Chapter 1
AI-Driven Decision-Making Applications in Pharmaceutical Sciences

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ABSTRACT

This chapter explores AI's influence on pharmaceutical sciences, highlighting its enhancement of traditional design methodologies. It explores AI's transformational role in key sectors, including drug discovery, virtual screening, and drug formulation development. AI's ability to efficiently identify potential drug candidates from large chemical libraries and its use of optimization algorithms in the selection of suitable excipients and dosage forms are discussed. The chapter also emphasizes AI's significance in improving pharmaceutical manufacturing processes through parameter refinement, quality outcome prediction, and real-time anomaly detection. The integration of traditional design methods with AI ensures robust, reliable, AI-driven processes that are compliant with regulations. In conclusion, the chapter highlights the potential of AI in pharmaceutical sciences and the importance of its integration with traditional design methods. This approach empowers scientists to innovate, speed up drug development, and improve patient outcomes.

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INTRODUCTION

The field of pharmaceutical sciences has traditionally placed great emphasis on studying decision-making processes to advance research. This promotes development and ensures the delivery of safe and effective medications to patients. However, in recent years, there has been a notable shift in this paradigm. This change is attributed to researchers integrating artificial intelligence (AI) into decision-making procedures, bringing about transformative effects not only in the pharmaceutical sector but also across various industries (Carou-Senra et al., 2023; Liu & Rudd, 2023; Malviya et al., 2023; Singh Sharma, 2023). AI-driven decision-making applications have emerged as powerful tools, enabling pharmaceutical scientists to make more informed and efficient decisions. The repercussions of this are evident in the accelerated pace of drug discovery, its optimization, and the enhancement of manufacturing processes (El-Naggar et al., 2023). Figure 1 offers a comprehensive visual representation of the key disciplines within the pharmaceutical sciences that AI-driven decision-making applications have profoundly impacted. The influence of AI is most pronounced in six primary areas: drug research and discovery, clinical development, personalized medicines, manufacturing and supply chain, launch and commercial activities, and postmarketing surveillance. AI-powered applications not only enhance decision-making but also elevate patient outcomes and improve the overall performance of the pharmaceutical industry. This highlights AI's transformative potential, positioning it as a pivotal catalyst for the future evolution of pharmaceutical sciences.

One of the foremost advantages of implementing AI in the domain of pharmaceutical sciences is its potential to expedite drug discovery and development. Traditional methods for identifying potential drug candidates have often been labor intensive, expensive, and filled with uncertainties (Khadela et al., 2023).

Figure 1. Areas of AI-driven decision-making applications in pharmaceutical sciences