# Machine Learning-Based Enhanced Drug Delivery System and Its Applications – A Systematic Review

Abhijeet Madhukar Haval [1*], Kumar Shwetabh [1], Sushree Sasmita Dash [1]

## Abstract

Machine Learning (ML) methods offer advanced algorithms and tools to enhance drug development. Quantitative Structure-Activity Relationship (QSAR) approaches have successfully predicted several physicochemical aspects of pharmaceuticals, including toxicity, intake, drug-drug interactions, carcinogenesis, and dispersion. ML, a branch of artificial intelligence, has demonstrated significant promise in drug development. The methods presented in this study can model non-linear databases and handle big data that is becoming more extensive and intricate. Diverse ML methodologies are currently employed for making forecasts of drug targets, modeling the framework of drug targets, forecasting binding sites, conducting ligand-based similarity searches, designing novel ligands with specific properties, creating scoring algorithms for molecular docking, constructing QSAR models for predicting biological reactions, and forecasting the pharmacokinetic and pharmacodynamic characteristics of ligands. The findings of this study illustrate the widespread utilization of ML techniques in drug discovery, suggesting a favorable outlook for these advances. These findings have the potential to facilitate further exploration of ML in connection with drug discovery and growth by researchers, learners, and pharmaceutical companies.

**Keywords:** Drug Delivery, Pharmaceutical Industry, Machine Learning, Applications

***Significance*** | Machine Learning (ML) transforms drug development, predicting drug properties, targets, interactions, and facilitating efficient exploration for researchers and pharmaceutical companies.

*Correspondence. Abhijeet Madhukar Haval, Faculty of CS & IT, Kalinga University, Naya Raipur, Chhattisgarh, India.
E-mail: ku.abhijeetmadhukarhaval@kalingauniversity.ac.in

Editor Fouad Saleh Resq Al-Suede And accepted by the Editorial Board Jan 22, 2024 (received for review Nov 13, 2023)

## 1. Introduction

Life is inherently dynamic, and people strive to influence these fluctuations, particularly in health and medicine. These fields concentrate on generating or identifying chemical substances, combinations, and usage to alleviate distress. For several years, the production of pharmaceuticals has been overseen by a system that ensures the finished goods by examining the primary materials used throughout the production, the features of the finished item, batch-based activities, and consistent processing conditions (Caban, Stepnowski, 2021) (Bavumiragira and Yin, 2022).

Drug and biopharmaceutical companies have served as a significant source of innovative and original inventions or machines and have spearheaded the advancement of new concepts or links in chemical and physical design Dagenais et al. (2022). The pharmaceutical sector requires urgent mechanical development to facilitate the development of drugs for human consumption Xu et al. (2021). The development and production of intricate pharmaceuticals that are safe for human use and can be manufactured on a large scale have proven difficult due to the current constraints on technical resources. Existing prescription medications rely on a universal strategy, but certain crucial areas of medicine necessitate innovative techniques and the creation of new pharmacological procedures Bochicchio et al. (2021).

**Author Affiliation.**
[1] Faculty of CS & IT, Kalinga University, Naya Raipur, Chhattisgarh, India.

**Please cite this article.**
Abhijeet Madhukar Haval, Kumar Shwetabh, Sushree Sasmita Dash, (2024). Machine Learning-Based Enhanced Drug Delivery System and Its Applications – A Systematic Review, Journal of Angiotherapy, 8(1), 1-9, 9480

Advancements in genetics and diagnosis have facilitated the development of innovative treatments and strategies, utilizing state-of-the-art analytical devices and accurate dosages. Customized medications specifically designed to match the patient's biological characteristics will enhance the efficacy of this sector Mazarura et al. (2022). The current level of progress in medical planning and manufacturing of these products needs to be improved to meet the requirements of personalized medicine. The pharmaceutical industry necessitates novel manufacturing assembly systems that facilitate the flexible production of bespoke apparatus and technologies Bannigan et al. (2021).

