

make an impact, subsequent books on combinatorial chemistry will have to be more specialized and detailed than these.

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**Guidebook on Molecular Modeling in Drug Design.** Edited by N. Claude Cohen (Ciba-Geigy, Ltd.). Academic Press: San Diego, 1996. xix + 361 pp. \$59.95. ISBN 0-12-178245-X.

This book presents a survey of many of the computer techniques used in drug design. It also provides a useful discussion of X-ray crystallography and nuclear magnetic resonance.

The book is intended to be a guide for advanced students and chemists who are entering the field of computer-assisted molecular design, either as practitioners or as collaborators. Emphasis is on the design of potent ligands using the 3D structure of the target biomolecule. Chapters include a 17 page perspective by N. C. Cohen, a 36 page discussion of the hardware and software for molecular modeling by R. E. Hubbard, a 39 page introduction to molecular modeling of small molecules by T. Gund, a 45 page discussion of molecular docking and computer de novo design of new molecules by A. Itai, M. Mizutani, Y. Nishibata, and N. Tomioka, a 79 page review of the techniques of X-ray crystallography and NMR, structure databases, and searching of 3D information by J. P. Priestle and C. G. Paris, a 17 page discussion of management views and issues in incorporating computer techniques into industrial programs by P. Gund, G. Maggiora, and J. P. Snyder, and a 102 page review of techniques for modeling drug-receptor interactions and examples of the use of modeling techniques in lead optimization by K. F. Koehler, S. N. Rao, and J. P. Snyder. The extensive index and 19 page glossary (compiled by J. P. Tollenaere) of terms used in molecular modeling enhance the usefulness of the book for self-study. As might be expected, many of the chapters are summaries that suggest additional reading, although most references are from 1995 or earlier. Although it is a guidebook in molecular modeling, its impact is lessened by the lack of color figures. Readers can judge for themselves if these negative features lessen the utility of the book for self-study.

The book is unusual in that most of the authors work in industry rather than academia. They represent experience in U.S. companies (Merck, MSI, Pharmacia-Upjohn, and Searle) and European companies (Ciba-Geigy, Janssen Pharmaceutica, and IRBM), as well as academic research in the U.S. (NJ Institute of Technology and Emory University), U.K. (York University), and Japan (The University of Tokyo). The authors are all acknowledged experts in their fields and provide insights helpful to those not already involved in the field.

The title, *Guidebook on Molecular Modeling in Drug Design*, is misleading because it barely mentions a major effort in the field, namely, QSAR and 3D-QSAR. Although more than 500 CoMFA analyses have been published, only seven sentences are devoted to this topic! Reference is made to some of the other 3D-QSAR methods, but neither they nor traditional QSAR is discussed in any detail. On the other hand, both the chapter by T. Gund and that by Koehler et al. discuss in some detail the techniques of pharmacophore mapping and computer-assisted drug design in the absence of the 3D structure of the target biomolecule.

Overall, this is a book that is well suited for study by students or newcomers. The index and glossary make it handy for reference. It probably is too superficial to be useful to experienced practitioners.

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**Carbohydrate Analysis: High Performance Liquid Chromatography and Capillary Electrophoresis.** Edited by Ziad El Rassi (Oklahoma State University). Elsevier: Amsterdam, 1995. xix + 668 pp. \$242.75. ISBN 0-444-89981-2.

The increasing recognition of the myriad of diverse roles played by carbohydrates in biological systems has resulted in a substantial demand for rapid efficient techniques for their separation. The analysis of these

water-soluble uncharged species that typically lack observable chromophores or fluorophores has traditionally made chromatographic analysis of underivatized samples a daunting task. Further complicating matters is the issue of glycoconjugates: frequently carbohydrates of biomedical interest exist not as free saccharides but rather as glycoproteins or glycolipids. Separation of these species was more accurately described as an art form than a science, and removal of the aglycon was frequently required for manageable analysis.

*Carbohydrate Analysis* carefully puts the past 20 years of methodological developments in HPLC and capillary electrophoretic separations into perspective in a single volume readily accessible to both novice and expert alike. The work, volume 58 in the Journal of Chromatography Library series, covers a variety of preparative and analytical separations of virtually every class of carbohydrate, including mono-, oligo- and polysaccharides, glycolipids, and glycoproteins, each from a variety of natural sources. The volume is broadly divided into three sections, covering sample preparation, chromatographic separation, and solute detection. Together the 17 chapters, representing contributions from 13 laboratories, provide all of the protocols required to design a separation for virtually any carbohydrate from any biological matrix.

