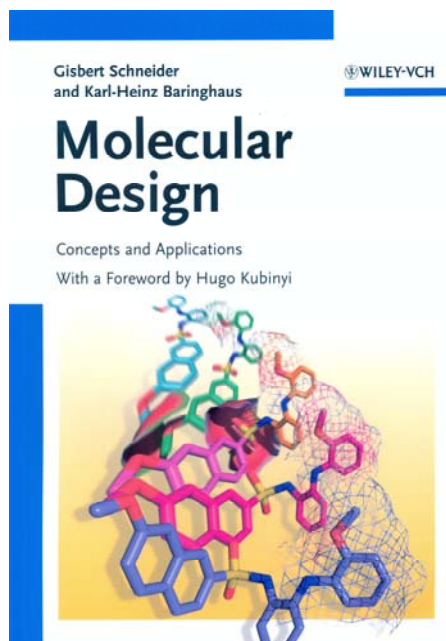


GISBERT SCHNEIDER AND KARL-HEINZ BARINGHAUS

# MOLECULAR DESIGN CONCEPTS AND APPLICATIONS



**John Wiley & Sons**  
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This first introductory-level textbook on molecular design is written with the first-time user in mind. Aimed at students and scientists alike, it provides computer-based methods to design and analyze drugs, enzyme inhibitors, probes and markers for biomolecules. Both authors are leading experts in the field with extensive practical experience. They provide insight into what can be achieved by computer-assisted design through proper modeling approaches.

The book guides the readers from basic principles to state-of-the-art techniques in virtual screening and molecular design with the help of carefully selected practical examples and case studies. The first two chapters present a basic introduction to molecular modeling. The following two chapters deal with computer-assisted design and screening while the final chapter concludes with design constraints and machine learning for lead finding and optimization.

The result is a textbook that places emphasis on design techniques and provides in-depth view on the subject which is equally suitable for teaching and self-learning.

## Table of Contents

Foreword  
Preface

### 1. Molecular Objects and Design Objectives

- 1.1. What is a Molecule?
- 1.2. Simplistic Molecular Representations
- 1.3. The Molecular Surface
- 1.4. Molecular Shape
- 1.5. The Topological Molecular Graph
- 1.6. Molecular Properties and Graph Invariants
- 1.7. The Drug-likeness Concept
- 1.8. Scaffolds, Linkers, and Side-chains
- 1.9. Substructure Similarity and "Privileged Motifs"
- 1.10. Molecules as Strings
- 1.11. Constructing Molecules from Strings
- 1.12. From Elements to Atom Types
- 1.13. Entering the Third Dimension: Automatic Conformer Generation
- 1.14. The "Bioactive" Conformation

### 2. Receptor–Ligand Interaction

- 2.1. The Thermodynamics of Protein–Ligand Interaction
- 2.2. The Entropic Contribution
- 2.3. From Theory to Experiment:  $K_i$  and  $IC_{50}$
- 2.4. QSAR: Estimating Quantitative Structure–Activity Relationships
- 2.5. Types of Receptor–Ligand Interaction
- 2.6. The "Biophore" Concept
- 2.7. Potential Pharmacophoric Points
- 2.8. The Correlation Vector Approach to Pharmacophore Modeling
- 2.9. "Hard Sphere" and "Fuzzy" Pharmacophore Models
- 2.10. Lessons from Automated Ligand Docking and Scoring: What Works and What Does Not
- 2.11. Fits Like a Glove: Alternative Ligand Binding Modes and Induced Fit Effects

### **3. Creating the Design**

- 3.1. Why We Need Computer-assisted Molecular Design
- 3.2. The Number of Drug Targets is Limited
- 3.3. Ligand Binding Sites
- 3.4. Ligand-based Design of Compound Libraries
- 3.5. Similar Compounds Do Not Necessarily Interact with Their Target in Similar Ways
- 3.6. The Same Ligand Can Adopt Multiple Binding Modes
- 3.7. GPCRs Represent a Challenging Target Family
- 3.8. Natural Products Are a Source of Inspiration
- 3.9. Transition State Analogs Are Potent Enzyme Inhibitors
- 3.10. New Targets Sometimes Require a New Ligand Design Concept
- 3.11. De novo Design Concepts
- 3.12. Primary and Secondary Constraints in de novo Design

### **4. Virtual Screening Triage**

- 4.1. The Drug Discovery Pipeline
- 4.2. High-throughput Screening (HTS): Why Is It Successful?
- 4.3. From Hit to Lead
- 4.4. Rationalizing the Design Process
- 4.5. From High to Low Diversity

- 4.6. Quantifying Diversity is Difficult
- 4.7. From Negative Design to Positive Design
- 4.8. Watch Out for Frequent Hitters!
- 4.9. Shape-matching: A Coarse-grained Filtering Step
- 4.10. The Ultimate Goal: Scaffold-hopping
- 4.11. Assessing Chemotype Diversity in Focused Libraries
- 4.12. It Works! Examples of Successful Scaffold-hops Found by Virtual Screening
- 4.13. Case Studies

### **5. Secondary Design Constraints and Machine Learning**

- 5.1. Physicochemistry and Pharmacokinetics
- 5.2. The "Rule of 5"
- 5.3. Pharmacokinetics
- 5.4. Absorption
- 5.5. Distribution
- 5.6. Metabolism
- 5.7. Elimination
- 5.8. Toxicity
- 5.9. Prodrugs and Bioisosteres
- 5.10. Machine Learning Methods Support Lead Finding and Optimization
- 5.11. An Important Step: Data Scaling
- 5.12. Application of Machine Learning to Compound Library Design
- 5.13. A "Pharmacophore Road Map"
- 5.14. Case Studies