Chapter 3
Artificial Intelligence and Machine Learning in Drug Discovery and Development

Sakshi Garg
KIET School of Pharmacy, KIET Group of Institutions, India

Kunal Arora
Sawmi Vivekanand Subharti University, India

Sumita Singh
Sawmi Vivekanand Subharti University, India

K. Nagarajan
KIET School of Pharmacy, KIET Group of Institutions, India

ABSTRACT

Over the past decade, artificial intelligence (AI) has significantly reshaped formulation development, drug discovery, and delivery processes. This study examines how AI and its technologies are enhancing efficiency and precision in pharmaceutical research. Crafting novel medications is crucial in the journey of drug development, offering the potential for enhanced bioavailability and targeted distribution. The conventional trial-and-error approach to formulation development, however, demands extensive resources and time-consuming in vitro and in vivo experiments. This article outlines the role of machine learning workflows in optimizing medication formulation processes, with a focus on structure-based and ligand-based drug design. Nanotechnology's potential for revolutionizing healthcare, including drug delivery and microscopic interventions, hinges on data science. Moreover, the exciting prospect of AI-powered nanobots holds promise for targeted drug delivery and tumor treatment with minimal patient impact.

1. INTRODUCTION

In 1956, John McCarty came up with the concept of "Artificial Intelligence" (AI), which he defined as the "science and technology of making intelligent machines." In 1950, Alan Turing made the bold pre-

DOI: 10.4018/979-8-3693-0368-9.ch003

diction that in the not-too-distant future, computers will be able to be trained to mimic human behaviour and intelligence. AI systems make use of algorithms such as use algorithms such as these, which are sufficiently intelligent and pre-programmed. In its place, it uses machine learning (ML) methods, such as deep learning (DL) neural networks and underlying learning algorithms. Without being specifically programmed, a computer system can use machine learning to learn from past experiences and use those learning to make predictions about the future or judgments based on those experiences.

Artificial intelligence is gaining ground in every discipline when it comes to improving the quality of human life. Artificial intelligence essentially refers to any tool that can 'mimic' human intelligence (Ramesh, 2004). Computers are programmed to perform complex and fresh functions in various areas to lower human workload, enhance preciseness, and make any task largely operative and quick (Miles & Walker, 2006).

Using cognitive science, artificial intelligence can perform tasks only humans can, such as reasoning, natural communication, and problem-solving. This involves making machines that learn and improve.

However, nanotechnology creates tiny materials and devices. Sometimes this involves working with atoms and molecules. Nanotechnology can make lightweight, solid materials and tiny machines and sensors.

2. AI IN DRUG DISCOVERY AND DEVELOPMENT

Methods such as molecular docking, quantum mechanics, and statistical learning are utilized in the process of mining chemical databases for the discovery of novel inhibitors. Both strategies have seen significant use in the process of drug development, with the end goal of locating potentially useful lead molecules. This field of research is also known as computational drug design, computer-aided molecular design, computer-aided molecular modelling, rational drug design, *in silico* drug design, and computer-aided rational drug design. *In silico* drug, design refers to the process of designing drugs entirely within a computer simulation environment. All of these terms refer to the same thing: designing drugs using computers. During the entirety of this investigation, the term "computer-assisted drug discovery and development" (CADDD) will be utilized to refer to the overall process. It is not impossible to combine computational and experimental methodologies. One of the most important and crucial areas in which artificial intelligence have shown to be of the utmost significance is the field of drug research and development. In today's world, when more and more diseases are posing a threat to people's lives and there is an ever-increasing demand for more and more medicines to combat these diseases, there is an ever-increasing need to identify innovative therapeutic molecules at a faster rate and with greater precision. This is because the number of diseases that threaten people's lives is also increasing. It is possible that the data sets given to pharmaceutical businesses for the purpose of medical development contain millions of molecules; hence, it is impossible for a typical machine-learning system to process these molecules. As a result, the process of drug discovery and development calls for increasingly sophisticated AI systems (Yang & Siau, 2018).

The process of researching and developing a new medicine can take anywhere from ten to fifteen years and cost up to two and a half billion and fifty-eight hundred million dollars. The multi-step process that begins with the selection of an appropriate pharmacological target and is validated by a breakthrough in the discovery of the first candidate, the optimization of the first molecule, and preclinical and clinical research are the following steps in the process that began with the choice of a suitable pharmacological