AI-Driven Nanopharmacology: Intelligent Nano systems Transforming Drug Discovery and Therapeutic Delivery

Dr. Muchukota Sushma [1], Bharathi Bhogenahalli Venkatappa [2*], Dr. Bestha Chakrapani [3], Dr. Muchukota Babu [4], Dr. Narayana Goruntla [5]

[1] Associate Professor, Department of Pharmacy Practice, Aditya Bangalore Institute of Pharmacy Education and Research (ABIPER), Yelahanka, Bangalore, Karnataka, India.

[2] Pharm D Intern, Department of Pharmacy Practice, Aditya Bangalore Institute of Pharmacy Education and Research (ABIPER), Kogilu cross, Yelahanka, Bangalore-64, India.

[3] Assistant Professor, Department of Pharmacology, Oil Technological Pharmaceutical Research Institute -Jawaharlal Nehru Technological University, Anantapur - Andhra Pradesh

[4] Professor and HOD, Dept of Forensic Medicine, Govt. Medical College, Kadapa, Andhra Pradesh, India

[5] Associate Professor & Research Co-ordinator, Department of Clinical Pharmacy & Pharmacy Practice, School of Pharmacy, Kampala International University, Uganda.

* Corresponding Author: **Bharathi Bhogenahalli Venkatappa**

Article Info

ISSN (online): 3049-0421
Volume: 02
Issue: 06
November - December 2025
Received: 29-09-2025
Accepted: 30-10-2025
Published: 28-11-2025
Page No: 12-19

Abstract

The artificial intelligence (AI) and nanotechnology coming together have created a game-changing horizon in drug discovery, formulation, and delivery of therapy. AI-based nanopharmacology is a machine learning (ML), deep learning (DL), and intelligent computational science approach to designing, optimizing and assessing nanoscale drug systems with unprecedented accuracy. The present paper is a review of recent developments in AI-driven nanoparticle design, autonomous nanosystems and applications of nanomedicine in the clinic. In the present day, AI algorithms make it possible to rapidly predict the effects of molecular interactions, screen the compatibility between drugs and nanocarriers in high throughput, and optimize the search of physicochemical parameters to achieve targeted delivery. Simultaneously, intelligent nanosystems e.g. stimuli-responsive nanocarriers, programmable nanoformulations, and early-stage therapeutic nano robots are transforming clinical pharmacology through the ability to release drugs in a controlled manner, real-time biosensing and individual pharmacokinetic modelling. Although great strides have been achieved, there are still several issues of data integrity, model bias, translational safety and ethical concerns in implementing autonomous nanosystems. It is predicted that future directions will involve AI-based digital twins, predictive nano-AI systems, and completely autonomous nanotherapeutic systems with the capacity to adjust their own responses to patient-specific biomarkers. This review has identified the possibility of AI-driven nanopharmacology to transform contemporary therapeutics, providing new avenues of precision medicine and pharmacological efficacy and personalized treatment of patients.

DOI: https://doi.org/10.54660/IJPGRR.2025.2.6.12-19

Keywords: Nanopharmacology, Artificial Intelligence, Smart Nanocarriers, Nanomedicine, Machine learning, Deep learning, Precision Medicine

1. Introduction

Nanotechnology has become one of the most powerful tools in the contemporary pharmaceutical sciences as it permits the exact control of materials at the size that are directly involved with the biological systems. In line with this development, artificial intelligence (AI) has rapidly evolved into an authoritative computational framework that can investigate complicated data, forecast the actions of molecules, and instruct therapeutic breakthroughs.

Historically, development and drug discovery were both time consuming and resource intensive processes that entailed a series of cycles of experimentation on different stages. These limitations can be surmounted by the introduction of AI into nanotechnology to create the interdisciplinary field called AI-driven nanopharmacology which can drive faster innovation in therapeutic applications [1].

AI introduces significant benefit to nanotechnology through better nanoparticle design, predictive toxicity data, better surface chemistry, and novel drug-nanocarrier interactions. Machine learning algorithms are able to analyse huge experimental data to reveal relationships that cannot be observed in the traditional analysis. Deep learning models, including graph neural networks (GNNs) and convolutional neural networks (CNNs), can be used to improve the accuracy of prediction about nanoparticle behaviour at physiological conditions. These properties allow the rational design of the nanosystems, instead of using trial-and-error techniques [2].

At the same time, nanotechnology has also increased the therapeutic opportunities, through its ability to deliver therapies, improve solubility, provide sustained delivery, and increase biocompatibility. Liposomes, polymeric nanoparticles, metallic nanoshells, and dendrimers are nanocarriers that provide regulated drug delivery and better disease targeting. Such platforms can be tailored to a particular patient group or disease phenotype with the help of AI-guided optimization, which enables personalized medicine [3].

