Computational biology is a rapidly expanding field, and the number and variety of computational methods used for DNA and protein sequence analysis is growing every day. These algorithms are extremely valuable to biotechnology companies and to researchers and teachers in universities. This book explains the latest computer technology for analyzing DNA, RNA, and protein sequences. Clear and easy to follow, designed specifically for the non-computer scientist, it will help biologists make better choices on which algorithm to use. New techniques and demonstrations are elucidated, as are state-of-the-art problems, and more advanced material on the latest algorithms. The primary audience for this volume are molecular biologists working either in biotechnology companies or academic research environments, individual researchers and the institutions they work for, and students. Any biologist who relies on computers should want this book. A secondary audience will be computer scientists developing techniques with applications in biology. An excellent reference for leading techniques, it will also help introduce computer scientists to the biology problems. This is an outstanding work which will be ideal for the increasing number of researchers and the institutions they work for, and students. Any biologist who relies on computers should want this book. A secondary audience will be computer scientists developing techniques with applications in biology. An excellent reference for leading techniques, it will also help introduce computer scientists to the biology problems. This is an outstanding work which will be ideal for the increasing number of scientists moving into computational biology.

Providing systematic technical expositions of the computational methods for major aspects of protein structure analysis, prediction and modelling, this work focuses on the basic characterisation of known protein structures as well as structure prediction from protein sequence information.

A Step-by-Step Guide to Describing Biomolecular Structure Computational and Visualization Techniques for Structural Bioinformatics Using Chimera shows how to perform computations with Python scripts in the Chimera environment. It focuses on the three core areas needed to study structural bioinformatics: biochemistry, mathematics, and computation. Understand Important Concepts of Structural Bioinformatics The book covers topics that deal primarily with protein structure and includes many exercises that are grounded in biological problems at the molecular level. The text encourages mathematical analysis by providing a firm foundation for computations. It analyzes numerous Python scripts for the Chimera environment, with the scripts and other materials available on a supplementary website. Build Python Scripts to Extend the Capabilities of Chimera Through more than 60 exercises that involve the development of Python scripts, the book gives you concrete guidance on using the scripting capabilities of Chimera. You'll gain experience in solving real problems as well as understand the various applications of linear algebra. You can also use the scripts as starting points for the development of similar applications and use classes from the structBio toolkit for computations, such as structure overlap, data plotting, thiệnchographies, and display of residue networks.

Proteins: Structure and Function is a comprehensive introduction to the study of proteins and their importance to modern biochemistry. Each chapter addresses the structure and function of proteins with a definitive theme designed to enhance student understanding. Opening with a brief historical overview of the subject the book moves on to discuss the ‘building blocks’ of proteins and their respective chemical and physical properties. Later chapters explore experimental and computational methods of comparing proteins, methods of protein purification and protein folding and stability. The latest developments in the field are included and key concepts introduced in a user-friendly way to ensure that students are able to grasp the essentials before moving on to more advanced study and analysis of proteins. An invaluable resource for students of Biochemistry, Molecular Biology, Medicine and Chemistry providing a modern approach to the subject of Proteins. 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 much improved picture of its molecular function. This realization 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 tests 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.

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 methods to study protein structures and residues. A valuable reference, this
book reflects current trends in the effort to solve new structures arising from genome initiatives, details methods to detect and identify errors
in the prediction of protein structural models, and outlines challenges in the conversion of routine processes into high-throughput platforms.

Protein-protein interactions underlie all biological processes and are a field of study that has wide implications throughout many other fields
including medicine, genetics, biology, and ecology. Proteins are the building blocks and primary actors of life. They work together to
accomplish virtually every task within a cell, including, metabolism, signal propagation, immune responses, and cell signaling. This problem is
a logical successor to the Human Genome Project: now that we know so much about the DNA of living organisms, how do we advance our
knowledge? The Human Genome and other DNA sequencing efforts have provided complete genetic sequences for more than 180 living
organisms. However, these efforts fall short of describing or predicting life processes because the sequence of a protein is not enough to
evaculate its function. Knowing this, the National Institute of Health started the Protein Structure Initiative, which seeks to increase knowledge
of protein structure and has led to an increase in the number of known protein structures. Unfortunately, even these efforts fall short as
there are over 80,000 known protein structures but the function of many is completely unknown. The fledgling field of interface prediction
seeks to use this wealth of structural information to be able to describe protein function and drastically increase our understanding of life
processes. Presented herein is a novel methodology for solving the protein-protein interface prediction problem leveraging a variety of
Computer Science techniques. Specifically detailed is a process for decomposing this 3-dimensional problem into a feature extraction and
classification problem using algorithms from computer vision and machine learning.

