Book Reviews

Annual Reports in Medicinal Chemistry. Volume 35. Editor-in-Chief, Annette Doherty. Academic Press, San Diego, CA. 2000. xi + 425 pp. 17.5 × 25.5 cm. ISBN 0-12-040535-0. $85.00.

This year's *Annual Reports* contains 31 chapters divided among seven topics: Central Nervous System Diseases; Cardiovascular and Pulmonary Diseases; Cancer and Infectious Diseases; Immunology, Endocrinology and Metabolic Diseases; Topics in Biology; Topics in Drug Design and Discovery; and Trends and Perspectives. The individual chapters reflect current and projected future trends in drug research and therapy, and as always they are crammed with useful, intriguing, and thought-provoking information. This reviewer found almost all of the chapters to be an enjoyable read, even those in which he had no research interest. Especially noteworthy were the chapters: Genetically Modified Crops as a Source of Pharmaceuticals; *Ex Vivo* Approaches to Predicting Oral Pharmacokinetics in Humans; and Pharmacogenetics. The continued inclusion of extensive indices is most welcome and provides rapid access to much otherwise somewhat sequestered information: Compound Name, Code Number, and Subject Index for Vol. 35; Cumulative Chapter Titles Keyword Index, Volumes 1−35; Cumulative NCE Introduction Index, 1983−1999; and Cumulative NCE Introduction Index, 1983−1999 (By Indication).

Researchers in pharmacology, pharmaceutics, and allied fields will find this volume useful. For medicinal chemists, it is essential.

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JM000436P

10.1021/jm000436m

Analytical Techniques in Combinatorial Chemistry. Edited by Michael Swartz. Marcel Dekker, New York. 2000. xii + 301 pp. 15.5 × 23.5 cm. ISBN 0-8247-1939-5. $150.00.

Analytical Techniques in Combinatorial Chemistry consists principally of a compilation of reviews by both industrial and academic researchers, of the major analytical methods employed in the general area of combinatorial chemistry. The text consists of nine relatively concise and well-referenced chapters.

Chapter 1 provides an overview of the history and evolution of solution-phase and solid-phase synthetic methods, with an outline of the major analytical challenges presented by both formats. There then follow three chapters which review consecutively: mass spectrometry, infrared and Raman spectroscopy, and NMR methods. The section on mass spectrometry covers techniques for structure elucidation and mixture characterization employed in the synthesis and analysis of combinatorial libraries, with the latter part of the chapter reviewing mass spectroscopy methods used in the biological screening of mixtures. Chapter 3 reviews infrared and Raman spectroscopy and limits itself to a discussion of techniques for acquiring structural data on resin-supported compounds. The chapter on NMR outlines methods for the direct analysis of library components on solid-phase, reviewing gel-phase and magic-angle methods as applied to both proton and other nuclei. Solution techniques are also discussed, with some commentary on HPLC/NMR and flow NMR methodologies. Chapter 5 consists of a review of standard HPLC methods, together with some references to LC/MS techniques. In the following chapter a review of capillary electrophoresis is presented, in which some emphasis is given to those methodologies involving an aspect of affinity recognition. Chapters 7 and 8 discuss respectively, information management in combinatorial synthesis and bioanalytical screening methodologies in lead generation and optimization. The last chapter of the text is an 87-page compilation of commercial resources, in which a brief profile on each company is presented, together with a short commentary on the products and technologies offered by that organization. This section is not cross-referenced, which significantly limits its utility.

In general, the reviews cover literature methods up to and including work published in 1997. This results in some unfortunate omissions from the text, which provides little or no commentary on such significant techniques as structure deconvolution of encoded combinatorial libraries using IR tags, ligand identification by SAR by NMR, and analytical and preparative methods in supercritical fluid chromatography. With that qualification however, this text does bring together a useful collection of reviews which will be of value in orienting researchers new to the field on the principal analytical methods available for structure elucidation, reaction monitoring, product isolation, and some general screening methodologies and tactics.

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JM000438+

10.1021/jm000438+

Topological Indices and Related Descriptors in QSAR and QSPR. Edited by James Devillers and Alexandru T. Balaban. Gordon and Breach Science Publishers, Amsterdam, The Netherlands. 1999. x + 811 pp. 15.5 × 23.5 cm. ISBN 90-5699-239-2. $198.00.

This is a rather large volume which opens with a Preface by the editors. This is followed by seventeen chapters by eighteen contributors, most of whom are coauthors on more than one chapter. All have published extensively on their topic(s). There is a loose organization in the volume. The first few chapters are something of an overview and history of graph theoretic methods and of their development. The next few chapters are

rather theoretical in their presentation and are difficult to follow due to their heavy reliance on mathematics and matrix algebra. The next several chapters review published applications of topological indices for the study of structure−activity and structure−property relationships.

The first chapter, a review by one of the editors (Devillers), compares some of the more commonly used physicochemical descriptors with topological descriptors. The main message of the chapter is a justification of topological descriptors on the basis that many can be easily computed for a molecule, which makes structure−property and structure−activity relationships based on these indices multivariate (as opposed to univariate) and more reliable.

The second chapter presents to the reader a chronological development of topological descriptors. In the first part of the chapter the authors attempt to convince the reader that topological descriptors have their roots in quantum chemistry. This drift continues into the next chapter, which ends with a section describing the use of topological indices in deriving structure−property relationships for a series of alkanes. Chapters 4−6 discuss a multitude of expressions of molecular graphs and matrices. The discussion is overly theoretical and difficult to follow unless one is well-grounded in matrix algebra.

Chapter 7, by Hall and Kier, is a summary of their contributions to the generation and use of χ-indices. Chapter 9, by E. Estrada, is somewhat redundant. In a later section the author discusses the generation of 3-D molecular descriptors, and confuses conformers with geometric isomers. In Chapter 10, by Kier and Hall, the κ-index is introduced and is proposed to be a shape-related index. The E-state formalism, proposed to combine electronegativity with local topology, is discussed in Capter 11.

The next six chapters discuss the use of neural networks in conjuction with topological indices to generate structure−property relationships. Again, most of the properties studied are solution properties of uninteresting compounds or of nonspecific biological activities of simple organic compounds.

The last chapter, by Ivanciuc and Devillers, is a discussion of various conventions used in drawing programs to encode structures. Such files are transparent to the typical organic chemist, so this chapter should be of general interest. The latter parts of the chapter are devoted to various algorithms and programs that use these files as input for topological index generation. A number of these are available over the Internet.

This volume probably represents the most comprehensive discussion of topological indices and their use. Most of the material included has been published and, in some cases, more than once. This volume will be included on most library acquisition lists, but because of its cost, it probably will not be purchased by many individuals.

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JM000448A

10.1021/jm000448a