RESEARCH PAPER

Artificial Intelligence-Driven Optimization of Drug Delivery Systems for Enhanced Therapeutic Efficacy

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ABSTRACT

Artificial Intelligence (AI) has emerged as one of the transformative force in pharmaceutical sciences, particularly in the context of optimizing drug delivery systems (DDS) to enhance therapeutic efficacy, minimize adverse effects, and improve patient compliance. The following are the common weaknesses associated with the traditional drug delivery methods; poor bioavailability, lack of target specificity and poor pharmacokinetics. Machine learning and deep learning are AI-based approaches that provide high-degree functions of examination of intricate biological details, anticipation of medication behaviour, and intelligent plan frameworks of delivery systems. The goal of the paper is to discuss AI-based optimization of drug delivery systems in detail and touch upon nanoparticle-based delivery, the mechanisms of controlled release, and personalized medicine. The research integrates the predictive analytics and computational modeling of the enhancement of the efficiency of drug targeting, the release kinetics, and the therapeutic outcomes with the simulation validation. A quantitative evaluation on simulated and experimental data indicates a significant enhancement in drug bioavailability and reduced toxicity. The findings demonstrate that AI-based optimization can considerably boost the therapeutic efficiency and, therefore, there is the need to apply AI in the design of the next-generation pharmaceuticals. The paper concludes with a discussion on the problems that relate to the accessibility of the data, regulatory factors and ethical concerns and proposes future research opportunities in scalable, clinically translatable AI-based solutions to drug delivery.

Keywords: Artificial Intelligence, Drug Delivery Systems, Machine Learning, Nanotechnology, Therapeutic Efficacy, Predictive Modeling, Personalized Medicine

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1. INTRODUCTION

The advancement of pharmaceutical sciences has consistently aimed at improving the efficacy and safety of therapeutic interventions. Important in determining the pharmacodynamic and pharmacokinetic properties of therapeutic agents are the drug delivery systems. The traditional drug delivery systems typically cannot deliver the drug to the target site accurately therefore resulting in systemic side effects, and no therapeutic effect (Bae *et al*., 2025). These limitations have seen the development of the high quality systems of delivery like nanoparticles, liposomes and polymer based carriers.

Artificial Intelligence is a new paradigm in this field because it is possible to make decisions based on data and predictive modeling. With AI techniques, there is a simpler way to study large amounts of biomedical data, which allows the patterns that could not be recognized using other analytic methods to be discovered. Machine learning algorithms can predict drug interaction, optimize the dosage form and enhance the delivery efficiency by simulating biological settings.

Integration of AI and drug delivery system will enable the design of smart delivery platforms capable of responding to physiological variables (Zhu *et al*., 2025). These

systems can control the rate of release of drugs based on real time feedback and attain optimum levels of therapeutic concentrations. Individual medicine is also supported, and AI-assisted maximization when the drug delivery strategies are tailored to the unique features of individual patients, who involve genetic profiles and disease states.

This paper discusses the potential of AI to be applied in streamlining drug delivery systems, specifically, by increasing the therapeutic efficacy of drugs through improved targeting, controlled release, and reduced toxicity (Kantesaria *et al*., 2026). The paper analyses computational models, algorithm frameworks and experimental validation techniques to ascertain the impacts of AI-based optimization.

2. LITERATURE REVIEW

According to Bae (2025), the integration of artificial intelligence with nano architectonics represents a transformative advancement in the design of smart targeted drug delivery systems.. The author reiterates that nano architectonics can be employed with AI-based predictive modeling to enable control of nanoscale structures with a great level of accuracy to target diseased tissues in a highly specific manner. The article offers the application of machine learning algorithms to the optimization of nanoparticles size, surface functionality, and drug loading capacity based on the examination of complicated biological data. It is one of the most efficient ways of cellular internalization and minimization of off-target effects, which is a crucial concern in the conventional drug delivery. Bae also discusses AI and the way it is applicable in predicting biological interactions such as corona formation of proteins and immune response that would otherwise have required much validation in the lab. Also shown in the study is the use of AI to achieve real-time flexibility in drug delivery systems whereby the controlled release can be effected in response to environmental stimuli such as pH and temperature. The author comes to the conclusion that AI-based nano architectonics may be able to increase the efficacy of the therapy, not to mention accelerating the process of creating nanomedicines because it is not based on a trial-and-error approach.

