REVIEW ARTICLE

A Review Analysis of Drug Delivery System Using Artificial Intelligence

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Abstract

According to the President of the United Nations, AI holds enormous promise for accelerating progress towards numerous United Nations Sustainable Development Goals (SDGs). This paper focuses on various applications of technologies such as artificial neural networks (ANN) and deep learning (DL) in the development of pharmaceutical solid dosage forms. DL is a subset of machine learning (ML) that utilizes extensive experimental data to learn through advanced methods like artificial neural networks. ANNs can analyze patient data to generate customized drug delivery regimens based on genetic and medical histories. A range of AI technologies, including neural networks, fuzzy logic, and evolutionary algorithms, are employed for creating solid dosage formulations. Support vector machine (SVM), a unique machine learning approach, was applied to predict oral drug absorption in humans using descriptors derived from chemical structure. ANNs are capable of forecasting drug dissolution profiles, predicting particle flowability, anticipating storage stability, and designing stable dosage forms. The study evaluates the accuracy of ANN, CNN, and SVM in oral solid dosage forms, drug release prediction, virtual screening, and pharmacokinetics/pharmacodynamics in drug delivery systems.

Keywords: artificial intelligence, drug delivery systems, machine learning, pharmaceutical formulation.

1 Introduction

According to WHO guidance on artificial intelligence to improve drug delivery system, this year the World Drug Report is comprised of two items for the first time since its inception: a collection of booklets and a web-based component. Although booklet 1 is an executive summary based on analysis of the important results of the online segment and Booklet 2 focuses on several additional modern issues in addition to offering a thorough examination of significant advancements and new trends in specific drug markets [1]. In today's fast changing drugs delivery system sector using artificial intelligence (AI) holds enormous promises for accelerating progress towards numerous united Nations Sustainable Development Goals (SDGs). SDGs health in well-being, industry, infrastructure and accountable production and consumption are all related to this. Traditional DDSs include giving

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the medication orally or intravenously, and the body's natural processes of absorbance, deposition, consumption, and mechanics of discharge [2].

The introduction of intelligent drug delivery systems, such as Janus micro- or nanoparticles that can transport many medications, is made possible by the application of microfluidic technology electronic parts, wireless correspondence gear, and a power supply have all been integrated into a microchip implant for controlled medication delivery [3]. Beyond these technologies, advanced targeting strategies like cell-mediated drug delivery systems have emerged as a powerful approach to enhance the precision of drug delivery to specific sites in the body, such as tumors [5]. The relationship between AI and Drugs delivery system is to provide practical answers for a range of supply chain problems, it also synthesises a number of AI research initiatives over the last several decades. Supply chain activities in the pharmaceutical business are going to undergo a major change due to the introduction of artificial intelligence. Artificial intelligence (AI) systems can give detailed complex relationships between pharmaceutical properties, physiological factors, and formulation components to predict drug activity at all scales. This promotes the development of efficient drug delivery devices [4].

The contribution of the study as follows:

1. Implantable microchips have been used for medication delivery in osteoporotic patients in a preliminary clinical study [6].

2. Controlled insulin administration combined with ongoing glucose monitoring may greatly lessen the difficulties associated with diabetes. Integration of the insulin delivery system, glucose sensors, control algorithms, and mathematical models is useful in this situation.

3. An insulin pump, dosage calculator, and glucose metre have all been integrated into a single device to provide an automatic system for glucose monitoring and insulin delivery.

Targeted distribution, stability of medications, and order of modification of dosage should all be considered when developing intelligent delivery systems. Appropriate algorithms ought to be used in conjunction with self-monitoring delivery devices to regulate the quantity and time of medication release.

2 Overview of Drug Delivery System

Artificial Intelligence's Contribution to Drug Delivery System Modernisation

This extended explanation looks at how advanced Drug Delivery Systems (DDSs), which are increasingly being built and optimised with the help of Artificial Intelligence (AI) and Machine Learning (ML), are addressing the shortcomings of conventional drug administration.

2.1 Traditional Drug Delivery's Challenge

Reaching a particular location in the body at the appropriate concentration for the appropriate duration is the main objective of any medicine. But conventional approaches frequently fail to achieve this objective.

2.1.1 Drawbacks of Traditional Approaches

After administration, a drug does not directly reach the target site; instead, it undergoes a complex journey within the body governed by four principal processes collectively referred to as ADME. Initially, the drug is absorbed into the bloodstream, followed by distribution throughout tissues and bodily fluids. It is then subjected to metabolic transformation, in which it is chemically modified by the body. Finally, the drug and its metabolites are eliminated through excretion. These processes together determine the pharmacokinetic profile and therapeutic efficacy of the drug [7, 8].

2.1.2 Developments in Contemporary DDS

Scientists created sophisticated drug delivery systems to address these problems. These are specially designed technologies that regulate a drug's release to increase both its safety and effectiveness. Making sure the medication is released at the appropriate time, location, and pace is the aim [9].

Formulations with sustained release are made to release a medication gradually over a long period of time. By doing this, the drug concentration in the bloodstream is kept constant and effective, avoiding the peaks and valleys that are typical of regular pills [10].

Tablets with an enteric coating are protected from stomach acid by a unique coating. This is important for medications that can irritate the stomach lining or be damaged by the low pH of the stomach. To guarantee that the medication is absorbed in the right area of the digestive system, the coating doesn't disintegrate until it reaches the small intestine's less acidic environment [11].

2.2 Foundations of Artificial Intelligence and Machine Learning

AI opens the door to more intelligent DDS design by offering the computational capacity to examine the incredibly complicated drug-body interactions [12].

