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BOOK REVIEW

Frontiers in Computational Chemistry (Volume 1)

edited by

Zaheer Ul-Haq & Jeffry D. Madura

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In their preface, the editors say that the focus of this book is to present material on molecular modeling techniques used in drug discovery and the drug development process. In this book, they collected eight different perspectives in the application of computational methods towards drug design. These contributions are written by a total of 30 authors. They quote over 1100 references, indicating that this book is scientifically very rich. The chapters in the book are the following:

1. *Computational Strategies to Incorporate GPCR Complexity in Drug Design*
2. *Knowledge–Based Drug Repurposing: A Rational Approach towards the Identification of Novel Medical Applications of Known Drugs*
3. *Tuning the Solvation Term in the MM-PBSA/GBSA Binding Affinity Predictions*
4. *Recent Advances in the Discovery and Development of Protein–Protein Interaction Modulators by Virtual Screening*
5. *Computational Design of Biological Systems: From Systems to Synthetic Biology*
6. *Considering the Medium when Studying Biologically Active Molecules: Motivation, Options and Challenges*
7. *Novel Coarse–Grained Description of Protein Structure and Folding by UNRES*
8. *Force Field and Discrete Nonlinear Schrödinger Equation. Computational Chemistry Strategies Tackling Function and Inhibition of Pharmaceutically Relevant Targets*

In the first two chapters, the authors review various computational approaches to G protein–coupled receptors (GPCRs) and the use of cheminformatics and bioinformatics in identifying new insights about known drugs, respectively.

In the third chapter, the authors point out that in order to obtain good, reliable results, the MM–PBSA or MM–GBSA methods need to be tuned for a particular system. In particular, they focus on interior dielectric constant as well as the PB and GB solvers, and report studies on the optimization of the non-electrostatic contributions.

The intention of Chapter 4 is to rationalize the computational calculations with experimental data. In this chapter, a review of the use of virtual screening in protein–protein interactions is provided, as well as its role in drug discovery. This study leads to a significant breakthrough in this young and exciting field of study.

Chapter 5 describes the development and use of computational methods on large biological data sets to potentially engineer circuits. These challenges are very important and have potential uses in biotechnology and in the development of strategies to treat various diseases such as cancer. The authors suggest that a synchronized effort should be strengthened to extend synthetic biology circuit construction strategies, which may prove crucial for the development of next generation therapeutics.

In Chapter 6, the authors touch a very critical field of study. This study concerns with the implementation of the environment in computational calculations. Within this chapter the authors yield some insight into how to appropriately include the environment into the study of a particular biological system.

Chapters 7 and 8 review the use of coarse–graining in the study of protein folding and the application of various tools from first principles to empirical methods in the discovery and development of new compounds that potentially lead or become the next drug, respectively.

The book ends with a detailed Subject Index.

In summary: the book presents useful and clear information on various details of computational chemistry, including studies of biological systems and drug design. It will be useful for the chemical, biological, and pharmaceutical areas, especially where these fields touch each other. In addition, this book offers valuable information for both beginners and experts.

Dr. Zaki Safi, Ivan Gutman