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Original Article

Artificial Intelligence in Pharmacy: A Boon for Drug Delivery & Drug Discovery

Sayali Gandhi, Varsharani Avhad, Kalyani Raut, Nalini Javane, Meet Shah, Swapnil Katkhade

Arihant College of Pharmacy, Kedgaon, Ahilyanagar, Maharashtra, India 414005

ABSTRACT

Artificial Intelligence (AI) is increasingly recognized as a game-changer in the pharmaceutical industry, especially in the fields of drug discovery and drug delivery. The integration of Artificial Intelligence (AI) into pharmacy practices represents a transformative advancement in drug delivery systems. Recent pharmaceutical research shows that significantly evolved artificial intelligence (AI) and machine learning Techniques are promising to facilitate the drug delivery system development. The intersection of artificial intelligence (AI) and pharmacy has ushered in a new era of drug delivery, marked by unprecedented precision, efficiency, and personalization. AI, with its ability to process vast amounts of data, identify patterns, and make intelligent decisions, is revolutionizing various aspects of drug development, manufacturing, and distribution. This paper explores the profound impact AI technologies are having on the optimization of pharmaceutical delivery mechanisms. By examining recent innovations and case studies, this presentation elucidates how AI is revolutionizing drug delivery, offering a substantial boon to pharmaceutical practice and patient care. AI can process big data, reveal potential correlations, provide accurate predictions, and navigate in a high-dimensional space, offering great potential to change the drug delivery research paradigm. Data-driven approaches can be applied to all aspects of the pharmaceutical field, across preformulation studies, formulation screening, and precision medicine in the clinic. Personalized medicine approaches can be facilitated through AI algorithms that analyze real-world patient data, leading to more effective treatment outcomes and improved patient adherence. Artificial Intelligence (AI) is revolutionizing the field of drug discovery by enhancing the efficiency, accuracy, and speed of identifying potential drug candidates. AI technologies, such as machine learning, deep learning, and natural language processing, are being increasingly integrated into various stages of drug discovery, including target identification, compound screening, lead optimization, and clinical trial design. This review explores the transformative potential of AI, focusing on how it is revolutionizing both the discovery of new drugs and the optimization of drug delivery systems.

Keywords: Artificial intelligence, Drug Delivery Design, Drug Discovery, Pharmacokinetics, Pharmacodynamics, Machine learning, Deep Learning, Drug Delivery System.

INTRODUCTION

Drug delivery is entering the mainstream orbit of the pharmaceutical industry due to the dramatically increasing cost of developing new molecular entities (NMEs). Drug delivery is a technique of delivering medication to a patient in such a manner that specifically increases the drug concentration in some parts of the body as compared to others. The ultimate goal of any delivery system is to extend, confine and target the drug in the diseased tissue with a protected interaction. Drug discovery is a process through which new medications against diseases are discovered. Drug discovery, a complex and time-consuming process, has been significantly accelerated by AI. Traditional drug discovery processes are often time-consuming and costly, typically requiring over a decade and billions of dollars to bring a new drug to market. Machine learning algorithms can analyse vast datasets of chemical structures, biological assays, and clinical trial results to identify potential drug candidates. By predicting molecular properties, target interactions, and off-target effects, AI helps researchers prioritize compounds with higher likelihoods of success. Moreover, AI-powered generative models can design novel molecules with desired properties, expanding the chemical space and increasing the chances of discovering breakthrough drugs. AI's integration into pharmacy represents a significant advancement, potentially increasing the efficacy and efficiency of drug delivery systems and improving patient outcomes. The comprehensive review explores the wide-ranging applications of AI

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in drug discovery, drug delivery dosage form designs, process optimization, testing, and pharmacokinetics/pharmacodynamics (PK/PD) studies. 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 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. AI-driven approaches can analyze vast datasets-ranging from genetic information to clinical trial results-and identify complex patterns that may not be immediately evident to human researchers. This ability accelerates the identification of novel therapeutic targets and the prediction of drug interactions, reducing the time required for drug development. Furthermore, AI systems are capable of simulating drug behaviour in biological systems, which minimizes the need for extensive experimental testing in the initial phases.

