# DRUG DELIVERY SYSTEMS USING QUANTUM COMPUTING


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*Dear healthcare professionals,*
*We are dedicating this book to you. Our love for the profession shall live forever.*

# Contents

# Foreword

The origin of this unique book started in a conversation I had with Rishabha about ten years ago. He had just started his career in research and wished to make a contribution to pharmacy professionals. I knew he was going to be a star in his field as he had all the qualities of a high-flyer. Every story and every achievement were a performance. Today, I am writing this Foreword for his dream project.

Identifying and developing small molecules and macromolecules that might help cure illnesses and diseases is the core activity of pharmaceutical companies. Given its focus on molecular formations, the pharmaceutical industry is a natural candidate for quantum computing. Today's trendiest issues in technology are all related to quantum computing. Thanks to technology, computing issues that were once thought to be insurmountable are now being solved by individuals and businesses. This technology has had a substantial impact on many different domains, including healthcare, the pharmaceutical industry, drug discovery, and many more.

The development of this emerging technology, both by itself and in concert with other technologies, has the potential to make a significantly positive impact on society. The impact of quantum computing on the pharmaceutical industry relies on the development, manufacture, and delivery of molecules. This book explains the profound impact that quantum computing could have on the pharmaceutical industry and presents user examples of its application. I hope after reading this book, healthcare professionals and pharmaceutical companies will be well-advised to assess the quantum computing opportunity for themselves and begin laying the groundwork for securing their place in this new competitive and technological landscape.

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# Preface

The majority of drug candidates have low solubility, rapid blood clearance, poor targeting, and, usually, poor ability to penetrate cell membranes. Some of these obstacles can be addressed by drug delivery systems (DDSs) that improve drug delivery to the site of action. Drug delivery technology is advancing significantly, and controlling the precise level and/or location of a given drug in the body reduces adverse effects, lowers dosages, and makes new therapies possible.

Nevertheless, there are still significant obstacles to delivering certain medications to particular cells. Drug delivery methods change pharmacokinetic, pharmacodynamic, and drug release patterns to enhance product efficacy and safety, as well as patient convenience and compliance. Computational approaches in drug development enable quick screening of a vast chemical library and identification of possible binders by using modeling, simulation, and visualization tools. Quantum computing (QC) is a fundamentally new computing paradigm based on quantum mechanics rules that enables certain computations to be conducted significantly more rapidly and effectively than regular computing, and hence this has huge promise for the pharmaceutical sector.

Significant advances in computational simulation are making it easier to comprehend the process of drug delivery. This book explores an important biophysical component of DDSs, and how computer modelling may help with the logical design of DDSs with enhanced and optimized characteristics. The book concentrates on computational research for various important types of nanocarriers, including dendrimers and dendrons, polymers, peptides, nucleic acids, lipids, carbon-based DDSs, and gold nanoparticles.

This new technology's advancement promises a significant and positive effect on society, both independently and in conjunction with existing technologies. With ethical research, development, and implementation, the trickle-down consequences of the quantum revolution should enhance

the lives of many people. Understanding the effects that quantum computing could have on the pharmaceutical business is therefore crucial.

This book contains 14 chapters, written by top researchers from many parts of the world. The book is profusely referenced and copiously illustrated, and all chapters were deliberately reviewed and revised to meet the highest standard of publication. We are deeply grateful to everyone who helped with this book and greatly appreciate the dedicated support and valuable assistance rendered by Martin Scrivener and the Scrivener Publishing team during its publication.

**The Editors**
April 2024

# Acknowledgments

Writing a book seemed difficult, but working on this had been a delightful experience. It was more rewarding and motivating than I had imagined. I would like to begin by expressing my gratitude to the Almighty, whose unending blessings and supreme power enable us to accomplish all our goals.

Although this period of my life was filled with many ups and downs, I am eternally grateful to my family for their continuous support and encouragement that made it possible to complete this task.

I am deeply indebted to the management at Galgotias University. I want to thank you all for letting me serve, for being a part of our amazing organization, and for motivating me every day.

Many thanks to all contributors. Without their participation, this goal could not have been achieved. Last but not least, I would like to thank our publisher for their support, innovative suggestions, and guidance in bringing out this edition.

# 1

# Quantum Computational Concepts and Approaches in Drug Discovery, Development and Delivery

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## *Abstract*

The use of quantum computing approaches in drug discovery, development, and delivery is on rise. Quantum computing (QC) is becoming more popular as a cost-saving measure in the research, production, and manufacturing of drugs. The use of molecular dynamics and computation tasks has greatly enhanced drug design and optimization of drug delivery systems. This QC method aids in investigating several issues that are difficult to examine in laboratory studies. This chapter discusses how QC simulations can assign a specific drug target site by anticipating the target, resulting in a successful drug development process. It also highlights the important applications of several algorithms in drug delivery and disease diagnosis. Additionally, computational methodologies for various drug delivery systems and carriers are discussed. This chapter also discusses ongoing challenges in the pharmaceutical industry and concerns regarding the chances of accomplishment of QC concepts and technology.

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## 1.1 Introduction

Drug development and discovery to identify new chemical entities to treat or cure human diseases is a very long, complex, expensive, and tedious process that often fails [1]. Over the years, the scientific community has tried its best to decrease expenditure, speed up the process of drug development, and progress the accomplishment frequency of identifying drugs or molecules of natural or synthetic origin [2, 3]. In the late 20th century, the paradigm slowly shifted from Ethnopharmacology, a traditional discovery method from medicinal plants, to a computational chemistry-based technique called computer-aided drug design (CADD) to identify a lead molecule capable of binding to a target protein to exhibit favorable therapeutic effects and pharmacokinetic profile [4]. Discovery and optimization of lead molecules following the high-throughput screening (HTS) over hit libraries using a CADD approach can be done either by structured-based or ligand-based drug design [5]. While the latter is favored in the absence of target architectural data and uses a quantitative structure–activity relation (QSAR) model, the former approach is used when knowledge of the 3D structural information of the biological target is available for molecular docking (pharmacophore modeling). Although most of the drugs in the pipeline have been discovered using CADD, the higher computational cost to study the molecular dynamics of protein–ligand interactions and the reliability of the current statistical techniques available to study pharmacokinetic profile limits its usefulness [6–8]. The challenges and limitations of CADD could be overcome with the help of an emerging quantum computing (QC) technology that can handle and stimulate larger and more complex chemical structures more efficiently. QC application will certainly benefit the pharmaceutical industry from innovation in drug discovery to the manufacture and development of promising therapeutic modalities [8].

Constructing a new drug for a chronic illness in the medical context was mainly based on new pills. Various drugs for identifying energetic facets in conventional therapies like penicillin have recently been developed. In natural compounds, organic molecules that aid in medical purposes to discover ingredients such as cells or unbroken life forms are used in pharmaceutical manufacturing. This is known as traditional pharmacology. As the DNA sequence has enabled massive cloning techniques and improved protein refinement, HTS with various libraries has become