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Nota di contenuto	1. Introductory Chapter: Molecular Docking-The Transition from the Micro Nature of Small Molecules to the Macro World -- 2. Fundamentals of Molecular Docking and Comparative Analysis of Protein-Small-Molecule Docking Approaches -- 3. Molecular Docking: Metamorphosis in Drug Discovery -- 4. Molecular Docking in the Study of Ligand-Protein Recognition: An Overview -- 5. Development of Nucleic Acid Targeting Molecules: Molecular Docking Approaches and Recent Advances -- 6. Repurposing Drugs as Potential Therapeutics for the SARS-Cov-2 Viral Infection: Automatizing a Blind Molecular Docking High-throughput Pipeline -- 7. N1-(3-(Trifluoromethyl)Phenyl) Isophthalamide Derivatives as Promising Inhibitors of Vascular Endothelial Growth Factor Receptor: Pharmacophore-Based Design, Docking, and MM-PBSA/MM-GBSA Binding Energy Estimation.
Sommario/riassunto	Molecular docking is a widely used bioinformatics method in biology, medicine, and biochemistry. This method, which can model interactions between different receptors and their various ligands at the molecular level, can represent intermolecular interactions at an unprecedented resolution that may not be achieved by classical experimental approaches. This book describes different aspects of this method that can reveal the intermolecular biochemical and biophysical interactions and the affinities of partner molecules to each other. It is designed for academics, students, and professionals interested in this technique.