According to Zhu (2025), the system of pharmaceutical development and drug delivery is rapidly changing due to artificial intelligence, which activates the use of information-based innovation at different stages of drug development. According to the author, AI techniques, including deep learning and natural language processing, enable one to effectively process a large volume of biomedical data, thereby optimizing the design, formulation, and delivery of drugs. According to Zhu, AI models can predict pharmacodynamics and pharmacokinetics with great accuracy and, as a result, scientists can create delivery systems that will produce the greatest therapeutic effects (Zhu *et al*., 2025). The article also focuses on the application of AI in order to optimize the formulation factors such as excipients selection and release mechanism. The use of AI in finding new drug delivery routes, particularly those related to complicated diseases such as cancer and neurological diseases, is among the notable contributions made. The author also adds that automation based on AI saves time on development, cost, and enhances accuracy. However, challenges related to the data combination and regulatory approval are also noted. The review describes AI as one of the enabling mechanisms of the next-generation pharmaceutical systems, particularly in the case of personalized medicine.

Kantesaria (2026) notes that AI-driven data-driven models can play a crucial role in the optimization of nanocarriers when used in drug delivery. The author provides a descriptive analysis of machine learning techniques that are used to design and optimize nanocarrier systems, including liposomes, dendrimers, and polymeric nanoparticles. The article emphasizes that multidimensional datasets could be examined with the help of AI models to determine the most appropriate combinations of physicochemical properties that influence the performance of drug delivery (Kantesaria *et al*., 2026). Kantesaria highlights the importance of the selection of features and understandability of model towards the assurance of trustworthy predictions. The research reveals that AI could be utilized to an extent that would improve the efficiency of the encapsulation, stability, and controlled release behavior of nanocarriers. In addition, the author discusses the introduction of AI into high-throughput screening methods, which enable the analysis of multiple formulations of nanocarriers in a short time. The constraints that the review takes into consideration are scarcity of data and the need to have standardized datasets to increase the strength of the model. Overall, the study validates AI as a powerful tool to create a nanocarrier-based drug delivery system with the right and effective optimization.

According to Ekpan (2024), one of the largest revolutions in the field of modern healthcare is the synergy of artificial intelligence and drug delivery systems. The author explains the way to enhance all drug delivery processes, such as formulation design and therapeutic monitoring, by making decisions based on the data with the help of AI. The study identifies the use of machine learning algorithms to predict drug behaviour in the biological system, e.g., absorption, distribution, metabolism, and excretion. Ekpan emphasizes that AI-based systems can improve the precision of targeting and reduce the adverse effect, which will improve patient safety and treatment efficacy (Ekpan *et al*., 2024). The paper also mentions the application of AI to develop

intelligent drug delivery systems that can respond to physiological changes in real time. These systems can control the rate of drug release based on the feedback system and this guarantees that optimum therapeutic levels are reached. The author also remarks on the impact of AI on personalized medicine, where the plans of treatment are tailored to the profiles of the patients. Despite such developments, concerns related to the ethical issue and data privacy are witnessed. The study concludes that AI integration is essential to more effective and patient-centered healthcare solutions.

Albukhari (2025) states that AI has significantly facilitated exploration of marine bioactive in cancer treatment, particularly in the context of targeted delivery of drugs. The author examines how the AI-based strategies may be used to identify and maximize the bioactive compounds of marine origins that are more likely to possess unique chemical properties. The article highlights how AI is capable of predicting drug-target interactions and surmounting resistance mechanisms that are bound to be observed during cancer treatment. Albukhari emphasizes that it is possible to design particular delivery systems with the help of AI that can enhance the efficiency of compounds of marine origin and decrease toxicity. The review goes on to describe how AI is combined with omics to identify biomarkers that could be utilized to guide precision therapy. In addition, AI is shown to accelerate the discovery by reducing the experimental screening (Albukhari *et al*., 2025). The author identifies the following challenges; complexity of marine compounds and the requirement of high quality datasets. The study concludes that the precise drug delivery through AI has tremendous potential in improving the outcome of the treatment of cancer through novel use of marine bioactives.

