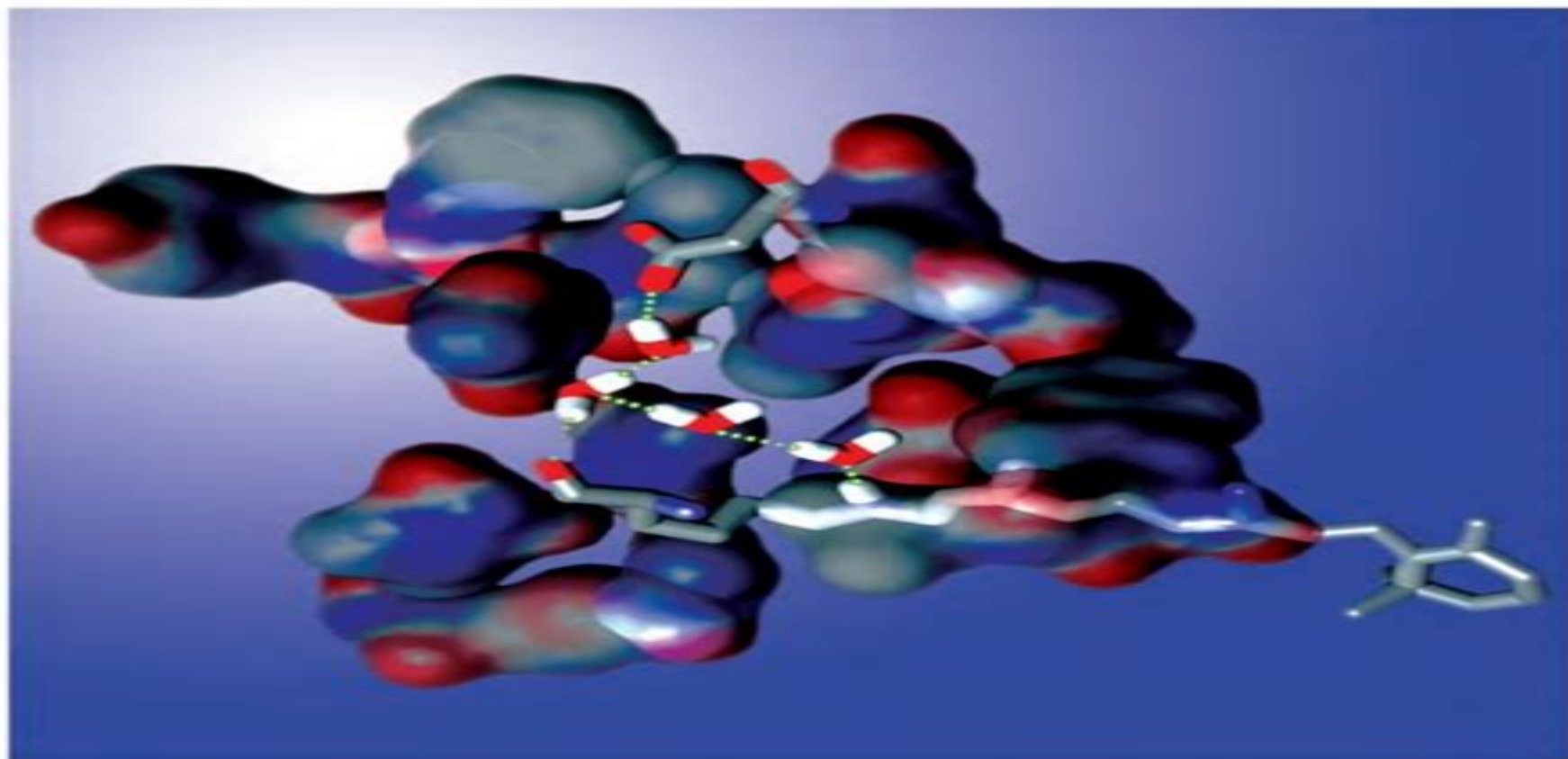


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Biophysical and Structural Aspects of Bioenergetics



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Biophysical And Structural Aspects Of Bioenergetics

