

Daniel J. Rigden
Editor

From Protein Structure to Function with Bioinformatics

From Protein Structure To Function With Bioinformatics
Author Daniel John Rigden Nov 201

Daniel John Rigden



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From Protein Structure to Function with Bioinformatics Daniel John Rigden, 2008-12-11 Proteins lie at the heart of almost all biological processes and have an incredibly wide range of activities Central to the function of all proteins is their ability to adopt stably or sometimes transiently structures that allow for interaction with other molecules An understanding of the structure of a protein can therefore lead us to a much improved picture of its molecular function This realisation has been a prime motivation of recent Structural Genomics projects involving large scale experimental determination of protein structures often those of proteins about which little is known of function These initiatives have in turn stimulated the massive development of novel methods for prediction of protein function from structure Since model structures may also take advantage of new function prediction algorithms the first part of the book deals with the various ways in which protein structures may be predicted or inferred including specific treatment of membrane and intrinsically disordered proteins A detailed consideration of current structure based function prediction methodologies forms the second part of this book which concludes with two chapters focusing specifically on case studies designed to illustrate the real world application of these methods With bang up to date texts from world experts and abundant links to publicly available resources this book will be invaluable to anyone who studies proteins and the endlessly fascinating relationship between their structure and function

Protein Structure Daniel Chasman, 2003-03-18 This text offers in depth perspectives on every aspect of protein structure identification assessment characterization and utilization for a clear understanding of the diversity of protein shapes variations in protein function and structure based drug design The authors cover numerous high throughput technologies as well as computational met Protein Bioinformatics M. Michael Gromiha, 2011-04-21 One of the most pressing tasks in biotechnology today is to unlock the function of each of the thousands of new genes identified every day Scientists do this by analyzing and interpreting proteins which are considered the task force of a gene This single source reference covers all aspects of proteins explaining fundamentals synthesizing the latest literature and demonstrating the most important bioinformatics tools available today for protein analysis interpretation and prediction Students and researchers of biotechnology bioinformatics proteomics protein engineering biophysics computational biology molecular modeling and drug design will find this a ready reference for staying current and productive in this fast evolving interdisciplinary field Explains all aspects of proteins including sequence and structure analysis prediction of protein structures protein folding protein stability and protein interactions Presents a cohesive and accessible overview of the field using illustrations to explain key concepts and detailed exercises for students **Protein Bioinformatics** Ingvar Eidhammer, Inge Jonassen, Willie R. Taylor, William R. Taylor, 2004-02-13 Pairwise global alignment of sequences Pairwise local alignment and database search Statical analysis Multiple global alignment and phylogenetic trees Scoring matrices Profiles Sequence patterns Structures and structure descriptions Superposition and Dynamic programming Geometric

techniques Clustering Combining local similarities Significance and assessment of structure comparisons Multiple structure comparison Protein structure classification Structure prediction Threading Basics in mathematics probability and algorithms Introduction to molecular biology *Prediction of Protein Structures, Functions, and Interactions* Janusz M.

Bujnicki, 2008-12-23 The growing flood of new experimental data generated by genome sequencing has provided an impetus for the development of automated methods for predicting the functions of proteins that have been deduced by sequence analysis and lack experimental characterization Prediction of Protein Structures Functions and Interactions presents a comprehensive overview of methods for prediction of protein structure or function with the emphasis on their availability and possibilities for their combined use Methods of modeling of individual proteins prediction of their interactions and docking of complexes are put in the context of predicting gene ontology biological process molecular function and cellular component and discussed in the light of their contribution to the emerging field of systems biology Topics covered include first steps of protein sequence analysis and structure prediction automated prediction of protein function from sequence template based prediction of three dimensional protein structures fold recognition and comparative modelling template free prediction of three dimensional protein structures quality assessment of protein models prediction of molecular interactions from small ligands to large protein complexes macromolecular docking integrating prediction of structure function and interactions Prediction of Protein Structures Functions and Interactions focuses on the methods that have performed well in CASPs and which are constantly developed and maintained and are freely available to academic researchers either as web servers or programs for local installation It is an essential guide to the newest best methods for prediction of protein structure and functions for researchers and advanced students working in structural bioinformatics protein chemistry structural biology and drug discovery **Introduction to Protein Structure Prediction** Huzefa Rangwala, George Karypis, 2011-03-16 A look at the methods and algorithms used to predict protein structure A thorough knowledge of the function and structure of proteins is critical for the advancement of biology and the life sciences as well as the development of better drugs higher yield crops and even synthetic bio fuels To that end this reference sheds light on the methods used for protein structure prediction and reveals the key applications of modeled structures This indispensable book covers the applications of modeled protein structures and unravels the relationship between pure sequence information and three dimensional structure which continues to be one of the greatest challenges in molecular biology With this resource readers will find an all encompassing examination of the problems methods tools servers databases and applications of protein structure prediction and they will acquire unique insight into the future applications of the modeled protein structures The book begins with a thorough introduction to the protein structure prediction problem and is divided into four themes a background on structure prediction the prediction of structural elements tertiary structure prediction and functional insights Within those four sections the following topics are covered Databases and resources that are commonly used for protein structure prediction The structure

