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International Journal of Artificial Intelligence and Machine Learning

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Artificial Intelligence in Precision Drug Delivery: From Machine Learning to Intelligent Nanomedicine

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Abstract

Artificial intelligence (AI) is rapidly transforming pharmaceutical research by enabling more precise, efficient, and patient-centered drug delivery strategies. The integration of machine learning, deep learning, and advanced computational techniques with nanotechnology has opened new opportunities for designing intelligent drug delivery systems capable of improving therapeutic outcomes while reducing adverse effects. AI-driven approaches support various stages of pharmaceutical development, including formulation optimization, prediction of drug-carrier interactions, controlled drug release, personalized dosing, and real-time therapeutic monitoring. These technologies also facilitate the development of advanced nanocarriers, targeted drug delivery platforms, and smart nanomedicine for complex diseases such as cancer and neurological disorders.

This review provides a comprehensive overview of recent advances in AI-assisted precision drug delivery, highlighting its applications in nanoparticle engineering, intelligent nanomedicine, pharmaceutical manufacturing, quality control, personalized medicine, and AI-enabled nanorobotics. The review further discusses current limitations related to data availability, algorithm transparency, regulatory considerations, ethical challenges, and clinical implementation. Finally, emerging trends such as explainable artificial intelligence (XAI), digital twins, generative AI, and autonomous nanotherapeutic systems are explored as promising directions for the next generation of precision medicine. Collectively, AI-driven technologies have the potential to reshape drug delivery by improving formulation design, enhancing therapeutic precision, accelerating pharmaceutical innovation, and supporting the transition toward personalized healthcare.

Keywords: Artificial intelligence, Machine learning, Deep learning, Precision drug delivery, Intelligent nanomedicine, Nanotechnology, Targeted drug delivery, Nanoparticles, Smart drug delivery systems, Personalized medicine, Nanorobotics, Drug formulation, pharmaceutical innovation, Precision medicine, Drug delivery systems.

1. Introduction

Artificial intelligence (AI) is a rapidly growing field that is transforming many industries, including the healthcare sector. Artificial intelligence is increasingly transforming agricultural practices by improving resource efficiency, crop management, forecasting, and decision-making. However, effective AI adoption also depends on managerial readiness, technological accessibility, organizational support, and appropriate institutional policies [1]. In recent years, Artificial intelligence (AI) has emerged as a promising technology in the field of drug delivery systems. John McCarthy coined the phrase "A.I." in 1956. AI can be used for drug discovery, drug design. The use of artificial intelligence in drug discovery is crucial [2]. In the field of drug delivery, many artificial network types, such as deep or neural networks, are used. In order to improve and provide a higher success rate for drug delivery, it is a fundamental technique to target the proteins utilised in drug delivery. The integration of AI with drug delivery systems has revolutionized the process of drug delivery systems [3]. AI-based drug delivery systems have the potential to revolutionize the pharmaceutical industry by optimizing drug delivery and reducing toxicity and has provided many benefits. AI in the field of drug delivery systems, enabling the development of more effective and precise drug delivery systems [4]

Cite This Paper: *Khandai M, Panda SK, Sahoo DK, Zankhwala FM, Raval MA, Suthar MA, Gupta MA, Khade MS. Artificial Intelligence in Precision Drug Delivery: From Machine Learning to Intelligent Nanomedicine. International Journal of Artificial Intelligence and Machine Learning. 2026 Sep 9;6(10s):56-68.* ***CORRESPONDING AUTHOR Dr. Madhusmruti Khandai**

