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Review Article

Artificial Intelligence in Pharmaceutical Research

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Abstract

Artificial intelligence (AI) is transforming the pharmaceutical industry by accelerating medication development and discovery. AI technologies, including machine learning and deep learning, are being applied in various areas, such as drug design, target discovery, preclinical research, and personalized medicine. AI can analyze vast amounts of data, identify patterns, and make predictions, thereby improving the efficiency and effectiveness of the drug development process. This review highlights the applications of AI in pharmaceutical research, including drug discovery, target identification, and preclinical research. We also discuss the challenges associated with AI in pharmaceutical research, such as data quality and integration, regulatory frameworks, and the need for skilled professionals. Also, the future directions of AI in pharmaceuticals, including the potential for AI to revolutionize personalized medicine and improve patient outcomes. Overall, AI has the potential to revolutionize the pharmaceutical industry by streamlining the drug development process, improving patient outcomes, and reducing costs.

Keywords: Artificial Intelligence, Machine Learning, Drug Discovery, Personalized Medicine, Target Discovery.

1. Introduction of AI in Pharmaceuticals:

Although machine learning, deep learning, and artificial intelligence (AI) are sometimes used interchangeably, they are actually hierarchical. The broad idea of artificial intelligence (AI) is the imitation of human intelligence by computer systems, which includes tasks like learning, reasoning, language processing, and displaying information or knowledge [1]. AI is the use of a computer to mimic intelligent behavior with little to no human intervention. Drug development and discovery have been transformed by artificial intelligence (AI) technologies. As of March 2023, at least 14 medications that are entirely AI-generated have started clinical trials, according to Deep Pharma Intelligence. Advances in generative AI have made it possible to develop new, intricate, and realistic models that can generate synthetic data with specific characteristics [2]. It is difficult to imagine how the genie will be placed back in the bottle now that artificial intelligence has arrived. AI is likely to be quickly and extensively adopted if it is perceived to offer a competitive advantage for drug discovery [3]. The repercussions of the industry's adaptation to this new reality will unavoidably materialize, and those who adopt the new methods of working later may feel pressured to do so out of concern that they would lose ground to others. Larger and more established players will have to change or die if they continue to fall behind [4].

AI can be used to address the time-consuming and costly medication development process that is limited by a lack of innovative technology. AI has the ability to identify hit and lead compounds, validate drug targets more quickly, and optimize drug structure design [5]. By better understanding structure-activity connections and forecasting macromolecular targets for compounds based on their chemical structures, a variety of artificial intelligence (AI) methodologies are being developed in the field of computational drug design that may assist address this difficulty. Two primary disciplines have historically predominated here. The subject of statistical modeling, known as quantitative structure activity relationship modeling, is concerned with determining relationships between chemical structure and biological activity [6]. Identification and validation of chemical compounds, target identification, peptide synthesis, assessment of drug toxicity and physiochemical properties, drug monitoring, drug efficacy and effectiveness, and drug repositioning are all created attainable by computational modeling rooted in AI and ML principles [7]. The greatest health care alternatives for doctors, patients, insurers, and regulators are being managed with the use of AI and ML. Statistics originates from an abundance of sources that include institutions of higher learning, manufacturing operations, research and development (R&D) groups, and regional and therapeutic chemists. To improve the healthcare system and medical treatment, AI and ML enable an improved means to organize the vast amounts of healthcare data [8].

2. Applications of AI in Pharmaceutical Research:

2.1Drug discovery and design:

