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Algorithms in Structural Molecular Biology Bruce R. Donald The MIT Press Cambridge, Massachusetts London, England . p Brief Contents Preface xxiii Acknowledgments xxxi 1 Introduction to Protein Structure and NMR 1 ... 17.1 NMR Structure Determination Algorithms Using Sparse RDCs 145

Algorithms in Structural Molecular Biology

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Algorithms in Structural Molecular Biology by Bruce R. Donald
Book Summary: Using the tools of information technology to understand the molecular machinery of the cell offers both challenges and opportunities to computational scientists.

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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 and other molecules, and the modeling of protein flexibility.

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1 Algorithmic Challenges in Structural Molecular Biology and Proteomics
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enabled us to collaborate with biological crystallographers to reveal the architecture of a parasite's en-zyme, which could help researchers reduce the threat of certain diseases among those with weak immune systems [17 ...

Physical Geometric Algorithms for Structural Molecular Biology

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of the cell offers both challenges and opportunities to computational scientists.

Protein design - Wikipedia

If your thesis area is not molecular or structural biological, to make sure your project proposal is acceptable -- make sure that in the proposal/project what you *mostly* write about are the computational biology algorithms you invent, use, and implement and how they worked -- what we don't want is a really long description that's 90 percent ...

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As an optimization problem. The goal of protein design is to find a protein sequence that will fold to a target structure. A protein

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design algorithm must, thus, search all the conformations of each sequence, with respect to the target fold, and rank sequences according to the lowest-energy conformation of each one,...

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An overview of algorithms important to computational structural biology that addresses such topics as NMR and design and analysis of proteins. Using the tools of information technology to understand the molecular machinery of the cell offers both challenges and opportunities to computational scientists.

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quick structural assays to speed data to the biologist early in an investigation, and could in principle be applied in an automation-like fashion to a large fraction of the proteome. 3.2 Algorithmic Approach Jigsaw consists of two main components: (1) graph-based secondary structure pattern identification in unas-

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