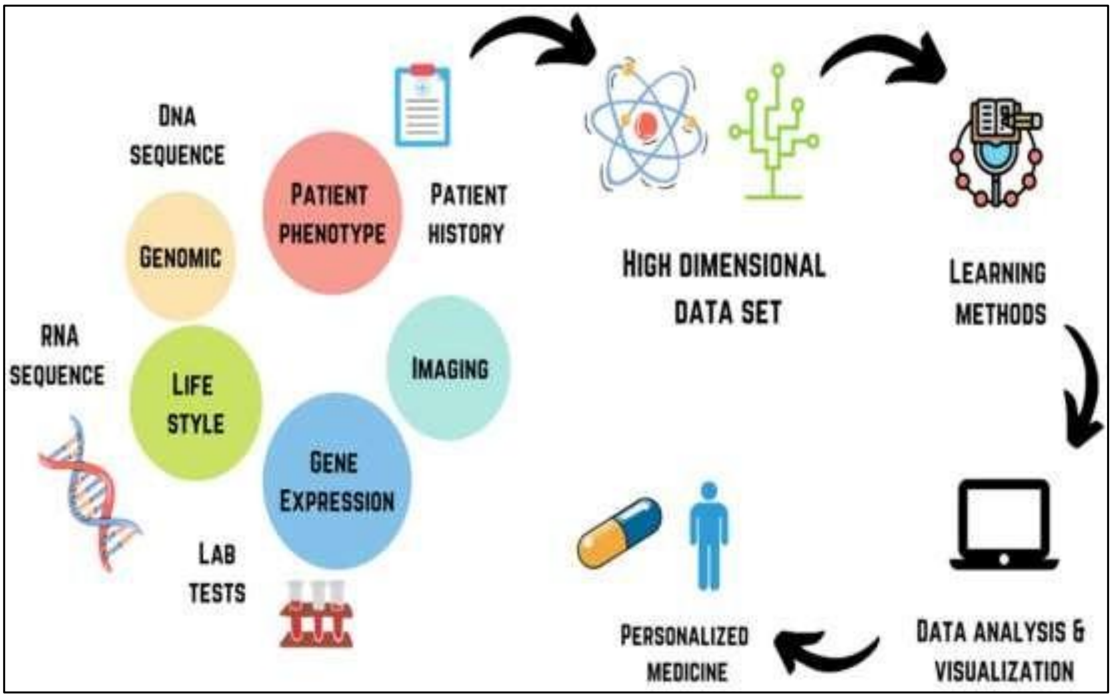

Figure 1 AI Based patient personalizing the treatment.

Drug delivery is the technique of administering the drug or pharmaceutical product, in order to obtain desired therapeutic impact. The technique with the aid of using which drug introduced is important, because it has tremendous impact on its efficacy [5]. Some drugs have an optimum concentration range within which maximum benefit is derived, and concentrations above or below this range can be toxic or produce no therapeutic benefit at all. On the other hand, the very slow progress in the efficacy of the treatment of severe diseases, has suggested a growing need for a multidisciplinary approach to the delivery of therapeutics to targets in tissues. From this, new ideas on controlling the pharmacokinetics, pharmacodynamics, non-specific toxicity, immunogenicity, biorecognition, and efficacy of drugs were generated [6]. These new strategies, often called drug delivery systems (DDS), are based on interdisciplinary approaches that combine polymer science, pharmaceutics, bio-conjugate chemistry, and molecular biology. Dramatic changes have in introduced, with new technology and new devices now on market. In some cases, traditional capsules and ointments have been replaced by osmotic pumps, wearable ambulatory pumps, electrically assisted drug delivery and host of other delivery methods based on various polymer technologies. In some cases, the new drugs require new delivery systems because the traditional systems are inefficient and ineffective [7].

Some therapies may become very site specific and require very high concentrations of drugs in selected sites of body, as more controlled drug delivery systems will be available very near future. New drug delivery system development is largely based on promoting the therapeutic effects of a drug and minimizing its toxic effects by increasing the amount and persistence of a drug in the vicinity of target cell and reducing the drug exposure of non-target cells. Novel drug delivery systems can include those based on physical mechanisms and those based on biochemical mechanisms [8].

Physical mechanisms also referred as controlled drug delivery systems include osmosis, diffusion, erosion, dissolution and electro transport. Biochemical mechanisms include monoclonal antibodies, gene therapy, and vector systems, polymer drug addicts and liposomes. Therapeutic benefits of some new drug delivery systems include optimization of duration of action of drug, decreasing dosage frequency, controlling the site of release and maintaining constant drug levels [9].

