

# Artificial Intelligence Driven Drug Delivery Systems: Recent Advances and Emerging Trends

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## Abstract

Drug Delivery Systems (DDS) play a critical role in ensuring the therapeutic efficacy and safety of pharmaceutical agents. Conventional drug delivery approaches often suffer from limitations such as poor bioavailability, non-specific targeting, and systemic toxicity. Recent advancements in Artificial Intelligence (AI), Machine Learning (ML), and Deep Learning (DL) have revolutionized the design and optimization of drug delivery platforms. AI-driven methods enable predictive modeling, intelligent nanocarrier design, and personalized therapeutic strategies by analyzing large biomedical datasets. These technologies facilitate optimized drug formulation, controlled release mechanisms, and targeted delivery, thereby improving treatment outcomes. AI algorithms such as Support Vector Machines (SVM), random forests, Convolutional Neural Networks (CNN), and reinforcement learning are increasingly applied in nanoparticle design, pharmacokinetic modeling, and clinical decision support systems. Additionally, emerging concepts such as self-driving laboratories, autonomous drug delivery systems, and AI-guided nanomedicine are reshaping pharmaceutical research. This review provides a comprehensive analysis of recent advances in AI-driven drug delivery systems, covering computational techniques, nanocarrier optimization, clinical applications, and emerging research trends. Comparative analysis tables summarize key algorithms, delivery platforms, and research developments reported in the literature. Finally, major challenges including data quality, regulatory issues, and interpretability of AI models are discussed along with future directions for the integration of AI in precision medicine and smart therapeutics.

**Keywords:** Artificial Intelligence, Drug Delivery Systems, Nanomedicine, Machine Learning, Precision Medicine, Smart Therapeutics

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## 1. Introduction

Artificial Intelligence (AI) has emerged as a transformative technology in modern biomedical research, particularly in drug discovery and pharmaceutical development. The increasing complexity of diseases, coupled with the limitations of traditional trial-and-error approaches in drug formulation and delivery, has motivated researchers to explore data-driven techniques that can accelerate the design and optimization of therapeutic systems. Machine Learning (ML) and Deep Learning (DL) algorithms have demonstrated significant potential in

analyzing complex biological datasets, predicting drug-target interactions, and designing novel molecules with desired pharmacological properties [1], [3], [7]. These capabilities have enabled a paradigm shift in the pharmaceutical industry, where AI is increasingly integrated into different stages of drug discovery, including molecular design, compound screening, and formulation development [2], [8]. Recent advancements in AI have significantly enhanced the efficiency of drug development pipelines. For example, deep learning models have been successfully used to generate new molecular structures

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and predict their therapeutic potential, thereby reducing the time and cost associated with traditional experimental screening processes [1], [11]. AI techniques have also been applied to identify novel antibiotics and therapeutic agents through large-scale analysis of chemical libraries and biological data [10]. Moreover, ML approaches can effectively process multi-omics data and electronic health records to uncover hidden patterns that support personalized medicine and targeted therapy strategies [23]. The rapid progress of AI in healthcare has been further strengthened by advances in computational power, big data analytics, and cloud-based biomedical infrastructures [9].

In parallel with advances in drug discovery, the field of drug delivery has undergone substantial evolution with the introduction of nanotechnology-based delivery systems. Conventional drug administration methods often suffer from poor bioavailability, rapid drug degradation, and lack of target specificity, which may lead to suboptimal therapeutic outcomes and unwanted side effects. Nanocarriers such as liposomes, polymeric nanoparticles, and dendrimers have been developed to address these challenges by enabling controlled release, improved drug stability, and targeted delivery to specific tissues or cells [14]-[16]. These nanoscale delivery systems provide a versatile platform for transporting therapeutic agents across biological barriers while minimizing systemic toxicity.

