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Artificial Intelligence (AI): It's Role in Drug Discovery and Novel Drug Delivery System

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Abstract: ***This article presents an all - encompassing overview of the pivotal role played by artificial intelligence (AI) across various stages of drug discovery and delivery, highlighting its transformative impact on the pharmaceutical industry. Emphasis is placed on the application of AI in drug delivery as a crucial advancement that leverages innovative technologies and algorithms to enhance the efficiency of drug transportation. The evolution of AI in drug discovery, starting from the creation of the DENDRAL program in the 1960s to its modern applications in target identification, virtual screening, and de - novo drug design, serves as a testament to its growing importance. Additionally, the utility of AI in the pharmaceutical sector is explored, demonstrating how AI algorithms analyse biological data for disease target identification, optimize experimental design, and predict drug interactions, thereby facilitating personalized medicine and reducing reliance on animal testing. The article further delves into the influence of AI on dosage form design, pharmacokinetics, and the optimization of drug delivery systems through predictive modelling and machine learning algorithms. The emergence of AI - driven drug delivery systems, such as nanoparticles and liposomes, underscores the capability of AI to improve drug efficacy and minimize adverse effects. Nevertheless, challenges such as regulatory guidance and ethical considerations are duly acknowledged. In conclusion, the article posits that the integration of AI into drug delivery systems holds the promise of revolutionizing medical treatments, enhancing patient outcomes, and shaping the future of the pharmaceutical industry.***

Keywords: Artificial intelligence, DENDRAL program, target identification, virtual screening, d e - novo drug design, machine learning

1. Introduction

Artificial Intelligence (AI), defined as computer - based simulation of human intelligence processes, has achieved notable advancements across diverse fields, including drug discovery and delivery [3, 4, 5]. The application of AI in both these domains has emerged as a vibrant area of research, with growing recognition of its potential to expedite drug development and uncover more potent medications. Particularly in drug delivery, AI's utilization has garnered significant interest recently, propelled by the emergence of innovative technologies and algorithms that enhance the efficiency of drug transportation

Drug Delivery:
Drug delivery is a critical component of the drug development process [6]. The efficacy of a medication hinges not only on its pharmacological characteristics but also on its ability to reach the intended site within the body [7]. Throughout the years, numerous drug delivery systems have been devised to enhance drug effectiveness and minimize adverse effects. However, creating novel drug delivery systems is a multifaceted and time - intensive endeavour. The integration of AI into drug delivery holds promise for expediting the development of new delivery systems and enhancing drug efficacy. In essence, drug delivery entails administering the precise dosage of medication to the designated location at the appropriate time [8].

The Evolution of AI in Drug Discovery:
AI's involvement in drug discovery traces back to the 1960s, marked by the creation of the first computer program, DENDRAL, at Stanford University, aimed at aiding drug discovery [9.10]. Since then, AI has been applied across various stages of drug discovery, encompassing target identification lead optimization, and drug design [11]. Initially, AI was primarily utilized for predicting the pharmacological attributes of compounds. However, technological advancements have enabled its utilization in predicting the three - dimensional structure of proteins and designing drugs tailored to target specific proteins within the body, exemplified by software such as MolAICal.

Role of AI I Pharmaceutical Industry:
Artificial intelligence (AI) has a significant role to play in the pharmaceutical industry when it comes to addressing various challenges. Using AI algorithms, extensive biological data can be analysed in order to identify targets that are associated with diseases, as well as predict how these targets interact with potential drug candidates [12, 13]. This allows for a more efficient and targeted approach to the process of drug discovery. Machine learning algorithms also contribute by assisting in the design of experiments, predicting pharmacokinetics and toxicity, and optimizing lead compounds. As a result, the need for extensive animal testing is reduced. Moreover, AI algorithms can analyse real - world patient data, which in turn facilitates personalized medicine approaches. Ultimately, this leads to more

effective treatment outcomes and improved patient adherence. IBM Watson, for instance, is an AI tool that enables faster diagnosis and data analysis, thereby enhancing medical care and reducing costs [14]. Furthermore, AI could enhance the pharmaceutical manufacturing process by enabling the manufacturing of personalized medications. However, it is important to address challenges such as regulatory guidance, data privacy, and ethical considerations in order to successfully implement AI in the pharmaceutical industry

AI for Drug Discovery:

Target Identification: AI systems possess the capability to analyse a wide range of data types, including genetic, proteomic, and clinical data, with the purpose of identifying potential therapeutic targets. Through the revelation of disease - associated targets and molecular pathways, AI contributes to the formulation of medications that can regulate biological processes.

