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Review Article

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Nanotechnology Enabled Drug Delivery System Leveraging Machine Learning Techniques

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Abstract

Integration of machine learning with nanotechnology has many benefits in a therapeutic manner as compared to classical treatment in areas like cancer, COVID-19, toxicity prediction and many others. Machine learning has proven to be instrumental in enabling personalized treatment approaches and effectively handling extensive datasets, presenting numerous advantages. Similarly, nanotechnology has garnered significant attention as a cutting-edge discipline, particularly in the realm of drug delivery systems, by facilitating targeted delivery exclusively to affected areas. This review paper aims to analyze the drug delivery system using nanotechnology with the integration of machine learning mainly in two areas, COVID-19, and cancer tumor cells. Additionally, it will emphasize the potential advantages of integrating machine earning into this field. Furthermore, it will explore the limitations associated with this approach and discuss the prospects for advancements in this area.

Keywords

Nanotechnology, Machine learning, Drug delivery system

Introduction

Machine learning is an integral aspect of artificial intelligence, enabling computers to learn and improve from experience without explicit programming. By employing algorithms and statistical models, machine learning enables systems to identify patterns, make decisions, and execute tasks based on data. Its versatile applications encompass diverse fields, ranging from image and speech recognition to natural language processing and recommendation systems. The adaptability of machine learning to assimilate new information makes it a powerful tool to address intricate challenges in today's world. Nanotechnology, on the other hand, is an interdisciplinary field that centers on manipulating and studying matter at the nanoscale level, equivalent to one billionth of a meter. This domain involves working with materials and structures at this scale, which exhibit distinctive properties. Nanotechnology finds practical applications in electronics, medicine, energy, and more, leading to advancements in targeted drug delivery. In the realm of drug delivery systems, the integration of machine learning and nanotechnology plays a pivotal role.

Machine learning enhances nanotechnology in drug delivery systems by optimizing nanoparticle design (by analyzing vast nanomaterial and biological data, machine learning optimizes the design of drug carrying nanoparticles. It enables drug delivery by predicting material behavior), enabling targeted delivery (machine learning leverages patient data and disease characteristics for developing targeted drug delivery system. It guides the design of nanoparticles, so can minimize the side effect of nanoparticle, and maximize the therapeutic effect), controlling drug release (machine learning algorithms optimize drug release kinetics from nanoparticles, considering environmental factor sand patient specific parameters to achieve desired therapeutic outcomes over time), predicting toxicity (machine learning models assess the toxicity of drug delivering nanoparticles [1]. Analyzing physicochemical properties and biological interactions helps ensure safer nanoscale drug delivery systems), supporting personalized medicine (Machine learning contributes to personalized drug delivery strategies. By utilizing patient data and treatment responses, it recommends tailored nanoparticle-based therapies for improved individual treatment outcomes). Figure 1 depicts nanoparticles in drug delivery systems enhanced by machine learning by optimizing nanoparticle design, enabling targeted delivery, controlling drug release, predicting toxicity, and supporting personalized medicine. This strategy offers effective and safer drug delivery, revolutionizing medical treatments.

Nanoparticles are extremely small materials, with sizes ranging from 1 to 100 nm [2]. Based on their characteristics, shapes, or sizes, they can be divided into many classifications [2]. By capitalizing on the unique characteristics exhibited by materials at the nanoscale, nanotechnology has revolutionized the field of drug delivery [3, 4], opening new avenues for enhanced therapeutic outcomes. One crucial factor that governs the effectiveness of a drug is its bioavailability, which refers to the rate and extent of drug absorption. The bioavailability of a drug is also influenced by its physicochemical properties, encompassing various attributes such as solubility, stability, and molecular size.

Pharmaceutical nanocarriers, such as polymeric, lipidic, and inorganic nanoparticles, liposomes, nanotubes, nanocomplexes, and niosomes, have emerged as versatile drug delivery vehicles with submicron dimensions [4-7]. Figure 2 depicts the same mentioned nanocarriers design. These nanocarriers offer distinct advantages over traditional drug delivery systems, primarily due to their ability to encapsulate and protect drugs, facilitate controlled release, and provide targeted delivery to specific sites within the body. Through surface modifications, ligands can be attached to nanocarriers [8], facilitating enhanced cellular uptake and site-specific delivery [9].

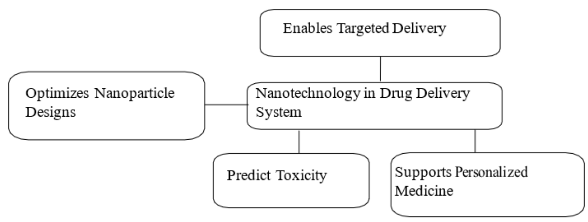

Figure 1: Nanotechnology in drug delivery system.

