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Nota di contenuto	Modeling Solvent Environments: Applications to Simulations of Biomolecules; Contents; Preface; List of Contributors; 1: Biomolecular Solvation in Theory and Experiment; 1.1 Introduction; 1.2 Theoretical Views of Solvation; 1.2.1 Equilibrium Thermodynamics of Solvation; 1.2.2 Radial Distribution Functions; 1.2.3 Integral Equation Formalisms; 1.2.4 Kirkwood-Buff Theory; 1.2.5 Kinetic Effects of Solvation; 1.3 Computer Simulation Methods in the Study of Solvation; 1.3.1 Molecular Dynamics and Monte Carlo Simulations; 1.3.2 Water Models; 1.3.3 Solvent Structure and Dynamics from Simulations 1.3.4 Free Energy Simulations1.4 Experimental Methods in the Study of Solvation; 1.4.1 X-Ray/Neutron Diffraction and Scattering; 1.4.2 Nuclear Magnetic Relaxation; 1.4.3 Optical Spectroscopy; 1.4.4 Dielectric Dispersion; 1.5 Hydration of Proteins; 1.5.1 Protein Folding and Peptide Conformations in Aqueous Solvent; 1.5.2 Molecular Properties of Water Near Protein Surfaces; 1.5.3 Water Molecules at Protein-Ligand and Protein-Protein Interfaces; 1.6 Hydration of Nucleic acids; 1.7 Non-Aqueous Solvation; 1.7.1 Alcohols; 1.7.2 Urea; 1.7.3 Glycerol; 1.8 Summary; References

2: Model-Free "Solvent Modeling" in Chemistry and Biochemistry Based on the Statistical Mechanics of Liquids
2.1 Introduction; 2.2 Outline of the RISM and 3D-RISM theories; 2.3 Partial Molar Volume of Proteins; 2.4 Detecting Water Molecules Trapped Inside Protein; 2.5 Selective Ion Binding by Protein; 2.6 Water Molecules Identified as a Substrate for Enzymatic Hydrolysis of Cellulose; 2.7 CO Escape Pathway in Myoglobin; 2.7.1 Effect of Protein Structure on the Distribution of Xe; 2.7.2 Partial Molar Volume Change Through the CO Escape Pathway of Myoglobin; 2.8 Perspective; References

3: Developing Force Fields From the Microscopic Structure of Solutions: The Kirkwood-Buff Approach
3.1 Introduction; 3.2 Biomolecular Force Fields; 3.3 Examples of Problems with Current Force Fields; 3.4 Kirkwood-Buff Theory; 3.5 Applications of Kirkwood-Buff Theory; 3.6 The General KBFF Approach; 3.7 Technical Aspects of the KBFF Approach; 3.8 Results for Urea and Water Binary Solutions; 3.9 Preferential Interactions of Urea; 3.10 Conclusions and Future Directions; Acknowledgments; References

4: Osmolyte Influence on Protein Stability: Perspectives of Theory and Experiment
4.1 Introduction
4.2 Denaturing Osmolytes
4.2.1 Does Urea Weaken Water Structure?;
4.2.2 Effect of Urea on Hydrophobic Interactions; 4.2.3 Direct Interaction of Urea with Proteins; 4.3 Protecting Osmolytes; 4.3.1 Do Protecting Osmolytes Increase Water Structure?; 4.3.2 Effect of Protecting Osmolytes on Hydrophobic Interactions; 4.4 Mixed Osmolytes; 4.5 Conclusions; Acknowledgments; References

5: Modeling Aqueous Solvent Effects through Local Properties of Water;
5.1 The Role of Water and Cosolutes on Macromolecular Thermodynamics; 5.2 Forces Induced by Water in Aqueous Solutions
5.2.1 Interactions in Water-Accessible Regions of Proteins

Sommario/riassunto

A comprehensive view of the current methods for modeling solvent environments with contributions from the leading researchers in the field. Throughout, the emphasis is placed on the application of such models in simulation studies of biological processes, although the coverage is sufficiently broad to extend to other systems as well. As such, this monograph treats a full range of topics, from statistical mechanics-based approaches to popular mean field formalisms, coarse-grained solvent models, more established explicit, fully atomic solvent models, and recent advances in applying ab initio me