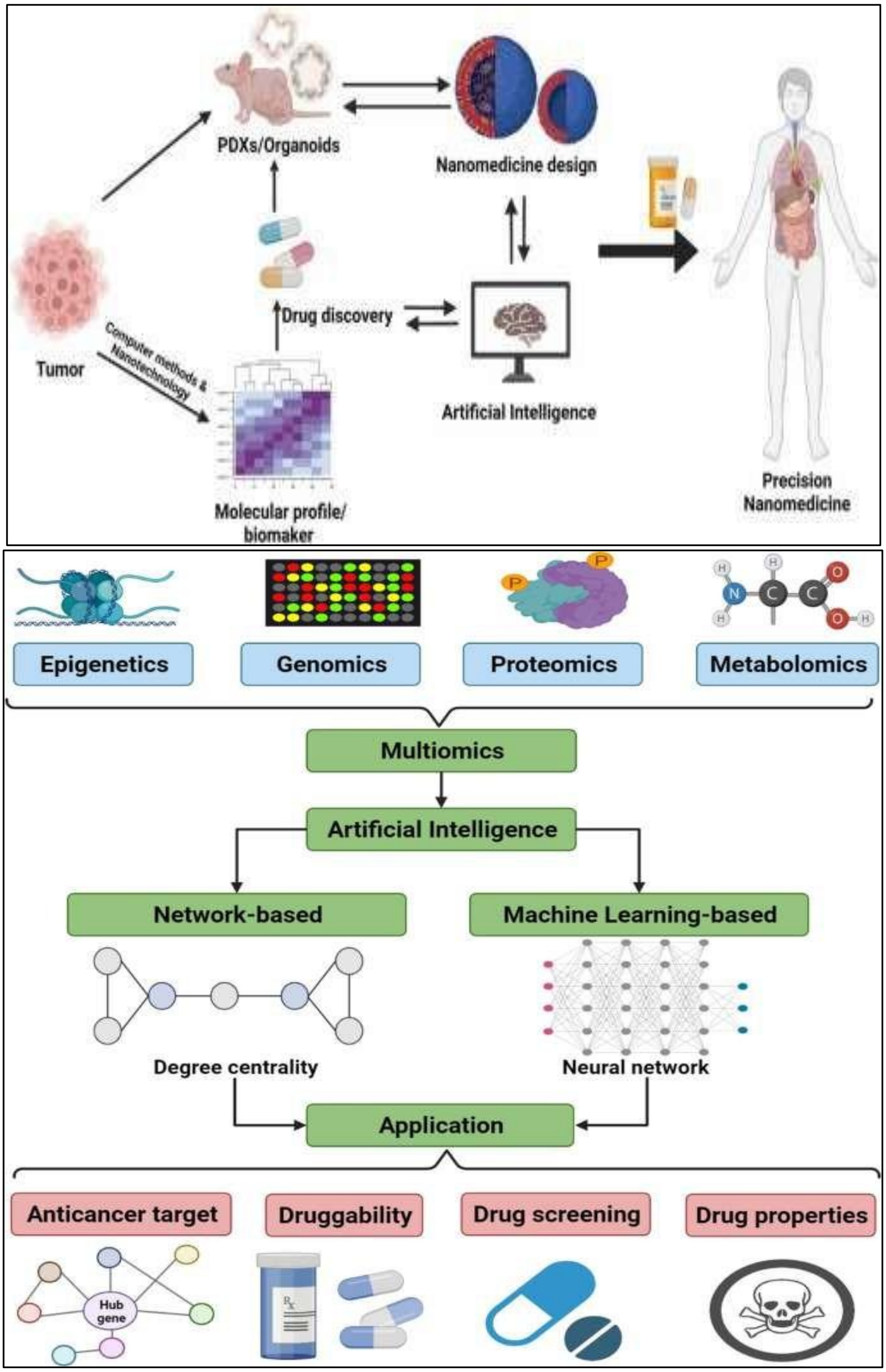

Figure 2 AI in cancer therapy

1.1 Drug Delivery System may be defined as a system comprising of

- Drug formulation
- Medical device or dosage form/technology to carry the drug inside the body
- Mechanism for the release

Conventional drug delivery involves the formulation of the drug into a suitable form, such as a compressed tablet for oral administration or a solution for intravenous administration. These dosage forms have been found to have serious limitations in terms of higher dosage required, lower effectiveness, toxicity and adverse side effects. New drug delivery systems have been developed or are being developed to overcome the limitation of the conventional drug delivery systems to meet the need of the healthcare profession [10].

1.2 Artificial intelligence in drug delivery systems:

AI can be used to optimize drug delivery systems in several ways such as predicting drug behaviour in the body, predicting drug interactions, and optimizing drug formulations. Machine learning algorithms can be used to analyse large datasets of drug behaviour in the body and predict drug response. This can be useful in designing drug delivery systems that are optimized for specific patient populations. One example of AI-assisted drug delivery systems is the use of machine learning algorithms to optimize drug formulations. Machine learning algorithms can be trained on large datasets of drug behaviour in the body to predict the optimal formulation for a specific drug. This can reduce the time and cost associated with formulation development and can lead to better drug efficacy [11].

AI-assisted drug delivery system is the use of neural networks to predict drug interactions. Neural networks can be trained on large datasets of drug interactions to predict potential interactions between different drugs. This can be useful in designing drug delivery systems that minimize drug interactions and reduce side effects. Artificial Intelligence in Drug Delivery Systems various drug delivery systems such as nanoparticles, liposomes, microspheres, dendrimers, and hydrogels. AI has played a significant role in the optimization of drug delivery systems by designing new drug carriers, predicting drug release profiles, and optimizing drug dosages [12].

Nanoparticles

Nanotechnology is science of matter and material that deal with the particle size in nanometres. The word “Nano” is derived from Latin word, which means dwarf (1nm $=10^{-9}$m). Nanoparticles are defined as particulate dispersions or solid particles with a size in the range of 10- 1000nm. The drug is dissolved, entrapped, encapsulated or attached to a nanoparticle matrix [13]. Nanoparticles offer some specific advantages such as they help to increase the stability of drugs/proteins and possess useful controlled release properties. It can be modified to achieve both active and passive targeting, drug loading is very high and can be administered by various routes such as parenteral, nasal, intra ocular and oral routes [14]. AI has been used to design and optimize nanoparticle drug delivery systems. For instance, machine learning algorithms have been used to predict the behaviour of nanoparticles in biological systems, enabling the optimization of drug release profiles and targeting of specific tissues. Additionally, AI algorithms have been used to design new drug carriers that can improve drug delivery efficacy and reduce toxicity [15].