The implication of AI-enabled nanopharmacology in the oncology, neurology, and the infectious disease field is especially high in the need to treat the disease in a targeted manner and decreased systemic toxicity. As the sphere of healthcare gets more and more dedicated to the concept of precision medicine, the intersection of AI and nanotechnology is a significant step toward the concept of smart therapeutics, one that can adapt to the preferences of a specific patient [4]. The paper discusses the use of AI in improving the process of nanotechnology-based drug discovery and the creation of smart nanosystems and clinical trials in the pharmaceutical field. It also deals with the existing challenges, ethical aspects and future views relating to fully autonomous therapeutics. Fig 1 shows a convergence of three fields in artificial intelligence, nanotechnology, and pharmacology, with their overlap in the same area, where intelligent smart nanocarriers are an integrated therapeutic innovation.

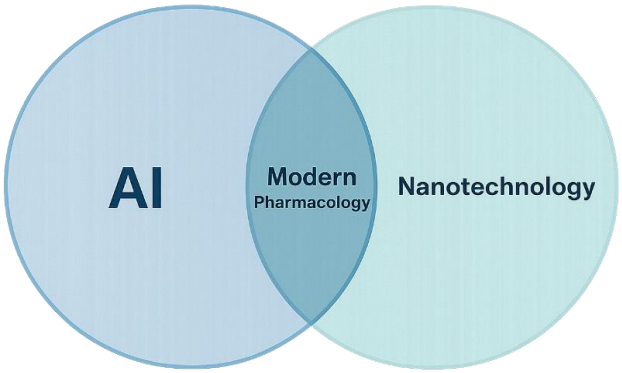

Fig 1: Convergence of AI and Nanotechnology in Modern Pharmacology

2. AI in Nanotechnology-Enhanced Drug Discovery

Machine learning (ML) is now an inherent technology in contemporary nanodrug discovery based on the rapid and data-driven prediction of molecular behaviours that used to need tedious experimentation. ML algorithms are used in nanotechnology to analyse multidimensional datasets of physicochemical properties of nanoparticles including size, surface area, zeta potential, hydrophobicity index, ligand density and core-shell architecture and correlate them with biological behaviours including cellular uptake, biodistribution, toxicity and drug-release kinetics [5].

Support Vector machines (SVMs), random forests (RF), gradient boosting, and XGBoost are the types of the supervised learning that are especially useful in classifying optimal nanoparticle design and predicting biological interactions. These models are able to identify trends that cannot be discovered using traditional methods of statistics. As an illustration, ML can be used to predict penetration of nanoparticles within the tumour microenvironment, across the blood-brain barrier or immune reactions [6].

ML models have been used in toxicity prediction, where the models are trained on historical cytotoxicity data to predict negative biological outcomes due to the generation of reactive oxygen species, the formation of corona on proteins or off-target binding. It is a critical ability that can greatly decrease the chances of choosing unsafe nanoformulations at an early phase of the development.

Uncontrolled ML approaches like clustering algorithms are useful in grouping nanoparticles into functional clusters according to their similarity in physicochemical activity, which simplifies the discovery of new nanocarrier families. Reinforcement learning (RL) is also becoming a technique to optimize iteratively, in which an algorithm is used to improve the attributes of nanoparticles over time with feedback on their performance.

In general, ML-based molecular prediction saves time, cost, and experimental overhead and allows the rational and evidence-based design of the next generation nanotherapies [7]. Table 1 is a summary of the key machine learning algorithms in nanodrug discovery, showing their main uses, strengths and weaknesses in nanoparticle behaviour, toxicity and therapeutic performance prediction.

Table 1: Summary of Machine Learning Algorithms used in Nanodrug Discovery

Machine Learning Algorithm	Primary Applications in Nanodrug Discovery	Key Strengths	Limitations
Support Vector Machines	Classification of nanoparticle toxicity; prediction of cellular uptake; nanocarrier-drug compatibility	High accuracy with small datasets; effective for binary classification	Requires feature engineering; struggles with very large datasets
Random Forests	Prediction of nanoparticle biodistribution, toxicity, and stability; feature importance ranking	Handles nonlinear relationships; robust to noise; interpretable	Can overfit with small datasets; less effective for highly correlated features
Gradient Boosting/ XG Boost	Optimization of nanoformulation parameters; prediction of encapsulation efficiency and release kinetics	High predictive accuracy; manages complex interactions	Sensitive to hyperparameters; computationally intensive
Unsupervised clustering	Grouping nanoparticles by physiochemical similarity; discovery of novel nanocarrier families	No labelled data required; uncovers hidden patterns	Limited interpretality; results depend on the selection of cluster numbers
Artificial Neural Networks (ANN)	Prediction of nanoparticle-cell interactions; modelling drug release profiles; toxicity forecasting	Learns nonlinear relationships; adaptable to various datasets	Needs a large dataset and is prone to overfitting
Deep Learning (CNNs, RNNs)	Analysis of microscopy images; prediction of nanoparticle morphology, aggregation, and degradation	Automatically extracts high-level features; excellent for image and time-series data	Computationally heavy with black-box interpretability issues

3. Deep Learning for Nanoparticle Design

Deep learning (DL) expands the ability to extract complex, nonlinear features of large and heterogeneous data and to do so automatically that is inherent to conventional machine learning. In nanoparticle engineering, the structural, chemical, and biological interaction data are analysed using the DL algorithms and are modelled and optimised to model nanoparticle morphology, composition and function [8].

