

## Book Reviews

### **Quantitative Structure–Activity Relationship (QSAR) Models of Mutagens and Carcinogens.**

Edited by Romualdo Benigni. CRC Press, Boca Raton, FL. 2003. x + 286 pp. 16 × 24.5 cm. ISBN 0-8493-1507-7. \$149.95.

In a field evolving as rapidly as QSAR, it is desirable periodically to take stock of what has been done and what most urgently needs to be done. To address this requirement for QSAR models of mutagenicity and carcinogenicity, the editor has assembled a first-rate team of contributors who are themselves active in the field and whose names will be mostly familiar to the volume's target audience. (Several contributors are fellow U.S. EPA employees.) In several chapters, the authors not merely are summarizing work and providing an overview of what it means but are the originators of much of the work they report.

The book's nine chapters consist of a general introduction to QSAR and eight special topics. I suspect that most readers who purchase this volume for the specialized chapters will already be familiar with much of the introductory chapter. Chapter 2 deals with mechanisms of action in chemical carcinogenesis and does a fine job of explaining why no single QSAR will ever suffice for the entire chemical universe. Carcinogenesis, and to a lesser extent mutagenesis, is not one process but many, and many QSARs are required to model it. Chapter 3 purports to be a summary of QSARs for individual classes of chemical mutagens and carcinogens. While it provides a good starting point, it is a rather bare-bones affair at best, and it makes no attempt at comparison or critical evaluation of the various models. It specifically omits aromatic amines, since these are the subject of Chapter 4. Again, while providing a good introduction, this chapter presents few actual models, much less makes any attempt to compare or evaluate them.

Chapter 5, which may be the most useful, lists, describes, and compares public sources of mutagenicity and carcinogenicity data. Somewhat surprisingly, this chapter also explicitly discusses the fact that the predictive accuracy of a QSAR cannot exceed the experimental reproducibility of the data on which it is based. This ought to be obvious, yet it is often overlooked in the QSAR literature. Chapter 6 describes the use of the commercial software MultiCASE in assessing carcinogenicity and relates the rationale of the MultiCASE approach. Chapter 7 presents case studies in the hierarchical use of different sets of molecular descriptors in constructing mutagenicity QSARs, a technique developed by the chapter's authors. This is one solution, a good one in my view, to the variable-selection problem created by throwing hundreds of descriptors at a model all at once.

Chapter 8 is not about mutagenicity and carcinogenicity at all but about aquatic toxicology. Nevertheless, the issues it discusses are mostly similar to the ones surrounding mutagenicity and carcinogenicity, particularly the use of QSARs in regulatory contexts. The final chapter treats mechanism of action and its relationship

to risk assessment. Especially valuable here is an explicit statement of rates of false positives and false negatives to be expected under various circumstances. I can certainly recommend this volume on the basis of the information it contains, although the price will probably restrict its ownership.

This review was written by Gordon Cash in his private capacity. No official support or endorsement by the Environmental Protection Agency is intended or should be inferred.

**Gordon G. Cash**

*United States Environmental Protection Agency  
Washington, D.C. 20460*

JM040146Z

10.1021/jm040146z

**Practice of Gas Chromatography. Fourth Edition.** Edited by Robert L. Grob and Eugene F. Barry. Wiley-Interscience, Hoboken, NJ. 2004. xi + 1045 pp. 16 × 24 cm. ISBN 0-471-2293-0. \$150.00.

It is a pleasure to review the fourth edition of what many regard as the "Bible" of gas chromatography. This review highlights the additions and changes from the third edition (1995).

