

terms, an introductory paragraph that defines the discussed topic and summarizes the article's contents, cross references to other topics in the encyclopedia, and a brief bibliography of key review articles and research papers. A subject index containing more than 10 000 entries is located at the end of Volume 3 and offers the most convenient way to access a specific subject. In addition, Volume 3 contains a complete glossary of key terms just preceding the subject index. Clearly, significant effort has gone into organizing the material in ways that will not only enable readers to quickly locate information on a specific topic but will also encourage them to browse and read other articles of interest throughout the encyclopedia.

Basic scientific research is continually revising and expanding our understanding of cancer, and an encyclopedia devoted to this disease must cover a wide range of fundamental topics (e.g. cell cycle control and differentiation, carcinogenesis, chemotherapy, drug resistance), as well as timely topics (e.g. gene therapy, chemoprevention). In this respect, the editor has succeeded admirably in assembling, in encyclopedic form, a comprehensive, well-chosen collection of topics, contributed by a group of highly regarded scientists. This encyclopedia should be of interest to a wide range of scientists, biologists and chemists alike. Medicinal chemists will find throughout the encyclopedia many valuable summaries of highly relevant subjects that relate to the biology and treatment of cancer. Students in various disciplines of life sciences will also find the encyclopedia useful because they can easily access authoritative articles on a wide range of topics related to cancer. The reasonable cost of this three-volume set should make it a feasible acquisition for departmental libraries.

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JM970387P

S0022-2623(97)00387-7

Molecular Modeling: Principles and Applications. By Andrew Leach. Longman, Edinburgh. 1996. xvi + 595 pp. ISBN 0-582-23933-8. \$35.00.

The book is a text covering the elements of the broad field called molecular modeling. It begins with a chapter on the useful concepts including potential energy surfaces, molecular graphics, coordinate systems, and associated mathematics. The second chapter is a review of quantum mechanical models. This is concise and well-written. This is followed by a chapter on empirical force fields in molecular mechanical applications. This is a wide-ranging review of the various terms in molecular mechanics calculations. Chapter four explores energy minimization as it relates to exploration of energy surfaces. It is well illustrated and clearly written. The next chapter describes computer simulation methods including molecular dynamics and Monte Carlo methods. Examples of simple thermodynamic properties that can be calculated are listed and

described. The following two chapters are devoted to detailed descriptions of molecular dynamics and Monte Carlo methods. This set of chapters is quite useful in presenting these dynamic simulation methods with good illustrations punctuating both chapters.

Chapter eight presents the subject of exploration of conformational space. Several methods are described, and it is a very good discussion of these subjects. Chapter nine addresses three challenges in molecular modeling, free energies, solvation, and simulation of reactions. Again the illustrations enhance this presentation. The final chapter reviews the use of molecular modeling to discover and design new molecules.

This book is an excellent piece of work that should be a part of the library of every graduate student in medicinal chemistry. This should be the new essence of medicinal chemistry graduate education supplanting the classical emphasis on synthesis.

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JM970383K

S0022-2623(97)00383-X

Neural Networks in QSAR and Drug Design.

Edited by J. Devillers. Academic Press, London. 1996. x + 284 pp. 15.5 × 23.5 cm. ISBN 0-12-213815-5. \$65.00.

This book is a collection of articles exploring the subject of neural networks as data processing tools in compound design. It assumes some prior orientation to the subject as it moves quickly into the back propagation algorithm in the first chapter, written by the book editor, J. Devillers. This is a thorough overview with illustrations, comparisons, and software sources. The next four chapters illustrate the applicability of neural networks in log *P* estimations, organic chemical biodegradation, odor relationships, and odor threshold modeling. These chapters reveal the potential for neural nets to organize information into useful patterns leading to predictive models. Copious references accompany each of these four chapters, providing the reader with a rich source of information for deeper involvement in this paradigm. The editor has brought in several authors for these chapters who have contributed significantly to neural net technology. All are well written. Chapter 6 explores the pattern recognition capability of the adaptive resonance theory of Grossberg. These classifiers are shown to be of significance in computer-aided molecular design.

Chapter 7 shows the value of neural nets in multivariate data display. Chapter 8 is a QSAR study of nicotinic agonists using neural nets. The last three chapters describe applications to the evaluation of molecular surface properties, nonlinear neural mapping, and fuzzy clustering to classify protein classes. All very well presented by authorities in these areas. This book, and others in these emerging areas of modeling, stand as signposts to the new approaches to molecular design. The medicinal chemist who aspires to professional success in the new millennium must have a rich back-