International Journal of Medical and Pharmaceutical Sciences
Open access peer-reviewed Journal
Volume 2, Issue 7, Page 389-403.
https://doi.org/10.5281/zenodo.21263928

Review Article

Artificial Intelligence-Driven Design and Optimization of Novel Drug Delivery Systems: Current Advances, Challenges, and Future Perspectives

Prachi Sharma*[1], Gagan Kaushal[1], Puja Gulati[2]

[1]*Associate Professor, Desh Bhagat University, School of Pharmacy, Mandi Gobindgarh, Punjab*
[2]*Principal, Desh Bhagat University, School of Pharmacy, Mandi Gobindgarh, Punjab*

The rapid advancement of artificial intelligence (AI) is transforming pharmaceutical research by introducing data-driven strategies that improve the design, optimization, and evaluation of novel drug delivery systems (NDDS). Conventional formulation development often relies on extensive experimental trials, making the process labor-intensive, time-consuming, and costly. AI-based technologies, including machine learning, deep learning, and predictive analytics, offer innovative solutions by accelerating formulation screening, optimizing critical formulation variables, and predicting the physicochemical and biopharmaceutical performance of drug delivery systems. These computational approaches have demonstrated significant potential in the development of liposomes, polymeric nanoparticles, solid lipid nanoparticles, nanostructured lipid carriers, hydrogels, microneedles, and other advanced delivery platforms. This review provides a comprehensive overview of the recent progress in AI-assisted pharmaceutical formulation development, highlighting the integration of predictive modeling, digital twins, and intelligent optimization tools throughout the drug development lifecycle. The article further discusses the growing role of AI in supporting Quality by Design (QbD), process optimization, personalized medicine, and real-time decision-making during pharmaceutical manufacturing. In addition, emerging applications of generative AI and digital twin technology are explored for their potential to improve formulation accuracy, reduce development timelines, and enhance product quality. Despite these promising advances, several challenges continue to hinder the widespread implementation of AI in pharmaceutical sciences, including limited availability of high-quality datasets, concerns regarding model transparency, regulatory uncertainty, data security, and the need for robust experimental validation. The review also outlines current regulatory considerations and future research directions that will facilitate the responsible adoption of AI in drug delivery research. Overall, AI-driven technologies are expected to reshape the future of NDDS by enabling more efficient, precise, and patient-centered pharmaceutical development, ultimately accelerating the translation of innovative drug delivery systems from laboratory research to clinical application.

Keywords: Artificial Intelligence; Machine Learning; Deep Learning; Novel Drug Delivery Systems; Predictive Modeling; Digital Twins; Quality by Design; Personalized Medicine; Pharmaceutical Formulation.

INTRODUCTION

Novel drug delivery systems (NDDS) have transformed modern pharmaceutical research by addressing many of the shortcomings associated with conventional dosage forms. Traditional drug delivery often suffers from poor aqueous solubility, limited bioavailability, rapid drug degradation, frequent dosing, and non-specific distribution, all of which may reduce therapeutic efficacy and increase adverse effects. To overcome these limitations, researchers have developed advanced delivery platforms such as liposomes, polymeric nanoparticles, solid lipid nanoparticles, nanostructured lipid carriers, niosomes, microneedles, hydrogels, dendrimers, and implantable systems that enable controlled, sustained, and targeted drug release (Vora et al., 2023; Jena et al., 2024). Although these technologies have significantly improved drug delivery, formulation development remains a challenging and resource-intensive process. The design of an optimized drug delivery system requires careful selection of excipients, optimization of formulation variables, evaluation of physicochemical characteristics, prediction of drug release behavior, stability assessment, and manufacturing optimization. Traditionally, these tasks rely heavily on iterative laboratory experiments and statistical optimization techniques, making pharmaceutical development both time-consuming and expensive. As drug molecules become increasingly complex, conventional experimental approaches alone are often insufficient to efficiently identify optimal formulations (Vora et al., 2023; Serrano et al., 2024). The rapid evolution of artificial intelligence (AI) has introduced a new paradigm in pharmaceutical sciences by enabling data-driven formulation design and predictive decision-making. AI refers to computational systems capable of learning from large datasets, recognizing complex patterns, generating predictions, and supporting intelligent decision-making with minimal human intervention. Modern AI encompasses several computational approaches, including machine learning (ML), deep learning (DL), natural language processing, reinforcement learning, and generative AI. These technologies are increasingly being integrated into pharmaceutical research to accelerate drug discovery, optimize formulations, improve manufacturing processes, and support precision medicine (Serrano et al., 2024; Vora et al., 2023). Among AI technologies, machine learning has emerged as one of the most valuable tools for pharmaceutical formulation development. Machine learning algorithms can analyze historical experimental data to establish relationships between formulation variables and product performance. Such models have demonstrated the ability to predict particle size, encapsulation efficiency, drug loading, dissolution behavior, permeability, stability, and pharmacokinetic characteristics before experimental validation. Deep learning further extends these capabilities by processing large multidimensional datasets, microscopic images, and molecular information to identify complex nonlinear relationships that are difficult to capture using conventional statistical methods (Jena et al., 2024; Panchpuri et al., 2025). Artificial intelligence is increasingly contributing to the rational design and optimization of novel drug delivery systems. Computational models can assist researchers in selecting appropriate lipids, polymers, surfactants, and stabilizers based on the physicochemical characteristics of active pharmaceutical ingredients. AI-driven optimization techniques can also identify optimal formulation compositions and manufacturing conditions while simultaneously predicting critical quality attributes such as particle size distribution, zeta potential, drug release profiles, and long-term stability. These capabilities have accelerated the development of liposomes, polymeric nanoparticles, nanostructured lipid carriers, hydrogels, microneedles, and stimuli-responsive nanocarriers, thereby reducing experimental workload and shortening formulation development timelines (Vora et al., 2023; Panchpuri et al., 2025). The integration of AI with Quality by Design (QbD) has further strengthened pharmaceutical product development by enabling intelligent optimization of formulation and manufacturing processes. Unlike conventional Design of Experiments (DoE), AI algorithms can analyze multidimensional datasets, identify critical material attributes (CMAs) and critical process parameters (CPPs), predict design spaces, and continuously improve formulation performance using real-time feedback. More recently, digital twin technology has emerged as an advanced computational approach in pharmaceutical manufacturing. A digital twin creates a virtual representation of a physical formulation or manufacturing process, allowing researchers to simulate formulation behavior, predict process deviations, optimize manufacturing conditions, and improve product quality while minimizing experimental costs (Vora et al., 2023; U.S. Food and Drug Administration, 2024). Another rapidly expanding application of AI is personalized medicine, where patient-specific clinical, genomic, proteomic, and pharmacological data are integrated to design individualized therapeutic strategies. AI models can predict treatment responses, recommend personalized dosage regimens, and facilitate the development of patient-specific drug delivery systems. Such intelligent approaches support the transition from conventional "one-size-fits-all" therapies to precision medicine, where treatment decisions are tailored according to individual biological characteristics and disease profiles. This shift is expected to improve therapeutic outcomes while minimizing adverse drug reactions (Panchpuri et al., 2025; Serrano et al., 2024). Despite its remarkable potential, the implementation of AI in pharmaceutical sciences is accompanied by several challenges. The availability of high-quality, standardized pharmaceutical datasets remains limited, which may affect model robustness and reproducibility. Additional concerns include algorithm transparency, interpretability, cybersecurity, data privacy, ethical considerations, and regulatory acceptance. Recognizing these challenges, regulatory agencies such as the U.S. Food and Drug Administration (FDA) have initiated discussions on the responsible application of AI and machine learning throughout the drug development lifecycle, emphasizing the importance of validation, transparency, risk assessment, and continuous model monitoring (U.S. Food and Drug Administration, 2024; Jena et al., 2024). Given the rapid advancements in AI technologies and their growing influence across pharmaceutical research, a comprehensive review of their applications in novel drug delivery systems is both timely and essential. This review critically discusses recent developments in AI-assisted formulation design, machine learning and deep learning algorithms, predictive modeling, digital twin technology, personalized medicine, and regulatory perspectives. Furthermore, it highlights the current challenges, emerging opportunities, and future directions that are expected to shape the next generation of intelligent drug delivery systems.

