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Review article

Harnessing the power of artificial intelligence in pharmaceuticals: Current trends and future prospects

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ABSTRACT

Introduction of artificial intelligence (AI) technology in the field of pharmaceutical industry has been driven to discovery and development of drugs, also personalized medicine. In this article The review investigates systematic trends facing AI-powered transformation. AI has improved efficiency by reducing the drug development time, costs and success rates due to machine learning (ML), deep learning (DL) and natural language processing (NLP). The literature search was conducted systematically, using core scientific databases to source data-mining research studies on predictive modelling, virtual screening, and automation in AI applications. Findings here underscore the critical role that AI plays in precision medicine, as well as process optimization in manufacture, but ethical issues and privacy of data and regulations add significantly to hurdles. The study confirms that AI presents unique opportunities for developing personalized healthcare and answering global health challenges, nonetheless its adoption involves overcoming ethical and regulatory issues beautiful collaboration and agreeing to industry wide standards. The next-generation products bring hope for low-cost, patient-centric solutions indicating pharmaceutical landscape phases of the paradigm.

1. Introduction

The phrase artificial intelligence (AI) describes the creative application of computer systems to carry out tasks that would normally need human intelligence. It is a compelling and transformative concept. These jobs require a broad range of skills, which AI systems perform with ease, including learning, analyzing, reasoning, and decision-making. Surprisingly, AI systems fall neatly into categories like rule-based expert systems and sophisticated machine learning methods like decision trees.[1]

Robotics is one example of how end-to-end solutions for dosage form manufacture might be facilitated. With the least amount of human intervention possible, these state-of-the-art systems efficiently manage the laborious task of loading refined pharmacological compounds into machines and simultaneously retrieving the finished goods. The pharmaceutical manufacturing industry has surely seen a revolution because to this outstanding usage of AI, which has streamlined and accelerated production processes like never before.[2] The goal of this work is to examine how artificial intelligence (AI) is altering drug research and development (*r*&D) procedures. It also explores the significant possibilities by which AI can be used to improve our knowledge of illnesses and, eventually, the health of humans and animals.[3]

Unquestionably, throughout the past few decades, the pharmaceutical industry's overall success in drug *r*&D and cost efficiency have gradually decreased. The pharmaceutical industry is facing a growing number of obstacles, including increased healthcare expenses.[4] This is the exact moment that artificial intelligence (AI) steps in as a game-changer. AI presents a previously unheard-of chance to improve the cost-effectiveness and success rate of research and development of new medications.[5,6]

The adoption of artificial intelligence (AI) by the pharmaceutical sector marks a turning point in our pursuit of improved health outcomes. With artificial intelligence, we have an opportunity to completely transform the pharmaceutical industry and bring in a new era of innovation, cost-effectiveness, and enhanced human and animal health.[7]

1.1. *Definition of artificial intelligence in pharmaceuticals*

Self-learning is a fundamental and pivotal component within the realm of artificial intelligence (AI), and owing to the perpetual and ever-changing nature of the pharmaceutical industry, this distinctive trait of AI renders it impeccably suited for this particular sector.[8] An intricate and protracted process of drug development, it typically requires a

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staggering span of approximately 12–15 years and incurs an exorbitant average cost of around $314 million to $4.46 billion per newly developed drug.[9] Astonishingly, a mere 2 out of 10 drugs will ultimately generate revenues surpassing or at the very least mirroring the research and development (*r*&D) costs. A prime example lies in the unequivocal collaboration between Pfizer and IBM in 2015, as they jointly embarked upon harnessing the unbridled capabilities of IBM's AI platform, Watson, with the aim of stimulating a more streamlined and efficient development of novel immuno-therapy drugs.[10] Watson strives towards this momentous objective through its ability to furnish an all-encompassing and immensely sophisticated artificial intelligence system, which not only facilitates the production of conclusive and incontrovertible data but also enables the formulation of pinpoint and meticulous recommendations.[11–14] The integration of AI is not without its challenges such as data privacy, algorithm bias, regulatory considerations, and ethical implications must be carefully navigated to ensure that the benefits of AI in pharmaceuticals are realized while minimizing potential risks.[15]

Nevertheless, with the rapid advancements in AI technology, the pharmaceutical industry has an unprecedented opportunity to transform and revolutionize itself in ways that were previously unimaginable.[16] By embracing and harnessing the power of AI, pharmaceutical companies can unlock new insights, accelerate the pace of drug discovery, and ultimately improve patient outcomes. As the possibilities and applications of AI continue to evolve, the future of the pharmaceutical industry looks brighter than ever before.[17,18]

1.2. Importance of artificial intelligence in pharmaceuticals

Firstly, the development of a hybrid application combining support vector machines and simulated annealing to create a predictive model for oral bioavailability of drugs represents an innovative approach that has tangibly contributed to enhancing the effectiveness and efficiency of the drug development process.[19] Secondly, a notable application involves the discovery of new enzymes for non-ribosomal peptide synthesis, a fundamental aspect of drug production, potentially leading to a remarkable expansion of therapeutic options available. Lastly, the introduction of an advanced robotic system has revolutionized the synthesis of small molecules in organic chemistry or chemical biology. This automation not only expedites the process but also significantly improves accuracy and reproducibility.[19]

These remarkable achievements achieved through the integration of AI in the pharmaceutical industry have sparked a growing interest and recognition of its immense potential among pharmaceutical researchers and executives.[20] In June 2009, it is intriguing to note that industry analyst Datamonitor predicted a significant surge in the pharmaceutical industry's investment in AI. The report projected that the industry's expenditure on AI would more than double, soaring from $880 million in 2008 to surpass an astounding $60 billion by 2030. This optimistic estimation further underscores the growing recognition of the invaluable role that AI can play in revolutionizing the pharmaceutical industry.[21] As the pharmaceutical industry unabashedly embraces AI, it is poised to revolutionize the pharmaceutical landscape, ultimately advancements in medical science that benefit humanity as a whole.[22]

