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Artificial Intelligence-The New Frontier In Drug Discovery: A Review

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Abstract

Artificial Intelligence (AI) is defined as a combination of human intelligence with computational algorithms that simulate technologies of convolutional neural networks (CNN) like machine learning (ML), deep learning, and artificial neural networks (ANN). It is primarily working on the development of the new methods and technologies that can solve the complexity of the formulation and processing in the pharmaceutical industry. AI devices are now developed that can help with their capacity to learn from experience and historical data, in analysing their immediate environment, carry out activities quickly, discern patterns, and recognise faces and things. Artificial intelligence is a procedure that uses a computational algorithm to mimic human intelligence. ANNs have number of applications in drug delivery research which consists of drug release prediction, pharmacokinetic modelling, targeted drug delivery, and formulation optimization. AI algorithms provide an understanding of drug delivery mechanisms, IV drug release profiles, and the knowledge of the current shelf life and deterioration of oral drugs. AI approach can be applied i.e., Convolutional neural network (CNN) that can ensure all the criteria required for automated analysis of the defects of tablet. Machine learning (ML), a branch of artificial intelligence, that provides a promising solution as its algorithms can "learn" from large datasets and can help in prediction of complex systems. AI simulated with computational algorithm is now widely accepted procedure to tackle these types of hurdles in the prediction of the PK parameter. Therefore, this needs to be developed in several areas to help the assessment and efficacy of the projects that are evolving in future.

Keywords: Artificial Intelligence; Drug Discovery; Technologies of AI; Solid Dispersions; Long Acting Injectables

1. INTRODUCTION

Artificial intelligence (AI)-based formulation development has shown to be a successful technique for supporting the pharma product development process. AI, which mimics human intellect through computational algorithms, is a powerful tool with numerous methods that may be used to a variety of situations. With increasing demand for AI, its applications are developing, particularly in clinical assessment and training. Furthermore, AI is critical for handling and interpreting big datasets, opening up new avenues for in-depth research [1]. The ability to process large amounts of data reduces human workload while increasing quality of life. The usual AI pipeline includes four main steps: data collection and preparation, AI modeling, simulation, testing, and deployment [3]. AI-based drug development has grown widely adopted in the pharmaceutical business, and it is currently seen as a dominating and powerful alternative to traditional

approaches [4]. Pharmaceutical corporations are increasingly investing in artificial intelligence, often forming joint ventures with AI startups, in order to develop more effective medication treatments and medical device [5].

AI focuses on creating intelligent systems capable of executing activities that would normally need human intelligence and cognition. These systems can learn from experience and past data, evaluate their surroundings, complete jobs quickly, recognize patterns, and even recognize faces and things. Machine Learning (ML), a subject of AI, is often divided into three categories: supervised learning, unsupervised learning, and reinforcement learning (Figure 1).

In supervised learning, algorithms expect target variables based on a set of input variables [6]. AI technology is expected to impact medication discovery and development as algorithms improve and clinical data is collected. AI is becoming increasingly important in all aspects of pharmacy, making it a necessary tool at every stage of developing new drugs. There are several methods for administering drugs, including transdermal, mucosal, oral solid dosages, and biologics, all with the goal of enhancing therapeutic effectiveness while decreasing side effects and taking into account patient demands. AI has shown promise in solving many medication delivery difficulties, including low dissolution, low permeability, increasing trial-and-error research, and poor patient compatibility.

2. TECHNIQUES OF ARTIFICIAL INTELLIGENCE

Artificial intelligence proves its benefits in various applications by using its several techniques (Figure 1Genetic algorithm provides its application in targeted drug delivery processes, for optimization the dosage of medicine for personal use, in drug delivery research, to understand the kinetics of drug release, aiding in modelling of PK models and in improving the patient and therapeutic compliance [7]. ANNs widely known technology referred as Artificial Neural Networks have number of applications in drug delivery research which consists of drug release prediction, pharmacokinetic modelling, targeted drug delivery, and formulation optimization. They also help in personalized drug dosing, quality control, and in silico screening of drug candidates. ANNs proved beneficial in increasing the process of drug delivery system development, in optimizing formulations that can provide efficient and targeted therapies. Support Vector Machines (SVM) are important because they can predict drug-target interactions, helps in improving formulations, simulate pharmacokinetics, and able for personalised medication delivery.

XGBoost aims mainly to estimate the area under curve (AUC) and for making accurate predictions by using pharmacokinetic (PK) datasets from individuals who had undergone kidney, liver, and heart transplants [8,9]. XGBoost is a very powerful machine learning algorithm that serves to finds applications in drug discovery and delivery. Its algorithm can also predict drug-target interactions, identifying potential drugs that mainly binds to their specific targets. Moreover, it imitates drug pharmacokinetics and pharmacodynamics, optimizing delivery strategies and dosage regimens. It is beneficial in prediction of toxic effects, in determining the selection of safe drug candidates. Additionally, it regulates drug formulations by considering such factors like solubility, stability, and bioavailability, leads for better delivery systems. It can predict individual responses to drugs, enabling personalized drug delivery by analysing patient data. Furthermore, it mimics drug release kinetics for sustained or controlled delivery from various systems.