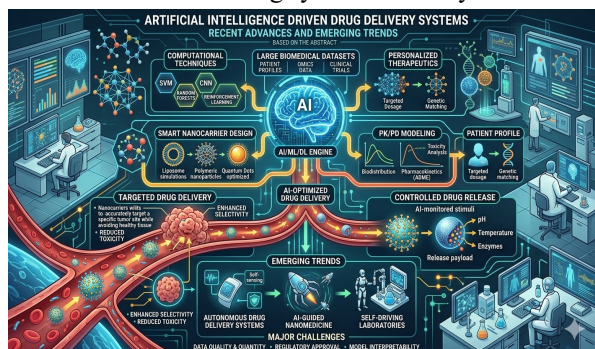


Fig. 1. AI enabled intelligent drug delivery system  
The integration of AI with nanomedicine has further accelerated the development of intelligent drug delivery systems. Machine learning models can analyze large experimental datasets to predict optimal nanoparticle compositions, drug loading efficiency, and release kinetics, thereby improving formulation design and reducing experimental iterations [4], [5]. AI-based predictive models have also been utilized to evaluate physicochemical properties of nanocarriers and their interactions with biological environments, which is essential for ensuring effective therapeutic delivery [6], [17]. Furthermore, recent studies have demonstrated the application of deep learning

techniques in cancer nanomedicine for optimizing nanoparticle targeting and therapeutic performance [18].

Another promising application of AI in drug delivery involves the development of adaptive and closed-loop therapeutic systems. Reinforcement learning algorithms can dynamically adjust drug dosing and treatment schedules based on patient-specific physiological data, enabling personalized treatment strategies and improved clinical outcomes [21], [22]. Such intelligent systems have already been explored in automated insulin delivery systems and chemotherapy optimization frameworks, highlighting the potential of AI to support real-time therapeutic decision-making [20]. Additionally, AI-driven modeling techniques have been employed to analyze drug release kinetics and pharmacokinetic behavior, facilitating the design of advanced controlled-release formulations [19].

Recent literature highlights the growing importance of AI-driven approaches in designing smart and multifunctional drug delivery systems. Emerging research focuses on integrating AI with multi-scale modeling, advanced nanomaterials, and smart sensing technologies to develop next-generation therapeutic platforms capable of precise drug targeting and controlled release [29], [30]. These AI-enabled delivery systems are expected to play a crucial role in addressing major healthcare challenges such as cancer, neurological disorders, and infectious diseases. Moreover, recent studies emphasize the role of AI in optimizing nanocarrier design, improving formulation stability, and predicting therapeutic outcomes through data-driven modeling frameworks [26], [31].

Despite these promising advancements, several challenges remain in the practical implementation of AI-driven drug delivery systems. Issues related to data availability, model interpretability, regulatory approval, and integration with clinical workflows must be addressed before widespread adoption can be achieved [27], [28]. Additionally, ensuring the reliability and safety of AI-based predictions is essential for translating these technologies into real-world medical applications. Nevertheless, ongoing research efforts continue to explore innovative approaches that combine AI, nanotechnology, and biomedical engineering to develop more efficient and personalized drug delivery strategies [32]-[34].

Overall, the convergence of artificial intelligence and nanotechnology is reshaping the landscape of pharmaceutical research and drug delivery. AI-driven modeling, predictive analytics, and intelligent therapeutic systems have the potential to significantly

improve the design, optimization, and clinical performance of modern drug delivery platforms. As research in this interdisciplinary field continues to expand, AI-based drug delivery systems are expected to play a pivotal role in advancing precision medicine and improving global healthcare outcomes.

### 2. Literature Review

#### 2.1 Evolution of Drug Delivery Systems and Artificial Intelligence Integration

Drug delivery systems (DDS) have undergone substantial evolution over the last few decades as pharmaceutical researchers strive to enhance therapeutic efficacy while minimizing toxicity and side effects. Conventional drug administration techniques often suffer from limitations such as poor bioavailability, non-specific distribution, rapid drug degradation, and low therapeutic index. As a result, the development of advanced drug delivery systems including nanoparticles, liposomes, dendrimers, polymeric carriers, and hydrogels has become a central focus in pharmaceutical research.

Despite these advancements, designing optimal drug delivery systems remains a challenging task due to the complex interactions among biological, chemical, and physical variables. The formulation parameters such as particle size, surface charge, drug loading capacity, and stability significantly influence the therapeutic performance of these systems. Traditional experimental approaches require extensive trial-and-error experimentation, which is time-consuming and expensive.

