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Review Article

Artificial Intelligence in Preclinical and Clinical Pharmacology

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ABSTRACT

Artificial Intelligence (AI) possesses the capacity to transform healthcare. By analysing vast Quantities of medical data, AI can improve disease diagnosis, accelerate drug discovery, optimize treatment plans, and enhance patient monitoring. Additionally, AI can help identify adverse drug reactions, extract valuable insights from real-world data, and personalize healthcare treatments. The overall outlook for AI in healthcare is good, with the potential to greatly enhance patient outcomes and healthcare efficiency, despite obstacles like data quality and privacy issues.AI can revolutionize healthcare by improving diagnosis, drug discovery, treatment, and patient monitoring. It can also identify adverse reactions, extract insights from real-world data, and personalize treatments. While there are challenges, the overall outlook for AI in healthcare is positive.

INTRODUCTION

The first time John McCarthy used the term "artificial intelligence" at the Dartmouth Conference in 1956 to make reference to "the science and engineering of making intelligent machines"[1]. With a few more specifics, McCarthy's initial description is still relevant today. AI, as a multidisciplinary field, needs to be integrated of insights from numerous academic fields, such as linguistics, neuroscience, psychology, mathematics, computer science, artificial psychology, as well as numerous others. Current engineering and intellectual developments have contributed to the development of intelligent systems that address issues in many facets of our lives, moving the discipline from purely theoretical research. Even though artificial intelligence (AI) may solve a wide range of issues, there are some fundamental techniques that are important in any situation. These include knowledge representation, acquisition and maintenance, solution searching, machine learning, and logic reasoning [2]. Early in the

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1930s, Alan Turing came up with the idea of a "universal Turing machine" that could mimic any kind of computer. In some ways, the history of artificial intelligence has followed the technological advancements in computer technology, with ups and downs as well as fits and starts. The first artificial intelligence computers were designed, such as STUDENT (1964), which was capable of implementing logical inference from statements and machine proofs of certain mathematical theorems. Another early example was the machine ELIZA (1966), which was capable of modest human discourse emulation [3, 4]. The 1950s and 1960s were the early heyday, driven by sheer optimization. During this time, man-machine interaction became possible, symbolic methods for semantic processing were introduced, as well as the concepts of heuristic searching and logical reasoning.AI peaked again in the early 1980s. Mathematical models connected to artificial intelligence have advanced significantly, such as Feed-forward neural networks with multiple layers and the backpropagation technique [5]. These technologies enable the creation of a world model in abstract form and offer a mechanism for updating the model in response to feedback or input. It was this combination that initially defeat a human player in chess, and it served as the model for a large portion of the research conducted in the field up to this point. Secondary structure prediction based on protein sequence data was the first excursion of such techniques into the fields of molecular biology and chemistry [6].

Artificial Intelligence Future:

Increasingly, artificial intelligence traction in a number of fields. It could potentially have a significant and positive impact on healthcare providers and patients. Due to its capacity to collect and evaluate enormous volumes of data, AI may be able to provide diagnoses that are significantly quicker and more precise for a greater number of people. This could benefit those who lack access to highly specialized healthcare [7]. Previous and more accurate diagnoses could lead to less expensive medical care. The AI poses hazards to the medical community as well as the patients. In order to guarantee artificial intelligence is providing precise diagnoses and suggestions for treatment, physicians will need to continue using their expertise and experience prior to the data warehouse being sufficiently highly qualified and large [8]. Artificial intelligence technologies have the potential to transform the way physicians observe their patients, increase the likelihood of identifying and managing diseases, lower healthcare expenses and improve medical treatment in areas with limited access to care. Ultimately, envisioning a data-driven and analytics-driven medical future shows promise, but further research is necessary to realize its full ability [9]. Artificial intelligence technology in preclinical and clinical pharmacology plays very important roles now days. In future it leads to the reason in development of preclinical and clinical pharmacology.

