Record Nr. UNINA9910877567303321 Computational methods for protein folding / / edited by Richard A. **Titolo** Friesner Pubbl/distr/stampa New York, : Wiley, 2002 **ISBN** 1-280-36766-0 9786610367665 0-470-34930-1 0-471-46523-2 0-471-22442-1 Descrizione fisica 1 online resource (546 p.) Collana Advances in chemical physics; ; v. 120 Altri autori (Persone) FriesnerRichard A Disciplina 541.305 541/.08 547.75 Soggetti Protein folding - Mathematical models Proteins - Conformation - Mathematical models Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Note generali Description based upon print version of record. Nota di contenuto COMPUTATIONAL METHODS FOR PROTEIN FOLDING A SPECIAL VOLUME VOLUME 120; INTRODUCTION; PREFACE; CONTENTS; STATISTICAL ANALYSIS OF PROTEIN FOLDING KINETICS; INSIGHTS INTO SPECIFIC

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AB INITIO PROTEIN STRUCTURE PREDICTION USING A SIZE-DEPENDENT 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

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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