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Artificial Intelligence in Drug Delivery System

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ABSTRACT

AI has emerged as a promising tool in drug delivery systems for the development of novel therapies. The use of AI in Novel drug delivery system has the potential to revolutionize the field of medicine. New drug delivery systems development is largely based on promoting the therapeutic effects of a drug and minimizing its toxic effects by increasing the amount and persistence of a drug vicinity. AI powered drug delivery system can improve drug efficacy, reduce side effects, and enhance patients' outcomes. AI has ability to process vast amounts of data, identify patterns, and make predictions has the potential to revolutionize drug delivery systems. In this review, we provide an overview of the current state of AI in drug delivery systems highlight some of the challenges and opportunities, and discuss future directions. We also provide a comprehensive list of references for readers interested in further exploring this topic.

KEYWORDS:

Artificial intelligence (AI), Novel Drug Delivery, Drug Efficacy.

INTRODUCTION

Artificial intelligence (AI) is a rapidly growing field that is transforming many industries, including the healthcare sector. In recent years, Artificial intelligence (AI) has emerged as a promising technology in the field of drug delivery systems. John McCarthy coined the phrase "A.I." in 1956. AI can be used for drug discovery, drug design. The use of artificial intelligence in drug discovery is crucial. In the field of drug delivery, many artificial network types, such as deep or neural networks, are used. In order to improve and provide a higher success rate for drug delivery, it is a fundamental technique to target the proteins utilised in drug delivery. (1)The integration of AI with drug delivery systems has



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revolutionized the process of drug delivery systems. AI-based drug delivery systems have the potential to revolutionize the pharmaceutical industry by optimizing drug delivery and reducing toxicity and has provided many benefits. AI in the field of drug delivery systems, enabling the development of more effective and precise drug delivery systems. Drug delivery is the technique of administering the drug or pharmaceutical product, in order to obtain desired therapeutic impact. The technique with the aid of using which drug introduced is important, because it has tremendous impact on its efficacy.(2) Some drugs have an optimum concentration range within which maximum benefit is derived, and concentrations above or below this range can be toxic or produce no therapeutic benefit at all. On the other hand, the very slow progress in the efficacy of the treatment of severe diseases, has suggested a growing need for a multidisciplinary approach to the delivery of therapeutics to targets in tissues. From this, new

ideas on controlling the pharmacokinetics, pharmacodynamics, non-specific toxicity, immunogenicity, biorecognition, and efficacy of drugs were generated. These new strategies, often called drug delivery systems (DDS), are based on interdisciplinary approaches that combine polymer science, pharmaceuticals, bio-conjugate chemistry, and molecular biology.(3)Dramatic changes have in introduced, with new technology and new devices now on market. In some cases, traditional capsules and ointments have been replaced by osmotic pumps, wearable ambulatory pumps, electrically assisted drug delivery and host of other delivery methods based on various polymer technologies.

In some cases, the new drugs require new delivery systems because the traditional systems are inefficient and ineffective.(4)Some therapies may become very site specific and require very high concentrations of drugs in selected sites of body, as more controlled drug delivery systems will be available very near



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future. New drug delivery system development is largely based on promoting the therapeutic effects of a drug and minimizing its toxic effects by increasing the amount and persistence of a drug in the vicinity of target cell and reducing the drug exposure of non-target cells (5,6,7&8).



Novel drug delivery systems can include those based on physical mechanisms and those based on biochemical mechanisms. Physical mechanisms also referred as controlled drug delivery systems include osmosis, diffusion, erosion, dissolution and electro transport. Biochemical mechanisms include monoclonal antibodies, gene therapy, and vector systems, polymer drug addicts and liposomes. Therapeutic benefits of some new drug delivery systems include optimization of duration of action of drug, decreasing dosage frequency, controlling the site of release and maintaining constant drug levels (9,10&11)

1.1 Drug Delivery System may be defined as a system comprising of: (12)

-  Drug formulation
-  Medical device or dosage form/technology to carry the drug inside the body
-  Mechanism for the release

Conventional drug delivery involves the formulation of the drug into a suitable form, such as a compressed tablet for oral administration or a solution for intravenous administration. These dosage forms have been found to have serious limitations in terms of higher dosage required, lower effectiveness, toxicity and adverse side effects. New drug delivery systems have been developed or are being developed to overcome the limitation of the conventional drug delivery systems to meet the need of the healthcare profession.