prediction flagship assessment CASP and the protein structure initiative PSI Definitions of recurring substructures and the computational approaches used for solving sequence problems Difficulties with contact map prediction and how sophisticated machine learning methods can solve those problems Structure prediction methods that rely on homology modeling threading and fragment assembly Hybrid methods that achieve high resolution protein structures Parts of the protein structure that may be conserved and used to interact with other biomolecules How the loop prediction problem can be used for refinement of the modeled structures The computational model that detects the differences between protein structure and its modeled mutant Whether working in the field of bioinformatics or molecular biology research or taking courses in protein modeling readers will find the content in this book invaluable

The Ten Most Wanted Solutions in Protein Bioinformatics Anna Tramontano, 2005-05-24 Utilizing high speed computational methods to extrapolate to the rest of the protein universe the knowledge accumulated on a subset of examples protein bioinformatics seeks to accomplish what was impossible before its invention namely the assignment of functions or functional hypotheses for all known proteins

The Ten Most Wanted Solutions in Protein Structure Prediction Mohammed Zaki, Chris Bystroff, 2007-09-12 This book covers elements of both the data driven comparative modeling approach to structure prediction and also recent attempts to simulate folding using explicit or simplified models Despite the unsolved mystery of how a protein folds advances are being made in predicting the interactions of proteins with other molecules Also rapidly advancing are the methods for solving the inverse folding problem the problem of finding a sequence to fit a structure This book focuses on the various computational methods for prediction their successes and their limitations from the perspective of their most well known practitioners

Invitation to Protein Sequence Analysis Through Probability and Information Daniel Graham, 2019-02-06 This book explores the remarkable information correspondences and probability structures of proteins Correspondences are pervasive in biochemistry and bioinformatics proteins share homologies folding patterns and mechanisms Probability structures are just as paramount folded state graphics reflect Angstrom scale maps of electron density The author explores protein sequences primary structures both individually and in sets systems with the help of probability and information tools This perspective will enhance the reader's knowledge of how an important class of molecules is designed and put to task in natural systems and how we can approach class members in hands on ways

Computational Methods for Protein Structure Prediction and Modeling Ying Xu, Dong Xu, Jie Liang, 2007-08-24 An ultimate goal of modern biology is to understand how the genetic blueprint of cells genotype determines the structure function and behavior of a living organism phenotype At the center of this scientific endeavor is characterizing the biochemical and cellular roles of proteins the working molecules of the machinery of life A key to understanding of functional proteins is the knowledge of their folded structures in a cell as the structures provide the basis for studying proteins functions and functional mechanisms at the molecular level Researchers working on structure determination have traditionally selected individual proteins due to their functional importance in a

biological process or pathway of particular interest Major research organizations often have their own protein X ray crystallographic or and nuclear magnetic resonance facilities for structure determination which have been conducted at a rate of a few to dozens of structures a year Realizing the widening gap between the rates of protein identification through DNA sequencing and identification of potential genes through bioinformatics analysis and the determination of protein structures a number of large scientific initiatives have been launched in the past few years by government funding agencies in the United States Europe and Japan with the intention to solve protein structures en masse an effort called structural genomics A number of structural genomics centers factory like facilities have been established that promise to produce solved protein structures in a similar fashion to DNA sequencing

Scalable Big Data Analytics for Protein Bioinformatics Dariusz Mrozek, 2018-09-25 This book presents a focus on proteins and their structures The text describes various scalable solutions for protein structure similarity searching carried out at main representation levels and for prediction of 3D structures of proteins Emphasis is placed on techniques that can be used to accelerate similarity searches and protein structure modeling processes The content of the book is divided into four parts The first part provides background information on proteins and their representation levels including a formal model of a 3D protein structure used in computational processes and a brief overview of the technologies used in the solutions presented in the book The second part of the book discusses Cloud services that are utilized in the development of scalable and reliable cloud applications for 3D protein structure similarity searching and protein structure prediction The third part of the book shows the utilization of scalable Big Data computational frameworks like Hadoop and Spark in massive 3D protein structure alignments and identification of intrinsically disordered regions in protein structures The fourth part of the book focuses on finding 3D protein structure similarities accelerated with the use of GPUs and the use of multithreading and relational databases for efficient approximate searching on protein secondary structures The book introduces advanced techniques and computational architectures that benefit from recent achievements in the field of computing and parallelism Recent developments in computer science have allowed algorithms previously considered too time consuming to now be efficiently used for applications in bioinformatics and the life sciences Given its depth of coverage the book will be of interest to researchers and software developers working in the fields of structural bioinformatics and biomedical databases

