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book reviews

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Protein structure prediction: methods and protocols. Edited by David M. Webster. Totawa: The Humana Press, Inc., 2000. Pp. × + 422. Price $89.50. ISBN 0-89603-637-5.

Our knowledge of protein structures has increased exponentially in the last 30 years or so. In 1970, there were only four protein structures known. By 1990, about 300 structures had been solved. Today more than 14 000 structures are stored in the Protein Data Bank and several hundred new ones are deposited every month. At the same time, however, our knowledge of protein sequences has increased at an even faster rate in recent years. Chemists, biochemists and biologists thus increasingly face the intellectual imperative of developing effective and rapid methods for prediction of protein structures.

In this volume, No. 143 in the well regarded series *Methods in Molecular Biology*, editor David M. Webster has assembled an eclectic but prodigious collection of articles on protein structure predictive methods that is likely to be regarded as a valuable addition to the series. The present volume describes established methods for prediction of secondary and tertiary structures of proteins, together with their theoretical bases. The mix of theoretical and practical aspects here is the result of Webster's attempts to target both novice and experienced researchers and to provide information that is not always immediately obvious in the primary scientific literature. It is fair to say that this excellent volume meets both these goals.

Articles in this volume range from basic to advanced and include the use of sequence alignment and *SAP* (the *Structure Alignment Program*), how to identify domains within protein sequences, comparative protein structure modeling, use of residue–residue mean-force potentials, genetic algorithms for protein folding, *ab initio* structure prediction methods, classification of protein folds, restrained molecular dynamics methods for modeling transmembrane helix bundles, predictive models of protein active sites and methods for peptide–protein and protein–protein docking. This list clearly covers a lot of ground, but at the same time one notices a surprising lack of coverage of both theoretical and experimental approaches to protein-folding algorithms. This may be intentional, as Volume 168 of this series, which was due out in March 2001, is tentatively titled *Protein Structure, Stability and Folding* (Kenneth P. Murphy, editor) and will presumably cover the exciting recent advances in the study of protein folding.

Each chapter in this volume is written by one or more of the experts working currently in that particular field. The result is state-of-the-art coverage of each of the topics presented. At the same time, the chapters differ from one another, in that some emphasize theory whereas others are much more practical in nature. The theoretical chapters provide valuable all-in-one-place presentations for novices and the practical articles provide useful step-by-step instructions, warnings of pitfalls and strategies for method optimization that will be valuable to anyone hoping to implement new methods in their own laboratory. The first six chapters of the book do a good collective job of covering the practical aspects of sequence alignment and comparative structure modeling. The article entitled *Genetic Algorithms and Protein Folding* by Steffen Schulze-Kremer contains useful source code (in C) for two-dimensional modeling of proteins, and the chapter *Comparative Protein Structure Modeling* by Roberto Sánchez and Andrej Šali provides a good introduction to *MODELLER*, along with information on how to obtain this free UNIX/LINUX program. Robert E. Bruccoleri's chapter *Ab Initio Loop Modeling and Its Application to Homology Modeling* provides detailed information on the use of *CONGEN*, a free UNIX-based program for homology modeling.

This is an eminently practical volume, one that will lead the interested reader logically and expeditiously through a field that has become complex and challenging in recent years. Its only fault may be that some of the articles were not carefully proofread prior to publication. For example, on p. 308, in the chapter on classification of protein folds, 'staphylococcal' is misspelled twice in Fig. 2 as 'staphococcyl' and on pp. 313 and 314 the legends for Figs. 4 and 5 are switched. These oversights notwithstanding, this book can be recommended enthusiastically to anyone who wishes to learn about either the theoretical or the practical aspects of protein structure prediction.

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