Content -

AI has made substantial strides in drug formulation optimization. Traditional methods of formulation development are often iterative and time-consuming. AI, on the other hand, can simulate various formulation parameters, such as excipients, pH, and temperature, to predict drug release profiles, stability, and bioavailability. By optimizing formulations, AI can enhance drug efficacy, reduce side effects, and improve patient compliance. Furthermore, AI can assist in the development of controlled-release systems, which can deliver drugs at predetermined rates, ensuring sustained therapeutic levels and minimizing dosing frequency. AI plays a crucial role in enabling personalized drug delivery. Moreover, AI can help identify counterfeit drugs and prevent their entry into the healthcare system, safeguarding public health. By analyzing patient genomics, electronic health records, and other relevant data, AI can identify biomarkers that predict drug response and toxicity. This information can be used to select the most appropriate drugs and dosages for each patient, maximizing efficacy while minimizing adverse events. Additionally, AI can assist in the development of targeted drug delivery systems, which can deliver drugs directly to the site of action, reducing systemic exposure and improving therapeutic outcomes. Supply chain management is another area where AI is making a significant impact. AI-powered analytics can optimize inventory levels, track drug shipments in real-time, and predict potential disruptions. By improving supply chain efficiency, AI can ensure that patients have access to the medications they need when they need them. Artificial intelligence (AI) has emerged as a powerful tool that harnesses anthropomorphic knowledge and provides expedited solutions to complex challenges. Companies and research institutions are leveraging AI to repurpose existing drugs for new indications, optimize drug combinations, and design new molecules with desired properties. As AI continues to advance, it holds the potential to reduce costs and improve the success rates of drug discovery, ultimately delivering more effective treatments to patients.

AI in Drug Delivery -

Artificial Intelligence (AI) has revolutionized various sectors, including the pharmaceutical industry. In drug delivery, AI offers numerous advantages, optimizing the process from drug design to patient-specific treatment. Here's how AI is proving to be a boon:

1. **Personalized Drug Delivery:** AI algorithms can analyze large datasets to predict how individual patients will respond to specific drugs. By integrating genetic, lifestyle, and environmental factors, AI helps in the creation of personalized treatment plans, ensuring that the right drug reaches the right patient in the most effective way.

Key Aspects:

- **Optimized Dosing:** AI can predict the exact dosage and timing for drug administration to maximize therapeutic outcomes while reducing the risk of adverse effects.
- **Real-Time Adjustments:** AI-powered systems can adapt the delivery of medication in real-time based on continuous monitoring of a patient's health metrics, such as blood glucose or blood pressure.
- **Improved Adherence:** AI can be used to develop wearable devices or smart pills that remind patients to take their medication, improving compliance with treatment regimens

