



Paper Type: Original Article

Machine Learning and Computational Insights into Nanoparticle-Based Drug Delivery

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Citation:

Received: 26 February 2025	Mar Cornelio, O. (2026). Machine learning and computational insights into nanoparticle-based drug delivery. <i>Biocompounds</i> , 3(1), 13-20.
Revised: 15 June 2025	
Accepted: 09 September 2025	

Abstract


Nanoparticle-based drug delivery systems have emerged as a promising strategy to overcome the limitations of conventional therapeutic approaches, including poor bioavailability, lack of target specificity, and systemic toxicity. The unique physicochemical properties of nanoparticles enable controlled drug release, enhanced targeting, and improved therapeutic efficacy. However, the design and optimization of these systems remain highly complex, requiring the integration of multiple physicochemical and biological parameters. In recent years, computational modeling and Machine Learning (ML) have gained significant attention as powerful tools to address these challenges. ML techniques facilitate the prediction of nanoparticle properties, optimization of formulation parameters, and analysis of nanoparticle–biological interactions. Moreover, data-driven approaches contribute to improved nanotoxicity assessment and more efficient drug delivery system design. This review provides a comprehensive overview of nanoparticle-based drug delivery, with a particular focus on computational methods, ML applications, available data sources, and recent case studies. Key challenges, including data scarcity, model interpretability, and reproducibility, are critically discussed. In addition, emerging trends such as personalized nanomedicine, generative artificial intelligence, and adaptive drug delivery systems are highlighted. Overall, the integration of ML with nanoparticle-based drug delivery offers a transformative pathway toward precision medicine, enabling the development of more effective, safe, and targeted therapeutic strategies.

Keywords: Nanoparticle, Drug delivery, Machine learning, Computational modeling, Nanotoxicity prediction.

1 | Introduction

Nanoparticle-based drug delivery systems have emerged as a transformative approach to overcome the limitations of conventional therapeutic strategies. Traditional drug delivery methods often suffer from poor bioavailability, lack of target specificity, systemic toxicity, and inefficient pharmacokinetics. These challenges significantly reduce therapeutic efficacy while increasing adverse side effects, particularly in complex diseases such as cancer and neurodegenerative disorders [1–3]. Consequently, there is a growing demand for advanced delivery platforms that can precisely transport therapeutic agents to targeted tissues while minimizing off-

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 <https://doi.org/10.48313/bic.vi.56>



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target interactions. Nanoparticles offer a promising solution due to their unique physicochemical properties, including tunable size, large surface area-to-volume ratio, and the ability to modify surface characteristics. Various classes of nanoparticles, such as liposomes, polymeric nanoparticles, dendrimers, and metallic nanoparticles, have been extensively investigated for drug delivery applications [4]. These systems enable controlled drug release, improved stability, and enhanced cellular uptake. Furthermore, surface functionalization allows for active targeting through ligand-receptor interactions, significantly improving delivery efficiency. Despite these advantages, the design and optimization of nanoparticle-based drug delivery systems remain highly complex. Multiple interdependent parameters, including particle size, surface charge, hydrophobicity, and material composition, collectively influence biological interactions, biodistribution, and therapeutic outcomes. Additionally, critical challenges such as nanotoxicity, immune system recognition, limited stability under physiological conditions, and scalability of production hinder clinical translation [5–8]. The traditional trial-and-error approach for nanoparticle design is time-consuming, resource-intensive, and often insufficient to fully explore the vast design space. To better understand these complexities, computational methods have been increasingly employed to model and predict nanoparticle behavior. However, even these approaches face limitations when dealing with high-dimensional, nonlinear biological systems [9]. This highlights the need for more advanced, data-driven methodologies to accelerate the design and optimization process. The following *Table 1* and *Fig. 1* summarize key types of nanoparticles, their advantages, and associated challenges in drug delivery applications:

Table 1. Types of nanoparticles and their advantages and challenges in drug delivery.

