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A Review: Role of Artificial Intelligence in Drug Research and Development

A.Divya[1], A.Revathi[2], B.Charu Hasini[3], B.Gowry Snehitha[4], K.Aaradhana[5], Dr.I.V.Ramarao[6]
NRI College of Pharmacy, Agiripalli Via Nunna, Vijayawada

Abstract-The pharmaceutical business is not an exception to how quickly artificial intelligence (AI) application is changing numerous sectors of the economy. From medication development through medicine administration, AI is rapidly being utilised to automate, optimise, and personalise many elements of the pharmaceutical sector. Machine learning and artificial intelligence are now advancing significantly. It has considerably increased quality of life while reducing human effort. Machine learning and artificial intelligence are now advancing significantly. It has considerably increased quality of life while reducing the workload for the human. This article explains how machine learning and artificial intelligence are being used to improve medication research and production. This article explains how artificial intelligence and machine learning are used to speed up and improve medication discovery and development: The screening, diagnosis, prognosis, survival estimation, and treatment of cancer as well as control measures remain significant public health issues and the world's top cause of death. The development of artificial intelligence (AI) and machine learning (ML) techniques, as well as their applications in a variety of sectors, have had a significant positive impact on cancer control. The field of medical devices has been interested in artificial intelligence (AI). In the past, formulators often used statistical formulations, depending on response surfaces to offer an optimisation process. We'll talk about the difficulties, advantages, and potential applications of neural computing. AI is a flexible tool with several algorithms that may be used in many situations. Among the most popular ways of administration are solid dosage forms, which include tablets, capsules, powder, granules, etc. Recently, AI has been acknowledged as a cutting-edge technique for developing pharmaceutical formulations that is attracting a lot of interest.

INTRODUCTION

The traditional pharmaceutical system is primarily reliant on manual tasks and human judgement, which can result in inefficiencies, mistakes, and delays. For instance, there are multiple manual procedures involved in filling a prescription, such as reading the prescription, giving the medication, and checking the dosage and frequency (1-3). The traditional pharmacy system has been successful in giving patients the necessary medications, but it has limitations due to its manual procedures and lack of customization. These drawbacks can be overcome by the introduction of AI-powered solutions like AI, which will improve patient outcomes by increasing the pharmacy system's effectiveness, accuracy, and personalization (4-7). The application of AI in pharmacy apps has enormous ramifications for consumers who use them at home and offers a number of benefits. Users may access medical advice, drug information, and instructions on dosage and usage from the comfort of their homes thanks to AI integration in pharmacy apps. For those living in rural areas or with mobility challenges, in particular, this can be helpful. Although AI has the potential to significantly improve the pharmacy system, there are some restrictions that must be taken into account. A human chemist can add empathy and a personal touch that an AI system might be unable to. This might be crucial in delicate circumstances where patients need emotional support.

AI's suggestions and counsel are only as reliable as the data it is given. The recommendations may be erroneous or incomplete if the data is inaccurate, lacking, or biassed. AI's ability to grasp language is dependent on the training data it has been given, therefore it might not be able to comprehend regional dialects, slang, or other linguistic nuances. Pharmacists can make educated decisions about whether or not to use AI in their practise by being aware of both its benefits and drawbacks. They can carefully weigh the possible advantages of AI, like increased productivity and a decreased risk of prescription errors, against its drawbacks, such the potential loss of human interaction and privacy-related ethical concerns. Pharmacists must carefully balance the benefits and drawbacks of AI and use it as a tool to supplement their knowledge, which will eventually improve patient outcomes.