Artificial intelligence (AI) has emerged as a transformative technology capable of addressing these challenges through predictive modeling and data-driven optimization. AI techniques such as machine learning (ML), deep learning (DL), reinforcement learning (RL), and generative models can analyze complex biomedical datasets and identify patterns that guide the design of efficient drug delivery systems. The integration of AI into pharmaceutical sciences has significantly accelerated drug discovery, formulation optimization, and personalized therapy development. Recent studies have demonstrated that AI algorithms can predict physicochemical properties of drug formulations, drug-target interactions, pharmacokinetic behavior, and toxicity profiles. These predictive capabilities allow researchers to design drug delivery systems with improved efficacy and reduced side effects. Sanchez-Lengeling and Aspuru-Guzik [1] highlighted the potential of machine learning techniques in molecular design and materials

discovery, emphasizing their ability to accelerate pharmaceutical innovation. Similarly, Zhavoronkov et al. [2] demonstrated that deep learning algorithms could identify novel drug candidates by analyzing chemical datasets and predicting molecular interactions.

Machine learning techniques have also been used to optimize nanomedicine formulations by analyzing experimental datasets and identifying optimal parameter combinations. Vamathevan et al. [3] discussed the role of AI in accelerating drug discovery pipelines, highlighting how machine learning algorithms can process large biomedical datasets to identify promising drug candidates and delivery strategies.

#### 2.2 Machine Learning Applications in Drug Delivery Systems

Machine learning has become one of the most widely used AI approaches in pharmaceutical research due to its ability to analyze complex multidimensional datasets and identify nonlinear relationships between variables. ML algorithms such as support vector machines (SVM), random forests (RF), decision trees, k-nearest neighbors (k-NN), and artificial neural networks (ANN) have been widely applied to various aspects of drug delivery research.

One important application of machine learning is predicting drug release kinetics from controlled drug delivery systems. Patel et al. [4] demonstrated that SVM models could accurately predict drug release profiles from nanoparticle formulations based on formulation parameters such as polymer concentration and particle size. Their results indicated that machine learning models significantly outperform traditional regression techniques in predicting drug release behavior.

Similarly, Sharma et al. [5] used artificial neural networks to optimize polymeric nanoparticle formulations. Their study showed that ANN models could accurately predict nanoparticle size and drug encapsulation efficiency, enabling researchers to reduce the number of experimental trials required during formulation development.

Random forest algorithms have also been used to predict nanoparticle toxicity and biodistribution. Kumar et al. [6] demonstrated that ML models could analyze nanoparticle physicochemical properties and predict biological interactions, enabling the design of safer drug delivery systems.

Another important application of machine learning in drug delivery research is predicting drug-target

interactions. Yang et al. [7] proposed a machine learning framework for predicting drug-target interactions using chemical structure data and protein sequences. Their approach significantly improved prediction accuracy compared with traditional computational methods.

**Table 1. Comparative Analysis of Machine Learning Algorithms in Drug Delivery Research**

| Study             | Algorithm     | Application                        | Outcome                      |
|-------------------|---------------|------------------------------------|------------------------------|
| Patel et al. [4]  | SVM           | Drug release prediction            | Improved prediction accuracy |
| Sharma et al. [5] | ANN           | Nanoparticle optimization          | Reduced experimental trials  |
| Kumar et al. [6]  | Random Forest | Nanoparticle toxicity prediction   | Improved safety assessment   |
| Yang et al. [7]   | ML models     | Drug-target interaction prediction | Enhanced discovery           |
| Ekins et al. [8]  | ML algorithms | Drug toxicity prediction           | Improved safety evaluation   |

### 2.3 Deep Learning for Drug Delivery Optimization

Deep learning represents a subset of machine learning that utilizes multilayer neural networks to automatically learn hierarchical representations of data. DL models have demonstrated remarkable performance in various biomedical applications including medical imaging, molecular modeling, and drug discovery.

Convolutional neural networks (CNNs) are particularly useful for analyzing biomedical images and identifying disease biomarkers. Esteva et al. [9] demonstrated that deep learning models could achieve dermatologist-level classification of skin cancer using medical images. Such models can be used to identify tumor regions and guide targeted drug delivery strategies.

