



(REVIEW ARTICLE)



AI-powered nano formulation: revolutionizing drug development and delivery

Amar Abubaker Edriss ¹, Sravani Yarra ^{1,*}, Joshua Anthony Vomo ², Kateregga Ismael ¹ and Yassin Babkir Elshiekh ³

¹ Department of Industrial Pharmacy, Raghavendra Institute of Pharmaceutical Education and Research, K.R. Palli Cross, Anantapur, Chiyvedu, Andhra Pradesh-515721-India.

² Department of Pharmacology, Raghavendra Institute of Pharmaceutical Education and Research, K.R. Palli Cross, Anantapur, Chiyvedu, Andhra Pradesh-515721-India.

³ Department of Pharmaceutics, Raghavendra Institute of Pharmaceutical Education and Research, K.R. Palli Cross, Anantapur, Chiyvedu, Andhra Pradesh-515721-India.

International Journal of Science and Research Archive, 2025, 14(02), 1501-1512

Publication history: Received on 07 January 2025; revised on 20 February 2025; accepted on 23 February 2025

Article DOI: <https://doi.org/10.30574/ijrsra.2025.14.2.0491>

Abstract

This study examines the revolutionary potential of AI-driven nanotechnology in redefining drug development and delivery systems. Nano formulations offer numerous advantages over traditional methods, including enhanced drug efficacy, targeted delivery, and reduced side effects. However, limitations like batch-to-batch variability hinder their widespread adoption. AI integration addresses these challenges by enabling data-driven design optimization, predictive modelling, and streamlined quality control in nano-formulation manufacturing processes. AI-powered algorithms can utilize large datasets to develop nanoparticles tailored for targeted drug delivery, and to foresee their interactions with biological entities. This approach can significantly accelerate the development of innovative nanomedicines and improve their clinical translation. Despite promising advancements, technical challenges related to data quality and regulatory hurdles remain. Additionally, ethical considerations regarding privacy, bias, and transparency in AI algorithms need to be addressed. The future of AI-driven nanomedicine holds exciting possibilities, such as autonomous nano formulation design and smart nanoparticles with controlled drug release. Further research focusing on advanced AI models, improved data integration, and interdisciplinary collaboration is crucial to fully realize the potential of this technology and bring us closer to achieving personalized and effective treatments.

Keywords: AI-Driven Nanotechnology; Drug Development; Targeted Drug Delivery; Nano-Formulation; Predictive Modelling

1. Introduction

Nanotechnology involves engineering materials at the nanoscale, a realm between 1 and 100 nanometres, and is a rapidly advancing field (1). This technology has found significant applications across various disciplines, including medicine, where it is referred to as nanomedicine. Nanotechnology holds immense potential for revolutionizing drug delivery systems(2).

Nanotechnology-powered drug delivery systems provide significant benefits compared to conventional methods. These systems can enhance the efficacy and safety of therapeutic agents by enabling targeted delivery to specific sites within the body, thereby reducing systemic side effects and improving patient outcomes(3). In one application, nanoparticles can be engineered to target cancer cells with drugs, sparing healthy tissue and improving the therapeutic potential of chemotherapy agents(4).

* Corresponding author: Sravani Yarra.

In the treatment of central nervous system (CNS) disorders, nanotechnology has shown great potential(5). Nanocarriers can penetrate the blood-brain barrier, a challenge in CNS drug delivery, providing a potential solution for treating neurological disorders like Alzheimer's, Parkinson's, and brain tumors (6). Additionally, polymeric nanoparticles have been developed to improve the oral bioavailability of peptide drugs and facilitate their passage through biological barriers(7).

Moreover, the versatility of nanomaterials allows for the development of multifunctional drug delivery systems(8). For example, chitosan nanoparticles are not only biocompatible and biodegradable but also offer controlled drug release and targeted delivery, making them suitable for a wide range of therapeutic applications, including cancer immunotherapy and theranostics (8).

Despite the promising advancements, there are challenges and concerns associated with nanotechnology in drug delivery. The potential risks and biological interactions of nanoparticles require comprehensive investigation to ensure safety and effectiveness. Nonetheless, the integration of nanotechnology with pharmacology and physiology holds the promise of innovative and highly effective therapeutic strategies(9).

Artificial Intelligence (AI) and nanotechnology are revolutionizing healthcare by enhancing precision medicine, particularly in cancer treatment(10). AI enhances the design of nanomaterials for diagnostic and therapeutic purposes, enabling patient-specific disease profiles and optimizing treatment outcomes(11). In the pharmaceutical sector, AI and nanotechnology are used to develop targeted drug delivery systems, identifying new therapeutic targets and optimizing clinical trials. AI-powered nanotechnology is used to develop advanced diagnostic tools, detecting diseases at early stages and monitoring treatment effectiveness in real-time.(12) AI also helps in optimizing nanomedicine by predicting interactions with biological systems, facilitating better disease management. AI automates tasks in healthcare, leading to faster, more accurate, and cost-effective solution(13)

This article aims to explore the transformative role of AI-powered nanotechnology in revolutionizing drug development and delivery systems. By integrating artificial intelligence with nanomedicine, this study seeks to evaluate how AI enhances the design, optimization, and targeting of nanocarriers for more efficient and precise drug delivery. The objective is to demonstrate the potential of AI to improve therapeutic outcomes, minimize systemic side effects, and address significant hurdles, such as drug resistance and the challenge of overcoming biological barriers, hinder the treatment of complex diseases like cancer and neurological disorders.

2. Nano formulation in Drug Development

Nano formulations are advanced drug delivery systems that utilize nanotechnology to enhance the efficacy, specificity, and safety of therapeutic agents(14). These formulations are designed to deliver drugs, genes, or other bioactive compounds to specific target sites in the body, thereby improving therapeutic outcomes and minimizing side effects(15)The unique properties of Nano formulations, such as their small size, large surface area, and ability to be functionalized, make them highly versatile and effective in various biomedical applications(16).

