Practical Application of Computer-Aided Drug Design

Paul S. Charifson (Ed.), (Vertex Pharmaceuticals Inc.), Marcel Dekker, New York, 1997. 552 pp. US$ 150.00, ISBN 0-8247-9885-6

This book is considered by its editor to be a comprehensive review of recent advances in the field of computer-aided drug design. It is divided into the following self explaining chapters. (1) Recent Successes and Continuing Limitations in Computer-Aided Drug Design, by Charifson and Kuntz, 38 pp., 143 references. (2) Recent Techniques and Applications in Pharmacophore Mapping, by Bures, 34 pp., 88 references. (3) Generation and Use of Three-Dimensional Databases for Drug Discovery, by DesJarlais, 32 pp., 70 references. (4) Three-Dimensional Quantitative Structure-Activity Relationship Analysis, by Hopfinger and Tokarski, 60 pp., 98 references. (5) Computational Approaches to Chemical Libraries, by Spellmeyer et al., 30 pp., 53 references. (6) Receptor Preorganisation for Activity and Its Role in Identifying Ligand-Binding Sites on Proteins, by Shoichet, 32 pp., 79 references. (7) Comparative Protein Modeling, by Peitsch, 16 pp. (plus 4 pages with color prints), 53 references. (8) Docking Conformationally Flexible Molecules into Protein Binding Sites, by Lambert, 62 pp., 239 references. (9) An Introduction to De Novo Ligand Design, by Murcko, 50 pp., 141 references. (10) Recent Advances in the Prediction of Binding Free Energy, by Ajay et al., 56 pp., 119 references. (11) Long-Range Electrostatic Effects, by Essmann and Darden, 60 pp., 220 references. (12) Metals in Molecular Mechanics Force Fields and Simulations, by Bartolotti and Pedersen, 24 pp., 89 references. (13) New Vistas in Molecular Mechanics, by Bowen and Liang, 44 pp., 85 references.

This recommendable book should be of great value for beginners as well as for active practitioners in the field of computer-aided drug design. The first group will get comprehensive information on the different points of view important for their future work; the latter will also use it as a reference and as a quick guide to original papers.

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Applied Surface Thermodynamics

A.W. Neumann and J.K. Spelt (Eds.), 646 pp. Marcel Dekker Inc. New York, 1996, $215, ISBN 0-8247-9096-0.

Surface phenomena are of great practical importance with widespread applications in different fields. Examples are stabilization and destabilization of emulsions and foams, flotation, wetting, adhesion, heterogeneous catalysis and semiconductor technology. In sharp contrast to the importance is the disregard in teaching surface science. Therefore, students usually are lacking a sound basis in this discipline. The book of Neumann and Spelt could be a remarkable step in improving this situation by providing a collection of scientific foundations of interfacial phenomena.

The book consists of 12 chapters from different authors, but later chapters are partly based on the former ones. In all cases, one of the editors acts as co-author, thus giving the book a unified style. The common idea of all chapters is the thermodynamic approach. This is most rigorously carried out in the first two chapters, entitled 'The generalized theory of capillarity' and 'Thermodynamics of axisymmetric capillary systems'. The generalized theory abandons the moderate curvature approximation used in the classical theory, introduces contact lines in addition and analogously to interphases in case of three phase systems, and culminates in the formulation and verification of a fundamental equation of surfaces. For axisymmetric systems the theory is further refined including compressible as well as incompressible interphases. It should not be concealed that it is hard work to read these first two chapters, but it will be rewarded by deeper insight into interphase phenomena.

