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THE IMPACT OF ARTIFICAL INTELLIGENCE ON PHARMA SECTOR: A COMPREHENSIVE REVIEW

Sk. Munthaz[1]*, Sk. Tanveer ul Haq[2], K. Nikitha[3], Y. Gnapthika[4]

B. Pharmacy 4th Year Students, Anurag Pharmacy College, Kodad, Telangana.

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***Corresponding Author: Sk. Munthaz**
B. Pharmacy 4th Year Students, Anurag Pharmacy College, Kodad, Telangana.
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ABSTRACT
Artificial intelligence use in pharmaceutical technology has increased over the years, and the use of technology can save time and money while providing a better understanding of the relationships between different formulations and processes parameters. Artificial intelligence is a branch of the computer science that deals with the problem-solving by the aid of symbolized programming. It has greatly evolved in to a science of problems-solving with the huge applications in Drug Discovery, pharma industry and health care, The review discusses the historical evolution of AI in pharma sector, its role in predicting drug effectiveness and safety, and its potential to streamline clinical trials and optimize pharmacokinetics and pharmacodynamics. Furthermore, the integration of AI in quality assurance and pharmacovigilance is examined, emphasizing its ability to process vast amounts of data and improve drug safety monitoring. As the pharmaceutical industry continues to embrace AI, the review underscores the future potential of these technologies to drive innovation, enhance patient outcomes, and reshape healthcare delivery.

KEYWORDS: Artificial Intelligence (AI), Pharmaceutical Industry, Drug Discovery, Machine Learning (ML), Drug Effectiveness, Drug Safety, Personalized Medicine.

INTRODUCTION
The scientific field of artificial intelligence (AI) combines intelligent machine learning, particularly intelligent computer programs that produce outcomes that are comparable to the attention process of a human.[1] This process generally consists of gathering data, creating effective systems to analyze the data, illustrating precise or approximate conclusions, and self-corrections/adjustments.[2]

In general terms, artificial intelligence (AI) is used to analyze machine learning to mimic human cognitive tasks. AI technology is also used to perform more accurate analyses and obtain insightful interpretation.[3] According to this perspective, artificial intelligence (AI) technology combines a number of statistical models with computational intelligence. The advancement and creativity of AI applications are frequently linked to fears regarding a risk of unemployment. However, practically every development in the use of AI technology is being praised due to the confidence that greatly enhances its effectiveness to the industry. AI technology has recently emerged as an essential part of industry due to its practical applications in many technical and research fields.[4]

The emergent initiative of accepting the applications of AI technology in pharmacy including drug discovery, drug delivery formulation development and other healthcare applications have already been shifted from hype to hope.[5,6] The uses of AI models also make possible to predict the in vivo responses, pharmacokinetic parameters of the therapeutics, suitable dosing, etc.[7] According to the importance of pharmacokinetic prediction of drugs, the uses of in silico models facilitate their effectiveness and inexpensiveness in the drug research.[8]

Artificial intelligence (AI) has been implemented progressively in many sectors of society, but especially in the pharmaceutical sector. In this review, we highlight the use of AI in various pharmaceutical industry sectors, such as drug development and marketing, pharmacovigilance, quality control, drug repurposing, enhancing pharmaceutical productivity, and clinical trials, the use of AI not only reduces the human workload but also quickly meets goals. We also talk about the future of AI in the pharmaceutical sector, ongoing difficulties and solutions, and crosstalk between the tools and techniques used in AI.

METHODOLOGY

We have used search strategy by using key words like health care, AI, pharmaceuticals, medicine in data bases of Google Scholar, NLM catalog, WOS and Scopus journals. We collected necessary data for the review from references cited.