2.1. Types of Nano formulations

2.1.1. Liposomes

Liposomes are spherical sacs formed by one or more phospholipid layers. They can carry both water-soluble and fat-soluble drugs(17). Liposomes are versatile drug delivery systems that enhance drug efficacy by stabilizing compounds, improving cellular and tissue uptake, and increasing drug biodistribution to target sites(18). They offer targeted delivery, high biocompatibility, biodegradability, and low toxicity, making them superior to traditional methods. Liposomes are used in various fields, including pharmaceuticals, cosmetics, food industries, and tissue engineering(19). They also serve as models for studying cell membranes and carriers for bioactive agents in vaccines, imaging, and regenerative medicine(20). Advances in liposome technology include PEGylated liposomes, ligand-functionalized liposomes, and stimuli-responsive liposomes. However, careful consideration of immunological and toxicological properties is essential for successful clinical application(21).

2.1.2. Micelles

Micelles are self-assembled colloidal structures formed by amphiphilic molecules in aqueous solutions. Micelles are colloidal aggregates formed by the self-assembly of amphiphilic molecules in aqueous solutions(22). They have significant applications in drug delivery, rheology, and biological systems. Micelles are characterized by their size, shape, and rheological properties, with giant micelles exhibiting unique shear thinning and complex flow phenomena. They

can encapsulate proteins, such as MG2, sIgA, lactoferrin, and lysozyme, and play a role in maintaining homeostasis in biological systems(23). Various techniques, such as small-angle neutron scattering, dynamic light scattering, cryo-TEM, and fluorescence correlation spectroscopy, help determine micelle size, shape, and interactions with biological environments. Advanced characterization techniques are essential for understanding micelle behavior and optimizing their applications(24).

2.1.3. Dendrimers

Dendrimers are tree-shaped macromolecules possessing a central core, hollow interiors, and a multitude of functional groups on their exterior(25). Dendrimers are highly branched macromolecules with unique properties, making them suitable for biomedical applications such as drug delivery, gene therapy, and diagnostic imaging(26). They exhibit cytotoxicity and haemolysis, with cationic dendrimers having lower toxicity and longer circulation times(27). Dendrimers with carboxylate terminal groups and those grafted with poly(ethylene oxide) show reduced cytotoxicity and haemolysis, making them more suitable for biological applications.(28) They can encapsulate or conjugate with therapeutic drugs, enhance drug delivery, and protect genetic materials from enzymatic degradation(29). Dendrimers can also be loaded with imaging agents, improving diagnostic accuracy. Their structural design and multifunctionality can be optimized for specific biomedical applications(30).

2.1.4. Quantum Dots

Quantum dots are tiny semiconductor particles that display distinctive optical and electrical behaviors due to quantum confinement(31). Their unique optical and electronic properties, driven by quantum confinement effects, make them useful in optoelectronics, bioimaging, and neurodegenerative diseases(32). Their electronic structure can be analyzed using various models and techniques, providing insights into excitonic processes(33). Quantum dots are increasingly used in biomedical imaging due to their bright fluorescence, long fluorescence lifetimes, and ability to be conjugated to proteins(33). Surface modification enhances solubility and reduces toxicity, making them suitable for drug delivery and pharmaceutical applications. However, toxicity and environmental impact remain critical considerations for safe and effective use(34).

2.1.5. Polymeric Nanoparticles

Polymeric nanoparticles are solid colloidal particles constructed from biodegradable and biocompatible polymers. Polymeric nanoparticles (NPs) have potential for targeted drug delivery and biomedical applications due to their customizable properties(35). They can release drugs in response to various stimuli, enhancing targeted drug delivery and anti-cancer efficacy(36). NPs with enzymatically degradable phosphate ester moieties can change their zeta potential, making them useful for targeted drug delivery systems(37). The size and surface chemistry of NPs significantly affect their cellular association and uptake, with larger NPs showing higher association under static conditions and lower under flow conditions. Protein binding affinity and cell membrane barrier play critical roles in NPs' pharmacokinetics. Understanding these interactions is essential for optimizing their performance in theranostic applications(38).

2.1.6. Carbon-Based Nanostructures

Carbon-based nanostructures include fullerenes, carbon nanotubes, graphene, and nanodiamonds(39). These nanostructures are used in drug delivery, imaging, and as scaffolds for tissue engineering. Carbon nanotubes (CNTs) have metallic and semiconducting properties, making them useful in nanodevices like metallic wires and electromechanical sensors. Carbon dots (CDs) have unique optical properties, making them suitable for sensors, anticounterfeiting, and energy devices(40). Carbon nanodots (CNDs) can be synthesized via top-down and bottom-up methods, offering tunable optical properties and high photostability. Carbon fibers have graphitic and amorphous components, with higher-modulus fibers showing extended sp² carbon layers. A new 2D carbon nanostructure with an orthorhombic superstructure and semiconductor character was constructed, suggesting potential in organic spintronic applications(41). Carbon nanomaterials, including fullerenes, carbon onions, carbon quantum dots, nanodiamonds, CNTs, and graphene, are extensively used in sensing due to their high specific surface area, electrical conductivity, and biocompatibility(42).

2.1.7. Gold Nanoparticles (AuNPs)

Gold nanoparticles are small gold particles with diameters in the nanometer range. AuNPs are used in drug delivery, imaging, and as therapeutic agents(43). Gold nanoparticles are gaining attention due to their unique properties and applications in medicine, catalysis, electronics, and materials science(44). They offer advantages such as precise control of size, shape, composition, and structure during synthesis, and can be tuned based on these characteristics(45). Gold

nanoparticles have a small size and high surface-to-volume ratio, allowing for distinctive physical, chemical, and biological behaviors(46). They can be used in drug and gene delivery, photothermal therapy, photodynamic therapy, radiation therapy, diagnosis, and imaging. They can bind to organic molecules with low toxicity levels, enabling the development of novel drug delivery systems(47).

3. Advantages of Nano formulations

3.1. Improved Solubility

Nano formulations significantly improve the water solubility of drugs that are poorly soluble, a frequent challenge in traditional drug delivery. For instance, nanocrystals and nano emulsions have been shown to increase the dissolution rate and saturation solubility of drugs, thereby improving their bioavailability. This is particularly beneficial for oral drug delivery, where poor solubility often leads to low and variable bioavailability(48).

3.2. Targeted Delivery

One of the most promising advantages of Nano formulations is their ability to deliver drugs specifically to targeted tissues or cells. Nanocarriers functionalized with targeting ligands can selectively bind to specific receptors expressed on the target cells. For example, smart responsive Nano formulations can respond to specific stimuli at the target site, such as pH or redox status, to release the drug precisely where it is needed, thereby reducing systemic side effects(49).