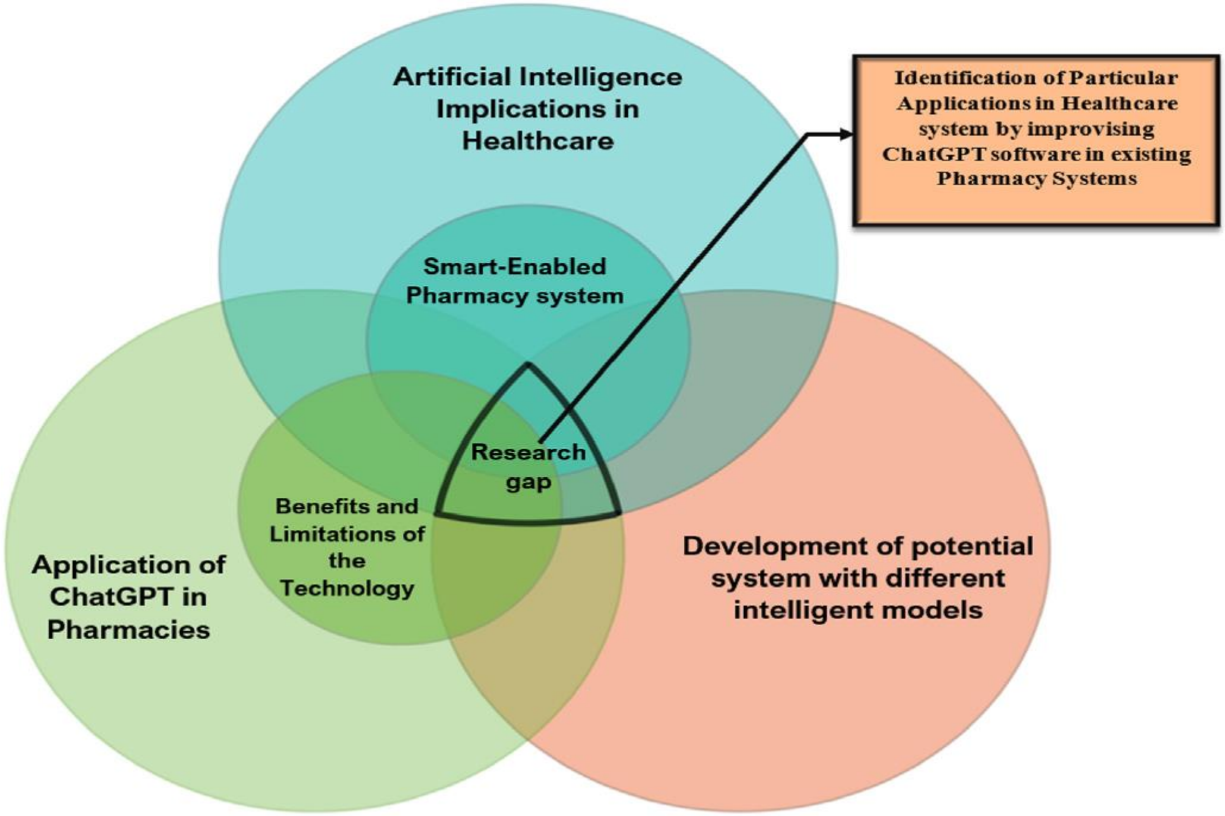


Fig. 1: illustrates the gaps in the research and obstacles for smart

The usage of a brand-new, sparsely investigated AI-powered pharmacy system is explored in the current research, which makes it novel.

The technology uses machine learning algorithms to process a variety of patient data, including genetic and medical history, to produce individualised treatment regimens. The application of AI in pharmacy shows potential, however as shown in Fig. 1, there are still a number of research gaps that need to be filled. These include the usability of the technology for both patients and chemists, long-term effects like the effect on medication adherence, ethical considerations like data privacy and potential biases, technical difficulties like data integration and system maintenance, and patient satisfaction with the technology. Researchers can better comprehend the effects of utilising AI in the pharmacy system by filling up these knowledge gaps, and they can create solutions that maximise its advantages and minimise its drawbacks while assuring ethical use. The potential for AI to completely transform the pharmacy system makes a study on the topic novel. While there have been prior research on the use of AI in healthcare, AI is a cutting-edge AI system that can respond to natural language inputs with human-like responses, enabling patients to engage in conversational interaction.

NECESSITY OF AI IN PHARMACY SYSTEM

The use of AI in pharmacy systems is gaining popularity, but it's vital to remember that any implementation of this technology should be well thought out and planned. While AI has the ability to completely transform the business by offering patients personalised medication management and round-the-clock support, it is crucial to use it responsibly and to address any potential obstacles and constraints. The integration of AI into the pharmacy system has the potential to improve the world in a number of ways. First off, by offering patients individualised medication management and round-the-clock support, it can enhance access to healthcare services [8,9]. As a

result, patients may be able to better manage their prescription regimens and cut back on the number of times they need to see a doctor. This can be especially helpful in places with scarce or inaccessible healthcare facilities. The growing population will benefit from the implementation of AI in
the pharmacy system as it can help address the increasing demand forhealthcare services. With personalized medication management and 24/7 support, AI can help patients manage their medications more effectively,reducing the need for frequent visits to healthcare providers. Thiscan the burden on the healthcare system and improve access patients.

The pharmaceutical system's AI research goals could include the following.

RO-1: To evaluate the viability of implementing AI in the pharmacy system to provide patients with 24/7 support and individualized medication management.

RO-2: To assess how AI affects patient outcomes such hospitalizations, drug responses, and general health condition, as well as medication adherence.

RO-3: To pinpoint any ethical issues that could arise from the application of AI in the pharmaceutical system, such as data privacy concerns and potential biases.

Data integration and system maintenance are two examples of technical difficulties that need to be identified and solved in RO-4.

RO-5: To evaluate the AI's usability for both patients and pharmacists and to pinpoint areas that need development.

RO-6: To assess the financial viability of AI in the pharmacy system and to compare

Although the use of AI in pharmacy systems is gaining popularity, it is crucial to remember that its deployment needs to be well thought out and planned. While tailored medicine management and round-the-clock patient support could change the business, it is crucial to make sure that AI is utilized ethically and that any possible issues are resolved.

