Additions and Corrections

Enantioselective Total Synthesis of Gracilins B and C Using Catalytic Asymmetric Diels–Alder Methodology [*J. Am. Chem. Soc.* **1995**, *117*, 9616–9617]. E. J. COREY* AND MICHAEL A. LETAVIC

Page 9617, column 2, line 5: 2-*endo*-hydroxy-3-*exo*-acetoxytetrahydrofuran should be 2-*endo*-acetoxy-3-*exo*-hydroxytetrahydrofuran.

Supporting Information: Corrected pages 3, 14, and 16 of the supporting information (3 pages). This material is contained in many libraries on microfiche, immediately follows this article in the microfilm version of the journal, can be ordered from the ACS, and can be downloaded from the Internet; see any current masthead page for ordering information and Internet access instructions.

JA955029V

Book Reviews

Enediyne Antibiotics as Antitumor Agents. Edited by D. B. Borders (BioSource Pharm, Inc.) and T. W. Doyle (OncoRx, Inc.). Dekker: New York. 1995. xii + 461 pp. $165.00. ISBN 0-582-06420-1.

The first reports in 1987 of the structures of esperamicin and calicheamicin came as an enormous surprise and boost for natural products chemistry in general. Since that time a large number a papers have appeared that describe the biology, structure, mechanism of action, and synthesis of enediynes. The once esoteric backwater of physical organic chemistry quite suddenly became the new lead structures for the design of antitumor agents. Predictable? Unfortunately not. Nature is well adhead of homosapiens in the design of biologically active molecules and will remain so for many generations of scientists to come.

With so much information being published in such a relatively short period of time, it is very pleasing to see the vast majority, if not all, of the key papers collected together and reviewed by experts in the area. The contents of this book are as follows: Part I. Calicheamicins, The Biochemical Induction Assay and its Application in the Detection of the Calicheamicins. Taxonomy, Fermentation, and Yield Improvement. Identification, Isolation, and Structure Determination. Disulfide Calicheamicins and the Chemistry of the Allylic Trisulfide Group. Preparations of Conjugates to Monoclonal Antibodies. Genetic Analysis of Calicheamicin Biosynthesis. Biological Activities of Calicheamicin. DNA-Cleaving Properties of Calicheamicin γ_1^I. Part II. Fermentation and Isolation of Esperamicins. Structure Determination of the Esperamicins. Biosynthesis of Esperamicin. Mechanism of Action and Molecular Modeling for Esperamicin A_1, Calicheamicin γ_1^I, and Dynemicin A. Biological Properties of Esperamicin and Other Enediyne Antibiotics. Part III. Dynemicins. Part IV. Neocarzinostatin: Chemical and Biological Basis of Oxidative DNA Damage. The Clinical Effects of Neocarzinostatin and its Polymer Conjugate, SMANCS. Part V. Synthetic Methodologies. Synthetic Studies of the Enediyne Antibiotics.

While one could quibble that the format of the book has been determined by the Bristol-Myers Squibb and Lederle groups describing their respective efforts on esperamicin and calicheamicin and that this could have been combined into a single chapter. However, it is a small point that in no way detracts from the usefulness that this book will have for chemists and biologists who are interested in enediyne compounds. There is the usual surfeit of structural drawing errors that abound with computerized drawing programs, but none is sufficiently bad as to be misleading. Overall, this is a timely and high-quality treatise which will be used by a relatively narrow audience, and hence the high price.

Philip D. Magnus, *The University of Texas at Austin*

JA955136P

Studies in Natural Products Chemistry, Vol. 15, Structure and Chemistry (Part C). By A. U. Rahman (University of Karachi, Pakistan). Elsevier: Amsterdam. 1994. xv + 577 pp. $322.75. ISBN 0-444-82083-3.

The fifteenth volume of the Atta-ur-Rahman series on natural products provides 14 chapters addressing a variety of elements from the tapestry that comprises this discipline including isolation, structure determination, structure–activity, detection, and biological activity.