2. **Enhancing Drug Formulations:** AI assists in optimizing drug formulations for better absorption and targeted delivery. Through machine learning models, AI can predict how different drug compositions will behave in the body, reducing the need for extensive experimental trials.
   Key aspects:
   - **Molecular Simulation:** AI-based algorithms can model how drug molecules will behave in various environments within the body.
   - **High-Throughput Screening:** AI can analyse vast amounts of data from high-throughput screening to identify the best drug candidates.
   - **Bioavailability Prediction:** AI tools can predict which formulations will maximize the bioavailability of a drug.
3. **Predicting Drug-Target Interactions:** AI can model complex biological interactions, enabling researchers to predict how drugs interact with specific cellular targets. This improves the accuracy of drug targeting and reduces side effects, making treatments more efficient.
4. **Optimizing Nanotechnology in Drug Delivery:** AI-driven simulations help design nanoparticles for targeted drug delivery systems. It aids in predicting the behaviour of Nano carriers in biological environments, enhancing the precision of therapies like cancer treatment.
   Key aspects:
   - **Nanotechnology:** AI can assist in designing nanoparticles that can carry drugs directly to specific tissues, improving efficacy and minimizing off-target effects.
   - **Molecular Targeting:** Machine learning algorithms can predict which molecules or receptors on target cells should be targeted by drug delivery systems.
   - **Dynamic Targeting:** AI can help adjust targeting strategies dynamically based on tumour progression or other changing conditions.
5. **Drug Release Optimization:** AI can optimize the release mechanisms of drug delivery systems to ensure that drugs are delivered in the right amounts at the right times. For example, AI can be used to design controlled release systems such as microspheres, liposomes, or implants that release drugs in a sustained or responsive manner
   Key aspects:
   - **Controlled Release Kinetics:** AI can predict the optimal release profile of drugs in various delivery systems.
   - **Responsive Delivery:** AI can optimize "on-demand" or "stimuli-responsive" drug release, where drug delivery is triggered by a specific condition (like temperature, pH, or enzyme activity)
   - **Long-Term Drug Release:** AI can assist in the design of drug delivery systems that provide sustained drug release over a prolonged period, reducing the need for frequent dosing.
6. **AI in Smart Drug Delivery Devices:** AI can be integrated with smart drug delivery systems like wearable devices or implantable pumps. These devices can autonomously adjust the drug dosage in response to real-time patient data, improving safety and effectiveness.
   Key aspects:
   - **Real-Time Monitoring:** AI-driven devices can track patient vitals and adjust drug delivery automatically.
   - **Controlled Release:** Using AI, these systems can ensure that drugs are delivered at the correct dose and timing.
   - **Wearables:** AI can power wearable devices like insulin pumps, transdermal patches, or inhalers that adjust drug delivery according to real-time data.
7. **Reducing Time and Costs in Drug Development:** Traditional drug development is time-consuming and costly. AI accelerates this process by analyzing vast datasets and running simulations to identify optimal drug candidates faster than conventional methods, reducing the overall cost of drug development.

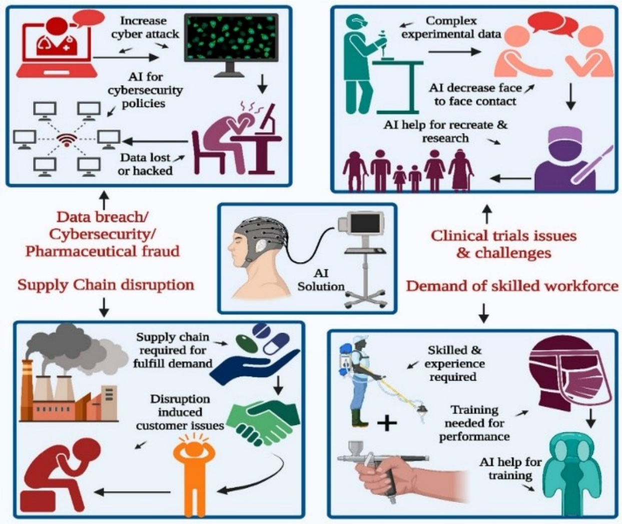

Fig 1 : Depicts a possible artificial intelligence (AI) solution to the pharmaceutical industry's challenges: acquiring a proficient workforce is a prerequisite in all sectors to leverage their expertise, proficiency, and aptitude in product innovation. The second pertains to supply chain disruption and clinical trial experimentation challenges. The incidence of cyberattacks is on the rise, with data breaches and security emerging as significant concerns for the industry.

The integration of AI and big data in the field of pharmaceutics has led to the development of computational pharmaceutics, which aims to enhance drug delivery processes by utilizing multiscale modelling approaches. Computational pharmaceutics employs AI algorithms and machine learning techniques to analyze large datasets and predict drug behaviour. By simulating drug formulation and delivery processes, researchers can evaluate various scenarios and optimize drug delivery systems without the need for extensive trial-and-error experiments. This accelerates the drug development timeline, reduces costs, and increases productivity. Computational pharmaceutics involves modelling drug delivery systems at different scales, ranging from molecular interactions to macroscopic behaviour. AI algorithms can analyze complex relationships between drug properties, formulation components, and physiological factors to predict drug behaviour at each scale. This allows for a more comprehensive understanding of drug delivery mechanisms and aids in designing efficient drug delivery systems. It helps in the prediction of the physicochemical properties of the drug, the in vitro drug release profile, and the stability of the drug. The same technology is also implemented for the better assessment of in vivo pharmacokinetic parameters and drug distribution along with in vivo-in vitro correlation studies. By utilizing the right set of AI tools, researchers can identify potential risks and challenges associated with drug delivery systems early in the development process. This allows for proactive modifications and adjustments to mitigate risks and optimize drug performance. The use of AI and computational modelling reduces the reliance on time-consuming and expensive trial-and-error experiments, minimizing the chances of unforeseen outcomes.