1.3 Current state of AI in drug delivery systems:

AI has the potential to transform drug delivery systems in several ways. For example, AI can be used to identify novel drug targets, optimize drug formulations, and predict drug efficacy and toxicity. One promising application of AI in drug delivery systems is the development of personalized medicine. By analysing patient data, including genetic and demographic information, AI algorithms can predict how an individual patient will respond to a particular drug, enabling the development of personalized therapies. Here are some key ways in which AI can be used in novel drug delivery system [16]

A. Prediction of drug release:[1]

AI can be used to predict drug release rates from various drug delivery systems, such as microspheres, nanoparticles, and liposomes. This information can be used to optimize drug dosages and to ensure that drugs are released at the appropriate times [17].

B. Formulation Design:

AI can be used to optimize the formulation of drug delivery systems, such as liposomes and nanoparticles, to enhance drug efficacy and reduce toxicity. AI algorithms can analyse data on the physicochemical properties of drugs and the characteristics of delivery systems to design optimized formulations. For instance, deep learning algorithms can be used to predict the properties of different formulations and identify the optimal conditions for drug loading and release [18].

C. Personalized Drug Delivery:

AI can be used to develop personalized drug delivery systems that are tailored to individual patients. AI algorithms can analyse patient data, such as genetic information, medical history, and lifestyle factors, to design personalized drug formulations and dosing regimens. For example, AI-based drug delivery systems have been developed for diabetes management that use continuous glucose monitoring and predictive algorithms to adjust insulin dosing in real-time [19].

D. Quality Control:

AI can be used to monitor the quality and consistency of drug delivery systems during production. AI algorithms can analyse data on manufacturing parameters, such as temperature, pressure, and flow rates, to detect and prevent quality defects. For instance, deep learning algorithms have been used to detect defects in pharmaceutical tablets by analysing images of the tablets during production [20].

Recent trends in artificial intelligence in novel drug delivery systems [2]

Artificial intelligence (AI) has the potential to revolutionize the field of drug delivery by optimizing drug design, improving drug targeting, and enhancing drug release. Here are some recent trends in AI-driven drug delivery systems:

A. Machine learning for drug discovery:

Machine learning algorithms are being used to analyse large datasets and identify potential drug targets, predict drug efficacy, and optimize drug properties. AI-powered drug discovery platforms can screen millions of compounds, drastically reducing the time and cost of drug development [21].

B. Nanoparticle-based drug delivery systems:

Nanoparticles can be engineered to deliver drugs to specific cells or tissues in the body. AI is being used to optimize the design of these nanoparticles to improve drug efficacy and reduce toxicity [22].

C. Predictive models for drug release:

AI models can predict how drugs will behave in the body and design drug delivery systems that release the drug in a controlled manner. This can help to ensure that drugs are released at the right time and in the right place in the body, improving therapeutic outcomes and reducing side effects [23].

D. Smart drug delivery systems:

AI-powered sensors can be used to monitor drug release in real-time, allowing doctorsm to adjust drug dosages and optimize treatment plans for individual patients [24].

E. Personalized medicine:

AI can be used to analyse patient data and design personalized drug delivery systems that are tailored to each individual's unique physiology and medical history. This can improve treatment outcomes and reduce the risk of adverse reactions [25].

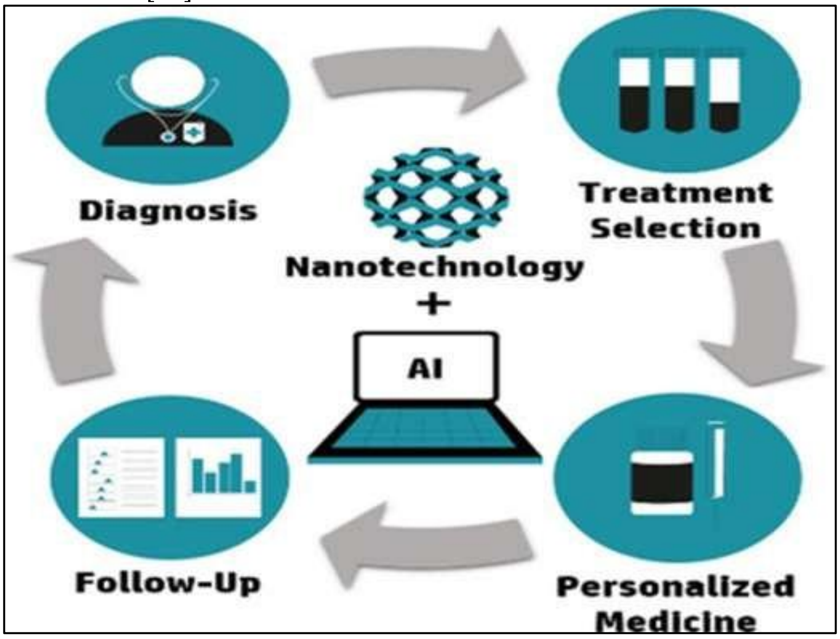

Figure 3 AI with Nanotechnology

Table 1. Applications of Artificial Intelligence in Precision Drug Delivery Systems [26-31]

Application Area	Role of Artificial Intelligence	Key Benefits	Representative References
Drug Discovery	AI and machine learning identify potential drug candidates, predict biological activity, and optimize lead compounds using large-scale datasets.	Reduced development time, lower cost, improved prediction accuracy	Kalyane et al., 2020, Lamberti, 2019, Gorska et al., 2020
Formulation Development	AI predicts optimal formulation composition and processing parameters using physicochemical and biological data.	Faster formulation optimization, reduced experimental workload	Joshi et al., 2022, Sharma et al., 2023

