Computer Software Reviews

Mathematica 4.1. Wolfram Research, Inc., 100 Trade Center Dr., Champaign, IL 61820-7237. www.wolfram.com. Suggested retail price: $1495. Mathematica for Students price: $139.95. Other academic pricing available.

The Mathematica software package allows a broad range of data analysis and graphics applications. The program runs under Linux, Windows 95, 98, Me, NT, and 2000, and Mac OS. Minimum system requirements include an 80386 compatible or higher processor and at least 200 MB of hard disk space. Additionally, 32 MB of RAM is recommended.

Mathematica comes with a short paperback entitled "Getting Started". Here, the most basic uses are explored, such as using proper mathematical notation for calculations, handling cells within notebooks, graphing functions, using and creating palettes for commonly required functions and variables, networking, and finding help elsewhere, whether in the thorough hardback documentation included with the software package or online.

Data entry in cells is straightforward and very well documented in the accompanying literature. However, the system is unable to recognize probable errors and instead treats mathematical expressions that look correct but fail to comply with the strict rules as constants. This is inconvenient and can be a source of a considerable loss of time for nontrivial entries. Mathematica also contains a variety of importing and exporting options. For example, spreadsheets and images can be read both from and to, once minor modifications are made for formatting purposes.

Despite the ease with which one can handle external data, the real strength of Mathematica rests in the fact that it can stand alone. The pull-down menus offer users the capability to manipulate entered data in a plethora of ways, and if these are not enough, there are many add-on packages available, including those for statistics, linear algebra, graphics and geometry, and calculus. In all, over a thousand additional functions are available.

In addition to data analysis, Mathematica is a powerful tool for graphical applications. Some of the options available are simple two-dimensional graphs, contour and density plots, and three-dimensional surface plots. The user is afforded the option of constructing graphics from functional or list input, which facilitates the construction of such output considerably. Furthermore, upon producing a figure of a given type, Mathematica allows quick conversion to all other applicable types. If a small number of graphs cannot detail enough information pertinent to a given function, Mathematica even contains animation capabilities to show evolution through a given variable.

All in all, Mathematica provides a very effective means of analyzing data and producing publication-quality output. Indeed, the scope of features present gives the experienced user little reason to utilize Mathematica's quick interfacing with other software.

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Book Reviews *

Advances in Chromatography, Volume 40. Edited by Phyllis R. Brown (University of Rhode Island) and Eli Grushka (Hebrew University of Jerusalem). Marcel Dekker, Inc.: New York. 2000. xxiv + 651 pp. $225.00. ISBN 0-8247-0018-X

The *Advances in Chromatography* series is a compilation of "current, critical reviews of the most important developments in separation science". Reviewing a new volume in this area is simultaneously an enjoyable and intimidating task: enjoyable in that each volume invariably contains several interesting chapters, but intimidating because each volume also makes one acutely aware of how fast the field of separation science is moving.

The current volume is no exception. It also appears to be the longest yet, in terms of the number of reviews in a single volume. There are 13 reviews—considerably more than in earlier volumes, which contained an average of eight—comprising approximately 640 pages of text, although most of the reviews in the current volume are somewhat shorter than those in older volumes in the series. The net result of these shorter reviews is that each appeals to a narrower audience. The topics range from the fundamental "Dispersion in Micellar Electrokinetic Chromatography" and "Fundamental Interpretation of the Peak Profiles in Linear Reversed-Phase Liquid Chromatography" to the more applied "Determination of Herbicides in Water Using HPLC-MS Techniques" and "Analysis of Oligonucleotides by ESI-MS".

The reviews are current, with only two reviews containing a significant number of references older than 1990. Indeed, the majority of the references date beyond the mid-1990s. Similarly, each of the reviews is, at least partially, an authoritative, exact, and careful evaluation of the relevant literature reports in a specialized area. One concern that might be raised, however, is that the references for several of the reviews are rather heavily weighted with citations of those authors' own work. While it is a virtual necessity that the author(s) of each review be actively publishing in that field, producing a critical review requires the objective evaluation of all work relevant to that area. The pattern of citations suggests that the prerequisite breadth, if not objectivity, is lacking.

The central question of whether the editors have compiled "reviews of the most important developments in separation science" can only be correctly answered with the passage of time. Certainly, any specialist in separations will find something of interest. This volume, as the other volumes in the series, belongs in every science and engineering library. However, my personal recommendation is that individuals only purchase this volume if they are directly working in one of the fields reviewed. In this reviewer's opinion, the narrow scope of each review limits the utility of the volume.

