WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
SJIF Impact Factor 8.453
Volume 13, Issue 5, 1426-1436. Research Article ISSN 2277–7105

ROLE OF ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND DEVELOPMENT

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Article Received on
17 January 2024,

Revised on 07 Feb. 2024,
Accepted on 27 Feb. 2024

DOI: 10.20959/wjpr20245-31605

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ABSTRACT

The current rise of artificial intelligence and machine learning has been remarkable. This reduced people's workload and greatly improved the quality of life. This article describes the use of artificial intelligence and machine learning to improve drug discovery and development. This study conducted a systematic review of studies; these were selected based on the previous knowledge of the authors and a keyword search of public databases filtered by relevant context, abstract, methodology, and full text. This task force supported the role of machine learning and artificial intelligence in facilitating drug discovery and development processes, making them more cost-effective or eliminating the need for clinical trials altogether, since these technologies can be used to run simulations. They also allowed scientists to study different molecules more widely without experiments. The results of this work demonstrate the general application of machine learning and artificial intelligence methods in drug development and indicate a promising future for these technologies. These results should allow researchers, students and the pharmaceutical industry to dive deeper into machine learning and artificial intelligence in the context of drug discovery and development.

INTRODUCTION

All aspects of life are constantly changing, and one of the main goals of people is to manage these changes to their advantag. For decades, pharmaceutical manufacturing has been guided by a regulatory framework that ensures the quality of end products by testing raw materials, in-process materials, end-product characteristics, batch-by-age performance and fixed process conditions. The pharmaceutical and biopharmaceutical industry has been a

source of limited ingenuity and new technologies or machinery and has led to the development of new principles or interpretations in the general chemical and machinery industry. The pharmaceutical industry is in dire need of mechanical inventions that facilitate the creation of medicines for human use. The creation and production of drugs with complex processes that are safe for humans on a commercial scale and their introduction into routine medical use has been difficult due to technical resource limitations.

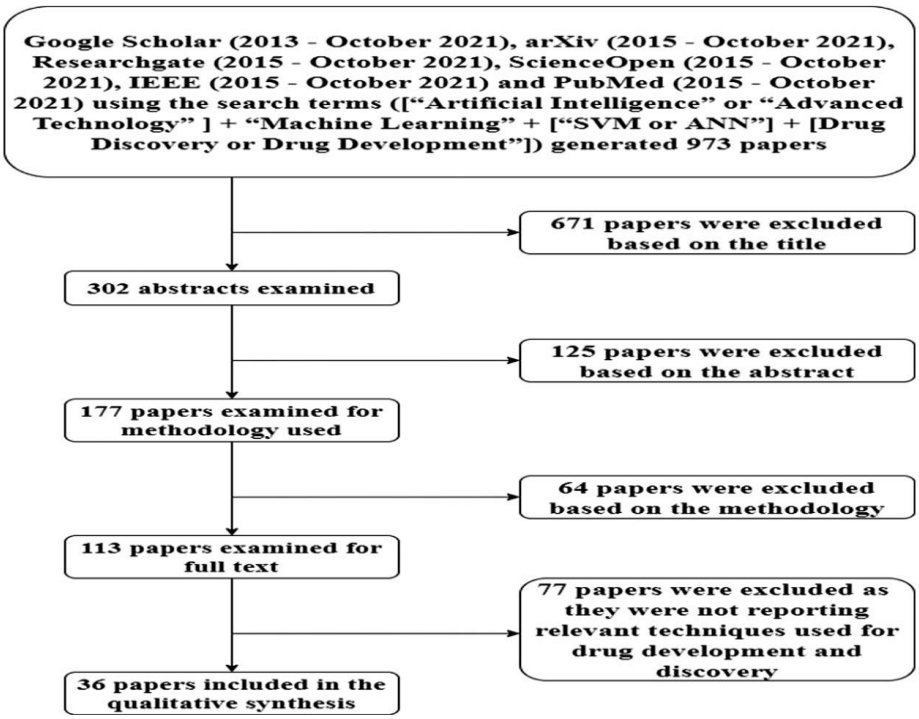
The use of artificial intelligence is rising and is likely to change the way clinical trials and training are conducted. Doctors can contribute to the development of this technology for use in the medical and pharmaceutical industries; this ensures that the potential of AI to outstandingly improve medical care is fulfilled. The artificial intelligence is currently used in 4,444 pharmaceutical industries in four main ways. The first is to assess the severity of the disease and predict whether a treatment will be successful in a given patient, even before it is administered. Second, it is used to prevent or resolve complications during treatment. The third main use is as an aid during the treatment or surgery of patients.