Nanoparticle Design	Machine learning models optimize nanoparticle size, surface characteristics, stability, drug loading, and targeting efficiency.	Enhanced bioavailability and targeted delivery	Sun et al., 2019, Das, 2023
Targeted Drug Delivery	AI predicts tissue-specific drug distribution and carrier interactions to improve site-specific delivery.	Reduced systemic toxicity and increased therapeutic efficacy	Li et al., 2023, Das, 2023
Controlled Drug Release	AI algorithms model drug-release kinetics and optimize sustained and stimuli-responsive release systems.	Improved therapeutic control and patient compliance	Joshi et al., 2022, Hu et al., 2021
Personalized Medicine	AI integrates genomic, clinical, and demographic information to personalize treatment and dosage regimens.	Precision therapy and improved clinical outcomes	Lamberti, 2019, Li et al., 2023
Cancer Nanomedicine	AI assists in biomarker discovery, nanoparticle optimization, and precision oncology applications.	Improved tumor targeting and treatment effectiveness	Li et al., 2023, Sun et al., 2019
AI-Enabled Nanorobotics	AI guides intelligent nanorobots for targeted drug delivery, minimally invasive surgery, and tissue repair.	High therapeutic precision and reduced collateral damage	Singh et al., 2021, Egorov et al., 2021
Pharmaceutical Manufacturing	AI supports process optimization, quality control, defect detection, and predictive maintenance.	Improved manufacturing efficiency and product quality	Sharma et al., 2023, Kalyane et al., 2020
Future Precision Medicine	AI integrates multimodal clinical data to support intelligent diagnostics, digital therapeutics, and autonomous drug delivery.	Personalized healthcare and improved decision-making	Gessner et al., 2020, Li et al., 2023

Artificial Intelligence in Nanomedicine

Nanomedicine, a rapidly growing field that combines physical, chemical, biological, and digital aspects, has made significant progress over the past three decades. It influences various medical fields and is a dynamic tool for developing therapeutics, medical imaging, nanotherapeutics, vaccines, and biomaterials [32]. The integration of AI and nanotechnology in nanomedicine has the potential to revolutionize various aspects of medicine, including drug delivery, imaging, and implants. To improve the design of nanotechnologies, AI algorithms can process vast datasets and recognize complicated patterns. Some of the drawbacks of fabrication and targeted drug delivery for cancer therapy can be solved with the use of AI [33]. Nanomedicine has been made a reality through the use of data science, high throughput, automatization, and AI. By accomplishing acquisition, the use of AI in the creation of nanotechnology-based goods may revolutionize the healthcare industry. The use of AI to nanotechnology has been started and is continually proving to be a successful and simple method. Since AI swiftly mines data and makes judgments, combining nanotechnology and AI results in more inventive technologies [34]. A scientific and technological revolution is being sparked by the convergence of biology, AI, and nanotechnology, even though the anticipated integration has not yet occurred. The discipline of nanomedicine has undergone a revolution as a result of the merging of AI with nanotechnology. Nanotechnologies for diagnosis and therapy can be designed and optimized with the help of AI. To maximize the therapeutic efficacy of materials, AI can also be used to predict interactions with the target drug, biological fluids, immune system, vasculature, and cell membranes [35]. Some of the obstacles to targeted medication delivery and manufacture for cancer therapy can be overcome with the aid of artificial intelligence (AI) in nanomedicine. In order to forecast how cells would behave under various conditions, AI systems can find patterns and relationships in cellular activity and interactions. More cuttingedge technologies may result from the combination of AI and nanotechnology. AI and other computational techniques are used in nano informatics for designing and implementing nanomaterials. Large-scale biomedical data can be analysed using AI algorithms to find current medications with potential therapeutic value for various diseases. AI can shorten the time and expense required for medical development by reusing already approved medications. The aim is to integrate artificial intelligence (AI) in nanomedicine to enhance various aspects of nanomedicine by leveraging the power of AI algorithms and techniques. This study tends to explore possible role of AI integration in precision cancer medicine, targeted drug delivery, data science, high throughput, and automatization in Nanomedicine. Based on this study, the following were discussed, Integration of AI in Nanomedicine, AI-based Diagnosis and Drug Discovery in Nanomedicine, AI-assisted Nanoparticle Synthesis and Drug Delivery, AI powered Imaging and Diagnostics in Nanomedicine, Integration of AI and Nanorobotics for Therapeutic Applications, Ethical and Safety Considerations in AI-Enabled Nanomedicine, and Future Directions and Implications in AI-based Nanomedicine Research [36-41].

