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pattern

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the
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density function

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structural model

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model

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Structures And Structure Determination

Hellmut G. Karge, Jens Weitkamp

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Structure Determination by X-Ray Crystallography Mark F.C. Ladd, Rex A. Palmer, 1994-04-30 This warmly received third edition is now available in an inexpensive softcover

Structure Determination from Powder Diffraction Data W. I. F. David, K. Shankland, L. B. McCusker, Ch. Baerlocher, 2006-08-03 The art of solving a structure from powder diffraction data has developed rapidly over the last ten years to the point where numerous crystal structures both organic and inorganic have been solved directly from powder data However it is still an art and in contrast to its single crystal equivalent is far from routine The art lies not only in the correct application of a specific experimental technique or computer program but also in the selection of the optimal path for the problem at hand Written and edited by experts active in the field and covering both the fundamental and applied aspects of structure solution from powder diffraction data this book guides both novices and experienced practitioners alike through the maze of possibilities

Algorithms in Structural Molecular Biology Bruce R. Donald, 2011-06-01 An overview of algorithms important to computational structural biology that addresses such topics as NMR and design and analysis of proteins Using the tools of information technology to understand the molecular machinery of the cell offers both challenges and opportunities to computational scientists Over the past decade novel algorithms have been developed both for analyzing biological data and for synthetic biology problems such as protein engineering This book explains the algorithmic

foundations and computational approaches underlying areas of structural biology including NMR nuclear magnetic resonance X ray crystallography and the design and analysis of proteins peptides and small molecules Each chapter offers a concise overview of important concepts focusing on a key topic in the field Four chapters offer a short course in algorithmic and computational issues related to NMR structural biology giving the reader a useful toolkit with which to approach the fascinating yet thorny computational problems in this area A recurrent theme is understanding the interplay between biophysical experiments and computational algorithms The text emphasizes the mathematical foundations of structural biology while maintaining a balance between algorithms and a nuanced understanding of experimental data Three emerging areas particularly fertile ground for research students are highlighted NMR methodology design of proteins and other molecules and the modeling of protein flexibility The next generation of computational structural biologists will need training in geometric algorithms provably good approximation algorithms scientific computation and an array of techniques for handling noise and uncertainty in combinatorial geometry and computational biophysics This book is an essential guide for young scientists on their way to research success in this exciting field

The Next Generation in Membrane Protein Structure Determination Isabel Moraes, 2016-08-23 This book reviews current techniques used in membrane protein structural biology with a strong focus on practical issues The study of membrane protein structures not only provides a basic understanding of life at the molecular level but also helps in the rational and targeted design of new drugs with reduced side effects Today about 60% of the commercially available drugs target membrane proteins and it is estimated that nearly 30% of proteins encoded in the human genome are membrane proteins In recent years much effort has been put towards innovative developments to overcome the numerous obstacles associated with the structure determination of membrane proteins This book reviews a variety of recent techniques that are essential to any modern researcher in the field of membrane protein structural biology The topics that are discussed are not commonly found in textbooks The scope of this book includes Expression screening using fluorescent proteins The use of detergents in membrane protein research The use of NMR Synchrotron developments in membrane protein structural biology Visualisation and X ray data collection of microcrystals X ray diffraction data analysis from multiple crystals Serial millisecond crystallography Serial femtosecond crystallography Membrane protein structures in drug discovery The information provided in this book should be of interest to anyone working in the area of structural biology Students will find carefully prepared overviews of basic ideas and advanced protein scientists will find the level of detail required to apply the material directly to their day to day work Chapters 4 5 6 8 and 9 of this book are published open access under a CC BY 4 0 license at link.springer.com

Bioactive Natural Products Detection, Isolation, and Structural Determination Steven M. Colegate, Russell J. Molyneux, 1993-09-29 Bioactive Natural Products covers all the aspects of bioactive natural product research from ethnobotanical investigations to modern technologically assisted isolation and structural determination of active compounds An internationally selected group of experts share their

knowledge of a wide range of bioactivities and chemical compound classes Topics in the chapters describing the modern application of detection isolation and structural determination techniques are strongly supported by chapters detailing and reviewing research involving various classes of bioactivity Research areas include the immunomodulatory antiviral cytotoxic anti inflammatory and insect behavior classes of bioactivity Extensive referencing throughout the text is helpful to those readers not familiar with this subject and serves as a critical review for more experienced researchers The book is also excellent for upper division or post graduate courses

Structure-based Study of Viral Replication R. Holland

Cheng,Tatsuo Miyamura,2008 This book addresses the innovative themes in characterizing the cellular membrane platforms and intracellular networking as well as the architectural aspects of cell compartments mediated by the entry and replication cycles of viruses The instrumentation of modern molecular and cellular biology provides a potent array of wave packets to image detect and manipulate major dynamics of macromolecular and subviral assemblies as in the host cellular context The book includes case studies presented with highly coherent and structured illuminations including microscopy spectroscopy and scanning probes The compilation and integration of the methodology provides time resolved observations on the reactivity of structures from near atomic resolution to various molecular or cellular levels of descriptors The book provides a broad introduction to the various fascinating virus systems and may be used as an advanced textbook by graduate students in biomedicine It provides adequate background material to explore further the research problems of epidemics in the 21st century

Genomics and Proteomics Sándor Suhai,2007-05-08 Genome research will certainly be one of the most important and exciting scientific disciplines of the 21st century Deciphering the structure of the human genome as well as that of several model organisms is the key to our understanding how genes function in health and disease With the combined development of innovative tools resources scientific know how and an overall functional genomic strategy the origins of human and other organisms genetic diseases can be traced Scientific research groups and developmental departments of several major pharmaceutical and biotechnological companies are using new innovative strategies to unravel how genes function elucidating the gene protein product understanding how genes interact with others both in health and in the disease state Presently the impact of the applications of genome research on our society in medicine agriculture and nutrition will be comparable only to that of communication technologies In fact computational methods including networking have been playing a substantial role even in genomics and proteomics from the beginning We can observe however a fundamental change of the paradigm in life sciences these days research focused until now mostly on the study of single processes related to a few genes or gene products but due to technical developments of the last years we can now potentially identify and analyze all genes and gene products of an organism and clarify their role in the network of life processes

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