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Study On The Dynamics Of Artificial Intelligence Innovations In The Pharmaceutical Industry

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Abstract

Artificial Intelligence (AI) is a powerful tool that provides rapid solutions to complex problems. Significant advances in AI technology have enabled the discovery of new drug formulations with fewer side effects. Using AI algorithms, vast biological data can be examined. This approach helps identify drugs more effectively and in a more targeted manner. AI can help reduce costs by optimizing research processes. This technology can predict the pharmacokinetics and toxicity of drugs, which leads to a reduction in the need for extensive and costly animal testing. Among the benefits of AI in the pharmaceutical industry are the prediction of toxicity, bioactivity, absorption, distribution, metabolism, and excretion properties, as well as physicochemical properties in drug screening. However, continued investment and research in AI bring exciting horizons for optimizing drug development processes. In this study, we first tried to classify artificial intelligence, then we discussed the importance of artificial intelligence in the health system, drug identification, drug delivery, dosage form design, and its disadvantages. Consequently, given the increasing importance and development of artificial intelligence in drug discovery and identification, this study examined the dynamics of artificial intelligence innovations in the pharmaceutical industry.

Keywords: “Artificial Intelligence”, “Drug Delivery”, “Pharmaceutical”, “Pharmacokinetic”.

Introduction

The pharmaceutical industry is one of the vital pillars that has a significant impact on saving human lives. Relying on continuous innovation and adopting new technologies, this industry solves global healthcare problems and responds to urgent medical needs [1]. New pharmaceutical innovations include a range of small drug molecules to biologics that have been targeted for the treatment of diseases due to better stability. The assessment of toxicity associated with new drugs is a matter of concern that necessitates extensive research and exploration. One of the primary goals is to provide drug molecules that offer optimal benefits for use in the healthcare industry. However, the pharmaceutical industry faces various challenges that require further advancements through technology-based approaches to meet global medical and healthcare needs [2]–[4]. AI systems can analyze various types of data, including genetic, proteomic, and clinical data, to identify potential therapeutic targets. By identifying disease-related targets and molecular pathways, AI helps design drugs that can regulate biological processes. By simulating chemical reactions and predicting molecular bonds, AI allows researchers to prioritize and select compounds for practical experiments, thus saving time and resources. Artificial intelligence models can establish relationships between the chemical structure of compounds and their biological activities. This allows researchers to improve the quality of drug candidates by designing molecules with desirable properties, such as high potency, selectivity, and favorable pharmacokinetic profiles. Using chemical libraries and experimental data, artificial intelligence helps expand the chemical scope and plays an effective role in the process of developing innovative drugs. Artificial intelligence algorithms can analyze and optimize drugs based on various factors, such as efficacy, safety, and pharmacokinetics. This capability allows researchers to adjust therapeutic molecules to increase their effectiveness while minimizing potential side effects. Artificial intelligence systems can predict drug toxicity by analyzing the chemical structure and properties of compounds. Machine learning algorithms trained on toxicology databases can identify harmful effects and detect dangerous structural properties. This allows researchers to prioritize safer chemicals and reduce the risk of adverse reactions in clinical trials [5]. The use of AI-based approaches in the drug research and development process allows for the

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identification, optimization, and design of new therapeutic candidates to be carried out more simply and rapidly, which will ultimately lead to the production of more efficient and effective drugs [6]. For example, in silico target fishing (TF) technology is used in pharmaceuticals to predict biological targets based on chemical structure. This information is provided based on data available in the chemical database. The conventional drug discovery methods used by various industries are very expensive. These methods involve several complex steps that need to be carefully considered to achieve the desired results. These steps include the selection and identification of target proteins as well as investigating the mechanism of action of small molecules in depth. To speed up this process, researchers introduced TF, which helped reduce the overall cost of testing during drug development processes. This technique was used to identify the high binding ability of diethylstilbestrol. It is a computational and proteomic-based approach that ranks data points based on their fusion similarity to drug targets. Furthermore, it is used to assess potential toxicities in ligand-based approaches used in drug discovery. Some of the drugs that have been successfully identified using this method include loperamide and emetine along with methadone. Also, the targets identified for these drugs include muscarinic, adrenergic, and neurokinin receptors [5], [7]–[9]. The field of drug discovery has made significant advances using artificial intelligence models and tools. Given the importance of artificial intelligence in the discovery of new drugs, in this study, we examined the dynamics of artificial intelligence innovations in the pharmaceutical industry.

