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Research Paper

Revolutionizing the pharmaceutical industry with artificial intelligence

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ABSTRACT

The pharmaceutical industry is one of the most important industries in the world. It provides essential medicines and treatments that help people live longer and healthier lives. The industry is also one of the most regulated and complex, with drugs taking years to develop and billions of dollars in investment. However, the emergence of artificial intelligence (AI) is transforming the way drugs are developed, tested, and brought to market. AI has the potential to revolutionize the pharmaceutical industry by accelerating drug discovery, reducing costs, and improving patient outcomes. In this article, we will explore the ways in which AI is transforming the pharmaceutical industry and how it is changing the way drugs are developed and delivered to patients. AI simplifies labour by analyzing, filtering, sorting, forecasting, scoping, and recognizing massive data volumes to follow the best implementation techniques for coming up with the optimum solution. Artificial intelligence has the potential to lower prices and provide new, effective medicines, but most significantly, it has the potential to save lives. It can be successfully applied to develop a robust, long-lasting pipeline of new medications. We would be able to produce medicines more quickly and affordably by utilizing the power of current technology.

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1. INTRODUCTION

A significant change must be made to the current drug discovery process and technologies in the pharma field. AI imitates human behaviour in terms of the thought processes involved in problem-solving. The pharmaceutical business has a genuine opportunity to change how it does research and development (R&D), making it more effective and dramatically raising the success of early drug development with the use of artificial intelligence (AI) and machine learning. Big pharma is using artificial intelligence to help with the research and development of new drugs to treat diseases that are challenging to treat. Using AI to analyze clinical data more effectively and understand it; speeding up the selection of reliable trial participants; and using robotic automated pharmacies to dispense medication, fill prescriptions, and oversee supply chains, logistics, and marketing.

Reading, observation, planning, interpretation, reasoning, correction, voice recognition, linguistics, and other approaches are among the strategies used in these procedures, which are drawn from the study of human cognition. By training machines from past experiences, relating actions and effort to results, finding and correcting errors, adapting to new and irregular input values, and doing human-like tasks with ease through careful scenario analysis, artificial intelligence (AI) streamlines employment. Artificial intelligence achieves this by employing Natural Language Processing to convert spoken language from humans into a language that computers can comprehend. Deep learning is also a requirement for AI to finish this assignment. By analyzing huge quantities of data and identifying new or recurring patterns in the data, AI trains computers to carry out certain tasks with the least amount of human participation [1].

