
Preface

Computational protein tertiary structure prediction has been extensively studied over the last two decades. Many approaches have been proposed, tested, and compared by researchers of various backgrounds who are attracted by this simple but fascinating protein structure prediction problem. We now see the field maturing, resulting in prediction methods able to produce sufficiently accurate structure models for many cases, although it is still far from the complete solution of the problem. As prediction methods become more practically useful, it becomes important to disseminate developed software to the research community so that researchers who are not necessarily familiar with computational tools can easily access and use them in their daily research activities. This software dissemination is also very beneficial for researchers who develop prediction methods because they can easily compare their methods with existing ones or integrate them as part of a pipeline of a prediction procedure. With this philosophy in mind, in the third edition of this book we focus on introducing software or Web servers which are available for researchers. This is a major difference from the second edition, which emphasized descriptive explanation of methods. Each chapter of the third edition provides practical step-by-step instructions of how to use a computational method with actual examples of prediction by the method. The chapters describe well-established methods developed by well-known researchers in this field.

The book starts by introducing three protein structure prediction/modeling methods. These methods take a single protein sequence as input and predict the tertiary structure of the input protein. The first chapter was written by Benjamin Webb and Andrej Sali on their extremely popular structure modeling tool, MODELLER. In the second chapter, Jinbo Xu and his colleagues present RaptorX, a template-based protein structure prediction server. In the third chapter, Jianlin Cheng and his colleagues provide a tutorial for their server, MULTICOM.

The next four chapters provide tools that are useful for subsequent steps of main-chain conformation prediction, which can be done by the methods introduced in Chapters 1–3. Chapter 4 deals with prediction of side-chain conformation of a protein structure model. Jiang Taijiao and his group members describe their method, RASP. The method takes the main-chain atom positions as input and builds side-chains of the protein. Chapter 5 details the use of Direct Coupling Analysis, a residue–residue contact prediction method written by Faruck Morcos, Terence Hwa, José N. Onuchic, and Martin Weigt. The method predicts physically contacting amino acid residues in the protein tertiary structure from a multiple sequence alignment. Contact prediction is useful for guiding protein structure modeling and also for selecting the most probable models from a pool of different structure models. ITScorePro, introduced in Chapter 6, is a scoring program for ranking different structure models of a target protein developed by Xiaoqin Zou's group. It is typical that a structure prediction method produces a large number of structure models, and thus identifying the most plausible model is a practically very important task in prediction. In Chapter 7, Liam James McGuffin and his colleagues describe how to use their model quality assessment server, ModFOLD. The server provides the estimated accuracy of a structure model,

i.e., overall accuracy and per-residue accuracy of a model. Estimated accuracy is helpful for practical use of a model as well as for choosing the most plausible models from a pool of different models.

When the structure of a protein is modeled, it is often of interest to find similar existing structures in a database, since structure similarity often provides insight into the function and evolution of the protein. Chapter 8 introduces 3D-SURFER, a server for real-time structure database search, which was developed by Daisuke Kihara and his group members. Yaoqi Zhou and his colleagues have extended their protein structure prediction methods for predicting protein–RNA complex structures in SPOT-Seq-RNA. Their method, described in Chapter 9, takes a protein sequence as input and predicts RNA sequences that would interact with the protein and the tertiary structure of the protein–RNA complex.

The subsequent two chapters are for prediction methods of intrinsic disordered regions. It has been found that many proteins have regions that are designed not to form a fixed structure and are thus called intrinsic disordered regions. These regions often have important functions such as serving as interaction sites to other proteins. In Chapter 10, Kana Shimizu describes how to use POODLE, while readers are introduced to MFDp2 by Marcin J. Mizianty, Vladimir Uversky, and Lukasz Kurgan in Chapter 11.

What follows is four chapters for protein–protein docking prediction. A protein–protein docking method predicts the complex structure of two (or more) protein structures. Chapter 12 was written by Gydo C. P. van Zudert and Alexandre M. J. J. Bonvin on their docking method, HADDOCK. In Chapter 13, the SwarmDock Web server developed by the Paul A. Bates group is introduced. The following chapter is about the DOCK/PIERR server by Ron Elber and his team. In Chapter 15, the LZerD docking program, which can perform pairwise as well as multiple protein docking, is reported by Daisuke Kihara and his lab members.

Finally, in Chapter 16, protocols for protein dynamics simulations with the CABS protein model are provided by Michal Jamroz, Andrzej Kolinski, and Sebastian Kmiecik. As you see now, this book covers a series of methods for protein structure prediction and related tools, model quality assessment, disordered region prediction, protein–protein docking, and protein dynamics. The diversity of the introduced methods shows the expansion of the computational protein structure prediction field. It will be my great pleasure if this book helps biology researchers with the use of computational methods for protein structure prediction and also serves as a bridge between computational and experimental biologists.

In closing, I would like to thank all of the authors of chapters in this book. This edition is very fortunate to have the leading experts of the field as the authors. I am also thankful to the series editor, Dr. John M. Walker for his patience and guidance and Ms. Kristen Johnson in my research group for her tremendous help in editing this book.

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