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| Descrizione fisica | 1 online resource (262 p.) |
| Altri autori (Persone) | GoodfellowJulia M |
| Disciplina | 574.880113<br>574.880285 |
| Soggetti | Molecular biology - Data processing<br>Molecular biology - Computer simulation |
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| Nota di bibliografia | Includes bibliographical references and index. |
| Nota di contenuto | Computer Modelling in Molecular Biology; Contents; Colour Illustrations; 1 Introduction to Computer Simulation: Methods and Applications; 2 Modelling Protein Structures; 3 Molecular Dynamics Simulations of Peptides; 4 Molecular Dynamics and Free Energy Calculations Applied to the Enzyme Barnase and One of its Stability Mutants; 5 The Use of Molecular Dynamics Simulations for Modelling Nucleic Acids; 6 Theory of Transport in Ion Channels; 7 Molecular Modelling and Simulations of Major Histocompatibility Complex Class I Protein-Peptide Interactions<br>8 Path Energy Minimization: A New Method for the Simulation of Conformational Transitions of Large MoleculesIndex |
| Sommario/riassunto | This book supplies an application-oriented introduction to molecular simulation techniques used to study a wide range of problems in molecular biology. Each chapter focuses in detail on one kind of application, including the scientific background, the appropriate methodology and the relationship to experimental results.The book contains many areas of interest to basic and industrial scientists, including:- flexibility of peptides- protein-peptide interactions- ion |

translocation across membranes- modelling protein and nucleic acid conformations- stability of muta