DISCUSSION

1. Role of AI in medicine

AI in medicine refers to the application of artificial intelligence methods, algorithms, and technologies in healthcare and medicine. In order to analyze medical data, make decisions, and carry out tasks that are typically performed by human healthcare professionals, specialized software and computer systems are used. By utilizing NLP, ML, and other AI techniques, medical AI seeks for improvements in effectiveness, efficiency, and accuracy of patient care, diagnosis, and treatment. Virtual health assistants, electronic health record management, drug discovery, disease diagnosis and prediction, medical image analysis, personalized treatment planning, and patient monitoring performed in many fields in which artificial intelligence is being used in the field of medicine. AI systems can assist healthcare professionals by processing vast amounts of patient data and medical literature, in making more up-to-date decisions, detecting patterns, and predicting patient outcomes, leading to better patient care and medical outcomes.

The use of AI-driven tools is expected to improve medical diagnoses, disease prevention, and treatment outcomes, ultimately leading to a more patient-centric and efficient healthcare system. The history of AI in medicine dates back several decades, with significant developments in both AI and medical sciences contributing to its evolution.[9]

2. HISTORY OF AI

Artificial intelligence (AI) is defined as ‘a field of science and engineering concerned with the computational understanding of what is commonly called intelligent behavior, and with the creation of artefacts that exhibit such behavior’. Aristotle attempted to formalize ‘right thinking’ (logic) through his syllogisms (a three part deductive reasoning). Much of the work in the modern era was inspired by this and the early studies on the operation of mind helped to establish contemporary logical thinking. Programs which enable computers to function in the ways, that make people seem intelligent are called artificial intelligent systems.

The British mathematician Alan Turing (1950) was one of the founders of modern computer science and AI. He defined intelligent behavior in a computer as the ability to achieve human-level performance in cognitive tasks, this later became popular as the ‘Turing test’. Since the middle of the last century, researchers have explored the potential applications of intelligent techniques in every field of medicine and pharmaceutical industry.[10]

Over the past few years, there has been a drastic increase in data digitalization in the pharmaceutical sector. However, this digitalization comes with the challenge of acquiring, scrutinizing, and applying that knowledge to solve complex clinical problems. This motivates the use of AI, because it can handle large volumes of data with enhanced automation.[11]

Milestones in Ai: The first use of the phrase- ‘Artificial Intelligence’ was appeared in 1956. However, the concept of AI was employed since 1950 with the uses of problem-solving as well as symbolic methodologies. Important milestones in the area of the AI uses are presented in Table 1.

Table 1: Important milestones in AI.

TABLE I: IMPORTANT MILESTONES IN THE AREA OF THE AL USES.

Years	Events
1943	Walter Pitts & Warren McCulloch proved that logical operations like "and", "or" or "not" can be done by neurons connected in network
1956	The term 'artificial intelligence' was first appeared.
1958	Frank Rosenblatt created neuronal networks called Perceptrons which can transmit information in one direction.
1974	Initiation of "First Al Winter".
1986	Georey Hinton promoted Back propagation algorithm design which is widely used in deep learning.
1987	Initiation of "Al winter".
2013	Google carried out efficient research on pictures by utilizing the British technology
2016	In this year, the Go Champion Lee Sedol was defeated by Google DeepMind, software AlphaGo

3. AI’s role in predicting drug effectiveness and safety

AI plays a crucial role in medicinal chemistry by predicting the effectiveness and safety of potential drug compounds. Traditional drug discovery methods often involve laborious experimentation to assess a compound’s impact on the human body, which is slow, costly, and uncertain. AI techniques, however, can address these challenges by analyzing vast amounts of data to uncover patterns and trends not easily discernible to human researchers. This accelerates the identification of new bioactive compounds with minimal side effects compared to conventional protocols.[12] Deep learning algorithms have shown promise in accurately predicting the activity of novel compounds based on training data of known drug compounds. AI models trained on extensive databases of toxic and non-toxic compounds have also made significant strides in preventing drug toxicity.[13]