This book provides a comprehensive overview of modern computer-based techniques for analyzing the structure, properties and dynamics of
biomolecules and biomolecular processes. It is organized in four main parts; the first one deals with methodology of molecular simulations;
the second one with applications of molecular simulations; the third one introduces bioinformatics and the use of experimental
information in molecular simulations; the last part reports on selected applications of molecular quantum mechanics. This second edition has
been thoroughly revised and updated to include the latest progress made in the respective field of research.

The aim this volume is to present the methods, challenges, software, and applications of this widespread and yet still evolving and maturing
field. Computational Protein Design, the first book with this title, guides readers through computational protein design approaches, software
and tailored solutions to specific case-study targets. Written in the highly successful Methods in Molecular Biology series format, chapters
include introductions to their respective topics, step-by-step, readily reproducible laboratory protocols, and tips on troubleshooting and
avoiding known pitfalls. Authoritative and cutting-edge, Computational Protein Design aims to ensure successful results in the further study
of this vital field.

Molecular Modeling of Proteins, Second Edition provides a theoretical background of various methods available and enables non-specialists
to apply methods to their problems by including updated chapters and new material not covered in the first edition. This detailed volume
opens by featuring classical and advanced simulation methods as well as methods to set-up complex systems such as lipid membranes and
membrane proteins and continues with chapters devoted to the simulation and analysis of conformational changes of proteins, computational
methods for protein structure prediction, usage of experimental data in combination with computational techniques, as well as protein-ligand
interactions, which are relevant in the drug design process. Written for the highly successful Methods in Molecular Biology series, chapters
include thorough introductions, step-by-step instructions and notes on troubleshooting and avoiding common pitfalls. Update-to-date and
authoritative, Molecular Modeling of Proteins, Second Edition aims to aid researchers in the physical, chemical and biosciences interested in
utilizing this powerful technology.

The second volume in a series which aims to focus on advances in computational biology. This volume discusses such topics as: statistical
analysis of protein sequences; progress in large-scale sequence analysis; and the architecture of loops in proteins.

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.
Since the first attempts to model proteins on a computer began almost thirty years ago, our understanding of protein structure and dynamics has dramatically increased. Spectroscopic measurement techniques continue to improve in resolution and sensitivity, allowing a wealth of information to be obtained with regard to the kinetics of protein folding and unfolding, and complementing the detailed structural picture of the folded state. Concurrently, algorithms, software, and computational hardware have progressed to the point where both structural and kinetic problems may be studied with a fair degree of realism. Despite these advances, many major challenges remain in understanding protein folding at both the conceptual and practical levels. Computational Methods for Protein Folding seeks to illuminate recent advances in computational modeling of protein folding in a way that will be useful to physicists, chemists, and chemical physicists. Covering a broad spectrum of computational methods and practices culled from a variety of research fields, the editors present a full range of models that, together, provide a thorough and current description of all aspects of protein folding. A valuable resource for both students and professionals in the field, the book will be of value both as a cutting-edge overview of existing information and as a catalyst for inspiring new studies.

Computational Methods for Protein Folding is the 120th volume in the acclaimed series Advances in Chemical Physics, a compilation of scholarly works dedicated to the dissemination of contemporary advances in chemical physics, edited by Nobel Prize-winner Ilya Prigogine.

This volume presents a diverse collection of methodologies used to study various problems at the protein sequence and structure level. The chapters in this book look at issues ranging from broad concepts like protein space to specifics like antibody modeling. Topics include point mutations, gene duplication, de novo emergence of new genes, pairwise correlated mutations, ancestral protein reconstruction, homology modelling, protein stability and dynamics, and protein-protein interactions. The book also covers a wide range of computational approaches, including sequence and structure alignments, phylogenies, physics-based and mathematical approaches, machine learning, and more. Written in the highly successful Methods in Molecular Biology series format, chapters include introductions to their respective topics, lists of the necessary materials and prerequisites, step-by-step, readily reproducible computational protocols (using command line or graphical user interfaces, sometimes including computer code), and tips on troubleshooting and avoiding known pitfalls. Cutting-edge and authoritative, Computational Methods in Protein Evolution is a valuable resource that offers useful workflows and techniques that will help both novice and expert researchers working with proteins computationally.

