

Book Reviews

Methods in Biotechnology 4: Natural Products Isolation. Edited by Richard J. P. Cannell. Humana Press, Totowa, NJ. 1998. x + 473 pp. 15 x 22.5 cm. ISBN 0-896-03362-7. \$89.50.

There can be little doubt that great progress has been made in isolation, structure elucidation, and discovery of biological effects of natural products. However, literature reports on natural products tend to emphasize chemical and biological aspects of these products once they have been isolated. Extraction and fractionation details are usually minimal and sometimes are lacking, and only the general techniques used are cited. Even when particular conditions of fractionation are reported, the reader's knowledge of the practical methodology used as well as the reasoning behind the conditions employed is assumed. *Natural Products Isolation* aims to provide a foundation for this knowledge. It is a concise, yet comprehensive, book in the *Methods in Biotechnology* series. The book offers some practical guidance in the processes of extraction and fractionation, utilizing modern purification techniques, to procure pure chemical entities. The book comprises 15 chapters, covering various aspects of the isolation process, authored by experts from industry and academia. The book begins and ends with two excellent chapters by the editor. The introductory chapter describes factors involved in approaching the isolation of small amounts of unidentified compounds from complex biological mixtures. The closing chapter, a follow-up of natural products isolation, covers contemporary aspects not covered in the earlier chapters, inter alia, preparation of minor analogues, gene expression, blocked and directed biosynthesis, novel biotransformation methodology, combinatorial synthesis, and combinatorial biosynthesis.

Other chapters addressing isolation methods include initial extraction and product capture and supercritical fluid extraction. Four chapters on chromatographic techniques include column chromatography, ion-exchange methods, planar chromatography, and high-speed counter current chromatography. These are followed by a chapter on crystallization. Two chapters address topics specifically associated with isolation of plant secondary metabolites and isolation of marine products. A chapter dealing with purification of water-soluble products also deals to a major extent with compounds of marine origin. There are also chapters on dereplication and on scale-up of natural products isolation.

Written by experienced experimentalists, the chapters provide references and/or suggested readings. Detailed hands-on methods are described, with background notes and examples of major techniques for various classes of novel products. The book contains a wealth of practical information, hints, and useful points. In several cases, stepwise instructions for a specific technique are included, and all chapters include specific examples of applications.

The book is aimed mainly at scientists with limited experience in natural products isolation and fractionation:

students embarking on natural products research and investigators from other chemical disciplines who wish to obtain pure natural products. However, the book is likely to be a useful reference for experienced natural products chemists. The book is an outstanding effort in presentation of well-written, clearly illustrated, and properly proofed chapters with a consistency of style and presentation. It will be an asset in any laboratory where natural products isolation is performed.

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Encyclopedia of Computational Chemistry. P. von R. Schleyer, Editor-in-Chief. John Wiley and Sons, Inc., Chichester, U.K. 1998. xxix + 3429 pp. 21 x 27.5 cm. ISBN 0-471-96588-X. \$2550.00.

How does one begin to encapsulate the important points of a stunning and comprehensive reference work that weighs in at 30 pounds and makes 1 foot of shelf space the most valuable real estate in the office? A time-honored place to start is "from the beginning" or ab initio, as it's said in Latin. Indeed, after some valuable preliminaries, this series of five hefty volumes offers almost 700 articles on literally all aspects of computers in chemistry—from ab initio to zeolites.

This new set of books is timely. The award of the 1998 Nobel prize for research in computational chemistry is indicative of the mainstream role that calculation has come to play in contemporary science. In the 14 years since the first Gordon Conference in Computational Chemistry, in 1985, we all have witnessed major changes in the application of computation to the chemical sciences. It has broadened to include more than simply energy calculations of small molecules. It has extended its reach down to the desktop of every chemist.

Leading edge thinkers in computation believed in the promise of the technique. In a public lecture at Harvard, in 1986, John Pople said: "These are the experimental data; and they're all by reputable people. So we have no reason to doubt them. And again, they're to be congratulated for getting the answers correctly."

