Book Reviews

Structure-Based Drug Design. Edited by Pandi Veerapandian. Marcel Dekker, Inc., New York. 1997. xiii + 647 pp. 16 × 23.5 cm. ISBN 0-8247-9869-4. $175.00.

The aim of this book is to act as a reference guide for the drug designer who is making extensive use of three-dimensional structural information in the process. The book has been divided into therapeutic areas or diseases which are highlighted by case studies of one or more molecular targets. A final section deals with emerging methodologies which have impact on the structure-based design approach for the future. Examples of the molecular targets covered include HIV-1 protease and reverse transcriptase, retroviral integrase, bradykinin receptors, purine nucleoside phosphorylase inhibitors, matrix metalloproteinase, protein kinases, aldose reductase, thrombin, sodium channels, catechol *O*-methyltransferase, neuraminidase, rhinoviral capsid binding sites, and interleukin-1 and interferon. Each chapter is well-referenced by leading researchers in their field and highlights numerous different structure-based techniques fully integrated into the drug discovery process. The range of examples spans a continuum of science from the mature, renin inhibition, to the emerging, interferon and interleukin systems. The illustrations are plentiful and generally well-placed relevant to the appropriate text. Sections in the novel methodologies arena touch on the utilization of combinatorial chemistry in structure-based design, on directed combinatorial chemistry, and on the incorporation of combinatorial approaches to computer-aided ligand design. Overall the book is well-planned and executed, succeeding in giving the reader a fairly broad and complete overview of the many facets of structure-based drug design. While the price of the book may deter many from buying it, this book certainly belongs in our libraries and should serve well as a general reference in the field.

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Asymmetric Synthesis. By Gary Proctor. Oxford University Press, Oxford, UK. 1997. 237 pp. 16 × 24 cm. ISBN 0-19-855726-3. $85.00.

Writing a monograph on a burgeoning field like asymmetric synthesis is, at best, a daunting task. The challenges in such an undertaking are numerous. The text must be comprehensive enough to cover important, basic concepts and their development into useful reagents and procedures. The material and references must be current enough to recommend the inclusion of the book into a practitioner's library. The organization of the material must be clear, and most importantly, the writing must be lucid and target the intended audience. Professor Proctor's book *Asymmetric Synthesis* meets each of these challenges with varying degrees of success.

In the Preface, Professor Proctor states that "... It is my hope that this book will be of some use to those involved in the preparation and teaching of such courses [in asymmetric synthesis], and to the students themselves. In addition, research workers starting out in this area might also find it of some interest..." The text is divided into seven chapters covering various reaction types, a chapter on the principles of asymmetric synthesis plus an introduction.

The chapter entitled "Principles" will probably be the most generally useful chapter for those involved in introducing the topic of asymmetric synthesis into an advanced undergraduate class. The chapter clearly and succinctly introduces many of the concepts which underpin the design of an asymmetric reaction or reagent. This chapter also illustrates one of the major shortcomings of this monograph, the dated references. The most recent reference in the monograph is ca. 1993! The author states, "I have attempted to make each chapter on reaction types stand alone, with the references presented at the end of each chapter." In this he succeeds; each chapter is generally well written. In a monograph of 237 pages it is difficult to decide what should be included or omitted; the author has generally chosen well. Examples of most of the major types of reactions used in asymmetric synthesis are covered with the notable exception of free radical chemistry. Important conceptual and mechanistic points are adequately supported with data from the primary literature. There is an emphasis on methods which allow good predictable asymmetric induction. However, if the student or neophyte researcher is to use a given chapter as a springboard into the area, there are few recent leading references to monographs or literature reviews provided for further in-depth reading.

The chapter "Additions to C−C double bonds" is interesting from the perspective of the wide range of reactions covered (the Michael reaction, the Diels Alder reaction, and 2 + 2, 3 + 2, and related 4 + 2 cycloadditions share the stage with methods such as hydroboration and carbeniod reactions)!! The grouping really works. The chapter "Reduction and oxidation" ought to have been separated into two chapters given the extensive literature. While the chapter "Hydrolysis and esterification" covers examples of some of the more "user friendly" enzymes in organic synthesis, the topic might have been better included in the chapter "Additions to the carbonyl" or in a chapter entitled "Enzymes in organic synthesis". Again, this is a case where more extensive referencing would be helpful.

Overall, this text's greatest advantage is to serve a design guide to lecturers involved in either presenting a unit on a topic in asymmetric synthesis or an entire course on the subject. Unfortunately, the dated referencing, coupled with the relatively high price of $85.00,

may limit the circulation of this text to library collections and faculty offices.