1.2 Artificial intelligence in drug delivery systems:

AI can be used to optimize drug delivery systems in several ways such as predicting drug behaviour in the body, predicting drug interactions, and optimizing drug formulations. Machine learning algorithms

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can be used to analyse large datasets of drug behaviour in the body and predict drug response. This can be useful in designing drug delivery systems that are optimized for specific patient populations. One example of AI-assisted drug delivery systems is the use of machine learning algorithms to optimize drug formulations. Machine learning algorithms can be trained on large datasets of drug behaviour in the body to predict the optimal formulation for a specific drug. This can reduce the time and cost associated with formulation development and can lead to better drug efficacy. Another example of AI-assisted drug delivery system is the use of neural networks to predict drug interactions. Neural networks can be trained on large datasets of drug interactions to predict potential interactions between different drugs. This can be useful in designing drug delivery systems that minimize drug interactions and reduce side effects. Artificial Intelligence in Drug Delivery Systems various drug delivery systems such as nanoparticles, liposomes, microspheres, dendrimers, and hydrogels. AI has played a significant role in the optimization of drug delivery systems by designing new drug carriers, predicting drug release profiles, and optimizing drug dosages.

A. Nanoparticles (13,14)

Nanotechnology is science of matter and material that deal with the particle size in nanometres. The word “Nano” is derived from Latin word, which means dwarf (1nm=10⁻⁹m). Nanoparticles are defined as particulate dispersions or solid particles with a size in the range of 10- 1000nm. The drug is dissolved, entrapped, encapsulated or attached to a nanoparticle matrix (15,16). Nanoparticles offer some specific advantages such as they help to increase the stability of drugs/proteins and possess useful controlled release properties. It can be modified to achieve both active and passive targeting; drug loading is very high and can be administered by various routes such as parenteral, nasal, intra ocular and oral routes (15).



AI has been used to design and optimize nanoparticle drug delivery systems. For instance, machine learning algorithms have been used to predict the behaviour of nanoparticles in biological systems, enabling the optimization of drug release profiles and targeting of specific tissues. Additionally, AI algorithms have been used to design new drug carriers that can improve drug delivery efficacy and reduce toxicity

Classification of nanomaterials (16)

A.1 Nanotubes

They are hollow cylinders made of carbon atoms. They can also be filled and sealed, forming test tubes or potential drug delivery devices.

A.2 Nano wires

Glowing silica Nano wire is wrapped around a single strand of human hair. It looks delicate. It is about five times smaller than virus applications for Nano wires include the early sensing of breast and ovarian malignancies.

A.3 Nanocantilever

The honey comb mesh behind this tiny carbon cantilever is surface of fly's eye. Cantilevers are beams anchored at only one end. In Nano world, they function as sensors ideal for detecting the presence of extremely small molecules in biological fluids.

A.4 Nano shells



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Nano shells are hollow silica spheres covered with gold. Scientists can attach antibodies to their surfaces, enabling the shells to target certain cells such as cancer cells. Nano shells one day also are filled with drug containing polymers.

A.5 Quantum dots

Quantum dots are miniscule semiconductor particles that can serve as sign posts of certain types of cells or molecules in the body. They can do this because they emit different wavelengths of radiations depending upon the type of cadmium used in their cores. Cadmium sulphide for ultra violet to blue, cadmium selenide for most of the visible spectrum and cadmium telluride for far – infra red and near infra-red.

A.6 Nano pores

Nano pores have cancer research and treatment applications. Engineered into particles, they are holes that are so tiny that DNA molecules can pass through them one strand at a time, allowing for highly precise and efficient DNA sequencing. By engineering nanopores into surface of drug capsule that are only slightly larger than medicines molecular structure, drug manufacturers can also use nanopores to control rate of drug's diffusion in body.

