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Accelerating Drug Development Process by Using AI/ML

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ABSTRACT-

Combining Artificial Intelligence (AI) and Machine Learning (ML) has transformed medicine research by accelerating the creation of novel medicines and changing traditional methods. This paper provides a thorough account of the ways in which these tools have transformed pharmaceutical research at every level, ranging from early target selection and clinical trial optimization to post-market surveillance. By utilising vast data warehouses, advanced algorithms, and predictive analytics, artificial intelligence and machine learning (AI and ML) have expedited the identification of potential therapeutic targets, enhanced our comprehension of intricate biological processes, and simplified the process of developing novel drugs. This synthesis also emphasises the difficulties in combining AI with the creation of pharmaceuticals, focusing on data protection, regulatory frameworks, ethical considerations, and the interpretability of AI-generated choices. Despite these challenges, the synthesis highlights the opportunities at the nexus of artificial intelligence (AI), machine learning (ML), and pharmaceutical research, imagining a time when innovation and precision medicine will combine to improve healthcare worldwide. This analysis addresses both the difficulties that demand careful attention and discussion for the advancement of treatments as well as the technologies' unmatched promise. It provides insights into the revolutionary influence of these technologies..

Keywords- Artificial Intelligence, Drug Discovery, Drug Development, Machine learning

Review of Literature

INTRODUCTION

Artificial intelligence (AI) advancements are updating many facets of our lives, but the pharmaceutical business is struggling to overcome high drug development attrition rates. To overcome obstacles, the pharmaceutical and AI sectors are working together. AI will increase the process of developing new drugs more efficiently (Mak & Pichika, 2019)

Many pharmacological compounds are developed as a result of the huge chemical space However, the discovery of new drugs is hampered by the absence of cutting-edge technologies which can be resolved by using AI (Paul et al., 2021)

Advances in AI, especially with the recent advances in digitization and machine learning, could help address the intractable search problem of discovering new drug candidates(Lou & Wu, n.d.)

There are several possible contributions AI can lessen the inefficiencies in the traditional medication discovery and development process. AI has improved target identification and validation, which is made feasible by genomics, which provides biochemical and histological data (*Artificial Intelligence in Oncology Drug Discovery and Development*, n.d.)

It has been determined that artificial intelligence (AI) will significantly impact drug development (Lamberti et al., 2019)

With the aid of enormous datasets, sophisticated algorithms, and predictive analytics, artificial intelligence (AI) and machine learning (ML) are speeding up the process of designing candidate molecules, finding new drug targets, and improving our knowledge of how drugs interact with biological systems (Gaudelet et al., 2021)

What is AI?

Artificial intelligence (AI) is a type of computer system that can perform actions and make decisions without being explicitly programmed to do so. It can learn from data and improve its performance over time, and it can even adapt to new situations (Tang et al., 2022).

What is ML?

Machine learning (ML) is a type of artificial intelligence that allows software to learn from data and improve predictions automatically, without being explicitly programmed. ML is a practical field with widespread applications in science, business, and engineering, leading to more informed decision-making(Holzinger et al., 2019).

ML can be separated into two groups: supervised and unsupervised ML, Using labeled data—also referred to as training data—the supervised machine learning model is built and then applied to new data to generate predictions. On the other hand, unsupervised machine learning involves the provision of unlabeled and uncategorized data without any prior knowledge(Arora et al., 2021a).

In particular, a variety of machine learning (ML) algorithms, including convolutional neural networks (CNN), gradient boosting decision trees (GBDT), artificial neural networks (ANN), and random forests (RF), have been used to build new scoring functions(Stanzione et al., 2021).

Convolutional, non-linearity, pooling, and fully linked layers are among the layers that make up CNN. Pooling and non-linearity layers lack parameters, but convolutional and fully-connected layers do. CNN performs exceptionally well in machine learning tasks(Bayat et al., n.d.)

What is Drug Development?

The complex and multidimensional process of developing a new pharmaceutical drug from the world of scientific discovery to the hands of patients in need is known as drug development. Although it can take tens of years and cost billions of dollars, the journey is lengthy, difficult, and costly, but it has great potential to improve human health and lessen suffering(Morgan et al., 2011).

The drug development process encompasses a series of meticulously designed and rigorously evaluated stages, each building upon the knowledge gained from the previous one. These stages can be broadly categorized into preclinical research and clinical research.(Lalonde et al., 2007).

