Review Article

Artificial Intelligence in Pharmacy

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ABSTRACT

Artificial Intelligence (AI) focuses in producing intelligent modelling, which helps in imagining knowledge, cracking problems and decision making. Artificial intelligence (AI) is changing the world we live in, and it has the potential to transform struggling healthcare systems with new efficiencies, new therapies, new diagnostics, and new economies. Artificial intelligence (AI) is rapidly transforming the field of pharmacy by improving the efficiency and accuracy of drug development, patient care, and medication management. This review article explores the various applications of AI in pharmacy, including drug discovery, personalized medicine, clinical decision-making, and pharmacy operations. AI algorithms can analyze vast amounts of medical data to identify potential drug targets and optimize drug design. Additionally, AI-powered diagnostic tools can help pharmacists make more informed treatment decisions based on patient data, medical history, and drug interactions. AI is also being used to optimize pharmacy operations, such as inventory management and medication adherence. Despite its many benefits, the integration of AI in pharmacy also poses challenges related to data privacy, ethical considerations, and regulatory compliance. This article concludes by discussing these challenges and outlining potential solutions to overcome them. Overall, AI has the potential to revolutionize the field of pharmacy and improve patient outcomes by enabling more precise, personalized, and efficient medication management.

Keywords: Artificial Intelligence, intelligent modelling, drug design.

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INTRODUCTION

Every aspect of life is constantly subject to change, and one of the main aims of humans is to control these changes for our benefit; this is especially true in the field of medicine and pharmaceuticals. These disciplines focus on the creation or discovery of chemical compounds and mixtures and their use to ease physical and psychological suffering. The drug and biopharmaceutical industries have been limited source of inventive and novel technologies or machinery, and have led the development of novel principles or interpretations in general chemical and mechanical engineering. The pharmaceutical industry is in critical need of mechanical innovation, easing the creation of medications for human use. Creating and manufacturing complex processes medications that are safe for humans on a commercial scale, and incorporating them into main stream therapeutic use, has been challenging, owing to existing limitations on technological resources. [1]

There are opportunities for AI to explore further in the field of pharmaceutical and healthcare research because of its ability to investigate enormous data from various modalities[2]. Artificial intelligence (AI), first described in 1955, is a combination of various intelligent processes and behavior, developed by computational models, algorithms or a set of rules which supports the machine to mimic the cognitive functions of humans such as learning, problem-solving, etc. [3-4]

The field of pharmacy has undergone numerous transformations over the years, with technological advancements being one of the primary drivers of these changes. Artificial intelligence (AI) is one such technology that has gained significant attention in recent years due to its potential to revolutionize the pharmaceutical industry.

AI technology is exercised to perform more accurate analyses as well as to attain useful interpretation. [5]

Artificial intelligence is a debatable subject because it involves topics like brain architecture and human intelligence, which we humans are oblivious to yet**.** Artificial intelligence is commonly used in computer systems using programs with proper computer hardware. [6]

The use of AI is increasing, and is likely to change how clinical examination and training is carried out. Doctors can participate in the development of this technology for use in the medical and pharmaceutical industries; this will ensure that the potential of AI to significantly improve medical care is fulfilled. [7]

Almost all advancements in the applications of AI technology are being celebrated on account of the confidence, which enormously contributes its efficacy to the industry. Recently, AI technology becomes a very

fundamental part of industry for the useful applications in many technical and research fields. The emergent initiative of accepting the applications of AI technology in pharmacy including drug discovery, drug delivery formulation development and other healthcare applications have already been shifted from hype to hope. [8-9]

AI in healthcare is already a reality. Healthcare providers are starting to embed the technology into their workflows and the decision-making processes at all stages of healthcare, bringing improvements for patients, providers, payers, and other healthcare stakeholders, as well as society at large. The benefits range from new treatment opportunities – such as in detecting suspicious lesions that may have otherwise been overlooked – to back-office areas such as claims management and instrument maintenance programs. [10]

AI can also help streamline pharmacy operations. For example, AI can be used to optimize inventory management, predict drug shortages, and automate medication dispensing. This can free up pharmacists to focus on patient care, ultimately improving patient outcomes.