Section I, covering sample preparation, provides methodology for isolating carbohydrate fractions from complex mixtures, cleavage of carbohydrates from glycoproteins and glycolipids, and both chemical and enzymatic digestion of complex samples into manageable fragments. The section provides detail on such methods at the level of solvent buffer compositions and commercial suppliers of reference compounds; extensive citations provide the reader with additional detail when required. Section II, detailing chromatographic separation of carbohydrates, covers a variety of methodologies from the traditional—reverse phase, silica, ion exchange, and size exclusion matrices—to specialized techniques more applicable to specific research applications, including lectin affinity chromatography. The level of detail in the eight chapters that comprise this section varies, but in general both the theoretical aspects of separation and practical aspects of carrying out procedures are covered. A chapter specifically devoted to preparative scale HPLC of carbohydrate derivatives will be of interest to a wide range of users, including synthetic chemists. The final section of the volume—detection of analytes—again covers techniques that the nonspecialist will likely have access to and those that will be of interest primarily to researchers involved in frequent laborious separations. Detection of underivatized carbohydrates by refractive index, mass spectroscopy, light scattering, electrochemical techniques, and polarimetry are covered thoroughly. Again, although the level of detail varies from chapter to chapter, both theoretical aspects of the technique and practical details required to actually effect detection are covered. Finally, detection techniques utilizing both chemical and enzymatic postcolumn modification are reviewed.

*Carbohydrate Analysis* has a copyright date of 1995, and the bulk of the references were published in the first three years of this decade. Most of the data and techniques presented here however are both fundamental and timeless. The volume provides a large amount of readily accessible practical information on chromatographic separations that will augment the collections of a wide range of chemists and biochemists with interests in carbohydrate chemistry.

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**Online Searching: A Scientist's Perspective. A Guide for the Chemical and Life Sciences.** By Damon D. Ridley (University of Sydney). John Wiley & Sons, Inc.: New York, 1996. xx + 344 pp. \$39.95 paperback. ISBN 0-471-96521-9.

This book fills the need of the literature retriever who would like an overview of STN (the online service that allows access to *Chemical Abstracts* and other chemical information databases). The author is well-qualified, having taught workshops and lectured on STN about 300 times in Australia and elsewhere. The author acknowledges, among others, Fred Winer (Chemical Abstracts Service, Columbus, OH), who may be more familiar to American audiences of the STN workshops.

The author effectively uses a pedagogical arrangement of each chapter, whereby he tells the reader what he will explain, he then explains it with explicit examples, and finally concludes with a summary of some key points of what has been explained. The book gives an

overview of the organization of several of the commonly used databases (files) among the 200 to which STN sells access. The reader will learn many of the sometimes cumbersome intricacies of designing text and structure search queries that will yield the most useful information. Pitfalls are pointed out. An outline of the book is available at <http://www.chem.usyd.edu.au/~dridley/tocframe.html>. The book has a pleasing paucity of misprints.

Although the individual scientist can clearly benefit from reading this textbook, the book's audience includes librarians. Essential concepts of chemistry are introduced assuming no prior knowledge. The author does an excellent job of teaching in one chapter the essence of (mainly organic) chemical structure conventions. On the other hand, some terminology of the CAS chemical information specialist, such as "bound phrases", "controlled term field", etc., are used with little or no attempt to explain what they mean. Unfortunately, the subject index is only 10 pages long and is rather incomplete, so it would be impractical to use this information-packed book as a quick reference. Much important material is listed in tables, but this information cannot be quickly refound because it is not indexed. A glossary of all the terms and acronyms encountered when using STN is sorely lacking.

One of the critical issues whenever using STN is to design the searches so as to maximize the relevance of the information retrieved while minimizing the cost of the searches. The author brings up this issue as early as page 20, but the introduction to the cost structure of STN is relegated to pages 163–166. The book claims it will help the user of other chemical information database providers, such as Knight Ridder (formerly Dialog) and Orbit/Questel. However, the two pages of appendix material devoted to some of the commands of the other systems are hardly adequate. Beilstein's online Crossfire system is not mentioned, and CAS's SciFinder is heralded briefly. Covering these other systems would have made the book too long. Most chemists probably will have their needs satisfied with STN. For STN structure searching, the author assumes the reader will have STN Express running on their PCs and Macs. Users having access to STN through other machines will have to follow the author's advice to obtain the relevant manuals from STN. The value of having STN reference books is brought up at several points in the book, but the postal, telephone, fax, and e-mail addresses of STN in Australia, the United States, or elsewhere are not given.

Librarians will certainly want to have this book on their shelves for themselves as well as their clients. The book will come in handy for librarians to loan to graduate students (or professors) when they come to the library asking for help on how to get started with the modern approach to literature searching. The book is no substitute for attending STN workshops but is highly recommended to the individual who is about attend a workshop.

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#### **Phthalocyanines: Properties and Applications, Volume 4.**

Edited by C. C. Leznoff and A. B. P. Lever (York University, Canada). VCH: New York, 1996. vi + 524 pp. \$150.00. ISBN 1-56081-916-2.

