

SERIES IN COMPUTATIONAL BIOPHYSICS

Nikolay V. Dokolyan, Series Editor

"The modeling of biological systems and processes has advanced remarkably in recent years, gradually becoming a legitimate field of research. ... Some of the progress in the field has been described in the scholarly articles compiled in this book. ... the present publication ... reflects the current developments in the field ..."

—From the Foreword by Nobel Laureate Ariel Warshel, Distinguished Professor of Chemistry and Biochemistry, University of Southern California

"The book is conveniently structured to simplify the preparation of a new graduate course on biomolecular simulations."

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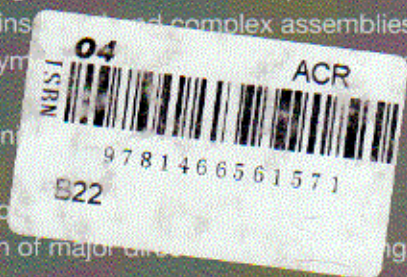
"... a comprehensive assessment of the methods for modeling protein dynamics and conformational heterogeneity across multiple spatial and time scales. Each contribution attempts to point the way toward connecting dynamics and heterogeneity to molecular function, thus making for a compelling read."

—Rohit V. Pappu, Department of Biomedical Engineering, Washington University, St. Louis

Computational Approaches to Protein Dynamics: From Quantum to Coarse-Grained Methods presents modern biomolecular computational techniques that address protein flexibility/dynamics at all levels of theory. An international contingent of leading researchers in biology, chemistry, and physics show how these advanced methods provide insights into dynamic aspects of biochemical processes.

Features

- Focuses on the dynamical aspects of biological functions with a special emphasis on intrinsically disordered proteins and complex assemblies
- Describes the methods and results of enzymatic reactions and protein-protein interactions of Ariel Warshel
- Explains how to apply computational techniques to solve major biological problems involving IDPs
- Discusses the experimental characterization of protein dynamics
- Gives a historical overview and description of major directions in modeling biological simulations



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