Record Nr. UNINA9910877602103321 Computer modelling in molecular biology / / edited by Julia M. **Titolo** Goodfellow Pubbl/distr/stampa Weinheim;; New York,: VCH, c1995 **ISBN** 1-281-75862-0 9786611758622 3-527-61533-4 3-527-61532-6 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 Description based upon print version of record. Note generali Includes bibliographical references and index. Nota di bibliografia 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 Molecules Index This book supplies an application-oriented introduction to molecular Sommario/riassunto 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,

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