Available online on 15.07.2026 at http://jddtonline.info

Journal of Drug Delivery and Therapeutics

Open Access to Pharmaceutical and Medical Research

Open Access Full Text Article

Review Article

Artificial Intelligence in Pharmaceutics and Drug Delivery: Current Applications and Future Perspectives

Ritika Sharma[1], Dr Harmeet Singh*[1]

[1] Faculty of Pharmaceutical Sciences, PCTE Group of Institutes, Near Baddowal Cantt., Ludhiana-142021

Article Info:

Article History:

Received 01 May 2026
Reviewed 18 May 2026
Accepted 02 June 2026
Published 15 July 2026

Cite this article as:

Sharma R, Singh H, Artificial Intelligence in Pharmaceutics and Drug Delivery: Current Applications and Future Perspectives, Journal of Drug Delivery and Therapeutics. 2026; 16(7):195-207 *DOI: https://doi.org/10.22270/jddt.v16i7.7845*

For Correspondence:

Ritika Sharma, Faculty of Pharmaceutical Sciences, PCTE Group of Institutes, Near Baddowal Cantt., Ludhiana-142021.

Abstract

Artificial intelligence (AI) is rapidly reshaping pharmaceutics and drug delivery, offering computational alternatives to traditional trial-and-error approaches in formulation design, nanocarrier engineering, and manufacturing. This review examines the current applications of machine learning, deep learning, reinforcement learning, and generative AI architectures across the pharmaceutical product lifecycle, from target identification and lead optimization to dosage form development and clinical translation. Particular attention is given to AI-driven prediction of excipient compatibility, formulation stability, and bioavailability, as well as the design of smart nanocarriers, stimuli-responsive delivery systems, and 3D-printed dosage forms enabled by graph neural networks, transformer-based models, and Bayesian optimization techniques. The review also traces the historical evolution of computational pharmaceutics, from early rule-based prediction systems to current high-throughput, automation-integrated platforms, and highlights emerging tools such as digital twins, federated learning frameworks, and AI-supported nanorobotics for targeted intracellular delivery. Despite these advances, significant challenges persist, including limited data availability and standardization, algorithmic opacity and the demand for explainable AI, and the absence of harmonized regulatory frameworks for validating AI-driven decision-making in drug development. The review further considers data quality and interpretability concerns specific to nanomedicine, alongside the regulatory and ethical considerations necessary for clinical adoption. Future directions emphasize the integration of multi-omics data, real-time adaptive drug delivery systems, and quantum-AI convergence to advance personalized medicine. Addressing these barriers through interdisciplinary collaboration, standardized data repositories, and transparent regulatory guidance will be essential to translating AI-enabled pharmaceutical innovations from computational design into safe, effective clinical therapeutics.

Keywords: Artificial intelligence; machine learning; drug delivery; nanomedicine; formulation design; personalized medicine; deep learning; pharmaceutics

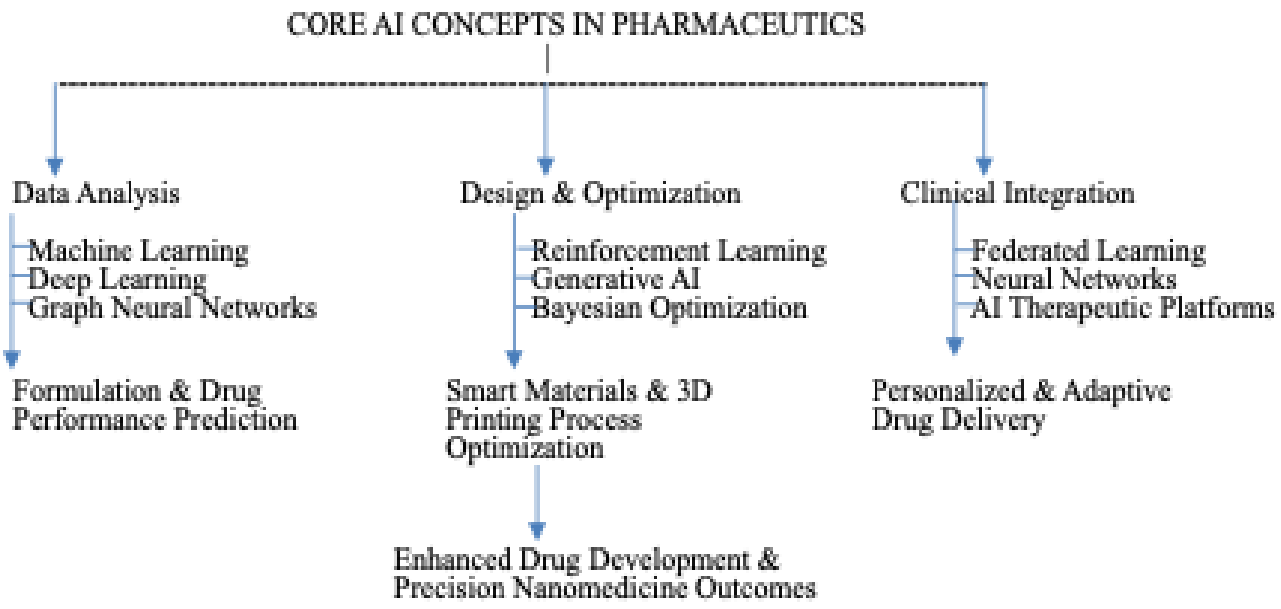
Introduction to AI

Artificial intelligence has transitioned from a theoretical computational tool to a fundamental driver of innovation, fundamentally altering the traditional paradigm of pharmaceutical research through the integration of machine learning and deep learning architectures [1,2]. These computational frameworks facilitate the analysis of high-dimensional biological datasets, enabling the rapid identification of therapeutic targets and the precise optimization of complex formulation designs [3,4]. By leveraging predictive modeling, these advanced algorithms effectively circumvent the limitations of traditional trial-and-error experimental methodologies, thereby enhancing the precision of pharmacokinetic and pharmacodynamic outcomes [5,6]. Furthermore, the implementation of these technologies extends to the strategic engineering of nanocarriers and smart drug delivery devices, which significantly improve therapeutic efficacy while minimizing systemic toxicity [7,8]. Beyond these design benefits, AI-driven platforms are increasingly utilized in intelligent manufacturing processes, such as three-dimensional printing, to ensure rigorous quality control and facilitate the realization of personalized medicine [9,10]. Despite these transformative capabilities, the widespread clinical integration of these technologies faces persistent barriers, including critical concerns regarding data interpretability, algorithmic bias, and the establishment of robust regulatory frameworks for automated decision-making [11,12]. To navigate these complexities, interdisciplinary collaboration and the development of explainable AI models are essential to ensure the safety, transparency, and ethical implementation of these systems in clinical practice [13,14]. Furthermore, the paradigm shift toward precision medicine requires the seamless integration of real-time monitoring and adaptive drug delivery systems, which can be dynamically tuned by machine learning to optimize patient-specific therapeutic responses [15]. This evolution necessitates a transition toward data-driven pharmacovigilance, where automated systems continuously analyze longitudinal patient health metrics to refine dosage regimens and mitigate adverse effects

in real-time [16,17]. The synthesis of AI with advanced fabrication techniques, such as 3D printing, further enables the precise control of drug release kinetics and facilitates the production of highly customized nanocomposite delivery systems.

Core AI Concepts

Foundational to this technological integration is the utilization of machine learning, which employs sophisticated algorithms to interpret complex pharmaceutical datasets and identify latent variables affecting formulation stability and bioavailability [18,19]. Concurrently, deep learning architectures leverage multi-layered neural networks to extract insights from vast, unstructured inputs, such as multi-omic profiles and imaging data, which are essential for refining patient-specific therapeutic outcomes [20]. Additionally, the deployment of reinforcement learning facilitates the autonomous optimization of synthesis pathways and experimental conditions, effectively minimizing the need for manual intervention during industrial manufacturing [21]. Furthermore, the adoption of graph neural networks has become increasingly pivotal for modeling the intricate chemical properties of nanocarrier surfaces, thereby improving the predictive accuracy of drug release profiles [22]. Moreover, the fusion of generative AI with these architectures is revolutionizing the intelligent design of materials and intelligent polymers, allowing for the autonomous adjustment of print parameters to maximize production scalability and ensure consistent quality in 3D-printed dosage forms [23]. Additionally, Bayesian optimization techniques are now being employed to navigate high-dimensional experimental spaces, significantly reducing the iterative laboratory cycles required to achieve desired critical quality attributes [24]. Beyond these computational design strategies, emerging innovations like federated learning are addressing data heterogeneity and security concerns, enabling collaborative model training across clinical institutions without compromising patient privacy [25]. Furthermore, these decentralized frameworks facilitate the incorporation of multi-omics and longitudinal clinical datasets to enhance the predictive modeling of nanoparticle behavior and patient stratification [26]. Complementary to these computational advancements, the application of artificial neural networks serves to elucidate the non-linear relationship between formulation components and process parameters, which is critical for establishing robust, controlled-release drug delivery systems [27]. Beyond static modeling, AI-driven platforms act as intelligent navigators capable of autonomously managing remote therapeutic transport and adjusting drug administration in response to real-time patient status [28]. By leveraging reinforcement learning, these adaptive systems can identify deformable nanomaterials capable of navigating dense biological barriers, such as tumor matrices, to ensure uniform drug distribution [29].



Historical Development Phases

The evolution of AI in pharmaceutical research began with rudimentary rule-based systems in the late 20th century, which initially focused on simple chemical structure property predictions [30]. These early computational models gradually matured into more sophisticated machine learning frameworks capable of analyzing larger datasets to optimize formulation pipelines and dissolution properties [31]. This progression catalyzed a shift from descriptive analytics toward predictive models that now enable the rational design of complex therapeutics and streamlined clinical trial simulations [32]. The subsequent integration of automated workflows has further accelerated this trajectory, enabling the rapid analysis of large-scale multivariate datasets to address the multifaceted challenges inherent in nanomedicine design [33]. Current efforts are now shifting toward the consolidation of these digital pipelines with high-throughput laboratory automation, which bridges the gap between theoretical structure-

function relationship extraction and the physical production of clinically viable nanocarriers [34]. Furthermore, the emergence of nanorobotics, supported by sophisticated computational frameworks, is revolutionizing internal drug delivery by enabling programmed navigation and targeted engagement with specific pathological markers. These autonomous systems utilize integrated sensors and power sources to detect and eliminate target sites while minimizing systemic exposure through pH-responsive navigation [35]. In parallel, the convergence of intelligent nanosystems and machine learning allows for the high-throughput screening of physicochemical parameters, facilitating the rapid assessment of molecular interactions between drugs and carriers [36]. By integrating these computational models, researchers can now anticipate the biological fate of nanocarriers, effectively mitigating off-target accumulation while enhancing therapeutic indices through precision engineering [37,38]. This paradigm shift towards "computational pharmaceutics" addresses the inefficiencies of conventional trial-and-error methodologies, thereby significantly reducing the time-consuming and error-prone nature of traditional formulation research [39]. Crucially, the establishment of comprehensive, high-quality datasets remains a fundamental prerequisite for the successful implementation of these automated workflows.