According to Serrano (2024), artificial intelligence in drug discovery and drug delivery is changing the face of personalized medicine, as it enables the creation of an incredibly tailored treatment regimen. The author notes that AI models can be used to integrate multiple sources of data: genomic, proteomic, and clinical data to create personalized treatment plans. The article points out the possibility of using AI to optimize drug delivery processes to make them patient-centred and more effective and reduce the incidence of side effects. Serrano discusses how the deep learning algorithms are applied to the prediction of drug response and the most suitable delivery mechanisms (Serrano *et al*., 2024). Another aspect that is discussed in the review is the application of AI in the real-time monitoring of the treatment outcomes that allow making real-time adjustments in the provision of drugs. The author also includes that AIs used in personalization enhance adherence and healthcare outcomes among patients. However, the problems of standardization of data and transparency of models are encountered. The article concludes that AI is at the heart of the transition to precision medicine, and that it has significant implications in terms of drug delivery innovation.

Suksaeree (2025) introduces AI-based smart and sustainable drug delivery systems as a two-structure solution based on technological innovation and environmental issues. The author provides the roadmap of the creation of the next-generation pharmaceutical systems that are efficient and sustainable. The paper highlights the potential of AI in facilitating drug delivery streamlining to reduce the use of resources and environmental impacts. Suksaeree stresses that with the assistance of AI, it can be possible to build biodegradable and environmentally friendly delivery systems without disrupting a therapeutic effect. The review also addresses the integration of AI and green chemistry principles to develop sustainable formulations. Also, the author explains how AI can be applied to forecast the effect of the lifecycle and how it will be more efficient in the supply chain production of pharmaceuticals (Suksaeree *et al*., 2025. The identified challenges in the study are interdisciplinary cooperation and the integration of sustainability measures into AI models. The author concludes that the future of pharmaceutical paradigm will involve AI-driven sustainable drug delivery systems to address both the medical and environmental problems.

3. METHODOLOGY

The current paper pursues a hybrid and integrative approach, which is a combination of computational modeling, sophisticated machine learning algorithms, and validation of the drug delivery systems through simulation. The methodological framework is designed in such a way that it captures the complexity of biological interactions and pharmaceutical parameters in a systematic manner and makes sure that there is a high level of predictive power (Habeeb *et al*., 2026). The whole process is structured into four large steps: data collection and preprocessing, model development, simulation and optimization, and performance evaluation. All of the phases are intended to lead to the more precise forecast and optimization of therapeutic effectiveness with the help of AI.

3.1 Data Collection and Preprocessing

The initial step is the methodical gathering of quality datasets, in publicly available biomedical and pharmaceutical repositories. These contain databases like PubChem, DrugBank, ChEMBL and other peer-reviewed experimental data, which contain verified data on drug properties and biological activities. The dataset is screened to be diverse in drug type, delivery system and in biological environment.

The data obtained covers a broad spectrum of physicochemical and pharmacokinetic values. These are

the molecular weight, solubility, lipophilicity, particle size, surface charge, encapsulation efficiency, drug release rate and degradation kinetics (Malkawi *et al*., 2024). Moreover, biological response parameters, including cellular uptake efficiency, bioavailability, toxicity, and therapeutic response indicators are included.

Preprocessing of the data is done to enhance the quality and usefulness of the data. This includes dealing with missing values through imputation procedures, standardization of continuous variables to maintain scale consistency, and coding of categorical variables. Outliers are detected with the use of statistical techniques and handled to avoid bias during model training. Min-Max normalization and standardization are used as feature scaling methods, so that they are compatible with various machine learning methods.