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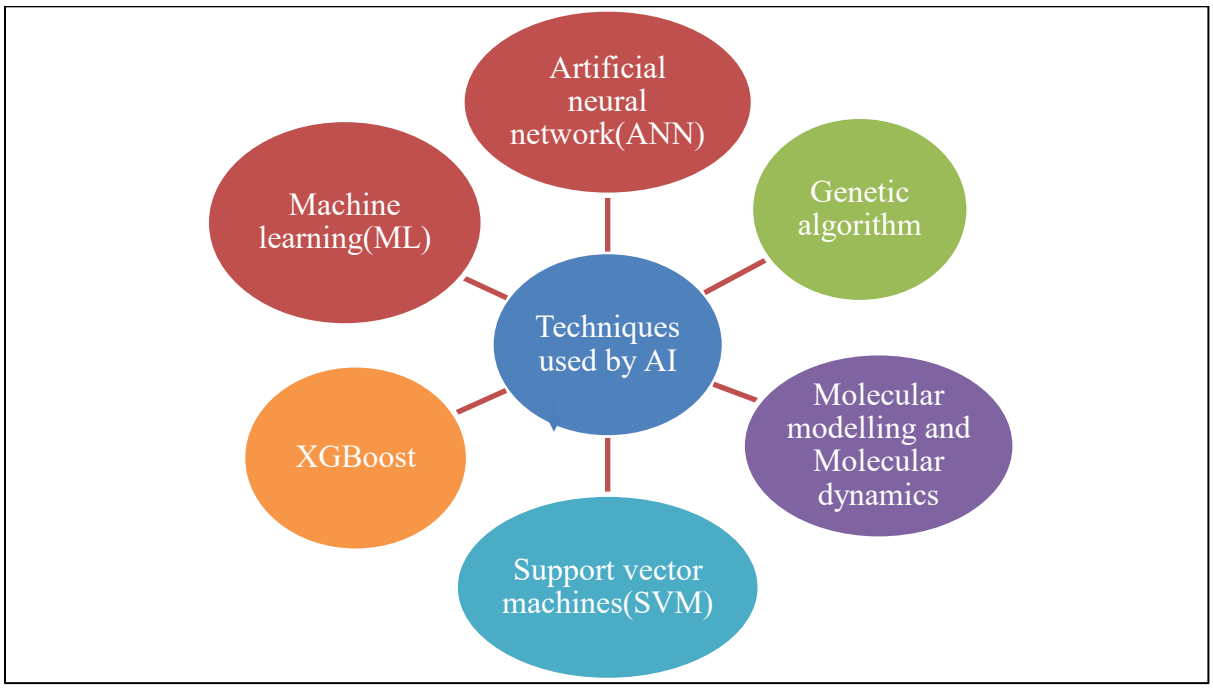

Figure 1. This figure illustrates key techniques in Artificial Intelligence, including Artificial Neural Networks (ANN), Machine Learning (ML), Genetic Algorithms, XGBoost, Support Vector Machines (SVM), Molecular Modelling, and Molecular Dynamics, showcasing their diverse applications in AI-driven problem solving.

Formulating drugs with low aqueous solubility poses a significant obstacle in the pharmaceutical industry, falling under the challenging biopharmaceutical classification system (BCS) classes II and IV [10]. Surprisingly, about 40% of commercial drug products and a staggering 90% of drugs in the developmental stage are plagued by poor water solubility [11]. Besides this, the formulation development process grapples with additional hurdles, such as poor powder flowability [12], a narrow therapeutic window [13], and susceptibility to chemical degradation during manufacturing [14].

Confronting these difficulties demands scientists to embark on numerous experiments to bridge the knowledge gap. However, these experiments are both labour-intensive and time-consuming, adding further complexity to the development process. Thankfully, artificial intelligence (AI) comes to the rescue as it provides an efficient and effective solution. In recent years, AI has significantly improved in power and flexibility, making it a compelling approach to tackle the challenges faced in formulation development. By leveraging AI's capabilities, researchers can streamline their efforts, accelerate experimentation, and ultimately devise innovative and optimized drug formulations to meet the needs of patients and the pharmaceutical market [15]. AI plays a crucial role in rectification of the development of systems of delivery of drug, transdermal, parenteral, mucosal, in biologics products development, nanomedicine, medical devices, pharmacokinetic and pharmacodynamic parameters (PKPD) assessment etc.

3. AI FOR SOLID ORAL DOSAGE FORM DEVELOPMENT

Solid dosage forms like tablets, capsules, powders are most popular due to their ease of self-administration, patient compliance, good stability, correct dosing, and simplicity of production, oral solid dosage forms are regarded as the most suitable type of drug delivery. Tablets rule the market among all solid dosage forms. By 2015, there will be a 100% rise in the use of AI for solving the issues stated above [16].

3.1 ROLES OF ARTIFICIAL INTELLIGENCE

AI predominantly helps in the product development phase, such as in predictions of drug behaviour, drug release through formulations, physical stability, detection of tablet defects, understanding the impact of QC parameters in the manufacturing of the product, and the manual resources used for trial-and-error experiments (Figure 2). AI algorithms provide an understanding of drug delivery mechanisms, IV drug release profiles, and the knowledge of the current shelf life and deterioration of oral drugs. It provides information on the detection of potential risks and challenges at an early stage [17].