Devices based on AI are bringing new sophistication to image analysis. Deep learning algorithms are currently used in mammography for breast cancer detection, in CT for colon cancer diagnosis, in chest radiographs for the detection of pulmonary nodules, in MRI for brain tumour segmentation and for the diagnosis of neurologic disorders, such as Alzheimer's disease. Algorithms can help dermatologists make better diagnoses, for example detecting 95% of skin cancers by learning from large sets of medical images. [11]

AI in pharma refers to use of automated algorithms to perform tasks which traditionally rely on human intelligence. Over the last five years the use of AI in pharma and biotech industries have redefined how scientists develop new drugs, tackle disease and more [12-13]. When AI solutions remotely assess a patient's symptoms and deliver alerts to clinicians only when patient care is needed, it reduces unnecessary hospital visits. It can also lessen the burden on medical professionals. AI can save 20% of nurses' time by averting unnecessary visits.

Innovative solutions making use of digital technologies can provide support for reforms in the organisation of healthcare and long-term care systems. The European Commission speaks of how "artificial intelligence and supercomputing offer new opportunities to transform healthcare systems"

The U.S. excels in technology and innovation, but continually lags far behind other countries in healthcare data access, transparency, organization, management, and analysis. Our healthcare organizational and programmatic imperatives in this current era should embrace **big data** and **data analytics/artificial intelligence** expertise to harvest meaningful medical data and its hidden information to the fullest extent in order to improve quality and outcome [14]. It is helping save lives by allowing emergency services to diagnose cardiac arrests or other conditions based on the sound of a caller's voice and AI is helping radiologists detect tumours more accurately by instantly comparing X-rays with a large amount of other medical data. Large-scale analysis of patient-reported symptoms or biometrics can suggest potential diagnoses and next steps for patients [15].

AI solutions have been developed that work with multiple data types, including patient-reported symptoms, biometric and biosensor data, imaging, and biomarker data, right through the patient care pathway from initial triage to monitoring of ongoing treatment. Sensors can detect symptoms at early stages and predict a potential health incident ahead of time, permitting preventive measures.

The AI technologies in the drug development, patient care and medication management include machine learning (ML), natural language processing (NLP), physical robots, robotic process automation, etc [16].

In ML, neural network models and deep learning with various features are being applied in imaging data to identify clinically significant elements at the early stages, especially in cancer-related diagnoses [17-18].

NLP uses computational techniques to comprehend human speech and derive its meaning. Lately, ML techniques are being widely incorporated in NLP for exploring unstructured data in the database and records in the form of doctors' notes, lab reports, etc. by mapping the essential information from various imagery and textual data which helps in decision making in diagnosis and treatment options [19].

The Food and Drug Administration (FDA) considers AI/ML-based software as a medical device. FDA would expect the AI innovators to comply with requirements of clinical, analytical, and technical validation, quality systems, good machine learning practice, assurance of safety and effectiveness, transparency, and real-world performance monitoring. Any new AI technology, which proposes to improve the efficiency of clinical trial design and conduct, should be validated by testing alongside the existing technology it claims to complement or substitute[20].

AI offers the promise of transforming crucial steps of clinical trial conduct-study design, planning, and execution. ML, DL, NLP, and OCR can be used for linking big and diverse datasets such as electronic medical records (EMRs), published medical literature, and clinical trial databases to improve recruitment by matching patient characteristics to selection criteria [21].

AI can increase the speed of data analysis and accuracy of decision-making in the medical area [22].

Figure 1: Artificial intelligence in pharmacy

AI IN PERSONALIZED MEDICINE

It is always a surprising problem seeing a drug work for some people and be less effective on others, or causing side effects in another. Another problem is the question of why some people develop some diseases e.g. cancers, while others do not. Genetic make-up and other differential factors such as age; lifestyle could be reasons for these problems.

Personalized medicine for treating diseases considers various factors, which can be referred to the genome of individuals, lifestyle, environmental factors, and characteristics of patients [23].

Personalized medicine as a branch or extension of Medical Sciences uses practice and medical decisions to deliver customized healthcare service to patients[24].

This includes their genetic makeup, lifestyle factors, and environmental influences. By taking a personalized approach to medicine, healthcare professionals can provide more effective treatments, reduce the risk of adverse reactions, and improve patient outcomes.