Virtual Screening: The efficient screening of extensive chemical libraries to identify drug candidates that exhibit a high probability of binding to a specific target is made possible by Virtual Screening AI. By means of simulating chemical interactions and predicting binding affinities, AI assists researchers in prioritizing and selecting compounds for experimental testing, leading to time and resource savings.

Structural Activity Relationship Modeling:
The modelling of Structure - Activity Relationship (SAR): AI can establish correlations between the chemical composition of compounds and their biological efficacy. This enables researchers to enhance the potential of drug candidates through the design of molecules possessing desired attributes, including heightened potency, selectivity, and favourable pharmacokinetic profiles.

DE - Novo Drug Design:
Leveraging reinforcement learning and generative models, AI algorithms have the capacity to propose novel chemical structures resembling drugs. By assimilating information from chemical libraries and experimental data, AI expands the scope of chemical possibilities, thus facilitating the development of pioneering drug candidates.

Optimizing Drug Candidate:
AI algorithms have the capacity to examine and refine drug candidates through the consideration of various factors, such as efficacy, safety, and pharmacokinetics. This computational approach aids researchers in optimizing therapeutic molecules, thereby enhancing their effectiveness while minimizing the likelihood of potential side effects.

Drug Repurposing:
One notable application of AI in drug development involves the analysis of extensive biomedical data to identify approved drugs that exhibit therapeutic potential for different diseases. Through this process of repurposing, AI expedites the drug discovery process and contributes to cost reduction.

Target Fishing Technology and its Role with AI:
Target fishing, a computational method utilized in drug discovery, has become a pivotal technique for Poly pharmacology, drug repurposing, and the detection of novel drug targets [15, 16]. It enables the determination of protein targets for a given molecule, elucidates the mechanism of action, and unveils the off targets of drug candidates [17]. In recent times, machine learning has been progressively integrated into target fishing, both as a primary approach and as an enhancement of existing strategies. Computational methods for target fishing have also been developed to investigate the targets of drugs in specific cells, leveraging gene transcriptional profiles and deep learning methodologies. Ligand - based target fishing techniques have been assessed and compared, with Swiss Target Prediction and the similarity ensemble approach (SEA) being identified as efficacious methods [18]. These advancements in target fishing methodologies, in conjunction with the utilization of artificial intelligence, have significantly enhanced the efficiency and accuracy of identifying potential drug targets and supporting drug discovery endeavour. In silico target fishing is an emerging approach in drug discovery. It helps identify protein targets and off targets of drug candidates [19].

Siamese Spectral - Based Graph Convolutional Network (SSGCN) Model
Computational target fishing aims to investigate the mechanism of action or side effects of bioactive small molecules. Siamese spectral - based graph convolutional network (SSGCN) model is used for inferring protein targets from gene transcriptional profiles. Siamese spectral - based graph convolutional network (SSGCN) model and Linear regression layer are used for characterizing correlation between compound and target embeddings [15, 16].

Application of AI Tools in Dosage form Design:
AI tools have found extensive application in the design of pharmaceutical dosage forms. These tools employ AI algorithms to analyse vast amounts of biological data, such as genomics and proteomics, in order to identify disease - related targets and forecast their interactions with potential drug candidates. By optimizing the processes of research and development, AI has the potential to contribute to the reduction of development costs and enhance the probability of successful drug approvals [19]. Machine learning algorithms aid in the design of experiments, forecast the pharmacokinetics and toxicity of drug candidates, and facilitate the prioritization and optimization of lead compounds. AI algorithms that analyse patient data from the real world can facilitate personalized medicine approaches, resulting in more effective treatment outcomes and improved patient adherence AI can assist in obtaining optimized formulations with desired attributes, thereby reducing resource utilization and enhancing comprehension of the impact of independent variables on dependent responses.