Fortunately, the following chapters can also be read without having studied the first ones. The third article gives a detailed report on contact angles, the Young equation, contact angle hysteresis, and the importance of line tension or linear tension for the interpretation of contact angles. This is followed by a comprehensive description of line tension including its measurement by two different methods: the dependence of contact angles on drop size and the analysis of contact line shape across a stripwise heterogeneous wall. In chapter five an equation of state is derived combining solid-liquid, solid-vapour and liquid-vapour tensions. The parameter in this equation is empirically determined from a lot of contact angle data and the validity of the equation is verified by means of different independent experiments. Chapters six and seven emphasize the theoretical and practical importance of solid surface tension. It is shown that methods based on the thermodynamic equation of state and on the measurements of contact angles are superior to other approaches in determining solid surface tension. Chapters eight, nine, and ten give a wonderful survey of the most powerful techniques used to measure contact angles and surface tensions.

Chapter 11 deals with the wettability of solid particles, an area of great technological interest. The same is true for 'The behaviour of particles at solidification fronts' treated in the last chapter. The behaviour of small inert particles at an advancing solid-liquid interface has important consequences for a lot of technological and biological phenomena, examples are crystal growth, and soil stability and vegetation in permafrost regions.

'Applied Surface Thermodynamics' is a valuable source of theory and experimental techniques for all working

actively in the fascinating field of 'wet' surfaces. (The book does not cover high-vacuum surfaces.) Each of the 12 chapters can be read independently, but cross-references are given, and a lot of references at the end of each chapter lead to the original literature. 'Applied Surface Thermodynamics' is not a textbook for beginners. Basic knowledge from, for example, Adamson's 'Physical Chemistry of Surfaces' is pre-supposed. Thus, the book is highly recommended for experts and also for students already experienced in surface science.

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Isolation Technology – A Practical Guide
T. Coles (Ed.), 322 pp. Interpharm Press, Buffalo Grove, IL, USA, 1998, ISBN 1-57491-059-0

Separating a working area from the operator, protecting the operator from a working process, creating a controlled work space of a well defined quality – all these issues are covered by the term Isolation Technology, which is now widely used at aseptic filling, sterility testing, pharmaceutical production of biologically active or toxic materials and hospital pharmacy work. Tim Coles' book provides, in 10 chapters, an overview of various aspects of isolation technology starting with the general concept on materials used for isolation, the air handling (filtration, pressure and flow regimes) and the methods by which the work inside an isolator can be assessed. The next section is devoted to a review of transfer methods including schematic illustrations of different types of lockchambers, waste and transfer ports as well as operational considerations concerning transfer of materials. An extra chapter emphasizes the importance of control systems and the isolator instrumentation, such as control and monitoring of temperature and humidity or the measure of air flow rates.

The author spends about one third of the book making the reader familiar with these basic concepts of isolation technology. The second part of the book focuses on detailed considerations for a design specification and project development to give an idea of what regulatory demands have to be achieved for the successful implementation of an isolation unit and what standards and guidelines have to be followed. Examples are given for operational qualification documents following the FDA-preferred format or for the points that should be included into a performance qualification to fulfil the overall design requirements.

Having discussed the setup of an isolator system the next chapter is concerned with the housekeeping of such a unit. A relatively broad room is given to the explanation of miscellaneous methods of sterilization by wet processes and fogging processes using different types of gasses. Decontamination problems with pathogens or recombinant DNA are only quickly mentioned because these matters are beyond the scope of the book.

After consideration of all stages of setup of an isolator facility the author continues with a short overview on operator training, how to validate the system physically and microbiologically and on the kind of process documentation. This special issue is in close context with regulatory affair aspects, which are outlined in the last but one chapter. Here, in detail, the FDA perspective on isolation technology is summarized.

In the final chapter two case studies are exemplarily described to give the reader an impression of real-life situations. The book closes with a literature list, which is only of restricted value, since many references refer to conference contributions or congress proceedings, which are not directly available. On the other hand, the literature list is followed by a very detailed glossary and an extensive list of world-wide resources, including consulting or validation support services.

In summary, the chapters are clearly arranged and the book is easily readable, so it can be used as guidance during the implementation of an isolation facility. It covers all important aspects of isolation technology and can be recommended to all those interested in this area.

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