1.3. Scope of the study

This review provides a comprehensive overview and detailed evaluation of the extensive application of artificial intelligence in pharmaceutical research and development. It identifies and explores the vast innovative potential for AI in various areas. Moreover, AI computer systems, including robotic automation, data analysis, and clinical trial management, are thoroughly examined to understand their profound impact on transforming the conventional methods of pharmaceutical discovery, development, and marketing. The review examines the balance between opportunity costs and the increased efficiency and productivity that AI technologies are expected to bring to the pharmaceutical industry, ultimately assessing whether these advancements will lead to a net socioeconomic benefit. Overall, this comprehensive review serves as a guiding resource for understanding the vast potential of AI in the pharmaceutical industry. It tackles various facets, including research, development, job market impact, and personalized medicine, while thoroughly analyzing the advantages and potential socio-economic implications.

1.4. Methods

A structured and exhaustive search strategy was implemented in this review to compile pertinent literature regarding the pharmaceutical industry's utilization of artificial intelligence (AI). A comprehensive search was carried out in order to find peer-reviewed articles published in the last ten years (2013–2023) throughout the main scientific databases, such as PubMed, Scopus, and Web of Science. To narrow down the search results, Boolean operators (AND, OR) were coupled with keywords like "AI in pharmaceuticals," "drug discovery with AI," "machine learning in healthcare," and "AI applications in drug development."

Studies that demonstrated AI technologies, such as machine learning, deep learning, and natural language processing, in fields like drug discovery, precision medicine, and pharmaceutical production were the main emphasis of the inclusion criteria. Included were studies that addressed implementation, ethical, and regulatory issues.

Articles that were not in English, had no bearing on AI applications in medicine, or were entirely theoretical without any scientific or technological analysis were excluded based on exclusion criteria.

Despite not adhering to the PRISMA guidelines, a complex and iterative method was employed for the selection of articles, which involved several rounds of screening full texts, abstracts, and titles to guarantee quality and relevance. Finding significant trends, technical developments, and their possible effects on the industry were the main goals of the data extraction process. This approach guaranteed a thorough examination of AI's revolutionary impact on medicines during the previous ten years.

2. Applications of artificial intelligence in pharmaceuticals

Clinical trials optimization is another area which AI has tremendous influence in. By harnessing the power of machine learning, AI can effectively identify suitable participants for clinical trials by matching them to a set of complex eligibility criteria.[23] Machine learning algorithms can compare potential candidates to a trial using pattern recognition and classify similar patients with common conditions or diseases. This breakthrough has improved the selection process and increasing the chances of successful trials.[24] Precision Medicine, the practice of tailoring treatments to individual patients. To create individualized treatments, meticulous data analysis plays a crucial role, and this is where machine learning algorithms excel.[25] This potential game-changer in precision medicine lies in the utilization of patient-specific data and the integration of this data with relevant treatment guidelines.[21] AI offers a myriad of applications in this field, including the repurposing of existing drugs for different conditions. Through the mining of vast data sets, AI can identify potential alternative uses for drugs, opening up new possibilities for treatment.[26] Additionally, AI's ability to conduct 'virtual screening' plays a vital role in drug discovery. AI accelerates the screening process, ultimately reducing the high rate of failure in drug development.[27] A remarkable example of AI's impact in drug development is IBM Watson. In collaboration with Pfizer, IBM Watson developed a machine learning model that compares gene mutations in cancer cells with data from cells exposed to a range of substances.[18,28–30]

2.1. Drug discovery and development

Artificial intelligence has been quite important in drug development and discovery of late. There are numerous technologies available to scientists, but the one that will be introduced in this essay is the application of artificial intelligence. This is because of the fact that artificial intelligence is a computational model designed to mimic human thought processes in an analytical manner.[31] There are no effective methods of prevention for running a global campaign and recruiting talent from around the world at all stages of drug development.[32] With an ever-growing database of genomics and drug discovery information, this area is pushing for new high-throughput screening, An example of this would be something like the influenza virus. It kills between 250,000 and 500,000 people globally each year, and current antiviral drugs are effective but rising rates of resistance are making them less effective.[15] High-throughput technology allows combinatorial chemistry and screening of a huge number of chemicals for their effectiveness in as short a time as possible. This can be coupled with an AI model that attempts to predict resistance and viral mutagenicity, in order to try and create drugs that will be effective longer term and cost less to develop. The approach is to use modern technology to model new methods of administration and drug effects on immunity, attempting to shift the balance from always trying to play catch up with vaccines and treatments, to one where disease prevention is viable for developing world demographics.[12]

Model-based technology all the way through to clinical trials will be necessary if these aims are to be achieved. By harnessing the power of AI and its ability to analyze vast amounts of data, researchers can expedite the drug discovery process, identify potential drug targets, and predict their efficacy with higher accuracy.[16] By analyzing patient data and genetic factors, it can tailor treatment plans to individual patients, ensuring the highest chance of success while minimizing adverse reactions.[33] Furthermore, the use of AI in drug development extends beyond traditional pharmaceuticals. It can be employed in the development of personalized medicine.[21]

The application of artificial intelligence in drug development holds tremendous promise for advancing medical research and improving global health outcomes.[34,35] Widely used AI model tools are described in Table 1.

Table 1
Description of popular AI model tools.

