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Role of Artificial Intelligence in Pharmaceutical Science

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ABSTRACT

Artificial intelligence (AI) has become an effective tool that utilizes personal knowledge and offers quicker fixes for difficult problems. Promising developments in artificial intelligence and machine learning offer a game-changing prospect for drug discovery, formulation, and dosage form testing. Through the application of AI algorithms that examine vast amounts of biological data, such as proteomics and genomes, scientists are able to pinpoint targets linked to disease and forecast how those targets may interact with possible therapeutic candidates. This makes it possible to approach drug discovery in a more effective and focused manner, which raises the possibility of successful drug approvals. Additionally, by streamlining research and development procedures, AI can help lower development costs. The pharmacokinetics and toxicity of potential drugs can be predicted using machine learning algorithms, which also help with experimental design. This review highlights the advantages and disadvantages of the several AI-based techniques used in pharmaceutical technology. However, the pharmaceutical industry's ongoing exploration and investment in AI present great opportunities for improving patient care and drug development procedures.

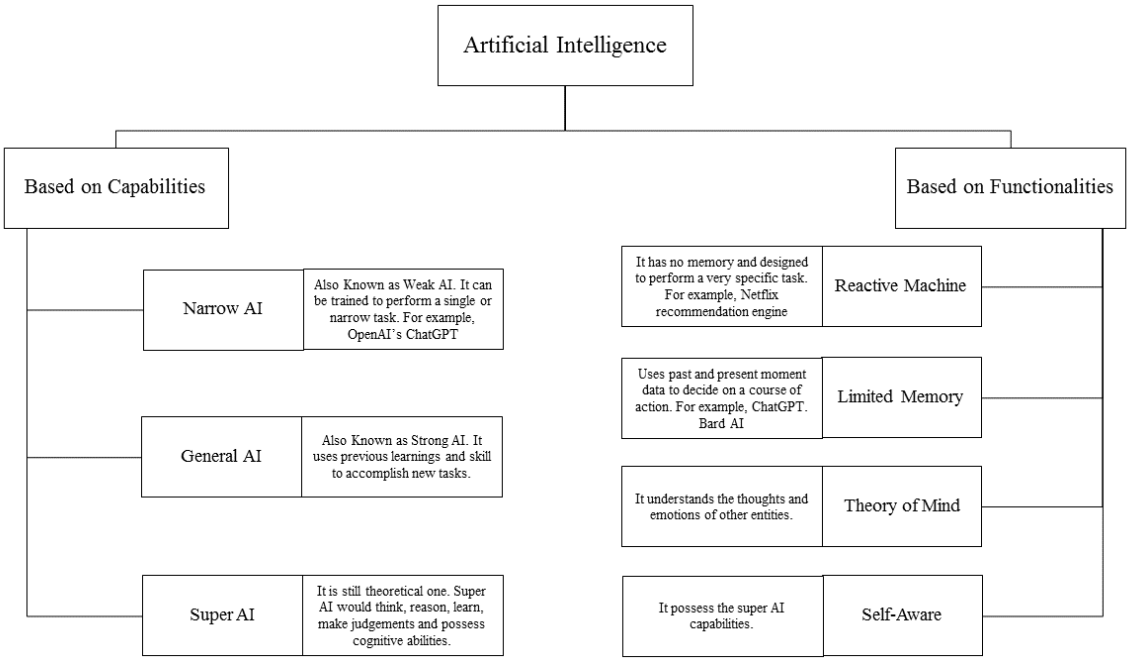
INTRODUCTION

Artificial intelligence (AI) has emerged as a transformative force in the field of pharmaceutical sciences, revolutionizing drug discovery, development, and healthcare delivery. With its ability to analyze vast amounts of data, identify patterns, and make predictions, AI offers unprecedented opportunities to accelerate the discovery of new drugs, optimize treatment regimens, and personalize medicine. This review explores the intersection of AI and pharmaceutical sciences, highlighting its potential to address complex challenges, enhance efficiency, and improve patient outcomes in the ever-evolving landscape of healthcare.

