1. Record Nr. UNINA9910897975903321

Autore	Satoh Hiroko
Titolo	Drug Development Supported by Informatics / / by Hiroko Satoh ; edited by Kimito Funatsu, Hiroshi Yamamoto
Pubbl/distr/stampa	Singapore : , : Springer Nature Singapore : , : Imprint : Springer, , 2024
ISBN	981-9748-28-3
Edizione	[1st ed. 2024.]
Descrizione fisica	1 online resource (XII, 357 p. 181 illus., 171 illus. in color.)
Disciplina	615.19
Soggetti	Medicinal chemistry Pharmacy Chemoinformatics Bioinformatics Medical informatics Machine learning Medicinal Chemistry Cheminformatics Health Informatics Machine Learning
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	The AI Trends in Chemical Space for Drug Discovery -- Screening Methods for Drugs Using Chemoinformatics Methods for Beginners -- Data-driven Molecular Structure Generation for Inverse QSPR/QSAR Problem -- Materials Informatics with Limited Data -- Primer on Graph Machine Learning -- Subgraph-based Molecular Graph Generation -- Language Models in Molecular Discovery -- Transformers and Large Language Models for Chemistry and Drug Discovery -- Drug Discovery and Drug Repositioning Using Computational Methods -- Two and Three-dimensional Molecular Representations in Ligand-based Approaches -- Electronic-Structure Informatics for Drug Development -- Data-Driven Chemistry for Developing Organic Synthesis Routes for Functional Chemicals -- “Quantum-Chemoinformatics” for Design and Discovery of New Molecules and Reactions -- Toxicity Prediction

System for Chemical Substances Based on Toxicity Expression Mechanisms - AI-SHIPS -- Data Assimilation to Integrate High-speed Atomic Force Microscopy with Biomolecular Simulations: Characterization of Drug Target Functions -- Potential of High-Spatiotemporal Resolution Live Cell Imaging for Drug Discovery and Development -- Design of Biomaterials Using Informatics -- Monitoring and Controlling in Continuous Manufacturing Process -- Formulation using Hansen Solubility Parameters.

Sommario/riassunto

This book describes the state-of-the-art of chemoinformatics, bioinformatics, materials informatics and measurement/metrology informatics to develop drugs with desired activity or physicochemical properties and to optimize the functionality, efficacy, safety and quality of the compounds for drugs. Recently, "AI drug discovery", drug discovery research utilizing artificial intelligence technology such as machine learning, has attracted much attention. This book provides an overview of the four applied informatics fields and their applications in drug development for a wide spectrum of readers from learners to professional scientists in academia and industry. It focuses on the basic research stage of drug development with contributions from experts at the forefront of these fields. The authors hope that this book will be of assistance to explore new opportunities for collaboration between pharmaceutical science and informatics.