AI Model Tools	Summary
DeepChem	An open-source library offering a large selection of drug discovery tools and models, such as generative chemistry, virtual screening, and deep learning algorithms for predicting chemical properties.
SMILES Transformer	A deep learning model that creates molecular structures from Standardized Molecular Input Line Entry System (SMILES) texts as input. Lead optimization and de novo drug development are two applications for it.
RDKit	An established open-source chemo-informatics library with many functions for handling molecules, finding substructures, and calculating descriptors. It can be included into drug discovery applications using machine learning frameworks.
Schrödinger Suite	A full-featured drug discovery software suite that includes a number of AI-powered capabilities. It has modules for drug design based on ligands and structures, virtual screening, molecular modeling, and predictive modeling.
ChemBERTa	A linguistic paradigm created especially for tasks involving drug development. Relying on the Transformer architecture, it can synthesize molecular structures, forecast attributes, and help optimize leads thanks to pre-trained data from a vast corpus of chemical and medicinal literature.
IBM RXN for Chemistry	Chemical reaction prediction using an artificial intelligence model. It helps in the development of new synthetic pathways and compound synthesis by generating possible reaction outcomes using deep learning algorithms as well as massive reaction databases.
GraphConv	An architecture for a model of deep learning that uses molecular graphs. By utilizing the structural data contained in the graphical representation of molecules, it has proved successful in predicting chemical attributes like toxicity and bioactivity.
scape-DB	A database called scape-DB (Extraction of Chemical and Physical Properties from the Literature-DrugBank) uses machine learning and natural language processing to extract biological and chemical information from scholarly publications. It offers useful data for studies on medication discovery.
AutoDock Vina	A well-known docking program that forecasts the binding affinity of small compounds and protein targets using machine learning approaches. It can help with lead optimization and virtual screening in the drug discovery process.
GENTRL (Generative Tensorial Reinforcement Learning)	A deep learning algorithm that builds new molecules with the desired properties by fusing generative chemistry and reinforcement learning. It has been applied to the optimization and de novo design of drugs.

2.2. Precision medicine

With machine learning techniques, computers have the ability to analyze vast amounts of data and unveil intricate relationships that might go unnoticed by human eyes. In the fields of genetics and molecular biology, which serve as the fundamental sciences of precision medicine, the data manifests in the form of gene sequences, expression levels, and an array of measurements.[36] On the other hand, the information embedded within medical records, in the form of unstructured text, ranging from progress notes to imaging and other test reports.[37,38] The ultimate objective of machine learning in the field of medicine is to discover the rules and logic that a decision maker would employ if they had ample time to meticulously analyze all the available evidence.[39,34] Precision medicine, which is also known as personalized medicine, represents an approach to patient care that enables doctors to select treatments with the highest likelihood of helping patients, based on a comprehensive understanding of the genetic aspects of their disease.[40] In order to achieve precision medicine, we must accumulate vast amounts of information about our individual patients and possess the capability to categorize patients and diseases in an exceedingly precise manner compared to our current practices.[41] This is where artificial intelligence (AI) and machine learning step in to enable us to gather diverse and disparate data, subsequently identifying intricate patterns and relationships that provide the necessary comprehension for precision medicine to flourish.[42,33]

2.3. Clinical trials optimization

In a futuristic world full of advanced technology and innovation, the realm of clinical trials is striving for swiftness, cost-effectiveness, and enhanced efficacy. Thankfully, the realm of artificial intelligence (AI) provides hope for the realization of this desire. Clinical trials stand as a crucial foundation for the evaluation and validation of novel treatments, making it imperative to identify and employ strategies that yield optimal results.[43] The journey of a clinical trial comprises multiple stages, each presenting its own unique challenges. These stages include study design, patient recruitment, data monitoring, and analysis, all playing pivotal roles in the course of a trial's progression.[44] Patient recruitment, in particular, has been a focal point, as it holds a high potential for failure when it comes to testing experimental drugs or therapies vis-à-vis their pre-existing counterparts.[45] However, with the advent of AI, a significant transformation in recruitment efficiency becomes conceivable, potentially revolutionizing the landscape of clinical trials.[46]

Despite the remarkable capacity of AI to enhance recruitment processes, challenges may arise when attempting to improve other stages of clinical trials. This is due to the inherent reliance on algorithms to analyze vast quantities of data for generating accurate insights.[47] Achieving success in these areas necessitates overcoming the conservative attitudes of clinicians who harbor a belief in their own capabilities, as well as addressing concerns regarding the costs and acceptance surrounding automation. Moreover, the complexity of fully comprehending algorithms poses a potential risk.[48] Thus, the development of AI in the scope of clinical trials mandates careful consideration and measures to ensure adequate comprehension and minimizing any inherent dangers.[49,50] However, various challenges must be addressed to extend AI's influence throughout all stages of clinical trials, necessitating the navigation of attitudinal barriers, cost considerations, and the risks associated with algorithmic reliance.[51]