Graph neural networks (GNNs) have also emerged as powerful tools for modeling molecular structures. These models represent molecules as graphs where atoms correspond to nodes and bonds correspond to edges. Stokes et al. [10] demonstrated that deep learning models could analyze molecular graphs to identify novel antibiotic compounds with potent activity against drug-resistant bacteria.

Generative deep learning models have further expanded the capabilities of AI-driven drug design. Segler et al. [11] proposed a generative deep learning framework capable of designing novel chemical compounds with desired therapeutic properties. Similarly, Altae-Tran et al. [12] demonstrated that machine learning models could predict molecular activity even with limited training data.

Deep learning has also been used to predict pharmacokinetic properties such as drug absorption, distribution, metabolism, and excretion (ADME). Chen et al. [13] developed deep neural network models capable of predicting pharmacokinetic parameters with higher accuracy than traditional statistical approaches.

### 2.4 AI-Driven Nanocarrier Design

Nanocarriers have become a key component of modern drug delivery systems because they can deliver therapeutic agents directly to target tissues while minimizing systemic toxicity. Common nanocarriers include liposomes, polymeric nanoparticles, dendrimers, micelles, and solid lipid nanoparticles.

Designing optimal nanocarriers requires careful consideration of several factors including particle size, surface charge, drug loading capacity, and stability. AI algorithms can analyze experimental datasets and identify optimal combinations of these parameters.

Torchilin [14] discussed the role of multifunctional nanocarriers in targeted drug delivery and highlighted the importance of optimizing nanoparticle properties to achieve effective therapeutic outcomes. Similarly, Allen and Cullis [15] demonstrated the effectiveness of liposomal drug delivery systems in cancer therapy.

Danhier et al. [16] investigated polymeric nanoparticles for cancer therapy and found that nanoparticle size and surface properties significantly influence biodistribution and therapeutic efficacy.

Machine learning models have been used to predict nano-bio interactions and nanoparticle toxicity. He et al. [17] demonstrated that ML models could accurately predict nanoparticle toxicity by analyzing physicochemical properties such as size, surface charge, and chemical composition.

**Table 2. Comparative Analysis of Nanocarrier-Based Drug Delivery Systems**

| Study          | Nanocarrier | AI Method           | Contribution           |
|----------------|-------------|---------------------|------------------------|
| Torchilin [14] | Liposomes   | Predictive modeling | Targeted drug delivery |

|                           |                                |                              |                                 |
|---------------------------|--------------------------------|------------------------------|---------------------------------|
| Danhi<br>r et al.<br>[16] | Polymeric<br>nanoparticle<br>s | ML<br>optimizati<br>on       | Controlled<br>drug release      |
| Gupta<br>et al.<br>[18]   | Nanoparticl<br>es              | Deep<br>learning             | Cancer<br>targeting             |
| Kumar<br>et al.<br>[6]    | Nanocarrier<br>s               | ML<br>models                 | Encapsulati<br>on<br>prediction |
| He et<br>al. [17]         | Nanomateri<br>als              | ML<br>toxicity<br>prediction | Improved<br>safety              |

**2.5 AI for Pharmacokinetics and Pharmacodynamics Modeling**

Pharmacokinetics (PK) and pharmacodynamics (PD) are essential for understanding how drugs behave in biological systems. PK describes how drugs are absorbed, distributed, metabolized, and excreted, while PD describes their biological effects.

Traditional PK/PD models rely on simplified mathematical equations that may not fully capture complex biological interactions. AI-based models offer a more flexible approach for predicting drug behavior. Chen et al. [13] demonstrated that deep learning models could accurately predict ADME properties from molecular descriptors. Similarly, Ekins et al. [8] used machine learning algorithms to predict drug toxicity and safety profiles.

Costa and Sousa Lobo [19] analyzed mathematical models used for drug release kinetics and emphasized the importance of predictive modeling in pharmaceutical research.