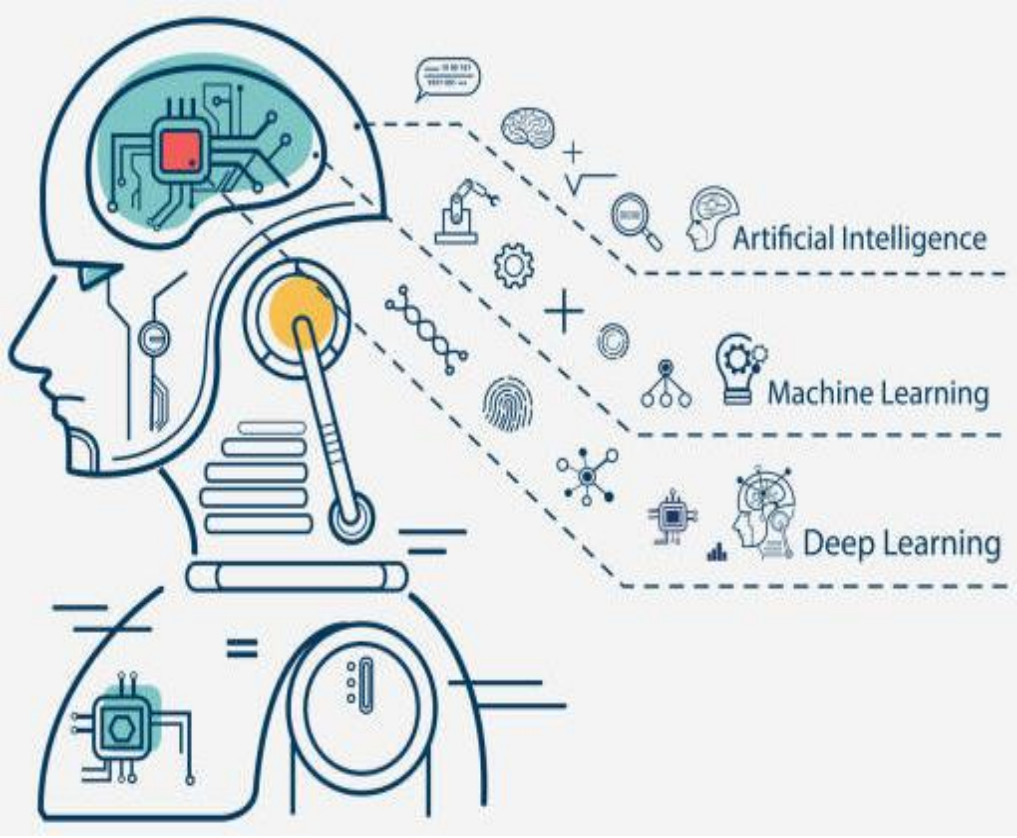


Figure 1. Development of AI

Most artificial intelligence systems utilized in healthcare today are built on human-made data science algorithms. The multivariate data analytics used in this type of AI are supported by previous experiential data. For example, it might recommend drug combinations and design therapy choices using clinical data, a patient's medical history, and population-based treatment outcomes.

Machine learning is a sort of AI that mimics the functioning of the human brain using so-called neural networks, though it may be able to make judgements far more quickly and accurately. Machine learning enables software programmes to create very accurate prediction skills without the necessity of explicit programming.

Deep learning, which is based on neural networks and is the next stage of AI, integrates numerous layers of calculations with integrated information. Deep learning offers enormous promise for diagnostic applications when paired with pathology data, past treatment results, and imagery [2].

1.1. Artificial Intelligence is divided into Seven Primary Categories

- The primary field of artificial intelligence (AI) is machine learning, which gives computers the ability to thoroughly examine, comprehend, and process data in order to provide accurate.
- Deep learning is the extraction and classification of various data components using a convolutional neural network with several layers.
- Technology for fundamental human-computer communication, natural language processing, has grown on its own. Conversational chatbots are its primary use.
- Creating, deploying, and controlling robots that mimic human behaviour and have human-to-human communication is the subject of
- Using logical notations and conditional operators, expert systems may learn from human decision-making and mimic it.
- Hypothesis testing, or fuzzy logic, shows how accurate a result is. The null hypothesis is deduced to be false, for example, if TRUE = 0 and the result is 1.
- The Random Forest technique, which aggregates several decision trees to assess output correctness, is sometimes referred to as an "ensemble" or "decision tree."

1.2. Technologies and Tools Used in AI

Natural language processing (NLP): program computers to process and analyze large amounts of natural language data [3], [4].

Support vector machine (SVM): Given labelled training data (supervised learning), the algorithm outputs an optimal hyperplane that categorizes new examples.

1.3. Artificial Neural Networks (ANN)

An information processing model that was first developed in the 1940s takes its cues from how biological nervous systems, like the brain, process information. A mathematical function is a synthetic neuron. In order to find solutions, ANN uses data samples rather than entire data sets, which saves both time and money.

1.4. Artificial Intelligence in Research and Development

Pharma companies all over the world are streamlining the drug development process with cutting-edge machine learning algorithms and AI-powered platforms. As a result of their ability to recognise complex patterns in vast datasets, these intelligent technologies can be utilised to address problems relating to sophisticated biological networks.

This ability is great for analysing the patterns of different diseases and figuring out which drug formulations would be most effective for treating particular characteristics of a given condition. The development of medications with the best odds of curing an illness or other medical condition can thus be funded by pharmaceutical corporations [5].

