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Titolo	Applications of Computational Tools in Drug Design and Development / / edited by S.N. Koteswara Rao G., Rajasekhar Reddy Alavala
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Livello bibliografico	Monografia
Nota di contenuto	Chapter 1. Computational simulation of drug delivery at the molecular level -- Chapter 2. Computational modelling for formulation design -- Chapter 3. Computational fluid dynamics-the revolutionary innovative methodology in pharmaceutical industry -- Chapter 4. Population Modelling -- Chapter 5. Design of Experiments: Understanding optimization -- Chapter 6. Computational modelling of pharmaceutical die filling processes -- Chapter 7. Inhalation Aerosol based Targeted Drug Delivery to upper airways: Computational fluid dynamics (CFD) Approach -- Chapter 8. Pharmaceutical inhalation compounds development by using in silico modelling tools -- Chapter 9. Computational tools employed in Cheminformatics -- Chapter 10. Computational simulations as preformulation perspective for the delivery of Drugs -- Chapter 11. Computational Tools for Solubility prediction -- Chapter 12. Advances in the Computational Prediction of Absorption of Pharmaceuticals -- Chapter 13. Protein Binding Prediction by Computational Methods -- Chapter 14. Physiologically

based Pharmacokinetic (PBPK) Modelling and Pharmacokinetic Pharmacodynamic (PKPD) Modelling -- Chapter 15. Prediction of Bio-permeability of Pharmaceuticals with advanced dynamic simulation studies -- Chapter 16. Accomplishment of Toxicity Prediction by CADD Tools -- Chapter 17. Metabolism Prediction: Identification of potential sites of metabolism in Lead molecules -- Chapter 18. Computer Assisted Simulation Studies for Identifying the Drug-Polymer Interactions -- Chapter 19. Recent Advances in Drug likeness screening by using the Software and Online tools -- Chapter 20. Mechanistic Understanding of the Anti-Alzheimer's Agents with Computational Studies -- Chapter 21. Advances in the design of novel antidiabetic agents by using in silico approaches -- Chapter 22. Towards the mechanistic understanding of Atherosclerosis Drug Design -- Chapter 23. Modern computational intelligence based drug repurposing for Cancer Therapeutics -- Chapter 24. Computational analyses of mechanism of action of Antiepileptic Agents -- Chapter 25. Rational Approaches and Designing Strategies for Antihypertensive Agents -- Chapter 26. Drug discovery and computational strategies in the Multi-Drug Resistant Tuberculosis -- Chapter 27. The Network Pharmacology Approach to Uncover the Pharmacological Mechanism of Natural Products.

Sommario/riassunto

This book provides a comprehensive overview of the role of computers and computational tools at different stages of drug discovery and development. Designed to meet the needs of a beginner to advanced learner, the book provides the information on the tools, how they work, with the latest reports on applications in drug design, drug delivery and building network pharmacology models. Part I explores the pharmacological aspects, covering computational simulation of drug delivery at the molecular level, modeling for formulation design, and the revolutionary use of computational fluid dynamics in pharmaceutical processes. Specific applications such as pharmaceutical die filling processes, inhalation aerosol-based targeted drug delivery, and the development of inhalation compounds using in silico modeling tools are discussed. The use of computational tools in cheminformatics and their application in preformulation perspectives for drug delivery are also included. Part II expands the scope to include solubility prediction, absorption prediction, protein binding prediction, bio-permeability prediction, toxicity prediction, and metabolism prediction. It covers the identification of potential sites of metabolism in lead molecules and computer-assisted simulation studies to understand drug-polymer interactions. Recent advances in drug likeness screening using software and online tools are also reviewed. Part III focuses on specific therapeutic areas. The chapters examine the mechanistic understanding of anti-Alzheimer's agents, the design of novel antidiabetic agents, and the exploration of drug design for atherosclerosis. It also covers modern computational intelligence-based drug repurposing for cancer therapeutics, computational analyses of the mechanism of action of antiepileptic agents, and rational approaches for designing antihypertensive agents. The final chapters explore drug discovery and computational strategies in the context of multi-drug-resistant tuberculosis and the network pharmacology approach to uncover the pharmacological mechanisms of natural products. The book will be a useful reference for researchers, students and professionals in the field of life sciences, chemistry, pharmaceutics and bioinformatics.

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Titolo	Visnyk Nacionalnoho universytetu Lvivska politechnika : = Journal of Lviv Polytechnic National University . [...] Naukovyj zurnal „Komp'juterni systemy ta merezi" : CSN = Scientific journal "Computer systems and networks"
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