2. Artificial Intelligence in Pharmaceutical Sciences

Artificial intelligence (AI) has emerged as one of the most transformative technologies in pharmaceutical sciences, fundamentally changing the way drugs are discovered, formulated, manufactured, and evaluated. Unlike conventional computational approaches that rely on predefined mathematical models, AI systems possess the ability to learn from historical data, identify hidden relationships, and generate accurate predictions with minimal human intervention. The integration of AI into pharmaceutical research has enabled scientists to process complex multidimensional datasets, optimize formulation variables, predict drug performance, and accelerate decision-making throughout the product development lifecycle (Vora et al., 2023; Serrano et al., 2024). The growing complexity of modern drug molecules and advanced drug delivery systems has increased the demand for computational tools capable of handling large volumes of experimental and molecular data. Traditional formulation development often involves repeated laboratory experiments to identify optimal formulation compositions and manufacturing conditions. This empirical approach is time-consuming, costly, and may delay the translation of promising drug candidates into clinical applications. AI offers an alternative by utilizing predictive algorithms that can rapidly analyze previous experimental outcomes, recognize formulation trends, and recommend optimized development strategies before laboratory validation (Jena et al., 2024). Consequently, AI has become an essential component of digital pharmaceutical research, supporting faster innovation while reducing development costs and experimental failures.

2.1 Evolution of Artificial Intelligence in Pharmaceutical Sciences

- **Artificial Intelligence**

Artificial intelligence refers to the capability of computer systems to simulate human cognitive functions such as learning, reasoning, problem-solving, and decision-making. In pharmaceutical sciences, AI is increasingly used to support drug discovery, pharmaceutical formulation, manufacturing optimization, quality assurance, and clinical decision support. Modern AI platforms can integrate chemical, biological, pharmaceutical, and clinical datasets to identify complex relationships that may remain undetected using traditional statistical methods (Serrano et al., 2024). Initially, AI applications in pharmacy were limited to expert systems and rule-based computational models that depended heavily on manually programmed knowledge. Although these systems improved data organization, they lacked the ability to adapt to new information. The availability of high-performance computing, cloud-based infrastructure, and large pharmaceutical datasets has significantly expanded AI capabilities, enabling adaptive learning and continuous model improvement. Today, AI is recognized as a key technology supporting Pharmaceutical Industry 4.0 and intelligent pharmaceutical manufacturing (Vora et al., 2023).

- **Machine Learning**

Machine learning (ML) represents one of the most widely applied branches of AI in pharmaceutical sciences. Rather than following fixed programming rules, ML algorithms learn directly from experimental data and continuously improve their predictive performance as additional information becomes available. These algorithms identify relationships between formulation variables and product characteristics, allowing researchers to predict formulation outcomes before conducting laboratory experiments (Jena et al., 2024). Machine learning has been successfully employed to optimize excipient selection, predict drug solubility, estimate encapsulation efficiency, forecast dissolution profiles, evaluate stability, and identify critical formulation variables. Supervised learning techniques such as Random Forest, Support Vector Machine (SVM), Decision Trees, and Gradient Boosting models have shown excellent performance in predicting pharmaceutical properties, whereas unsupervised learning methods assist in clustering formulations and identifying hidden patterns within complex datasets (Panchpuri et al., 2025).

- **Deep Learning**

Deep learning (DL) is an advanced subset of machine learning that utilizes multiple layers of artificial neural networks to process highly complex datasets. Compared with conventional ML algorithms, deep learning models are capable of extracting intricate nonlinear relationships without extensive manual feature engineering. This capability makes DL particularly valuable for pharmaceutical applications involving image processing, molecular modeling, spectroscopy, microscopy, and drug delivery optimization (Serrano et al., 2024). Convolutional Neural Networks (CNNs) are widely applied for microscopic image analysis, particle characterization, and pharmaceutical quality inspection, whereas Recurrent Neural Networks (RNNs) are useful for analyzing sequential pharmaceutical data. More recently, Graph Neural Networks (GNNs) have gained attention for predicting molecular interactions and nanoparticle behavior, providing valuable insights during the development of advanced drug delivery systems (Jena et al., 2024).