Phase I trials assess the drug's safety, tolerability, and pharmacokinetics in a small group of healthy volunteers. Phase II trials, involving a larger group of patients with the target disease, focus on determining the drug's efficacy and further evaluating its safety profile. Phase III trials, involving hundreds or thousands of patients, aim to confirm the drug's efficacy and safety in a larger and more diverse population(Ivy et al., 2010).

Artificial Intelligence and Machine Learning-Based Methods

KronRLS

Regularized least-square (RLS), or KronRLS, is an effective model that is applied to various applications. It has demonstrated exceptional performance when used to predict binary DTIs. SimBoost. Using gradient-boosting regression trees, a new non-linear technique called SimBoost has been created to predict DTBA as a regression job. DRUG-TARGET COMPATIBILITY (DTBA)(Thafar et al., 2019).

What are the challenges and opportunities of using AI/ML in drug development?

Over time, automation of some jobs in clinical trials, manufacturing, supply chains, medication research, and sales will occur; nevertheless, these tasks are all classified as "narrow AI," meaning that the AI must first be trained on a vast amount of data to be appropriate for a specific task. But since AI is already replacing monotonous tasks (Paul et al., 2021).

At the moment, selecting the best drug target or dosage for a particular patient group, as well as chemical structures (such as toxicity, side effects, or even intellectual property), represent the main obstacles in the drug discovery process(Zhavoronkov et al., 2020).

Because tensor learning models can precisely predict the dose-response matrices of drug combinations, which can be difficult to construct and screen, the most effective combinations can be prioritised for additional testing.(Aittokallio, 2022).

Medical Bias in AI can hurt disadvantaged populations. By using a variety of datasets, understandable tools, and open reporting, we may lessen prejudice and increase confidence in AI. For the safe, equitable, and responsible application of AI in medicine, there must be clearly defined roles and legal liability.(Rajpurkar et al., 2022).

Companies that are using AI/ML

AstraZeneca and Benevolent are utilising AI to combine genetic, chemical, and clinical data in an effort to identify novel potential treatment targets. GlaxoSmithKline (GSK) can access 23andMe's datasets and use machine learning to find new pharmacological targets by investing in the biotechnology company.(Quazi, 2022).

DeepMind is using artificial intelligence (AI) algorithms to forecast protein structures, which may be useful in locating novel therapeutic targets and creating medications with fewer adverse effects. AI is being used by Exscientia to design and develop novel pharmaceuticals; the company has already produced a number of candidates, one of which is a Phase 2 clinical trial candidate for Alzheimer's disease. Verily is leveraging artificial intelligence (AI) to create novel clinical trial tools, such as tools that use AI to anticipate trial outcomes and help find the best patients to enrol in studies.(Blanco-González et al., 2023).

AI/ML in drug discovery

Application of AI in Drug Discovery

Complex and state-of-the-art drug research pipelines can be created with the help of AI algorithms, potentially reducing down on the costly and time-consuming drug development process. Through the application of various supervised machine learning and deep learning algorithms on experimental data, these approaches have demonstrated a higher degree of success in the discovery of new drugs.(Arora et al., 2021b).

By anticipating drug qualities, repurposing current medications, and finding new targets, artificial intelligence is speeding up the process of finding and developing new drugs. By creating innovative biomarkers and therapeutic targets based on bionomics signals, AI is also enabling personalised medicine.(Mak & Pichika, 2019a).

Drug discovery: Artificial intelligence (AI) systems are being developed to find novel therapeutic candidates from enormous databases of data on already-approved medications that may be modified to target serious dangers like the Ebola virus. This might increase the effectiveness and success rate of drug development, hastening the process of releasing new medications in response to the threat of lethal diseases.(Wisetsri, 2021).

Early drug discovery uses AI/ML to forecast preclinical development outcomes, identify disease-related targets, and generate and optimise lead candidates. Artificial intelligence (AI) methods incorporate diverse data to comprehend molecular pathways and enhance virtual screening and de novo medication creation.(Vatansever et al., 2021).

Target Identification and Validation

The early discovery stage involves target identification and validation, hit discovery, lead molecule identification, and then optimization to achieve the desired characteristics of a drug candidate (Gaudelet et al., 2021).

Artificial Intelligence (AI) has revolutionized medication research by changing the way that pathways or targets are identified. This was made feasible by the integration of target tractability, biochemical characteristics, and genome data (Mak & Pichika, 2019b).

