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Crystallographic and Modeling Methods in Molecular Design



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Crystallographic And Modeling Methods In Molecular Design

Charles W. Carter, Robert M. Sweet



Crystallographic And Modeling Methods In Molecular Design:

Crystallographic and Modeling Methods in Molecular Design Charles E. Bugg, Steven E. Ealick, 2013-11-11 This book contains the papers that were presented at the Crystallographic and Modeling Methods in Molecular Design Symposium in Gulf Shores Alabama April 30 to May 3 1989 During the past few years there has been a burst of activity in this area especially related to drug design and protein engineering projects The purpose of the symposium and this book is to provide an up to date review of the most recent experimental and theoretical approaches that are being used for molecular design The book covers several recent examples of approaches for using crystallography in conjunction with forefront modeling methods for guiding the development of enzyme inhibitors and of peptides and proteins with modified biological and physical properties In addition this book contains discussions of new approaches for combining crystallographic data and advanced computational techniques for aiding in the design of enzyme inhibitors and other compounds that bind to selected biological targets This book is therefore of interest not only to molecular biologists and biochemists but is stimulating reading for anyone involved in structural biology pharmaceutical chemistry enzymology protein engineering and biotechnology The meeting was the third in a series of symposia initiated and sponsored by the Department of Biochemistry University of Alabama at Birmingham

Reviews in Computational Chemistry, Volume 17 Kenny B. Lipkowitz, Donald B. Boyd, 2003-04-24 Computational chemistry is increasingly used in most areas of molecular science including organic inorganic medicinal biological physical and analytical chemistry Researchers in these fields who do molecular modelling need to understand and stay current with recent developments This volume like those prior to it features chapters by experts in various fields of computational chemistry Two chapters focus on molecular docking one of which relates to drug discovery and cheminformatics and the other to proteomics In addition this volume contains tutorials on spin orbit coupling and cellular automata modeling as well as an extensive bibliography of computational chemistry books FROM REVIEWS OF THE SERIES Reviews in Computational Chemistry remains the most valuable reference to methods and techniques in computational chemistry JOURNAL OF MOLECULAR GRAPHICS AND MODELLING One cannot generally do better than to try to find an appropriate article in the highly successful Reviews in Computational Chemistry The basic philosophy of the editors seems to be to help the authors produce chapters that are complete accurate clear and accessible to experimentalists in particular and other nonspecialists in general JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Visualization of Receptors Gerard Morel, 1997-02-26 A multiplicity of methods for visualization are described in Visualization of Receptors This book of techniques covers immunocytology radioautography in situ hybridization plasmon resonance RT in vitro PCR and X ray crystal structure analysis Lecturers researchers practitioners technicians and students will find all the principles and protocols they require and the means of implementing them Topics discussed include localization of ligands in vitro or in vivo visualization of immunoreactivities of ligand and receptor proteins detection and quantification of mRNA expression

amplification of signals and determination of 3 D structure Details of protocols with illustrations of results and commentaries are provided throughout the book

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

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Physics Briefs, 1994

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Methodologies to Anticipate and Incorporate Protein Mutation in the INVENTON Molecular Invention System Michael Anthony Kappler, 1999

Synchrotron Radiation in the Biosciences Britton Chance, 1994 This book represents the edited proceedings of the 4th International Conference on Biophysics and Synchrotron Radiation held in Tsukuba Japan in 1992 It discusses advances in the application of synchrotron radiation to biophysics and medicine The papers have been selected by a distinguished international board after refereeing and edited for publication It discusses advances in the application of synchrotron radiation to biophysics and medicine of interest to researchers from many diverse fields Just a few of the topics covered are filamentous viruses angiography and solution X ray scattering

Protein Architecture Arthur M. Lesk, 1991

Modern computer graphics transforms protein structures into visually exciting images Protein Architecture A Practical Approach shows the reader how to visualize protein structures and how to design an illustration to help understand and appreciate the variety of protein folding patterns *Artificial Intelligence and Molecular Biology* Lawrence Hunter,1993 These original contributions provide a current sampling of AI approaches to problems of biological significance they are the first to treat the computational needs of the biology community hand in hand with appropriate advances in artificial intelligence The enormous amount of data generated by the Human Genome Project and other large scale biological research has created a rich and challenging domain for research in artificial intelligence These original contributions provide a current sampling of AI approaches to problems of biological significance they are the first to treat the computational needs of the biology community hand in hand with appropriate advances in artificial intelligence Focusing on novel technologies and approaches rather than on proven applications they cover genetic sequence analysis protein structure representation and prediction automated data analysis aids and simulation of biological systems A brief introductory primer on molecular biology and AI gives computer scientists sufficient background to understand much of the biology discussed in the book Lawrence Hunter is Director of the Machine Learning Project at the National Library of Medicine National Institutes of Health

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ES arrow right TI 1 We propose that upon deprotonation of His57 Ser195 undergoes a conformational change that is responsible for preventing the TI 1 arrow right ES back reaction Based on precise atomic positions obtained at sub ngstrom resolution we have concluded that the His57 Asp102 interaction is a standard ionic hydrogen bond in both the free enzyme and the acylation transition state and not a low barrier hydrogen bond as had been previously debated Instead I propose that transition state stabilization by chymotrypsin like serine proteases is achieved through a network of optimized hydrogen bonds that position the catalytic triad and stabilize the Ser195 substrate tetrahedral adduct In particular I identified a short ionic hydrogen bond between His57 and the amide of the substrate leaving group that may play the primary role in catalyzing the second step of the acylation reaction A surprising outcome from these studies was the discovery of a site of conformational strain that appears to be evolutionarily linked to alpha LP s kinetic stability Distortion of Phe228 a conserved residue in the protein core is estimated to account for 4 kcal mol in conformational energy The rearrangement and subsequent distortion of Phe228 by co evolved residues surrounding it supports the hypothesis that tight packing in alpha LP is a key component of alpha LP s folding energy landscape Subsequent mutational studies support this hypothesis confirming our discovery of the first known functionally relevant distortion

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