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Review Paper

Artificial Intelligence in Nanomedicine: Current Advances and Future Perspectives

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ABSTRACT

Nanoscale materials are used in nanomedicine to diagnose, treat and deliver medications for cancer, neurological diseases, and heart disease. Using artificial intelligence (AI) (such as machine learning and deep learning), nanomedicine can use AI to better design nanoparticles, predict how they will be distributed in the body, improve how sick patients can be diagnosed, and allow doctors to provide personalised treatment. Examples of AI advances include the use of computer screens to identify nanomaterials, the use of AI to identify and monitor patients at an early stage of neurological disease and the development of precision nanomedicine for cancer that uses molecular profiling and a reduction in toxicity. In addition, the integration of different types of biological information (also known as multi-omics data) with nanosensors is facilitated by AI, which supports the identification of disease-specific biomarkers and advances personalised medicine in many diseases and conditions. Although these advances are promising, many challenges remain, including data standardisation, model transparency, regulatory frameworks, and the ability to scale for use in clinical trials. Future development of nanomedicine will focus on interdisciplinary collaboration, consideration of ethical issues and development of a platform-agnostic AI tool to help accelerate the development of safe and effective nanomedicines through multiple disease processes..

INTRODUCTION

Complex diseases such as cancer, Alzheimer's, and cardiovascular disease are arising worldwide in such large numbers that standard diagnostics and therapies cannot address them. Integration of artificial intelligence (AI) into nanomedicine has the potential to provide new ways to discover and

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design novel nanomaterials for maximum efficacy, safety, and personalization using large datasets that include patient clinical and genetic data.[1] These datasets can also be used to identify and evaluate optimal drug delivery and dosing methods. Integrating AI with nanotechnology in the field of medicine supports precision medicine by utilizing AI-based methods to analyze the biological complexity and heterogeneity of patients through pattern analysis, predictive modeling, and optimizing nanocarrier properties for targeted therapy. Through the applications of nanotechnology, patients with neurodegenerative disease can experience advantages from early detection and targeted intervention with the assistance of AI as it increases the sensitivity of biomarkers and the stratification of patients. Data standardization, ethical and regulatory issues, and clinical translation remain challenges; however, interdisciplinary collaboration will help to mitigate these roadblocks.[2] Consequently, AI-based platforms for nanomedicine have the potential to deliver more precise, personalized, and adaptive treatments that will improve the overall outcomes of patients who experience a wide range of complex diseases.[3] The application of nanomedicine is the utilization of drug delivery systems and diagnostic tools that are designed and produced off-the-shelf using materials developed at the nanoscale (such as liposomes, polymeric nanoparticles, metallic nanoparticles, and dendrimers) to enhance both drug delivery and disease diagnosis. Artificial intelligence (AI) is defined here using computational techniques (e.g., machine learning, deep learning, reinforcement learning, and predictive modelling) applied to bioinformatics to advance nanomedicine development and provide better patient care. AI provides an opportunity to analyze large amounts of data to optimize nanoparticles for design and predict biological interactions when combining clinical and genetic data to personalize treatment [4]. The synergy of these 2 disciplines creates a pathway for delivery of precision medicine through improved diagnosis, targeted drugs, optimized dosing, and ongoing outcome monitoring of therapy . [5]While there has been progress over the last decade, challenges remain regarding the standardization of data, ethical issues associated with the use of AI, and the development of an appropriate regulatory framework for the implementation of AI-based nanomedicine . Overall, AI will serve as an important resource in aiding the rational design and clinical translation of nanomedicines that demonstrate increased efficiency and safety profiles. The emergence of numerous complex/chronic illnesses, including cancer, cardiovascular diseases, and neurodegenerative disorders, has exposed the disadvantages of traditional therapies and diagnostic methods.[6] In addition, there are many drug development problems that arise from poor solubility, low bioavailability, and improper targeting of APIs. APIs that fall under BCS Classes II and IV also have these issues. Therefore, new advanced delivery systems are needed to increase therapeutic effects while reducing systemic toxicity.[7]Nanomedicine is gaining popularity as an alternative to this issue by using engineered nanoscale materials to deliver drugs and to help diagnose diseases.[8] The field has rapidly evolved in the last several decades, evolving from early developments with conventional nanocarrier systems such as liposomes and polymeric nanoparticles, to more advanced systems such as dendrimers, metallic nanoparticles, and responsive ‘smart’ nanocarrier systems. The clinical approval of liposomal formulations (Doxil®) and other therapeutic agents using nanotechnology for drug delivery has resulted in improved pharmacokinetics, decreased toxicity, and enhanced targeting ability.[9]