2.4. Pharmacovigilance and adverse event monitoring

Regarding an original study, the term artificial intelligence (AI) was first present at a conference at Dartmouth College in 1956. By simulating intelligence through the use of computers and related technology, AI has the potential to greatly enhance problem-solving abilities, reasoning skills, and knowledge acquisition. Furthermore, AI has the capability to revolutionize the healthcare industry by providing meaningful pattern recognition and valuable insights from complex data. In fact, AI techniques have already proven their worth by being utilized for the development and analysis of data from research and development, as well as in identifying patterns in disease states and therapy through clinical research studies.[52] Researchers believe that AI could potentially analyze trial and error studies and patient records in order to predict which treatment options will be most effective for future patients with specific diseases.[53] Another area in which AI is making significant contributions is pharmacovigilance.[54,55] With the help of automated databases, AI has been able to facilitate and improve the drug safety surveillance process, especially in spontaneous reporting systems. These systems allow for the detection of signals indicating potential adverse effects from various data sources. AI applications in signal detection include Bayesian inference, data mining, knowledge-based systems, and information retrieval.[56] AI, particularly through the use of natural language processing and knowledge representation techniques, lays a solid foundation for the extraction of adverse event and safety data from large text-based data sources. This method, known as intelligent data analysis. It can be classified into two main types: statistical analyses and more advanced "hypothesis-generating" analyses.[57] Statistical analyses focus on finding relationships between drugs and outcomes, as well as quantifying them, while "hypothesis-generating" analyses are aimed at revealing new information about suspected associations or new drugs.[58,59]

3. Challenges and limitations of artificial intelligence in pharmaceuticals

One of the major concerns in the field of modern medicine is the interpretation of recent EU regulations and other regulatory measures in terms of their impact on it. This is particularly true of artificial intelligence (AI).[60] The development and deployment of AI applications in medicine can potentially revolutionize the entire health-care ecosystem and is facing a rapidly increasing number of vendors and stakeholders invested in its success.[61] This general lack of regulation means that developers often do not consider certain issues because they are not yet accustomed to thinking of AI as a method not a tool.[62,63] This lack of awareness led to a number of violations, and it is likely that the same thing will happen in AI development if developers are not given specific guidelines. The lack of standardization is related to the lack of regulation.[64,65] The introduction of AI algorithms into healthcare raises complex ethical questions regarding privacy, security, and the potential for biased outcomes. It is imperative that developers are equipped with the knowledge and tools to address these ethical concerns.[66] Finally, in order to share and aggregate data to train AI algorithms, there must be a unified system for data representation. This represents an order given the sheer variety of existing medical data.[67] Cooperation and collaboration among various stakeholders, including healthcare providers, researchers, and technology companies, will be essential to establish a standardized data representation framework.[68] Regardless, it is essential that the necessary measures are taken to ensure the responsible and effective implementation of AI in the medical field.[69]

3.1. Data privacy and security concerns

Privacy and integrity of information are critical issues in AI, machine learning, and data security. It is imperative to address concerns about the misuse and leakage of valuable proprietary data, especially within the pharmaceutical industry.[70] The potential disaster that can arise from the breach of sensitive information is a cause for alarm. Aside from the pharmaceutical sector, there are also worries surrounding the security of private medical and clinical trial data.[71] Looking ahead, there is a risk that data protection legislation in the future may inadvertently hinder the advancement of AI in healthcare and pharmaceuticals.[72] The tight restrictions imposed on the use of medical data could make it difficult to effectively train algorithms, thus limiting their potential in improving patient outcomes and revolutionizing the industry. A notable example of data protection legislation is the European Union's General Data Protection Regulation (GDPR), set to be enforced in 2018.[73] However, its impact on the field of AI in healthcare remains uncertain, leaving questions regarding its compatibility with technological advancements.[74] It is essential to continue exploring comprehensive solutions that prioritize both privacy and innovation, ensuring that future legislation aligns with the evolving landscape of AI and its potential contributions to the betterment of society[66,75,76]

3.2. Ethical considerations

An IBM research project, conducted by a team of dedicated scientists, delved into the intricate realm of machine learning as it pertains to medical decision support systems. This enlightening investigation uncovered compelling evidence of discrimination that can occur within these systems, particularly when catering to specific subpopulations.[35] Specifically, the study centered on a model designed to aid in treatment decisions for individuals grappling with complex chronic kidney disease. Surprisingly, the results revealed a disheartening disparity in the way the system responded to African American patients, even when there was an intentional omission of racial information from the algorithm.[77–79] The revolutionary capability to automate repetitive tasks or predictively intervene to mitigate disease progression presents an incredible opportunity for health systems to optimize efficiency and financial resources.[80] However, the ethical dilemma arises when the aforementioned cost savings become disproportionately burdened upon a specific group or individual as a result of decisions derived from AI. Such a scenario, where one group bears a greater share of the financial implications, is inherently perceived as unfair and inherently unethical.[81–83] Thus, this groundbreaking research serves as a clarion call to rectify the inherent biases and potential injustices embedded within the realms of machine learning and AI-driven decision-making. By addressing and mitigating these imbalances, we can strive towards a future where technological advancements truly serve humanity as a whole, ensuring equitable treatment and fostering a just society.[84–88]

3.3. Lack of standardization and regulation

Another major issue is the global nature of artificial intelligence (AI) and healthcare. The utilization of AI and data is not confined to any specific region, as they can easily cross borders.[68,88] However, this global nature of AI in healthcare poses challenges in terms of determining regulatory boundaries. It becomes difficult to discern what falls under regulatory oversight and what doesn't. Additionally, there is uncertainty about the applicability of data privacy and localization laws to various AI products and datasets.[89] They learn from their environment in unpredictable ways, making it challenging, if not impossible, to determine a fixed underlying mechanism.[90,91] Consequently, a drug or treatment developed using machine learning may not be a static product, but rather an ongoing subscription that provides updated recommendations. The conventional approach of pre-market clinical trials, designed to ensure the safety and efficacy of medical products, may have limited applicability to AI.[92] Artificial intelligence is increasingly finding applications in healthcare, particularly in the fields of drug development and personalized treatments.[93] The immense potential of AI in these areas necessitates the establishment of regulatory frameworks that account for the unique nature of healthcare data and recognize the potential consequences of AI product failures.[94] In 2017, the FDA introduced an innovation pathway with the aim of regulating AI and machine learning-based medical devices. This initiative involves the development of novel regulatory frameworks, tools, and assessment methods to evaluate these devices effectively.[95,96]

