

---

# Contents

<i>Preface</i> . . . . .	<i>v</i>
<i>Contributors</i> . . . . .	<i>ix</i>
1 Protein Structure Modeling with <i>MODELLER</i> . . . . .	1
<i>Benjamin Webb and Andrej Sali</i>	
2 RaptorX server: A Resource for Template-Based Protein Structure Modeling . . . . .	17
<i>Morten Källberg, Gohar Margaryan, Sheng Wang, Jianzhu Ma, and Jinbo Xu</i>	
3 The MULTICOM Protein Tertiary Structure Prediction System . . . . .	29
<i>Jilong Li, Debswapna Bhattacharya, Renzhi Cao, Badri Adhikari, Xin Deng, Jesse Eickholt, and Jianlin Cheng</i>	
4 Modeling of Protein Side-Chain Conformations with RASP . . . . .	43
<i>Zhichao Miao, Yang Cao, and Taijiao Jiang</i>	
5 Direct Coupling Analysis for Protein Contact Prediction . . . . .	55
<i>Faruck Morcos, Terence Hwa, José N. Onuchic, and Martin Weigt</i>	
6 ITScorePro: An Efficient Scoring Program for Evaluating the Energy Scores of Protein Structures for Structure Prediction . . . . .	71
<i>Sheng-You Huang and Xiaoqin Zou</i>	
7 Assessing the Quality of Modelled 3D Protein Structures Using the ModFOLD Server . . . . .	83
<i>Daniel Barry Roche, Maria Teresa Buenavista, and Liam James McGuffin</i>	
8 3D-SURFER 2.0: Web Platform for Real-Time Search and Characterization of Protein Surfaces . . . . .	105
<i>Yi Xiong, Juan Esquivel-Rodriguez, Lee Sael, and Daisuke Kihara</i>	
9 SPOT-Seq-RNA: Predicting Protein–RNA Complex Structure and RNA-Binding Function by Fold Recognition and Binding Affinity Prediction . . . . .	119
<i>Yuedong Yang, Huiying Zhao, Jibua Wang, and Yaoqi Zhou</i>	
10 POODLE: Tools Predicting Intrinsically Disordered Regions of Amino Acid Sequence . . . . .	131
<i>Kana Shimizu</i>	
11 Prediction of Intrinsic Disorder in Proteins Using MFDp2 . . . . .	147
<i>Marcin J. Mizianty, Vladimir Uversky, and Lukasz Kurgan</i>	

12	Modeling Protein–Protein Complexes Using the HADDOCK Webserver “Modeling Protein Complexes with HADDOCK” . . . . .	163
	<i>Gydo C.P. van Zundert and Alexandre M.J.J. Bonvin</i>	
13	Predicting the Structure of Protein–Protein Complexes Using the SwarmDock Web Server . . . . .	181
	<i>Mieczyslaw Torchala and Paul A. Bates</i>	
14	DOCK/PIERR: Web Server for Structure Prediction of Protein–Protein Complexes. . . . .	199
	<i>Shruthi Viswanath, D.V.S. Ravikant, and Ron Elber</i>	
15	Pairwise and Multimeric Protein–Protein Docking Using the LZerD Program Suite . . . . .	209
	<i>Juan Esquivel-Rodriguez, Vianney Filos-Gonzalez, Bin Li, and Daisuke Kihara</i>	
16	Protocols for Efficient Simulations of Long-Time Protein Dynamics Using Coarse-Grained CABS Model . . . . .	235
	<i>Michal Jamroz, Andrzej Kolinski, and Sebastian Kmiecik</i>	
	<i>Index</i> . . . . .	251

Protein Structure Prediction

Kihara, D. (Ed.)

2014, XI, 253 p. 64 illus., 48 illus. in color., Hardcover

ISBN: 978-1-4939-0365-8

A product of Humana Press