1.1.Artificial Intelligence (AI)

Artificial Intelligence (AI) is a branch of science related to intelligent machine learning and mainly consists of intelligent computer software that provides results similar to human attention processes. This process usually involves collecting information, designing effective systems to exploit the collected data, providing definitive or approximate results, and making corrections. In general, artificial intelligence is used to analyze machine learning to mimic the cognitive tasks of humans [10], [11]. Artificial intelligence technology is used to perform more accurate analyses and obtain useful interpretations. 3 Artificial intelligence technology has become a key component of industry and has found valuable applications in many research fields [10], [12]. The application of artificial intelligence technology in the pharmaceutical industry, including in the field of drug discovery, drug delivery formulation design, and other healthcare-related applications, is continuously developing and advancing [13], [14]. Applying artificial intelligence models allows us to predict in vivo responses, pharmacokinetic parameters of drugs, appropriate dosage, and other aspects [11], [13]. Due to the importance of predicting the pharmacokinetics of drugs, for example, the use of in silico models facilitates the process of drug research due to their efficiency and low cost. There are two main categories of AI technology advancements [13]. The first refers to common computing methods, including expert systems that are capable of simulating human experiences and can provide results based on the same principles as these systems [15]. The second includes systems that can simulate brain activity using artificial neural networks (ANN). In particular, different types of neural networks, including deep neural networks (DNNs) and recurrent neural networks (RNNs), have a significant impact on advances in artificial intelligence technology [13].

1.2.History of Artificial Intelligence

In 1956, the term "artificial intelligence" was first coined. However, the concept of artificial intelligence has been around since the 1950s. In 1958, Frank Rosenblatt created neural networks called perceptrons that could transmit information in one direction. In 1986, Georey Hinton promoted the design of the backpropagation algorithm, which is widely used in deep learning. In 1997, Garry Kasparov (Russian grandmaster) was defeated by IBM Deep Blue. In 2013, Google conducted effective research on images using British technology. In 2016, Go champion Lee Sedol was defeated by Google DeepMind's AlphaGo

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software [13]. From 2016 to today, i.e. 2025, artificial intelligence has brought tremendous advances to humanity in the world of science. The pharmaceutical industry has not been left behind by this progress.

1.3.Artificial Intelligence Classification

According to the capabilities, artificial intelligence can be divided into three categories. The first category is narrow AI (ANI) or weak AI, which is designed to perform specific and limited tasks. The second group is artificial general intelligence (AGI) or strong artificial intelligence. It performs all tasks both as a human and as an artificial intelligence with capabilities similar to human intelligence. This feature can help improve human mental abilities and is also able to perform unfamiliar tasks. The third group is called Artificial Super Intelligence (ASI). This type of intelligence is smarter than humans and performs much more tasks in areas such as design, mathematics, space, and other fields.

Based on the researchers' research, another classification can be presented that includes four groups. The first type is used for specific applications that cannot exploit past experiences because they lack a memory system. These types of systems are known as reactive machines. The second type has a limited memory and can use past experiences to solve various problems. The third type is based on "theory of mind". In other words, the choices that people make are influenced by their personal thoughts, goals, and desires. This type of system does not exist in artificial intelligence. The fourth type is self-awareness, which is also not present in artificial intelligence [16], [17].