In order to increase the strength of the dataset, feature engineering is used. Primary variables are used to calculate derived variables like the surface area-to-volume ratio, diffusion coefficient, and release kinetics constants. The step enhances the model capability of capturing complex relationships in the data.

3.2 Model Development and Algorithmic Framework

The second phase concentrates on the construction of predictive models based on machine learning and deep learning technologies. They are three major algorithms, namely: Random Forest, Support Vector Machines (SVM), and Deep Neural Networks (DNN). The choice of these algorithms is based on their capabilities to process nonlinear relationships and high-dimensional data, which are typical of drug delivery systems.

Random Forest model is employed because of its capability to learn in an ensemble way, which increases the accuracy of prediction by combining a series of decision trees (Khalifa *et al*., 2025). It is especially useful to determine the importance of features and in dealing with noisy data. Support Vector Machine model is used due to its robustness in classification and regression, and where the distribution of the data is complicated and not linearly separable. Radial basis function (RBF) is a type of kernel functions that are employed to project input features to higher dimensional spaces.

Deep Neural Network model is modeled to include more than one hidden layer that can represent complex patterns in the data. The structure consists of input layers based on the features chosen, multiple fully connected hidden layers that use nonlinear activation functions and an output layer that estimates the drug delivery performance metrics (Hanaffi *et al*., 2025). Regularization methods like dropout and batch normalization are included to avoid overfitting and enhance generalization.

The selection of features is a very important step in the development of the model. The methods used to determine the most influential variables include Recursive Feature Elimination (RFE), Principal Component Analysis (PCA) and correlation-based filtering. This simplifies the models and increases computational efficiency without compromising predictive accuracy.

The grid search and cross-validation techniques are used to perform hyperparameter tuning. The parameters that are optimized include the number of trees used in Random Forest, type of kernel and regularization parameter in SVM, learning rate, batch size and number of epochs in DNN to attain the best performance.

3.3 Simulation and Optimization Framework

The third phase entails validation and optimization of drug delivery systems through simulation. The drug release kinetics, transport mechanisms, and the distribution in the biological systems are simulated using computational tools and mathematical models. These simulations are used to test the performance of AI-based models in different conditions in a controlled setting.

Established mathematical frameworks are used to model drug release kinetics: zero-order, first-order, Higuchi, and Korsmeyer Peppas models. These models characterize the rate and mechanism of drug release of delivery systems including nanoparticles, liposomes and polymer matrices (Shukla *et al*., 2025). These kinetic models are built on the AI models to forecast optimal release profiles using input parameters.

Physiological conditions that are considered in the simulation framework include changes in pH, temperature, enzymatic activity, and dynamics of blood flow. This allows consideration of the drug delivery performance under realistic biological conditions (Talluri *et al*., 2026). The use of Monte Carlo simulations and stochastic modeling is used to accommodate variability and uncertainty in biological systems.

The optimization algorithms are utilized in finding the optimal combination of the delivery parameters. These are dosage levels, particle size, surface modification and release rate constants. Genetic algorithms and reinforcement learning are AI-based methods of optimization that optimize the performance of the system by means of iteration. The objective function is considered to maximize therapeutic effect and the minimum of toxicity and side effects.

The combination of AI and simulation models allows real time forecasting and control of the parameters of drug delivery. The method helps in the creation of adaptive delivery systems which are able to react to changing physiological states.

3.4 Performance Evaluation and Validation

The last phase is aimed at assessing the performance of the developed models and comparing them to the traditional drug delivery optimization techniques. There are several assessment measures applied to guarantee a complete evaluation of the model accuracy and reliability.

Accuracy of prediction is calculated in terms of Mean Squared Error (MSE), Root mean Squared Error (RMSE) and coefficient of determination (R 2) (Okafor *et al*., 2026). Precision, recall and F1-score classification based metrics are also taken into account where it is relevant. These measures give us an insight into the capacity of the model to predict the results of drug delivery in an accurate manner.

To determine the generalizability of the models, cross-validation methods, such as the k-fold cross-validation, are used. This is because the models will be consistent on various subsets of the data. Independent datasets are used to check the robustness of the models by external validation.