Drug Discovery Applications

AI-driven platforms are currently accelerating the identification of therapeutic candidates by analyzing vast chemical libraries to predict structure-activity relationships with unprecedented speed [40]. Moreover, these computational models streamline lead optimization and ADMET profiling, directly addressing historical bottlenecks related to high development costs and low clinical success rates [41]. By integrating machine learning with high-throughput screening, these methodologies enable the rapid generation and refinement of molecular candidates, which substantially mitigates the risks associated with early-stage attrition [42,43]. Furthermore, the implementation of deep learning architectures facilitates the precise prediction of cytotoxic profiles and metabolic outcomes, effectively narrowing the search space for potent and safe drug candidates [44,45]. Additionally, AI-driven drug repurposing leverages existing safety and pharmacokinetic profiles to identify new therapeutic uses for approved agents, providing a more cost-effective and expedited alternative to traditional de novo discovery [46,47]. This integration of predictive analytics into the drug development lifecycle significantly curtails both the temporal and financial burdens historically associated with bringing novel therapeutics to clinical application [48,49]. Beyond these primary discovery workflows, recent breakthroughs, such as the development of AlphaFold, have revolutionized structural biology by accurately predicting protein architectures to guide the design of functional biological therapeutics [50]. Additionally, these predictive frameworks have enabled the transition from empirical testing to data-driven formulation development, where machine learning models optimize excipient compatibility and design space parameters according to Quality by Design principles [51,52]. Specifically, AI-driven bioinformatics and systems biology network analysis facilitate the rapid identification and validation of disease-associated protein targets, substantially reducing the complexity of early-stage therapeutic development [53]. These computational methodologies further extend to de novo drug design, utilizing generative models to synthesize novel molecular structures with optimal pharmacokinetic, pharmacodynamic, and ADME profiles [54].

Molecular Modelling Tools

Advanced computational platforms like AtomNet employ structure-based drug design to effectively map ligand-protein interactions within high-dimensional chemical spaces [55]. These generative models, particularly variational autoencoders and diffusion frameworks, enable the exploration of vast chemical landscapes to identify novel compounds with sub-Ångström structural fidelity [56]. By learning intricate patterns from large-scale biological datasets, these algorithms facilitate the generation of synthetically feasible molecules specifically optimized for enhanced therapeutic potency and safety [57]. In parallel, these predictive frameworks facilitate drug repurposing by analyzing polypharmacological interactions, allowing researchers to uncover secondary therapeutic applications for already-approved medications [58,59]. Beyond structural modeling, deep learning architectures are increasingly employed to decipher complex biological pathways, enabling the prioritization of leads that possess favorable profiles for clinical transition [60,61]. Recent studies demonstrate that integrating AlphaFold-derived protein structures into these virtual screening workflows significantly improves hit rates, exemplified by the identification of novel CDK20 inhibitors in as little as 30 days [62,63]. Such methodologies extend beyond small molecules, as generative adversarial networks are now being utilized to predict the stability and assembly kinetics of lipid-based drug delivery systems [64]. Furthermore, these architectures allow for the optimization of particle morphology and encapsulation efficiency, which are critical for overcoming physiological barriers during systemic administration [65]. By leveraging graph-to-graph models that incorporate 3D spatial information, these systems can refine the design of macrocycles and molecular glues, expanding the potential interactome to include complex protein surface binding sites [66]. Moreover, the integration of multi-parameter optimization within these frameworks enables researchers to balance target affinity with synthetic accessibility, addressing the inherent limitations of traditional combinatorial chemistry [67]. This transformation is further bolstered by dual diffusion models that transcend the constraints of historical chemical databases, enabling the de novo generation of structures that reside outside the known chemical space.

Target Identification Processes

Computational workflows now leverage multi-omics data integration to map complex genetic and chemical interaction networks, pinpointing nodes whose modulation yields significant therapeutic benefits. This transition from single-gene hypotheses toward network-based, AI-assisted discovery allows for the mining of large unlabeled corpora and knowledge graphs to elucidate disease-associated mechanisms. By grounding these digital hypotheses in transcriptomic and proteomic signatures, researchers can achieve a more holistic understanding of the biological interactome, effectively navigating the complexities of disease states [68]. These integrative approaches further enhance druggability assessments by predicting protein structure-function relationships, thereby facilitating the rapid identification of novel therapeutic vulnerabilities [69]. Furthermore, the utilization of machine learning-based multi-property optimization enables researchers to prioritize candidates that exhibit not only high target affinity but also favorable ADME/Tox profiles throughout the lead optimization phase [70,71]. Moreover, the convergence of nanoarchitectonics and artificial intelligence allows for the engineering of stimuli-responsive delivery systems capable of autonomously adapting to the dynamic physiological microenvironment of targeted tissues [72]. These algorithms also assist in the systematic analysis of real-world evidence, such as electronic health records, to validate clinical targets and refine biomarker identification through complex biological network mapping [73]. Despite these advancements, the performance of such predictive models remains contingent upon the quality and comprehensiveness of training data, as significant gaps in protein-drug interaction maps can introduce localized biases [74].

Lead Optimization Strategies

The integration of generative models at this stage enables the iterative refinement of lead scaffolds by predicting substituent effects on binding kinetics and metabolic stability [75]. Furthermore, reinforcement learning algorithms autonomously navigate chemical space to optimize molecular properties, ensuring that synthesized candidates satisfy stringent bioavailability and toxicity constraints [76]. Additionally, network-based approaches such as knowledge graphs are increasingly deployed to impute novel protein-phenotype associations, allowing for the systematic prioritization of targets even when causative mechanisms remain partially obscured [77]. Specifically, hybrid computational techniques leverage both structural data and historic pharmacological databases to improve bioactivity predictions, effectively guiding the methodical assembly of fragment-based molecules into more potent lead compounds [78]. Concurrently, machine learning models analyze structure-activity relationship data to suggest precise modifications that enhance selectivity and reduce off-target effects, thereby streamlining the path to preclinical development. Predictive toxicology models further augment this phase by identifying potential safety concerns through the analysis of historical data, which facilitates the early mitigation of unforeseen toxicity risks before extensive in vivo testing. Understanding the underlying mechanisms of toxicity through these computational insights allows for the proactive modification of lead structures, ensuring that safety profiles are optimized well before clinical transition [79]. This synergy between de novo design and lead optimization facilitates the generation of molecules conditioned on specific substructures, thereby bridging the gap between theoretical potency and practical synthetic feasibility [80].

AI in Formulation Design

Recent advancements in this domain have shifted from heuristic, trial-and-error experimentation toward predictive models that leverage generative deep learning to optimize the physicochemical properties of drug delivery vehicles [81]. By training neural networks on high-throughput experimental datasets, these systems can predict the performance of lipid-based nanoparticles, polymeric micelles, and hydrogels, significantly reducing the time required for lead formulation [82]. These models further streamline manufacturing processes by integrating automated robotic workflows with real-time feedback loops to enhance encapsulation efficiency and optimize critical quality attributes [83]. By simulating the interactions between diverse therapeutic cargos and delivery matrices, these computational platforms facilitate the precise tuning of release kinetics to match specific physiological requirements [84]. These predictive frameworks also assess the stability and biocompatibility of nanocarriers, ensuring that formulated systems maintain structural integrity under varying environmental conditions [85]. Furthermore, deep learning algorithms are now being utilized to predict the long-term storage stability and degradation pathways of these complex formulations, which accelerates the selection of optimal excipient combinations [86,87]. By integrating vast experimental datasets with physicochemical and biological interaction parameters, these systems can explore complex formulation spaces that were previously inaccessible through conventional empirical testing [88]. These AI-driven strategies simultaneously improve drug bioavailability by navigating the challenges of poor solubility and chemical stability, thereby enabling the development of tailored drug administration protocols [89,90].

Predictive Excipient Selection

Computational platforms now employ quantitative structure-property relationship modeling to predict excipient-drug compatibility, effectively minimizing the risk of chemical incompatibilities that often compromise formulation stability [91]. Furthermore, these models utilize historical formulation data and molecular descriptors to identify synergistic excipient combinations that enhance the solubility and bioavailability of poorly water-soluble compounds [92,93]. Beyond simple compatibility, these tools facilitate the virtual screening of novel excipients, allowing researchers to rationally customize medication formulations to optimize metabolic profiles and

therapeutic effectiveness [94]. By coupling high-throughput screening with machine learning, researchers can now simultaneously optimize multiple compositional variables, such as lipid-to-drug ratios, to maximize the success rates of complex nanoparticle assembly [95]. Advanced transformer-based architectures, such as COMET, further extend these capabilities by integrating multi-component features to accurately predict the performance of non-canonical formulations in an end-to-end manner. These architectures significantly expand the explored design space for lipid nanoparticles by accounting for multimodal variables that traditional single-molecule algorithms often overlook [96]. Additionally, mechanistic and multiscale simulations, such as physiologically based pharmacokinetics and computational fluid dynamics, provide granular, in silico insights into how these complex systems behave during scale-up and dissolution [97]. These simulations effectively bridge the gap between bench-scale research and industrial manufacturing by predicting how fluctuations in processing conditions, such as temperature and shear stress, impact final product performance [98]. Moreover, the implementation of comprehensive, web-based platforms now allows for the systematic evaluation of key properties across diverse delivery systems, such as self-emulsifying formulations and nanocrystals, replacing labor-intensive, trial-and-error workflows with intelligent, data-driven optimization [99]. Current initiatives are now addressing the critical requirement for rigorous model validation by calibrating these computational frameworks against empirical, real-world experimental data [100].