- **Generative Artificial Intelligence**

Generative Artificial Intelligence (Generative AI) represents the latest advancement in AI technologies. Unlike conventional predictive models, generative AI can create new molecular structures, formulation compositions, optimization strategies, and scientific hypotheses based on previously learned information. Large Language Models (LLMs), generative adversarial networks (GANs), and diffusion models are increasingly being explored in pharmaceutical research to accelerate drug design and formulation development (Panchpuri et al., 2025). Within pharmaceutical sciences, generative AI has the potential to recommend novel excipient combinations, simulate formulation performance, design patient-specific dosage forms, and automate scientific literature analysis. When integrated with machine learning and experimental validation, these technologies may significantly reduce formulation development time while improving prediction accuracy and supporting personalized medicine initiatives (Vora et al., 2023).

2.2 Types of Artificial Intelligence Algorithms Used in Pharmaceutical Sciences

Different AI algorithms are selected according to the complexity of pharmaceutical datasets and the intended application. Some algorithms excel at prediction, whereas others are designed for classification, optimization, or image recognition. Table 1 summarizes commonly used AI algorithms and their major pharmaceutical applications.

Table 1. Common Artificial Intelligence Algorithms and Their Pharmaceutical Applications

AI Method	Principle	Major Pharmaceutical Applications
Machine Learning	Learns patterns from experimental datasets	Formulation optimization, solubility prediction, stability prediction
Deep Learning	Multi-layer neural network architecture	Microscopic image analysis, particle characterization, quality inspection
Artificial Neural Networks	Models complex nonlinear relationships	Drug release prediction, dissolution modeling, bioavailability estimation
Random Forest	Ensemble decision-tree algorithm	Excipient selection, formulation screening, stability prediction
Support Vector Machine (SVM)	Supervised classification algorithm	Classification of formulations, toxicity prediction, quality assessment
Reinforcement Learning	Learns optimal decisions through continuous feedback	Process optimization, autonomous manufacturing, adaptive process control
Bayesian Optimization	Probabilistic optimization technique	Quality by Design (QbD), formulation optimization, process parameter optimization

The integration of these algorithms has shifted pharmaceutical research from empirical experimentation toward predictive and data-driven development. Rather than relying solely on trial-and-error experimentation, researchers can now employ AI models to screen thousands of formulation combinations, predict product performance, and identify optimal manufacturing conditions before initiating laboratory studies. This approach substantially reduces development time, minimizes material consumption, and improves formulation success rates. As AI technologies continue to evolve alongside digital twins, robotics, and automated laboratories, they are expected to become indispensable tools for the development of next-generation intelligent drug delivery systems (FDA, 2024; Vora et al., 2023).

3. Artificial Intelligence in Novel Drug Delivery System Design

Artificial intelligence (AI) is revolutionizing the design and development of novel drug delivery systems (NDDS) by transforming conventional trial-and-error formulation approaches into data-driven and predictive processes. Traditional formulation development often requires numerous laboratory experiments to optimize excipients, manufacturing parameters, and product quality attributes, making the process expensive and time-consuming. AI algorithms can analyze large experimental datasets, identify hidden relationships among formulation variables, and predict formulation performance before experimental validation. Consequently, AI has become an important tool for accelerating pharmaceutical product development, reducing research costs, and improving formulation success rates (Vora et al., 2023; Jena et al., 2024).

3.1 AI-Assisted Formulation Development

One of the most significant applications of AI in pharmaceutical sciences is formulation development. The formulation of an effective drug delivery system requires careful selection of excipients, optimization of formulation composition, and evaluation of multiple quality attributes. AI enables researchers to make informed decisions by predicting formulation behavior using previously generated experimental data, thereby minimizing unnecessary laboratory trials (Panchpuri et al., 2025).

- **Excipient Screening**

Selecting suitable excipients is a critical step in formulation development because excipients directly influence drug stability, dissolution, bioavailability, and patient acceptability. Machine learning models can rapidly evaluate large databases of pharmaceutical excipients and identify the most compatible materials based on the physicochemical properties of the drug molecule. This computational approach significantly reduces formulation screening time and improves formulation efficiency (Vora et al., 2023).

- **Polymer Selection**

Polymers play an essential role in controlled and targeted drug delivery systems. AI-assisted predictive models help researchers select appropriate polymers by analyzing factors such as molecular weight, degradation characteristics, swelling behavior, and drug-polymer compatibility. Such predictions improve encapsulation efficiency, drug release profiles, and formulation stability while reducing experimental optimization (Jena et al., 2024).

- **Lipid Selection**

Lipid composition strongly influences the performance of liposomes, solid lipid nanoparticles (SLNs), and nanostructured lipid carriers (NLCs). AI algorithms can evaluate lipid physicochemical properties, drug-lipid interactions, and formulation stability to recommend suitable lipid combinations. This approach facilitates the development of lipid-based nanocarriers with improved drug loading and sustained release characteristics (Vora et al., 2023).

- **Solubility Prediction**

Poor aqueous solubility remains one of the major challenges in pharmaceutical development. Machine learning models can predict drug solubility based on molecular descriptors and physicochemical characteristics before experimental testing. Accurate solubility prediction assists researchers in selecting suitable formulation strategies such as nanoparticles, lipid carriers, or amorphous solid dispersions, thereby shortening formulation development time (Serrano et al., 2024).

- **Drug Loading Prediction**

Drug loading capacity determines the therapeutic efficiency of many nanocarrier systems. AI models predict encapsulation efficiency and drug loading by evaluating formulation variables, polymer properties, lipid composition, and manufacturing conditions. These predictions reduce formulation failures and enable researchers to optimize formulations more efficiently (Panchpuri et al., 2025).

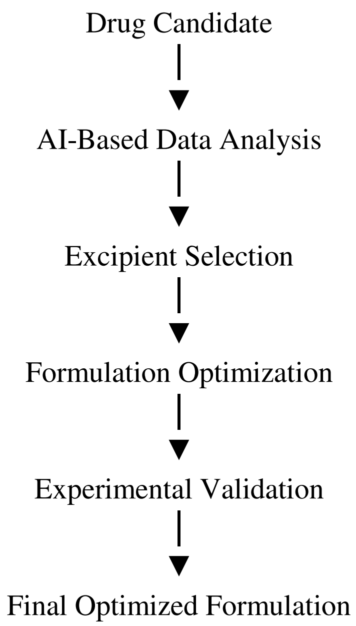


Figure 1. AI-Assisted Formulation Development Workflow

3.2 AI-Based Optimization of Different Novel Drug Delivery Systems

AI has been successfully integrated into the optimization of various advanced drug delivery platforms. By analyzing experimental datasets and predicting formulation outcomes, AI improves formulation accuracy while reducing experimental workload. Lipid-based systems, polymeric nanoparticles, hydrogels, microneedles, and transdermal patches have particularly benefited from AI-assisted optimization (Jena et al., 2024).

