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Record Nr.	UNINA9910143872903321
Titolo	Mathematical Methods for Protein Structure Analysis and Design : Advanced Lectures / / edited by Concettina Guerra, Sorin Istrail
Pubbl/distr/stampa	Berlin, Heidelberg : , : Springer Berlin Heidelberg : , : Imprint : Springer, , 2003
ISBN	3-540-44827-6
Edizione	[1st ed. 2003.]
Descrizione fisica	1 online resource (XI, 157 p.)
Collana	Lecture Notes in Bioinformatics ; ; 2666
Disciplina	572/.633/015118
Soggetti	Mathematics Algorithms Computer science—Mathematics Database management Computer graphics Optical data processing Mathematics, general Algorithm Analysis and Problem Complexity Discrete Mathematics in Computer Science Database Management Computer Graphics Image Processing and Computer Vision
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Bibliographic Level Mode of Issuance: Monograph
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Protein Structure Comparison: Algorithms and Applications -- Spatial Pattern Detection in Structural Bionformatics -- Geometric Methods for Protein Structure Comparison -- Identifying Flat Regions and Slabs in Protein Structures -- OPTIMA: A New Score Function for the Detection of Remote Homologs -- A Comparison of Methods for Assessing the Structural Similarity of Proteins -- Prediction of Protein Secondary Structure at High Accuracy Using a Combination of Many Neural Networks -- Self-consistent Knowledge-Based Approach to Protein Design -- Protein Structure from Solid-State NMR -- Learning Effective Amino-Acid Interactions -- Proteinlike Properties of Simple Models.

Sommario/riassunto

The papers collected in this volume reproduce contributions by leading scharstoaninternationalschoolandworkshopwhichwasorganizedandheldwith thegoaloftakinga snapshotofadiscipline undertumultuous growth. Indeed, the area of protein folding, docking and alignment is developing in response to needs for a mix of heterogeneous expertise spanning biology, chemistry, mathematics, computer science, and statistics, among others. Some of the problems encountered in this area are not only important for the scientific challenges they pose, but also for the opportunities they disclose intermsofmedicalandindustrialexploitation. Atypicalexampleisofferedby protein-drug interaction (docking), a problem posing daunting computational problems at the crossroads of geometry, physics and chemistry, and, at the same time, a problem with unimaginable implications for the pharmacopoeia of the future. The schoolfocused on problems posed by the study of the mechanisms - hind protein folding, and explored different ways of attacking these problems under objective evaluations of the methods. Together with a relatively small core of consolidated knowledge and tools, important reflections were brought to this effort by studies in a multitude of directions and approaches. It is obviously impossible to predict which, if any, among these techniques will prove completely successful, but it is precisely the implicit dialectic among them that best conveys the current flavor of the field. Such unique diversity and richness inspired the format of the meeting, and also explains the slight departure of the present volume from the typical format in this series: the exposition of the current sediment is complemented here by a selection of qualified specialized contributions.