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Methods; Hamiltonian; Monte Carlo Simulations; Molecular Dynamics Simulations; Thermodynamic Perturbation; Thermodynamic Integration Thermodynamic CyclesPotentials of Mean Force; Free Energy Evaluations in Practice; Hamiltonian Coupling; Creation and Annihilation of Atoms; Constraints; Conformational Isomeric States; Long-Range Interactions; Boundary Conditions; Error Analysis; Sensitivity of Calculated Free Energies to Force Field Parameters; Electronic Polarization; Atomic Replacement Calculations; Recommendations; Free Energy Methodology; Choice of Pathway; Standard Protocol; Analysis of Results; Conclusion; Acknowledgment; References
The Application of Molecular Modeling Techniques to the Determination of Oligosaccharide Solution ConformationsIntroduction; Carbohydrate Conformational Analysis: The Motivation and the Challenge; Electronic Effects and Carbohydrate Conformation; Carbohydrate Force Fields: An Overview; Hard Sphere Exo-Anomeric (HSEA) and Monte Carlo Methods; MM2/MM3; Macromolecular Force Fields and Molecular Dynamics Simulations; Role of Water-Sugar Interactions; Conclusions; References; Molecular Mechanics Calculated Con formational Energies of Organic Molecules: A Comparison of Force Fields; Introduction
The Principles of Molecular MechanicsForms of Potential Energy Functions; Bond Stretching/Compression Functions; Bond Angle Bending Functions; Torsional Functions; Van der Waals Functions; Electrostatic Functions; Cross-Terms; Conjugated Systems; Parameterization; Comparisons of Calculated Conformational Energies; Reproducibility of Conformational Energies; Summary and Conclusions; Acknowledgments; References; Molecular Shape Descriptors; Introduction; Hierarchical Levels of Molecular Shape and Shape Descriptors; Some Notions Regarding Molecular Shape and Scaling Classification of Molecular Models and Shape Descriptors

Sommario/riassunto

A select group of scientists from around the world join in this volume to create unique chapters aimed at both the novice molecular modeler and the expert computational chemist. Chapter 1 shows how molecular modeling of peptidomimetics plays a key role in drug discovery. Specific examples of successful computer-aided drug design are spelled out. Chapter 2 is a definitive exposition on thermodynamic perturbation and thermodynamic integration approaches in molecular dynamics simulations. Three additional chapters elucidate molecular modeling of carbohydrates, the best empirical force fields to u