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