belongs in all science libraries of every professional working in these areas.

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Protein NMR Techniques, Volume 60 Methods in Molecular Biology. Edited by David G. Reid. Humana Press, Totowa, NJ. 1997. x + 418 pp. 16 x 23.5 cm. ISBN 0-89603-309-0. $79.50.

The book contains 12 chapters covering a wide range of topics from instrumental concerns to the theory of molecular modeling written by acknowledged leaders in each area. Each chapter is well-written and well-referenced. This is an excellent text, with several chapters that will be of particular interest to graduate students and researchers new to the area.

Chapter 1 presents an introduction to the application of NMR to the investigation of protein structure. Topics discussed in this chapter include sample considerations, the "technique of sequence-specific resonance assignment", the role of isotropic labeling, and NOEs that are important in the characterization of secondary structure. The second chapter provides an overview of the most commonly used three- and four-dimensional double- and triple-resonance experiments for the determination of protein structure. The chapter concludes with a review of the assignment strategies which use these methods to determine the three-dimensional structure of a protein. Chapter 3 presents a detailed discussion of how protein structure affects chemical shift. The application of ^{13}C and ^{1}H chemical shift indexing for predicting protein secondary structure is also discussed. Chapter 4 presents an excelelnt discussion of processing NMR data. This chapter is an excellent guide for students and researchers who are just learning how to process NMR data. Topics discussed include preparation of the data, on-line vs off-line processing, format conversion, processing strategy and data structure, sampling and quadrature detection schemes, apodization, zero-filling, and a review of available processing software. The chapter is very well-referenced with 388 literature citations. Chapter 5 is again an excellent introductory chapter for graduate students and researchers new to the area. In this chapter, a detailed discussion of the calculation of protein structures from NMR data is presented. The chapter begins with a basic outline of the procedures used to convert NMR data into a three-dimensional structure. The relationships between NOEs and coupling constants obtained from the NMR experiment and the dihedral angles and distance restraints used in molecular modeling calculations are clearly defined. The two major calculation methods, distance geometry and molecular dynamics simulated annealing, are discussed. Methods for structure analysis and refinement of the originally calculated structure are also discussed. Chapter 6 provides a discussion on the application of NMR to study protein−ligand interactions. In this chapter, NMR parameters and methods that can provide information on protein−ligand interactions are discussed, including NMR detected titration, transfer-NOE experiments, isotope editing, chemical shift, relaxation parameters, and NOE effects. The effect of the time scale of the binding process for NMR detection is also discussed. The chapter concludes with selected applications. Chapter 7 presents an excellent discussion on NMR of paramagnetic proteins. In Chapter 8, an excellent overview of the application of liquid and solid NMR methods for the studies of membrane-associated proteins and peptides is presented. Of particular interest is the discussion of the application of the solid-state methods REDOR (rotational-echo double-resonance) and RF-Driven recoupling experiment to the determination of protein structure. Chapter 9 is the third chapter in the text which should be of particular interest to graduate students. In this chapter, an excellent discussion of application of metal NMR for the study of metelloproteins is given. Topics discussed include theoretical and experimental considerations, exchange effects, quadropolar ions, and dipolar ions. Chapter 10 provides an overview of the methods for the production and characterization of recombinant proteins. Topics discussed include labeling methods, bacterial expression, yeast expression, baculovirus expression, and mammalian cell expression. Chapter 11 provides an excellent summation for the text. In this chapter, a case history of the NMR studies of a small protein ω-conotoxin MVIIA is presented. This discussion present here illustrates how the material presented in the previous 10 chapters comes together to yield the complete story of a protein structure. For students or researchers new to this area, this chapter, in my opinion, provides an excellent research outline from which to build their own NMR studies. The last chapter should be required reading for all students using an NMR instrument. This chapter provides clear and detailed insight into the operation and calibration of an NMR spectrometer. Topics include basic principles and procedures, calibration of hard pulses, spin−lock pulses, decoupler pulses, and X-nucleus pulses, solvent suppression, calibration of pulse field gradient pulses, how to use pulse field gradient pulses, selective exctiation using shaped pulses, and how to implement new pulse sequences.