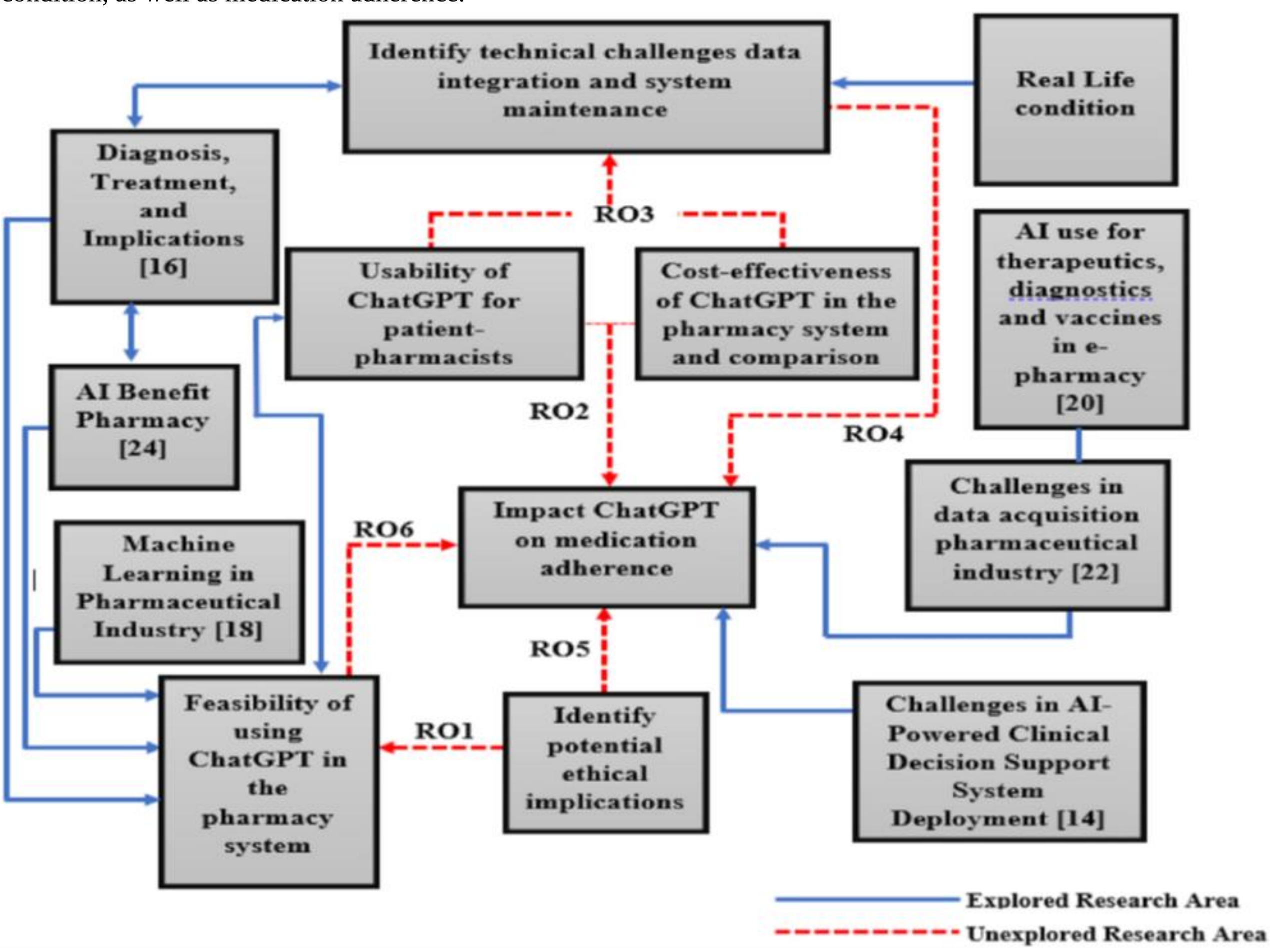
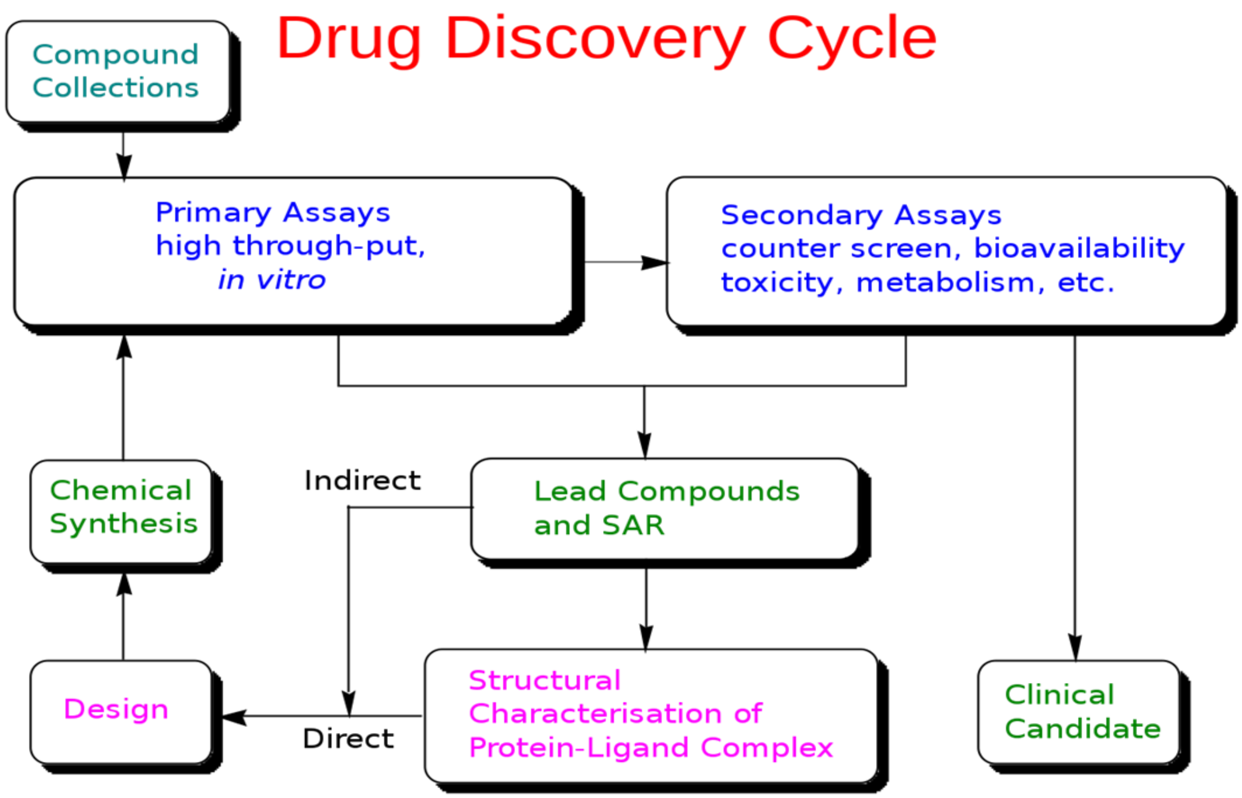