2.2.1 *Introducing Deep Learning (DL), Machine Learning (ML), and Artificial Intelligence*

Although distinct, the concepts of artificial intelligence (AI), machine learning (ML), and deep learning (DL) are closely related. AI represents the broadest domain, encompassing the development of computational systems capable of performing tasks such as problem solving, learning, and decision-making, which traditionally require human intelligence [13]. Within this domain, ML constitutes a subset in which systems are not explicitly programmed with predefined rules but are instead trained on large datasets to recognize patterns and make predictions. A further specialization within ML is DL, which leverages complex, multi-layered neural networks to approximate human-like learning and thereby advances machine learning systems closer to the realization of true AI.

2.2.2 *Artificial Neural Networks (ANNs) as Core Architectures*

The computational systems at the core of deep learning are artificial neural networks. The structure of the human brain served as the model for its creation. An artificial neural network (ANN) is made up of interconnected nodes, or "neurons," arranged in layers, much like the billions of interconnected neurons in human brain that process information. The weight assigned to each connection is changed as learning progresses. The network uses these layers to handle new data and generate an output, like a classification or prediction. They are also known as "connectionist systems" since the strength of the connections between nodes determines how well they work.

2.2.3 *Convolutional Neural Networks (CNNs)*

A crucial example One well-known and potent kind of ANN is a convolutional neural network. CNNs work very well for visual data analysis. They are the technology that powers a wide range of image recognition applications, including as detecting cancers in medical scans and facial recognition on your phone. Their architecture learns spatial feature hierarchies from photos automatically and adaptively. They are therefore perfect for any issue involving intricate, image-driven pattern identification, which is a frequent difficulty in drug research and medical diagnostics [15].

2.3 AI's Effect on Personalized Medicine and Drug Delivery

Healthcare is entering a new era of accuracy and personalization by fusing advanced DDS technology with potent AI algorithms.

2.3.1 *AI-Powered Analysis for Forecasting and Enhancement*

Fundamentally, AI analyzes vast amounts of data in a way that is well above human capability by using computer algorithms and machine learning. Clinical trial outcomes, patient medical histories, genetic data, and molecular interaction data are examples of this type of data in medicine. AI can generate extremely precise predictions about the behavior of a medication or a delivery system by analyzing this data. AI turns DDS design and treatment optimization from a trial-and-error procedure into a predictive science by offering a variety of tools [16].

2.3.2 *Important Therapeutic Uses*

Artificial intelligence (AI) is increasingly finding practical applications in pharmacology, with its scope of use continuing to expand. One major area is drug discovery, where AI facilitates the rapid screening of millions of candidate compounds to identify those with the highest potential therapeutic efficacy against specific diseases. In dosage optimization, AI enables the analysis of patient-specific variables to determine the optimal dosing regimen that maximizes therapeutic benefit while minimizing the risk of toxicity. Furthermore, AI contributes to combination therapy design by predicting which drug combinations are most effective for complex conditions such as cancer. In addition, AI is employed in the enhancement of drug delivery systems (DDSs), allowing researchers to model and optimize the interactions of novel platforms, such as nanoparticles, with the human body even before these systems advance to clinical trials [17].

2.3.3 *The future Personalized Medicine Driven by AI*

Real tailored medicine is the ultimate aim of combining AI with DDS. The emphasis now is on treating the patient rather than a condition. An individual's genetic profile and medical history are among the unique data that AI algorithms can examine to generate a fully personalized drug distribution plan. This individualized approach guarantees that the

treatment is planned to be as effective as possible for that particular individual. The adoption of more AI-based health solutions will have a significant impact on healthcare in the future, improving treatment outcomes and reducing side effects for patients everywhere [18].

3 Oral Solid Dosage Form

Recent advances in artificial intelligence (AI) have introduced novel algorithmic approaches that significantly enhance the design and optimization of solid pharmaceutical dosage forms. By leveraging computational power, AI enables the rapid analysis of complex formulation variables, thereby facilitating more efficient development processes and improved product performance. Fundamentally, AI represents an interdisciplinary convergence of computer science, data analytics, and mathematics, which together provide the methodological framework necessary for addressing the multifactorial challenges inherent in pharmaceutical formulation [19].

3.1 Drug Formulation Using Machine Learning Techniques

3.1.1 Machine Learning Categories

In the field of artificial intelligence, three principal learning paradigms are commonly applied to pharmacological research and development. Supervised learning involves the use of labeled input data to predict specific target or output variables, enabling accurate modeling and outcome forecasting [20, 21]. In contrast, unsupervised learning focuses on detecting intrinsic structures, patterns, or clusters within unlabeled datasets, thereby uncovering hidden relationships without prior guidance. A third paradigm, reinforcement learning, operates through iterative feedback and reward mechanisms, allowing the system to progressively refine its strategies and identify optimal solutions. Together, these learning approaches provide complementary methodologies that significantly enhance the capacity of AI to address complex problems in pharmaceutical sciences.

3.1.2 Uses for Designing Solid Dosage Forms

Artificial intelligence has shown considerable potential in the design and optimization of solid dosage forms, particularly in the refinement of manufacturing processes and dosage parameters. By integrating predictive modeling and data-driven algorithms, AI can identify optimal formulation conditions, streamline production variables, and ensure consistent product quality. Such approaches not only enhance efficiency and reduce development costs but also contribute to achieving precise control over critical attributes, including drug release profiles and bioavailability.

