

Drug Delivery Systems

Drug delivery is arguably one of the most extensive and dynamic fields of present-day research. It is also one of the most multidisciplinary areas of research, with inputs from medicine, pharmacology, chemistry, biology, biochemistry, materials science, and physics. Consequently, it is not easy to assemble a comprehensive book and to clearly communicate the knowledge to all the professionals of the diverse disciplines involved. In this book the editor has collected together detailed descriptions of selected important technologies used in drug-delivery systems. The book is structured to provide guidelines for specific applications in drug delivery, with emphasis on the techniques involved for the development of drug-delivery systems rather than on detailed descriptions of physicochemical properties or recent theories. The reader interested in the latter aspects can find further information in the list of references provided at the end of every chapter.

The chapters are well documented and written in clear language for the specialists of each discipline involved. However, the chapters are not grouped by topics or even slightly related, and the index does not compensate for this drawback by cross-referencing between them.

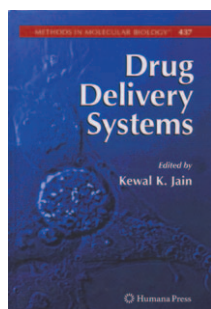
In accordance with the layout of the series *Methods in Molecular Biology*, most of the chapters begin with a brief description of the fundamental aspects, followed by the methods used to prepare or evaluate the drug-delivery system under discussion. The book starts with an extensive introduction that discusses many different drug-delivery approaches and their adoption by the pharmaceutical industry. However, only a few of the technologies introduced there are reviewed in the main body of the book. Moreover, some of the references in the introduction might not be readily available for all readers.

The second chapter is a succinct description of the role of virus capsids in gene transfer, including complete protocols for the production of adeno-associated viral vectors. The third chapter reviews small interfering RNA delivery systems, but does not cover the methodology. In Chapter 4, chronic drug delivery to the brain through a catheter is explained, with practical details. In Chapter 5, the authors discuss transdermal drug delivery, including the skin abrasion method. In Chapter 6, pulmonary release of peptides is described, and this is followed in Chapter 7 by a detailed description of the preparation of protein particles for lung delivery. Chapter 8 gives a meticulous description of an in vitro model to test drug transport through the blood–brain barrier, which is exemplified by an

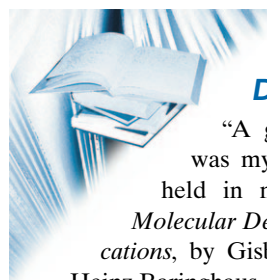
analysis of the transport of a nontoxic mutant protein of the diphtheria toxin. Chapter 9 is a brief summary of the basic methods for the preparation of liposomes loaded with an anticancer drug. Chapter 10 is merely a review of the state of the art in the use of pH-sensitive nanoparticles for the delivery of drugs to cancer patients; the design of such drug-delivery systems is not included. Finally, Chapter 11 describes examples of oral drug delivery using monolithic matrices for extended drug release.

This volume could serve as a source of information for the development of novel drug-delivery systems, not only for scientists working in academia but also for executives in charge of research and development in companies. Nevertheless, it probably will not be useful as a straightforward tool for the rational design of more advanced drug-delivery formulations by establishing structure–activity performance relationships. However, the reader seeking solutions to a specific practical problem that comes within the scope of the highly topical chapter titles will obtain a quick overview of the current state of knowledge and a concise description of the methods used. The value of the book will depend on whether the interests of the reader are as diverse as the contents.

Horacio Cabral
Graduate School of Medicine
University of Tokyo (Japan)



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Molecular Design

“A good book for teaching” was my impression when I first held in my hand the new book *Molecular Design: Concepts and Applications*, by Gisbert Schneider and Karl-Heinz Baringhaus. On 262 pages, the authors

introduce the reader to the complex field of creating novel molecules with desired biological effects. Molecular design is a highly interdisciplinary field, touching areas of science that range from medicine, pharmacology, chemistry, and biology to computational disciplines such as bioinformatics and chemoinformatics. There are several books available that deal with closely related topics such as molecular modeling and chemoinformatics applications, but books that aim to cover the whole process of molecular design for pharmaceutical applications are rare. Twelve years after the famous book *Wirkstoffdesign* by Böhm, Klebe, and

Kubinyi appeared, the time was ripe for a fresh look at this exciting field.

The first two chapters of the book deal with molecular objects, design objectives, and receptor–ligand interactions, which are the foundation of every molecular design project. The authors start where the story begins. The foundations of molecular design cannot be covered in depth by just these two chapters, but they are enough to introduce important concepts and terms dealing with molecular representations, properties, and interactions. Scientists working in the field of molecular design are well aware of how important it is to speak a common language. The introductory chapters are therefore important for everyone approaching the subject of molecular design.

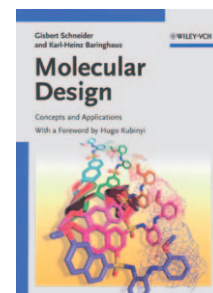
The next three chapters cover the main aspects of molecular design, starting with a look at the available data sources (Chapter 3). Proteins as drug targets and their chemical and geometrical properties are discussed, as well as small molecules and compound libraries. The authors are careful to achieve a good balance between the description of methods and that of their applications. Important aspects of molecular design such as the challenge presented by multiple binding modes are explained with the help of examples. Chapter 4 summarizes the virtual screening approach. Starting with fundamental questions such as the role of screening in drug design or the importance of library diversity, important virtual screening techniques such as shape-based and descriptor-based screening are described. Many examples and success stories are presented to illustrate the usefulness as well as the difficulties of virtual screening. It is a little surprising for the experienced reader that the important topic of structure-based virtual screening is not really covered. Lastly, Chapter 5 discusses methods for the optimization of pharmacologically important molecular properties that go beyond just achieving activity towards a particular target protein. The ADMET parameters are introduced, including examples of how to predict them by computer-based methods. With the help of introductory text boxes, the authors cover many aspects of this complex topic, including machine-based learning techniques, and describe practical examples.

After reading the book, it becomes increasingly clear that it is very difficult to summarize a highly interdisciplinary field like molecular design. The extent of previous knowledge, the interests, and the expectations of scientists entering the field of molecular design are as widely varied as the disciplines from which they come. Schneider and Baringhaus have done a pretty good job of writing an introductory textbook on molecular design. It should be seen as an appetizer that demonstrates the complexity of the problems but emphasizes the power of the methods already available today.

The book is not intended to be a complete reference source. Sometimes the assignment of topics to chapters seems a little inconsistent, as also does the varying depth of treatment. For example, a more complete description of the SMILES and SMARTS language in Chapter 1 would be really helpful for scientists who are mainly interested in applications, whereas a mathematical formulation of PCA and PLS is clearly beyond the scope of the book. However, as the collection of topics is generally well chosen, and many literature references are given, it is a very good starting point for entering the field. Compared to many multi-author compilations, the book is easy to read, because of the excellent writing style combined with many high-quality figures and numerous examples. Especially for chemists and biologists whose work brings them into contact with modelers and chemoinformatics specialists, this is an excellent book to gain a basic understanding of molecular design. And for teaching? For students who aim to specialize in bio- and chemoinformatics the level of methodological detail is probably too low. On the other hand, for including molecular design as a part of a life sciences course, it is certainly an excellent choice.

Matthias Rarey
Zentrum für Bioinformatik
Universität Hamburg

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