The utilization of Machine Learning (ML) is on the rise and is expected to revolutionize the methods employed in clinical evaluation and training Chang et al. (2023). Medical professionals have the opportunity to contribute to the advancement of this technique for application in the healthcare and pharmaceutical sectors, therefore ensuring that the full potential of ML to enhance healthcare is realized. ML is being employed in the pharmaceutical industry for primary purposes Boso et al. (2020). One aspect is evaluating the extent of the illness and forecasting the likelihood of therapy efficacy for a specific patient, even before it is given. It is employed to avert or resolve issues that arise throughout treatment. One of its primary applications is as a gadget for medical operations or surgeries on participants Bertolini et al. (2021) Rai et al. (2021). The rationales for using specific devices or compounds in therapy and devising or inferring novel applications for gadgets or chemicals to enhance safety and effectiveness.

ML also plays a broader role in the handling and examination of large datasets. Big data refers to obtaining and analyzing massive datasets, which leads to discovering or understanding new information. As the volume of data in the pharmaceutical sector grows, conventional storage solutions must be updated Kibria et al. (2023). Big data presents a significant opportunity for conducting more comprehensive research through mining data in the industry Zhang et al. (2021). This can enhance the production of pharmaceuticals by implementing a three-step data handling procedure after acquiring the information. The process involves extracting and compiling diverse and scattered information, configuring the information to ensure consistent design, and analyzing the information using different analytical systems Carpenter et al. (2018). The outcome of this evaluation can inform decisions regarding the development of chemicals or medication, as well as the selection of processes to maximize efficiency Bao et al. (2023).

The medication and development sectors aggressively use ML-enabled technologies to address small yet critical challenges. This is owing to the innovations, growth, and use of large volumes of information, which allows for generating relevant insights Mozafari et al. (2023). Hence, the research recognizes the necessity of creating a thorough ML and big data impact on drug discovery and growth. This article will encompass the most recent technology, advancements, and innovative studies conducted in this domain. It will also explore the potential future implications for the pharmaceutical sector when it effectively integrates modern machine-learning techniques.

The subsequent sections are organized in the specified sequence: Section 2 provides an overview and review of the existing research and literature on the medication delivery mechanism. Section 3 examines the techniques employed in drug distribution, as well as the many applications of drug delivery. Section 3 also addresses the difficulties and potential future opportunities of medication delivery applications. Section 4 demonstrates the culmination of the drug delivery applications using ML.

## 2. Literature review of drug delivery systems

This section comprehensively examines and evaluates drug delivery methods by reviewing relevant literature. Below, the research will review the current methodologies, their advantages, and the outcomes obtained.

De Oliveira et al. formulated and analyzed particles that included babassu oil alone or combined with Moderate-Chain Triglycerides (MCT) in the central region de Oliveira et al. (2023). The purpose was to investigate various Hydrophilic-Lipophilical Balance (HLB) values and assess the encapsulation of a representative water-soluble molecule. Multiple methodologies were employed to analyze the properties of all products, namely their size and dispersion. An in vitro drug release study was also conducted using the dialysis method. The results indicate that the nanoparticles enhance the encasement of a model hydrophilic compound. Multiple elements are assessed to modify the hydrophilic ability of the core and the immersion of chemicals.

Palugan et al. sought to provide a concise overview of the progression of intravesical medication administration, emphasizing the advancement of delivery methods that can sustain optimal levels of bioactive substances in the bladder for specific durations Palugan et al. (2021). Significant attention was given to solid dose forms that remain in the body for an extended period, focusing on 3D and 4D printed gadgets.

Diniz et al. discuss advanced techniques, such as polyclonal antigens, monoclonal antigen-drug mixtures, and nanomaterials, that precisely and carefully target tumor-related carbohydrates in malignant tissues Diniz et al. (2022). Utilizing nanomaterials in drug delivery involves innovative applications in cancer treatment, such as vaccinations enclosed in artificial nanomaterials and specialized nanomaterials that selectively target glycoproteins or glycan-binding enzymes.

Sheng et al. provide a new method for delivering methotrexate (MTX) and Asp to individuals with colon cancer. This method

involves using $CaCO_3$ microspheres-entrapped hydrogels for chemotherapy and pain management Sheng et al. (2021). The findings of the in vitro release study and viability of cells test indicate that the suggested Dual-Drug Delivery Strategy (DDDS) effectively safeguards the anti-cancer medication MTX against absorption in the stomachs and small intestines. The drug remains potent and effective, specifically at the intended location in the colorectum.

