

Daniel J. Rigden  
*Editor*

# From Protein Structure to Function with Bioinformatics



Springer

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

**Gregory Petsko, Dagmar Ringe**



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

**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 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 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

**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

**Jnl Proteins: Structure, Function & Genetics** Thomas G. Chasteen, Bruce Coburn Richardson, 1990-06-03 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

*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

**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

On protein structure, function and modularity from an evolutionary perspective Robert Pilstål, 2018-05-23 We are compounded entities given life by a complex molecular machinery When studying these molecules we have to make sense of a diverse set of dynamical

nanstructures with vast and intricate patterns of interactions Protein polymers is one of the major groups of building blocks of such nanostructures which fold up into more or less distinct three dimensional structures Due to their shape dynamics and chemical properties proteins are able to perform a plethora of specific functions essential to all known cellular lifeforms The connection between protein sequence translated into protein structure and in the continuation into protein function is well accepted but poorly understood Malfunction in the process of protein folding is known to be implicated in natural aging cancer and degenerative diseases such as Alzheimer s Protein folds are described hierarchically by structural ontologies such as SCOP CATH and Pfam all which has yet to succeed in deciphering the natural language of protein function These paradigmatic views centered on protein structure fail to describe more mutable entities such as intrinsically disordered proteins IDPs which lack a clear defined structure As of 2012 about two thirds of cancer patients was predicted to survive past 5 years of diagnosis Despite this about a third do not survive and numerous of successfully treated patients suffer from secondary conditions due to chemotherapy surgery and the like In order to handle cancer more efficiently we have to better understand the underlying molecular mechanisms Elusive to standard methods of investigation IDPs have a central role in pathology dysfunction in IDPs are key factors in cellular system failures such as cancer as many IDPs are hub regulators for major cell functions These IDPs carry short conserved functional boxes that are not described by known ontologies which suggests the existence of a smaller entity In an investigation of a pair of such boxes of c MYC a plausible structural model of its interacting with Pin1 emerged but such a model still leaves the observer with a puzzle of understanding the actual function of that interaction If the protein is represented as a graph and modeled as the interaction patterns instead of as a structural entity another picture emerges As a graph there is a parable from that of the boxes of IDPs to that of sectors of allosterically connected residues and the theory of foldons and folding units Such a description is also useful in deciphering the implications of specific mutations In order to render a functional description feasible for both structured and disordered proteins there is a need of a model separate from form and structure Realized as protein primes patterns of interaction which has a specific function that can be defined as prime interactions and context With function defined as interactions it might be possible that the discussion of proteins and their mechanisms is thereby simplified to the point rendering protein structural determination merely supplementary to understanding protein function

Människan byggs upp av celler de i sin tur består av mindre beständsdelar livets molekyler Dessa fungerar som mekaniska byggstenar likt maskiner och robotar som sliter vid fabriken band envar utförandes en absolut nödvändig funktion för cellens och hela kroppens fortsatta verksamhet De av livets molekyler som beskrivs centralt i den här avhandlingen är proteiner vilka i sin tur består utav en lång kedja med olika typer av länkar som likt garn lindar upp sig i ett nystan av en mer eller mindre bestämd struktur som avgör dess roll och funktion i cellen Intrinsiskt oordnade proteiner IDP går emot denna enkla skildring de är proteiner som saknar struktur och beter sig mer likt spaghetti i vatten än en maskin IDP är en funktionell och bör spela centrala roller i cellens maskineri exempelvis oncoproteinet c

Myc som agerar gaspedal för cellen fel i c-Myc:s funktion leder till att cellerna löper amok delar sig hejdlöst och vi får cancer. Man har upptäckt att c-Myc har en ombytlig struktur vi inte kan se studier av punktvisa förändringar/mutationer i kedjan av byggstenar hos c-Myc visar att många länkar har viktiga roller i funktionen. Detta ger oss bättre förståelse om cancer men samtidigt är laboratoriearbetet både komplicerat och dyrt här kan evolutionen hjälpa oss och avslöja hemligheterna snabbare. Molekylär evolution studeras genom att beräkna variation i proteinkedjan mellan beslötade arter som finns lagrade i databaser detta visar snabbt via nätverksanalys och grafteori vilka delar av proteinet som är centrala och kopplade till varandra av nätverksmängd för artens fortlevnad. Påvisar här evolutionen oss att förstå proteinfunktioner via modeller baserade på proteinernas interaktioner snarare än deras struktur. Samma modeller kan nyttjas för att förstå dynamiska flöden och skillnader mellan normala och patologiska varianter av proteiner. Mutationer kan uppstå i vår arvsmassa som kan leda till sjukdom. Genom analys av proteinernas kopplingsnätverk i grafmodellerna kan man bättre förstå vilka mutationer som är farligare än andra. Dessutom har det visat sig att en sådan representation kan ge bättre förståelse för den normala funktionen hos ett protein än vad en proteinstruktur kan. Här introduceras även konceptet proteinprimär vilket är en abstrakt representation av proteiner centrerad på deras interaktiva mönster snarare än på partikulär form och struktur. Det är en förhoppning att en sådan representation skall förklara diskussionen anbelangande proteinfunktioner till den grad att strukturbestämelse av proteiner som är en mycket kostsam och tidskrävande process till viss mån kan anses vara sekundär i betydelse jämfört med funktionellt modellerande baserat på evolutionär data extraherade ur våra sekvensdatabaser.