The process of drug innovation and discovery has been revolutionized by intelligent technology (AI) technologies. As of March 2023, at least 14 medications that are entirely AI-generated have started clinical trials, according to Deep Pharma Intelligence. Advances in generative AI have made it possible to develop new, intricate, and realistic models that can generate synthetic data with the appropriate characteristics [2]. AI has the ability to detect hit and leads materials, evaluate therapeutic targets better quickly as well as optimize drug structure design. However, the medication development process is limited by the absence of sophisticated technology, which makes it a costly and time-consuming operation that AI can help with [5]. AI/ML techniques are used in preclinical development to optimize absorption, distribution, metabolism, and excretion toxicity (ADME-T) profiles and produce prediction models of physicochemical features by processing vast amounts of chemical data efficiently [9]. Finding suitable drugs or drug-like molecules that can interfere with these targets is the first and most important step in drug discovery. We now have access to a variety of biomedical data repositories that can assist us in this process [7]. The initial action in the development of drugs is the recognition of compatible targets (e.g., genes, proteins) associated with disease pathophysiology into Metabolomics, also enables the direct detection of manufactured elements, regardless of their particular structures are unidentified, although genomic mining strategies could point to biosynthetic potential. However, it is far from simple to deduce molecular structures and substructures from mass spectrometry (MS) data. Thus, to address frequent issues in MS-based metabolome mining, AI has been used [6]. Artificial intelligence models are able to connect a compound's chemical makeup to its biological action. By inventing compounds with desirable properties including high potency, selectivity, and attractive pharmacokinetic characteristics, researchers can optimize therapeutic candidates [10]. A one-shot learning approach was used for the last stage of model training, which established the iterative refinement of long short-term memory architecture and yielded significant predictive power results that are relevant for low-data drug discovery [8]. Overcoming regulatory obstacles is also necessary to guarantee medication safety, effectiveness, and price. These unmet demands have driven the quest for novel solutions, and AI has emerged as a potent tool to revolutionize the drug discovery process [11]. Therefore, computational drug design in conjunction with traditional chemistry-oriented drug discovery and development concepts offers an excellent foundation for future study [7]. The process of creating molecules, which is the foundation of drug design, consists of two levels of tasks: (i) realistic molecule generation, which involves creating molecules that adhere to the rules of chemistry, and (ii) goal-directed molecule generation, which entails creating chemically sound molecules with the desired characteristics [12].

2.2 Target Discovery:

Unprecedented changes have been brought about in drug research and development, particularly in drug target discovery, by the quick advancement of deep learning and artificial intelligence technologies [13]. Prioritizing candidate targets, determining which targets contribute to the pathophysiology of the disease, and evaluating therapeutic efficacy are all steps in the target discovery process. To understand the molecular mechanisms behind illness phenotypes and identify patient-specific changes, however, this procedure frequently calls for more thorough techniques that combine existing heterogeneous data and information due to the complexity of human diseases [9]. It has been stated that toxicity and a lack of clinical efficacy are the main reasons why medications fail in the clinic. To determine if targeting a specific RNA (or RNA-protein complex) will be effective in treating the disease or preventing its progression, it is imperative to establish a target RNA-disease link from the start of a drug discovery program [14].

2.3 Preclinical Research:

To avoid negative consequences, it is fundamental to predict the harmful effects of each medicinal properties component. The cost of drug development is increased by the frequent use of cell-based in vitro assays as preliminary research, which are then followed by animal trials to determine a compound's toxicity. LimTox, pkCSM, admetSAR, and Toxtree are available to a few web-based tools that aid in cost reduction [5]. 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 [12]. Identification and validation of chemical compounds, target identification, peptide synthesis, assessment of drug toxicity and physiochemical properties, drug monitoring, drug efficacy and effectiveness, and drug repositioning are all made possible by computational modeling grounded in AI and ML principles[7]. Pharmacokinetics and pharmacodynamics have undergone a revolution thanks to AI-based techniques. Compared to conventional experimental techniques, they have a number of benefits. Predicting pharmacokinetic parameters, simulating drug distribution and clearance in the body, and optimizing medication dosage and administration routes are all possible with AI-based models [10].

2.4 Automated Drug Synthesis:

To accomplish the synthesis of 14 distinct small molecules, organic synthesis would be transformed into a machine-driven process through the application of automated systems [15]. A more recent study described an automated polypeptide synthesis process. While manual input and process development are still necessary, the tools and platforms we outlined here marked a significant step toward completely automated synthesis [16]. The domain of contagious conditions which are already underdeveloped in drug development investment portfolios, is a specific field where AI/ML provides potential for healthcare. Lower to middle-income countries (LMICs), the majority of which are in the Global South, are most affected by infectious diseases[17].