Table 2. Applications of AI in Different Novel Drug Delivery Systems

Drug Delivery System	AI Application
Liposomes	Optimization of lipid composition and drug encapsulation
Niosomes	Prediction of vesicle size and entrapment efficiency
Polymeric nanoparticles	Polymer selection and particle size optimization
Solid Lipid Nanoparticles	Prediction of encapsulation efficiency and stability
Nanostructured Lipid Carriers	Stability prediction and lipid ratio optimization
Microneedles	Mechanical strength and drug release optimization
Hydrogels	Swelling behavior and controlled drug release prediction

Transdermal patches	Drug permeation and release kinetics modelling

For liposomal formulations, AI predicts the optimal lipid ratio required to maximize drug encapsulation while maintaining vesicle stability. In polymeric nanoparticles, machine learning assists in selecting biodegradable polymers and estimating particle size and drug release behavior. Similarly, AI models improve the mechanical strength of microneedles, optimize hydrogel swelling characteristics, and predict drug permeation across biological membranes in transdermal delivery systems (Vora et al., 2023; Panchpuri et al., 2025). These applications demonstrate the ability of AI to accelerate formulation development while improving product quality and reproducibility.

3.3 AI in Quality by Design (QbD)

Quality by Design (QbD) is a systematic approach to pharmaceutical development that emphasizes predefined objectives, scientific understanding, and risk-based process control. AI has strengthened the QbD framework by enabling rapid analysis of multidimensional datasets and improving formulation optimization (FDA, 2024). AI-assisted Design of Experiments (DoE) enables researchers to evaluate numerous formulation variables simultaneously and identify the most influential factors affecting product quality. Machine learning models can accurately predict **Critical Material Attributes (CMAs)**, such as polymer concentration and lipid composition, as well as **Critical Process Parameters (CPPs)**, including mixing speed, temperature, homogenization pressure, and drying conditions. By integrating these variables, AI predicts the formulation **Design Space**, allowing researchers to manufacture pharmaceutical products with consistent quality and reduced variability (Jena et al., 2024). Unlike conventional QbD, which primarily relies on statistical models, AI-QbD continuously updates predictive models using newly generated experimental data. This adaptive capability improves process understanding, enhances manufacturing efficiency, and supports continuous process optimization throughout the product lifecycle (Vora et al., 2023).

Traditional QbD

↓

AI-Assisted QbD

↓

Continuous Process Optimization

Figure 2. AI-Integrated Quality by Design Framework

Overall, the integration of AI into formulation development and Quality by Design represents a significant advancement in pharmaceutical sciences. By enabling predictive modeling, intelligent optimization, and data-driven decision-making, AI reduces development time, lowers experimental costs, and improves the quality and consistency of novel drug delivery systems. As computational tools continue to evolve, AI is expected to become an indispensable component of future pharmaceutical research and advanced drug delivery technologies (Panchpuri et al., 2025; FDA, 2024).

4. Predictive Modeling In Drug Delivery

Predictive modeling has become one of the most promising applications of artificial intelligence (AI) in pharmaceutical sciences. It involves the use of computational algorithms and mathematical models to predict the behavior and performance of drug delivery systems before laboratory experimentation or clinical evaluation. Unlike traditional formulation development, which relies heavily on repeated experimental trials, predictive modeling analyzes historical experimental data, molecular descriptors, and physicochemical properties to estimate formulation outcomes with high accuracy. This data-driven approach enables researchers to identify optimal formulation conditions, minimize experimental failures, reduce development costs, and accelerate the translation of innovative drug delivery systems into clinical practice (Vora et al., 2023; Serrano et al., 2024). The growing complexity of novel drug delivery systems (NDDS), including liposomes, polymeric nanoparticles, microneedles, hydrogels, and lipid-based nanocarriers, has generated vast amounts of formulation and process data. AI-based predictive models are capable of processing these multidimensional datasets and identifying nonlinear relationships among formulation variables that are often difficult to detect using conventional statistical methods. Machine learning algorithms such as Random Forest, Artificial Neural Networks (ANNs), Support Vector Machines (SVMs), Gradient Boosting, and Deep Neural Networks (DNNs) are increasingly employed to predict formulation performance, optimize process parameters, and improve product quality (Jena et al., 2024).

4.1 Prediction of Drug Solubility and Bioavailability

Poor aqueous solubility remains one of the major causes of formulation failure and low oral bioavailability. Nearly 40–70% of newly discovered drug molecules exhibit poor water solubility, making formulation optimization particularly challenging. AI-driven predictive models analyze molecular descriptors, chemical structures, lipophilicity, and physicochemical characteristics to estimate drug solubility before experimental evaluation. These predictions assist formulation scientists in selecting suitable delivery strategies such as lipid nanoparticles, amorphous solid dispersions, polymeric carriers, or nanoemulsions to enhance drug dissolution and absorption (Serrano et al., 2024). Predictive modeling also estimates oral bioavailability by integrating factors such as molecular weight, permeability, solubility, and metabolic stability. Early prediction of bioavailability enables researchers to prioritize promising drug candidates and optimize formulation strategies during the initial stages of pharmaceutical development (Panchpuri et al., 2025).

4.2 Prediction of Drug Release Profiles

Controlled drug release is a critical quality attribute for many advanced drug delivery systems. AI algorithms can accurately predict drug release kinetics by analyzing formulation composition, particle characteristics, polymer degradation, lipid composition, and environmental conditions. Machine learning models establish relationships between formulation variables and release behavior, enabling researchers to simulate dissolution profiles before conducting laboratory studies (Vora et al., 2023). Artificial Neural Networks and Deep Learning models have shown excellent predictive performance for sustained-release tablets, polymeric nanoparticles, hydrogels, transdermal patches, and lipid-based formulations. These computational tools facilitate the design of formulations with desired release characteristics while minimizing experimental optimization (Jena et al., 2024).