3.3. Reduced Toxicity

Nano formulations can reduce the toxicity of drugs by ensuring that the drug is released only at the target site, thereby minimizing exposure to healthy tissues. This targeted approach optimizes therapeutic efficacy and minimizes unwanted side effects associated with traditional drug delivery methods. For instance, in cancer therapy, natural product-based Nano formulations have been shown to specifically target tumor cells, thereby reducing the systemic toxicity and improving patient outcomes(50).

3.4. Enhanced Bioavailability

Nano formulations improve the bioavailability of drugs by enhancing their absorption and permeability. Various Nano systems, such as nanocrystals, solid lipid nanoparticles, and polymeric nanoparticles, have been developed to improve the oral bioavailability of poorly soluble drugs. These Nano formulations can increase the maximum plasma concentration and in vivo residence time of the drugs, thereby enhancing their therapeutic efficacy(51).

3.5. Limitation of the Nano formulation

Traditional Nano formulation techniques, while transformative, face several significant limitations that hinder their widespread adoption and consistent performance in drug development. One of the most prominent challenges is batch-to-batch variability. Even slight variations in the production process can lead to inconsistent particle sizes, surface properties, and drug encapsulation efficiency. This variability impacts the reproducibility and reliability of the Nano formulations, complicating clinical outcomes and regulatory approvals(52).

Additionally, the need for maintaining strict conditions to preserve the nanoscale characteristics adds to the overall burden. These limitations highlight the need for innovative approaches, such as AI-powered solutions, to overcome these hurdles, making nano formulation more efficient, cost-effective, and scalable for broader therapeutic use(52).

4. AI in Drug Development

The pharmaceutical industry struggles to maintain drug development programs due to escalating research and development costs and diminished efficiency. However, the rapid advancements in artificial intelligence and machine learning technologies have opened up new avenues for revolutionizing the drug discovery and development process(53). Artificial intelligence (AI) technologies, such as machine learning and deep learning, can be used to tackle complex challenges in drug development.

AI-powered tools have the potential to revolutionize drug development by optimizing each stage, from target identification and lead optimization to clinical trials and post-market surveillance. One of the key advantages of utilizing AI in drug development is the ability to handle and analyze large volumes of data. The pharmaceutical industry

possesses abundant data, such as chemical compounds, biological assays, and clinical trial results, which AI algorithms can process to identify potential drug candidates, predict drug properties, and optimize the development process(54).

AI-powered drug discovery platforms are already being employed by pharmaceutical companies and biotechnology firms to accelerate the identification of new drug targets and lead compounds. In the field of drug discovery, the pace of innovation can often be slowed down by the time it takes to identify potential targets for disease treatment. With AI's advanced capabilities, the process of target identification, molecule design, lead optimization, and screening processes has been greatly accelerated(55).

Target identification is a critical step in the drug discovery process as it focuses on finding proteins or genetic sequences that are responsible for a particular disease(56). With AI, researchers can now analyze vast amounts of biological and clinical data to pinpoint the most promising targets for disease treatment. Machine learning algorithms can process this data and identify patterns that are not easily discernable through traditional methods, resulting in a more efficient and accurate target identification process(57).

Once a target has been identified, the next step is to design a molecule that can bind to the target and potentially treat the disease(58). AI has revolutionized molecule design by enabling researchers to predict the structure and function of new molecules with high accuracy and efficiency(59). Natural language processing (NLP) and machine learning algorithms can be used to mine large databases of existing molecules and rapidly generate novel compounds that have the desired properties for drug development. These algorithms can also predict the toxicity and pharmacokinetic properties of the molecules to help researchers identify the best lead candidates for further optimization(59).

The lead optimization process involves refining the molecular structure to maximize its efficacy against the target molecule while minimizing side effects. AI technologies such as deep learning and robotics automation can significantly streamline the lead optimization process by quickly identifying the most promising compounds for further testing. Machine learning algorithms can analyze large datasets of previously tested molecules and predict the potential success of new molecules before they are synthesized, allowing scientists to focus on the most promising candidates(60).

AI-powered personalized medicine is advancing treatment strategies by empowering healthcare professionals to choose the best therapeutic options for individual patients, leveraging their genetic makeup, lifestyle habits, and medical history(61).

5. AI Integration in Nano formulation Design

Nanomedicine has transformed drug delivery, significantly improving the efficacy, safety, and bioavailability of medications. AI-driven design and development of Nano formulations further enhances these benefits, enabling data-driven optimization, predictive modelling, and streamlined manufacturing quality control(62).

Table 1 AI Techniques Applied in Nano formulation

AI Technique	Application in Nano formulation
Machine Learning	Predicting physicochemical properties of nanoparticles
Deep Learning	Image analysis for nanoparticle characterization
Reinforcement Learning	Optimizing synthesis parameters for desired properties

5.1. Data-Driven Design and Optimization

The use of AI algorithms in optimizing nanoparticle properties, such as size, surface charge, and shape, has been a game-changer in enhancing the efficiency of drug delivery. Machine learning techniques can analyse extensive datasets, including experimental results and simulations, to identify the most favorable nanoparticle characteristics for targeted drug delivery(63). These algorithms can rapidly explore multidimensional parameter spaces, accelerating the identification of optimal Nano formulation designs, which would be prohibitively time-consuming using traditional methods(64).

5.2. Predictive Modelling

AI also plays a crucial role in predicting the interaction between nanocarriers and biological systems. Sophisticated machine learning models can simulate the complex interplay between nanoparticles and their target cells, tissues, and organs, allowing for the prediction of pharmacokinetics, biodistribution, and therapeutic efficacy. These predictive tools can facilitate the rational design of nano formulations, reducing the reliance on costly and time-consuming in vitro and in vivo studies(64,65).

5.3. Quality Control and Manufacturing

The integration of AI into the production of nano formulations can ensure consistency, scalability, and quality throughout the manufacturing process. AI-powered systems can monitor critical process parameters, detect anomalies, and optimize operating conditions, thereby improving batch-to-batch reproducibility and reducing the risk of product variability(66).

