



Molecular Modeling

Hans-Dieter Höltje, Wolfgang Sippl, Didier Rognan, Gerd Folkers

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Written by experienced experts in the field, this book describes the basics to the extent necessary for reliably judging the results from molecular modeling calculations.

Without unnecessary overhead, it leads readers from simple calculations on small molecules to the modeling of proteins and other relevant biomolecules. Beginners are guided through their first modeling experiment, while routine users of modeling software are provided with invaluable troubleshooting hints. A unique resource for students, researchers and lecturers, now available in this all-new, enlarged edition.

"If the currently popular 'Dummies' series of computer books were to publish a volume on molecular modeling this would be it" (Journal of the American Chemical Society)

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