Ma et al. introduced an innovative method for simulating the pharmacokinetics (PK) and PK-pharmacodynamics (PK-PD) of an injectable nano-drug delivering device Ma et al. (2023). This methodology is designed to forecast the speed and dispersion of free-drugs and encapsulating drugs precisely. The novel technique will significantly contribute to advancing scutellarin emulsified as a prototype for drug delivery systems. It will offer a valuable understanding of the practical application of nanotechnologies in clinical settings and offer promising prospects for the future of personalized health and individualized healthcare.

Sharma et al. provided a concise overview of the latest nanostructure-integrated Extracellular Vesicles (EVs) advancements for medication administration, therapies, and the real-time tracking of disease development Sharma et al. (2021). This paper examines the exosomal vehicles, varied drug delivering framework, and biomimetic nanomaterials related to targeted drug administration. It also discusses the requirements and difficulties associated with EV-related biomimetic nanomaterials and offers a further perspective on the proposed solutions.

He et al. aim to assess the importance, fundamental principles, and commonly used Artificial Intelligence (AI) methods in medication administration to manage infectious diseases (He, Leanse, Feng, 2021). The research will concentrate on the accomplishments and significant discoveries of current studies in the field. The research will explore how AI is utilized in drug delivery for the entire antimicrobial therapy process. This will include creating medications, optimizing treatment regimens, designing drug delivery systems and governance routes, and predicting drug delivery outcomes.

To decrease the computational expenses associated with a completely fluctuating Large Eddy Simulation flow area, Calmet et al. devised a method to generate a time-averaged frozen place Calmet et al. (2023). They then conducted a time-integrated analysis of particle pathways within the flow growing to ascertain the deposition of particles in four specific anatomical areas of the nasal passageway for every of the 384 spray fields. The present research examined the impact of six spraying input variables on the coating efficiency in four anatomical areas.

Harrison et al. employed Convolutional Neural Networks to extract per-cell information during the initial time points Harrison et al. (2021). These characteristics were merged and investigated utilizing either a Long Short-Term Memory (LSTM) or time series extraction of features and gradient boost machinery. The findings emphasize the advantage of including time dynamics in analyzing medication distribution through high-content imagery.

The current literature needs more sophisticated machine-learning techniques for drug discovery, delivery, and other pharmacology applications. The following section explores the utilization of machine learning in medication delivery applications.

## 3. Drug delivery systems and applications of machine learning

This section discusses the drug delivery system with ML for drug production and other possible applications. Figure 1 depicts a streamlined sequence of events that occur during the integration of ML in the pharmaceutical business, particularly in the domains of creation and manufacture. It illustrates the fundamental workings of ML. The information has many elements, including orthogonal information, applicability area, and termination information.

The data is inputted into a pre-existing system considering model selections, selection operations, and orthogonal calculations. The method produces outcomes and iterative enhancements to the existing technique and processes to enhance efficiency and dependability. The approach undergoes modifications, and this iterative process continues until a definitive product is conceived and produced.

Figure 2 illustrates the integration of ML into vaccine research and growth procedures and the innovative uses of ML in the pharmaceutical sector. The drug discovery process comprises four components: drug development, polypharmacology, reusing drugs, and vaccine evaluation. The main usage of ML is in determining medicinal qualities, potentially decreasing the requirement for clinical studies and research. This would bring about economic and ethical advantages. This section discusses the papers in this study that endorse ML use in the drug development process to enhance efficiency, precision, and production.

### 3.1 Prediction of 3D structure

Proteins are commonly selected as drug targets in most drug discovery endeavors, aiming to develop treatments. Various supervised and unsupervised ML methods have been employed to predict the design of proteins at different levels of evaluation, including the structural characteristics in the main pattern of amino acids, the spatial arrangement of amino acids, the three-dimensional form of the proteins, and the performance of multiple protein subunits. ML techniques are employed to forecast the secondary framework, solvent availability, structure, and contact mapping. These forecasts are then utilized to construct a 3D model of the targets. ML-based prediction method for drug delivery is shown in Figure 3.

