

Biological Magnetic Resonance

17

Edited by
N. Rama Krishna
and **Lawrence J. Berliner**

Structure Computation and Dynamics in Protein NMR



Biological Magnetic Resonance Vol 17 Structure Computation And Dynamics In Protein Nmr

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Nuclear Magnetic Resonance of Biological Macromolecules, Part B ,2001-07-12 This volume and its companion Volume 338 supplement Volumes 176 177 239 and 261 Chapters are written with a hands on perspective That is practical applications with critical evaluations of methodologies and experimental considerations needed to design execute and interpret NMR experiments pertinent to biological molecules

Optimization in Computational Chemistry and Molecular Biology Christodoulos A. Floudas, Panos M. Pardalos, 2013-06-29 Optimization in Computational Chemistry and

Molecular Biology Local and Global Approaches covers recent developments in optimization techniques for addressing several computational chemistry and biology problems A tantalizing problem that cuts across the fields of computational chemistry biology medicine engineering and applied mathematics is how proteins fold Global and local optimization provide a systematic framework of conformational searches for the prediction of three dimensional protein structures that represent the global minimum free energy as well as low energy biomolecular conformations Each contribution in the book is essentially expository in nature but of scholarly treatment The topics covered include advances in local and global optimization approaches for molecular dynamics and modeling distance geometry protein folding molecular structure refinement protein and drug design and molecular and peptide docking Audience The book is addressed not only to researchers in mathematical programming but to all scientists in various disciplines who use optimization methods in solving problems in computational chemistry and biology

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Modern Techniques in Protein NMR N. Rama Krishna, Lawrence J. Berliner, 2006-03-16 Volume 16 marks the beginning of a special topic series devoted to modern techniques in protein NMR under the Biological Magnetic Resonance series This volume is being followed by Volume 17 with the subtitle Structure Computation and Dynamics in Protein NMR Volumes 16 and 17 present some of the recent significant advances in biomolecular NMR field with emphasis on developments during the last five years We are honored to have brought together in these volumes some of the world s foremost experts who have provided broad leadership in advancing this field Volume 16 contains advances in two broad categories the first Large Proteins Complexes and Membrane Proteins and second Pulse Methods Volume 17 which will follow covers major advances in Computational Methods and Structure and Dynamics In the opening chapter of Volume 16 Marius Clore and Angela Gronenborn give a brief review of NMR strategies

including the use of long range restraints in the structure determination of large proteins and protein complexes In the next two chapters Lewis Kay and Ron Venters and their collaborators describe state of the art advances in the study of perdeuterated large proteins They are followed by Stanley Opella and co workers who present recent developments in the study of membrane proteins A related topic dealing with magnetic field induced residual dipolar couplings in proteins will appear in the section on Structure and Dynamics in Volume 17 *Biological Magnetic Resonance* Lawrence J.

Berliner, Jacques Reuben, 1978 Nuclease Methods and Protocols Catherine H. Schein, 2008-02-03 Nucleases enzymes that restructure or degrade nucleic acid polymers are vital to the control of every area of metabolism They range from housekeeping enzymes with broad substrate ranges to extremely specific tools 1 Many types of nucleases are used in lab protocols and their commercial and clinical uses are expanding The purpose of *Nuclease Methods and Protocols* is to introduce the reader to some well characterized protein nucleases and the methods used to determine their activity structure interaction with other molecules and physiological role Each chapter begins with a mini review on a specific nuclease or a nuclease related theme Although many chapters cover several topics they were arbitrarily divided into five parts Part I Characterizing Nuclease Activity includes protocols and assays to determine general processive distributive or specific mechanisms Methods to assay nuclease products identify cloned nucleases and determine their physiological role are also included here Part II Inhibitors and Activators of Nucleases summarizes assays for measuring the effects of other proteins and small molecules Many of these inhibitors have clinical relevance Part III Relating Nuclease Structure and Function provides an overview of methods to determine or model the 3 D structure of nucleases and their complexes with substrates and inhibitors A 3 D structure can greatly aid the rational design of nucleases and inhibitors for specific purposes Part IV Nucleases in the Clinic summarizes assays and protocols suitable for use with tissues and for nuclease based therapeutics

Nuclear Magnetic Resonance G A Webb, 2007-10-31 As a spectroscopic method Nuclear Magnetic Resonance NMR has seen spectacular growth over the past two decades both as a technique and in its applications Today the applications of NMR span a wide range of scientific disciplines from physics to biology to medicine Each volume of *Nuclear Magnetic Resonance* comprises a combination of annual and biennial reports which together provide comprehensive coverage of the literature on this topic This Specialist Periodical Report reflects the growing volume of published work involving NMR techniques and applications in particular NMR of natural macromolecules which is covered in two reports NMR of Proteins and Acids and NMR of Carbohydrates Lipids and Membranes For those wanting to become rapidly acquainted with specific areas of NMR this title provides unrivalled scope of coverage Seasoned practitioners of NMR will find this an invaluable source of current methods and applications Specialist Periodical Reports provide systematic and detailed review coverage in major areas of chemical research Compiled by teams of leading authorities in the relevant subject areas the series creates a unique service for the active research chemist with regular in depth accounts of progress in particular fields of chemistry Subject coverage within

different volumes of a given title is similar and publication is on an annual or biennial basis **Protein NMR** Lawrence Berliner, 2015-08-24 This book covers new techniques in protein NMR from basic principles to state of the art research It covers a spectrum of topics ranging from a toolbox for how sequence specific resonance assignments can be obtained using a suite of 2D and 3D NMR experiments and tips on how overlap problems can be overcome Further topics include the novel applications of Overhauser dynamic nuclear polarization methods DNP assessing protein structure and aspects of solid state NMR of macroscopically aligned membrane proteins This book is an ideal resource for students and researchers in the fields of biochemistry chemistry and pharmacology and NMR physics Comprehensive and intuitively structured this book examines protein NMR and new novel applications that include the latest technological advances This book also has the features of A selection of various applications and cutting edge advances such as novel applications of Overhauser dynamic nuclear polarization methods DNP and a suite of 2D and 3D NMR experiments and tips on how overlap problems can be overcome A pedagogical approach to the methodology Engaging the reader and student with a clear yet critical presentation of the applications

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