

wondering about details of the method. He also fails to give the reader an appreciation of the difficulty of applying the transition-state seeker to chemical mechanisms in general. The book ends with a discussion of half a dozen applications that will give the reader some flavor of recent applications of calculational methods to problems of chemical interest.

Although the book is well written, it is not clear what its primary intended audience would be. Unfortunately, the level of treatment is such that there is considerably more mathematical detail than the experimentalist interested in using the book as a compilation of what can be gained from using calculations would likely be interested in, but it is not sufficiently detailed to meet the needs of the person interested in mathematical aspects of the computations. It is probably best suited for use in an advanced undergraduate or beginning graduate course designed to introduce students to molecular modeling.

J. W. Viers

Department of Chemistry  
Virginia Polytechnic Institute and State University  
Blacksburg, Virginia 24061-0212

NP9606355

S0163-3864(96)00635-0

### Computer-Aided Molecular Design: Applications in Agrochemicals, Materials and Pharmaceuticals.

Edited by C. H. Reynolds (Rohm and Haas Company), M. K. Holloway (Merck Research Laboratories), H. K. Cox (Zeneca Ag Products). American Chemical Society, Washington, DC. 1995. x + 428 pp. 15 × 22.5 cm. \$109.95. ISBN 0-8412-3160-5.

Computer-Aided Molecular Design (CAMD) consists of many different methods aimed at solving a variety of chemical problems. As a collection, these methods form a set of powerful tools that are being used in a number of industrial and academic laboratories to design and develop new chemical products. This book brings together a number of examples in which CAMD has increased the mechanistic understanding and/or provided energetic and structural information that has assisted in the design of new drugs, agrochemicals, and materials. The book is well organized and referenced (ca. 850), and each chapter is lucid. The balance between the theoretical bases behind the methods, the application of the methods, and results is well maintained.

Chapter one provides a short historic overview of computational chemistry and provides the reader with a brief description of the various CAMD techniques. The description covers the scientific underpinning of each method, what type of information can be obtained, and computational cost relative to other methods. In addition, modeling paradigms that have been found to be of general use such as structure-based design, novel lead generation, protein homology modeling, and catalysis simulation are discussed. The remainder of the book is divided into three sections. The sections contain case studies aimed at the understanding of the underlying mechanisms and/or design of new products in pharmaceutical, agrochemical, and material sciences. Molec-

ular dynamics studies are presented on backbone-modified antisense oligodeoxynucleotides, drug diffusion in biomembranes, polyelectrolyte adsorption on mineral surfaces, and the behavior of organic molecules in zeolites. Studies using Genetic Algorithms (GA) to design a screen for antihistamine agents and new materials are reported. In addition, case studies using Quantitative Structure Activity Relationships (QSAR), structure-based design, de novo design, and quantum mechanics are reported.

Overall, this book will be most useful to chemists who wish to apply CAMD to their own research. It provides a collection of examples that clearly demonstrate how CAMD can be used to assist in moving a project forward without setting up unrealistic expectations.

David R. Langley

Bristol-Myers Squibb  
Pharmaceutical Research Institute  
5 Research Parkway  
Wallingford, Connecticut 06492

NP960637P

S0163-3864(96)00637-4

### Chemistry and Toxicology of Diverse Classes of Alkaloids.

Edited by Murray S. Blum (University of Georgia). Alaken Incorporated, Fort Collins, CO. 1996. v + 386 pp. 15 × 22.5 cm. \$99.50. ISBN 1-880293-06-4.

Five chapters on the chemical and toxicological properties of alkaloids from terrestrial and marine sources and one chapter describing alkaloids as anticancer agents comprise this book edited by M. S. Blum. *Chemistry and Toxicology of Diverse Classes of Alkaloids* is a companion volume to *The Toxic Action of Marine and Terrestrial Alkaloids* published recently by Alaken, Inc., which was reviewed in this journal (*J. Nat. Prod.* **1996**, 59, 1218–1219).

In this book, G. T. Tan and J. M. Pezzuto describe *Toxic Alkaloids Pertinent to Cancer Chemotherapy* (711 references); Atta-ur-Rahman and M. I. Choudhary discuss *Toxic Alkaloids and Other Nitrogenous Compounds from Marine Plants* (87 references); M. S. Blum elaborates the *Chemistry and Toxicology of Arthropod Alkaloids* (112 references); W. Z. Antkowiak details *The Chemistry and Toxicology of Mushroom Alkaloids* (387 references); J. M. Jacyno delineates *The Chemistry and Toxicology of the Diterpene Alkaloids* (100 references); and T. Higa and J.-I. Tanaka survey *Bioactive Marine Alkaloids from Okinawan Waters* (125 references).

The chapter by Tan and Pezzuto focuses on specific alkaloids from the 15 families of antitumor alkaloids that have demonstrated clinical antitumor activity. Their survey provides insight into botanical source and occurrence, chemistry and structure–activity relationships, proposed biochemical mechanisms of cytotoxic/antitumor activity, clinical pharmacology and pharmacokinetics, clinical applications and toxicology, and mechanism of resistance to antitumor alkaloids. Pertinent alkaloids discussed include *Vinca* alkaloids, aronycine, camptothecin, *Cephalotaxus* alkaloids, ellipticine, indicine *N*-oxide, and swainsonine. This richly detailed presentation is accompanied by over 700 citations.