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Bentham Science Publishers, United States, 2015. Paperback. Book Condition: New. 235 x 191 mm. Language: English . Brand New Book. Frontiers in Computational Chemistry, originally published by Bentham and now distributed by Elsevier, presents the latest research findings and methods in the diverse field of computational chemistry, focusing on molecular modeling techniques used in drug discovery and the drug development process. This includes computer-aided molecular design, drug discovery and development, lead generation, lead optimization, database management, computer and molecular graphics, and the development of new computational methods or efficient algorithms for the simulation of chemical phenomena including analyses of biological activity. In Volume 2, the authors continue the compendium with nine additional perspectives in the application of computational methods towards drug design. This volume covers an array of subjects from modern hardware advances that accelerate new antibacterial peptide identification, electronic structure methods that explain how singlet oxygen damages DNA, to QSAR model validation, the application of DFT and DFRT methods on understanding the action of nitrogen mustards, the design of novel prodrugs using molecular mechanics and molecular orbital methods, computational simulations of lipid bilayers, high throughput screening methods, and more. Brings together a wide range of research into a single collection to help researchers keep up with new methodsUniquely focuses on computational chemistry approaches that can accelerate drug designMakes a solid connection between experiment and computation, and the novel application of computational methods in the fields of biology, chemistry, biochemistry, physics, and biophysics.

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