Dosage Form Optimization

Machine learning models, including neural networks and regression ensembles, are increasingly employed to refine the physicochemical attributes of complex systems such as self-emulsifying drug delivery systems and solid-state dosage forms [101]. These computational approaches facilitate the prediction of drug supersaturation levels and solubility enhancements upon dispersion, effectively narrowing the search space for optimal lipid-based composition ratios. Furthermore, the integration of molecular dynamics with machine learning algorithms allows for the precise mapping of self-emulsification regions, providing insights into the spatial distribution of excipients within the carrier matrix [102]. By utilizing random forest models to evaluate non-covalent interaction potentials, these platforms can effectively select excipient combinations that maintain drug loading capacity and formulation stability [103]. Simultaneously, deep neural networks are being leveraged to optimize three-dimensional printing parameters and microfluidic configurations, ensuring consistent drug release profiles and structural integrity in personalized additive manufacturing [104]. These innovations are further complemented by digital twins, which offer real-time monitoring and predictive control of manufacturing processes to ensure high-fidelity production outcomes [105]. Moreover, the transition toward continuous manufacturing is bolstered by these diagnostic models, which can identify deviations in critical quality attributes before they manifest as batch failures [1]. These advanced methodologies effectively overcome existing data scarcity by utilizing federated learning frameworks, which allow for the collaborative training of robust models across decentralized pharmaceutical datasets without compromising proprietary security [106]. Additionally, the deployment of IoT-enabled sensor arrays facilitates the continuous collection of process data, enabling the real-time adjustment of critical quality attributes within the manufacturing loop [107]. Furthermore, the adoption of generative adversarial networks is facilitating the *de novo* design of specialized carriers, enabling researchers to explore chemical spaces for novel drug delivery vehicles with predefined pharmacokinetic targets [108], [4]. These models optimize the architecture of nanocarriers for targeted delivery, significantly reducing the development time for complex therapeutic systems [109].

Nanotechnology and Delivery

The integration of artificial intelligence into nanomedicine research represents a paradigm shift, transitioning the field from traditional, labor-intensive trial-and-error methodologies to an era of intelligent, data-driven design [5,110]. Computational algorithms now enable the rational engineering of smart nanocarriers, such as AI-optimized liposomes, which can be precisely tailored to address unique patient physiological needs while maximizing targeted therapeutic delivery [13]. By leveraging machine learning, researchers can now simulate the interactions between nanocarriers and specific biological barriers, enabling the prediction of cellular uptake and systemic circulation times with unprecedented precision [3]. These predictive models further enhance the stability and bioavailability of nanoparticle-based carriers by continuously optimizing their structural parameters and surface functionalization [9,15]. Furthermore, AI-driven predictive modeling is essential for forecasting the toxicity of these nanomaterials and their specific interactions with biological entities, thereby streamlining the safety assessment process during early-stage development [111,112]. Concurrent advancements in high-throughput screening and automated data acquisition are now enabling the construction of large-scale, diverse datasets that overcome the historical limitations of data sparsity in nanomedicine research [113,114]. For instance, autonomous platforms now utilize machine learning-driven Bayesian optimization to dynamically adjust nanoprecipitation parameters, reducing synthesis time from days to mere minutes while ensuring high reproducibility [115].

Nanocarrier Design Parameters

Predictive algorithms now systematically analyze multidimensional datasets to determine optimal particle size, drug loading efficiency, and surface charge, which are critical for enhancing stability and circulation duration [116]. Beyond these physical characteristics, these models effectively simulate complex interactions with the immune system, vasculature, and lipid membranes, allowing for the fine-tuning of drug release

kinetics and therapeutic efficacy. Furthermore, the utilization of graph neural networks and deep learning architectures has proven instrumental in modeling the complex, high-dimensional data generated from these interactions, ultimately refining pharmacokinetic and dose-response forecasts [22]. Moreover, the application of multiscale machine-learned infrastructure and physiologically based pharmacokinetic models allows for a more accurate estimation of biodistribution and nanotoxicity, facilitating the translation of these systems into clinical settings [117]. Beyond these foundational design aspects, machine learning-assisted single-vessel analysis techniques now provide critical guidance for optimizing the targeted permeability of nanodrugs within tumor vasculature [118]. This high-throughput capability, exemplified by automated image segmentation, enables researchers to decipher distinct transport mechanisms across diverse tumor models, thereby informing the development of next-generation nanotheranostics [119].

Controlled Release Modeling

Advanced computational frameworks are currently being deployed to decipher the nonlinear relationship between formulation variables and drug release kinetics, addressing the inherent challenges of high-throughput experimental screening where property interactions are difficult to isolate. By integrating reinforcement learning with physical degradation models, these frameworks can dynamically forecast release profiles across varying physiological pH and temperature gradients [120]. These predictive systems further facilitate the design of stimuli-responsive nanocarriers by optimizing the coupling of specific biological triggers with the therapeutic payload release rate [121,122]. Specifically, reinforcement learning agents can iteratively refine formulation characteristics in a closed-loop manner, effectively optimizing drug delivery systems against real-time performance metrics [29]. In addition, the application of machine learning techniques has enabled the systematic prediction of drug release success by evaluating various molecular and coating descriptors [123]. Furthermore, deep reinforcement learning has emerged as a robust approach for optimizing the complex pharmacokinetics of these systems, allowing for the precise calibration of biodistribution, metabolism, and clearance profiles [124]. Additionally, these computational methodologies allow for the exploration of autonomous drug administration systems, where AI-mediated navigation and intelligent patching technologies adapt to patient-specific symptoms in real time [28]. Building on these advancements, the utilization of artificial neural networks has become pivotal in deciphering the intricate relationships between physicochemical properties and the resulting drug release profiles from sophisticated nanoplatforms [30].

Clinical Translation Challenges

Despite the potential of these models to streamline preclinical stages, the poor delivery efficiency of nanoparticles to solid tumors remains a primary barrier to successful clinical implementation [33]. The integration of AI-driven platforms, such as in silico tumor microenvironment simulations, is critical for addressing these physiological hurdles by enabling real-time assessment of nanoparticle behavior within complex, patient-specific vascular architectures [125]. However, the path to clinical integration is further complicated by the urgent need for regulatory standardization and the establishment of robust, transparent frameworks to ensure manufacturing reproducibility across heterogeneous therapeutic platforms [126]. Addressing these hurdles requires the adoption of advanced omics and large-scale data integration to refine nanomedicine design through rigorous, standardized validation protocols [127]. Moreover, bridging the gap between computational prediction and clinical approval necessitates the creation of interpretable models that elucidate the complex dependencies between nanomaterial attributes and in vivo biological performance [128]. Such transparency is essential for overcoming data limitations and fostering trust in automated design, as model interpretability directly influences the ability of researchers to translate optimized nanocarriers into validated clinical therapeutics [129]. Furthermore, the implementation of federated learning strategies can mitigate data heterogeneity concerns by enabling collaborative model training across international research consortia without compromising patient data privacy [25].

Data Quality Issues

The reliability of these computational frameworks is frequently constrained by the limited availability of experimental data and the inherent variability in nanomaterial structural properties [130]. To mitigate these discrepancies, the scientific community must prioritize the development of large-scale, well-structured public repositories that standardize metadata regarding morphology, surface composition, and biological response [131]. Such efforts must concurrently address data privacy and the lack of comprehensive sharing protocols among pharmaceutical entities to ensure that predictive models remain representative of complex biological environments [21]. Furthermore, establishing standardized reporting guidelines for preclinical studies is essential to resolve the significant discrepancies often observed between animal model outcomes and clinical patient data [132,133]. To facilitate this shift, it is strongly recommended that the field adopts a centralized, annotated database architecture—modeled after successful initiatives like The Cancer Genome Atlas—to catalog nanomaterial compounds, their physicochemical characteristics, and their specific interactions with diverse tissue microenvironments [134,135]. By testing thousands of nanomaterials in vivo and understanding how strain- and species-dependent biological factors influence delivery, these large-scale datasets may significantly improve the predictive accuracy of preclinical models for human clinical outcomes [136]. Moreover, addressing the high-dimensionality of these datasets and the scarcity of *in vivo* results is imperative to minimize risks such as overfitting and to demonstrate the generalizability of predictive models to diverse clinical applications [137].

Regulatory Compliance Standards

The implementation of AI-driven pharmaceutical solutions necessitates rigorous adherence to emerging regulatory frameworks that prioritize safety, efficacy, and explainability [138]. Beyond these safety protocols, regulatory bodies must address the challenge of validating deep learning models that often function as "black boxes," hindering the transparent clinical decision-making required for drug approval [139]. To mitigate these concerns, policymakers must advocate for the implementation of explainable AI methodologies that allow researchers to map model predictions directly back to biological determinants [31]. Furthermore, developing comprehensive ethical and regulatory frameworks is essential to address concerns regarding algorithmic bias, data accountability, and informed consent in AI-enabled healthcare systems [54]. The current absence of standardized governance poses a significant risk, as the rapid technological trajectory of these systems consistently outpaces the evolution of traditional regulatory policies [140]. In response to this latency, regulatory agencies such as the FDA are actively developing roadmaps for integrating *in silico* methodologies, including AI, into preclinical safety assessments to provide more human-representative data [141]. Consequently, the future of AI-enhanced nanomedicine relies on fostering high-quality, accessible datasets that facilitate the robust validation of these computational tools [38,142]. Future advancements may also involve the synergistic combination of AI with quantum computing, which could further accelerate the discovery of innovative nanocarriers capable of achieving high-precision, personalized therapeutic outcomes [143]. Establishing such interdisciplinary governance and oversight committees will be paramount to addressing the current lack of science-informed regulatory guidance regarding biocompatibility, systemic clearance, and long-term toxicity [144].

Future Research Directions

Future investigations should prioritize the integration of multi-omics data with machine learning algorithms to decipher the intricate feedback loops between nanocarriers and systemic physiological responses [26]. Integrating Explainable AI into these predictive frameworks will be essential to provide human-understandable insights into the key biological mechanisms governing therapeutic efficacy and safety [145]. Additionally, researchers must establish robust data-sharing frameworks and promote interdisciplinary collaboration to overcome regional disparities in standardized experimental protocols, which currently act as a bottleneck for algorithmic development [146]. Furthermore, prioritizing the development of predictive models that account for patient-specific variability will be critical for transitioning from generalized nanocarrier designs to truly personalized nanomedicine strategies [147]. This transition necessitates the realization of intelligent closed-loop platforms that harmonize diagnostic data with therapeutic evaluation to refine the design of nanotheranostics [148]. Moreover, the convergence of these platforms with bioengineered carriers, such as exosome-mimetic systems and cell membrane-coated nanoparticles, promises to enhance biocompatibility and immune evasion capabilities [149]. Furthermore, investigating the influence of the albumin corona on the nano-bio interface will be crucial for refining the accuracy of toxicity predictions and ensuring the sustainable translation of these systems into clinical practice [150,151]. Beyond material optimization, future research must also explore the integration of immunotherapy with nanocarrier design to leverage the immune system's potential in targeting and destroying malignant cells [152].