Furthermore, AI-driven quality control measures can automate the characterization of nanoparticle properties, streamlining the evaluation of critical quality attributes and accelerating the release of qualified drug products(67). The advancements in AI-driven nano formulation design and development have the potential to revolutionize the pharmaceutical industry, leading to more effective, safer, and personalized drug therapies. The increasing adoption of AI technologies in the pharmaceutical industry, including their application in drug discovery, repurposing, and structural biology, as exemplified by the COVID-19 pandemic(68).

6. Case Studies and Current Applications

AI-powered nano formulations have shown promising results in both preclinical and clinical trials. One notable example is the use of AI and machine learning (ML) to optimize the design and development of nanomedicines(69). These technologies can significantly improve drug safety and efficacy profiles by automating the experimental processes and generating high-quality datasets. This approach has the potential to accelerate the development of innovative nanomedicines and improve their clinical translation(70).

The pharmaceutical industry is increasingly embracing AI-driven technologies, leading to numerous partnerships and collaborations. For instance, pharmaceutical companies, AI developers, and research institutions are working together to integrate AI into the clinical trial process. AI tools are being used to optimize patient selection, matching, and enrollment, which can reduce the complexity and costs associated with clinical trials. These collaborations have shown encouraging results, although more studies are needed to validate these tools and facilitate their widespread adoption(71).

The integration of AI technologies, such as deep learning, neural networks, and Bayesian nonparametric models, is accelerating pharmaceutical and healthcare research (72). These tools are being utilized for a wide range of applications, including disease diagnosis, digital therapeutics, personalized medicine, and drug discovery (73). This rapid advancement is expected to lead to more efficient and cost-effective healthcare solutions, ultimately benefiting the general public. AI and ML technologies can address many of the traditional obstacles in drug formulation and clinical trials, accelerating the development of innovative and effective therapies (74).

Table 2 Overview of AI-Powered Nano formulation in Drug Development and Delivery

Aspect	Description	Key Examples/Tools	Advantages	Challenges
AI in Drug Discovery	Utilizes machine learning to identify drug candidates and predict interactions	Deep learning, QSAR models	Reduces time and cost	Requires high-quality training data
Nano formulation Design	Optimizes nanoparticles' size, shape, and surface properties for efficient drug encapsulation and release.	Nanoparticle simulation software (e.g., COMSOL	Enhances bioavailability and targeting	Complex manufacturing processes

Drug Delivery Optimization	AI predicts and improves pharmacokinetics and biodistribution of Nano formulated drugs	AI-driven pharmacokinetic modelling	Personalized drug delivery	Validation in diverse biological systems
Case Studies	AI-enhanced Nano formulations for specific diseases.	AI-designed liposomal drugs for cancer	Demonstrates real-world applications	Limited translational studies
Regulatory Considerations	Addresses ethical and safety concerns for AI-driven Nano formulations to meet regulatory standards	FDA guidelines for AI in drug development	Ensures compliance and public trust	Regulatory frameworks still evolving

7. Challenges and Ethical Considerations

7.1. Technical Challenges

The integration of AI into existing healthcare technologies presents several technical challenges(75). One major issue is data quality, as AI systems require large, diverse, and high-quality datasets to function effectively. Poor data quality can lead to inaccurate predictions and biased outcomes, which can be detrimental in a healthcare setting. Additionally, integrating AI with existing healthcare technologies involves logistical difficulties, such as data standardization and interoperability across multiple platforms(76). These challenges must be addressed to ensure seamless integration and functionality. Interdisciplinary collaboration is also crucial, as the development and implementation of AI in healthcare require expertise from various fields, including computer science, medicine, and ethics(77).

7.2. Regulatory Hurdles

The regulatory landscape for AI-driven nano formulations in healthcare is complex and evolving. In the United States and Europe, there are ongoing efforts to develop regulatory frameworks that balance innovation with patient safety(78). Regulatory bodies must ensure that AI systems are rigorously tested and validated before they are approved for clinical use. Post-market surveillance is also essential to monitor the performance and safety of AI-driven technologies once they are in use(79). The current regulatory environment emphasizes the need for transparency in algorithm design and the importance of maintaining high standards for data protection and privacy. A new regulatory model that focuses on the process of AI design, rather than just the final product, may be necessary to address these challenges effectively(80).

7.3. Ethical Issues

The ethical implications of AI in healthcare are profound and multifaceted. Privacy concerns are significant, as AI systems frequently require access to large volumes of confidential patient data. Ensuring data security and protecting patient privacy are critical to maintaining trust in AI-driven healthcare(81). Potential biases in AI algorithms are another significant ethical issue inherent in the training data or the algorithms themselves can lead to unjust or discriminatory results. Addressing these biases is essential to prevent healthcare disparities and ensure equitable treatment for all patients. The ethical implications of AI also extend to issues of transparency, responsibility, and trust. Explainable AI (XAI) is crucial for ensuring that healthcare providers and patients understand how AI-generated predictions are made, which can help build trust in these systems(82). Ultimately, the ethical use of AI in healthcare needs a collaborative effort among policymakers, developers, practitioners, and patients to tackle these complex issues(83).

8. Future Directions and Opportunities

8.1. AI and Nano formulation Trends

Emerging trends in AI-driven nanomedicine are significantly impacting the treatment of rare diseases, cancer, and gene therapy. The integration of AI with nanotechnology is enabling precision medicine by tailoring treatments to individual patients. For instance, AI is being used to optimize the design of nanomaterials for cancer treatment, improving diagnostic accuracy and therapeutic outcomes by analyzing complex patient data and predicting interactions with biological systems. Additionally, smart nanoparticles are being developed for targeted drug delivery and theranostic applications, which combine therapy and diagnostics in a single platform. These advancements are particularly

promising for cancer therapy, where AI-driven nanomedicine can address the high heterogeneity of tumours and patient-specific responses to treatment(84)

The future of nanomedicine holds exciting possibilities, such as autonomous nano formulation design, where AI algorithms could independently design and optimize nanoparticles for specific therapeutic needs. Smart nanoparticles that can respond to environmental triggers within the body, such as pH or temperature changes, are also on the horizon. These nanoparticles could release drugs in a controlled manner, enhancing treatment efficacy and reducing side effects. Theranostic applications, which integrate diagnostic and therapeutic functions, are another area of potential innovation. These platforms could enable real-time monitoring of treatment responses and adjust therapy accordingly, providing a more dynamic and personalized approach to disease management(85).

