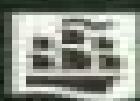


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MOLECULAR MODELLING PRINCIPLES AND APPLICATIONS



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Computational Chemistry and Molecular Modeling K. I. Ramachandran, Gopakumar Deepa, Krishnan Namboori, 2008-05-20 Computational chemistry and molecular modeling is a fast emerging area which is used for the modeling and simulation of small chemical and biological systems in order to understand and predict their behavior at the molecular level. It has a wide range of applications in various disciplines of engineering sciences such as materials science, chemical engineering, biomedical engineering, etc. Knowledge of computational chemistry is essential to understand the behavior of nanosystems; it is probably the easiest route or gateway to the fast growing discipline of nanosciences and nanotechnology which covers many areas of research dealing with objects that are measured in nanometers and which is expected to revolutionize the industrial sector in the coming decades. Considering the importance of this discipline computational chemistry is being taught presently as a course at the postgraduate and research level in many universities. This book is the result of the need for a comprehensive textbook on the subject which was felt by the authors while teaching the course. It covers all the aspects of computational chemistry required for a course with sufficient illustrations, numerical 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 in related fields such as biomedical engineering, computational drug designing, etc., has been added. *Molecular Modeling* Hans-Dieter Höltje, 2003

Conceptual Density Functional Theory and Its Application in the Chemical Domain Nazmul Islam, Savas Kaya, 2018-06-13 In this book, new developments based on conceptual density functional theory (CDFT) and its applications in chemistry are discussed. It also includes discussion of some applications in corrosion and conductivity and synthesis studies based on CDFT. The electronic structure principles such as the electronegativity equalization principle, the hardness equalization principle, the electrophilicity equalization principle, and the nucleophilicity equalization principle along with studies based on these electronic structure principles are broadly explained. In recent years, some novel methodologies have

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Martín-Santamaría,2017-10-25 The rapid development of efficient computational tools has allowed researchers to tackle biological problems and to predict analyse and monitor at an atomic level molecular recognition processes This book offers a fresh perspective on how computational tools can aid the chemical biology research community and drive new research Chapters from internationally renowned leaders in the field introduce concepts and discuss the impact of technological advances in computer hardware and software in explaining and predicting phenomena involving biomolecules from small molecules to macromolecular systems Important topics from the understanding of biomolecules to the modification of their functions are addressed as well as examples of the application of tools in drug discovery glycobiology protein design and molecular recognition Not only are the cutting the edge methods addressed but also their limitations and possible future development For anyone wishing to learn how computational chemistry and molecular modelling can provide information not easily accessible through other experimental methods this book will be a valuable resource It will be of interest to postgraduates and researchers in the biological and chemical sciences medicinal and pharmaceutical chemistry and theoretical chemistry

Chemical Applications of Molecular Modelling Jonathan M. Goodman,1998

This book explores the molecular modeling enabling the nonspecialist to appreciate the power as well as the limitations of the computational tools available and giving a background to the methods used and how they were developed It also provides examples of how molecular modeling has been used to address chemical questions commonly asked by the experimental chemist and includes practical examples and case studies 143 illus

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Molecular Modelling for Beginners Alan Hinchliffe,2005-12-17

Presenting a concise basic introduction to modelling and computational chemistry this text includes relevant introductory material to ensure greater accessibility to the subject Provides a comprehensive introduction to this evolving and developing field Focuses on MM MC and MD with an entire chapter devoted to QSAR and Discovery Chemistry Includes many real chemical applications combined with worked problems and solutions provided in each chapter Ensures that up to date treatment of a variety of chemical modeling techniques are introduced

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BOOK JACKET Methods for Molecular Interactions and Large-scale Simulations Byoungseon Jeon,2008 **Chemistry and Industry** ,2012

Fundamental Principles of Molecular Modeling Anton Amann,Jan C.A. Boeyens,W. Gans,2013-06-29 Molecular similarity has always been an important conceptual tool of chemists yet systematic approaches to molecular similarity problems have only recently been recognized as a major contributor to our understanding of molecular properties Advanced approaches to molecular similarity analysis have their foundation in quantum similarity measures and are important direct or indirect contributors to some of the predictive theoretical computational and also experimental methods of modern chemistry This volume provides a survey of the foundations and the contemporary mathematical and computational methodologies of molecular similarity approaches where special emphasis is given to applications of similarity studies to a range of practical and industrially significant fields such as pharmaceutical drug design The authors of individual chapters are leading experts in various sub fields of molecular similarity analysis and the related fundamental theoretical chemistry topics as well as the relevant computational and experimental methodologies Whereas in each chapter the emphasis is placed on a different area nevertheless the overall coverage and the wide scope of the book provides the reader with a general yet sufficiently detailed description that may serve as a good starting point for new studies and applications of molecular similarity approaches The editors of this volume are grateful to the authors for their contributions and hope that the readers will find this book a useful and motivating source of information in the rapidly growing field of molecular similarity analysis

Macromolecules, Volume 3 Hans-Georg Elias,2005 Providing a broad survey of the entire field Macromolecules integrates representations of chemistry physics and technology as well as including precise descriptions of basic phenomena and balanced treatments of facts and theory

QSAR and Molecular Modeling Studies in Heterocyclic Drugs II S.P. Gupta,2006-06-22

Computational Evaluation of Noncovalent Interactions in Biomimetic Polymers and Small Molecules Laurie

Anne Christianson,1997 *Journal of the Physical Society of Japan* Nihon Butsuri Gakkai,2011 *Computer Aided Design of Selective Cytochrome P450 Inhibitors* Andreas Verras,2005 I have generated a virtual library of imidazole based compounds and used an altered form of the DOCK algorithm CovDOCK to screen these compounds against heme containing proteins I was able to generate high affinity ligands for P450cam An L244A mutant of P450cam was generated and used to test our ability to generate selective ligands Using our methods I was able to generate ligands which only inhibit the mutant enzyme The library was expanded with more substituted imidazoles and screened against a viable drug target *Mycobacterium tuberculosis* CYP51 After one round of compound development I was able to find micromolar inhibitors I also demonstrated that the methods and library are easily applicable to new protein systems To explore differences of the imidazole compounds in binding and inhibition I carried out stopped flow kinetics experiments and further UV spectroscopic studies I find that mono and disubstituted imidazoles bind distinctly to wild type P450cam The natural substrate also affects both classes of ligands uniquely To explore the mitigated affinity for imidazole of the L244A mutant I have done crystallography studies I report the structures of the substrate free mutant and imidazole co crystallized wild type and mutant proteins I present a possible explanation for the mitigated imidazole affinity based on structural factors observed when juxtaposing the wild type and mutant structures *Calculating Precise and Accurate Free Energies in Biomolecular Systems* Michael R. Shirts,2004

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