References

1. Serrano DR, Luciano FC, Anaya BJ, Öngoren B, Kara A, Molina G, et al. Artificial Intelligence (AI) Applications in Drug Discovery and Drug Delivery: Revolutionizing Personalized Medicine. Pharmaceutics [Internet]. 2024 Oct 14 [cited 2026 Mar];16(10):1328–1328. Available from: https://doi.org/10.3390/pharmaceutics16101328

2. SHahreza MS, Naeimi F. A Mini-Review on Machine Learning Framework for Drug Delivery Applications. Journal of advanced materials and processing [Internet]. 2026 Feb 2 [cited 2026 Feb]; Available from: https://doi.org/10.71670/jmatpro.2024.1232710

3. B SDM, Kamala G, G H, M AVDSP, N SSD, Ketha J. Utilization of Artificial Intelligence in Pharmaceutical Sciences for Teaching, Learning, and Clinical Practice. Journal of Pharma Insights and Research [Internet]. 2026 Feb 5 [cited 2026 Mar];4(1):69–77. Available from: https://doi.org/10.69613/dw5jnw67

4. Vora LK, Gholap AD, Jetha K, Singh TRR, Solanki HK, Chavda VP. Artificial Intelligence in Pharmaceutical Technology and Drug Delivery Design. Pharmaceutics [Internet]. 2023 July 10 [cited 2026 Jan];15(7):1916–1916. Available from: https://doi.org/10.3390/pharmaceutics15071916

5. Darekar PB Krushi Pradhan, Janvi Patil, Dr Avinash. Artificial Intelligence in Drug Delivery Systems: Revolutionizing Pharmaceutical Formulation, Optimization, and Personalized Therapeutics. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2025 Nov 14 [cited 2025 Nov]; Available from: https://doi.org/10.5281/zenodo.17611150

6. Wu Y, Wang N, Xiong P, Wang R, Deng J, Ouyang D. Artificial intelligence for drug delivery: Yesterday, today and tomorrow. Acta Pharmaceutica Sinica B [Internet]. 2025 Sept 1 [cited 2026 Feb]; Available from: https://doi.org/10.1016/j.apsb.2025.09.022

7. Darekar PB Krushi Pradhan, Janvi Patil, Dr Avinash. Artificial Intelligence in Drug Delivery Systems: Revolutionizing Pharmaceutical Formulation, Optimization, and Personalized Therapeutics. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2025 Nov 14 [cited 2025 Nov]; Available from: https://doi.org/10.5281/zenodo.17611149

8. Swami AAS, Shruti SS, Kansal PK, S GS, Bhide AB. Artificial Intelligence in Pharmacology and Pharmaceutics: From Drug Discovery to Clinical Translation. Journal of Pharmaceutical Research and Integrated Medical Sciences [Internet]. 2026 Mar 17 [cited 2026 Mar];17–31. Available from: https://doi.org/10.64063/3049-1681.vol.3.issue3.2

9. Zhu T, Liu B, Chen N, Liu Y, Wang Z, Xue T. Artificial Intelligence-Driven Innovations in Pharmaceutical Development and Drug Delivery Systems. Current Topics in Medicinal Chemistry [Internet]. 2025 Apr 25 [cited 2025 Nov];25(25):2937–51. Available from: https://doi.org/10.2174/0115680266373236250411060857

10. Noorain, Srivastava V, Parveen B, Parveen R. Artificial Intelligence in Drug Formulation and Development: Applications andFuture Prospects. Current Drug Metabolism [Internet]. 2023 Sept 1 [cited 2026 Feb];24(9):622–34. Available from: https://doi.org/10.2174/0113892002265786230921062205

11. Joshi S, Sheth S. Artificial Intelligence (AI) in Pharmaceutical Formulation and Dosage Calculations. Pharmaceutics [Internet].

2025 Nov 7 [cited 2026 Mar];17(11):1440–1440. Available from: https://doi.org/10.3390/pharmaceutics17111440

12. Gouma AGA, Alhaj AAK, Karar OMFA, Mahgoub MAI, Saleh A. The convergence of AI and pharmaceutics a new era of data-driven drug development. International Journal of Science and Research Archive [Internet]. 2025 Feb 18 [cited 2025 Dec];14(2):947–60. Available from: https://doi.org/10.30574/ijsra.2025.14.2.0478

13. Aundhia C, Parmar G, Talele C, Shah N, Talele D. Impact of Artificial Intelligence on Drug Development and Delivery. Current Topics in Medicinal Chemistry [Internet]. 2024 Aug 13 [cited 2025 Nov];25(10):1165–84. Available from: https://doi.org/10.2174/0115680266324522240725053634

14. kawale* K patil A. Applications of Artificial Intelligence in Pharmaceutical Sciences: A Review. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2026 Feb 3 [cited 2026 Feb]; Available from: https://doi.org/10.5281/zenodo.18464413

15. Jena GK, Patra CN, Jammula S, Parhi R, Chand S. Artificial Intelligence and Machine Learning Implemented Drug Delivery Systems: A Paradigm Shift in the Pharmaceutical Industry. Journal of Bio-X Research [Internet]. 2024 Jan 1 [cited 2025 Dec];7. Available from: https://doi.org/10.34133/jbioxresearch.0016

16. Jadge VP Sonam Babaso Kamble, Dr Dhanraj Raghunath. Artificial Intelligence in Pharmaceutics: Applications and Future Perspectives. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2025 Nov 8 [cited 2025 Nov]; Available from: https://doi.org/10.5281/zenodo.17556719

17. Jadge VP Sonam Babaso Kamble, Dr Dhanraj Raghunath. Artificial Intelligence in Pharmaceutics: Applications and Future Perspectives. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2025 Nov 8 [cited 2025 Nov]; Available from: https://doi.org/10.5281/zenodo.17556720

18. Bhelkar N. Role of Artificial Intelligence in Formulation Design. International Journal For Multidisciplinary Research [Internet]. 2026 Jan 30 [cited 2026 Mar];8(1). Available from: https://doi.org/10.36948/ijfmr.2026.v08i01.67247

19. Pawar V, Patil A, Tamboli FA, Gaikwad D, Mali DP, Shinde AJ. Harnessing the Power of AI in Pharmacokinetics and Pharmacodynamics: A Comprehensive Review. International Journal of Pharmaceutical Quality Assurance [Internet]. 2023 June 25 [cited 2025 Oct];14(2):426–39. Available from: https://doi.org/10.25258/ijpqa.14.2.31

20. Petković K, Strika Z, Likić R, Lucijanić M. Spotlight commentary: Integrating artificial intelligence in clinical pharmacology: Opportunities, challenges and ethical imperatives. British Journal of Clinical Pharmacology [Internet]. 2024 Sept 5 [cited 2026 Mar];90(11):2700–4. Available from: https://doi.org/10.1111/bcp.16241

21. Elmahboub Y, Albash R, Ahmed S, Salah S. The Road to Precision Nanomedicine: An Insight on Drug Repurposing and Advances in Nanoformulations for Treatment of Cancer. AAPS PharmSciTech [Internet]. Springer Science+Business Media; 2025 Oct 6 [cited 2025 Oct];26(8). Available from: https://doi.org/10.1208/s12249-025-03233-1

22. Sarhan OM, Gebril MI, Elsegaie D. Artificial intelligence-enabled nanomedicine: enhancing drug design and predictive modeling in pharmaceutics. Journal of Pharmacy and Pharmacology [Internet]. 2025 Oct 23 [cited 2026 Mar];78(3). Available from: https://doi.org/10.1093/jpp/rgaf113

23. Mishra N, Dasari A. Artificial intelligence and 3D printing in pharmaceuticals: A new frontier in personalized drug manufacturing. International Journal of Pharmacy and Pharmaceutical Science [Internet]. 2025 Jan 1 [cited 2025 Nov];7(2):15–22. Available from: https://doi.org/10.33545/26647222.2025.v7.i2a.188

24. Suksaeree J. A Review of Artificial Intelligence (AI)-Driven Smart and Sustainable Drug Delivery Systems: A Dual-Framework Roadmap for the Next Pharmaceutical Paradigm. Sci [Internet]. 2025 Dec 3 [cited 2026 Mar];7(4):179–179. Available from: https://doi.org/10.3390/sci7040179

25. Akhtar M, Nehal N, Gull A, Parveen R, Khan SI, Khan SI, et al. Explicating the transformative role of artificial intelligence in designing targeted nanomedicine. Expert Opinion on Drug Delivery [Internet]. 2025 May 5 [cited 2026 Mar];22(7):971–91. Available from: https://doi.org/10.1080/17425247.2025.2502022

26. Kataria S. AI-Guided Design of Personalized Nanomedicine: A Review of Data-Driven Approaches in Nanoparticle Formulation. International Journal For Multidisciplinary Research [Internet]. 2025 Aug 13 [cited 2025 Dec];7(4). Available from: https://doi.org/10.36948/ijfmr.2025.v07i04.53283

27. Ros H, Chan N, Cook MT, Shorthouse D. Artificial intelligence and machine learning guided optimization in drug delivery. Advanced Drug Delivery Reviews [Internet]. 2026 Jan 22 [cited 2026 Mar];232:115781–115781. Available from: https://doi.org/10.1016/j.addr.2026.115781

28. Sun L, Liu H, Ye Y, Yang L, Islam R, Tan S, et al. Smart nanoparticles for cancer therapy. Signal Transduction and Targeted Therapy [Internet]. Springer Nature; 2023 Nov 3 [cited 2025 Aug];8(1). Available from: https://doi.org/10.1038/s41392-023-01642-x

29. Nag S, Ong YS, Narayanan K, Subramaniyan V, Naidu R. Mechanistic Insights into Nanomaterials and Advanced Drug Delivery Platforms for the Theranostic Management of Hepatic Cancer: A Comprehensive Update. BioNanoScience [Internet]. 2025 Oct 20 [cited 2025 Oct];15(4). Available from: https://doi.org/10.1007/s12668-025-02175-z

30. Das KP, Chandra J. Nanoparticles and convergence of artificial intelligence for targeted drug delivery for cancer therapy: Current progress and challenges. Frontiers in Medical Technology [Internet]. Frontiers Media; 2023 Jan 6 [cited 2025 Oct];4. Available from: https://doi.org/10.3389/fmedt.2022.1067144