3.2 Deep Learning for Use in Medicine

3.2.1 Deep Learning (DL) Role

Deep learning (DL) has emerged as a powerful approach in medical applications, primarily owing to its ability to handle large-scale experimental datasets and to leverage advanced architectures such as artificial neural networks (ANNs) [22]. By employing multi-layered neural network structures, DL is capable of performing complex non-linear data transformations, thereby enabling the extraction of subtle patterns and relationships from highly heterogeneous biomedical data. This capability makes DL particularly well suited for tackling challenges in diagnostics, treatment planning, and drug development where conventional computational methods are limited.

3.2.2 Algorithms in Deep Learning

Within the medical and pharmaceutical domains, several deep learning (DL) algorithms have demonstrated remarkable utility. Convolutional neural networks (CNNs) are widely applied in tasks such as particle flowability assessment, drug defect detection, biomedical image processing, and dissolution profile prediction, owing to their strong capacity for feature extraction from spatially structured data [23, 24]. In parallel, recurrent neural networks (RNNs) provide unique advantages in handling sequential or time-series data, making them particularly valuable in drug development processes that require the analysis of dynamic pharmacokinetic and pharmacodynamic patterns [23]. Collectively, these algorithmic approaches extend the scope of DL by offering tailored solutions to diverse challenges in pharmaceutical research and clinical practice.

3.2.3 DL Applications in the Formulation of Solid Dosage Forms

Deep learning (DL) has gained increasing relevance in the formulation and quality control of solid dosage forms. One key application is the prediction of drug dissolution profiles, where DL models can capture complex, non-linear relationships between formulation variables and release behavior, thus reducing the reliance on extensive experimental trials. DL has also been employed to predict the stability of pharmaceutical products during storage, enabling

early identification of factors that may compromise product quality and shelf life. In addition, DL algorithms are effective in detecting flaws in tablets, such as cracks, coating irregularities, or content non-uniformity, thereby supporting automated quality assurance processes. Collectively, these applications highlight the capacity of DL to enhance both efficiency and reliability in solid dosage form development.

3.3 Algorithms Based on AI That Go Beyond DL

In addition to deep learning, several other artificial intelligence (AI)–based algorithms have demonstrated substantial utility in pharmaceutical sciences. Artificial neural networks (ANNs) are frequently applied to improve the precision of dosage formulation predictions, enabling more reliable control over critical quality attributes [25]. Evolutionary algorithms, which mimic natural selection processes, have been employed to optimize formulation parameters and manufacturing conditions, as well as to forecast complex outcomes in drug development [25]. Furthermore, fuzzy logic models provide a valuable framework for enhancing the understanding of nonlinear relationships between process inputs and outputs, thereby supporting more robust decision-making in formulation and process design. Together, these approaches extend the scope of AI beyond deep learning, offering complementary methodologies to address multifactorial challenges in the development of pharmaceutical dosage forms.

3.4 Excipients' Function in Solid Dosage Forms

Tablets remain the most widely used type of oral solid dosage form, largely due to their convenience, stability, and cost-effectiveness [18]. Within their formulation, excipients play indispensable roles, not only as inert components but also as functional contributors to product performance and manufacturability. For example, lubricants and glidants are crucial for facilitating smooth tablet compression and preventing manufacturing defects, thereby expediting the production process. More recently, artificial intelligence (AI) algorithms have been introduced to support excipient selection, enabling researchers to optimize formulations by assessing compatibility, functionality, and performance requirements. This data-driven approach improves both efficiency and precision in the design of robust solid dosage forms.

3.5 Complex Applications of Machine Learning

Machine learning (ML) techniques have been increasingly applied to address complex challenges in pharmaceutical sciences, particularly in the development of oral solid dosage forms. For instance, support vector machines (SVMs) have been employed to predict the absorption behavior of orally administered drugs, offering a valuable tool for early-stage screening and formulation design. These models often leverage molecular descriptors derived from chemical structures within large-scale datasets, enabling more accurate and generalizable predictions across diverse compound libraries [24]. Such approaches exemplify the growing role of ML in enhancing drug formulation research by integrating chemical informatics with predictive modeling. The comparative performance of various AI technologies applied to oral solid dosage form development is summarized in Table 1.

4 Prediction of drug release formulation

4.1 AI in Batch Optimization and Drug Release

Artificial intelligence (AI) has become an essential tool in optimizing batch production and characterizing drug release behavior in solid dosage forms. By

Table 1. Oral solid dosages form.

Reference	Technology	Accuracy	Description
[22]	ANN	60%	ANNs is used for drug release from multiple dosage form. They can ensure solving best formulation for prediction of the release behaviour in alive of active pharmaceutical various element under different situation.
[23]	CNN	97.56%	CNNs have been used extensively for image recognition and object perception.
[24]	SVM	60%	Using those five descriptors derived just from the chemical structure, SVM, a unique machine learning go towards, was applied to predict the oral absorption of a drug for human usage for a vast and multiple data set.

applying advanced predictive models, AI can facilitate accurate forecasting of drug release profiles, thereby reducing the need for extensive in vitro experimentation. Moreover, AI-driven approaches support disintegration time analysis, enabling precise assessment of formulation performance and patient-centric outcomes. In large-scale pharmaceutical manufacturing, AI further contributes to efficient batch selection, ensuring consistent quality, minimizing variability, and enhancing overall process efficiency [28]. These applications highlight the transformative role of AI in bridging formulation science with large-scale production demands.