**Reinhard Grisshammer, Susan K
Buchanan**



Biophysical And Structural Aspects Of Bioenergetics:

Biophysical and Structural Aspects of Bioenergetics Mårten Wikström, 2007-10-31 Bioenergetics is a term used to describe the events of primary energy transduction in biology. The field has seen tremendous advances in recent years thanks to developments in the biophysical and computational techniques used to solve the three dimensional structures of the membrane bound proteins which often act as catalysts in these reactions. This has enabled researchers to bring otherwise static structures to life and decipher the dynamic function of these intriguing systems. *Biophysical and Structural Aspects of Bioenergetics* brings together contributions from internationally respected experts all of whom helped shape and develop the field of bioenergetics. It provides a representative snapshot of the very latest key developments in this multidisciplinary subject with an emphasis on molecular structure and how this changes during the bioenergetic function. Offering a comprehensive overview of the current state of the art and complete with extensive citations in each chapter, this book is the ideal reference for both biochemists and biophysicists studying this fascinating topic.

The Purple Phototrophic Bacteria C.N. Hunter, Fevzi Daldal, Marion C. Thurnauer, J. Thomas Beatty, 2008-10-11 Here is a comprehensive survey of all aspects of these fascinating bacteria, metabolically the most versatile organisms on Earth. It compiles 48 chapters written by leading experts who highlight the huge progress made in studies of these bacteria since 1995.

Comprehensive Biophysics, 2012-04-12 Biophysics is a rapidly evolving interdisciplinary science that applies theories and methods of the physical sciences to questions of biology. Biophysics encompasses many disciplines including physics, chemistry, mathematics, biology, biochemistry, medicine, pharmacology, physiology, and neuroscience, and it is essential that scientists working in these varied fields are able to understand each other's research. *Comprehensive Biophysics Nine Volume Set* will help bridge that communication gap. Written by a team of researchers at the forefront of their respective fields under the guidance of Chief Editor Edward Egelman, *Comprehensive Biophysics Nine Volume Set* provides definitive introductions to a broad array of topics uniting different areas of biophysics research from the physical techniques for studying macromolecular structure to protein folding, muscle and molecular motors, cell biophysics, bioenergetics, and more. The result is this comprehensive scientific resource, a valuable tool both for helping researchers come to grips quickly with material from related biophysics fields outside their areas of expertise and for reinforcing their existing knowledge. Biophysical research today encompasses many areas of biology. These studies do not necessarily share a unique identifying factor. This work unites the different areas of research and allows users regardless of their background to navigate through the most essential concepts with ease, saving them time and vastly improving their understanding. The field of biophysics counts several journals that are directly and indirectly concerned with the field. There is no reference work that encompasses the entire field and unites the different areas of research through deep foundational reviews. *Comprehensive Biophysics* fills this vacuum, being a definitive work on biophysics. It will help users apply context to the diverse journal literature, offering aid in identifying areas for

further research Chief Editor Edward Egelman E I C Biophysical Journal has assembled an impressive world class team of Volume Editors and Contributing Authors Each chapter has been painstakingly reviewed and checked for consistent high quality The result is an authoritative overview which ties the literature together and provides the user with a reliable background information and citation resource

Structural Biology of Membrane Proteins Reinhard

Grisshammer, Susan K Buchanan, 2007-10-31 In the last few years there have been many exciting and innovative developments in the field of membrane protein structure and this trend is set to continue Structural Biology of Membrane Proteins is a new monograph covering a wide range of topics with contributions from leading experts in the field The book is split into three sections the first discusses topics such as expression purification and crystallisation the second covers characterisation techniques and the final section looks at new protein structures The book will hence have wide appeal to researchers working in and around the field and provide an up to date reference source Introductory sections to each topic are accompanied by more detailed discussions for the more experienced biochemist Detailed descriptions of experimental methods are included to demonstrate practical approaches to membrane protein structure projects The book also offers an up to date reference source in addition to descriptions of new and emerging developments including state of the art techniques for solving membrane protein structures Structural Biology of Membrane Proteins encompasses both basic introductions and detailed descriptions of themes and should appeal to a wide range of biochemical scientists both experienced and beginner