1.4. Artificial intelligence in the healthcare system

Keeping the medical records of patients is a complex process. However, with the use of artificial intelligence systems, data collection, standardization, storage, and tracking become significantly easier. Google Deep Mind Health Project, designed by Google, helps to analyze medical records in a short time. Using artificial intelligence technology, it is possible to design effective treatment plans. In critical situations where choosing an appropriate treatment plan becomes difficult, the use of artificial intelligence systems is essential to manage the patient's condition. In this process, all information, previous reports, clinical expertise, and other data are carefully reviewed to design an optimal treatment plan [17]. In recent years, the use of artificial intelligence technology in health support services and the provision of pharmaceutical assistance has been recognized as an effective method. Molly, a virtual nurse designed by a startup, serves patients with a pleasant voice and a friendly face. The goal of this system is to assist patients in managing their treatments as well as to support people who are facing chronic diseases, especially in the time between medical visits. Ai Cure is an app that is installed on the webcam of smartphones and monitors patients and helps them manage their condition. Artificial intelligence helps people in the healthcare field and can collect data and compare them using social awareness algorithms [14].

1.5.Artificial intelligence in the identification of medicines

The drug discovery process begins with the use of results from a variety of sources, including high-throughput screening modeling, computational modeling, and available reported data [4], [18]. In the drug discovery process, the structural features of drug molecules can be investigated directly or indirectly through computer-aided design methods. These molecules are then synthesized. Molecules and pharmaceutical compounds synthesized in the early stages are subjected to high-throughput screening. These compounds are then evaluated

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in secondary experiments with successful structure-activity relationship (SAR) analysis. Humans cannot exploit all the available information to advance scientific research. However, AI supercomputers can receive and analyze data to identify relationships between compounds and come up with new drug molecules [13], [19]. Applications of artificial intelligence in the drug discovery process are related to the exploitation of the chemical space [4], [19]. This space helps in identifying new molecules because it is possible to determine the molecules of interest computationally. In addition, it can help identify effective molecules with a specific target [20]. Selecting a new and successful drug molecule from a large number of active chemical compounds is a very challenging process. Artificial intelligence is being used to process fewer molecules with much greater confidence. In this context, the new design requires an understanding of organic chemistry for the synthesis of in silico molecules and virtual screening modeling. This method is used as an alternative option for many biochemical and biological tests and is effective in evaluating efficiency and toxicity [21]–[24]. The purpose of de novo design in the drug discovery process is to produce new and active molecules independently and without dependence on reference molecules [22]. Finally, active learning algorithms can identify new molecules that can affect disease or disorder targets. Several methods, including ligand-based design and molecular structure-based design approaches, can be employed using available information on structural biology features [20]. In Table 1, a list of the main AI-based computer tools used in the drug discovery process is presented.

Table 1. Artificial intelligence-based computer tools used in the drug discovery process [13].

Rout number	Computer tools based on AI in the drug discovery process	Applications
1	Chemputer	Further standardization for chemical synthesis reporting.
2	ODDT	For use in chemistry informatics and molecular modeling.
3	ORGANIC	Molecular generation tool to create molecules with desired properties.
4	DeepChem	Python-based AI tool for drug discovery prediction.
5	DeepNeuralNet-QSAR	Molecular activity prediction.
6	Neural Graph Fingerprints	Predicting the properties of new molecules.
7	Hit Dexter	Machine learning models to predict molecules that may react to biochemical tests.
8	NNScore	Neural network-based scoring function analysis for protein-ligand interactions.
9	DeepTox	Toxicity and biocompatibility prediction.
10	PotentialNet	Predicting the affinity of a graft based on a convolutional graph neural network.
11	REINVENT	Novel molecular design using RNN and reinforcement learning.
12	DeltaVina	Scoring function for retrieving protein-ligand binding affinity.
13	AlphaFold	Predicting the three-dimensional structure of a protein

1.6.Artificial intelligence in drug delivery

In recent years, there has been increased focus on developing innovative systems to deliver treatments in a targeted manner with maximum effectiveness and minimal side