Early in the drug development process, drug target identification benefits from AI innovation capabilities(Lou & Wu, n.d.).

GSK and the business powered by AI Insilico Medicine collaborated on a study to explore the potential applications of Insilico's artificial intelligence (AI) capabilities in identifying novel biological targets and routes important to business (Yang et al., 2019).

The lead discovery phase is the next crucial stage once the biological targets have been found and verified. There are three parts to this: lead optimization, hit-to-lead phase, and hit detection lead optimization, hit detection, and the hit-to-lead phase come in that order.(*Artificial Intelligence in Oncology Drug Discovery and Development*, n.d.)

Algorithms using AI and ML have several benefits for drug discovery. They accelerate the search for novel medications by processing data at amazing speeds, Increasing effectiveness, and cost-effectiveness of AI/ML may reduce the total costs related to drug development, making it a promising tool in the search for novel drugs(Selvaraj et al., 2022).

Hit Identification and Lead optimization

Phase of hit-to-lead and lead optimization

The goal of this transitional stage is to create a molecule or compounds with improved characteristics and pharmacokinetics appropriate for one or more in vivo application models. This process often entails a sequence of relationship-building exercises (SAR) studies for every hit molecule, aiming to quantify the activities and selectivity of every substance.(*Artificial Intelligence in Oncology Drug Discovery and Development*, n.d.)

Artificial intelligence (AI) can identify hit and lead compounds, expedite the confirmation of the drug target, and optimize the design of the drug structure(Paul et al., 2021b)

Virtual screening (VS) can be used to assist in hit identification and lead optimization (biologically, active compounds are transformed into appropriate drugs by improving their physicochemical properties), Virtual screening (VS) can help with lead optimization and hit identification(Maia et al., 2020)

AI/ML in Denovo synthesis Big data in drug discovery

A collection of data sets that are too huge and complex to handle with conventional data analysis methods is referred to as "big data". Big data is becoming more and more popular in research domains other than clinical investigations that are driven by biological data(Gilson MK, 2016).

A publicly available online database of drug-target binding information, represented as measured binding affinities, is called the Binding Database (BindingDB) (50). Proteins and enzymes that are The targets indicated in BindingDB are thought to be therapeutic targets. For present, BindingDB is(Maia et al., 2020).

AI is streamlining antiviral and antimicrobial drug discovery by designing new molecules with desired properties and predicting QSBRs(Méndez-Lucio et al., 2020)

But now that artificial intelligence (AI) has advanced to a new level, it is conceivable to mine our current knowledge base to discover practically infinite chemical space and create new tiny molecules with the appropriate physicochemical and biological features. New antibacterial compounds have recently been developed using AI-based techniques.(Blaschke et al., 2020).

However, with the most recent advancements in artificial intelligence (AI), it is possible to use this data to find and make new, small molecules with the required physicochemical and biological characteristics. Notably, new antibacterial molecules have recently been developed using AI-based techniques. (Méndez-Lucio et al., 2020).

AI/ML in clinical trials

A medication developed with artificial intelligence, commences clinical trials.

According to reports, DSP-1181 is the first drug of this type created by AI to enter clinical testing. The development of DSP-1181 by Exscientia, in partnership with Sumitomo Dainippon Pharma of Japan, took less than a year from the beginning to the end, compared to four years using typical processes (Sumitomo Dainippon Pharma 2020).) (Harrer et al., 2019).

AI in drug manufacturing and post-marketing surveillance

Artificial intelligence could be used in the industrial manufacturing of pharmaceuticals to make them far more flexible, efficient, high-quality, and agile. This could emerge from the industrial revolution and the application of these technologies.(Arden et al., 2021).

Investing in AI skills can sustain production productivity. Applications of AI include robotic manufacturing and process automation. AI may therefore improve decision-making and eventually result in the creation of innovative, superior pharmaceuticals.s(Damiati, 2020).

Since the introduction of electronic health records, it has been possible to assess the value of AI approaches in automating PV operations and the application of machine-learning techniques to the development of practice-based clinical pathways, probabilistic clinical risk stratification models, and disease models. This has been made possible by the application of AI approaches to publicly accessible consumer data.(Schmider et al., 2019)

Drug safety (DS) experts require help from assistive technologies like artificial intelligence (AI) to manage the increasing volume and complexity of their work as the number of individual case safety reports rises.(Danysz et al., 2019).