Artificial intelligence also plays a more general role in big data management and analysis. Big data is a new paradigm that describes the acquisition of extremely large amounts of data and combines it with advanced analysis that enables new information or insights from that data.[4,5] In the pharmaceutical industry, traditional data storage methods have therefore become obsolete as the amount of data increases. Big data offers a huge opportunity for further research as a result of data mining in this field and can increase drug production using a three-step data management process after acquisition, which includes the following steps: extraction and aggregation. large amount of distributed and heterogeneous data; configure data to ensure consistent format; and finally data analysis using various analytical platforms to produce a final output, the interpretation of which can inform which compounds or drugs to develop or which processes to use to maximize effectiveness.

AI-enabled technology is actively being adopted to solve small but critical problems in the pharmaceutical and development industries, driven by advances, growth and the adaptation of additional data available to generate meaningful insights. Therefore, the authors see the need for a comprehensive article that looks at the contribution of artificial intelligence, machine learning and big data to drug discovery and development, consisting of the latest technology, advances and new research by researchers in the field. and what the future of the pharmaceutical industry will look like if it practically includes the latest artificial intelligence.

2. Search methodology and article selection

As machine learning is used to solve important problems in drug discovery and development, we aim to provide an in-depth review of the latest technology, advances and new research from researchers in the field. As shown in Figure 1, we systematically searched recent literature using keywords related to this field (including [Artificial Intelligence or Advanced Technology] + Machine Learning + [SVM or ANN] + [Drug Discovery or Drug Development]) in publicly available databases such as Google Scholar (January 2013–October 2021), arXiv (January 2015–October 2021), Researchgate (January 2015–October 2021), Science20Open (October 1, 2013, IE) (January 2015–October 21), 5 January 2015-October (2015-October 2021), -October 2021). After filtering based on relevant context, abstract and methodology, approximately 36 studies were considered for inclusion in the literature review.



CONCLUSION

Advanced technologies in drug discovery

The results of our literature search revealed that there are a number of different technologies and techniques currently being used in the pharmaceutical industry to aid in drug discovery and manufacturing. (Absorption, Distribution, Metabolism and Excretion) in silico platform (Bayer, Leverkusen, Germany. This method models pharmacokinetic and physicochemical endpoints in the development of new drug substances. In theory, two distinctly different

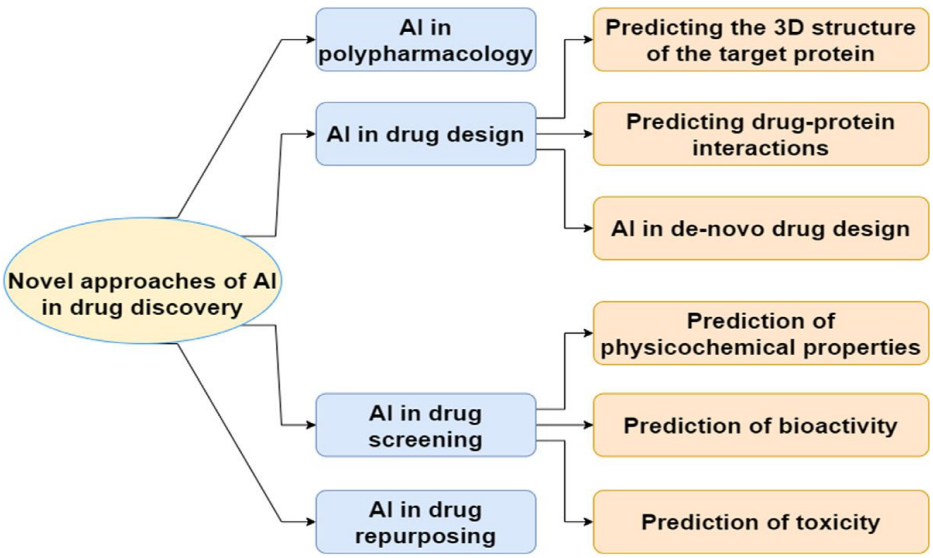
methods can be used to implement this technology. The first measures these results in the context of interactions between compounds of interest and defined proteins. he disadvantage of this approach is that it requires single proteins whose effects are clearly related to ADMET results, such as: changes in cognition, safety and measured cost-effectiveness; A high-resolution, three-dimensional (3D) image of the protein under study is also required.

