



## Computer-Aided Drug Discovery (Hardback)

By -

Humana Press Inc., United States, 2016. Hardback. Condition: New. 1st ed. 2016. Language: English . Brand New Book. This detailed volume examines computer-aided drug discovery (CADD), a crucial component of modern drug discovery programs that is widely utilized to identify and optimize bioactive compounds for the development of new drugs. With a focus on the methods that are commonly used in the early stage of drug discovery, chapters explore computer simulation, structure prediction, conformational sampling, binding site mapping, docking and scoring, in silico screening, and fragment-based drug design. In addition to the state-of-the-art theoretical concept, this book also includes step-by-step, readily reproducible computational protocols as well as examples of various CADD strategies. The limitations and potential pitfalls of different computational methods are discussed by experts, and tips and advice for their applications are suggested. Practical and thorough, Computer-Aided Drug Discovery serves as an ideal addition to the Methods in Pharmacology and Toxicology series, guiding researchers toward their lab s goals with this exciting and versatile technology.



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