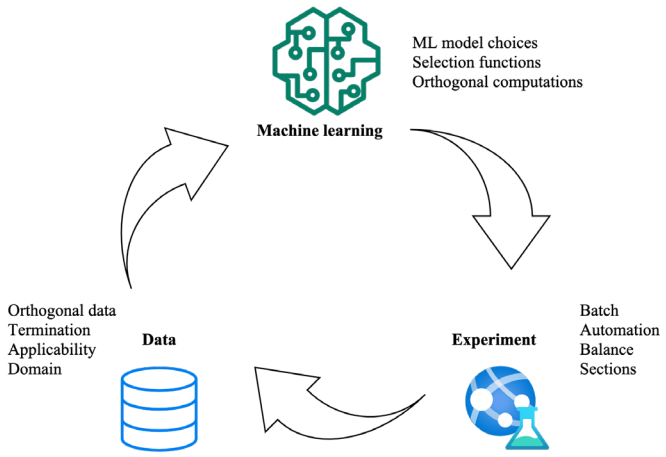


Figure 1. Pharmaceutical Industry Cyclic Process

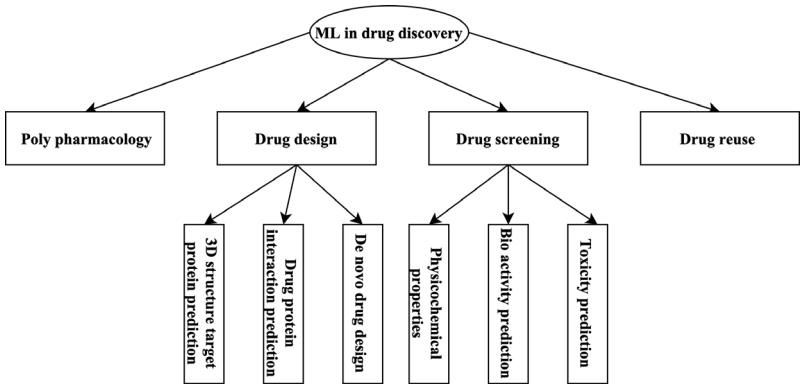


Figure 2. Ml-Based Drug Discovery Methods

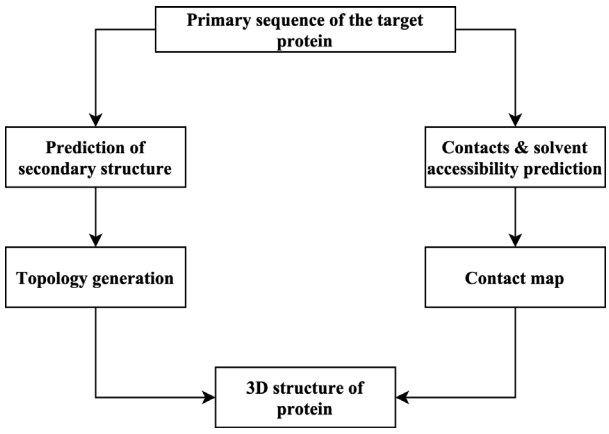


Figure 3. Ml-Based Prediction Method For Drug Delivery

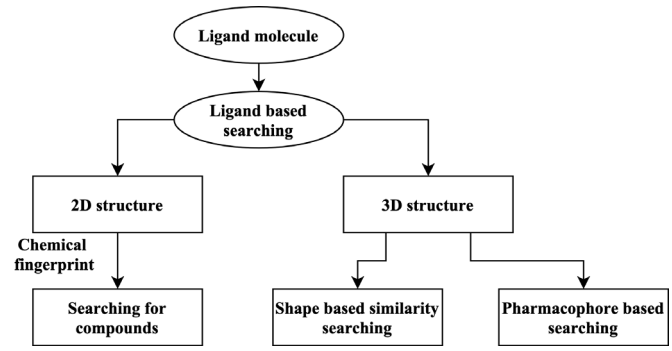


Figure 4. Ligand Molecule-Based Approaches

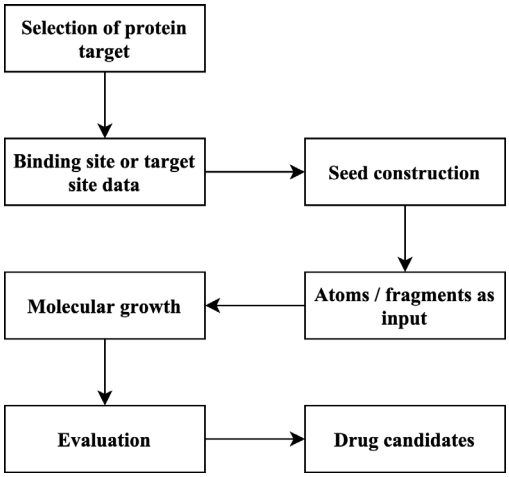


Figure 5. Drug Design Process

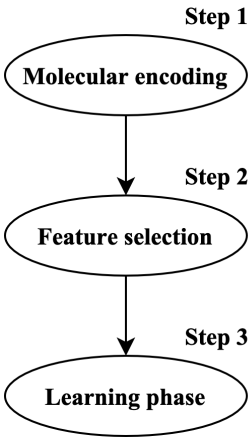


Figure 6. ML-Based Drug Delivery System Process

The Support Vector Machine (SVM) and Decision Tree (DT) were employed to generate rules for predicting secondary patterns in training data sets. Artificial Neural Networks (ANN) are used to forecast the distances separating pairs of amino acid groups. This information is then employed to build the possibility of mean power, which is crucial for developing the structure of a protein. ML techniques are also used for fold identification and model validation. The conjugate slope descent and Monte Carlo procedures are optimization strategies for constructing three-dimensional models. During model creation, many potential models are created and organized into clusters using k-means clustering based on the designs' similarities. ML techniques have also been employed to rank the algorithms and evaluate the accuracy of the predicted architecture.

3.2 Ligand-based similarity searching and virtual screening

One bioactive ligand can be employed as a source to query an extensive collection of analogous chemicals from a chemical repository. ML techniques, such as kernel discriminating and naïve Bayesian classification techniques, have been employed to do virtual screening by examining the characteristics of a bioactive compound. The process involves searching, scoring, and screening comparable compounds related to their distance-based similarities and functional category compatibility with the input bioactive chemical. In a chemical resemblance search that relies on distance, the resemblance between two substances is calculated using the Tanimoto factor of their molecular fingerprinting. The functional group similarities are encoded as a binary vector of features. Chemical fingerprints, form, and pharmacophore-based similarity methods are employed to explore an extensive collection of molecules similar to a given input component. The categorization and grouping techniques are employed in the virtual screening of compounds. The categorization involves using binary classification techniques, such as active and inactive, to categorize the ligands. The grouping clusters the ligands together depending on their resemblance or distance measurements. Figure 4 shows the Ligand molecule-based approaches.

