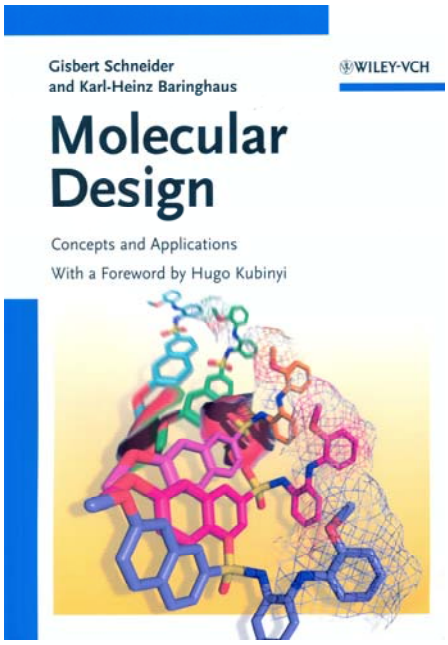
GISBERT SCHNEIDER AND KARL-HEINZ BARINGHAUS

MOLECULAR DESIGN
CONCEPTS AND APPLICATIONS



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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.

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