4.2 Formulation Design Using Machine Learning

Machine learning (ML) has emerged as a valuable tool for modern formulation design, complementing the expertise of pharmaceutical scientists by reducing experimental workload and accelerating decision-making. Through the integration of physicochemical properties of excipients and active pharmaceutical ingredients (APIs), along with critical process parameters, ML algorithms can generate predictive models that forecast formulation performance with high accuracy [29]. Such approaches enable rational formulation design by identifying optimal variable combinations without exhaustive trial-and-error experimentation. Moreover, when combined with mechanistic understanding of formulation systems, ML can further enhance the design of advanced drug delivery platforms. For instance, Li et al. [14] summarized strategies for encapsulating and controlling the release of small hydrophilic molecules using carriers such as cyclodextrins, highlighting the importance of excipient–drug interactions in achieving effective delivery. Incorporating such mechanistic insights into ML-driven models holds great promise for improving prediction accuracy and guiding the rational selection of excipients in formulation development. Collectively, these applications underscore the growing role of ML in the systematic and efficient design of pharmaceutical formulations.

4.3 Applications of Deep Learning

4.3.1 Predicting Protein Structure

Deep learning (DL) has demonstrated significant promise in structural biology, particularly in the prediction of three-dimensional protein structures directly from amino acid sequences. By learning the complex spatial and physicochemical relationships among residues, DL models are capable of achieving highly accurate structural predictions, thereby advancing drug discovery and molecular design. In addition, DL frameworks increasingly incorporate reinforcement learning techniques to forecast reaction outcomes and optimize chemical processes, providing a data-driven strategy for improving efficiency in both protein engineering and pharmaceutical development [27]. Together, these approaches highlight the transformative role of AI in bridging molecular-level understanding with practical therapeutic applications.

4.3.2 Artificial Neural Networks (ANNs)

Artificial neural networks (ANNs) are widely applied in pharmaceutical research due to their ability to transform complex formulation problems into optimized solutions through iterative learning. Owing to their high computational capacity, ANNs can store and analyze extensive molecular structural databases, enabling the identification of hidden relationships among chemical features and formulation outcomes. Moreover, they play a critical role in enhancing predictive accuracy and facilitating the design of novel molecular structures, thereby accelerating the discovery and optimization of innovative drug candidates and delivery systems [28]. Collectively, these features make ANNs a versatile and powerful tool in modern pharmaceutical development.

4.3.3 Convolutional Neural Networks (CNNs)

Convolutional neural networks (CNNs) represent a class of deep neural networks specifically designed for classification and regression tasks, characterized by the presence of at least one convolutional layer [29]. Their architecture allows for the reduction of image size without loss of critical features, making them highly effective in processing complex visual data. CNNs have been successfully applied in diverse fields, including posture estimation, visual saliency detection, object recognition, and scene labeling, where robust feature extraction and hierarchical learning are essential. In pharmaceutical sciences, CNNs are increasingly utilized for image-based applications such as defect detection in solid dosage forms, surface morphology analysis, and dissolution profile prediction. The comparative performance of various AI technologies in drug release prediction formulations is summarized in Table 2.

Table 2. Prediction of drug release formulation.

Reference	Technology	Accuracy	Description
[28]	ANN	74.27	ANN is used to predict the formulation, and reduce the complex formula into easy one. ANN helps to reduce the vast formulation and to give the best output. It has help to store the large amount of formula and molecular structure. ANN help to make more molecular structure
[29]	CNN	6.85	CNN helps to reduce scale of picture without disturbing its information. It should also be suggested to introduce CNNs into many other domains, such as posture estimation, visual saliency detection, object identification, and scene labelling. Deep neural networks with at least one convolutional layer that are well-suited for challenging regression or classification tasks are known as convolutional neural networks, or CNNs
[18]	SVM	<4.47	The procedures of data analysis and dissolution profile prediction employ the support machine vector (SVM).

5 Virtual Screening

5.1 AI for Virtual Screening

Artificial intelligence (AI) has become an indispensable tool in virtual screening, enabling the systematic evaluation of vast chemical libraries to identify promising therapeutic candidates with high efficiency. By leveraging advanced algorithms, AI can rapidly analyze molecular features, binding affinities, and structural compatibilities, thereby prioritizing compounds for experimental validation. This approach not only accelerates the early stages of drug discovery but also significantly reduces associated costs and resource demands by narrowing the pool of candidates to those most likely to succeed in subsequent testing [31]. As a result, AI-driven virtual screening is reshaping traditional workflows, bridging computational prediction with laboratory experimentation in a more integrated and cost-effective manner.

5.2 Machine Learning Principles for Drug Development

Machine learning (ML) provides a powerful framework for predictive modeling in drug development, wherein functions are derived from training inputs and outputs to forecast outcomes for new, unseen data. The theoretical foundation of ML in this context is grounded in the Structural Risk Minimization (SRM) principle, which seeks to achieve an optimal balance between model complexity and predictive accuracy [32]. By minimizing the risk of overfitting to training data while ensuring the capacity to generalize to novel datasets, SRM enables the development of models that are both robust and reliable. This balance is achieved through the careful trade-off between dependency on model complexity and the observed risk, measured as the error rate. In drug development, adherence to these principles is essential for building predictive tools that can reliably guide decision-making across diverse stages, from compound screening to clinical outcome forecasting.

5.3 Artificial Neural Networks (ANN) in Machine Learning

Artificial neural networks (ANNs) are a core component of machine learning, designed to simulate cognitive processes through interconnected artificial neurons, analogous to learning mechanisms in the human brain. Their architecture often incorporates hidden layers, which enhance the network's capacity to capture complex, non-linear relationships in data, even when such patterns are not explicitly reflected in the training output. Learning within ANNs is further refined through the backpropagation algorithm, which iteratively adjusts connection weights to minimize prediction errors and improve overall model performance [33]. These features make ANNs particularly powerful in pharmaceutical research, where they are increasingly employed for tasks such as formulation optimization, property prediction, and drug–excipient interaction modeling.