The major goal of ‘Expanding Frontiers in Polypeptide and Protein Structural Research’ has been to bring the various avenues for the exploration of protein structures to a single forum. The idea of organizing the symposium was conceived by one of the editors, V. Renugopalakrishnan, during the 9th International Biophysics Congress satellite symposium at Kibbutz Nof Ginosar, Israel in 1987. It was originally supposed to dwell on 2D NMR and molecular dynamics of polypeptides and proteins. During the earlier part of the last decade, these two approaches began to emerge as powerful tools to probe protein structures at the atomic level in solution. The developments in molecular biology ushered in the capability to design polypeptides and proteins for specific application in science and technology. The emergence of 2D NMR and molecular dynamics was greatly facilitated by contemporary developments in molecular biology and protein engineering. Therefore an international symposium devoted exclusively to 2D NMR and molecular dynamics studies of proteins was felt necessary to bring two major approaches in a single forum. In addition to emphasis on 2D NMR and molecular dynamics simulation, the scope of the symposium included optical spectroscopy, protein design, and new horizons in protein structure. The symposium consisted of five plenary sessions devoted to NMR and optical spectroscopy as probes for protein structure, protein dynamics, computational methods in protein design, and new horizons in protein structure. In addition, five workshops in related areas, viz,

This book discusses topics related to bioinformatics, statistics, and machine learning, presenting the latest research in various areas of bioinformatics. It also highlights the role of computing and machine learning in knowledge extraction from biological data, and how this knowledge can be applied in fields such as drug design, health supplements, gene therapy, proteomics and agriculture.

Understanding sequence-structure relationships of proteins is a central theme of computational structural biology. To create accurate mapping between sequences and structures is a big computational challenge, because the inherent dynamics of protein molecules requires any structure to be seen as an ensemble containing a large number of structural states. In this thesis, I focus on developing new structural modeling methods representing two routes towards efficient sequence-structure mapping that are compatible with this ensemble view of structures. First, I will show that the relationships between the sequence and the structural ensemble of a protein can be revealed by breaking down the protein into constituent structural fragments, for which ensemble statistics can be obtained from the protein structure database. Second, sequence-structure relationships can be also extracted by combining explicit atomistic modeling of ensembles and statistical tools reducing the overall computational cost. Implications in structure prediction, mutational analysis, and design of protein-interaction modulators will be presented and discussed, showing the great promise held by these methods in further improving the state-of-the-art in a broad spectrum of applications in computational structural biology.

The International Conference of Computational Methods in Sciences and Engineering (ICCMSE) is unique in its kind. It regroups original contributions from all fields of the traditional Sciences, Mathematics, Physics, Chemistry, Biology, Medicine and all branches of Engineering. The aim of the conference is to bring together computational scientists understanding the synthesis, structures and functions of proteins draws vital attention in computational biology as proteins participate in virtually every cellular function in an organism. In appropriate environment, a protein folds spontaneously into unique three dimensional structure of minimum energy termed as native state. Protein Structure Prediction (PSP) refers to the computational approach of predicting protein tertiary structure from amino acid sequence. Protein synthesis, on the other hand, is a multi-step process where nuclear DNA is transcribed into protein-coding messenger RNA (mRNA), which is then translated into unique amino acid sequence. MicroRNAs (miRNAs) bind to target mRNAs through complementary base-pairing and regulate protein production by translational repression or target degradation. A miRNA can bind to another mRNA from a potentially large mRNA pool and computational prediction of such target mRNA set is referred to as miRNA Target Prediction. - Incomplete knowledge of folding mechanism, absence of an established perfect energy function, and apparently complex and irregular tertiary structure make the PSP problem ever so difficult, which encourages researchers adopting simplified lattice and energy models to ease the computational hardness of the problem so as to explain essential functional properties of
Computational Methods for Protein Folding seeks to illuminate recent advances in computational modeling of protein folding in a way that will be useful to physicists, chemists, and chemical physicists. Covering a broad range of topics, the book is organized into thirteen sections, each 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.

