

Table of contents

- **Preface** (p. v)
- **Section I Structure Prediction and Assessment Methods** (p. 1)
- **Chapter 1 Protein Structure Modeling** (p. 3)
- **Chapter 2 Protein Fold Recognition and Threading** (p. 37)
- **Chapter 3 Scoring Functions for Protein Structure Prediction** (p. 61)
- **Chapter 4 Assessment of Protein Structure Predictions** (p. 89)
- **Chapter 5 The Biological Applications of Protein Models** (p. 111)
- **Section II From Structure to Function to Design** (p. 129)
- **Chapter 6 Evolution of Protein Folds** (p. 131)
- **Chapter 7 Classification of Protein Structures** (p. 153)
- **Chapter 8 Methods to Characterize the Structure of Enzyme Binding Sites** (p. 189)
- **Chapter 9 Atomistic Simulations of Reactions and Transition States** (p. 223)
- **Chapter 10 Functional Motions in Biomolecules: Insights from Computational Studies at Multiple Scales** (p. 253)
- **Chapter 11 Protein-Protein Interactions and Aggregation Processes** (p. 299)
- **Chapter 12 Modeling and Simulation of Ion Channels** (p. 325)
- **Chapter 13 Milestones in Molecular Dynamics Simulations of RNA Systems** (p. 363)
- **Chapter 14 Computational Protein Design** (p. 401)
- **Chapter 15 Prediction and Identification of B Cell Epitopes Using Protein Sequence and Structure Information** (p. 425)
- **Chapter 16 Computational Antibody Engineering** (p. 445)
- **Section III Drug Discovery and Pharmacology** (p. 467)
- **Chapter 17 Small Molecule Docking** (p. 469)
- **Chapter 18 Structure-based Pharmacophores and Screening** (p. 501)
- **Chapter 19 Molecular Dynamics-based Free Energy Simulations** (p. 513)
- **Chapter 20 Structure-based Computational Pharmacology and Toxicology** (p. 549)
- **Chapter 21 Structure-based Computational Approaches to Drug Metabolism** (p. 573)
- **Section IV New Frontiers in Experimental Methods** (p. 599)
- **Chapter 22 New Frontiers in X-ray Crystallography** (p. 601)
- **Chapter 23 New Frontiers in High-Resolution Electron Microscopy** (p. 623)
- **Chapter 24 New Frontiers in Characterizing Structure and Dynamics by NMR** (p. 655)
- **Section V Selected Topics** (p. 681)
- **Chapter 25 Docking for Neglected Diseases as Community Efforts** (p. 683)
- **Chapter 26 Protein Structure Databases** (p. 705)
- **Chapter 27 Molecular Graphics in Structural Biology** (p. 729)