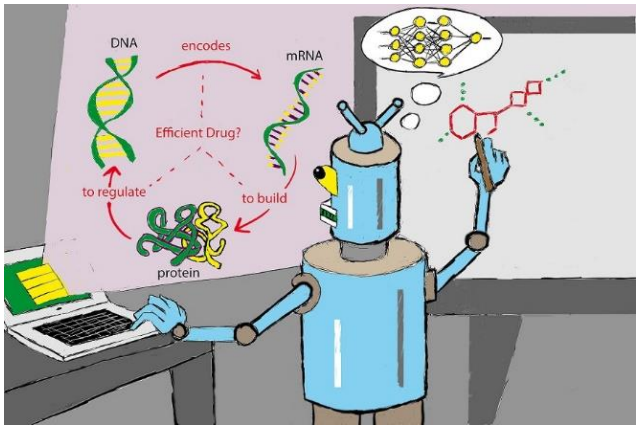


Figure 2: Artificial intelligence in personalized medicine

It is opposed to a one-size-fits-all approach, in which disease treatment and prevention techniques are advanced for the average individual with much less attention for the variations among individuals

Artificial Intelligence has been successfully able to classify problems using different algorithms and solve precision medicine problems e.g. accurate disease diagnosis, disease detection and prediction, treatment optimization.

It can further be used to predict the risk of a disease, identification of the disease response and outcomes on the individual patients based on their own characteristics.

Personalized medicine is an approach to healthcare that tailors medical treatment to the individual characteristics of each patient. AI algorithms can analyse genetic, imaging, and other data to identify potential biomarkers or treatment options that are tailored to individual patients.

AI can generate insights from genetic information, biomarkers, and other physiological data to predict how a patient will respond to different treatment options, which may help avoid adverse reactions, reduce the use of expensive or unnecessary treatments on patients that are unlikely to respond, and ultimately reduce hospitalisation and outpatient costs.

The human genome contains more than three billion base pairs, and analysing this data can be incredibly time-consuming and complex, with the help of AI, healthcare professionals can analyse vast amount of genomic data quickly and accurately, identifying genetic variations that may be linked to specific diseases or conditions.

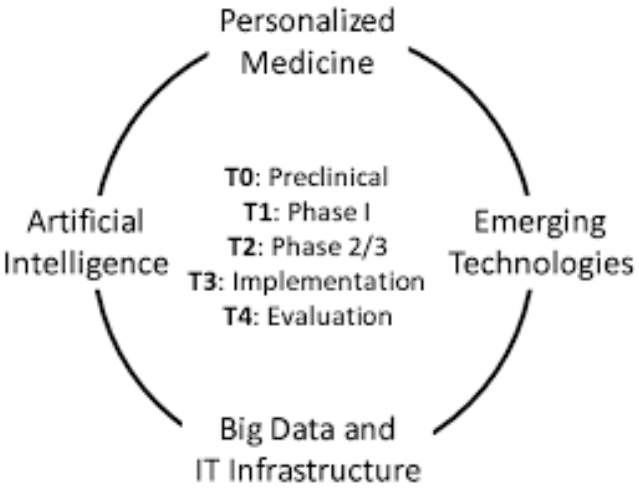
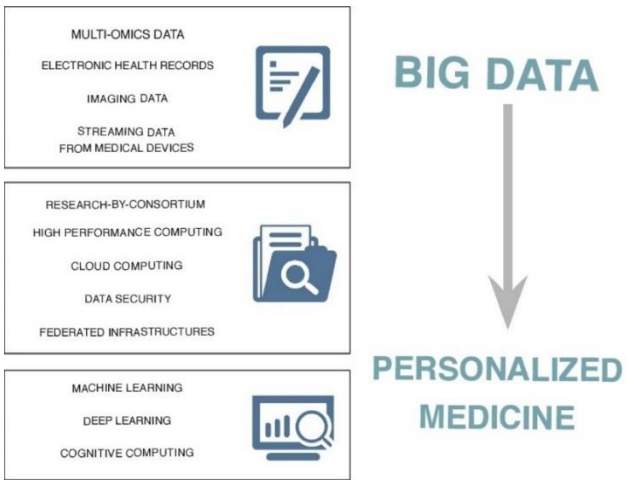


