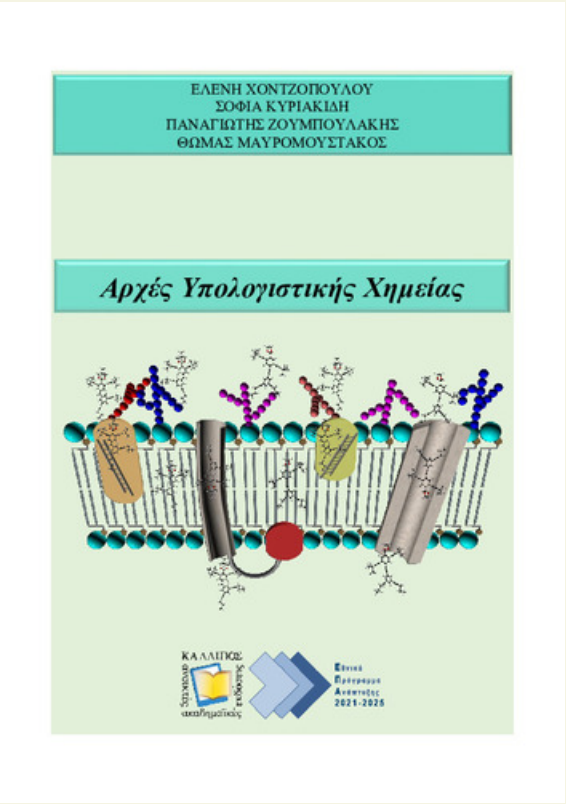

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Abstract

In this book, the research sector of Molecular Modeling is defined and its contribution to experimental chemistry is extensively analyzed (Chapter 1). Moreover, the importance of computational analysis in the Rational Drug Design of novel compounds is described, as well as its role in complementing the experimental results (Chapter 3). In particular, the contribution of Molecular Dynamics, Extended analysis, Energy Minimization (Chapter 4), and Monte Carlo methods (Chapter 8) to the drug design process is thoroughly discussed. Quantum (Chapter 6) and Molecular mechanical approaches (Chapter 8) are analyzed for the energy calculation and the conformational search of chemical compounds. Furthermore, the forces that govern the interactions of the pharmaceutical molecules with their macromolecule targets are discussed. In the same chapter, the developing algorithms which are used to describe molecular binding are illustrated (Chapter 7). Peptidomimetics is a separate chapter because of its major importance in synthesizing and designing new pharmaceutical molecules. The main example in the history of peptidomimetics resides in the renin-angiotensin system (Chapter 5). In addition, the book includes a specific chapter for the molecular modeling of lipid bilayers and transmembrane receptors, since they act as potent targets for a variety of different drugs (Chapters 2 & 9). Finally, Chapter 10 illustrates some general examples and future insights for the Molecular Modeling research sector. The chapters are accompanied by many questions, exercises, and tests, so the students can understand computational chemistry concepts. Answers are also offered for some of the questions, to aid the students understand the studying material of each chapter. We are sure that the adequate number of questions, examples, and exercises is quite helpful for both the professors and the students in understanding the concepts of Computational Chemistry and Molecular Modeling.

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