PMS, or post-marketing surveillance, is the practise of keeping an eye on the effectiveness and safety of medications and medical devices once they have been given the go-ahead to be sold. PMS research is undergoing a significant transformation thanks to artificial intelligence (AI) and machine learning (ML). Large datasets of PMS data can be analysed using AI/ML algorithms to find patterns and trends that can point to safety or efficacy issues. This can assist in recognising and addressing adverse occurrences before they significantly affect patients.(Zinchenko et al., 2022).

By improving error detection, patient stratification, and drug management, artificial intelligence (AI) can help improve patient safety. It can also be used to predict drug dosages, identify medication errors, monitor stroke patients and track their medication intake, review clinical notes, and spot signs of opioid abuse (Choudhury & Asan, 2020).

Predictive analytics, powered by artificial intelligence, is a novel approach that forecasts future events using data that is currently accessible. Prescriptive modeling, predictive analytics modelling, and descriptive modelling are also utilized (Basile et al., 2019).

AI/ML for rare diseases

AI technologies can be especially helpful for rare diseases (RDs), which are notably underrepresented in basic and clinical research, The development of novel medications could be speed up by artificial intelligence's capacity to understand RDs. AI applications in many RD fields, including (a) prognosis and diagnosis, (b) disease classification and characterization, (c) therapeutic strategies, and (d) patient registries and medical records (Brasil et al., 2019).

AI is used for diagnosis, risk assessment, and treatment recommendations, an artificial intelligence agent correctly diagnoses and makes treatment recommendations for congenital cataracts in an in silico test, a website-based study, a "finding a needle in a haystack" test, and in other scenarios a multicenter clinical experiment (Long et al., 2017).

AI/ML in cancer drug development

Machine learning models can accurately predict the drug sensitivity of patients with endometrial, gastric, and ovarian cancer, Artificial intelligence (AI) can also advance cancer research by enhancing cancer imaging, cancer screening and diagnosis, cancer treatment, and cancer medication. Cancer imaging should currently be the most advanced use of AI in the field of cancer (Liang et al., 2020).

Pfizer and IBM Watson Health, an AI platform, collaborated to improve Pfizer's search for immuno-oncology therapies (Linton-Reid, 2020).

AI/ML in infectious diseasese

One of the top 10 infectious diseases that kill men worldwide is tuberculosis (TB), In developing nations, traditional techniques are employed for tuberculosis diagnosis. Artificial intelligence (AI) algorithms have advanced significantly, particularly in recognizing tuberculosis (TB) symptoms, A number of attempts were undertaken to come up with methods for improving the accuracy of TB diagnosis classifications through the use of AI and machine learning(How Government Can Use AI and ML to Identify Spreading Infectious Diseases, 2018).

Role of AI/ML in Covid vaccine

DeepMind and AlphaFold: This technology is a promising technique in healthcare that can address the needs of researchers and scientists in the creation of antiviral medications and vaccines. DeepMind uses the AlphaFold library to predict the protein structures of COVID(Kannan et al., 2020).

Building an effective surveillance system requires an integrated modelling strategy that incorporates many individual data model types, such as trip data, mobile phone location monitoring, and epidemiological and behavioural pattern data. In order to limit the transmission of illness, this modelling approach necessitates an understanding of the target population both individually and, crucially, during large gatherings.(Arora et al., 2021c).

AI/ML for personalized medicine

Personalized medicine, including illness diagnosis, treatment, and detection, depends on AI algorithms. This paper assesses the problem-solving performance of ANNs, SVMs, fuzzy logic, and Naïve Bayes in customised medicine. This encourages more study and advancement in this area. (Awwalu et al., 2015).

Big Data is revolutionising biomedical research, but analysis and interpretation are made more difficult by the volume, variety, and complexity of the data. Significant scientific and technological advances along with new computational techniques are required to create reliable systems for utilising biomedical Big Data in customised medicine.(Cirillo & Valencia, 2019).

AI/ML for drug repurposing

Drugs are being repurposed for SARS-CoV-2 at a fast rate thanks to AI/ML. The most well-known example is baricitinib, although numerous other intriguing contenders are in the works. Pharmacological targets are being prioritised and anti-SARS-CoV-2 effects are being predicted from molecular structure using AI/ML models. This study is hastening the identification of novel COVID-19 therapies.(Levin et al., 2020).