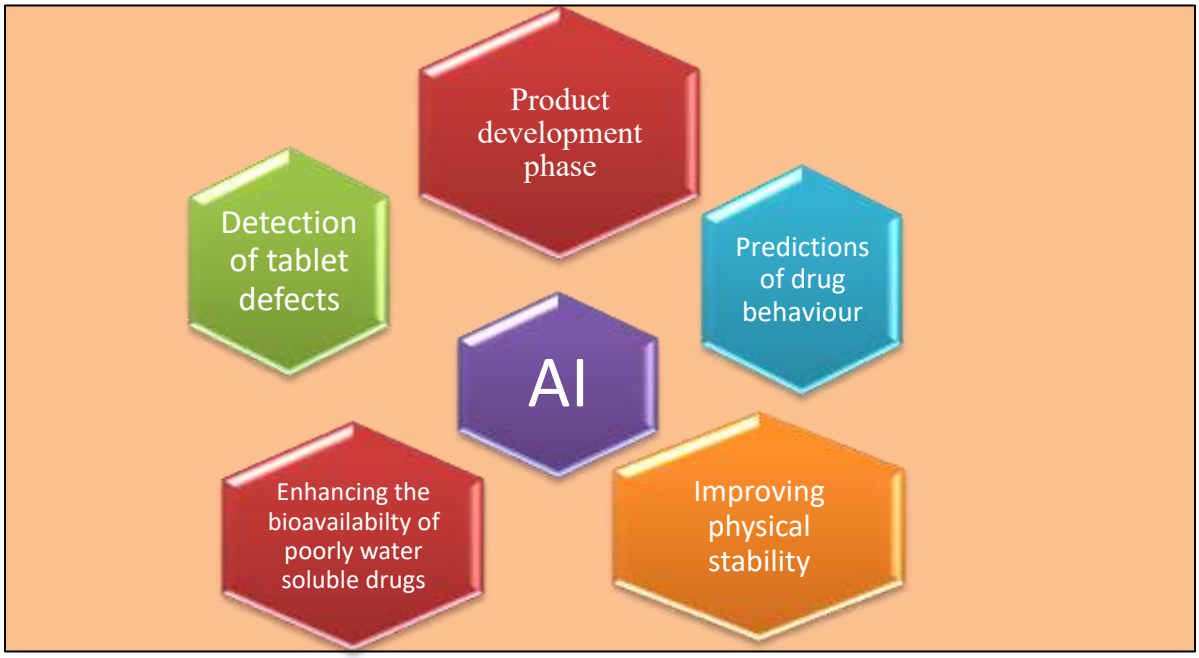

Figure 2. The roles of Artificial Intelligence in pharmaceutical product development, including the detection of tablet defects, predictions of drug behavior, improvement of physical stability, and enhancement of the bioavailability of poorly water-soluble drugs.

1.1. BIOAVAILABILITY OF POORLY WATER-SOLUBLE DRUGS

Artificial Intelligence (AI) has significant promise in improving the oral bioavailability of poorly water-soluble drugs using supersaturating drug delivery systems (SDDS) [18-21]. AI can optimize SDDS formulation parameters, like carrier materials and release rates, to enhance drug solubility and availability. AI-based predictive models can also identify suitable precipitation inhibitors ("parachutes") [22]. They help in sustaining the supersaturated state in the gastrointestinal tract, leading to improved drug absorption and effectiveness when taken orally [23].

1.1.1. MACHINE LEARNING IN SOLID DISPERSIONS

Amorphous solid dispersion (SD) has gathered major beneficial interest for its potential to enhance drug solubility. Major challenge for economization is due to the physical stability of solid dispersions. The current stability testing process is time-consuming and unpredictable, that lacks the progress. The specified mechanism of Solid dispersions stability still poorly understood. Many theoretical models have been established, but they require extensive physicochemical data and expertise of professional results in limiting their predictive capabilities.

Machine learning (ML), a branch of artificial intelligence, that provides a promising solution as its algorithms can "learn" from large datasets and can help in prediction of complex systems. In pharmaceutical research, ML has shown success in areas such as quantitative structure-activity relationship (QSAR), drug-drug interaction, drug discovery, and pharmacogenomics [24-29]. In development of formulation the models of ML have been developed that possess high accuracy for prediction of disintegration time, dissolution curves, and binding free energy of drug complexes [30]. By

using the techniques of ML, ability to insights into the physical stability of solid dispersions and help in the development of stable drug delivery systems for pharmaceutical applications can improved. The result is evaluated by comparing the true values with predictive value for each considered datasets - training set, validation set and testing set by ANN and DNN. Most accurate neural technology will be considered for prediction of further datasets [31]. Two crucial steps were followed in ML:

1. **Data extraction**: Solid dispersions-related data were gathered using the keywords "solid dispersions" and "physical stability" from the databases of the Web of Science.
2. **Dataset classification**: The dataset was split into three subsets via using machine learning techniques training set, validation set and testing set [31].

As compared with previous data selection methods maximum dissimilarity algorithm (MD-FIS) in R language is the best choice. Both Artificial neural network (ANN) and deep neural networks (DNN) are the most widely used neural network technologies. In comparison of ANN, DNN provides information with more accuracy and detect minute variation with complicated parameters of network [32]. Data were taken from internal Merck data by Junshui Ma et al. and comprised on-target and absorption, distribution, metabolism, and excretion (ADME), with each molecular characteristic being defined as serious. Deep neural networks were utilised to analyse QSAR in the end, and the outcome was superior to that of the widely used random forest [33]. Each layer of network consists of several epochs that indicates how many times a dataset is used for training. The are many primary distinctions between Artificial Neural Networks (ANN) and Deep Neural Networks (DNN), some of them are summarized in the Table 1:

Artificial Neural Network	**Deep Neural Network**
It is defined as Artificial neural network.	It is defined as Deep neural network.
ANN consists of one or two hidden layers of neural networks	DNN consist of multiple hidden layers of neural network.
ANN is commonly used for basic tasks such as regression and classification problems.	DNN is used for more complex tasks, such as identification of image, natural language analysis, and other tasks that require understanding complex relationships in the data.

