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ARTIFICIAL INTELLIGENCE BASED SYSTEM TO DIRECT THE DRUGS TO THE FAULTY DNA SEQUENCES AND TAILORING THE GENE SEQUENCES

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Abstract
Machine learning and artificial intelligence are now advancing significantly. It has considerably raised quality of life while reducing human effort. This article explains how artificial intelligence and machine learning are used to speed up and improve medication research and development. In this study, papers were evaluated systematically. These studies were chosen based on the authors' prior knowledge and a keyword search in freely accessible databases that were filtered based on related context, abstract, methodology, and full text. This body of study highlighted the roles of artificial intelligence and machine learning in expediting the drug research and development processes, making them more affordable or even removing the need for clinical trials. They also made it possible for broad, trial-free research on many compounds. The findings of this paper show how machine learning and artificial intelligence methods are frequently used in drug discovery and point to a bright future for these technologies. These findings should allow researchers, students, and the pharmaceutical industry to learn more about machine learning and artificial intelligence in the context of drug discovery and development.
Keywords: Drug discovery Artificial intelligence Machine learning

Introduction

One of the fundamental goals of humans is to regulate these changes for our advantage. This is especially true in the fields of medicine and pharmaceuticals, which are continually undergoing change.
These fields concentrate on the synthesis or discovery of chemical substances and combinations, as well as their use to alleviate both physical and mental pain. A regulatory framework that protects the quality of finished goods through testing of raw materials, in-process materials, end-product characteristics, batch-based operations, and set process conditions has been in place for many decades now regulates the production of medicinal products [1]. The development of new ideas or interpretations in general chemical and mechanical engineering has been driven by the drug and biopharmaceutical sectors, which have been a restricted supply of imaginative and original technologies or machines. Mechanical innovation is urgently needed in the pharmaceutical sector to facilitate the production of drugs for human use. Because to the current restrictions on technological resources, it has been difficult to develop and manufacture complicated processes drugs that are safe for humans on a commercial scale, and to incorporate them into mainstream therapeutic usage [1]. The "one size fits all" philosophy underlies current prescription practices; nonetheless, numerous crucial fields of medicine demand fresh approaches, necessitating new pharmaceutical development procedures.
New and innovative pharmaceutical goods and procedures, based on new analytic tools and precise portions, are now possible because to recent advancements in genetics and diagnostics. The effectiveness of this sector would increase with the development of drugs like these that are adapted to the biology of the patient. The challenges of personalized medication cannot be solved with the level of progress in medical planning and assembly of these goods currently available. The pharmaceutical

business needs novel manufacturing assembly arrangements and tools that allow for the flexible assembly of specialized equipment and technologies [1].
Artificial intelligence (AI) is being used more often, which will probably alter how clinical evaluation and training are conducted. To guarantee that the promise of AI to dramatically enhance medical care is realized, doctors may collaborate in the development of this technology for application in the medical and pharmaceutical sectors [2]. There are now four primary methods that AI is applied in the pharmaceutical sector. The first is in determining the extent of the illness and forecasting, even before the therapy is started, if it will be effective for a certain patient. Second, it is employed to avoid or resolve issues that may arise during therapy. Its third primary application is as an aid during medical procedures or surgeries on patients in order to ascertain the rationale for the use of certain instruments or chemicals during treatment and to invent or extrapolate new uses for instruments or chemicals to increase safety and efficacy.
In the administration and analysis of huge data, AI also plays a more general function [3]. The term "big data" refers to a relatively new paradigm that describes the gathering of very large datasets and its pairing with advanced analytics to provide new knowledge or insights [4-5]. So, as data volumes grow, conventional data storage techniques in the pharmaceutical business are rendered outdated. As a result of data mining in this business, big data presents a significant possibility for more in-depth study and may enhance pharmaceutical manufacture by adopting a three-step data management method after collection that involves the following steps: large-scale data extraction and collation from a variety of sources; data configuration to guarantee consistent formatting.
Due to developments, expansion, and the adaptation of excess amounts of data accessible for producing useful insights, AI-enabled technology is actively being used to handle small yet significant concerned issues in the medication and development sectors. As a result, the authors feel that it is necessary to compile a thorough article that examines how AI, machine learning, and big data have contributed to drug discovery and development. This article will cover the most recent developments, research advances, and novel studies made by researchers in this area as well as what the future will hold for the pharmaceutical industry when it successfully applies the latest AI developments to it.