Artificial intelligence (AI) is a combination of various intelligent processes and behavior, developed by computational models, algorithms, or a set of rules which supports the machine to mimic the cognitive functions of humans such as learning, problem-solving, etc. [1].

Artificial Intelligence is being utilised in pharmaceutical product development to select the right development process, pick the right excipients, and make sure all requirements are met in accordance with compliance. AI is frequently utilised to reduce the amount of time and improve drug design processes. AI rooted from the development of theorem-proving program in 1955-1956 by Allen Newell, J. Clifford Shaw, and Herbert Simon of the RAND Corporation and Carnegie Mellon University [2].

2. Classification of Artificial Intelligence [3]



Regarding AI, the methodology employed involves the utilization of machine learning or its subsets, such as deep learning and natural language processing. The learning process can be either supervised or unsupervised, and the type of algorithm employed is also a crucial factor. Supervised learning is a machine learning methodology that involves the use of known inputs (features) and outputs (labels or targets), as opposed to unsupervised learning, which deals with unknown outputs. The supervised approach involves the prediction of output, such as labels or targets, based on multiple inputs or features. On the other hand, unsupervised classification aims to create groups that are homogeneous in terms of features [4].

3. AI for Drug Delivery

Using multiscale modelling approaches, with integration of AI and large datasets paved a way for computational pharmaceutics. Various AI algorithms and ML techniques are used to analyse those datasets and predict the drug behaviour. Simulation of drug formulation and delivery processes to evaluate and optimize drug delivery system made trial-and-error experiments negligible [5, 6].

3.1. Solid Oral Dosage Form

One of the major dosage form in this class is tablets, while designing AI is utilised for optimization of the formula. Technologies such as Artificial Neural Network (ANN), fuzzy logics along with genetic algorithms are utilised in understanding the inputs and outputs for processing and operations.

Various type of excipients are used in the preparation of tablets to get the desired output parameters such as disintegration, dissolution and drug release. These factors are optimised using AI integrated softwares. The drug release is predicted using Support Machine Vector (SVM) along with regression analysis. Data for these analysis are obtained through process analytical technology (PAT) and critical material attributes.

Solid oral dosage forms has solubility as a rate-limiting step on absorption and other pharmacokinetic steps. Using random forest algorithm integrated machine learning various researchers predicted the solid dispersion stability. They also used to distinguish between the spring and parachute type dissolution profile [7, 8].

Artificial Intelligence (AI) has revolutionized the detection of tablet defects in pharmaceutical manufacturing. Traditional methods like X-ray computed tomography are

time-consuming and affect rapid production. Deep learning, combined with X-ray tomography, has been used to identify defects. Researchers used three models, including UNetA, Module 2 (uses augmented analysis), and UNetB (detects internal cracks), to improve accuracy and reduce time, financial costs, and workload [9, 10].

Dong et al. used AI to predict dissolution and dissolution rate for 50 active pharmaceutical ingredients and 25 polymers. They used algorithms like SVM, LightGBM, and XGBoost, which help with unstructured data. The study used molecular computational software for descriptors (API and polymers), and the dissolution rate was considered as the research output. Temperature, drug loading and volume are selected as input variables, and the dissolution rate was considered as the research output [11].

3.2. Nano medicine

AI in nanomedicine can accelerate the development of novel nanoscale interventions, improve diagnostics, enhance drug delivery, and advance personalized medicine. AI algorithms aid in designing and optimizing nanoparticles, and predicting their properties, stability, and efficacy [12, 13].

AI intervention enhances therapeutic nanocarriers for specific cell types for tumor treatment. AI is used to create a database repository for nanocarriers, aiding in 3D structure determination, physical and chemical property investigations, and collaborating with structural nanobiology [14-17].

A study performed by Lutz Nuhn found that AI helped to identify the heterogenous vascular permeablitiy for the prepared nanoparticles by analysing single blood vessels [18]. Zhoumeng Lin et al. utilized AI for improved assessment using a PBPK modeling approach in the effective study of cancer medicine [19].