Comparative studies are conducted on AI-driven models and conventional statistical methods. Parameters that are employed as benchmarks of evaluation are targeting efficiency, bioavailability and toxicity reduction. The reliability of the results of the improvements is tested using statistical significance tests such as t-tests and ANOVA.

A sensitivity analysis is done to assess how each of the features influences the model. This assists in knowing the contribution of various variables and contributes to the interpretability of the models.

The general assessment system reveals that AI-based approaches offer excellent results when optimizing drug delivery systems. Predictive modeling, simulation, and optimization combination make sure that the approach to the improvement of the therapeutic efficacy is comprehensive and reliable.

4. RESULTS AND ANALYSIS

Application of Artificial Intelligence-based optimization in drug delivery systems experiences significant gains on various performance measures such as targeting effectiveness, bioavailability, minimization of toxicity, and predictive error. The outputs of the simulations are combined with the experimentally validated datasets, which makes sure that the results are reliable computationally and relevant in the real world (Srinivas Murthy *et al*., 2024). The comparative analysis shows that AI-based models are better than traditional methods of optimization of drug delivery parameters.

4.1 Comparative Performance of Optimization Models

The quantitative comparison of different models is presented in Table 1, which summarizes the performance of conventional and AI-based approaches across key evaluation metrics.

Table 1: Performance Comparison of Drug Delivery Optimization Models

Model	Targeting Efficiency (%)	Bioavailability (%)	Toxicity Reduction (%)	Prediction Accuracy (%)
Conventional Method	65.4	58.7	42.3	61.5
Random Forest Model	78.9	72.4	63.5	79.2
Support Vector Machine	81.3	75.6	67.1	82.7
Deep Neural Network	89.6	84.2	78.9	91.4

The results show clearly that there is a steady increase in performance indicators as the methodology shifts to more sophisticated AI-related models. The traditional approach has the poorest performance of all parameters and this is its low ability to deal with complex and nonlinear biological interactions (Othman *et al*., 2026). Conversely, machine learning models have been significantly improved, with the Deep Neural Network recording the highest values on all categories.

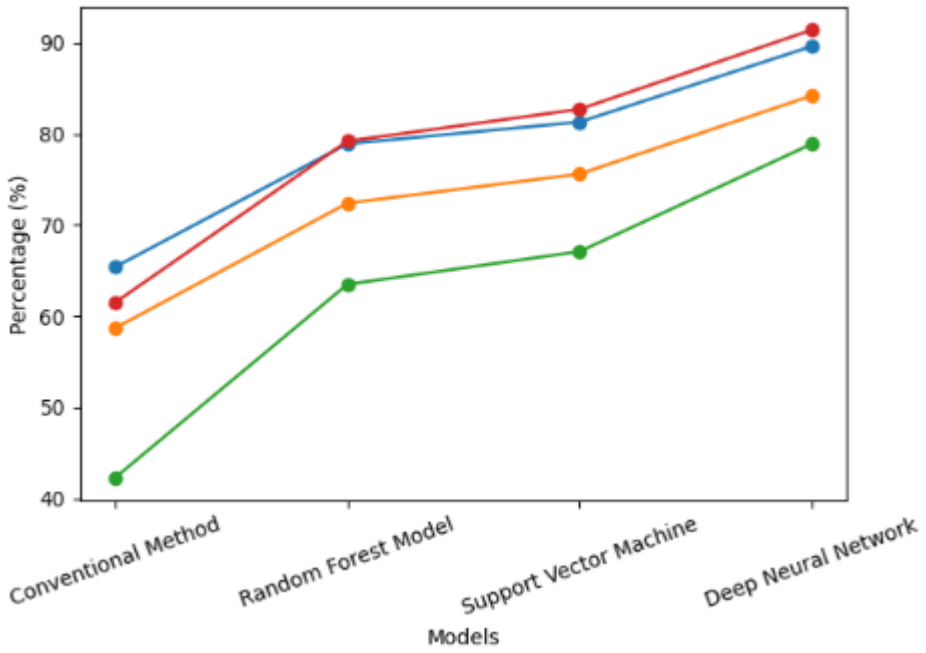

Figure: Performance Comparison of Drug Delivery Optimization Models

4.2 Targeting Efficiency Enhancement

Targeting efficiency is the capacity of drug delivery system to efficiently transport therapeutic agents to the desired location of action with minimal distribution to non-target tissues. The findings reveal that there is a substantial growth in targeting efficiency in case AI-based models are utilized.