31. Castro BM, Elbadawi M, Ong JJ, Pollard TD, Song Z, Gaisford S, et al. Machine learning predicts 3D printing performance of over 900 drug delivery systems. Journal of Controlled Release [Internet]. 2021 July 30 [cited 2025 Aug];337:530–45. Available from: https://doi.org/10.1016/j.jconrel.2021.07.046

32. Dey H, Arya N, Mathur H, Chatterjee N, Jadon R. Exploring the Role of Artificial Intelligence and Machine Learning in Pharmaceutical Formulation Design. International Journal of Newgen Research in Pharmacy & Healthcare [Internet]. 2024 June 30 [cited 2026 Mar];30–41. Available from: https://doi.org/10.61554/ijnrph.v2i1.2024.67

33. Kapoor DU, Sharma JB, Gandhi S, Prajapati BG, Thanawuth K, Limmatvapirat S, et al. AI-driven design and optimization of nanoparticle-based drug delivery systems. Science, Engineering and Health Studies [Internet]. 2024 Dec 6 [cited 2025 Oct];24010003–24010003. Available from: https://doi.org/10.69598/sehs.18.24010003

34. Heydari S, Masoumi N, Esmaeeli E, Ayyoubzadeh SM, Ghorbani-Bidkorbeh F, Ahmadi M. Artificial intelligence in nanotechnology for treatment of diseases. Journal of drug targeting [Internet]. 2024 Aug 19 [cited 2025 Nov];32(10):1247–66. Available from: https://doi.org/10.1080/1061186x.2024.2393417

35. Ali KA, Mohin S, Mondal P, Goswami S, Ghosh S, Choudhuri S. Influence of artificial intelligence in modern pharmaceutical formulation and drug development. Future Journal of Pharmaceutical Sciences [Internet]. 2024 Mar 29 [cited 2025 Oct];10(1). Available from: https://doi.org/10.1186/s43094-024-00625-1

36. Sushma M, Venkatappa BB, Chakrapani B, Babu MCL, Goruntla N. AI-Driven Nanopharmacology: Intelligent Nano systems Transforming Drug Discovery and Therapeutic Delivery. International Journal of Pharma Growth Research Review [Internet]. 2025 Jan 1 [cited 2026 Mar];2(6):12–9. Available from: https://doi.org/10.54660/ijpgrr.2025.2.6.12-19

37. Sanjay KD, Gadekar PS, Patil KVT. Transforming Drug Discovery: The Impact of Artificial Intelligence and Machine Learning from Initial Screening to Clinical Trials. International Journal for Research in Applied Science and Engineering Technology [Internet]. 2024 Aug 15 [cited 2025 Oct];12(8):503–8. Available from: https://doi.org/10.22214/ijraset.2024.63936

38. Chou W, Canchola A, Zhang F, Lin Z. Machine Learning and Artificial Intelligence in Nanomedicine. Wiley Interdisciplinary

Reviews Nanomedicine and Nanobiotechnology [Internet]. 2025 July 1 [cited 2026 Mar];17(4). Available from: https://doi.org/10.1002/wnan.70027

39. Sultana A, Maseera R, Rahamanulla A, Misiriya A. Emerging of artificial intelligence and technology in pharmaceuticals: review. Future Journal of Pharmaceutical Sciences [Internet]. 2023 Aug 8 [cited 2025 Sept];9(1). Available from: https://doi.org/10.1186/s43094-023-00517-w

40. Garg S, Arora K, Singh S, Nagarajan K. Artificial Intelligence and Machine Learning in Drug Discovery and Development. In: Advances in computational intelligence and robotics book series [Internet]. IGI Global; 2023 [cited 2025 Nov]. p. 42–61. Available from: https://doi.org/10.4018/979-8-3693-0368-9.ch003

41. Pandey V. Artificial Intelligence and Machine Learning in Drug Discovery: Transformative Applications and Interdisciplinary Integration with Nanotechnology and Robotics. International Journal For Multidisciplinary Research [Internet]. 2025 Oct 9 [cited 2026 Mar];7(5). Available from: https://doi.org/10.36948/ijfmr.2025.v07i05.57130

42. Gupta K, Sharma M, Sharma I, Shukla S. Next-Generation Pharmaceutics: AI-Assisted Drug Design, Nanotechnology, and Advanced Therapeutic Delivery Systems [Internet]. Zenodo (CERN European Organization for Nuclear Research). European Organization for Nuclear Research; 2025 [cited 2026 Mar]. Available from: https://doi.org/10.5281/zenodo.18815117

43. Gupta K, Sharma M, Sharma I, Shukla S. Next-Generation Pharmaceutics: AI-Assisted Drug Design, Nanotechnology, and Advanced Therapeutic Delivery Systems [Internet]. Zenodo (CERN European Organization for Nuclear Research). European Organization for Nuclear Research; 2025 [cited 2026 Mar]. Available from: https://doi.org/10.5281/zenodo.18815118

44. Mottaghi-Dastjerdi N, Soltany-Rezaee-Rad M. Advancements and Applications of Artificial Intelligence in Pharmaceutical Sciences: A Comprehensive Review. Iranian journal of pharmaceutical research [Internet]. 2024 Oct 15 [cited 2026 Mar];23(1). Available from: https://doi.org/10.5812/ijpr-150510

45. Narayanan RR, Durga N, Nagalakshmi S. Impact of Artificial Intelligence (AI) on Drug Discovery and Product Development. Indian Journal of Pharmaceutical Education and Research [Internet]. 2022 Sept 6 [cited 2025 Sept];56. Available from: https://doi.org/10.5530/ijper.56.3s.146

46. Sunil DS. ArtificialIntelligenceInDrugDiscoveryAndFormulation:Transforming PersonalizedMedicine. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2026 Mar 6 [cited 2026 Mar]; Available from: https://doi.org/10.5281/zenodo.18885510

47. Sunil DS. ArtificialIntelligenceInDrugDiscoveryAndFormulation:Transforming PersonalizedMedicine. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2026 Mar 6 [cited 2026 Mar]; Available from: https://doi.org/10.5281/zenodo.18885509

48. Arora P, Behera M, Saraf SA, Shukla R. Leveraging Artificial Intelligence for Synergies in Drug Discovery: From Computers to Clinics. Current Pharmaceutical Design [Internet]. 2024 June 14 [cited 2025 Nov];30(28):2187–205. Available from: https://doi.org/10.2174/0113816128308066240529121148

49. Medhi B, Sharma H, Kaundal T, Prakash A. Artificial Intelligence: A Catalyst for Breakthroughs in Nanotechnology and Pharmaceutical Research. International Journal of Pharmaceutical Sciences and Nanotechnology [Internet]. 2024 Aug 15 [cited 2025 Dec];17(4):7439–45. Available from: https://doi.org/10.37285/ijpsn.2024.17.4.1

50. Kanakia A, Sale M, Zhao L, Zhu Z. AI In Action: Redefining Drug Discovery and Development. Clinical and Translational Science [Internet]. 2025 Feb 1 [cited 2026 Mar];18(2). Available from: https://doi.org/10.1111/cts.70149

51. jadhav SSP Vishwjit Kisan Rathod, Nagane Abhijeet Ramesh, Mujawar suhana salim*, Dr Rahul ishwara. ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING IN PHARMACEUTICAL RESEARCH: TRANSFORMING DRUG DISCOVERY, FORMULATION DEVELOPMENT, AND QUALITY ASSURANCE. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2026 Mar 2 [cited 2026 Mar]; Available from: https://doi.org/10.5281/zenodo.18838484

52. jadhav SSP Vishwjit Kisan Rathod, Nagane Abhijeet Ramesh, Mujawar suhana salim*, Dr Rahul ishwara. ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING IN PHARMACEUTICAL RESEARCH: TRANSFORMING DRUG DISCOVERY, FORMULATION DEVELOPMENT, AND QUALITY ASSURANCE. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2026 Mar 2 [cited 2026 Mar]; Available from: https://doi.org/10.5281/zenodo.18838485

53. Krishnan PS, Krishnan NJS, Dey A, Sivakumar S, Ravichandran S, Bharathi MPG. TECH-DRIVEN TRUST: THE ROLE OF AI AND EMERGING TECHNOLOGIES IN PHARMACEUTICAL QUALITY ASSURANCE. International Journal of Applied Pharmaceutics [Internet]. 2025 Sept 7 [cited 2025 Sept];122–31. Available from: https://doi.org/10.22159/ijap.2025v17i5.54474

54. Carini C, Seyhan AA. Tribulations and future opportunities for artificial intelligence in precision medicine. Journal of Translational Medicine [Internet]. BioMed Central; 2024 Apr 30 [cited 2025 Oct];22(1). Available from: https://doi.org/10.1186/s12967-024-05067-0

55. Jarallah SJ, Almughem FA, Alhumaid NK, Fayez NA, Alradwan I, Alsulami KA, et al. Artificial intelligence revolution in drug discovery: A paradigm shift in pharmaceutical innovation. International Journal of Pharmaceutics [Internet]. 2025 May 30 [cited 2026 Jan];680:125789–125789. Available from: https://doi.org/10.1016/j.ijpharm.2025.125789

56. Liu Y, Zhang L, Jiang Z, Xia T, Li P, Wu P, et al. Applications of Artificial Intelligence in Biotech Drug Discovery and Product Development. MedComm [Internet]. 2025 July 30 [cited 2025 Nov];6(8). Available from: https://doi.org/10.1002/mco2.70317

57. Robert K, Kaium O, Alasa L. Generative AI and Pharmaceutical Innovation: Accelerating Drug Discovery with Deep Learning and Predictive Analytics. International Journal of Multidisciplinary Evolutionary Research [Internet]. 2025 Jan 1 [cited 2025 Nov];6(2):44–52. Available from: https://doi.org/10.54660/ijmer.2025.6.2.44-52

58. Husnain A, Rasool S, Saeed A, Hussain HK. Revolutionizing Pharmaceutical Research: Harnessing Machine Learning for a Paradigm Shift in Drug Discovery. International Journal of Multidisciplinary Sciences and Arts [Internet]. 2023 Sept 27 [cited 2025 Oct];2(2):149–57. Available from: https://doi.org/10.47709/ijmdsa.v2i2.2897

59. Nwankwo EI, Emeihe EV, Ajegbile MD, Olaboye JA, Maha CC. AI in personalized medicine: Enhancing drug efficacy and reducing adverse effects. International Medical Science Research Journal [Internet]. 2024 Aug 23 [cited 2025 Sept];4(8):806–33. Available from: https://doi.org/10.51594/imsrj.v4i8.1453

