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Nota di bibliografia	Includes bibliographical references at the end of each chapters and index.
Nota di contenuto	1 Hybrid QM/MM Methods: Treating Electronic Phenomena in Very Large Molecular Systems -- 2 Structure, Thermodynamics and Energetics of Drug-DNA Interactions: Computer Modeling and Experiment -- 3 Formation of DNA Lesions, Its Prevention and Repair -- 4 DNA dependent DNA Polymerases as Targets for Low-Weight Molecular Inhibitors: State of Art and Prospects of Rational Design -- 5 Molecular structures, relative stability, and proton anities of nucleotides: Broad view and novel findings -- 6 Quantum Chemical Approaches in Modeling the Structure of Quadruplex DNA and Its Interaction with Metal Ions and Small Molecules -- 7 Density Functional Theory Calculations of Enzyme-Inhibitor Interactions in Medicinal

Chemistry and Drug Design -- 8 Molecular Dynamics Simulations of Lipid Bilayers with Incorporated Peptides -- 9 Polyphenol Glycosides as Potential Remedies in Kidney Stones Therapy. Experimental Research Supported by Computational Studies -- 10 Quantum-Chemical Investigation of Epoxidic Compounds Transformation. Application for In Vitro and In Vivo Processes Modeling -- 11 Computational Toxicology in Drug Discovery: opportunities and limitations -- 12 Consensus Drug Design Using it Microcosm -- 13 Continuous Molecular Fields Approach Applied to Structure-Activity Modeling -- 14 Quantitative Structure-Pharmacokinetic Relationships of Drugs within the Framework of Biopharmaceutics Classification System by Using Simplex Representation of Molecular Structure -- 15 (How to) Profit from Molecular Dynamics-based Ensemble Docking -- 16 Cheminformatics on Crossroad of Eras.

Sommario/riassunto

The current volume provides both fundamental and detailed information about the computational and computational-experimental studies which improve our knowledge of how leaving matter functions. It also covers research areas related to structures and properties of drugs (including the calculation and the design of new ones), and the development of completely new ways of treating numerical diseases. Whenever it is possible, the interplay between theory and experiment is emphasized. The book features computational techniques such as quantum-chemical and molecular dynamic approaches supplemented by a discussion on quantitative structure–activity relationships. The initial chapters describe the state-of-the art computational approaches for molecular biology, molecular pharmacy, and molecular medicine performed with the use of pure quantum-chemical techniques. The central part of the book illustrates the status of computational techniques that utilize hybrid, so called QM/MM approximations. In addition, the results of the QSAR studies, which now are the most popular in predicting drugs' efficiency, are discussed. The last chapter reveals the current state of chemoinformatics and discusses new problems and experimental perspectives related to both chemical and biological characteristics of molecules.