3.3. Parenteral Products

AI can enhance parenteral product production by identifying and adjusting process factors affecting product quality through real-time analysis of process data. Thus, product consistency, batch failures, and manufacturing productivity increase. AI was utilized for particle inspection to determine if particles were swimming, sinking, or sticking to the inner side of the container. The optical setup, strategy, algorithm, and inspection were

recommended for proper particle inspection, using particle tracking algorithm and image subtraction for floating particle analysis [20].

The availability and promise of state-of-the-art machine learning (ML) technologies in the pharmaceutical and materials science fields are highlighted by Bannigan et al. They illustrate how machine learning (ML) might hasten the creation of novel drug delivery methods by precisely forecasting the in vitro release of drugs from long-acting injectables (LAIs) [21].

4. AI for Pharmacokinetics and Pharmacodynamics

The ideal dosage, mode of administration, and safety of a medicine in the body are all determined by pharmacokinetics and pharmacodynamics, which are important components of drug development. Conventional experimental techniques for pharmacokinetics and pharmacodynamics research can be costly and time-consuming, and they might not always yield reliable estimates of the safety and efficacy of drugs [22].

Computational models and artificial intelligence (AI) techniques have been developed to circumvent these constraints and forecast medication pharmacokinetics and pharmacodynamics more accurately, quickly, and affordably.

Pharmacokinetic parameter prediction is one area where machine learning (ML) and deep learning (DL) algorithms are widely used.

Various ML algorithms, including the Bayesian model, random forest, support vector machine, artificial neural network, and decision tree, have been employed to forecast drug absorption, distribution, metabolism, and excretion (ADME) characteristics. DL algorithms, including convolutional neural networks (CNNs), long short-term memory (LSTM), and recurrent neural networks (RNNs), are commonly employed in the prediction of various pharmacokinetic parameters, such as drug absorption, bioavailability, clearance, volume of distribution, and half-life [23-25].

4.1. AI in PBPK Modeling

To replicate how drugs are distributed and cleared from the body, PBPK models are frequently employed. Because of their complexity, these models need a lot of data and processing power to create. AI-based computational techniques can also optimize the PBPK model's parameters, reducing the necessity for human clinical trials and animal research [26-28].

Table. 1: Software used for the development of AI models for various PKPD

Target	Software	Limitation	Reference
Sample-based on individual patient profile	Support Vector Machine	Less accurate	[29]
Handle data below the limit of quantification	Bayesian/WinBUGS	Consumes time	[30]
Prediction of drug concentration, ideal dose, and dose intervals for a new patient	Support Vector Machine/Drug Administration Decision Support System (DADSS) and Random Sample Consensus RANSAC	Interference of noise from datsets	[31]
Therapeutic drug monitoring of kidney transplant recipient	Support Vector Machine/Profile Dependent SVM	Time consuming Large datasets	[32]
Estimation of drug area under the curve (AUC)	XGBoost	Not possible to calculate the probability of target attainment and accurate dosing	[33,34]
To validate the interaction between drugs and target	Deep Long Short-Term Memory (DeepLSTM)	Large datasets	[35]
Identification of the drug-target interactions	Drug Target Interaction Convolutional Neural Network (DTICNN)	Large datasets	[36]

4.2. Drug Release and Absorption

AI models are able to estimate the rate and extent of drug release over time by taking into account many aspects, including the drug's physicochemical qualities, formulation features, and the delivery system's release mechanism. The release kinetics of medications from

various drug delivery methods, including oral tablets, transdermal patches, and inhalers, can also be predicted using AI based models [37].

To determine how well a medicine is absorbed into the bloodstream, these model scans analyse the physicochemical characteristics of the drug, such as lipophilicity and molecular weight, and relate them with absorption data [38,39].

4.3. Metabolism and Excretion

Artificial intelligence systems are capable of predicting a drug's metabolic pathways by examining its physicochemical features and molecular structure. AI models are able to recognize structural characteristics linked to particular metabolic transformations by training on extensive datasets of known drug metabolism information. These models offer insights into the main enzymes involved in drug metabolism as well as the ability to anticipate possible metabolites [40].

5. Limitations

AI-based models offer benefits but have limitations like large datasets, biases, and interpretability. Combining them with traditional experimental methods ensures drug safety and efficacy.