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Studies in Natural Products Chemistry. Volume 21. Bioactive Natural Products (Part B). Edited by Atta-ur-Rahman (University of Karachi). Elsevier: Amsterdam. 2000. xiii + 812 pp. $432.00. ISBN 0-444-50469-9.

This book is a collection of 14 individually authored chapters dealing with an unconnected series of topics in natural products chemistry. The only "unifying" theme, if one needed to find one, would be that most of the structures covered have some type of known biological activity. The specific chapters are as follows: Chapter 1, Interference of Alkaloids with Neuroreceptors and Ion Channels; Chapter 2, Chemistry and Biological Activity of Natural and Semisynthetic Chromone Alkaloids; Chapter 3, Prodrugs of Natural Anthracyclines Suited for Antibody Directed Enzyme Prodrug Therapy (ADEPT) and Prodrug Monotherapy (PMT); Chapter 4, Bioactive Metabolites from Soil-borne Fungi: Natural Fungicides and Biocontrol Agents; Chapter 5, Structure—Activity Relationships of Bioactive Metabolites from some Indo-Pacific Marine Invertebrates; Chapter 6, Biosynthesis of Bioactive Marine Natural Products; Chapter 7, Cyanide and Thiocyanate-Derived Functionality in Marine Organisms—Structures, Biosynthesis and Ecology; Chapter 8, Natural Products with Polyene Amide Structures; Chapter 9, Phytochemicals as Potential Hypoglycemic Agents; Chapter 10, Analysis of Procyanidins; Chapter 11, Biological Activity of Essential Oils and Their Constituents; Chapter 12, Bioactive Saponins from Plants: An Update; Chapter 13, Biologically Active Diterpenoids from *Scoparia dulcis* L. (Scrophulariaceae); and Chapter 14, Some Bioactive

*Unsigned book reviews are by the Book Review Editor.

Natural Products from Chinese Medicinal Plants. Few of the references in any given chapter reach beyond 1997.

Most of the chapters cover natural products isolated from either marine or terrestrial sources and discuss pertinent biological activity and some semisynthetic modifications. One chapter, "Natural Products with Polyene Amide Structures", presents a fair bit of total synthesis work on a diverse structural array of natural products that contain polyene amides. There is an index at the end of the book that contains both compound names and genus + species names of producing organisms, as well as other terms cited throughout the book. While individual chapters might be useful to the specialist, the book as a whole summons little in the way of a coherently useful book for the organic chemist or natural products chemist.

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Surface and Colloid Science. Progress in Colloid and Polymer Science 116. Edited by V. Razumas (Institute of Biochemistry, Linius, Lithuania), B. Lindman (University of Lund), and T. Nylander (University of Lund). Springer-Verlag: Berlin, Heidelberg, New York. 2001. viii + 158 pp. DM 249. ISBN 3-540-67814-X.

This book contains the proceedings of the First Nordic-Baltic Meeting on Surface and Colloid Science held in Lithuania in August 1999. The wide range of topics covered—from adhesion to functionalized surfaces for bio- and chemosensors—is organized into the following sections: Self-Assembly of Lipids, Macromolecules and Surfactants; Disperse Systems; Interfacial Processes; and Biosensor Applications.

JA015242T

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Greenhouse Gas Carbon Dioxide Mitigation: Science and Technology. By Martin M. Halmann (Weizmann Institute of Science, Israel) and Meyer Steinberg (Brookhaven National Laboratory). Lewis Publishers: Boca Raton, FL. 1999. xix + 568 pp. $99.95. ISBN 1-56670-284-4

The pernicious effect of carbon dioxide on global temperatures will eventually force us to change our methods of power generation, our means of transportation, and the feedstocks from which we manufacture chemical products. The goal of presenting and evaluating these alternatives has been admirably achieved in the two halves of this timely book.

Technological alternatives are presented in the first half, written by Steinberg, so as to be readable by a general audience with little chemical knowledge. After a quick summary of the greenhouse effect, Steinberg covers mitigative responses to CO_2 accumulation, technologies for improving the efficiency of energy conversion and utilization, the removal and disposal of CO_2, and methods of decarbonization of fossil fuels. Interestingly, the power requirement for CO_2 removal, recovery, and disposal from stationary power generation is predicted to be only 11−16% of the power-generating capacity of most regions of the United States. Thus, given sufficient motivation, society can significantly reduce CO_2 emissions from stationary sources without a crippling loss in power production.

The chemistry of CO_2 fixation is the subject of the second half of the book, written in a manner more appropriate for a chemically literate audience. Halmann presents a fairly comprehensive overview of the chemical reactions that consume CO_2, emphasizing those reactions that either have or could eventually have industrial application and that therefore could reduce CO_2 emissions. The chapters include biochemistry, thermochemical reactions, carboxylations, CO_2 reforming and hydrogenation, and photochemical and electrochemical reduction. Particularly appealing is the use of biomass as a CO_2-neutral fuel and the use of CO_2 as a phosgene replacement for the preparation of polycarbonates, which could be a long-term sink for CO_2.