Objectives and scope of the review

1. To study the role of AI in nanocarrier design.
2. To optimize nanoparticle formulations using machine learning.
3. To predict drug loading and release kinetics using AI.
4. To analyze AI-based prediction of biodistribution.
5. To evaluate AI in medical imaging (MRI, PET).
6. To improve tumor detection and disease diagnosis using AI.
7. To develop AI-driven targeted drug delivery systems.
8. To explore stimuli-responsive nanocarriers for theranostics.
9. To identify challenges in clinical translation and regulation.
10. To assess future trends in AI-based personalized nanomedicine**.** [10,11]

Theoretical and methodological background

Nanomedicine utilizes various machine learning and artificial intelligence techniques including supervised learning, which can perform a range of tasks related to predicting toxicity for nanoparticles, determining how well a nanoparticle will target tissues or specific cells, and forecasting how well a specific nanoparticle treatment will work for individual patients. CNNs, RNNs and transformers are also commonly used for medical image evaluation including MRI, histology, and microscopy.[12] Unsupervised learning methods can help identify previously unknown relationships in complex datasets, whereas reinforcement learning can be used to develop adaptive dosing regimens and identify new nanoparticle materials by optimizing the decisions made over time.[13]The AI models that use nanomedicine integrate multiple datasets, including multi-omics data including genomics, transcriptomics, proteomics; electronic health record (EHR) data; imaging data; and high-throughput experiments of nanoparticle libraries to create a complete picture of the biological and clinical information available for developing a given nanomedicine.[14] The AI-nanomedicine workflow typically consists of many steps, including collecting data, developing features and models, conducting in silico analyses, performing in vitro and/or animal studies, and ultimately obtaining regulatory approval prior to clinical use. While there has been significant progress in these areas, ongoing hurdles such as standardizing data for review, making models interpretable, and ensuring that models are acceptable to regulators will need to be addressed before AI will be fully utilized for developing nanomedicines.[15]

Methodology

Literature was collected from PubMed, Scopus, and Google Scholar using keywords such as AI, nanomedicine, and drug delivery. Recent articles (last 10 years) were included.

AI Techniques in Nanomedicine[16]

AI Technique	Application	Example
Machine Learning	Toxicity prediction	QSAR models
Deep Learning (CNN)	Medical imaging	Tumor detection
Reinforcement Learning	Dose optimization	Adaptive therapy
NLP	Literature mining	Drug discovery
Generative Models	Nanoparticle design	Novel nanostructures

AI-guided design and optimization of nanomedicines

Nanomedicines can be customized and optimized using AI and machine learning to identify important characteristics like size, ζ potential, PEGylation and drug loading that are significant contributors to their therapeutic outcome in vivo.[17] Generative models and inverse design techniques allow for the generation of novel nanoparticle structures at scale through exploration of enormous physical chemical spaces compared to classical methods of trial-and-error.[18]The use of Bayesian optimization and surrogate modelling has permitted the optimization of synthesis parameters (e.g., solvent type, temperature, and amount of reactant) such that there is a major reduction in experimental trials at scale as compared to the use of classical methods .[19] The use of QSAR-type ML models has allowed for the prediction of toxicity and biocompatibility-related effects through use of ensemble learning-based predictions of potential for cytotoxicity, hemolysis, immunogenicity, and multi-endpoint toxicity risk during the early stages of development to improve safety profiling along the development life cycle of nanomedicines .[20] AI also aids in modelling of complex nano-bio interactions (e.g., protein corona formation) which impacts the immunogenicity and cellular uptake of nanoparticles, ultimately refining design for clinical translation . To date, there are still challenges associated with the implementation of AI in nanomedicine for personalized and precision therapeutics including heterogeneity of data, model interpretability, limitations with regulatory frameworks, and ethical issues associated with the use of AI in implementing personalized and precision medicine in combination with nanomedicine**.**[21]

