Virtual screening : principles, challenges, and practical guidelines

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Drug discovery is all about finding small molecules that interact in a desired way with larger molecules, namely proteins and other macromolecules in the human body. If the three-dimensional structures of both the small and large molecule are known, their interaction can be tested by computer simulation with a reasonable degree of accuracy. Alternatively, if active ligands are already available, molecular similarity searches can be used to find new molecules. This virtual screening can even be applied to compounds that have yet to be synthesized, as opposed to "real" screening that requires cost- and labor-intensive laboratory testing with previously synthesized drug compounds. Unique in its focus on the end user, this is a real "how to" book that does not presuppose prior experience in virtual screening or a background in computational chemistry. It is both a desktop reference and practical guide to virtual screening applications in drug discovery, offering a comprehensive and up-to-date overview. Clearly divided into four major sections, the first provides a detailed description of the methods required for and applied in virtual screening, while the second discusses the most important challenges in order to improve the impact and success of this technique. The third and fourth, practical parts contain practical guidelines and several case studies covering the most important scenarios for new drug discovery, accompanied by general guidelines for the entire workflow of virtual screening studies. Throughout the text, medicinal chemists from academia, as well as from large and small pharmaceutical companies report on their experience and pass on priceless practical advice on how to make best use of these powerful methods.