
PREFACE

Since the arrival of information technology, biochemistry has evolved from an interdisciplinary role to becoming a core program for a new generation of interdisciplinary courses such as bioinformatics and computational biochemistry. A demand exists for an introductory text presenting a unified approach for the combined subjects that meets the need of undergraduate science and biomedical students.

This textbook is the introductory courseware at an entry level to teach students biochemical principles as well as the skill of using application programs for acquisition, analysis, and management of biochemical data with microcomputers. The book is written for end users, not for programmers. The objective is to raise the students' awareness of the applicability of microcomputers in biochemistry and to increase their interest in the subject matter. The target audiences are undergraduate chemistry, biochemistry, biomedical sciences, molecular biology, and biotechnology students or new graduate students of the above-mentioned fields.

Every field of computational sciences including computational biochemistry is evolving at such a rate that any book can seem obsolete if it has to discuss the technology. For this reason, this text focuses on a conceptual and introductory description of computational biochemistry. The book is neither a collection of presentations of important computational software packages in biochemistry nor the exaltation of some specific programs described in more detail than others. The author has focused on the description of specific software programs that have been used in his classroom. This does not mean that these programs are superior to others. Rather, this text merely attempts to introduce the undergraduate students in biochemistry, molecular biology, biotechnology, or chemistry to the realm of computer methods in biochemical teaching and research. The methods are not alternatives to the current methodologies, but are complementary.

This text is not intended as a technical handbook. In an area where the speed of change and growth is unusually high, a book in print cannot be either comprehensive or entirely current. This book is conceived as a textbook for students who have taken biochemistry and are familiar with the general topics. However, the book aims to reinforce subject matter by first reviewing the fundamental concepts of biochemistry briefly. These are followed by overviews on computational approaches to solve biochemical problems of general and special topics.

This book delves into practical solutions to biochemical problems with software programs and interactive bioinformatics found on the World Wide Web. After the introduction in Chapter 1, the concept of biochemical data analysis and management is described in Chapter 2. The interactions between biochemists and computers are

the topics of Chapter 3 (Internet resources) and Chapter 4 (computer graphics). Computational applications in structural biochemistry are described in Chapter 5 (biochemical compounds) and then in Chapters 14 and 15 (molecular modeling). Dynamic biochemistry is treated in Chapter 6 (biomolecular interactions), Chapter 7 (enzyme kinetics), and Chapter 8 (metabolic simulation). Information biochemistry that overlaps bioinformatics and utilizes the Internet resources extensively is discussed in Chapters 9 and 10 (genomics), Chapters 11 and 12 (proteomics), and Chapter 13 (phylogenetic analysis).

I would like to thank all the authors who elucidate sequences and 3D structures of nucleic acids as well as proteins, and they kindly place such valuable information in the public domain. The contributions of all the authors who develop algorithms for free access on the Web sites and who provide highly useful software programs for free distribution are gratefully acknowledged. I thank them for granting me the permissions to reproduce their web pages, online and e-mail returns. I am grateful to Drs. Athel Cornish-Bowden (Leonora), Tom Hall (BioEdit), Petr Kuzmic (DynaFit), and Pedro Mendes (Gepasi) for the consents to use their software programs. The effort of all the developers and managers of the many outstanding Web sites are most appreciated. The development of this text would not have been possible without the contribution and generosity of these investigators, authors, and developers. I am thankful to Dr. D. R. Wiles for reading parts of this manuscript. It is my pleasure to state that the writing of this text has been a family effort. My wife, Alice, has been most instrumental in helping me complete this text by introducing and continuously coaching me on the wonderful world of microcomputers. My son, Willis, and my daughter, Ellie, have assisted me in various stages of this endeavor. The credit for the realization of this textbook goes to Luna Han, Editor, and Danielle Lacourciere, Associate Managing Editor, of John Wiley & Sons. This book is dedicated to Alice.

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