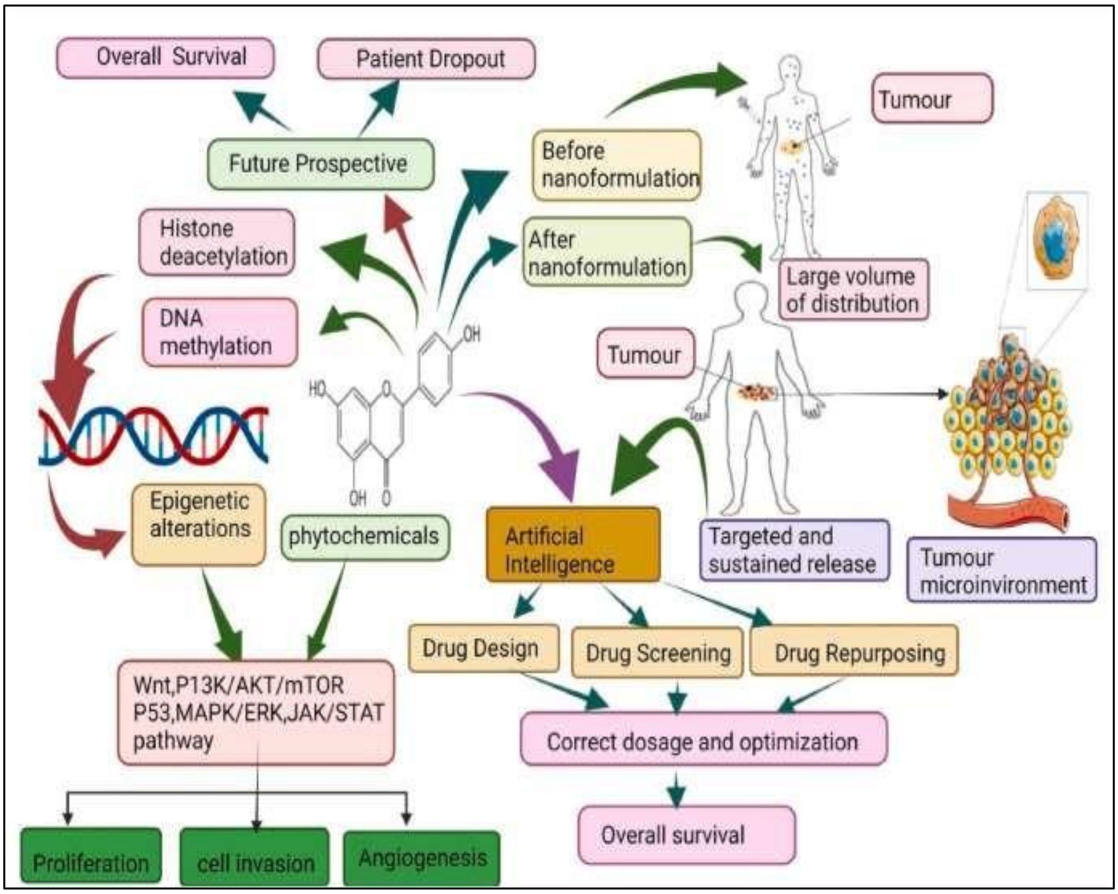

Figure 4 Integration of AI and nanotechnology in nanomedicine

Integration of AI and Nanorobotics for Therapeutic Applications

Incorporating AI (Artificial Intelligence) and nanorobotics for therapeutic purposes is an intriguing and incredibly hopeful junction of two cutting-edge technological fields. By enabling focused, minimally invasive, and accurate therapies, this synergy has the potential to change medicine. AI includes several different types of technology, such as deep learning, machine learning, and natural language processing. Massive amounts of data may be processed and analysed by AI systems, which can also spot patterns and base predictions or choices on them. Small machines or gadgets with dimensions at the nanoscale (usually below 100 manometers) are known as nanorobots[3]. These nanoscale robots can be created for a number of purposes, including the delivery of drugs, surgery, and tissue healing [41-46]. The integration of AI with nanorobotics has a great deal of potential for medical applications. Collectively, these two disciplines can offer therapies that are accurate, individualized, and minimally intrusive, vastly increasing patient outcomes [47]. Realizing this promise will require addressing the accompanying difficulties, such as safety, control, and ethical issues. Exciting developments in healthcare are predicted to result through continuing research and development in the fields of artificial intelligence (AI) and nanorobotics [48].

Therapeutic applications, especially in targeted medication administration and precision medicine, have the potential to be revolutionized by the merging of AI with nanorobotics. Even though there are obstacles to be solved, current innovations in engineering and bio-nanotechnology offer encouraging progress in incorporating intelligent sensors, power, and AI in nanorobots [49]. The integration provides unmatched diagnostic and therapeutic precision while limiting harm to healthy tissue. Nanorobots can provide these customized remedies after AI analyses a patient's genetic and health data. Nanorobots can complete tasks without the need for large incisions, minimizing patient suffering and speeding up healing [50-51].

