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Molecular Modelling - Imperial College London

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cal examples, applications,and exercises.For a computationalchemist, scientist, or researcher,this bookwill be highlyusefulin understandingandmasteringthe artof chemical computation. Familiarization with common and commercial software in molecular modeling is also incorporated.Moreover,the application of the concepts

Molecular modelling: principles and applications | Andrew ...

Molecular Modelling. Principles and Applications, A. R. Leach, Longman, 1996.

ISBN 0-582-23933-8; Introduction to Computational Chemistry, by Frank Jensen, Wiley, 1999 (ISBN 0-471-98425-6).

Introduction to Theoretical Organic Chemistry and Molecular Modellingby William B. Smith. ISBN:

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Molecular Modeling | Methods and Principles in Medicinal ...

Hans-Dieter H ö ltje is director of the Institute of Pharmaceutical Chemistry at the Heinrich-Heine-Universit ä t D ü sseldorf, where he also holds the chair of Medicinal Chemistry. His main interest is the molecular mechanism of drug action. He is especially interested in modeling G-Protein-Coupled receptors, cytochromes, enzymes of therapeutic importance and phospholipid membranes.

Molecular Modeling: Principles and Applications 2nd ...

The book will also be useful to researchers in academia and in the pharmaceutical and chemical industries and to those teaching or attending courses in molecular modelling.

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This new edition provides background theory in the techniques of molecular modelling, illustrated with applications from the physical, chemical and biological sciences.

Molecular Modeling: Basic Principles and Applications | Wiley

Molecular modelling encompasses all methods, theoretical and computational, used to model or mimic the behaviour of molecules. The methods are used in the fields of computational chemistry, drug design, computational biology and materials science to study molecular systems ranging from small chemical systems to large biological molecules and material assemblies.

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