Chapters on structural diversity by Capon (marine sesquiterpenes and quinones) and Tsantrizos (*Phompsis* metabolites) reveal the ever-expanding variety of natural products from all sources. This overview is strengthened by chapters describing specific classes of natural products and their structural variations from defined sources. In this area, the chapters by Minale bring together a valuable extensive collection of structural information on saponins from the Echinoderms; by Takeda and Ghisalbeti, on terpenoids from *Rabdisia* and from *Eremophila*; by Takayama and Saito, on alkaloids; and by McInerney, on biologically active dihydroisocoumarins.

A third theme on the isolation and detection of natural products is illustrated by chapters on saponin structural elucidation which nicely complements that of Minale's on structural variation and a report on the circular dichroism of carbohydrate complexes. Finally, consideration of the biological activity of natural products is provided by reviews on natural products with pronounced sweet taste by Kinghorn; on the antimicrobial activity of amphibian venoms by Habermehl; on cardenolide detection by ELISA by Yoshimatsu; and on oncogene function inhibitors by Umezawe.

Each of the chapters is produced by a recognized expert in their respective field and there is a wide variation in presentation styles from a catalog of natural products to incisive commentary.

This book and others in the series are characterized by a broad approach to the many classes of natural products, and each contain chapters that will be standard references for many years. On the other hand, one wonders if is this the best format for the publication of extensive spectral data at 56 cents per page!

The book is produced from camera-ready copy leading to a sometimes disturbing, variety of formats. It would be best if the editors required submission to future volumes in a standard format.

In summary, this series continues to produce a number of extremely good contributions to the natural products review literature. It is doubtful if individual researchers would buy this, but libraries committed to the accumulation of natural products literature would be wise to continue with this volume.

John W. ApSimon, *Carleton University*

JA955167K

Polymer Science and Technology Series. Computer Simulation of Polymers. Edited by E. A. Colbourn (Oxford Science Park, Oxfordshire). Longman Scientific and Technical: Essex, England. 1994. vii + 343 pp. $185.00. ISBN 0-582-08374-5.

This book provides a good introduction to the state of the art of computer simulation of polymers. The eight chapters present methods of computer simulation of polymer molecules, physical and chemical properties, amorphous polymers, polymer blends, crystalline polymers and crystallization, deformation and failure, phase diagrams, networks, and biopolymers. Although the time when this diverse array of subjects can be brought together into one well-connected and easy to use ensemble in cyberspace is still in the future, it is reassuring to see them skillfully herded together in this well-written, carefully edited, and optimistic book. Each chapter serves as a useful gateway to the special approaches, defined parameters, collections of data, and phenomena of general interest that have been brought together by the pioneers of the past decade or so to create beachheads aimed at the solution of the large problem of computing useful properties of polymers from knowledge of the chemical constitution and structure of polymer molecules. If you intend to look at only one book on computer simulation of polymers, and wish to obtain a broad view of what is going on, in terms used by the specialists in each area, with a good set of references, this is the book for you this year.

E. A. Colburn and J. Kendrick describe how interchain packing can affect the geometry of typical chains. Their computer simulation aids in the understanding of X-ray diffraction data and other data that reveal information about the conformation of segments of the molecules. They include a useful section on the role of conformational defects that are constrained in otherwise translationally symmetric polymer crystals. They predict an accelerating use of the techniques of molecular dynamics to describe the onset of disorder in crystalline polymers.

A. J. Hopfinger and M. G Koehler describe an approach the assigns properties to groups of atoms in a polymer chain, for example, by relating torsion angles of sequences of bonds in a group of atoms to properties of interest. Their approach seeks to use such information in a neural network formalism which connects structural information to measured properties of polymers.

J. H. R. Clark and D. Brown's approach simplifies the molecular level description of polymer molecules in order to extend the time and ensemble size that can be treated by the procedures of molecular dynamics. K. Binder has created a coarse grained model that involves effective bond lengths and produces models of the long-wavelength degrees of freedom of collective phenomena in dense polymer systems.

G. Goldbeck-Wood brings thermodynamics and the geometry of chain-folded polymer crystals together in the computer to provide insight into the morphological and dynamical properties of crystalline polymers.