Another approach involves the collection and compilation of secondary data based on the aforementioned parameters on various compounds used in protein synthesis; Based on this information, complex/hybrid deep learning models can be developed using machine learning algorithms and artificial intelligence. However, this approach requires a lot of manual maintenance and attention to detail; small design mistakes can lead to incorrect results and conclusions, which is expensive and time-consuming. Even if no mistakes are made, this approach still takes a lot of time because large amounts of data must be monitored, moderated and manually deleted. Another technology used in this industry is blockchain. A blockchain is a data structure based on collecting and compiling records and turning them into blocks, which are then chained together in chronological order of creation; hence the name blockchain. Blockchain has several different characteristics that allow it to be used in the pharmaceutical industry. These factors include permanence, decentralization, immediacy and recognition. Persistence refers to the immutability and immutability of blockchain data. Decentralization describes the fact that several entities can be responsible for processing data in a system. Immediacy refers to the transparency of the information stored on the blockchain and the fact that the user can see all the information stored on the blockchain. Traceability is the ability of a blockchain user to track data stored on the blockchain with indisputable timestamps. In the pharmaceutical industry, these factors ensure that drug manufacturers can review and control their data and transactions at any time. According to various studies, the blockchain made it possible to carry out drug tests and clinical trials more efficiently and made the distribution chain of pharmaceutical companies more efficient and easier to monitor. However, blockchain has some disadvantages. For example, because it is a new and cutting-edge technology, it comes with huge installation and maintenance costs that smaller companies cannot afford, thus limiting its usefulness. Due to the cost barrier, very few people have the experience and knowledge of how to use this type of technology, limiting its use to wealthier geographies. Thus, there is still a long way to go before expensive technologies such as blockchain can be widely adapted to fulfill their great potential. The third innovative technology currently used in the pharmaceutical industry is 3D printing. More innovative

methods of this technology use blue light instead of white, which increases accuracy due to its extended impedance transmission capability. These updates allow you to configure the reproduction of objects incrementally; Advances in 3D printing enable on-site and on-demand production of products for a wide variety of people and industries due to the widespread availability and practicality of advanced 3D printing. Overall, we have identified gaps and issues affecting the utility, effectiveness and overall impact of these new technologies in the pharmaceutical industry. Future inventions may overcome this by lowering prices, increasing efficiency and increasing consumer-friendliness, enabling wider adoption and use for human health.

Artificial intelligence in drug discovery

Improved computing power and the development of innovative techniques in the field of artificial intelligence could be used to innovate drug discovery and development processes. At the time of this literature review, the pharmaceutical industry is facing a reduction in the effectiveness of drug development programs and at the same time increasing research and development costs. In recent years, the digitization of information in the pharmaceutical industry has radically expanded; Effective acquisition, research and application of this knowledge to solve complex clinical problems is a current challenge. Thanks to updated computerization, artificial intelligence can process a huge amount of information .This section discusses the main uses of artificial intelligence to improve the efficiency of the drug development cycle.



The above shows how and where AI can be integrated into drug discovery and development processes and new applications of AI in the pharmaceutical industry. Drug discovery can be divided into four parts: drug development, polypharmacology, drug purification and drug screening. Artificial intelligence is mostly used to predict drug properties, potentially reducing the need for clinical trials and real-time research participants, which would be beneficial from both an economic and ethical perspective. This section discusses the research identified in this review that supports the integration of artificial intelligence into the drug development process to improve efficiency, accuracy and productivity.