High-Performance Computational Solutions in Protein

Bioinformatics Dariusz Mrozek, 2014-06-04 Recent developments in computer science enable algorithms previously perceived as too time consuming to now be efficiently used for applications in bioinformatics and life sciences This work focuses on proteins and their structures protein structure similarity searching at main representation levels and various techniques that can be used to accelerate similarity searches Divided into four parts the first part provides a formal model of 3D protein structures for functional genomics comparative bioinformatics and molecular modeling The second part focuses on the use of multithreading for efficient approximate searching on protein secondary structures The third and fourth parts

concentrate on finding 3D protein structure similarities with the support of GPUs and cloud computing Parts three and four both describe the acceleration of different methods The text will be of interest to researchers and software developers working in the field of structural bioinformatics and biomedical databases

Practical Protein Bioinformatics Florencio Pazos, Mónica Chagoyen, 2014-11-28 This book describes more than 60 web accessible computational tools for protein analysis and is totally practical with detailed explanations on how to use these tools and interpret their results and minimal mentions to their theoretical basis only when that is required for making a better use of them It covers a wide range of tools for dealing with different aspects of proteins from their sequences to their three dimensional structures and the biological networks they are immersed in The selection of tools is based on the experience of the authors that lead a protein bioinformatics facility in a large research centre with the additional constraint that the tools should be accessible through standard web browsers without requiring the local installation of specific software command line tools etc The web tools covered include those aimed to retrieve protein information look for similar proteins generate pair wise and multiple sequence alignments of protein sequences work with protein domains and motifs study the phylogeny of a family of proteins retrieve manipulate and visualize protein three dimensional structures predict protein structural features as well as whole three dimensional structures extract biological information from protein structures summarize large protein sets study protein interaction and metabolic networks etc The book is associated to a dynamic web site that will reflect changes in the web addresses of the tools updates of these etc It also contains QR codes that can be scanned with any device to direct its browser to the tool web site This monograph will be most valuable for researchers in experimental labs without specific knowledge on bioinformatics or computing

Jnl Proteins: Structure, Function & Genetics Thomas G. Chasteen, Bruce Coburn Richardson, 1990-06 3 Nobel laureates contributed to this invaluable collection of high quality articles extracted from the much praised R A Meyer's Encyclopedia With sections on Structure Modeling Expression Analysis and others this book covers a wide range of topics in protein research

Protein Structure Prediction David Webster, 2008-02-03 The number of protein sequences grows each year yet the number of structures deposited in the Protein Data Bank remains relatively small The importance of protein structure prediction cannot be overemphasized and this volume is a timely addition to the literature in this field Protein Structure Prediction Methods and Protocols is a departure from the normal Methods in Molecular Biology series format By its very nature protein structure prediction demands that there be a greater mix of theoretical and practical aspects than is normally seen in this series This book is aimed at both the novice and the experienced researcher who wish for detailed information in the field of protein structure prediction a major intention here is to include important information that is needed in the day to day work of a research scientist important information that is not always decipherable in scientific literature Protein Structure Prediction Methods and Protocols covers the topic of protein structure prediction in an eclectic fashion detailing aspects of prediction that range from sequence analysis a starting

point for many algorithms to secondary and tertiary methods on into the prediction of docked complexes an essential point in order to fully understand biological function As this volume progresses the authors contribute their expert knowledge of protein structure prediction to many disciplines such as the identification of motifs and domains the comparative modeling of proteins and ab initio approaches to protein loop side chain and protein prediction **Protein Bioinformatics** Cathy H. Wu,Cecilia N. Arighi,Karen E. Ross,2017 This volume introduces bioinformatics research methods for proteins with special focus on protein post translational modifications PTMs and networks This book is organized into four parts and covers the basic framework and major resources for analysis of protein sequence structure and function approaches and resources for analysis of protein PTMs protein protein interactions PPIs and protein networks including tools for PPI prediction and approaches for the construction of PPI and PTM networks and bioinformatics approaches in proteomics including computational methods for mass spectrometry based proteomics and integrative analysis for alternative splice isoforms for functional discovery Written in the highly 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 laboratory or computational protocols and tips on troubleshooting and avoiding known pitfalls Cutting edge and thorough Protein Bioinformatics From Protein Modifications and Networks to Proteomics is a valuable resource for readers who wish to learn about state of the art bioinformatics databases and tools novel computational methods and future trends in protein and proteomic data analysis in systems biology This book is useful to researchers who work in the biotechnology and pharmaceutical industries and in various academic departments such as biological and medical sciences and computer sciences and engineering OCLC

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