

Sequence Based Prediction Of Protein Solubility

In Gene Sharing and Evolution Piatigorsky explores the generality and implications of gene sharing throughout evolution and argues that most if not all proteins perform a variety of functions in the same and in different species, and that this is a fundamental necessity for evolution.

This thorough volume explores predicting one-dimensional functional properties, functional sites in particular, from protein sequences, an area which is getting more and more attention. Beginning with secondary structure prediction based on sequence only, the book continues by exploring secondary structure prediction based on evolution information, prediction of solvent accessible surface areas and backbone torsion angles, model building, global structural properties, functional properties, as well as visualizing interior and protruding regions in proteins. Written for the highly successful Methods in Molecular Biology series, the chapters include the kind of detail and implementation advice to ensure success in the laboratory. Practical and authoritative, Prediction of Protein Secondary Structure serves as a vital guide to numerous state-of-the-art techniques that are useful for computational and experimental biologists.

Detailed characterization of fuzzy interactions will be of central importance for understanding the diverse biological functions of intrinsically disordered proteins in complex eukaryotic signaling networks. In this volume, Peter Tompa and Monika Fuxreiter have assembled a series of papers that address the issue of fuzziness in molecular interactions. These papers provide a broad overview of the phenomenon of fuzziness and provide compelling examples of the central role played by fuzzy interactions in regulation of cellular signaling processes and in viral infectivity. These contributions summarize the current state of knowledge in this new field and will undoubtedly stimulate future research that will further advance our understanding of fuzziness and its role in biomolecular interactions.

Volume Two of this two-volume sequence presents a comprehensive overview of protein structure prediction methods and includes protein threading, De novo methods, applications to membrane proteins and protein complexes, structure-based drug design, as well as structure prediction as a systems problem. A series of appendices review the biological and chemical basics related to protein structure, computer science for structural informatics, and prerequisite mathematics and statistics.

Summing up almost a decade of biomedical research, this topical and eagerly awaited handbook is the first reference on the topic to incorporate recent breakthroughs in amyloid research. The first part covers the structural biology of amyloid fibrils and pre-fibrillar assemblies, including a description of current models for amyloid formation. The second part looks at the diagnosis and biomedical study of amyloid in humans and in animal models, while the final section discusses pharmacological approaches to manipulating amyloid and also looks at its physiological roles in lower and higher organisms. For Biochemists, Molecular Biologists, Neurobiologists, Neurophysiologists and those working in the Pharmaceutical Industry.

Proteins continuously interact with each other to determine cell fate. Consequently, an examination of just when such protein-protein interactions occur and how they are controlled is essential for understanding the molecular mechanism of biological processes, elucidating the molecular basis of diseases, and identifying potential targets for therapeutic interventions. In Protein-Protein Interactions: Methods and Applications, leading experts describe in detail their highly successful biochemical, biophysical, genetic, and computational techniques for studying these interactions. Their readily reproducible methods demonstrate how to identify protein interaction partners, qualitatively or

quantitatively measure protein-protein interactions, monitor protein-protein interactions as they occur in living cells, and determine interaction interfaces. The techniques described utilize a variety of cutting-edge technologies, including surface plasmon resonance (SRP), fluorescence resonance energy transfer (FRET), fluorescence polarization (FP), isothermal titration calorimetry (ITC), circular dichroism (CD), protein fragment complementation assays (PCA), various two-hybrid systems, and proteomics- and bioinformatics-based approaches, such as the Scansite program for computational analysis. Each time-tested protocol includes a background introduction outlining the principle behind the technique, lists of equipment and reagents, and tips on troubleshooting and avoiding known pitfalls. Authoritative and highly practical, *Protein-Protein Interactions: Methods and Applications* offers both beginning and experienced investigators a full range of the powerful tools needed for deciphering how proteins interact to form biological networks, as well as for unraveling protein-protein interactions in disease in the search for novel therapeutic targets.