Since the first attempts to model proteins on a computer began almost thirty years ago, our understanding of protein structure and dynamics has dramatically increased. Spectroscopic measurement techniques continue to improve in resolution and sensitivity, allowing a wealth of information to be obtained with regard to the kinetics of protein folding and unfolding and to the detailed structural picture of the folded state. Concurrently, algorithms, software, and computational hardware have progressed to the point where both structural and kinetic problems may be studied with a fair degree of realism. Despite these advances, many major challenges remain in understanding protein folding at both the conceptual and practical levels. Computational Methods for Protein Folding seeks to illuminate recent advances in computational modeling of protein folding in a way that will be useful to physicists, chemists, and chemical physicists. Covering a broad range of computational methods and practices culled from a variety of research fields, the editors present a full range of models that, together, provide a thorough and current description of all aspects of protein folding. A valuable resource for both students and professionals in the field, the book will be of value both as a cutting-edge overview of existing information and as a catalyst for inspiring new studies.

The Latest Developments on the Role of Dynamics in Protein Functions Computational Approaches to Protein Dynamics: From Quantum to Coarse-Grained Methods presents modern biomolecular computational techniques that address protein flexibility/dynamics at all levels of theory. An international contingent of leading researchers in chemistry, physics, and biology show how these advanced methods provide...
insights into dynamic aspects of biochemical processes. A particular focus is on intrinsically disordered proteins (IDPs), which lack a well-defined three-dimensional structure and function as dynamic ensembles. The book covers a wide spectrum of dynamics, from electronic structure-based to coarse-grained techniques, via models at different levels. After an introduction to dynamics and historical overview of basic methodologies, the book addresses the following issues: Is there a quantitative relationship between enzymatic catalysis and protein dynamics? Which are the functionally relevant motions of proteins? How can structural properties and partner recognition mechanisms of IDPs be simulated? How can we speed up molecular dynamics? How can we describe conformational ensembles by the synergistic effort of computations and experiments? While dynamics is now considered essential for interpreting protein action, it is not yet an integral component in establishing structure–function relationships of proteins. Helping to reshape this classical view in biochemistry, this groundbreaking book explores advances in computational methodology and contributes to the new, ensemble way of studying proteins.

This book presents applications of bioinformatics tools that experimental research scientists use in "daily practice." Its interdisciplinary approach combines computational and experimental methods to solve scientific problems. The book begins with reviews of computational methods for protein sequence-structure-function analysis, followed by methods that use experimental data obtained in the laboratory to improve functional predictions.

Despite significant advancement being made during the recent past in predicting structure of proteins using computational methods, these techniques often cannot achieve sufficiently high level of accuracy to fully appreciate biological function and to serve as a reliable starting point for rational drug design efforts to develop novel therapeutics. Bringing these low-resolution models as close as possible to the native structure, called the protein structure refinement problem, however, has remained largely unsolved. Existing approaches in protein structure refinement suffer from two key challenges: (1) lack of consistency and (2) failure to produce meaningful degree of refinement. This thesis is composed of three major contributions. First, we propose a consistent and computationally efficient computational optimization protocol called 3Drefine. Next, we further improve the 3Drefine algorithm by developing an iterative version of the protocol, named i3Drefine. Finally, we present a novel conformation ensemble-based iterative refinement method, REFINEpro, aimed at producing pronounced degree of refinement. All of these methods were benchmarked in large-scale benchmark datasets and achieved consistent refinement in both global and local structural quality measures. In particular, 3Drefine was ranked as the best protein structure refinement server method in recent Critical Assessment of Protein Structure Prediction experiment. All of these methods are freely available to the scientific community in the form of software and web-servers.

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.

Membrane proteins play key roles in numerous cellular processes, in particular mediating cell-to-cell communication and signaling events that lead to a multitude of biological effects. Membrane proteins have also been implicated in many critical diseases such as atherosclerosis, hypertension, diabetes and cancer. In Membrane Protein Structure Predictions: Methods and Protocols, expert researcher in the field detail the advances in both experimental and computational approaches of the structure, dynamics and interactions of membrane proteins dividing the volume into two sections. The first section details the procedures used for measurements of structure and dynamics of membrane proteins. While the second section contains a survey of the computational methods that have played a critical role in membrane protein structure prediction as well as in providing atomic level insight into the mechanism of the dynamics of membrane receptors. Written in the highly successful Methods in Molecular BiologyTM series format, the chapters include the kind of detailed description and implementation advice that is crucial for getting optimal results in the laboratory. Thorough and intuitive, Membrane Protein Structure Predictions: Methods and Protocols seeks to aid scientists in the further study of membrane protein structure and function.

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.

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