In summary, this is a very good reference text and study guide for students and the experienced researcher.

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Reviews in Computational Chemistry, Volume 9. Edited by Kenny B. Lipkowitz and Donald B. Boyd (Indiana University−Purdue University at Indianapolis). Wiley/VCH, New York. 1996. xxxiii + 282 pp. ISBN 1-56081-930-8. $110.00.

This is the ninth volume in this on-going series and continues the excellent efforts by these editors to bring together applications of state-of-the-art computational chemistry methods. This volume contains five chapters that address computational problems of specific chemical types and include peptides, oligosaccharides, and organic molecules, as well as the calculation of free energies and molecular shape descriptors. Chapter 1, Peptide Mimetic Design with the Aid of Computational Chemistry, by James Damewood, Jr., presents 31 case studies, encapsulated in 80 well-documented pages. These examples are a good resource for didactic lessons of successful applications of peptidomimetic design. A prerequisite to the success of these studies was the availability of X-ray crystal structures for the target proteins upon which the modeling studies were performed. In most cases, standard applications of a variety of computational programs were carried out. Chapter 2, Free Energy by Molecular Simulation, by R. P. Straatsma, reviews the advantages and disadvantages in the use of thermodynamic perturbation and thermodynamic integration methods in the calculation of relative free energy differences. In many cases, the choice is predicated on the availability of computational resources which engenders a choice between adequate methods and the practicality of the calculations. The review provides numerous examples of the pitfalls these methods entail. Chapter 3, The Application of Molecular Modeling Techniques to the Determination of Oligosaccharide Solution Conformations, by Robert J. Woods, focuses on the choice of parameters for the description of oligosaccharides as their variable degree of flexibility dictates whether a statistically accurate ensemble of conformations or a single conformer is appropriate. Because counterions for oligosaccharides are important, explicit treatment of solvent is crucial. Chapter 4, Molecular Mechanics Calculated Conformational Energies of Organic Molecules: A Comparison of Force Fields, by Ingrid Pettersson and Tommy Liljefors, reviews the relative merits and limitations of various molecular mechanics force fields. Each of the components of the force field is defined, and a comparison is made with each of several typically available force field programs with their reliability to describe specific functional molecular features. On the basis of these data, those force fields which are derived from MMFF93, MM2, and MM3 have the best overall results. Chapter 5, Molecular Shape Analysis, by Gustavo A. Arteca, provides an overview of shape parameters and a guide to their key applications, along with criteria for choosing the appropriate shape parameters. A large part of the chapter deals with scaling and dimensionality of the descriptors. These methods can be powerful tools for the description of several independent geometrical or topological properties. This book will serve those looking for new perspectives in the field and is a recommended addition to every structural biology and computer modeling laboratory library.

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From Ion Channels to Cell-to-Cell Conversations. Edited by R. Latorre and J. C. Saez. Plenum Press, New York and London. 1997. 16 × 23.5 cm. xxvii + 504 pp. ISBN 0-306-45605-2. $135.00.

As major cellular, cell-to-cell, and intracellular portals of information, ion channels fully deserve the attention they get. This multiauthored volume of some 28 chapters covers both the channels of plasma membranes and the gap junction intercellular channels. The topics included range from issues around activation, inactivation, and gating mechanisms, to channel regulation, subunit interaction, and odoront mechanisms. At the intracellular level, chapters cover topics ranging from lens gap junctions, gap junctions in liver during CCl_4-induced injury, and connexins to sex hormone regulation of smooth muscle gap junctions.

Given the diversity of topics covered, there is something for everyone here. However, it is not clear for whom the book is intended. It is too diverse to serve either as a text for new workers or as a reference volume for experts. It is probably too expensive for the individual buyer, and I cannot easily recommend it for libraries save for those in institutions with a major commitment to ion channel research.

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