AI-driven diagnostics and imaging in nanomedicine

Deep learning is being utilized to create AI-based diagnostics for nanomedicine to segment and quantify nanoparticles within imaging modalities, including MRI, CT, PET, and fluorescence, providing information that can define the biodistribution, accumulation of tumors, and elimination pathways. Nanoparticle-mediated imaging and AI provide a unique capability of early detection through the use of contrast-enhancing nanoprobes and advanced pattern recognition within multimodal imaging to detect subtle pathological changes, with applications to brain disease, cancer, and cardiovascular disease. Liquid biopsy methods using nanoparticles or nanosensors combined with machine learning provide multiple opportunities for the early detection of disease through the analysis of blood- or cerebrospinal fluid-based biomarkers, thus enhancing diagnostic sensitivity/specificity for neurodegenerative disease and cancer.[22] AI is also enhancing the development of intelligent nanocarriers that can respond to cues from the tumor microenvironment to provide targeted drug delivery and improve diagnostic accuracy through imaging-guided theranostics. Despite these advancements, challenges related to data heterogeneity, model interpretability, nanoparticle manufacturing scalability, and regulatory impediments pose substantial obstacles to the clinical translation of these technologies. The continuing integration of nanomedicine with AI may provide a means of personalized, adaptive diagnostic and therapeutic approaches that could significantly improve the management of complex diseases, such as brain tumors and neurodegenerative diseases.[23]

AI-enabled targeted therapy and nanotherapeutics

The use of AI-driven targeted therapies and nanotherapeutics to develop personalized, patient-centred therapies utilizing ML will predict individual patients' pharmacokinetics/pharmacodynamics (PK/PD) and tumor microenvironment characteristics for optimal individualised drug delivery, dosing schedules, and NP release kinetics. Also, AI will aid in designing combination therapies and multi-agent nanosystems by identifying synergistic drug combinations as well as optimal NP formulations.[24] In combination with reinforcement learning, AI would allow for adaptive therapy regimens based on longitudinal patient data. In terms of CNS disorders, ML will enable optimising the design of blood-brain barrier (BBB) penetrating nanocarriers for diseases such as glioblastoma, Alzheimer's, Parkinson's and multiple sclerosis; and AI-guided imaging will allow for the development of localized delivery systems and characterisation of the therapeutic action of the active pharmaceutical ingredient (API).[25] The combination of AI with nanoarchitectures will enable more precise surface engineering procedures and in silico modelling, allowing for enhanced targeting specificity and systemic distribution, and facilitating and accelerating progress beyond the empirical design approaches towards mechanism-driven design. There are still many challenges remaining to achieving clinical translation of AI-based nanomedicines; these include data heterogeneity, regulatory gaps, batch-to-batch variability, scalability, and ethical issues that need to be resolved. In summary, the application of AI to nanomedicines could revolutionise precision medicine through improved efficacy, safety, and flexibility of treatments for cancer and neurological disease.[26]