Nanoparticle Type	Key Advantages	Major Challenges
Liposomes	Biocompatibility, the ability to encapsulate hydrophilic and hydrophobic drugs	Stability issues, rapid clearance
Polymeric nanoparticles	Controlled release, structural versatility	Potential toxicity, complex synthesis
Dendrimers	Precise structure, high drug loading capacity	Costly production, toxicity concerns
Metallic nanoparticles	Unique optical and magnetic properties	Long-term toxicity, accumulation in tissues

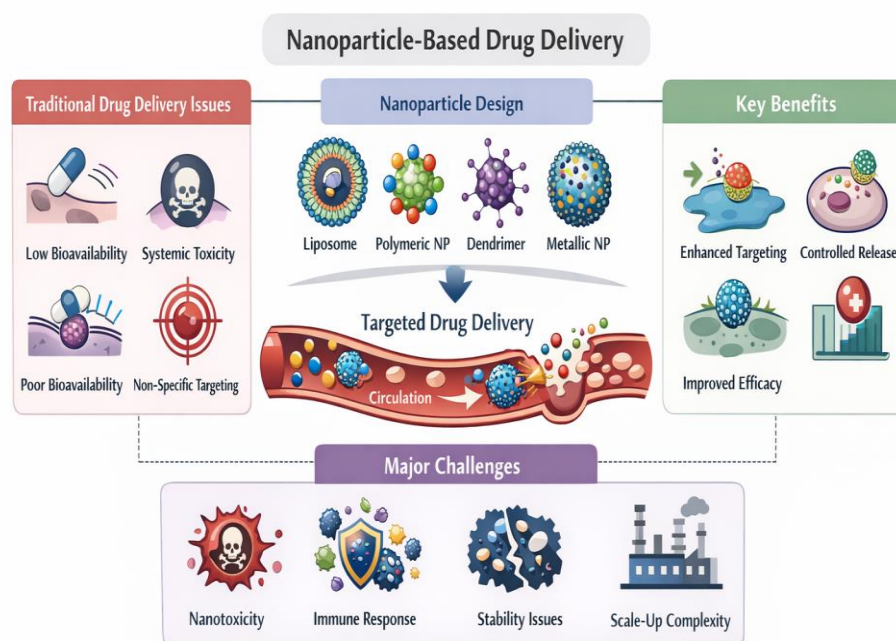


Fig. 1. Schematic illustration of nanoparticle-based drug delivery highlighting design, targeting mechanisms, advantages, and key challenges.

2 | Computational Methods in Nanoparticle-Based Drug Delivery

The increasing complexity of nanoparticle-based drug delivery systems has necessitated the adoption of advanced computational approaches to understand better, predict, and optimize their behavior in biological environments. Traditional experimental methods alone are insufficient to explore the vast design space defined by physicochemical parameters such as particle size, morphology, surface charge, ligand density, and material composition [10]. Computational modeling provides a powerful complementary framework to systematically investigate these parameters and their interactions at multiple scales. At the molecular level, Molecular Dynamics (MD) simulations are widely used to study the structural stability, drug encapsulation, and release mechanisms of nanoparticles. MD simulations enable atomistic insights into nanoparticle drug and nanoparticle membrane interactions, helping to elucidate mechanisms governing cellular uptake and intracellular trafficking. Similarly, molecular docking techniques are employed to evaluate the binding affinity between nanoparticle surface ligands and biological targets such as receptors or proteins, which is crucial for targeted drug delivery. Another important computational approach is the use of Quantitative Structure-Activity Relationship (QSAR) models, which establish correlations between nanoparticle properties and their biological effects, including toxicity, cellular uptake, and biodistribution. QSAR models are particularly valuable for screening large libraries of nanomaterials and identifying promising candidates without extensive experimental testing [11], [12]. Furthermore, multiscale modeling techniques integrate information across different spatial and temporal scales from quantum-level interactions to macroscopic biological behavior (Table 2). These models allow researchers to bridge the gap between nanoscale design and system-level responses, providing a more comprehensive understanding of nanoparticle performance in vivo. Despite their advantages, computational methods face several limitations, including high computational cost, dependence on accurate input parameters, and challenges in modeling complex biological environments. Nonetheless, they form a critical foundation for the integration of data-driven approaches such as Machine Learning (ML), which further enhances predictive capabilities.

Table 2. Overview of computational methods in nanoparticle drug delivery.