60. Kiriiri GK, Njogu P, Mwangi A. Exploring different approaches to improve the success of drug discovery and development projects: a review. Future Journal of Pharmaceutical Sciences [Internet]. Springer Science+Business Media; 2020 June 23 [cited 2025 Oct];6(1). Available from: https://doi.org/10.1186/s43094-020-00047-9

61. A SI, N. BS. Artificial Intelligence Drug Discovery and Development. Asian Journal of Pharmaceutical Research and Development [Internet]. 2025 Dec 15 [cited 2026 Mar];13(6):119–29. Available from: https://doi.org/10.22270/ajprd.v13i6.1657

62. Bilgin GB, Bilgin C, Burkett BJ, Orme JJ, Childs DS, Thorpe M, et al. Theranostics and artificial intelligence: new frontiers in personalized medicine. Theranostics [Internet]. Ivyspring International Publisher; 2024 Jan 1 [cited 2025 Oct];14(6):2367–78. Available from: https://doi.org/10.7150/thno.94788

63. Gangwal A, Ansari MA, Ahmad I, Azad AK, Kumarasamy V, Subramaniyan V, et al. Generative artificial intelligence in drug discovery: basic framework, recent advances, challenges, and opportunities. Frontiers in Pharmacology [Internet]. 2024 Feb 7 [cited 2025 Oct];15. Available from: https://doi.org/10.3389/fphar.2024.1331062

64. Bhosale SZ Tanuja Tandale, Dr Sujit Kakade, Dr Ashok. Review on Artificial Intelligence (AI) in Pharmaceutical Field. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2026 Feb 22 [cited 2026 Feb]; Available from: https://doi.org/10.5281/zenodo.18730245

65. Bhosale SZ Tanuja Tandale, Dr Sujit Kakade, Dr Ashok. Review on Artificial Intelligence (AI) in Pharmaceutical Field. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2026 Feb 22 [cited 2026 Feb]; Available from: https://doi.org/10.5281/zenodo.18730246

66. Atz K, Cotos L, Isert C, Håkansson M, Focht D, Hilleke M, et al. Prospective de novo drug design with deep interactome learning. Nature Communications [Internet]. 2024 Apr 22 [cited 2025 Oct];15(1). Available from: https://doi.org/10.1038/s41467-024-47613-w

67. Hinkson IV, Madej BD, Stahlberg E. Accelerating Therapeutics for Opportunities in Medicine: A Paradigm Shift in Drug Discovery. Frontiers in Pharmacology [Internet]. 2020 June 30 [cited 2025 Oct];11. Available from: https://doi.org/10.3389/fphar.2020.00770

68. Li X, Xing J, Zhang S, Zhou J. Editorial: Advancing drug discovery with AI: drug–target interactions, mechanisms of action, and screening. Frontiers in Pharmacology [Internet]. 2025 Oct 24 [cited 2026 Mar];16:1721323–1721323. Available from: https://doi.org/10.3389/fphar.2025.1721323

69. Ocaña A, Pandiella A, Privat C, Bravo I, Luengo-Oroz M, Amir E, et al. Integrating artificial intelligence in drug discovery and early drug development: a transformative approach. Biomarker Research [Internet]. 2025 Mar 14 [cited 2026 Jan];13(1):45–45. Available from: https://doi.org/10.1186/s40364-025-00758-2

70. Hasselgren C, Oprea TI. Artificial Intelligence for Drug Discovery: Are We There Yet? The Annual Review of Pharmacology and Toxicology [Internet]. Annual Reviews; 2023 Sept 22 [cited 2025 Aug];64(1):527–50. Available from: https://doi.org/10.1146/annurev-pharmtox-040323-040828

71. Potineni B. Generative AI in drug discovery: Accelerating the search for new therapeutics. World Journal of Advanced Engineering Technology and Sciences [Internet]. 2025 Apr 26 [cited 2025 Nov];15(1):1784–94. Available from: https://doi.org/10.30574/wjaets.2025.15.1.0298

72. Bae H, Ji H, Konstantinov K, Sluyter R, Ariga K, Kim YH, et al. Artificial Intelligence-Driven Nanoarchitectonics for Smart Targeted Drug Delivery. Advanced Materials [Internet]. 2025 Aug 7 [cited 2025 Nov];37(42). Available from: https://doi.org/10.1002/adma.202510239

73. Niazi SK. The Coming of Age of AI/ML in Drug Discovery, Development, Clinical Testing, and Manufacturing: The FDA Perspectives. Drug Design Development and Therapy [Internet]. 2023 Sept 1 [cited 2025 Aug];2691–725. Available from: https://doi.org/10.2147/dddt.s424991

74. Pushkaran AC, Arabi AA. From understanding diseases to drug design: can artificial intelligence bridge the gap? Artificial Intelligence Review [Internet]. 2024 Mar 11 [cited 2025 Oct];57(4). Available from: https://doi.org/10.1007/s10462-024-10714-5

75. Crucitti D, Míguez CP, Arias JÁD, Prada DBF, Orgueira AM. De novo drug design through artificial intelligence: an introduction. Frontiers in Hematology [Internet]. 2024 Jan 25 [cited 2025 Oct];3. Available from: https://doi.org/10.3389/frhem.2024.1305741

76. Bilotta M, Rocca R, Alcaro S. Next-generation drug discovery: The AI revolution in pharmaceutical research. Artificial Intelligence in the Life Sciences [Internet]. 2025 Nov 27 [cited 2025 Dec];8:100149–100149. Available from: https://doi.org/10.1016/j.ailsci.2025.100149

77. Zhavoronkov A, Vanhaelen Q, Oprea TI. Will Artificial Intelligence for Drug Discovery Impact Clinical Pharmacology? Clinical Pharmacology & Therapeutics [Internet]. Wiley; 2020 Jan 20 [cited 2025 Oct];107(4):780–5. Available from: https://doi.org/10.1002/cpt.1795

78. Naithani U, Guleria V. Integrative computational approaches for discovery and evaluation of lead compound for drug design. Frontiers in Drug Discovery [Internet]. 2024 Apr 5 [cited 2025 Oct];4. Available from: https://doi.org/10.3389/fddsv.2024.1362456

79. Udegbe FC, Ebulue OR, Ebulue CC, Ekesiobi CS. MACHINE LEARNING IN DRUG DISCOVERY: A CRITICAL REVIEW OF APPLICATIONS AND CHALLENGES. Computer Science & IT Research Journal [Internet]. Fair East Publishers; 2024 Apr 17 [cited 2025 Sept];5(4):892–902. Available from: https://doi.org/10.51594/csitrj.v5i4.1048

80. Zhang O, Lin H, Zhang H, Zhao H, Huang Y, Hsieh C, et al. Deep Lead Optimization: Leveraging Generative AI for Structural Modification. Journal of the American Chemical Society [Internet]. American Chemical Society; 2024 Nov 5 [cited 2025 Oct];146(46):31357–70. Available from: https://doi.org/10.1021/jacs.4c11686

81. Khan MK, Raza MA, Shahbaz M, Hussain I, Khan MF, Xie Z, et al. The recent advances in the approach of artificial intelligence (AI) towards drug discovery. Frontiers in Chemistry [Internet]. 2024 May 31 [cited 2025 Aug];12. Available from: https://doi.org/10.3389/fchem.2024.1408740

82. Bahekar S, Bhosale T. Artificial Intelligence in Drug Discovery. The Journal of Medical Research [Internet]. 2025 Sept 22 [cited 2026 Jan];11(6):135–6. Available from: https://doi.org/10.4103/jmr.jmr_26_25

83. Honey E, Khan A. Artificial Intelligence in Drug Discovery & Development. International journal of research and scientific innovation [Internet]. 2025 Nov 6 [cited 2026 Mar];12(10):1337–49. Available from: https://doi.org/10.51244/ijrsi.2025.1210000118

84. Zeb S, FNU N, Abbasi N, Fahad M. AI in Healthcare: Revolutionizing Diagnosis and Therapy. International Journal of Multidisciplinary Sciences and Arts [Internet]. 2024 Aug 17 [cited 2025 Oct];3(3):118–28. Available from: https://doi.org/10.47709/ijmdsa.v3i3.4546

85. Unogwu OJ, Ike M, Joktan OO. Employing Artificial Intelligence Methods in Drug Development: A New Era in Medicine. Mesopotamian Journal of Artificial Intelligence in Healthcare [Internet]. 2023 Oct 20 [cited 2025 Oct];2023:52–6. Available from: https://doi.org/10.58496/mjaih/2023/010

86. Mehran MJ, Mohammadzadeh S, Bolideei M, Barzigar R, Haider KH, Jadgal N, et al. Artificial Intelligence in Drug Discovery: Integrative Advances From Data to Therapeutic Innovation. Drug Development Research [Internet]. 2026 Feb 2 [cited 2026 Feb];87(2). Available from: https://doi.org/10.1002/ddr.70229

87. Mintaş Ş, Sevimli-Gür C. Artificial Intelligence Applications in Drug Discovery and Research. DergiPark (Istanbul University) [Internet]. 2024 Nov 18 [cited 2025 Oct]; Available from: https://dergipark.org.tr/en/pub/jaida/issue/89048/1587347

88. Raut1 SMR. Revolutionizing Formulation Design: The Power of Ai-Driven De Novo Approaches. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2026 Mar 3 [cited 2026 Mar]; Available from: https://doi.org/10.5281/zenodo.18851647

89. Kumar PKK, Yadagiri PY, Eswaramoorthi ME, Jaganathan S, Saravanan J, M V. **Artificial Intelligence (AI): Drug Design and Formulation** . Indian Journal of Pharmaceutical Chemistry and Analytical Techniques [Internet]. 2026 Feb 24 [cited 2026 Mar];2(1):1–10. Available from: https://doi.org/10.64062/ijpcat.vol2.issue1.1

90. Raut1 SMR. Revolutionizing Formulation Design: The Power of Ai-Driven De Novo Approaches. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2026 Mar 3 [cited 2026 Mar]; Available from: https://doi.org/10.5281/zenodo.18851648

91. Bandgar. SC kale* Sayali S More, DrSA. THE FUTURE OF DRUG AND FORMULATION INNOVATION: AI-DRIVEN STRUCTURE-BASED DE NOVO DESIGN PARADIGMS. In: Zenodo (CERN European Organization for Nuclear Research) [Internet]. European Organization for Nuclear Research; 2026 [cited 2026 Jan]. Available from: https://doi.org/10.5281/zenodo.18225162