Methodology and choice of articles for searches

We set out to perform a thorough analysis of the most recent developments, advancements, and original studies carried out by researchers in this sector since machine learning is being used to address critical difficulties in drug development and discovery. As depicted in Figure 1, we carried out a thorough search of recent literature using key words associated with this field (such as ["Artificial Intelligence" or "Advanced Technology"] + "Machine Learning" + "SVM or ANN"] + [Drug Discovery or Drug Development"]) in openly accessible databases like Google Scholar (January 2013-October 2021), arXiv (January 2015-October 2021), Research gate (January 2015-October 2021), Science Open (January After filtering based on pertinent context, abstract, and technique, about 36 papers were taken into consideration for our literature evaluation.

Results

Advanced technologies in drug discovery

According to the findings of our literature search, several different technologies and methods are now employed in the pharmaceutical sector to help with medication development and production. One of these innovations is the in silico absorption, distribution, metabolism, and excretion (ADMET) platform

from Bayer in Leverkusen, Germany. With the use of this method, novel pharmaceutical compounds may be produced with accurate pharmacokinetic and physicochemical endpoint modelling [6].
Two fundamentally different techniques might theoretically be applied while using this technology. In the first, these results are evaluated in relation to interactions between relevant chemicals and specified proteins [6]. This method's disadvantage is that it calls for a single protein with effects that are directly connected to ADMET outcomes, such as changes in cognition, safety, and measurable cost-effectiveness. It also calls for high-definition and three-dimensional (3D) imaging of the protein under investigation. The second method entails gathering secondary data for numerous chemical substances used to generate proteins depending on the aforementioned parameters. Based on this data, complex/hybrid deep learning models may be created with the use of machine learning algorithms and AI [6]. This method calls for a lot of manual upkeep and meticulousness, though; even minor design errors can result in costly and time-consuming errors in findings and conclusions. Even if there are no errors.
Block chain is another another piece of technology utilized in the pharmaceutical sector. A particular sort of data structure called blockchain relies on gathering and compiling records, putting them into blocks, and connecting those blocks in chronological sequence to build. The term "block chain" refers to a chain. Blockchain may be used in the pharmaceutical sector due to a variety of various features. These characteristics include constancy, decentralization, clarity, and recognize ability [7]. Permanence describes how the data on the blockchain cannot be changed or altered. Decentralization refers to the possibility of a system's data handling being handled by a number of different organizations. The term "straightforwardness" refers to the fact that data stored in a blockchain is transparent and that every user may see all data.
The capacity of a blockchain user to follow the data contained in the blockchain with unquestionable timestamps is known as recognize ability. These elements make it possible for drug producers to examine and monitor their data and transactions at any time [7] in the pharmaceutical industry. Many studies have found that blockchain has improved the efficiency of drug testing and clinical trials, as well as the effectiveness and transparency of pharmaceutical businesses' supply chains [7]. Blockchain does have certain drawbacks, though. For example, because it is a novel and cutting-edge technology, it has high installation and maintenance expenses that are insurmountable for smaller businesses, which limits its use.
3D printing is a third cutting-edge innovation that is now applied in the pharmaceutical sector [8]. More advanced applications of this technology use blue light instead of white light, which increases accuracy because of its increased impedance transfer capability. These developments allow for the gradual configuration of item reproduction; moreover, because to the widespread accessibility and usefulness of modern 3D printing, a wide variety of individuals and companies are now able to produce goods locally and on demand [9]. We discovered a consistent pattern of flaws and issues that have an influence on the value, efficacy, and overall impact of these breakthrough technologies employed by the pharmaceutical sector. Future technological advancements may circumvent this by lowering costs, boosting efficacy, and improving consumer-friendliness, permitting more broad acceptance and use that will improve human health.

using machine learning to find new drugs

The pharmaceutical business is increasingly utilizing machine learning in several areas, including drug development, which has improved the sector as a whole. The growing number of businesses whose business models depend heavily on machine learning is evidence of the technology's success. Several pharmaceutical organizations have reportedly looked into using machine learning techniques for

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medication research and development [10]. Given the capabilities of machine learning and their value in the field of drug discovery, it is essential that they be included into any future developments in this area. The objective is to lessen the asset and work severity of drug disclosure via the use of high-throughput screening technology. The need for live animal testing might one day be reduced, if not entirely, thanks to machine learning [10]. These findings show that machine learning is a highly helpful technique for finding new drugs.