The first three chapters (introduction, theory, and columns) are basically the same as in the previous edition. Chapter 4 on optimization of separations has a new author, John V. Hinshaw. It focuses primarily on capillary columns, acknowledging that the majority of laboratories do only capillary GC. It provides a very practical approach to optimization, recognizing the limits of one's individual GC system. Useful suggestions are provided to approach a specific goal, i.e., decreased analysis time versus improved peak resolution. Chapter 5 is an added new chapter by Richard D. Sacks on high-speed GC. Although not as common as high-speed LC, this chapter is an important addition to address the push toward high-throughput analyses. All components of the GC system are covered. Detectors are particularly important, with MS predominating because of sample size limitations. The topic of autonomous microchromatographs is also presented. Chapter 6 on detectors is a revision of the former Chapter 5, with new authors Luis A. Colon and Lisa J. Baird. It focuses on all available detectors except MS. Chapter 7 is an update of the former Chapter 6 on techniques for GC/MS and includes a section on high-speed GC/MS. Chapter 8 on qualitative and quantitative analysis is a moderate revision of former Chapter 7, with new authors editor Robert L. Grob and Mary A. Kaiser. Chapter 9 on inlet systems is a slight revision of former Chapter 7 by new author Nicholas H. Snow. Chapter 10 on gas management by Reginald J. Bartram is a new and important addition concerning this critical component of GC systems. Chapter 11 on sample preparation techniques by Nicholas H. Snow and Gregory C. Slack is another excellent addition of an important topic covering all the

techniques for gas-phase sample introduction from neat samples to complex extraction devices. Chapter 12 on physicochemical measurements is a slight revision of the previous Chapter 9 by the same authors, Mary A. Kaiser and Cecil R. Dybowski. Chapter 13 on petroleum and petrochemical analysis by Edward F. Smith with two added coauthors, Mark E. Craig and Clifford C. Walters, is an update of former Chapter 10. Chapter 14 on clinical and pharmaceutical analysis by Juan G. Alvarez is basically unchanged from the former Chapter 12. Chapter 15 on environmental applications is a substantial revision and update, by new author John R. Snyder, of former Chapter 14. Chapter 16 on forensic applications is a revision and update by Thomas A. Brettell of his former Chapter 13. Chapter 17 on validation and QA/QC by Thomas A. Brettell and Richard E. Lester is a welcome new addition. Also added is Appendix C on useful hints for gas chromatography, which to even the experienced gas chromatographer is a reminder of what it takes to get quality results.

The first ten chapters of this new edition will continue to make this an outstanding textbook for beginning and advanced courses in chromatography, and the remaining chapters with newly added material will make this a must-have book on the shelves of all laboratories doing gas chromatographic analyses.

**John F. Fitzloff**

*Department of Medicinal Chemistry and Pharmacognosy  
College of Pharmacy  
University of Illinois at Chicago  
833 S. Wood Street, M/C 781  
Chicago, Illinois 60612*

JM040152V

10.1021/jm040152v

**Medicinal and Aromatic Plants of Indian Ocean Islands.** By Ameenah Gurib-Fakim and Thomas Brendler. Medpharm Scientific Publishers, Stuttgart, Germany. 2004. viii + 567 pp. 20 × 28 cm. ISBN 3-88763-094-7. \$169.95.

The Indian Ocean Islands of Madagascar, Mascarenes, Comoros, and Seychelles are a habitat to flora and fauna of wide diversity. However, currently these represent a fraction of the number of species in existence even 50 years ago, before exploitation and cultivation changed the face of the islands radically and permanently. According to the authors, despite its unique diversity, the region is (with the exception of Madagascar) heavily under-represented in current scientific literature. With the publication of this book, they hope to fill a gap in existence since the 1960s.

Monographs of some 350 medicinal and aromatic plants of the region have been selected on the basis of their usefulness, popularity, and rarity with emphasis on plants from Seychelles and Comoros being described for the first time. However, the list is not inclusive of every medicinal plant in the region. Rather, it aims to concentrate on those endemic plants that are rare and less well-known because their successful use in local traditional medicine has caused them to become vulnerable or even virtually extinct.

For each plant the description, as and when available, is given under the following categories: general information, family, synonyms, vernacular names, etymology, botanical description, distribution and ecology, conservation status, drug specification, chemistry of the active or unique constituents including their structures, pharmacological studies, and use in traditional medicine. Sixteen pages covering over 800 references are included. An indication index is covered in eight pages. A names index of plants is provided in 21 pages. The provision of a general index would have been a helpful feature to readers. In addition, titles of the referenced articles would have also been useful.

