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1 Computational Biology and Biochemistry -- 2 Cheminformatics I: Ligand-Based Molecular Modeling -- 3 Cheminformatics II: Structure-Based Molecular Modeling and Drug Design -- 4 Bioinformatics -- 5 Machine Learning, Artificial intelligence, and Big Data.

Sommario/riassunto

The Springer Handbook of Chem- and Bioinformatics provides an introduction as well as a detailed description of the application of various techniques used in chemo- and bioinformatics. It covers basic topics such as a discussion of computational techniques used in the predictions of structures, properties, and dynamics of small compounds, macromolecules, and their complexes. Diverse applications of Quantitative structure-activity relationships (QSAR) methods are also revealed. Various chapters offer specifics of current methodologies used by research labs in the pharmaceutical industry for drug design. Modern computational approaches taking advantage of searching big data, using artificial intelligence and machine learning are discussed, while the necessity of applying such advanced novel techniques for bio- and chemo-informatics is revealed. This handbook combines nicely together discussion and assessment of both closely related fields of modern informatics. It is a welcome addition to the university libraries, research institutes, as well as to basic textbook resources of individual researchers. The target audience includes students (both graduate and advanced undergraduate), university researchers, scientists working in private and governmental laboratories as well as a large group of developers from pharmaceutical and medical institutes and related industrial research centers.