The use of convolutional neural networks (CNNs) is quite useful in the analysis of microscopy and imaging data that enables automatic classification of shapes of nanoparticles, determination of aggregation modes, and prediction of stability in biological conditions. The recurrent neural networks (RNN) like the long short-term memory (LSTM) networks handle sequential or time-dependent data, e.g. drug-release data or nanoparticle degradation. Transformer architectures that were initially used in natural language processing are now used to represent relationships between nanoparticle components in a self-attention model [9].

Graph neural networks (GNNs) have gained significant motivation due to the possibility of visualizing nanoparticles in the form of a graph, in which nodes are atoms or functional groups and edges are chemical bonds or interactions. GNNs are hence able to predict the effect of small structural changes on drug-loading efficiency, surface reactivity or immune recognition [10].

The variational autoencoders (VAEs) and generative adversarial networks (GANs) are generative deep learning models that can be used to design nanoparticles de novo. With these models, entirely new nanostructures with the preferred properties such as increased drug encapsulation, optimal circulation time or preferential targeting ligand distribution can be created [11].

DL speeds up the innovation process by making less use of trial-and-error experimentation and enables virtual exploration of millions of variations of nanoparticles prior to the synthesis process. This radically reduces the time of design and presents a novel avenue of customized nanoformulations.

4. AI-Based Screening of Nanocarrier–Drug Interactions

Conventional screening of drug-nanocarrier interactions is performed by labour intensive synthesis, loading and characterization experiments on a formulation-by-formulation basis. The AI makes this process revolutionized as it can be used to screen at high throughput in silico and identify the most promising drug-nanocarrier combinations without performing laboratory experiments [12].

The virtual screening models based on AI are used to screen the compatibility of the molecule, considering the molecular weight, polarity, hydrophobic/hydrophilic ratio, hydrogen bonding, nanoparticle surface chemistry, and predicted affinity. These models are used to determine how an individual drug molecule is type fitted into the internal matrix of a nanocarrier or with its surface ligands.

Multi objective optimization algorithms evaluate multiple variables at the same time such as, encapsulation efficiency, loading capacity, release kinetics, plasma stability, and biodegradation profiles. The further refinements with Bayesian optimization and Monte Carlo simulations are used to estimate the uncertainties and determine the designs that are most likely to succeed in a clinical trial [13].

Moreover, AI can be used to predetermine the impact of the physiological conditions, including pH variations in the tumour tissue, the enzymatic activity of gastrointestinal tract, or the oxidative conditions on the stability and behaviour of the nanocarrier-drug complex.

The prioritization of promising candidates allows AI to reduce the number of wet-lab experiments required, reduces the development time, and increases chances of success in the nanoformulations. This method of computing improves accuracy and lowers the time taken in early discovery to preclinical testing [14]. Table 2 outlines the role of AI-based screening approaches in evaluating drug–nanocarrier interactions, highlighting key computational models, screening parameters, predicted outcomes, and representative therapeutic examples.

Table 2: AI-Based Screening of Drug-Nanocarrier Interactions

Nanocarrier Type	AI/Computational Model used	Screening Parameters Assessed	Predicted Outcomes	Example Drug
Liposomes	Support Vector Machines, Random Forests	Lipid composition, charge, bilayer fluidity, hydrophobic–hydrophilic balance	Encapsulation efficiency, membrane stability, leakage rate	Doxorubicin
Polymeric Nanoparticles (PLGA, PEG-PLGA)	Artificial Neural Networks (ANN), Bayesian Optimization	Polymer ratio, molecular weight, degradation rate, particle size	Release kinetics, biodegradation profile, loading capacity	Paclitaxel
Dendrimers	Gradient Boosting, XG Boost	Surface charge, generation number, ligand density	Binding affinity, toxicity prediction, cellular uptake	siRNA
Nanogels / Hydrogel-based NPs	Reinforcement Learning (RL), Unsupervised Clustering	Cross-linking density, swelling ratio, polymer chemistry	Drug–matrix interaction strength, diffusion rate	Insulin
Solid Lipid Nanoparticles (SLNs)	Genetic Algorithms, ANN	Lipid melting point, surfactant type, crystal structure	Loading efficiency, long-term stability, polymorphic transition	Amphotericin B
Lipid Nanoparticles (LNPs) for mRNA	Deep Learning (CNNs, Transformer Models)	Ionizable lipid pKa, PEG-lipid %, particle size	mRNA protection efficiency, endosomal escape probability, in vivo expression	mRNA Vaccines

4.1. Intelligent Nanosystems for Targeted Drug Delivery

Smart nanocarriers are among the most revolutionary transformations in the contemporary nanomedicine. Compared to the typical nanocarriers, smart nanoparticles are not passive (they may deliver drugs by diffusion and circulation patterns) but stimuli-responsive i.e. and can release therapeutic molecules under specific biological situations. Examples of such stimuli include pH gradient (in tumour microenvironment or endosomal compartments), temperature variation, enzyme overexpression, oxidative stress, or external stimulus, such as magnetic field, ultrasound, or near-infrared (NIR) light. Intelligent nanocarriers are able to help in delivering drugs in a stable state when in circulation and release selectivity and rapidly at diseased destinations with the assistance of these cues [15]. Table 3 gives a comparative review of different smart nanocarriers, their unique modes of stimulus responsiveness, e.g. pH, temperature, enzymes and light stimulated, and their potential in targeted and controlled delivery of drugs.