2.5 Personalized Medicine:

The practice of personalized medicine involves adjusting medical care to each patient's unique needs. Pharmacogenomics, the study of how genes influence a person's reaction to medications, is one of the main uses of AI in personalized medicine [18]. By providing insightful information on outcome prediction and enhancing individualized health care the goal of theranostics AI applications in other complex domains like radiomics, genomics, or transcriptomics may hasten improvements in patient management [19]. The problem of evaluating vast volumes of data to create individualized treatment regimens is what artificial intelligence (AI) in personalized medicine seeks to address. The intricacy of evaluating the enormous volumes of data required to develop a customized treatment plan limits the use of traditional personalized medicine techniques [20]. Machine learning (ML) has the potential to advance precision medicine in rheumatology by improving patient profiling and treatment customization. In fact, a personalized treatment approach may be developed in the future by using the investigation of oral microbial alterations as a screening biomarker for rheumatic disorders as well [21]. Such a strategy would enable the assignment of customized treatment routes based on individualized diagnoses, but it would require a thorough multimodal data collection [22]. Personalized medicine is a more effective approach that may be employed in the treatment process if the development of genomic profiles is the basis for the diagnosis and treatment of cancer in individuals [23]. AI holds promise for better patient outcomes, reduced medical errors, and enhanced efficiency. Thirdly, a chance to further inform and encourage primary and secondary cardiovascular health prevention for patients who are processing more and more of their own data [24]. Together with clinical, biochemical, and histological data, radiomic analysis offers a wealth of extra imaging information that can be utilized to create more precise predictive models for more individualized therapy and surveillance planning [25]. By simulating trajectories, this could allow us to fully manage the pathophysiology of each individual patient in perioperative medicine and the potential effects on the results of our medical interventions. This is crucial because the aim of surgery is to restore the patient's functionality to its preoperative level, or at least as close to it as possible [26]. Personalized care and artificial intelligence are viewed as essential components of diabetes control in the future. AI is capable of analyzing enormous volumes of data to create individualized treatment regimens and forecast a person's likelihood of acquiring diabetes. Furthermore, depending on the unique circumstances of each patient, individualized care can offer customized management and treatment plans [27]. The production of medications and treatments in the context of personalized medicines might necessitate subtle features based on patient profiles, necessitating real-time design and crafting rather than mass production, storage, and distribution when needed. This subject will be covered in a later section that focuses on "Integration and the Personalized Medicine Workflow" [28]. The AI system's ability to identify cardiovascular risk factors unique to athletes will boost personalized therapy. In professional athletic therapy, this systematic method ensuring AI predictions are accurate understandable and usable [29]. Achieving the goal requires more investment in this field is necessary. Prioritizing this area of research might help us move closer to a day when personalized patient care is not just a potential but a reality [30].

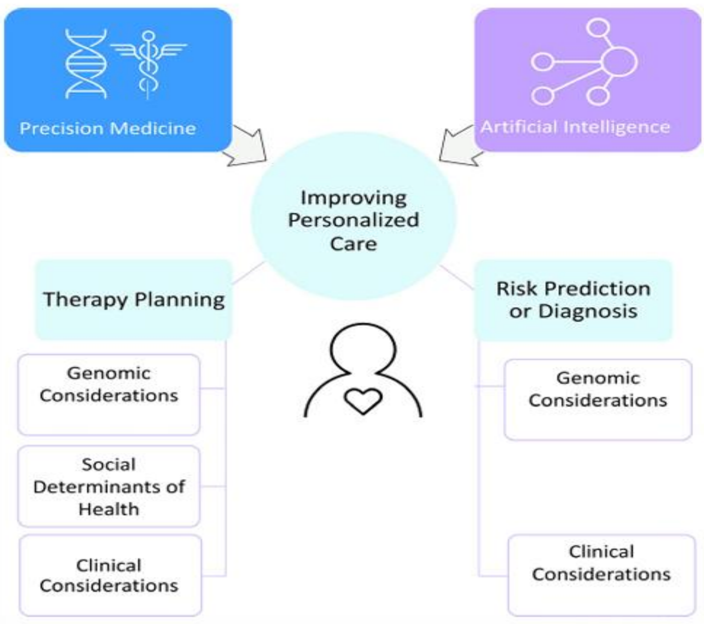

Figure 1: Dimensions of Synergy between AI and Precision Medicine[31]

