

1. Record Nr.	UNINA9910130843903321
Titolo	Virtual screening [[electronic resource]] : principles, challenges, and practical guidelines // edited by Christoph Sotriffer
Pubbl/distr/stampa	Weinheim, : Wiley-VCH, 2011
ISBN	1-283-14059-4 9786613140593 3-527-63332-4 3-527-63333-2 3-527-32636-7
Descrizione fisica	1 online resource (551 p.)
Collana	Methods and principles in medicinal chemistry ; ; v. 48
Altri autori (Persone)	SotrifferChristoph
Disciplina	615.1900113
Soggetti	High throughput screening (Drug development) - Computer simulation Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
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

2. Record Nr.	UNINA9910346925403321
Autore	Oertel HerbertKrittian, SebastianSpiegel, Kathrin
Titolo	Modelling the human cardiac fluid mechanics. 3rd ed
Pubbl/distr/stampa	KIT Scientific Publishing, 2009
ISBN	1000011015
Descrizione fisica	1 online resource (80 p. p.)
Soggetti	Technology: general issues
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Sommario/riassunto	The third edition of this article on the modelling and simulation of the flow in human hearts supplements earlier editions. It discusses the flow-structure coupled heart model KAHMO FSI (Karlsruhe Heart Model) and examines patient-specific clinical application of the heart model for cardiac surgery. The KAHMO heart model can be used to predict flow losses and flow structures due to pathological ventricle defects. These are considered before and after surgery.