1.5. AI in Pharmaceutical Manufacturing

The pharmaceutical industry is the latest sector to adopt AI, and it is already showing promising results. AI has the potential to transform drug discovery, development, and delivery to patients. The use of AI in drug development is already showing promise, with AI-powered drug discovery platforms identifying potential drug candidates faster and more accurately than traditional methods.

In the pharmaceutical industry, AI is being used to analyze large amounts of data from various sources, including clinical trials, medical records, and scientific publications. This data analysis allows researchers to identify patterns and insights that would not be visible with traditional methods.

Modern manufacturing systems are attempting to automate human knowledge because of the complexity of production processes as well as the rising need for efficiency and higher product quality. The use of AI in manufacturing may be advantageous to the pharmaceutical sector. [6] The complexity of production processes is increasing, along with consumer demands for better efficiency and higher-quality products, and modern manufacturing systems are attempting to transfer human expertise to robots [7].

Heuristics are mental shortcuts that ease the cognitive load of making a decision.

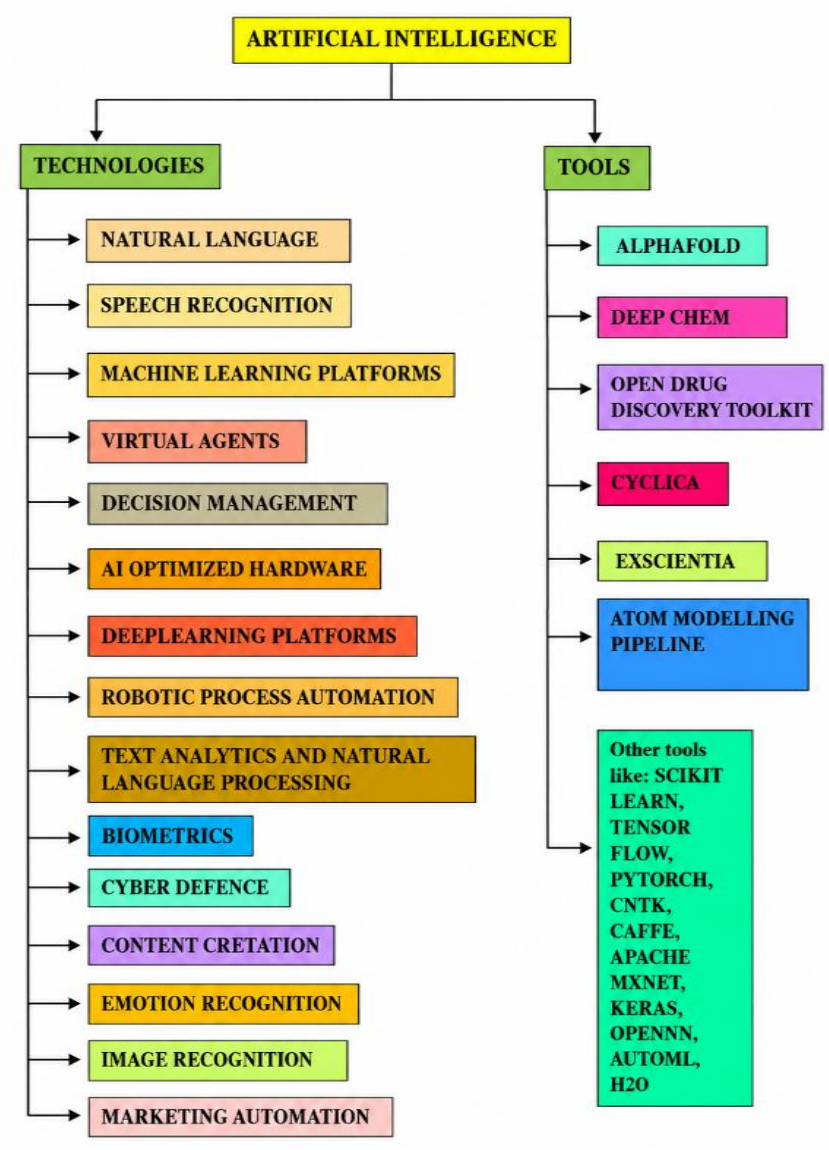


Figure 2. Various Tools and Technologies in AI

1.6. AI in Health Care

Artificial intelligence (AI) technologies are being adopted progressively by the healthcare industry, just as they are in daily life and modern business. Artificial intelligence (AI) has several applications in the healthcare industry, including administrative and patient care. They will be able to build on existing fixes and find answers more quickly with this help. Hospitals and other healthcare organizations may employ very varied implementation tactics, despite the fact that the bulk of AI and healthcare technologies are very relevant to the healthcare industry.

1.7. AI in Drug Design

AI can help with structure-based drug development by predicting the 3D protein structure since the design is in line with the chemistry of the target protein site. This makes it easier to predict, before synthesis or manufacture, a compound's impact on the target as well as any safety issues. Using the AI tool Alpha Fold, which is based on DNNs, the 3D target protein structure was predicted by evaluating the distances between nearby amino acids and the corresponding angles of peptide bonds. 25 out of 43 structures were successfully predicted by this approach, which yielded good results [8].

1.8. De Novo Design Using Artificial Intelligence

De novo design, which means from scratch, » was developed about 25 years ago with the intention of creating new active chemicals. There are numerous available techniques and software programmes. De novo design hasn't been widely utilised in the drug discovery process yet. This is caused, at least in part, by the creation of chemicals that are difficult to obtain synthetically. The field of artificial intelligence has experienced a minor rebirth as a result of recent developments. The variational autoencoder, which combines an encoder network with a decoder network made of neural networks, is an intriguing algorithm. In order to create a latent space—a real-value continuous vector—the encoder network converts the chemical structures specified by SMILES.

