1. Record Nr. UNINA9910506382103321

Titolo	Biophysical and Computational Tools in Drug Discovery / / edited by Anil Kumar Saxena
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2021
ISBN	3-030-85281-4
Edizione	[1st ed. 2021.]
Descrizione fisica	1 online resource (405 pages)
Collana	Topics in Medicinal Chemistry, , 1862-247X ; ; 37
Disciplina	615.1
Soggetti	Pharmaceutical chemistry Physical biochemistry Biology - Technique Chemistry - Data processing Chemistry, Physical and theoretical Biophysics Medicinal Chemistry Biophysical Chemistry Biological Techniques Computational Chemistry Physical Chemistry Biophysical Methods
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Kinetic profiling of fragments by TR-FRET -- Role of Structural biology in drug discovery with emphasis on X-ray crystallography -- A computational search for peptide vaccines using novel mathematical descriptors of sequences of emerging pathogens -- Solution NMR methods in Drug Discovery for the series -- Applications of Mass Spectrometry in Herbal Drug Research -- Generative machine learning for drug discovery -- Structure and ligand based virtual screening in drug discovery -- Quantum Chemical and Quantum Dynamics Techniques for Drug Discovery Including Bioinorganic Compounds.
Sommario/riassunto	This book reviews recent physicochemical and biophysical techniques

applied in drug discovery research, and it outlines the latest advances in computational drug design. Divided into 10 chapters, the book discusses about the role of structural biology in drug discovery, and offers useful application cases of several biophysical and computational methods, including time-resolved fluorometry (TRF) with Förster resonance energy transfer (FRET), X-Ray crystallography, nuclear magnetic resonance spectroscopy, mass spectroscopy, generative machine learning for inverse molecular design, quantum mechanics/molecular mechanics (QM/MM,ONIOM) and quantum molecular dynamics (QMT) methods. Particular attention is given to computational search techniques applied to peptide vaccines using novel mathematical descriptors and structure and ligand-based virtual screening techniques in drug discovery research. Given its scope, the book is a valuable resource for students, researchers and professionals frompharmaceutical industry interested in drug design and discovery.