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"Role of AI in Drug Discovery- Application,Techniques and Algorithm, Various Tools, Various databases- An Updated Review"

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Abstract: The integration of artificial intelligence (AI) into drug discovery and development marks a significant advancement in the pharmaceutical industry, addressing the longstanding challenges of traditional methods. These traditional approaches are often characterized by high costs, prolonged timelines, and low success rates, with drug development typically taking over a decade and costing billions of dollars. Despite substantial investments, the success rate for candidate compounds gaining regulatory approval is less than 10%. AI, particularly through machine learning (ML) and deep learning (DL) techniques, offers a versatile and efficient solution across various stages of drug development, from target identification to clinical trial design. By harnessing vast biomedical datasets, AI facilitates the identification of novel insights, optimization of lead compounds, and refinement of patient stratification, thereby accelerating decision-making and resource allocation. This review provides a comprehensive overview of AI's transformative role in pharmaceutical research, highlighting recent advancements in AI technologies, their applications in drug development, and the associated opportunities and challenges. The findings emphasize AI's potential to revolutionize the drug discovery process, making it more efficient, cost-effective, and successful. To fully realize this potential, it is essential to address data quality, ensure ethical AI use, and promote interdisciplinary collaboration. By integrating AI methodologies with traditional approaches and human expertise, significant advancements in healthcare and therapeutic innovation are anticipated.

Key words: Artificial Intelligence (AI),Drug Discovery and development,AI Technologies,Healthcare Innovation

