Defining the scope: Drug prediction interaction system

Drug interactions play a vital role in drug research. However, they may also cause adverse reactions in patients, with serious consequences. Manual detection of drug interactions is time-consuming and expensive, so it is urgent to use computer methods to solve the problem.There are two ways for computers to identify drug interactions: one is to identify known drug interactions, and the other is to predict unknown drug interactions. In this paper, we review the research progress of machine learning in predicting known drug interactions.

The scope of the " Drug prediction interaction system " project encompasses the range of activities, functionalities, and objectives that the project aims to achieve. It outlines the boundaries and limitations of the project in terms of features, target users, technologies, and expected outcomes.

Drug-drug interactions (DDIs) and their associated adverse drug reactions (ADRs) represent a significant detriment to the public health.Existing research on DDIs is primarily focused on pairwise DDIdetection and prediction. It is highly needed to develop effectivecomputational tools for high-order DDI prediction.

The introduction of AI-models in DDIs recognition, many efforts have been applied to boost the predictive powerof algorithms by putting forward more complex systems, turningthese models into those called ‘‘black-box AI” that hinder the ability of users to explain how these models work. Specifically,higher performance models are associated with more sophisticatedsystems, but lower performance tools with simple approaches areeasier to comprehend. Despite various benefits given by widespread industrial adoption of machine learning (ML) models, a critical domain as healthcare should be taken more seriously due to itsimmense value to humans. Additionally, from a human-orientedresearch angle, the ambiguity of complicated models in makingpredictive decisions hamper its successful adoption in medical settings as unable-to-interpreted systems are difficult to be trusted.Since the fundamental application of AI in drug treatment mustfirst do with DDIs, explainable DDIs-AI models are pivotal for clinicians and patients to understand and trust their prediction.Prediction of drug-drug interactions (DDIs) can prevent unexpected adverse drug events (ADEs). ADEs can damage people’s health and bring about economic losses to the society.Existing methods usually adopt the dataset of the adverse drug reports (ADRs) to build the DDIprediction statistical mode. Clinical trials are time-consuming, expensive, and infeasible when facing the large-scale data and limitations of experimental conditions. Therefore, the researchers introducea lot of computational methods to accelerate the prediction process. Developing algorithms and models to predict potential DDIs based on various factors, including pharmacokinetics, pharmacodynamics, chemical structures, and patient characteristics.

Utilizing various data sources, including biomedical literature, pharmacovigilance databases, clinical trials data, chemical databases, and electronic health records (EHRs), to gather information on known and potential drug interactions. Employing machine learning, data mining, and computational techniques to build predictive models that can identify and classify DDIs. These models may use features such as drug properties, patient demographics, and co-prescription patterns. . Nowadays, combining multiple drugs is the optimal therapy to decelerate the pathologic process, which contains various underlying adverse effects due to drug-drug interactions (DDIs). Artificial intelligence (AI) has the potential to evaluate the interaction, pharmacodynamics, and possible side effects between drugs. Over the past years, many AI-based DDI prediction techniques, including both machine learning and deep learning, that harness available big data have been presented.

Defining appropriate metrics and benchmarks to assess the performance of DDI prediction models, including sensitivity, specificity.Addressing the challenges associated with patients taking multiple medications (polypharmacy) and considering the cumulative effects of drug interactions in treatment plans.Personalizing DDI predictions based on individual patient characteristics, including genetics, age, gender, comorbidities, and concomitant medications.Integrating DDI prediction systems into electronic health records (EHRs) and clinical decision support systems to provide real-time guidance to healthcare professionals during prescription and medication management.Contributing to the labelling of pharmaceutical products with clear information on potential interactions, as well as educating patients and healthcare providers about safe medication use.

Continuously monitoring drug interactions in post-marketing settings and updating prediction models as new information becomes available. The final DDI prediction between a drug pair is based on the interactions between pairs of their (learned) substructures, each pair weighted by a relevance score to the final DDI prediction output.

Search strategy: On the basis of existing related works and accumulated experience, relevant data has been organized and various databases have been constructed.

ChEMBL is a manually curated database of bioactive molecules with drug-like properties. It brings together chemical, bioactivity and genomic data to aid the translation of genomic information into effective new drugs.

SIDER contains information on marketed medicines and their recorded adverse drug reactions. The information is extracted from public documents and package inserts. The available information includes side effect frequency, drug and side effect classifications as well as links to further information, for example drug–target relations.

The Anatomical Therapeutic Chemical (ATC) classification system is used for the classification of drugs. It is published by the World Health Organization (WHO). The classification is based on therapeutic and chemical characteristics of the drugs.

Drug Bank database: Drug Bank combines detailed drug data (i.e., chemical, pharmacological, and pharmaceutical) with comprehensive target information (i.e., sequence, structure, and pathway). Database describes not only clinical information on drugs, namely drug side effects and drug-drug interactions, but also contains molecular-level data, such as chemical structures of drugs and proteins targeted by drugs (Wishart et al., 2008). One significant function of Drug Bank is that it supports comprehensive and complex searches, so it is used widely by the pharmaceutical industry, medicinal chemists, pharmacists, physicians, students and the general public.

Drug Bank is one of the most popular databases and has been widely used as a drug reference resource. This database was first released in 2006. As a database both in bioinformatics and cheminformatics, Drug Bank contains detailed drug data with comprehensive drug target information. The DTI relationships in Drug Bank were originally collected from textbooks, published articles and other electronic databases. All data can be freely downloaded from Drug Bank.

STITCH: STITCH not only includes experimentally validated drug–target interaction data, but also integrates predicted drug– target relationships (Kuhn et al., 2007). This website can clearly depict the protein–protein interactions, protein–compound interactions, and the strength of the interactions.

OpenChem: OpenChem is a pytorch-based deep learning toolkit for computational chemistry and drug design.

We use the MINER DTI dataset from BIOSNAP collection. Itconsists of 4,503 drug nodes and 2,182 protein targets, and 15,138 drug-targetinteraction pairs from DrugBank. BIOSNAP dataset only contains positivedrug target interaction pairs. For negative pairs, we sample from the unseenpairs. We obtain a balanced dataset with equal positive and negative samples.We use DrugBank database toobtain target sequence, and hence, we filter out target/drug that do not havetarget sequences from Drug Bank.

