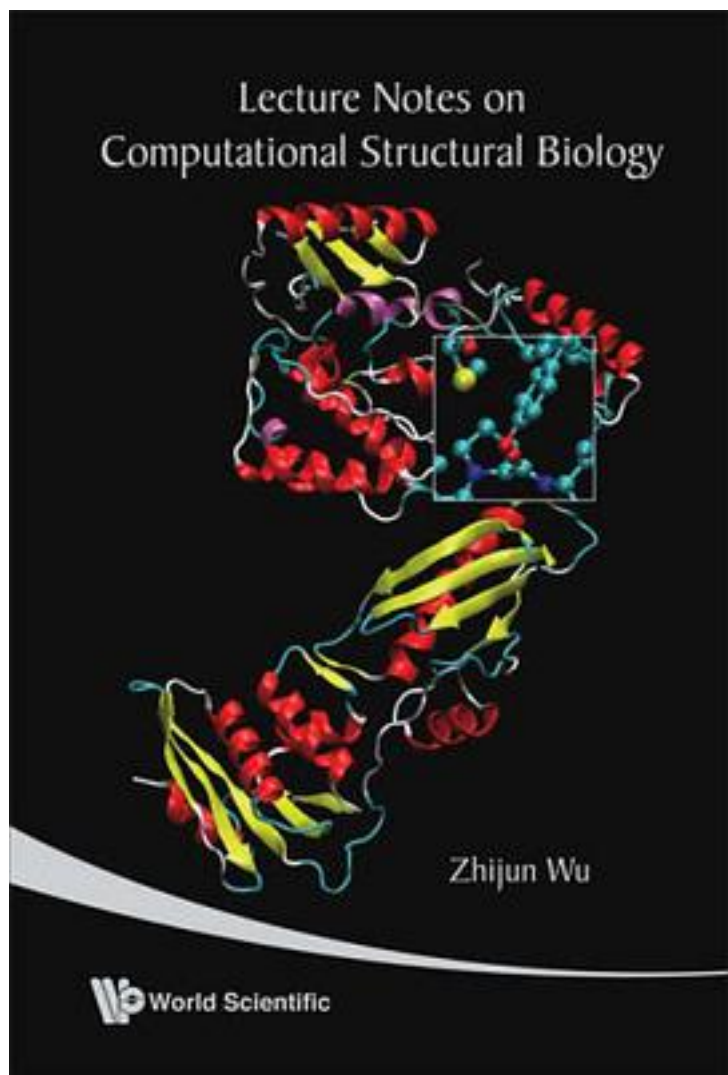


Lecture Notes on Computational Structural Biology



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出版者:World Scientific Pub Co Inc

出版时间:2008-6

装帧:HRD

isbn:9789812705891

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 Iowa State University, the book is in essence a comprehensive summary of computational structural biology based on the author's own extensive research experience, and a review of the subject from the perspective of a computer scientist or applied mathematician. Readers will gain a deeper appreciation of the biological importance and mathematical novelty of the research in the field.

Contents: X-ray Crystallography Computing NMR Structure Determination Potential Energy Minimization Molecular Dynamics Simulation Knowledge-based Protein Modeling Appendices: Design and Analysis of Computer Algorithms Numerical Methods.

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