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AI In Pharmaceutical Research

Sumit Nehe, Sarika Ahire, Sunil kakad
[1,2]*Student, SCES's Indira College of Pharmacy, Tathawade, Pune-411 033,* [3]*Associate Professor, SCES's Indira College of Pharmacy, Tathawade, Pune-411 033 Corresponding Author: Sumit P. Nehe*

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ABSTRACT:
Artificial Intelligence (AI) has emerged as a revolutionary technology in the pharmaceutical industry, transforming traditional methods of drug development, manufacturing, and healthcare delivery. AI uses advanced technologies such as machine learning, deep learning, natural language processing, and predictive analytics to analyze large volumes of data and support faster, more accurate decision-making. It plays a significant role in various pharmaceutical applications, including drug discovery, drug design, formulation development, clinical trials, quality control, pharmacovigilance, personalized medicine, and supply chain management. AI helps reduce the time and cost involved in developing new medicines while improving their safety, quality, and effectiveness. It also enhances disease diagnosis and enables personalized treatment based on individual patient data. Despite challenges such as data privacy, regulatory requirements, and the need for high-quality datasets, AI continues to show great potential in advancing pharmaceutical research and healthcare. This review highlights the major applications, advantages, challenges, and future prospects of AI in the pharmaceutical industry, emphasizing its growing importance in improving healthcare outcomes and accelerating pharmaceutical innovation.

KEY WORDS: Artificial Intelligence (AI), Drug Discovery, Machine Learning, Pharmaceutical Research, Computer-Aided Drug Design (CADD)

I. INTRODUCTION:

While artificial intelligence (AI), deep learning, and machine learning are commonly used interchangeably, they are actually hierarchical. Artificial intelligence (AI) is the general term for computer systems that simulate human intelligence in tasks like learning, reasoning, language processing, and information or knowledge display (1). Artificial intelligence (AI) is the use of a computer to simulate intelligent behavior with little to no human involvement. Artificial intelligence (AI) technologies have altered drug development and discovery. According to Deep Pharma Intelligence, at least 14 fully AI-generated drugs had begun clinical testing as of March 2023. New, complex, and realistic models that can produce synthetic data with certain properties have been made possible by developments in generative AI (2). With the arrival of artificial intelligence, it is hard to see how the genie will be put back in the bottle. If AI is thought to provide a competitive edge for drug research, it is likely to be swiftly and widely implemented (3). AI can help with the expensive and time-consuming drug development process that is constrained by a lack of cutting-edge technologies. AI can find hit and lead compounds, validate drug targets faster, and improve drug structure design (4). Computational modeling based on AI and ML principles enables the identification and validation of chemical compounds, target identification, peptide synthesis, evaluation of drug toxicity and physiochemical properties, drug monitoring, drug efficacy and effectiveness, and drug repositioning (5). The goal of artificial intelligence (AI), a subfield of computer science, is to build intelligent machines that will play a crucial role in the technology sector. AI has significantly altered every aspect of the healthcare sector. This technology is the result of combining computer processing with human intellect. It is a sophisticated form of computer-aided technique that involves gathering data from multiple sources, creating guidelines to be adhered to when handling the necessary data, and sketching potential outcomes to ascertain suitable outcomes and procedures that can mimic human behavior. It includes elements that make dealing with neural processes easier, including machine learning and deep learning (6)(7)(8). The relevance of AI in the pharmaceutical industry cannot be overlooked because of its broader applications at different stages. It is clear that AI has an impact on pharmaceutical products at every level, from product management to medication development. ML, deep learning, AI-based quantitative structure–activity relationship (QSRL) technologies, QSLRML, virtual screening (VS), support vector machines (SVMs), deep virtual screening, deep neural networks (DNNs), recurrent neural networks (RNNs), etc. are just a few of the algorithms used in drug discovery. AI neural networks are modelled after biological neural networks, which process input data and produce an output. AI is being utilized in pharmaceutical product development to identify the right excipients, choose the development procedure, and make sure the specifications are met in accordance with compliance throughout the process. Pharmaceutical product development makes use of ANNs, model expert systems (MES), etc. AI is used in manufacturing to match manufacturing faults to define limitations in automated and customized manufacturing. To attain the required quality in the finished product, AI technologies like tablet classifiers and meta classifiers are utilized (9). AI is used in clinical trials to assist with participant selection and trial monitoring, which lowers dropout rates. Clinical studies are using machine learning (10). Product positioning, product costing, and market analysis all make use of AI technology like machine learning and natural language processing (9).