Method	Scale	Applications	Limitations
MD	Atomic	Drug loading, membrane interaction	High computational cost
Molecular Docking	Molecular	Ligand–receptor binding	Simplified assumptions
QSAR Models	Molecular/Statistical	Toxicity prediction, screening	Requires high-quality data
Multiscale Modeling	Multi-level	System-level behavior	Model complexity

3 | Machine Learning Applications in Nanoparticle-Based Drug Delivery

ML has emerged as a transformative tool in the design and optimization of nanoparticle-based drug delivery systems. By leveraging large datasets and advanced algorithms, ML enables the identification of complex, nonlinear relationships between nanoparticle properties and biological outcomes, which are often difficult to capture using traditional modeling approaches. One of the primary applications of ML is the prediction of nanoparticle physicochemical properties. ML techniques, including Random Forest, Support Vector Machines (SVMs), and deep learning models, have demonstrated significant capability in predicting nanoparticle behavior and optimizing formulations, as summarized in Table 3. These predictive capabilities significantly reduce the need for iterative experimental trials [13]. Another critical application is the optimization of nanoparticle formulations. ML algorithms can analyze multidimensional datasets to determine optimal combinations of materials, synthesis conditions, and functionalization strategies. Techniques such as Bayesian optimization and genetic algorithms are particularly effective in navigating complex design spaces. ML is also extensively used to model nanoparticle biological interactions, including cellular uptake, biodistribution, and pharmacokinetics. By integrating experimental and clinical data, ML models can predict how nanoparticles behave in different biological environments, enabling more precise targeting strategies. A

particularly important area is the prediction of nanotoxicity. ML-based toxicity models utilize features such as size, shape, surface chemistry, and composition to assess potential adverse effects. These models are crucial for improving the safety profile of nanomedicines and accelerating regulatory approval processes. Recent advances in deep learning and Graph Neural Networks (GNNs) have further expanded the capabilities of ML in this field. GNNs, in particular, are well-suited for representing nanoparticle structures and capturing complex relationships between their components. Additionally, deep learning models can process high-dimensional data from imaging, omics, and simulation outputs, providing deeper insights into nanoparticle behavior [14]. However, the application of ML is not without challenges. Issues such as data scarcity, lack of standardization, model interpretability, and reproducibility remain significant barriers. Addressing these challenges is essential for the successful integration of ML into nanoparticle drug delivery research.

Table 3. ML techniques and their applications.

ML Technique	Application	Advantages	Challenges
Random Forest	Property prediction	Robust, handles nonlinear data	Limited interpretability
SVM	Classification, toxicity prediction	High accuracy	Sensitive to parameters
Neural Networks	Complex prediction tasks	Captures nonlinear patterns	Requires large datasets
Deep Learning	Imaging, feature extraction	High performance	Computationally intensive
GNNs	Structural modeling	Captures relationships	Emerging, limited datasets

4 | Case Studies: Machine Learning in Nanoparticle-Based Drug Delivery

In recent years, ML has been increasingly applied to address key challenges in nanoparticle-based drug delivery. These approaches enable the prediction of complex biological interactions, optimization of nanoparticle formulations, and improvement of therapeutic performance. Several representative case studies are presented below to illustrate the practical impact of ML techniques in this field.

4.1 | Prediction of Nanoparticle Cellular Uptake

A significant study conducted by Walkey et al. [15] explored the relationship between nanoparticle physicochemical properties and cellular uptake. By applying ML techniques, the study demonstrated that the formation of the protein corona plays a critical role in mediating nanoparticle cell interactions. The results indicated that surface chemistry, particularly hydrophobicity and functional group composition, strongly influences cellular internalization. The developed models were able to predict uptake efficiency with high accuracy, providing valuable insights for the rational design of nanoparticle systems.

4.2 | Machine Learning for Nanotoxicity Prediction

Research by Cohen et al. [16] applied QSAR-based ML models to evaluate nanoparticle cytotoxicity. Using descriptors such as particle size, surface area, and chemical composition, the study established predictive relationships between nanoparticle properties and biological effects. The findings highlighted the ability of ML models to capture nonlinear relationships and improve prediction accuracy compared to traditional statistical methods, thereby contributing to safer nanoparticle design.

