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TERTIARY FOLDING POTENTIALDETERMINISTIC GLOBAL OPTIMIZATION AND AB INITIO APPROACHES FOR THE STRUCTURE PREDICTION OF POLYPEPTIDES, DYNAMICS OF PROTEIN FOLDING, AND PROTEIN-PROTEIN INTERACTIONS; DETECTING NATIVE PROTEIN FOLDS AMONG LARGE DECOY SITES WITH THE OPLS ALL-ATOM POTENTIAL AND THE SURFACE GENERALIZED BORN SOLVENT MODEL; AUTHOR INDEX; SUBJECT INDEX

Sommario/riassunto

Since the first attempts to model proteins on a computer began almost thirty years ago, our understanding of protein structure and dynamics has dramatically increased. Spectroscopic measurement techniques continue to improve in resolution and sensitivity, allowing a wealth of information to be obtained with regard to the kinetics of protein folding and unfolding, and complementing the detailed structural picture of the folded state. Concurrently, algorithms, software, and computational hardware have progressed to the point where both structural and kinetic problems may be studied with a fair d