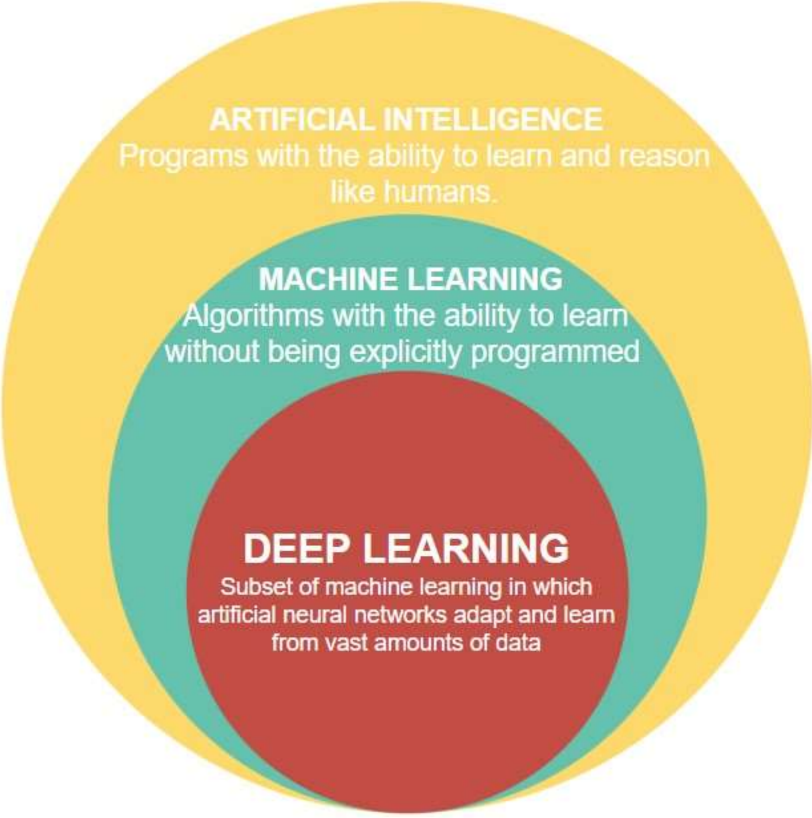
1. INTRODUCTION

The importance of drug discovery and development cannot be underestimated, as they serve as the driving force behind healthcare innovation and progress. It involves a rigorous process that encompasses identifying potential therapeutic targets and bringing effective medications to the market with far-reaching implications for public well-being. However, traditional methods of drug discovery are often characterized by high cost, lengthy timelines, and low success rates. Typically, the process extends for over a decade, from target identification to regulatory approval, and entails expenses ranging from hundreds of millions to billions of dollars per approved drug. Despite significant investments, only a small portion of candidate compounds that enter clinical trials are ultimately granted regulatory approval, with estimates suggesting a success rate of less than 10%. The presented data highlight the substantial challenges inherent in drug discovery, such as identifying viable drug targets, optimizing lead compounds for efficacy and safety, navigating intricate regulatory pathways, and addressing unforeseen obstacles throughout the development process. In this context, the emergence of artificial intelligence (AI) in pharmaceutical research has resulted in a paradigm shift, providing transformative solutions to longstanding challenges. AI-powered algorithms and machine learning techniques are transforming every stage of the drug discovery and development process, from target identification and lead optimization to clinical trial design and patient stratification.By leveraging the vast amounts of data generated in life sciences, AI enables researchers to uncover novel insights, expedite decision-making, and optimize resource allocation.The objective of this review is to provide a comprehensive overview of the integration of AI into pharmaceutical research, emphasizing its potential to revolutionize drug discovery and development. The subject matter encompasses the most recent advancements in artificial intelligence technologies, their applications across various stages of the drug development process, and opportunities and challenges associated with their adoption. By examining this information, we aim to shed light on the transformative effect of AI in the pharmaceutical industry and open the door for future innovations in healthcare.

The use of artificial intelligence (AI) in medicinal chemistry has garnered significant attention in recent years as a means of potentially revolutionizing the pharmaceutical industry. Drug discovery, the process of identifying and developing new medications, is a complex and time-consuming endeavor traditionally reliant on labor-intensive techniques such as trial-and-error experimentation and high-throughput screening. However, AI techniques such as machine learning (ML) and natural language processing offer the potential to accelerate and improve this process by enabling more efficient and accurate analysis of large database. The successful application of deep learning (DL) to predict the efficacy of drug compounds with high accuracy has been highlighted by recent studies. AI-based methods have also demonstrated the ability to predict the toxicity of drug candidates. These and other research efforts underscore the capacity of AI to enhance the efficiency and effectiveness of drug discovery processes. Nonetheless, the use of AI in developing new bioactive compounds is not without challenges and limitations. Ethical considerations must be taken into account, and further research is necessary to fully understand the advantages and limitations of AI in this field. Despite these challenges, AI is expected to significantly contribute to the development of new medications and therapies in the coming years.

In the realm of drug design, artificial intelligence (AI) leverages computer software programs that analyze, learn from, and interpret pharmaceutical-related big data to discover new medicinal molecules. By integrating advancements in machine learning (ML) in a highly systematic and automated manner, AI paradigms have established a significant presence in drug design, driven by data-centric computational processes. Unlike traditional methods, ML-driven approaches, as a branch of AI, do not rely on the theoretical progression of complex physico-chemical principles but instead focus on transforming vast biomedical data into new insights and sustainable expertise. Common ML algorithms include Logistic Regression (LR), Naive Bayesian Classification (NBC), k Nearest Neighbor (KNN), Multiple Linear Regression (MLR), Support Vector Machine (SVM), Probabilistic Neural Network (PNN), Binary Kernel Discrimination (BKD), Linear Discriminant Analysis (LDA), Random Forest (RF), Artificial Neural Network (ANN), Partial Least-Squares (PLS), and Principal Component Analysis (PCA).

In recent times, AI technologies, particularly Deep Learning (DL) paradigms, have shown immense potential in drug design due to their superior generalization and feature extraction capabilities. Conventional ML approaches use manually crafted features, whereas DL approaches can automatically learn features from input data, reorganizing simple attributes into complex characteristics through multi-layer feature extractio. Furthermore, DL approaches often exhibit lower generalization errors compared to traditional ML techniques, allowing for more advantageous outcomes in various benchmarks and competitive evaluations. For example, George Dahl's team won the Merck Molecular Activity Challenge by applying DL algorithms. Due to these advantages, DL techniques have shown great promise in the field of drug design. DL paradigms typically include Deep Neural Networks (DNN), Convolutional Neural Networks (CNN), Recurrent Neural Networks (RNN), autoencoders, and Restricted Boltzmann Machines (RBM). Comprehensive reviews of DL algorithms are available elsewhere, with a thorough introduction to DL methodologies provided in the book "Deep Learning." This review introduces AI models relevant to drug design, with a particular focus on the application of DL algorithms in new drug discovery and development.