In order to improve and develop machine learning technologies for drug discovery and development, several chemical and biological information-related aspects are required. By using the conclusions gained from the data, this data would aid in the creation of more sophisticated and precise systems [11]. These data will need to be gathered by utilizing assays that quantify medicinal properties such cellular toxicity, cell structure heterogeneity, animal model effectiveness, on-target activity, pharmacokinetic endpoints, microsomal stability, and cytochrome P450 (CYP) inhibitory values [11].

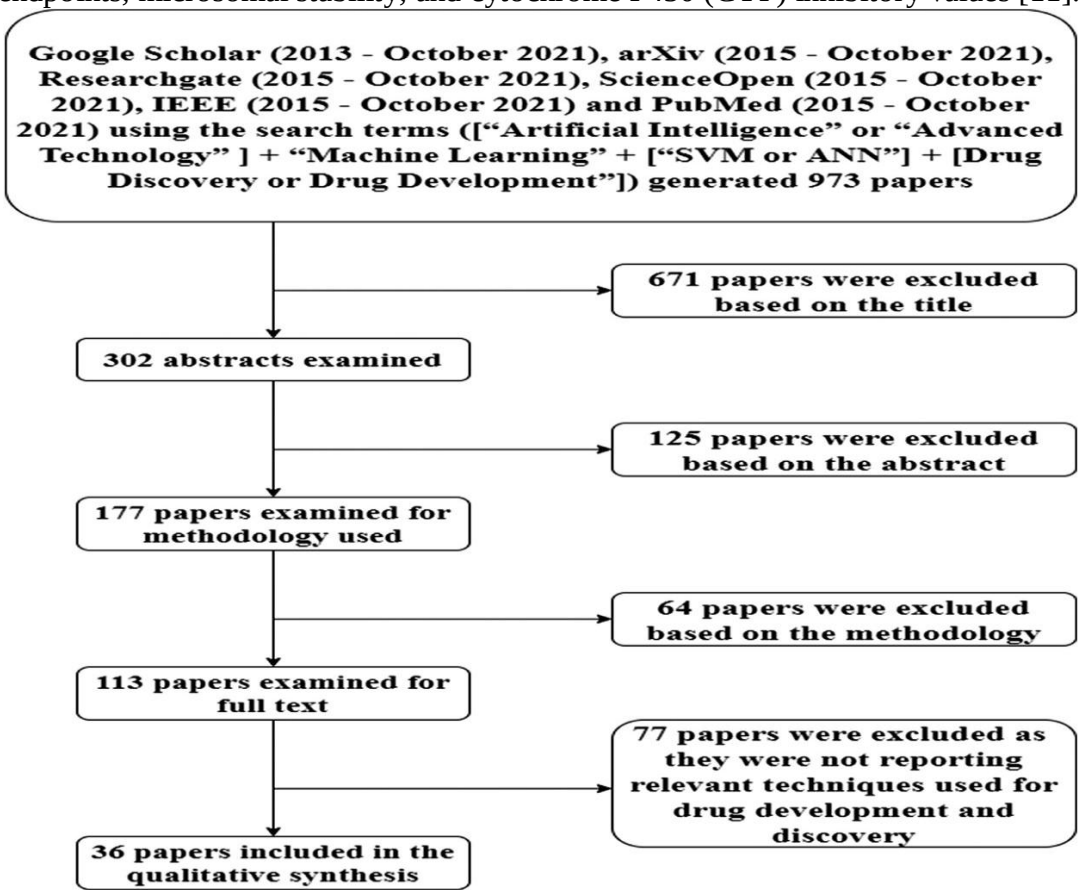

Figure 1. Criteria for study selection flowchart.