Application Of artificial intelligence (AI) in Drug Delivery:

- It involves leveraging advanced algorithms, machine learning, and data analytics to optimize the design, development, and administration of pharmaceutical agents.
- AI can be utilized to predict drug interactions, personalize drug regimens, and identify optimal drug delivery systems.
- It enhancing therapeutic efficacy while minimizing side effects.
- Additionally, AI-driven models can be employed in the development of Nano carriers, improving the targeted delivery of drugs to specific cells or tissues, thereby advancing precision medicine. By delving into vast datasets, AI can ultimately facilitate faster drug discovery and more effective treatment strategies.

Challenges Of Artificial intelligence (AI) in Drug Delivery:

- The effectiveness of drug delivery can vary greatly across individuals due to factors like genetics, age, gender, and comorbidities.
- Any error in drug dosing, delivery, or prediction of adverse effects could have serious consequences, making validation and testing a critical step.
- Successful drug delivery systems require collaboration between multiple disciplines, including AI, pharmacology, materials science, and clinical medicine. Coordinating these areas effectively can be challenging.
- AI-powered drug delivery systems in healthcare requires significant investment in both technology and infrastructure.

Fig 2 : Conventional Drug Delivery System and their limitations

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, Since then, AI has been applied cross various stages of drug discovery, encompassing great Identification lead optimization, and drug design. 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.

AI in Drug Discovery:

One of the most important baseline for a pharmaceutical industry is the drug discovery. The average time taken for a drug to reach the market is about 14 years, with a whopping cost of an average $2.6 billion. Moreover, the selection of a new successful drug molecule is the toughest task from the cluster of prospective pharmacological active chemical entities (lead molecules). With the help of AI, researchers are able to select few clinically effective candidates out of thousands of molecules with the help of computer- aided drug design software in a lesser amount of time, whereas, traditional methods may require years together.

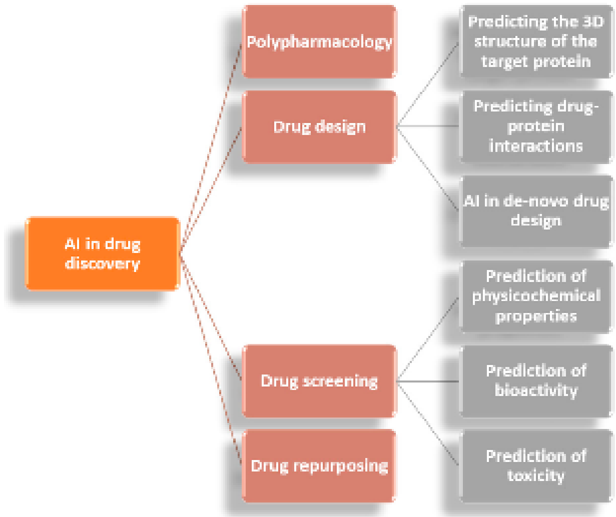

Fig 3: Application Of AI in Drug Discovery

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

2. 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.

3.Structural Activity Relationship Modelling: 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.

4. 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.

5. 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.

6. 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.

7. Hit Identification and Lead Optimization: Virtual screening using AI helps researchers identify potential "hits" from large chemical libraries more efficiently. It also assists in optimizing lead compounds by predicting their binding affinity, bioavailability, and toxicity. This helps in narrowing down the best candidates for further development.

8. Clinical Trials: AI is used to optimize the design of clinical trials by predicting patient responses, identifying suitable participants, and determining optimal dosing strategies. This can reduce the time and cost of clinical trials while increasing success rates.