2. Application of Artificial Intelligence in drug discovery

The development of new drugs is an extremely challenging task, and identifying successful drugs is the most difficult aspect of drug development.This is because of the large size of the chemical space, which is estimated to contain 1060 molecules.Fortunately, AI technology has become a versatile tool that can be universally applied across various stages of drug development, such as identifying and validating drug targets, designing new drugs, repurposing drugs, improving R&D efficiency, aggregating and analyzing biomedical information, and refining the decision-making process to recruit patients for clinical trials.These potential applications of AI provide a unique opportunity to address the inefficiencies and uncertainties associated with traditional drug development methods while minimizing bias and human intervention in the process.

The use of AI in drug development encompasses a range of applications, including the prediction of feasible synthetic routes for drug-like molecules, pharmacological properties, protein characteristics, efficacy, drug combination, drug-target association, and drug repurposing.Additionally, AI enables the identification of new pathways and targets through the generation of novel biomarkers and therapeutic targets, personalized medicine based on omics markers, and discovery of connections between drugs and diseases.

DL has demonstrated exceptional success in identifying potent drug candidates and accurately predicting their properties and potential toxicity risks.AI methods have enabled the circumvention of past problems in drug development, such as the analysis of large datasets, laborious screening of compounds while minimizing standard error, and the requirement of substantial R&D cost and time, which previously exceeded US$2.5 billion in a decade.With the assistance of AI technology, new studies can be conducted to aid the identification of new drug targets, rational drug design, and drug repurposing.