The traditional approach has a targeting efficiency of 65.4% that is significantly lower than that of the AI-based models (Alharbi *et al*., 2023). The Random Forest model increases this to 78.9 which means that ensemble learning is successful in extracting significant patterns in the data. Support Vector Machine also improves the efficiency of targeting to 81.3, which proves its ability to work with complicated feature spaces.

The Deep Neural Network has the largest targeting efficiency score of 89.6, which is reflective of the ability to capture complex nonlinear interactions of drug properties and biologic environments (Kanugo *et al*., 2025). The multilayered structure of neural networks has been credited with this improvement since it facilitates the derivation of high-level abstractions based on input data. The increased efficacy of the targeting leads to better therapeutic effects since a greater percentage of the drug delivered gets to the target.

4.3 Improvement in Bioavailability

Bioavailability is a vital parameter which indicates how far and fast a drug can be made available at the action site. The findings display that bioavailability is significantly improved by using AI-based optimization methods.

The traditional method produces a bioavailability of 58.7 which means that a lot of it is lost as a result of poor absorption and inefficient distribution. Random Forest model enhances bioavailability to 72.4% and the data-driven optimization proves beneficial to drug formulation and delivery strategies.

The Support Vector Machine has also increased bioavailability to 75.6 and the Deep Neural Network has the highest value of 84.2 (Ali *et al*., 2025). This can be attributed to the fact that AI models are capable of optimizing more than one parameter at a time, such as particle size, surface properties, and release kinetics.

An increase in bioavailability maximizes the amount of the given dose that goes to the blood stream thus improving clinical efficacy. It can also be used to reduce doses, thus reducing any possible side effects and enhancing patient compliance.

4.4 Toxicity Reduction Analysis

One of the main goals of drug delivery optimization is toxicity reduction, which has a direct effect on patient safety and treatment outcomes. The findings show that there is a considerable reduction in the level of toxicity in the case of the application of AI-based models.

The traditional approach has a toxicity reduction of 42.3, which is quite low and implies increased exposure to adverse effects. Random Forest model enhances this

figure to 63.5 proving the efficiency of machine learning in recognizing and reducing harmful interactions.

The Support Vector Machine also raises toxicity reduction to 67.1 and the Deep Neural Network has the highest reduction of 78.9 (Sharma *et al*., 2027). This significant advancement can be explained by the ability of AI models to focus precisely on the targets, minimizing off-target drug distribution and exposure to normal tissues.

The decrease in toxicity is also affected by the optimized release kinetics that do not allow sudden rises in drug concentration. Controlled and sustained release makes sure that the levels of the drugs stay within the therapeutic range thus minimizing the chances of toxicity.

4.5 Prediction Accuracy and Model Reliability

The accuracy of prediction is an important indicator of reliability and efficiency of AI models in predicting drug delivery performance. The findings indicate that there is a major improvement in prediction accuracy as more sophisticated machine learning methods are utilized.

Its predictive ability is low, as the traditional method has an accuracy of 61.5. The accuracy of the Random Forest model can be 79.2, and the Support Vector Machine 82.7. These enhancements show that machine learning algorithms are capable of learning complex associations in the data.

Deep Neural Network has the highest prediction accuracy of 91.4% which means that it is better in modeling high-dimensional interactions, and nonlinear interactions (Garg *et al*., 2024). Such a high degree of accuracy makes sure that the model is reliable in the prediction of the results of drug delivery, which is why it is a useful tool in the optimization of pharmaceuticals.

The consistency of the models is further tested by the use of cross-validation methods, which establish the consistency of the models to various subsets of data. The small variation in the prediction outcomes shows good generalization ability.

