



## Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery (Hardback)

By -

Humana Press Inc., United States, 2004. Hardback. Condition: New. 2004 ed.. Language: English . Brand New Book \*\*\*\*\* Print on Demand \*\*\*\*\*.In the literature, several terms are used synonymously to name the topic of this book: chem-, chemi-, or chemo-informatics. A widely recognized definition of this discipline is the one by Frank Brown from 1998 (1) who defined chemoinformatics as the combination of all the information resources that a scientist needs to optimize the properties of a ligand to become a drug. In Brown's definition, two aspects play a fundamentally important role: decision support by computational means and drug discovery, which distinguishes it from the term chemical informatics that was introduced at least ten years earlier and described as the application of information technology to chemistry (not with a specific focus on drug discovery). In addition, there is of course chemometrics, which is generally understood as the application of statistical methods to chemical data and the derivation of relevant statistical models and descriptors (2). The pharmaceutical focus of many developments and efforts in this area-and the current popularity of gene-to-drug or similar paradigms-is further reflected by the recent introduction of such terms as discovery informatics...



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