Computational and Structural Approaches to Drug Discovery Robert M. Stroud, Janet

Finer-Moore, 2008 1 Facing the Wall in Computationally Based Approaches to Drug Discovery Janet S Finer Moore and Jeff Blaney and Robert M Stroud 2 The Changing Landscape in Drug Discovery Hugo Kubinyi 3 Purine Nucleoside Phosphorylase Yang Zhang and Steven E Ealick 4 Application and Limitations of X Ray Crystallographic Data in Structure Guided Ligand and Drug Design Andrew M Davis and Simon J Teague and Gerard J Kleywegt 5 Dealing with Bound Waters in a Site Do they Leave or Stay Donald Hamelberg and J Andrew McCammon 6 Knowledge Based Methods in Structure Based Design Marcel L Verdonk and Wijnand T M Mooij 7 Combating Drug Resistance Identifying Resilient Molecular Targets and Robust Drugs Celia A Schiffer 8 Docking Algorithms and Scoring Functions State of the Art and Current Limitations Gregory L Warren and Catherine E Peishoff and Martha S Head 9 Application of Docking Methods to Structure Based Drug Design Demetri T Moustakas 10 Strength in Flexibility Modeling Side Chain Conformational Change in Docking and Screening Leslie A Kuhn 11 Avoiding the Rigid Receptor Side Chain Rotamers Amy C Anderson 12 Computational Prediction of Aqueous Solubility Oral Bioavailability P450 Activity and hERG Channel Blockade David E Clark 13 Shadows on Screens Brian K Shoichet and Brian Y Feng and Kristin E D Coan 14 Iterative Docking Strategies for Virtual Ligand Screening Albert E Beuscher IV and Arthur J Olson 15 Challenges and Progresses in Calculations of Binding Free Energies What Does it Take to Quantify Electrostatic Contributions to Protein Ligand Interactions Mitsunori Kato and Sonja Braun Sand and Arie Warshel 16

Discovery and Extrapolation of Fragment Structures towards Drug Design Alessio Ciulli and Tom L Blundell and Chris Abell 17 A Link Means a Lot Disulfide Tethering in Structure Based Drug Design Jeanne A Hardy 18 The Impact of Protein Kinase Structures on Drug Discovery Chao Zhang and Sung Hou Kim *Innovations in Biomolecular Modeling and Simulations* Tamar Schlick, 2012 The chemical and biological sciences face unprecedented opportunities in the 21st century A confluence of factors from parallel universes advances in experimental techniques in biomolecular structure determination progress in theoretical modeling and simulation for large biological systems and breakthroughs in computer technology has opened new avenues of opportunity as never before Now experimental data can be interpreted and further analysed by modeling and predictions from any approach can be tested and advanced through companion methodologies and technologies This two volume set describes innovations in biomolecular modeling and simulation in both the algorithmic and application fronts With contributions from experts in the field the books describe progress and innovation in areas including simulation algorithms for dynamics and enhanced configurational sampling force field development implicit solvation models coarse grained models quantum mechanical simulations protein folding DNA polymerase mechanisms nucleic acid complexes and simulations RNA structure analysis and design and other important topics in structural biology modeling The books are aimed at graduate students and experts in structural biology and chemistry and the emphasis is on reporting innovative new approaches rather than providing comprehensive reviews on each subject **Recent Developments in Biomolecular NMR** Marius Clore, Jennifer Potts, 2012 NMR spectroscopy is widely used in biomolecular science particularly for structure determination of proteins nucleic acids and carbohydrates Much of the innovation within NMR spectroscopy has been within the field of protein NMR spectroscopy an important technique in structural biology Filling a gap in the literature this book draws together experts in the field to discuss the real advances in NMR methods that have occurred or have an impact on the biomolecular field in the last few years The coverage includes recent developments in using NMR for determination of protein structures membrane proteins the dynamics of RNA and advances in NMR in drug discovery Edited by leading biological NMR spectroscopists the book is essential reference for researchers in industry and academia interested in or joining this bioanalytical field **Molecular Simulations and Biomembranes** Mark S. P. Sansom, Philip Charles Biggin, 2010 The need for information in the understanding of membrane systems has been caused by three things an increase in computer power methodological developments and the recent expansion in the number of researchers working on it worldwide However there has been no up to date book that covers the application of simulation methods to membrane systems directly and this book fills an important void in the market It provides a much needed update on the current methods and applications as well as highlighting recent advances in the way computer simulation can be applied to the field of membranes and membrane proteins The objectives are to show how simulation methods can provide an important contribution to the understanding of these systems The scope of the book is such that it covers simulation of membranes and

