-07 Phytochemicals as Lead Compounds for New Drug Discovery presents complete coverage of the recent advances in the discovery of phytochemicals from medicinal plants as models to the development of new drugs and chemical entities Functional bioactive compounds of plant origin have been an invaluable source for many human therapeutic drugs and have played a major role in the treatment of diseases around the world These compounds possess enormous structural and chemical diversity and have led to many important discoveries This book presents fundamental concepts and factors affecting the choice for plant based products as well as recent advances in computer aided drug discovery and FDA drug candidacy acceptance criteria It also details the various bioactive lead compounds and molecular targets for a range of life threatening diseases including cancer diabetes and neurodegenerative diseases Written by a global team of experts Phytochemicals as Lead Compounds for New Drug Discovery is an ideal resource for drug developers phytochemists plant biochemists food and medicinal chemists nutritionists and toxicologists chemical ecologists taxonomists analytical chemists and other researchers in those fields It will also be very valuable to professors students and researchers in this domain Presents fundamental concepts and factors affecting choice for plant based products Details the FDA drug candidacy acceptance criteria including bottlenecks and way forward Highlights recent advances in computational based drug discovery Focuses on the discovery of new drugs and potential druggable targets for the treatment of chronic diseases of world importance **Proceedings of the 1st International**

Conference on Recent Advancements in Materials Science and Technology, Volume II P. Sakthivel,Mangalaraja Ramalinga Viswanathan,K. Ravichandran,2024-11-26 This book presents peer reviewed and selected papers from the 1st International Conference on Recent Advancements in Materials Science and Technology held at Karpagam Academy of Higher Education in Coimbatore India on 29 30 January 2024 Experts across the world share the latest developments in their respective fields within materials science including nanomaterials biomaterials optical materials construction materials

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