Fig. 2 shows the intelligent pharmacy system's focus areas and the associated research goals.

PROCESSING OF DRUG DEVELOPMENT

The feedback-driven drug development process begins with results already gathered from a variety of sources, including high-throughput compound and fragment screening, computer modeling, and information found in the literature. In this method, induction and deduction are alternated. Ultimately, this inductive-deductive cycle produces optimized hit and lead compounds. By automating some steps in the cycle, randomness and errors are reduced, increasing the effectiveness of medication development. For in silico compound synthesis and virtual screening models that serve as substitutes for biochemical and biological testing of efficacy and toxicity, de novo design procedures call upon an understanding of organic chemistry [10].Hit expansion is carried out by medicinal chemists utilizing tried-and-true organic chemistry methods. Chemists concentrate on a particular reaction or collection of reactions to swiftly assemble building blocks to produce a succession of analogues in order to boost the synthetic throughput.



A molecule with a reactive functional group and atoms that engage the active site of a biological target is referred to as a "building block." The biological target's active site is a particular area where the substance (or substrate) binds with interaction forces.[11,12].. The better than Beatles factor provides an analogy to convey the implausible idea of creating a novel treatment with pharmacological activity superior to any of the currently approved drugs for a specific ailment. The challenges described here pertain to what will happen to any new medication that has a more effective therapeutic impact. The stakes increase with each new medicine, and here is where R&D inefficiency occurs because it is harder and harder to get past the ever-rising barriers. The risk tolerance for new pharmaceuticals is being gradually reduced, and a guide for drugs with safer profiles is being developed. While this is good for consumers, it significantly raises R&D costs. The throw money at it tendency then follows, when R&D facilities boost their hiring of personnel and other resources in the expectation of receiving a strong return on investment by being the first to market a new drug. The increase in R&D costs as well as high attrition rates in the development process of a new drug pose challenges to the pharmaceutical industry. The underlying causes and possible measures to reduce attrition rates have previously been reviewed [13,14]. In Phase IIb and Phase III clinical trials, over 62% of novel chemical entities (NCEs) fail to enter the clinic. Clinical safety and efficacy are the primary underlying causes of attrition in late clinical phases, followed by formulation, pharmacokinetics and bioavailability, and toxicity. Due to the abundance of available treatments for a certain condition, there is a lower chance that a new follow-up therapy will become a blockbuster drug, which lowers the return on R&D expenditure.

A further contributing cause for a drop in the return on R&D investments is the prolonged approval cycle brought on by the FDA's strict approval standards. The scientific literature, which shows that different therapeutic areas have variable success rates, suggests that these criteria are not universal. A chemical substance called a lead has the potential to be developed into a novel medicine that might be used to treat a condition. The abundance of available treatments for a given condition lowers the return on R&D investment and lowers the likelihood that a new follow-up drug will become a blockbuster medication. Compounds with novel mechanisms of action attrit more quickly than those with established mechanisms of action. As a way to balance the overall success and lower attrition rates, pharmaceutical companies can average out the many treatment areas with differing success rates.

USE OF AI IN THE MEDICATION DEVELOPMENT

The tasks of finding successful new drugs is daunting and predominantly the most difficult part of drug development. This is caused by the vast size of what is known as chemical space, which is estimated to be in the order of 1060 molecules [15]. The technologies that incorporate AI have become versatile tools that can be applied ubiquitously in various stages of drug development, such as identification and validation of drug targets, designing of new drugs, drug repurposing, improving the R&D efficiency, aggregating and analysing biomedicine information and refining the decision-making process to recruit patients for clinical trials [16-18]DL has exhibited exceptional success in suggesting powerful medication ideas and correctly predicting their characteristics and potential toxicity hazards. Using AI methodologies, it is now possible to avoid previous issues in drug development, such as analysis of enormous datasets, arduous compound screening while minimizing standard error, and needing large amounts of R&D cost and time of over US$2.5 billion and a more than a decade.