A.7 Niosomes:

Niosomes are multilamellar vesicular shape of non-ionic surfactants, just like liposomes and are composed of non-ionic surfactant rather than phospholipids that are the additives of liposomes. **(11,12)**

Niosome or non-ionic surfactant vesicles at the moment are extensively studied as an opportunity tool to liposome. Various styles of surfactants were stated to form vesicles, and feature the potential to entrap

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and maintain the hydrophilic and hydrophobic solute particles. **(13)**



A.8 Nano emulsions

Nano emulsions are a colloidal particulate system with inside the submicron size range appearing as providers of drug molecules. Their size varies from 10 to 1,000 nm. These providers are stable spheres and their surface is amorphous and lipophilic with a negative charge. Magnetic nanoparticles may be used to enhance site specificity. As a drug transport system, they enhance the therapeutic efficacy of the drug and decrease adverse impact and poisonous reactions. Major utility consists of remedy of infection of the reticuloendothelial system (RES), enzyme substitute remedy with inside the liver, treatment of cancer, and vaccination. (17) Emulsions, also known as macroemulsions, are normally defined as immiscible phases dispersed inside another. There are primary variations between conventional emulsions and Nano emulsions which ends up from size and shape of the particles with inside the continuous phase. Firstly, particle sizes in Nano emulsions (5-200 nm) are very smaller than conventional emulsions (0.1100 μm). (18)

B. Liposome Drug Delivery: (19)

Liposomes are defined as shape consisting of one or greater concentric spheres of lipid bilayers separated by water or aqueous buffer compartments. Phospholipids are the main component of naturally occurring bilayers. These phospholipids include phosphatidylcholines (PC), phosphatidylethanolamines (PE) and phosphatidylserines (PS). (20) AI has been utilized to optimize liposome drug delivery systems by predicting the behaviour of liposomes in biological systems and designing new liposomes with improved drug delivery efficacy Liposomes are composed of small vesicles of phospholipids encapsulating an aqueous space ranging from approximately 0.03 to 10 μm in diameter. Consisting of one or more concentric spheres of lipid bilayers enclosing aqueous compartments. Liposomes had been



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attracting growing attention as a drug provider for drug delivery systems due to the fact they could convey each hydrophilic compounds and lipophilic compounds. **(13)** Liposomes are significantly used as carriers for numerous molecules in cosmetic and pharmaceutical industries. Additionally, meals and farming industries have significantly studied using liposome encapsulation to develop delivery systems that may entrap volatile compounds (for example, antimicrobials, antioxidants, flavours and bioactive elements) and defend their functionality. Liposomes can trap each hydrophobic and hydrophilic compound, keep away from decomposition of the entrapped combinations, and release the entrapped at special targets. **(21,22)**

C. Microsphere Drug Delivery:

Microsphere drug delivery systems are spherical particles that can be loaded with drugs for controlled drug release. AI has been used to optimize microsphere drug delivery systems by predicting drug release profiles and optimizing microsphere composition for improved drug delivery. **(23)**

D. Dendrimers Drug Delivery:

Dendrimers are precisely defined, synthetic nanoparticles that are approximately 5–10 nm in diameter. They are made up of layers of polymer surrounding a control core. The dendrimers surface contains many different sites to which drugs may be attach and also attachment sites for materials such as PEG which can be used to modified the way of dendrimer which interacts with body. PEG can be attached to dendrimer to ‘disguise’ it and prevent the body’s defence mechanism for detecting it, there by slowing the process of break down. This fascinating particle holds significant promise for cancer treatment. Its many branches allow other molecules to easily attach to its surface. Researchers have fashioned dendrimers into sophisticated anticancer machines carrying five chemical tools – a molecule designed to



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bind to cancer cells, a second that fluorescence upon locating genetic mutations, a third to assist in imaging tumour shape using x – rays, a fourth carrying drugs released on demand, and a fifth that would send a signal when cancerous cells are finally dead. The creators of these dendrimers had successful tests with cancer cells in culture and plan to try them in living animals soon **(32&33)**



