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Altri autori (Persone)	SotrifferChristoph
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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	pt. 1. Principles -- pt. 2. Challenges -- pt. 3. Applications and practical guidelines -- pt. 4. Scenarios and case studies : routes to success.
Sommario/riassunto	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