5.4 Convolutional Neural Networks (CNNs)

Convolutional neural networks (CNNs) are a specialized class of deep learning models that employ filters of varying sizes to extract shared

Table 3. Data collection of Virtual screening.

Reference	Technology	Accuracy	Description
[35]	ANN	1%	ANNs from combinatorial libraries may be employed in the VS pipeline, demonstrating how choosing descriptors is crucial for ANN evaluation.
[36]	CNN	75%	It was demonstrated that CNN could identify chemical functional groups, which are crucial components of a compound's capacity to bind.
[32]	SVM	0.547-0.647%	the SVM create an ideal boundary that splits the data into two groups. These Section are often preset since supervised learning is where SVM is most frequently employed.

features from input tensors, thereby enabling efficient representation of complex data. Their architecture is particularly advantageous in image processing and advanced data analysis, especially when dealing with repeated or hierarchical structures. In pharmaceutical research, CNNs have been applied extensively for pattern recognition and data classification tasks, such as detecting tablet defects, analyzing microscopy images, and classifying molecular structures [34]. These capabilities highlight CNNs as powerful tools for translating high-dimensional biomedical and pharmaceutical data into actionable insights.

5.5 Support Vector Machines (SVM)

Support vector machines (SVMs) are a widely used class of machine learning algorithms that represent input data as feature vectors in high-dimensional space, allowing for the identification of optimal separating hyperplanes. By constructing these decision boundaries, SVMs can effectively classify data into distinct groups, even in cases where the relationships between variables are highly complex. While SVMs are most commonly applied in supervised learning, recent advances have also highlighted their potential for certain unsupervised learning tasks, such as clustering and anomaly detection [32]. In pharmaceutical sciences, SVMs have been employed in areas such as compound classification, bioactivity prediction, and formulation analysis. A comparative overview of the performance of AI technologies in virtual screening applications is presented in Table 3.

Figure 1: this figure shows that how the virtual screening works on solid dosage forms of medicines. And show virtual screening of the drugs implementation of pharmacodynamics and pharmacokinetic works.

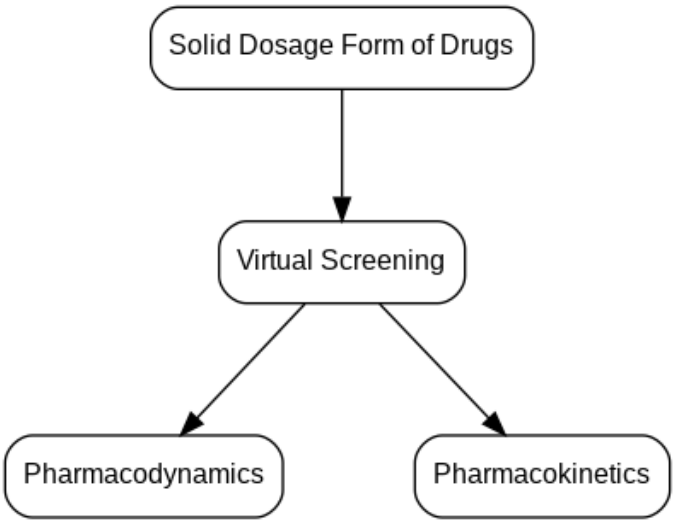

Figure 1. Flow chart of virtual screening.

6 Pharmacokinetics and Pharmacodynamics

6.1 The Function of Artificial Intelligence in PK/PD Prediction

Artificial intelligence (AI) has emerged as a powerful approach for improving the prediction of pharmacokinetics (PK) and pharmacodynamics (PD), offering faster, more accurate, and cost-effective alternatives to conventional modeling strategies. By integrating large-scale biological, chemical, and clinical datasets, AI enables the identification of complex, non-linear relationships that govern drug absorption, distribution, metabolism, excretion, and therapeutic response. With continuous advances in computational power and the refinement of machine learning (ML) methodologies, AI has become a reliable tool for forecasting and optimizing PK/PD models, thereby supporting rational drug design, individualized therapy, and streamlined clinical development [37].

6.2 Applying Machine Learning to PK/PD Modeling

Machine learning (ML) has been increasingly applied to pharmacokinetic/pharmacodynamic (PK/PD) modeling, where it offers substantial improvements in both efficiency and predictive accuracy. By leveraging complex datasets that integrate physicochemical, biological, and clinical variables, ML algorithms can capture non-linear patterns that traditional statistical models often fail to address. These capabilities not only accelerate the drug development process by reducing reliance on labor-intensive experimentation but also contribute to improved therapeutic efficacy through more precise predictions of drug behavior in diverse patient populations [38]. Consequently, ML-based PK/PD modeling represents a key step toward more data-driven and patient-tailored pharmaceutical development.

6.3 Artificial neural networks (ANNs)

Artificial neural networks (ANNs) have proven particularly valuable in pharmacokinetic/pharmacodynamic (PK/PD) modeling, owing to their ability to predict time-dependent PK/PD parameters from patient-specific data. By capturing complex, nonlinear relationships, ANNs provide a more accurate representation of inter-individual variability, thereby supporting personalized dosing strategies. In addition, ANNs have been applied to tablet formulation and the prediction of drug absorption, distribution, metabolism, and excretion (ADME), offering insights that improve both formulation design and therapeutic performance [39]. These applications highlight the versatility of ANNs in bridging formulation science with clinical pharmacology, reinforcing their role as a transformative tool in modern drug development.