4.3 Prediction of Drug Loading and Encapsulation Efficiency

Drug loading capacity and encapsulation efficiency directly influence the therapeutic performance of nanocarrier-based drug delivery systems. Experimental optimization of these parameters often requires extensive screening of formulation variables, including polymer concentration, lipid composition, surfactant ratio, solvent selection, and manufacturing conditions. AI models analyze previous experimental datasets to predict optimal formulation compositions capable of achieving maximum drug loading and encapsulation efficiency. Such predictive capabilities reduce formulation failures and enable rapid optimization of liposomes, solid lipid nanoparticles (SLNs), nanostructured lipid carriers (NLCs), polymeric nanoparticles, and niosomes (Vora et al., 2023; Jena et al., 2024).

4.4 Pharmacokinetic and Pharmacodynamic Prediction

Artificial intelligence has significantly improved the prediction of pharmacokinetic (PK) and pharmacodynamic (PD) behavior of pharmaceutical formulations. Machine learning algorithms integrate molecular properties, formulation characteristics, and biological data to estimate drug absorption, distribution, metabolism, excretion (ADME), and therapeutic response. These predictive models assist researchers in identifying potential pharmacokinetic limitations before animal studies or clinical trials. AI also supports dose optimization by predicting plasma drug concentrations, therapeutic windows, and drug exposure under different physiological conditions. Such applications reduce experimental costs and contribute to more efficient drug development (Serrano et al., 2024).

4.5 Stability Prediction

Long-term stability is an essential requirement for pharmaceutical products. Stability studies are traditionally performed under different environmental conditions over several months, making them expensive and time-consuming. AI-based predictive models utilize historical stability data together with environmental variables such as temperature, humidity, light exposure, and packaging characteristics to estimate formulation stability and shelf life. Machine learning algorithms can identify degradation pathways, predict chemical instability, and recommend appropriate storage conditions before long-term stability studies are completed. These capabilities significantly shorten formulation development timelines and support regulatory documentation (Panchpuri et al., 2025).

4.6 Toxicity and Safety Prediction

Safety assessment represents another important application of predictive modeling. AI algorithms evaluate molecular descriptors, physicochemical characteristics, and biological interactions to predict cytotoxicity, organ toxicity, immunogenicity, and adverse drug reactions. Early toxicity prediction enables researchers to eliminate unsuitable formulations during preclinical development, thereby reducing unnecessary animal experiments and improving research efficiency. In nanomedicine, predictive models are increasingly used to evaluate nanoparticle toxicity, biodistribution, cellular uptake, and interactions with biological membranes. These computational approaches contribute to the development of safer and more effective nanocarrier systems (Jena et al., 2024).

4.7 Digital Predictive Models for Intelligent Drug Delivery

Recent advances in AI have facilitated the integration of predictive modeling with digital twins and smart pharmaceutical manufacturing systems. Digital predictive models continuously receive experimental and manufacturing data, enabling real-time monitoring of formulation performance and manufacturing processes. These systems can predict process deviations, recommend corrective actions, and optimize production parameters throughout the product lifecycle. When combined with sensors, automation, and cloud computing, predictive models support intelligent pharmaceutical manufacturing by improving process robustness, minimizing batch failures, and ensuring consistent product quality. Such technologies represent an important step toward the implementation of Pharmaceutical Industry 4.0 and personalized medicine (FDA, 2024).

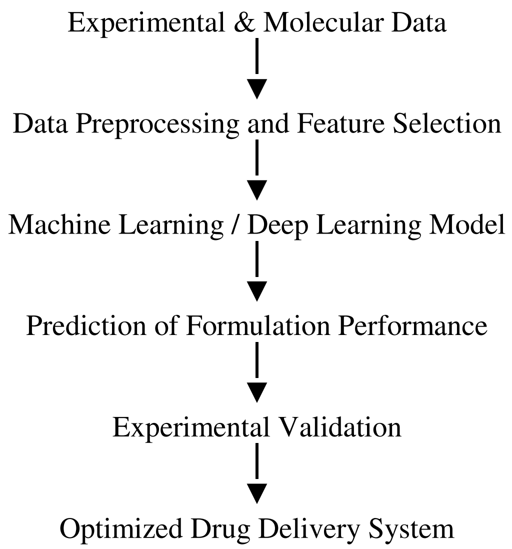


Figure 4. AI-Based Predictive Modeling Workflow in Drug Delivery

Table 4. Major Applications of Predictive Modeling in Drug Delivery

Predictive Model	Predicted Parameter	Pharmaceutical Benefit
Solubility Prediction	Drug solubility	Selection of suitable formulation strategy
Drug Release Modeling	Release kinetics	Controlled and sustained drug delivery
Encapsulation Prediction	Drug loading efficiency	Improved nanocarrier performance
Stability Modeling	Shelf life and degradation	Reduced stability studies
Pharmacokinetic Modeling	ADME profile	Dose optimization
Toxicity Prediction	Safety profile	Early identification of formulation risks
Bioavailability Prediction	Drug absorption	Improved therapeutic efficacy

Overall, predictive modeling has transformed pharmaceutical formulation development from an empirical process into a knowledge-driven strategy supported by artificial intelligence. By accurately forecasting formulation characteristics, drug release behavior, stability, pharmacokinetics, and safety, AI enables researchers to make informed decisions before conducting extensive laboratory experiments. The integration of predictive modeling with machine learning, deep learning, and digital manufacturing technologies is expected to further accelerate the development of safer, more effective, and patient-centered drug delivery systems. As pharmaceutical datasets continue to expand, predictive modeling will remain a cornerstone of intelligent formulation design and next-generation precision medicine (Vora et al., 2023; Panchpuri et al., 2025).

