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## Preface

One of the most important challenges in molecular biology is to figure out how the one-dimensional (1D) sequence of amino acid residues in a protein at a physiological condition specifies its unique, functional three-dimensional (3D) structure. Despite more than 50 years of effort, reliable computational protein models with experimental resolution remain out of reach, except for homology models that are based on the structures of highly similar sequences. To overcome the challenge of prediction from 1D to 3D, many 1D to 1D methods have been developed as an intermediate step or a substitute for 1D to 3D prediction. These 1D quantities can be either structural or functional properties characterized by a one-dimensional vector along the protein sequence. One prominent example is protein secondary structure where protein backbone structure is annotated by a few states such as helices, sheets, or coils. Protein backbone structure can also be characterized by torsion angles. In addition to backbone structural properties, protein structures can be characterized by global structural properties: Properties that depend on interactions between multiple residues that are far apart in the sequence. One such example is the solvent accessible surface area, relevant to tertiary packing and function of proteins. More recently, predicting one-dimensional functional properties (functional sites in particular) from protein sequences has received increasing attention.

This book starts from secondary structure prediction based on sequence only (GOR, Chapters 1 and 2 and single helix prediction, Chapter 3), followed by secondary structure prediction based on evolution information (CDM, Chapter 4, SPINE-X, Chapter 5, and SPIDER2, Chapter 6). In addition to secondary structure, SPINE-X and SPIDER2 also predict solvent accessible surface areas and backbone torsion angles. The latter is reviewed in Chapter 7. Predicted secondary structures are utilized in model building (Chapters 8 and 9). Next, a few chapters focus on global structural properties (solvent accessibility in Chapter 10; intrinsically disordered regions in Chapters 11 and 12; and protein flexibility in Chapter 13). Functional properties are predicted in Chapter 14 (DNA/RNA-binding sites), Chapter 15 (RNA-binding residues), Chapter 16 (protein-binding sites), Chapter 17 (B-cell epitopes), Chapter 18 (phosphorylation sites), and Chapter 19 (post-translation modifications). Chapter 20 describes a tool for visualizing interior and protruding regions in proteins. These chapters represent a fraction of the excellent methods available in the literature. We hope that this collection will provide a guide to a few current state-of-the-art techniques that are useful for computational and experimental biologists.

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