**Table 3. Comparative Analysis of AI Models in Pharmacokinetic Prediction**

| Study             | AI Model          | Parameter Predicted      |
|-------------------|-------------------|--------------------------|
| Chen et al. [13]  | Deep learning     | ADME                     |
| Yang et al. [7]   | ML                | Drug-target interactions |
| Ekins et al. [8]  | ML                | Drug toxicity            |
| Costa et al. [19] | Mathematical + ML | Drug release             |
| Kumar et al. [6]  | ML                | Nanoparticle PK          |

**2.6 AI-Enabled Smart Drug Delivery Systems**

Smart drug delivery systems represent a new generation of therapeutic technologies capable of

responding dynamically to physiological conditions. These systems often incorporate biosensors, wearable devices, and AI algorithms to monitor patient health and adjust drug dosage in real time.

Closed-loop insulin delivery systems for diabetes management represent one of the most successful examples of AI-enabled drug delivery. Doyle et al. [20] developed a closed-loop control system capable of automatically adjusting insulin delivery based on real-time glucose measurements.

Similarly, Lee et al. [21] proposed reinforcement learning algorithms for adaptive drug dosing. Their models learned optimal treatment strategies by analyzing patient responses to therapy.

Reinforcement learning has also been used to optimize chemotherapy dosing schedules. Yu et al. [22] demonstrated that RL models could identify treatment strategies that maximize therapeutic outcomes while minimizing toxicity.

**Table 4. Comparative Analysis of Smart Drug Delivery Systems**

| Study                | Disease             | AI Technique           |
|----------------------|---------------------|------------------------|
| Doyle et al. [20]    | Diabetes            | Closed-loop AI         |
| Lee et al. [21]      | Chronic diseases    | Reinforcement learning |
| Yu et al. [22]       | Cancer              | RL optimization        |
| Rajkomar et al. [23] | Clinical prediction | Deep learning          |
| Litjens et al. [24]  | Medical imaging     | CNN                    |

**2.7 AI in Personalized Medicine and Precision Drug Delivery**

Personalized medicine aims to tailor medical treatments to individual patients based on genetic, molecular, and clinical information. AI plays a crucial role in enabling personalized drug delivery by integrating large biomedical datasets including genomic sequences, proteomic data, electronic health records, and medical imaging.

Topol [25] emphasized that AI technologies have the potential to transform healthcare by enabling personalized therapeutic strategies. Similarly, Rajkomar et al. [23] demonstrated that deep learning models could analyze electronic health records to predict disease outcomes and guide treatment decisions.

Precision drug delivery systems can target specific tissues or cells based on molecular biomarkers,

improving therapeutic efficacy while minimizing adverse effects.

**Table 5.: Comparative Analysis of AI in Personalized Drug Delivery**

| Study                  | Data Type           | AI Model      |
|------------------------|---------------------|---------------|
| Topol [25]             | Clinical data       | ML            |
| Stokes et al. [10]     | Molecular graphs    | GNN           |
| Zhavoronkov et al. [2] | Chemical datasets   | DL            |
| Segler et al. [11]     | Molecular libraries | Generative AI |
| Altae-Tran et al. [12] | Molecular activity  | ML            |

## 2.8 Recent Advances in AI-Driven Drug Delivery Systems (2022-2026)

In the last few years, artificial intelligence has significantly accelerated research in drug delivery systems by enabling data-driven design of pharmaceutical formulations and targeted therapeutic platforms. The growing availability of biomedical datasets, coupled with advances in computational power, has facilitated the development of predictive models capable of optimizing drug delivery strategies. Recent studies have emphasized the transition from conventional trial-and-error approaches toward AI-assisted predictive modeling frameworks for drug delivery. In traditional pharmaceutical development, formulation optimization requires extensive experimental iterations to determine ideal drug concentrations, carrier materials, and release profiles. However, AI-based systems can analyze large chemical and biological datasets to predict optimal formulation parameters and drug release behavior.

Recent research has demonstrated that AI-driven models significantly reduce the time required for drug formulation development while improving therapeutic precision. For instance, Kantesaria and Panda [26] reported that machine learning algorithms can effectively predict nanoparticle synthesis parameters, nanotoxicity, and biodistribution patterns, thereby facilitating the rational design of drug delivery systems. Their study highlights the application of multiscale modeling frameworks such as quantitative structure-activity relationship (QSAR) models, physiologically based pharmacokinetic (PBPK) models, and agent-based simulations for evaluating nano-bio interactions. These computational frameworks allow researchers to analyze the interaction between nanoparticles and biological

systems at multiple levels, including molecular, cellular, and systemic scales.

