Algorithms in Structural Molecular Biology (Hardback)

By Bruce R. Donald

MIT Press Ltd, United States, 2011. Hardback. Book Condition: New. 229 x 203 mm. Language: English . Brand New Book. Using the tools of information technology to understand the molecular machinery of the cell offers both challenges and opportunities to computational scientists. Over the past decade, novel algorithms have been developed both for analyzing biological data and for synthetic biology problems such as protein engineering. This book explains the algorithmic foundations and computational approaches underlying areas of structural biology including NMR (nuclear magnetic resonance); X-ray crystallography; and the design and analysis of proteins, peptides, and small molecules. Each chapter offers a concise overview of important concepts, focusing on a key topic in the field. Four chapters offer a short course in algorithmic and computational issues related to NMR structural biology, giving the reader a useful toolkit with which to approach the fascinating yet thorny computational problems in this area. A recurrent theme is understanding the interplay between biophysical experiments and computational algorithms. The text emphasizes the mathematical foundations of structural biology while maintaining a balance between algorithms and a nuanced understanding of experimental data. Three emerging areas, particularly fertile ground for research students, are highlighted: NMR methodology, design of proteins...

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