well as acadamic researchers. It also shows that the different philosophies involved in industrial and academic research can be reconciled to create new momentum. Browsing through the chapters yet again leaves me looking forward to the third workshop, to be held in the Netherlands in the autumn of 1994.

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SSDI 0008-6215(94)00142-3

Reviews in Computational Chemistry, Edited by Kenny B. Lipkowitz and Donald B. Boyd, VCH, Weinheim, 1993. Vol. 3, ISBN 1-56081-619-8, pp 271, 128 DM; Vol. 4, ISBN 1-56081-620-1, pp 280, 138 DM; and Vol. 5, ISBN 1-56081-658-9, pp 458, 179 DM.

Carbohydrate Research gives a regular demonstration of the increasing use of computational methodologies in carbohydrate chemistry. So where texts become available which review the techniques commonly used, they are likely to be of interest to a wide range of readers from students up to the experts actively involved in developing the next levels of application.

We are still in an environment of rapid progress in computer hardware and software development so it is no easy task to produce books that can maintain a useful lifespan against this background. In this series we have the latest volumes of reviews designed to begin "from ground zero and provide for you a minitutorial on how to implement various computational methods to solve problems". The editors also hope that the publication will allow the reader "to use this series to learn how to solve problems using computational methods and be able to locate key references quickly".

Although these selected volumes from the series on Computational Chemistry do not specifically address carbohydrates, there is much of interest.

The opening chapter of Volume 3 by Tamar Schlick, *Optimization Methods in Computational Chemistry*, looks at the use of numerical minimisation algorithms as provided in many molecular modelling packages, as well as other simulation procedures. These are often poorly detailed by software suppliers and are easily used and abused, but this review introduces the concepts well and gradually progresses through the mathematical preliminaries to a discussion of the merits and drawbacks of several methods. It is supported with numerical examples and numerous references.

Following on from this, partly as an application of the types of minimisation

techniques described by Schlick, and expansion to envelope other considerations is *Predicting Three-Dimensional Structures of Oligopeptides* by Harold Scheraga. The review begins with an introduction which seems over complicated, making it clumsy in places. This is followed by a very full, technical, and historical view of modelling techniques for peptides starting from basic geometry considerations, assessment of potentials, optimisation techniques, and their applications to simple peptide systems. Several methods of addressing the multiple minima problem are reviewed before a discussion on expanding the techniques for use with larger peptides and proteins. There was one annoying discontinuity that, having been introduced to the techniques in Chapter 1, Harold Sheraga, in consideration of optimisation methods says "The one that has been judged to be most efficient in our laboratory..." is one that Schlick does not refer to. It would perhaps have been better if this type of omission could have been avoided.

In the third chapter, *Molecular Modeling Using Nuclear Magnetic Resonance Data* by Andrew E. Torda and Wilfred F. van Gunsteren, the authors intentionally avoided detailed description of NMR techniques and data collection and concentrated more on the use of the data generated in the context of molecular modelling. This makes for a much more readable chapter. The reader is taken from initial structure generation through the use of NMR data in modelling, distance restraints, averaging, NOE refinement, dihedral restraints, refinement, minimisation, molecular dynamics... and so on with appropriate assessment of systematic errors, forcefield considerations, and other relevant issues.

The final chapter, *Computer-Assisted Methods in the Evaluation of Chemical Toxicity* by David F.V. Lewis, gives a contrasting topic to round off the volume. Rather than look at modelling techniques *per se* the subject turns to considering molecular characteristics that may be relevant to their chemical toxicity. Using the cytochromes P450 superfamily of enzymes to demonstrate examples, the major programs in use are critically assessed and compared in a very interesting review, which provides recommendations regarding which software packages used together can give the most useful information. For completeness, addresses are supplied at the end for each package discussed.

Volume 4. This has a similar thematic approach with an opening chapter by Jerzy Cioslowski, *Ab Initio Calculations on Large Molecules: Methodology and Applications*, which gives a concise introduction to the methodology used in the two subsequent chapters, *Computing Reaction Pathways on Molecular Potential Energy Surfaces* by Michael McKee and Michael Page, and *Computational Molecular Dynamics of Chemical Reactions in Solution* by Robert M. Whitnell and Kent R. Wilson.

Volume 5. This also has chapters of general interest on the historical development of Computational Chemistry in the United States (John D. Bolcer and Robert B. Hermann) from the 1950's, the applications of Post-Hartree–Fock methods (Rodeny J. Bartlett and John F. Stanton) and distance geometry (Jeffrey M. Blaney and J. Scott Dixon). The final chapter, *A Perspective of Modern Methods*

in Computer Aided Drug Design by Lisa M. Balbes et al., in one way brings us back to carbohydrates. It describes the important targeted pharmacophore method and the several algorithms for this now being investigated by the pharmaceutical industry. Methods are discussed for finding the optimal arrangement of functional groups within a protein binding site. These are then computationally arranged on a skeleton molecule of the correct dimensions picked from 3D-structural libraries. Although not mentioned in this chapter, the latter search often alights on oligosaccharides as the optimal skeleton molecule.

In common with previous volumes in this series, those reviewed here have an appendix, *Compendium of Software for Molecular Modeling* by Donald B. Boyd. This gives a very useful overview of available molecular modelling packages and will prove useful for potential purchasers. However, these are similar in each volume and it would be more useful for there to be additional information on which algorithms are available within the packages discussed for the particular applications in each review. But these are minor points. Overall the series is to be recommended.

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SSDI 0008-6215(94)00174-E

β-Glucosidases Biochemistry and Molecular Biology, Asim Esen (Ed.), ACS Symposium Series 533, American Chemical Society, Washington, D.C., 259 pp, ISBN 0-8412-2697-0

This book is an attempt to bring together the current state of knowledge regarding β-glucosidases. These ubiquitous enzymes are finding increasing medical and commercial importance, and are being shown to be key enzymes in a variety of biochemical processes. Sixteen chapters cover a wide spectrum of interests from catalysis and specificity through to the genetics and the medical relevance of the enzyme. I would consider this book to be an essential reference work for workers in the field of β-glucosidase research. For those, such as myself, on the fringes of this field the book contains the inevitable mixture of good, bad, relevant, and irrelevant articles. The sections on catalytic mechanisms describe some rather elegant chemistry and are excellent, the chapter by Trimbur and colleagues especially so. Later chapters focus on genetics, enzymology, and the medical aspects of β-glucosidases and its relevance to Gaucher's disease. Five chapters are dedicated to the study of cyanogenic β-glucosidases. In short, this book is indis-