8.2. Recommendations for Research

To fully realize the potential of AI-driven nanomedicine, several areas require further research: Firstly, Improved. Developing Sophisticated AI: Building highly complex AI models to address the complexities of biological systems is crucial. These models should be capable of integrating diverse data types, including genomic, proteomic, and clinical data, to provide more accurate predictions and personalized treatment plans.

Secondly, Better Data Integration: Effective integration of large datasets from different sources is essential for the success of AI in nanomedicine. This includes developing standardized protocols for data collection, storage, and sharing to facilitate collaboration and improve the robustness of AI predictions.

Lastly, Interdisciplinary Approaches: Collaboration between experts in AI, nanotechnology, biology, and medicine is vital to address the multifaceted challenges of developing effective nanomedicines. Interdisciplinary research can lead to innovative solutions and accelerate the translation of laboratory findings into clinical applications. By focusing on these areas, researchers can enhance the capabilities of AI-driven nanomedicine and bring us closer to achieving truly personalized and effective treatments for a wide range of diseases.

9. Conclusion

AI-powered nano formulation represents a paradigm shift in drug development and delivery. By harnessing the unique properties of nanomaterials and the analytical prowess of AI, researchers are creating targeted and efficient therapeutic solutions. AI algorithms optimize nanoparticle design, predict interactions with biological systems, and streamline manufacturing processes, leading to improved drug efficacy, reduced side effects, and enhanced patient outcomes. The future of AI-driven nanomedicine is brimming with possibilities. We can expect the development of autonomous nano formulation design, smart nanoparticles that respond to internal stimuli, and theranostic platforms that combine diagnostics and treatment. These advancements hold immense potential for personalized medicine, particularly in tackling complex diseases like cancer. To fully realize this potential, further research is crucial. We need more sophisticated AI models that can integrate diverse data types and account for biological complexity. Effective data sharing and standardized protocols are essential for robust AI predictions. Additionally, fostering interdisciplinary collaboration between AI experts, nanotechnologists, biologists, and medical professionals will accelerate the translation of research findings into clinical applications. By investing in AI-powered nanomedicine and fostering collaborative research, we can unlock a new era of personalized and effective healthcare, empowering us to deliver targeted therapies and improve patient outcomes for a wide range of diseases. This technology has the potential to revolutionize how we treat illness, offering a future where medicine becomes more precise and patient-centric. Let us embrace this opportunity and work together to shape the future of healthcare.

Compliance with ethical standards

Acknowledgments

The authors are extremely thankful to management of Raghavendra Institute of Pharmaceutical Education and Research-Autonomous

Disclosure of conflict of interest

No conflict of interest to be disclosed.

References

- [1] Nasrollahzadeh M, Sajadi SM, Sajjadi M, Issaabadi Z. An Introduction to Nanotechnology. In: Interface Science and Technology [Internet]. Elsevier; 2019 [cited 2024 Oct 27]. p. 1–27. Available from: <https://linkinghub.elsevier.com/retrieve/pii/B9780128135860000018>
- [2] Mahendra Kumar S, Rajni Y, Sandeep Prasad T. Recent advances in nanotechnology. *Int J Nanomater Nanotechnol Nanomedicine*. 2023 Sep 15;9(2):015–23.
- [3] Liang W, Zhou C, Jin S, Fu L, Zhang H, Huang X, et al. An update on the advances in the field of nanostructured drug delivery systems for a variety of orthopedic applications. *Drug Deliv*. 2023 Dec 31;30(1):2241667.
- [4] Sanjay SS, Pandey AC. A Brief Manifestation of Nanotechnology. In: Shukla AK, editor. *EMR/ESR/EPR Spectroscopy for Characterization of Nanomaterials* [Internet]. New Delhi: Springer India; 2017 [cited 2024 Oct 27]. p. 47–63. (Advanced Structured Materials; vol. 62). Available from: http://link.springer.com/10.1007/978-81-322-3655-9_2
- [5] Martinelli C, Pucci C, Battaglini M, Marino A, Ciofani G. Antioxidants and Nanotechnology: Promises and Limits of Potentially Disruptive Approaches in the Treatment of Central Nervous System Diseases. *Adv Healthc Mater*. 2020 Feb;9(3):1901589.
- [6] Nguyen TT, Dung Nguyen TT, Vo TK, Tran NMA, Nguyen MK, Van Vo T, et al. Nanotechnology-based drug delivery for central nervous system disorders. *Biomed Pharmacother*. 2021 Nov;143:112117.
- [7] Smith ES, Porterfield JE, Kannan RM. Leveraging the interplay of nanotechnology and neuroscience: Designing new avenues for treating central nervous system disorders. *Adv Drug Deliv Rev*. 2019 Aug;148:181–203.
- [8] Chung YH, Cai H, Steinmetz NF. Viral nanoparticles for drug delivery, imaging, immunotherapy, and theranostic applications. *Adv Drug Deliv Rev*. 2020;156:214–35.
- [9] Sharma D, Sharma N, Pathak M, Agrawala PK, Basu M, Ojha H. Nanotechnology-based drug delivery systems. In: *Drug Targeting and Stimuli Sensitive Drug Delivery Systems* [Internet]. Elsevier; 2018 [cited 2024 Oct 27]. p. 39–79. Available from: <https://linkinghub.elsevier.com/retrieve/pii/B9780128136898000021>
- [10] Sahu M, Gupta R, Ambasta RK, Kumar P. Artificial intelligence and machine learning in precision medicine: A paradigm shift in big data analysis. In: *Progress in Molecular Biology and Translational Science* [Internet]. Elsevier; 2022 [cited 2024 Oct 27]. p. 57–100. Available from: <https://linkinghub.elsevier.com/retrieve/pii/S1877117322000436>
- [11] Tajunisa M, Sadath L, Nair RS. Nanotechnology and Artificial Intelligence for Precision Medicine in Oncology. In: *Artificial Intelligence* [Internet]. 1st ed. Boca Raton: CRC Press; 2021 [cited 2024 Oct 27]. p. 103–22. Available from: <https://www.taylorfrancis.com/books/9781003095910/chapters/10.1201/9781003095910-8>
- [12] Dhanalakshmi M, Das K, Iqbal M, Mohanan VP, Dave S. Artificial Intelligence – The Imperative Tool in Healthcare Innovations Employing Nanotechnology. In: *Nanomaterials and Point of Care Technologies* [Internet]. 1st ed. Boca Raton: CRC Press; 2024 [cited 2024 Oct 27]. p. 195–213. Available from: <https://www.taylorfrancis.com/books/9781003316435/chapters/10.1201/9781003316435-8>
- [13] Habeeb M, You HW, Umapathi M, Ravikumar KK, Hariyadi, Mishra S. Strategies of Artificial intelligence tools in the domain of nanomedicine. *J Drug Deliv Sci Technol*. 2024 Jan;91:105157.
- [14] Kingsley JD, Dou H, Morehead J, Rabinow B, Gendelman HE, Destache CJ. Nanotechnology: A Focus on Nanoparticles as a Drug Delivery System. *J Neuroimmune Pharmacol*. 2006 Sep;1(3):340–50.
- [15] Peng Y, Chen L, Ye S, Kang Y, Liu J, Zeng S, et al. Research and development of drug delivery systems based on drug transporter and nano-formulation. *Asian J Pharm Sci*. 2020 Mar;15(2):220–36.
- [16] Sahu T, Ratre YK, Chauhan S, Bhaskar LVKS, Nair MP, Verma HK. Nanotechnology based drug delivery system: Current strategies and emerging therapeutic potential for medical science. *J Drug Deliv Sci Technol*. 2021 Jun;63:102487.
- [17] Tyagi RK, Garg N, Shukla R, Singh Bisen P, editors. *Role of Novel Drug Delivery Vehicles in Nanobiomedicine*. Erscheinungsort nicht ermittelbar: IntechOpen; 2020. 1 p.
- [18] Guimarães D, Cavaco-Paulo A, Nogueira E. Design of liposomes as drug delivery system for therapeutic applications. *Int J Pharm*. 2021 May;601:120571.
- [19] Cheng R, Liu L, Xiang Y, Lu Y, Deng L, Zhang H, et al. Advanced liposome-loaded scaffolds for therapeutic and tissue engineering applications. *Biomaterials*. 2020 Feb;232:119706.

