in vacuo. The residue was partitioned between chloroform and water. After drying with magnesium sulfate, the chloroform layer was evaporated to dryness in vacuo, giving the product as a syrup. Trituration with ether and cyclohexane gave a glass: yield 43 mg (67%); UV λ_{max} at pH 1, 245 (9.07); at pH 7 and pH 13, 264 (11.2); ^{1}H NMR ($CDCl_3$) δ 1.38 and 1.62 (2 s, CH_3 of IP), 1.44 (cyclohexane), 2.52 and 2.58 (2 s, 4-CH_3 and CH_3CO), 3.9 (m, CH_2), 4.35 (m, H-4'), 4.74 (m, H-2'), 4.88 (s, OH), 4.96 (m, H-3'), 6.48 (d, H-1', $J_{1'2'}$ = 2 Hz), 8.33 (H-2); ^{13}C NMR ($CDCl_3$) δ 16.91 (4-CH_3), 25.55 and 27.34 (CH_3 of IP), 26.96 (cyclohexane), 30.12 (CH_3CO), 61.71 (CH_2), 79.76 (C-3'), 86.89 and 87.21 (C-2' and C-4'), 93.14 (C-1'), 114.15 (C of IP), 127.50 and 147.60 (C-4 and C-5), 139.44 (C-2), 188.62 (CO); mass spectrum (FAB) m/e 173 (sugar)$^+$, 297 (M + 1)$^+$. Anal. Calcd for $C_{14}H_{20}N_2O_5 \cdot 0.12C_6H_{12} \cdot 0.47H_2O$: C, 56.15; H, 7.16; N, 8.90. Found: C, 56.13; H, 7.02; N, 8.80.

4(*R*)-(1-Hydroxyethyl)-5-methyl-1-β-D-ribofuranosylimidazole (10). Method A. To a cold (ice bath) solution of 4-acetyl-5-methyl-1-β-D-ribofuranosylimidazole (**5**; 100 mg, 0.39 mmol) in 15 mL of anhydrous ethanol was added a solution of sodium borohydride (22.3 mg, 0.59 mmol) in 2.23 mL of anhydrous ethanol. After 4 h at ambient temperature, the solution was acidified (pH 2) with 1 N hydrochloric acid and evaporated to dryness. The residue was purified by preparative thin-layer chromatography (3:1 chloroform/methanol) on silica gel. The product was obtained by methanol extraction. Evaporation of the solvent gave a syrup that crystallized on standing; yield 52 mg (51%).

The analytical sample was obtained by absorbing an aqueous solution of the material on rexyn 101 (H) ion-exchange resin and eluting with 50% aqueous ammonium hydroxide. The solid thus obtained was recrystallized from ethanol: mp 170–172 °C; mass spectrum (EI) m/e 258 (M$^+$); ^{1}H NMR (Me_2SO-d_6) δ 1.32 (d, CH_3CHOH, J = 7 Hz), 2.19 (s, 4-CH_3), 3.55 (m, CH_2), 3.85 (m, H-4'), 4.02 (m, H-3'), 4.2 (m, H-2'), 4.5-5.5 (OH), 4.64 (m, CH_3CHOH), 5.4 (d, H-1', $J_{1'2'}$ = 6 Hz), 7.7 (s, H-2); assignments of CH_3CHOH and H-2' verified by spin-decoupling. Anal. Calcd for $C_{11}H_{18}N_2O_5 \cdot 0.15H_2O$: C, 50.63; H, 7.07; N, 10.73. Found: C, 50.63; H, 7.24; N, 10.72.

Method B. A solution of 4-acetyl-5-methyl-1-β-D-ribofuranosylimidazole (**5**; 100 mg, 0.39 mmol) in ethanol (25 mL) containing Raney Nickel catalyst (25 mg) was hydrogenated at ambient temperature and 30 psi for 48 h, then filtered, and evaporated to dryness in vacuo. The residue was purified by flash chromatography on Merck silica gel 60 (70–230 mesh, 20 g) using chloroform/methanol (3:1) as the eluting solvent to give 82 mg of a glass. A crystalline solid was obtained from ethanol; yield 51 mg (51%). A solution of 20 mg of this material in ethanol (5 mL) was allowed to evaporate slowly at ambient temperature. A crystalline residue identical with that obtained by the borohydride reduction was obtained.