5. Artificial Intelligence for Personalized Medicine

Personalized medicine, also known as precision medicine, is transforming healthcare by shifting treatment strategies from a generalized "one-size-fits-all" approach to individualized therapies based on a patient's genetic profile, physiological characteristics, lifestyle, and disease condition. Advances in genomics, proteomics, metabolomics, and digital health technologies have generated large volumes of patient-specific data, creating new opportunities for individualized therapeutic interventions. However, the interpretation of these complex datasets exceeds the capabilities of conventional analytical methods. Artificial intelligence (AI) has emerged as a powerful solution by integrating multidimensional biological and clinical information to support personalized diagnosis, treatment planning, dosage optimization, and drug delivery system design (Panchpuri et al., 2025; Serrano et al., 2024). In pharmaceutical sciences, AI-driven personalized medicine aims to deliver the right drug, at the right dose, through the most appropriate delivery system for each patient. By analyzing patient-specific variables such as age, body weight, genetic polymorphisms, disease severity, organ function, and biomarker profiles, AI algorithms can predict therapeutic responses and recommend individualized treatment strategies. This approach has the potential to improve treatment efficacy, reduce adverse drug reactions, and enhance patient compliance, particularly in chronic diseases requiring long-term therapy (Topol, 2019; Vora et al., 2023).

5.1 AI in Patient Stratification

Patient populations often respond differently to the same medication because of variations in genetic makeup, metabolism, disease progression, and environmental factors. AI algorithms can analyze electronic health records (EHRs), laboratory findings, medical imaging, and genomic data to classify patients into clinically meaningful subgroups with similar therapeutic characteristics. This process, known as patient stratification, enables clinicians to identify individuals who are most likely to benefit from a particular drug or drug delivery system (Rajkomar et al., 2019). Machine learning models have demonstrated considerable success in identifying disease subtypes and predicting treatment outcomes in conditions such as cancer, diabetes, cardiovascular disorders, autoimmune diseases, and neurological disorders. These predictive capabilities facilitate evidence-based therapeutic decision-making and support the development of targeted treatment strategies (Panchpuri et al., 2025).

5.2 AI-Guided Personalized Drug Delivery Systems

Artificial intelligence is increasingly being incorporated into the design of personalized drug delivery systems. Conventional formulations are generally developed for average patient populations and may not adequately address individual variations in pharmacokinetics and pharmacodynamics. AI enables researchers to optimize formulation composition and dosage according to patient-specific physiological and genetic characteristics. For example, AI algorithms can recommend the most suitable nanoparticle formulation, polymer composition, lipid carrier, or transdermal patch based on predicted drug absorption, metabolism, and therapeutic requirements. Personalized formulations may include modified drug release profiles, patient-specific doses, and optimized administration routes that maximize therapeutic benefit while minimizing toxicity (Vora et al., 2023). Three-dimensional (3D) printing technologies combined with AI have further expanded the possibilities of personalized drug delivery. AI-assisted 3D printing can design individualized dosage forms with customized drug doses, release profiles, tablet geometries, and combination therapies tailored to individual patient requirements. Such technologies are expected to play an important role in future hospital pharmacies and personalized pharmaceutical manufacturing (Panchpuri et al., 2025).

5.3 Pharmacogenomics and AI

Pharmacogenomics examines how genetic variations influence individual responses to medications. Genetic polymorphisms affecting drug-metabolizing enzymes, transport proteins, and receptors often explain differences in drug efficacy and toxicity among patients. AI algorithms can rapidly analyze genomic datasets and identify clinically significant genetic markers associated with therapeutic outcomes. Integrating pharmacogenomic information with AI allows healthcare professionals to predict patient responses before treatment begins. This enables selection of appropriate drugs, optimization of dosing regimens, and avoidance of adverse drug reactions. AI-supported pharmacogenomic analysis is particularly valuable in oncology, psychiatry, cardiology, and infectious diseases, where genetic variability strongly influences therapeutic success (Topol, 2019; Serrano et al., 2024).

5.4 AI and Wearable Health Technologies

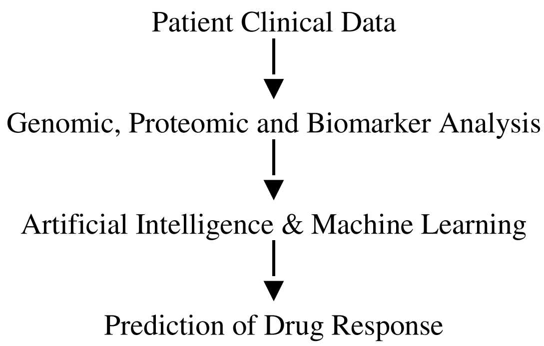
The increasing availability of wearable medical devices has created new opportunities for continuous health monitoring and personalized therapy. Smartwatches, biosensors, glucose monitoring systems, blood pressure monitors, and implantable sensors continuously collect physiological information such as heart rate, physical activity, blood glucose levels, body temperature, oxygen saturation, and sleep patterns. Artificial intelligence analyzes these real-time datasets to monitor disease progression, predict clinical deterioration, and recommend individualized treatment adjustments. For patients receiving controlled drug delivery systems, AI can dynamically modify dosing schedules according to physiological responses and treatment effectiveness. Such adaptive therapeutic approaches improve disease management while reducing unnecessary medication exposure (Esteva et al., 2019).

5.5 AI in Precision Oncology

Cancer treatment represents one of the most successful applications of personalized medicine. Tumor heterogeneity often limits the effectiveness of standardized chemotherapy regimens. AI integrates genomic sequencing, histopathological imaging, molecular biomarkers, and clinical information to identify personalized treatment strategies for individual patients. AI also supports the development of targeted nanocarrier systems capable of delivering anticancer drugs directly to tumor tissues while minimizing damage to healthy cells. Machine learning algorithms optimize nanoparticle size, ligand selection, drug loading, and targeting efficiency based on tumor-specific characteristics. These intelligent delivery systems improve therapeutic efficacy while reducing systemic toxicity and treatment-related adverse effects (Panchpuri et al., 2025).

5.6 Challenges in AI-Driven Personalized Medicine

Despite its enormous potential, several challenges continue to limit the widespread implementation of AI in personalized medicine. One major concern is the availability of high-quality, standardized, and representative clinical datasets. Incomplete or biased datasets may reduce prediction accuracy and limit the generalizability of AI models across diverse patient populations. Additional challenges include data privacy, cybersecurity, ethical considerations, algorithm transparency, and regulatory acceptance. Healthcare organizations must ensure that AI systems comply with data protection regulations while maintaining patient confidentiality and informed consent. Furthermore, clinicians require explainable AI models that provide transparent reasoning behind clinical recommendations to improve trust and facilitate regulatory approval (FDA, 2024).