DeepDDI is composed of 1,710 drugs and 86 different interaction types from DrugBank capturing 192,284drug-drug pairs as samples. 99.87% of drug-drug pairs only have one type of DDI.Decagon is composed of 637 drugs and 200 different interaction types from the TWOSIDES dataset capturing1,121,808 drug-drug pairs as samples. We follow common practice by sampling 200 medium frequency DDI typesranging from Top-600 to Top-800, ensuring that every DDI type has at least 90 drug combinations. 73.27% of drug-drug pairs have more than one type of DDI

PROMISCUOUS was established in 2011 and proposed as a database for network-based drug repositioning. This database contains three different types of data: drugs, proteins, and side effects. The protein data are extracted from UniProt and incorporated with the 3D structure information from Protein Data Bank (PDB). Drugs and side effects are extracted and incorporated from SuperDrug and SIDER, respectively. In addition to DTIs and drug side effects linkages, PROMISCUOUS also includes data on drug–drug similarities.

SuperDRUG2 is proposed as a one-stop data source thatoffers all crucial features of approved and marketed drugs. Thedrug items in SuperDRUG2 are classified into two categories:small molecules and biological/other drugs. Several publicresources like US FDA, CFDA and EMA, etc. were used fordrug collections. Drug target information in SuperDRUG2 was extracted from Drug Bank, TTD and ChEMBL. Besides these drugs and targets information, SuperDRUG2 alsoprovides 2D and 3D structure information of small moleculedrugs, drug side effects, drug–drug interactions and drug pharmacokinetic parameters.

PDID was released in 2014 and covers all known protein–drug interactions and predicted protein–drug interactions for theentire structural human proteome. The known interactions wereextracted from Drug Bank, Binding DB and PDB. The predictions were made by using three different software's(i.e.,IL bind , SMAP and eFindSite).

The FEARS dataset has 6,338 drug combinations from 826 drugs, including 2,981 2-drug combinations, 1,555 3-drug combinations, 6524-drug combinations, 323 5-drug combinations, 220 6-drug combinations, 1577-drug combinations and 450 combinations with morethan 7 drugs. The maximum number of drugs in a combinationis 52, and the average is 3.6. The drug combinations are selectedbased on their odds ratios of inducing myopathy among a largecollection of spontaneous reports to FDA2. The detailed descriptionof drug combination selection and dataset construction is availablein the Materials section in Chiang et al. We collected 4 types ofinformation for the drugs, including chemical substructure fingerprints (FP), side-effect profiles (SE), therapeutic-indication profiles(TI) and target profiles (TG). Unfortunately, we cannot find all the 4types of features for each drug.

The BMC has 48,584 drug pairs from 548 drugs with 9 differenttypes of drug features, including chemical substructures denotedas FP, drug target profiles denoted as TG, transporter profiles denoted as TP, enzymes denoted as EM, pathways denoted as PW,drug indications denoted as TI, side effects denoted as SE, off-sideeffects denoted as OSE and the drug-drug interaction profiles.

To analyse the efficacy of our study, we employ the benchmark dataset proposed by Ryu et al. that covers 86 DDIs types classified from the gold standard dataset holding 192,284 DDIs contributed by 191,878 drug pairs in Drug Bank. This dataset contained the molecular form of each molecule used, and we did not apply any pre-processing.

The primary purpose for maintaining the FDA/Centre for Veterinary Medicine Adverse Drug Experiences (ADE) database is to provide an early warning or signalling system to the centre for adverse effects not detected during pre-market testing of FDA-approved animal drugs and for monitoring the performance of drugs not approved for use.

ChemSpider is not primarily a database for drug-drug interaction (DDI) prediction. Instead, it is a chemical database that provides information about chemical compounds, including their structures, properties, and identifiers. ChemSpider is valuable for chemists, researchers, and professionals who need information about individual chemical substances, but it does not specifically focus on drug interactions or DDI prediction. ChemSpider may be helpful for obtaining chemical structure information about the drugs involved in DDI studies, but it is not the primary source for interaction prediction.

PubChem is not primarily a database for drug-drug interaction (DDI) prediction. Instead, PubChem is a freely accessible repository of chemical information provided by the National Center for Biotechnology Information (NCBI). It contains data on the chemical properties, structures, and activities of a wide range of chemical compounds, including drugs. PubChem can be a useful resource for obtaining chemical information about drugs, which can be a component of DDI prediction efforts, but it is not a dedicated DDI prediction database.

SuperCYP: SuperCYP is a database that focuses on drug metabolism and the cytochrome P450 enzyme system, which plays a crucial role in drug interactions and metabolism.

Drug Interaction Knowledge Base (DIKB): The Drug Interaction Knowledge Base (DIKB) is a specialized database that provides structured information about drug interactions, including their mechanisms, clinical relevance, and supporting evidence. While DIKB is not a primary tool for predicting drug-drug interactions (DDIs) in real-time or on a large scale, it is a valuable resource for researchers and experts in the field of pharmacology and drug safety.

The STRING database, which stands for "Search Tool for the Retrieval of Interacting Genes/Proteins," is primarily designed for the prediction and exploration of protein-protein interactions. While it is not a dedicated database for drug-drug interaction (DDI) prediction, it can be a valuable resource when researching potential DDIs, especially those related to the molecular mechanisms of drug action.

TWOSIDES is a database that combines data from electronic health records to identify potential drug-drug interactions associated with adverse effects.

Selection Criteria: The dataset of drug compounds and their interaction, representing a wide range of chemical and pharmacological properties, to enhance the accuracy and generalizability of the AI-driven prediction system.

Frequency and nature of drug-drug interactions in the intensive care unit

Publication Date: February 18, 2013.

Drug-drug interactions (DDIs) may compromise patient safety. However, there are no good estimates of their frequency or understanding of their nature in the intensive care unit (ICU). The objective of this study was to determine the frequency and nature of potential DDIs (pDDIs) in the ICU when assessed in light of documented and perceived clinical relevance.

We developed a computerized algorithm to identify pDDI occurrence in ICU admissions with medication administration, on the basis of the Dutch national drug database. A panel of nine local pharmacists and intensivists completed questionnaires to classify the perceived relevance of the identified pDDI types for the ICU. A focus group discussed the conflicting classifications of relevance to reach consensus. For the pDDI types classified as relevant, we calculated their number and frequency per admission days.Out of 9644 admissions, 3892 had at least one pDDI. The pDDIs corresponded to 85 types, 36 of which were deemed relevant on the basis of the survey and focus group. These 36 types corresponded to 16 122 pDDIs (rate: 33.6 per 100 admission days) and 1084 unique admissions. PDDIs occurred in 11% of admissions to the general ICU, after limiting analysis to severe and relevant DDI types. The most frequently encountered drug classes were antithrombotic agents and antibacterials for systemic use.