Another vital application of AI in drug discovery is identifying drug-drug interactions, which can lead to altered effects or adverse reactions when multiple drugs are combined. AI-based approaches analyse large datasets of known drug interactions to recognize patterns and trends, facilitating the prediction of interactions between novel drug pairs. Furthermore, AI contributes to personalized medicine by identifying potential drug-drug interactions tailored to individual patients based on their genetic profile and medication response. This allows for the development of personalized treatment plans to minimize adverse reactions. The literature showcases how AI enhances pharmaceutical research by improving the prediction of drug efficacy and toxicity, ultimately leading to the development of safer and more effective medications while expediting the drug discovery process.[14]

AI is employed in pharmaceutical research for pinpointing targets, refining leads, and designing clinical trials. It sifts through extensive data sets to forecast drug characteristics, pinpoint possible drug targets, and expedite the entire drug development process, enhancing the efficiency and efficacy of pharmaceutical discovery.[15,16]

4. AI in quality control and quality assurance

Manufacturing of the desired product from the raw materials includes a balance of various parameters Quality control tests on the products, as well as maintenance of batch-to-batch consistency, require manual interference. This might not be the best approach in each case, showcasing the need for AI implementation at this stage.[17] The FDA amended the Current Good Manufacturing Practices (cGMP) by introducing a 'Quality by Design' approach to understand the critical operation and specific criteria that govern the final quality of the pharmaceutical product.[18]

AI technologies are also transforming product or quality control, an essential aspect of pharmaceutical manufacturing in the pharmaceutical industry. Ensuring the safety and effectiveness of products requires careful attention to detail. Conventional quality control methods, although efficient, can be laborious and susceptible to human errors. The incorporation of AI technologies, specifically in ML and computer vision, has triggered a fundamental change in quality control. AI systems can quickly and accurately detect flaws, irregularities, and deviations from established standards in pharmaceutical production and packaging.[19]

5. AI in clinical filed

Clinical trials are directed toward establishing the safety and efficacy of a drug product in humans for a particular disease condition and require 6–7 years along with a substantial financial investment. However, only one out of ten molecules entering these trials gain successful clearance, which is a massive loss for the industry.[20]

The ensuing the impact of the expensive clinical studies on patient therapy expenses is also a concern. The most costly and time-consuming phase of the drug discovery process is conducting clinical trials. The Food and Drug Administration (FDA) only approves a small number of clinical trials, despite the time and money invested in them.[21]

There are several potential obstacles in clinical investigations that might lead to the experiment's failure. Some of these bottlenecks include a shortage of volunteers, study dropouts, severe medication reactions, or contradicting data. Should this type of failure occur later in clinical trials more precisely, in phases III and IV the sponsor will be compelled to shoulder a significant financial cost.[22] Another worry is how the costly clinical trials would affect the cost of the patient's care in the aftermath. These failures can result from inappropriate patient selection, shortage of technical requirements, and poor infrastructure. However, with the vast digital medical data available, these failures can be reduced with the implementation of AI. With the help of AI and digitization, these challenges in the clinical trial have been transforming.[23]

6. AI for drug discovery

AI has revolutionized drug research and discovery in numerous ways. Some of the key contributions of AI in this domain include the following:

6.1. Target Identification

AI systems can analyze diverse data types, such as genetic, proteomic, and clinical data, to identify potential therapeutic targets. By uncovering disease-associated targets and molecular pathways, AI assists in the design of medications that can modulate biological processes.

6.2. Virtual Screening

AI enables the efficient screening of vast chemical libraries to identify drug candidates that have a high likelihood of binding to a specific target. By simulating chemical interactions and predicting binding affinities, AI helps researchers prioritize and select compounds for experimental testing, saving time and resources.

6.3. Structure-Activity Relationship (SAR) Modeling

AI models can establish links between the chemical structure of compounds and their biological activity. This allows researchers to optimize drug candidates by designing molecules with desirable features, such as high potency, selectivity, and favorable pharmacokinetic profiles.