Figure 2 depicts a condensed cycle of the actions that take place when machine learning is applied to the pharmaceutical business, in particular to its development and production sectors, and it also demonstrates how machine learning works in general [12].

The data are made up of many elements, including termination data, applicability domain data, and orthogonal data. These data are fed into an algorithm that has been previously developed, taking into consideration model selections, selection functions, and orthogonal calculations. The algorithm produces

outcomes as well as iterative enhancements to the present methodology and practices to make them more dependable and efficient. Until a final product is conceived and produced, the process is updated and the cycle is repeated.

Margulis and colleagues' [13] work, which examines how highly bitter compounds may be found with the use of machine learning in the early phases of drug development, is one example of how machine learning is applied in the field of drug discovery.

The goal was to establish if a certain machine learning algorithm could be used in place of animal testing to forecast the bitterness of various compounds used in pharmaceuticals. This investigation was successful, as 80% of the bitter molecules were found to match those found in a short access taste aversion (BATA) trial. The BATA experiment's findings showed that, contrary to what was previously believed, toxicity and bitterness are not necessarily correlated.

This illustrates that machine learning was able to deliver findings that were both adequately accurate and new knowledge. Raschka et alresearch .'s [14–15] illustrates how machine learning may be incorporated into the detection of GPCR ligands, a crucial step in the drug development process. Their study sought to ascertain if machine learning might take the place of the outdated technology employed in trials to suppress the Sea Lamprey Receptor 1 (SLOR1) receptor signal, utilizing those tests to verify the outcomes of the machine learning algorithm. The program's output closely matched the performance that was thought to be the baseline, showing that the new algorithm could take the place of the previous technology for recognizing the properties of other molecules.

Pereira and colleagues conducted a further investigation demonstrating the usefulness of machine learning in this situation. The study's goal was to ascertain whether a machine learning system could distinguish between and rank docking receptors with the appropriate ligands, among other substances or chemicals. The outcomes demonstrated that the machine learning technique performed better than the typical docking receptor ranking mechanism. This demonstrated the potential of machine learning for a variety of tasks, including creating molecular databases and libraries and determining the pharmacokinetic characteristics of novel medications.

They conducted research to anticipate the antifungal and antibacterial effects of various medicines and compounds based on how well they worked against different bacteria and fungi. Several diverse descriptors, including stimulants, depressants, hallucinogens, dissociative, opioids, inhalants, and cannabis, were integrated using a linear description analysis algorithm. The findings added to the body of data supporting the use of machine learning in the drug development process by demonstrating that this way of evaluating drug properties had greater success rates than other non-linear methods.

Another research demonstrating the benefits of machine learning investigated if deep learning (neural networks) and machine learning algorithms might be used to analyze the therapeutic and preventive effects of various medications on genes. Findings revealed that, compared to the baseline model, predictions of drug categories were much more accurate, and they were categorized more accurately as well, increasing the accuracy %. The increased accuracy demonstrates that the usefulness of this classification method was enhanced by the integration of deep learning neural networks with machine learning algorithms, which more effectively identified medications with different pharmacodynamic and pharmacokinetic features.

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Two experiments that show two distinct subcategories of machine learning—conducted by Rantanen and Khinast [16] and Turki and Taguchi [17]—can be effectively contrasted. While Zhavoronkov and Mamoshina used transfer learning (a research problem in machine learning (ML) that focuses on storing knowledge gained while solving one problem and applying it to a different but related problem), Turki and Taguchi's study used reinforcement learning (one of the three basic machine learning paradigms, alongside supervised learning and unsupervised learning) to speed up the process used to identify