Structural Bioinformatics Jenny Gu, Philip E. Bourne, 2011-09-20 Structural Bioinformatics was the first major effort to show the application of the principles and basic knowledge of the larger field of bioinformatics to questions focusing on macromolecular structure such as the prediction of protein structure and how proteins carry out cellular functions and how the application of bioinformatics to these life science issues can improve healthcare by accelerating drug discovery and development. Designed primarily as a reference the first edition nevertheless saw widespread use as a textbook in graduate and undergraduate university courses dealing with the theories and associated algorithms resources and tools used in the analysis prediction and theoretical underpinnings of DNA RNA and proteins. This new edition contains not only thorough updates of the advances in structural bioinformatics since publication of the first edition but also features eleven new chapters dealing with frontier areas of high scientific impact including sampling and search techniques use of mass spectrometry genome functional annotation and much more. Offering detailed coverage for practitioners while remaining accessible to the novice Structural Bioinformatics Second Edition is a valuable resource and an excellent textbook for a range of readers in the bioinformatics and advanced biology fields. Praise for the previous edition: This book is a gold mine of fundamental and practical information in an area not previously well represented in book form. Biochemistry and Molecular Education destined to become a classic reference work for workers at all levels in structural bioinformatics recommended.

with great enthusiasm for educators researchers and graduate students BAMBED a useful and timely summary of a rapidly expanding field Nature Structural Biology a terrific job in this timely creation of a compilation of articles that appropriately addresses this issue Briefings in Bioinformatics 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 **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 **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

**Computational Methods for Protein Structure Prediction and Modeling** Ying Xu,Dong Xu,Jie Liang,2007-08-24 Volume One of this two volume sequence focuses on the basic characterization of known protein structures and structure prediction from protein sequence information Eleven chapters survey of the field covering key topics in modeling force fields classification computational methods and structure prediction Each chapter is a self contained review covering definition of the problem and historical perspective mathematical formulation computational methods and algorithms performance results existing software strengths pitfalls challenges and future research

Structural Bioinformatics of Membrane Proteins D. Frishman,2011-01-22 This book is the first one specifically dedicated to the structural bioinformatics of membrane proteins With a focus on membrane proteins from the perspective of bioinformatics the present work covers a broad spectrum of topics in evolution structure function and bioinformatics of membrane proteins focusing on the most recent experimental results Leaders in the field who have recently reported breakthrough advances cover algorithms databases and their applications to the subject The increasing number of recently solved membrane protein structures makes the expert coverage presented here very timely Structural bioinformatics of membrane proteins has been an active area of research over the last three decades and proves to be a growing field of interest

*Bioinformatics* Christine Orengo,David Jones,Janet Thornton,2003-12-16 Bioinformatics the use of computers to address biological questions has become an essential tool in biological research It is one of the critical keys needed to unlock the information encoded in the flood of data generated by genome protein structure transcriptome and proteome research Bioinformatics Genes Proteins Computers covers both the more traditional approaches to bioinformatics including gene and protein sequence analysis and structure prediction and more recent technologies such as datamining of transcriptomic and proteomic data to provide insights on cellular mechanisms and the causes of disease

*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

**Protein Structure Prediction** Anna Tramontano, 2006-02-20 While most textbooks on bioinformatics focus on genetic algorithms and treat protein structure prediction only superficially this course book assumes a novel and unique focus Adopting a didactic approach the author explains all the current methods in terms of their reliability limitations and user friendliness She provides practical examples to help first time users become familiar with the possibilities and pitfalls of computer based structure prediction making this a must have for students and researchers

*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

**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

**Protein Structure and Function** Gregory Petsko, Dagmar Ringe, 2008-05-29 Protein Structure and Function provides a critical survey of our current understanding protein structure and function in the age of genomics Moving from sequence to structure and structure to function the book also explores the link between sequence and function in a series of case studies in structural and functional genomics

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