9. Target Fishing Technology and its Role with AI: Target fishing, a computational method utilized in drug discovery, has become a pivotal technique for Polypharmacology, drug repurposing, and the detection of novel drug targets. It enables the determination of protein targets for a given molecule, elucidates the mechanism of action, and unveils the off targets of drug candidates. 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. 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 emerging approach in drug discovery. It helps identify protein targets and off targets of drug candidates.

Application of AI in Drug Discovery:

- Drug repurposing
- De novo drug design
- Biomarker discovery
- Personalized medicine
- Another important application of AI in drug Discovery is the identification of drug-drug interactions that take place when several drugs are combined for the same or different diseases in the same patient, resulting in altered effects or adverse reactions

Challenges Of AI In Drug Discovery -

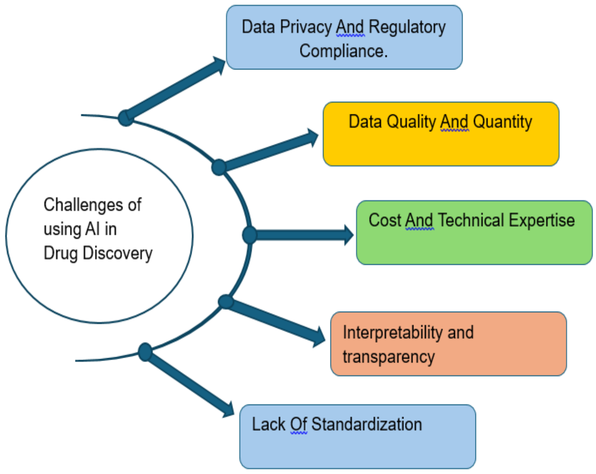

Fig 4: Challenges of AI in Drug Discovery

CONCLUSION

In conclusion, Artificial Intelligence (AI) is a powerful tool in pharmacy, revolutionizing both drug delivery and drug discovery. AI enhances drug delivery by enabling personalized, targeted, and efficient systems that improve treatment precision and reduce side effects. In drug discovery, AI accelerates the identification of promising drug candidates, optimizes clinical trials, and aids in drug repurposing. Despite challenges such as data privacy and regulatory concerns, AI's potential to improve drug efficacy, safety, and development timelines marks a significant advancement in pharmaceutical practices, ultimately benefiting patient care and healthcare outcomes.

REFERENCE

1. Chowdhury, A., "Artificial Intelligence: Transforming Drug Delivery Systems," Journal of Advanced Drug Delivery Science, 2021.