II. APPLICATIONS OF AI IN PHARMACEUTICAL RESEARCH;

A] Drug Discovery

Intelligent technology (AI) has completely changed the drug discovery and innovation process. According to Deep Pharma Intelligence, at least 14 fully AI-generated drugs had begun clinical testing as of March 2023. New, complex, and realistic models that can produce synthetic data with the right properties have been made possible by developments in generative AI (2). AI can identify hit and lead materials, assess therapeutic targets more rapidly, and improve drug structure design. However, the lack of advanced technology limits the pharmaceutical development process, making it an expensive and time-consuming procedure that AI can assist with (9). By effectively analyzing enormous volumes of chemical data, AI/ML algorithms are utilized in preclinical research to enhance absorption, distribution, metabolism, and excretion toxicity (ADME-T) profiles and generate prediction models of physicochemical properties (11). The first and most crucial stage in drug discovery is to identify appropriate medications or drug-like compounds that can interfere with these targets. Numerous biomedical data repositories are now at our disposal to help us with this procedure (5). The chemical composition of a molecule and its biological effect can be linked using artificial intelligence models. Researchers can maximize therapeutic prospects by creating molecules with desirable qualities like high potency, selectivity, and appealing pharmacokinetic features (12). Ensuring the safety, efficacy, and cost of medications also requires overcoming regulatory challenges. AI has become a powerful instrument to transform the drug discovery process as a result of these unfulfilled demands driving the search for new solutions (13). Therefore, a great starting point for further research is provided by combining computational drug design with conventional chemistry-oriented drug discovery and development techniques (5).

Lack of suitable technology makes it difficult to produce a large number of drug molecules from a chemical space; this can be overcome by utilizing AI in the drug development process (14)(15). With AI-based QSAR techniques, QSAR is prepared for the possible use of the drug candidate (16)(17). The biological activity found and developed may take a decade to regulate if the conventional methods are used to achieve the statistical differences (18). When creating a new medication, the drug's solubility, partition coefficient, degree of ionization, and inherent permeability all influence target receptor binding (19). To predict the binding qualities, algorithms use molecular descriptors like the Simplified Molecular Input Line Entry System (SMILES) (20). The six physicochemical properties are often determined using a quantitative structure–property relationship (QSPR) called the Estimation Program Interface Suite (21). The lipophilicity and solubility of different substances have been predicted using deep learning and neural networks based on the ADMET predictor and ALGOPS software (22). A lot of undirected graphs are used for estimating solubility (23). When predicting a new chemical entity, factors including surface area, mass, hydrogen count, refractivity, volume, log P, surface area, sum of the indices, solubility index, and rotatable bonds are taken into account (24).

B] Target discovery

The rapid growth of deep learning and artificial intelligence technology has brought about unprecedented advances in drug research and development, especially in therapeutic target discovery (25). The target discovery process includes prioritizing candidate targets, identifying which targets contribute to the pathophysiology of the disease, and assessing therapeutic efficacy. However, because human diseases are complicated, this process often requires more comprehensive methods that integrate existing heterogeneous data and information in order to comprehend the molecular mechanisms behind illness symptoms and discover patient-specific changes (11).