Clinical translation, regulatory, and ethical aspects

AI facilitates the clinical application of nanomedicine faster through optimization of preclinical testing, diminished dependency on animal models, and enhancement of trial design via predictive modeling and data integration. The first stages of clinical trials utilizing AI-assisted nanotechnology reveal promise, but there exist several problems surrounding data quality, standardization, and reproducibility of predictions — all of which are essential components for obtaining approval from regulatory agencies.[27] Since deep learning models' "black boxes" prevent access to their internal workings, it will be necessary to create and implement a framework for the development of explainable AI (XAI) systems to instill transparency and trust in all regulatory filings and decisions made based on these systems. In addition, ethical dilemmas regarding use of data privacy and biased data (that may intensify current health disparities) raise concern for equitable access to AI-based nanomedicines amongst various patient populations. Regulatory policies are being amended; however at present, they remain reactionary to the rapid advance of AI technologies, thus creating a critical need for developing standardized guidelines to provide proper balance between innovation and patient safety, accountability, and equity. For these issues to be addressed by all parties involved (i.e., clinicians, ethicists, regulators, technologists) there needs to be collaborative teamwork to accomplish the responsible incorporation of AI into nanomedicine in order to support public trust while maximizing patient welfare.[28]

Nanocarriers and AI Applications

Nanocarrier	AI Application	Outcome
Liposomes	Drug loading prediction	Improved bioavailability
Polymeric NP	Stability optimization	Enhanced circulation
Metallic NP	Imaging enhancement	Better diagnosis
Dendrimers	Targeted delivery	Reduced toxicity

Future perspectives and emerging trends

Nontheranostics with advanced artificial intelligence supported solid technologies are being developed to provide clinicians with more accurate, sophisticated, and faster treatment options. As AI continues to advance, smart nanoparticles will use their knowledge of the body and microenvironment, to program themselves to deliver specific doses at the appropriate time through targeted delivery systems. These types of nanoparticles will also have the ability to adjust to changing microenvironments in order to provide the best therapeutic outcome possible for each cancer patient. Current research in federated AI systems allows researchers from different institutions to collaborate on developing models without requiring access to sensitive patient data. In addition, federated AI will ensure that AI-based models can be created without disclosing sensitive information regarding patients or patient populations. There is an increasing emphasis on the use of nanomedicine to enhance clinical research and improving patient care through AI. Through the use of AI algorithms, nanomaterials are being designed to be biodegradable, recyclable, and low in toxicity in order to reduce their negative impact on the environment. AI algorithms are also increasingly being integrated into nanomedical platforms to improve the drug development and delivery process. Many companies are developing their own nanomedical platforms that are consistent with these goals, allowing for the discovery and delivery of new and repurposed drugs to patients faster and with greater precision. However, the rapid advancements being made in AI nanomedicine are also creating challenges with standardization, regulatory compliance, ethical considerations, and further clinical application; therefore, interdisciplinarity will be critical in providing the resources and tools needed to maximize benefits from the adoption of AI-based therapeutic applications.

CONCLUSION

Nanoparticle design has made great strides in its development due to the ability of artificial intelligence (AI) to rapidly screen and optimise the different physicochemical properties of those particles, predict biodistribution based on readily available databases, and provide better outcomes from precision medicine by providing AI-optimised personal regimens for patients. Additionally, AI modelled biomarkers improve the detection and analysis of imaging biomarker studies, allowing for earlier detection of disease and better monitoring of disease progression. The use of AI models to design nanocarriers that can be used for targeted delivery (to a specific area) have the added benefit of being able to adjust to the biological conditions of the host, produce less toxicity, and provide controlled drug delivery, thus facilitating more efficient clinical trials of nanocarriers. While these accomplishments of using AI have been significant for the field, there are still challenges to overcome related to standardising data for use with models developed for use in the development of nanomedicine, developing models that can be used in different biological conditions, establishing appropriate regulatory frameworks, and addressing ethical issues before we will see widespread clinical use of AI in nanomedicine. Roadmaps for the next decade include developing robust clinically validated AI models that are tightly integrated with engmnanered nanomaterials to help ensure reproducibility and safety of these innovations for all patients. The collaboration between investigators, clinical practitioners, and regulatory agencies will be critical to translating AI-mediated innovation in nanomedicine into clinically effective, precision-fine therapies.

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