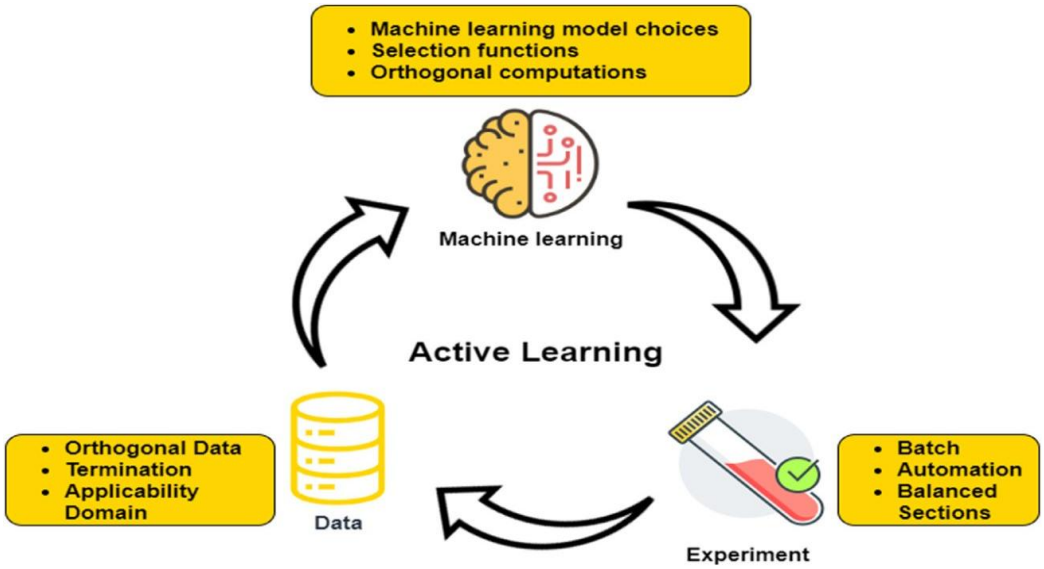

Figure 2. Machine learning in drug discovery [12] .

potentially useful drugs. Turki and Taguchi showed that the drug discovery process took just 46 days, which is a significant reduction from the time required by traditional methods. In comparison to their base readings, the study's results by Zhavoronkov and Mamoshina showed higher prediction accuracy.

Zhavoronkov and Mamoshina concluded that the algorithm's scope should be expanded (by using hybrid models and deep learning models) as the data collected for individuals is not applicable to a wider group of people. Turki and Taguchi concluded that there are still some algorithm coding improvements to be made in order to ensure that synthesized compounds have different formulas from current market products. Table 1 [18–22]

Artificial intelligence in the search for new drugs

Processes for drug discovery and development may be changed by increased processing capacity and the creation of novel AI tools. The pharmaceutical industry is now dealing with a decline in the effectiveness of its medication improvement efforts and concurrent increases in research and development expenses [23]. The pharmaceutical sector has experienced a significant growth in the digitization of information in recent years; one ongoing difficulty is to effectively gather, examine, and utilize this information to address complicated clinical challenges. AI is capable of handling massive amounts of data with improved computerization [24]. To boost productivity and efficiency, it may also incorporate and apply machine learning techniques. The primary applications of AI to increase efficacy are discussed in this section.

The unique uses of AI in the pharmaceutical sector are depicted in Figure 3 above, along with examples of how and where they may be incorporated into drug research and development procedures [25]. Drug design, poly pharmacology, drug repurposing, and drug screening are the four segments that may be meaningfully divided into drug discovery. AI is mostly used to anticipate pharmacological qualities,

which may eliminate the need for clinical trials and human research subjects, which would be advantageous from a financial and ethical perspective.

This section discusses the papers found in the review that back the incorporation of AI into the drug discovery process in order to increase productivity, accuracy, and efficiency. Using a Res Net neural network, Cui and Zhu [26] investigated whether AI can predict the physicochemical characteristics (solubility, partition coefficient, and dissociation constant) of several medicines. The longer extraction time and higher yield of polysaccharides from Many studies found that when compared to other non-AI based models, this network was more accurate in predicting the solubility of the compounds. This demonstrated that AI may be used into the medicine development process to increase its effectiveness.

Using a recursive neural network to predict the solubility of various chemical and biological compounds in water, Lusci and colleagues [27] conducted a second investigation to highlight the advantages of AI in this situation. Regarding the research done by Cui and Zhu, it revealed that the AI model gave findings that were more accurate than those attained using traditional methods, demonstrating its value in drug development.

Polykovskiy and colleagues' work [28], which looked at the ability of AI to anticipate the activity of various synthesized compounds, is another example of how AI may increase efficiency.

