American Journal of
Biomedical Science & Research

www.biomedgrid.com
ISSN: 2642-1747

Mini review

Artificial Intelligence in Drug Discovery and Development

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To Cite This Article: *Amal Abdulrahim Abdullah Althubiti*. Artificial Intelligence in Drug Discovery and Development. Am J Biomed Sci & Res. 2023 20(4) AJBSR.MS.ID.002732,* DOI: 10.34297/AJBSR.2023.20.002732

Received: November 09, 2023; **Published:** November 16, 2023

Abstract

Artificial intelligence accelerates the drug discovery and development process and reduces the cost, with enormous amounts of successful applications from language modeling to improvement in the pharmaceutical sector. The deep-learning approach has been used throughout the drug discovery steps as the drug-related data increase. In this mini-review, I gave a general description of AI and its application in drug discovery and development. Computer-aided drug discovery and ligand-based quantitative structure-activity and property (QSAR/ QSPR) and De Novo drug design, integration with single cell technology, drug metabolism, and excretion, and discuss recent advancement in colorectal cancer and tooth loss, integration of plant-based traditional medicine, and showing AI-assisted platform used to discover serotonin 5-HT1A drug, which is reaching the clinical trial in less than 12 months which is far less than conventional method that needs four years of drug discovery process.

Keywords: Artificial intelligence, Machine learning, Computer-aided drug discovery, Drug discovery and development

Introduction

Innovation of the artificial intelligence approach has made remarkable improvements in various fields, particularly biological technologies, to reduce the drug discovery and development cost and time and failure-rate processes [1].

Developing an effective system to deliver therapeutic agents to the desired target while minimizing their harmful effects and maximizing their efficiency was challenging among drug discovery scientists [2]. In addition, novel therapeutic agents need more time, effort, and a high-cost process, hence, traditional computational approaches, including molecular docking and Virtual Screening (VS), are utilized as an alternative to overcome those limitations [2]. However, their inefficiency and inaccuracy emphasize the need for new techniques to solve these hurdles.

The lengthy drug discovery process is known to take around 12 years, starting from a preclinical study such as Hit and lead discovery and optimization all through clinical trials of phase l, ll, lll, until the final drug approval to be officially used in humans, with the need of high cost of around 1.2 billion dollars of the whole process, challenged by the drugs withdraw from the market due to their side and adverse effects on human. Consequently, a sophisticated system such as Artificial Intelligence (AI), including Machine Learning (ML) and Deep Learning (DL), has successfully decreased the cost and accelerated the drug discovery process [3,4].

Artificial intelligence AI, which is referred to as machine intelligence, is human intelligence simulation, by which a machine mimics cognitive behavior associated with the human brain during learning and problem-solving [5], using software and systems that, when learning and interpreting from input data, facilitate independent decisions-making for specific aims [6]. There is a variance in the definition of Artificial Intelligence and machine learning. Artificial Intelligence is a computer science branch of engineering and statistics that uses models or algorithms to complete tasks and obtain behaviors like prediction and decision-making. Machine learning, on the other hand, does not have to be explicitly programmed. The deep learning approach uses a neural network algorithm to

direct the input data entered into the machine, thus improving the accuracy and minimizing the system's bias.

As part of AI, machine learning models use data analysis in ML training algorithms to develop efficient ML models. These ML tools assist the 3-dimensional structure prediction of the target protein, which is crucial in drug discovery [2]. Recently, Alpha Fold, an AI-based tool that predicts 3D protein structure based on amino acid sequences, has been detected by Google's DeepMind (*https://github.com/deepmind*), which uses PDB structural data as a training set [7,8]. *Jessica Vamathevan, et al.,* have illustrated the application of machine learning in drug discovery and development, from target identification and biomarker prediction to small molecule design [9].

In this mini-review, I will briefly investigate the artificial intelligence applications and the limitations and future perspectives of this remarkable computational approach.

Artificial Intelligence Applications

One of the critical AI breakthroughs was IBM Watson, whose development led to DeepQA software, a computer system that mimics successful competition at the quiz show Jeopardy compared to top players at Jeopardy! Quiz show (www.jeopardy.com). They used unstructured and structured data to answer questions logically through natural language- processing such as DeepQA, which utilizes various models that scored based on a training set using multilayer logistic regression and screening through a testing set [10]. In the drug discovery field, this IBM Watson system has been extensively used by Pfizer to accelerate the search for drugs of immuno-oncology conditions.