- [20] Han X, Alu A, Liu H, Shi Y, Wei X, Cai L, et al. Biomaterial-assisted biotherapy: A brief review of biomaterials used in drug delivery, vaccine development, gene therapy, and stem cell therapy. *Bioact Mater.* 2022 Nov;17:29–48.
- [21] Eroğlu İ, İbrahim M. Liposome–ligand conjugates: a review on the current state of art. *J Drug Target.* 2020 Mar 15;28(3):225–44.
- [22] Bu X, Ji N, Dai L, Dong X, Chen M, Xiong L, et al. Self-assembled micelles based on amphiphilic biopolymers for delivery of functional ingredients. *Trends Food Sci Technol.* 2021 Aug;114:386–98.
- [23] Larsson J, Sanchez-Fernandez A, Leung AE, Schweins R, Wu B, Nylander T, et al. Molecular structure of maltoside surfactants controls micelle formation and rheological behavior. *J Colloid Interface Sci.* 2021 Jan;581:895–904.
- [24] Li L, Qu J, Liu W, Peng B, Cong S, Yu H, et al. Advancements in Characterization Techniques for Microemulsions: From Molecular Insights to Macroscopic Phenomena. *Molecules.* 2024 Jun 18;29(12):2901.
- [25] Wang J, Li B, Qiu L, Qiao X, Yang H. Dendrimer-based drug delivery systems: history, challenges, and latest developments. *J Biol Eng.* 2022 Dec;16(1):18.
- [26] Mukherjee S, Mukherjee S, Abouehab MAS, Sahebkar A, Kesharwani P. Exploring dendrimer-based drug delivery systems and their potential applications in cancer immunotherapy. *Eur Polym J.* 2022 Aug;177:111471.
- [27] Pan J, Attia SA, Filipczak N, Torchilin VP. Dendrimers for drug delivery purposes. In: *Nanoengineered Biomaterials for Advanced Drug Delivery* [Internet]. Elsevier; 2020 [cited 2024 Oct 27]. p. 201–42. Available from: <https://linkinghub.elsevier.com/retrieve/pii/B9780081029855000103>
- [28] Naharros-Molinero A, Caballo-González MÁ, De La Mata FJ, García-Gallego S. Direct and Reverse Pluronic Micelles: Design and Characterization of Promising Drug Delivery Nanosystems. *Pharmaceutics.* 2022 Nov 28;14(12):2628.
- [29] Gahrooe TR, Abbasi Moud A, Danesh M, Hatzikiriakos SG. Rheological characterization of CNC-CTAB network below and above critical micelle concentration (CMC). *Carbohydr Polym.* 2021 Apr;257:117552.
- [30] Bober Z, Bartusik-Aebisher D, Aebisher D. Application of Dendrimers in Anticancer Diagnostics and Therapy. *Molecules.* 2022 May 18;27(10):3237.
- [31] Nair A, Haponiuk JT, Thomas S, Gopi S. Natural carbon-based quantum dots and their applications in drug delivery: A review. *Biomed Pharmacother.* 2020 Dec;132:110834.
- [32] Badilli U, Mollarasouli F, Bakirhan NK, Ozkan Y, Ozkan SA. Role of quantum dots in pharmaceutical and biomedical analysis, and its application in drug delivery. *TrAC Trends Anal Chem.* 2020 Oct;131:116013.
- [33] Samimi S, Ardestani MS, Dorkoosh FA. Preparation of carbon quantum dots- quinic acid for drug delivery of gemcitabine to breast cancer cells. *J Drug Deliv Sci Technol.* 2021 Feb;61:102287.
- [34] Ruzycka-Ayoush M, Kowalik P, Kowalczyk A, Bujak P, Nowicka AM, Wojewodzka M, et al. Quantum dots as targeted doxorubicin drug delivery nanosystems in human lung cancer cells. *Cancer Nanotechnol.* 2021 Dec;12(1):8.
- [35] Begines B, Ortiz T, Pérez-Aranda M, Martínez G, Merinero M, Argüelles-Arias F, et al. Polymeric Nanoparticles for Drug Delivery: Recent Developments and Future Prospects. *Nanomaterials.* 2020 Jul 19;10(7):1403.
- [36] Zielińska A, Carreiró F, Oliveira AM, Neves A, Pires B, Venkatesh DN, et al. Polymeric Nanoparticles: Production, Characterization, Toxicology and Ecotoxicology. *Molecules.* 2020 Aug 15;25(16):3731.
- [37] Zhang W, Mehta A, Tong Z, Esser L, Voelcker NH. Development of Polymeric Nanoparticles for Blood–Brain Barrier Transfer—Strategies and Challenges. *Adv Sci.* 2021 May;8(10):2003937.
- [38] Gagliardi A, Giuliano E, Venkateswararao E, Fresta M, Bulotta S, Awasthi V, et al. Biodegradable Polymeric Nanoparticles for Drug Delivery to Solid Tumors. *Front Pharmacol.* 2021 Feb 3;12:601626.
- [39] Debnath SK, Srivastava R. Drug Delivery With Carbon-Based Nanomaterials as Versatile Nanocarriers: Progress and Prospects. *Front Nanotechnol.* 2021 Apr 14;3:644564.
- [40] Henna TK, Raphey VR, Sankar R, Ameena Shirin VK, Gangadharappa HV, Pramod K. Carbon nanostructures: The drug and the delivery system for brain disorders. *Int J Pharm.* 2020 Sep;587:119701.
- [41] Kumar N, Chamoli P, Misra M, Manoj MK, Sharma A. Advanced metal and carbon nanostructures for medical, drug delivery and bio-imaging applications. *Nanoscale.* 2022;14(11):3987–4017.

