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Titolo	Computer-Aided and Machine Learning-Driven Drug Design : From Theory to Applications / / edited by Vinícius Gonçalves Maltarollo
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Collana	Computer-Aided Drug Discovery and Design, , 2730-5465 ; ; 3
Altri autori (Persone)	Maltarollo
Disciplina	615.6
Soggetti	Drug delivery systems Machine learning Drugs - Design Artificial intelligence Computer simulation Drug Delivery Machine Learning Structure-Based Drug Design Artificial Intelligence Computer Modelling
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Echoes from the past, visions from the future: a journey into the Medicinal Chemistry and the Computational Drug Discovery -- Molecular Databases -- A Brief Introduction to Pharmacogenomics and Personalized Medicine in the Drug Design Context -- Machine Learning and Neural Networks Methods Applied to Drug Discovery -- Clustering of Small Molecules -- QSAR and Machine learning predictors -- Molecular docking: state-of-art scoring functions and search algorithms -- Drug Design in Motion: concepts and applications of classical Molecular Dynamics simulations -- Conformational sampling of proteins: methods for simulate protein plasticity and ensemble docking -- Free energy perturbation and free energy calculations ap-plied to drug design -- Ultra-large-scale Virtual Screening --

Experimental assays: chemical properties, biochemical and cellular assays, and in vivo evaluations -- Challenges faced in the development of computational methods for predicting pharmacokinetics behavior -- Exploring the Significance of Experimental and Computational Methods in Protein Structure Determination -- Molecular modeling strategies in drug design, development, and discovery targeting proteases -- Computational study of conformational changes in nuclear receptors upon ligand binding -- An Overview on Computational Methods Targeting the Endocannabinoid System -- Kinase Inhibitors and Computer-aided Drug Design Methods -- Prediction of Drug Metabolism with In Silico Models: A Case Study of Doping Detection.

Sommario/riassunto

The computer-aided drug design research field comprises several different knowledge areas, and often, researchers are only familiar or experienced with a small fraction of them. Indeed, pharmaceutical industries and large academic groups rely on a broad range of professionals, including chemists, biologists, pharmacists, and computer scientists. In this sense, it is difficult to be an expert in every single CADD approach. Furthermore, there are well-established methods that are constantly revisited, and novel approaches are introduced, such as machine-learning based scoring functions for molecular docking. This book provides an organized update of the most commonly employed CADD techniques, as well as successful examples of actual applications to develop bioactive compounds/drug candidates. Also includes is a section of case studies that cover certain pharmacological/target classes, focusing on the applications of the previously described methods. This part will especially appeal to professionals who are not as interested in the theoretical aspects of CADD. This is an ideal book for students, researchers, and industry professionals in the fields of pharmacy, chemistry, biology, bioinformatics, computer sciences, and medicine who are seeking a go-to reference on drug design and medicinal chemistry.

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Descrizione fisica	1 online resource (volumes)
Soggetti	Statistics Statistics as Topic Periodicals.
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Livello bibliografico	Periodico
Note generali	Refereed/Peer-reviewed