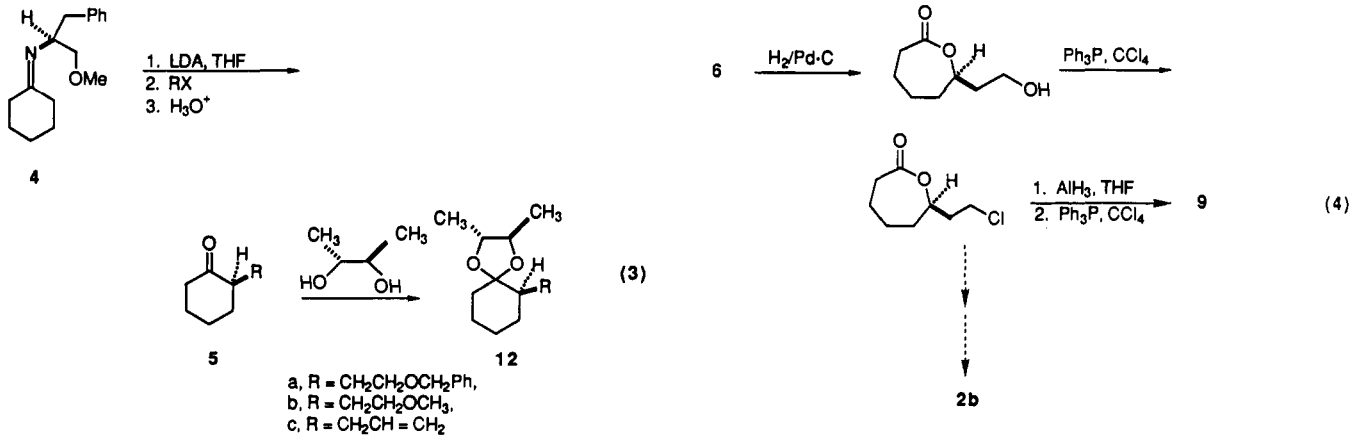

Book Reviews

Concepts and Applications of Molecular Similarity. Edited by M. A. Johnson and G. M. Maggiora. Wiley-Interscience, New York, 1990. xix + 393 pp. 16.5 × 25 cm. ISBN 0-471-62175-7. $65.00.

What could be as subjective as the notion of similarity, depending as it does on personal experience? Yet, as this volume makes clear, no concept is more fundamental to the scientific method, nor to our assimilating the overwhelming amount of data we must process. Indeed, as indicated in the scholarly chapter by Dennis Rouvray, the advancement of science, from taxonomic classification in biology to the periodic table of the chemical elements and the structural theory of matter, can be read as progress in developing objective criteria of similarity. Fortunately, *molecular* similarity lends itself to expression by mathematical methods which are objective and quantitative. An introductory chapter by the editors defines the current mathematical representations of molecules in terms of descriptors, and introduces mathematical operations on the descriptors as unifying themes for the following chapters.

Based on a symposium on computer-based methods of molecular similarity at the fall 1988 American Chemical Society National Meeting in Los Angeles, this book aims (according to the preface) to provide "definitive overviews" of topics related to the definition, computation, and application of molecular similarity and to promote and focus research efforts in this area. It succeeds admirably in these aims.

A major focus of the book is the development of molecular descriptors from topological (graph–theoretic, fragment-based) to topographical (shape and surface-based). From chapters 3 (by Peter Willett) and 4 (by David Bawden), describing methods for searching large databases of 2-D and 3-D molecular structures by similarity, to chapter 7 (by A. J. Hopfinger and B. J. Burke) on molecular shape analysis to quantitatively establish spatial molecular similarity, to chapter 8 (by Philip Dean) on molecular similarity in ligand–receptor interaction, to chapter 11 (by Paul Mezey) on similarity of molecular shapes and molecular surfaces, there is a progression in complexity and sophistication of concepts. Other topics covered include an extensive review of topological measures of similarity in chapter 5 (by Milan Randic) including an interesting attempt to extend these concepts to a 3-dimensional connectivity index, quantum mechanics derived measures of molecular similarity in chapter 6 (by R. Carbo and B. Calabuig), application of graph theoretic and matrix methods to description of chemical reaction similarity and stereochemical similarity in chapter 9 (by Ivar Ugi and co-workers), a formalism for modeling similarity in chemical transformation pathways in chapter 10 (by Mark Johnson, Eric Gifford, and C.-c. Tsai), and finally, the foundations of a mathematical theory of molecular similarity in chapter 12 (by Robert Rosen).