The decoder component can transform the vectors of this latent space into chemical structures. Artificial intelligence (AI) tremendously facilitates the creation of novel medications. Artificial intelligence (AI) tremendously facilitates the creation of novel medications. Deep neural networks, recurrent networks, and other artificial neural networks are among the leading competitors in this field.

The technology's strength in quantitative structure-property relationships (QSPR) or quantitative structure-activity correlations is supported by the large number of applications in property or activity predictions, including physicochemical and ADMET attributes that have just recently emerged (QSAR). By using artificial intelligence, de novo design guides the creation of important new physiologically active molecules towards desired traits [9].

1.9. Improved Clinical Trial Study Design

AI is being used to improve the design and analysis of clinical trials. AI can analyse patient data to identify potential participants who are more likely to respond to a treatment, reducing the number of patients needed for a trial. This can significantly reduce the time and cost of clinical trials.

To ascertain the efficacy and safety of a therapeutic therapy in people for a particular clinical disease, clinical trials typically last 6-7 years and require a significant financial commitment. However, because only one out of every ten molecules that enter these trials is approved, the industry still experiences a large loss. These failures may be caused by poor patient selection, a lack of technological requirements, or insufficient infrastructure. With the help of AI, these failures can be decreased, despite the abundance of digital medical data already available.

1.10. AI for Quality Assurance and Quality Control

A variety of characteristics must be balanced in order to produce the desired result from the raw ingredients. Manual intervention is required to keep the items consistent from batch to batch and to perform quality control tests on the goods. Although it may not always be the best course of action, this shows that AI deployment is necessary at this moment. To better understand the critical process and specific requirements that affect the ultimate quality of the pharmaceutical product, the FDA modified current good manufacturing practises (cGMP) by adopting a quality by design approach.

1.11. AI in Nanomedicine

Nanomedicines are drug- and nanotechnology-based therapies for the detection, management, and monitoring of complex illnesses like HIV, cancer, malaria, asthma, and many inflammatory disorders. Drug administration by nanoparticle modification has lately gained relevance in the therapeutic and diagnostic domains because of its enhanced therapeutic effectiveness and diagnostic value. Numerous issues with formulation development may be solved by combining AI with nanotechnology.