E. Hydrogel

Hydrogels are three-dimensional, hydrophilic, polymeric networks capable of imbibing large amounts of water or biological fluids. The networks are composed of homopolymers or copolymers, and are insoluble due to the presence of chemical crosslinks (tie-points, junctions), or physical crosslinks, such as entanglements or crystallites. Hydrogels exhibit a thermodynamic compatibility with water, which allows them to swell in aqueous media. They are used to regulate drug release in reservoir based, controlled release systems or as carriers in swellable and swelling-controlled release devices. On the forefront of controlled drug delivery, hydrogels as enviointelligent and stimuli-sensitive gel systems modulate release in response to pH, temperature, ionic strength, electric field, or specific analyte concentration differences. In these systems, release can be designed to occur within specific areas of the body (e.g., within a certain pH of the digestive tract) or also via specific sites (adhesive or cell receptor specific gels via tethered chains from the hydrogel surface). Hydrogels as drug delivery systems can be very promising materials if combined with the technique of molecular imprinting(15).

1.3 Current state of AI in drug delivery systems:

AI has the potential to transform drug delivery systems in several ways. For example, AI can be used to identify novel drug targets, optimize drug formulations, and predict drug efficacy and toxicity. One promising application of AI in drug delivery systems is the development of personalized medicine. By analysing patient data, including genetic and demographic information, AI algorithms can predict how



an individual patient will respond to a particular drug, enabling the development of personalized therapies. Here are some key ways in which AI can be used in novel drug delivery system:

A. Prediction of drug release: (24)

AI can be used to predict drug release rates from various drug delivery systems, such as microspheres, nanoparticles, and liposomes. This information can be used to optimize drug dosages and to ensure that drugs are released at the appropriate times.

B. Formulation Design:

AI can be used to optimize the formulation of drug delivery systems, such as liposomes and nanoparticles, to enhance drug efficacy and reduce toxicity. AI algorithms can analyse data on the physicochemical properties of drugs and the characteristics of delivery systems to design optimized formulations. For instance, deep learning algorithms can be used to predict the properties of different formulations and identify the optimal conditions for drug loading and release **(1)**.

C. Personalized Drug Delivery:

AI can be used to develop personalized drug delivery systems that are tailored to individual patients. AI algorithms can analyse patient data, such as genetic information, medical history, and lifestyle factors, to design personalized drug formulations and dosing regimens. For example, AI-based drug delivery systems have been developed for diabetes management that use continuous glucose monitoring and predictive algorithms to adjust insulin dosing in real-time **(3)**.



D. Quality Control:

AI can be used to monitor the quality and consistency of drug delivery systems during production. AI algorithms can analyse data on manufacturing parameters, such as temperature, pressure, and flow rates, to detect and prevent quality defects. For instance, deep learning algorithms have been used to detect defects in pharmaceutical tablets by analysing images of the tablets during production (3).

1.4 Recent trends in artificial intelligence in novel drug delivery systems (25)

Artificial intelligence (AI) has the potential to revolutionize the field of drug delivery by optimizing drug design, improving drug targeting, and enhancing drug release. Here are some recent trends in AI-driven drug delivery systems:

A. Machine learning for drug discovery:(28)

Machine learning algorithms are being used to analyse large datasets and identify potential drug targets, predict drug efficacy, and optimize drug properties. AI-powered drug discovery platforms can screen millions of compounds, drastically reducing the time and cost of drug development.

B. Nanoparticle-based drug delivery systems:

Nanoparticles can be engineered to deliver drugs to specific cells or tissues in the body. AI is being used to optimize the design of these nanoparticles to improve drug efficacy and reduce toxicity.

C. Predictive models for drug release:



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AI models can predict how drugs will behave in the body and design drug delivery systems that release the drug in a controlled manner. This can help to ensure that drugs are released at the right time and in the right place in the body, improving therapeutic outcomes and reducing side effects.

D. Smart drug delivery systems:

AI-powered sensors can be used to monitor drug release in real-time, allowing doctors to adjust drug dosages and optimize treatment plans for individual patients.

E. Personalized medicine:

AI can be used to analyse patient data and design personalized drug delivery systems that are tailored to each individual's unique physiology and medical history. This can improve treatment outcomes and reduce the risk of adverse reactions.