Application of *AI*-assisted computational models in drug discovery *investigated by José Jiménez-Luna. et al.,* in ligand-based quantitative structure-activity and property (QSAR/ QSPR) and *De Novo* drug design. In the case of QSAR/QSPR, the prediction of pharmacokinetic parameters and biological activity showed successful progress and molecular descriptors are used to present machine-readable numbers that are indicative of molecules' structural features such as functional groups, pharmacophore distribution, and physicochemical properties [11]. Computer-assisted *de novo* drug design is challenging, with ligand and/or structure-based being the most known approach to designing novel molecular profiles with effective pharmacological potency and properties [12,13]. AI can identify hit and lead compounds with faster validation of the drug target and can also assist in predicting a targeted protein 3D structure [14]. PDB bind is a database that details the protein-ligand structure complex [15]. Leveraging artificial intelligence AI and machine learning with the biology knowledge of a single cell level can produce unprecedented solutions in drug discovery and development by enhancing biomarker prediction and the discovery of drug candidates with high-quality and disease-associated targets; for this purpose, HiFiBiO Therapeutics has established a novel translational platform of Drug Intelligence Science (DIS) integrating AI/ML with single-cell technology [16], resulting in the translation of high-resolution outcomes related to drugs, targets and patients.

AI in drug research and discovery can enhance the effectiveness and safety of drugs in both animals and human by increasing their metabolism and excretion. Regulation of metabolism and excretion is crucial to release toxic substances from our body and prevent their accumulation, which can result in metabolic diseases and liver and kidney organ damage. Understanding the importance of these process regulations and the consequences of their disturbances, predicting drug metabolism and excretion, helps researchers to design novel compounds with enhanced efficacy and pharmacokinetics and decreased toxicity. Noticeably, multidrug resistance in cancer chemotherapy and infectious illnesses is also affected by drug metabolism. Recent research showed the AI's utility in predicting the metabolism and excretion of medication [17].

Ryza Rynazal, et al., has used a local explanatory method instead of a global one to personalize specific bacteria strains potential as biomarkers for Colo Rectal Cancer (CRC) [18] and has suggested the potential role of this method in future personalized treatments in other conditions.

Khan, et al., has reviewed integrating traditional medicine and AI in drug discovery and provided a framework for plant-based traditional medicine with a drug discovery platform, in which AI assists. Plant-derived traditional medicine has been used widely in various conditions that chemical therapy has not been discovered yet, and it is also less toxic, less time-consuming, and cheaper than modern medicine. [19].

Chin-Chang-Chen, et al., have developed a model of AI-based detection based on Convolutional Neural Networks (CNN), which can be beneficial for the diagnosis and treatment by dental professionals through estimation of radiographic of RBL and interproximal alveolar bone level [20].

Sumitomo Dainippon Pharma (Japan), in cooperation with Ex Scientia by using their AI-assisted platform, has invented the first AI- drug molecule DSP-1181, a serotonin 5-HT1A receptor agonist, has reached human trial for obsessive-compulsive disorder in less than 12 months compared to 4 years of conventional therapy [21]. The strong alignment of the experiences and knowledge in pharmacology and chemistry on monoamine G-protein coupled receptor G-PCR drug discovery resulted in the success of their project.

Limitations and Future Perspectives

Despite the enormous advancement of AI in the advancement of drug discovery and innovation, the lack of accountability might hinder this technology as it is claimed to produce false information and safety concerns by generating threatening content. In addition, the automation of special tasks can lead to job displacement; however, augmented capabilities of humans pave the way for new job opportunities and productivity enhancement. Implication of AI may also encounter ethical issues regarding bias and data privacy. Hence, considerable care should be taken for the data used to train

the model; nevertheless, AI/ML has no ethical concern for drug development [3].

Conclusion

Real-world applications of AI/ML demonstration are crucial for the transformation of the pipeline of drug discovery and development process and in the enhancement of the reliable decision-making abilities of humans. Deep learning in AI with Computer-Aided Drug Discovery (CADD) methods has been extensively utilized to expedite drug discovery of valuable results. In this mini-review, I have briefly revised the recent research achievements in the application of artificial intelligence in the drug discovery and development era.

Acknowledgement

None.

Conflict of Interest

The author declares no conflict of interest.

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