The goal was to ascertain whether utilizing AI, the reliability of the drug screening process could be improved by increasing accuracy. To forecast activity, an adversarial auto-encoder was employed. The results obtained with a recurrent neural network-based generative model approach differ from those obtained with the de novo molecular design to generate random drug-like compounds and another to generate target-biased compounds, indicating that the two approaches can be used in conjunction with one another. Moreover, it provided crucial details about the molecule-target, indicating that AI not only increases procedural speed and accuracy but also facilitates new discoveries.

Another research by Daynac and colleagues [29] investigated if artificial neural networks might be used to predict the antibacterial characteristics of diverse compounds, making the procedure quicker, less expensive, and more accurate. The outcomes demonstrated that the neural network had a very tiny error margin and could correctly predict more than 70% of the antibacterial activity (10 mm). Also, it was able to forecast the behavior of two or three molecules simultaneously, which cut down on the amount of time needed for processing in general.

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Table 1 An overview of additional studies that used machine learning for drug discovery

Technique	Application	Methods	Accuracy
Traditional reinforcement learning [18]	New drug development	Integrating a number of machine learning techniques to create new molecules	Very accurate (95% of molecules were found to be feasible)
Transfer learning [19]	Emulating biological processes	Using regression-based transfer learning to model responses to anticancer medication	Very accurate
Multitask learning [20]	Drug development and testing	Using genetic and medicinal data to monitor the signals between the pathways where the molecules of the drug travelled	Accurate
Multitask analysis [21]	Drug–target interaction	Using a number of machine learning algorithms and sub-categories in order to analyze and monitor the interactions of the drug with its target	Accurate
Multitask learning [22]	Post-manufacture drug reviews	Using multitask learning and analysis algorithms in order to analyze data in bulk	Very accurate (4,200 reviews in a very short span of time)

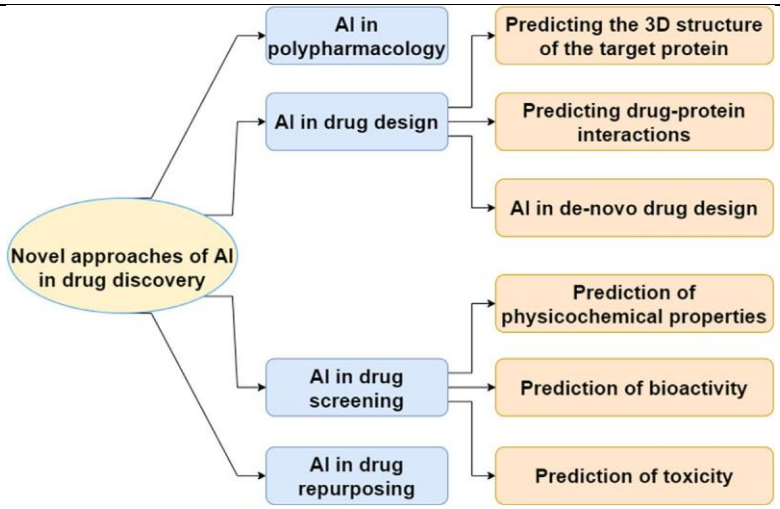

Figure 3. Applications of artificial intelligence in drug discovery [25] .

Pu and colleagues' research [30] is the most recent one in our literature review to report on the utility of AI. The authors sought to accelerate the current procedure and do away with the need for clinical trials by using an AI algorithm, eToxPred, to forecast the degrees of toxicity of various synthetic and biological chemicals. The outcomes demonstrated that the AI model was sufficiently accurate to possibly replace clinical trials since it could correctly predict the hazardous qualities more than 72% of the time with only a 4% total error rate.

Kadura and colleagues used adversarial auto-encoders and adversarial networks to speed up the drug screening process for anticancer molecules, while Al-Safarini and El-Sayed used a variety of AI processes to predict the biological activity of various molecules when they come into contact with

various cell types. These two studies, by Kadura and colleagues [31] and Maram and Hamdy [32], used two different subcategories of AI networks, respectively. The initial study's findings showed how effective this technology is by showing that it can screen around 72 million anticancer compounds. The outcome of the second investigation showed a low error margin and better accuracy (71.9%) when compared to the base readings (RF: 62.6% and SVM: 66.0%). Both studies present various elements of the usefulness of AI in a pharmaceutical Table 2 [33–37]

Challenges

The introduction and integration of AI and machine learning algorithms into the drug development process particularly, as well as the pharmaceutical business in general, still faces numerous challenges. This is true even if these technologies have advanced.