3.3 De novo design of molecules

Computational methods can produce chemical compounds with specific physicochemical and biological characteristics. Supervised learning methods are employed to assist the model in generating chemically viable sequences and evaluating the physical characteristics of molecules. Reinforcement Learning for Structural Evolution is an algorithm that uses deep reinforcement learning to develop and evaluate the biological aspects of newly created molecules. A ligand-generating model utilizing Recurrent Neural Networks (RNNs) has been made. This model extracts pertinent chemical and physical data from many known bioactive compounds. The process of creating new drug alternatives with specific features depending on the target's binding location is illustrated in Figure 5.

3.4 Quantitative structural-activity relationships (QSAR)

QSAR is founded on the idea that the arrangement of an atom could impact its physical, substance, and biological characteristics. QSAR has been employed for four decades in several branches of chemistry, such as agrochemistry, pharmaceutical chemicals, toxicity, and other related fields. QSAR has successfully simulated several physiochemical aspects, including toxicity, digestion, drug interactions, and carcinogenesis. The initial QSAR designs, such as Hansch and free-Wilson evaluation, employed regression techniques to establish a relationship between potency and several architectural and chemical features. These qualities include chelation, substitution structure, surface action, hydrophobicity dissolution, and electrical variables. The rigorous examination has resulted in the creation of molecule and atom-based characteristics and characteristics obtained from quantum chemical computations and fluorescence. The construction of QSAR modeling for developing drugs has been methodically organized and comprises many modular processes that use chemo-informatics and machine-learning approaches. The initial stage in QSAR modeling is molecular encryption, wherein the chemical arrangement of the drug molecules is utilized to generate chemical traits and attributes.

