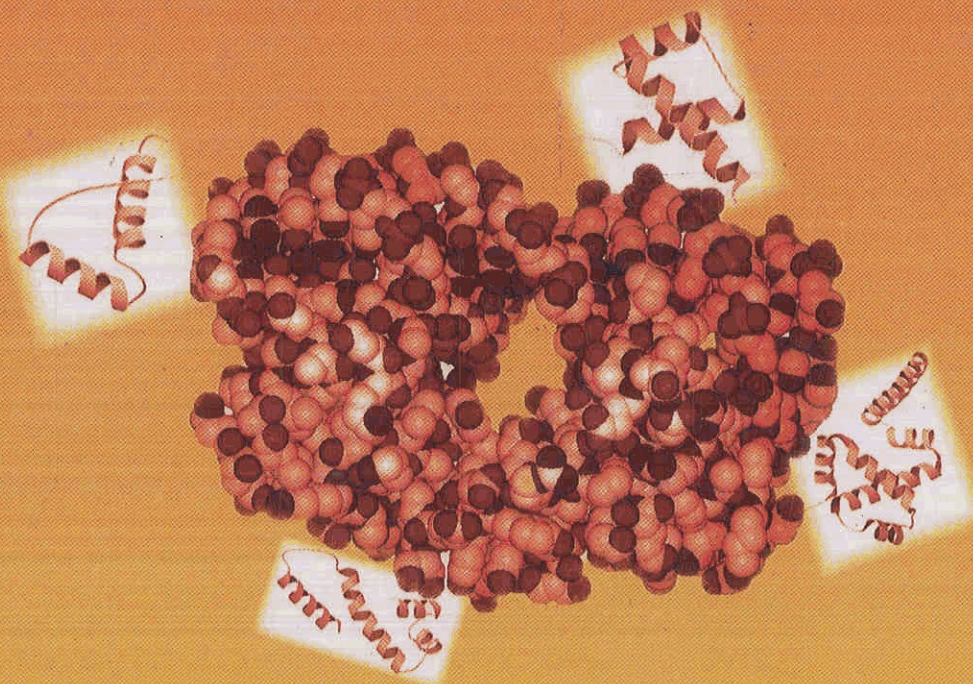


Bioinformatics

Volume II

Structure, Function and Applications



Edited by

Jonathan M. Keith

Contents

<i>Preface</i>	v
<i>Contributors</i>	ix
<i>Content of Volume I</i>	xiii

SECTION I: STRUCTURES

1. UNAFold: <i>Software for Nucleic Acid Folding and Hybridization</i>	3
<i>Nicholas R. Markham and Michael Zuker</i>	
2. Protein Structure Prediction	33
<i>Bissan Al-Lazikani, Emma E. Hill, and Veronica Morea</i>	
3. An Introduction to Protein Contact Prediction	87
<i>Nicholas Hamilton and Thomas Huber</i>	
4. Analysis of Mass Spectrometry Data in Proteomics.	105
<i>Rune Matthiesen and Ole N. Jensen</i>	
5. The Classification of Protein Domains	123
<i>Russell L. Marsden and Christine A. Orengo</i>	

SECTION II: INFERRING FUNCTION

6. Inferring Function from Homology.	149
<i>Richard D. Emes</i>	
7. The Rosetta Stone Method	169
<i>Shailesh V. Date</i>	
8. Inferring Functional Relationships from Conservation of Gene Order	181
<i>Gabriel Moreno-Hagelsieb</i>	
9. Phylogenetic Profiling	201
<i>Shailesh V. Date and José M. Peregrín-Alvarez</i>	
10. Phylogenetic Shadowing: <i>Sequence Comparisons of Multiple Primate Species</i>	217
<i>Dario Boffelli</i>	
11. Prediction of Regulatory Elements	233
<i>Albin Sandelin</i>	
12. Expression and Microarrays	245
<i>Joaquín Dopazo and Fátima Al-Shahrour</i>	
13. Identifying Components of Complexes	257
<i>Nicolas Goffard and Georg Weiller</i>	
14. Integrating Functional Genomics Data	267
<i>Insuk Lee and Edward M. Marcotte</i>	

SECTION III: APPLICATIONS AND DISEASE

15. Computational Diagnostics with Gene Expression Profiles	281
<i>Claudio Lottaz, Dennis Kostka, Florian Markowitz, and Rainer Spang</i>	

16.	Analysis of Quantitative Trait Loci	297
	<i>Mario Falchi</i>	
17.	Molecular Similarity Concepts and Search Calculations	327
	<i>Jens Auer and Jürgen Bajorath</i>	
18.	Optimization of the MAD Algorithm for Virtual Screening	349
	<i>Hanna Eckert and Jürgen Bajorath</i>	
19.	Combinatorial Optimization Models for Finding Genetic Signatures from Gene Expression Datasets	363
	<i>Regina Berretta, Wagner Costa, and Pablo Moscato</i>	
20.	Genetic Signatures for a Rodent Model of Parkinson's Disease Using Combinatorial Optimization Methods	379
	<i>Mou'ath Hourani, Regina Berretta, Alexandre Mendes, and Pablo Moscato</i>	
SECTION IV: ANALYTICAL AND COMPUTATIONAL METHODS		
21.	Developing Fixed-Parameter Algorithms to Solve Combinatorially Explosive Biological Problems	395
	<i>Falk Hüffner, Rolf Niedermeier, and Sebastian Wernicke</i>	
22.	Clustering	423
	<i>Geoffrey J. McLachlan, Richard W. Bean, and Shu-Kay Ng</i>	
23.	Visualization	441
	<i>Falk Schreiber</i>	
24.	Constructing Computational Pipelines.	451
	<i>Mark Halling-Brown and Adrian J. Shepherd</i>	
25.	Text Mining	471
	<i>Andrew B. Clegg and Adrian J. Shepherd</i>	
	<i>Index</i>	493