Table 1: Comparison between Artificial Neural Network (ANN) and Deep Neural Network (DNN), highlighting differences in their structure, applications, and complexity.

1.1.2. AI IN TABLET DEFECTS

UNet is a convolutional neural network (CNN), that is based on the image segmentation analysis. The "U" in **U-Net** refers to the shape of the network architecture. It was previously used for image segmentation of cell and tissue in biomedical. It is known as UNet because of its U-shaped form, which consists of an encoder element and a decoder part. Mainly two convolutional neural networks were used UNetA and UNetB. Current application of UNet is detection of tablet defects, requires a images dataset which includes both defective and non-defective tablets, simultaneously with the truth that masks indication of the regions of defects. AI is trained by a large dataset of labelled images of previous collection of defects of images to produce the result. The process of detecting the tablet defects via UNet is consisit of several steps that are shown in Figure 3.

Tablet defects can arise during manufacturing or storage that results into impure products that may have cracks, chips, and capping like defects that leads to deterioration of structure. Defects like lamination, hardness variation, and weak bonding can cause defects in appearance and functional parameters. Content non-uniformity defects effects consistency of dosage. Major defects like Sticking, mottling, swelling, double impression, and softening can result potential reduction in quality. So, QC measures are important to produce safe and effective tablets. Traditional methods like X-ray microcomputed tomography (XRCT) mainly used for identification of analysis of the internal

image and for identification of damage [34]. The use of XRCT to automatically determine internal tablet faults has been hold back due to its inability to accurately measure the internal cracks of tablet. But an AI approach can be applied i.e., Convolutional neural network (CNN) that can ensure all the criteria required for automated analysis of the defects of tablet.

Mainly two convolutional neural networks were used UNetA and UNetB.

The process of detecting the tablet defects via UNet

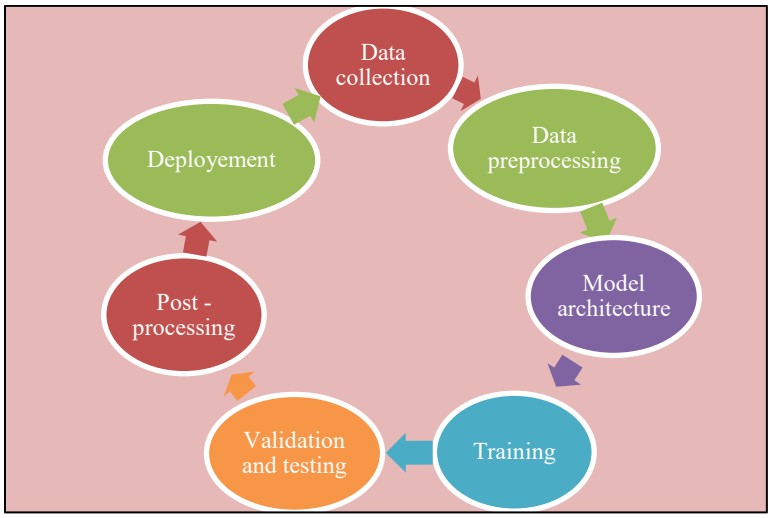

Figure 3. Workflow for Detecting Tablet Defects Using U-Net: This process involves data collection, preprocessing, model architecture design, training, validation/testing, post-processing, and deployment. Each step is essential to ensure the accurate identification of defects, utilizing U-Net's encoder-decoder structure for segmentation.

1.1.3. AI in parenteral drug delivery

Artificial Intelligence (AI) is defined as a combination of human intelligence with computational algorithms that simulate technologies of convolutional neural networks (CNN) like machine learning (ML), deep learning, and artificial neural networks (ANN). The usefulness of AI is well seen in every aspect of the pharmaceutical field, mainly in the development and manufacturing of sterile preparations such as parenteral and biologic products (vaccine, sera, antibodies, immunomodulators, etc.). Parenterals are considered the most widely used form of drug delivery after oral dosage forms as they provide several advantages [35]. Parenteral route of drug administration generally includes: Intravenous (IV), Subcutaneous (SC), Intramuscular (IM) and Intradermal. Parenteral drug delivery is the process of injecting drugs or other chemicals straight into the circulation or other body tissues, eliminating the need for the digestive system. So, sterility and stability are crucial to determine before administering them into the patient's body.

It offers several advantages, like being suitable for patients who are unable to take oral drugs, offering a rapid start to action and accurate dose control, avoiding the first-pass effect, and providing 100% bioavailability. As far as the benefits, parenteral hold several limitations, such as the fact that the presence of any other particles can cause capillary emboli, skilled or trained professionals are required for administration, and there is the possibility of tissue irritation or a blood coagulation cascade. Automation actually makes it possible to increase safety, lessen exposure to dangerous drugs, guarantee excellent repeatability, and establish tracking of each step in the manufacturing process. Because it provides a secure alternative for manual labour [35]. The evolving importance of AI in the manufacturing and development of injectables is increasing rapidly, as it plays a quite significant role in the determination of physical stability, small particle detection, long-acting injectables (LAI) in vitro release of drug, quality, efficiency, and variability of parenteral products. Therefore, based on this neural network, it is necessary to decrease down on the time spent on manufacturing preparations and to enhance work dynamics.