92. Saha G. Artificial Intelligence (AI) in Formulation Development. In 2024 [cited 2025 Nov]. p. 459–81. Available from: https://doi.org/10.69613/tkh3gv85

93. G.3 HH *1 Kottai Muthu A 2, Alagu Manivasagam. Artificial Intelligence and Machine Learning in Drug Formulation Development. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2025 Nov 12 [cited 2025 Nov]; Available from: https://doi.org/10.5281/zenodo.17589193

94. Chauhan SB, Singh I, Singh M, Jain chirag. AI-Powered Excipient Innovation: Transforming Drug Design, ADMETProfiling, and Formulation Developmen. Current Topics in Medicinal Chemistry [Internet]. 2026 Mar 27 [cited 2026 Mar];26. Available from: https://doi.org/10.2174/0115680266431788260223072453

95. Zhang Z, Xiang Y, Laforêt J, Spasojević I, Fan P, Heffernan A, et al. TuNa-AI: A Hybrid Kernel Machine To Design Tunable Nanoparticles for Drug Delivery. ACS Nano [Internet]. 2025 Sept 11 [cited 2026 Mar];19(37):33288–96. Available from: https://doi.org/10.1021/acsnano.5c09066

96. Chan A, Kirtane AR, Qu QR, Huang X, Woo J, Subramanian DA, et al. Designing lipid nanoparticles using a transformer-based neural network. Nature Nanotechnology [Internet]. 2025 Aug 15 [cited 2025 Oct]; Available from: https://doi.org/10.1038/s41565-025-01975-4

97. Bais SDP Yogesh B Raut, Sanjay K. RECENT ADVANCEMENT IN USE OF COMPUTER IN PHARMACEUTICAL FORMULATION DEVELOPMENT. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2025 Dec 10 [cited 2025 Dec]; Available from: https://doi.org/10.5281/zenodo.17878680

98. Bais SDP Yogesh B Raut, Sanjay K. RECENT ADVANCEMENT IN USE OF COMPUTER IN PHARMACEUTICAL FORMULATION DEVELOPMENT. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2025 Dec 10 [cited 2025 Dec]; Available from: https://doi.org/10.5281/zenodo.17878681

99. Dong J, Wu Z, Xu H, Ouyang D. FormulationAI: a novel web-based platform for drug formulation design driven by artificial intelligence. Briefings in Bioinformatics [Internet]. 2023 Nov 22 [cited 2025 Dec];25(1). Available from: https://doi.org/10.1093/bib/bbad419

100. Siepmann J, Basit AW, Rades T. Pharmaceutical Technology in Europe. International Journal of Pharmaceutics [Internet]. 2021 Dec 30 [cited 2025 Aug];613:121441–121441. Available from: https://doi.org/10.1016/j.ijpharm.2021.121441

101. Tanga S, Ramburrun P, Aucamp M. From Liquid SNEDDS to Solid SNEDDS: A Comprehensive Review of Their Development and Pharmaceutical Applications. The AAPS Journal [Internet]. Springer Science+Business Media; 2025 Oct 30 [cited 2025 Nov];28(1). Available from: https://doi.org/10.1208/s12248-025-01167-x

102. Zaslavsky J, Allen C. A dataset of formulation compositions for self-emulsifying drug delivery systems. Scientific Data [Internet]. 2023 Dec 20 [cited 2025 July];10(1). Available from: https://doi.org/10.1038/s41597-023-02812-w

103. Reker D, Rybakova Y, Kirtane AR, Cao R, Yang JW, Navamajiti N, et al. Computationally guided high-throughput design of self-assembling drug nanoparticles. Nature Nanotechnology [Internet]. 2021 Mar 25 [cited 2025 Oct];16(6):725–33. Available from: https://doi.org/10.1038/s41565-021-00870-y

104. Pan Y, Mi R, Bian W, Wang Z, Zhao M, Li Z, et al. Harnessing the Power of Artificial Intelligence for Pharmaceutics: From Pharmacokinetics Prediction, Formulation, to Manufacturing. Pharmaceutical Fronts [Internet]. 2026 Feb 27 [cited 2026 Mar];8(1). Available from: https://doi.org/10.1055/a-2790-6937

105. Nagpure N, Askar D, Kale DS, Raut H, Rasala T. In-silico pharmaceutics: Quantum simulations for next-generation dosage form design. International Journal of Pharmaceutical Research and Development [Internet]. 2025 July 1 [cited 2026 Mar];7(2):398–405. Available from: https://doi.org/10.33545/26646862.2025.v7.i2e.201

106. G.3 HH *1 Kottai Muthu A 2, Alagu Manivasagam. Artificial Intelligence and Machine Learning in Drug Formulation Development. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2025 Nov 12 [cited 2025 Nov]; Available from: https://doi.org/10.5281/zenodo.17589192

107. Askr H, Elgeldawi E, Ella HA, Elshaier YAMM, Gomaa MM, Hassanien AE. Deep learning in drug discovery: an integrative review and future challenges. Artificial Intelligence Review [Internet]. 2022 Nov 17 [cited 2025 Aug];56(7):5975–6037. Available from: https://doi.org/10.1007/s10462-022-10306-1

108. Research MJ of M. Artificial Intelligence in pharmaceutical sciences: Transforming drug discovery, formulation, and manufacturing. Zenodo (CERN European Organization for Nuclear Research) [Internet]. 2025 Dec 15 [cited 2025 Dec]; Available from: https://doi.org/10.5281/zenodo.17945148

109. Wu P, Zang P. Artificial Intelligence in Pharmaceutical Formulation: A Comprehensive Review. Applied Artificial Intelligence Research [Internet]. 2025 Dec 2 [cited 2026 Mar];1(3). Available from: https://doi.org/10.65455/nshrsr55

110. Wei Z, Zhuo S, Zhang Y, Wu L, Gao X, He S, et al. Machine learning reshapes the paradigm of nanomedicine research. Acta Pharmaceutica Sinica B [Internet]. 2025 May 1 [cited 2026 Mar]; Available from: https://doi.org/10.1016/j.apsb.2025.05.014

111. Malik MN, Mali S, Surve P, Londhe P, Komarol H. Artificial intelligence as an innovative tool in nanotechnology for drug delivery. International Journal of Pharmacy and Pharmaceutical Science [Internet]. 2026 Mar 1 [cited 2026 Mar];8(3):59–63. Available from: https://doi.org/10.33545/26647222.2026.v8.i3a.333

112. Edriss AA, Yarra S, Vomo JA, Ismael K, Elshiekh YB. AI-powered nano formulation: revolutionizing drug development and delivery. International Journal of Science and Research Archive [Internet]. 2025 Feb 28 [cited 2025 Dec];14(2):1501–12. Available from: https://doi.org/10.30574/ijsra.2025.14.2.0491

113. Prusty A, Panda SK. The Revolutionary Role of Artificial Intelligence (AI) in Pharmaceutical Sciences. Indian Journal of Pharmaceutical Education and Research [Internet]. 2024 Aug 10 [cited 2025 Aug];58. Available from: https://doi.org/10.5530/ijper.58.3s.78

114. Abdalla Y, Taub MA, Hilton E, Akkaraju P, Milanovic A, Orlu M, et al. VECT-GAN: A variationally encoded generative model for overcoming data scarcity in pharmaceutical science. arXiv (Cornell University) [Internet]. 2025 Jan 15 [cited 2025 Sept]; Available from: http://arxiv.org/abs/2501.08995

115. Baena JC, Victoria J, Toro-Pedroza A, Aragón CC, Ortiz-Guzman J, García-Robledo JE, et al. Smart CAR-T Nanosymbionts: archetypes and proto-models. Frontiers in Immunology [Internet]. Frontiers Media; 2025 Aug 12 [cited 2025 Oct];16. Available from: https://doi.org/10.3389/fimmu.2025.1635159

116. Han Y, Kim DH, Pack SP. Nanomaterials in Drug Delivery: Leveraging Artificial Intelligence and Big Data for Predictive Design. International Journal of Molecular Sciences [Internet]. 2025 Nov 17 [cited 2026 Mar];26(22):11121–11121. Available from: https://doi.org/10.3390/ijms262211121

117. Kantesaria R, Panda HS. A Review on AI-Based Data-Driven Models for Optimization of Nanocarriers as Drug Delivery Systems. ACS Biomaterials Science & Engineering [Internet]. 2026 Feb 11 [cited 2026 Mar];12(3):1397–418. Available from: https://doi.org/10.1021/acsbiomaterials.5c01998

118. Huang Y, Guo X, Wu Y, Chen X, Feng L, Xie N, et al. Nanotechnology's frontier in combatting infectious and inflammatory diseases: prevention and treatment. Signal Transduction and Targeted Therapy [Internet]. Springer Nature; 2024 Feb 21 [cited 2025 Oct];9(1). Available from: https://doi.org/10.1038/s41392-024-01745-z

119. Wei XX, Jiang Y, Chenwu F, Li Z, Wan J, Li Z, et al. Synergistic Ferroptosis–Immunotherapy Nanoplatforms: Multidimensional Engineering for Tumor Microenvironment Remodeling and Therapeutic Optimization. Nano-Micro Letters [Internet]. Springer Science+Business Media; 2025 Sept 2 [cited 2025 Sept];18(1). Available from: https://doi.org/10.1007/s40820-025-01862-6

120. Sahu RC, Arora S, Kumar D, Agrawal AK. Machine Learning for Predictive Modeling in Nanomedicine-Based Cancer Drug Delivery. Med Research [Internet]. 2025 Nov 17 [cited 2026 Mar];2(1):130–56. Available from: https://doi.org/10.1002/mdr2.70043

121. Okafor NI, Igbokwe NN, Onohuean H, Faya M, Choonara YE. Artificial Intelligence-Driven Development and Characterization of

Nanomedicine. BioNanoScience [Internet]. 2026 Mar 17 [cited 2026 Mar];16(4). Available from: https://doi.org/10.1007/s12668-026-02476-x

122. Gao XJ, Gao XJ, Ciura K, Ma Y, Mikołajczyk A, Jagiełło K, et al. Toward the Integration of Machine Learning and Molecular Modeling for Designing Drug Delivery Nanocarriers. Advanced Materials [Internet]. 2024 Sept 10 [cited 2026 Mar];36(45). Available from: https://doi.org/10.1002/adma.202407793