Figure 3: Actual practice of personalized medicine

The actual practice of personalized medicine can be seen as involving an analogous process to the develop of drugs and health devices. Thus, P0 activity involves making a diagnosis or determining an individual's risk of diseases; P1 activity involves identifying the key pathophysiologic processes, if not known, that are causing (or likely to cause) a disease that might be amenable to modulation by an appropriate intervention; P2 considers the identification of an appropriate intervention given what was identified in the P0 and P1 stages; P3 involves testing the intervention on the relevant individual undergoing the diagnosis and pathobiology assessment; and P4 involves warehousing the result in appropriate databases so that the insights and information obtained on a patient can be exploited in examinations of further patients or used in broader data mining initiatives to find further clinically-meaningful patterns[25].

The use of Artificial Intelligence techniques in setting up or building personalized medicine is important in terms of precision and accuracy of disease discovery, treatment, and drug administration. The control of adverse drug reactions and enzymes metabolism which results in some people having issues eliminating drugs from their bodies, hence leading to overdose; while others eliminate the drug from the body before it gets the chance to work[26].

Research associated with each of these themes is often pursued independently of the others because of the very specialized expertise required. For example, there are scientific journals devoted to Personal Medicine (e.g., 'Personalized Medicine,' 'Journal of Personalized Medicine'), emerging assays (e.g., 'Nature Biotechnology,' 'Nature Digital Medicine'), big data (e.g., 'Big Data,' 'Journal of Big Data,' 'Gigascience'), and artificial intelligence (e.g., 'IEEE Transactions on Neural Networks and Learning Systems,' 'IEEE Transactions on Pattern Analysis and Machine Intelligence') that publish very focused studies.



CHALLENGES:

AI algorithms require vast amount of patient data to learn and make accurate predictions, which means that data quality and accessibility are critical. There is also a need for greater transparency in how AI systems make decisions, to AI-generated insights.

One of the significant challenges of AI in personalized medicine is the need of high-quality data. Personalized medicine requires access to large amounts of patient data, including medical histories, genetic information, and lifestyle factors. Ensuring that data is accurate, complete, and secure is essential for the success of AI in personalized medicine. Privacy concerns also need to be addressed to protect patient data while still allowing AI systems to access the necessary information.

AI IN DRUG DISCOVERY:

Artificial intelligence (AI) is revolutionizing the drug discovery process, enabling researchers to develop new drugs faster, more efficiently, and with greater precision.

The use of AI in drug discovery is transforming the pharmaceutical industry, providing a range of benefits that could lead to the development of more effective drugs and improved patient outcomes.

The traditional process of drug discovery involves years of research and experimentation, with a low success rate and high costs. the entire process for one approved drug takes approximately 13.5 years, namely 5.5 years before clinical trials (drug discovery) and eight years for the remaining process (drug development) [27].

However, with the application of AI, the process can be accelerated, resulting in quicker development of new drugs that are safer, more effective, and affordable.

AI algorithms are trained on large datasets of molecular and biological data, allowing them to identify patterns and relationships that are not easily discernible to humans. AI can be used at every stage of drug discovery process, from identifying new drug targets to predicting the safety and efficacy of new compounds.

Popular applications of AI in drug discovery include virtual screening[28], de novo drug design[29], retro synthesis and reaction prediction[30], and de novo protein design[31], among others, which can be reduced to two categories, i.e., predictive and generative tasks.

With the help of AI, researchers can analyse vast amounts of data and make predictions about which molecules are most likely to succeed in clinical trials. AI is also helping researchers to identify new drug targets and to optimize the design of clinical trials.

Drug Discovery Process:

The drug discovery process is a complex and time-consuming process that involves the identification and validation of drug targets, the optimization of lead compounds, and the evaluation of drug efficacy and safety.

Traditionally, drug discovery has relied on trial and error, with researchers testing large numbers of compounds in the hopes of finding a viable drug candidate. However, this process can be slow and inefficient, and may potential drug candidates fail to progress beyond the preclinical stage.

AI can be used at various stages of drug discovery, from target identification to preclinical and clinical development.

AI in target identification:

Identifying new drug targets is a critical first step in drug discovery, which are biological pathways or molecules that are involved in a disease process. AI can be used to analyse large datasets of molecular and biological information, identifying new drug targets that were previously unknown or overlooked. Machine learning algorithms can learn from existing data to identify patterns and predict which targets are most likely to be successful.

