ADVANCES IN CHEMICAL PHYSICS VOLUME 120
I. PRIGOGINE and STUART A. RICE, Series Editors

Edited by RICHARD A. FRIESNER

COMPUTATIONAL METHODS FOR PROTEIN FOLDING

CONTENTS

STATISTICAL ANALYSIS OF PROTEIN FOLDING KINETICS By Aaron R. Dinner, Sung-Sau-So, and Martin Karplus	1
Insights into Specific Problems in Protein Folding Using Simple Concepts By D. Thirumalai, D. K. Klimov, and R. I. Dima	35
PROTEIN RECOGNITION BY SEQUENCE-TO-STRUCTURE FITNESS: BRIDGING EFFICIENCY AND CAPACITY OF THREADING MODELS By Jaroslaw Meller and Ron Elber	77
A Unified Approach to the Prediction of Protein Structure and Function By Jefferey Skolnick and Andrzej Kolinski	131
Knowledge-Based Prediction of Protein Tertiary Structure By Pierre-Jean L'Heureux, Benoit Cromp, Éric Martineau, and John Gunn	193
AB INITIO PROTEIN STRUCTURE PREDICTION USING A SIZE-DEPENDENT TERTIARY FOLDING POTENTIAL By Volker A. Eyrich, Daron M. Standley, and Richard A. Friesner	223
DETERMINISTIC GLOBAL OPTIMIZATION AND AB INITIO APPROACHES FOR THE STRUCTURE PREDICTION OF POLYPEPTIDES, DYNAMICS OF PROTEIN FOLDING, AND PROTEIN-PROTEIN INTERACTIONS By John L. Klepeis, Heather D. Schafroth, Karl M. Westerberg, and Christodouls A. Floudas	265
DETECTING NATIVE PROTEIN FOLDS AMONG LARGE DECOY SITES WITH THE OPLS ALL-ATOM POTENTIAL AND THE SURFACE GENERALIZED BORN SOLVENT MODEL By Anders Wallqvist, Emilio Gallicchio, Anthony K. Felts, and Ronald M. Levy	459
AUTHOR INDEX	487
Subject Index	507

xiii