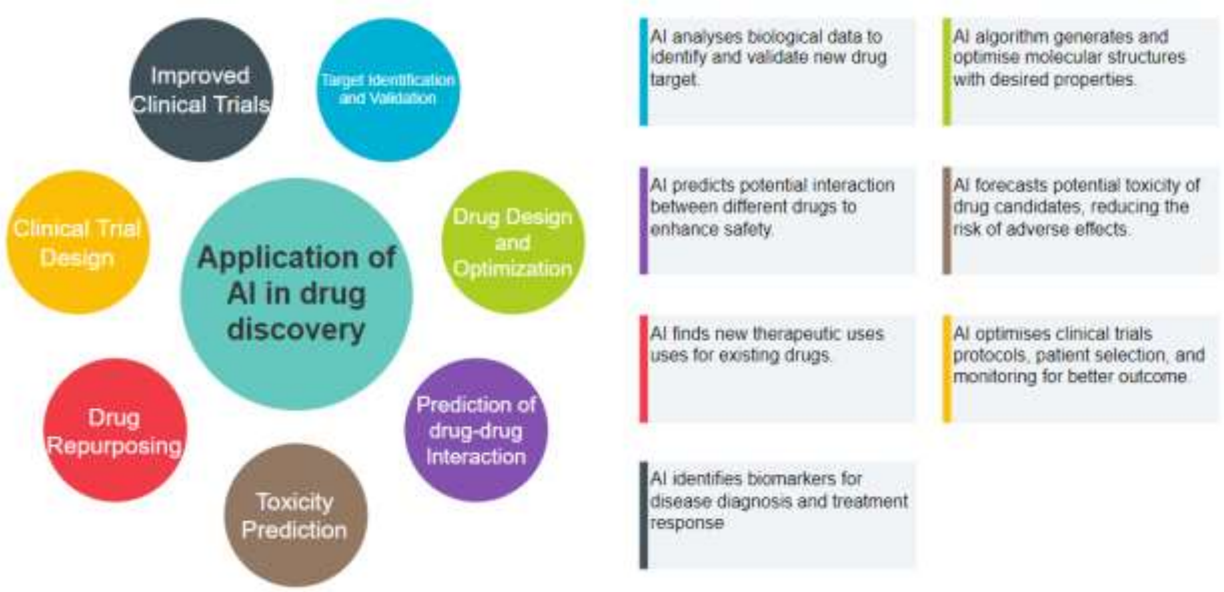


Figure no : 01 Application of AI in drug discovery

3. Techniques and Algorithm in AI for drug discovery

In contemporary pharmaceutical research, the integration of Artificial Intelligence (AI), particularly its subfields of Machine Learning (ML) and Deep Learning (DL), has emerged as a transformative force in drug discovery.These AI-driven methodologies offer a spectrum of techniques and algorithms that significantly enhance the efficiency and precision of drug development.AI technologies play indispensable roles throughout various stages of drug discovery, including virtual screening, de novo drug design, prediction of physicochemical and pharmacokinetic properties, drug repurposing, and anticipation of drug-target interactions. By leveraging predictive models and computational algorithms, researchers can swiftly screen molecular libraries, design novel compounds with predefined properties, forecast critical drug attributes, repurpose existing drugs for new indications, and elucidate complex drug-target interactions. The amalgamation of AI, ML, and DL not only accelerates the identification of promising drug candidates, but also streamlines decision-making processes, ultimately advancing therapeutic innovation and drug development efforts.

3.1 Machine Learning

Machine learning (ML) algorithms have advanced the field of drug discovery significantly, providing significant benefits to pharmaceutical companies.These algorithms have been employed to develop various models to predict the chemical, biological, and physical characteristics of compounds used in drug discovery. They can be incorporated into all stages of the drug discovery process, from finding new uses for existing drugs to optimizing the bioactivity of molecules. ML algorithms widely used in drug discovery include Random Forest (RF), Naive Bayesian (NB), and support vector machines (SVM).

Machine learning (ML) algorithms and techniques are not monolithic homogeneous subsets of artificial intelligence (AI). They can be classified into two primary types: supervised and unsupervised.Supervised learning involves training samples with known labels to determine the labels for the new samples.By contrast, unsupervised learning recognizes patterns in a set of samples without labels. Before recognizing patterns in high-dimensional data, unsupervised learning algorithms transform the data to a lower dimension. Dimension reduction is useful not only because unsupervised learning is more efficient in a low-dimensional space but also because the recognized pattern can be more easily interpreted. Supervised and unsupervised learning can be combined into semi-supervised and reinforcement learning, in which both functions can be utilized for various datasets.

In the field of drug discovery, extensive data volumes are crucial for the development, evolution, and viability of ML algorithms.Reliance on big high-quality data and well-defined training sets is critical in precision medicine and therapies for drug discovery.Precision medicine requires a comprehensive characterization of all related pan-omics data, such as genomic, transcriptomic, and proteomic data, to aid in the development of truly effective personalized medicines.

The widespread use of high-throughput screening and sequencing, online multi-omics databases, and ML algorithms over the past two decades has created a thriving environment for many aspects of data generation, collection, and maintenance required for drug development. Advancements in data analytics have successfully described and interpreted the generated data. This project, which incorporates machine learning techniques and integrated databases via various software/web tools, has become an integral part of drug discovery at all stages.The combination of new data analytics with traditional methods and prior hypotheses has proven to be beneficial in applications such as repositioning, target discovery, small-molecule discovery, and synthesis.The data generated in the medical and multi-omics fields are complex and multidimensional, often noisy, and heterogeneous in nature and source.By utilizing machine learning methods such as generalized linear models through Naive Bayes, the challenges of analyzing and interpreting multidimensional data can be addressed.Other commonly used machine-learning techniques and models in these areas of analysis include regression, clustering, regularization, neural networks (NNs), decision trees, dimensionality reduction, ensemble methods, rule-based methods, and instance-based methods.