C] Preclinical research

Predicting the detrimental effects of each component of therapeutic characteristics is essential to preventing bad outcomes. The frequent use of cell-based in vitro tests for basic research, followed by animal studies to assess a compound's toxicity, raises the expense of medication development. Some web-based programs that help with cost reduction include LimTox, pkCSM, admetSAR, and Toxtree (9). When there are no medications for a condition or when the medications that are available have poor efficacy and/or high toxicity, drug development is an endeavor that is driven by these circumstances (26). Computational modeling based on AI and ML principles enables the identification and validation of chemical compounds, target identification, peptide synthesis, evaluation of drug toxicity and physiochemical properties, drug monitoring, drug efficacy and effectiveness, and drug repositioning (5). AI-based methods have revolutionized pharmacokinetics and pharmacodynamics. They have several advantages over traditional experimental methods. AI-based models can predict pharmacokinetic parameters, simulate drug distribution and clearance in the body, and optimize drug dosage and administration routes (12).

D] Automated drug synthesis

By using automated technologies, organic synthesis would become a machine-driven process to achieve the synthesis of fourteen different tiny compounds (27). An automated polypeptide synthesis procedure was reported in a more recent work. The tools and platforms we described here were a major step toward fully automated synthesis, even though manual input and process development are still required (28). One particular area where AI/ML has potential for healthcare is the subject of infectious diseases, which are currently undeveloped in drug development investment portfolios. Infectious diseases are particularly prevalent in lower to middle-income countries (LMICs), most of which are located in the Global South (29).

E] Personalized medicine

Personalized medicine entails tailoring medical treatment to the particular requirements of every patient. One of the primary applications of AI in personalized medicine is pharmacogenomics, the study of how genes affect a person's response to drugs (30). The aim of theragnostic AI applications in other complicated fields like radiomics, genomics, or transcriptomics may accelerate advancements in patient management by offering insightful information on outcome prediction and improving tailored health care (31). Artificial intelligence (AI) in personalized medicine aims to solve the challenge of analyzing enormous amounts of data to provide customized treatment plans. Traditional personalized medicine approaches are limited by the complexity of analyzing the massive amounts of data needed to create a specific treatment plan (32). AI can analyze massive amounts of data to estimate a person's risk of developing diabetes and develop customized treatment plans. Additionally, individualized care can provide tailored management and treatment regimens based on each patient's particular circumstances (33). In the context of customized pharmaceuticals, the creation of drugs and therapies may require nuanced aspects depending on patient profiles, requiring real-time design and crafting instead of mass production, storage, and distribution when necessary. A later section on "Integration and the Personalized Medicine Workflow" will address this topic (34). More funding in this area is required to reach the objective. Making this field of study a priority could help us get closer to the day when individualized patient care is a reality rather than just a possibility (35).

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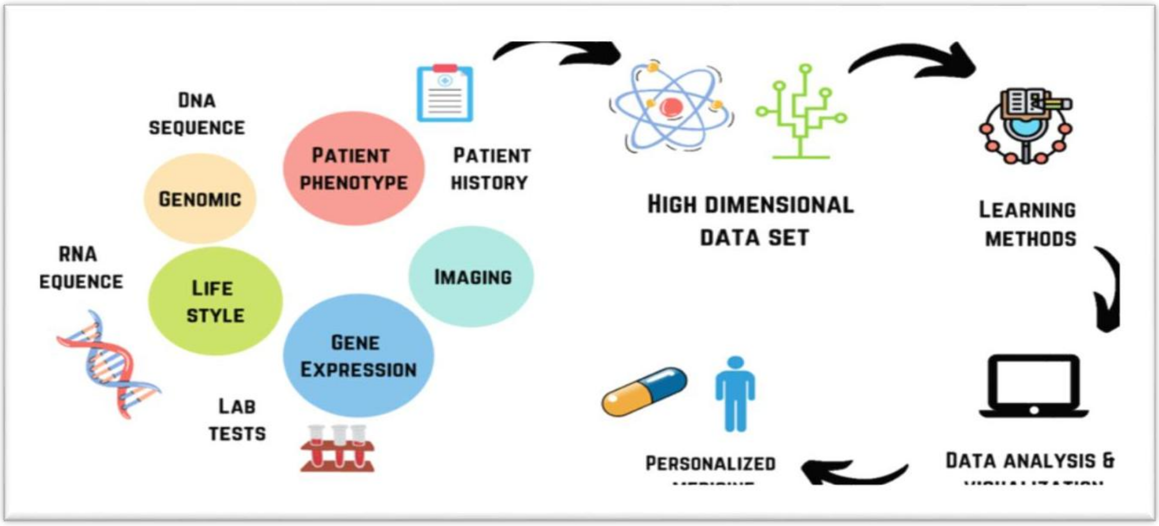