Drug-drug interactions (DDIs) are a common concern in healthcare, occurring with varying frequencies and encompassing a diverse range of natures. The prevalence of DDIs is notably higher in individuals taking multiple medications, often referred to as polypharmacy. This risk is especially pronounced in elderly patients managing chronic health conditions. DDIs are a frequent occurrence in hospital settings, where patients are exposed to diverse drug regimens. However, they are not limited to inpatient care; outpatient settings also witness DDIs, especially among those with long-term medication requirements.

AI in drug-drug interactions prediction

Publication Date: March 12, 2022.

AI plays a crucial role in drug-drug interactions (DDIs) prediction, which is a critical aspect of drug safety and pharmacovigilance. DDIs occur when two or more drugs interact with each other in a way that affects their efficacy or safety. Predicting and managing these interactions are vital to ensure patient safety and the effectiveness of drug therapies.

Artificial Intelligence (AI) is ubiquitous today, many AI prediction models have been developed to predict DDIs to support clinicians in pharmacotherapy-related decisions. However, even though DDI prediction models have great potential for assisting physicians in polypharmacy decisions, there are still concerns regarding the reliability of AI models due to their black-box nature. Building AI models with explainable mechanisms can augment their transparency to address the above issue. Explainable AI (XAI) promotes safety and clarity by showing how decisions are made in AI models, especially in critical tasks like DDI predictions.

In this review, a comprehensive overview of AI-based DDI prediction, including the publicly available source for AI-DDIs studies, the methods used in data manipulation and feature preprocessing, the XAI mechanisms to promote trust of AI, especially for critical tasks as DDIs prediction, the modeling methods, is provided.

The advanced computer science development and growing network pharmacology approaches, the development of a traditional ML-based model using multi-dimensional drug properties has been widely applied as a promising strategy to predict unknown DDIs. Single ML algorithm-based predictive model, Support vector machine (SVM) was a common algorithm used to predict DDIs due to its high performance with a broad range AUC value of 0.565 – 0.985 [6,19,54,84-87], Ensemble learning predictive model, this method use multiple learning algorithms to obtain better predictive performance than separate models in DDIs prediction.

Artificial intelligence (AI) paving critical role in drug discovery, drug designing and studying drug-drug interactions.

Publication Date: June 22, 2023.

All this data is collected from the Adobe Analytics and Altimetric APIs.
AI is a system based on technology involving several modern tools and networks mimicking intelligence of human. Side by side there is no threat of replacement of physical presence of human completely due to AI. Potential applications of AI are being extended in the field of pharmaceuticals continuously and developing pharmaceutical products from bench to the side of bed is imaginably provided. AI can help in designing of drug rationally, assist in decision making, helps in determination of correct therapeutic management of the patients, and be wisely exploited for developing drugs in future.
Various case studies have identified potential use of AI in discovery of drugs. AI is being successfully used for identification of novel compounds for treating cancer. Researchers have trained a deep learning (DL) algorithm upon a huge dataset of known compounds related to cancer and their corresponding activity biologically. Novel compounds with greater potential for treatment of cancer have been obtained as an output. This demonstrates the capability of the method for discovering new candidates for new therapy.
For prediction of the desired chemical structure of a compound, several parameters viz., predictive models, the molecular similarity, process of generation of molecules and the utilization of approaches in silico can be done. A new approach known as multi-objective replacement algorithm (automated) for optimizing the potency profile of an inhibitor of cyclin-dependent kinase-2 by assessment of its similarity in shape, biochemical action, and physiochemical features.AI has a great role to play for revolutionizing the process of drug discovery, can offer better accuracy and efficiency. AI can also accelerate the process of development of drugs and has got the ability of developing more efficacious and personalized medicines and therapies.

Artificial Intelligence in Drug Interactions Prediction

Publication Date: July 17, 2023.

We aim to provide a comprehensives overview of drug interaction prediction. The first section introduces commonly used databases and presents an overview of current research advancements and techniques across three domains of DDI. Additionally, we introduce classical machine learning techniques for predicting undirected drug interactions and provide a timeline for the progression of the predicted drug interaction events.
Based on the differences among these prediction problems, we have divided the DDI forecasts into three categories These categories include undirected DDI prediction,
the prediction of drug-drug interaction events, and asymmetric drug interaction prediction.

- **Undirected DD**: Undirected binary classification, this is all about to check whether there are interactions between drugs.
- **Asymmetric DDI:** Directional binary classification, this category focus on the direction of drug-drug interactions.
- **DDI Events:** Undirected multiclassification, the side-focus of DDI Events was to detect the types of drug interactions that may occur.

The dataset of META-DDIE method includes a greater number of types of drug interaction events compared to previous ones, with the top ten types of drug interactions accounting for 74.77% of the total number of interactions relationships.
Artificial Intelligence (AI) has emerged as a transformative force in the field of drug interactions prediction. Leveraging vast datasets from electronic health records, clinical trials, scientific literature, and adverse event reporting systems, AI systems have revolutionized our ability to foresee and manage drug interactions. These systems utilize machine learning algorithms to create predictive models, ranging from binary classifiers indicating the presence or absence of interactions to models that predict the severity of these interactions.
Utilizing the advancements in Artificial Intelligence (AI) is essential for achieving accurate forecasts of DDIs. In this review, DDI prediction tasks are classified into three types according to the type of DDI prediction: undirected DDI prediction, DDI events prediction, and Asymmetric DDI prediction.

Data Extraction: Extract the Drug Attributes and the drug properties, including chemical structures, molecular weights, and mechanisms of action and Clinical Data are patient-specific data, such as medical histories, concomitant

medications, and treatment durations and also Biological Pathways are enzyme activities, protein-protein interactions, and metabolic pathways.

ADeep attention neural network framework named DANN-DDI to predict potential interactions between drug-drug pairs in multiple drug feature networks.

Key Findings and Methodologies
Drug-Drug Interaction Prediction: Al models analyse potential interactions between medications. Personalized Medication Plans: Al suggests tailored treatment regimens to avoid adverse effects. Real-time Alerts: Al-generated notifications for healthcare providers and patients about potential interactions.

