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Virtual Screening in Drug Discovery (Drug Discovery Series)

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Virtual screening can reduce costs and increase hit rates for lead discovery by eliminating the need for robotics, reagent acquisition or production, and compound storage facilities. The increased robustness of computational algorithms and scoring functions, the availability of affordable computational power, and the potential for timely structural determination of target molecules, have provided new opportunities for virtual screening, and made it more practical. Why then, isn't everyone using virtual screening? Examining the scope and limitations of this method, **Virtual Screening in Drug Discovery** explores the algorithms involved and how to actually use them.

Part I offers perspectives on both ligand-based and docking-based virtual screens. The authors of these chapters frame many of the challenges currently facing the field. *Part II* considers the choice of compounds that are best suited as drug leads. *Part III* discusses ligand-based approaches, including descriptor-based similarity, traditional pharmacophore searching, and similarity based 3D-pharmacophore fingerprints. The final two sections are devoted to molecular docking. *Part IV* outlines some important and practical considerations relating to the energetics of protein-ligand binding and target-site topography, whereas specific docking algorithms and strategies are discussed in *Part V*.

Notwithstanding this list of subjects, the book does not overwhelm you with more information than you need—many of the strategies outlined will transcend the specifics of any given method. Nor does the book purport to offer single best ways to use the programs. What it does is provide a snapshot of virtual screening that gives you easy access to strategies and techniques for lead discovery.

Daniel E. Levy, editor of the *Drug Discovery Series*, is the founder of DEL BioPharma, a consulting service for drug discovery programs. He also maintains a blog that explores organic chemistry.

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