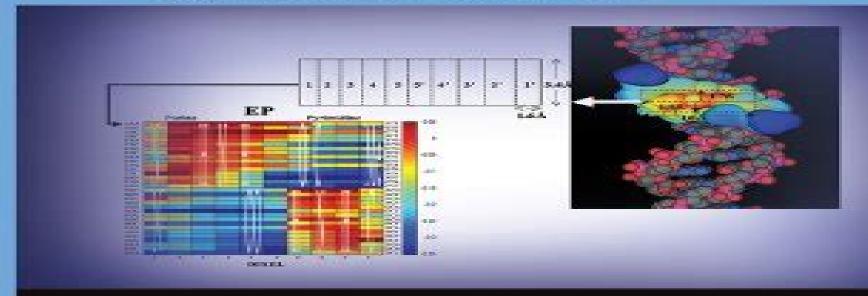
Computational Approaches in Cheminformatics and Bioinformatics

Educator Rajarshi Guba and Andreas Bender





Computational Approaches In Cheminformatics And Bioinformatics

Rajarshi Guha, Andreas Bender

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terms of the number of new molecular entities NMEs Amongst the reasons noted for this are the adverse side effects and reduced efficiency of many of the potential compounds This is a problem both for the pharmaceutical industry and for those suffering from diseases for which there are no or few available treatments Advances in computational chemistry computer science structural biology and molecular biology have all contributed to improved drug design strategies and reduced the time taken for drug discovery By interfacing cheminformatics and bioinformatics with systems biology we can create a powerful tool for understanding the mechanisms of patho physiological systems and identifying lead molecules for various diseases This integration of drug design approaches can also play a crucial role in the prediction and rationalization of drug effects and side effects improving safety and efficacy and leading to better approval rates Addressing the lack of knowledge on the fundamental aspects of the various computational tools for drug discovery this book is a compilation of recent bioinformatics and cheminformatics approaches and their integration with systems biology Written primarily for researchers and academics in chem and bioinformatics it may also be a useful resource for advanced level students **Computational** Approaches in Biotechnology and Bioinformatics Pranav Deepak Pathak, Roshani Raut, Sebastian Jaramillo-Isaza, Pradnya Borkar, Rutvij H. Jhaveri, 2024-05-27 Volume 1 of Computational Approaches in Bioengineering Computational Approaches in Biotechnology and Bioinformatics explores many significant topics of biomedical engineering and bioinformatics in an easily understandable format It explores recent developments and applications in bioinformatics biomechanics artificial intelligence AI signal processing wearable sensors biomaterials cell biology synthetic biology biostatistics prosthetics big data and algorithms From applications of biomaterials in advanced drug delivery systems to the role of big data AI and machine learning in disease diagnosis and treatment the book will help readers understand how these technologies are being applied across the areas of biomedical engineering bioinformatics and healthcare The chapters also include case studies on the role of medical robots in surgery and the determination of protein structure using genetic algorithms. The contributors are all leading experts across multiple disciplines and provide chapters that truly represent a complete view of these state of the art technologies FEATURES Covers a wide range of subjects from biomedical engineering like wearable devices biomaterials synthetic biology phytochemical extraction and prosthetics Explores AI machine learning big data analysis and algorithms in biomedical engineering and bioinformatics in an easily understandable format Includes case studies on the role of medical robots in surgery and the determination of protein structure using genetic algorithms Discusses genetic diagnosis classification and risk prediction in cancer using next generation sequencing in oncology This book is ideally designed for biomedical professionals biomedical engineers healthcare professionals data engineers clinicians physicians medical students hospital directors clinical researchers and others who work in the field of artificial intelligence bioinformatics and computational biology Chemoinformatics and Advanced Machine Learning Perspectives: Complex Computational Methods and Collaborative Techniques Lodhi, Huma, Yamanishi, Yoshihiro, 2010-07-31 This book is a timely compendium of

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