Healthcare Databases
CHEMBL is a manually curated database of bioactive molecules with drug-like properties. It brings together chemical, bioactivity and genomic data to aid the translation of genomic information into effective new drugs.
SIDER contains information on marketed medicines and their recorded adverse drug reactions. The information is extracted from public documents and package inserts. The available information includes side effect frequency, drug, and side effect classifications as well as links to further information, for example drug–target relations. Drug Bank database: Drug Bank combines detailed drug data (i.e., chemical, pharmacological, and pharmaceutical) with comprehensive target information (i.e., sequence, structure, and pathway). Database describes not only clinical information on drugs, namely drug side effects and drug-drug interactions, but also contains molecular-level data, such as chemical structures of drugs and proteins targeted by drugs (Wishart et al., 2008). One significant function of Drug Bank is that it supports comprehensive and complex searches, so it is used widely by the pharmaceutical industry, medicinal chemists, pharmacists, physicians, students, and the general public.

DDIs information retrieved from text-based sources.

This method involves extracting DDIs information in the form of biomedical text, especially in scientific literature since these sources represent valuable information for the retrieval of knowledge about the interaction between drugs. The amount of biomedical literature, which holds a vast amount of DDIs, has been growing over the past years and facilitating many DDIs extracting studies.

In these DDIs extraction approaches, feature preprocessing is essential. Tokenization and lower casing are the first vital steps in reducing the sparsity of feature space. Also, many dimensionally reduction text preprocessing techniques have been used for DDIs extraction. Some compression techniques such as sentence pruning, and anaphora resolution have been applied. Encoder Representations from Transformers (BERT) that relies on attention mechanism to capture high-quality contextual information.

Molecule-based input data and feature preprocessing for DDIs prediction

Usually, DDIs studies utilize chemical, molecular, and pharmacological properties information to elucidate drug interactions insights. In detail, the chemical properties of drugs are typically described via the simplified molecular-input line-entry system (SMILES). This flexible chemical notation allows the generation of computer-feedable input. pharmacological properties such as targets, transporters, genes and proteins, interaction pathways like enzymes and transporters can also be manipulated to represent drugs features through a set of descriptors.

Conventional ML-based prediction models of DDIs
Given the advanced computer science development and growing network pharmacology approaches, the development of a traditional ML-based model using multi-dimensional drug properties has been widely applied as a promising strategy to predict unknown DDIs.

Single ML algorithm-based predictive model

A single machine learning (ML) algorithm-based predictive model is a fundamental approach used across various domains to make predictions, classifications, or decisions based on data patterns. In this approach, a specific ML algorithm is selected and trained on a dataset to learn the underlying relationships and patterns within the data. This trained model can then be used to make predictions on new, unseen data points.

SVM was a common algorithm used to predict DDIs due to its high performance with a broad range AUC value of 0.565 – 0.985. Due to the growing demand for adverse DDIs (ADDIs) signal detection, Bayesian network framework and

domain knowledge were combined to identify direct associations between a combination of medicines and the target. Furthermore, gradient boosting-based algorithm XGBoost was employed to achieve robust DDI prediction even for drugs whose interaction profiles were completely unseen during training. XGBoost performed better or comparable to other algorithms, such as SVM, random forest, and the standard gradient boosting in terms of predictive performance and speed in DDIs prediction.
While single ML algorithm-based models are effective for many tasks, their choice depends on the specific problem and dataset characteristics. The success of such models relies on factors like feature engineering, data quality, and hyperparameter tuning.

Ensemble learning predictive model

Ensemble methods use multiple learning algorithms to obtain better predictive performance than separate models in DDIs prediction Combined ML algorithms using Lib-LINEAR, which consists of linear SVM, Naïve Bayes, and Voting Perceptron classifiers, outperformed the original (unbalanced) train corpora model based on F-score (70.4% vs. 69.0%) a heterogeneous network-assisted inference (HNAI) framework consisting of five different ML algorithms, including Naive Bayes (NB), decision tree (DT), k-nearest neighbours (k-NN), LR, and SVM, was proposed to detect the unknown DDIs.

Ensemble techniques in drug prediction help address the complexity and multidimensionality of drug-related data. By combining the predictions from multiple models, ensemble methods reduce the risk of overfitting and improve the model's ability to generalize to new and unseen drug compounds. This is especially critical in drug discovery, where the goal is to identify potential drug candidates with desired properties while minimizing false positives and negatives.
Ensemble learning has also been employed in drug-drug interaction prediction, toxicity prediction, and drug response modelling. In these applications, the combination of various models allows for a more holistic and accurate assessment of drug behaviour in complex biological systems. As the field of drug discovery continues to rely on data-driven approaches, ensemble learning remains a valuable tool for improving the reliability and precision of drug-related predictions, ultimately advancing the development of safer and more effective medications.

Artificial neural network (ANN)

ANN is a data-driven algorithm that seeks hidden functional relations from the dataset. In ANN, many neurons are connected in complex interconnections to solve linear or nonlinear problems. The two layers ANN model has been used a feed-forward neural network with fully connected layers and the RELU activation function was used between layers of the model as a sigmoid activation function for the output layer. An XGBoost classifier used for the DDIs classification, which output a binary value representing whether there is an interaction between the drug pairs or not.

In drug prediction, ANNs are utilized to perform tasks such as compound screening, target identification, and pharmacokinetics modelling. ANNs can analyze extensive chemical and biological data to predict the likelihood of a chemical compound's effectiveness against a specific target or disease. This accelerates the identification of potential drug candidates, reducing the time and cost associated with traditional drug development processes. Moreover, ANNs can predict a drug's pharmacokinetic behaviour, including absorption, distribution, metabolism, and elimination within the human body, providing critical information for optimizing drug dosages and administration.

In the context of drug-drug interactions (DDIs), ANNs excel in forecasting potential interactions between multiple drugs. They can process complex datasets that include drug properties, patient profiles, and biological mechanisms to identify possible adverse effects or synergistic actions when drugs are used together. This capability is crucial for ensuring patient safety and preventing harmful interactions, particularly in patients with polypharmacy or complex medical conditions. While ANNs offer remarkable predictive capabilities in drug discovery and interaction analysis, challenges remain, including the need for large and high-quality datasets, interpretability of complex models, and potential overfitting. Nevertheless, ongoing advancements in deep learning techniques, coupled with domain expertise and robust data integration, continue to enhance the accuracy and applicability of ANNs in the pharmaceutical industry, contributing to the development of safer and more effective medications.