The book is heavy on definitions of molecular descriptors to be compared, as is appropriate for one oriented toward computer implementation of the concepts; it is somewhat light on presentation of significant chemical applications of the approaches, although there are plenty of such examples cited. There are a number of current research frontiers covered, with many 1989 references, and several chapters give proposals for future research. Particularly interesting research directions, to this reviewer's mind, include the concept of "self-similarity" (chapter 2), searching for critical fragments and for the optimal structure (chapter 5), determining "optimal similarity" and similarity of part structures (chapter 7), "blind searching" for common motifs and automatic creation of novel ligands containing these motifs (chapter 8), and treatment of molecular electrostatic, accessibility, and dynamic shape similarity (chapter 11). The book is oriented to small molecules; thus, similarity of peptide sequences is only obliquely addressed in chapters 5 and 12, and similarity of macromolecular structures does not appear to be addressed at all.

In summary, this volume constitutes an admirable review and synthesis of concepts and accomplishments in this fast-moving field of research and points directions for future progress. Several of the chapters can be read with profit by practicing medicinal chemists wishing to improve their understanding of molecular similarity concepts. For practitioners of computational chemistry, this volume is a must.

There is a detailed table of contents and a good subject index. There is no author index.

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Reductions by the Alumino- and Borohydrides in Organic Synthesis. By J. Seyden-Penne. VCH Publishers, New York. 1991. xiii + 193 pp. 16 × 24 cm. ISBN 1-56081-099-8. $65.00.

Since the earliest days of organic chemistry, functional-group reduction has constituted one of the most useful and frequently used tools in the synthetic chemist's armamentarium. The development of hydrides of aluminum and boron, beginning in the late 1930s and continuing unabated through the present day, has revolutionized the field, greatly expanding the number of functional groups which may be conveniently reduced and introducing an extraordinary degree of chemo-, regio-, and stereoselectivity. Unfortunately, the very profusion of these reagents, and the lack

of a systematic tabulation of their properties and uses, has often made the selection of the ideal hydride reagent for a particular application difficult for the nonspecialist. The present volume solves this problem nicely.

Based on a preparatory Ph.D. course taught at Orsay, the book has three parts. The first section contains brief descriptions and characteristics of the commercially available hydrides of boron and aluminum. These descriptive passages are cross-referenced to part 2, which assembles and organizes the available data for the reduction of organic functional groups by these reagents. It is this section which is the heart of the book. Organized by type of functional group reduced, it presents an enormous amount of literature information in a readily accessible form. While the discussions are brief, excellent literature references allow one to rapidly proceed to more detailed descriptions and procedures. Issues of solvent effects, reagent stoichiometry, and selectivity are noted wherever relevant and are nicely illustrated with examples from the synthetic literature. The references themselves are quite up-to-date; most are from the 1980s and many are as recent as 1988–1990. Part 3 recapitulates the basic reactions in the form of synoptic tables organized by substrate and reaction product; these are again cross-referenced to the appropriate sections of part 2. A conventional index at the end of the book further facilitates retrieval of information on specific reagents, substrates, or reactions.

This excellent little book is written with the practicing chemist in mind. It deserves a place on the laboratory bookshelf of every synthetic organic chemist.

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Neurotransmitters and Drugs. Third Edition. By Zygmunt L. Kruk and Christopher J. Pycock. Chapman & Hall, New York. 1991. ix + 204 pp. 15.5 × 23.5 cm. ISBN 0-412-36110-8 pbk. $25.00.

This book follows the format of the previous editions. The initial chapter introduces the biology and pharmacology of neurotransmission. Subsequent chapters are devoted to synthesis, storage, release, receptors, and inactivation of neurotransmitters. In addition, therapeutic utility and mechanisms of adverse effects associated with substances that modulate nerve transmission are described. Specific neurotransmitters that are discussed are acetylcholine, norepinephrine, dopamine, serotonin, histamine, inhibitory amino acids, excitatory amino acids, and neuropeptides.