We all believed back then that ab initio numbers, at the highest levels, were approaching experimental accuracy. But where would most regular scientists get access to supercomputers, to solve small but important scientific problems? In the 1980s, the arcane knowledge and specific expertise required were a significant barrier to the everyday application of theory.

Today, the picture has changed dramatically. One can perform calculations at will, even for pedagogical purposes in a high school curriculum. In the pharmaceutical industry, computational chemistry, rational design, and

molecular simulation are regarded as mainstream. This important transformation is due, in no small part, to explosive technological advances in the microcomputer hardware and software industries, which have placed powerful computational tools in the hands of everyday scientists.

Due to the global nature of the computational chemistry enterprise, Paul Schleyer, the Editor-in-Chief, has pulled together the content of this encyclopedia under the able leadership of five Editors: Norman L. Allinger, Tim Clark, Peter A. Kollman, Henry F. Schaefer III, and Johann Gasteiger and an Associate Editor/Project Coordinator: Peter R. Schreiner. They have managed to assemble a momentous and impressive set of articles, falling into three categories: (1) regular articles, (2) definition entries, and (3) descriptions of software packages.

Each of these is written by specialists in the field—more often than not, important names that I recognize from 25 years of scanning the literature.

The selection of topics for the articles leaves very little additional information to be desired. Practically every branch of chemistry is represented by a tie-in to computation. Some titles that stand out in my mind include: Drug Design; Diversity of Chemical Libraries; Combinatorial Chemistry; Charmm; Cambridge Structural Database; Electronegativity; Electrostatic Potential; Force Fields; Genetic Algorithms; Graph

Theory; History; Hydrogen Bonding; LFER; 3D Structure; Topological Indices; Wavelet Transforms; NMR; Neural Networks; Protein Structure; QSAR; Sweeteners; Tanimoto Index; X-Ray Crystallographic Analysis; and Zeolites.

True to the definition of an encyclopedia, this series of five volumes provides information on every branch of computational chemistry and many other scientific and technological topics which are germane to the present-day use of computers in the chemical sciences. Coverage of contemporary subjects illustrates just how far we have come since the early days of molecular modeling. These include: Teaching Computational Chemistry to Undergraduate Students; CAS; Electronic Lab Notebooks; Electronic Publishing; Experimental Design; Internet; JAVA; C++; LIMS; and Structural Similarity Measures.

The amazing editorial scope of this set was achieved by an innovative approach to the international collaboration—totally electronic submission and refereeing of the manuscripts. Timeliness of the subject matter was thus assured by the fast execution and production of the project. This methodology is said to promise fast updates in the future.

Each volume features 4 pages of symbols and abbreviations, listed inside the covers; synopses of important branches of computational chemistry, by the editors; a complete listing of the contents of the entire series; and the topical articles, themselves, listed in alphabetical order. Each article or definition is accompanied by cross-references (bold italics) to other articles in the book. Longer entries are written in the format of review articles. Each includes its own bibliography.

The excellent and very readable page layout is further enhanced by the use of multicolor graphics. Beyond

what would be expected in molecular model pictures, color is used to good advantage in figures and diagrams, where it enhances the interpretation and readability. The article on Cambridge Structural Database is exemplary in this regard.

At the end of Volume 5, there is an excellent author index, which keys to the contributed articles in the volumes as well as current institutional affiliation. The final section is a very complete 28-page subject index.

The encyclopedia aims to introduce the full sweep of science and technology of computational chemistry to a wide variety of practicing scientists, beyond just those individuals who specialize in molecular structure calculations. Indeed, the computational chemistry subject matter is at the leading edge of scientific practice. The volumes fold in important, related subject matter which is growing in practical importance to the broader group of scientists, e.g., Chemical Abstracts searching; the internet; electronic notebooks; combinatorial chemistry; electronic publishing; and experimental design.

