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| 1. Record Nr. | UNINA9911019984903321 |
| Titolo | Computer modelling in molecular biology / / edited by Julia M. Goodfellow |
| Pubbl/distr/stampa | Weinheim ; ; New York, : VCH, c1995 |
| ISBN | 9786611758622 9781281758620 1281758620 9783527615339 3527615334 9783527615322 3527615326 |
| Descrizione fisica | 1 online resource (262 p.) |
| Altri autori (Persone) | GoodfellowJulia M |
| Disciplina | 574.880113 574.880285 |
| Soggetti | Molecular biology - Data processing Molecular biology - Computer simulation |
| Lingua di pubblicazione | Inglese |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| Note generali | Description based upon print version of record. |
| 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 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