The INDI framework for novel DDI prediction. They introduce a method for computing similarity scores between target interaction edges to known interaction edges based on the given drug–drug similarities. For each target drug-pair, each pair wise combination of similarities is considered for computing the similarity score to the most similar known drug interaction. The procedure effectively performs nearest neighbour search using different similarity distance measures. Each score is then used as a feature to train a logistic regression classifier.
We can obtain DDI data from Drug Bank. Among the 5 major interaction categories in Drug Bank, we can consider the first category as they were clearly defined as adverse DDIs. Non-interacting drug pairs were constructed by taking all other combinations using the same set of drugs, removing drug pairs also appearing in other categories in Drug Bank, TWOSIDES, or a complete dataset of DDIs compiled from a number of sources. This minimizes the chance of having actual adverse DDIs in the non-interacting set given the absence of a gold standard set of non-interacting drug pairs. From Drug Bank, we also collected human protein targets of drugs and their sequences.

Organization: Certainly, here's a coherent organization of sources for AI-driven drug interaction prediction systems, organized thematically, along with a brief explanation in paragraph form:

The research in this category delves into the historical development of AI-driven drug interaction prediction systems. Early works focused on rule-based approaches and knowledge bases. They laid the foundation for later machine learning-based methods. These sources provide valuable insights into the evolution of this field.

This category encompasses research that emphasizes the application of various machine learning techniques, including decision trees, support vector machines, and neural networks, in DDI prediction. These sources highlight the effectiveness of data-driven approaches in capturing complex drug interactions.NLP and text mining techniques have gained prominence in recent years. Researchers in this category explore how NLP can extract valuable information from biomedical literature and electronic health records, contributing to more comprehensive DDI prediction models.

Identifying gaps in drug-drug interaction (DDI) prediction systems is crucial for advancing drug safety and patient care. One major challenge lies in the quality and availability of data, with the need for comprehensive and up-to-date datasets encompassing various drugs and interactions. Additionally, the complexity of interactions, including less-studied mechanisms and rare interactions, presents a significant gap in current DDI prediction systems.

The technological limitations of current AI systems for drug interaction prediction. Include topics like algorithm accuracy, computational resources, and model interpretability. Provide examples of instances where AI may struggle to predict interactions accurately. Moreover, individual variability in drug metabolism due to genetic differences is often overlooked, leading to limitations in personalization. Emerging drugs and novel combinations continuously enter the market, requiring adaptable prediction systems. The integration of diverse data sources, from electronic health records to clinical trials, is an ongoing challenge that, if addressed effectively, can enhance prediction accuracy.

With the increasing availability of healthcare data, research sources in this category focus on handling and integrating diverse data sources, such as genomics data, patient records, and drug databases. They discuss the challenges and benefits of working with big data in DDI prediction.

These sources emphasize the importance of rigorous validation and evaluation of AI-driven DDI prediction models. They provide insights into the metrics used to assess model performance, ensuring that predictions are reliable and clinically relevant. Research in this category explores the challenges and considerations of implementing AI-based DDI prediction systems in clinical practice. Ethical concerns, regulatory approvals, and strategies for integrating these tools into healthcare settings are discussed.

Recent trends in research emphasize the need for patient centric DDI prediction. These sources discuss tailoring predictions to individual patient profiles, considering genetic factors, lifestyle, and preferences to optimize medication regimens. Sources in this category provide insights into the future of AI-driven DDI prediction, highlighting ongoing gaps in research. They discuss the need for continuous learning models, improved real-time predictions, and collaborative efforts among researchers, pharmacologists, and clinicians.

Some sources delve into drug interactions that extend beyond medications, considering dietary choices, lifestyle factors, and environmental influences. These sources emphasize the need to broaden the scope of AI-driven prediction systems to encompass these multifaceted interactions, which can significantly impact patient outcomes.

Another thematic cluster of sources highlights the shift towards patient-centric approaches in AI-driven DDI prediction. They discuss the importance of tailoring predictions to individual patient profiles, considering genetics, comorbidities, and lifestyle choices, to provide personalized healthcare solutions and enhance.

Certain sources focus on the challenges posed by polypharmacy, where patients take multiple medications simultaneously. They explore the complexities of predicting interactions among numerous drugs and the need for scalable AI models that can handle these intricate scenarios effectively.

Additional sources delve into the economic aspects of AI-driven DDI prediction systems. They conduct cost-benefit analyses to assess the potential savings in healthcare costs resulting from reduced adverse drug reactions and hospitalizations. These sources offer insights into the financial implications of implementing AI solutions.

A distinct group of sources discusses the integration of AI-driven DDI prediction tools into clinical practice. They examine the practical aspects of deploying AI systems in healthcare settings, addressing issues related to user interfaces, clinician adoption, and decision support.

Lastly, some sources emphasize the importance of patient education and communication in the context of AI-driven DDI prediction. They explore strategies for effectively conveying potential drug interactions to patients, ensuring their active participation in medication management.

In summary, the sources are organized thematically to provide a coherent understanding of the historical development, current trends, and future directions in AI-driven drug interaction prediction systems. This organization helps researchers and practitioners navigate the evolving landscape of DDI prediction effectively.

Synthesis: Undirected DD: Undirected binary classification, this is all about to check whether there are interactions between drugs.

Asymmetric DDI: Directional binary classification, this category focus on the direction of drug-drug interactions.
DDI Events: Undirected multiclassification, the side-focus of DDI Events was to detect the types of drug interactions that may occur.
Despite their initial success, there are still limitations for existing computational approaches. For example, they only focus on binary predictions, which correspond to whether a DDI would happen. There is a detailed type (e.g., hepatic failure, cough, dizziness, etc.)associated with each DDI. Obtaining the actual DDI typesmay help us understand better the mechanistic underlying. The DDI and take proper preventative actions. They typically use drug features alone in the predictive model (e.g., logistic regression). However, the interactions among different chemical compounds arealso important factors that lead to DDIs.

In the era of big data, machine learning methods are designed to generate predictive modelsbased on some underlying algorithm and a given big data set. For biological and biomedicalresearch, machine learning plays a pivotal role in filtering large amounts of data into patterns [24–27]. The general machine learning workflow in DTI prediction can be divided into three steps. First, preprocessing the input data of the drug and the target; second, training the underlying model basedon a set of learning rules; third, utilizing the predictive model to make predictions for a test data set.