Table 3: Comparison of Smart Nanocarriers and their Trigger Mechanisms

Smart Nanocarrier Type	Primary Trigger Mechanism	Common Therapeutic Cargo	Advantages	Challenges
pH-Sensitive Liposomes	Acidic microenvironment (tumour pH 6.5, endosomal pH 5.5)	Chemotherapeutics (e.g., doxorubicin)	High selectivity for tumour tissues; reduces systemic toxicity	Premature leakage; stability issues in bloodstream
Redox-Responsive Polymeric Nanoparticles	High intracellular glutathione levels (GSH)	Anticancer drugs, siRNA	Excellent intracellular release; high biocompatibility	Variable GSH levels between tissues; synthesis complexity
Enzyme-Responsive Nanoparticles	Tumour-associated proteases (MMPs), hyaluronidase, lipases	Proteins, peptides, anticancer drugs	High specificity; favourable for tumour microenvironment targeting	Enzyme overexpression varies by patient; slower release rate
Thermo-Responsive Nanogels	Local hyperthermia (40–45 °C), externally induced heat	Peptides, insulin, anticancer drugs	Non-invasive external control; reversible swelling/shrinkage	Heat penetration limits; risk of thermal damage
Magnetic-Responsive Nanocarriers	External magnetic field	Chemotherapeutics, thrombolytics	Precise spatial targeting; deep tissue penetration	Need specialized equipment; risk of overheating
Light/NIR-Responsive Nanoshells	Near-infrared (NIR) irradiation	Photothermal agents, anticancer drugs	High temporal control; minimally invasive	Limited tissue penetration; potential phototoxicity
Ultrasound-Responsive Nanobubbles/Nanodroplets	Focused ultrasound waves	Genes, siRNA, anticancer drugs	Enhanced permeability; image-guided delivery	Instability in circulation; requires ultrasound access
Glucose-Responsive Nanocarriers	Changes in blood glucose levels	Insulin, antidiabetic molecules	Ideal for closed-loop diabetes therapy	Sensitivity may vary; risk of hypoglycaemia
Logic-Gated Nanocarriers	Multiple simultaneous stimuli	Multi-drug combinations	Ultra-high precision; minimizes off-target effects	Complex fabrication; high cost; early-stage technology

One benefit of smart nanocarriers is that they reduce systemic toxicity particularly with chemotherapeutic agents that have low therapeutic indices. Indicatively, pH-sensitive liposomes do not breakdown in the blood (pH 7.4) but change structurally in the acidic tumour areas (pH 6.5) such that they release the payload. On the same note, the degradation of redox-responsive polymeric nanoparticles occurs in high-glutathione conditions, typical of cancer cells [16].

Controlled, pulsatile, or sustained drug release can also be supported using smart nanosystems, which is why they are

suitable in chronic diseases where long-term exposure to therapeutic agents is required. Scientists have come up with glucose sensitive nanocarriers that deliver insulin, thermo-responsive nanogels that utilize hyperthermia-assisted oncology therapies, and enzyme-responsive nanoparticles that take advantage of tumour-associated proteases. Upcoming platforms are the logic-gated design, in which several stimuli have to take place concurrently to increase accuracy and minimize off-target consequences [17].

4.2. AI-Guided Optimization of Nanoformulations

The optimization of nanoformulation design using artificial intelligence has been able to significantly improve the speed of specificating a system nanoformulation by combining experimental data (large parameters) with predictive computational models. The conventional formulation development is also reliant on both time and lab resources because it involves a lot of trial-and-error experimentation. AI does not have these restrictions and can be used to analyse more complicated data sets, such as those involving nanoparticle size, shape, polymer composition, zeta potential, encapsulation efficiency, and surface modifications, determining the best combinations to boost therapeutic activity [18].

Random forests, artificial neural networks, Bayesian optimization, and genetic algorithms are machine learning algorithms that allow the use of accurate prediction of formulation behaviour despite not having experimental confirmation. The models can also determine the interactions of nanoformulations with biological environments and can predict biodistribution, cytotoxicity, rate of cellular uptake, degradation, and systemic circulation time. As an example, prediction tools based on AI can be used to determine the shape of a nanoparticle (spherical, rod-like, cubic) that will give optimal tumour penetration or the type of polymer blend to achieve an improved blood-brain barrier.

An alternative significant innovation is the adoption of AI-based Design of Experiments (AI-DOE), which greatly minimizes the number of experiments to be conducted in order to find the most effective formulation conditions [19]. This technique assists researchers to quickly lock on the optimal nanoparticle structure by proposing focused combinations of experiments as compared to random searching.