AI IN ROUTE UNDERSTANDING OR MOLECULAR TARGET DISCOVERY

AI has revolutionized the approaches of disease target or pathway identification in medication development. This was made achievable by using genetic data, biochemical characteristics, and target tractability Using a platform made out of gene-disease association data, 'Open Targets' is a computer prediction tool that was used in one study to test the plausibility of predicting therapeutic targets. By reducing the quantity of synthesized compounds that are later examined in in vitro or in vivo systems, AI systems can lower attrition rates and R&D costs.

AI IN LEAD OR HIT DETECTION

The data on small-molecule modulator probes or their structural biology can be employed with a range of in silico strategies for profile selection, such as virtual ligand or structure-based design approaches. By reducing the quantity of synthesized compounds that are later examined in in vitro or in vivo systems, AI systems can lower attrition rates and R&D costs. The data on small-molecule modulator probes or their structural biology can be employed with a range of in silico strategies for profile selection, such as virtub.al ligand or structure-based design approaches.[19,20]

SYNTHESIZING DRUGS WITH ARTIFICIAL INTELLIGENCE

Molecules that conform to Lipinski's rule of five are those that are drug-like: 500 Da for the molecular weight, 5 for H-bond donors, 10 for H-bond acceptors, and 5 for the computed Log P (cLogP) value. Chemists frequently employ retrosynthesis for the synthesis of drug-like compounds. The target compounds are recursively analyzed as the initial step in the retrosynthetic technique, after which they are successively broken down into smaller fragments or attainable building components. Finding the processes that will transform these pieces into the desired chemicals is the second stage.

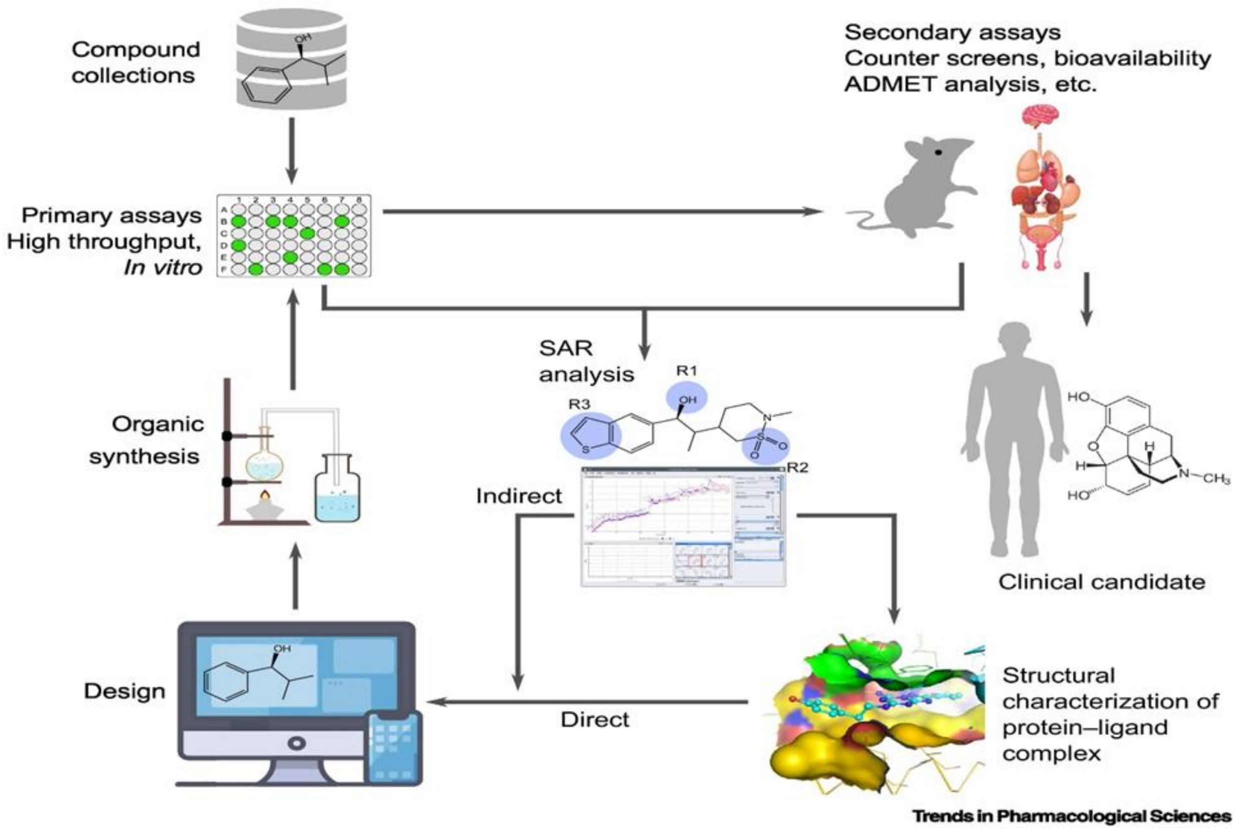


Fig.3. Synthesizing drugs with AI[21]

The second stage is the most difficult since it is difficult for the human brain to sort through the enormous number of pertinent organic reactions that are available in the literature in order to select the most likely response. For the synthesis of the target molecules, this platform may filter out the most promising building blocks and choose only well-known reactions. It has been demonstrated that the platform, 3NMCTS, is significantly quicker and more effective than conventional computer-assisted retrosynthesis techniques. In a decent amount of time, the platform was able to provide workable synthesis paths without needless steps. Interrogating the relationship between human-relevant biomarkers and in vitro phenotypes affords a more predictable, quantifiable assessment of the uncertainty of therapeutic responses in a specific patient. The development of AI approaches to identify and predict human-relevant biomarkers of disease allows the recruitment of a specific patient population in Phase II and III clinical trials. The AI predictive modelling in selection of a patient population would increase the success rate in clinical trials [22,23].

