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Nota di contenuto	1. Introduction. 1.1. Protein structure. 1.2. Structure determination. 1.3. Dynamics simulation. 1.4. The myth of protein folding -- 2. X-ray crystallography computing. 2.1. The phase problem. 2.2. Least squares solutions. 2.3. Entropy maximization. 2.4. Indirect methods -- 3. NMR structure determination. 3.1. Nuclear magnetic resonance. 3.2. Distance geometry. 3.3. Distance-based modeling. 3.4. Structural analysis -- 4. Potential energy minimization. 4.1. Potential energy function. 4.2. Local optimization. 4.3. Global optimization. 4.4. Energy transformation -- 5. Molecular dynamics simulation. 5.1. Equations of motion. 5.2. Initial-value problem. 5.3. Boundary-value problem. 5.4. Normal mode analysis -- 6. Knowledge-based protein modeling. 6.1. Sequence/structural alignment. 6.2. Fold recognition/inverse folding. 6.3. Knowledge-based structural refinement. 6.4. Structural computing and beyond.
Sommario/riassunto	While the field of computational structural biology or structural bioinformatics is rapidly developing, there are few books with a relatively complete coverage of such diverse research subjects studied in the field as X-ray crystallography computing, NMR structure determination, potential energy minimization, dynamics simulation, and knowledge-based modeling. This book helps fill the gap by providing such a survey on all the related subjects. Comprising a

collection of lecture notes for a computational structural biology course for the Program on Bioinformatics and Computational Biology at Iow