Moreover, the AI models can help in estimating long-term stability of the formulation, such as the aggregation, oxidative, or storing degradation. The use of deep learning algorithms is being adopted more to mimic nano-bio interaction and understand the behaviour of nanoparticles in different physiological conditions [20].

When applied to designing rational formulations, AI-controlled optimization can facilitate the design of predictive analytics with laboratory experimentation, lowering the cost of development, and shortening the time needed to bring nanomedicines to the bedside.

4.3. Autonomous Nanorobots and Microbots

The next generation of nanorobotics in the area of precision therapeutics is autonomous nanorobots and microbots, in which control of navigation, sensing, and targeted delivery of drugs to the cell or molecular level can be exerted. The miniature systems (10-1000 nm) are designed to travel in the biological fluids, to interrelate with the tissues and to react to real-time biological cues [21].

Concept vehicles Early versions use magnetic propulsion, in which external magnetic fields are used to control the movement of nanorobots within a blood vessel or tissue matrix. The other systems are based on the chemical propulsion technique where endogenous gradients, like the concentration of hydrogen peroxide, pH difference, or glucose metabolism generating the movement, are used. Light-responsive nanobots are nanobots that use the near-infrared stimulus to produce a movement or release a drug.

The important role of AI is that it facilitates independent decision-making in these nanosystems. Nanorobots are capable of sensing disease biomarkers e.g. tumour antigens, inflammatory cytokines, or an abnormal metabolite and changing their course or dispensing cargo with the help of embedded sensors and onboard algorithms [22]. The reinforcement learning models have the potential to enable nanorobots navigate complicated biological environments, circumvent obstacles as well as optimize their routes to their target's tissues.

This could be used in high-precision cancer therapy, where nanorobots can be used to target tumour tissues with chemotherapeutic drugs; thrombus dissolution, where nanorobots can deliver clot-dissolving drugs to blocked blood vessels; and in microsurgery, where nanorobots would be used to repair tissues or pathological material with minimal invasiveness [23].

Even though the clinical nanorobotics still remain in their early development phases, the rate at which material science, micromotors, and AI-powered control systems have advanced is quickly making clinical nanorobotics viable. Autonomous nanorobots can become the future of customized and ultra-targeted medicine as the technologies become more mature.

5. AI-Integrated Nanomedicine in Clinical Pharmacology

The precision pharmacokinetic and pharmacodynamic (PK/PD) modelling based on AI has become a critical part of maximizing the clinical performance of nanoformulated therapeutics. Contrary to traditional medications, nanocarriers possess complicated biological properties that depend on aging things like surface chemical, aggregation propensities, receptive routes by cells, and opsonization by immunoproteins. AI models use these variables and patient-specific ones including hepatic and renal functionality, age, condition of disease, and comorbidities to make personalized predictions of PK/PD [24].

Preclinical and clinical study large datasets can be analysed by machine learning algorithms, specifically neural networks and support the whole ensemble learning models to predict absorption, biodistribution, metabolism, elimination, and therapeutic effect of nanomedicines. These models can detect nonlinear interactions that the conventional PK/PD equations might not capture, e.g. the effect of nanoparticle size or surface PEGylation on circulation half-life of various patient groups [25].

AI-based modelling also allows modelling dose-response curves, predicting interpatient variability, and finding the optimal dosing period. In the case of drugs exhibiting a small therapeutic index e.g. chemotherapeutics carried using nanoparticles these models minimize the chances of toxicity by more precisely predicting maximum tolerated doses.

Forming a combination of practical patient data and mechanistic insights, AI-based interventions into PK/PD modelling can offer a solid basis of personalized dosage plans

and help a physician to optimize the use of nano-based therapies to reduce the number of adverse effects and maximize their efficacy [26].

5.1. Real-Time Therapeutic Monitoring via Nanosensors

Precision medicine also requires real-time monitoring of therapeutic efficacy, which is done by nanosensors that offer a superior platform of continuous, non-invasive evaluation of drug dynamics in the body. These nanosensors can also be integrated into nanocarriers, or implanted in tissues to detect drug levels, pH, oxidative stress, enzyme activity, and inflammatory biomarkers. Their sensitivity is very high such that they are able to pick up any small biochemical variations that precede therapeutic response or toxicity [27].

AI algorithms allow decoding the enormous dynamic data of nanosensors. Fluctuations in therapeutic levels, the formation of new resistance patterns and the evaluation of local tissue reactions can be analysed with the help of machine learning models. Using sensor output together with past patient data, AI systems create real-time feedback loops, modulating drug release profiles or inducing smart nanocarrier controlled dosing.

This will facilitate adaptive therapy, in which a treatment regimen will be adjusted automatically, responding to physiological feedback, instead of being fixed to a fixed dosing schedule. By way of an illustration, glucose-sensitive nanosensors with AI algorithms can be used to control the amount of insulin released into diabetic patients and keep the glycaemic index within normal limits. On the same note, hypoxia or enzyme overexpression can be detected by tumour microenvironment-responsive sensors, which initiates the targeted release of anticancer drugs [28]. Table 4 compares the main nanosensors used to perform real-time monitoring of therapeutic applications which includes the principle of detection, analyte of interest, and the potential applications of the device in drug delivery that is personalized and adaptive.