1. Artificial Intelligence in Preclinical Pharmacology:

1.1 Drug discovery:

Drug discovery is a drawn-out procedure with a large pipeline and numerous selection stages. The procedure starts with a big number of compounds containing lead, but as it moves down the development pipeline, a strict selection process is used to identify the promising substances, eventually resulting in the administration of one molecule that is approved for the market. The cost of creating a new medicine rises as the quantity of things that require testing. Examining the characteristics and structure of the chemical, artificial intelligence can be applied to assist choose the compounds that are most likely to succeeding. There are several different ways AI has been used in medication discovery. Drug development can be halted before costly trials have begun if it is possible to predict throughout the process's initial phases whether a compound will fail due to unfavourable absorption, distribution, metabolism, and excretion (ADME) characteristics or failure to bind to the intended target. Numerous pharmaceutical organizations currently routinely use these AI applications, to the point where businesses like Cytoreason were established expressly to create and provide models to pharmaceutical corporations for use in disease and medication route research. A novel compound's toxicity profile must be evaluated later in the development cycle. This necessitates large datasets containing in vivo information collected in clinical studies. However, because structure of chemicals has a significant impact When toxicity is present, the same methods to drug discovery might be used. Hepatotoxicity and cardiotoxicity are major toxicities assessed during medication development. As a result, being able to forecast if a compound produces some toxins at the beginning of the development pipeline would significantly lower the likelihood of compound failure, and numerous organizations have used AI techniques to do so [10]. Mamoshina and colleagues examined the viability developing a model based on AI to forecast the cardiotoxicity of various drugs. Based on medication features gleaned from the general public accessible information (e.g., Drug bank and med DRA), they created a model to predict cardiotoxicity. By categorizing medications as safe or dangerous, the model might forecast cardiotoxicity using good preciseness (area under the curve [AUC] 79% for validation data and AUC 66% for unknown data) [11]. Similar methods been employed to forecast medication-caused liver impairment, with 89% of correct classifications based on drug properties, achieving even greater accuracies [12].AI can be used for more than only choosing the best drug and estimating it in vivo activity. Additionally, it can be used to identify novel uses for currently available medications with a known risk/benefit ratio. This shifting of the drug is especially helpful for tiny populations of patients, for which clinical studies are impractical and drug development expenses are sometimes deemed excessively exorbitant. Drug repositioning takes many distinct forms, all of which necessitate extensive computer analysis and enormous datasets. Using An approach centered on drugs, new and current medications are first compared to find compounds with similar qualities that could be effectively utilized to address the therapeutic indications of the comparator medication. Secondly, a disease-focused approach seeks to find drugs that are effective for diseases that share Comparable characteristics through disease comparison pathways and characteristics. The most common way to integrate these two approaches is to look for a match by comparing the patterns of gene expression of various medications with the illness profiles. This combinatorial method was employed by Al- taie et al. to find novel treatments for colorectal cancer (CRC) [13]. Using the clinical studies information, an Artificial intelligence model was instructed to recognize subgroups. Subsequently, each subgroup's distinct gene profiles were cross-referenced with the medication database to determine plausible candidates for repurposing. Twelve of the sixteen most popular drugs discovered in this manner are linked to cancer, eight of which have been authorized for use in the care of colorectal cancer, demonstrating the potential of this strategy [14]. AI models have also been applied in similar ways to other disease areas. For instance, 103 hits were found in a study on Alzheimer's disease, and three of those hits had validation studies conducted on a population [15].

Zhang and colleagues used a technique to find possible therapeutic diabetes targets before identifying drugs that are recognized to have an impact on these targets. Consequently, 58 medications were discovered, nine of which included determined to be significant based on gene expression profile connection [16].

1.2 Drug toxicity and safety:

An important development in toxicology and pharmacology is the incorporation of Artificial intelligence, which provides deep insights into pharmacological effects, environmental implications and safety profiles. The power of artificial intelligence to handle massive datasets, spot trends, and forecast results is transforming these domains and offering a thorough comprehension of toxicological risk assessment and pharmaceutical research. The article's contribution to various fields is explained in this section [17].

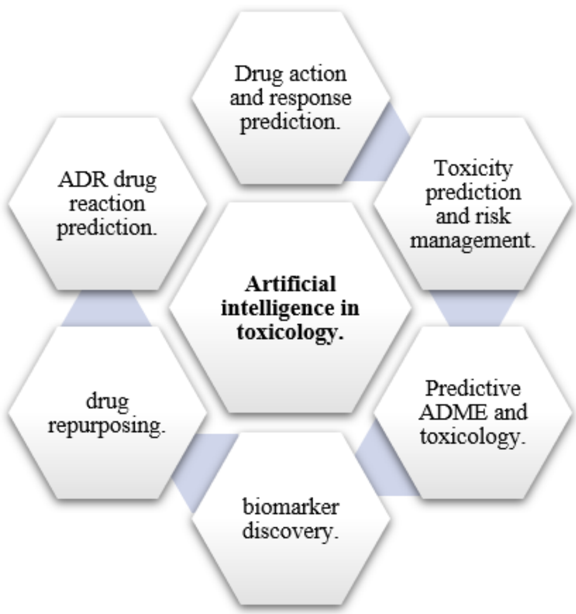

Figure 1. Artificial intelligence in toxicology [17].