Ineffective data integration is one issue. This issue arises from the diversity of datasets, which may include candidate data, processed data, raw data, or metadata. There is presently no standardized procedure for gathering and assembling these datasets for effective analysis. This is necessary before the drug discovery process starts since the output of the machine learning algorithms would be erroneous without properly prepared data. Hence, more effective techniques are needed to incorporate existing data into data banks before the drug development process starts [38].

Another issue is the immobility of occupations and skill sets. Many people now employed in the pharmaceutical sector lack the training or credentials required to run AI systems. Although many people are specialists in data science and others in molecular biology and chemistry, very few possess the necessary expertise in both fields to apply artificial intelligence (AI) in a pharmaceutical setting. To create suitable algorithms, one has to understand the underlying chemistry, and vice versa [38].

A third, related issue is the pharmaceutical industry's scepticism of machine learning and AI due to ignorance of the algorithms' technique, or the "black box" phenomenon, and mistrust of the outcomes produced.

Skeptics may be hesitant to exploit the data produced by AI and machine learning, wasting time and resources and hindering the efficiency of the sector [24].

The absence of funding for AI development in the pharmaceutical business is a result of this mistrust of AI. Money invested in this technology may be resisted due to scepticism regarding its function and outcomes in medication development procedures. This might result in research and development that is slower and less effective than it could be, which would hinder the advancement of AI in the pharmaceutical sector.

Future scope

AI's key promise in the pharmaceutical sector is to lower costs and boost productivity [39]. Several studies have shown that dynamic learning may identify AI models with a high degree of accuracy while utilizing half or less information than conventional AI and information subsampling techniques. It seems that less repetition and predisposition, as well as acquiring more relevant knowledge to overcome decision restrictions, are critical factors in this greater execution, even if the cause of this higher productivity is not entirely known. As a result, screening costs look to be lowered by up to 90% without accounting for the anticipated mechanical overhead for actually carrying out dynamic learning activities. [12].

Writing business applications has benefited from the ability of machine learning algorithms to handle difficult analyses with large, diverse, and high-dimensional information sets without the need for user input. Using machine learning, especially deep learning, in conjunction with human expertise and

experience may be the most effective approach to organize several massive data warehouses. Computer aided medication regimens that combine numerous clinical aspects are superior than fragmentary information and can speed up prescription procedures thanks to the incredible information-mining capabilities of AI innovation. AI innovation is anticipated to allow many elements of drug research and development and become the norm for computer-supported medication plans as clinical data is collected further and AI calculations are improved. The synchronized growth of mechanization and technological developments should result in improvements in the analysis of massive and complicated datasets, which in turn should result in advances in medicine. The ultimate objective of using AI in this setting is to shorten drug development cycles, lower costs, and increase success rates [40–41].

Conclusion

In conclusion, a variety of criteria affect how successfully AI and machine learning are used into pharmaceutical business processes such as ploy pharmacology, drug design, drug screening, and drug repurposing. Technology advancements, especially those based on artificial intelligence (AI), will always be needed to boost productivity and save time and money spent on R&D and manufacturing. This comprehensive analysis of the literature demonstrated how artificial intelligence (AI) and machine learning may increase the effectiveness and precision of medication development. These technologies not only improve process efficiency but in some cases reduce or eliminate the need for clinical trials by performing simulations in their place. They also enable researchers to study molecules more thoroughly without using human subjects, which lowers costs and alleviates ethical concerns. Although integrating AI and machine learning is predicted to revolutionize drug research in the future, there are still a number of obstacles that may stand in the way, including the need to clean up unstructured and diverse datasets and occasional computer hardware incompetence. As these obstacles are overcome, advances in AI and machine learning may be adopted and enhanced more widely, indicating the beginning of a new age for the pharmaceutical industry.

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