membrane proteins but also covers the more recent methodological developments such as coarse grained molecular dynamics and multiscale approaches in systems biology Applications embrace a range of biological processes including ion channel and transport proteins The book is wide ranging with broad coverage and a strong coupling to experimental results wherever possible including colour illustrations to highlight particular aspects of molecular structure With an internationally respected list of authors its publication is timely and it will prove indispensable to a large scientific readership

Structure-Based Drug Discovery Roderick E Hubbard, 2007-10-31 Structure based drug discovery is a collection of methods that exploits the ability to determine and analyse the three dimensional structure of biological molecules These methods have been adopted and enhanced to improve the speed and quality of discovery of new drug candidates After an introductory overview of the principles and application of structure based methods in drug discovery this book then describes the essential features of the various methods Chapters on X ray crystallography NMR spectroscopy and computational chemistry and molecular modelling describe how these particular techniques have been enhanced to support rational drug discovery with discussions on developments such as high throughput structure determination probing protein ligand interactions by NMR spectroscopy virtual screening and fragment based drug discovery The concluding chapters complement the overview of methods by presenting case histories to demonstrate the major impact that structure based methods have had on discovering drug molecules Written by international experts from industry and academia this comprehensive introduction to the methods and practice of structure based drug discovery not only illustrates leading edge science but also provides the scientific background for the non expert reader The book provides a balanced appraisal of what structure based methods can and cannot contribute to drug discovery It will appeal to industrial and academic researchers in pharmaceutical sciences medicinal chemistry and chemical biology as well as providing an insight into the field for recent graduates in the biomolecular sciences

Ribozymes and RNA Catalysis David Malcolm James Lilley, Fritz Eckstein (Professor.), 2008 Takes the reader through the origins of catalysis in RNA and necessarily includes significant discussion of structure and folding The main focus of the book concerns chemical mechanism with extensive comment on how despite the importance of RNA catalysis in the cell its origins are still poorly understood and often controversial The reader is given an outline of the important role of RNA catalysis in many aspects of cell function including RNA processing and translation

Metabolomics, Metabonomics and Metabolite Profiling William J. Griffiths, 2008 In this comprehensive resource the Editor draws together experts from the field and provides an insightful introduction into the technology and methodology

Protein Folding, Misfolding and Aggregation Victor Muñoz, 2008 Protein folding and aggregation is the process by which newly synthesized proteins fold into the specific three dimensional structures defining their biologically active states It has always been a major focus of research in biochemistry and has often been seen as the unsolved second part of the genetic code In the last 10 years we have witnessed a quantum leap in the research in this exciting area Computational methods

have improved to the extent of making possible to simulate the complete folding process of small proteins and the early stages of protein aggregation Experimental methods h RNA Polymerases as Molecular Motors Henri C. Buc, Terence Strick, 2009-04-16 This book focuses on two aspects of the transcription cycle the recognition of the promoter by the enzyme and the achievement of consecutive translocation steps during elongation of the RNA product *Therapeutic Oligonucleotides* Jens Kurreck, 2008 This book provides a compelling overall update on current status of RNA interference