Utilizing AI and ML techniques for the repurposing of drugs

In machine learning models, orthogonal drug-target space deconvolution is used in drug-target interaction prediction algorithms, where the chemical structures of the medications and targets serve as recommendations for the in-silico predictions. Another line of research has successfully predicted target activity for kinase inhibitors using crowdsourcing-based AI and ML techniques..(Tanoli et al., 2021).

AI-based medication repurposing can reduce clinical trial failures and is a quicker, less expensive, and more efficient method. Without first going through toxicity testing and trials, the repurposed medicine might go straight into the advanced phase for testing. Even though AI-powered medication repurposing is still in its infancy, this method holds promise for the creation of future COVID-19 treatment medications.(Mohanty et al., 2020).

The economic impact of AI/ML in drug development

Drug discovery costs might be lowered by up to 50% and the time to market could be shortened by up to 10% with AI/ML. Pharmaceutical corporations might save billions of dollars as a result, and patients could profit from faster release of innovative medications.(Panch et al., 2018).

Benefits of using AI/ML for drug target identification

There are various benefits to using AI/ML for drug target discovery, including:

Drug discovery algorithms that make use of AI and ML offer various advantages. They process data at incredible speeds, which expedites the search for new drugs. Their accuracy in identifying drug targets reduces the possibility of inaccurate outcomes, boosting efficacy. Additionally, the affordability of AI/ML may lower the overall expenses associated with drug research, making it a promising tool in the hunt for new medications.(Selvaraj et al., 2022).

Collaboration between Humans and Machines:

Exploring the synergy between human researchers and AI/ML algorithms in drug development

For drug development to advance, technology and people must work together. AI/ML algorithms enable automation, improved accuracy, decreased risk, and enhanced innovation. However, there are challenges that need to be addressed, such as gaining government approval, changing cultural norms, and improving data quality and accessibility.(Dara et al., 2022).

Regulatory aspects of using AI/ML in drug development

It is imperative to integrate the regulatory aspects pertaining to digital health technologies when evaluating pharmaceuticals that are created using data-driven methodologies. There are clear obstacles to regulatory licencing for clinical trials using machine learning-based technologies, highlighting the importance of transparent algorithms and high-quality data. To guarantee reliable AI in clinical trials, a number of important regulatory issues need to be addressed during the assessment process.(Massella et al., 2022).

Regulatory bodies are concentrating on several crucial aspects of AI/application ML's in drug research, such as validation, transparency of models, and data quality. In order to make sure that their AI/ML models adhere to all relevant regulations, sponsors should thoroughly study the (Ivy et al., 2010)

METHODOLOGY

- The literature search was limited to articles published from 2007-2023. The search for articles was done online by using the search words '' Artificial intelligence (AI), Machine learning (ML) Drug discovery, Drug development, Target identification, Drug design, Clinical trials, Post-marketing surveillance'' in the title and keywords in research databases at Wiley, Elsevier, Taylor & Francis, ERIC, Springer, SAGE, Frontiers.

