

# Chapter 10

## The Application of AI in Drug Discovery: Challenges, Opportunities, and Strategies

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### ABSTRACT

*The integration of artificial intelligence (AI) into drug discovery represents a transformative milestone in the field of healthcare. With the advent of AI technologies, researchers are equipped with unprecedented tools to address the intricate challenges that inherent in drug development. This chapter explores the profound impact of AI on revolutionizing the pharmaceutical industry, offering novel solutions to*

DOI: 10.4018/979-8-3693-5468-1.ch010

*enhance research and development (R&D) performance and accelerate therapeutic innovation. The chapter also highlights the critical role of AI-enabled platforms in identifying promising drug prospects and presents a roadmap for effective integration strategies. Additionally, it delves into emerging techniques and applications at the forefront of AI-enabled drug research, offering insights into future opportunities and advancements in the field.*

## **1. INTRODUCTION**

The integration of artificial intelligence (AI) into drug discovery heralds a revolution in medicine, offering novel solutions to the multifaceted challenges plaguing healthcare. While reproduction results, AI has given researchers unprecedented tools to navigate the complexities of drug development. As the pharmaceutical industry harnesses the power of generative AI to gain insights from vast amounts of data, predict complex drug interactions, and rapidly develop new therapies with tangible clinical implications the pharmaceutical industry stands at the end of a period of change (Alam & Khan, 2022, 2020).

This paradigmatic shift to a data-driven approach underscores the critical role of nascent AI in increasing Research and Development (R&D) performance and unprecedented growth in the healthcare industry as we embark on a journey to unlock dynamic AI potential applications in drug discovery. The key challenges, we do so underscore the transformation the power of AI in creating new ways to succeed (Naitali et al., 2023).

This paper will highlight the critical role of AI-enabled parenting in identifying new drug candidates, and provide a roadmap for effective integration strategies. Moreover, this chapter will highlight what is at the forefront of AI-enabled drug research. Many other opportunities will also be discussed.

## **2. EVOLUTION OF DRUG DISCOVERY**

In this section we will discuss about the evolution of drug discovery with time.

### **2.1 Early Practices and Philosophies in Medicine**

- **Early phase:** Since ancient times, drugs have been utilized for physical remedies, often mixed with religious and spiritual practices. Initially,

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