- [42] Sajjadi M, Nasrollahzadeh M, Jaleh B, Soufi GJ, Iravani S. Carbon-based nanomaterials for targeted cancer nanotherapy: recent trends and future prospects. *J Drug Target*. 2021 Aug 9;29(7):716–41.
- [43] Mirkin CA, editor. *Spherical nucleic acids*. Singapore: Jenny Stanford Publishing; 2020. 1 p.
- [44] Hammami I, Alabdallah NM, Jomaa AA, Kamoun M. Gold nanoparticles: Synthesis properties and applications. *J King Saud Univ - Sci*. 2021 Oct;33(7):101560.
- [45] Mikhailova EO. Gold Nanoparticles: Biosynthesis and Potential of Biomedical Application. *J Funct Biomater*. 2021 Dec 3;12(4):70.
- [46] Bansal SA, Kumar V, Karimi J, Singh AP, Kumar S. Role of gold nanoparticles in advanced biomedical applications. *Nanoscale Adv*. 2020;2(9):3764–87.
- [47] Amina SJ, Guo B. A Review on the Synthesis and Functionalization of Gold Nanoparticles as a Drug Delivery Vehicle. *Int J Nanomedicine*. 2020 Dec 7;15:9823–57.
- [48] Abu Hajleh MN, Abu-Huwaij R, AL-Samydai A, Al-Halaseh LK, Al-Dujaili EA. The revolution of cosmeceuticals delivery by using nanotechnology: A narrative review of advantages and side effects. *J Cosmet Dermatol*. 2021 Dec;20(12):3818–28.
- [49] Yetisgin AA, Cetinel S, Zuvin M, Kosar A, Kutlu O. Therapeutic Nanoparticles and Their Targeted Delivery Applications. *Molecules*. 2020 May 8;25(9):2193.
- [50] Ahmar S, Mahmood T, Fiaz S, Mora-Poblete F, Shafique MS, Chattha MS, et al. Advantage of Nanotechnology-Based Genome Editing System and Its Application in Crop Improvement. *Front Plant Sci*. 2021 May 28;12:663849.
- [51] Wang Y, Pi C, Feng X, Hou Y, Zhao L, Wei Y. The Influence of Nanoparticle Properties on Oral Bioavailability of Drugs. *Int J Nanomedicine*. 2020 Aug 24;15:6295–310.
- [52] Yang M, Byrn SR, Clase KL. An Analytic Investigation of the Drug Formulation-Based Recalls in the USA: See More Beyond the Literal. *AAPS PharmSciTech*. 2020 Jul 16;21(5):198.
- [53] Tiwari PC, Pal R, Chaudhary MJ, Nath R. Artificial intelligence revolutionizing drug development: Exploring opportunities and challenges. *Drug Dev Res*. 2023 Dec;84(8):1652–63.
- [54] Mak KK, Wong YH, Pichika MR. Artificial Intelligence in Drug Discovery and Development. In: Hock FJ, Pugsley MK, editors. *Drug Discovery and Evaluation: Safety and Pharmacokinetic Assays* [Internet]. Cham: Springer International Publishing; 2024 [cited 2024 Oct 28]. p. 1461–98. Available from: https://doi.org/10.1007/978-3-031-35529-5_92
- [55] Sahu A, Mishra J, Kushwaha N. Artificial Intelligence (AI) in Drugs and Pharmaceuticals. *Comb Chem High Throughput Screen*. 2022 Sep;25(11):1818–37.
- [56] Jiménez-Luna J, Grisoni F, Weskamp N, Schneider G. Artificial intelligence in drug discovery: recent advances and future perspectives. *Expert Opin Drug Discov*. 2021 Sep 2;16(9):949–59.
- [57] Malandraki-Miller S, Riley PR. Use of artificial intelligence to enhance phenotypic drug discovery. *Drug Discov Today*. 2021 Apr;26(4):887–901.
- [58] Mohanty S, Harun Ai Rashid M, Mridul M, Mohanty C, Swayamsiddha S. Application of Artificial Intelligence in COVID-19 drug repurposing. *Diabetes Metab Syndr Clin Res Rev*. 2020 Sep;14(5):1027–31.
- [59] David L, Thakkar A, Mercado R, Engkvist O. Molecular representations in AI-driven drug discovery: a review and practical guide. *J Cheminformatics*. 2020 Sep 17;12(1):56.
- [60] Walters WP, Barzilay R. Critical assessment of AI in drug discovery. *Expert Opin Drug Discov*. 2021 Sep 2;16(9):937–47.
- [61] Zhavoronkov A, Vanhaelen Q, Oprea TI. Will Artificial Intelligence for Drug Discovery Impact Clinical Pharmacology? *Clin Pharmacol Ther*. 2020 Apr;107(4):780–5.
- [62] Noorain, Srivastava V, Parveen B, Parveen R. Artificial Intelligence in Drug Formulation and Development: Applications and Future Prospects. *Curr Drug Metab*. 2023 Sep;24(9):622–34.
- [63] Tao H, Wu T, Aldeghi M, Wu TC, Aspuru-Guzik A, Kumacheva E. Nanoparticle synthesis assisted by machine learning. *Nat Rev Mater*. 2021 Aug;6(8):701–16.
- [64] Lin Z, Chou WC, Cheng YH, He C, Monteiro-Riviere NA, Riviere JE. Predicting Nanoparticle Delivery to Tumors Using Machine Learning and Artificial Intelligence Approaches. *Int J Nanomedicine*. 2022 Mar 24;17:1365–79.