Analysis

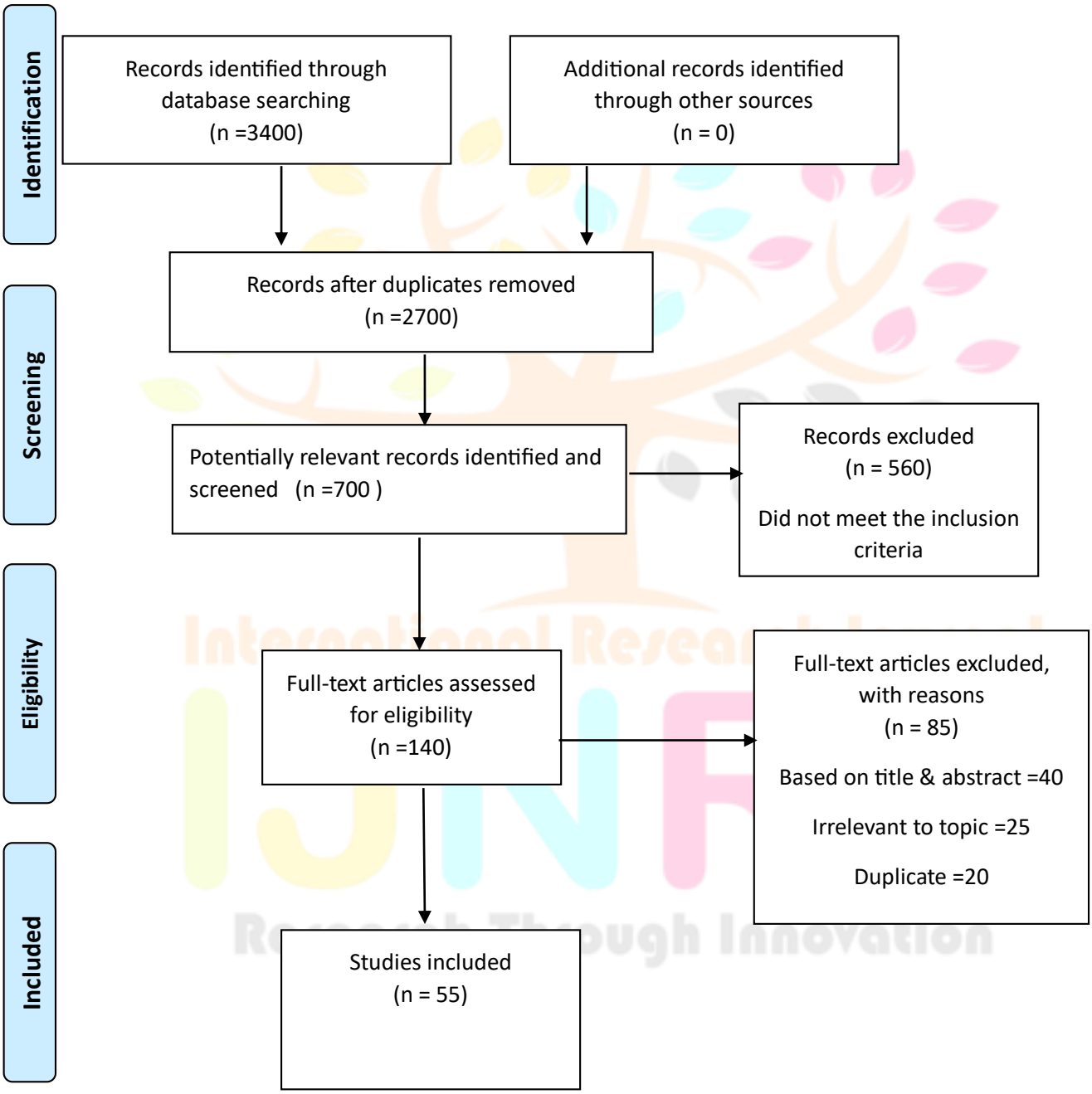
The method used is the Preferred Reporting Item for Systemic Reviews and Meta analytic (PRISMA) method. All articles that have passed the selection process were then reviewed and summarised based on the objectives, year of publication, number of citations and suggestions for further research.

Inclusion & Exclusion criteria

The be included in current study, studies have to meet some criteria

(a) Studies have included some kind of selection criteria (Academic procrastination, work place). These criteria limited the number of studies (b) Accordingly excluded the studies in which it based on irrelevant information there is no proper Title, Abstract & Review.

PRISMA Flow Diagram



The research database search resulted in all keywords search results obtained 4000 research articles. After scanning the title, there was the same article in two different databases. The results after deducting the duplicates are 3005 articles. A total of 700 articles were screened. 560 Articles excluded that they not meet the inclusion criteria.

Articles accessed for eligibility are 140 articles. A Total number of 80 articles excluded based on title and abstract (40) Irrelevant to topic (15) Duplicate (15).

The final data set consists of 60 articles.

The oldest included study was published in the year 2005 and the most recent study was conducted on 2021.

The Entire process is shown in the figure

Conclusion

In conclusion, exploring AI and ML in drug development shows that these technologies have the potential to change how we do pharmaceutical research. The readings we looked at give a good overview of how artificial intelligence and machine learning are used at different stages of discovering and developing drugs. As this area keeps progressing, it's becoming clear that AI/ML isn't just an extra tool; it's changing the whole way we approach pharmaceutical research.

They use fancy algorithms, like KronRLS and SimBoost, which help understand the tricky relationships between drugs and their targets. Also, they're bringing in things like convolutional neural networks (CNN) and gradient boosting decision trees (GBDT) to make better predictions in drug discovery. This shows that there's a real effort to make these models better for finding effective drugs.

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