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Nota di contenuto	Chapter 1: Fundamentals of Computational Drug Design Approaches (CADD) -- Chapter 2: Molecular and Computational Modeling in Drug Design -- Chapter 3: Bioinformatics/Chemo-informatics Tools and Database in Drug Discovery -- Chapter 4: Computational Screening of Phytochemicals/Natural Products in Drug Discovery -- Chapter 5: Virtual Screening in Lead Discovery and Optimization -- Chapter 6: Target-based Screening (SBDD) in Lead Discovery -- Chapter 7: Pharmacophore-based and Similarity Search (LBDD) Screening in Lead Discovery -- Chapter 8: Receptor-based De Novo and Fragment-based Drug Design -- Chapter 9: Artificial Intelligence and Machine Learning in Drug Discovery -- Chapter 10: Network Pharmacology and System Biology Approaches -- Chapter 11: In Silico Pharmacology and Drug

Sommario/riassunto

This book updates knowledge on recent advances in computational and bioinformatics tools/techniques and their practical applications in modern drug design and discovery programme. Also it encompasses fundamental principles, advanced methodologies and applications of various CADD approaches including several cutting-edge areas; presenting recent developments covering ongoing trends in the field of computer-aided drug discovery. Having contributions by a global team of experts, the book is expected to be an ideal resource for drug discovery scientists, medicinal chemists, pharmacologists, toxicologists, phytochemists, biochemists, biologists, R&D personnel, researchers, students, teachers and those working in the field of drug discovery. It will fill the knowledge gaps that exist in the current CADD approaches and methodologies/ protocols being widely used in both academic and research practices. Further, a special focus on current status of various computational drug design approaches (SBDD, LBDD, De-novo drug design, Pharmacophore-based search), bioinformatics tools and databases, computational screening and modeling of phytochemicals/natural products, artificial intelligence and machine learning, and network pharmacology and system biology would certainly guide researchers, students or readers to conduct their research in the emerging area(s) of interest. It is also expected to be highly beneficial to different stakeholders working in the pharmaceutical and biotechnology industries (R&D), the academic as well as research sectors. .