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effects [25]–[27]. Controlled drug delivery and overcoming the challenges associated with traditional drug delivery systems, including systemic toxicity, therapeutic limitations, and dose adjustment in long-term treatments, are the main focus of extensive research [26], [27]. Using microfabrication technology to produce implantable microchips that deliver drugs in a controlled manner looks promising [28]. Microfabricated drug delivery systems include drug reservoirs with various shapes and capacities that can be opened based on specific commands and provide the drug in a continuous or pulsatile manner [11]. To provide targeted and controlled treatments, the use of implantable drug delivery systems that are capable of automatically adjusting drug concentration and release time is considered a promising method to increase the efficacy and safety of treatment [29]. This is especially important in relation to chronic diseases that require timely treatment and continuous monitoring. Designing implantable drug delivery systems requires consideration of several factors, including dose adjustment, targeted delivery, sustained release, and intelligent control systems. In the design of control systems, neural networks, fuzzy logic, integrators, and differentiators have been utilized [11], [30]. Drug delivery methods include the use of focused ultrasound, micropump systems, and targeted delivery using microrobots [11], [31]. The use of microfluidic platforms is considered a promising method for producing nanoparticles for drug delivery [32], [33]. To deliver the drug in a controlled manner, electronic components, wireless communication hardware, and power supply are combined into a microchip implant. The technology was used in the first clinical trial to deliver drugs to patients with osteoporosis [34]. Regular insulin injections and constant monitoring of glucose levels can significantly reduce the complications of diabetes. In this area, the combination of glucose sensors, insulin delivery systems, mathematical models, and control algorithms can be very efficient. By combining an insulin pump and glucometer into one device, an automated system for monitoring glucose levels and delivering insulin has been created [11]. In designing smart delivery systems, it is necessary to consider adjustments based on demand for dose or drug release rate, along with targeted delivery and drug stability [35]. Information technology, wireless communications, and artificial neural networks (ANN) are helping to develop intelligent drug delivery systems that can perform better against the challenges of traditional treatment methods. Wireless communications allow drug delivery devices to be more flexible [11]. Artificial Neural Networks consist of interconnected processing components that are created through network simulation of model neurons. These networks have been used to develop software to mimic biological processes, generate control algorithms, model pharmacodynamics and pharmacokinetics, control drug delivery, and evaluate the effectiveness of therapeutic strategies [11]. Therefore, the use of artificial intelligence methods can be very effective in predicting drug dose efficiency and drug delivery capability in a variety of dosage delivery systems.

1.7.AI in Dosage Form Design

One of the most important metrics for monitoring a drug delivery system is the penetration rate based on the route of administration. Physicochemical barriers are crucial for biological compartments and can be implemented depending on the mode of

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drug delivery in the body [5]. Drug interactions with biological components and drug availability in biological environments have a great impact on the fate of the drug in the body. This process is controlled by the molecular characteristics of the drug. For many small molecules, passive diffusion is inefficient and requires a specific drug delivery system. The process of active diffusion is driven by membrane transport and depends on complex biological interactions. This complex process requires investigation using numerous specific parameters through calculations and systematic modeling methods [17], [36]–[38]. All of these are related to drug interactions with membranes and can be better analyzed by the modeled environment, as presented in Figure 1 [5]. The accuracy of the analysis helps to better understand the research units. Artificial intelligence is an advanced technology that is capable of analyzing multi-layered data. To better train AI in the biological environment, a proper understanding of drug-biological interactions is essential. Pharmacokinetic studies can be performed using many new artificial intelligence technologies, such as artificial neural networks. Many artificial intelligence databases, such as chemical, genomic, and phenotypic databases, are being used to better understand drug interactions. Some methods are used to study the effect of drug delivery systems on pharmacokinetics, to gain a better understanding of the disposition and toxicity of drugs. Many modern methods in drug delivery systems address the design of quality features along with critical properties and examine their impact on the results of real experiments [5]