AI in Lead Optimization:

Once a promising drug target has been identified, researchers need to design molecules that can interact with the target and produce a therapeutic effect. AI can help to optimize these molecules by predicting their properties and optimizing their structure. For example, machine learning algorithms can predict the solubility, stability, and bioavailability of a molecule based on its structure. They can also predict the likelihood of the molecule being toxic or producing unwanted side effects. This can save time and money by identifying promising leads early on and reducing the number of compounds that need to be synthesized and tested.

AI in clinical Trials:

AI can also play a significant role in optimizing clinical trials. By analysing patient data and identifying subgroups of patients who are most likely to benefit from a particular treatment, AI can researchers to design more efficient and effective clinical trials. This can reduce the time and costs associated with clinical trials and improve the chances of success. AI can also be used to identify potential safety concerns early on, allowing researchers to modify the trial design or stop the trial if necessary.

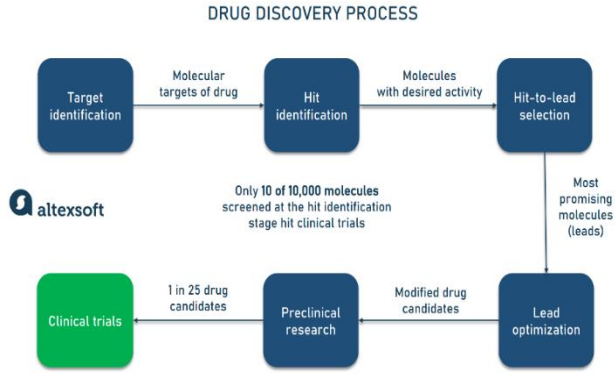


Figure 4: Key steps of drug discovery

CHALLENGES:

Despite the potential benefits of AI in drug discovery, there are also challenges that must be addressed. One of the primary challenges is the lack of standardization in data formats, which can hinder the integration of different data sources and limit the effectiveness of AI algorithms. Another challenge is the need for regulatory frameworks to ensure the safety and effectiveness of AI applications in drug discovery.

Additionally, the use of AI in drug discovery may raise ethical questions regarding the use of personal data and the potential consequences of AI generated drugs.

One of the main challenges is the need for high-quality data. AI algorithms rely on large datasets to make accurate predictions, and if the data is biased or of poor quality, the results may not be reliable.

RECENT RESEARCHES IN DRUG DISCOVERY USING AI:

1. In 2021, researchers from the university of California, San Francisco, used AI to identify potential new drugs for treating COVID-19. The researchers used a machine learning algorithm to screen over 1 billion compounds and identify those that could potentially inhibit the SARS-CoV-2 virus.
2. In 2020, researchers from the university of Cambridge used AI to design a new drug for treating kidney disease. The researchers used a deep learning algorithm to analyze the 3D structure of protein that is involved in the disease, and then used this information to design a molecule that could potentially bind to the protein and block its activity.
3. In 2019, researchers from the university of North Carolina at Chapel Hill used AI to design new antibiotics that could potentially combat antibiotic-resistant bacteria. The researchers used a machine learning algorithm to analyze the chemical structures of known antibiotics and identify common patterns, which they then used to design new antibiotics with different chemical structures.
4. In 2018, researchers from Stanford University used AI to predict the activity of potential drug candidates for cancer treatment. The researchers used deep learning algorithm to analyze the chemical structures of known cancer drugs and predict the activity of new compounds.
5. "Deep learning enables rapid identification of potent DDR1 kinase inhibitors" (Nature Communications, 2022) – This study used deep learning algorithms to identify potential inhibitors of the DDR1 kinase, a promising drug target for cancer treatment. The researchers screened a large library of compounds and used machine learning models to predict their binding affinity to the target, leading to the discovery of several potent DDR1 inhibitors.
6. "Deep learning-based virtual screening for novel mTOR inhibitors" (bioorganic chemistry,2021) – This study used deep learning models to screen a large library of compounds for potential inhibitors of the mTOR kinase, a key regulator of cell growth and proliferation. The researchers identified several promising compounds with high predicted binding affinity to the target, which were validated through in vitro assays.
7. "Artificial intelligence for drug discovery in Alzheimer`s disease" (Expert Opinion on Drug Discovery, 2021) – This review article discusses the potential of AI-based approaches for drug discovery in Alzheimer`s disease, a neurodegenerative disorder with no effective cure. The authors describe various AI techniques, such as deep learning and network analysis, and their applications in drug discovery,

including target identification, lead optimization, and repurposing of existing drugs.

