## REVIEWS

**Index Nominum 1980.** 10th ed. The Swiss Pharmaceutical Society. 1979. xiv + 913 pp. 21 x 29.5 cm. (Available from Drug Intelligence Publications, Dept. C78, Hamilton, IL 62341.) (*Introduction in French, German, and English; text in French.*)

Index Nominum 1980 is an alphabetical list of generic and trade names of internationally available drug products containing one active substance. Information is given on International Nonproprietary Names (INN) and other generic names, trade names and manufacturers, chemical names and structures, pharmacopeial monographs on each drug, and main therapeutic uses. The 1980 edition lists approximately 3800 compounds and derivatives, approximately 200 of which are new. More than 26,000 references are given.

As with the previous edition, Index Nominum 1980 is a single volume with a single alphabet; readers never have to look up more than one cross-reference to find the main entry. Among the other convenient features retained in this edition are the listing of monograph titles from pharmacopeias of international importance and the distinction of new substances published for the first time by a point preceding the name or synonym.

*Staff Review*

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**Selective Toxicity: The Physico-Chemical Basis of Therapy, 6th ed.** By ADRIEN ALBERT. Wiley, One Wiley Drive, Somerset, NJ 08873. 1979. 662 pp. 15 × 23 cm. Price $42.50.

The first edition of this book appeared in 1951, and the sixth edition, published recently, is approximately 10% larger than the fifth edition, which was published in 1973.

The book is divided into two parts. The first part is entitled Topics of General Interest and consists of seven chapters (269 pages). The first chapter briefly discusses the principle of selectivity, and the second chapter outlines various steps in correlating chemical structure with biological activity. This account deals mainly with the concept of receptors followed by a discussion of how minor molecular modifications by methyl or methylene groups may affect biological properties. Chapters 3–5 (129 pages) deal with three general principles of selectivity: differences in the distribution of compounds between "economic and uneconomic cells," a comparison of the biochemistry between the same metabolic routes in different biological systems, and comparisons between the structures of different cells and cellular components. Chapter 6 describes some principles of chemotherapy, including a succinct account of drug resistance. This chapter is prefaced by a short but interesting account of various aspects of the history of chemotherapy. The first section of this book concludes with a chapter on pharmacodynamics (70 pages), in which the theme of selective toxicity of a compound in one organism is amplified.

The second section, Studies, in Depth, of Topics from Part I (285 pages), commences with a chapter on the nature of chemical bonding and absorption followed by a chapter on metabolites and antimetabolites. Chapters 10 and 11 are particularly valuable and emphasize the importance of ionization and chelation of compounds in eliciting biological responses. They are followed by two chapters on the covalent bond and stereochemistry. Chapter 14 discusses surface activity. The next chapter deals with biological activity that is not related to chemical structure. A chapter not appearing in previous editions, entitled The Perfection of a Discovery (approximately 5 pages), emphasizes multiple regression analyses, molecular orbital calculations, and molecular conductivity. Four appendixes follow the second section.

On the positive side, many medicinal chemists, pharmacologists, biochemists, and toxicologists will derive some benefit from portions of this book. A number of recent developments in medicinal chemistry are incorporated into this monograph, including certain aspects of cancer, opioid receptors, and robust metal complexes. The bibliography is excellent, and many recent references are included.

On the negative side, although it is difficult to deal adequately with every facet of selective toxicity, there are areas where the present work is lacking. While the author states that regression analysis and other mathematical models are much used, he gives only a brief account of them. Thus, although he deals with this subject on pages 70–75 and 557–562, this account will be considered by some to be a somewhat cursory treatment. Furthermore, a somewhat truncated summary of information is available on prodrugs. Another criticism is the fragmentation of information throughout the book; although it is understood that the classification of the vast amount of information recorded in this book is a difficult art, the value of dividing the book into two parts is not clear to this reviewer. Why go back in Part II and resurrect a theme that was started in Part I? For example, the subject of receptors is introduced on pages 23–39, mentioned briefly again on pages 250–261, and outlined again in Chapter 13. The same approach is used not only for stereochemistry, which is described initially on pages 39–46 and then becomes the subject of an entire chapter, but also for regression analyses, as noted earlier. Presumably, the author would maintain that it is an unreasonably large jump, and, thus, the book may be regarded as too undergraduate oriented for those who are experienced in the chemical–biological interface.

In summary, this book is valuable reading to those interested in chemicals producing biological responses, but medicinal chemists and others will have to delve into other monographs in many cases to obtain a fuller treatment of the subject.

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**Atlas of the Three-Dimensional Structure of Drugs, Vol. 1.** By J. P. TOLLENAERE, H. MOEREELS, and L. A. RAYMAEKERS. Elsevier/North-Holland Inc., 52 Vanderbilt Ave., New York, NY 10017. 1979. 322 pp. 17 × 24.5 cm. Price $36.50.