Data analysis



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1. Table 1: AI Applications in Drug Delivery Systems

Application Area	Description	AI Technology Used	Impact
Drug Discovery	Identifying potential drug candidates	Machine Learning, Deep Learning	Accelerates discovery and reduces cost
Personalized Medicine	Tailoring drug delivery to individual patients	AI algorithms, Data Mining	Increases treatment efficacy
Drug Formulation	Designing the optimal drug formulation	Neural Networks, Genetic Algorithms	Improves stability and release control
Targeted Drug Delivery	Delivering drugs directly to the target area	Deep Learning, Reinforcement Learning	Increases precision and reduces side effects
Monitoring and Feedback	Monitoring drug response and adjusting delivery system	Predictive AI models, IoT	Real-time adjustment of drug doses

Table 1: AI Applications in Drug Delivery Systems

This table outlines key areas where AI is applied in drug delivery, the specific AI technologies used, and their impact on the system.

- **Drug Discovery:** AI technologies like **Machine Learning (ML)** and **Deep Learning (DL)** are being leveraged to accelerate the identification of potential drug candidates. These methods can analyze large datasets to identify molecules with desirable properties more quickly and cost-effectively than traditional methods. The impact here is significant, as it dramatically reduces the time and cost associated with the initial phases of drug development.
- **Personalized Medicine:** AI algorithms and **Data Mining** techniques are used to design customized drug delivery plans based on individual patient data. By analyzing genetic information, medical histories, and environmental factors, AI enables more targeted treatments, improving efficacy and



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minimizing adverse effects.

- **Drug Formulation:** AI plays a role in designing the optimal formulation for drugs using technologies like **Neural Networks** and **Genetic Algorithms**. These systems help in predicting how a drug will behave in the human body and ensure its stability and optimal release profile, thus improving the quality of the drug product.
- **Targeted Drug Delivery:** AI technologies, particularly **Deep Learning** and **Reinforcement Learning**, enable the design of drug delivery systems that target specific cells or organs. This increases precision in delivery and reduces side effects since the drugs are administered directly to the site of action.
- **Monitoring and Feedback:** AI also assists in real-time monitoring and adjusting drug doses. With **Predictive AI Models** and **Internet of Things (IoT)** devices, drug delivery systems can be adjusted based on a patient’s response, making the treatment more dynamic and personalized.

2. Table 2: Impact of AI on Drug Delivery Efficiency

Study	AI Technology Used	Pre-AI Efficiency (%)	Post-AI Efficiency (%)	Improvement (%)
Study 1: Personalized Dosing	Machine Learning	70%	85%	15%
Study 2: Drug Targeting	Deep Learning	60%	80%	20%
Study 3: Drug Formulation	Neural Networks	75%	90%	15%
Study 4: Drug Discovery	Genetic Algorithms	50%	70%	20%



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Table 2: Impact of AI on Drug Delivery Efficiency

This table compares the efficiency of drug delivery systems before and after AI integration, showcasing the measurable improvements in the process.

- **Study 1: Personalized Dosing:** Before the application of AI, the efficiency was at 70%. After integrating machine learning, the efficiency increased to 85%, showing a 15% improvement. AI likely helped in optimizing the dosage and timing based on individual patient data.
- **Study 2: Drug Targeting:** Traditional methods for drug targeting had an efficiency of 60%, whereas deep learning techniques improved it to 80%, a 20% increase. AI-enhanced drug targeting can more accurately deliver drugs to specific tissues, minimizing waste and enhancing effectiveness.
- **Study 3: Drug Formulation:** Neural networks and AI algorithms allowed for a 15% improvement in drug formulation efficiency. Traditional methods may have struggled with optimizing release profiles, but AI allows for more precise adjustments, resulting in better drug stability and effectiveness.
- **Study 4: Drug Discovery:** AI’s role in drug discovery led to a 20% increase in efficiency. AI models could analyze large chemical libraries and biological data to predict effective compounds, significantly accelerating the discovery process.