Table 4: Nanosensors used in Real-Time Therapeutic Monitoring

Type of Nanosensor	Target Biomarker	Detection Modality	Clinical Application	AI Integration
Electrochemical Nanosensors	Glucose, lactate, electrolytes, drug levels	Current/voltage change	Diabetes monitoring, drug plasma-level estimation	AI models analyse temporal fluctuation patterns and predict dose adjustments
Fluorescent Nanosensors (quantum dots, dye-loaded nanoparticles)	pH, ROS, protease activity	Fluorescence intensity/wavelength shift	Tumour microenvironment sensing, oxidative stress monitoring	ML algorithms classify microenvironmental states and trigger smart drug-release responses
Optical Nanosensors (plasmonic gold nanoshells, photonic nanostructures)	Biomarker binding events, molecular interactions	Surface plasmon resonance (SPR), Raman scattering	Cancer biomarker detection, infection monitoring	AI-assisted signal deconvolution improves detection accuracy and reduces noise
Magnetic Nanosensors (superparamagnetic iron oxide nanoparticles)	Inflammatory markers, enzyme activity	Magnetic relaxation changes (MRI)	Monitoring inflammatory diseases and targeted therapy response	AI enhances MRI signal interpretation and biomarker prediction
FRET-Based Nanosensors	Drug concentration, enzymatic cleavage	Energy transfer efficiency changes	Real-time tracking of drug release from nanocarriers	DL models forecast release kinetics and adjust therapy adaptively
Nanosensor-Integrated Smart Wearables	Sweat biomarkers, temperature, metabolites	Electrochemical/optical hybrid signal	Chronic disease monitoring, chemotherapy toxicity tracking	AI aggregates multisensor data for continuous health status prediction
Implantable Micro–Nanosensors	Local tissue oxygenation, pH, cytokines	Wireless optical/electrical output	Post-surgical monitoring, tumour response assessment	AI enables real-time, closed-loop therapeutic modulation

5.2. Clinical Applications

Nanomedicine AI is the fast-track to the clinical practice of providing specific, effective, and personalized medicine and surgery in various domains. In oncology, nanoparticles designed using AI optimize size, charge and surface ligands to enhance tumor targeting, take advantage of EPR effect and detect cancer-specific biomarkers resulting in enhanced intratumoral drug delivery and reduced cytotoxicity. AI-controlled nanocarriers are effective in the neurobiological field in enhancing the delivery of therapeutic agents into the brain across the blood-brain barrier in the treatment of Alzheimer disease, Parkinson disease, epilepsy, and brain tumours [29].

In the case of infectious diseases, nanosystems increase antimicrobial efficacy through stability improvement, biofilms targeting, and resistance. AI-based formulation devices can find nanoparticles that can enhances uptake in intracellular pathogens and improves vaccine development as was found in lipid nanoparticles with mRNA vaccines. In addition to these fields, AI-enabled nanotechnology can be applied in precision cardiovascular therapy, immunomodulation, gene delivery, and regenerative medicine, meaning that it can be used to stratify patients, predict outcomes, and optimize the formulation design to achieve safer and more personalized therapy [30].

6. Difficulties and Moral Laws

Combining AI and nanosystems has some significant advantages to therapy, and it also presents vast challenges. Nanomedicine datasets are usually small and inconsistent scientifically which limits model reliability and reproducibility. The problem of algorithmic bias can result in unfair treatment choices in a variety of populations, whereas AI-generated nanoformulations need to be thoroughly experimentally validated to be accurate in the real world. Safety issues continue, of particular concern long-term

toxicity of nanoparticles, and erratic behaviour of autonomous nanosystems [31].

Ethically, challenges like the transparency of algorithms, the trust of the clinicians, and confidentiality of the sensitive data of the patients are still urgent. The regulators also find it difficult to assess the adaptive and learning-based AI-nanotechnology platforms, which casts doubts on the standards, liabilities, and continuous monitoring.

7. Future Directions

Intelligent, adaptive, and highly personalized systems will change the future of the AI-driven nanomedicine. The predictive nano-AI systems will combine mechanistic models and deep learning to predict the behaviour of nanoparticles, optimise designs and predict patient responses. With the growth of multimodal datasets these models will give much more accurate predictions of therapeutic results [32].

Digital twins made in real-time will also be used to revolutionize care through the simulation of drug distribution, tissue interactions, and pharmacodynamic effects based on continually updated clinical and sensor data. Combined with nanosensors feedback, they will make it possible to plan treatment proactively and optimize it in real-time.

The first important frontier is the appearance of autonomous nanosystems nanocarriers and nanorobots able to sense information and respond and control the release of drugs independently. The nanomachines of the future are also able to target diseased cells, avoid normal tissue and even carry out micro-scale procedures including plaque removal, neural repair or eliminating tumor cells [33].

