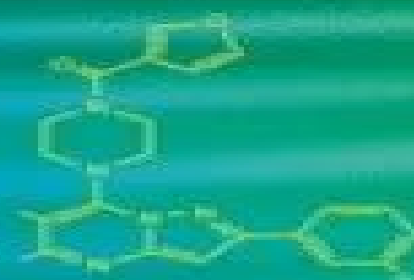


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Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences Navneet Sharma, Himanshu Ojha, Pawan Raghav, Ramesh K. Goyal, 2021-05-21 Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences brings together two very important fields 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

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Jagtap,2023-09-07 This second edition provides new and updated methods and techniques for identification of drug target binding sites prediction high throughput virtual screening lead discovery and optimization conformational sampling prediction of pharmacokinetic properties using computer based methodologies Chapters also focus on the application of the latest artificial intelligence technologies for computer aided drug discovery Written in the format of the highly successful Methods in Molecular Biology series each chapter includes an introduction to the topic lists necessary methods includes tips on troubleshooting and known pitfalls and step by step readily reproducible protocols Authoritative and cutting edge Computational Drug Discovery and Design Second Edition aims to effectively utilize computational methodologies in discovery and design of novel drugs Bioinformatics and Drug Discovery Richard S. Larson,2005-10-01 A collection of readily reproducible bioinformatic methods to advance the drug discovery process from gene identification to protein modeling to the identification of specific drug candidates The authors demonstrate these techniques including microarray analysis the analysis of genes as potential drug targets virtual screening and in silico protein design and cheminformatics in a variety of practical situations Because these technologies are still emergent each chapter contains an extended introduction that explains the theory and application of the technology and techniques described BIOINFORMATICS: METHODS AND APPLICATIONS S. C. RASTOGI,NAMITA MENDIRATTA,PARAG RASTOGI,2013-05-22 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 *Modern Methods of Drug Discovery* Alexander Hillisch, Rolf Hilgenfeld, 2002-12-11 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 discovery Quite often companies favor one of these relatively new approaches over the other e g screening over rational design or vice versa but we believe that an intelligent and concerted use of several or all methods currently available to drug discovery will be more successful in the medium term What has changed most significantly in the past few years is the time available for identifying new chemical entities Because of the high costs of drug discovery projects pressure for maximum success in the shortest possible time is higher than ever In addition the multidisciplinary character of the field is much more pronounced today than it used to be As a consequence researchers and project managers in the pharmaceutical industry should have a solid knowledge of the more important methods available to drug discovery because it is the rapidly and intelligently combined use of these which will determine the success or failure of preclinical projects *Computational Approaches in Cheminformatics and Bioinformatics* Rajarshi Guha, Andreas Bender, 2012-01-04 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 **BIOINFORMATICS, FIFTH EDITION RASTOGI,**

S.C., RASTOGI, PARAG, MENDIRATTA, NAMITA, 2022-04-05 Designed as a comprehensive text for students and professionals pursuing careers in the fields of bioinformatics molecular biology pharmacy and drug research the Fifth Edition continues to offer a fascinating and authoritative treatment of the entire spectrum of bioinformatics covering a wide range of high throughput technologies The content can be used for four core courses bioinformatics fundamentals genomics proteomics and drug discovery and design The Fifth Edition takes a completely new pedagogical approach and the book is divided into eight distinct Units for the ease of learning Bioinformatics Fundamentals Sequence Alignment Phylogenetic Analysis Genomics Protein Structure and Function Drug Discovery Methods Drug Design and Development and Integrative Topics Accordingly all the chapters are revised and updated in the new edition besides introduction of seven new chapters and another seven completely re written chapters As a student friendly text it embodies several pedagogical features such as detailed examples numerous tables a large number of diagrams flow charts and web resources The book in its present edition should prove an invaluable asset to the students and researchers in the fields of bioinformatics biotechnology computer aided drug design information technology medical diagnostics molecular biology and pharmaceutical sciences NEW TO THE FIFTH EDITION Re written chapters Biological database search and data retrieval Pair wise alignment of sequences PSSMs and Hidden Markov Models Gene Mapping Gene Prediction Protein Structure Overview and Protein Structure Prediction Inclusion of new chapters Scoring Matrices Gene Sequencing Regulatory Elements Prediction Comparative Genomics Protein Structure Databases Protein Function Prediction and Potential Drug Targets KEY FEATURES Covers the field of bioinformatics in a complete and integrated approach moving from the fundamentals to theory and practical applications State of the art technologies for gene identification molecular modeling and monitoring of cellular processes Data mining data curation and analysis classification interpretation and efficient structure determination of genomes and proteomes Companion website provides useful resources for the teachers as well as for the students So visit Learning Centre https://www.phindia.com/bioinformatics_mendiratta_rastogi to have access of Lecture notes solutions manual MCQs problems set for practice glossary of important terms etc TARGET AUDIENCE UG and PG Students of Bioinformatics Biotechnology Molecular Biology and Pharmacy

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