↓

Personalized Formulation and Dose Selection

↓

Targeted Drug Delivery

↓

Continuous Monitoring and Treatment Optimization

Figure 5. AI Workflow in Personalized Medicine

Table 5. Applications of Artificial Intelligence in Personalized Medicine

AI Application	Role in Personalized Medicine	Clinical Benefit
Patient Stratification	Identification of patient subgroups	Improved treatment selection
Pharmacogenomic Analysis	Prediction of genetic drug response	Reduced adverse drug reactions
Dose Optimization	Individualized dosage prediction	Enhanced therapeutic efficacy
Wearable Device Analytics	Real-time physiological monitoring	Continuous treatment adjustment
Nanocarrier Optimization	Patient-specific drug delivery design	Improved targeting and reduced toxicity
Clinical Decision Support	AI-assisted treatment recommendations	Faster and evidence-based clinical decisions
Predictive Analytics	Disease progression prediction	Early intervention and improved outcomes

In summary, artificial intelligence is redefining personalized medicine by enabling data-driven treatment decisions and individualized drug delivery strategies. Through the integration of genomic information, clinical records, wearable technologies, and predictive analytics, AI supports the design of patient-specific formulations that improve therapeutic efficacy while minimizing toxicity. Although challenges related to data quality, ethical considerations, and regulatory acceptance remain, continued advances in AI and digital health technologies are expected to accelerate the clinical implementation of precision medicine and establish a new era of intelligent pharmaceutical care.

6. Current Challenges and Future Perspectives

Artificial intelligence (AI) has emerged as a transformative technology in pharmaceutical sciences and has demonstrated remarkable potential in improving the design, optimization, and manufacturing of novel drug delivery systems (NDDS). Nevertheless, several scientific, technical, regulatory, and ethical challenges continue to limit its widespread implementation. One of the major obstacles is the limited availability of high-quality pharmaceutical datasets. Most formulation datasets are generated under different experimental conditions, contain relatively small sample sizes, and often exclude unsuccessful experiments, making it difficult to develop robust and highly generalizable AI models. Furthermore, the absence of standardized data formats and harmonized reporting practices restricts data sharing among academic institutions, healthcare organizations, and pharmaceutical industries, thereby reducing the predictive capability of machine learning algorithms (Vora et al., 2023; Jena et al., 2024). Another significant concern is the limited interpretability of advanced AI models, particularly deep learning algorithms, which frequently function as "black-box" systems. Although these models achieve high prediction accuracy, their inability to explain the reasoning behind predictions creates uncertainty among formulation scientists and regulatory authorities. The development of Explainable Artificial Intelligence (XAI) is therefore receiving increasing attention because it improves model transparency, facilitates scientific interpretation, and enhances confidence in AI-assisted decision-making (Panchpuri et al., 2025). In addition, AI-generated predictions require extensive laboratory validation before clinical or industrial implementation, as computational models cannot completely replace experimental investigations. Variations in raw materials, manufacturing processes, and environmental conditions may influence formulation performance, emphasizing the importance of integrating AI with experimental research rather than using it as a standalone approach (Serrano et al., 2024). Regulatory acceptance also remains an important challenge because AI-based pharmaceutical products must comply with stringent quality, safety, efficacy, and data integrity requirements. Regulatory agencies such as the U.S. Food and Drug Administration (FDA) and the European Medicines Agency (EMA) are actively developing frameworks to guide the validation, monitoring, and lifecycle management of AI-enabled pharmaceutical technologies while addressing concerns related to patient privacy, cybersecurity, algorithm bias, and ethical use of clinical data (FDA, 2024). Moreover, the implementation of AI requires advanced computational infrastructure, cloud-based platforms, high-performance computing facilities, and interdisciplinary expertise in pharmaceutical sciences, bioinformatics, computer science, and data analytics, resources that may not be readily available in many research laboratories and small pharmaceutical organizations. Despite these challenges, the future of AI in novel drug delivery systems is exceptionally promising. Continuous advances in machine learning, deep learning, generative AI, robotics, digital twins, and cloud computing are expected to transform pharmaceutical development from an empirical process into an intelligent, predictive, and patient-centered discipline. Generative AI has the capability to design novel formulation compositions, recommend optimal excipient combinations, and identify manufacturing conditions that satisfy predefined quality objectives while substantially reducing formulation development time (Panchpuri et al., 2025). Similarly, digital twin technology is anticipated to revolutionize pharmaceutical manufacturing by creating virtual replicas of formulations and production processes, enabling real-time monitoring, simulation, process optimization, predictive maintenance, and continuous quality assurance throughout the product lifecycle (FDA, 2024). Future pharmaceutical research will increasingly integrate AI with pharmacogenomics, electronic health records, wearable biosensors, and multi-omics technologies to facilitate personalized medicine and individualized drug delivery systems tailored to each patient's biological characteristics. Patient-specific nanoparticles, intelligent transdermal patches, smart hydrogels, implantable delivery systems, and AI-assisted three-dimensional (3D) printed dosage forms are expected to improve therapeutic efficacy while minimizing adverse drug reactions and enhancing patient compliance (Vora et al., 2023). Furthermore, autonomous laboratories combining robotics with AI-driven experimentation may accelerate formulation screening, optimize manufacturing parameters, and significantly reduce human intervention and experimental variability. The establishment of standardized global pharmaceutical databases, explainable AI models, collaborative research networks, and harmonized regulatory guidelines will further strengthen the reliability and industrial acceptance of AI technologies. Overall, artificial intelligence is poised to become an indispensable component of next-generation pharmaceutical research by enabling predictive formulation design, intelligent manufacturing, precision therapeutics, and continuous process optimization. As technological innovations continue to evolve alongside regulatory frameworks and interdisciplinary collaboration, AI-driven drug delivery systems are expected to deliver safer, more effective, and highly personalized therapies, ultimately transforming the future landscape of pharmaceutical sciences and healthcare (Vora et al., 2023; Serrano et al., 2024; Panchpuri et al., 2025).