Quantum Tunnelling in Enzyme-catalysed Reactions Rudolf Konrad Allemann, Nigel S. Scrutton, 2009 In recent years there has been an explosion in knowledge and research associated with the field of enzyme catalysis and H tunneling Rich in its breath and depth this introduction to modern theories and methods of study is suitable for experienced researchers those new to the subject Edited by two leading experts and bringing together the foremost practitioners in the field this up to date account of a rapidly developing field sits at the interface between biology chemistry and physics It covers computational kinetic and structural analysis of tunnelling and the synergy in combining these methods with a major focus on H tunneling reactions in enzyme systems The book starts with a brief overview of proton and electron transfer history by Nobel Laureate Rudolph A Marcus The reader is then guided through chapters covering almost every aspect of reactions in enzyme catalysis ranging from descriptions of the relevant quantum theory and quantum classical theoretical methodology to the description of experimental results The theoretical interpretation of these large systems includes both quantum mechanical and statistical mechanical computations as well as simple more approximate models Most of the chapters focus on enzymatic catalysis of hydride proton and H transfer an example of the latter being proton coupled electron transfer There is also a chapter on electron transfer in proteins This is timely since the theoretical framework developed fifty years ago for treating electron transfers has now been adapted to H transfers and electron transfers in proteins Accessible in style this book is suitable for a wide audience but will be particularly useful to advanced level undergraduates postgraduates and early postdoctoral workers *Nucleic Acid-metal Ion Interactions* Nicholas V. Hud, 2009 Provides a perspective on nucleic acid metal ion interactions with an emphasis on experimental biophysical studies which will prove indispensable to biophysicists and molecular biologists **Sequence-specific DNA Binding Agents** Michael J Waring, 2007-10-31 The binding of antibiotics and drugs to DNA is a fast developing area of research with important applications in medicine particularly the treatment of cancer Sequence specific DNA Binding Agents uniquely discusses key aspects of this topic providing a novel perspective on the subject Written by experts in the field this book discusses diverse modes of binding of antibiotics and drugs to DNA emphasising matters that are important or promising for cancer treatment Chapters discuss established agents like actinomycin D but also look at novel drugs with strong potential in chemotherapy such as new topoisomerase inhibitors telomerase inhibitors peptide nucleic acids and triple helix forming oligonucleotides There are also sections discussing methodological advances including computational methods slow kinetics melting curve analysis and approaches to medicinal

chemistry Finally there is a section on RNA structure and its potential as a drug target The book is ideal for researchers in industry and academia who require a comprehensive source of reference to this rapidly expanding subject

Physicochemical and Environmental Plant Physiology Park S. Nobel, 2009-05-13 Physicochemical and Environmental Plant Physiology Fourth Edition is the updated version of an established and successful reference for plant scientists The author has taken into consideration extensive reviews performed by colleagues and students who have touted this book as the ultimate reference for research and learning The original structure and philosophy of the book continue in this new edition providing a genuine synthesis of modern physicochemical and physiological thinking while entirely updating the detailed content This version contains more than 40% new coverage five brand new equations and four new tables with updates to 24 equations and six tables and 30 new figures have been added with more than three quarters of figures and legends improved Key concepts in plant physiology are developed with the use of chemistry physics and mathematics fundamentals The book is organized so that a student has easy access to locate any biophysical phenomenon in which he or she is interested More than 40% new coverage Incorporates student recommended changes from the previous edition Five brand new equations and four new tables with updates to 24 equations and six tables 30 new figures added with more than three quarters of figures and legends improved Organized so that a student has easy access to locate any biophysical phenomenon in which he or she is interested Per chapter key equation tables Problems with solutions presented in the back of the book Appendices with conversion factors constants coefficients abbreviations and symbols

Protein-Nucleic Acid Interactions Phoebe A. Rice, Carl C. Correll, 2008-05-22 The structural biology of protein nucleic acid interactions is in some ways a mature field and in others in its infancy High resolution structures of protein DNA complexes have been studied since the mid 1980s and a vast array of such structures has now been determined but surprising and novel structures still appear quite frequently High resolution structures of protein RNA complexes were relatively rare until the last decade Propelled by advances in technology as well as the realization of RNA's importance to biology the number of example structures has ballooned in recent years New insights are now being gained from comparative studies only recently made possible due to the size of the database as well as from careful biochemical and biophysical studies As a result of the explosion of research in this area it is no longer possible to write a comprehensive review Instead current review articles tend to focus on particular subtopics of interest This makes it difficult for newcomers to the field to attain a solid understanding of the basics One goal of this book is therefore to provide in depth discussions of the fundamental principles of protein nucleic acid interactions as well as to illustrate those fundamentals with up to date and fascinating examples for those who already possess some familiarity with the field The book also aims to bridge the gap between the DNA and the RNA views of nucleic acid protein recognition which are often treated as separate fields However this is a false dichotomy because protein DNA and protein RNA interactions share many general principles This book therefore includes relevant examples from both sides and frames