Parenterals drug delivery is classified into various groups given below:

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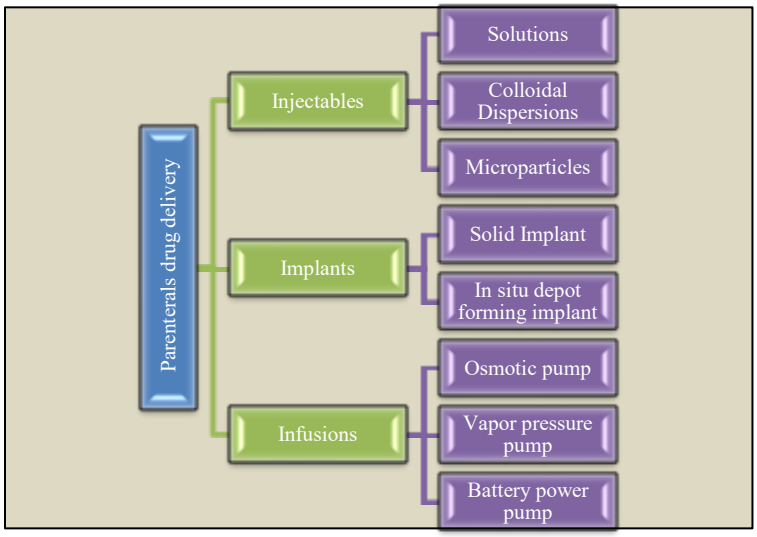

Figure 4. Types of Parenteral Drug Delivery Systems: This figure illustrates various parenteral drug delivery methods, including injectables (solutions, colloidal dispersions, and microparticles), implants (solid implants and in situ depot forming implants), and infusions (osmotic pump, vapor pressure pump, and battery-powered pump).

1.1.4. USE OF ML IN LONG ACTING INJECTABLES (LAI)

Machine learning algorithm is most widely used in long acting injectables (LAI) for improving the rate of drug delivery. LAI are considered beneficial as they improve patient's compliance of not administering the medication again and again as they release their cargo number of medications over an extended period of time and improve therapeutic outcomes [36]. Neural networks simulation helps in predictions of in vitro drug release via collection of data by tree-based method and instance-based methods. The data is then proceeded for testing, development of models, validation and in last for training them for future predictions [37].

2. TECHNIQUES USED BY AI TO REMOVE THE ISSUES

4.1 PARTICLE TRACKING ALGORITHM:

Particle tracking algorithm is used for the determination of the small molecules that floats in the parenteral formulation and cause a limitation in the drug delivery. It works with the of image subtraction or imaging data obtained via previous analysis. These algorithms use innovative computer vision techniques to efficiently and precisely analyse microscopic images by automatically recognising and tracking particles. It helps in checking and analysing through AI-based tracking that may improve the effectiveness of QA and procedures used in production of pharmaceutical. Particle tracking algorithm involves several steps in the process that are illustrated in the Figure 5. AI significantly reduces the need for human involvement in key areas of pharmaceutical research and production. It is instrumental in particle detection and tracking analysis, streamlining the process and boosting efficiency. By utilizing AI, the likelihood of errors is greatly diminished, as the technology can reliably execute tasks with high precision. Additionally, AI improves the reproducibility of results, ensuring that experiments and processes produce consistent outcomes each time, which minimizes variability and enhances the overall reliability of the data. This results in more accurate and efficient processes, leading to higher-quality products and improved decision-making in drug development.

As the measurement of the particles, bubbles, minute contamination can affect the quality index of the parenteral and the route of administration, drug delivery processes are also affected. Particle tracking algorithm with the use of AI provides the acceptable quality level (AQL) simulated with the previous record. If the presence of these adherent molecule is below than the AQL then the products are considered safe and effective [38].

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2.1.1. Process of particle tracking algorithm:

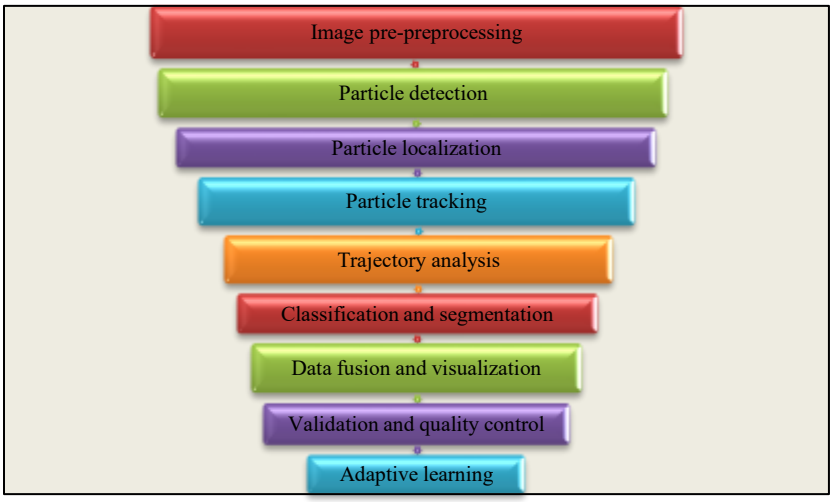

Figure 5. Process Flow of Particle Analysis in Pharmaceutical Research: This figure illustrates the steps involved in particle analysis, starting from image pre-processing, through particle detection, localization, and tracking, followed by trajectory analysis, classification, and segmentation. It also includes data fusion and visualization, validation and quality control, and concludes with adaptive learning to improve accuracy and efficiency over time.