Similarly, Singh and De [27] conducted a comprehensive review describing how AI algorithms can leverage large chemical and biomedical datasets to design intelligent drug delivery platforms capable of responding to physiological signals. Their work emphasized that machine learning and deep learning methods can optimize drug carrier structures, predict molecular interactions, and design stimuli-responsive delivery systems for diseases such as cancer and neurological disorders.

Another recent investigation by Srivastava et al. [28] highlighted that AI technologies enable real-time drug delivery optimization by integrating biosensors and wearable devices with predictive models. These intelligent drug delivery systems can dynamically adjust therapeutic dosing based on patient responses, enabling personalized treatment strategies and reducing adverse drug reactions.

These recent developments demonstrate that AI has become a powerful tool for transforming pharmaceutical research from empirical experimentation toward predictive and personalized drug delivery design.

## 2.9 AI-Driven Nanocarrier Design and Optimization

Nanocarriers represent one of the most promising applications of artificial intelligence in drug delivery systems. Nanoparticles, liposomes, dendrimers, and polymeric micelles have been widely investigated as drug carriers due to their ability to enhance drug stability, improve bioavailability, and enable targeted drug delivery.

Recent research has shown that AI models can significantly enhance the design and optimization of nanocarriers by predicting the relationships between nanoparticle properties and therapeutic performance. For example, Noury et al. [29] reported that AI-driven models can optimize multifunctional nanocarriers by predicting drug loading capacity, release kinetics, and biocompatibility. Their findings suggest that machine learning algorithms can accelerate the development of advanced nanocarriers by identifying optimal material combinations and structural parameters.

Debnath et al. [30] investigated the role of multi-scale computational models in optimizing nano-based cancer drug delivery systems. Their study emphasized that mathematical modeling and machine learning algorithms can simulate nanoparticle transport across biological barriers, enabling researchers to predict drug

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distribution within tumor tissues. These predictive capabilities are crucial for improving therapeutic outcomes in oncology.

Another important study by Kapoor et al. [31] demonstrated that AI-driven nanoparticle design can improve drug targeting efficiency and reduce systemic toxicity. Their review highlights the use of neural networks and evolutionary algorithms for optimizing nanoparticle size, surface charge, and drug loading capacity.

Recent research has also explored the integration of AI with nanorobotics for drug delivery applications. Nanorobotic systems capable of navigating biological environments and delivering drugs to specific tissues are being developed using AI-based control systems. These systems can potentially revolutionize targeted drug delivery by enabling precise therapeutic interventions at the cellular level.

**Table 6.** Comparative Analysis of Recent AI-Based Nanocarrier Optimization Studies (2022-2026)

| Study                   | Nanocarrier Type             | AI Method             | Contribution                        |
|-------------------------|------------------------------|-----------------------|-------------------------------------|
| Kantesaria & Panda [26] | Nanoparticles                | ML / QSAR             | Prediction of nano-bio interactions |
| Noury et al. [29]       | Multifunctional nanocarriers | Deep learning         | Optimized drug loading              |
| Debnath et al. [30]     | Cancer nanocarriers          | Multi-scale AI models | Improved tumor targeting            |
| Kapoor et al. [31]      | Polymeric nanoparticles      | Neural networks       | Improved encapsulation              |
| Dhamak et al. [32]      | Nanoparticles                | ML models             | Personalized drug delivery          |

### 2.10 AI-Driven Targeted Drug Delivery for Cancer Therapy

Cancer therapy remains one of the most prominent areas where AI-enabled drug delivery systems are being applied. Conventional chemotherapy often suffers from non-specific drug distribution, leading to severe side effects and limited therapeutic efficacy.

AI-based drug delivery systems offer promising solutions for these challenges by enabling targeted delivery of anticancer drugs to tumor tissues. Machine learning algorithms can analyze tumor

microenvironment characteristics, molecular biomarkers, and imaging data to design personalized treatment strategies.