discussions of the fundamentals in terms that are relevant to both. The monograph approaches the study of protein nucleic acid interactions in two distinctive ways. First, DNA-protein and RNA-protein interactions are presented together. Second, the first half of the book develops the principles of protein nucleic acid recognition, whereas the second half applies these to more specialized topics. Both halves are illustrated with important real-life examples. The first half of the book develops fundamental principles necessary to understand function. An introductory chapter by the editors reviews the basics of nucleic acid structure. Jen Jacobsen and Jacobsen discuss how solvent interactions play an important role in recognition, illustrated with extensive thermodynamic data on restriction enzymes. Marmorstein and Hong introduce the zoology of the DNA-binding domains found in transcription factors and describe the combinatorial recognition strategies used by many multiprotein eukaryotic complexes. Two chapters discuss indirect readout of DNA sequence in detail. Berman and Lawson explain the basic principles and illustrate them with in-depth studies of CAP, while in their chapter on DNA bending and compaction, Johnson, Stella, and Heiss highlight the intrinsic connections between DNA bending and indirect readout. Horvath lays out the fundamentals of protein recognition of single-stranded DNA and single-stranded RNA and describes how they apply in a detailed analysis of telomere end-binding proteins. Nucleic acids adopt more complex structures. Lilley describes the conformational properties of helical junctions and how proteins recognize and cleave them. Because RNA readily folds due to the stabilizing role of its 2' hydroxyl groups, Li discusses how proteins recognize different RNA folds, which include duplex RNA. With the fundamentals laid out, discussion turns to more specialized examples taken from important aspects of nucleic acid metabolism. Schroeder discusses how proteins chaperone RNA by rearranging its structure into a functional form. Berger and Dong discuss how topoisomerases alter the topology of DNA and relieve the superhelical tension introduced by other processes such as replication and transcription. Dyda and Hickman show how DNA transposases mediate genetic mobility, and Van Duyne discusses how site-specific recombinases cut and paste DNA. Horton presents a comprehensive review of the structural families and chemical mechanisms of DNA nucleases, whereas Li, in her discussion of RNA-protein recognition, also covers RNA nucleases. Lastly, Ferré-D'Amar shows how proteins recognize and modify RNA transcripts at specific sites. The book also emphasises the impact of structural biology on understanding how proteins interact with nucleic acids, and it is intended for advanced students and established scientists wishing to broaden their horizons.

Exploiting Chemical Diversity for Drug Discovery Paul A. Bartlett, Michael Entzeroth, 2007-10-31. Conceptual and technological advances in chemistry and biology have transformed the drug discovery process. Evolutionary pressure among the diverse scientific and engineering disciplines that contribute to the identification of biologically active compounds has resulted in synergistic improvements at every step in the process. *Exploiting Chemical Diversity for Drug Discovery* encompasses the many components of this transformation and presents the current state of the art of this critical endeavour. From the theoretical and operational considerations in generating a collection of compounds to screen to the design and implementation of high

capacity and high quality assays that provide the most useful biological information this book provides a comprehensive overview of modern approaches to lead identification Beginning with an introductory overview subsequent chapters address topics that include the design of chemical libraries and methods for optimizing their diversity automated and accelerated chemistry high throughput assay design and detection techniques and strategies for data analysis and property optimization Written by experts in the field both academic and industrial and illustrated in full colour this book provides an excellent overview for current practitioners and will also serve as a stimulating resource for future generations Researchers in organic and medicinal chemistry the biological and pharmacological sciences as well as those interested in allied computational and engineering disciplines will value the comprehensive and up to date coverage

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