Challenges

Industry back in terms of efficiency. Despite the advances in artificial intelligence and machine learning algorithm technologies applied in the pharmaceutical industry, there are still many challenges in implementing and integrating these technologies into the drug development process in particular and the pharmaceutical industry in general. One problem is inefficient data integration. This problem arises from the diversity of data sets, which may include raw data, processed data, metadata, or candidate data. These datasets need to be collected and combined to ensure effective analysis, but currently there is no established method for this. This is necessary before drug discovery begins, because without properly formatted data, the output of machine learning algorithms will be inaccurate. Therefore, more efficient methods are needed to integrate existing information into data banks before the drug development process begins. Another problem is immobility of professional and skills: many people currently working in the pharmaceutical industry lack the skills or qualifications to use AI systems. Many people are good at data science and others at molecular chemistry and biology, but few are experts in both and have the right mix of skills to apply AI in a pharmaceutical context. Knowledge of the underlying chemistry is required to create appropriate algorithms and vice versa. A third but related difficulty is the skepticism of machine learning and artificial intelligence in the pharmaceutical industry, because the methodology of the algorithms is not known as a "black box" phenomenon, and the lack of trust in the resulting results. Those who are skeptical may be reluctant to use data generated by artificial intelligence and machine learning, which waste time and money and hold the development of artificial intelligence in the pharmaceutical industry. Skepticism about the role and results of artificial intelligence and machine learning in drug development processes can cause hesitation to invest in this technology. This can lead to slower, less efficient R&D compared to potential, which in turn leads to a decline in AI-related developments in the

pharmaceutical industry. These are the various barriers that stand in the way of actual development, and these are the challenges that must be overcome to integrate AI into drug development processes.

Future scope

The main potential of artificial intelligence in the pharmaceutical industry is to reduce costs and increase efficiency. Extensive research has shown that dynamic learning can distinguish deeply accurate AI models using half or less data than traditional AI and data subsampling methods. Although the reason for this increased productivity is not fully understood, it appears that reduced repetitions and biases, as well as the acquisition of more relevant information to cross selection boundaries, are key factors in this improved performance. As a result, examination costs appear to be reduced by up to 90% when the expected mechanical overhead of dynamic learning is not taken into account. Machine learning techniques can handle complex analyzes of huge, heterogeneous and multidimensional data sets without manual input, which has proven useful for writing business applications. Combining machine learning, especially deep learning, with human skills and experience may be the best way to coordinate many data repositories. The amazing data mining power of AI innovations has given new importance to computerized medication plans that cover multiple clinical aspects better than fragmented data that can speed up prescribing processes. Thanks to improvements in clinical data collection and artificial intelligence calculations, AI innovations are enabling many aspects of drug discovery and development and becoming a standard computerized drug planning strategy. The coordinated development of mechanization and innovation resulting from the convergence of technologies should lead to advances in medicine through better analysis of large and complex data. This is necessary to shorten drug development cycles, reduce costs and increase success.

Summary

In summary, many factors influence the successful integration of artificial intelligence and machine learning into drug discovery and development and pharmacology, drug design, drug screening, and drug repurification in the pharmaceutical industry. Technological development, including development based on artificial intelligence, is always necessary to reduce the time and money spent on research, development and production activities and to increase efficiency. This systematic literature review demonstrated that artificial intelligence and machine learning can improve the efficiency and accuracy of drug discovery and

development. These techniques not only increase the efficiency of the process, but in some cases reduce or eliminate the need for clinical trials by running simulations instead, and allow researchers to study molecules more broadly without experiments, thus reducing costs and ethics. worries The integration of artificial intelligence and machine learning is likely to revolutionize drug development over time, but there are still several obstacles such as cleaning unstructured and heterogeneous datasets, random qualification of the computing device, etc. it can be prevented. Once these barriers are removed, advances in artificial intelligence and machine learning can be adopted and improved more broadly, marking the beginning of a new era for the pharmaceutical industry.

Abbreviations

AI: Artificial Intelligence

FDA: Food and Drug Administration;

PAAB: Pharmaceutical Advertising Advisory Board;

UGC: user-generated content.

Conflicts of Interest

The author declares no conflict of interest.

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