Essential Bioinformatics is a concise yet comprehensive textbook of bioinformatics, which provides a broad introduction to the entire field. Written specifically for a life science audience, the basics of bioinformatics are explained, followed by discussions of the state-of-the-art computational tools available to solve biological research problems. All key areas of bioinformatics are covered including biological databases, sequence alignment, genes and promoter prediction, molecular phylogenetics, structural bioinformatics, genomics and proteomics. The book emphasizes how computational methods work and compares the strengths and weaknesses of different methods. This balanced yet easily accessible text will be invaluable to students who do not have sophisticated computational backgrounds. Technical details of computational algorithms are explained with a minimum use of mathematical formulae; graphical illustrations are used in their place to aid understanding. The effective synthesis of existing literature as well as in-depth and up-to-date coverage of all key topics in bioinformatics make this an ideal textbook for all bioinformatics courses taken by life science students and for researchers wishing to develop their knowledge of bioinformatics to facilitate their own research.

Researchers in many disciplines face the formidable task of analyzing massive amounts of high-dimensional and highly-structured data. This is due in part to recent advances in data collection and computing technologies. As a result, fundamental statistical research is being undertaken in a variety of different fields. Driven by the complexity of these new problems, and fueled by the explosion of available computer power, highly adaptive, non-linear procedures are now essential components of modern "data analysis," a term that we liberally interpret to include speech and pattern recognition, classification, data compression and signal processing. The development of new, flexible methods combines advances from many sources, including approximation theory, numerical analysis, machine learning, signal processing and statistics. The proposed workshop intends to bring together eminent experts from these fields in order to exchange ideas and forge directions for the future.

This book presents the latest developments in bioinformatics, highlighting the importance of bioinformatics in genomics, transcriptomics, metabolism and cheminformatics analysis, as well as in drug discovery and development. It covers tools, data mining and analysis, protein analysis, computational vaccine, and drug design. Covering cheminformatics, computational evolutionary biology and the role of next-generation sequencing and neural network analysis, it also discusses the use of bioinformatics tools in the development of precision medicine. This book offers a valuable source of information for not only

beginners in bioinformatics, but also for students, researchers, scientists, clinicians, practitioners, policymakers, and stakeholders who are interested in harnessing the potential of bioinformatics in many areas.

Given the immense progress achieved in elucidating protein-protein complex structures and in the field of protein interaction modeling, there is great demand for a book that gives interested researchers/students a comprehensive overview of the field. This book does just that. It focuses on what can be learned about protein-protein interactions from the analysis of protein-protein complex structures and interfaces. What are the driving forces for protein-protein association? How can we extract the mechanism of specific recognition from studying protein-protein interfaces? How can this knowledge be used to predict and design protein-protein interactions (interaction regions and complex structures)? What methods are currently employed to design protein-protein interactions, and how can we influence protein-protein interactions by mutagenesis and small-molecule drugs or peptide mimetics? The book consists of about 15 review chapters, written by experts, on the characterization of protein-protein interfaces, structure determination of protein complexes (by NMR and X-ray), theory of protein-protein binding, dynamics of protein interfaces, bioinformatics methods to predict interaction regions, and prediction of protein-protein complex structures (docking and homology modeling of complexes, etc.) and design of protein-protein interactions. It serves as a bridge between studying/analyzing protein-protein complex structures (interfaces), predicting interactions, and influencing/designing interactions.

Probabilistic models are becoming increasingly important in analysing the huge amount of data being produced by large-scale DNA-sequencing efforts such as the Human Genome Project. For example, hidden Markov models are used for analysing biological sequences, linguistic-grammar-based probabilistic models for identifying RNA secondary structure, and probabilistic evolutionary models for inferring phylogenies of sequences from different organisms. This book gives a unified, up-to-date and self-contained account, with a Bayesian slant, of such methods, and more generally to probabilistic methods of sequence analysis. Written by an interdisciplinary team of authors, it aims to be accessible to molecular biologists, computer scientists, and mathematicians with no formal knowledge of the other fields, and at the same time present the state-of-the-art in this new and highly important field.

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.

Sequence - Evolution - Function is an introduction to the computational approaches that play a critical role in the emerging new branch of biology known as functional genomics. The book provides the reader with an understanding of the principles and approaches of functional genomics and of the potential and limitations of computational and experimental approaches to genome analysis. Sequence - Evolution - Function should help bridge the "digital divide" between biologists and computer scientists, allowing biologists to better grasp the peculiarities of the emerging field of Genome Biology and to learn how to benefit from the enormous amount of sequence data available in the public databases. The book is non-technical with respect to the computer methods for genome analysis and discusses these methods from the user's viewpoint, without addressing mathematical and algorithmic details. Prior practical familiarity with the basic methods for sequence analysis is a major advantage, but a reader without such experience will be able to use the book as an introduction to these methods. This book is perfect for introductory level courses in computational methods for comparative and functional genomics.