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Monosaccharide Sugars. By Zoltán Györgydeák and István F. Pelyvás. Academic Press, San Diego, CA. 1998. xviii-508 pp. 15.5 × 23.5 cm. ISBN 0-12-550360-1. $89.95.

This book is a compendium of the literature on methods for C−C bond formation, degradation, and epimerization of monosaccharides. It contains approximately 1700 references and is divided into three parts. The first and largest part, 370 pages, describes the ascending synthesis of monosaccharides by long-known methods, such as the formose or cyanohydrin reactions, as well as more recent methodologies using nitroalkanes, malonesters, phosphoranes, and organometallics. The second part, 95 pages, covers the degradation of monosaccharides and related acids to smaller chiral synthons. The final part, 20 pages, deals with sugar epimerization.

Each chapter is illustrated by relevant examples taken from fields as diverse as *C*-saccharide, antibiotic, nucleoside, and isotopically labeled saccharide synthesis. Despite these useful examples, little or no mechanistic information is given on the reactions presented. Collections of known sugar derivatives are summarized in many tables, and the influence of experimental conditions on the reaction products is briefly discussed. Suitable experimental protocols are given for each type of transformation. While this is helpful, particularly for older chemistry published in difficult to obtain or foreign language journals, it is likely that most chemists would want to return to the original literature before attempting a synthesis.

Although the authors use systematic carbohydrate nomenclature, recently established by IUPAC, it would have been helpful for the authors to have included a primer on carbohydrate nomenclature for the nonexpert. There is no author or compound index, limiting the value of the compendium as a fast reference. The subject index is very simple and generally useful to find syntheses of a given type of sugar or examples of particular reactions. While some references are quite old (1860s), more recent, important references (1995−1997) are discussed in a brief addendum.

The utility of this book is as a general overview and compendium, comparing useful strategies for synthesis of higher-carbon sugars and related chiral synthons from simple carbohydrate derivatives. This book has little value for the carbohydrate chemist, focused primarily on oligosaccharide targets of biological and pharmaceutical importance, as constituent monosaccharides must be designed and protected with a specific target in mind. This book is somewhat more useful for the medicinal and synthetic chemists wishing to investigate the use of monosaccharides as chiral building blocks to prepare more complex targets.

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Reviews in Computational Chemistry, Volume 11. Edited by Kenney B. Lipkowitz and Donald B. Boyd. Wiley-VCH, Inc., New York, NY. 1997. xxiv + 431 pp. 16 x 24 cm. ISBN 0-471-19248-1. $120.00.

The book is number 11 in the series started in the mid-1980s to cover recent advances in the burgeoning field of computational chemistry. In the decade since the first Gordon Conference on computational chemistry, we have witnessed amazing advances in the field. It is fair to say that computational chemistry as an element of the discovery process for new materials and drugs has become mainstream. With some refinements, and more powerful machines and algorithms, we use essentially the same force fields as a decade ago and the same fundamental theory in ab initio calculations. The bigger strides in recent years are in the application of computational methods and the linkage of thermodynamic theory to quantities like receptor structure, ligand structure, and molecular electronic properties.

The preface of the book starts with a philosophical note by explaining that the theme of the volume is "computer aided ligand design" and "modeling of biomolecules". It is further explained that "ligand design", not "drug design", is the proper nuance for what is being described, because the design of a drug encompasses a large number of downstream scientific analyses and disciplines beyond the strictly computational. The editors assert: "One of the best ways for the computational chemist to influence the drug discovery process is to supply essential information and good ideas, which, when implemented help drive a pharmaceutical project toward a successful conclusion." Thus the thrust of the book is how to optimize the role of computational chemistry in drug discovery.

Briefly, Chapters 1 and 2 discuss the multitude of new methods which have been developed for de novo design of ligands. Chapters 3 and 4 survey and discuss current advances in 3-D QSAR methods. In Chapter 5, the emphasis is on using computational methods to calculate partition coefficients, which are important in classical drug design work. Chapter 6 details recent work in the treatment of counterions in the modeling and simulation of DNA structures. Finally, the volume is concluded with an appendix entitled "Compendium of Software and Internet Tools for Computational Chemistry."

The book appropriately begins with two complementary chapters on de novo design of ligands. The first chapter provides a general introduction. The author systematically reviews and explains each of six major classes of methods: fragment location, site point con-