1.12. AI in the Pharmaceutical Market

Pharmaceutical companies are turning to AI to lower the associated financial expenses and failure risks of VS. The market for artificial intelligence is expected to reach $5 billion by 2024, up from US$200 million in 2015 and US$700 million in 2018. (10) With a 40% growth rate from 2017 to 2024, AI is expected to upend the pharmaceutical and healthcare sectors. Numerous pharmaceutical companies have invested in AI and are still doing so. To develop essential healthcare solutions, they have also collaborated with AI companies.

An illustration of this is the collaboration between the Royal Free London NHS Foundation Trust and Google subsidiary DeepMind Technologies for the treatment of acute renal injury [10].

1.13. Ethical Considerations for Using AI in Pharmaceuticals

The use of AI in the pharmaceutical industry raises significant ethical considerations. One of the main concerns is the use of patient data. AI algorithms require vast amounts of data to train and improve their performance, and this data often includes sensitive patient information.

There are also concerns about the potential for bias in the algorithms used. AI algorithms can be biassed based on the data used to train them, leading to unfair or discriminatory outcomes.

Finally, there are concerns about the impact of AI on the workforce. The use of AI in the pharmaceutical industry could lead to job losses for skilled personnel, particularly in areas such as drug discovery and development.

1.14. AI Applications in Personalized Medicine

Personalized medicine involves tailoring medical treatments to individual patients based on their genetic makeup, medical history, and other factors. AI has the potential to revolutionize personalized medicine by analyzing vast amounts of patient data to identify personalized treatment options.

AI can be used to identify patients who are more likely to respond to a particular treatment and to predict potential side effects or interactions with other drugs. This personalised approach can lead to better patient outcomes and reduced side effects.

1.15. AI and Regulatory Compliance

Another challenge in implementing AI in the pharmaceutical industry is regulatory compliance. The pharmaceutical industry is heavily regulated, and any new technology must comply with strict regulations and guidelines.

The use of AI in drug development and clinical trials raises significant regulatory challenges, particularly in areas such as data privacy and patient safety. Regulatory bodies such as the FDA are working to develop guidelines for the use of AI in the pharmaceutical industry, but there is still a long way to go.

1.16. Accelerated Drug Discovery

AI is being used in drug discovery to identify potential drug candidates faster and more accurately than traditional methods. This is because AI algorithms can analyze vast amounts of data and identify patterns that would be impossible for humans to detect. AI-powered drug discovery platforms are already being used to identify potential treatments for diseases such as cancer, diabetes, and Alzheimer's disease.

According to a research report, the development of a molecule takes an average of 10 to 12 years from discovery to commercialization. In a different study, the average cost of the research and development (R&D) process for a single medicine rose to $2.168 billion, nearly double the $1.188 billion number from 2010. A similar decline was seen in the average predicted peak sales for assets in the therapeutic pipeline, which fell by 50% from $816 million in 2010 to $407 million in 2018. The estimated return on investment from drug research has consequently declined progressively, falling from 11% in 2010 to 1.9% in 2018. The entire business must figure out how to reduce the cost of putting new pharmaceuticals on the market. One of the things that can increase throughput in the discovery process is having a thorough understanding of the three-dimensional structures of substances and targets and their binding affinities (specificity), which ultimately influence the efficacy of pharmacological action and efficient drug delivery. The area in

which the market for this method is concentrating its efforts is the application of AI to improve the accuracy, predictability, and speed of drug development [11].

