# In Silico Drug Discovery and Design: Theory, Methods, Challenges, and Applications

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***In Silico* Drug Discovery and Design: Theory, Methods, Challenges, and Applications** provides a comprehensive, unified, and in-depth overview of the current methodological strategies in computer-aided drug discovery and design. Its main aims are to introduce the theoretical framework and algorithms, discuss the range of validity, strengths and limitations of each methodology, and present applications to real world problems in the drug discovery arena. Special emphasis has been given to the emerging and most pressing methodological challenges in *in silico* drug discovery and design.

The book assumes a basic knowledge of physical principles and molecular modeling. Particular attention has been paid to outline the underlying physico-chemical foundation of the methods described, thus providing the necessary background to avoid a "black-box" approach. In each self-contained chapter, this is presented together with the latest developments and applications, and the challenges that lie ahead.

Assembling a unique team of experts to weigh in on the most important issues influencing modern computational drug discovery and design, this book constitutes both a desktop reference to academic and industrial researchers in the field, and a textbook for students in the area of molecular modeling and drug discovery.

Comprised of 18 chapters and divided into three parts, this book:

- Provides a comprehensive, unified, and in-depth overview of the current methodological strategies in computer-aided drug discovery and design
- Outlines the underlying physico-chemical foundation of the methods described
- Presents several applications of computational methods to real world problems in the drug design field
- Helps to avoid a "black-box" approach to *in silico* drug discovery
- Constitutes an actual textbook for students in the area of molecular modeling and drug discovery
- Gives the reader the adequate background to face the current challenges of the field

*In Silico* Drug Discovery and Design: Theory, Methods, Challenges, and Applications describes the theoretical framework, methods, practical applications and case examples relevant to computer-aided drug lead discovery and design. This text will surely aid in understanding the underlying physical foundation of computational tools and their range of application, thus facilitating the interpretation of simulation results.

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