4.3 | Optimization of Nanoparticle Formulations

A more recent investigation by Li et al. [17] focused on optimizing lipid nanoparticle formulations through ML. By integrating experimental data with ML algorithms such as Random Forest and Bayesian optimization, the study efficiently explored complex formulation spaces. This approach enabled the identification of optimal compositions that enhanced drug delivery efficiency while significantly reducing experimental workload and development time.

4.4 | Deep Learning for Targeted Drug Delivery

In another study, Chun Chou et al. [18] utilized deep learning models to predict nanoparticle targeting efficiency in cancer therapy. The model incorporated multimodal data, including imaging features, nanoparticle characteristics, and biological parameters. The results demonstrated that deep learning approaches can effectively capture complex interactions and significantly improve predictive performance in targeted drug delivery applications.

4.5 | Graph Neural Networks for Nanoparticle Design

Recent work by Zhang et al. [19] introduced GNNs as a novel framework for modeling nanoparticle structures. In this approach, nanoparticles are represented as graph-based systems, allowing for a more accurate representation of structural relationships. This method enhances the ability to predict nanoparticle behavior and provides a powerful tool for the design of next-generation nanomedicines with improved functionality and targeting capabilities (*Table 4*).

Table 4. Summary of case studies in ML-based nanoparticle drug delivery.

Study	ML Method	Application	Key Outcome
Walkey et al. [15]	ML models	Cellular uptake	Role of surface chemistry and protein corona
Cohen et al. [16]	QSAR/ML	Nanotoxicity	Improved toxicity prediction
Li et al. [17]	Random Forest, Bayesian	Formulation optimization	Efficient design space exploration
Chun Chou et al. [18]	Deep Learning	Targeting efficiency	Enhanced predictive accuracy
Zhanget al. [19]	GNN	Nanoparticle design	Structural relationship modeling

5 | Limitations and Challenges of Machine Learning in Nanoparticle-Based Drug Delivery English Version

Despite the remarkable progress in applying ML to nanoparticle-based drug delivery, several critical limitations and challenges remain that hinder its widespread adoption and clinical translation. These challenges arise from both data-related issues and inherent limitations of current ML methodologies when applied to complex biological systems. One of the most significant challenges is data scarcity and quality. High-quality, standardized datasets are essential for training reliable ML models; however, experimental data in nanomedicine are often limited, heterogeneous, and inconsistently reported. Variability in experimental protocols, differences in measurement techniques, and incomplete documentation of nanoparticle properties can introduce significant noise and bias into datasets. As a result, ML models trained on such data may exhibit poor generalization and limited reproducibility [8–12]. Another major limitation is data imbalance and representativeness. Existing datasets are often skewed toward specific types of nanoparticles, such as lipid-based or polymeric systems, while other classes remain underrepresented. This imbalance can lead to biased predictions and restrict the applicability of ML models to a narrow range of nanomaterials. A further challenge lies in the interpretability of ML models. Many advanced models, particularly deep learning architectures, operate as “black boxes,” making it difficult to understand how input features influence predictions. In the context of drug delivery, where safety and regulatory compliance are critical, the lack of interpretability can hinder trust and acceptance among researchers and clinicians [20].

The integration of multimodal and heterogeneous data also presents a significant obstacle. Nanoparticle-based drug delivery involves diverse data types, including physicochemical properties, biological responses, imaging data, and omics datasets. Combining these data sources into a unified ML framework is complex and often requires sophisticated preprocessing and data fusion techniques.

In addition, overfitting and model robustness remain persistent concerns. Due to limited dataset sizes, ML models may capture noise rather than underlying patterns, leading to overfitting and reduced predictive

performance on unseen data. This issue is particularly critical in biomedical applications, where model reliability is essential. From a practical perspective, reproducibility and standardization are also major challenges. Differences in data collection, preprocessing pipelines, and model evaluation metrics make it difficult to compare results across studies. The absence of standardized benchmarks further complicates the validation of ML models in this field [12].

Finally, computational cost and scalability can limit the application of advanced ML techniques. Training deep learning models or integrating large-scale simulation data requires significant computational resources, which may not be accessible to all research groups. These challenges collectively highlight the need for robust, interpretable, and generalizable ML frameworks that can effectively bridge the gap between computational predictions and real-world clinical applications, as summarized in *Table 5*.

Table 5. Key challenges in ML-based nanoparticle drug delivery.