Therapeutic Applications of AI-Nanorobotics include [52-56]

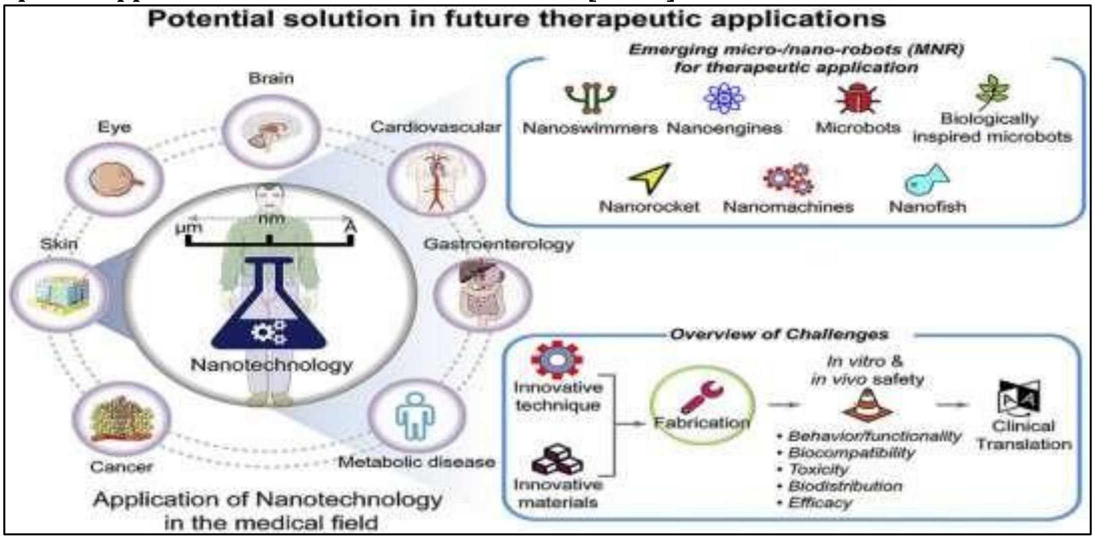

Figure 5 FUTURE THERAPEUTICS APPLICATION

1. Drug Delivery: Drugs can be transported and delivered by nanorobots to specific parts of the body. They can be guided to the desired location by AI, resulting in precise and effective drug delivery [57].
2. Cancer Therapy: By fusing AI and nanorobots, highly focused cancer therapies are possible. While nanorobots directly deliver therapeutic payloads to cancer cells, AI can analyse imaging data to identify cancer cells [58-59].
3. Surgery: Minimally invasive surgeries can be carried out by nanorobots, and AI can help in planning and directing these procedures to increase precision.
4. Tissue Repair: Nanorobots can assist in repairing damaged tissues at the cellular level, and AI can monitor the healing process [60].
5. Diagnostic and Imaging: Nanorobots can be used to carry out on-site diagnostic testing or supply contrast chemicals for medical imaging, and AI can evaluate medical images to find irregularities [61].
6.

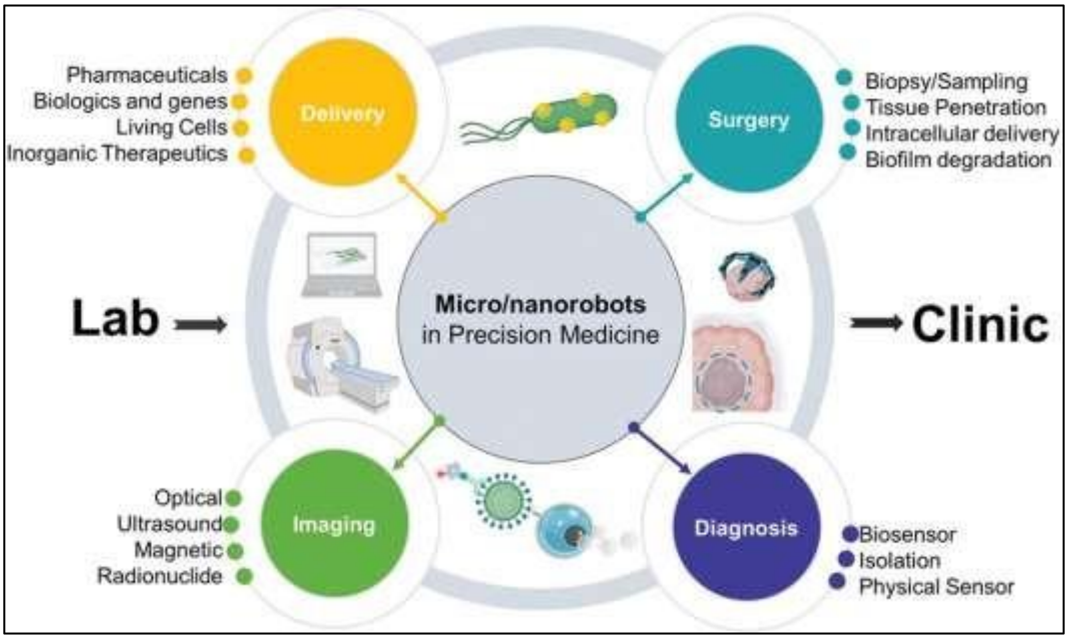

Figure 6 Schematic of the current trends of micro/nanorobotics in precision medicine, including delivery, surgery, diagnosis, and medical imaging applications.