Homology modeling is an extremely useful and versatile technique that is gaining more and more space and demand in research in computational and theoretical biology. This book, "Homology Molecular Modeling - Perspectives and Applications", brings together unpublished chapters on this technique. In this book, 7 chapters are intimately related to the theme of molecular modeling, carefully selected and edited for academic and scientific readers. It is an indispensable read for anyone interested in the areas of bioinformatics and computational biology. Divided into 4 sections, the reader will have a didactic and comprehensive view of the theme, with updated and relevant concepts on the subject. This book was organized from researchers to researchers with the aim of spreading the fascinating area of molecular modeling by homology.

"In this book, Andy Baxevanis and Francis Ouellette . . . have undertaken the difficult task of organizing the knowledge in this field in a logical progression and presenting it in a digestible form. And they have done an excellent job. This fine text will make a major impact on biological research and, in turn, on progress in biomedicine. We are all in their debt." —Eric Lander from the Foreword Reviews from the First Edition
"...provides a broad overview of the basic tools for sequence analysis ... For biologists approaching this subject for the first time, it will be a very useful handbook to keep on the shelf after the first reading, close to the computer." —Nature Structural Biology "...should be in the personal library of any biologist who uses the Internet for the analysis of DNA and protein sequence data." —Science "...a wonderful primer designed to navigate the novice through the intricacies of in scripto analysis ... The accomplished gene searcher will also find this book a useful addition to their library ... an excellent reference to the principles of bioinformatics." —Trends in Biochemical Sciences
This new edition of the highly successful *Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins* provides a sound foundation of basic concepts, with practical discussions and comparisons of both computational tools and databases relevant to biological research. Equipping biologists with the modern tools necessary to solve practical problems in sequence data analysis, the Second Edition covers the broad spectrum of topics in bioinformatics, ranging from Internet concepts to predictive algorithms used on sequence, structure, and expression data. With

chapters written by experts in the field, this up-to-date reference thoroughly covers vital concepts and is appropriate for both the novice and the experienced practitioner. Written in clear, simple language, the book is accessible to users without an advanced mathematical or computer science background. This new edition includes: All new end-of-chapter Web resources, bibliographies, and problem sets
Accompanying Web site containing the answers to the problems, as well as links to relevant Web resources
New coverage of comparative genomics, large-scale genome analysis, sequence assembly, and expressed sequence tags
A glossary of commonly used terms in bioinformatics and genomics
Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins, Second Edition is essential reading for researchers, instructors, and students of all levels in molecular biology and bioinformatics, as well as for investigators involved in genomics, positional cloning, clinical research, and computational biology.

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.

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.

An introduction to machine learning methods and their applications to problems in bioinformatics Machine learning techniques are increasingly being used to address problems in computational biology and bioinformatics. Novel computational techniques to analyze high throughput data in the form of sequences, gene and protein expressions, pathways, and images are becoming vital for understanding diseases and future drug discovery. Machine learning techniques such as Markov models, support vector machines, neural networks, and graphical models have been successful in analyzing life science data because of their capabilities in handling randomness and uncertainty of data noise and in generalization. From an internationally recognized panel of prominent researchers in the field, Machine Learning in Bioinformatics compiles recent approaches in machine learning methods and their applications in addressing contemporary problems in

bioinformatics. Coverage includes: feature selection for genomic and proteomic data mining; comparing variable selection methods in gene selection and classification of microarray data; fuzzy gene mining; sequence-based prediction of residue-level properties in proteins; probabilistic methods for long-range features in biosequences; and much more. Machine Learning in Bioinformatics is an indispensable resource for computer scientists, engineers, biologists, mathematicians, researchers, clinicians, physicians, and medical informaticists. It is also a valuable reference text for computer science, engineering, and biology courses at the upper undergraduate and graduate levels. Molecular Toxinology has been consolidated as a scientific area focused on the intertwined description of several aspects of animal toxins. In an inquiring biotechnological world, animal toxins appear as an invaluable source for the discovery of therapeutic polypeptides. Animal toxins rely on specific chemical interactions with their partner molecule to exert their biological actions. The comprehension of how molecules interact and recognize their target is essential for the rational exploration of bioactive polypeptides as therapeutics. Investigation on the mechanism of molecular interaction and recognition offers a window of opportunity for the pharmaceutical industry and clinical medicine. Thus, this book brings examples of two interconnected themes - molecular recognition and toxinology concerning to the integration between analytical procedures and biomedical applications.