Innovation will be faster with improvements in genomics, biosensing, soft robotics, and biodegradable materials, which will allow the development of mutation-specific therapies and have the highest level of diagnostic nanodevices. The governance systems will be modified to meet dynamic, learning-based nanosystems, focusing on real time monitoring, transparency and ethical governance. This will heavily depend on tight cooperation between clinical, engineering, data science and policy fields to achieve successful translation [34].

8. Conclusion

The field of nanopharmacology based on AI is revolutionizing drug discovery and drug delivery by combining the AI predictive power with the nanoscale engineering accuracy. Nanotechnology can be used to achieve targeted delivery, controlled release and reduced toxicity- major shortcomings of traditional pharmacology-AI can accelerate molecular screening and nanoparticle optimization and assist in overcoming such limitations. Such convergence underpins high personalization, adaptive, genetically informed, disease-biological, and real-time physiological-informed therapies enhanced through advances such as nanosensors, digital twins, and autonomous nanorobots.

There are still some challenges such as bias in data, regulatory loopholes, safety concerns in the long term, and transparency and privacy ethics. To deal with them, multidisciplinary collaboration will be needed. Nevertheless, the challenges do not prevent the development of AI-enhanced nanomedicine, which is the paradigm shift of the more precise, efficient, and personalized healthcare.

Author Contributions:

Bharathi Bhogenahalli Venkatappa conducted the literature review and drafted the manuscript. Muchukota Sushma provided methodological input, supervised the work, and refined the final content. Both authors reviewed and approved the final manuscript.

Fundings:

No external funding was received for conducting this study or preparing this manuscript. The research and writing activities were entirely self-supported by the authors.

Acknowledgement:

The authors sincerely thank the Department of Pharmacy Practice, Aditya Bangalore Institute of Pharmacy Education and Research (ABIPER) for providing academic support, access to scientific resources, and an encouraging research environment. The authors also acknowledge the valuable insights provided by mentors and peers during manuscript development.

Conflict of Interest:

The authors declare no conflict of interest related to the content, preparation, or publication of this manuscript.

9. References:

1. Patra JK, Das G, Fraceto LF, Campos EVR, Rodriguez-Torres MDP, Acosta-Torres LS, *et al*. Nano based drug delivery systems: recent developments and future prospects. J Nanobiotechnology. 2018;16(1):71.
2. Khemani B, Patil S, Kotecha K, Tanwar S. A review of graph neural networks: concepts, architectures, techniques, challenges, datasets, applications, and future directions. J Big Data. 2024;11(1):18.
3. Asl FD, Mousazadeh M, Taji S, Bahmani A, Khashayar P, Azimzadeh M, *et al*. Nano drug-delivery systems for management of AIDS: liposomes, dendrimers, gold and silver nanoparticles. Nanomedicine (Lond). 2023;18(3):279-302.
4. Jamalinia M, Weiskirchen R. Advances in personalized medicine: translating genomic insights into targeted therapies for cancer treatment. Ann Transl Med. 2025;13(2):18.
5. Kopac T. Leveraging artificial intelligence and machine learning for characterizing protein corona, nanobiological interactions, and advancing drug discovery. Bioengineering (Basel). 2025;12(3):312.
6. Chen Y, Chen H, Harker A, Liu Y, Huang J. A supervised machine learning tool to predict the bactericidal efficiency of nanostructured surface. J Nanobiotechnology. 2024;22(1):748.
7. Dou B, Zhu Z, Merkurjev E, Ke L, Chen L, Jiang J, *et al*. Machine learning methods for small data challenges in molecular science. Chem Rev. 2023;123(13):8736-80.
8. Sarker IH. Deep learning: a comprehensive overview on techniques, taxonomy, applications and research directions. SN Comput Sci. 2021;2(6):420.
9. Bian Q, Wang X. Machine learning-driven design of fluorescent materials: principles, methodologies, and future directions. Nanomaterials (Basel). 2025;15(19):1495.
10. Choudhary K, DeCost B, Chen C, Jain A, Tavazza F, Cohn R, *et al*. Recent advances and applications of deep learning methods in materials science. NPJ Comput