8. "AI-assisted design of antiviral peptides targeting the SARS-CoV-2 spike protein" (Nature Communications,2020) – This study used AI-based algorithms to design and optimize short peptides that can inhibit the entry of the SARS-CoV-2 virus into the host cells by targeting the spike protein. The researchers used a combination of deep learning and molecular dynamics simulations to identify and refine the most promising peptides, which showed potent antiviral activity in cell-based assays.

9. "Deep Graph Convolutional Encoder-Decoder Network for de novo Drug Discovery" published in the journal of chemical information and Modelling in 2021. The study developed a novel deep learning framework that can generate new molecules with desired properties for drug discovery.

10. "Accelerating drug discovery for Alzheimer`s disease through an AI-powered platform" published in Nature Communications in 2021. The study developed an AI platform that can rapidly screen and predict potential drug candidates for Alzheimer`s disease, reducing the time and cost of drug discovery.

11. "Deep learning enables rapid identification of potent DDR1 kinase inhibitors" published in Nature Communications in 2020. The study used deep learning algorithms to predict the binding affinity of small molecules to DDR1 kinase, leading to the identification of potent and selective inhibitors that could be developed into new cancer drugs.

12. "Design of Anti-HER2 Antibody-Drug Conjugates by Optimizing Payload-Conjugation Sites with Machine learning" published in ACS Central Science in 2020. The study developed a machine learning model to predict the optimal sites for conjugating chemotherapy drugs to antibodies for targets cancer therapy.

WILL AI REPLACE SCIENTISTS?

No, AI will not replace scientists. While AI can certainly assist scientists in many ways, such as helping to analyse large datasets, simulate experiments, or automate certain tasks, it cannot replace the creativity, intuition, and judgement of human scientists. Science is a dynamic and complex field that involves not only data analysis and computation, but also hypothesis generation, experimental design, interpretation of results, and communication of findings. These are all skills that require human sight, critical thinking, and collaboration. Moreover, science is not just about finding answers to specific questions, but also about asking new questions, exploring new areas of research, and challenging established assumptions. AI can certainly contribute to these efforts, but it cannot replace the curiosity, imagination, and passion of human scientists.

Kai-Fu Lee, AI expert, has predicted that AI will automate and potentially eliminate 40% of jobs within 15 years[32].

He says that AI will surely replace 'repetitive' jobs, e.g., those tasks that are being automated by robots in factories. Further, he predicts that AI will potentially replace many 'whitecollar' tasks in the fields of accounting, healthcare, marketing, law, hospitality and other areas.

As researchers, we pride ourselves on the novelty and creativity of our work. Thus, a critical issue for us is whether AI can and will replace our major activity, research, or even us researchers. This issue of how AI will impact researchers is not only relevant for the research community itself, but is also pertinent in the broader context of research institutions and universities[33].

In short, AI is a powerful tool that can augment and enhance scientific research, but it cannot replace the human element that is essential for creativity, innovation, and scientific discovery.

Moreover, the field of pharmacy involves not only the scientific aspects of drug development, but also the ethical and regulatory considerations that are essential for ensuring patient safety and efficacy of drugs. These complex issues require human judgement, and AI alone cannot provide the necessary insights and solutions.

CONCLUSION

In conclusion, the integration of artificial intelligence in pharmacy has the potential to revolutionize the field and improve patient outcomes. From drug discovery and development to personalized medicine and patient care, AI is at present making an impact in the pharmacy industry. However, it is important to note that AI is not a replacement for human expertise and judgement, but rather a tool to enhance and support decision making. As AI continues to evolve and improve, it will undoubtedly play an even greater role in the field of pharmacy. It is therefore essential for pharmacists and other healthcare professionals to stay up-to date with the latest developments in AI and to embrace this technology to improve patient care.

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