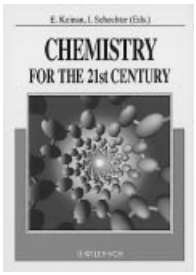
The Shape of Things to Come

Chemistry for the 21st Century. Edited by *Ehud Keinan* and *Israel Schechter*. Wiley-VCH, Weinheim 2001. xiv + 293 pp., softcover € 39.90.—ISBN 3-527-30235-2

Where is chemical research going, and what should be the chemist's research targets in the present age of interdisciplinary science? These are the questions considered by Ehud Keinan and Israel Schechter in *Chemistry for the 21st Century*. The book contains a wide-ranging collection of articles by well-known scientists representing different fields of work, and it provides an impressive demonstration of the rich variety of chemical research that crosses subject boundaries. The 15 chapters discuss the resulting benefits in the areas of supramolecular chemistry, chemical synthesis, drug design, heterogeneous catalysis, protein research, nitrogen chemistry, combinatorial chemistry, prebiotic chemistry, molecular modeling, and quantum chemistry, and they extrapolate from what has already been achieved to identifying the tasks for the future. They cover topics as varied as protocols for total syntheses of epothilones, methods for the biological testing of synthetic compounds with therapeutic potential, and examples of the conformational control of biological function.



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Guidelines for the development of efficient catalysts are indicated, and there are discussions about the importance of biological sources of nitrogen and ways of using them. The close interweaving of chemistry and biology is emphasized, especially in the chapter "Drugs for a New Millenium". Advances in the understanding of biological processes and of factors that affect them have made it possible to develop specific strategies for the design and synthesis of active agents. Combinatorial chemistry extends the scope of interaction further to include inorganic chemistry and the materials sciences. The use of combinatorial methods for drug design has generated interest in applying inorganic chemistry to the development of suitable solid phases as support materials for molecular libraries. The chapter on protein chain folding goes hand in hand with the chapter on theoretical chemistry, which defines the ever-more precise characterization of the spectroscopic and dynamic properties of large molecules, such as proteins, as an important frontier of modern quantum chemistry. *Chemistry for the 21st Century* is a rich pool of ideas for research on challenging current problems, as for example in the discussions about homochirality of biomolecules and theories about its origins in prebiotic chemistry.

The book is certainly not a comprehensive treatment of all the research topics centered around chemistry. Nevertheless, the examples chosen will serve to give the attentive reader an impression of the wide-ranging nature of chemical research and its important intermeshing with other disciplines. A look at the list of contents is enough to appreciate the broadness of the range of topics and to arouse one's curiosity. Although a few of the authors have tended to put more emphasis on reviewing their own subject than on identifying new directions of research, taken as a whole the 15 chapters serve to point the way ahead for chemistry-related interdisciplinary work in the modern age.

The book is not only of interest to chemists—scientists in related disciplines such as physics and biology will also derive useful ideas from it. Students will certainly find it stimulating, and it may also give them a broader outlook to help in deciding on their preferred area of research. Although the book generally assumes some scientific education on the part of the reader, even some without a background in natural science may benefit from reading one or another of the chapters.

Ehud Keinan and Israel Schechter have put together nice collection of chemical research topics, which are bound together by the common element of cooperative research and mutual enrichment across interdisciplinary boundaries. We can look forward with anticipation to the two further volumes that are to complement this one in the series *Science for the 21st Century*.

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Virtual Screening for Bioactive Molecules. Edited by *Hans-Joachim Böhm* and *Gisbert Schneider*. Wiley-VCH, Weinheim 2000. xviii + 307 pp., hardcover € 129.00.—ISBN 3-527-30153-4

Virtual screening is a computer-based method for arriving at a systematic selection of compounds from a large number of molecules, as the editors explain in defining the subject of this book. It consists of 12 chapters describing the different approaches to virtual screening. The authors of the individual chapters are drawn mainly from industrial research and development groups,

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as one expects in view of the importance of these methods to the pharmaceutical industry. As can be seen from the literature references cited, many books and review articles dealing with aspects of virtual screening have appeared in the last few years. That is especially evident in Chapter 4, which is concerned with similarity searches. The authors have incorporated into this book most of the work that they have published in the primary literature.

