Chapter 5
Applications of AI in Computer-Aided Drug Discovery

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ABSTRACT

Drug discovery is the process in which healthcare is approached through identification of potential new therapeutic agents. CADD provides solutions at every stage of drug discovery including the leading challenges of cost and time. CADD has provided an effective solution to this challenge. AI has enabled multiple aspects of drug discovery, including the analysis of high content screening data and the design and synthesis of new molecules. The use of transparent methodologies like AI is crucial, particularly in drug repositioning/repurposing in rare diseases. An abundant variety of methods, in particular the concepts of deep learning, have been used for protein modelling and ligand-based drug discovery along with artificial neural networks for QSAR modelling. Structure-based ligand identification via AI modelling is also explored. AI presents the scientific community and the biopharma industry and its established processes for discovering and developing new medicines with new challenges.

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INTRODUCTION

Computer Aided Drug Discovery and design is an arena of Computational Biology that is being explored more and more with major improvements being made in the past decade. The amalgamations of AI and ML with existing CADD technologies has led to the numerous successful outcomes of CADD. Before delving into the concepts of CADD and its applications with AI, it is important to gain an understanding of what AI and ML are as follows.

Artificial Intelligence and Machine Learning

It is essentially the development of such machines and models that are "intelligent". What one means by this is that these machines and models use deduction processes inspired from the way a human thinks. AI which is often erroneously confused with Machine Learning is a method derived from the concepts of ML and deep learning to enable the user to understand problems rationally and to come up with possible solutions. One may define Machine Learning as a subset of AI, fundamentally the generation of such analytical models which accepts enormous data as input and can successfully sort through this data to establish the presence of any patterns and make decisions based on this. As mentioned above, AI is the development of such machines and models that are "intelligent". When the avenue of artificial intelligence was first explored, researchers had aimed to essentially duplicate the way humans think through a machine. Over the years, scientists have adopted new definitions and explored new arenas of AI and aim at developing systems that don't just think like humans but can have deduction powers personalised for a number of simulated conditions to come up with optimum solutions for the given problem. (Leighton et al., 2022)

These AI systems use the concepts of ML and neural networks to do what might be understood as mimicking human decision-making patterns in a way that these decisions are a series of yes or no questions. The aforementioned concept of Machine Learning and AI finds its application in many spheres. Biology and Life Sciences is one such field that has significantly benefited from AI and ML. Biological and Life Sciences research has led to an abundance of biological data that has been generated (omics data). AI and ML has enabled researchers to analyse the vast amount of biological data and draw inferences from the patterns recognized in the data using AI and ML. AI and ML has enormous applications in a very important are of life sciences which deals with medicine and healthcare. Some of the noteworthy examples that have been highlighted further. Antibody Discovery and Antibody selection is a notable example of AI in healthcare (Artificial intelligence turns to antibody selection, 2022). ML has also been used to design antibodies by