Select Agents are defined in regulations through a list of names of particularly dangerous known bacteria, viruses, toxins, and fungi. However, natural variation and intentional genetic modification blur the boundaries of any discrete Select Agent list based on names. Access to technologies that can generate or 'synthesize' any DNA sequence is expanding, making it easier and less expensive for researchers, industry scientists, and amateur users to create organisms without needing to obtain samples of existing stocks or cultures. This has led to growing concerns that these DNA synthesis technologies might be used to synthesize Select Agents, modify such agents by introducing small changes to the genetic sequence, or create entirely new pathogens. Amid these concerns, the National Institutes of Health requested that the Research Council investigate the science and technology needed to replace the current Select Agent list with an oversight system that predicts if a DNA sequence could be used to produce an organism that should be regulated as a Select Agent. A DNA sequence-based system to better define when a pathogen or toxin is subject to Select Agent regulations could be developed. This could be coupled with a 'yellow flag' system that would recognize requests to synthesize suspicious sequences and serve as a reference to anyone with relevant questions, allowing for appropriate follow-up. Sequence-Based Classification of Select Agents finds that replacing the current list of Select Agents with a system that could predict if fragments of DNA sequences could be used to produce novel pathogens with Select Agent characteristics is not feasible. However, it emphasized that for the foreseeable future, any threat from synthetic biology and synthetic genomics is far more likely to come from assembling known Select Agents, or modifications of them, rather than construction of previously unknown agents. Therefore, the book recommends modernizing the regulations to define Select Agents in terms of their gene sequences, not by their names, and called this 'sequence-based classification.'

Sequence-based Prediction of Protein-protein Interactions
Study on Sequence Based Prediction of Protein B-factors
Prediction of Protein Structures, Functions, and Interactions
John Wiley & Sons

This book is intended for those wishing to acquire a working knowledge of orthogonal transforms in the area of digital signal processing. The authors hope that their introduction will enhance the opportunities for interdisciplinary work in this field. The book consists of ten chapters. The first seven chapters are devoted to the study of the background, motivation and development of orthogonal transforms, the prerequisites for which are a basic knowledge of Fourier series transform (e.g. via a course in differential equations) and matrix algebra. The last three

chapters are relatively specialized in that they are directed toward certain applications of orthogonal transforms in digital signal processing. As such, a knowledge of discrete probability theory is an essential additional prerequisite. A basic knowledge of communication theory would be helpful, although not essential. Much of the material presented here has evolved from graduate level courses offered by the Departments of Electrical Engineering at Kansas State University and the University of Texas at Arlington, during the past five years. With advanced graduate students, all the material was covered in one semester. In the case of first year graduate students, the material in the first seven chapters was covered in one semester. This was followed by a problems project-oriented course directed toward specific applications, using the material in the last three chapters as a basis.

This volume presents a collection of computational and experimental protocols pertaining to the creation, characterization, and utilization of RNA nanostructures. The chapters in this book cover topics such as ion effects in RNA folding; design and crystallography of self-assembling RNA nanostructures; x-aptamer selection and validation; RNAi in HIV-infected cells; and preparation of a conditional RNA switch. 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 protocols, and tips on troubleshooting and avoiding known pitfalls. Cutting-edge and thorough, RNA Nanostructures: Methods and Protocols is a valuable resource for the design and production of RNA nanostructures. Researchers and scientists sharing these detailed protocols is important for sustained progress in the field.

This is a comprehensive introduction to Landau-Lifshitz equations and Landau-Lifshitz-Maxwell equations, beginning with the work by Yulin Zhou and Boling Guo in the early 1980s and including most of the work done by this Chinese group led by Zhou and Guo since. The book focuses on aspects such as the existence of weak solutions in multi dimensions, existence and uniqueness of smooth solutions in one dimension, relations with harmonic map heat flows, partial regularity and long time behaviors. The book is a valuable reference book for those who are interested in partial differential equations, geometric analysis and mathematical physics. It may also be used as an advanced textbook by graduate students in these fields.