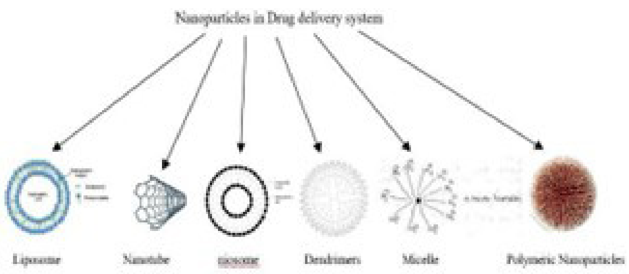

Figure 2: Nanocarriers.

When administered intravenously, drugs achieve a bioavailability of 100% as they directly enter the supporting personalized medicine. This strategy offers effective and safer drug delivery, revolutionizing medical bloodstream. The intravenous route of administration ensures that the site of drug administration aligns with the site of absorption, allowing for rapid and efficient systemic distribution. In contrast, nanotechnology offers a paradigm shifting approach by enabling precise and targeted drug delivery to specific areas of interest [10]. Whether it is delivering therapeutics to the tumor site in cancer treatment or targeting specific organs or tissues, nanocarriers can navigate physiological barriers and reach the intended destination, minimizing off target effects and reducing systemic toxicity. Cancer treatment stands out as a notable beneficiary of nanotechnology enabled drug delivery [11, 12]. By leveraging the unique properties of nanocarriers, therapeutic agents can be selectively delivered to cancer cells, while sparing healthy cells from unnecessary damage. This targeted approach not only improves the efficacy of treatment but also mitigates the adverse side effects associated with conventional chemotherapy [13]. Nanocarriers can be engineered to carry a payload of anticancer drugs, guided by surface modifications or specific ligands that recognize and bind to cancer cells, thus enhancing drug accumulation and uptake at the tumor site.

Incorporating machine learning into the realm of drug delivery systems adds another dimension of advancement and optimization. There are numerous ways that machine learning can be applied to nanomedicine [14-16]. By harnessing the power of machine learning algorithms, complex and diverse datasets can be analyzed to uncover valuable insights and patterns. These models can be trained on vast amounts of data, enabling them to interpret and predict optimal drug release profiles, dosage regimens, and treatment strategies. Machine learning algorithms can utilize patient specific information, such as genetic profiles, clinical history, and lifestyle factors, to personalize treatment approaches, tailoring therapies to individual patients for maximum efficacy and safety. By combining machine learning with nanotechnology-based drug delivery systems, the potential for precise, targeted, and patient specific treatments becomes a tangible reality, revolutionizing the field of precision medicine.

Nanotechnology in COVID-19

The relentless impact of COVID-19 has galvanized scientists to seek novel treatment avenues [17]. The convergence of nanotechnology and machine learning holds the promise of revolutionizing drug delivery systems. Nanoparticles, liposomes, and various other types of nanomaterials have emerged as versatile platforms for delivering therapeutic agents with precision [18]. It showcases strategies for optimizing drug encapsulation, controlled release, and enhanced bioavailability. The integration of machine learning techniques, encompassing virtual screening, molecular docking, and quantitative structure activity relationship modeling, has expedited the identification of potential drug candidates. By synergistically merging machine learning with nanotechnology, the design process for drug loaded nanoparticles is streamlined. Through the deployment of machine learning algorithms, the prediction of optimal nanoparticle formulations becomes a reality by comprehensively considering physicochemical attributes and release kinetics. This predictive modeling expedites the developmental phase of formulations, reduces the need for extensive trial-and-error iterations and facilitates the seamless translation from laboratory experiment to clinical application.

Machine learning, adapted at distilling valuable insights from extensive datasets, significantly facilitates the identification of biomarkers pivotal for precise targeted drug delivery. The collaborative prowess of nanotechnology and machine learning empowers the creation of bespoke nanocarriers meticulously tailored to specific cellular or tissue types. This approach serves to minimize off target effects while heightening therapeutic efficacy.

However, the author's focus centers around three key challenges in the field of nanomaterial systems and their corresponding solutions to enhance productivity, table 1 depicts the major issues that need to be resolved and the suggested remedies to promote continuous innovation and increase efficiency in the creation of nano delivery systems [2]. So, the analysis done on 315 nanotechnology research manuscripts published from 2006 to 2019, the focus was on iron oxide, gold, and silica nanoparticles [2].