The process of experimental analysis of drug delivery using ML is shown in Figure 6. Empirical data is also taken into account for structural design. Next, choosing features involves utilizing unsupervised learning approaches to identify the most pertinent attribute. Feature selection begins with a dataset measured via molecular encoding and constructs valuable features that aim to facilitate and reduce complexity. In the final and crucial stage, a supervised learning approach is employed to discover an empirical function that creates an appropriate relationship among input vectors of features and their corresponding biological reactions. The selection of SAR databases for training and validating models is crucial for constructing a precise QSAR algorithm. It is essential to meticulously separate the learning and test databases while creating the first model and to evaluate the test databases without bias to assess the ultimate performance of the algorithm.

3.5 Recent advances and limitations

Given the vast quantity of organic substances exceeding forty million, it is necessary to establish a comprehensive database to hold data about their structure and physical, biological, chemical, and toxicological characteristics. These databases are particularly crucial in drug discovery since they provide a thorough knowledge of the effectiveness of a collection of structurally related compounds versus a specific pharmacological target by studying and comprehending the Structure-Activity Relationship (SAR). The agriculture business has utilized in silico methods to discover

pesticides. Computing methods have been used in the medical field and in studying many chemical processes, such as C-H stimulation, acid-base responses, and enzymatic reactions. These methods have been employed to gain insights into these events' mechanisms, energies, and kinetics. This theoretical method aids in forecasting and investigating the potential use of a chemical as a medication and pesticide, eliminating the necessity for conducting chemical operations and separating the intermediary and final goods. This adheres to the principles of green chemistry, which promotes reducing waste production and avoiding harmful compounds.

Protein architectures are crucial in drug discovery for molecular bioinformatics, and ML methods assist in accurately evaluating model precision for determining the structures of proteins. X-ray crystallography is used to identify structures in protein molecules, but purifying and crystallizing proteins are challenging and time-consuming. To address these issues, ML techniques have been employed to develop computer-based protein forecasting systems. ML approaches are highly successful in natural language and imaging processing, recognizing speech, and computerized vision. ML techniques classify proteins, determine their structure, and assess the affinity between proteins and ligands. Both methodologies utilize physiochemical, energetic, and statistical components to integrate various data types. ML methodologies are crucial in representing the three-dimensional architecture of the target molecule employed in drug development initiatives. In molecular protein forecasting, 2021 stands out as a significant milestone due to the exceptional precision attained by Alphafold, a deep learning approach. The advent of Alphafold2 has revolutionized the field of structural computational biology.

ML techniques provide several benefits, including the ability to quickly identify patterns, automation without human intervention, processing of multidimensional information, and ongoing improvement in precision and effectiveness across a wide range of applications. Despite the numerous benefits, there are still several constraints. ML necessitates impartial, high-quality information for management. It also demands significant time to analyze the incoming message with notable accuracy. Significant obstacles include high susceptibility to errors and the need to interpret outcomes carefully. ML must execute the data through multiple algorithms to choose the optimal method. The accuracy of the results obtained chiefly determines the selection process. This is a time-consuming process that has an impact on the operation. ML methods are unsuitable for complex, abstract thinking or strategic decision-making, which poses challenges in comprehending the nuances of natural language.

3.6 Future scope

The primary promise of ML in the pharmaceutical sector lies in its ability to decrease expenses and enhance operational effectiveness. Numerous studies have shown that dynamic modeling may differentiate highly accurate ML models by utilizing 50% or less data compared to classic ML and data subsampling methods. While the exact cause of this heightened productivity is not entirely comprehended, decreased repetition and propensity and acquiring more substantial knowledge to navigate decision boundaries are crucial elements in this enhanced performance. Excluding the anticipated mechanical costs associated with implementing dynamic study, screening costs decrease by as much as 90%.

ML algorithms can handle intricate analyses involving large, diverse, and high-dimensional datasets without manual input. This capability has shown to be advantageous in developing commercial applications for the industry. Integrating ML with human expertise and experience might be optimal for managing several vast data repositories. The remarkable data-extraction capability of ML technology has enhanced the significance of computer-assisted medicine regimens that integrate many clinical factors, surpassing fragmented data and expediting prescription procedures. As medical information accumulates and ML algorithms improve, ML technology is anticipated to facilitate several areas of drug study and development, becoming the prevailing computer-assisted medicine design approach. The synchronized progress of mechanization and technological integration is expected to drive improvements in medicine through enhanced analysis of extensive and intricate information. Implementing ML is crucial for shortening drug creation cycles, lowering costs, and improving successing rates, which is the final goal.