This volume details several important databases and data mining tools. Data Mining Techniques for the Life Sciences, Second Edition guides readers through archives of macromolecular three-dimensional structures, databases of protein-protein interactions, thermodynamics information on protein and mutant stability, "Kbdock" protein domain structure database, PDB_REDO databank, erroneous sequences, substitution matrices, tools to align RNA sequences, interesting procedures for kinase family/subfamily classifications, new tools to predict protein crystallizability, metabolomics data, drug-target interaction predictions, and a recipe for protein-sequence-based function prediction and its implementation in the latest version of the ANNOTATOR software suite. 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 protocols, and tips on troubleshooting and avoiding known pitfalls. Authoritative and cutting-edge, Data Mining Techniques for the Life Sciences, Second Edition aims to ensure successful results in the further study of this vital field.

This book constitutes the refereed proceedings of the First International Symposium on Computational Life Sciences, CompLife 2005, held in Konstanz, Germany in September 2005. The 21 revised full papers presented together with 3 papers of a workshop on Distributed Data Mining in the Life Sciences (LifeDDM) were carefully reviewed and selected from 49 initial submissions. The papers cover areas ranging from high-level system biology to data analysis related to mass spec traces and are organized in topical sections on systems biology, data analysis and integration, structural biology, genomics, computational proteomics, molecular informatics, molecular structure determination and

simulation, and distributed data mining.

In this, the post-genomic age, our knowledge of biological systems continues to expand and progress. As the research becomes more focused, so too does the data. Genomic research progresses to proteomics and brings us to a deeper understanding of the behavior and function of protein clusters. And now proteomics gives way to neuroproteomics as we begin to unravel the complex mysteries of neurological diseases that less than a generation ago seemed opaque to our inquiries, if not altogether intractable. Edited by Dr. Oscar Alzate, *Neuroproteomics* is the newest volume in the CRC Press Frontiers of Neuroscience Series. With an extensive background in mathematics and physics, Dr. Alzate exemplifies the newest generation of biological systems researchers. He organizes research and data contributed from all across the world to present an overview of neuroproteomics that is practical and progressive. Bolstered by each new discovery, researchers employing multiple methods of inquiry gain a deeper understanding of the key biological problems related to brain function, brain structure, and the complexity of the nervous system. This in turn is leading to new understanding about diseases of neurological deficit such as Parkinson's and Alzheimer's. Approaches discussed in the book include mass spectrometry, electrophoresis, chromatography, surface plasmon resonance, protein arrays, immunoblotting, computational proteomics, and molecular imaging. Writing about their own work, leading researchers detail the principles, approaches, and difficulties of the various techniques, demonstrating the questions that neuroproteomics can answer and those it raises. New challenges wait, not the least of which is the identification of potential methods to regulate the structures and functions of key protein interaction networks. Ultimately, those building on the foundation presented here will advance our understanding of the brain and show us ways to abate the suffering caused by neurological and mental diseases.

A multi-discipline, hands-on guide to microarray analysis of biological processes *Analyzing Microarray Gene Expression Data* provides a comprehensive review of available methodologies for the analysis of data derived from the latest DNA microarray technologies. Designed for biostatisticians entering the field of microarray analysis as well as biologists seeking to more effectively analyze their own experimental data, the text features a unique interdisciplinary approach and a combined academic and practical perspective that offers readers the most complete and applied coverage of the subject matter to date. Following a basic overview of the biological and technical principles behind microarray experimentation, the text provides a look at some of the most effective tools and procedures for achieving optimum reliability and reproducibility of research results, including: An in-depth account of the detection of genes that are differentially expressed across a number of classes of tissues Extensive coverage of both cluster analysis and discriminant analysis of microarray data and the growing applications of both methodologies A model-based approach to cluster analysis, with emphasis on the use of the EMMIX-GENE procedure for the clustering of tissue samples The latest data cleaning and normalization procedures The uses of microarray expression data for providing important prognostic information on the outcome of disease

A guide to machine learning approaches and their application to the analysis of biological data. An unprecedented wealth of data is being generated by genome sequencing projects and other experimental efforts to determine the structure and function of biological molecules. The demands and opportunities for interpreting these data are expanding rapidly. Bioinformatics is the development and application of computer methods for management, analysis, interpretation, and prediction, as well as for the design of experiments. Machine learning approaches (e.g., neural networks, hidden Markov models, and belief networks) are ideally suited for areas where there is a lot of data but little theory, which is the situation in molecular biology. The goal in machine

learning is to extract useful information from a body of data by building good probabilistic models—and to automate the process as much as possible. In this book Pierre Baldi and Søren Brunak present the key machine learning approaches and apply them to the computational problems encountered in the analysis of biological data. The book is aimed both at biologists and biochemists who need to understand new data-driven algorithms and at those with a primary background in physics, mathematics, statistics, or computer science who need to know more about applications in molecular biology. This new second edition contains expanded coverage of probabilistic graphical models and of the applications of neural networks, as well as a new chapter on microarrays and gene expression. The entire text has been extensively revised.