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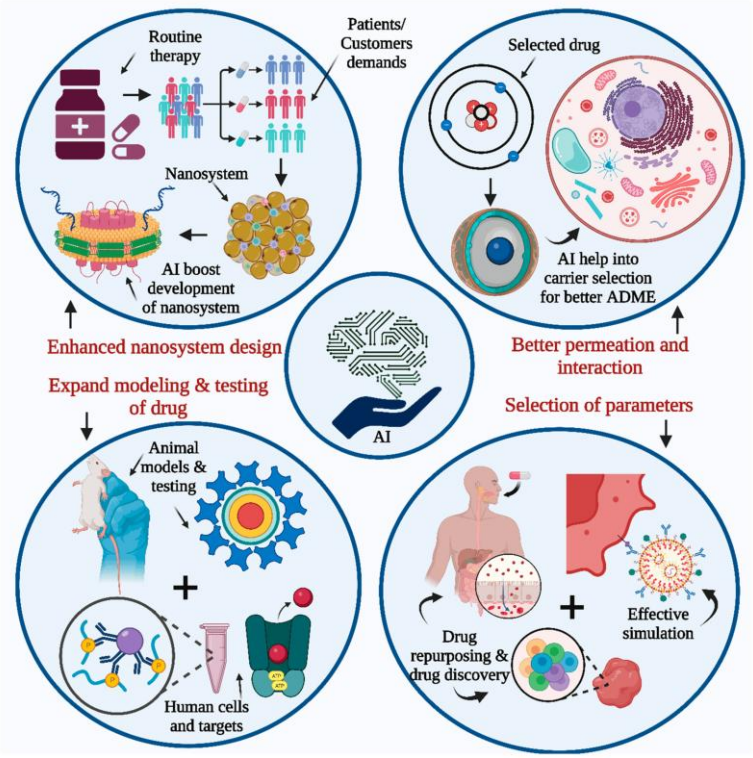

Figure 1. The role of artificial intelligence in drug development and research [5].

1.8. Disadvantages of AI Technology

The disadvantages of artificial intelligence technology include the following.

a) Launching artificial intelligence requires spending a lot of money. The complex design of equipment, as well as its maintenance and

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repair, entails significant costs. To design an AI system, the research and development department needs a lot of time. These systems constantly require software updates. Additionally, the process of reinstalling and restoring devices is time-consuming and involves significant costs.

b) Robots equipped with artificial intelligence technology, due to their human-like thinking ability and lack of emotions, perform assigned tasks more accurately and continue their work without judgment. However, when faced with unknown challenges, these robots cannot make decisions and may provide incorrect information.

c) Human resources can improve through their experiences, but this is not possible for machines equipped with AI technology.

d) Humans can hear, see, feel, and think. They can use their creativity and ideas. These features are not accessible through machines.

e) The widespread use of AI technology in all fields may lead to widespread unemployment [14], [17], [39].

Results Discussion

Artificial intelligence can transform the pharmaceutical industry in the future and accelerate the process of drug discovery and development. Using artificial intelligence, scientists can design new compounds that help improve drug effectiveness and reduce side effects. Artificial intelligence algorithms will revolutionize the safety assessment process by predicting drug side effects and toxicity. The use of AI in various areas of healthcare is increasingly increasing [5], [40]. The large amount of time and money spent on drug research and development makes the need to employ innovative methods and strategies inevitable [41]. Artificial intelligence has transformed the pharmaceutical industry by combining formulations, optimizing dose ratios, accelerating drug development, predicting biological and drug interactions, cellular responses, and the efficacy of treatments [5], [42]. Drug development is a complex process that involves various stages, including drug discovery, preclinical research, clinical trials, and obtaining regulatory approvals [43]. Artificial intelligence has demonstrated remarkable capabilities in the fields of pharmacokinetics, pharmacodynamics, and drug discovery [44]. With the emergence of advanced computational algorithms and machine learning, artificial intelligence is recognized as an effective tool for predicting and optimizing the pharmacokinetics and pharmacodynamics of drugs [45], [46]. Overall, advances in artificial intelligence, especially deep neural network models, can help address some of the current challenges. This in turn can improve the efficiency of modeling and simulation in the process of drug discovery and development [47].