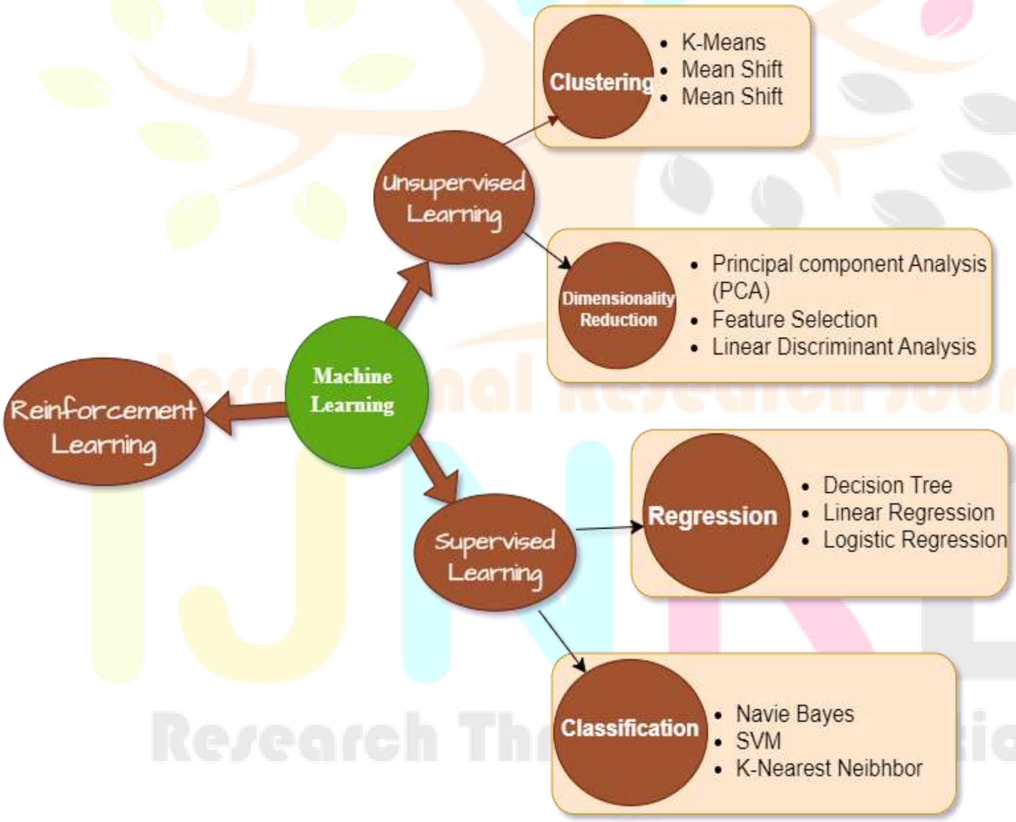


Figure2:Machine learning algorithm

3.1.1 Supervised learning

Supervised machine learning (SML) techniques have become increasingly essential in the field of drug discovery as they enable the extraction of valuable insights from data and the generation of predictions about future events, which is critical for the development of new pharmaceuticals.These techniques, including support vector machines (SVM), neural networks, and random forests (RF), are applied to analyse and interpret complex datasets, such as those derived from genomics and proteomics, to identify potential drug candidates and predict their efficacy and toxicity. In supervised machine learning algorithms, a labeled training dataset is initially used to train the underlying algorithm. The trained algorithm was then applied to the unlabeled test dataset to categorize them into similar groups.

In the context of supervised learning, consider a dataset comprising various entities, such as fish, pears, and apples, each annotated with their respective labels by ansupervisor. In this scenario, the supervisor utilizes a supervised learning algorithm to classify and segregate the data based on the provided labels. This algorithm learns from the input-output pairs in the training data to accurately assign labels to new, unseen instances.

Supervised learning involves training a model on a labeled dataset, where the input data (features) and the corresponding output labels (targets) are known. The algorithm iteratively adjusts its parameters to minimize the discrepancy between its predictions and the actual labels, effectively learning the mapping from inputs to outputs. Once trained, the model can generalize this learnedmapping to classify or predict labels for new data points, thereby ensuring that entities such as fish, pears, and apples are correctly identified and separated based on their predefined categories.

This approach is fundamental in various applications, including object recognition, natural language processing, and predictive analytics, where accurate labeling and classification of data are crucial.