AI FOR CLINICAL TRIAL POPULATION SELECTION

A perfect AI tool for clinical trials assistance should be able to recognize the condition in patients, identify the gene targets, and forecast the effects of the intended drug as well as any off-target consequences. A novel AI platform called AiCure was also developed as a mobile application to measure medication adherence in a Phase II trial of subjects suffering from schizophrenia, where it was reported that AiCure increased adherence 25% compared with the traditional 'modified directly observed therapy[24]. A clinical trial's patient selection procedure is an essential step. Examining the connection between in vitro phenotypes and human-relevant indicators enables a more quantified, predictable assessment of the uncertainty of therapy responses in a given patient. The recruitment of a particular patient group in Phase II and III clinical trials is made possible by the development of AI techniques to detect and forecast human-relevant illness biomarkers. The success rate of clinical trials would increase with the use of AI predictive modeling in patient population selection

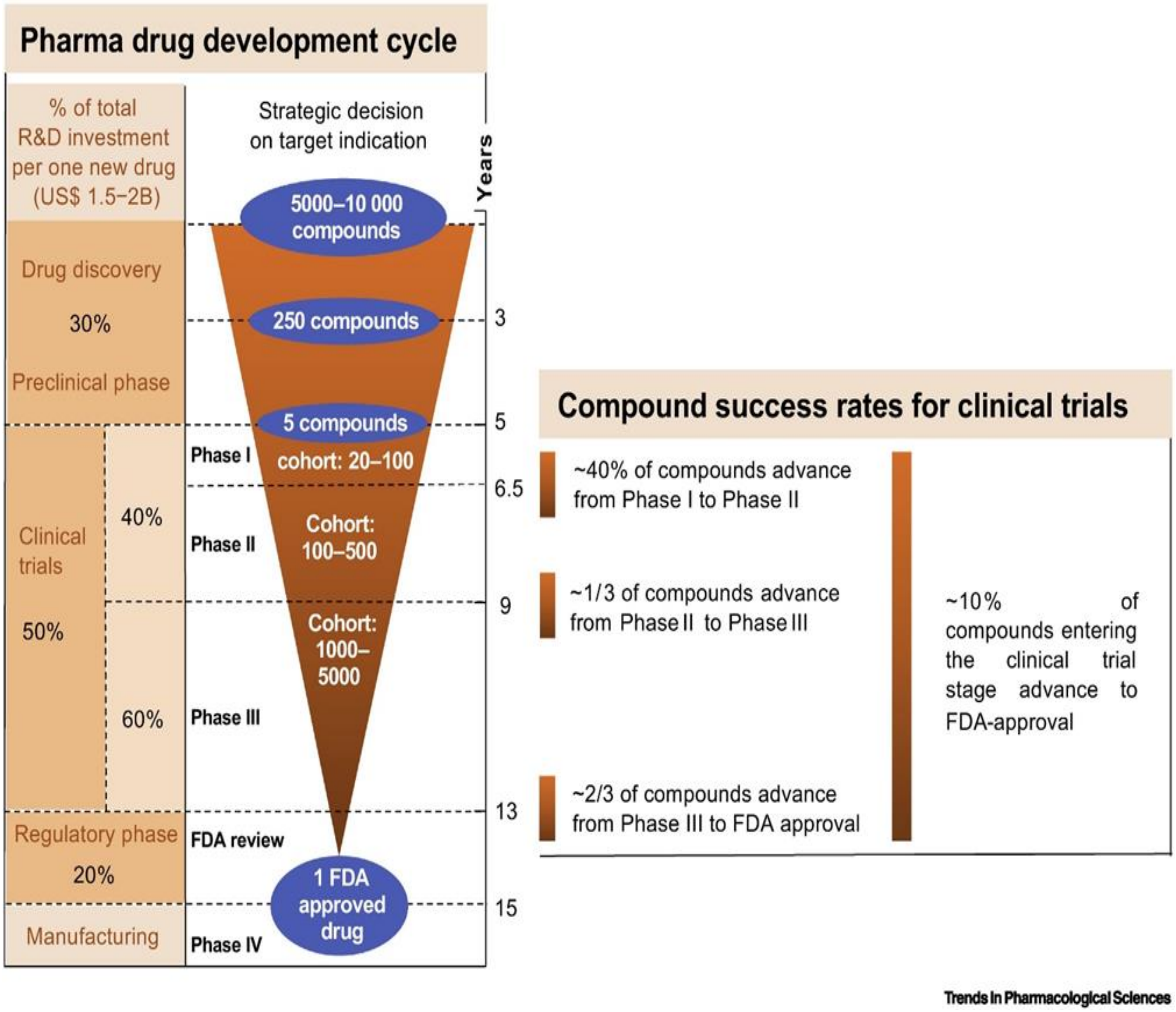


Fig.4.AI for clinical trial population selection[25]