4. Current trends in artificial intelligence in pharmaceuticals

Current machine learning strategies could use these methods and make utilization of real datasets regarding the compound in order to learn the most predictive function. This ranges from general supervised strategies to support vector machines, to more particular methods, for example, simulated event of the function inside a specific environment.[97] To understand this-a given compound influences the disease, the approach utilized as a part of predictive learning through step 2 has been to connect between features of the compound and its impact on the disease using a function, frequently graphically.[98] Coming these methods will lessen the time and cost for new drug development by determining the best probability of success for specific compounds prior to testing them. At that point, the methodology would recognize specific features of promising compounds to known successful drugs.[99] Step three – to understand the significance of machine learning to pharmaceuticals. This is just a study of an algorithm to determine its effects on a given environment in this way it could be straightforwardly connected. Coming above, this could run simple S.E.A (Side Effect Assessment) on adverse/side effect of a few potential drugs for a given disease.[100] The most compelling space is simulation of a given drug to some state of a disease and its potential impact. This clearly determines a wide range of discoveries with the aim to reinforce that AI, particularly machine learning, and is becoming progressively imperative in pharmaceuticals.[101] By leveraging advanced algorithms and real-world data sets, we can unlock the potential of predictive functions that bridge the gap between compound features and their impact on diseases.[102] Implementing these cutting-edge methodologies will not only expedite the drug development process but also significantly reduce costs.[33] By accurately assessing the likelihood of success for specific compounds before extensive testing, valuable resources can be allocated more efficiently. Machine learning serves as a vital tool for algorithmic analysis, providing invaluable insights into the effects of various compounds within specific environments.[2] This allows for the seamless application of simple S.E.A (Side Effect Assessment) on potential drugs for a given disease. Additionally, simulating the interaction between a drug and a diseased state offers tremendous potential for discovering novel treatments and interventions. By harnessing its capabilities, we stand on the brink of a new era, where innovation and precision converge to yield transformative advancements in healthcare.[103]

In the area of drug development, the prediction of potential new drugs to diseases is currently receiving a significant amount of attention, and for good reason.[97] By accurately predicting the effectiveness of a drug, researchers and scientists can not only save substantial amounts of money on research and development costs, but also drastically reduce the time it takes to bring a new drug to the market.[104] Historically, this prediction process has been divided into two distinct stages. The first stage involves conducting tests to determine if a compound has a natural impact on a particular disease. These tests can range from traditional wet lab biology methods to more innovative approaches such as data mining techniques that utilize a vast amount of diverse data, including gene and protein sequences from disease-affected tissues.[105] The wide range of methodologies available for this stage makes it incredibly versatile and suitable for comprehensive data analysis. However, it is important to note that despite the diversity of approaches, their ultimate goal remains the same – to identify compounds that have a real potential to combat the targeted disease. Once a compound has been identified as having a potential impact, it progresses to the second stage.[106] This stage involves developing a method for the compound to be tested or utilized as a drug for the specific disease. This step is crucial in the drug development process as it lays the foundation for further testing and validation.[107,108] The overall process of drug development is intricate and multifaceted, requiring collaboration between experts from various fields, such as biology, chemistry, and medicine.[109] The success of each stage heavily relies on the accurate analysis of data and the implementation of innovative techniques.[16] As technology continues to advance, the field of drug development further evolves, paving the way for more efficient and effective approaches to predicting and developing new drugs for diseases.[3,11,12]

4.1. Machine learning and predictive analytics

In the pharmaceutical industry, the rapid growth in the abundance of biomedical data has sparked a significant demand for applications of artificial intelligence (AI).[14] Among the various domains, machine learning stands out as a field capable of making remarkable advancements. By employing sophisticated algorithms to learn from data, machine learning enables the generation of predictions and informed decisions.[98] Within the pharmaceutical landscape, this technology can be effectively utilized to construct models that identify patterns within data. Consequently, these findings can be leveraged to discover novel drug targets or ascertain which patients are likely to respond favorably to specific treatments.[110] Thus, it serves as a crucial element in the development of personalized medicine.[111] Early initiatives in this sphere include a groundbreaking study aiming to predict the likelihood of schizophrenia diagnosis by analyzing pertinent health conditions in patients. Furthermore, a pioneering model has been created to determine the probability of drug withdrawal from the market by evaluating its properties and adverse events reported.[112] Notably, both of these notable examples utilize publicly available data derived from clinical trials, epidemiological studies, and adverse event databases.[113] Within the pharmaceutical industry, machine learning finds wider application in the realm of *in-silico* modeling. This comprehensive term encompasses an extensive range of mathematical modeling techniques that facilitate the simulation or prediction of drug behavior and/or disease states.[12] For instance, a model has been developed to forecast the probability of encountering adverse cardiac events associated with new drugs.[114] This innovation has the potential to proactively detect safety concerns during drug development or even eliminate unnecessary safety warnings for drugs with low associated risks.[115] Through these transformative applications, machine learning continues to revolutionize the pharmaceutical industry, fostering advancements in drug discovery, safety evaluation, and personalized healthcare.[116]

