Book Reviews

Computational Medicinal Chemistry for Drug Discovery. Edited by Patrick Bultinck, Hans De Winter, Wilfried Langenaeker, and Jan P. Tollenaere. Marcel Dekker, New York. 2004. xiv + 794 pp. 18 × 26 cm. ISBN 0-8247-4774-7. $195.00.

Some people aspire to managerial positions because, besides the increased pay and power, managers often have the luxury of sitting in judgment of other people's ideas and work rather than having to produce the ideas and work themselves. As a reviewer, I have the luxury of making a judgment about the book I have been asked to review. But as a former editor, I can appreciate all the hard work involved in creating an exemplary tome like this. Of the 27 chapters, fully a third were written by authors who also wrote chapters, generally on similar subjects, for the book series *Reviews in Computational Chemistry*.

The first seven chapters of the book examine core computational chemistry: force field, molecular orbital, and density functional methodologies. The next several chapters deal with how computational chemistry describes the interaction of molecules. The latter half of the book blossoms into many of the computational chemistry approaches that are used in attempts to discover medicinally interesting molecules. Many of these latter approaches rest on the ideas of quantitative structure−activity relationships (QSAR).

The editors taught a workshop on Computational Medicinal Chemistry in 2002. Although well qualified to write many of the chapters themselves, the editors have chosen to enlist a phalanx of outstanding computational chemists to write the chapters. Almost 30% of the authors are from industry, which brings some fundamental realism to the book. Authors with experience in the pharmaceutical industry have actually faced the difficult task of evaluating and designing synthetic targets in a fast-paced, high-pressure working environment. Hence, these authors can share their perspectives with newcomers.

Among the many illuminating chapters are those on molecular mechanics, generation of three-dimensional molecular structures, structure-based drug design, docking, pharmacophore modeling, QSAR descriptors, three-dimensional QSAR modeling, and databases. One cannot help but notice that some of the quantum theory chapters show an almost religious-like reverence for the standard equations of quantum mechanics. These chapters could have benefited from a greater attempt to bridge the communication gap with medicinal chemists.

The bulk of the references in the chapters dates from the mid-1990s through 2001. Color plates of figures are provided at the end of some chapters. The subject index (26 pages) is designed mainly to help the reader find computational methods rather than classes of compounds. Indexing of common receptors is spotty. If a therapeutic target is mentioned in a heading, it is likely to be indexed. If the mention is only in the text, the occurrence is unlikely to appear in the index. Regrettably, the editors have not compiled an index of cited authors, so an avenue for tracking down work in a particular area of research is shut off. Also missing are e-mail addresses of the editors and authors. All modern books should provide this information to facilitate communication between the readers and the writers.

Some topics not receiving much attention in this already thick book are as follows. There is only a limited mention of cheminformatics, which may be the fastest growing facet of computational chemistry at the present time. As the editors explain in their preface, there is little in the book on molecular simulations and free energy perturbation calculations because these are not usually practical (except for the most academic molecular design projects). To its credit, the book describes a few examples of successful drug discovery aided by computational chemistry and X-ray crystallography. There are more examples known, but they are not discussed. Overall, however, the book has many appealing strengths.

All the editors and about half the authors are European (another 40% are American). This is fine and brings to mind the report in *Modern Drug Discovery* (July 2004) pointing out that the number of new molecular entities (NMEs) launched in Europe fell from 81 for the period 1993−1997 to 44 NMEs for the period 1998−2002. In contrast, the number of NMEs launched in the U.S. jumped from 48 for the period 1993−1997 to 85 for the period 1998−2002. Canada is not mentioned. Pharmaceutical R&D has been moving to the U.S. Tipping the scales in favor of the U.S. is not because the U.S. produces more scientists or clinicians. In 2000, for instance, Europe produced about three scientifically or technologically trained people to every two produced in the U.S. The decline in NMEs in Europe is also not because of differing levels of science or desire on the part of clinicians and scientists. Rather, we should recognize that the freer entrepreneurial environment in the U.S. has fostered the flow of more therapeutic products down through the "funnel" reaching from the discovery laboratories to the patients who need the innovative molecules. Patients in the U.S., as well as patients throughout the world who consume U.S.-discovered medicines, should be concerned if the entrepreneurial climate in the U.S. were to be torpedoed by shortsighted public-policy decisions.

