

utilizing this method. The next chapter describes a procedure for construction of atomic-level receptor site models in the absence of a receptor crystal structure. Applications are extended to molecular recognition and chemical structure handling in the next chapter. Chapter ten describes genetic selection of aromatic substituents for designing test series. Neural networks and genetic algorithms are integrated into property prediction and structure construction from properties. The final chapter uses neural nets and a genetic algorithm to design biodegradable molecules.

The book is an essential part of a library of the medicinal chemist and drug design specialist who aspires to be at all creative in the new millennium. Computer-assisted design and *in silico* experiments are the ingredients of a productive approach to new drugs and, with the help of books like this, become more prominent in graduate curricula.

**Lemont B. Kier**

*Department of Medicinal Chemistry  
Virginia Commonwealth University  
Richmond, Virginia 23298-0540*

JM970382S

S0022-2623(97)00382-8

**Biological NMR Spectroscopy.** Edited by John L. Markley and Stanley J. Opella. Oxford University Press, New York, 1997. x + 360 pp. 16 × 24 cm. ISBN 0-19-509468-9. \$65.00.

This excellent text is the result of a Symposium on Biological NMR held at Stanford University in March of 1994 to honor the 65th birthday of one of the great pioneers in the area, Professor Oleg Jardetzky. The Epilogue of Professor Jardetzky's chapter highlighting the history of the application of NMR techniques to biological problems is in itself noteworthy. In his epilogue he discusses the importance to daydream and to be an explorer of science, and not to be just an exploiter of existing knowledge. Professor Jardetzky leaves us with these words, "A society that increasingly thinks only in terms of directing and channeling craftsmanship in the pursuit of clearly visible goals is cutting itself off from the source of all innovation." His thought-provoking epilogue should be required reading for all scientists, particularly those who sit on grant review panels.

The text is divided into four sections containing 23 chapters dealing with all areas of NMR related to the investigation of biological problems. The first section discusses the history of biological NMR spectroscopy. These four chapters provide an insight into the major challenges which have been overcome in the past 30–40 years. For the graduate student and recent Ph.D. who are accustomed to and familiar with the application of modern NMR techniques for the determination of protein structure, these chapters provide an insight into the process of the development of these techniques. This historical perspective provides a valuable insight into the creativity, as well as the hard work, which went into the development of these powerful techniques. The second section, which is divided into 13 chapters, is devoted to a discussion of the application of NMR to

protein structural studies. The application of both solution and solid state NMR methods to determine protein structure, protein folding, protein specificity, ligand receptor binding, and enzyme action are discussed in a clear and concise manner. The third section contains three chapters devoted to the study of nucleic acids. Topics discussed include determination of the structure of ribosomal RNA, characterization of DNA, and determination of conformational transitions. The fourth and final section presents a discussion of *in vivo* spectroscopy. These three chapters discuss the application of MRI methods to the study of the brain, and cancer cell metabolism.

This text should be required reading for all scientists interested in, or involved with, the application of NMR to biological problems. The text provides not only a clear overview of the state of the art in the field but also, in my opinion, an equally important overview of the history of the field.

**Rickey P. Hicks**

*Department of Chemistry  
Mail Stop 9573  
Mississippi State University  
Mississippi State, Mississippi 39762*

JM970386X

S0022-2623(97)00386-5

**Encyclopedia of Cancer. Volumes 1–3.** Edited by Joseph R. Bertino. Academic Press, Inc., San Diego, CA, 1997. xxxviii + 2134 pp. 22.5 × 28.5 cm. ISBN 0-12-093-230-X. \$475.00 (3 volume set).

The *Encyclopedia of Cancer* is an ambitious three-volume compendium containing 163 articles on various topics relating to the disease of cancer, including its molecular and genetic processes, its epidemiology, its prevention, and its treatment. As defined in the glossary of this encyclopedia, cancer is "a multistep genetic disease resulting from specific alterations in the function of one or more genes, disrupting the control of cellular growth and differentiation, with the outcome of uncontrolled cellular proliferation and transformation to a neoplastic state." This description provides sufficient detail of the underlying complexities which make this disease a worthy subject for an encyclopedic collection of knowledge.

The encyclopedia is thoughtfully organized and presented, and includes at the very beginning a brief, helpful Guide to Using the Encyclopedia. All articles are arranged alphabetically by title. Each volume contains two complete Tables of Contents for the entire encyclopedia. One Table of Contents lists articles as they are arranged in the encyclopedia, alphabetically by title. A second, more useful Table of Contents lists articles alphabetically by subject area. Fourteen specific subjects are presented in this second Table of Contents: Antisense, Ribozymes; Biological Treatment; Biology of Cancer; Chemical Carcinogenesis; Chemoprevention; Chemotherapy; Drug Resistance; Epidemiology/Tumor Genetics; Gene Therapy; Invasion and Spread of Cancer; Oncogenes; Radiation Therapy; Tumor Suppressor Genes; and Viral Carcinogenesis.

A uniform format for each article includes a brief outline of the general content, a short glossary of key

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.

**Janice R. Sufrin**

*Department of Experimental Therapeutics  
Grace Cancer Drug Center  
Roswell Park Cancer Institute  
Buffalo, New York 14263*

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.

**Lemont B. Kier**

*Department of Medicinal Chemistry  
Virginia Commonwealth University  
Richmond, Virginia 23298-0540*

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-