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ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING IN DRUG DESIGN

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ABSTRACT : Artificial Intelligence (AI) and Machine Learning (ML) have transformed drug discovery, significantly improving efficiency, accuracy and speed in drug research and development. Compared to the older, time-consuming, and expensive traditional approach, AI-driven methodologies optimize molecular design, predict drug-target interactions and streamline clinical trial processes to the potential saving of both costs and timelines. AI-powered computational tools, such as virtual screening, de novo drug design, and structure-based drug development, have also helped enhance the selection of more accurate drug candidates to be brought to development, improving success in drug development. AI has also affected prediction in Drug-Drug Interactions (DDIs) and adverse drug reactions (ADRs), enhancing safety due to patient improvements from advanced techniques in data analysis like Natural Language Processing (NLP) and network-based modeling. Optimistic to this notion, clinical trials have become improved through AI: better patient selection, adaptive design and constant monitoring, maximizing efficiency while trimming costs. Currently, challenges encountered encompass data quality model interpretability along with ethical debates, yet research in pharmaceutical fields continues with momentum. Quantum Computing, automated laboratories and more such drugs repurposing by AI make it all work the faster way it is meant. This advancement of AI will continue to shape health care, hasten drug development, and enhance patients' outcomes and therefore, is essential in modern medicine.

Key words : Artificial intelligence (AI), Machine learning (ML), Drug-Drug interactions (DDIs), virtual screening, de novo drug design.

Introduction

Drug discovery is the sophisticated process of inventing, finding, and producing new pharmaceuticals to improve human health and combat disease. This comprehensive journey, which is critical for putting effective medications into medical practice, includes numerous steps ranging from target identification and lead compound discovery to optimization, rigorous preclinical testing and meticulous clinical trials (Rantanen and Khinast, 2015). Historically, this approach has required tremendous time and resources, taking an average of 12 years and costing US\$2.6 billion to progress a single molecule from conception to FDA clearance. Despite these efforts, the process is characterized by high attrition rates, considerable adverse effects of contemporary medications, and ongoing difficulty in treating chronic diseases like as diabetes and cancer. The introduction of AI represents a paradigm shift in drug discovery, providing a range of advanced computer tools designed to supplement rather than replace