6.4. De Novo Drug Design

Using reinforcement learning and generative models, AI algorithms can propose novel drug-like chemical structures. By learning from chemical libraries and experimental data, AI expands the chemical space and aids in the development of innovative drug candidates.

6.5. Optimization of Drug Candidates

AI algorithms can analyze and optimize drug candidates by considering various factors, including efficacy, safety, and pharmacokinetics. This helps researchers fine-tune therapeutic molecules to enhance their effectiveness while minimizing potential side effects.

6.6. Drug Repurposing

AI techniques can analyze large-scale biomedical data to identify existing drugs that may have therapeutic potential for different diseases. By repurposing approved drugs for new indications, AI accelerates the drug discovery process and reduces costs.

6.7. Toxicity Prediction

AI systems can predict drug toxicity by analyzing the chemical structure and characteristics of compounds. Machine learning algorithms trained on toxicology databases can anticipate harmful effects or identify hazardous structural properties. This helps researchers prioritize safer chemicals and mitigate potential adverse responses in clinical trials.

Overall, AI-driven approaches in drug research and development offer the potential to streamline and expedite the identification, optimization, and design of novel therapeutic candidates, ultimately leading to more efficient and effective medications.[24]

Table 2: Popular AI model tools used for drug discovery.

AI Model Tools	Summary
DeepChem	An open-source library offering a large selection of drug discovery tools and models, such as generative chemistry, virtual screening, and deep learning models for predicting chemical properties.
Scape-DB	scape-DB (Extraction of Chemical and Physical Properties from the Literature-DrugBank) is a database that combines natural language processing and machine learning to extract chemical and biological data from the scientific literature. It provides valuable information for drug discovery research.
RDKit	A widely used open-source cheminformatics library that Offers various functionalities for molecule handling, substructure searching, and Descriptor calculation.It can be integrated with machine learning frameworks for drug discovery applications.
AutoDock Vina	A popular docking software that uses machine learning techniques to predict the binding affinity between small molecules and protein targets. It can assist in virtual screening and lead optimization for drug discovery.

7. Artificial intelligence for pharmacokinetics & pharmacodynamics

The development of medications involves various stages, such as drug discovery, preclinical assessments, clinical trials, and regulatory clearance. Understanding pharmacokinetics and pharmacodynamics is pivotal in determining the appropriate dosage, administration method, and safety profile of a medication within the body.[25-27] Traditional experimental approaches for studying pharmacokinetics and pharmacodynamics can be time-consuming, costly, and sometimes fail to provide precise forecasts regarding a drug’s effectiveness and safety.[28]

Traditionally, investigations into pharmacokinetics and pharmacodynamics have relied on experimental techniques like animal studies and human clinical trials. However, these methods pose significant challenges, including ethical considerations, limitations in sample size, and variations among individuals. Additionally, they may not consistently offer accurate projections of how drugs will behave within human systems. To address these constraints, computational models and AI techniques have been developed to forecast drug pharmacokinetics and pharmacodynamics more swiftly, economically, and accurately.[29,30]

AI signifies immense promise in the field of pharmacokinetics, pharmacodynamics, and drug development. With the advancements in machine learning algorithms and computing power, AI has emerged as a valuable asset for predicting and enhancing drug pharmacokinetics and pharmacodynamics. Despite challenges related to handling extensive datasets and ensuring data reliability, AI holds the potential to revolutionize pharmacokinetics-pharmacodynamics studies and therapeutic interventions impacts.[31]

7.1 Prediction of Drug Release and Absorption Parameters

AI-based models have been successfully employed to predict drug release and absorption parameters. AI algorithms can analyze data from various drug delivery systems and predict the release kinetics of drugs. By considering factors such as the drug's physicochemical properties, formulation characteristics, and release mechanism of the delivery system, AI models can estimate the rate and extent of drug release over time. AI-based models can also predict the release kinetics of drugs from different drug delivery systems, such as oral tablets, transdermal patches, and inhalers.[32]

7.2. Prediction of Drug Metabolism and Excretion Parameters

Drug interactions with transporters involved in metabolism, excretion, distribution, and absorption can be predicted using AI models. AI models may evaluate the possibility of drug–drug interactions or altered pharmacokinetics as a result of transporter-mediated effects by taking into account the physicochemical parameters of the drug and the transporter. Understanding drug disposition and improving medication formulations are made easier with this knowledge.

