Preface

Computational technologies have been applied in drug discovery for decades and are gaining increasingly in popularity, implementation, and appreciation due to the recent advances in computational methodologies and the fast growth of low-cost high performance computing techniques. Computer-aided drug discovery (CADD) has become a crucial component of modern drug discovery programs and is widely utilized to identity and optimize bioactive compounds for the development of new drugs. The intent of this book is to provide a practical guide for solving drug discovery-related problems using computational techniques.

CADD is a diverse discipline where various aspects of applied and basic research merge and stimulate each other. Computational strategies thus need to be frequently adjusted for different drug discovery purposes. A wide variety of computational approaches have been used in different stages of drug discovery and development, as well as in clinical studies. It is not possible to comprehensively cover such a broad field in one volume. Therefore, this book focuses on the methods that are commonly used in the early stage of drug discovery, including computer simulation, structure prediction, conformational sampling, binding site mapping, docking and scoring, in silico screening, and fragment-based drug design. In addition to the state-of-the-art theoretical concept, this book also includes step-by-step, readily reproducible computational protocols as well as examples of various CADD strategies. The limitations and potential pitfalls of different computational methods are discussed by experts, and tips and advice for their applications are suggested.

It has been a great privilege to work with the many experts in the CADD field. I very much appreciate the patience of the authors who carefully worked on their chapters and took into consideration my comments to make them a part of a coherent picture.

I would like to dedicate this book to my dearly beloved grandfather, whose wisdom, dedication, and passion for life has always been an inspiration for me.

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