4.2 CONVOLUTIONAL NEURAL NETWORKS (CNNS)

CNNs is a most widely used method of deep learning algorithm which provides understanding of finding and differentiating between chemical molecules that are composed in parenteral products by the use picture analysis. This technique combines the knowledge of collection of large amounts of labelled microscopic pictures that represents molecules that are highlighted in between molecules these materials. The data is then forwarded for preprocessing confirmation to improve the efficacy of the collected data.

The data is processed randomly from images that are already uploaded by collecting data from sites like 'web of science' by the use of these CNN layers. By this way they extract out the most suitable methods for learning the algorithm and then the model is trained by previous data to rewind the patterns of molecules from dataset.

4.3 LIGHT GRADIENT BOOSTING MACHINE (LGBM)

LightGBM is one of the mostly used algorithms of AI for analysis of fractional drug release by the use of random search. it is used for the identification of potential features like PDI prediction and analysis of size by properly assessing, refining and optimization. LightGBM and related algorithms proved to be very useful like its technique of prediction of modelling used for various purposes like to calculate the drug release kinetics, absorption profiles, pharmacokinetic data for long-acting parenteral formulations, and enhancing drug delivery methods for therapeutic effects are critical aspects of drug development (Figure 6).

An experiment performed to evaluate the accuracy of various learning methods along with LGBM by formation of nanocrystals by three different methods BMW, HPS, ASP of three hydrophobic drugs – CEL, GLP and DOC were selected. Over various applied machine learning methods LGBM shows higher efficacy, superior predictive performance for predicting the size of nanocrystal and shows least mean absolute error (MAE) [39].

4.3.1 ADDITIONAL EXTENDED USES OF LGBM:

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Figure 6. Applications of Light Gradient Boosting Machine (LGBM) in Pharmaceutical Research: This figure outlines the uses of LGBM in pharmaceutical development, including predictive modelling for drug release kinetics, formulation optimization, release profile customization, drug stability predictions, accelerating drug development, and optimizing in-vitro studies.

4.5 ROLE OF AI IN PK AND PD

Artificial intelligence (AI) serves role in advancement in almost every field such as drug discovery, drug development, drug delivery, predicts PK parameters (study of the effect of what body does to the drug after administration (ADME), drug release, absorption parameters, metabolism, excretion and PD-pharmacodynamic parameters (study of what body does to the drug).

5. AI BASED COMPUTATIONAL METHODS FOR PHYSIOLOGICAL BASED PHARMACOKINETIC MODELS (PBPK).

PBPK refers to Physiological based pharmacokinetic and simulation modelling in which preclinical data from animal testing is used to analyse the pharmacokinetic behaviour of drugs in humans. It also provides a brief information about the effects of factors like age, diversity, sex, disease status and contribute in the determination of the dosing regimen, optimal dose to produce effect and risk associated to the drug [40]. These models were designed on the basis of hypothetical compartments that consider body's organs and tissues. Body can be divided into one, two or various departments depends on the perfusion rate limited and permeability rate limited.

Models which have the basis of AI are capable of recognizing the major hazards which may be sourced by results of improper interactions between the enzyme and substrate, inappropriate knowledge of the kinetics of drugs, enzymes and the rate of metabolism. Collectively every hazard mentioned above can be detected beforehand with the help of AI generated models by the means of the datasets and reports of clearance of the drug and its efficacy by thoroughly analysing and calculating the factors such as levels of enzyme expression, genetic variations, and drug- drug interactions [41]. AI generated models provide benefits such as reduction in timeline, saving cost.

The growth of these kinds of models are a little compounded which needs a huge amount of data and statistical sources but on the other hand AI based statistical algorithm practice can make the processes and all the issues which are connected to these kinds of model easier. Several methods are employed to design these models via AI based technologies:

a. **Bayesian/WinBUGS:** This approach uses probability distributions to define parameters of the model and estimates to convey uncertainty. It is typically used to deal with data below the limit of quantification [42].
b. **Support Vector Machine/Least Square (SVM):** SVM is employed to analyse drug concentration in a sample based on the profile of a certain patient [43].

c. **Random Sample Consensus and Support Vector Machine (SVM)/Drug Administration Decision Support System (DADSS) RANSAC**: It is used to estimate medication concentration, determine the ideal dose, and improve the intervals between doses for a new patient [44].
d. **Support Vector Model Combined with Random Forest Model:** Its goal is to identify pharmacodynamic medication interactions based on targeted protein connectedness (TPC), chemical resemblance and side-effect homology (SES). It precisely forecasts PDI with an AUC value of 79.96% and a certainty of 89.93%. and safeguarding time, cash, and other assets that would otherwise be used for experimentation and failure experiments [45]. Understanding drug delivery processes, IV drug dispersion profiles, plus the durability of oral solid intake versions are all made possible by AI algorithms. It offers details on how to identify potential hazards and difficulties at an early stage.
e. **Linear Regressions (LASSO)/Gradient Boosting Machines/ XGBoost/Random Forest:** These algorithmic combinations are used to predict plasma concentration variation over time and the region underneath the concentration relative time curve (AUC) from 0 to 24 h following repeated drug dosage. It provides time-efficient analytical benefits and enhances the covariate selection approach [46].
f. **Drug Target Interaction Convolutional Neural Network (DTICNN):** Primarily used for predicting new drug compounds and identifying drug-target interactions [47].
g. **Deep Long Short-Term Memory (DeepLSTM):** This technique uses computers to verify how medications interact with their intended recipients [48].