This detailed volume explores the continuing techniques of studying RNA-protein complexes and interactions as research in these areas expand. After an introductory chapter, the book continues with ways to purify RNA-protein complexes assembled in cells or in isolated cellular extracts, methods for measuring various biochemical activities of RNA-interacting proteins or ribonucleoproteins, biochemical methods for measuring direct RNA-protein contact, as well as various new or innovative methods pertinent to the subject. Written for the highly successful *Methods in Molecular Biology* series, chapters contain brief introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible laboratory protocols, and tips on troubleshooting and avoiding known pitfalls. Authoritative and up-to-date, *RNA-Protein Complexes and Interactions: Methods and Protocols* provides a set of useful protocols, both basic and advanced, designed to inspire researchers working with RNA and RNA-interacting proteins.

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.

Ranging from the evolution of pathogenicity to oceanic carbon cycling, the many and varied roles that bacteriophages play in microbial ecology and evolution have inspired increased interest within the scientific community. *Bacteriophages: Methods and Protocols* pulls together the vast body of knowledge and expertise from top international bacteriophage researchers to provide both classical and state-of-the-art molecular techniques. With its well-organized modular design, *Volume 2: Molecular and Applied Aspects* examines a multitude of topics, including the bacteriophage genomics, metagenomics, transcriptomics, and proteomics, along with applied bacteriophage biology. Written in the highly successful *Methods in Molecular Biology*™ series format, chapters consist of brief introductions to the subject, lists of the necessary materials and reagents, readily reproducible laboratory protocols, and a Notes section which details tips on troubleshooting and avoiding known pitfalls. Thorough and cutting-edge, *Bacteriophages: Methods and Protocols* is a valuable reference for experienced bacteriophage researchers as well as an easily accessible introduction for newcomers to the subject.

The prediction of the conformation of proteins has developed from an intellectual exercise into a serious practical endeavor that has great promise to yield new stable enzymes, products of pharmacological significance, and catalysts of great potential. With the application of prediction gaining momentum in various fields, such as enzymology and immunology, it was deemed time that a volume be published to make available a thorough evaluation of present methods, for researchers in this field to expound fully the virtues of various algorithms, to open the field to a wider audience, and to offer the scientific public an opportunity to examine carefully its successes and failures. In this manner the practitioners of the art could better evaluate the tools and the output so that their expectations and applications could be more realistic. The editor has assembled chapters by many of the main contributors to this area and simultaneously placed their programs at three national resources so that they are readily available to those who wish to apply them to their personal interests. These algorithms, written by their originators, when utilized on personal or larger computers, can instantaneously take a primary amino acid sequence and produce a two- or three-dimensional artistic image that gives satisfaction to one's esthetic sensibilities and food for thought concerning the structure and function of proteins. It is in this spirit that this volume was envisaged.

Protein folding is a process by which a protein structure assumes its functional shape of conformation, and has been the subject of research since the publication of the first software tool for protein structure prediction. Protein folding *in silico* approaches this issue by introducing an *ab initio* model that attempts to simulate as far as possible the folding process as it takes place *in vivo*, and attempts to construct a mechanistic model on the basis of the predictions made. The opening chapters discuss the early stage intermediate and late stage intermediate models, followed by a discussion of structural information that affects the interpretation of the folding process. The second half of the book covers a variety of topics including ligand binding site recognition, the "fuzzy oil

drop" model and its use in simulation of the polypeptide chain, and misfolded proteins. The book ends with an overview of a number of other ab initio methods for protein structure predictions and some concluding remarks. Discusses a range of ab initio models for protein structure prediction Introduces a unique model based on experimental observations Describes various methods for the quantitative assessment of the presented models from the viewpoint of information theory

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