3. AI-Driven Technologies in Pharmaceuticals:

3.1 Machine Learning Algorithms:

The aim of machine learning, a branch of artificial intelligence, is to enable computers to learn on their own and get better with practice without explicit programming. A collection of AI techniques known as machine learning enables computers to recognize trends and connections between data and relevant results [1]. Although machine learning (ML) has been utilized extensively in drug discovery, translational research, and the pre-clinical phase, its application in clinical trial operations and data analysis has been slower during the past two decades due to its increasing sophistication [3]. Beyond that, machine learning (ML) involves feeding data into the machine along with algorithms that help it learn without explicit programming, such as Naïve Bayes, decision trees (DT), hidden Markov models (HMM), and others. Later, when neural networks advanced, robots were able to categorize and arrange input data in a manner similar to that of the human brain, demonstrating even more progress in artificial intelligence [7]. In medicine, supervised machine learning is most common. In supervised learning, an algorithm is trained on labeled datasets to accurately categorize data. Any correlation between independent and dependent variables is inferred from the labeled data to train an algorithm [32]. ML models can help achieve proper polypharmacy, which is particularly common in the highly comorbid PAD population and match preventative efforts to patients who may benefit the most from new or existing medications [33]. Lack of racial diversity in ML algorithms has been discussed extensively in dermatology as a possible source of bias that can sustain health inequities for people of color [34]. To develop a supervised ML model, the dataset is divided into a training set (70%-80% of data) and a test set (20% 30% of data) [35]. Based on a head model and neural inputs that resemble the central nervous system (CNS), machine learning applications in neurology and neuroimaging use statistical codes, weights, and coefficients to predict pathology [36]. Additionally, bibliometric methodologies were used to examine wearable gadget applications in sports. Machine learning was employed in addition to bibliometric techniques to analyze citation details, keywords, co-authors, and significant subjects in the context of sports [37]. Numerous problems in pathology and laboratory medicine can be resolved with supervised machine learning, including forecasting test costs based only on specific patient attributes and test outcomes [38]. Machine learning algorithms (MLAs) are rarely used to diagnose TPE, and there haven't been any comparisons made between the diagnostic capabilities of different algorithmic models. Additionally, there has been no comparison of the diagnostic capabilities of MLAs and pleural fluid adenosine deaminase (pfADA) [39]. For machine learning to be effective, large volumes of data are required. Safeguarding patient information is crucial in the medical field. The incidents surrounding DeepMind and the Royal Free London Trust, in which patient data was not adequately protected before being sent to Google DeepMind, serve as an example of this [40]. The initial goal of U-Net was to address issues with biomedical pictures. U-Net's outstanding performance has led to its widespread usage in biology and chemistry, including the design of drugs and materials, the prediction of protein structures, and other areas including satellite image segmentation and the detection of industrial defects [41]. By using algorithms, the influence of confounding variables on the classification of diseases is lessened. According to one study, without the assistance of a medical expert, an ML algorithm can lessen the influence of confounding variables like age, which can lower the homogeneity of study groups (clusters) [42]. To identify correlations from enormous quantities of data, artificial intelligence systems emulate the way it works of the brains of humans. These algorithms correctly identify and categorize prostate tissue in WSIs when used for cancer [43]. The assessment of machine learning yields trustworthy data and aids in enhancing medical decision-making procedures. AI's primary objective is to enable automated learning without the need for human judgment [44]. In machine learning, pixel analysis is used to evaluate medical images so that specific values can be taken straight out of the picture. Pixel-based machine learning does not require feature segmentation or calculation. As a result, processing to extract information will not be hampered by even a low contrast image [45].