Finding indicated a significant lack of important information, for iron oxide nanoparticles 68% did not report the size, shape, or zeta potential with only 1% providing pharmacokinetics profiles and 32% including dosing information, similarly for gold and silica nanoparticles 51%and 45% of manuscript respectively were missing complete physicochemical characteristics. So, it is not fulfilling the complete information.

Here, machine learning holds significant potential in nanotechnology by facilitating the creation and extraction of nanotechnology databases [19]. Through the integration of natural language processing and deep learning techniques, machine learning aids in generating comprehensive and reliable datasets for statistical modeling. These data sets serve as the foundation for developing machine learning tools that enable efficient experiment prioritization, predictive modeling, and innovative design of composite nano-delivery systems. This synergy between machine learning and nanotechnology promises to advance research and implementation in the field, leading to breakthroughs in drug delivery and other nanotechnology applications.

Table 1: Challenges and solutions of issues to increase efficiency in the creation of nano-delivery.

Challenges	Solution
Inadequate composition, insufficient pro-filing, insufficient methods, multidisciplinary field, and terms.	Standardize (e.g., MIRIBEL) composition reports phys chem reports, bioassay reports, pharmacokinetics reports, methods description.
Nonexistence of public data repository, missing information.	Encouraging the collection of additionaldatasets text mining.
Nonexistence of canonical form, Absenceof custom-tailored nanomaterials.	Artificial intelligence-oriented language, machine learning for prognostication of assets using FAIR instruments.

However, the forthcoming trajectory of this study encompasses exploring the potential of machine learning tools in shaping the landscape of composite nano-delivery systems within the healthcare domain. By harnessing machine learning's capabilities, this research aims to advance the design and implementation of innovative nanotechnological approaches to improve drug delivery and healthcare outcomes.

However, the author explored the significance of nanomaterial databases in nanotechnology research [3]. These databases provide standardized information on nanomaterial nomenclature, physicochemical properties, and quantitative structure activity relationships [20], enabling a better understanding of their efficacy and toxicity.

In some studies, the authors analyzed around 56 papers to understand the composition of protein coronas. They used a random forest model to accurately identify key proteins in protein coronas of different nanoparticles. Surface modification was found to significantly influence protein interactions. Factors influencing corona formation were found to have a heterogeneous distribution. Protein compositions showed strong correlations with uptake efficiencies, proinflammatory markers, and immune disturbances [21]. Protein compositions were closely associated with absorption rates, proinflammatory indicators, and immunological abnormalities (R^2 values of 0.8) [21]. This model can predict the physicochemical properties of protein coronas and guide nanoparticle design for complex biological environments and specific biological activity.

However, there are difficulties in incorporating curated nanomaterial datasets into machine learning studies [3]. These databases receive little attention and are rarely used. It costs money to convert important features into machine learning training sets. Standardization attempts are hampered by the absence of standardized measures for comparing nanomaterials.

So, collaboration and automation can enhance dataset quality and data curation. For nanomedicine to advance, cooperation between researchers, developers, and artificial intelligence professionals is essential. For curated databases to be successful in the development of nanomedicine, standardized data formats, reporting processes, and metrics are necessary. Machine learning offers solutions to challenges in integrating curated nanomaterial databases. It raises awareness, translates key features into usable training sets, and establishes standardized metrics. Additionally, it handles data heterogeneity and improves dataset quality through automation. Collaboration between researchers and artificial intelligence experts leverages data analytics for nanomedicine development, while standardized data formats ensure consistency and advance nanomedicines [3].

Nanotechnology in Tumor

Machine learning facilitates the creation of nanoparticles with unprecedented specificity for cancer cells. By identifying key molecular attributes crucial for binding to cancer cells, machine learning guides the design of nanoparticles coated with matching molecules. Consequently, these nanoparticles possess the ability to homing in on cancer cells, enabling the targeted delivery of therapeutic payloads directly to the tumor site. The controlled release of therapeutic agents from nanoparticles is pivotal for maximizing treatment outcomes. Machine learning algorithms analyze intricate relationships between drug properties, nanoparticle characteristics, and desired release profiles. In doing so, they pave the path towards achieving standardized reporting of information, thereby addressing the existing lack of uniformity prevalent in nanomedicine and nanotoxicology. This concerted effort toward standardization serves to mitigate the observed variability [22].

However, to improve research quality and reusability researchers used artificial intelligence and machine learning dependent reporting standards like MIRIBEL (Minimum information reporting for bio nano experimental literature) framework [22].

