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Hans-Dieter Höltje is director of the Institute of Pharmaceutical Chemistry at the Heinrich-Heine-Universität Düsseldorf, 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 Modelling - Imperial College London

Molecular Modeling Applications The starting point for many computer assisted molecular modeling studies is generally a two-dimensional drawing of a required molecule. These diagrams can range from note-book sketches to electronically stored connection tables in which one defines the types of atoms in the molecule, their hybridization and how they are bonded to each other.

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Molecular Modelling Principles And Applications

Molecular modelling: principles and applications Andrew Leach Preface to the Second Edition The impetus for this second edition is a desire to include some of the new techniques that have emerged in recent years and also extend the scope of the book to cover certain areas that were under-represented (even neglected) in the first edition.

Molecular Modelling: Principles and Applications: Leach ...

Molecular Modeling: Principles and Applications By Andrew R. Leach. Addison Wesley Longman Limited: Essex, England, 1996. 595 pp. ISBN 0-582-23933-8. \$35

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cal examples, applications, and exercises. For a computational chemist, scientist, or researcher, this book will be highly useful in understanding and mastering the art of chemical computation. Familiarization with common and commercial software in molecular modeling is also incorporated. Moreover, the application of the concepts

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