Figure 1. AI in acquiring and analyzing data of a patient in personalizing the treatment.

F] AI in Cancer

AI has become more significant in the fields of cancer diagnosis and treatment due to its enormous application. A multilayer perceptron neural network was used to predict the non-Hodgkin lymphoma subtypes using gene expression data. 20,863 genes make up the input layer of the neural network, whereas lymphoma subtypes make up the output layer. Mantle cell lymphoma (MCL), follicular lymphoma, diffuse large B-cell lymphoma (DLBCL), marginal zone lymphoma, and Burkitt lymphoma are examples of lymphoma subtypes. The lymphoma subtypes have been accurately predicted by an AI neural network (36). Using gene expression data, an artificial neural network was utilized to find new prognostic markers for MCL. The results showed that 58 genes accurately predicted survival, 10 genes were linked to bad survival, and 5 genes were linked to favorable survival (37). Four genes are correlated with favorable survival and three with unfavorable survival for DLBCL, according to the Multilayer Perceptron (MLP) with multivariate analysis of gene expressions (38).

The prognosis and overall survival of patients with follicular lymphoma (FL) were predicted using MLP and radial basis function (RBF) neural networks. Following the analysis of 22,215 genes, it was found that 18 genes were linked to a poor prognosis and 43 genes were linked to the prediction of overall survival (39). Using genetic and transcriptional data from RNA-Seq on a next-generation sequencing (NGS) platform, an AI deep learning technique was used to classify the cell-of-origin (COO) of DLBCL. AI made assays for categorization and future clinical use repeatable, effective, and reasonably priced (40).

AI is utilized to diagnose cancer with great accuracy while cutting down on time. AI-based PET imaging of lymphoma is utilized to assess the tumor burden, which is then used for tumor characterization, heterogeneity measurement, and treatment response prediction (41). Colorectal cancer (CRC) screening technology is used to assess the malignancy in patients with gastrointestinal cancer (42). and visual nocturnal detection of Helicobacter pylori infection are important indicators of the development of stomach cancer (43). Cancer progression can be influenced by early diagnosis using appropriate blood tests, endoscopic imaging, and artificial intelligence (42). However, only retrospective evidence may be collected because AI lacks the necessary randomization and blinding controlled research (44). Additionally, there have been studies where the prognosis of cancers was not supported by the prediction models. Subsequently, a number of models, including the random survival forest algorithm, the Cox survival regression algorithm, and the multi-task logistic regression algorithm, have gained several facets and likely predictive outcomes (24).

These developments have made it possible to automate the diagnosis of cancer through gastroenterology, not only for classification but also for endocytoscopy-based detection and magnification, which has not yet been applied in actual practice (45). AI is a versatile clinical aid for lung cancer detection in early stages and screening purposes. Because deep learning and machine learning AI techniques can accurately characterize

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pulmonary nodules and maintain large amounts of data, they provide a supportive measure in lung cancer screening (46)(47). The changes in this area are preliminary and have many limits such as absence of large public datasets, requirement of high-quality images, ROI annotating dependence, difficulty in binary classification, inability in handling multiple tasks at the same time. Thus, the innovations of AI tools including DL-based CAD are still at an early level due to the absence of enough public data sets for training the deep convolutional neural networks (DCNNs) (48).