REPURPOSING DRUGS WITH AI

With AI, the drug repurposing process becomes more attractive and pragmatic. The concept of applying an existing therapeutic to a new disease is advantageous because the new drug is qualified go directly to Phase II trials for a different indication without having to pass through Phase I clinical trials and toxicology testing again [26,27].Thus, this platform can perform remarkable tasks beyond analysing data, such as imagining or creating new data modelled on real data. Essentially, the GAN technique is an adversarial game between two DNNs where, principally, one DNN evalu- ates the output of the other iteratively and, in that adversarial game, the two networks learn how to generate more perfect molecules [28,29].A new business model is therefore required, and AI presents such a chance. These partnerships show the value of AI technology in enabling us to explore a much larger design space and find uncommon compounds with features that go beyond what would be found using only traditional HTS.

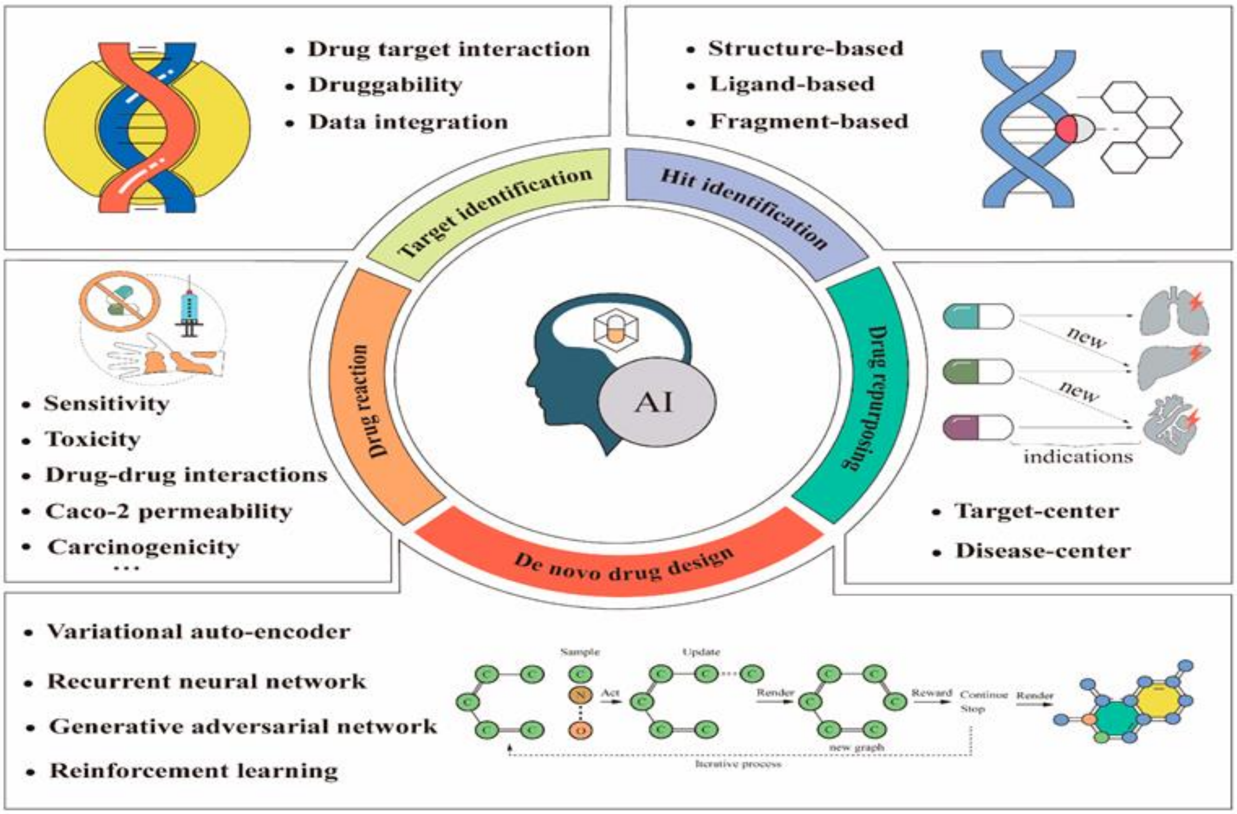


Fig 5.Repurposing drugs with AI[30]

PARTNERSHIPS BETWEEN PHARMACEUTICAL BUSINESS AND AI COMPIAN

companies with the rapid introduction of AI in healthcare, especially in the years It is thought that the resulting graphs, which include extremely intricate interactions, can reveal information or point out new connections or knowledge gaps that can lead to new theories. AI utilizes the disease-agonistic method, which allows for the impartial views of scientific facts that lead to unbiased hypotheses, in contrast to human intervention where bias is present and have joint ventures with AI companies in the hopes of developing better healthcare tools. These include the improvements in diagnostics or biomarkers and the identification of drug targets and designing new drugs. The analyses of these underlying data combined with ML or DL are then put into algorithms, making a significant contribution to current, progressive healthcare that uses AI. As a result, significant global partnerships between the pharmaceutical and artificial intelligence industries have recently been created The UK's 100,000 Genomes Project, a global initiative in partnership with Roche, Berg, Merck, and Biogen, uses data and AI from NHS patients with rare disorders. It utilises the strategy of text mining to analyse the available patents and other genetics and biological information to extrapolate the relation-ships between those entities to create highly informative graphs consisting of dynamic maps with over one billion relationships. In contrast to human intervention, where bias is inherent, AI employs the disease-agonistic approach, allowing for impartial interpretations of scientific data that result in unbiased hypotheses[31].