123. Wu C, Xu Y, Fang J, Li Q. Machine Learning in Biomaterials, Biomechanics/Mechanobiology, and Biofabrication: State of the Art and Perspective. Archives of Computational Methods in Engineering [Internet]. 2024 May 4 [cited 2025 Oct]; Available from: https://doi.org/10.1007/s11831-024-10100-y

124. Padmini S, Amaran S, Sreekumar K, Kalaivani J, Iniyan S. Artificial Intelligence-Enhanced Nanomedicine Design and Deep Reinforcement Learning in Pharmacokinetics. In: Advances in medical technologies and clinical practice book series [Internet]. IGI Global; 2024 [cited 2025 Dec]. p. 135–68. Available from: https://doi.org/10.4018/979-8-3693-3212-2.ch006

125. Kumar A, Qasim S, Sharma A, Gugulothu D, Verma S. Machine Learning Algorithm for Nanomedicine: AI Curated Nanocarriers for Cancer Treatment. Current Pharmaceutical Design [Internet]. 2026 Mar 12 [cited 2026 Mar];32. Available from: https://doi.org/10.2174/0113816128413703251124110442

126. Aundhia C, Parmar G, Talele C, Kumari M, Gupta G. Personalized Nanocomposite-based Drug Delivery Systems: Integration of AI and 3D Printing. Current Drug Targets [Internet]. 2026 Jan 19 [cited 2026 Jan];27. Available from: https://doi.org/10.2174/0113894501430905251210054617

127. Li H, Yue F, Luo Q, Li Z, Li X, Gan H, et al. Stimuli-activatable nanomedicine meets cancer theranostics. Theranostics [Internet]. Ivyspring International Publisher; 2023 Jan 1 [cited 2025 Aug];13(15):5386–417. Available from: https://doi.org/10.7150/thno.87854

128. Yousfan A, Rahwanji MJA, Hanano A, Al-Obaidi H. A Comprehensive Study on Nanoparticle Drug Delivery to the Brain: Application of Machine Learning Techniques. Molecular Pharmaceutics [Internet]. 2023 Dec 7 [cited 2025 Aug];21(1):333–45. Available from: https://doi.org/10.1021/acs.molpharmaceut.3c00880

129. Azimi S. Intelligent nanoparticle design: Unlocking the potential of AI for transformative drug delivery. Current Opinion in Biomedical Engineering [Internet]. 2025 Oct 15 [cited 2026 Jan];36:100625–100625. Available from: https://doi.org/10.1016/j.cobme.2025.100625

130. Singh AV, Varma M, Laux P, Choudhary S, Datusalia AK, Gupta N, et al. Artificial intelligence and machine learning disciplines with the potential to improve the nanotoxicology and nanomedicine fields: a comprehensive review. Archives of Toxicology [Internet]. Springer Science+Business Media; 2023 Mar 7 [cited 2025 Oct];97(4):963–79. Available from: https://doi.org/10.1007/s00204-023-03471-x

131. Mendes BB, Conniot J, Avital A, Yao D, Jiang X, Zhou X, et al. Nanodelivery of nucleic acids. Nature Reviews Methods Primers [Internet]. 2022 Apr 14 [cited 2025 Oct];2(1). Available from: https://doi.org/10.1038/s43586-022-00104-y

132. Đorđević S, Medel M, Conejos-Sánchez I, Carreira B, Pozzi S, Acúrcio RC, et al. Current hurdles to the translation of nanomedicines from bench to the clinic. Drug Delivery and Translational Research [Internet]. Springer Science+Business Media; 2021 July 23 [cited 2025 Oct];12(3):500–25. Available from: https://doi.org/10.1007/s13346-021-01024-2

133. Waheed S, Li Z, Zhang F, Chiarini A, Armato U, Wu J. Engineering nano-drug biointerface to overcome biological barriers toward precision drug delivery. Journal of Nanobiotechnology [Internet]. BioMed Central; 2022 Aug 31 [cited 2025 Oct];20(1). Available from: https://doi.org/10.1186/s12951-022-01605-4

134. Bardhan NM. Nanomaterials in diagnostics, imaging and delivery: Applications from COVID-19 to cancer. MRS Communications [Internet]. Springer Nature; 2022 Oct 17 [cited 2025 Sept];12(6):1119–39. Available from: https://doi.org/10.1557/s43579-022-00257-7

135. Leong HS, Butler KS, Brinker CJ, Azzawi M, Conlan RS, Dufès C, et al. On the issue of transparency and reproducibility in nanomedicine [Internet]. Vol. 14, Nature Nanotechnology. Nature Portfolio; 2019 [cited 2025 Aug]. p. 629–35. Available from: https://doi.org/10.1038/s41565-019-0496-9

136. Paunovska K, Loughrey D, Sago CD, Langer R, Dahlman JE. Using Large Datasets to Understand Nanotechnology. Advanced Materials [Internet]. 2019 Aug 20 [cited 2025 Oct];31(43). Available from: https://doi.org/10.1002/adma.201902798

137. Jones D, Ghandehari H, Facelli JC. A review of the applications of data mining and machine learning for the prediction of biomedical properties of nanoparticles. Computer Methods and Programs in Biomedicine [Internet]. Elsevier BV; 2016 Apr 30 [cited 2025 Sept];132:93–103. Available from: https://doi.org/10.1016/j.cmpb.2016.04.025

138. Tade RS, Jain SN, Satyavijay JT, Shah PN, Bari TD, Patil TM, et al. Artificial Intelligence in the Paradigm Shift of Pharmaceutical Sciences: A Review. Nano Biomedicine and Engineering [Internet]. 2023 Dec 8 [cited 2025 Oct];16(1):64–77. Available from: https://doi.org/10.26599/nbe.2023.9290043

139. Crisafulli S, Ciccimarra F, Bellitto C, Carollo M, Carrara E, Stagi L, et al. Artificial intelligence for optimizing benefits and minimizing risks of pharmacological therapies: challenges and opportunities. Frontiers in Drug Safety and Regulation [Internet]. Frontiers Media; 2024 Mar 18 [cited 2025 Sept];4. Available from: https://doi.org/10.3389/fdsfr.2024.1356405

140. Somara S, Joshi AM, Mitra K, Desai S, Lundberg MS, Bhasin S, et al. Artificial Intelligence in Biotechnology and Pharmaceuticals: Evolution, Applications, and Regulatory Frontiers. Current Stem Cell Reports [Internet]. 2025 Nov 1 [cited 2025 Nov];11(1). Available from: https://doi.org/10.1007/s40778-025-00249-y

141. Health TLD. Fixing cracks in the artificial intelligence drug development pipeline. The Lancet Digital Health [Internet]. 2025 July 1 [cited 2026 Feb];7(7):100897–100897. Available from: https://doi.org/10.1016/j.landig.2025.100897

142. Zaslavsky J, Bannigan P, Allen C. Re-envisioning the design of nanomedicines: harnessing automation and artificial intelligence. Expert Opinion on Drug Delivery [Internet]. 2023 Jan 16 [cited 2025 Nov];20(2):241–57. Available from: https://doi.org/10.1080/17425247.2023.2167978

143. Mazumdar H, Khondakar KR, Das S, Harder A, Kaushik A. Artificial intelligence for personalized nanomedicine; from material selection to patient outcomes. Expert Opinion on Drug Delivery [Internet]. 2024 Dec 8 [cited 2025 Nov];22(1):85–108. Available from: https://doi.org/10.1080/17425247.2024.2440618

144. Gupta YD, Mackeyev Y, Krishnan S, Bhandary S. Mesoporous silica nanotechnology: promising advances in augmenting cancer theranostics. Cancer Nanotechnology [Internet]. 2024 Jan 31 [cited 2025 Oct];15(1). Available from: https://doi.org/10.1186/s12645-024-00250-w

145. Haramshahi SMA, Hamblin MR, Ravesh RK, Sadr H, Ahmadirad N, Mehrabi F, et al. Biomaterials for CNS disorders: a review of development from traditional methods to AI-assisted optimization. Journal of Materials Science Materials in Medicine [Internet]. Springer Science+Business Media; 2025 Oct 14 [cited 2025 Oct];36(1). Available from: https://doi.org/10.1007/s10856-025-06947-7

146. Sampene AK, Nyirenda F. Evaluating the effect of artificial intelligence on pharmaceutical product and drug discovery in China. Future Journal of Pharmaceutical Sciences [Internet]. 2024 Apr 7 [cited 2025 Oct];10(1). Available from: https://doi.org/10.1186/s43094-024-00632-2

147. Sarkar S, Das D. Artificial Intelligence in Nanomedicine Formulation and Applications. In: BENTHAM SCIENCE PUBLISHERS eBooks [Internet]. 2025 [cited 2026 Jan]. p. 171–200. Available from: https://doi.org/10.2174/9798898813123125010012

148. Zhou H, Xu J, Qin X, Zhang J, Zou W, Shakouri M, et al. New Frontiers in AI-Nano Converged Platforms for Intelligent Diagnostics, Therapeutics, and Safety Evaluation. Chem & Bio Engineering [Internet]. 2026 Mar 28 [cited 2026 Mar]; Available from: https://doi.org/10.1021/cbe.5c00188

149. Hwang N, Lim DC, Goh TS, Kang J, Kim J, Kim S, et al. Recent advances in theranostic nanomaterials for overcoming traumatic brain injury. Journal of Nanobiotechnology [Internet]. BioMed Central; 2025 Oct 29 [cited 2025 Oct];23(1). Available from: https://doi.org/10.1186/s12951-025-03685-4

150. Zhang P, Guo Z, Ullah S, Melagraki G, Afantitis A, Lynch I. Nanotechnology and artificial intelligence to enable sustainable and precision agriculture. Nature Plants [Internet]. Nature Portfolio; 2021 June 24 [cited 2025 Aug];7(7):864–76. Available from: https://doi.org/10.1038/s41477-021-00946-6

151. Singh AV, Bhardwaj P, Upadhyay AK, Pagani A, Upadhyay J, Bhadra J, et al. Navigating regulatory challenges in molecularly tailored nanomedicine. 2024 Apr 25 [cited 2025 Oct];1(2):124–34. Available from: https://doi.org/10.37349/ebmx.2024.00009

152. Chehelgerdi M, Chehelgerdi M, Allela OQB, Pecho RDC, Narayanan J, Rao DP, et al. Progressing nanotechnology to improve targeted cancer treatment: overcoming hurdles in its clinical implementation. Molecular Cancer [Internet]. BioMed Central; 2023 Oct 9 [cited 2025 Aug];22(1). Available from: https://doi.org/10.1186/s12943-023-01865-0