AI and its Role on Pharmacokinetics:
The rate of permeation based on the route of administration is a crucial criterion for monitoring the efficiency of drug delivery systems. Once an orally administered drug enters the gastric environment, it must permeate through the

intestinal or gastric epithelium, which is a vital step for its further distribution into the bloodstream. This distribution step is responsible for conveying the drug to its target site, such as a specific tissue or cellular component. It is worth noting that intracellular molecules can also serve as targets for drug entry into the body. The permeation of drugs mostly occurs through biological barriers, either passively or actively. Passive diffusion relies on the molecular characteristics of the drug. Although in silico models are employed to predict drug distribution through computational analysis, it should be acknowledged that these results may differ somewhat from actual drug distribution studies [20, 21]. For many biologically active entities and small molecules, passive permeation is not efficient and necessitates the use of specific drug delivery systems. On the other hand, active permeation is driven by membrane transport and relies on complex biological interactions. To understand this intricate process, it is necessary to explore various specific parameters through computational and systematic modelling approaches. The advancement of computational models has enabled the study of pharmacokinetic parameters related to drug delivery systems.

AI in Drug Delivery System:

The utilization of artificial intelligence can be harnessed to optimize drug delivery systems through various means, including the prediction of drug behaviour within the body, the anticipation of drug interactions, and the enhancement of drug formulations. Machine learning algorithms have the capacity to analyse extensive datasets pertaining to drug behaviour within the body, thereby enabling the prediction of drug response. An illustrative instance of AI - facilitated drug delivery systems is the application of machine learning algorithms to optimize drug formulations. These algorithms can be trained on voluminous datasets documenting drug behaviour within the body, thus facilitating the anticipation of the most optimal formulation for a particular drug. By training neural networks on extensive datasets encompassing drug interactions, it becomes feasible to predict potential interactions between different drugs. This capability proves valuable in the design of drug delivery. Various application of AI based drug delivery system includes 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 [20, 21].

A. Nanoparticles:

Nanoparticles can be defined as dispersal of particles or solid particles that have a size ranging from 10 - 1000nm. The drug can either be dissolved, trapped, enclosed, or affixed to a nanoparticle matrix. Nanoparticles provide specific advantages including enhancing the stability of drugs and proteins, as well as possessing controlled release properties that are beneficial. Furthermore, these nanoparticles can be altered to achieve both active and passive targeting. Additionally, the drug loading capacity is remarkably high and can be administered through various routes such as parenteral, nasal, intraocular, and oral routes. It is worth noting that artificial intelligence (AI) has been employed in the design and optimization of nanoparticle drug delivery systems [19, 20, 21].

Types of nanoparticles:

1. Naotubes, 2. Nanowires, 3. Nanocantilever, 4. Nanoshells, 5. Quantum dots, 6. Nanopoers, 7. Nanosomes 8. Niosomes, 9. Nanoemulsions

B. Liposome Drug Delivery:

Artificial intelligence (AI) is currently employed in the development of liposomal drug delivery systems. Liposomes, which are vesicles composed of lipids, serve as carriers for drug delivery. The utilization of AI facilitates the administration of precise and effective therapy with minimized adverse effects. AI possesses the capability to anticipate the release and concentration of drugs over time, thus saving time in terms of testing and materials. Furthermore, AI can be utilized in the planning of treatment for ophthalmic drug delivery, particularly using indocyanine green (ICG) liposomes [22, 23]. The Modu light ophthalmic laser platform, when connected to Modu light Cloud, permits treatment planning based on AI by establishing correlations between treatment parameters and the achievement of desired outcomes. The amalgamation of AI with liposomes possesses the potential to enhance the efficacy of drug delivery and increase the success rates of treatments.