The book is intended for students of medicine, pharmacy, and other biological disciplines. It is well-suited for this purpose; however, more advanced scientists will find the relatively large number of small errors, e.g., "Pirbedil" (Table 4.2), "8-hydroxydipropyl amino tetraline", "retanserine" (p. 120), "ketanserine", "phenylbiguanid" (p. 121), placement of the δ antagonist naltrindole under κ receptors, and omission of norbinaltorphine, the κ antagonist (Table 9.4), disconcerting. Also, the lack of structural formulas, although perhaps needed to save space, is disappointing. Chemists with limited biological orientation will, nonetheless, find this book to be a very good introduction to neurotransmitters.

Staff

Alkaloids. Chemical and Biological Perspectives. Volume 7. Edited by S. William Pelletier. Springer-Verlag, New York. 1991. xv + 591 pp. 16.5 × 24 cm. ISBN 0-387-97290-0. $98.00.

This book focuses on three groups of alkaloids—the *Homoerythrina* group and related compounds (I.R.C. Bick and S. Panichanun), steroidal alkaloids (P. K. Agrawal, S. K. Srivastava, and W. Gaffield), and norditerpenoid alkaloids (S. W. Pelletier and B. S. Joshi). All these authors are concerned with chemistry rather than biology, and in my opinion the unifying theme is the imposition of order on bodies of data growing at an explosive rate.

The *Homoerythrina* chapter summarizes the current state of chemical knowledge of these curious compounds, whose existence had been predicted before any had been isolated as natural products, and which are related to compounds known to have powerful physiological activity without appearing themselves to be very noteworthy in this respect. They have been the subjects of important structural, synthetic, and biosynthetic investigations and these are dealt with expertly in this review.

The chapters on steroidal alkaloids and norditerpenoid alkaloids are mostly compilations of the spectral data, principally ^{13}C NMR data, which are the principal means by which structures are assigned to new alkaloids in these families. Investigators already in the field, or those entering it to discover new compounds, will appreciate the full coverage of alkaloids and the way in which the authors are keeping the literature honest by either making assignments themselves or altering previous assignments from the primary papers.

This book will be interesting to all alkaloid chemists and essential for many.

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Nuclear Magnetic Resonance; Vol 20; Specialist Periodical Reports. *Edited by G. A. Webb.* The Royal Society of Chemistry, Cambridge, U.K. 1991. XXII + 602 pp. 15 × 22 cm. ISBN 0-85186-432-5. £140.00.

The Specialist Periodical Reports (SPRs) are an outgrowth of the *Annual Reports* published by the Royal Chemical Society for over 80 years to cover yearly developments in chemistry. Currently, three volumes of the *Annual Reports* in the areas of inorganic, organic and physical chemistry are intended for more general coverage while 11 SPRs deal with more specialized fields of chemistry that are currently experiencing rapid growth. Nuclear Magnetic Resonance has been one of the most successful members of the SPR series. This 20th volume, in which G. A. Webb is the Senior Reporter, covers the literature between June 1989 and May 1990 and has the same format used in the previous volumes. There are 15 chapters, the first of which lists all books and reviews having NMR as their principal theme. The other chapters cover theoretical and physical aspects of nuclear shielding, applications of nuclear shielding, theoretical aspects of spin–spin coupling, applications of spin-spin couplings, nuclear spin relaxation in liquids and gases, solid-state NMR, multiple pulse NMR, natural macromolecules, synthetic macromolecules, conformational analysis, NMR spectroscopy of living systems, NMR imaging of living systems, NMR of paramagnetic species, and NMR of liquid crystals and micellar solutions. Each chapter is covered by one or more individual reporters and has a very extensive list of references including titles. The volume also includes a complete author index as well as a listing of symbols and abbreviations as an aid to the reader.

This is an excellent reference manual which provides the reader with a bird's-eye view of all the recent developments in this fast-growing field. Practitioners of NMR as well as more casual users should find it informative regarding current methods and applications. As with the previous volumes, the reports are written clearly and succinctly. The literature is generally covered quite thoroughly and the lag time between the literature cited and the appearance of this volume is reasonable. The shortcomings, which include the dissimilarity in format between the different chapters, the small script and/or densely packed layout of certain chapters, and the very sparse use of illustrations, should not seriously detract from the value of this very useful publication, which is a must for every library.

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Fidia Research Foundation Symposium Series. Volume 5. Excitatory Amino Acids. Edited by Brian S. Meldrum, Flavio Moroni, Roger P. Simon, and James H. Woods. Raven Press, New York. 1991. xxxiii + 780 pp. 16 × 24 cm. ISBN 0-88167-701-9. $174.00.