Full-color photographs of 192 plants and 588 black and white figures of most of the plants and structures are described in the monographs. Errors were noted in some structures presented in the book. For example, the chromene derivative 7-methoxy-2,2-dimethylchromene, first isolated in the mid-1950s and biologically evaluated in the 1970s, is well-known in the literature as precocene I. However, on pages 100 and 101 precocene I is identified as 6-angeloyloxy-7-methoxy-2,2-dimethylchromene, the isolation of which was reported in the mid-1990s. On page 107 the structure of aloe-emodin (1,8-dihydroxy-3-hydroxymethylanthraquinone) is given. However, the compound is identified as aloe-emodin anthrone. The structure of the iridoid glycoside paederoside is shown on pages 357 and 358 as a thioacetate. The correct structure is the *S*-methylthiocarbonate (Kapadia, G. J.; et al. *Tetrahedron Lett.* **1979**, No. 22, 1937–1938).

Nevertheless, this volume combines a rich source of ancient local biodiversity and knowledge with a Western approach to preserving both knowledge and environment. It provides a useful and fascinating reference work that captures the interest in traditional medicine as well as the potential for the development of new drugs. The comprehensive volume is recommended to those working in the field of medicinal plants as researchers, educators, or other professionals with an interest in plants as medicines or sources of medicines.

**Govind J. Kapadia**

*Department of Pharmaceutical Sciences  
School of Pharmacy, Howard University  
Washington, D.C. 20059*

JM040147R

10.1021/jm040147r

**Managing Scientists. Leadership Strategies in Scientific Research. Second Edition.** By Alice M. Sapienza. Wiley-Liss, Hoboken, NJ. 2004. xiii + 246 pp. 15.5 × 23.5 cm. ISBN 0-471-22614-9 (Paperback). \$39.95.

This is the second edition of a book specifically written as an aid to leaders of scientific research in biotechnology and in pharmaceutical research and development industries. It is written with the recognition that most managers of this research are scientists with training in their specific scientific discipline but in most instances with no management training and relatively little practical managerial experience. The author notes

that poor leadership most often results in poor productivity and a lack of creativity. Conversely, good leadership can make a major difference to result in a superbly creative laboratory. The book is intended to assist managers of scientific research in enhancing their leadership skills.

The second edition includes conclusions derived from surveys of scientists on their perceptions of being led. These surveys emphasize the attributes of leaders supporting creative research, the hindrance to creativity and effective collaboration resulting from the negative climate created by ineffective leaders, the need for quick and effective resolution of conflicts, and the importance of active listening skills. Balancing scientific and administrative responsibilities, dealing with personality differences, motivating subordinates, and in effective communications are problems noted by many leaders of scientific research. In addition to addressing these topics, this book treats many other leadership issues, including the special problems faced by minority scientists in industry and academia.

Following an introductory chapter describing the general rationale of the book, there are nine additional chapters that address issues of importance to leaders of scientific research. The second chapter is new; it focuses on the special challenges with which women scientists must deal. Chapter 3 considers the importance of motivation and includes material on motivation theory. The fourth chapter addresses leadership styles and theories of leadership. In Chapter 5 the critical significance of effective communication is considered. Recognizing that no organization is without conflict at some time or another, Chapter 6 addresses potential

sources of conflict and the challenge of conflict resolution. Chapter 7, entitled "Creativity: Influence of Structure, Size, and Formal Systems" considers a number of factors that influence creativity. The uniqueness and special considerations required to manage a project, which is defined as "a temporary endeavor undertaken to create a unique product or service," are topics of Chapter 8. In Chapters 9 and 10 the author addresses organizational culture and organizational change; she notes that organizational culture and individual personality share two attributes; i.e., both have a profound effect on the work environment and both are very difficult to change. Chapter 9 considers the first of these, i.e., the influence of organizational culture on the work environment. The final chapter addresses the second, i.e., the role of leadership in organizational change. Each of the 10 chapters is followed by an extensive list of notes and references, and the book concludes with an adequate subject index.

A major premise for this book is the very reasonable assumption that better leadership in scientific research will increase productivity and creativity. As the career paths of many scientists proceed through the laboratory to leadership and administrative positions, with little or no intermediate leadership training, this book will provide beneficial insights to these scientists as they progress through the ranks.

**Carl Kaiser**

*8470 Woodland Road  
Millersville, Maryland 21108-1756*

JM040150A

10.1021/jm040150a