The first thing that caught my eyes was the appropriate choice for the color of the book cover, i.e. about the same blue as on my lab coat and equipment after working with phthalocyanines. This book is the fourth of a series started in 1989. It deals with the preparation, characterization, properties, and applications of phthalocyanines. Chapters are written by different authors from various parts of the world. The topics presented cover a wide range of substituted species and applications. The breadth of aspects regarding phthalocyanines makes this book a worthwhile addition to any science library, and more particularly to anyone with an interest on phthalocyanines. Chapter length varies considerably, from 18 pages for Chapter 1 to 102 for Chapter 3. The quality of the print and of the figures is pretty uniform and makes the book enjoyable to read. Most of the references are recent, up to 1995 for most chapters, which makes the book well up to date.

The stated purpose of the book is to discuss the properties and applications of phthalocyanines. These objectives seem to have been reached. Different chapters deal with chemical properties, for example,

synthesis and chromatographic separation, acid–base and coordination, encapsulation in zeolites, molecular orbitals and electronic spectra, and single-atom bridge dimers. Others are concerned with physical properties, such as nonlinear optical properties and epitaxial growth of ultrathin films. A variety of applications are presented, including the use of the nonlinear optical (NLO) properties of metallophthalocyanines (MPcs) in photonics, their use in the fabrication of organic photovoltaic junctions, and the use of phthalocyanines and their derivatives for catalyzing various types of reactions. Examples of use in catalysis include hydrocarbon activation, chemical fixation and photoreduction of carbon dioxide, and metal–oxo chemistry as mimic of the P-450 enzyme. The application of molecular beam epitaxy for the epitaxial growth of ultrathin films of phthalocyanines is also described. Good electrical conduction properties have been obtained by appropriate stacking to give low-dimensional solids with special charge transport properties along the chain. Biomedical and biological applications are also found in the book, which describes medical imaging and therapy using radiolabeled phthalocyanines, the use of hemoproteins reconstituted with phthalocyanines for studying the biological functions of the proteins, and developments in photobiology for their tumoricidal effects, ophthalmic photodynamic applications, antihyperplasia activity, inactivation of viral pathogens, antibiotic and antifungal effects, and use as photodynamic sensitizers for treating highly pigmented lesions.

In Chapter 1, the synthesis of new unsymmetrically substituted phthalocyanines includes the Diels–Alder reaction with [60]fullerene to give unsymmetrical enophilic phthalocyanines. Chromatography is used to separate tetrasubstituted and unsymmetrically substituted phthalocyanines. The acid–base properties of azaporphyrins is presented in Chapter 2. This includes acid ionization, the methods used for estimating quantitatively the acidity or basicity, and the influence of acid–base properties on aromaticity, addition reactions, complexation reactivity, and protonation. Metal-free azaporphyrins and a theoretical approach are also given. In the very long Chapter 3, the NLO properties of MPcs are presented, including their second-order and third-order NLO, and ultrafast optical nonlinearities properties in relation to molecular symmetry and crystal symmetry, second-harmonic generation (SHG) and degenerate four-wave mixing (DFWM) for measuring the optical nonlinearities. The short Chapter 4 discusses the use of phthalocyanines for the catalytic oxidation of hydrocarbons, thiols, phenols, and indoles and for the homolytic activation of hydrocarbons. Chapter 5 describes briefly the chemical fixation and photoreduction of carbon dioxide catalyzed by phthalocyanine derivatives. Chapter 6 explains the fabrication of thin films of molecular organic semiconductors, their characterization, and their use in Schottky cells, n/p-junction cells, and photoelectrochemical cells. Chapter 7 discusses another very interesting application in catalysis: the encapsulation of metallophthalocyanines in the pores of zeolites, without chemical bonding ("ship-in-a-bottle complexes"), prevents aggregation of the catalyst in solution, or its deactivation by dimerization, and results in highly selective (including cis/trans stereospecificity) enhanced reactions. Chapter 8 discusses the epitaxial growth of ultrathin films of phthalocyanines by Organic Molecular Beam Epitaxy and compares the results to inorganic films grown by the same method, in terms of substrate/film lattice mismatch and of weak intermolecular interactions, and their implications on the strain in the films and their elastic constants. Chapter 9 is much more theoretical and provides an in-depth presentation of molecular orbital calculations and electronic spectra of phthalocyanines analogues, including deprotonated and metal-free tetraazaporphyrins and species containing carbon and/or nitrogen at the meso positions. The Symmetry-Adapted Perturbation Method in evaluating symmetry-lowering effects are also used. Chapter 10 gives recent results on metal phthalocyanine single-atom bridged dimers, with stacking properties leading to unidimensional electrical conduction and possible use as precursors for the formation of linearly elongated aggregates with interesting charge transfer properties. Characterization includes also X-ray crystal structures and Mössbauer spectroscopy. Chapters 11, 12, and 13 describe biological and biomedical applications. Labeling metallophthalocyanines with radioisotopes provides novel diagnostic and therapeutic agents in nuclear medicine and biology, particularly for cancers. The chemical modification of heme in proteins by removing the native prosthetic group and coupling the resultant apoprotein with artificial hemins, including phthalocyanines, provides an elegant method for investigating the molecular mechanism of the function. The preferential binding of some dyes to tumor, viruses, bacteria, fungi, and parasites cause their accumulation. Then, using their photosensi-