

Daniel J. Rigden  
*Editor*

# From Protein Structure to Function with Bioinformatics



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# From Protein Structure To Function With Bioinformatics

## Author Daniel John Rigden May 2009

**Z.H. Zaidi, D.L. Smith**



## **From Protein Structure To Function With Bioinformatics Author Daniel John Rigden May 2009:**

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

**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

**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 *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 **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 nanostructures 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

M niskan byggs upp av celler de i sin tur best r av n mindre best ndsdelar livets molekyler Dessa fungerar som mekaniska byggstenar likt maskiner och robotar som sliter vid fabrikens band envar utf randes en absolut n dv ndig funktion f r cellens och hela kroppens fortsatta verlevnad De av livets molekyler som beskrivs centralt i den h r avhandling r proteiner vilka i sin tur best r utav en l ng kedja med olika typer av l nkar som likt garn lindar upp sig i ett nystan av en mer eller mindre best md struktur som avg r dess roll och funktion i cellen Intrinsiellt oordnade proteiner IDP g r emot denna enkla sk dning de r proteiner som saknar struktur och beter sig mer likt spaghetti i vatten n en maskin IDP r nd funktionella och b r p centrala roller i cellens maskineri exempel r oncoproteinet c Myc som agerar gaspedal f r cellen fel i c Myc s funktion leder till att cellerna l per amok delar sig hejdl st och vi f r cancer Man har uppt ckt att c Myc har en ombytlig struktur vi inte kan se studier av punktvisa f r ndrningar mutationer i kedjan av byggstenar hos c Myc visar att m nga l nkar har viktiga roller i funktionen Detta ger oss b ttre f rst else om cancer men samtidigt r laboratoriearbetet b de komplicerat och dyrt h r kan evolutionen v gleda oss och avsl ja hemligheterna snabbare Molekyl r evolution studeras genom att ber kna variation i proteinkedjan mellan besl ktade arter som finns lagrade i databaser detta visar snabbt via n tverksanalys och grafteori vilka

delar av proteinet som är centrala och kopplade till varandra av en dyndighet för artens fortlevnad. På så vis hjälper evolutionen oss att först proteinfunktioner via modeller baserade på proteinernas interaktioner snarare än deras struktur. Samma modeller kan nyttjas för att först dynamiska flöpp och skillnader mellan normala och patologiska varianter av proteiner. Mutationer kan uppstå i vår arvs massa 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 förstelse 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 evolutionära data extraherade ur våra

sekvensdatabaser **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 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. **Introduction to Protein Structure** Carl-Ivar Brändén, John Tooze, 1999

This new edition gives an up to date account of the principles of protein structure with examples of key proteins in their biological context illustrated in colour to illuminate the structural principles described in the text. **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      **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      *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      The Structure and Function of Biological Networks Daniel Duanqing Wu, Xiaohua Hu, 2010  
*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

**Protein Structure — Function Relationship** Z.H. Zaidi,D.L. Smith,1996-10-31 Although many pursue understanding of the relationship between protein structure and function for the thrill of pure science the pay off in a much broader sense is the ability to manipulate the Earth s chemistry and biology to improve the quality of life for mankind Immediately goals of this area of research include identification of the life supporting functions of proteins and the fundamental forces that facilitate these functions Upon reaching these goals we shall have the understanding to direct and the tools required to implement changes that will dramatically improve the quality of life For example under standing the chemical mechanism of diseases will facilitate development of new therapeutic drugs Likewise understanding of chemical mechanisms of plant growth will be used with biotechnology to improve food production under adverse climatic conditions The challenge to understand details of protein structure function relationships is enormous and requires an international effort for success To direct the chemistry and biology of our environment in a positive sense will require efforts from bright imaginative scientists located throughout the world Although the emergence of FAX e mail and the World Wide Web has revolutionized international communication there remains a need for scientists located in distant parts of the world to occasionally meet face to face

*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

*Practical Protein Bioinformatics* Florencio Pazos,Mónica Chagoyen,2014-12-11 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      *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      **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

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