3.2 Data Analytics:

The data can be examined using a variety of analytical techniques, including data mining and artificial intelligence. Big data analytics techniques can be applied to find the anomalies that arise from merging vast amounts of data from many sources [46]. The emergence of new analytical methods that enable us to analyze data more quickly using larger, dynamic databases has led to improvements in digital data storage, new methods for data collection, and faster computers and algorithms for data analysis [47]. Visual analytics aims to accomplish analysis tasks and uses data as its object. To facilitate visual analysis of food safety hazards, analysts can choose the best data analysis methodologies and visualization approaches by having a thorough understanding of the data sources, data features, and analysis tasks in the food safety domain [48]. The amount of computing power needed to evaluate big, integrated datasets must also be considered. Whenever feasible, it is important to think about how to make the model work with parallel computing [49].

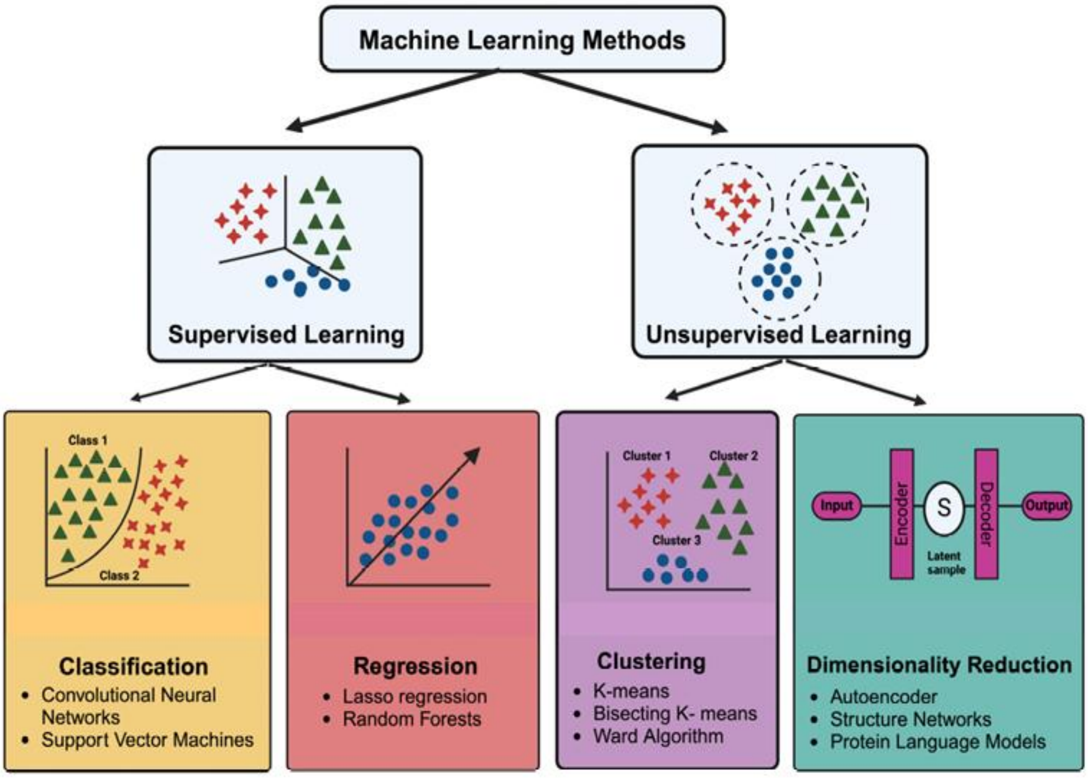

Figure 2: Classification of ML and Examples of algorithms[11]