1.17. Currently AI Being Used in the Pharmaceutical Field

- By 2025, almost half of all healthcare organisations in the world will have adopted AI strategies, and some business analysts think that this will have a significant impact on future business practises.
- According to the research, 72% of businesses believe AI will be essential to their future business practises, and 62% of healthcare organisations aim to invest in AI shortly.
- Researchers claim that the application of these technologies improves decision-making, maximises creativity, increases the efficacy of clinical trials and research, and creates new tools that are beneficial to physicians, patients, insurers, and regulators.
- Leading pharmaceutical firms including Roche, Pfizer, Merck, AstraZeneca, GSK, Sanofi, AbbVie, Bristol-Myers Squibb, and Johnson & Johnson have already used or purchased AI technology [12].
- Massachusetts Institute of Technology (MIT) joined forces with Novartis and Pfizer in 2018 to create the Machine Learning for Pharmaceutical Discovery and Synthesis consortium, which aims to revolutionize the drug design and manufacturing process by bringing together academics and industry to identify and address the most pressing problems in
- GSK and Cloud Pharmaceuticals worked together to speed up the creation of novel medication candidates. Further, GSK and Vir Biotechnology teamed up in April 2020 to enhance COVID-19 drug development through the use of clustered, regularly interspaced short palindromic repeats and AI.
- Two months later, Roche and Owkin, a machine learning platform for medical research, teamed up to hasten the discovery, development, and clinical testing of a new drug.
- Abbott most recently unveiled an artificial intelligence-powered technology for coronary imaging. The platform could detect vessel diameter and evaluate the severity of calcium-based obstructions in order to increase the precision of decision-making during coronary stenting procedures.
- "There is a significant unmet need for pharmaceuticals. There is a revolution happening in the healthcare sector. According to a statement from a Johnson & Johnson representative, "We are learning new methods and therapies faster thanks to artificial intelligence than we ever could have imagined ten years ago.
- Pharmaceutical firms are looking towards AI as a new approach to reduce expenses connected with research and development while avoiding costly mistakes since drug discovery has become more expensive and competitive over time.
- AI has the potential to revolutionise drug discovery by accelerating research and development.
- Additionally, the technology can help in the repurposing of novel medications, particularly in light of the COVID-19 pandemic. This will make medications more accessible and increase the likelihood that they will be approved by the FDA.
- AI and machine learning algorithms are able to discover molecules that may have failed in clinical trials in order to forecast how the same chemicals may be used to treat different.
- AI offers a variety of opportunities to streamline processes in drug development and production.
- In fact, artificial intelligence (AI) can perform quality control, reduce material waste, boost production reuse, and do predictive maintenance. Machine learning may assist with production line and supply chain concerns in addition to forecasting demand and avoiding it from being too high or too low.
- When establishing a diagnosis, medical experts take a patient's symptoms, diagnostic tests, prior knowledge, and other factors into account. Based on this information, the doctor will present the patient with personalised therapy alternatives [13].
- Artificial intelligence and machine learning can considerably help with diagnostic assistance by providing a more data-driven approach to patient categories.
- To provide individualised patient care, the FDA has approved a significant number of AI systems throughout the year. Some of the platforms were employed for remote patient monitoring, as well as for the detection of brain haemorrhage on a CT scan and irregular heart rhythms on an Apple Watch.

- Mobile applications with health assessment and remote monitoring capabilities can employ AI to enhance the medical treatment process. It's easier to anticipate a result during a medical operation than it is to make a proposal to modify that result. Personal data collected by the applications can improve both the effectiveness of therapies and research and development.
- In the middle of April, the FDA gave the GI Genius, a medical gadget that employs AI to assist doctors in identifying colon cancer signs, marketing approval.
- GI Genius uses an AI system based on machine learning to identify sections of the colon during a colonoscopy that may contain a possible lesion, such as polyps or suspected tumours.

1.18. The Future of AI in the Pharma Industry

The use of AI in the pharmaceutical industry is still in its early stages, but it is already showing promising results. The future of AI in the pharmaceutical industry is likely to involve the continued development of AI-powered drug discovery platforms and the use of AI in personalized medicine.

