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	Through ALK Receptor-Targeted Drug Metabolism and Pharmacokinetics -- Targeting Intrinsically Disordered Proteins (IDPs) in Drug Discovery : Opportunities and Challenges.
Sommario/riassunto	Comprehensive resource covering computational tools and techniques for the development of cost-effective drugs to combat diseases, with specific disease examples Computational Methods for Rational Drug Design covers the tools and techniques of drug design with applications to the discovery of small molecule-based therapeutics, detailing methodologies and practical applications and addressing the challenges of techniques like AI/ML and drug design for unknown receptor structures. Divided into 23 chapters, the contributors address various cutting-edge areas of therapeutic importance such as neurodegenerative disorders, cancer, multi-drug resistant bacterial infections, inflammatory diseases, and viral infections. Edited by a highly qualified academic with significant research contributions to the field, Computational Methods for Rational Drug Design explores topics including: * Computer-assisted methods and tools for structure- and ligand-based drug design, virtual screening and lead discovery, and ADMET and physicochemical assessments * In silico and pharmacophore modeling, fragment-based design, de novo drug design and scaffold hopping, network-based methods and drug discovery * Rational design of natural products, peptides, enzyme inhibitors, drugs for neurodegenerative disorders, anti-inflammatory therapeutics, antibacterials for multi-drug resistant infections, and antiviral and anticancer therapeutics * Protac and protide strategies in drug design, intrinsically disordered proteins (IDPs) in drug discovery and lung cancer treatment through ALK receptor-targeted drug metabolism and pharmacokinetics Helping readers seamlessly navigate the challenges of drug design, Computational Methods for Rational Drug Design is an essential reference for pharmaceutical and medicinal chemists, biochemists, pharmacologists, and phytochemists, along with molecular modeling and computational drug discovery professionals.