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Revisiting biomolecular NMR spectroscopy for promoting small-molecule drug discovery Authors (first, second and last of 4) Hiroyuki Hanzawa; Takashi Shimada; Hideo Takahashi; Content type: Perspective; Published: 18 April 2020

Journal of Biomolecular NMR | Online first articles
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This timely book, entitled Biomolecular NMR Spectroscopy, focuses on the latest state-of-the-art NMR techniques for characterization of biological macromolecules in the solid and solution state. The editors, Dr. Andrew Dingley (University of Auckland, New Zealand) and Dr. Steven Pascal (Massey University, New Zealand) have organized the book into four sections, covering the following topics: (i) sample preparation, (ii) structure and dynamics of proteins, (iii) structure and dynamics of ...

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NMR Spectroscopy and its Application to Biomedical ...
Description. Biomolecular Structure and Function covers the proceedings of the 1977 Cellular Function and Molecular Structure: Biophysical Approaches to Biological Problems symposium. It summarizes the application of several biophysical techniques to molecular research in biology. This book starts by describing the use of deuterium-labeled lipids, as monitors of the degree of organization of membrane lipids.

Biomolecular Structure and Function - 1st Edition
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Applications of NMR Spectroscopy: Volume 3 - 1st Edition
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In principle, NMR and EPR spectroscopy can be used to investigate the conformation and dynamics of biological macromolecules in living cells. The development of in/cell magnetic resonance techniques has demonstrated the feasibility of this approach.

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Next-Generation Heteronuclear Decoupling for High-Field ...
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The technique of nuclear magnetic resonance (NMR) spectroscopy is an important tool in biochemistry and biophysics for the understanding of the structure and ultimately, the function of biomolecules. This textbook explains the salient features of biological NMR spectroscopy to undergraduates and postgraduates taking courses in NMR, biological NMR, physical biochemistry, and biophysics. Unlike other books in the general field of NMR (except the advanced treatises), the approach here is tointroduce and make use of quantum mechanical product operators as well as the classical vector method of explaining the bewildering array of pulse sequences available today. The book covers two- dimensional, three- dimensional, and four- dimensional NMR and their application to protein and DNA structure determination. A unique feature is the coverage of the biological aspects of solid- state NMR spectroscopy. The author provides many selected examples from the research literature, illustratingthe applications of NMR spectroscopy to biological proteins.

Edited by leading biological NMR spectroscopists, this book will cover the new developments that have occurred in biomolecular NMR over the last few years.

Nuclear Magnetic Resonance (NMR) spectroscopy is the most powerful technique for characterization of biomolecular structures at atomic resolution in the solution state. This timely book, entitled "Biomolecular NMR Spectroscopy," focuses on the latest state-of-the-art NMR techniques for characterization of biological macromolecules in the solid and solution state. The editors, Dr. Andrew Dingley (University of Auckland, New Zealand) and Dr. Steven Pascal (Massey University, New Zealand) have organized the book into four sections, covering the following topics: sample preparation, structure and dynamics of proteins, structure and dynamics of nucleic acids and protein-nucleic acid complexes, and rapid and hybrid techniques--

NMR spectroscopy has proven to be a powerful technique to study the structure and dynamics of biological macromolecules. Fundamentals of Protein NMR Spectroscopy is a comprehensive textbook that guides the reader from a basic understanding of the phenomenological properties of magnetic resonance to the application and interpretation of modern multi-dimensional NMR experiments on 15N/13C-labeled proteins. Beginning with elementary quantum mechanics, a set of practical rules is presented and used to describe many commonly employed multi-dimensional, multi-nuclear NMR pulse sequences. A modular analysis of NMR pulse sequence building blocks also provides a basis for understanding and developing novel pulse programs. This text not only covers topics from chemical shift assignment to protein structure refinement, as well as the analysis of protein dynamics and chemical kinetics, but also provides a practical guide to many aspects of modern spectrometer hardware, sample preparation, experimental set-up, and data processing. End of chapter exercises are included to emphasize important concepts. Fundamentals of Protein NMR Spectroscopy not only offer students a systematic, in-depth, understanding of modern NMR spectroscopy and its application to biomolecular systems, but will also be a useful reference for the experienced investigator.

