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Recent progress in high-throughput screening, combinatorial chemistry and molecular biology has radically changed the approach to drug discovery in the pharmaceutical industry. New challenges in synthesis result in new analytical methods. At present, typically 100,000 to one million molecules have to be tested within a short period and, therefore, highly effective screening methods are necessary for today's researchers - preparing and characterizing one compound after another belongs to the past. Intelligent, computer-based search agents are needed and "virtual screening" provides solutions to many problems. Such screening comprises innovative computational techniques designed to turn raw data into valuable chemical information and to assist in extracting the relevant molecular features.

This handbook is unique in bringing together the various efforts in the field of virtual screening to provide the necessary methodological framework for more effective research. Leading experts give a thorough introduction to the state of the art along with a critical assessment of both successful applications and drawbacks. The information collated here will be indispensable for experienced scientists, as well as novices, working in medicinal chemistry and related disciplines.

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