Challenge	Description	Impact
Data scarcity	Limited availability of high-quality datasets	Reduces model accuracy
Data heterogeneity	Variability in experimental conditions	Introduces noise and bias
Data imbalance	Overrepresentation of certain nanoparticle types	Limits generalization
Model interpretability	Black-box nature of complex models	Reduces trust and usability
Overfitting	Poor generalization to new data	Decreases reliability
Data integration	Difficulty combining multimodal data	Increases model complexity
Reproducibility	Lack of standardization	Limits validation
Computational cost	High resource requirements	Restricts accessibility

6 | Future Perspectives in Nanoparticle-Based Drug Delivery

The integration of ML with nanoparticle-based drug delivery systems is expected to revolutionize the future of precision medicine. As both fields continue to evolve, several emerging trends and technological advancements are poised to address current limitations and unlock new opportunities for more efficient, personalized, and adaptive therapeutic strategies [5–9]. One of the most promising directions is the development of AI-driven nanoparticle design frameworks. By combining ML with high-throughput experimentation and computational modeling, researchers can create autonomous or semi-autonomous platforms capable of designing, testing, and optimizing nanoparticle formulations with minimal human intervention. These systems significantly accelerate the discovery process and enable exploration of vast design spaces that are otherwise impractical to investigate experimentally. Another key area is the advancement of personalized nanomedicine. Future drug delivery systems are expected to be tailored to individual patient characteristics, including genetic profile, disease state, and immune response. ML models trained on patient-specific data can predict optimal nanoparticle properties for targeted therapy, thereby improving treatment efficacy and reducing adverse effects. This approach aligns closely with the broader vision of precision medicine. The integration of multimodal data and digital health technologies will also play a crucial role. Combining data from genomics, proteomics, imaging, and clinical records allows for a more comprehensive understanding of disease mechanisms and nanoparticle interactions. ML models capable of handling such heterogeneous data will enable more accurate predictions and better-informed therapeutic decisions [2–6]. In addition, the emergence of real-time and adaptive drug delivery systems represents a significant future direction. By incorporating biosensors and feedback mechanisms, nanoparticle systems can dynamically respond to physiological changes within the body. ML algorithms can process real-time data to adjust drug release profiles, ensuring optimal therapeutic outcomes. Another transformative development is the concept of digital twins in nanomedicine. A digital twin is a virtual representation of a patient or biological system that can simulate the behavior of nanoparticles *in vivo*. By integrating ML with computational modeling, digital twins can be used to predict treatment outcomes, optimize dosing strategies, and reduce reliance on trial-and-error approaches. Advances in generative artificial intelligence, such as Generative Adversarial Networks (GANs) and diffusion models, are also expected to play an important role. These

techniques can be used to design novel nanomaterials with desired properties, thereby expanding the range of available drug delivery platforms. Despite these promising developments, achieving these goals will require overcoming existing challenges related to data availability, model interpretability, and regulatory acceptance. Collaboration between interdisciplinary fields, including materials science, biology, data science, and clinical research, will be essential to drive innovation and ensure successful clinical translation [20–23]. These emerging trends and future directions are summarized in *Table 6*.

Table 6. Future trends in ML-driven nanoparticle drug delivery.

Future Direction	Description	Potential Impact
AI-driven design	Automated nanoparticle optimization	Faster discovery
Personalized nanomedicine	Patient-specific drug delivery	Higher efficacy, side effects
Multimodal data integration	Combining omics, imaging, and clinical data	Improved prediction accuracy
Adaptive systems	Real-time responsive drug delivery	Dynamic treatment optimization
Digital twins	Virtual patient modeling	Reduced experimental cost
Generative AI	Design of novel nanomaterials	Innovation in drug carriers

Authors' Contributions

All aspects of the research and manuscript preparation were carried out by the author. The author has read and approved the final version of the manuscript.

Data Availability

All data are included in the text.

Funding

This study did not receive any specific funding from public, commercial, or non-profit funding agencies.

Conflict of Interest

The author declares that he does not have any conflict of interest.

Consent for Publication

The author has given consent for the publication of this manuscript.

Ethics Approval and Consent to Participate

This study does not involve any research conducted on human participants or animals.

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