5.1. Lack of Transparency

AI models use complex algorithms and are often referred to as “black boxes”. It is challenging to understand how an AI model arrives at a prediction. Because of this lack of transparency, it may be difficult to convince regulators to approve AI-based drug development tools and difficult to prove the model is producing trustworthy and accurate predictions. Moreover, a lack of transparency may also contribute to a lack of confidence in the model's predictions, especially if those predictions differ from what researchers or physicians would expect [41,42].

5.2. Limited Availability of Data

For AI models to make accurate predictions, an enormous quantity of data is needed. But occasionally, there might not be enough information available for a particular drug or demographic, which could produce biased or less precise results. Furthermore, not all data types are easily accessible, such as real-world evidence or longitudinal data, which can

restrict the use of AI models. These drawbacks emphasise how important it is to give careful thought to the representativeness and quality of the data utilised in the creation of AI models.

5.3. Biases in Data

Predictions that are made as a result of incomplete or biassed data may likewise be biassed. The model may not be able to accurately forecast the drug's efficacy in a given population if a particular demographic or disease state is not sufficiently represented in the training dataset. It is crucial to ensure that the training data used to build AI models are reliable, complete, and unbiased and that they are representative of the population for which the model will be employed [43,44].

5.4. Interpretation of Results

Clinicians and researchers may find it difficult to understand and interpret the results if the models are unable to clearly explain how they came to their conclusions. It could occasionally be challenging to interpret the data into useful information for drug development or clinical practice. Therefore, to ensure that AI models' predictions can be understood and applied effectively, they must be made more interpretable and explicable [45,46].

5.5. Lack of Clinical Expertise

AI models that primarily focus on statistical connections have challenges due to the complicated nature of treatment decisions, which are influenced by a variety of individual conditions [47]. As a result, AI's capacity to fully understand the crucial elements and impacts of particular parameters may be restricted.

6. Current Pharmaceutical Challenges and the Role of AI

The pharmaceutical industry is exploring small molecules for improved products and customer satisfaction due to their simplicity and cost-effectiveness. However, competition from generic molecules and complex data requirements increase the pressure for innovation. Despite this, the biomolecular drug industry continues to grow rapidly. Successful products like insulin and adalimumab have complex pharmacokinetic aspects, with infusion being the preferred method. New technological advancements can help address these challenges [48,49] . AI has potential in drug delivery innovation and discovery, but it faces limitations such as algorithm bias, inactive molecules, and system bias. Human intervention is needed for interpretation and decision-making, as well as cross-verifications to rule out system bias.

Despite these challenges, extensive work could reduce AI's limitations and make it more effective and reliable [50].

7. Current trends in AI

7.1. Precision Medicine: Artificial intelligence (AI) algorithms can help with personalized medical decision-making by identifying patient subgroups and predicting therapy responses by analyzing patient data, including genomes, proteomics, and clinical records.

7.2. Drug Repurposing: AI have the capacity to repurpose licenced drugs for new therapeutic purposes and identify possible drug-disease interaction by analysing massive datasets and biological knowledge. This method provides a more efficient and quicker path to drug development.

7.3. Drug Formulation and Delivery: AI is also applied in the development of drug delivery systems and technologies that increase patient convenience and adherence.

7.4. Regulatory Compliance and Safety: AI algorithms can monitor postmarketing drug safety and identify any safety risks by analyzing real-world data, adverse event reports, and literature. AI is also useful for signal detection, adverse event prediction, and pharmacovigilance.

8. Conclusion:

With AI's powers in data analysis, pattern identification, and optimization, medical practitioners and pharmaceutical researchers can reduce adverse effects, optimize therapeutic efficacy, and enhance patient outcomes. Computer aided drug design has replaced traditional drug design techniques in recent years. Artificial Intelligence is being used widely to enhance drug design methods and time requirements. AI-based models can mimic drug distribution and clearance in the body, predict pharmacokinetic parameters, and optimise drug dosage and administration methods. The development of PBPK models can be made simpler and their parameters optimised by the use of AI-based computational approaches. All things considered, the use of AI technologies has enormous potential to expedite drug development, enhance patient outcomes, and completely reshape the pharmaceutical sector.

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