There are a fair number of typographical errors and an unfortunate inconsistency in the choice of units: BTU, lb, and °F in the first half of the book, kJ, g, and °C in the second. References are current to 1997. The book is already showing its age, especially in the chapter on global warming, although this is to be expected in such a rapidly changing field.

The financial costs of failing to curb CO_2 emissions are likely to become the motivation for adoption of many of the alternative technologies described. As the political and ultimately financial debate continues, all parties to the debate would do well to acquaint themselves with the available alternatives, as most handily compiled by the authors of this readable volume.

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High-Throughput Synthesis. Principles and Practices. Edited by Irving Sucholeiki (Solid Phase Sciences Corp., Medford, MA). Dekker: New York, Basel. 2001. xxiv + 366 pp. $175 ($75 for orders of 5 or more for classroom purposes). ISBN 0-8247-0256-5

The goal of Irving Sucholeiki in editing this book was to create a kind of combinatorial cookbook—a practical, hands-on laboratory manual "that would describe the mechanics of how to make large numbers of compounds". To this end, most of chapters begin with a brief overview of the subtopic, such as purification strategies, followed by a number of case studies that illustrate the different methods that can be used. To make the book accessible to graduate students and scientists who are not familiar with the field of combinatorial chemistry, an introductory section of two chapters has been included, covering the theory and methods in solid-phase organic synthesis. The remaining chapters are organized into the following sections: High-Throughput Synthesis for Drug Discovery; High-Throughput Synthesis of New Materials and Catalysts; and New Directions in High-Throughput Synthesis.

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Virtual Screening for Bioactive Molecules. Edited by H.-J. Böhm and G. Schneider (F. Hoffmann-La Roche, Ltd). Wiley-VCH: Weinheim. 2000. xviii + 308 pp. $125.00. ISBN 3-527-30153-4.

This book provides a good introduction to the combined topics of high-throughput screening (HTS) and bioinformatics. The pharmaceutical chemist almost certainly would be familiar with the topics covered, but other chemists would find the book informative at various levels. First, it provides an overview into a rapidly advancing area in which major changes occur from year to year. Second, it provides valuable insights into important unsolved chemical problems. Until recently, HTS had to deal with either the lack of availability of precursors, limited ways to make intermediates or products, or ineffective procedures to analyze combinational libraries. We simply did not know if any of the compounds missing from the library were good candidates for pharmaceuticals or not. With the creation of virtual libraries, we may now have increasing confidence in our predictions, but we find ourselves examining structures predicted to have high activity which are currently unknown. Some of these may be accessible from known chemical platforms (synthons). Almost certainly, however, numerous predicted structures will appear that will require considerable innovation and thus present a challenge to the synthetic organic chemist.

The bioinformatics aspect is burgeoning. The rapidly growing list of sequenced genomes will challenge the molecular biologist to generate the corresponding proteomes. Binding predictions of candidate agents, real or virtual, will be important when searching for possible drugs against pathogens. The completion of the sequencing of the human genome is going to increase the demand for success in predicting the binding of ligands to the yet unknown list of proteins. The reality is that because virtual libraries can outpace HTS-based libraries, as their predictive effectiveness increases, virtual libraries will not so much supplant as guide the creation of combinational libraries for evaluation at the bench.

Much of the book is devoted to the adaptation of existing predictors to virtual screening and to the identification of druglike properties or

characteristics useful in agriculture. Screening databases is important and recognized as being hampered by the lack of access to the proprietary structures that exist in the collections of pharmaceutical companies. However, considerable progress has been made in the screening of public databases, such as the World Drug Index and Comprehensive Medicinal Chemistry. The ultimate goal here is successful modeling of structure−activity relationships because the development of good predictive methods allows useful virtual libraries to be created. These libraries differ from the current combinatorial libraries in that the computationally generated candidate structures are not restricted to known compounds that are prepared through either published or "in-house" methodologies.

The various approaches to the generation of useful parameters are covered adequately. However, the authors make it clear that no relevant criteria should be neglected. Just as Mother Nature has sampled a miniscule fraction of molecular structural space, so must pharmaceutical chemists identify useful structures out of an impossibly large list to examine by current computational means. In one approach, molecular diversity is broken down into three main components: (1) diversity metrics, which attempts to quantify relationships of molecular similarity and chemical distance, (2) diversity spaces, which defines molecular characteristics in terms of chemical distance, and (3) diversity sampling, which uses methodology to find maximum diversity in representative subsets of a large virtual collection. Thus sampling, using techniques such as the Monte Carlo method, is essential.