From our research, study [28] is the first work that applies machine learning to protein-chemicalinteraction prediction. This work establishes a SVM analysis framework of amino acid sequence data, chemical structure data and mass spectrometry data. This pioneering study has inspired subsequentstudies. Machine learning for drug discovery has become a field of long-standing and growing interestsince then.
We formulate the problem of predicting whether high-order drug combinations induce a particular ADR asa binary classification problem and solve the classification problem within the framework of kernel methods and support vector machines (SVMs).

Deep learning is becoming more and more popular given itsgreat performance in many areas, such as speech recognition, image recognition and natural language processing. Applyingdeep leaning methods to drug discovery has been consistentlyincreasing in recent years.Deep learning approaches appear to overcome certain limitations by reducing the loss of feature information in predictingDTIs. One of the drawbacks in using deep learning methodslays in the fact that there is not always sufficient information available to perform deep learning methods.

Over the past years, several machine learning and deep learning approaches have been proposed to embed DDI knowledge graphs for predicting unknown DDIs. Firstly, training a KG embedding model requires negative samplesand

there are no confirmed negatives in the original DDI datasets. In order to conveniently generate enough negativesamples to train the model.

The vast majority of existing DDI prediction methods represent drugs using molecular fingerprints, andother drug profiles such as side effects, binding targets, transporters, enzymes, pathways, or the combination of two or more of these features. Molecular fingerprints are binary vectors whose elements indicate the presence or absence of a specific chemical substructure.

The limitations of drug-drug interaction (DDI) prediction systems have been explored in various research studies. Here are some common limitations identified:

- Data Quality and Availability: Many DDI prediction systems rely on diverse data sources, but data quality and completeness can be inconsistent, leading to inaccuracies. Additionally, data on rare or newly introduced drugs may be limited.
- Incomplete Knowledge: DDI databases and knowledge bases may not encompass all potential interactions, especially for novel drugs. This can result in false negatives, where important interactions are missed.
- Complexity of Interactions: DDIs can be highly complex, involving multiple drugs and mechanisms. Existing models may not capture these intricate relationships accurately.
- Patient Variability: Individual patient characteristics, such as genetics and health status, play a role in DDI outcomes. Many DDI prediction systems do not account for this variability adequately.
- Lack of Long-term Data: Predicting chronic or long-term DDI effects can be challenging due to the limited availability of longitudinal patient data.
- Temporal Aspects: The timing of drug administration can influence interactions. Some systems may not consider the timing factor in their predictions.
- Polypharmacy: Patients often take multiple medications simultaneously (polypharmacy). Predicting interactions among multiple drugs can be challenging, and current models may not scale well for these scenarios.
- False Positives: Overly sensitive DDI prediction models can generate many false-positive alerts, leading to potential over-caution and unnecessary medication changes.
- Clinical Relevance: Not all predicted DDIs are clinically significant. Distinguishing between minor and major interactions can be difficult.
- Limited Validation: Many DDI prediction systems lack extensive validation using real-world clinical data, which is crucial for assessing their real-world performance.
- Ethical and Privacy Concerns: The use of patient data for DDI prediction raises ethical and privacy concerns. Balancing the need for data with patient privacy is an ongoing challenge.
- Regulatory Approval: Obtaining regulatory approval for DDI prediction tools can be complex and time-consuming, limiting their adoption in clinical practice.
- Bias in Data: Data used to train DDI prediction models may contain biases, potentially leading to biased predictions, particularly concerning underrepresented patient populations.
- Interactions Beyond Drugs: Some DDIs involve factors beyond drugs, such as dietary choices or lifestyle. These factors are often not considered in prediction models.
- Constantly Changing Landscape: The field of pharmacology is dynamic, with new drugs and interactions emerging regularly. Keeping prediction systems up to date is a continuous challenge.

To address these limitations, ongoing research is focused on improving data quality, refining prediction models, considering patient-specific factors, and enhancing the clinical relevance of DDI predictions. Additionally, collaborations between researchers, clinicians, and regulatory bodies are essential to ensure the safe and effective use of DDI prediction systems in healthcare.

Synthesizing the field of Drug-Drug Interaction (DDI) prediction involves a comprehensive approach that combines the strengths of data science, pharmacology, and clinical expertise. At its core, DDI prediction aims to bridge the gap between drug development and patient safety by providing insights into how different medications may interact within the human body. This synthesis begins with the integration of diverse data sources, ranging from clinical trials and electronic health records to the chemical properties of drugs and adverse event reports. Feature engineering plays a pivotal role in identifying relevant attributes, allowing for the creation of accurate predictive models.

Machine learning algorithms, including classification and regression techniques, are then applied to these features, enabling the development of predictive models that learn from historical data and patterns. However, true efficacy in DDI prediction lies in the incorporation of pharmacological knowledge, encompassing drug metabolism pathways, targets, and underlying biological mechanisms. This domain expertise enhances the interpretability and clinical

relevance of predictions. DDI prediction involves a comprehensive amalgamation of heterogeneous data sources, including chemical properties of drugs, patient demographics, and clinical records.

DDI prediction is expanding to encompass not only the identification of interactions but also the prediction of potential adverse events stemming from these interactions, facilitating a more comprehensive approach to patient safety. Ethical considerations, including privacy and responsible data usage, remain paramount in this synthesis, ensuring that DDI prediction is not only accurate but also conducted in an ethical and privacy-respecting manner. Overall, the synthesis of DDI prediction represents a dynamic and evolving field that converges data science, pharmacology, clinical care, and ethics to enhance medication safety and optimize patient outcomes in healthcare.

The synthesis also entails the integration of pharmacological knowledge, incorporating insights into drug metabolism, molecular interactions, and pharmacokinetics, providing a holistic understanding of DDIs. Furthermore, robust validation methodologies and clinical integration into decision support systems are imperative, enabling real-time alerts and recommendations to healthcare professionals during the prescription process.

Identify gaps: Identifying gaps in drug-drug interaction (DDI) prediction systems is crucial for advancing drug safety and patient care. One major challenge lies in the quality and availability of data, with the need for comprehensive and up-to-date datasets encompassing various drugs and interactions. Additionally, the complexity of interactions, including less-studied mechanisms and rare interactions, presents a significant gap in current DDI prediction systems.

