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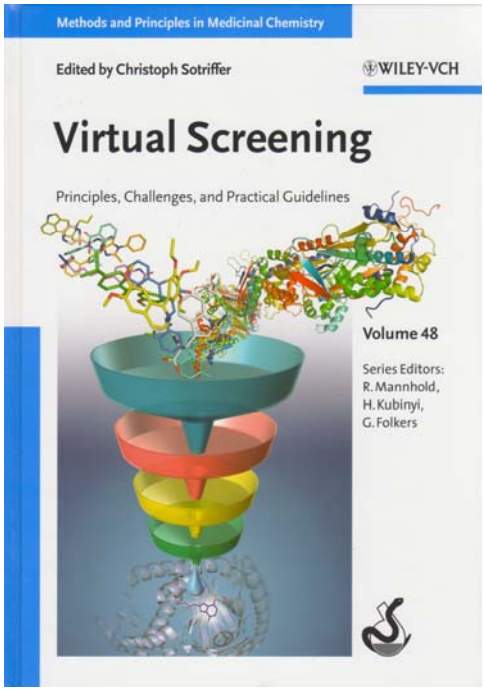
VIRTUAL SCREENING: PRINCIPLES, CHALLENGES, AND PRACTICAL GUIDELINES



WILEY-VCH
ISBN: 978-3-527-32636-5
Hardcover
550 pages
January 2011

Virtual Screening: Principles, Challenges, and Practical Guidelines offers a comprehensive and up-to-date overview and can be used both as a desktop reference and as practical guide for virtual screening applications in drug discovery. In a logical and didactic way, this volume is organized in four parts covering principles, challenges, practical guidelines, and case studies under different scenarios. Chapters of *Part One* are dedicated to virtual screening of chemical space, processing of small molecule databases for virtual screening, ligand-based and target-based virtual screening, virtual screening with 3D pharmacophore models, and docking methods. Challenges discussed in *Part Two* comprise affinity prediction, fragment-based approaches, handling of protein flexibility, as well as consideration of water and solvation effects, as well as parallel virtual screening for compound profiling and prediction of off-target effects. The *third* and *fourth*, practically oriented 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. In these parts medicinal chemists from both academia and pharmaceutical companies report on their experience and pass on priceless practical advice on how to make best use of these powerful methods.

All above-mentioned aspects of virtual screening are discussed by a team of leading experts. The book is well suited both for all practitioners in medicinal chemistry and for graduate students who want to learn how to apply virtual screening methodology.

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