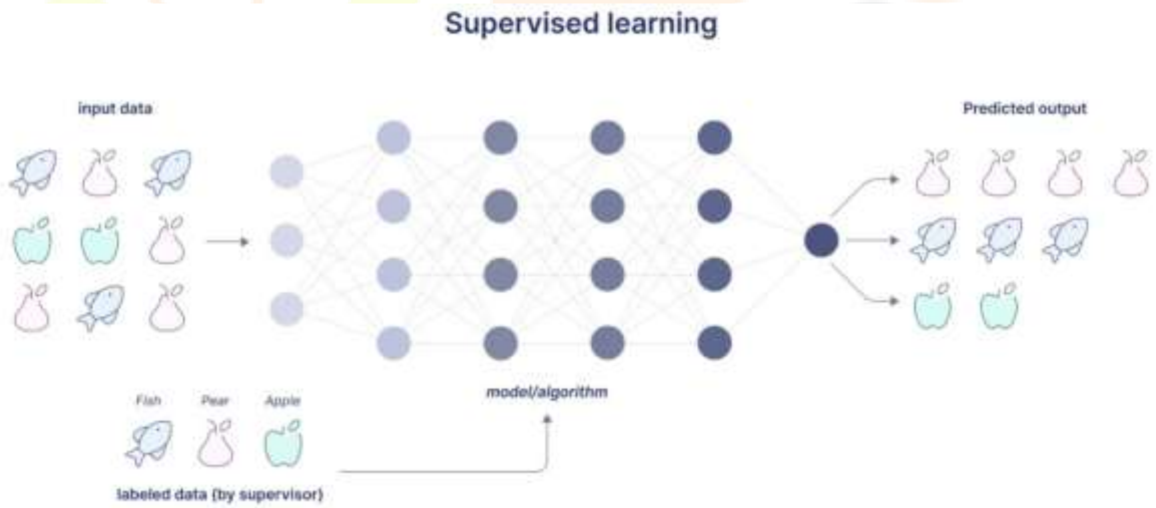


Figure no. 3: supervised learning

3.1.1 Unsupervised learning

Unsupervised learning is a pivotal component in drug discovery and development because of its ability to extract meaningful patterns from vast datasets without the need for labeledinformation.By employing clustering techniques, such as K-means or hierarchical clustering, molecules with similar characteristics can be grouped together, thereby facilitating the identification of potential drug candidates or patient subgroups with similar responses to treatments.Dimensionality reduction methods, such as PCA or t-SNE, aid in visualizing complex molecular data and identifying crucial features relevant to drug discovery.Additionally, anomaly detection algorithms help identify unexpected molecular structures or rare drug responses, potentially leading to the discovery of new therapeutic targets or adverse effects.Association rule learning uncovers the relationships between molecular properties and biological activities, shedding light on potential drug-target interactions.Furthermore, unsupervised generative models, such as VAEs or GANs, assist in the creation of novel molecular structures with desired properties, offering avenues for the design and optimization of drug candidates.Unsupervised learning techniques provide invaluable insights into complex biological systems, guiding researchers towards more effective drug discovery and development strategies.

In the context of unsupervised learning, consider a dataset comprising various entities such as fish, pears, and apples, but without any labels or annotations provided by an supervisor. In this scenario, an unsupervised learning algorithm is employed to identify inherent patterns or groupings within the data, without prior knowledge of the categories.

Unsupervised learning entails analysing the structure of the input data to discern hidden patterns, relationships, or clusters. The algorithm does not have access to labeled outputs; instead, it relies on the features of the data to group similar items together. For instance, the algorithm might identify clusters of data points that share common characteristics, thereby grouping the fish, pears, and apples into distinct clusters based on their similarities and differences in features such as shape, size, or colour.

This approach is particularly beneficial in exploratory data analysis, anomaly detection, and clustering tasks, where the objective is to uncover the underlying structure of the data without pre-existing labels. By harnessing unsupervised learning, one can gain insights into the natural groupings within the dataset, facilitating further analysis and decision-making processes.