G] AI in Clinical Trials

Clinical trials are the most time-consuming and expensive part of drug discovery. Despite the time and capital invested in clinical trials, the success rate is only marginal for those that obtain approval from the Food Drug Administration (FDA) (49). There are numerous bottlenecks in clinical trials, and those can contribute to failure of the trial. Those bottlenecks include the insufficient number of participants, drop-outs during the experiment, negative effects of the test medicine, or conflicting data. If such failure occurs in late phases of clinical trials, such as in phase-III and phase-IV, the sponsor needs to endure an extraordinarily significant fiscal burden (50). The clinical trials which are associated with high costs also have subsequent effects on therapeutic costs for patients. Due to this rationale, biopharma companies attach R&D expenditures of failed studies into the pricing of approved products to hold out the profit (51). The method of implementation and conduct of clinical trials involves clinical trial design, patient recruitment/selection, location selection, monitoring, data gathering and analysis. Out of these steps, patient recruitment and selection is the burdensome process where 80% of the studies exceed the enrolment deadline, and 30% of phase-III trials are prematurely stopped due to patient enrolment issues. Trial monitoring in a multicentered worldwide trial is a very expensive and time-consuming activity. Other obstacles in clinical trials are the length from the “last subject last visit” to data submission to regulatory authorities, which are enormous data collection and analysis operations. With the use of AI and digitization, these issues in the clinical trial have been addressed (52).

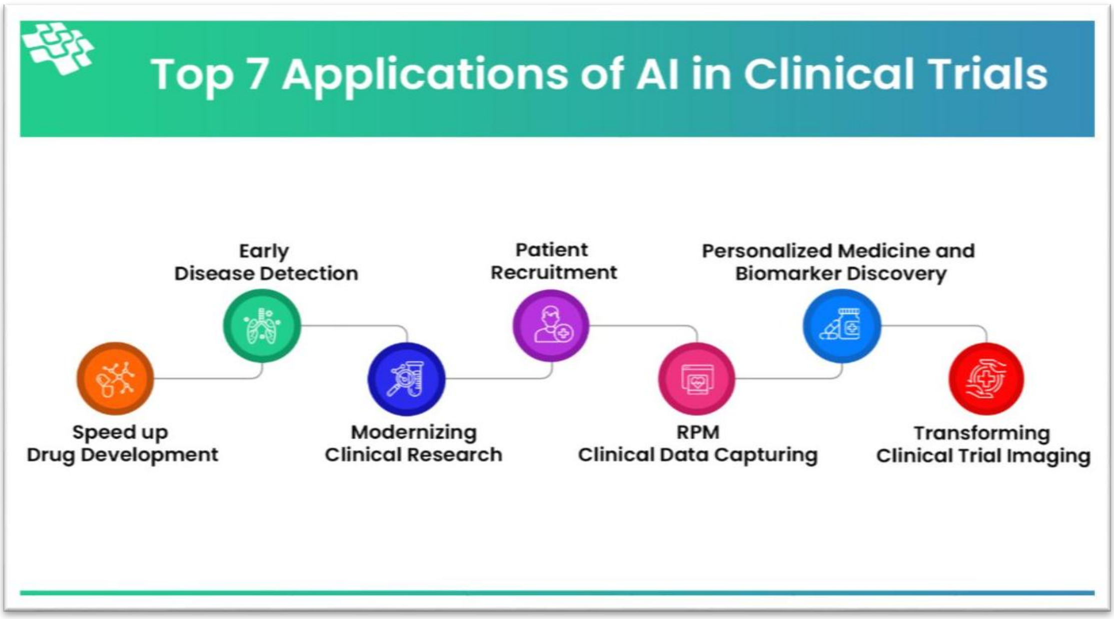

Figure 2. Application of AI in Clinical Trails

III] AI-DRIVEN TECHNOLOGIES IN PHARMACEUTICALS:

A] Machine Learning Algorithms:

The goal of machine learning, a subfield of artificial intelligence, is to make it possible for computers to learn independently and improve with practice without the need for explicit programming. Computers can identify patterns and relationships between data and pertinent outcomes thanks to a set of AI algorithms called machine learning (1). Although machine learning

(ML) has been widely used in pre-clinical research, drug development, and translational research, its implementation in clinical trial operations and data analysis has been slower during the past 20 years due to its growing sophistication (3)

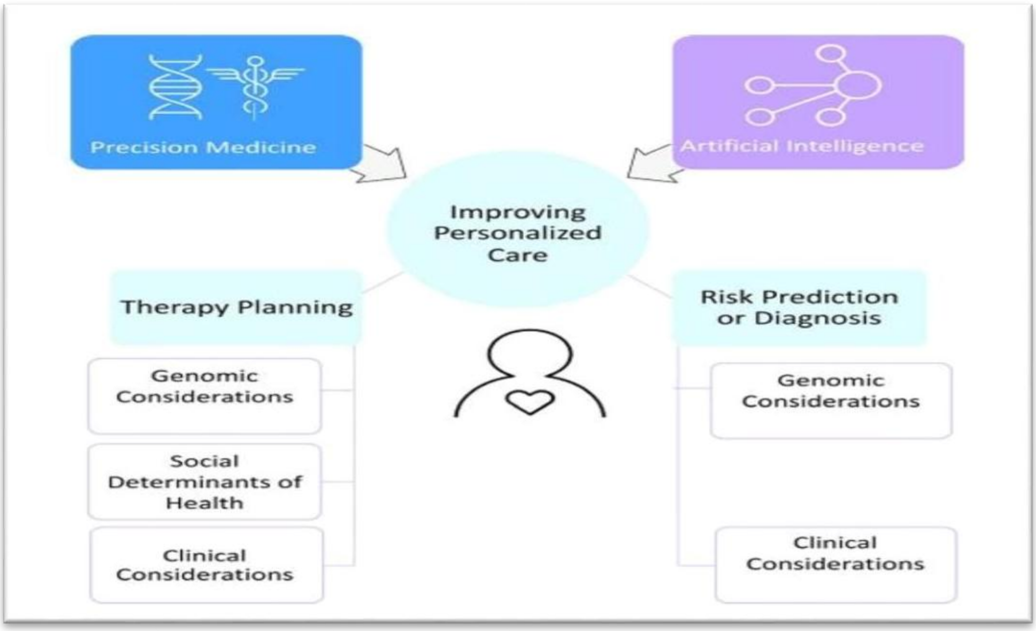

Figure 3. Application of AI in Personalizes Medicine

Beyond that, machine learning (ML) entails providing the machine data along with methods like Naïve Bayes, decision trees (DT), hidden Markov models (HMM), and others that aid in learning without explicit programming. Later, as neural networks developed, robots showed even greater advancements in artificial intelligence by classifying and organizing input data similarly to the human brain (5). Supervised machine learning is most prevalent in the medical field. An algorithm is trained on labeled datasets to precisely classify data in supervised learning. To train an algorithm, any correlation between independent and dependent variables is deduced from the labeled data (53).

IV] CONCLUSION:

Artificial Intelligence (AI) is changing the pharmaceutical industry by making drug discovery, development, manufacturing, quality control, and patient care faster, more accurate, and cost-effective. AI helps researchers analyze large amounts of data, predict drug behavior, identify new drug candidates, and improve clinical trials. It also supports better decision-making, reduces human errors, and increases productivity.

Despite its many benefits, AI also has some challenges, such as the need for high-quality data, concerns about data privacy and security, high implementation costs, and regulatory and ethical issues. These challenges must be addressed to ensure the safe and effective use of AI in the pharmaceutical field.

In conclusion, AI has become a powerful tool in the pharmaceutical industry and is expected to play an even greater role in the future. With proper regulations, skilled professionals, and continuous technological advancements, AI will help develop safer, more effective medicines and improve healthcare outcomes worldwide

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