S.N	Tools and software	Description	Method	Feature	Year	Reference
1	**ChemDes**	An integrated web-based platform for molecular descriptor and	Pybel, CDK, RDKit, BlueDesc, Chemopy, PaDEL and jCompoundMapper	Format converting, MOPAC optimization and fngerprint similarity	2015	https://doi.org/10.1021/acs.jcim.9b00295
2	**Pred-binding**	Large-scale protein–ligand binding afnity prediction	Support vector machine and random forest	589 molecular descriptors and 1080 protein descriptors in 9948 ligand–protein pairs predicted DTIs that were quantifed by Ki values. The cross-validation coefcient of determination of 0.6079 for	2016	https://doi.org/10.3109/14756366.2016.
3	**ChemSAR**	An online pipelining platform for molecular SAR modeling	An online pipelining platform for molecular SAR modelling	Generating SAR classifcation models that will beneft cheminformatics and other biomedical users	2017	ChemSAR

4	**LS-align**	An atom-level, fexible ligand structural alignment algorithm for high-throughput virtual screening.	Machine learning	Generate fast and accurate atom-level structural alignments of ligand molecules	2018	https://doi.org/10.1093/bioinformatics/bty081
5	**DLIGAND2**	Improved knowledge-based energy function for protein–ligand interactions.	Distance-scaled	Best performance as a parameter-free statistical potential and among the best in all performance measures	2019	https://doi.org/10.1186/s13321-019-0373-4
6	**StackCBPred**	A stacking-based prediction of protein-carbohydrate binding sites from the sequence.	Machine learning	Predicted structural properties of amino acids to efectively train a Stacking-based machine learning method for the accurate prediction of protein-carbohydrate binding sites	2019	https://doi.org/10.1016/j.carres.2019.107857
7	**AutoGrow4**	De novo drug design and lead optimization.	Genetic algorithm	The predicted binding modes of the AutoGrow4 compounds mimic those of the known inhibitors, even when AutoGrow4 is seeded with random small molecules	2020	https://doi.org/10.1186/s13321-020-00429-4
8	**LigGrep**	A tool for fltering docked poses to improve	Machine learning	It can improve the hit rates of test VS targeting H. sapiens	2021	https://doi.org/10.1093/bib/bbaa321
9	**ChemDes**	An integrated web-based platform for	Pybel, CDK, RDKit, BlueDesc, Chemopy, PaDEL,	Format converting, MOPAC	2015	https://doi.org/10.1021/acs.jcim.9b00295

		molecular descriptor and fingerprint computation	and jCompoundMapper	optimization, and fingerprint similarity calculation		
10	**Pred-binding**	Large-scale protein–ligand binding affinity prediction	Support vector machine and random forest	589 molecular descriptors and 1080 protein descriptors, Ki values, SVM and RF models	2016	https://doi.org/10.3109/14756366.2016.
11	**ChemSAR**	An online pipelining platform for molecular SAR modeling	SAR modeling pipeline	Generates SAR classification models for cheminformatics and biomedical users	2017	ChemSAR
12	**LS-align**	An atom-level, flexible ligand structural alignment algorithm for high-throughput virtual screening	Machine learning	Accurate atom-level structural alignments of ligand molecules	2018	https://doi.org/10.1093/bioinformatics/bty081
13	**DLIGAND2**	Improved knowledge-based energy function for protein–ligand interactions	Distance-scaled	Parameter-free statistical potential for protein-ligand interactions	2019	https://doi.org/10.1186/s13321-019-0373-4
14	**StackCBPred**	A stacking-based prediction of protein-carbohydrate binding sites from the sequence	Machine learning	Predicts structural properties of amino acids for protein-carbohydrate binding site prediction	2019	https://doi.org/10.1016/j.carres.2019.107857
15	**AutoGrow4**	De novo drug design and lead optimization	Genetic algorithm	Predicts binding modes of compounds and optimizes lead structures	2020	https://doi.org/10.1186/s13321-020-00429-4
16	**LigGrep**	A tool for filtering docked poses to improve virtual-screening hit rates	Machine learning	Improves hit rates in virtual screening targeting specific proteins	2021	https://doi.org/10.1093/bib/bbaa321

17	**DeepDock**	A deep learning-based molecular docking approach	Deep learning	Predicts binding affinity and docking poses	2021	https://doi.org/10.1093/bib/bbab230
18	**ChemProp**	A graph convolutional neural network for molecular property prediction	Graph neural network	Predicts molecular properties and bioactivity	2021	https://doi.org/10.1016/j.jmgm.2020.07.012
19	**AlphaFold**	DeepMind's AI system for protein structure prediction	Deep learning	Predicts 3D protein structures with high accuracy	2020	https://doi.org/10.1126/science.abj8754
20	**DeepChem**	A deep learning library for drug discovery	Deep learning	Supports bioinformatics and cheminformatics tasks	2019	https://doi.org/10.1021/acs.jcim.9b00719

Table 2. List of Tools and Software for Pharmaceutical Research and Drug Discovery: This table provides an overview of various tools and software used in drug discovery and development, including molecular descriptor calculation, protein-ligand binding prediction, virtual screening, SAR modeling, and de novo drug design. It also includes methods, features, year of release, and corresponding references for each tool or software used in pharmaceutical research.