In order to forecast the modes of action and pharmacological effects of medications, artificial intelligence algorithms examine intricate datasets. This capacity predicts how drugs will interact with biological systems, enabling the creation of more specialized and efficient treatments [18, 19]. AI is essential to toxicology because it can forecast a substance's possible toxicity. ML algorithms can forecast the level of toxicity of novel substances by examining chemical compositions and past toxicity data, which lessens the need for intensive in vivo testing [20,21]. Predicting and modelling ADMET characteristics, which are essential in drug discovery, is greatly aided by artificial intelligence. AI models also mimic pharmacodynamics (PD) and PK, which aid in understanding how drugs behave in the body and optimizing dosage to ensure safety and efficacy [22,23]. By identifying uncommon but serious side effects, artificial intelligence can forecast adverse drug reactions (ADRs) by analysing patient input and medical records [24]. Drug repositioning, another name for drug repurposing, entails looking for novel therapeutic uses for licensed medications that are already on the market. It is a successful strategy in discovering the medicinal compounds with novel indications for treatment. Drug recycling is a cost-effective and time-saving strategy because of the widely available and well-established safety of the already licensed medications. Drug repositioning and drug discovery heavily rely on the identification of drug–target interactions (DTIs) [25]. AI techniques have been shown to be essential for premarketing drug safety, especially in the area of toxicity evaluation. A critical step in the drug design process is identifying the adverse effects (AEs) of compounds on humans, animals, plants, and the environment. Toxic medications must be stopped before they enter clinical trials through preclinical assessments. High toxicity, however, still plays an important role in drug failure, contributing to one-fifth of unsuccessful therapeutic trials and two-thirds of post-marketing drug withdrawals. As a result, precise toxicity assessments might shorten the time and expense required to develop and introduce novel medications to the market while also guaranteeing drug safety. In the past, using animal research has been the most common method for determining toxicity. Nevertheless, time, money, and ethical constraints limit this research. Many computational, in silico methods have shown promise in determining the toxicity of potential drugs [25].

Relevant studies:

Recent studies demonstrate how AI is revolutionizing toxicology and pharmacology. For example, research has examined the therapeutic and prognostic implications of different genes in gastric cancer and the function of miRNAs in glioblastoma regulation. Clinical and genetic data have been integrated through the use of machine learning algorithms to predict clinical reactions to anti-epileptic medications and adverse drug reactions. AI's increasing significance in preclinical drug discovery is shown by developments in chemical language models for toxicity prediction and its application in ADMET modelling [26,27].

2. Artificial Intelligence in Clinical Pharmacology:

2.1 Clinical trials:

Clinical pharmacy is using artificial intelligence more and more to help improve patient care. Clinical pharmacies can apply more precise, effective, and personalized techniques by leveraging AI's skills in data analysis, pattern recognition, and forecasting. This section offers a thorough examination of how artificial intelligence is being incorporated into clinical pharmacy. AI can improve a number of clinical pharmacy functions, such as medication delivery and patient counselling. [28]. Six to seven years are needed for clinical studies, and a significant financial dedication, are intended to determine the effectiveness and safety of a drug product in humans for a specific disease state. Nevertheless, the industry suffers a significant loss because only one out of ten compounds that undergo these trials are successfully cleared [29]. These shortcomings can be caused by insufficient infrastructure, absence of technological needs, improper patient selection. However, by using artificial intelligence, the wealth of digital medical data already available can help to reduce these issues [30]. Enrolling participants takes about a third of the clinical trial's duration. Finding the right patients is crucial to the success of a clinical study, as failure cases account for about 86% of all cases [31]. Through patient-specific analysis of the genome-exposome profile, AI can assist in selecting only a specific affected group for participation in Phase II and III clinical trials. This can help identify potential treatment targets in the selected patients early on. Preclinical molecule discovery and lead compound prediction before clinical trials begin using other AI components, such as predictive machine learning and other reasoning techniques, enables early prediction of lead molecules that would pass clinical trials with consideration of the selected criteria. Patient dropouts cause 30% of clinical trials to end in failure, wasting time and money and requiring additional recruitment to finish the trial. This can be avoided by keeping a careful eye on the patients and helping them follow the intended clinical trial protocol.[32]. Ai Cure developed software for mobile devices that monitored the regular medication intake of patients with schizophrenia in a Phase II study. This ensured the successful completion of the research trial and increased patient adherence by 25% [33].

2.2 Treatment optimization:

The best pharmaceutical dosage for each patient is determined aided by artificial intelligence. It considers a variety of factors, including weight, age, kidney function, and particular patient circumstances to recommend dosages that maximize effectiveness while reducing adverse effects [34]. Customizing the treatment is beneficial and crucial for many commercially available medications. To individualize the dose, therapeutic drug monitoring (TDM) is utilized for medications that have a narrow therapeutic window. To ascertain drug exposure and optimal treatment practices, methods for extrapolating TDM data are often based on statistical prediction models. Compared to drug discovery, this area of use of AI is less developed. This is mostly because substantial clinical datasets are required for model training and are not easily accessible [35]. As an example, Labriffe et al. trained several XGBoost models to replicate the PK traits of everolimus patients. An XGBoost model is a kind of supervised learning that combines multiple (weak) decision trees to create a powerful overall model. At three distinct timepoints (predose, one, and two hours), the models were trained using a variety of combinations of simulated and real patient PK profiles and everolimus TDM measurements. 5016 simulated PK profiles were used to train the best-performing model (n = 114, R2 = 0.956, root mean squared error [RMSE] = 10.3%), which was then able to predict the everolimus AUC for an external validation set [36,37].