AI is also likely to be used to improve the design and analysis of clinical trials, leading to faster and more cost-effective drug development. However, there are significant challenges to the widespread adoption of AI in the pharmaceutical industry, including the need for large amounts of high-quality data and the shortage of skilled personnel.

AI has been used more frequently recently in the pharmaceutical industry, and this trend doesn't seem to be slowing down. A recent study indicates that by 2025, the vast majority of international healthcare organisations want to implement AI programmes and use the technology extensively. [14] The search for novel therapies for oncology and chronic diseases will receive increased funding from international pharmaceutical and drug development businesses. In the US, chronic diseases account for the bulk of fatalities. As a result, companies are using AI more and more to improve chronic illness management, lower expenses, and improve patient health. The main chronic ailments that AI will eventually treat are idiopathic pulmonary fibrosis, cancer, diabetes, and chronic kidney disease.

By enhancing the candidate selection procedures for clinical trials, AI will eventually have an influence on the pharmaceutical industry. AI encourages adoption by giving the most qualified candidates access to trials by swiftly analysing patient data and selecting the most appropriate participants for a specific study. The technology also helps to eliminate possible obstacles to clinical trials, which eliminates the requirement for a large trial population to make up for such obstacles. Artificial intelligence will boost different fields and develop processes. AI will change the future of development in a new way and make it more powerful in all fields and processes.

2. CONCLUSION

Pharmaceutical companies have challenges that are continuously being addressed by the development of AI and its incredible capabilities, which affect both the process of developing new medications and the longevity of the final product. The increase in new businesses in this sector may be explained by this. The healthcare sector today confronts a variety of difficult difficulties, such as the growing cost of pharmaceuticals and therapies, and society needs specific big advances in this area. By creating personalised medications with the required dose, release parameters, and other components using AI in the pharmaceutical product production process, patients' unique demands may be addressed.

The use of the most recent AI-based innovations will increase the relevance of automation, which will not only reduce the time it takes for products to reach the market but will also improve product quality, increase overall production cycle safety, better utilise existing resources, and be cost-effective. The biggest concern with using these technologies is the potential loss of jobs and the stringent rules required for AI implementation.

These systems, however, are not meant to entirely replace people; rather, they are just meant to make labour easier. In addition to assisting in the rapid and simple discovery of hit compounds, AI can also anticipate the required chemical structure, recommend methods for producing these molecules, and assist in understanding drug-target interactions and its SAR.

AI may greatly contribute to the further inclusion and optimisation of the found medicine in its proper dosage form, in addition to helping with quick decision-making.

By doing this, the production of higher-quality goods will be sped up while maintaining uniformity from batch to batch. Through detailed market research and forecasting, AI can help determine a product's safety and effectiveness in clinical trials, as well as ensure proper market placement and pricing. It is anticipated that AI will soon turn into a precious tool in the pharmaceutical industry, and it will be a more powerful tool in all fields and processes compared to all other technologies available.

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Author Contributions Statement

Name of Author	C	M	So	Va	Fo	I	R	D	O	E	Vi	Su	P	Fu
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Gururaj S Kulkarni		✓	✓	✓	✓		✓		✓	✓	✓	✓		✓
Yogaraj R	✓	✓	✓	✓		✓		✓	✓	✓	✓		✓	
Padmaa M Paarakh		✓	✓	✓	✓		✓		✓	✓	✓	✓		✓

C : **C**onceptualization
M : **M**ethodology
So : **So**ftware
Va : **Va**lidation
Fo : **Fo**rmal analysis
I : **I**nvestigation
R : **R**esources
D : **D**ata Curation
O : Writing - **O**riginal Draft
E : Writing - Review & **E**diting
Vi : **Vi**sualization
Su : **Su**pervision
P : **P**roject administration
Fu : **Fu**nding acquisition

Conflict of Interest Statement

The authors declare that there are no conflicts of interest regarding the publication of this paper.

Informed Consent

All participants were informed about the purpose of the study and their voluntary consent was obtained prior to data collection.

Ethical Approval

Not applicable.

Data Availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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