

1. Record Nr.	UNINA9911006567103321
Titolo	Drug design strategies : computational techniques and applications // edited by Lee Banting, Timothy Clark
Pubbl/distr/stampa	Cambridge, : RSC Pub., 2012
ISBN	9781621981398 1621981398
Edizione	[1st ed.]
Descrizione fisica	1 online resource (251 p.)
Collana	RSC drug discovery series, , 2041-3203 ; ; 20
Altri autori (Persone)	BantingLee ClarkTimothy
Disciplina	615.19 615.1900113
Soggetti	Drugs - Design - Computer simulation
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	i-iv; v-vi; vii-x; 1-26; 27-55; 56-86; 87-106; 107-119; 120-163; 164-183; 184-209; 210-231; 232-240
Sommario/riassunto	This book documents the latest research into the theory and application of force-fields, semi-empirical molecular orbital, density functional and ab initio calculations, Quantum Mechanical (QM) based modelling, Atoms in Molecules (AIM) approach, and biomolecular dynamics. It also covers theory and application of 2D cheminformatics, QSAR/QSPR, ADME properties of drugs, drug docking/scoring protocols and approaches, topological methodology, and modelling accurate inhibition constants of enzymes. Finally, the book gives the theory and applications of multiscale modelling of proteins and biomolecu