4.2. Natural language processing and text mining

One of the main difficulties involved in extracting information from clinical notes is the wide range of language used by healthcare professionals, which includes complex medical terminology. Clinical text consists of various ambiguous terms, abbreviations, acronyms, as well as instances of negation and speculation.[117–119] For example, consider the following sentence: “It is possible that the patient may have early-stage pneumonia." The context in which this sentence is expressed is extremely important.[120] The mention of possibility implies that the diagnosis is still uncertain and could change. Ongoing research in Natural Language Processing (NLP) aims to develop tools that can identify such terms and automatically transform the text into a representation that preserves the information while getting rid of the original wording.[121] In recent years, due to remarkable technological advancements, there has been a significant increase in the amount of clinical data that is available.[122] A large proportion of this data is in the unstructured form. By applying NLP techniques to this type of data, it becomes possible to convert unstructured information into well-organized structured data.[123] This process not only simplifies the analysis of medical information but also enables making accurate predictions about potential negative reactions to medications, medical procedures, and a wide range of other medical outcomes.[124] However, clinical notes present numerous challenges, these challenges require extensive exploration and implementation of advanced NLP algorithms to ensure accurate extraction and interpretation of clinical data,[125] ultimately leading to improved healthcare outcomes and patient care.[126]

4.3. Image recognition and computer vision

Computer vision, as a subset of software engineering, offers numerous advantages compared to traditional image processing techniques. This makes it highly suitable for applications in the pharmaceutical and medical fields.[127] However, the aim is to replace macroscopic and microscopic examinations with more efficient and informed diagnostic tools through the use of extensive medical image databases.[128] The primary focus lies on automating the analysis of intricate image data, thus significantly reducing the burden on healthcare professionals.[129] High content screening (HCS), a technique that enables the simultaneous evaluation of multiple cellular parameters, generates an overwhelming number of images in a single experiment, often described as "extracting a phenotypic readout".[130] This flood of data requires sophisticated and highly efficient image analysis algorithms to extract meaningful information and patterns.[131] On the other hand, we are also deeply interested in examining clinical data, including images of tissue samples, for disease diagnosis.[132] Although the translation of these processes into clinical practice is still in the early stages, there is immense potential for revolutionizing healthcare and improving patient outcomes.[133–136]

5. Future prospects of artificial intelligence in pharmaceuticals

Community well-being programs established through the gathering and analysis of collective data, automatically taxonomize and stored with subsequent retrieval possibilities, can also become an AI learning experience.[137] AI would thus implement an effective community health management plan by providing people resources and information on implementing lifestyle changes to better public and individual health.[138] Wearable devices and software programs that utilize AI to derive data obtained from various patient sources will steer humanity towards more efficient illness prevention and management of current health conditions.[139,140] A patient similarity AI model developed by BioXcel used unsupervised learning to analyze data from 70,000 patients, including unstructured data from patient history reports.[141] This led to the development of an algorithm that could rapidly match patients with appropriate clinical trials or treatments.

With AI virtual simulation, concept testing, and other AI algorithm methods, this is predicted to increase efficacy and confidence by reducing development time and cost by up to 70 %, with a higher 10 % increase in approval rates of new drugs.[142,143] Future prospects of AI in pharmaceuticals are bright. The current new drug development platform is time-consuming, high-costing, and inefficient. It takes an average of 12 years from discovery to market.[144] The cost of new drug development is estimated to range from $109 million to $2 billion, with not even a 100 % success rate on human or animal tests. Considering only 5 in 5000 drugs progress to pre-clinical trials. This is largely due to the limitations of human clinical trials and error.[145,146]

5.1. Integration of artificial intelligence with internet of things (IoT)

The Internet of Things (IoT) refers to the interconnection of computing devices embedded in everyday objects that enable them to send and receive data. Current trends show that homes, cars, and consumer products are just a few examples of items that are becoming part of the IoT ecosystem.[147] In healthcare, there is much interest in IoT and how it can be used to improve patient care. With the growing number of individuals with chronic diseases and conditions, healthcare is shifting from hospital-based care to home and community-based care.[148] A shift to home-based care means a greater burden of disease management is being placed on the patient who is often ill-equipped for the task. IoT devices designed to aid in disease management could provide a bridge for this gap in care. For the pharmaceutical industry, more patient-generated data means a greater opportunity to understand the patient and the effects of treatments in the real world.[149] AI and IoT can be integrated in multiple ways to track and analyze data in patients with chronic diseases.

One simple example is the tracking of medication adherence. It is well understood that adherence to medications for chronic diseases is poor, with roughly 50 % of patients not taking their medications as prescribed.[81] Missed doses directly lead to increased disease complications and hospitalizations, which are costly to the patient and the healthcare provider. Smart pill bottles are an example of an IoT device that could be used to track adherence.[150] The bottle can detect when it has been opened and closed and relay that information to an application that stores the data.[83] AI can be applied to analyze this data and send reminders to patients who have missed doses. In a case study involving stroke patients, it was found that simple mobile phone reminders significantly increased adherence.[86] AI can take this a step further and analyze when patients are missing doses and look for patterns as to why the doses are being missed. In this way, interventions can be designed to target specific problems in individual patients.