2.3 Pharmacovigilance:

The treatment and prevention of diseases have been revolutionized by drugs and vaccines. Although pharmaceutical products provide benefits, they can also have negative or unexpected side effects. Pharmacovigilance is the study and practice of identifying, assessing, understanding, and preventing side effects or any other problem related to drugs or vaccines. All drugs and vaccines must pass rigorous clinical trials to guarantee their safety and effectiveness before being authorized for use. Nevertheless, the process of conducting a clinical study comprises a brief period of time spent researching these goods in a comparatively a few carefully selected participants. Some negative consequences may not show up until after these products have been used for an extended amount of period and by a wide range of people, such as those who are co-ill with other conditions [38]. In pharmacovigilance, artificial intelligence is increasingly being used. The subject of artificial intelligence in pharmacovigilance, or AIPV, is expanding quickly, according to a MEDLINE search conducted using the terms "artificial intelligence" and "pharmacovigilance". Even while this figure's recent increase is merely a rough indicator of the amount of growing interest, it is consistent observing the agendas of scientific meetings and related actions. AI, for instance, is the focus of a subgroup under the recently established Drug

Safety Research Unit International Working Group on Signal Detection and Evaluation. In order to detect potential adverse drug reactions (ADRs) and drug mistakes, artificial intelligence applications track and evaluate data from many sources, offering an active strategy for pharmacovigilance. This procedure improves medication profiles and increases patient safety [39,40].

2.4 Real word evidence:

In the context of life science and healthcare, real-world data (RWD) is defined as patient health or healthcare delivery data that is gathered outside of randomized clinical trials (RCTs). In addition to claim procedures, product and sickness registries, and patient-generated data (such settings for at-home use or mobile devices), this information is collected via a patient's electronic health record (EHR) in a hospital or from a health insurance provider. Large-scale or granular data can be obtained from RWD sources in almost real-time, and This information can be used to support a variety of clinical trial designs, such as observational studies, pragmatic clinical trials, large-scale trials and RCTs [41]. The recorded EHR data can be divided into two categories: unstructured data (such as doctor notes) and structured data (such as International Classification of Diseases codes, lab results, and prescriptions). While structured data do not require this kind of processing, unstructured data which comprise the majority of recorded data—need to undergo extensive processing before statistical tests and machine learning tasks can be completed. The examination of RWD yields Real-World Evidence (RWE), which is clinical data regarding the application, possible hazards, and advantages of a pharmaceutical. However, a substantial amount of RWD must be gathered and converted into an analysable format with a certain level of data accuracy and reliability guaranteed in order to produce high quality RWE that is appropriate for regulatory use and other decision-making applications. This is beyond the capacity of humans alone. Consequently, the study of RWD is increasingly utilizing AI skills [42].

2.5 Precision medicine:

In order to adapt healthcare solutions to each patient's specific needs, artificial intelligence technologies are employed to evaluate and interpret massive datasets, including genetic information, lifestyle characteristics, and environmental exposures. The term "AI-driven personalised medicine" refers to this procedure. Personalized medicine powered by AI offers hope for overcoming some of the most serious difficulties faced by the medical industry. Preventive measures can drastically alter people's health outcomes since AI-driven personalised medicine can identify individuals who are at-risk before diseases manifest symptoms. Medical research is accelerated by AI's ability to analyse and learn from massive amounts of data, leading to a better knowledge of complex diseases and a quicker search for new remedies [43].

Relevant studies

The use of AI in clinical settings for risk assessment, diagnosis, screening, and treatment of various situations was explored by Yin et al. in 51 studies that were published between 2010 and 2020. By combining real-world evidence with expert knowledge, the xDECIDE system illustrates the importance of AI in personalized oncology care. AI can be employed in drug repurposing and tailored treatment, as demonstrated by other studies such as the DRIAD framework for Alzheimer's disease [44].

CONCLUSION:

Artificial Intelligence (AI) is transforming healthcare via the analysis of enormous volumes of medical data. It can improve disease diagnosis, accelerate drug discovery, personalize treatments, and enhance patient monitoring. While challenges like data quality and bias exist, AI's potential to significantly improve healthcare outcomes and make it more efficient and affordable is promising.

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