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Registry No. **1**, 23328-91-8; **2**, 40554-98-1; **3**, 13035-61-5; **5** (β anomer), 98483-23-9; **5** (α anomer), 98483-24-0; **6**, 98483-25-1; **8**, 31281-18-2; **9**, 31281-20-6; **10**, 98483-26-2; adenosine deaminase, 9026-93-1.

Book Reviews

Biologically Active Principles of Natural Products. Edited by W. Voelter and G. D. Daves, Jr. Georg Thieme Verlag, Stuttgart. 1984. 310 pp. 16 × 23.5 cm. $26.00

Nothing on the title page of this volume reveals that it is a Festschrift honoring Karl Folkers and that it was assembled by the editors following a symposium at Lehigh University toward the end of 1981, which celebrated Karl Folker's 75th birthday.

In their preface the editors state that Dr. Folkers's life-long research interests have dealt with "chemical regulation of life processes", which might not have been a bad title for a book, that deals with the chemistry, biochemistry, and some clinical aspects of vitamins. hormones, and antibiotics. In his own contribution the Festschrift—which would have made an excellent opening chapter—Dr. Folkers reflects on some of his teachers and their influence on his research. Among those guidelines is one that characterizes this book well, namely the attempt to bring chemistry and medicine closer together. The remarkable aspect of Folkers's research career and hence of the Festschrift is the fact that "medicine" is not equivalent to biochemistry, molecular biology, or physiology, but to clinical medicine.

The 27 contributions cover a wide spectrum of biomedical topics, among them coenzyme Q_{10}, vitamins B_6 and B_{12}, biosynthesis, structure–activity relationships, and even organic synthesis and analysis. Slightly over half of the contributions are mini-reviews by single authors, as one would expect for a symposium celebrating a scientist and his career. Chapters with post-1981 references are the exception rather than the rule, despite the 3-year interval between symposium and publication dates, which according to the editors was needed to update the symposium lectures.

Festschriften are no substitutes for the periodical literature or for monographs. However, they are valuable markers in the history of science and often are fun to read. In this case, the breadth of the topics provides added stimulation for scientists and students of many disciplines in the biomedical research community, particularly for those who would, with Karl Folkers, like to forge a closer link between chemistry and medicine.

The book, which is produced by offset printing, includes author and subject indices and some good-quality black and white photographs. Its modest price should make it an attractive addition to many personal libraries—this despite the inexcusable typo in the preface, where Folkers becomes Folker—not once but twice!

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Minimum Steric Difference. The MTD Method for QSAR Studies. Vol. 7 in the Chemometrics Series. By Z. Simon, A. Chiriac, S. Holban, D. Ciubotaru and G. I. Mihalas. Ed. by D. Bawden. Wiley, New York. 1984. ix + 173 pp. 15 × 23.5 cm. ISBN 0471-90438-4. $47.95.

The ultimate goal of a QSAR study is to get a picture of the interaction between the receptor and the effector substance. In Volume 1 of *The Chemometrics Series* the distance geometry method of mapping receptor–effector interactions was presented. In Volume 7 the editor returns to this important topic. The five authors present their approach to the receptor mapping problem—the MSD and MTD methods. The aim of the two methods is to reduce the large number of structure descriptors necessary for describing the receptor–effector interaction to a single number, which is then used as a variable in traditional multiple-regression QSARs. Such a tremendous reduction of the description of the molecular structure seems somewhat hazardous. The authors could have avoided this problem by the use of modern methods of multivariate analysis.

The book contains six chapters and two appendices. Chapter 1 is a short and trivial introduction to QSAR and the MTD method. Chapter 2 is the highlight of the book. It is a careful and well-organized overview covering receptor–effector interactions and how they can be described in physical terms. The authors point out the importance of steric effects for the receptor–effector interaction and make comparisons with other interactions like hydrophobic and polar forces. They point out that within a specific set of data it might be difficult to separate the various interactions.

Chapter 3 is a detailed description of the MSD and MTD methods. The interaction of each of the substrate atoms with the receptor is evaluated as being either beneficial, nonimportant, or detrimental. In the evaluation a crossvalidation procedure is used for evaluating the significance of the regression results. It is somewhat difficult to follow how the final classification of the substrate atoms into the three classes is made even though some examples are shown.

