



Application of Computational Techniques in Pharmacy and Medicine (Challenges and Advances in Computational Chemistry and Physics)

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The proposed volume provides both fundamental and detailed information about the computational and computational-experimental studies which improve our knowledge of how living matter functions, the different properties of drugs (including the calculation and the design of new ones), and the creation of completely new ways of treating numerical diseases. Whenever it is possible, the interplay between theory and experiment is provided. The book features computational techniques such as quantum-chemical and molecular dynamic approaches and quantitative structure–activity relationships.

The initial chapters describe the state-of-the art research on the computational investigations in 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 as well as the results of the QSAR studies which now are the most popular in predicting drugs' efficiency. The last chapters describe combined computational and experimental investigations.

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