

However, it is not a book for beginners: prerequisites are strong molecular biology, mathematics, statistics and solid computer science with at least some intermediate programming skills. The increasing body of computer scientists who are looking at moving into bioinformatics will find this a fabulous resource (so long as it is used alongside a friendly practising bioinformatician!), as will instructors of graduate level bioinformatics programmes. Biologists keen to get into computational biology research should only look at this reference once they have had their mathematics and computational capabilities tested. In the meantime, if some rapid scripting is all you need to string together existing applications, look at other references on perl or other languages such as python. As James Tisdall says the question is no longer 'shall we program?' but rather 'who's going to do the programming?' ('Why Biologists Want to Program Computers; http://www.oreilly.com/news/perlbio_1001.html). The trick is knowing *how much* you need to program.

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Structural Bioinformatics

Philip E. Bourne and Helge Weissig
John Wiley & Sons, Chichester,
UK; ISBN: 0 471 20199 5; 649
pp.; \$69.95, £46.95; 2003

Structure mediates function in the biological processes that occur in nature. Structural biology is an established area of research where scientists have developed a variety of experimental and modelling techniques to determine the form, or structure, for biological molecules. The techniques have matured to a point where determination of large numbers of structures for proteins and nucleic acids is now possible. The exponentially increasing amount of structural data, combined with other kinds of single

molecule as well as genomic/proteomic data, has led to the advent of informatics approaches being used to represent, characterise, analyse and manipulate the data, giving us the field of structural bioinformatics.

Structural bioinformatics lies at the interface of structural biology and informatics, each of which derive their principles from the basic areas of computing science, mathematics, physics, chemistry and biology. It is therefore highly interdisciplinary and requires a particular kind of specialisation in the area of protein and/or nucleic acid structures that goes beyond traditional bioinformatics knowledge. A fundamental challenge then for an educator or a research advisor in this field is to provide students or trainees with a proper background in structural biology that appropriately illustrates the informatics aspects. Phil Bourne and Helge Weissig provide an excellent response to that challenge by presenting us with 'Structural Bioinformatics'.

The book is composed a collection of articles written by experts in diverse fields. These articles describe the basics of protein and nucleic acid structures; experimental methods to determine such structures as well as computational methods to predict them; representation, comparison and analysis of structures; assigning function from structure; structure–structure interactions; drug discovery using structure; and large-scale structure determination and prediction. The vast majority of the articles have a consistent feel to them, and are written in a lucid, easy-to-understand manner. In most cases, an exhaustive list of references is provided for readers wishing to pursue topics of interest for further detailed study.

The first chapter provides a very good introduction to the field, in part by appropriately defining it in a clear and concise manner. The next chapters provide detail on the fundamentals of DNA, RNA and protein structure. This is followed by excellent descriptions of

structure determination by X-ray crystallography, nuclear magnetic resonance (NMR) spectroscopy and electron microscopy. The book then turns to the issue of data representation with articles describing the Protein Data Bank (PDB) and the Nucleic Acid Database (NDB). The next chapters describe how the data can be used, by introducing us to methods for protein structure comparison, databases that compare and relate all known protein structures, and structural validation.

Ultimately, the goal of obtaining structures for biological molecules is so that they will provide us with a detailed atomic-level understanding of their functional mechanism. The technical aspects of the book then lead into the more scientific aspects that include chapters on protein secondary structure assignment, identification of protein structural domains, inferring protein function from structure, and protein-protein interactions.

The next chapters focus on how the technical aspects can be combined with the scientific aspects to aid pragmatically for drug design and the discovery of drug targets. The book closes with giving us an idea of the state of art in two highly active subfields: blind protein secondary and tertiary structure prediction and determination of protein structures in large numbers (structural genomics).

Particularly unusual contributions in this book are chapters on visualisation, on structure-based databases other than the PDB and NDB, and the role of electrostatics in protein interactions.

This book is highly relevant for any scientist interested in the area of bioinformatics as it relates to biological structure, particularly those that have already had some training in informatics and wish to obtain knowledge about structure in an easily accessible manner. The book is also relevant to those setting policy in the area of bioinformatics and computational biology, and would be appropriate in an upper-level undergraduate or graduate class in

computational aspects of structural biology.

Besides the research articles, the book provides insight into the future stability and prospects for the field of structural bioinformatics. The introduction, the first chapter, and the last section provide a feel for the resources and interest invested into structural bioinformatics by the broader scientific community, as well as near- and long-term goals that are expected to be accomplished.

It is to the credit of Bourne and Weissig, and the individual authors of the articles, that the most topical material is presented to give the reader a clear picture of where the field stands currently. This is no easy task given that structural bioinformatics is a rapidly changing field, and that the production time for a book is significant. While the introductory material in the book will be relevant for a long time to come, details of the cutting-edge research in structural bioinformatics are likely to change in the near future.

The book would have been greatly strengthened by the inclusion of chapters on how structures can be related to other kind of genomic and proteomic expression and interaction data, and how they can contribute to our understanding of biological systems. Even though this issue is touched upon in some of the chapters, it is of particular importance since the book promotes a forward-looking vision, seeking to influence educators, researchers and policy.

Chapters on large macromolecular structure determination would also give readers an appreciation for handling difficult structure determination problems and how they can provide knowledge about the intricate workings of biological machinery. Both of these are minor criticisms since reading the entire book in itself provokes thought on frameworks to integrate the structural data with functional information, and how the structures can be used to assemble larger complexes.

The advent of large-scale high-

throughput approaches to understand organismal genomes and proteomes has resulted in an unprecedented revolution in the biological sciences, a revolution that is still going on. The structural aspects of bioinformatics are neglected because it requires a detailed knowledge of tertiary structure of proteins and other biological molecules, beyond the traditional computational expertise. This knowledge

is necessary for a thorough understanding and application of the concepts involved to obtain insight into the function of these molecules. Bourne and Weissig have done a terrific job in this timely creation of a compilation of articles that appropriately addresses this issue.

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