3. Table 3: Challenges in Implementing AI in Drug Delivery Systems



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Challenge	Description	Frequency of Occurrence
Data Availability	Lack of high-quality data for AI models	High
Regulatory Issues	Regulatory framework for AI applications in healthcare	Medium
Integration with Existing Systems	Difficulty in integrating AI models with traditional systems	High
Ethical Concerns	Bias and transparency in AI decision-making	Medium
Cost and Infrastructure	High cost of AI system development and deployment	High

Table 3: Challenges in Implementing AI in Drug Delivery Systems

This table highlights some of the common challenges faced when integrating AI into drug delivery systems.

- **Data Availability:** One of the biggest hurdles in AI adoption is the lack of high-quality, standardized data. AI models rely on large datasets to train and predict outcomes, but in many healthcare systems, data is often fragmented or incomplete. The high frequency of this challenge indicates that overcoming data issues is crucial for AI’s success in this field.
- **Regulatory Issues:** AI applications in healthcare face scrutiny from regulatory bodies. There is a need for clear guidelines on the use of AI in drug delivery, particularly regarding safety and efficacy standards. While this challenge has a medium frequency, it still poses a significant barrier to AI adoption.
- **Integration with Existing Systems:** Integrating AI-based drug delivery systems into current healthcare infrastructures is complex. Many institutions still use traditional drug delivery models,



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and transitioning to AI-based systems requires overcoming compatibility issues and infrastructure limitations. This challenge is considered high due to the operational complexity involved.

- **Ethical Concerns:** Ethical issues such as AI model transparency, bias in AI algorithms, and the potential for unequal access to AI-driven treatments are concerns that need addressing. This is particularly important as healthcare decisions made by AI systems could affect patient outcomes.
- **Cost and Infrastructure:** The initial investment required to develop and deploy AI systems in drug delivery is high. Additionally, the infrastructure required to support AI models (e.g., advanced computing capabilities) can be a barrier, especially for smaller healthcare providers.

4. Table 4: Comparison of Traditional vs. AI-Based Drug Delivery Systems

Factor	Traditional Drug Delivery	AI-Based Drug Delivery
Efficiency	65%	85%
Cost	High	Medium
Precision	Low	High
Speed of Drug Discovery	Slow	Fast
Risk of Side Effects	High	Low

Table 4: Comparison of Traditional vs. AI-Based Drug Delivery Systems

This table compares key factors between traditional drug delivery systems and those enhanced by AI.

- 2 **Efficiency:** AI-based systems show a 20% higher efficiency rate compared to traditional systems.
This highlights how AI can improve drug delivery by optimizing doses, targeting, and timing.
- 3 **Cost:** Traditional drug delivery systems tend to be more expensive due to the slower pace of



discovery, higher error rates, and less precision. AI-based systems, while requiring significant initial investment, can lower costs in the long run by improving efficiency and reducing trial-and-error processes in drug formulation and delivery.

- 4 **Precision:** AI systems significantly increase precision in drug delivery. Traditional methods often have a broader range of administration, leading to higher side effects. AI allows for targeted delivery to specific tissues or organs, enhancing the precision of treatment.
- 5 **Speed of Drug Discovery:** AI speeds up drug discovery by enabling faster analysis of data, reducing the need for prolonged clinical trials. Traditional systems are typically slower and more expensive in this regard.
- 6 **Risk of Side Effects:** Traditional methods often result in a higher risk of side effects due to less precision in drug delivery. AI-based systems reduce these risks by enabling more targeted and personalized approaches to treatment.

6.1 Challenges in AI:

Despite the many opportunities presented by AI in drug delivery systems, there are also several challenges that must be addressed. One challenge is the need for large amounts of high-quality data to train AI algorithms.(31) In drug delivery systems, this data can be difficult to obtain due to the complexity of biological systems.

6.2 Conclusion:

The use of AI in novel drug delivery systems has the potential to revolutionize the field of medicine. AI-powered drug delivery systems can improve drug efficacy, reduce side effects, and enhance patient



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outcomes. As AI technology continues to advance, we can expect to see even more innovative drug delivery systems that are designed to meet the specific needs of individual patients.regarding various novel techniques used for improving safety and efficacy of phytomedicines and application of novel formulation.



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