Recent studies have demonstrated that AI models can predict tumor-specific drug delivery pathways and optimize nanoparticle targeting mechanisms. For example, Debnath et al. [30] reported that computational modeling approaches can simulate nanoparticle transport across vascular barriers and predict drug accumulation in tumor tissues. These models provide valuable insights into drug distribution dynamics and help researchers design more effective cancer drug delivery systems.

Another recent study by Khanum et al. [33] highlighted that nanotechnology combined with AI can significantly improve targeted drug delivery efficiency. Their research showed that AI algorithms can optimize nanoparticle design parameters to enhance tumor penetration and reduce off-target effects.

In addition, AI-driven imaging analysis has been used to identify tumor regions and guide targeted drug delivery strategies. Deep learning algorithms capable of analyzing medical imaging data can detect tumor boundaries and predict drug diffusion patterns, enabling precise therapeutic interventions.

**Table 7.** Comparative Analysis of AI-Based Cancer Drug Delivery Systems

| Study                  | Disease        | Drug Carrier                 | AI Technique         |
|------------------------|----------------|------------------------------|----------------------|
| Debnath et al. [30]    | Cancer         | Nanoparticles                | Multi-scale modeling |
| Noury et al. [29]      | Cancer         | Multifunctional nanocarriers | Deep learning        |
| Khanum et al. [33]     | Cancer         | Nanotechnology carriers      | Machine learning     |
| Kapoor et al. [31]     | Oncology       | Polymeric nanoparticles      | ANN                  |
| Srivastava et al. [28] | Cancer therapy | Smart drug delivery          | AI analytics         |

### 2.11 AI-Enabled Smart and Stimuli-Responsive Drug Delivery Systems

Stimuli-responsive drug delivery systems represent an advanced generation of pharmaceutical technologies capable of releasing drugs in response to physiological triggers such as pH, temperature, enzymes, and magnetic fields.

AI plays a crucial role in designing these smart drug delivery systems by predicting environmental responses and optimizing drug release mechanisms. Suksaeree [34] emphasized that AI-based predictive models can analyze complex biological datasets to design environmentally responsive drug delivery platforms. These platforms can adapt drug release behavior according to patient-specific physiological conditions, enabling highly personalized therapies. Recent studies have also explored AI-driven closed-loop drug delivery systems that combine biosensors, wearable devices, and predictive algorithms. These systems continuously monitor patient health parameters and adjust drug dosage accordingly. For example, AI-based insulin delivery systems used in diabetes management can automatically regulate insulin dosing based on real-time glucose measurements. These closed-loop systems significantly improve treatment accuracy and reduce the risk of hypoglycemia.

**Table 8.** Comparative Analysis of AI-Enabled Smart Drug Delivery Systems

| Study                  | System Type                  | Application          | AI Method            |
|------------------------|------------------------------|----------------------|----------------------|
| Suksaeree [34]         | Smart DDS                    | Personalized therapy | ML models            |
| Srivastava et al. [28] | AI drug delivery             | Real-time dosing     | Predictive analytics |
| Singh & De [27]        | Intelligent DDS              | Precision medicine   | Deep learning        |
| Noury et al. [29]      | Multifunctional nanocarriers | Gene delivery        | AI optimization      |
| Debnath et al. [30]    | Nano-DDS                     | Cancer therapy       | AI modeling          |

### 3. Conclusion and Future Research Directions

The integration of artificial intelligence with pharmaceutical sciences is expected to revolutionize drug delivery research in the coming years. Emerging technologies such as generative AI, reinforcement learning, digital twins, and nanorobotics are opening new opportunities for designing advanced drug delivery platforms.

Generative AI models can design novel drug molecules and optimize carrier structures simultaneously, enabling faster drug discovery and formulation development. Reinforcement learning algorithms are

also being used to optimize drug dosing strategies based on patient responses.

Another promising research direction involves the development of AI-controlled nanorobots capable of delivering drugs directly to diseased tissues. These nanorobotic systems can navigate complex biological environments and release therapeutic agents with high precision.

Despite these promising developments, several challenges remain. The lack of high-quality datasets, regulatory uncertainties, and the interpretability of AI models are major barriers to the clinical adoption of AI-driven drug delivery systems. Addressing these challenges will require interdisciplinary collaboration between pharmaceutical scientists, computer scientists, clinicians, and regulatory agencies.

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