APPLICATIONS

1 Drug Discovery Process and Design

➢ The use of AI in the pharmaceutical industry for the design and development of drugs is increasing. From making small molecules to determining novel biological targets, AI plays a prominent role in drug target identification and validation. It is widely used for multi-target drug innovation and biomarker identification in an efficient way with great accuracy.

- For example, researchers in pharmaceutical can identify and verify novel cancer drugs using data such as longitudinal EMR records (Electronic Medical Records) and other omic data. The AI systems using ML and other data analytics algorithms will extract insights from EMR data and creates the best formulations to design and develop drugs that cure tumors well.[32].

2 R&D

- Pharma companies across the globe are using advanced AI-powered tools and ML algorithms to smoothen the drug research, development, and innovation process. These technology tools are designed to detect complex patterns in large datasets. Therefore, AI in pharma industry can be used to resolve problems associated with the research and development process.
- This ability to study patterns of various diseases and to determine which composite formulations are best suited for the treatment of specific symptoms of a particular disease is excellent. Pharma industries can invest in the R&D of such drugs that are more likely to treat a disease or medical condition successfully.[32]

3 Disease Prevention

- Pharmaceutical organizations can use Artificial intelligence to develop medicines Parkinson's and Alzheimer's and very rare diseases.
- As per Global Genes, it is a fact that almost 95% of rare diseases do not have more drugs to treat and cure faster. However, thanks to the innovative capabilities of AI and ML. The use of AI in the pharmaceutical industry will completely transform this scenario and ensure the most-advanced models for detecting hazardous diseases in the early stage and improve patient outcomes.[32]

4 Next-Level Diagnosis

- Physicians can use advanced machine learning systems to gather, process, and analyze patient health care data. Healthcare professionals across the globe are using deep learning and ML to securely store patient data in the centralized storage system or cloud. It is called Electronic Medical Records (EMR).
- Physicians may refer to these health records when they need to understand the effect of a specific genetic trait on a patient's health or how medicine treats it. Machine Learning systems can use data stored in EMRs to generate real-time estimates for diagnostic purposes and to indicate appropriate treatment for the patient.[32]

5 Epidemic Prediction

- Pharma companies and healthcare industries are using ML and AI technologies to monitor and assess the spread of infections worldwide. These modern technologies are used for consuming data collected from various resources, analyzing several environmental, biological, and geographical factors on the population health of diverse geographical regions, and deriving data insights to reduce the impact of epidemics in the future.
- Artificial intelligence and machine learning models are particularly beneficial for underdeveloped economies that lack medical infrastructure and financial framework to combat the spread of infection.[32]

6 Identifying Clinical Trials

- It is one of the key pharmaceutical use cases for embracing AI into existing models. The use of AI in the pharmaceutical industry for identifying drug candidates which are under final clinical trials from vast clinical data is on the rise.

AI in Pharmaceutical Industry will help companies in analyzing thousands of samples in minutes and automatically logs data related to how patients are responding during clinical trials.

Here are a few advantages of using AI in pharma industry for clinical trials:

- AI applications or systems analyze historic clinical data
- AI apps help in monitoring drug performance and evaluating drug responses
- With the integration of speech recognition technologies, AI apps for pharma will be helpful for recording patients' oral text during drug trial phases. It means that AI applications will record patients' responses.[32]

7 Drug Adherences and Dosage

- The adoption of AI in Pharmaceuticals and Healthcare is increasing at a rapid pace for identifying the right amount of drug intake to ensure the safety of drug consumers. AI technology will monitor patients during clinical trials and suggest the right amount of dosage at regular intervals.
- These AI trends & use cases in pharma will assist drug development and healthcare companies in ensuring efficacy across end-to-end production lines and delivering top-notch performance in front of the FDA.[32]

CONCLUSION

Currently, there are no developed drugs that have utilised AI approaches but, based on the advances described in this review, it is likely that it will take a further 2–3 years for a drug to be developed. Interestingly, experts strongly believe that AI will permanently change the pharmaceutical industry and the way drugs are discovered. However, for an individual to be efficient in drug development using AI, the individual should know how to train algorithms, requiring domain expertise. More significantly, we grouped various pharmacological formulations and listed the AI prediction models that may be used to predict them in the published literature. A few studies conducted experimental validations prospectively, whereas the majority of recent studies used retrospective experimental validation. We therefore think that the pharmaceutical research community faces both a challenge and an opportunity in extending the utility of AI in pharmaceutical solid dose formulations.

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