5.2. Personalized medicine and treatment planning

In the realm of personalized medicine, these innovative methods must undergo extensive and stringent clinical testing and regulatory scrutiny in order to ensure their safety and efficacy.[147] This groundbreaking potential would undoubtedly bring about a profound and transformative shift in the landscape of evidence-based medicine, blurring the boundaries that have traditionally delineated the realms of AI and clinical research.[148] Renowned expert Peter Szolovits of MIT envisions a future where the practice of medicine undergoes a revolutionary transformation. He asserts, "In the long run, we cannot simply continue practicing medicine as we have done so far. The solution lies in harnessing the power of computerization and extracting meaningful and actionable conclusions from the vast amount of information available to us.".[149] Therefore, it seems highly likely that these advanced technologies will gradually assume greater decision-making responsibilities in various domains of healthcare.[150] Over recent years, there has been a noticeable and discernible shift towards tailoring treatment regimens and therapeutic approaches to suit the unique genetic makeup and specific disease characteristics of individual patients. This increasingly popular approach, commonly referred to as personalized medicine, recognizes that each patient is distinct and requires a personalized analysis and treatment plan.[151] This is precisely where the immense potential of artificial intelligence comes to the front.[152] Artificial intelligence has already demonstrated significant promise and potential in aiding the interpretation, integration, and analysis of complex data derived from sources such as the human genome, disease chemistry, and biological responses to treatments.[153] In particular, machine learning approaches have showcased their remarkable ability to identify intricate patterns, extract crucial attributes, and discover valuable insights from data that would otherwise elude human analysts.[154] These data-centric and AI-driven approaches have the potential to revolutionize personalized disease treatment by closely aligning with the analysis of intricate datasets in order to derive and foster the most optimal and evidence-based clinical decisions.[155,156]

5.3. Intelligent drug delivery systems

The implementation of artificial intelligence (AI) in drug delivery is now a reality and marks the beginning of a revolutionary shift. Micro particles are commonly used to transport drugs to their intended sites, but automating this process using conventional programming methods has been challenging.[157] However, with the use of neural networks, motion can be programmed in micro particles, allowing for precise and complex movements under varying external conditions. Pohly's essay demonstrates the effectiveness of using neural networks and fuzzy logic to control the movement of simulated micro robots and particles in a Java program. Additionally, the study highlights the increased accuracy and reliability of drug release compared to conventional methods.[158] The ability to program step-by-step drug release through changes in the microenvironment is also a promising application. While this level of micro drug release is still in development, the potential of this technique is significant.[159,160]

It is evident that smart drug delivery systems combine bio-compatible devices and/or appliances with drug delivery systems to automate and regulate the medicine administration process in the body.[161] Through advancements in neural networks, the motion of micro particles can be programmed to ensure targeted drug release. This ability to simulate precise and complex movements under varying external conditions enhances the efficiency and reliability of drug delivery.[162] One notable application is the use of AI in intelligent drug delivery systems, which integrate bio-compatible devices and/or appliances with drug delivery systems to automate and regulate medicine administration in the body.[159] The emergence of smart drug delivery systems represents a significant advancement in pharmaceutical technology. This integration of intelligent technology addresses the challenges of precise drug targeting and personalized medicine administration, ultimately improving treatment outcomes and patient care through automation and regulation.[158]

In this section, the role of the healthcare professional is set to change with the use of AI tools, the diagnostic process and therapeutic decision making will become more data driven.[161,162] It should result in the prevention of adverse events, the avoidance of misdiagnosis and the generation of tailored treatment plans.[163] However, this change to evidence-based practice will require healthcare professionals to have a broad of the methodologies used to derive conclusions in specific AI applications. Treatment plans which are based on complex data analysis may be difficult to comprehend for the patient.[78] This would make it hard to obtain informed consent for the treatment process. With specific reference to clinical research, AI tools have the potential to automate clinical trials, through intelligent trial design, patient recruitment, and data collection and analysis.[164] The use of historical data in this context has both positive and negative implications. The ability to learn from past mistakes to improve trial design and the analysis of large-scale data to find new insights into diseases, are clear benefits.[165] However, the automation of aspects of the clinical trial may lead to a loss of clinical research posts and less opportunity for research training.

5.4. Impact on healthcare professionals

Healthcare practitioners must adapt to the integration of AI in their daily responsibilities. To effectively utilize AI, healthcare professionals must place their trust in the technology and recognize it as a reliable tool for generating data.[166] It is crucial to demonstrate that technology and humans can collaborate to deliver optimal healthcare. This can be accomplished by incorporating AI education into medical school curricula and integrating AI into continuing education programs for practicing healthcare professionals.[167,168] For instance, AI can be utilized to analyze patient electronic health records and propose a diagnosis for a patient complaint.[169] However, it is imperative for healthcare practitioners to comprehend the extent of AI's role and not rely solely on it to perform tasks that they are capable of completing themselves.[170]

Lastly, healthcare professionals must consider the implications that AI will bring to patient care. This encompasses both the potential benefits and drawbacks it may have for their patients, as well as how it might impact their approach to patient care.[133,171,172]

5.5. Economic and business considerations

There are many ways in which AI can help reduce costs, but one of the largest areas is through the process of clinical trials.[32] One article suggests that using AI in the drug development stage could have a significant impact on costs.[157] Drug development makes up a third of total clinical trial expenditure, suggesting that around $37 billion would be saved on an annual basis by implementing AI. This would not only reduce the cost of healthcare for the patient, it could also increase the speed at which drugs are developed.[173] The added speed of drug development can be attributed to the fact that AI can perform tasks much faster than a human and has the capacity to multitask.[172] An example of this would be the system developed by Berg Health, which can scan the vast knowledge contained within biology in order to form and test the main hypotheses of a clinical trial in a fraction of the time that it would take a team of researchers.[174]

An increase in the speed of drug development and a decrease in costs of clinical trials could lead to an overall decrease in drug prices. This could however lead to a decrease in revenue for the top pharmaceutical companies.[117] Increased mergers and acquisitions may in fact increase industry efficiency by maximizing the strength of combining companies and ridding the industry of weaker ones.[35,117,175] This is already evident through the combination of AI and big data approaches to form a virtual brain trust of several companies with the common goal of bringing collective knowledge to a singular industry.[176–178]