Chapter 1 gives an introduction to high-throughput screening (HTS) and virtual screening. Although it contains a brief summary of the current state of the art in HTS, it fails to provide the reader with a comparison and evaluation of the various virtual screening methods used in the development of pharmaceutical agents. Chapter 3 deals with the subject of predicting physicochemical properties, the great importance of which is clearly emphasized in the opening sentences. Although an active agent may have a high affinity for binding to the receptor, that is of no use if it turns out to be ineffective in vivo because of insufficient solubility and bioavailability. This chapter is concerned with calculating lipophilicity, solubility, pK value, and protein-binding efficiency. Several references in this chapter give the impression that a paragraph is missing.

In Chapter 5 on the modeling of structure–activity correlations and in Chapter 12 on measurements of molecular diversity some mathematical formulas were unavoidable. In Chapter 5, for the benefit of readers with only limited mathematical knowledge, some statistical methods are explained in the appendix.

Chapter 7 describes the identification of pharmacophores in biologically active compounds and their use in virtual screening. The applications range from the screening of already existing data bases to the design of compound libraries. In the discussions much space is devoted to problems associated with the conformational flexibility of molecules. For identifying pharmacophores one can use various computer programs that are commercially available. Chapter 11 includes tables listing programs for dealing with docking and for de novo design of pharmaceutical agents, and discusses ligand–receptor interactions in the context of predicting binding constants. As well as the question of the conformational flexibility of molecules, the chapter discusses problems of protein flexibility and the role of water molecules in the docking experiment. Several examples of interesting pharmaceutical projects are described.

If the crystal structure of the biological target is known, one can carry out docking or superposition experiments with the ligands to achieve a virtual screening with selection. In Chapter 10 a university-based research group explains this principle. The examples described illustrate its relevance to pharmaceutical development.

Who will benefit from this book? What group of readers is it intended for? For medical chemists involved in the synthesis of active agents the book provides an excellent survey of the methods that are currently available for virtual screening. A particular advantage of the book is that the various aspects of virtual screening (library filtering, drug-likeness, ADME, QSAR, etc.) are considered from different viewpoints by the authors of the individual chapters. In that way the reader with only a limited knowledge of the subject can appreciate the concepts from a variety of different standpoints. However, the book has a few weaknesses, some of which are mentioned above, and inevitably the chapters vary in quality.

To summarize, the book resembles a collection of short stories of varying interest rather than a coherent novel.

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Nuclear and Radiation Chemical Approaches to Fullerene Science. (Series: Developments in Fullerene Science, Vol. 1.) Edited by *Tibor Braun*. Kluwer Academic Publishers, Dordrecht 2000. 204 pp., hardcover £ 60.00.—ISBN 0-7923-6524-0

Fullerene research is clearly not at present a field that gets a mention every month in the popular press. Despite that, the enthusiasm of the scientist whose satisfaction comes from discovering new types of carbon structures, thoroughly investigating their properties, and gaining new scientific insights remains undiminished, provided that he or she courageously and successfully resists the currently prevailing attitudes. Against that background it is to be welcomed that the well-known Hungarian scientist Tibor Braun has succeeded by his tenacity in persuading a major publishing house to begin a new series on fullerene research, and to courageously choose for the first volume a topic that does not promise sensational developments. Instead the book begins the series in a way that emphasizes the broad scope of fullerene research.

The subject *Nuclear and Radiation Chemical Approaches to Fullerene Science* is, of course, the editor's special area of interest, and thus he has been able to bring together a collection of articles reporting contributions to fullerene research that have not been given the recognition that they deserve in other review publications and conference volumes.

The articles by C. S. Sundar on positron annihilation and by E. J. Ansaldo on muon spectroscopy review the relatively small numbers of publications on their respective topics. Ansaldo emphasizes the advantages of the latter form of spectroscopy for determining surface states. However, for both these methods of characterization the scope for applications in fullerene research will remain narrowly defined. Klenscár and Vértes discuss the use of Mössbauer spectroscopy, and report the first studies on determining the structures of fullerene–metal complexes and metallofullerenes. Although only a small number of elements can be observed by Mössbauer spectroscopy, the method yields important information about the redox states and mobilities of the ions, and therefore it is to be hoped that its use in fullerene research will grow. In the following chapter Nakahar and Sueki describe the use of radionuclides and their decay processes in studies of metallofullerenes, with particular emphasis on the scandium group elements and the rare earth metals, which are especially important in work on endohedral fullerenes. After describing the preparation of endohedral fullerenes, the authors discuss methods for isolating them, and emphasize

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