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This thorough book provides a collection of techniques used in the emerging field of computational chemogenomics, which is an integration of chemoinformatics, bioinformatics, computer science, statistics, automated pattern recognition and modeling, database usage with data retrieval, and systems integration. [Computational Chemogenomics | J.B. Brown | Springer](#) This book provides a collection of techniques used in the emerging field of computational chemogenomics, an integration of chemoinformatics, bioinformatics, computer science, statistics, automated pattern recognition and modeling, database usage with data retrieval, and systems integration.

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Computational chemogenomics is expected to increase the quality and productivity of drug discovery and lead to the discovery of new medicines. Students and academics in chemistry, bioinformatics and pharmaceutical sciences

Chemogenomics - Wikipedia

Chemogenomics, or chemical genomics, is the systematic screening of targeted chemical libraries of small molecules against individual drug target families (e.g., GPCRs, nuclear receptors, kinases, proteases, etc.) with the ultimate goal of identification of novel drugs and drug targets.

Computational systems pharmacology analysis of cannabidiol ...

Integrated computational methodologies, including homology modeling, molecular docking, and molecular dynamics simulation, were used to evaluate the protein-CBD binding modes. A CBD-preferred pocket consisting of a hydrophobic cavity and backbone hinges was proposed and tested for CBD-class A GPCR binding.

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