- [65] Lv H, Chen X. Intelligent control of nanoparticle synthesis through machine learning. *Nanoscale*. 2022 May 16;14(18):6688–708.
- [66] Day AL, Wahl CB, Dos Reis R, Liao W keng, Dravid VP, Choudhary A, et al. Automated Nanoparticle Image Processing Pipeline for AI-Driven Materials Characterization. In: *Proceedings of the 33rd ACM International Conference on Information and Knowledge Management [Internet]*. Boise ID USA: ACM; 2024 [cited 2024 Oct 28]. p. 4462–9. Available from: <https://dl.acm.org/doi/10.1145/3627673.3680100>
- [67] Jayaraman A, Lu S. *Machine Learning for Analysis of Structural Characterization*. In: *The Digital Transformation of Product Formulation*. CRC Press; 2024.
- [68] Nandipati M, Fatoki O, Desai S. Bridging Nanomanufacturing and Artificial Intelligence—A Comprehensive Review. *Materials*. 2024 Apr 2;17(7):1621.
- [69] Singh AV, Rosenkranz D, Ansari MHD, Singh R, Kanase A, Singh SP, et al. Artificial Intelligence and Machine Learning Empower Advanced Biomedical Material Design to Toxicity Prediction. *Adv Intell Syst*. 2020 Dec;2(12):2000084.
- [70] Singh AV, Ansari MHD, Rosenkranz D, Maharjan RS, Kriegel FL, Gandhi K, et al. Artificial Intelligence and Machine Learning in Computational Nanotoxicology: Unlocking and Empowering Nanomedicine. *Adv Healthc Mater*. 2020 Sep;9(17):1901862.
- [71] Serov N, Vinogradov V. Artificial intelligence to bring nanomedicine to life. *Adv Drug Deliv Rev*. 2022 May;184:114194.
- [72] Moraffah B. Bayesian Nonparametrics: An Alternative to Deep Learning [Internet]. arXiv; 2024 [cited 2024 Oct 28]. Available from: <https://arxiv.org/abs/2404.00085>
- [73] Westermann P, Evins R. Using Bayesian deep learning approaches for uncertainty-aware building energy surrogate models. *Energy AI*. 2021 Mar;3:100039.
- [74] Kolluri S, Lin J, Liu R, Zhang Y, Zhang W. Machine Learning and Artificial Intelligence in Pharmaceutical Research and Development: a Review. *AAPS J*. 2022 Jan;24(1):19.
- [75] Lee D, Yoon SN. Application of Artificial Intelligence-Based Technologies in the Healthcare Industry: Opportunities and Challenges. *Int J Environ Res Public Health*. 2021 Jan 1;18(1):271.
- [76] Singh RP, Hom GL, Abramoff MD, Campbell JP, Chiang MF, on behalf of the AAO Task Force on Artificial Intelligence. Current Challenges and Barriers to Real-World Artificial Intelligence Adoption for the Healthcare System, Provider, and the Patient. *Transl Vis Sci Technol*. 2020 Aug 11;9(2):45.
- [77] Wang Q, Su M, Zhang M, Li R. Integrating Digital Technologies and Public Health to Fight Covid-19 Pandemic: Key Technologies, Applications, Challenges and Outlook of Digital Healthcare. *Int J Environ Res Public Health*. 2021 Jun 4;18(11):6053.
- [78] Da Silva RGL. The advancement of artificial intelligence in biomedical research and health innovation: challenges and opportunities in emerging economies. *Glob Health*. 2024 May 21;20(1):44.
- [79] Serrano DR, Luciano FC, Anaya BJ, Ongoren B, Kara A, Molina G, et al. Artificial Intelligence (AI) Applications in Drug Discovery and Drug Delivery: Revolutionizing Personalized Medicine. *Pharmaceutics*. 2024 Oct 14;16(10):1328.
- [80] Dey H, Arya N, Mathur H, Chatterjee N, Jadon R. Exploring the Role of Artificial Intelligence and Machine Learning in Pharmaceutical Formulation Design. *Int J Newgen Res Pharm Healthc*. 2024 Jun 30;30–41.
- [81] Prakash S, Balaji JN, Joshi A, Surapaneni KM. Ethical Conundrums in the Application of Artificial Intelligence (AI) in Healthcare—A Scoping Review of Reviews. *J Pers Med*. 2022 Nov 16;12(11):1914.
- [82] Elendu C, Amaechi DC, Elendu TC, Jingwa KA, Okoye OK, John Okah M, et al. Ethical implications of AI and robotics in healthcare: A review. *Medicine (Baltimore)*. 2023 Dec 15;102(50):e36671.
- [83] Al-kfairy M, Mustafa D, Kshetri N, Insiew M, Alfandi O. Ethical Challenges and Solutions of Generative AI: An Interdisciplinary Perspective. *Informatics*. 2024 Aug 9;11(3):58.
- [84] Heydari S, Masoumi N, Esmaeeli E, Ayyoubzadeh SM, Ghorbani-Bidkorpeh F, Ahmadi M. Artificial intelligence in nanotechnology for treatment of diseases. *J Drug Target*. 2024 Aug 27;1–20.
- [85] Hristova-Panusheva K, Xenodochidis C, Georgieva M, Krasteva N. Nanoparticle-Mediated Drug Delivery Systems for Precision Targeting in Oncology. *Pharmaceutics*. 2024 May 24;17(6):677.