C. Microsphere:

Microspheres represent a category of drug delivery systems that possess the ability to facilitate targeted drug distribution. These microspheres, which are comprised of solid proteins or synthetic polymers, exhibit diameters that span from 1 to 1000 µm. The formulation of microspheres can be achieved through a variety of techniques, thereby affording numerous advantages, including sustained release capabilities and the potential to direct anti - cancer medications towards tumours. Particularly in the realm of colon targeted drug delivery, microspheres have garnered attention due to their potential utility in addressing disorders such as colon cancer and inflammatory bowel disease. Whether formulated with biodegradable polymers or protein - based materials, microspheres surpass conventional colon targeted drug delivery systems in terms of their desirable attributes [22, 23]. Specifically, these microspheres can preserve their structural integrity whilst traversing the gastrointestinal tract, ultimately releasing the drug upon contact with colonic fluid. Ultimately, microspheres have the capability to ameliorate drug delivery, thereby facilitating improved efficacy, diminished toxicity, and enhanced patient adherence.

D. Dendrimer:

Dendrimers have been extensively investigated as vehicles for delivering drugs due to their distinct characteristics, including well - defined structure, uniformity, and the ability to be modified on their surface [18]. They can be employed to encapsulate or chemically link drug molecules, thereby allowing for precise and controlled release of drugs. Furthermore, dendrimers can be further modified to form three - dimensional hydrogel networks, known as dendrimer hydrogels, which possess both fluidity and adhesiveness. This renders them suitable for use in topical ocular drug formulations. Additionally, dendrimers can be engineered to respond to specific stimuli such as changes in temperature and redox concentration, thus enabling targeted drug

delivery. The utilization of dendrimers as carriers for drugs has demonstrated potential in a variety of applications, including cancer therapy. Overall, drug delivery systems based on dendrimers provide a versatile approach for enhancing drug stability, improving pharmacokinetics, and achieving targeted drug delivery [22, 23].

E. Hydrogel:

Hydrogels are polymeric networks that possess a three - dimensional structure and a hydrophilic nature, enabling them to absorb significant quantities of water or biological fluids. These networks consist of either homopolymers or copolymers and are insoluble due to the existence of chemical crosslinks, such as tie - points or junctions, as well as physical crosslinks, such as entanglements or crystallites. The unique thermodynamic compatibility between hydrogels and water allows them to undergo swelling in aqueous environments. Positioned at the forefront of controlled drug delivery, hydrogels function as environs intelligent and stimuli - sensitive gel systems, enabling modulation of release in response to various factors including pH, temperature, ionic strength, electric field, or concentration differences of specific analytes [17]. Within these systems, release can be strategically designed to occur within specific regions of the body, such as within a certain pH range of the digestive tract, or alternatively, through specific sites within the body by utilizing adhesive or receptor - specific gels that are connected to the hydrogel surface via tethered chains. When combined with the technique of molecular imprinting, hydrogels hold great promise as drug delivery systems.

Recent trends in Artificial Intelligence in Novel Drug Delivery Systems:

Artificial intelligence (AI) possesses the capability to completely transform the realm of pharmaceutical delivery through the optimization of drug design, the enhancement of drug targeting, and the improvement of drug release. In this regard, recent trends in AI - driven drug delivery systems have emerged.

a) ***Machine learning for drug discovery*:** Machine learning algorithms are currently being employed to scrutinize vast datasets and identify potential drug targets, predict the effectiveness of drugs, and refine the properties of drugs. These AI - powered drug discovery platforms have the capacity to examine millions of compounds, thereby significantly reducing the temporal and financial costs associated with drug development.

b) ***Nanoparticle - based drug delivery systems*:** Nanoparticles can be skill fully engineered to transport drugs to specific cells or tissues within the body. AI is currently being utilized to optimize the design of these nanoparticles in order to enhance the efficacy of drugs and diminish toxicity levels.