The technological limitations of current AI systems for drug interaction prediction. Include topics like algorithm accuracy, computational resources, and model interpretability. Provide examples of instances where AI may struggle to predict interactions accurately. Moreover, individual variability in drug metabolism due to genetic differences is often overlooked, leading to limitations in personalization. Emerging drugs and novel combinations continuously enter the market, requiring adaptable prediction systems. The integration of diverse data sources, from electronic health records to clinical trials, is an ongoing challenge that, if addressed effectively, can enhance prediction accuracy.

Machine learning models used in DDI prediction often lack interpretability, hindering their acceptance and trust among healthcare professionals. Real-time alerts in clinical decision support systems (CDSS) need improvement to provide immediate guidance to prescribers. Establishing standardized benchmarks and validation processes is essential for comparing different prediction systems reliably. Expanding DDI prediction to include the prediction of adverse events resulting from interactions is a critical gap that demands attention. Addressing these gaps in DDI prediction systems will contribute to safer and more effective medication management in healthcare.

Data integration also remains a gap. Efficiently harnessing diverse data sources, such as electronic health records, clinical trial data, and adverse event reporting systems, into a unified prediction framework is essential to enhance prediction accuracy.

Below are several key gaps in the project:

Data Quality and Quantity Insufficient Data Many drug interactions are rare, and there may not be enough data available to train accurate AI models for these interactions. Datasets used for training AI models may be biased towards commonly prescribed drugs or certain populations, leading to biased predictions. There may be gaps in data related to drug properties, patient characteristics, and historical interactions, limiting the comprehensiveness of predictions.

Model Accuracy and Generalization Existing AI models may not consistently provide highly accurate predictions, leading to false positives or negatives. Models may struggle to generalize across diverse patient populations, making it challenging to predict interactions in various clinical settings.

Complexity of interactions: Predicting interactions among multiple drugs (polypharmacy) is highly complex and often overlooked in AI models. Some drug interactions depend on specific combinations, and models may not account for these nuances effectively. Interpretable Models Many AI models used for drug interaction predictions, like deep learning models, are often regarded as black boxes, making it difficult to interpret their decisions. The inability to explain why a specific prediction was made can hinder the trust and adoption of AI-driven predictions in clinical practice. Real-World Application, Integrating AI predictions into clinical workflows and electronic health records (EHRs) can be challenging due to the need for seamless and user-friendly interfaces. Physicians may be reluctant to trust AI predictions, and there is a need for education and training to facilitate adoption.

Regulatory and Ethical Challenges: AI-driven drug interaction prediction systems may require regulatory approval, and the regulatory landscape for such systems is still evolving. Privacy concerns, especially those related to patient data, need to be addressed to ensure ethical AI-driven drug interaction predictions. Rare and Emerging Drug Interactions: AI models may struggle to predict rare or newly discovered drug interactions due to limited historical data. The rapid introduction of new drugs requires continuous model updates and adaptation to capture interactions with these drugs.

Clinical Validation and Feedback Loop: There is a need for rigorous clinical validation studies to assess the real-world performance of AI-driven drug interaction prediction systems. Establishing mechanisms for healthcare professionals to provide feedback on system predictions can help improve model accuracy. Interdisciplinary Collaboration, Bridging the gap between AI researchers, pharmacologists, and clinicians is crucial for the development and deployment of effective drug interaction prediction systems. Scalability and accessibility. Ensuring that AI-driven systems can scale to accommodate a large volume of drug interactions and diverse patient populations. Making AI-driven predictions accessible to healthcare providers in resource-limited settings.

Temporal Dynamics: AI models often focus on short-term interactions but may overlook the long-term effects of drug combinations, which are essential for chronic conditions. Patient conditions change over time, and their medication needs evolve. AI models should account for dynamic changes in drug interactions.Patient-Specific Predictions, Current AI models often provide generalized predictions, but personalized medicine requires tailoring predictions to individual patient profiles, genetics, and health histories. Patients exhibit varying responses to drug interactions, and AI systems should consider these variations, Adverse Event Prediction. While predicting drug interactions is vital, AI should also focus on predicting potential adverse events, allowing for proactive intervention.

Integration with Decision Support Systems: The seamless integration of AI predictions into existing clinical decision support systems (CDSS) is essential for real-world applicability. CDSS should support real-time updates to AI models to keep up with emerging knowledge. Interactions Beyond pharmaceuticals. AI models often focus on drug interactions but should also consider interactions with food, dietary supplements, and lifestyle factors, which can also impact treatment outcomes. Regulatory Standardization, Developing standardized frameworks for evaluating the performance of AI-driven drug interaction prediction systems is crucial for consistent quality assessment and comparison.

Resource Allocation: Some AI models require significant computational resources, hindering their widespread adoption in resource-constrained settings. There is a need for more resource-efficient models. Educational Initiatives, Training healthcare professionals to understand and interpret AI-driven predictions is essential to bridge the knowledge gap and promote trust.

Longitudinal Data Collection: Collecting longitudinal data on patient drug interactions and health outcomes is crucial for refining AI models and understanding the full spectrum of interactions. Patient Involvement, Involving patients in the development and validation of AI-driven systems can enhance user acceptance and provide valuable insights into patient-specific concerns. A transparency and Accountability Establishing mechanism for algorithmic transparency and accountability is critical to building trust in AI-driven predictions. Insufficient Data, One of the significant technological gaps is the availability of insufficient data for training accurate AI models.

Many drug interactions are rare: and data on these interactions may be limited. Without enough data, AI models may struggle to identify and predict these rare interactions, leading to incomplete and potentially inaccurate predictions. Data Bias, Datasets used for training AI models may be biased towards commonly prescribed drugs or certain patient populations. Bias in training data can result in AI models that are not representative of the broader patient population, leading to skewed predictions and potentially overlooking important interactions. Missing Data, There can be gaps in data related to drug properties, patient characteristics, and historical interactions. Missing data can limit the comprehensiveness of predictions. If essential data elements are missing, AI models may not provide a holistic understanding of drug interactions.

Algorithmic Accuracy: Achieving high accuracy in predicting drug interactions can be difficult due to the complexity of biological systems and the myriad factors that influence drug responses. Inaccurate predictions can lead to false positives or negatives, which can have significant clinical consequences, such as ineffective treatments or adverse reactions. Model Generalization: AI models often need to generalize across diverse patient populations and clinical settings. Models that do not generalize well may provide accurate predictions in some contexts but fail in others, limiting their usefulness in real-world clinical practice. Complexity of drug interactions, Predicting interactions among multiple drugs (polypharmacy) and accounting for specific drug combinations is highly complex. Neglecting these complexities can result in incomplete predictions, as some interactions may only manifest when specific drugs are combined.

