BOOKS

X-ray Crystallography and Drug Action. Edited by A. S. HORN and C. J. DE RANTER. Oxford University Press, 200 Madison Avenue, New York, NY 10016. 1984. 514 pp. 16 × 24 cm. Price: $59.00.

The International School of Crystallography at the Ettore Majorana Centre in Erice, Sicily, sponsors an annual week-long course devoted to one of the various interdisciplinary subdivisions of crystallography. In the spring of 1983, the ninth course was devoted to the subject of X-ray crystallography and drug action. This book is a collection of the twenty-seven papers presented at the course.

The first six papers are general reviews of the ways in which the results of both small molecule and macromolecular crystal structure determinations are applied to problems in pharmaceutical chemistry. Discussions of selected basic principles of crystal structure determination and of quantum chemical calculations are included. They are technically sound, but not so rigorous as to encourage a noncrystallographer to pass on to the next paper. The last four papers in the book are similarly comprehensive in their coverage of aspects of graphics and molecular modeling.

Most of the volume is devoted to presentations of research studies of a variety of biological systems. Pharmacologists, biochemists, and crystallographers interact in many mutually supportive ways. Two papers on the dihydrofolate reductase-thymidylate synthetase system as a therapeutic target for the treatment of a variety of diseases describe this relationship with exceptional clarity. Analgesics and neuroactive drugs are treated with similar thoroughness. The remaining presentations are so broad in scope that no summary of reasonable length could do them justice.

As with any effort involving many authors, there are places where this book falls short of its potential. The reader is denied the benefit of summaries of what must have been exciting discussions after each presentation. No single paper is concerned primarily with polymorphism, an omission which will disappoint pharmaceutical chemists. Perhaps an even more serious omission is that, with several of the contributions discussing enantiomeric effects upon drug activity, crystallographic studies of spontaneous resolution in drugs are not even considered in the review papers.

From a technical point of view, the book is extremely well produced. The typescripts provided by the authors are generally clear. Very few typographical errors were discovered. For the most part, the figures are well done and clearly labeled. A few of the stereoscopic pairs are so closely set that some individuals may encounter difficulty in achieving stereopsis, even with the aid of a viewer. The subject index could have been more complete and consistent, particularly with reference to citations of drugs by name. Computer programs are indexed by name rather than by function. This is unnecessarily confusing, since the former might well be obscure to the noncrystallographer, as well as being unrelated to the latter.

When one considers the price of this volume in relation to others of similar coverage, it is certainly modestly priced. Even with the omissions and technical shortcomings noted, the overall strength of the discussions of structure activity relationships in proteins, enzymes, and their complexes with smaller molecules makes this book a worthwhile addition to the personal library of most pharmaceutical chemists.

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Fungal Metabolites. Vol. II. By W. B. TURNER and D. C. ALDRIDGE. Academic Press, 111 Fifth Avenue, New York, NY 10003. 1983. 631 pp. 16 × 23.5 cm. Price: $80.00.

As a frequent and happy user of the first volume of *Fungal Metabolites* by Turner, it was a great pleasure to see the publication of this second volume in 1983. The first volume, published in 1971, is an extensive compilation of secondary (specific) metabolites of fungi organized into chapters largely on the basis of their biogenesis. Volume II is essentially a 10-year update that includes nearly 2,000 new metabolites. Chapters 1 and 2 from Volume I dealt with primary and secondary metabolism, and aspects of cultivation and secondary metabolism. These chapters are not included as separate topics in the new book, but the few developments in these areas are covered in other sections where appropriate. References to labeling experiments used in Volume I have

been deleted, but Volume II contains much new important information on carbon-13 isotopic labeling experiments extensively utilized during the past decade in the elucidation of biosynthetic pathways.

The 1983 edition of *Fungal Metabolites* is divided into seven chapters of varying length. Chapters describe groups of metabolites which are: not from acetate (40 pp.—215 references); from fatty acids (10 pp.—59 references); from polyketides (168 pp.—731 references); from terpenes (141 pp.—593 references); from tricarboxylic acid cycle intermediates (16 pp.—75 references); from amino acids (72 pp.—389 references); miscellaneous compounds (37 pp.—180 references); and an addendum chapter (62 pp.—281 references). References for all but the last chapter date largely in the 1970's with a few citations from the 1960's and 1980. The addendum chapter is essentially an update of information on all classes of fungal metabolites covered in earlier chapters, and it includes literature citations from 1980, 1981, and a few into 1982.

The bulk of this book is loaded with useful illustrations and references, and the text provides good concise coloring for the structures shown. The empirical formula, organism, and subject indices make the book practically useful. This is especially so, since the authors took great care to maintain the same organization used in the original volume. It is also easy to cross-reference between the two volumes. This is an outstanding reference-work and it is a must for any laboratory seriously engaged in research on the topic of fungal metabolites.

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Pattern Recognition Approaches To Data Interpretation. By DIANE D. WOLFF and MICHAEL L. PARSONS. Plenum Press, 233 Spring St., New York, NY 10013. 1983. 223 pp. 17 × 26 cm. Price: $29.50.

This book is a "how to" description of the use of multivariate statistical packages in the evaluation of large arrays of chemical data. The authors focus primarily on techniques popularized in recent years under the general term, "pattern recognition" with a major emphasis on how to use and interpret ARTHUR (B. R. Kowalski, Laboratory of Chemometrics, Seattle, WA), SPSS (SPSS, Inc., Chicago, IL), and BMDP (Health Sciences Computing Facility, Los Angeles, CA). SAS (SAS Institute Inc., Cary, NC) and CLUSTAN (Scotland) are described to a somewhat lesser degree. The book is intended for investigators with little or no prior experience with data analysis nor with the above-mentioned statistical packages. Program descriptions, strengths, and implementation are linked to the particular versions of the packages used by the authors. For example, users of the 1977 and later versions of the ARTHUR program would be advised to refer to the manuals for those programs for program description and implementation and to the book for suggestions on problem statement, analysis, and interpretation.

Through the example of a single set of pollution data, the authors take the reader through the steps of data analysis from problem statement and data coding to final evaluation. The numerical techniques described and applied to the pollution data include data mapping, supervised and unsupervised learning algorithms, and univariate and bivariate statistics. The excellent discussion and demonstration of preliminary data evaluation and variable relationships is the major strength of this book. A minor weakness is that the opinions expressed by the authors concerning the utility-specific numerical techniques seem to be based on their experiences rather than rigorous statistical studies. The comparison of numerical techniques available in two or more packages will certainly be valued by chemists who are uncertain as to which packages better address a particular application.

Pattern Recognition Approaches to Data Interpretation is a long overdue addition to the wealth of monographs on chemometrics published over the past few years. It is unique in its applications oriented approach. The book is a recommended reader for novices and a resource for more experienced investigators.

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