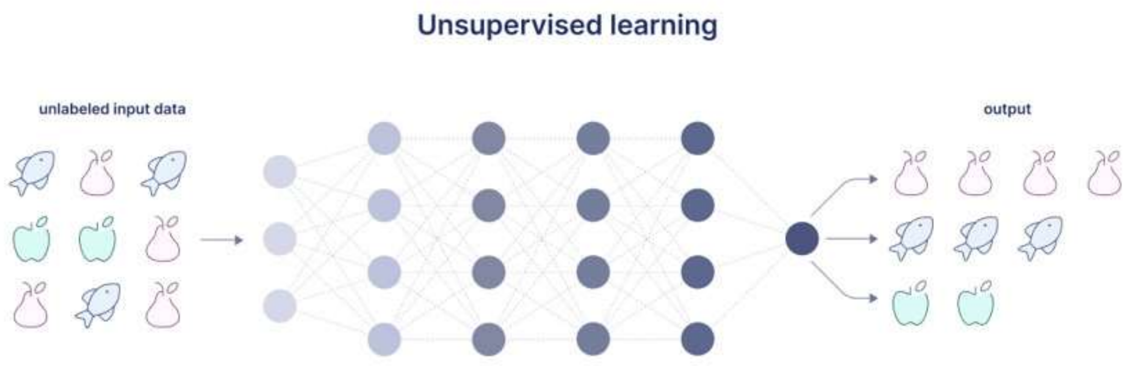


Figure no. 4: Unsupervised learning

4. Various AI tools used for drug discovery and drug development

AI tools are employed in various aspects of the drug discovery process, including real-time image-based cell sorting, cell classification, quantum mechanics calculations, compound property analysis, computer-aided organic synthesis, de novo molecule design, assay development, and prediction of 3D structures of target proteins, among others.It is worth noting that traditional experimental structural biology methods often require several years to determine protein structure. In contrast, AI-based structure predictions can be completed in a few hours to a few days, making the process significantly more time efficient.

The use of machine learning algorithms in the pharmaceutical industry can lead to a range of benefits, including identifying new drug applications, predicting drug-protein interactions, determining drug efficacy, verifying safety biomarkers, and optimizing molecular bioactivity. By employing various models to predict the chemical, biological, and physical properties of compounds, pharmaceutical companies can automate and optimize their R&D process.

Various AI tools used in drug discovery and drug development

Table No – 01 Ai Tool & Function

AI TOOL NAME	FUNCTION
Deep Chem	MLP model that uses a python-based AI system to find a suitable candidate in drug discovery.
Chemputer Software	Helps to report procedure for chemical synthesis in a standardized format.
Deep Neural Net- QSAR	Python-based system driven by computational tools that aid detection of the molecular activity of compounds.
Deep Tox	Software that predicts the toxicity of a total of 12 000 drugs.
DeltaVina	A scoring function for rescoring protein-ligand binding affinity.
ODDT	A comprehensive toolkit for use in chemo-informatics and molecular modelling.
ORGANIC	An efficient molecular generation tool that helps to create molecules with desired properties.
PotentialNet	Ligand-binding affinity prediction based on a graph convolutional neural network (CNN).
PPB2	Used for poly-pharmacology prediction.
QML	A Python toolkit for quantum ML.
REINVENT	Molecular de novo design using RNN (recurrent neural network) and RL (reinforcement learning).
SCScore	A scoring function to evaluate the synthesis complexity of a molecule.
SIEVE-Score	An improved method of structure-based virtual screening via interaction-energy-based learning.

Various databases used for target discovery

Table No – 02 Database & Function

Database	Function
BRENDA	Enzyme and enzyme-ligand information source.
PubChem	Database for encompassing information on chemicals and biological activities.
DrugBank	Detailed drug data and drug-target information database.
TDR targets	Database containing chemogenomic information for neglected tropical diseases.
Gene Expression Omnibus	Database of raw microarray datasets.
UniProt	Encompassing protein information.
InterPro	Database of protein domain information.
ChEMBL	Database of drug-like small molecules with predicated bioactive properties.
ChemSpider	Encompassing database of over 64 million chemical structures.
DrugCentral	Database containing relevant drug information of activity, chemical identity, mode of action, etc.

