Contents

Protein Structure Comparison: Algorithms and Applications
Giuseppe Lancia, Sorin Istrail 1
1 Introduction 1
2 Preliminaries 4
3 Applications of Structure Comparisons 6
4 Software and Algorithms for Structure Comparison 11
5 Problems Based on Contact Map Representations 20
6 Acknowledgements 30
References 30

Spatial Pattern Detection in Structural Bionformatics
Haim J. Wolfson 35
1 Introduction 35
2 Protein Shape Representation 37
3 Protein Structural Alignment 38
4 Protein-Protein Docking 46
5 Summary 52
References 53

Geometric Methods for Protein Structure Comparison
Carlo Ferrari, Concettina Guerra 57
1 Introduction 57
2 Protein Description 59
3 Structural Comparison: Problem Formulation 62
4 Representation of Rigid Transformations 63
5 Determination of 3D Rigid Transformations 68
6 Geometric Pattern Matching 71
7 Indexing Techniques 73
8 Graph-Theoretic Approaches 76
9 Integration of Methods for Protein Comparison Using Different Representations 77

10 Conclusions 78
11 Acknowledgements 79
References 79

Identifying Flat Regions and Slabs in Protein Structures
Mary Ellen Bock, Concettina Guerra 83
1 Introduction 83
2 A Geometric Algorithm 85
3 An Improved Geometric Algorithm 87
4 Hough Transform 88
5 Performances of the Two Algorithms 90
6 Plane Detection in Proteins 92
7 Acknowledgements 95
References 96

OPTIMA: A New Score Function for the Detection of Remote Homologs
Maricel Kann, Richard A. Goldstein 99
1 Abstract 99
2 Introduction 99
3 Methods 100
References 107

A Comparison of Methods for Assessing the Structural Similarity of Proteins
Dean C. Adams, Gavin J.P. Naylor 109
1 Introduction 109
2 The DALI Algorithm 109
3 The Root Mean Square Algorithm 110
4 Geometric Morphometrics 111
5 Comparison of Methods 111
6 Discussion 113
References 114

Prediction of Protein Secondary Structure at High Accuracy Using a Combination of Many Neural Networks
Claus Lundegaard, Thomas Nordahl Petersen, Morten Nielsen, Henrik Bohr, Jacob Bohr, Søren Brunak, Garry Gippert, Ole Lund 117
1 Summary 117
2 Introduction 117
3 Methods 118
4 Results 119
References 121

Self-consistent Knowledge-Based Approach to Protein Design
Andrea Rossi, Cristian Micheletti, Flavio Seno, Amos Maritan 123
1 Introduction 123
2 The Design Strategy 124
3 Results and Discussion 125
4 Summary 127
References 128

Protein Structure from Solid-State NMR
John R. Quine, Timothy A. Cross 131
1 Discrete Curves 131
2 Tensors and NMR 133
3 Structure from Orientational Constraints 134
4 Acknowledgment 136
References 136

Learning Effective Amino-Acid Interactions
Flavio Seno, Cristian Micheletti, Amos Maritan, Jayanth R. Banavar . . 139
1 Introduction 139
2 Models and Techniques 141
3 Results 142
4 Conclusions 144
References 144

Proteinlike Properties of Simple Models
Yves-Henri Sanejouand, Georges Trinquier 147
1 The 3x3x3 Cubic Lattice Model 147
2 N-Soft-Spheres Models 151
References 152

List of Participants 155