Standardized reporting improves data interpretation, prediction of safer cell particle interactions, and facilitates safe manufacturing of nanomaterials. Computational methods, such as density functional theory calculations, are valuable in studying nano bio-interactions and predicting nanomaterial properties. The adsorption of proteins by nanomaterials can be characterized using the BSAI approach. These approaches contribute to understanding nanotoxicity and developing effective and nontoxic nanomaterials.

However, it does not address potential challenges or ethical considerations associated with the use of nanotechnology.

Nanotechnology has the potential to contribute to the development of rapid and sensitive diagnostic tools for early detection of viral infections. Integration of nanotechnology with other emerging technologies, such as artificial intelligence and gene editing, may lead to innovative approaches for combating infectious diseases.

However, in some studies, the authors employed machine learning and artificial intelligence techniques to analyze the impact of nanoparticle properties, tumor models, and cancer types on nanoparticle tumor delivery efficiency [23]. They utilized a recently published Nano Tumor Database containing 376 datasets generated from a physiologically based pharmacokinetic model. Results revealed that a deep neural network model outperformed other methods, accurately predicting nanoparticle delivery efficiency across different tumors. Methods used were Random Forest, Support Vector Machine, Linear Regression, and bagged model, their (R^2) were found 0.70,0.46, 0.33 and 0.63. Cancer type was found to be a significant determinant, contributing 19 - 29% to the model's performance. Among the studied physicochemical properties, the zeta potential and core material played pivotal roles, surpassing factors like type, shape, and targeting strategy.

The suboptimal delivery efficiency of nanoparticles to tumors poses a significant challenge in cancer nanomedicine. Enhancing nanoparticles tumor delivery efficiency is a crucial area that requires further investigation and exploration.

So, machine learning takes center stage by constructing a robust quantitative model that combines deep learning and physiologically based pharmacokinetic approaches [23]. This model enables the accurate prediction of tumor delivery efficiency for various nanoparticles, considering their physicochemical properties, cancer type, and tumor model. By leveraging machine learning and artificial intelligence techniques, this research represents a significant advancement in cancer nanomedicine, empowering scientists to make informed decisions regarding the selection of nanoparticles for preclinical trials. This innovative framework not only optimizes nanomedicine design but also reduces and refines animal studies, aligning with ethical research practices. Beyond cancer nanomedicine, this methodology's versatility extends to other domains, including small molecular drug development, environmental health risk assessment, and animal derived food safety evaluation, demonstrating the transformative potential of machine learning/artificial intelligence in diverse applications.

Miscellaneous

The rapid growth of nanomedicine has led to increased complexity at the nanoscale level [24]. To address this, artificial intelligence has been employed for data analysis and inference. This article focuses on the application of artificial intelligence in nanomedicine, specifically in nanodrug screening and development, brain-machine interfaces [25], and nanotoxicology. AI serves as a valuable tool to enable advancements in these areas of nanomedicine.

The goal of precision medicine is to provide customized treatments for each patient [26]. It faces difficulties in tailoring nanoparticle probes and nanodrugs for molecular targets.

Artificial intelligence and machine learning algorithms can significantly advance nanomedicine by predicting biocompatibility, surface binding properties, and membrane interactions [27]. Machine learning algorithms enable drug candidate identification and design of immunomodulatory nanostructures. Artificial intelligence facilitates image analysis for treatment monitoring and personalized glucose level monitoring in diabetes therapy. The integration of artificial intelligence with nanomedicine holds promise for personalized therapies, standardized quantification, and toxicity testing.

The future of nanomedicine lies in harnessing the power of machine learning algorithms to improve patient outcomes and drive healthcare advancements [28].

Discussion

This concise review explores the fusion of machine learning and nanotechnology in drug delivery systems, targeting COVID-19, cancer, and in brain-machine interface regulation at some level. By leveraging machine learning algorithms, nanoparticle design, drug release, and toxicity prediction are optimized, while nanotechnology enables precise drug delivery. This integration promises personalized treatments, targeted therapies, and transformative healthcare advancements. Nonetheless, challenges and limitations are addressed, and prospects are discussed to propel the field forward.

Conclusion

Nanotechnology has revolutionized drug delivery by capitalizing on the unique characteristics of materials at the nanoscale. Nanocarriers offer advantages such as targeted delivery, controlled release, and protection of drugs. By integrating machine learning, personalized treatment approaches can be developed for maximum efficacy and safety. However, challenges in composition profiling and standardization need to be addressed. Further research is needed to validate the efficacy of nanotechnology in various fields, including cancer treatment and infectious diseases. Overall, nanotechnology holds immense potential in precision medicine and improving patient outcomes.

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None.

Conflict of Interest

None.

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