Bioinformatics, Chemoinformatics, and Drug Design

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Informatics and computers have not yet become as pervasive in chemistry as they have in physics and biology. Drawing analogies from bioinformatics, key ingredients for progress in chemoinformatics are the availability of large, annotated databases of compounds and reactions, algorithms to efficiently search these databases and to predict the physical, chemical, and biological properties of new compounds and reactions. We will describe the development of: (1) a large public database of compounds and reactions (ChemDB); (2) machine learning kernel methods to predict molecular properties; and (3) the applications of these methods in drug screening/design to identify new leads against a major disease.