Scientific development in the area of excitatory amino acid mediated neuronal processes continues to expand at an explosive rate. This volume, which is the fifth in a series of Fidia Research Foundation sponsored symposia, highlights the proceedings of

a most recent conference on this important field of study held in Montegrotto Terme, Italy, May 21–26, 1990.

Over 80 papers from the more than 200 presentations featured at this international symposium have been organized into 11 sections which span a wide range of disciplines engaged in excitatory amino acid (EAA) research. Progress in the localization and distribution of EAA receptor subtypes and putative transmitters by immunocytochemical techniques are discussed in a section on anatomy. This is followed by a group of papers dealing with recent developments in the expanding area of molecular biology of EAA receptor proteins. In particular, the characterization, cloning, and expression of various non-NMDA-binding proteins are discussed. Several papers describing advances in electrophysiology, pharmacology, and signal transduction mechanisms as related to EAA receptor subtypes are presented in the following section. Of particular note are those dealing with second messenger activation, allosteric modulators of NMDA receptors, and heterogeneity of EAA receptor subtypes. Topics such as long-term potentiation and synaptic plasticity, mechanisms and patterns of excitotoxicity, behavioral pharmacology (mostly dealing with NMDA receptor agents), and neuropathologies underlying epilepsy and ischemia and related disorders are updated in individual sections.

It was gratifying to find a separate section, albeit short, devoted to kynurenate and quinolinate, two endogenous modulators of EAA receptors. While the role of these compounds in neurodegenerative as well as immunological disorders still remains to be delineated, advances toward understanding the importance of these neuromodulators and the neurochemical mechanisms regulating their existence are presented.

A medicinal chemistry section, which by no means attempts to be comprehensive in its coverage of EAA receptor active molecules, touches upon various structural classes that have been generated in the development of synthetic modulators of EAA receptor transmission. Particular attention has been paid to the description of structure–activity relationship (SAR) studies. Included in this section are papers dealing with natural and synthetically modified arthropod toxins, MK-801 and PCP analogues, various NMDA receptor ligands (cyclopropylglutamates, piperidine and tetrahydroisoquinoline phosphonates, and tetrazoles), non NMDA receptor ligands (isoxazole- and quinoxaline-based) and putative polyamine antagonists (ifenprodil and SL 82.0715). Somewhat surprisingly, NMDA-associated, strychnine-insensitive glycine receptor ligands are not discussed in this context. Descriptions of SAR studies of antagonists of this modulatory site would have been a welcomed addition to this section.

Overall, the book is well organized and edited. References provide broad literature coverage, particularly between 1987 and 1989, though several citations through 1990 were also noted. The subject index is extensive and quite adequate. The average lengths of individual papers are approximately 8–10 pages, making the chapters easy to read. Though the high cost of this book will likely preclude its addition to personal collections, it would be a valuable addition for institutional libraries. Due to the diverse range of disciplines included, this book should appeal to a wide range of scientists.

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Books of Interest

Organic Syntheses. Volume 69. Edited by Leo A. Paquette. John Wiley & Sons, Inc., New York. 1991. xx + 328 pp. 15.5 × 23.5 cm. ISBN 0-471-54560-0. $34.95.

HPLC in the Pharmaceutical Industry. Volume 47. Edited by Godwin W. Fong and Stanley K. Lam. Marcel Dekker, Inc., New York. 1991. viii + 309 pp. 16 × 23.5 cm. ISBN 0-8247-8499-5. $99.75.

Carbohydrate Chemistry. Volume 23. A Specialist Periodical Reports. Monosaccharides, Disaccharides, and Specific Oligosaccharides. A Review of the Literature Published in 1989. Senior Reporter R. J. Ferrier. Royal Society of Chemistry, Cambridge, U.K. 1991. xvi + 308 pp. 14.5 × 22.5 cm. ISBN 0-85186-172-5. £95.00.

Second Supplements to the 2nd Edition of Rodd's Chemistry of Carbon Compounds. Volume 1: Aliphatic Compounds. Part A,B: Hydrocarbons; Halogen Derivatives; Monohydric Alcohols, Their Ethers and Esters; Sulphur Analogues; Nitrogen Derivatives; Organometallic Compounds. Edited by M. Sainsbury. Elsevier Science Publishers B.V., The Netherlands. 1991. xviii + 620 pp. 16 × 23.5 cm. ISBN 0-444-88157-3. $303.00.