6.4 Convolutional Neural Networks (CNN)

Convolutional neural networks (CNNs) have gained increasing importance in pharmacokinetic/pharmacodynamic (PK/PD) research due to their capacity to analyze chemical and molecular structure data with high efficiency. By extracting hierarchical features from complex input data, CNNs can support drug formulation development and facilitate the recognition of critical molecular structures relevant to drug behavior. Moreover, CNNs are increasingly applied to the analysis of biological datasets, enabling the identification of correlations between drug characteristics, pharmacological effects, and patient-specific responses [40]. These applications underscore the role of CNNs as a powerful tool for integrating molecular, biological, and clinical data in order to advance predictive modeling and personalized therapy.

6.5 Support Vector Machines (SVM)

Support vector machines (SVMs) are increasingly applied in pharmacokinetic/pharmacodynamic (PK/PD) modeling, particularly for predicting drug toxicity levels and evaluating key pharmacological processes, including absorption, distribution, metabolism, and elimination (ADME). By mapping input data into high-dimensional feature spaces, SVMs construct optimal decision boundaries that enable the classification and prediction of complex biological responses. However, two persistent challenges in SVM applications are feature selection, which determines the most relevant variables for accurate modeling, and boundary optimization, which ensures generalizability without overfitting [41]. Despite these challenges, SVMs remain a robust and versatile tool for drug development, offering valuable predictive insights across multiple PK/PD processes. A comprehensive comparison of ANN, CNN, and SVM applications in PK/PD prediction is summarized in Table 4.

7 Result

Figure 2: illustrates the comparative analysis of accuracy obtained using three prominent AI-based technologies: Artificial Neural Networks (ANNs), Convolutional Neural Networks (CNNs), and Support Vector Machines (SVMs). The study covers research publications from 2017 to 2024, and the average values across different application domains were considered to generate the findings. This comparative visualization enables a clearer understanding of how different AI models perform in drug delivery applications.

Figure 2: The results show that ANN obtained accuracies of 60% (OSDF), 74.27% (PODRF), 1% (VS), and 63% (P&P), with an overall average of 49.56%. In comparison, CNN outperformed in most areas, scoring 97.56% (OSDF), 6.85% (PODRF), 75% (VS), and 90% (P&P), for an average accuracy of 67.35%. SVM, while good in P&P (92.03%), underperformed in PODRF (4.47%) and VS (0.597%), resulting in the lowest average accuracy of 39.27% among the three models.

Figure 3: depicts the total average accuracy of the three

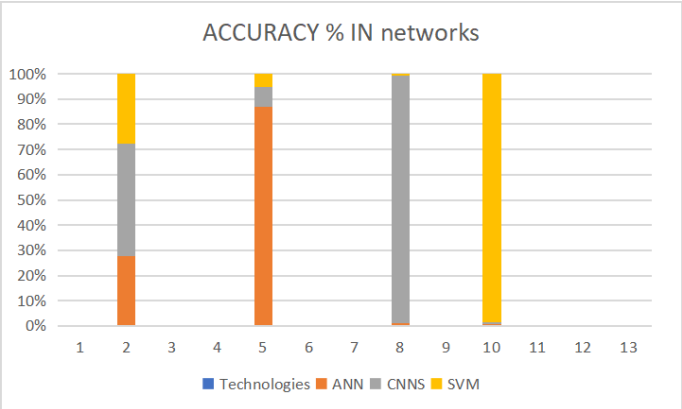

Figure 2. Accuracy % in ANN, CNN, SVM.

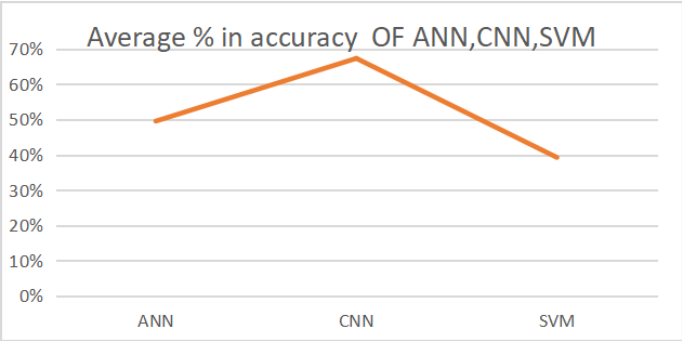

Figure 3. Average % in accuracy of ANN, CNN, SVM.

AI technologies—Artificial Neural Networks (ANNs), Convolutional Neural Networks (CNNs), and Support Vector Machines (SVMs)—based on their performance in four domains: OSDF, PODRF, VS, and P&P.

The comparative results indicate that:

- CNN earned the greatest overall average accuracy of 67.35%, proving its strength and adaptability across a wide range of pharmaceutical applications.
- ANN achieved a respectable average of 49.56%, indicating reasonable performance in PODRF (74.27%) and P&P (63%), but was considerably hampered by its poor VS accuracy (1%).
- SVM, despite outperforming in P&P (92.03%), had the lowest overall average of 39.27% due to poor results in PODRF (4.47%) and VS (0.597%).

The results in Figure 3 clearly show that CNNs beat ANNs and SVMs in terms of average predicted accuracy. While ANNs and SVMs have domain-specific strengths (e.g., ANN in drug release formulation prediction and SVM in pharmacokinetics/pharmacodynamics), their inconsistency across domains limits their efficiency. In contrast, CNNs regularly perform well in OSDF, VS, and P&P, making them the most trustworthy model for drug delivery system applications.

Figures 2 and 3 show that CNN is the superior AI model for drug delivery systems. Its capacity to work with complex data structures, molecular recognition, and image-based analysis provides it a considerable advantage in pharmaceutical applications. While ANN and SVM are useful for specific tasks, their limited generalizability makes them less suitable for use in integrated drug development pipelines than CNN.

