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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