

researcher currently using or seriously contemplating the use of capillary electrophoresis.

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The Combinatorial Index. By Barry A. Bunin. Academic Press, New York, NY. 1998. xvii + 322 pp. 18 × 26 cm. ISBN 0-12-141340-3. \$79.95.

Surely virtually everyone now knows that combinatorial chemistry is a rapidly growing multidisciplinary field in medicinal chemistry. The present rate of publication of research articles exceeds two papers daily, and the literature is widely scattered. Consequently it is becoming difficult for all but the most dedicated to keep abreast of current findings in an organized way. This book is a welcome aid to this process. It is an easy to use collection of reliable literature methods for all phases of medicinal chemical laboratory transformations using combinatorial techniques and places a particular emphasis on resin-based methods and the preparation of small, druglike libraries.

The book is divided into chapters describing particular laboratory transformations and procedures starting with a general background chapter and going on in turn to chapters dealing with linker technologies, specific reactions for preparing libraries, analytical methods, and solution/mixed solid-phase–solution reactions. This is followed by a series of appendixes keyed back into the preceding chapters covering a summary of functional group transformations, classification of heterocyclization reactions, unnatural biopolymers, oligosaccharides, a list of abbreviations, and then useful author and subject indexes. Each reaction covered is described in sufficient detail that a reasonably experienced chemist could perform the reaction described or use the description as the basis for developing an analogous reaction. Each reaction is also commented upon bringing out specific points of interest and ranges of utility, and each reaction or process is referenced at the point of discussion.

On the whole; this book is a very useful and practical “cook book” that many chemists will keep close at hand and refer to often. It is clearly organized and well-written and is comparatively inexpensive. Despite the magnitude of the task, it is hoped that Bunin will be able to follow through on his desire to keep the book up to date with supplements on or off the net.

All chemists who work in this key area will want to have a copy near at hand and will wear it out through constant resort. It is not, however, the sort of book that chemists will read from cover to cover. Those medicinal

chemists who are not actively engaged as yet in combinatorial work will find it an excellent way to learn about it.

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Practical Application of Computer-Aided Drug Design. Edited by Paul S. Charifson. Marcel Dekker, Inc., New York, NY. 1997. x + 52 pp. 16 × 23.5 cm. ISBN 0-8247-9885-6. \$150.00.

Practical Application of Computer-Aided Drug Design is an impressive compilation of chapters covering not only computational drug discovery techniques but also related fields in structural biology and biophysical chemistry. The authors of the various chapters have had considerable experience in their respective areas and many times provide lucid explanations of respective approaches to drug discovery. In general, the text is well-referenced and should be a valuable resource for interested researchers and students. Recent Successes and Limitations in Computer-Aided Drug Design, the topic of the first chapter; authored by Paul S. Charifson and Irwin D. Kuntz, provides a key take home message that the more “simplistic methods” have been the most successful. The fundamental concepts and techniques emphasized include molecular graphics applications, the calculation of interacting energies, molecular docking, QSAR, and pharmacophore modeling. The authors conclude that the simplistic method provides a multidisciplinary “buy-in” early in the design process and allows rapid evaluation of ideas studies permitting early incorporation of synthesis and bioavailability considerations. Clearly stated is the author’s bias that structure-based approaches possess the greatest overall potential.

The second chapter on Recent Techniques and Applications in Pharmacophore Mapping by Mark G. Bures highlights in some detail recent pharmacophore mapping techniques. There are 88 references that range from very specific examples such as the work on sigma 1 pharmacophores by Richard Glennon to the more general approaches using superposition methods (DISCO) developed by Yvonne Martin and colleagues at Abbott.

The Generation and use of 3D Databases for Drug Discovery is reviewed by Renée L. DesJarlais. The chapter provides general information on the sources of 3D structures and on how to assess the quality of structure data bases as well as a review of different search methods and specific applications including pharmacophore searching (auxin transport and protein kinase C inhibitors), caveat (cyclosporine analogues and major histocompatibility complex peptides), and DOCK (HIV-1 protease, thymidylate synthetase, influenza hemagglutinin, and inhibitors of parasitic proteases). The chapter, although of interest and well-presented, covers a smaller segment of the literature than the other chapters with only 20 references.

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