

A. J. Hopfinger and John S. Tokarski summarize 3-D QSAR Analysis COMFA, Distance Geometry, and Receptor Dependent 3-D QSARS. This is an extensive, detailed, and well-reviewed contribution. Validation of 3D QSARS methods is stressed. There are 98 references. Computational Approaches to Chemical Libraries is covered by David C. Spellmeyer, Jeffrey M. Blaney, and Eric Martin. This is another well-written chapter focused on the general aspects of chemical library design. The chapter is informing without detailed specific examples (53 references). Receptor Preorganization for Activity and Its Role in Identifying Ligand-Binding Sites on Proteins (Brian K. Shoichet) briefly covers broad areas such as protein–ligand interfaces, the role of conformational change, and specificity of binding sites. Experimental and computational methods for identifying binding sites is reviewed with brief discussions on each methodology (79 references).

Manuel C. Peitsch provides a short chapter on Comparative Protein Modeling. Although protein modeling does not directly relate to computer-aided drug design, the techniques and programs discussed provide information of interest to computational chemists in an important related field (53 references). Docking Conformationally Flexible Molecules into Protein Binding Sites is covered extensively by Millard H. Lambert with a prodigious 239 references. In this chapter DOCK and distance geometry play a central role as well as Monte Carlo minimization and conformer buildup approaches. This chapter is very helpful for understanding and reviewing this important area.

Mark A. Murcko contributes an Introduction to De Novo Ligand Design. This is a very well-written and an informative addition. There are clearly described “how-to’s” and an evaluation of progress in this computational field. This is another excellent contribution with 141 references. Ajay and Mark A. Murcko and Peter F. W. Stouten review Recent Advances in the Prediction of Binding Free Energy. This is a most interesting area of computational chemistry that is not often covered. The chapter is well-written, complete, and descriptive (119 references). Long Range Electrostatic Effects (Ulrich Essmann and Thomas A. Darden), 220 references, and Metals in Molecular Mechanics Force Fields and Simulations (Libero J. Bartolotti and Lee G. Pedersen), 89 references, follows. Both chapters provided needed information. It is very important to include both areas which are not often emphasized (especially long range electrostatic effects) and often needed (especially metals in force fields). The latter topic is assembled by category including most useful tables with references. The last chapter, New Vistas in Molecular Mechanics (J. Phillip Bowne and Guyan Liang), 88 references, makes this book complete.

The editor Paul S. Charifson deserves credit for putting together an outstanding review of essential topics in this field. All chapters have similar formats and make the text user-friendly. This reviewer highly recommends the text for anyone interested in computational chemistry or structure-based drug design,

especially students. Unfortunately the high cost may make it primarily a library acquisition, which is a shame.

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The Laboratory Companion: A Practical Guide to Materials, Equipment, and Technique. By Gary S. Coyne. John Wiley & Sons, New York. 1997. xviii + 527 pp. 18 × 26 cm. ISBN 0-4711-8422-5. \$59.95.

This book is an updated version of the previously published *The Laboratory Handbook of Materials, Equipment, and Technique* (1992). As the word “practical” in the title of the current version implies, this book concentrates on common laboratory methods and materials used on a daily basis in most chemistry laboratories. It is this focus which sets this book apart from other general purpose laboratory manuals which might provide more complete coverage, but often in a sketchy fashion.

The author, a scientific glassblower, covers laboratory glassware in nice detail throughout the book in chapters entitled Materials in the Lab; Joints, Stopcocks and Glass Tubing; Cleaning Glassware; and The Gas-Oxygen Torch (for those who might want to perform some simple glass manipulation in the laboratory). Flexible tubing, O-rings, and other miscellaneous items (often neglected, until a problem arises) are also discussed. The unique chapter dedicated to vacuum systems is of particular note. Topics range from vacuum pumps (aspirators to diffusion pumps) and gauges to leak detection. Chapters on Measurement; Compressed Gases; and High and Low Temperature will seem familiar to practicing bench chemists. However, beginning chemists will find these chapters very informative, and experienced chemists will find them a useful resource.

Each topic is introduced from a historical perspective, followed by a brief discussion of theory. A generous, comprehensible text (accompanied by abundant illustrations and tabular data) provides comprehensive technical details, applications, and numerous handy tips. Tables containing useful data and practical comments are routinely used to summarize the sections. Safety issues are stressed throughout the book.

This book is highly recommended for those beginning their laboratory careers. More seasoned, time-impaired chemists will find this compilation of information very

helpful, and supervisors will find that a "lab copy" will pay for itself in short-order.

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Emerging Drugs. The Prospect for Improved Medicines. Annual Executive Briefing. Volume 3.

Edited by W. C. Bowman, J. D. Fitzgerald, and J. B. Taylor. Ashley Publications Ltd., London. 1998. vi + 397 pp. 21 x 29.54 cm. ISSN 1361-9195. \$690.00.

Volume 3 of this series consists of 25 well-written reviews concentrated in the cardiovascular and cancer areas but including other topics such as pain, inflammation, therapeutic vaccines, and antisense oligonucleotides. Each chapter is written by well-qualified mostly industrial investigators actively engaged in the area under discussion. Each entry is between 12 and 25 pages long and contains the following sections: summary, background, medical need, therapeutic class review, current research goals, scientific rationale, competitive environment, potential development issues, editorial analysis, and bibliography. The articles are sufficiently in depth for a pharmaceutically literate reader to get a good sense of the importance of the particular field, the rationale and current status of the approaches being followed as revealed in the literature,

and some of the unique problems of developing a marketed drug in that area. The articles appear to be current with 1997 literature references. For those of us who have difficulty keeping the alphabet soup jargon straight, there is an extensive glossary. There is also a company index which references for each company those areas covered in this volume in which they may be active.

In summary, this volume consists of in-depth reviews of some active areas of research and development, targeting the future potential of a given hypothesis and the data describing its present status, with emphasis on compounds in the various stages of development. As indicated by the subtitle of the series, "Annual Executive Briefing", and its price, this series is not targeted specifically toward the individual laboratory investigator. As stated in the foreword to Volume One 1996, it could "provide a critical guide for those working in strategic marketing, licensing department and health-care planning". However, it could also serve to give researchers a broad picture of a research area and provide data to suggest how their project relates. I would recommend that pharmaceutical company libraries consider acquiring this book, not only for the use of executives but also for those involved in the research and development process.

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