8 Methadology

The proposed methodology emphasizes the use of Artificial Intelligence (AI) techniques such as Artificial Neural Networks (ANN), Convolutional Neural Networks (CNN), and Support Vector Machines (SVM) to improve drug formulation,

Table 4. Pharmacokinetics and Pharmacodynamics.

Reference	Technology	Accuracy	Description
[39]	ANN	63%	ANN is used to forecast the time period in pharmacokinetics and pharmacodynamics on the bases of characteristics associated with the patients ANN is also used in tablet formulation in pharmacokinetics
[40]	CNN	90.00%	CNN help in the analyzing the biological data of a patient. It makes valuable tools that helps in understanding relationship between the drug behaviour in pharmacokinetics and pharmacodynamics
[41]	SVM	92.03%	Support vector machine is a numerical education technology that has been used to predict the toxicity level and essential quality of absorbance diffusion, consumption and elimination of new drug Further, there are two Problem associated with: quality choice and boundary choice

drug release prediction, virtual screening, and pharmacokinetics/pharmacodynamics modeling.

The process can be broken into the following stages:

Step 1: Data collection and preprocessing.
The initial stage involves the systematic collection of datasets that integrate multiple dimensions of pharmaceutical information, including drug molecular structures, excipient and formulation parameters, pharmacokinetic and pharmacodynamic (PK/PD) profiles, as well as toxicity and absorption properties. To ensure data quality and suitability for machine learning applications, a rigorous preprocessing phase is required. This includes the removal of missing or incomplete values, normalization of continuous variables to achieve comparability across scales, and the transformation of chemical descriptors into standardized numerical feature vectors. Finally, the curated dataset is partitioned into training, validation, and testing subsets, thereby enabling robust model development, hyperparameter tuning, and independent performance evaluation.

Step 2: Feature Development
In this phase, the focus shifts to the systematic extraction of critical formulation features that serve as inputs for predictive modeling. These features typically encompass molecular descriptors—such as molecular size, weight, energy values, and hydrophobicity—as well as process parameters, including temperature, solubility, and concentration. Additionally, patient-specific biological parameters are incorporated to account for inter-individual variability in pharmacokinetic and pharmacodynamic responses. To manage the often high-dimensional nature of these datasets, dimensionality reduction techniques such as principal component analysis (PCA) or autoencoders are employed. This not only enhances computational efficiency but also helps retain the most informative features, thereby improving the robustness and generalizability of the model.

Step 3: Model Development.
Following feature development, appropriate machine learning models are selected and trained to address the specific requirements of pharmaceutical formulation and PK/PD prediction. Artificial neural networks (ANNs) are widely applied to forecast formulation outcomes, as their multi-layered structure allows them to approximate non-linear relationships and simplify complex mathematical equations. For tasks involving structural and image-related data, such as molecular graphs or compound images, convolutional neural networks (CNNs) are employed owing to their strong feature extraction and pattern recognition capabilities. Meanwhile, support vector machines (SVMs) are particularly effective for classification tasks, including toxicity prediction and the categorization of drug absorption behaviors. Collectively, these models provide complementary strengths, and their integration into the training process ensures a robust and versatile predictive framework.

Step 4: Model Training and Validation.
In this stage, predictive models are systematically trained using the designated training datasets, allowing them to learn underlying patterns and relationships within the data. For neural network–based models such as ANNs and CNNs, learning is refined through backpropagation algorithms, which iteratively adjust network weights to minimize prediction error. In contrast, support vector machines (SVMs) rely on kernel optimization techniques to construct effective decision boundaries in high-dimensional feature spaces. Following training, models are assessed on validation datasets using performance metrics such as accuracy, precision, recall, and the F1-score, thereby ensuring that the predictive framework not only fits the training data but also generalizes effectively to new, unseen inputs.

Step 5: Comparative Analysis.
The final stage involves a systematic comparison of model performance across the different algorithms employed, such as ANNs, CNNs, and SVMs. This comparative evaluation highlights the relative strengths and limitations of each approach, ensuring that the chosen model is optimally aligned with the task requirements. For instance, CNNs are often more effective for formulation prediction tasks involving structural or image-based data, whereas ANNs demonstrate strong performance in patient-specific dosing predictions due to their ability to model complex, non-linear relationships. Conversely, SVMs are particularly advantageous for toxicity classification and absorption categorization, where robust boundary optimization enhances predictive accuracy. Through this process, the most effective algorithm is selected and tailored to each specific application in drug formulation and delivery.

Step 6: Deployment
In the final stage, the selected AI model is integrated into a decision-support system designed to assist pharmaceutical scientists and clinicians in real-world applications. Once deployed, the model can generate

predictions across multiple domains, including the optimization of pharmaceutical formulations, the forecasting of drug release profiles, and the modeling of pharmacokinetic and pharmacodynamic (PK/PD) behaviors. Additionally, the system can provide early warnings by predicting toxicity levels and potential adverse effects, thereby supporting risk assessment and patient safety. Through this integration, AI functions not only as a research tool but also as a practical framework for evidence-based decision-making in pharmaceutical development and therapeutic practice. Pseudo code for the methodology:

Algorithm 1: Drug Delivery AI Model

Data: Dataset D
Result: Improved drug formulation predictions and accuracy outcomes.
Begin with Step 1: Data Preprocessing;
Load Dataset D;
Clean missing or incomplete values;
Normalize and standardize features;
Convert molecular structures to numerical vectors;
Split data into TrainSet, ValidationSet, and TestSet;
Step 2: Feature Engineering;
Extract molecular descriptors and process parameters;
Reduce dimensionality (e.g., PCA/Autoencoder);
Step 3: Model Initialization;
Initialize ANN for formulation prediction;
Initialize CNN for molecular structure analysis;
Initialize SVM for toxicity classification;
Step 4: Model Training;
foreach *model in* {*ANN, CNN, SVM*} **do**
    Train on TrainSet;
    Validate on ValidationSet;
    Record performance (accuracy, precision, recall, F1);
end
Step 5: Comparative Analysis;
Compare ANN, CNN, SVM results to select *Best_Model*;
Step 6: Deployment;
Use *Best_Model* to:;
    Predict drug release;
    Forecast PK/PD behavior;
    Classify toxicity risk;
    Recommend optimal formulation;

9 Discussion and Recommendation

In this part, we explore the recommendations for applications in drug delivery system as part of future work, based on the study discussed above. Here are some essential suggestions:

According to the studies this paper Suggest that, the AI algorithms that are being used till now for drug delivery system can be improved, to enhance drug delivery strategies, forecast drug behaviour, and get a better understanding of DDSs, researchers have to keep experimenting with and refining different simulation methodologies. Combining several simulation methods, oral solid dosage form, formulations, virtual screening, Pharmacokinetics and Pharmacodynamics and give a deeper comprehension of DDSs. Become greater the use of component in the drug delivery sector and enhancing the dependability of simulation findings need the creation of more precise and verified models.

More personalization and training will be required for AI/ML enabled devices and applications in the future in order to forecast data more accurately. As artificial intelligence (AI) gains traction in the drug deliver industry, it will require more personalization and training to yield accurate outcomes. These devices can comprehend a person's requirements, preferences, and behaviour better when AI is given the freedom to be customized. In addition to increasing customer pleasure, personalization enables AI to provide more individualized ideas and recommendations. When AI systems are consistently taught to adjust to changing user preferences and behaviours, the prediction accuracy and overall usefulness of AI-enabled devices are eventually improved.

Ethical issues related to economics, justice, privacy, and other aspects of integrating AI into drug delivery system. AI integration in drug delivery raises a number of ethical issues that should be carefully explored. Economic considerations are significant because they have the potential to restrict access to AI-powered drug delivery services, perhaps exacerbating already-existing gaps in drug delivery system availability. When it comes to the equitable allocation of AI drug delivery system resources, concerns of justice arise since it ensures that people with less money should benefit equally. Working with legislators, medical practitioners, technologists, and ethical academics is crucial to addressing these ethical concerns and making sure AI improves healthcare outcomes while upholding ethical norms.

AI has the ability to improve drug delivery system outcomes by increasing the effectiveness and precision of medical diagnosis, treatment plans, and decision-making. With the application of AI, which has the potential to improve the precision and efficacy of a range of medical treatments, AI might undergo a significant transformation. Additionally, AI-powered predictive analytics may be used to adopt preventive, improving patient outcomes. AI-enabled drug delivery system workers reduce diagnostic inaccuracy, streamline procedures, and enhance treatment protocols. In the end, these advantages lead to better patient care. AI has a lot of promise to be a very useful tool for enhancing the provision of drug delivery system.

Machine learning algorithms may be able to evaluate vast amounts of patient data to identify patterns and trends that might result in an earlier diagnosis and course of treatment. Machine learning algorithms are capable of analyzing large amounts of patient data, which are then used to find patterns and trends that may indicate an early diagnosis. The combination of natural language processing (NLP) and machine learning (ML) has significantly advanced in drug delivery by enabling effective patient data management that maximizes clinical decision-making.

Further, in order to improve simulation speed and efficiency, researchers must also address computational constraints and keep creating new technologies and AI algorithms. In order to guarantee the correctness of simulation findings and boost the dependability of Component based predictions, it is important to validate and confirm simulation models. Researchers should keep looking at the ways that simulations might be used to examine the effectiveness and safety of cutting-edge drug delivery system, including gene and cell therapies. Developing new algorithm and models to give personalize treatment to the patients. The researcher should create more AI tools for getting the accurate and better outcomes, for creating more new drugs and designs. The researcher should create new technologies for improving accuracy and side effects

10 Conclusion

After evaluating a large number of referenced articles and research studies, it is possible to conclude that incorporating artificial intelligence (AI) into drug delivery systems has enormous potential to transform current healthcare. AI technology can prevent adverse drug reactions, optimize dosing regimens, and provide vital insights into the interaction between pharmaceuticals and patient-specific biological responses. By analyzing large datasets, AI allows researchers to reduce chemical structures, streamline formulation design, and improve the efficiency of pharmaceutical development pipelines.

Furthermore, AI allows for a better knowledge of the interaction between medications and their pharmaceutical behavior in patients, which is essential for adapting treatments to specific needs. This not only improves therapeutic outcomes but also reduces the hazards associated with traditional, one-size-fits-all drug administration methods. The use of AI-driven models like ANN, CNN, and SVM has already resulted in quantifiable gains in accuracy, prediction, and efficiency across several stages of drug delivery research.

In a larger sense, the incorporation of AI into medicine delivery systems supports and advances numerous United Nations Sustainable Development Goals (SDGs). AI helps to achieve global goals such as Good Health and Well-Being (SDG 3) and Industry, Innovation, and Infrastructure (SDG 9). Furthermore, AI-driven advances in pharmaceutical research have the potential to contribute to Responsible Consumption and Production (SDG 12) by improving the sustainability of medicine formulation and distribution.

To summarize, artificial intelligence (AI) is both a technological innovation and a transformational tool in healthcare. Its ongoing incorporation into drug delivery systems promises to result in safer, more effective, and patient-centered medicines, ultimately transforming the future of medicine.

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Conflicts of Interest

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Ethical Approval and Consent to Participate

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