In 2025, Jin et al achieved significant results in fields such as automatic identification of drug molecular structures, interpretation of drug action mechanism maps, and health guide content generation. This study not only demonstrated the scope of The application of artificial intelligence in the field of popular pharmaceutical sciences but also provided a strategic reference for optimizing methods of knowledge dissemination and promoting the safe public use of medicines [48]. In 2025, Vinothini et al found that artificial machine intelligence (AMI) has emerged as a revolutionary force in pharmaceutical research and development, fundamentally transforming traditional approaches to drug discovery, formulation science, and therapeutic applications. They also found that integrating AMI into pharmaceutical processes significantly increased data processing efficiency and predictive accuracy in drug efficacy evaluation. In their review,

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they found that significant advances have been made in vaccine development, where AMI accelerates antigen selection and immune response prediction. Despite these advances, the pharmaceutical sector faces challenges, including ethical considerations, in implementing AMI. As AMI continues to evolve, strategic implementation and ethical considerations will be critical in maximizing its potential for healthcare innovation [49]. In 2024, Singh et al found that AI is increasingly being used to optimize and personalize various aspects of the pharmaceutical industry, especially in drug discovery. Traditional drug development methods are time-consuming, costly, and less efficient, often taking about a decade and costing billions of dollars. Integrating artificial intelligence (AI) techniques addresses these challenges. Furthermore, it plays an important role in drug screening by predicting toxicity, bioactivity, ADME (absorption, distribution, metabolism, and excretion) properties, physicochemical properties, and more [50]. In 2024, Bhatt et al found that artificial intelligence is useful in optimizing clinical trials, thereby improving trial design and cost-effectiveness and enhancing patient safety. Notable in their study were AI-based strategies for enhancing drug delivery, creating smart drug delivery systems engineered to target specific cells or organs, leading to increased efficacy while simultaneously reducing adverse side effects. The findings of this study underscored the enormous potential of artificial intelligence in reshaping the pharmaceutical industry and thus increasing the quality of life of patients worldwide [51]. In 2024, Garg et al. examined how artificial intelligence and its technologies are increasing efficiency and accuracy in pharmaceutical research. This study demonstrated the role of machine learning workflows in optimizing drug formulation processes, with a focus on structure- and ligand-based drug design. They found that the potential of nanotechnology to revolutionize health care, including drug delivery and microscopic interventions, depends on the science. In addition, they showed the exciting prospect of nanorobots equipped with artificial intelligence, showing promise for targeted drug delivery and tumor therapy [52]. Based on the research conducted, we can conclude that artificial intelligence (AI) has had a significant impact on the pharmaceutical industry. This technology can analyze huge amounts of biological and chemical data to identify drug compounds, which leads to a reduction in time and costs. However, continued investment and research in AI bring exciting horizons for optimizing drug development processes.

Conclusions

In general, it can be concluded that artificial intelligence in the pharmaceutical industry can be used in areas such as new drug discovery, drug side effect prediction, drug design, disease diagnosis, and also pharmacological research. This technology improves the drug design process by improving the efficiency and accuracy of predicting drug behavior, interactions, and properties. This approach significantly reduces the costs of clinical trials, which leads to the development of more effective drugs. The creation of new drugs is very important in drug development and offers the potential to increase bioavailability and targeted delivery. However, the traditional trial-and-error approach to formulation development requires extensive resources and time-consuming in vivo and laboratory experiments, and this technology has somewhat facilitated these challenges. Considering the increasing progress of artificial intelligence, we suggest

that in the future, research should be carried out to identify more features of artificial intelligence to discover drugs.

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Conflicts of interest

None declared.

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