Drug pharmacokinetics can be better understood by using AI-based models to predict drug metabolism and excretion parameters. Drugs' physicochemical characteristics and molecular structure can be analyzed by AI systems to forecast their metabolic routes. AI models may recognize structural characteristics linked to certain metabolic transformations by training on large datasets of known drug metabolism data. These models include information on the major enzymes involved in drug metabolism as well as the ability to predict potential metabolites.[33]

Table 3: Algorithms used for development of AI models for various PKPD studies along with their advantages.

ALGORITHMS USED FOR THE DEVELOPMENT OF AL MODELS FOR VARIOUS PKPD STUDIES ALONG WITH THEIR ADVANTAGES

Algorithm/Software	Aim/Target	Advantage	PK/PD/Both
Bayesian/WinBUGS	To handle data below the limit of quantification	• Prior information from the literature can be directly used for model-fitting • Easy implementation	Both
Bayesian/ PKBUGS (vl.I) /WinBUGS (v I.3)	Pharmacokinetic analysis of sirolimus concentration data for therapeutic drug monitoring	• Easy incorporation of prior information with current data • Identification of possible covariate relationship	PK
Support Vector Machine/Least Square-SVM	Drug concentration analysis of sample drug based on individual patient profile	• Personalized model for every new patient • SVM-based approaches are more accurate than the PK modeling method for predicting drug concentration	PK
Support Vector Machine/Drug Administration Decision Support System (DADSS) and Random Sample Consensus RANSAC	Prediction of drug concentration, ideal dose, and dose intervals for a new patient	• More flexible and structurally adjustable	PK

8. Artificial intelligence in pharmaceutical marketing

Modern manufacturing systems are attempting to transfer human expertise to machines, continuously changing production procedures in response to the increasing complexity of manufacturing processes and the growing need for improved efficiency and product quality. The pharmaceutical industry has a bright future with the use of AI in manufacturing.[34]

Tools like Computational Fluid Dynamics (CFD) leverage Reynolds-Averaged Navier-Stokes solvers technology to analyze the effects of agitation and stress levels in various equipment, such as stirred tanks, streamlining the automation of numerous pharmaceutical operations. Similarly, systems like direct numerical simulations and large eddy simulations employ sophisticated methods to address complex flow challenges in manufacturing.[35-37]

The Innovativ Chapter platform facilitates digital automation for molecule synthesis and manufacturing, employing diverse chemical codes and operating through a scripting language termed Chemical Assembly32. This platform has demonstrated success in the synthesis and production of medications like sildenafil, diphenhydramine hydrochloride, and rufinamide, yielding purity and efficiency levels akin to manual synthesis. AI technologies enable efficient estimation of granulation completion in granulators ranging from 25 to 600 liters. By employing technology and neuro-fuzzy logic, critical variables are correlated with their respective responses, yielding polynomial equations for predicting the requisite proportion of granulation fluid, optimal speed, and impeller diameter in both geometrically similar and dissimilar granulators.[38]

9. The future of AI in the pharmaceutical industry

The future of AI in the pharmaceutical industry is brimming with potential; it is poised to revolutionize drug discovery, pharmaceutical product development, industry management, regulatory affairs, and PMS. AI algorithms can analyze vast amounts of biological data to identify potential drug targets and accelerate drug discovery. AI-driven simulations can be implemented in drug development to predict the interactions between compounds and biological systems, facilitating more efficient and cost-effective clinical trials. In addition, AI-driven tools can optimize supply chain management, maximize regulatory compliance, and streamline formulation development and manufacturing processes.

