

Clustering in Bioinformatics and Drug Discovery (Chapman & Hall/CRC Mathematical and Computational Biology)

John David MacCuish, Norah E. MacCuish



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With a DVD of color figures, **Clustering in Bioinformatics and Drug Discovery** provides an expert guide on extracting the most pertinent information from pharmaceutical and biomedical data. It offers a concise overview of common and recent clustering methods used in bioinformatics and drug discovery.

Setting the stage for subsequent material, the first three chapters of the book introduce statistical learning theory, exploratory data analysis, clustering algorithms, different types of data, graph theory, and various clustering forms. In the following chapters on partitional, cluster sampling, and hierarchical algorithms, the book provides readers with enough detail to obtain a basic understanding of cluster analysis for bioinformatics and drug discovery. The remaining chapters cover more advanced methods, such as hybrid and parallel algorithms, as well as details related to specific types of data, including asymmetry, ambiguity, validation measures, and visualization.

This book explores the application of cluster analysis in the areas of bioinformatics and cheminformatics as they relate to drug discovery. Clarifying the use and misuse of clustering methods, it helps readers understand the relative merits of these methods and evaluate results so that useful hypotheses can be developed and tested.

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