Challenges and Limitation

Despite the potential benefits of AI in drug discovery, several challenges and limitations need to be addressed. One key challenge is the availability of suitable data . AI-based approaches require large volumes of high-quality information for training . However, accessible data may be limited, low in quality, or inconsistent, which can impact the accuracy and reliability of AI models . Additionally, ethical considerations pose another significant challenge . AI can raise concerns about fairness and bias, particularly if the training data is biased or unrepresentative, leading to inaccurate or unfair predictions . Ensuring the ethical and fair use of AI in developing new therapeutic compounds is crucial.Several strategies can help overcome these obstacles. One approach is data augmentation , which involves generating synthetic data to enhance existing datasets, thereby increasing the quantity and diversity of data available for training machine learning (ML) algorithms and improving their accuracy and reliability . Another approach is the use of explainable AI (XAI) methods . XAI aims to provide transparent and interpretable explanations for ML predictions, addressing concerns about bias and fairness and offering a better understanding of the underlying mechanisms and assumptions.

It is important to note that current AI-based approaches are not substitutes for traditional experimental methods, nor can they replace the expertise and experience of human researchers. AI can only generate predictions based on the available data, and these predictions must be validated and interpreted by human experts . However, integrating AI with traditional experimental methods can enhance the drug discovery process. By combining the predictive power of AI with the expertise of human researchers, it is possible to optimize drug discovery and accelerate the development of new medications.

Future Direction

AI is already playing a significant role in drug discovery, aiding in identifying pharmacological targets, searching data libraries for suitable molecules, suggesting chemical modifications, and identifying candidates for drug repurposing. However, several challenges must be addressed in the near future. As Mitchell pointed out, "new techniques in drug development often get overhyped, much like combinatorial chemistry did a few years ago, and failing to manage unrealistic expectations can lead to disappointment. It is better to expect modest improvements and possibly be pleasantly surprised than to promise a revolution that never materializes.

While AI has the potential to revolutionize chemistry, there are several obstacles and limitations to overcome. One major challenge is the need for high-quality data. The effectiveness of AI models hinges on the data they are trained with, and high-quality chemistry data can be scarce. Another difficulty is understanding complex models. Deep learning models, in particular, can be hard to interpret and explain, which may lead to chemists having difficulty trusting their predictions. Additionally, there are social and ethical concerns. While AI can be used to develop new medications and substances, it can also be misused to create dangerous materials such as weapons. Therefore, the use of AI in chemistry must be ethical and responsible, with a focus on beneficial outcomes.

Looking ahead, AI is expected to significantly advance personalized and precision medicine, potentially becoming standard practice even for treating minor illnesses.

Discussion

The integration of artificial intelligence (AI) into drug discovery and development marks a significant advancement in the pharmaceutical industry. This review underscores the transformative potential of AI technologies in tackling the substantial challenges of traditional drug discovery methods, which are often plagued by high costs, lengthy timelines, and low success rates.

Key Findings and Implications

AI, particularly machine learning (ML) and deep learning (DL) algorithms, offers robust solutions across various stages of drug development, from target identification and lead optimization to clinical trial design and patient stratification. The ability of AI to process vast amounts of biomedical data and uncover novel insights has led to significant improvements in efficiency and accuracy. For instance, DL techniques have demonstrated superior generalization and feature extraction capabilities compared to traditional ML methods, enabling more accurate predictions of drug efficacy and toxicity.

Furthermore, AI tools such as Deep Chem, DeltaVina, and PotentialNet illustrate how AI-driven methodologies can streamline decision-making processes and optimize resource allocation in drug discovery. The application of AI in virtual screening, de novo drug design, and the prediction of pharmacokinetic properties highlights its pivotal role in contemporary pharmaceutical research. These advancements not only expedite the drug development process but also reduce costs and increase the likelihood of success in clinical trials.

conclusion

In conclusion, AI has the transformative potential to revolutionize drug discovery and. development, addressing long-standing challenges and enabling more efficient, cost-effective, and successful pharmaceutical research. However, to fully realize this potential, it is essential to address data quality issues, ensure the ethical use of AI, and foster interdisciplinary collaboration. By combining AI with traditional methodologies and leveraging human expertise, the pharmaceutical industry can anticipate significant advancements in healthcare and therapeutic innovation.

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