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.

Govind J. Kapadia

School of Pharmacy
College of Pharmacy, Nursing, and Allied Health Sciences
Howard University
Washington, D.C. 20059

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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.

Emile M. Bellott

Pharm-Eco Laboratories, Inc.
128 Spring Street
Lexington, Massachusetts 02421-7800

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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