## 4. Conclusion

Several variables influence the effective incorporation of ML into delivering drugs, manufacturing, and the pharmaceutical business, particularly in polypharmacology, drug creation, drug assessment, and drug reinventing. The continual need for technological advancements, particularly those rooted in machine learning, arises from minimizing the resources allocated to study, growth, and manufacturing while enhancing efficiency.

The findings of this study demonstrate that utilizing ML techniques can enhance the effectiveness and precision of drug research and development processes. These innovations improve process efficiency and, in certain instances, replace the necessity for clinical trials by conducting simulators. They also enable studies to thoroughly examine molecules without difficulties, resulting in reduced costs and ethical problems. The integration of ML can potentially transform medication research significantly in the future. However, several obstacles hinder this progress, such as the need to clean unstructured and diverse datasets and occasional limitations of computing devices. The pharmaceutical business

embraces and enhances machine learning upon eliminating these obstacles, ushering in a new era of progress and innovation.

## Author contribution

A.M.H., K.S., S.S.D. wrote, reviewed and edited the article. All authors read and approve for publication.

## Acknowledgment

The authors are grateful to the Kalinga University to support their study.

## Competing financial interests

The authors have no conflict of interest.

## References

Bannigan, P., Aldeghi, M., Bao, Z., Häse, F., Aspuru-Guzik, A., & Allen, C. (2021). Machine learning directed drug formulation development. Advanced Drug Delivery Reviews, 175, 113806.
https://doi.org/10.1016/j.addr.2021.05.016

Bao, Z., Bufton, J., Hickman, R. J., Aspuru-Guzik, A., Bannigan, P., & Allen, C. (2023). Revolutionizing drug formulation development: The increasing impact of machine learning. Advanced Drug Delivery Reviews, 115108.
https://doi.org/10.1016/j.addr.2023.115108

Bavumiragira, J.P., Yin, H. (2022). Fate and transport of pharmaceuticals in water systems: A processes review. Sci. Total Environ. 823, 153635.
https://doi.org/10.1016/j.scitotenv.2022.153635

Bertolini, M., Mezzogori, D., Neroni, M., Zammori, F. (2021). Machine Learning for industrial applications: A comprehensive literature review. Expert Syst. Appl. 175, 114820.
https://doi.org/10.1016/j.eswa.2021.114820

Bochicchio, S., Lamberti, G., Barba, A.A. (2021). Polymer-lipid pharmaceutical nanocarriers: innovations by new formulations and production technologies. Pharm. 13(2), 198.
https://doi.org/10.3390/pharmaceutics13020198

Boso, D. P., Di Mascolo, D., Santagiuliana, R., Decuzzi, P., & Schrefler, B. A. (2020). Drug delivery: Experiments, mathematical modelling and machine learning. Computers in biology and medicine, 123, 103820.
https://doi.org/10.1016/j.compbiomed.2020.103820

Caban, M., Stepnowski, P. (2021). How to decrease pharmaceuticals in the environment? A review. Environ. Chem. Lett. 19, 3115-3138.
https://doi.org/10.1007/s10311-021-01194-y

Calmet, H., Dosimont, D., Oks, D., Houzeaux, G., Almirall, B.V., Inthavong, K. (2023). Machine learning and sensitivity analysis for predicting nasal drug delivery for targeted deposition. Int. J. Pharm. 123098.
https://doi.org/10.1016/j.ijpharm.2023.123098

Carpenter, K. A., & Huang, X. (2018). Machine learning-based virtual screening and its applications to Alzheimer's drug discovery: a review. Current pharmaceutical design, 24(28), 3347-3358.
https://doi.org/10.2174/1381612824666180607124038

Chang, V., Bailey, J., Xu, Q.A., Sun, Z. (2023). Pima Indians diabetes mellitus classification based on machine learning (ML) algorithms. Neural. Comput. Appl. 35(22), 16157-16173.
https://doi.org/10.1007/s00521-022-07049-z

Dagenais, S., Russo, L., Madsen, A., Webster, J., Becnel, L. (2022). Use of real-world evidence to drive drug development strategy and inform clinical trial design. Clin. Pharmacol. Ther. 111(1), 77-89.
https://doi.org/10.1002/cpt.2480

de Oliveira, J.V.R., Silveira, P.L., Spingolon, G., Alves, G.A.L., Peña, F.P., Aguirre, T.A.S. (2023). Polymeric nanoparticles containing babassu oil: A proposed drug delivery system for controlled release of hydrophilic compounds. Chem. Phys. Lipids. 253, 105304.
https://doi.org/10.1016/j.chemphyslip.2023.105304