5.6. Patient empowerment and engagement

AI chatbots are an emerging technology with great potential for engaging patients. This is evident from the increasing use of chatbots in fields like eCommerce and customer service.[179] Wearable devices can collect a wider range of data about a patient's daily habits and physiological state passively. This data can then be used to provide personalized feedback to the patient in a timely manner. Particularly in certain populations like the elderly or those with memory impairment, who may struggle to input data into an app, these devices can be extremely beneficial.[180] Mobile apps, on the other hand, hold great promise in helping patients understand and manage their medical conditions. Patients can easily track their symptoms, medications, and health metrics, and receive personalized information about their condition through these apps.[181,182]

However, the concept of patient empowerment has gained importance in healthcare due to the rising prevalence of chronic diseases. Patients believe that the healthcare system should be more focused on meeting their needs.[183] Extensive research indicates that empowered patients achieve better health outcomes and incur lower healthcare costs.[184] Patients who are better informed and involved take more responsibility for their health, communicate better with their healthcare providers, and seek more information and assertiveness in their interactions with the healthcare system.[185–187]

5.7. Recommendations for industry adoption of AI in pharmaceuticals

To accelerate the integration of Artificial Intelligence (AI) into the pharmaceutical industry, the following concrete recommendations are proposed:

Pilot Programs and Feasibility Studies: Launch pilot initiatives in particular stages of drug research, such predictive modeling or virtual screening. With this strategy, businesses may evaluate AI's capabilities in safe settings and compare the results to those obtained using more conventional techniques.

Collaborative Ecosystems: Form alliances between academic institutions, regulatory agencies, pharmaceutical businesses, and AI technology companies. These kinds of partnerships help fill knowledge gaps in the use of AI by combining resources, encouraging creativity, and facilitating information transfer.

Infrastructure Development: Make investments in cutting-edge computational infrastructure, including cloud-based platforms and high-performance computing (HPC) devices. These are necessary for effectively organising huge datasets and executing intricate AI algorithms.

Regulatory Readiness: To guarantee adherence to changing standards, involve regulatory bodies early in the AI development process. Approvals for AI-driven approaches can be accelerated by creating validation frameworks tailored to AI.

Skill Development: Employees should be trained to effectively operate AI systems and interpret their results. Professionals in *r*&D, production, and quality assurance should be the focus of upskilling programs in order to close the knowledge gap between domain expertise and AI.

Data Governance: To guarantee data security, quality, and adherence to privacy laws, implement strong data governance principles. AI models will be able to produce trustworthy and objective findings if data collecting and annotation procedures are standardized.

Ethical and Transparent AI Deployment: Create policies that handle ethical issues like decision openness, data privacy, and algorithmic bias. In addition to fostering trust, ethical AI methods will reduce the likelihood of unfavourable consequences.

Phased Implementation: Before branching out to more intricate and resource-intensive fields like personalized medicine, start with AI applications that offer an instant return on investment, such virtual screening in drug discovery or predictive maintenance in manufacturing.

Performance Metrics: Define precise, quantifiable standards for assessing the effectiveness of AI applications. To show the value of AI, metrics like shorter development times, cost savings, and increased predictive accuracy should be monitored.

Open Innovation Platforms: Establish or take part in open-access platforms that allow stakeholders to exchange insights, datasets, and algorithms. This collaborative approach can drive collective progress and reduce duplication of efforts in AI research.

By adopting these strategies, the pharmaceutical industry can harness AI's full potential to enhance innovation, optimize resource utilization, and improve global health outcomes.

6. Conclusion

The recent years of rapid development in the area of artificial intelligence and related areas, including data mining, image analysis, and robotics, have provided abundant opportunities for the utilization of AI in pharmaceutical research and development. As the field continues to evolve, the advancements in AI are paving the way for groundbreaking innovations in various domains within the pharmaceutical industry.[188,189] The work presented in this paper, while significant, is just a glimpse into the vast potential of AI in pharmaceutical research and development. It represents only a spectrum of the ongoing efforts in this rapidly growing field.

The interest in data mining and knowledge discovery for use in decision support has also gained considerable momentum in recent years. This trend highlights the importance of leveraging AI to extract meaningful information from massive datasets and using it to inform critical decisions in medicine.[190] To achieve this, the implementation of computer-based methods at multiple stages of the research and development process is indispensable.[168] AI-powered tools and techniques will empower researchers to navigate the immense complexity of biological systems and accelerate the discovery of innovative therapies.[191,192] However, the journey of AI in the pharmaceutical industry is not without challenges. Additionally, the validation and regulatory approval of AI-driven solutions pose unique considerations that need to be addressed to ensure patient safety and the efficacy of the developed treatments.[193,194] The true testing ground for AI lies in its ability to comprehensively analyze complex interactions and pathways at a molecular level.[195,196] The achievements in these endeavors will shape the future landscape of the pharmaceutical industry and determine the perceived value of AI for the industry as a whole.[197,198] Exciting times lie ahead as we witness AI's transformative influence on healthcare and its profound implications for improving patient outcomes.

CRediT authorship contribution statement

Saha Aritra: Writing – original draft, Conceptualization. **Singh Indu:** Writing – review & editing.

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The English language of the article was improved with ChatGPT, OpenAI's large-scale language-generation model. Upon generating draft language, the author reviewed, edited, and revised the language to their own liking and takes ultimate responsibility for the content of this publication. The authors declare no conflict of interest in the preparation and publication of this review article, “Harnessing the Power of Artificial Intelligence in Pharmaceuticals: Current Trends and Future Prospects.”

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Data availability

This is a review article, and therefore, no new data were generated or analysed in the course of this study. All information and data discussed are derived from previously published works, as cited within the article.

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