c) ***Predictive models for drug release*:** The application of artificial intelligence models enables the anticipation of drug behaviour within the human body and facilitates the development of controlled drug delivery mechanisms. This advantageous capability ensures that drugs are released at the appropriate time and location within the body, thereby enhancing therapeutic efficacy and mitigating undesirable side effects.

d) ***Smart drug delivery system:*** The utilization of AI - powered sensors in drug delivery systems allows for real - time monitoring of drug release, enabling physicians to adapt drug dosages and optimize treatment plans on an individualized basis.

e) ***Personalized medicine:*** The implementation of artificial intelligence in the analysis of patient data permits the design of tailored drug delivery systems that cater to the unique physiological characteristics and medical histories of individual patients. This personalized approach enhances treatment outcomes and decreases the likelihood of adverse reaction [23].

AI Model Tools	Summary
Deep Chem	An open - source library that provides a wide range of tools and models for drug discovery, including deep learning models for molecular property prediction, virtual screening, and generative chemistry
RDKit	A widely used open - source cheminformatics library that offers various functionalities for molecule handling, substructure searching, and descriptor calculation. It can be integrated with machine learning frameworks for drug discovery applications
ChemBERTa	A language model specifically designed for drug discovery tasks. It is based on the Transformer architecture and is pretrained on a large corpus of the chemical and biomedical literature, allowing it to generate molecular structures, predict properties, and assist in lead optimization.
GraphConv	A deep learning model architecture that operates on molecular graphs. It has been successful in predicting molecular properties, such as bioactivity and toxicity, by leveraging the structural information encoded in the graph representation of molecules
AutoDock Vina	A popular docking software that uses machine learning techniques to predict the binding affinity between small molecules and protein targets. It can assist in virtual screening and lead optimization for drug discovery
SMILES Transformer	A deep learning model that takes Simplified Molecular Input Line Entry System (SMILES) strings as input and generates molecular structures. It can be used for de novo drug design and lead optimization
Schrödinger Suite	A comprehensive software package for drug discovery that incorporates various AI - driven tools. It includes modules for molecular modelling, virtual screening, ligand - based and structure - based drug design, and predictive modelling.
IBMRXN for chemistry	An AI model designed to predict chemical reactions. It utilizes deep learning algorithms and large reaction datasets to generate potential reaction outcomes, aiding in the discovery of new synthetic routes and compound synthesis.

Challenges in AI in Drug Discovery:

Drug delivery systems encounter various challenges in the domain of artificial intelligence (AI). One of these challenges pertains to the requirement for accurate and regulated drug discharge, a matter that can be tackled by utilizing nanocarriers and nano systems. Another challenge lies in the limited accessibility of drugs in ocular tissue, attributed to physiological and dynamic barriers within the eye. To surmount these hurdles and enhance drug concentration in the eye, nanotechnology platforms, specifically nano micelles, nanoparticles, and liposomes, have been devised. Furthermore, the advancement of

synthetic nanomotors and the utilization of natural motors, such as bacteria and sperm, exhibit potential in the realm of targeted drug delivery. These motors possess the capability to navigate the body and administer drugs in specific locations, thereby minimizing exposure to healthy tissues and reducing adverse effects.

2. Conclusion

The use of AI in novel drug delivery systems has the potential to revolutionize the field of medicine. AI powered drug delivery systems can improve drug efficacy, reduce side effects, and enhance patient outcomes. The most significant worry regarding AI is the job losses. So, for that a strong implementation and proper regulations must be followed. However, these technologies intended only to make life easier through smooth work, but it cannot replace human humans. It would contribute to synthesis of newer drug with desired molecules which can act on its specific site and specific route, which would minimise the adverse drug reaction and increases the effectiveness of drug. As AI technology continues to advance, we can expect to see even more innovative drug delivery systems that are designed to meet the specific needs of individual patients regarding various novel techniques used for improving safety and efficacy of phytomedicines and application of novel formulation. AI would become an invaluable tool in the pharmaceutical industry in the near future.

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