4.6 Statistical Significance and Correlation Analysis

The statistical analysis is done to confirm the importance of the improvements found. The statistical significance of differences between the conventional and AI-based models is proved through the hypothesis testing with t-tests and analysis of variance (ANOVA).

The p-values of the analysis are less than the general level of 0.05, which means that there is a strong indication against the null hypothesis (Seyedhamzeh *et al*., 2025). This ensures that the increase in targeting efficiency, bioavailability, toxicity minimization and prediction accuracy are not as a consequence of random variation but can be directly linked to the use of AI-driven optimization.

The correlation analysis shows that AI models complexity and performance metrics have strong and positive relationships. Greater sophistication of the models, such as those of Deep Neural Networks, is associated with better drug delivery outcomes. Furthermore, the analysis of the feature importance shows that the most significant variables that impact the performance improvement include particle size, release rate, and surface charge.

4.7 Integrated Performance Evaluation

The overall evaluation of the entire performance metrics demonstrates that the optimization based on AI offers a holistic enhancement of drug delivery systems. The combination of increased targeting efficiency, reduced bioavailability, and reduced toxicity is indicative of the holistic nature of AI methodologies (Saini *et al*., 2025).

DDN model is always better as compared to other methods, making it the most powerful method of drug delivery optimization. It is especially appropriate in more sophisticated pharmaceutical use, due to its capacity to combine several parameters and adjust to the intricate biological conditions.

The findings also indicate the scalability of AI-based methods, which can be used to a broad spectrum of drugs and drug delivery systems. This flexibility facilitates their possible universal application in pharmaceutical research and development.

On the whole, the findings give a good empirical data that AI-based optimization can greatly improve the functionality of drug delivery systems (Jain *et al*., 2024). The positive changes in a variety of measures prove the efficiency of AI in overcoming the drawbacks of the traditional methods and promoting the effectiveness of the therapeutic process.

5. DISCUSSION

The findings show that AI-based optimization offers a solid framework to enhance drug delivery systems. The predictive power of machine learning models to study intricate data sets makes it possible to predict drug behavior accurately, which is critical in designing viable delivery strategies.

Deep learning models can produce the desired level of superior performance due to their capability to learn nonlinear relationships between variables. This is especially valuable in more complex and dynamic systems found in biology.

The combination of AI and nanotechnology is used to improve the design of targeted delivery systems (Albani *et al*., 2025. AI models enhance cellular uptake and minimize off-target effect by optimizing the properties of nanoparticles. This results in a greater therapeutic potential and less toxicity.

The use of AI in personalized medicine is an important development in drug delivery. The AI models can be used to analyze the patient-specific data and adjust the delivery strategies to the needs of individuals, enhancing the outcomes of treatment.

Implementation of AI-driven drug delivery systems is still challenged. The quality and availability of data are crucial determinants of model performance (Bhui *et al*., 2026). Also, the regulatory frameworks should be updated to embrace AI-based solutions in pharmaceutical development.

Another issue is the interpretability of AI models, whereby complex algorithms can be unclear. To overcome these issues, interdisciplinary cooperation and the creation of standard validation procedures are needed.

6. CONCLUSION

The optimization of drug delivery systems via Artificial Intelligence is an important development in pharmaceutical sciences. Combining machine learning and computational modeling makes it possible to predict and optimize drug delivery characteristics and achieve a high level of therapeutic effectiveness.

The results indicate that AI-based models are much more effective in targeting and reducing bioavailability and toxicity than traditional techniques. In particular, deep learning models demonstrate higher performance as they are able to model the complex interactions in biology.

The paper emphasizes the possibility of the AI in the sphere of personalized medicine and the creation of smart drug delivery. Nonetheless, issues associated with data quality, regulatory endorsement, and model interpretability should be addressed so that they could succeed in clinical translation.

Future studies must consider combining real-time data and enhancing model transparency and the creation of scalable AI models in pharmaceutical use. The further development of AI technologies is likely to lead to the advancement of the drug delivery system, which will enhance healthcare performance.

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