2. Mack, K. K., Pichika, M. R., "Artificial Intelligence in Drug Development: Present and Future," Drug Discovery Today, 2019.
3. Vamathevan, J., et al., "Applications of Machine Learning in Drug Discovery and Development," Nature Reviews Drug Discovery, 2019.
4. Schneider, P., Walters, W. P., & Plowright, A. T. (2020). Rethinking drug design in the artificial intelligence era. Nature Reviews Drug Discovery, 19(5), 353-364.
5. Vamathevan, J., Clark, D., Czodrowski, P., Dunham, I., Hackett, B., Millan, M. J., ... & Zhao, S. (2019). Applications of machine learning in drug discovery and development. Nature Reviews Drug Discovery, 18(6), 463-477.
6. Zhavoronkov, A., et al. (2019). Deep learning enables rapid identification of potent DDR1 kinase inhibitors. Nature Biotechnology, 37(9), 1038-1040.
7. Hassanzadeh P, Atyabi F, Dinarvand R. The significance of artificial intelligence in drug delivery system design. Advanced drug delivery reviews. 2019 Nov 1;151:169-90
8. Luo M, Feng Y, Wang T, Guan J. Micro-/nan robots at work in active drug delivery. Advanced Functional Materials. 2018 Jun;28(25):1706100.
9. Dara, S.; Dhamercherla, S.; Yadav, S.S.; Babu, C.M.; Ahsan, M.J. Machine Learning in Drug Discovery: A Review. Artif. Intell. Rev. 2022, 55, 1947–19
10. Colombo, S. (2020). Applications of artificial intelligence in drug delivery and pharmaceutical development. Artificial Intelligence in Healthcare, 85–116. https://doi.org/10.1016/B978-0-12-818438-7.00004-6
11. Buntz, B. 6 Signs AI Momentum in Drug Discovery Is Building. Available online: https://www.drugdiscoverytrends.com/six-signs-ai-driven-drug-discovery-trends-pharma-industry
12. Wirtz BW, Weyerer JC, Geyer C. Artificial intelligence and the public sector—applications and challenges. International Journal of Public Administration. 2019 May 19;42(7):596-615.
13. Blasius A, Khong J, Kee T. CURATE. AI: optimizing personalized medicine with artificial intelligence. SLAS technology. 2020 Apr 1;25(2):95-105.
14. Baronzio G, Parmar G, Baronzio M. Overview of methods for overcoming hindrance to drug delivery to tumours, with special attention to tumour interstitial fluid. Frontiers in oncology. 2015 Jul 23;5:165
15. Mack KK, Pichika MR. Artificial intelligence in drug development: present status and future prospects. Drug discovery today. 2019 Mar 1;24(3):773-80.
16. Mishra V. Artificial intelligence: the beginning of a new era in pharmacy profession. Asian Journal of Pharmaceutics (AJP). 2018 May 30;12(02).
17. Sell wood MA, Ahmed M, Segler MH, Brown N. Artificial intelligence in drug discovery. Future medicinal chemistry. 2018 Sep;10(17):2025-8.
18. Zhu H. Big data and artificial intelligence modelling for drug discovery. Annual review of pharmacology and toxicology. 2020 Jan 1;60:573
19. Chan HS, Shan H, Dahoun T, Vogel H, Yuan S. Advancing drug discovery via artificial intelligence. Trends in pharmacological sciences. 2019 Aug 1;40(8):592-604.
20. Pereira JC, Caffarena ER, Dos Santos CN. Boosting docking-based virtual screening with deep learning. Journal of chemical information and modeling. 2016 Dec 27;56(12):2495-506.
21. Yang X, Wang Y, Byrne R, Schneider G, Yang S. Concepts of artificial intelligence for computer-assisted drug discovery. Chemical reviews. 2019 Jul 11;119(18):10520-94.
22. Kumar R, Sharma A, Siddiqui MH, Tiwari RK. Prediction of human intestinal absorption of compounds using artificial intelligence techniques. Current drug discovery technologies. 2017 Dec 1;14(4):244-54.
23. Presides A. The benefits of drug repositioning. Drug Discovery World. 2011;12:9-12.
24. Reddy AS, Zhang S. Polypharmacology: drug discovery for the future. Expert review of clinical pharmacology. 2013 Jan 1;6(1):41-7.
25. Schneider G, Clark DE. Automated de novo drug design: are we nearly there yet?. Angewandte Chemie International Edition. 2019 Aug 5;58(32):10792-8
26. Paul D, Sanap G, Shenoy S, Kalyane D, Kalia K, Tekade RK. Artificial intelligence in drug discovery and development. Drug discovery today. 2021 Jan;26(1):80.

27. Hassanzadeh P, Atyabi F, Dinarvand R. The significance of artificial intelligence in drug delivery system design. Advanced drug delivery reviews. 2019 Nov 1;151:169-90.
28. Vora LK, Gholap AD, Jetha K, Thakur RRS, Solanki HK, Chavda VP. Artificial Intelligence in Pharmaceutical Technology and Drug Delivery Design. Pharmaceutics.2023 Jul 10; 15 (7): 1916.
29. Alshawwa SZ, Kassem AA, Farad RM, Mostafa SK, Labib GS. Nano carrier Drug Delivery Systems: Characterization, Limitations, Future Perspectives and Implementation of Artificial Intelligence. Pharmaceutics.2022 Apr 18; 14 (4): 883.
30. Das KP, J C. Nanoparticles and convergence of artificial intelligence for targeted drug delivery for cancer therapy: Current progress and challenges. Front Med Technol.2023 Jan 6; 4: 1067144.

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