Mater. 2022;8(1):59.
11. Ghebrehiwet I, Zaki N, Damseh R, Mohamad MS. Revolutionizing personalized medicine with generative AI: a systematic review. Artif Intell Rev. 2024;57(5):128.
12. Benko A, Medina-Cruz D, Vernet-Crua A, O'Connell CP, Świętek M, Barabadi H, *et al*. Nanocarrier drug resistant tumor interactions: novel approaches to fight drug resistance in cancer. Cancer Drug Resist. 2021;4(2):264-83.
13. Greif L, Hübschle N, Kimmig A, Kreuzwieser S, Martenne A, Ovtcharova J. Structured sampling strategies in Bayesian optimization: evaluation in mathematical and real-world scenarios. J Intell Manuf. 2025:1-31. doi: 10.1007/s10845-025-02234-8.
14. Bas TG. Innovative formulation strategies for biosimilars: trends focused on buffer-free systems, safety, regulatory alignment, and intellectual property challenges. Pharmaceuticals (Basel). 2025;18(6):908.
15. Ciftci F, Özarslan AC, Kantarci IC, Yelkenci A, Tavukcuoglu O, Ghorbanpour M. Advances in drug targeting, drug delivery, and nanotechnology applications: therapeutic significance in cancer treatment. Pharmaceutics. 2025;17(1):121.
16. Brito B, Price TW, Gallo J, Bañobre-López M, Stasiuk GJ. Smart magnetic resonance imaging-based theranostics for cancer. Theranostics. 2021;11(18):8706-27.
17. Qin W, Quan G, Sun Y, Chen M, Yang P, Feng D, *et al*. Dissolving microneedles with spatiotemporally controlled pulsatile release nanosystem for synergistic chemo-photothermal therapy of melanoma. Theranostics. 2020;10(18):8179-94.
18. Takechi-Haraya Y, Ohgita T, Demizu Y, Saito H, Izutsu KI, Sakai-Kato K. Current status and challenges of analytical methods for evaluation of size and surface modification of nanoparticle-based drug formulations. AAPS PharmSciTech. 2022;23(5):150.
19. Hamdia KM, Zhuang X, Rabczuk T. An efficient optimization approach for designing machine learning models based on genetic algorithm. Neural Comput Appl. 2021;33(6):1923-33.
20. Alalmaie A, Alshahrani HT, Alqahtani M, Alshahrani Z, Alahmari S, Asiri A, *et al*. Integrating computational insights in gold nanoparticle-mediated drug delivery: enhancing efficacy and precision. Front Med Technol. 2025;7:1528826.
21. Das T, Sultana S. Multifaceted applications of micro/nanorobots in pharmaceutical drug delivery systems: a comprehensive review. Futur J Pharm Sci. 2024;10(1):2.
22. Kong X, Gao P, Wang J, Fang Y, Hwang KC. Advances of medical nanorobots for future cancer treatments. J Hematol Oncol. 2023;16(1):74.
23. Khan Z, Khan N, Geetha M, Veettil RP, Kasote DM, Hasan A, *et al*. Therapeutic applications of nanobots and nanocarriers in cancer treatment. Anal Sci. 2025:1-20. doi: 10.1007/s44211-025-00567-9.
24. Mottaghi-Dastjerdi N, Soltany-Rezaee-Rad M. Advancements and applications of artificial intelligence in pharmaceutical sciences: a comprehensive review. Iran J Pharm Res. 2024;23(1):e150510.
25. Dhaliwal A, Ma J, Zheng M, Lyu Q, Rajora MA, Ma S, *et al*. Deep learning for automatic organ and tumor segmentation in nanomedicine pharmacokinetics. Theranostics. 2024;14(3):973-89.
26. Kulesza A, Couty C, Lemarre P, Thalhauser CJ, Cao Y. Advancing cancer drug development with mechanistic mathematical modeling: bridging the gap between theory and practice. J Pharmacokinet Pharmacodyn. 2024;51(6):581-604.
27. Liu Y, Lin Z, Wang Y, Chen L, Wang Y, Luo C. Nanotechnology in inflammation: cutting-edge advances in diagnostics, therapeutics and theranostics. Theranostics. 2024;14(6):2490-516.
28. Anto M, Mukherjee K, Mukherjee K. Nano bio-robots: a new frontier in targeted therapeutic delivery. Front Robot AI. 2025;12:1639445.
29. Fahim YA, Hasani IW, Kabba S, Ragab WM. Artificial intelligence in healthcare and medicine: clinical applications, therapeutic advances, and future perspectives. Eur J Med Res. 2025;30(1):848.
30. Leong KY, Tham SK, Poh CL. Revolutionizing immunization: a comprehensive review of mRNA vaccine technology and applications. Virol J. 2025;22(1):71.
31. Młynarska E, Bojdo K, Frankenstein H, Kustosik N, Mstowska W, Przybylak A, *et al*. Nanotechnology and artificial intelligence in dyslipidemia management—cardiovascular disease: advances, challenges, and future perspectives. J Clin Med. 2025;14(3):887.
32. Hassan YM, Wanas A, Ali AA, El-Sayed WM. Integrating artificial intelligence with nanodiagnostics for early detection and precision management of neurodegenerative diseases. J Nanobiotechnology. 2025;23(1):668.
33. Wasilewski T, Kamysz W, Gębicki J. AI-assisted detection of biomarkers by sensors and biosensors for early diagnosis and monitoring. Biosensors (Basel). 2024;14(7):356.
34. Hazra RS, Hasan Khan MR, Kale N, Tanha T, Khandare J, Ganai S, *et al*. Bioinspired materials for wearable devices and point-of-care testing of cancer. ACS Biomater Sci Eng. 2022;9(5):2103-28.

How to Cite This Article
Muchukota S, Venkatappa BB, Chakrapani B, Muchukota B, Goruntla N. AI-Driven Nanopharmacology: Intelligent Nano systems Transforming Drug Discovery and Therapeutic Delivery. Int J Pharma Growth Res Rev. 2025 Nov-Dec;2(6):12-19. doi: 10.54660/IJPGRR.2025.2.6.12-19.