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Book Review: Computational Tools for Chemical Biology Edited by Sonsoles Martín-Santamaría

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From ligand-based [1-4] to structure-based[5-7] drug design and from comprehension of reaction mechanisms [8-10] to the simulation of complex systems [11], computational techniques are actually an important part of our research group. When we talk about computer scientist the most important thing is to remember that is only thanks to different Nobel Prize (e.g. Martin Karplus, Michael Levitt and AriehWarshel) and to the incredible power of computer of nowadays that today computer scientist took literally chemicals experiment into cyberspace. Nowadays computational tools are strictly specialized into a particular aspect of the simulation, some of them are good for example to simulate a protein and non-covalent interaction with a ligand or another protein, and others are better studied for the chemical reactivity of molecules. It is exciting and challenging that the computation tools are so different and specialized, but on the other hand, the entry-level user always needs a direction to the vast world of computational chemistry. It is only thanks book like this: *Computational Tools for Chemical Biology* edited by Sonsoles Martín-Santamaría, that scientist can easy see at this intricate environment in a clearly and simple way and can easily find the best solution for their own research problems. As part of the series "Chemical Biology", which includes other interesting titles that deal with different aspects of different areas at the interface between chemistry and biology, the book aims to give the reader an understanding of the fundamental methodologies, theories and applications of computational techniques in chemical biology. Each chapter is written by internationally renowned leaders in the field. Important topics from the understanding of the dynamic of biomolecules to the modification of their functions and drug design are addressed, as well as examples of the application of tools in enzyme design and molecular recognition. Not only are the cutting-the-edge methods addressed, but also their limitations and possible future development. For anyone wishing to learn how computational chemistry and molecular modelling can provide information and explain data not easily accessible through other experimental methods, this book will be a valuable resource. It will be of interest to postgraduates and researchers in the chemical sciences as well as biology and medicinal/pharmaceutical chemistry, and theoretical chemistry.

The book is divided into total 13 different chapters. In chapter 1 the different techniques in bio molecular simulations are described as well as how to predict the structure of a protein and a description of computer-based drug design. Chapter 2 is devoted to molecular dynamics simulations of a biological system, particularly interesting is a section in this chapter in which are described different methods how to extract Information from molecular dynamics. Chapters 3 and 4 are dedicated to the design of chemical tools with computational chemistry and to computational design of protein function, respectively. Always fascinating and useful is the section in chapter 4 which describe the QM/MM (ONIOM) approach to enzyme design. Chapter 5 is the continuation of chapter 4, this is entitled *Computational Enzymology: Modelling Biological Catalysts,* and in this chapter, the computational Enzymology is deeply described. In chapters 6–8 the attention is related to different biological entities: Glycobiology, Nucleic Acids, and G protein, for the three chapters, respectively. In each chapter, the different available computational tool for each class of molecule are describes as well as how to solve common research question arise from these classes of molecules. Chapter 9 is devoted to the molecular recognition process, from the modeling of the dynamic of the proteins to the homology modeling and the prediction of protein/protein interaction. In chapter 10 the membrane transport is the subject of interest, of course how to model biological membrane and how to computationally simulate transport across membranes are the topic of interest. Chapters 11 and 12 are dedicated to the lead discovery process and to the drug discovery targets, respectively. The final chapter is entitled *The Polypharmacology Gap between Chemical Biology and Drug Discover.* In this chapter, the concepts of Polypharmacology and Drug-target network are discussed and different cases study is presented. Every chapter has a small introduction, where the reader can find information about a topic enclosed in the chapter. At the end of each chapter, there is a paragraph with conclusions, challenges and perspectives of

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the subject treated and the list of references. The topics covered in the book are aimed to graduate students and researchers in various fields, who want to understand how to apply different computational techniques to understand and rationalize some chemical biology problems at the molecular level and "resolve and understand" some intricate aspects of life.(Figure 1)

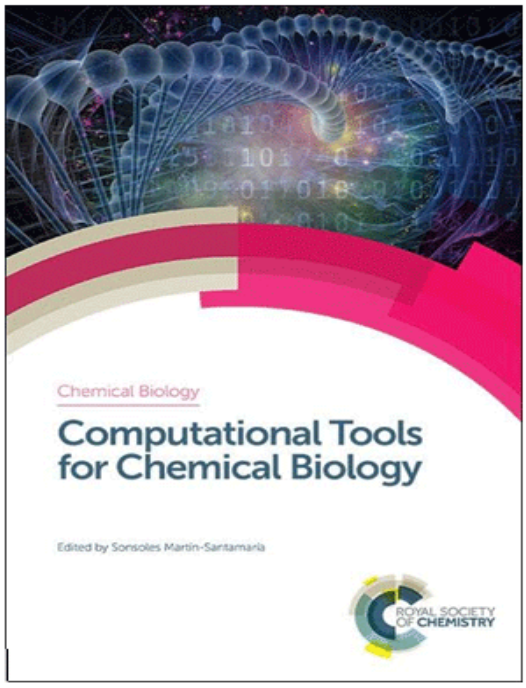

Figure 1: Cover of Computational Tools for Chemical Biology Edited by Sonsoles Martín-Santamaría

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