Y. Termonia describes intuitively appealing models of the failure process in solids composed of linear polymers, on the one hand, and cross-linked polymers on the other. His models show the response of a loose network of entangled or cross-linked polymer molecules to elongational strain that first break Van der Waals bonds according to rate theory, producing localized failures within the material, and finally breaking the backbone bonds of molecules in a probabilistic way that is related to the stress in each molecule.

S. Kumar describes two Monte Carlo simulation methods for calculating the free energies of polymer systems. One method is appropriate for short chains and the other for long chains. Each scale requires its own parameters to provide satisfactory calculation of the thermodynamic parameters.

B. E. Eichinger and O. Akgiray show how simple modeling techniques that encompass significant molecular detail can lead to improved understanding of complicated systems such as bimodal networks, adhesives, and natural rubber.

D. J. Osguthorpe and P. Dauber-Osguthorpe provided a brief summary of the massive amount of computer simulation work that has been applied to biopolymers and compared this effort to the work described in the other chapters.

I found the promise that is implicit in the work described in this book exhilarating, and the amount of work that will be required to bring it all together quite daunting. This collection is a useful look at the landscape of the 1990s, with infectious enthusiasm and optimism for the future.

Darrell H. Reneker, *The University of Akron*

JA945055D

Fluorine-Containing Amino Acids—Synthesis and Properties. Edited by V. P. Kukhar' and V. A. Soloshonok (National Academy of Sciences of Ukraine). John Wiley and Sons: New York. 1995. x + 411 pp. $140.00. ISBN 0-471-95203-6.

The goals of editors Kukhar' and Soloshonok in putting together this broad, comprehensive, and well-referenced treatise dealing with the synthesis and properties of fluorine-containing amino acids (FAA's) have certainly been accomplished with the publishing of this volume. The book, as advertised, presents a thorough and up-to-date review of virtually every aspect of the synthesis, chemistry, and properties of this very important class of biologically-significant molecules. The book should be of great interest to workers in the field; indeed, it should be indispensable to them. In fact, just about anyone interested in either amino acids or how to incorporate fluorine into multifunctional molecules should find this book a very useful addition to their library.

The early chapters deal with general synthetic methodology. Chapter 1 presents an excellent, well-organized, review of amino acid synthetic methodology and how one can apply these methods to make FAA's. Just reading this chapter is certain to get the creative juices going in most readers. Chapter 2 comes at the same subject from a different angle. It focuses on the methodology of organofluorine chemistry and how it has been applied to the synthesis of amino acids. This concisely-written chapter should provide a good starting point for those researchers interested in simply how to put fluorine into molecules, whether they be amino acids or not. Chapter 3 provides a nicely-written elaboration on one specific synthetic method which is particularly useful in amino acid synthesis, that of the utilization of homogeneous catalysis in hydroformulation and carbalkoxylation processes. Chapter 4, which focuses on the synthesis of β-fluorine-containing amino acids, adds to and again touches on most of the methodolgies introduced in the earlier chapters, with an emphasis on their application to this biolofically very important class of compounds.

As with any class of biologically-active molecules, the preparation of optically active compounds is of extreme importance. Thus, considerable attention is given to this subject in this volume. Chapter 5 (and part of Chapter 3) presents an excellent review of C−C and C−H bond-forming reactions which have utilized asymmetric induction to provide optically-active FAA's, while Chapter 6 discusses the application of enzymatic asymmetric synthesis of such compounds. Two chapters on the enzymatic and chromatographic resolution of racemic FAA's bring this excellent synthesis section to a satisfying finish.

The next two chapters provide a bit of additional spice to the book by discussing the unique and diverse properties of FAA's, particularly with respect to their biological activities. Chapter 9 presents an excellent discussion of the general features of such biological activity, while Chapter 10 elaborates on one specific example, that of renin inhibitors which contain FAA derivatives. The final chapter, quite fittingly, extends the discussion to fluorine-containing peptides and proteins. This lengthy chapter provides an excellent review of both the synthetic and the application aspects of this important subject.

To summarize, this is an excellent book which should prove indispensable to those specialists who are interested in fluorinated amino acids, but should also comprise a very useful reference work for any organic or biochemist who would like to learn how to incorporate fluorine into multifunctional organic compounds and to gain some understanding of the effect of such incorporation on the properties of such compounds.

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