Book Reviews

Recent Developments in Theoretical Studies of Proteins. Edited by Ron Elber. World Scientific Publishing Co. Pte. Ltd., Singapore. 1996. viii + 399 pp. 16 × 22 cm. ISBN 981-02-2196-7. $78.00.

This text contains six chapters, one of which was written by the editor. With the exception of Chapter 3, which is an excellent review (with 156 references) of algorithms for the optimization of proteins, the chapters mostly focus on each author's own work.

In the first chapter, molecular dynamics is applied to an investigation of globins. The first half of the chapter describes atomic fluctuations and ligand binding/escape pathways. Concise discussion is provided to explain the steps involved in setting up a molecular dynamics simulation and analyzing the resulting trajectories. The second half of the chapter deals with more advanced topics including free energy perturbation methods. Although comparable information could be found elsewhere, this chapter is well-written, is logical, and serves as a good introduction to the most routine uses of the molecular dynamics technique.

Chapter 3 is a lucid review of algorithms that are useful for the optimization of proteins. Many are described in good detail, yet the discussion is not overly complex. The chapter ends with comments about future directions and a list of 156 references. This chapter, together with Chapter 1, almost justifies owning the book by itself.

The remaining chapters cover interesting special topics but are not aimed toward the beginner and, in some cases, seemed out of place given the title of this book. For example, most of Chapter 2 is dedicated to a detailed analysis of reaction path studies, and the author makes little attempt (and shows few examples) to tie it together with proteins. The latter portion of Chapter 2 briefly mentions interesting ideas using mean field simulations to study ligand diffusion in leghemoglobin and an approach for the determination of reaction coordinates which is not dependent on minimum energy pathways. These latter topics seemed well-suited for the book but were covered only superficially.

Although most chapters in the book are written in a conceptual form, Chapter 4 delivers a rigorous mathematical analysis of the formation of secondary structures in globular proteins and of the freezing transitions of various random heteropolymer models. The style and tone of this chapter are quite unique with respect to the remainder of the book. The chapter is very good, but reading it will require extensive familiarity with high-level statistical mechanics.

The final chapter of this book is not a review, but instead describes a statistical approach to the optimization of the Hamiltonian for sequence−structure alignment. In addition, a particular form of the Hamiltonian is described which is based on local interactions. Results of this methodology are also presented and discussed in a concise and interesting fashion. At the conclusion of this chapter, I wished the author had included a mini review of this rapidly emerging area such that the presented work could be considered in context.

In summary, this book is interesting in that it showcases the efforts of several groups on a broad range of topics. Each chapter was apparently written in the 1994−1995 time frame so it may not be completely current. It is not a book for beginners and is perhaps too diverse for a course, although the review in Chapter 3 is excellent. The issues raised and the topics presented are forward-looking, so the book is probably most useful to investigators who are up to speed with this literature, know the techniques, and are actively participating in the field of protein simulation.

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ACCORD. Synopsys Scientific Systems Ltd., United Kingdom. Version 2.0 for Windows. £495 (£295 academic price).

Accord is an add-in for Microsoft Excel that allows management of structural data in a spreadsheet format; hence, Accord is referred to as a chemical spreadsheet. Using a Windows platform (Windows 3.1 or Windows 95) a Chemistry menu item appears on the main Excel menu once Accord is installed. This provides access to an Accord toolbar. A Macintosh version is also available. Accord workbooks can be set up much in the same manner as Excel workbooks. Chemical structures (molecules, reactions, and substituents) can be created and inserted into worksheet cells. Thus, chemical objects in cells can be handled in the same way as other data types typically employed by Excel. The chemical objects can be displayed as structures or as chemical names (with interchangeable views), and data analysis can be performed regardless of which of the two is displayed. Structures can be drawn with the Draw Picture command, created from a SMILES string, or imported from other programs via a clipboard with the Paste command, and resulting structures can be resized, renamed, moved, and/or edited.

Once a spreadsheet has been created, a number of very useful functions can be performed. Data can be manually entered for each entry (such as, for example, melting points, biological data), or the Lookup command can be used to automatically enter properties associated with substituent groups (e.g., σ values, π values for about 300 substituents). Molecular formulas, molecular weights, and elemental compositions can also be entered automatically with the push of a button. Chemical data analysis can be performed by sorting tables based on property values or other data, and regression analysis

can be conducted. Chemical tables can also be searched for exact structures, substructures, and structural similarity. The program can handle stereochemistry, organometallic molecules, and inorganic molecules and allows for extensive customization. Accord, although a spreadsheet and not a database, allows for entry of hundreds if not thousands of chemical structures.

One of the seemingly most useful features is R-Group analysis. An R-Group table can be created using a general (i.e., generic or core) structure with one or more appended R groups (e.g., R1, R2, etc...). Various R groups can be entered, and these are then automatically associated with the core structure; related data can be added (manually or automatically) for each entry in the table. R-Group analysis can be performed on the completed table. (This reviewer had difficulty creating and analyzing R-Group tables, and the 134-page User's Guide was not found to be particularly useful for solving problems. Likewise, the Help command never seemed to provide all the solutions to problems that were encountered. It might be noted, however, that Accord training courses are available for users.)

Accord promises to be an incredibly useful Excel add-in. Although the program is relatively easy to install and run, it is likely that practice will be necessary to reduce early frustration and to avail oneself of the full power of Accord. Additional documentation would have been a welcomed feature. Nevertheless, given its potential usefulness, Accord is certainly something worth exploring.

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HPLC Methods for Pharmaceutical Analysis. By George Lunn and Norman R. Schmuff. John Wiley and Sons, Inc., New York. 1997. xxii + 1609 pp. 19 × 26 cm. ISBN 0-471-18176-5. $150.00.

This extensive compilation of HPLC methods for drugs has made available a concise presentation of methods published roughly between 1980 and 1996. A well-standardized format has been used throughout, with abbreviations defined and a good discussion of the monograph structure, abstract, abstract conventions, extraction from biological matrices, and working practices following the Preface. Also following the Preface are listings of PIC reagents, matrices, suppliers, and trademarks. The monographs appear alphabetically by United State Adopted Name (USAN). The indexes include a name index, molecular formula index, cross-listing with the Merck Index (12th edition), and cross-reference to *The Organic Chemistry of Drugs*.

This book is also available in a CD-ROM version, which would be more valuable to the busy analyst, by assisting in rapid access to the essentials of methods of interest. Typical methods development begins with a literature search of methods for compounds of similar structure and chemistry. The authors appear to have already done a thorough search of the primary literature data bases, as well as putting the information from the original publication in a standard format.

The book/CD-ROM combination is highly recommended to any laboratory that is doing methods development. It is also a useful reference book for industrial and university libraries.

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