Medicinal chemists should welcome this volume since it is a successful effort to relate appropriate crystallography to the representation of the molecular architecture of compounds from a variety of pharmacological classes.

Representative compounds from the following categories are included: muscarinic agonists and antagonists; nicotinic agonists and antagonists; phenethylamines, catecholamines, and related compounds; $H_1$- and $H_2$-histamine receptor agonists and antagonists; opiate receptor agonists and antagonists; serotonin and related compounds; hallucinogens; local anesthetics; antiarrhythmic agents; $Ca^{2+}$-antagonists; anticonvulsants and sedative hypnotics; diuretics; nonsteroidal anti-inflammatory agents; and anthelmintic, antifungal, and antiprotozoal agents.

The primary objective was to compare and classify the compounds within each class with respect to geometric and conformational characteristics by using crystallographic data, but it was necessary to visualize molecular structures rather than merely rely on interpretations of numerical data in terms of distances and torsion angles. To determine the optimal orientation of so many molecules, interactive computer techniques were used; an APL (A Programming Language) function PROJ was developed to generate numerous orientations from which the final selection was made. Rotation angles around defined $x$, $y$, and $z$ axes, the scale, and viewing distance then were transferred and used in the ORTEP (Oak Ridge Thermal Ellipsoid Program), which draws the picture on a CALCOMP plotter. The ORTEP drawings of the molecular structures then were retouched slightly and thus appear very artistically in the book.

The authors emphasize the idea of pharmacological class relationship by representing molecular structure in space in such a manner that common moieties within each class can be recognized. In many cases, a compromise had to be made between strictly analogous orientation of key moieties and clarity of the representation and the authors' attempt to show the intrinsic beauty of molecular architecture. Due to this compromise, not only medicinal chemists who have expertise in crystallography and three-dimensional structural studies, but also most connoisseurs of fine art and fine science will appreciate the beauty of the struc-

tural representations, with one structure per page covering most of the page.

The introduction includes very helpful, brief explanations regarding the structural data bearing on groups, classes, and subclasses of the compounds. Although these comments are not intended to provide complete explanations, they strengthen the perception of intra- and interclass relationships and differences which are reflected by the pictorial representations.

The authors' intent was for this book "to serve as a bridge between crystallographers and structural chemists and those engaged in drug research." This reviewer concludes that the book does in fact provide such an effective bridge. This book therefore is recommended not only to medicinal chemists but also to graduate and undergraduate students in medicinal chemistry and pharmacology.

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**Computer-Assisted Drug Design.** Edited by E. C. OLSON and R. E. CHRISTOFFERSEN. (ACS Symposium Series 112.) American Chemical Society, 1155 16th St., N.W., Washington, DC 20036. 1979. 619 pp. 15 × 23 cm. Price $40.00.

This book is a collection of 26 presentations made at a recent American Chemical Society symposium entitled "Computer-Assisted Drug Design." The articles cover a few of the theoretical structure–activity relationship methods in use for drug design. The book is divided into four sections covering the assessment of several techniques, drug receptor modeling, examples of some techniques, and applications. A 15-page index completes the book.

A number of articles stand out and deserve comment. In the first section, a review of a few of the general structure–activity relationship methods is attempted. Unfortunately, it is incomplete in its coverage. An article by Topliss *et al.* is a useful description of chance factors in dealing with structure–activity relationship statistics.

In the second section on drug receptor modeling, Andrews briefly discusses transition state analogs. Articles by *Cole et al.*, Marshall *et al.*, and Humber *et al.* on mapping and modeling are of interest. An article by Loew *et al.* on interaction studies on the opiate receptor is well written and of quality. Rohrer *et al.* describe the use of PROPHET in the same section.

In the third section on examples of techniques, articles by Magee, Bersohn, Weintraub, and Stuper *et al.* present useful descriptions of computer-assisted methods of analysis.

The fourth section on applications in drug design contains a refreshingly thorough and accurate review of theoretical structure–activity relationship contributions over the past 15 years by Grunewald *et al.* Articles by Gund *et al.*, Petit *et al.*, and Hodes reveal computer-based applications of theoretical structure—activity relationships.

A number of problems apparent with this book are common to similar efforts to publish quickly everything presented at a symposium. Because of the requirement for speed, there is little opportunity for screening or review, leading to a wide range of scholarship and quality. Since every presentation is published, the amount of background material that can accompany each article is restricted. As a result, a reader outside of the area is not sufficiently informed. In contrast, an investigator in the field probably would turn to the original journal articles of the authors.

The book should be examined by anyone involved or interested in theoretical structure–activity relationship studies in medicinal chemistry.

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