6. ROLE OF AI IN PK PD MODELLING

Pharmacokinetic -PK parameters are known to be the most crucial parameters for optimizing any drug during its development and discovery phase. These parameters are used to understand that what body does to the drug after its administration into the human system, it comprises mostly of four parameters: absorption, distribution, metabolism and excretion commonly known as ADME. A PK study plays a vital role in understanding the rate, route of administration and excretion, safety and efficacy associated with certain drug formulations.

The process of determination of PK parameters requires in- vivo animal and human testing for the determination of safety and efficacy of the drug. As this in-vivo testing process requires large number of datasets of pre-clinical and clinical testing that may cause certain serious health effects on humans and require consent and permission to proceed the testing. PBPK modelling is used for understand in vivo behaviour of animals testing which further extend to the in- vivo understanding of human experimental testing but these modelling are time consuming and so much expensive to conduct [49]. AI simulated with computational algorithm is now widely accepted procedure to tackle these types of hurdles in the prediction of the PK parameter. Machine learning (ML) is the main method of AI that is used for prediction of PK properties that significantly reduces the number of designs make test analyse cycle [49].

Recent developments in AI and ML have enabled the accurate prediction and optimization of PK and PD parameters with much larger datasets, which are the result of these cutting-edge technologies. In silico chemical discovery and property prediction allow for fast screening of compounds and their possible interactions, which reduces the requirement for long experimental testing and expensive processes. High-throughput synthesis and screening techniques speed this process even further by enabling rapid production and testing of large compound libraries for promising drug candidates. In addition, bioanalytical methods

like whole-genome DNA sequencing, RNASeq, single-molecule array assays, and array-based mRNA expression profiling yield detailed molecular and genomic data to better understand the genetic and cellular basis of drug responses. Mass spectrometric methods offer valuable insights into small molecule quantification, proteomics, methylation profiling, and metabolomics, facilitating the analysis of drug metabolism, interactions, and efficacy.

7. AI ADVANCEMENT FOR COMPOUND PK PREDICTION

Machine learning plays a pivotal role in optimizing drug delivery and predicting PK/PD parameters through various approaches. These include optimization of formulation by ML models which suggest the optimal drug composition in order to maximize solubility and stability; in-silico modelling enables virtual simulation of drug behaviour inside the body which reduces the animal trials needed to be conducted on animals. Drug delivery is targeted by ML and can predict which tissues or organs drugs will act on, which ensures that the drugs are efficiently delivered to the target sites. Dosing regimen optimization is another area where ML is highly effective, as it helps predict the ideal dosage and timing to maximize therapeutic effect while minimizing side effects. Additionally, real-time monitoring of drug levels in patients using wearable technologies or sensors allows for dynamic adjustments to dosing regimens. Drug-device interactions can be optimized by leveraging AI to better understand how the drug and delivery system interact, ensuring proper efficacy [49]. Nanoparticle design is increasingly assisted by ML models to develop nanoparticles that improve drug absorption and bioavailability, especially for poorly soluble compounds. Finally, personalized medicine benefits from AI by tailoring drug treatment plans based on an individual's genetic makeup and health data, ensuring that therapies are more effective and safer for each patient.

Together, these advances in AI, ML, and data collection methods are transforming drug development by enhancing the precision, efficiency, and safety of drug therapies, enabling the creation of highly targeted treatments tailored to individual patient needs.

8. APPLICATIONS OF ARTIFICIAL INTELLIGENCE (AI)

Artificial intelligence (AI) is transforming the pharmaceutical industry by improving various aspects of drug development, manufacturing, and optimization. It helps predict pharmacokinetic (PK) and pharmacodynamic (PD) parameters of drug molecules, simulating how drugs behave to fine-tune dosing regimens [50]. AI also plays a crucial role in determining how quickly tablets disintegrate, which is vital for ensuring proper dissolution and optimal absorption [51]. Furthermore, AI techniques are instrumental in detecting and reducing tablet defects, thereby enhancing quality control during production[52-53]. In addition, AI supports the creation of capsule-based formulations [54], predicts interactions between compounds and proteins, and helps mitigate drug toxicity and errors in the early phases of drug development [55-56]. For long-acting parenterals (LAI), AI can forecast drug release profiles, ensuring therapeutic levels are maintained over extended periods [57-59]. The technology is also essential for assessing particle size and polydispersity index (PDI), which are critical for maintaining consistency in drug performance [60]. By minimizing the need for trial-and-error approaches, AI streamlines the processes of drug formulation and optimization [61-64]. It further improves the development of sterile preparations by ensuring quality control and reducing contamination risks. AI enhances the physical stability of solid dispersions and boosts the bioavailability of poorly water-soluble drugs by optimizing particle size and delivery systems. Additionally, AI advances drug delivery methods by predicting absorption, distribution, metabolism, and elimination, making these systems more efficient. In drug discovery, AI speeds up the identification of candidates, predicts toxicity, and identifies targets, facilitating the design of safer and more effective medications. It also models complex relationships and variables in drug development, providing insights into how different factors interact and affect outcomes [65]. Lastly, AI is significantly involved in image-based tasks, such as identification.

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Conflict of interest-

The writers say they have no competing interest.

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