Book Reviews

Molecular Modeling: Basic Principles and Applications. Third Edition. By Hans-Dieter Höltje, Wolfgang Sippl, Didier Rognan, and Gerd Folkers. Wiley-VCH, Weinheim, Germany. 2008. x + 310 pp. 17 × 24 cm. ISBN 978-3-527-31568-0. $90.00.

The focus of this book is explained in its subtitle: Basic Principles and Applications. This third edition of Molecular Modeling is the best executed of the series and will be met with more enthusiasm than the previous editions by virtue of its broader scope (inclusion of chemical genomics), greater depth (more bioinformatics in the comparative protein modeling), and extensive pertinent references to basic modeling principles and appropriate illustrative examples. The fully elaborated case study (Chapter 8) of the nuclear hormone receptor, constitutive androgen receptor (CAR), demonstrates the interplay of bioinformatic tools with classical techniques of structure-based design and X-ray crystallography. Each step in the modeling process is prefaced with the rationale, and the integration of the methods is clearly delineated on pp 265−298.

The first two chapters give an overview of the historical development of molecular modeling and the repertoire of computational chemistry methods associated with computer-assisted drug design and modeling (CADD or CAMM). Fundamentals of pharmacophore analysis, comparative molecular field analysis (CoMFA), and electrostatics are presented concisely but at a level that would serve as an introductory volume for industry scientists of any discipline, as well as a text for upper level undergraduates or graduate students exploring applications of computational chemistry. The QSAR case study of the dopamine D_3 receptor antagonists provides insights into the integration of computational techniques that focus on discovering and optimizing small molecule properties key to intrinsic activity.

Chapter 4 begins the transition into protein modeling, with sections on protein structure, homology, solvation, electrostatics, and hydrophobicity. The interface between chemical libraries/collections and structure-based design, that is, virtual screening and docking, is the subject of Chapters 5 and 6. Tables of libraries suitable for virtual screening, docking programs, and successful screening studies from the 2003−2006 literature highlight Chapter 5, which is replete with 143 references.

Chapter 7 delivers the most dramatic enhancement over the previous versions of this text, with a thoroughly illustrated discourse on ligand space, target space, annotated libraries, privileged structures, binding site target analysis, and in silico screening.

With very few exceptions, molecular modeling books tend to be written by experts for experts. Overall, this book is an excellent resource as an introduction to molecular modeling techniques as practiced primarily in the pharmaceutical or biotechnology industries. The substantial number of references will assist the novice in the learning experience. The expert reader may be frustrated somewhat by the lack of an author index, although the subject index is extensive. I can particularly recommend this book to academics who are looking for an anchor text for an upper level undergraduate/graduate special topics course in computational chemistry.

Salvatore Profeta, Jr.

Department of Chemistry and Biochemistry
DePauw University
602 South College Avenue
Greencastle, Indiana 46135

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Annual Review of Pharmacology and Toxicology. Volume 48. Edited by Arthur Cho, Terrence Blaschke, Paul Insel, and Horace Loh. Annual Reviews, Palo Alto, CA. 2008. viii + 701 pp. 19 × 24 cm. ISBN 978-0-8243-0448-5. $84.00.

This text is a broad collection of reviews covering prominent topics of modern pharmacology. The majority of the review articles are well written, and they cover relevant advances in understanding from the past decade. The various authors cite recent literature with well over half of the references to communications published since 2000. As with all review collections, the subject matter and level of depth vary widely from one chapter to the next, and the editors had the unenviable task of organizing these in a consistent manner. This is one of the shortcomings of the book. For example, several articles discuss G-protein-coupled receptors; these might well have been grouped together. However, the title listing by subject matter at the end of the book does classify titles from volumes 44−48 according to topic.

The book contains discussions of G-protein-coupled and other receptor systems, signal transduction, transporters (neurotransmitter and xenobiotic), therapeutic targeting of isozyme variants, carcinogenesis, clinical therapeutics, drug development, and inflammation. There are no chapters relating the role of genomics and proteomics to pharmacology and toxicology, disappointing given recent major advances in these areas and their growing role.

This volume is obviously of interest and value to researchers in drug discovery and development; additionally, I have used the book to introduce some advanced undergraduate students to research topics that they might wish to pursue as future Ph.D. candidates.

Michael LaFontaine

School of Osteopathic Medicine
Pikeville College
147 Sycamore Street
Pikeville, Kentucky 41501

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