



Computer Aided Molecular Design

Jean-Pierre Doucet, Jacques Weber



Computer Aided Molecular Design:

Computer-Aided Molecular Design Jean-Pierre Doucet, Jacques Weber, 1996-03-05 The computer aided design of novel molecular systems has undoubtedly reached the stage of a mature discipline offering a broad range of tools available to virtually any chemist However there are few books covering most of these techniques in a single volume and using a language which may generally be understood by students or chemists with a limited knowledge of theoretical chemistry The purpose of this book is precisely to review in such a language both methodological aspects and important applications of computer aided molecular design CAMD with a special emphasis on drug design and protein modeling Using numerous examples ranging from molecular models to shapes surfaces and volumes Computer Aided Molecular Design provides coverage of the role molecular graphics play in CAMD The text also treats the very notion of the structure of molecular systems by presenting both the various experimental techniques giving access to it and the most common model builders based on force fields Separate chapters are devoted to other important topics in CAMD such as Monte Carlo and molecular dynamics simulations most common quantum chemical methods derivation and visualization of molecular properties and molecular similarity Finally strategies used in protein modeling and drug design such as receptor mapping and the pharmacophore approach are presented and illustrated by several examples The book is addressed to students and researchers who wish to enter this new exciting field of molecular sciences but also practitioners in CAMD as a comprehensive source of refreshing information in their field Key Features Presents a comprehensive introduction to computer aided molecular design Describes applications of CAMD through the use of numerous examples Emphasizes strategies used in protein modeling and drug design Includes separate chapters devoted to other important topics in CAMD such as Monte Carlo and molecular dynamics simulations Common quantum chemical methods Derivation and visualization of molecular properties Molecular similarity

Computer Aided Molecular Design Luke Achenie, Venkat Venkatasubramanian, Rafiqul Gani, 2002-11-20 CAMD or Computer Aided Molecular Design refers to the design of molecules with desirable properties That is through CAMD one determines molecules that match a specified set of target properties CAMD as a technique has a very large potential as in principle all kinds of chemical bio chemical and material products can be designed through this technique This book mainly deals with macroscopic properties and therefore does not cover molecular design of large complex chemicals such as drugs While books have been written on computer aided molecular design relating to drugs and large complex chemicals a book on systematic formulation of CAMD problems and solutions with emphasis on theory and practice which helps one to learn understand and apply the technique is currently unavailable This title brings together the theoretical aspects related to Computer Aided Molecular Design the different techniques that have been developed and the different applications that have been reported Contributing authors are among the leading researchers and users of CAMD First book available giving a systematic formulation of CAMD problems and solutions

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Developed from a symposium sponsored by the Division of Computers in Chemistry and the Division of Agrochemicals at the 207th National Meeting of the American Chemical Society San Diego California March 13 17 1994 Computer Aided Molecular Design David M. Ricketts, 1986 *Computer Aided Molecular Design with Combined Molecular Modeling and Group Contribution* Peter M. Harper, Rafiqul Gani, Petr Kolar, American Institute of Chemical Engineers, American Institute of Chemical Engineers. Annual Meeting, 1998 *Journal of Computer-aided Molecular Design*, 1987 *Molecular Docking for Computer-Aided Drug Design* Mohane S. Coumar, 2021-02-18 Molecular Docking for Computer Aided Drug Design
Fundamentals Techniques Resources and Applications offers in depth coverage on the use of molecular docking for drug design The book is divided into three main sections that cover basic techniques tools web servers and applications It is an essential reference for students and researchers involved in drug design and discovery *Computer Aided Molecular Design* David M. Ricketts, 1986 **Handbook of Chemoinformatics Algorithms** Jean-Loup Faulon, Andreas Bender, 2010-04-21 Unlike in the related area of bioinformatics few books currently exist that document the techniques tools and algorithms of chemoinformatics Bringing together worldwide experts in the field the Handbook of Chemoinformatics Algorithms provides an overview of the most common chemoinformatics algorithms in a single source After a historical perspective
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Current Trends in Computer Aided Molecular Design Luke E. K. Achenie,Manish

Sinha,American Institute of Chemical Engineers,1999

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