Large data and information databases are indispensable for the training and development of AI algorithms. Over a thousand research articles and reviews have been published in the last 5 years on the use of AI in pharmaceutical applications. This indicates the value of enhancing and accelerating current research processes and protocols. Nevertheless, the best AI-driven applications and technologies for practical implementation or commercialization will ultimately be identified. As technology continues to advance, the integration of AI into various aspects of the pharmaceutical industry will undeniably drive innovation, improve patient outcomes, and reshape the future of healthcare and pharma sector.

9.1. Pharma companies collaboration with AI technology

Table 4:- Pharma companies collaboration with ai technology

Pharmaceutical company	AI company/technology	Collaboration scope
Pfizer	IBM Watson Concerto Health AI Catalia Health	Using AI to analyze vast datasets and used in drug discovery To employ artificial intelligence and real-world data in oncology
Novartis	Google Deepmind	Clinical trials: Applying AI algorithms to optimize patient selection, treatment protocols, and data analysis during clinical trials.
GSK	Insilico Medicine	AI~Driven drug design: utilising AI to design and optimization of Drug molecule for enhancing potency and safety.
Astrazeneca	Benevolent Ai	Use ML &AI to find potential novel medications for chronic renal disease and idiopathic pulmonary fibrosis.
Sanofi	ORKIN	AI is being used to stratify patient groups to provide more targeted and effective therapies.

10. AI in Pharmacovigilance

10.1. Overview of Pharmacovigilance

The objective of PV is to reduce the incidence and the risk associated with the use of medicines at the earliest by processing suspected adverse reaction reports and extraction of health data to identify drug safety signals. Worldwide post marketing safety reports of medical products have been collected through spontaneous reporting system in a structured and systematic way by means of individual case safety reports (ICSRs). Electronic health-care records, periodic safety update reports, published medical literature, registries, and pharmacoepidemiology studies are complementary data sources for routine PV practices, nonetheless, having unstructured text.

There has been exponential growth in the number of suspected adverse event (AE) reports in the PV database. Processing of the enormous volume and variety of data sources, making its sensible use and separating “needles from haystack,” is a challenge for key stakeholders such as pharmaceutical firms, regulatory authorities, medical and PV experts, and National Pharmacovigilance Program managers.

10.2. The Role of AI in Enhancing Data Processing

The AI tool has been proposed to be beneficial for the manual repetitive and routine task of data entry, identifying AE, drug–drug interactions, subtle data patterns, and review of single cases.[39,40 In addition, AI can convert the unstructured, free-text format of drug safety data and hand-written documents into machine-readable format. Further, the tool can automate the Medical Dictionary for Regulatory Activities coding, check duplicate reports, categorize reports into physician or consumer reports, identify serious reports, and exclude non serious reports.[41]

10.3. Impact on Data Quality and Speed

A recent survey reports that the use of AI tools processes the data very fast, speeds up computations that were not previously feasible, and saves scientists time and money. With the large amount of drug safety data being stored in an electronic manner, the adoption of AI tools will reduce the efforts, time, and cost of case processing, improve data quality, and possibly be a game changer for PV activities.[42]

CONCLUSION

In conclusion, the integration of artificial intelligence into the pharmaceutical sector represents a significant advancement that promises to enhance various aspects of drug development and healthcare delivery. AI's ability to analyze large datasets, predict drug interactions, and streamline clinical trials has the potential to reduce costs and improve the efficiency of the drug discovery process. As AI technologies continue to evolve, they will play a crucial role in addressing the challenges faced by the pharmaceutical industry, including the need for personalized medicine and improved pharmacovigilance. However, the successful implementation of AI in this field will require ongoing collaboration between pharmaceutical companies, regulatory bodies, and technology developers to ensure that these innovations are effectively integrated into existing workflows. Ultimately, the future of AI in the pharmaceutical industry is bright, with the potential to significantly improve patient care and reshape the landscape of healthcare.

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