Diniz, F., Coelho, P., Duarte, H.O., Sarmento, B., Reis, C.A., Gomes, J. (2022). Glycans as targets for drug delivery in cancer. Cancers. 14(4), 911.
https://doi.org/10.3390/cancers14040911

Harrison, P.J., Wieslander, H., Sabirsh, A., Karlsson, J., Malmsjö, V., Hellander, A., Spjuth, O. (2021). Deep-learning models for lipid nanoparticle-based drug delivery. Nanomed. 16(13), 1097-1110.
https://doi.org/10.2217/nnm-2020-0461

He, S., Leanse, L.G., Feng, Y. (2021). Artificial intelligence and machine learning assisted drug delivery for effectively treating infectious diseases. Adv. Drug Deliv. Rev. 178, 113922.
https://doi.org/10.1016/j.addr.2021.113922

Kibria, M. R., Akbar, R. I., Nidadavolu, P., Havryliuk, O., Lafond, S., & Azimi, S. (2023). Predicting efficacy of drug-carrier nanoparticle designs for cancer treatment: a machine learning-based solution. Scientific Reports, 13(1), 547.
https://doi.org/10.1038/s41598-023-27729-7

Ma, M., Huang, S., Liu, S., Lv, X., Zhu, J., Liu, K., Xiong, F. (2023). A novel approach of modeling pharmacokinetics and pharmacokinetics-pharmacodynamics for

the intravenous nano drug delivery system. J Drug Deliv Sci Technol. 89, 105071.
https://doi.org/10.1016/j.jddst.2023.105071

Mazarura, K.R., Kumar, P., Choonara, Y.E. (2022). Customized 3D printed multi-drug systems: an effective and efficient approach to polypharmacy. Expert Opin Drug Deliv. 19(9), 1149-1163.
https://doi.org/10.1080/17425247.2022.2121816

Mozafari, N., Mozafari, N., Dehshahri, A., & Azadi, A. (2023). Knowledge gaps in generating cell-based drug delivery systems and a possible meeting with artificial intelligence. Molecular Pharmaceutics, 20(8), 3757-3778.
https://doi.org/10.1021/acs.molpharmaceut.3c00162

Palugan, L., Cerea, M., Cirilli, M., Moutaharrik, S., Maroni, A., Zema, L., Gazzaniga, A. (2021). Intravesical drug delivery approaches for improved therapy of urinary bladder diseases. Int. J. Pharm. X, 3, 100100.
https://doi.org/10.1016/j.ijpx.2021.100100

Rai, R., Tiwari, M.K., Ivanov, D., Dolgui, A. (2021). Machine learning in manufacturing and industry 4.0 applications. Int. J. Prod. Res. 59(16), 4773-4778.
https://doi.org/10.1080/00207543.2021.1956675

Sharma, S., Masud, M.K., Kaneti, Y.V., Rewatkar, P., Koradia, A., Hossain, M.S.A., Salomon, C. (2021). Extracellular vesicle nanoarchitectonics for novel drug delivery applications. Small. 17(42), 2102220.
https://doi.org/10.1002/smll.202102220

Sheng, Y., Gao, J., Yin, Z.Z., Kang, J., Kong, Y. (2021). Dual-drug delivery system based on alginate and sodium carboxymethyl cellulose hydrogels for colorectal cancer treatment. Carbohydr. Polym. 269, 118325.
https://doi.org/10.1016/j.carbpol.2021.118325

Xu, J., Wang, X., Liu, F. (2021). Government subsidies, R&D investment and innovation performance: analysis from pharmaceutical sector in China. Technol Anal Strateg Manag. 33(5), 535-553.
https://doi.org/10.1080/09537325.2020.1830055

Zhang, J.Z., Srivastava, P.R., Sharma, D., Eachempati, P. (2021). Big data analytics and machine learning: A retrospective overview and bibliometric analysis. Expert Syst. Appl. 184, 115561.
https://doi.org/10.1016/j.eswa.2021.115561