In conclusion, this substantial book, if carefully read, can be of considerable value to scientists hoping to embark on a career or who are engaged in a career of using computational chemistry to discover molecules that alleviate the suffering of mankind.

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Organic Spectroscopic Analysis. By Rosaleen J. Anderson, David J. Bensell, and Paul W. Groundwater. Royal Society of Chemistry, Cambridge, U.K. 2004. vi + 175 pp. 19 × 24.5 cm. ISBN 0-85404-476-0. £14.95.

This is the 22nd book in the *Tutorial Chemistry Text* series begun by the Royal Society of Chemistry. This volume covers the basics of organic spectroscopy used for structure determination. The text does not provide the reader with large numbers of correlation tables for every form of spectroscopy used by organic chemists nor does it provide an in-depth explanation of the physical processes that occur when molecules interact with electromagnetic radiation. Rather, the text provides an overview of the spectroscopic methods used currently in structure elucidation of organic compounds. The text contains sections on ultraviolet−visible spectroscopy, infrared spectroscopy, nuclear magnetic resonance spectroscopy, and mass spectrometry. Suggested further readings and useful Web sites are also included, as well as answers to practice problems in the text. Many of the examples address simple organic molecules and natural products and describe how the generated spectra are characteristic of each of the molecular structures. Fundamentally, the book is not likely to be of utility to practicing organic chemists. However, it does an excellent job of providing the beginning student with an understanding of how different spectroscopic methods can be used to elucidate chemical structures. The material is presented in a clear and concise manner, and the book would be an excellent addition to the library of undergraduates, as well as students who are beginning their graduate studies.

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Bioconjugation Protocols. Strategies and Methods. Volume 283 in Methods in Molecular Biology. Edited by Christof M. Niemeyer. Humana Press, Totowa, NJ. 2004. xi + 330 pp. 16 × 24 cm. ISBN 1-588-29-098-0. $125.00.

Bioconjugates have continuously drawn attention for the past several decades not only because of their pivotal links between chemistry and biology but also because of their association with emerging novel applications in bioscience and pharmaceutics. A bioconjugate with desirable function relies on control over attachment site and orientation between entities down to molecular level. This book summarizes updates in both the classic skills and newer approaches as a technical conjunction among advanced organic synthesis, molecular biology, and material science.

This book is divided into four parts. Part I has seven chapters and illustrates several protocols for the syntheses and characterizations of antibody and enzyme conjugates. The specific biorecognition between biotin and streptavidin was demonstrated under either a protein or a polymer matrix environment. Part II contains seven chapters with a focus on various approaches to the syntheses of nucleic acid conjugates and molecular probes for applications in microarray and immunopolymerase chain reactions. The six chapters in part III elucidate approaches in synthesizing glycosyl and lipid conjugates anchored with peptide and proteins. Chemical coupling of Ras lipoproteins and conjugation of synthetic glycopeptide to a recombinant human interleukin-2 protein fragment were demonstrated. The last part contains three protocols on the biofunctionalization between nucleic acid and inorganic surfaces with cognizable applications in microarray and atomic force microscopy imaging.

The protocols presented in this volume are particularly valuable because they provide concrete pathways for scientists in designing bioconjugates toward a wide variety of research. The references are mostly updated through all the chapters; however, only limited references were cited for some of them. Despite that, the Note section at the end of each chapter addresses practical details in laboratory procedure that will lead scientists to master these techniques. I think this book therefore provides highlights for scientists who are pioneering in the synthesis of biofunctional macromolecules, as well as providing resources to all levels of scientists who are engaged in the fields of diagnostics, biomaterials, and pharmacotherapeutics.

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