This text is aimed at people who have some familiarity with high-resolution NMR and who wish to deepen their understanding of how NMR experiments actually work. This revised and updated edition takes the same approach as the highly-acclaimed first edition. The text concentrates on the description of commonly-used experiments and explains in detail the theory behind how such experiments work. The quantum mechanical tools needed to analyse pulse sequences are introduced set by step, but the approach is relatively informal with the emphasis on obtaining a good understanding of how the experiments actually work. The use of two-colour printing and a new larger format improves the readability of the text. In addition, a number of new topics have been introduced: How product operators can be extended to describe experiments in AX2 and AX3 spin systems, thus making it possible to discuss the important APT, INEPT and DEPT experiments often used in carbon-13 NMR. Spin system analysis i.e. how shifts and couplings can be extracted from strongly-coupled (second-order) spectra. How the presence of chemically equivalent spins leads to spectral features which are somewhat unusual and possibly misleading, even at high magnetic fields. A discussion of chemical exchange effects has been introduced in order to help with the explanation of transverse relaxation. The double-quantum spectroscopy of a three-spin system is now considered in more detail. Reviews of the First Edition iFor anyone wishing to know what really goes on in their NMR experiments, I would highly recommend this book! Chemistry World [...] warmly recommend for budding NMR spectroscopists, or others who wish to deepen their understanding of elementary NMR theory or theoretical tools! Magnetic Resonance in Chemistry

Steering clear of quantum mechanics and product operators, "Pocket Guide to Biomolecular NMR" uses intuitive, concrete analogies to explain the theory required to understand NMR studies on the structure and dynamics of biological macromolecules. For example, instead of explaining nuclear spin with angular momentum equations or Hamiltonians, the books describes nuclei as "bells" in a choir, ringing at specific frequencies depending on the atom type and their surrounding electromagnetic environment.This simple bell analogy, which is employed throughout the book, has never been used to explain NMR and makes it surprisingly easy to learn complex, bewildering NMR concepts, such as dipole-dipole coupling and CPMG pulse sequences. Other topics covered include the basics of multi-dimensional NMR, relaxation theory, and Model Free analysis. The small size and fast pace of iPocket Guide to Biomolecular NMRi makes the book a perfect companion to traditional biophysics and biochemistry textbooks, but the book's unique perspective will provide even seasoned spectroscopists with new insights and handy ithoughti short-cuts.

NMR spectroscopy has undergone a revolution in recent years with the advent of several new methods overcoming the problems of sensitivity and resolution. Recent developments in biotechnology have made it easier and economical to introduce 13C, 15N and 2H into proteins and nucleic acids. At the same time, there has been an explosion in the number of NMR experiments that utilize such isotope labeled samples. Thus, a combination of isotopic labeling and multidimensional, multinuclear NMR has opened up new avenues for structural studies of proteins, nucleic acids and their complexes. This book will focus on recent developments in isotope labeling methods for structural studies of small molecules, peptides, proteins and nucleic acids. The aim of the book is to serve as a compendium of isotope labeling for the biomolecular NMR community providing comprehensive coverage of the existing methods and latest developments along with protocols and practical hints on the various experimental aspects. The book will cover a wide range of topics in isotope labeling under one title including emerging areas of metabolonomics and solid state NMR.

NMR is one of the most powerful methods for imaging of biomolecules. This book is the ultimate NMR guide for researchers in the biomedical community and gives not only background and practical tips but also a forward looking view on the future of NMR in systems biology.

From complex structure elucidation to biomolecular interactions - this applicationoriented textbook covers both theory and practice of modern NMR applications. Part one sets the stage with a general description of NMR introducing important parameters such as the chemical shift and scalar or dipolar couplings. Part two describes the theory behind NMR, providing a profound understanding of the involved spin physics, deliberately kept shorter than in other NMR textbooks, and without a rigorous mathematical treatment of all the physico-chemical computations. Part three discusses technical and practical aspects of how to use NMR. Important phenomena such as relaxation, exchange, or the nuclear Overhauser effects and the methods of modern NMR spectroscopy including multidimensional experiments, solid state NMR, and the measurement of molecular interactions are the subject of part four. The final part explains the use of NMR for the structure determination of selected classes of complex biomolecules, from steroids to peptides or proteins, nucleic acids, and carbohydrates. For chemists as well as users of NMR technology in the biological sciences.

Protein NMR Spectroscopy, Second Edition combines a comprehensive theoretical treatment of NMR spectroscopy with an extensive exposition of the experimental techniques applicable to proteins and other biological macromolecules in solution. Beginning with simple theoretical models and experimental techniques, the book develops the complete repertoire of theoretical principles and experimental techniques necessary for understanding and implementing the most sophisticated NMR experiments. Important new techniques and applications of NMR spectroscopy have emerged since the first edition of this extremely successful book was published in 1996. This updated version includes new sections describing measurement and use of residual dipolar coupling constants for structure determination, TROSY and deuterium labeling for application to large macromolecules, and experimental techniques for characterizing conformational dynamics. In addition, the treatments of instrumentation and signal acquisition, field gradients, multidimensional spectroscopy, and structure calculation are updated and enhanced. The book is written as a graduate-level textbook and will be of interest to biochemists, chemists, biophysicists, and structural biologists who utilize NMR spectroscopy or wish to understand the latest developments in this field. Provides an understanding of the theoretical principles important for biological NMR spectroscopy Demonstrates how to implement, optimize and troubleshoot modern multi-dimensional NMR experiments Allows for the capability of designing effective experimental protocols for investigations of protein structures and dynamics Includes a comprehensive set of example NMR spectra of ubiquitin provides a reference for validation of experimental methods