Chapter 4 contains a number of examples of QSARs established with the method. The examples are carefully evaluated and discussed in detail. Also, the meaning of atom assignments is discussed in great detail, although the authors state on page 26 "one must be cautious with the interpretation of results, in particular with the significance of vertex assignments". In Chapter 5 the MTD method is compared to other receptor mapping methods like molecular shape analysis and the distance geometry method. Both of these methods are more complex than the MTD method and thus demand much more computer capacity, a difference that is rapidly becoming unimportant. Chapter 6 highlights some concluding remarks that could as well have been included in the preceding text.

Appendix 1 reviews some additional QSARs and is a natural complement to Chapter 4. Most examples in the book seem to come from the work of the authors themselves, and another one or two from geographically close contacts, as far as can be judged from the list of references. This highlights the fact that the MTD method has not been widely accepted despite the fact that most of the basic work seems to have been done about 10 years ago.

Appendix 2 is a thorough presentation and listing of the computer program used by the authors.

In summary, the book gives an open and honest presentation of the subject. It is mostly well written but would have gained from a more precise description of how the significance of the assignments of the effector atoms was evaluated.

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QSAR in Design of Bioactive Compounds. Proceedings of the First International Telesymposium on Medicinal Chemistry. Edited by M. Kuchar. J. R. Prous Publishers, Barcelona, Spain. 1984. xi + 458 pp. 18.5 × 25 cm. ISBN 84-499-6941-7.

This book is a collection of 32 papers authored by 76 specialists in the field of quantitative structure–activity relationships (QSAR). The papers were presented as contributions to the First International Telesymposium on Medicinal Chemistry, Feb 29, 1984. The Telesymposium was defined as an exchange of opinions or a series of contributed papers submitted and discussed *from a distance* among scientists from different countries working in the same area of specialization. Most of the contributions reflect the more traditional concept of QSAR, but four of the papers are concerned with computer graphics and three-dimensional drug design. An important feature of the book is the discussion of the papers, which consists of questions or comments and the author's response. Eighteen of the papers have such a Discussion, which is valuable in helping to clarify and enlarge on specific aspects of the presentations. Unfortunately, the Discussion is "hidden" at the end of the book, and the editor does not draw attention to this fact. It is only when one looks for an index (which is missing) that one finds the Discussion.

Each contribution is organized with a Summary, an Introduction, Results, Discussion, and often a Conclusion. All the papers have many references to the original literature, and since many of the conributions are very technical in nature, these references are very useful and often necessary. The papers are in no way a summary or simplification of the topics discussed—rather they are a fascinating collection of individual papers as in a journal—each is of interest in its own way, but there is no attempt to connect the papers with each other. In most cases the individual papers present in technical detail a specific aspect of the author's current work. For readers new in the area it will be necessary to go back to the original literature to view a new concept in perspective. Without an index, this book is not a reference text, but it is a fascinating place to browse to see most of the current approaches to QSAR.

The Introduction asks the question "Wither QSAR?". The author, Stephen Ungar, supplies an answer with the statement that "QSAR provides a rationale for investigation of more novel side chains and increased potencies or improved properties are the result."

The papers are arranged in four Sections: Section I is entitled "Characteristics of Physico-Chemical Properites in QSAR" and is chaired by J. C. Dearden. The diverse topics discussed are liposome/saline partitioning, the estimation of melting points, a molecular conductivity study, and hydrophobic substituent constants for pyridine derivatives.

Section II entitled "Practical Results of QSAR in Various Active Groups" is chaired by V. Rejholec and M. Kuchar. This section contains 12 chapters, each describing an application of QSAR to the correlation of biological activity with the physical properties of a particular class of compounds. There is such a wide variety of topics here that anyone interested in QSAR will find several papers that are relevant to a special field.

Section III is entitled "Three Dimensional Drug Design and Computer Graphic Methods" and is chaired by M. S. Tute. This section has only four papers, which hardly do justice to such a rapidly growing area. However, the papers are already over 1 year old, and each in its own way provides a useful view of a special aspect of this field. The subjects treated are the antifolates, electrostatic potentials, DNA binding, and applications of molecular shape analysis.

Section IV, "New Mathematical Approaches to QSAR—Multivariate Techniques in Prediction of New Drugs", is chaired by W. P. Purcell. The papers in this section provide a valuable glimpse of the application of modern mathematical techniques. Included among the topics are drug distribution, multivariate techniques, the bilinear model, principal component analysis, the Free–Wilson model, the MASCA model, autocorrelation, and nonparamatric methodology. The section ends with an open letter discussion by P. P. Magee of the factors to be considered in quantitative correlation analysis.

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