Some chapters in this book are more technical than others, relying heavily on mathematical approaches. For example, the statistical approach of virtual screening is presented without mathematical derivations, and the discussion of neural networks is given with little background. The latter topic is directed to readers who understand the basics of graph theory and neural routing. Unfortunately, most of the equations and mathematical model representations are given without explanation. The complexity of the theory behind molecular modeling makes the more technical chapters difficult to read or interpret. All the chapters, however, appear to be well referenced so that the reader can pursue any relevant topic in depth.

In conclusion, this well-edited book not only provides a good introduction to the major strategies under development for the pharmaceutical world but also identifies important avenues of research for the chemist. To go from the best virtual structure to a compound for testing will undoubtedly provide significant challenges for the experimentalist.

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Block Copolymers. Edited by Francisco J. Balta Calleja (Instituto de Estructura de la Materia, CSIC, Madrid, Spain) and Zbigniew Roslaniec (Technical University of Szczecin, Szczecin, Poland). Marcel Dekker: New York and Basel. 2000. xi + 584 pp. $195.00. ISBN 0-8247-0382-0

At present the chemical industry is actively developing new block copolymers and new applications for them. The field is expanding as traditional styrenic triblock copolymers and polyurethane multiblock copolymers are being joined by a host of new materials that use a wider range of monomeric units to provide improved mechanical, thermal, and optical properties. This new book, edited by Calleja and Roslaniec, is directed toward this substantial audience.

The broad title is appropriate for this compilation of 20 chapters. Topics include synthesis, dynamics, characterization methods, blends containing block copolymers, and applications, although thin films are omitted. Commensurate with this breadth, references from a variety of journals and patents are incorporated. The breadth is also reflected in the variety of block copolymers covered that have architectures ranging from simple block, diblock, triblock, multiblock, and graft as well as chemistries involving styrenics, urethanes, ethers, esters, amides, natural compounds, and more.

As with most compiled books, the chapters vary in balance. For example, Chapters 7 and 9, describing block copolymer characterization by microhardness and ultrasonic measurements, respectively, provide a synopsis of research from the authors' groups, as evidenced by nearly 50% of the references. These summaries provide a unified view that a reader would otherwise have to piece together from a dozen or more journal articles. Other chapters provide a more balanced view of the field, most notably Chapters 6, 13, and 20 on viscoelastic properties, block copolymer/homopolymer blends, and future trends, respectively. The chapters also vary in their timeliness, as evaluated by the proportion of recent references; some chapters have fewer than five references from 1997 and beyond. Because the topical and chemical breadth of this book's content has been accomplished almost exclusively by European authors, however, the book is likely to connect the reader with previously unknown bodies of work, particularly for the American reader.

Block Copolymers provides a broad synopsis of the field with an emphasis on European contributions. It is written for researchers or graduate students already familiar with block copolymers, but eager to broaden their horizons.

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Handbook of Molecular Descriptors. Methods and Principles in Medicinal Chemistry Series. Volume 11. By Roberto Todeschini and Viviana Consonni (Universita degli Studi di Milano-Bicocca). Edited by R. Mannold, H. Kubinyi, and H. Timmerman. Wiley-VCH: Weinheim and New York. 2000. xxi + 668 pp. 498 DM. ISBN 3-527-29913-O

The book is composed of an introduction by the authors, a user's guide that provides a key to the hierarchical organization of the topics, a section with notations and symbols, and a section of acronyms or abbreviations. These are followed by over 500 pages of definitions of descriptors listed in alphabetical order and three appendices. The appendices contain the Greek alphabet, symbols of molecular descriptors, and a software list. The last appendix contains the names and sources of some of the common software packages that have been introduced over the past 25−30 years. Most are no longer supported or available, however. The last section of the book features a bibliography, which is extensive and covers approximately 140 pages.

The publication of this work was a monumental undertaking and has led to the most complete listing of molecular descriptors that has been published. They range from the most obscure to the most widely used. One fault of the volume is that it is completely noncritical. A large number of the descriptors defined are so-called "topological" descriptors, which can be generated in large numbers and have found very limited utility.

Finally, the name of this book is somewhat misleading. It is, in this reviewer's opinion, a dictionary or encyclopedia of molecular descriptors, rather than a handbook. "Handbook" implies a "how-to" discussion of the titled concepts, whereas this volume is really an alphabetical listing of published descriptors. This is not to distract from the value of the book, however. Because of its cost, it is doubtful that the book will be purchased by individual researchers, but it should find itself in most reference libraries.

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