This series would be a most welcome addition to industrial and academic libraries and research groups/departments involved in the general area of application of computers to chemistry. I can see an important service to scientists and students who need to learn more about many important topics in which they are not directly involved with their own work, or to gain a concise high-level, high-quality foothold in a particular subject area. The downside of the encyclopedia's price point is accessibility at smaller institutions and companies, who could use the information but need to conserve their cash. Perhaps a way could be found to offer per-article access via the internet or an abbreviated edition on CD ROM.

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Thin-Layer Chromatography. Fourth Edition. Chromatographic Science Series Volume 81. By Bernard Fried and Joseph Sherma. Marcel Dekker, Inc., New York. 1999. viii + 499 pp. 16 x 23.5 cm. ISBN 0-8247-0222-0. \$195.00.

Thin-layer chromatography (TLC) involves the application of a sample to a thin sorbent layer (stationary phase) on a plate followed by the movement of a solvent (mobile phase) through the stationary phase. The variety of stationary and mobile phases available enables resolution of a vast number of compounds. This admirable book has two sections: the first on theory and practice and the second on applications to important classes of compounds. The writing is clear and rigorous, suited to students as well as established investigators. There is a 12-page subject index and a glossary with 162 entries. Table 8.1 lists 51 detection reagents along with directions for their preparation and the expected color of the compounds detected. Commercial sources for standards, TLC instruments, plates, and reagents

are provided. Each chapter is thoroughly referenced, mainly with material from 1985–1997. It is pointed out that TLC is reviewed every 2 years in the Fundamental Reviews Issue of *Analytical Chemistry*.

The section on theory and practice of TLC has 11 chapters including history, theory, materials, instrumentation, detection, and quantitation. The applications section has 10 chapters including those on organic dyes, natural pigments, lipids, amino acids, carbohydrates, steroids, and pharmaceuticals. Each of these 10 chapters has a detailed description of experiments suitable for a student laboratory.

Of major interest to medicinal chemists is the chapter on pharmaceuticals which has sections on barbiturates, tricyclic antidepressants, benzodiazepines, theophylline, aspirin, cardiac glycosides, and antiarrhythmic drugs. A detailed experiment is provided on separation of drugs of abuse from urine and another on the determination of aspirin and caffeine in analgesic tablets. Although not given a separate section in this book, TLC is widely used to monitor the course of chemical syntheses.

The enthusiasm of the authors for TLC and the thoroughness of their presentation makes a reader who has not used this technique wish to try it for fun in addition to the useful results likely to accrue.

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Principles of Chemical Nomenclature. A Guide to IUPAC Recommendations. Edited by G. J. Leigh. Blackwell Science, Oxford, U.K. 1998. viii + 133 pp. 19 x 27 cm. ISBN 0-86542-685-6. \$28.50.

This is a very nice, brief discussion of the rules of nomenclature for the major classes of molecules with which the medicinal or organic chemist may deal. A

variety of examples are given for most of the rules, such that it is relatively easy to learn to apply the rules in different situations. Many of these types of nomenclature questions are not always well-remembered or perhaps not yet learned (in the case of students). The book begins with discussion of the use and representation of formulas and progresses to consideration of complex nomenclature of organic, inorganic, and organometallic compounds. A book of this brevity omits coverage of some types of compounds. While these omissions are not always insignificant, it is probably impossible to cover all types of compounds in a brief guide such as this. The reader is directed to several in-depth volumes for a more complete guide to nomenclature.

While I noticed no errors, there are a few aspects that American readers may find confusing. For example, *LithAl* is (to me) an unfamiliar British acronym for lithium aluminum hydride.

One of the real pluses of the book is the tables of names of ions, groups, ligands, and ligand abbreviations. The table of names of ions and groups (Table 4.1) comprises 14 pages of the various common and IUPAC names. For most organic chemists, remembering the abbreviations of ligands for inorganic compounds is not always second nature, and this book contains a helpful compilation of such abbreviations. One minor error in Table 4.5 is the listing of *Bzl* as an abbreviation for benzyl (PhCH₂). Most journals use *Bn* for benzyl and *Bz* for benzoyl.

I strongly recommend this book to all medicinal and organic chemists, both students and practitioners. For its modest price, this is a great little book for one's personal bookshelf.

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