

CONTENTS

PREFACE	vii
CONTRIBUTORS	xi
1 INTRODUCTION TO PROTEIN STRUCTURE PREDICTION <i>Huzefa Rangwala and George Karypis</i>	1
2 CASP: A DRIVING FORCE IN PROTEIN STRUCTURE MODELING <i>Andriy Kryshchak, Krzysztof Fidelis, and John Moult</i>	15
3 THE PROTEIN STRUCTURE INITIATIVE <i>Andras Fiser, Adam Godzik, Christine Orengo, and Burkhard Rost</i>	33
4 PREDICTION OF ONE-DIMENSIONAL STRUCTURAL PROPERTIES OF PROTEINS BY INTEGRATED NEURAL NETWORKS <i>Yaoqi Zhou and Eshel Faraggi</i>	45
5 LOCAL STRUCTURE ALPHABETS <i>Agnel Praveen Joseph, Aurélie Bornot, and Alexandre G. de Brevern</i>	75
6 SHEDDING LIGHT ON TRANSMEMBRANE TOPOLOGY <i>Gábor E. Tusnády and István Simon</i>	107
7 CONTACT MAP PREDICTION BY MACHINE LEARNING <i>Alberto J.M. Martin, Catherine Mooney, Ian Walsh, and Gianluca Pollastri</i>	137
8 A SURVEY OF REMOTE HOMOLOGY DETECTION AND FOLD RECOGNITION METHODS <i>Huzefa Rangwala</i>	165
9 INTEGRATIVE PROTEIN FOLD RECOGNITION BY ALIGNMENTS AND MACHINE LEARNING <i>Allison N. Tegge, Zheng Wang, and Jianlin Cheng</i>	195

10	TASSER-BASED PROTEIN STRUCTURE PREDICTION	219
	<i>Shashi Bhushan Pandit, Hongyi Zhou, and Jeffrey Skolnick</i>	
11	COMPOSITE APPROACHES TO PROTEIN TERTIARY STRUCTURE PREDICTION: A CASE-STUDY BY I-TASSER	243
	<i>Ambrish Roy, Sitao Wu, and Yang Zhang</i>	
12	HYBRID METHODS FOR PROTEIN STRUCTURE PREDICTION	265
	<i>Dmitri Mourado, Bostjan Kobe, Nicholas E. Dixon, and Thomas Huber</i>	
13	MODELING LOOPS IN PROTEIN STRUCTURES	279
	<i>Narcis Fernandez-Fuentes, Andras Fiser</i>	
14	MODEL QUALITY ASSESSMENT USING A STATISTICAL PROGRAM THAT ADOPTS A SIDE CHAIN ENVIRONMENT VIEWPOINT	299
	<i>Genki Terashi, Mayuko Takeda-Shitaka, Kazuhiko Kanou and Hideaki Umeyama</i>	
15	MODEL QUALITY PREDICTION	323
	<i>Liam J. McGuffin</i>	
16	LIGAND-BINDING RESIDUE PREDICTION	343
	<i>Chris Kauffman and George Karypis</i>	
17	MODELING AND VALIDATION OF TRANSMEMBRANE PROTEIN STRUCTURES	369
	<i>Maya Schushan and Nir Ben-Tal</i>	
18	STRUCTURE-BASED MACHINE LEARNING MODELS FOR COMPUTATIONAL MUTAGENESIS	403
	<i>Majid Masso and Iosif I. Vaisman</i>	
19	CONFORMATIONAL SEARCH FOR THE PROTEIN NATIVE STATE	431
	<i>Amarda Shehu</i>	
20	MODELING MUTATIONS IN PROTEINS USING MEDUSA AND DISCRETE MOLECULE DYNAMICS	453
	<i>Shuangye Yin, Feng Ding, and Nikolay V. Dokholyan</i>	
	INDEX	477