CONCLUSION

The field of nanomedicine is rapidly evolving, and versatile drug carriers are being evaluated for their effectiveness in reaching the targeted tumour sites and improving localized drug delivery. Furthermore, combining nano therapies with hybrid approaches is continuously evaluated to enhance treatment efficacy for cancer patients. However, these approaches are confronted by various challenges of conventional drug development and delivery methods. While it is essential to understand drug synergies, identifying individual patient profiles based on their unique molecular signatures has become critical in ensuring the ultimate success of targeted drug delivery. These are necessities because the rate of treatment failures and lack of response to treatments continue to remain high. At the same time, to improve cancer treatments, more clinical parameters are required to minimize treatment failures and chances of cancer recurrence. In this context, intelligent computational models can process complex data and produce accurate results successfully. Therefore, AI plays a crucial role in devising a roadmap to assess real-time monitoring of drug delivery procedures, classifying patients according to molecular signatures, and also provide actionable insights on treatment response, ability to quantify clinical information. Although several techniques have been evaluated in pharmaceutical and nanotechnology domains over the years, the studies focusing on AI for targeted drug delivery have remained limited. Therefore, this study aimed to provide a pathway on how the integration of AI can help overcome some of the limitations of fabrication techniques and the likely impact on nanoparticle imaging, patient profiling, and cancer biomarker detection to help enhance the outcomes of nanotechnology-based therapeutics. Future works may lead to building intelligent solutions for biomarker detection and nanoparticle tracking and analysis systems by taking critical insights from the survey.

Abbreviations

AI - Artificial Intelligence
ANN - Artificial Neural Network
API - Active Pharmaceutical Ingredient
AUC - Area Under the Curve
CNN - Convolutional Neural Network
DDS - Drug Delivery System
DL - Deep Learning
FDA - Food and Drug Administration
GAN - Generative Adversarial Network
ML - Machine Learning
NLP - Natural Language Processing
NP - Nanoparticle
PEG - Polyethylene Glycol
PK - Pharmacokinetics
PD - Pharmacodynamics
QbD - Quality by Design
RNA - Ribonucleic Acid
SVM - Support Vector Machine
XAI - Explainable Artificial Intelligence

Future Perspectives

Artificial intelligence is expected to transform precision drug delivery by enabling the design of intelligent nanomedicines capable of real-time adaptation, personalized therapeutic optimization, and predictive clinical decision-making. The integration of machine learning, digital twins, wearable biosensors, and Internet of Medical Things (IoMT) platforms will facilitate continuous patient monitoring and dynamic dose adjustment. Future developments are anticipated to focus on explainable AI, federated learning, multimodal data integration, and regulatory-compliant AI frameworks to improve transparency, reproducibility, and clinical acceptance. Moreover, AI-assisted autonomous formulation development, smart stimuli-responsive nanocarriers, and closed-loop drug delivery systems are likely to redefine precision therapeutics. Continued interdisciplinary collaboration among pharmaceutical scientists, clinicians, engineers, regulatory agencies, and data scientists will be essential for translating these innovations into safe, effective, and globally accessible healthcare solutions.

Acknowledgements

The authors sincerely acknowledge their respective institutions for providing academic support, research facilities, and encouragement during the preparation of this review article. The authors also appreciate the valuable contributions of researchers worldwide whose published work has significantly advanced the fields of artificial intelligence, machine learning, and precision drug delivery.

Funding

The authors declare that no specific funding was received from any public, commercial, or not-for-profit funding agency for the preparation of this review article.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this manuscript.

Author Contributions

Dr. Madhusmruti Khandai: Conceptualization, Supervision, Writing - Original Draft, Review & Editing.
Dr. Susanta Kumar Panda: Literature Review, Writing - Original Draft, Data Curation.
Dr. Dillip Kumar Sahoo: Validation, Scientific Review, Writing - Review & Editing.
Fayeja M. Zankhwala: Literature Search, Data Collection, Visualization.
Mr. Amar M. Raval: Writing - Original Draft, Figure Development, Critical Review, Reference Management.
Ms. Astha Suthar: Literature Review, Manuscript Editing, Formatting.
Mr. Ayush Gupta: Data Interpretation, Technical Validation, Proofreading.
Ms. Shubhada Milind Khade: Literature Review, Visualization, Final Manuscript Review.
All authors have read and approved the final version of the manuscript.

Data Availability Statement

No new datasets were generated or analyzed during the preparation of this review article. All information presented is derived from previously published literature cited in the reference section.

Ethical Approval

This article is a review of previously published studies and does not involve human participants, animals, or identifiable personal data. Therefore, ethical approval was not required.

Informed Consent

Not applicable.

Declaration of Generative AI and AI-Assisted Technologies

The authors declare that artificial intelligence-assisted tools were used solely to improve language, grammar, formatting, and readability during manuscript preparation. All scientific interpretation, critical analysis, literature evaluation, and final manuscript content remain the sole responsibility of the authors.

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