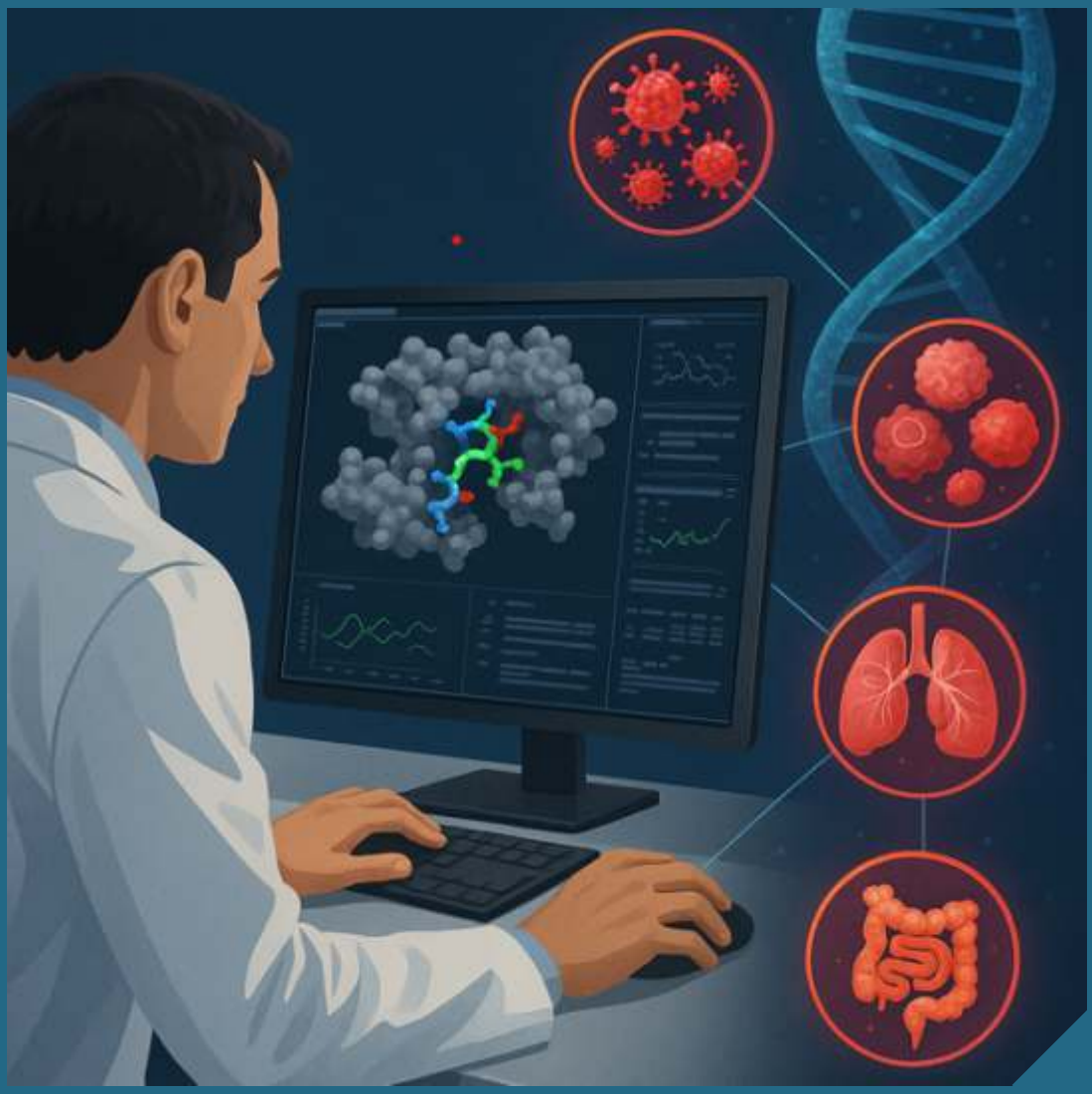

Computer-Aided Drug Design: In-silico Tools and Techniques

DeepScience

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Preface

The field of rational drug design has transformed how we approach the discovery and development of novel therapeutics. Depending only on trial-and-error approaches, in which innumerable chemicals were created and tested with no clear understanding of their molecular interactions. Researchers may now build and improve pharmacological compounds with remarkable precision and efficiency because to advances in computational tools and procedures.

This book aims to provide a complete understanding of the rational drug design process, including the underlying principles, methodologies, and tactics employed in the area. Our mission is to provide students, researchers, and professionals with the knowledge and abilities they need to develop and discover novel therapeutic compounds that can solve the complex issues of modern medicine. The book is organized into chapters, with each concentrating on an important topic of rational drug design. We begin by discussing lead molecule design and discovery, emphasizing the significance of understanding the molecular causes of disease and the function of drug design in the drug discovery process. The following chapters cover the basics of Quantitative Structure-Activity Relationship (QSAR) and molecular docking, which provide a solid framework for understanding the intricate interactions between medicines and their targets.

One of the book's main merits is its emphasis on practical applications. We give extensive explanations of the many tactics utilized to create novel drug-like compounds, such as molecular modeling software and computational tools. Working through the examples and case studies in this book, readers will receive hands-on experience developing and optimizing drug compounds, preparing them for the challenges of real-world drug development.

The subject of rational drug design is fast changing, with new methodologies and technology constantly appearing. This book seeks to provide a thorough understanding of the ideas and methods of rational drug design, while simultaneously highlighting the most recent breakthroughs and trends in the area. Our goal is to provide readers with the knowledge and skills they need to help develop breakthrough therapeutic agents that will improve human health and quality of life. Finally, this book is intended to be a useful resource for anybody interested in rational drug design, including students, researchers, and pharmaceutical industry personnel. We hope that the knowledge and insights offered in this book will inspire and enable readers to make significant contributions to

the field, resulting in the development of safer, more effective, and more tailored medicinal agents.

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Chapter 1: Drug Discovery and Development: From Lead Discovery to Analog-Based Design

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Abstract

Drug discovery and development is a complex process involving the identification and optimization of potential therapeutic agents. An outline of the phases is given in this chapter, with an emphasis on lead finding and analog-based design. Random and non-random screening, and clinical observation are some of the lead discovery techniques. While random screening employs high-throughput screening of sizable compound libraries, traditional medicine focuses on identifying active compounds from natural materials. chemicals that share structural or functional similarities with known chemicals are the focus of non-random screening. Analog-based design maximizes the qualities of a lead compound after it has been identified. By substituting atoms or functional groups with comparable characteristics, bioisosterism enhances pharmacokinetics, potency, and selectivity. There are two types of bioisosteres: classical and non-classical. By improving the characteristics of lead compounds, bioisosteric replacement creates novel therapeutic medicines with better safety and efficacy profiles. Although creating new medications necessitates a large expenditure in research and development, a successful discovery can have a positive impact on both human health and the economy. This chapter emphasizes how crucial it is to comprehend lead discovery and analog-based design concepts in order to create novel therapeutic medicines. Effective drug discovery and development require a multidisciplinary strategy that involves cooperation between chemists, biologists, pharmacologists, and clinicians. Researchers can create therapeutic agents that answer complicated patient and healthcare system needs by utilizing bioisosterism and other design principles. This chapter highlights important phases, methods, and tactics in drug discovery and development, making it an invaluable resource for researchers. The ultimate objective is to create novel therapeutic agents in order to enhance human health. Researchers can advance treatments for a variety of ailments by contributing to