4. Challenges associated with AI in pharmaceutical Research:

4.1 Data Quality and Integration:

The knowledge and experience of human researchers cannot be replaced by current AI-based techniques, nor can they take the place of conventional experimental techniques. AI can only make predictions based on the facts at hand; human researchers must then verify and explain the findings. However, the drug development process can potentially be improved by combining AI with conventional experimental techniques [50]. In the integration phase, integrative model development was done after basic models and neural networks were built using each kind of omic data [51]. A computational model's requirements are obviously unique to each individual and business; there is no "one size fits all" solution. A model must be interpretable and offer insights into certain chemical properties that contribute to the measured endpoint to be most helpful in a medicinal chemistry setting (the "Computer Aided Drug Design" view) [52]. Another barrier for the completely application of AI inside the pharmacological and healthcare areas is the lack of experienced workers to manage the artificial intelligence (AI) platforms. Job losses result from small organizations' limited budgets and the use of AI and ML tools to replace human workers in large corporations like pharmaceutical businesses. In certain situations, the black box phenomenon may cause the data produced by AL to be implausible [53]. ATOM has created the ATOM Modeling Pipeline, an AI-based cheminformatics platform that accesses molecular characteristics, bioassay data, and past drug discovery data on 500 unsuccessful glycogen synthase kinase (GSK) medications. Big data and machine learning adaption, integration, and application in Partially Matched Crossover (PMX) are still in the early stages of development [54]. The next step for researchers is to determine the operational point, or the probability that should be utilized to differentiate between positives and negatives. In various configurations of the AI clinician cooperation, different operating points may yield ideal results because they correlate to the sensitivity and specificity of the AI-based tool [55]. It is challenging to anticipate attributes for every individual with any degree of accuracy. It can be challenging to forecast how a drug will be metabolized and eliminated in various populations due to genetic variations in these enzymes that can cause individual disparities in drug metabolism and clearance. Numerous enzymes and pathways are involved in the intricate metabolic processes of many medications [56]. Therapeutics and medical science are intricate and dynamic fields. There is no uniform or established procedure for evaluating individual case safety reports (ICSRs) that can be automated. Human intervention and clinical evaluation are usually necessary for decision-making due to differences in the patients' clinical presentations and side effects [57].

4.2 Regulatory Framework:

Gene expression profiling: This technique is now frequently used to screen for tumor treatment sensitivity. However, batch effects, heterogeneity, and differences in sequencing depth between technologies and labs have made it difficult to analyze single-cell RNA sequencing (scRNA-seq) data [58]. The incapacity of the scanners to focus on tissue, their inability to reflect negative or dim staining, and the lengthy setup time required by human technologists for scanning are among the main problems relating to the immunoassay sliding detectors currently available currently in the scene [59]. Small changes in measurement might lead to major errors in derived variables (such LVEF), which could have serious therapeutic repercussions by reclassifying healthy patients as sick or the other way around [60]. In the field of drug discovery, selecting the best models to fulfill research task criteria is difficult due to the large number of ML model designs and the ongoing appearance of new ones [61]. Continued development and the resolution of existing issues with the use of ML in pregnancy complicated by autoimmune rheumatic diseases (Preg-ARDs) can provide important data and sources for furthering this area. Effectively addressing these issues requires actions like encouraging uniformity in sample data entry, strengthening researchers capacity to choose appropriate model techniques, and expanding model interpretability [62].

5. Future Directions:

AI has the potential to transform the pharmaceutical sector in the future by speeding up medication development and discovery. Virtual screening methods will speed up lead compound identification by quickly analyzing massive chemical libraries and identifying therapeutic candidates with the necessary characteristics [10]. Future research should concentrate more on a model's influence on treatment choices, clinical and patient-reported outcomes, and cost-effectiveness in addition to its accuracy, as these factors may be more significant to patients, healthcare providers, and organizers [22]. Furthermore, converting research into useful applications and developing precision oncology would require improved cooperation between computer scientists, biologists, physicians, and pharmacologists [58]. It is anticipated that autonomous AI-assisted review preparation will soon play a crucial role in the AI-assisted drug discovery process [50]. Future research on the economic assessment of clinical AI has a lot of potential [55].

Conclusion:

AI is poised to revolutionize the pharmaceutical industry by transforming the way medications are developed and discovered. The applications of AI in pharmaceutical research are vast, ranging from drug design and target discovery to preclinical research and personalized medicine. While there are challenges associated with AI in pharmaceutical research, such as data quality and integration, regulatory frameworks, and the need for skilled professionals, the potential benefits of AI in improving patient outcomes and reducing costs are significant. With the ongoing evolution of AI technology, we expect substantial progress in targeted medicine, enhanced patient outcomes, and reduced healthcare expenditures. Future research needs to focus on overcoming the issues related to AI in pharmaceutical research and investigating novel uses of AI to enhance patient care. Utilizing AI facilitates the development of a more efficient, effective, and customized healthcare system that advantages both patients and healthcare professionals.

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