CONCLUSION

Artificial intelligence (AI) is redefining the landscape of pharmaceutical sciences by introducing intelligent, data-driven approaches to the design, optimization, and manufacturing of novel drug delivery systems (NDDS). As highlighted throughout this review, AI technologies—including machine learning, deep learning, predictive modeling, and generative AI—have significantly enhanced formulation development by enabling rapid excipient selection, optimization of formulation variables, prediction of drug release profiles, encapsulation efficiency, stability, and bioavailability. The integration of AI with advanced pharmaceutical technologies such as nanocarriers, lipid-based delivery systems, microneedles, hydrogels, transdermal patches, and Quality by Design (QbD) has reduced reliance on conventional trial-and-error experimentation, thereby accelerating product development while improving formulation quality and reproducibility. Furthermore, emerging innovations such as digital twins, autonomous laboratories, and AI-assisted personalized medicine demonstrate the growing potential of intelligent pharmaceutical systems capable of delivering patient-specific therapies with improved therapeutic efficacy and safety. Despite these promising advances, several challenges continue to hinder the widespread implementation of AI in pharmaceutical development. Limitations related to data quality, model transparency, experimental validation, regulatory acceptance, cybersecurity, and ethical considerations must be addressed before AI can be routinely integrated into industrial manufacturing and clinical practice. Collaborative efforts among pharmaceutical scientists, computational researchers, clinicians, regulatory authorities, and industry partners will be essential to establish standardized datasets, develop explainable and trustworthy AI models, and create harmonized regulatory frameworks that ensure the safe and responsible application of AI technologies. Looking ahead, the convergence of artificial intelligence with nanotechnology, digital health, multi-omics, robotics, cloud computing, and precision medicine is expected to transform the future of drug delivery. Intelligent drug delivery systems capable of continuously adapting to patient-specific physiological conditions may become an integral component of next-generation therapeutics. As computational capabilities continue to advance and interdisciplinary collaboration strengthens, AI is likely to evolve from a supportive analytical tool into a central driver of pharmaceutical innovation. Ultimately, the successful integration of AI into novel drug delivery system design has the potential to accelerate drug development, improve manufacturing efficiency, reduce healthcare costs, and deliver safer, more effective, and highly personalized therapies, marking a significant step toward the realization of precision pharmaceutical medicine.

REFERENCES

1. Vora LK, Gholap AD, Jetha K, Thakur RR, Tekko IA, Donnelly RF. Artificial intelligence in pharmaceutical technology and drug delivery. Pharmaceutics. 2023;15(7):1916.
2. Jena GK, Kumar S, Sharma N, et al. Artificial intelligence and machine learning implemented in drug delivery systems. Journal of Bio-X Research. 2024;7(1):1–20.
3. Panchpuri M, Painuli R, Kumar C. Artificial intelligence in smart drug delivery systems: A step toward personalized medicine. RSC Pharmaceutics. 2025.
4. Topol EJ. High-performance medicine: The convergence of human and artificial intelligence. Nature Medicine. 2019;25(1):44–56.
5. Rajkomar A, Dean J, Kohane I. Machine learning in medicine. New England Journal of Medicine. 2019;380(14):1347–1358.
6. Esteva A, Robicquet A, Ramsundar B, et al. A guide to deep learning in healthcare. Nature Medicine. 2019;25(1):24–29.
7. U.S. Food and Drug Administration. Using Artificial Intelligence and Machine Learning in the Development of Drug and Biological Products: Discussion Paper. Silver Spring, MD: FDA; 2024.
8. European Medicines Agency. Reflection Paper on the Use of Artificial Intelligence in the Medicinal Product Lifecycle. Amsterdam: EMA; 2024.
9. ICH Harmonised Guideline Q8(R2). Pharmaceutical Development. International Council for Harmonisation of Technical Requirements for Pharmaceuticals for Human Use; 2009.
10. ICH Harmonised Guideline Q9(R1). Quality Risk Management. International Council for Harmonisation; 2023.
11. ICH Harmonised Guideline Q10. Pharmaceutical Quality System. International Council for Harmonisation; 2008.
12. Yu LX. Pharmaceutical quality by design: Product and process development, understanding, and control. Pharmaceutical Research. 2008;25(4):781–791.
13. Paul D, Sanap G, Shenoy S, et al. Artificial intelligence in drug discovery and development. Drug Discovery Today. 2021;26(1):80–93.
14. Mak KK, Pichika MR. Artificial intelligence in drug development: Present status and future prospects. Drug Discovery Today. 2019;24(3):773–780.
15. Zhavoronkov A. Artificial intelligence for drug discovery, biomarker development, and generation of novel chemistry. Molecular Pharmaceutics. 2018;15(10):4311–4313.
16. Ekins S, Puhl AC, Zorn KM, et al. Exploiting machine learning for end-to-end drug discovery

and development. Nature Materials. 2019; 18:435–441.
17. Stokes JM, Yang K, Swanson K, et al. A deep learning approach to antibiotic discovery. Cell. 2020;180(4):688–702.
18. Jumper J, Evans R, Pritzel A, et al. Highly accurate protein structure prediction with AlphaFold. Nature. 2021; 596:583–589.
19. Schmidhuber J. Deep learning in neural networks: An overview. Neural Networks. 2015; 61:85–117.
20. LeCun Y, Bengio Y, Hinton G. Deep learning. Nature. 2015; 521:436–444.
21. Goodfellow I, Bengio Y, Courville A. Deep Learning. Cambridge (MA): MIT Press; 2016.
22. Breiman L. Random forests. Machine Learning. 2001; 45:5–32.
23. Cortes C, Vapnik V. Support-vector networks. Machine Learning. 1995; 20:273–297.
24. Sutton RS, Barto AG. Reinforcement Learning: An Introduction. 2nd ed. Cambridge (MA): MIT Press; 2018.
25. Frazier PI. A tutorial on Bayesian optimization. arXiv. 2018:1807.02811.

Cite: Prachi Sharma*, Gagan Kaushal, Puja Gulati, Artificial Intelligence-Driven Design and Optimization of Novel Drug Delivery Systems: Current Advances, Challenges, and Future Perspectives, Int. J. Med. Pharm. Sci., 2026, 2 (7), 389-403. https://doi.org/10.5281/zenodo.21263928