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MOLECULAR MODELING BASIC PRINCIPLES AND APPLICATIONS

H.-D. Höltje, W. Sippl, D. Rognan, WILEY-VCH

Molecular Modeling

Basic Principles and Applications

Third, Revised and Expanded Edition



Ideal for beginners, this book explains the basics of modeling in a competent yet easily understandable way. Following complete sections on the modeling of small molecules, protein modeling and chemogenomics, completely worked-out examples show the way to the reader's first modeling experiment.

This new, third edition features a new chapter on chemogenomics, reflecting the trend towards 'chemical biology', as well as the completely rewritten protein modeling example providing a better 'feel' of modeling complex biomolecules.

The authors are experienced university lecturers and as a result of their teaching practices the textbook provides teachers with a tried-and-tested learning material. The text is equally valuable to experts since it offers an evaluation of the strengths and limitations of the molecular modeling techniques and the software currently available.

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