Model Interpretability: Many AI models used for drug interaction prediction, such as deep learning models, are often regarded as black boxes. Lack of interpretability hinders clinicians' ability to understand and trust model decisions, potentially leading to scepticism and reduced adoption. Real-World Application, Integrating AI predictions into clinical workflows and electronic health records (EHRs) can be technologically challenging. If not seamlessly integrated, AI predictions may not reach the healthcare professionals who need them, limiting their practical impact on patient care.

Critical Evaluation:. The critical evaluation of drug-drug interaction prediction systems is paramount to their successful implementation in healthcare. These systems, while promising, face several crucial considerations. Firstly, the quality and quantity of data used for training are pivotal, as inaccurate or incomplete data can lead to erroneous predictions. Striking a balance between sensitivity and specificity is another challenge, as overly sensitive systems might generate excessive false positives, while overly specific ones could miss clinically relevant interactions. Clinical significance is vital, and the prioritization of interactions based on potential severity is crucial for patient care. Integration into existing healthcare infrastructure and interoperability with electronic health records are essential for seamless adoption by healthcare professionals. Continual learning and updates to stay current with evolving pharmacology are imperative, as is the development of interpretable AI models. Validation through real-world clinical data and rigorous testing is essential to ensure practical utility, while ethical considerations and cost-effectiveness analyses must guide their implementation. In conclusion, while the potential benefits of AI-driven drug interaction prediction systems are substantial, addressing these critical aspects is essential to realizing their full potential and ensuring their impact on patient safety and healthcare outcomes potential impact on patient safety. And alsoevaluating the user interface's ease of use, clarity of predictions. A critical evaluation of drug-drug interaction prediction systems is essential to understand their strengths and limitations in the context of healthcare and pharmaceuticals.

Discussion: Each machine learning model possesses its unique advantages as well as disadvantages. Therefore, in this review we can only evaluate the advantages and disadvantages of each method category based on DDI prediction context. A number of supervised models have been already proven feasible for DDI prediction.

In the past decade, many methods have been developed for predicting DDIs based on various types of features. In this study, we have incorporated a novel feature, namely genetic interaction, to build a gradient boosting-based model for fast and accurate adverse DDI prediction. We have shown that our classifier can robustly predict drug-drug interactions even for drugs whose interaction profiles are completely unseen during training. Furthermore, we have predicted 432 novel DDIs, with additional evidence supporting our top predictions, demonstrating the usefulness of our approach.

The occurrence of DDI affects the treatment of patients and has become a serious problem for patient safety and drug management. The harm caused by DDI will be greatly reduced if machine learning can be used to efficiently predict DDI. To this end, it is urgent to develop better-performing machine learning approaches. This article describes existing machine learning-based approaches for predicting DDI. In the past 10 years, machine learning has been widely applied in bioinformatics and achieved good results. Under most of the existing approaches, drug similarity is taken as the most fundamental starting point for better prediction of DDI, assisted by a variety of other means. However, most current DDI predictions are limited to the interactions between two drugs. In the future work, we should not only pursue the accuracy of predicting the probability of drug-drug interactions, but also pursue the ability to accurately predict the types of drug-drug interactions. However, because the use of multiple drugs has become a trend in clinical medicine, it is urgent to develop methods to predict interactions between multiple drugs. It is our opinion that a number of excellent ways to solve this problem will be available in the near future.

Researchers in the field of AI-driven DDI prediction are dedicated to enhancing drug safety and optimizing patient care. Their work focuses on harnessing the capabilities of artificial intelligence, particularly machine learning and natural language processing, to predict potential drug interactions more accurately and efficiently. To achieve this, they leverage a multitude of data sources, including electronic health records, drug databases, scientific literature, and genomic data, allowing for comprehensive analysis. These dedicated experts develop sophisticated AI models, carefully considering model architecture and feature selection, which are crucial for accurate predictions. Rigorous validation is an integral part of their research, ensuring that the AI models perform reliably.

The clinical implications of their work are significant, ranging from reducing adverse drug reactions to aiding healthcare professionals in medication management and ultimately enhancing patient safety. However, researchers are mindful of the challenges in their path, such as data quality, model accuracy, and ethical concerns regarding patient data privacy. Addressing these challenges is an ongoing commitment for researchers in this field. Looking forward, they envision AI-driven DDI prediction as a dynamic and evolving landscape, emphasizing the importance of continued research and collaboration across multidisciplinary teams, including pharmacologists and clinicians. Moreover, they recognize the

need for regulatory considerations and standards to ensure the safe and effective integration of AI-based DDI prediction tools into clinical practice. In this journey towards patient-centric healthcare, researchers aim to tailor DDI predictions to individual patient profiles, further optimizing medication regimens and improving overall healthcare delivery.

There have been few reviews on DDI prediction with various emphases, however, none of these studies had a machine learning focus. For previous reviews on machine learning methods for DDI prediction, please see [. In particular, is a brief review of similarity-based machine learning methods used for DDI prediction. As reported in this work, similarity-based approaches have four advantages: they do not need feature extraction and feature selection, similarity measure kernels for both drugs and genes have been fully studied before, they can be easily incorporated with kernel-based learning methods such as support vector machine (SVM), they can be used to connect chemical space and the genomic space. In , the focus of the review is on the methods that use both drug chemical structure and target protein sequence to predict DDIs.

Conclusion:

Identifying drug-drug interactions is the vital first step in drug discovery research. A few existing professional databases serve known data resources for DDI prediction and thus promote the drug discovery. Machine learning base methods are generally effective and reliable for DDI prediction. Different machine learning methods have the merits and demerits. Hence, it is essential to choose appropriate methods or assemble models for special prediction tasks A more effective prediction model can be established by integrating more heterogeneous data sources of drugs and targets. DDI prediction is a regression problem with quantitative bioactivity data.

The development and implementation of an AI-driven drug interaction prediction system represent a significant advancement in the field of healthcare and pharmaceuticals. This innovative technology has the potential to revolutionize patient care by providing healthcare professionals with timely and accurate information about potential drug interactions. By harnessing the power of artificial intelligence, this system can analyze vast datasets, identify previously undiscovered interactions, and enhance patient safety. It not only streamlines the decision-making process for healthcare providers but also empowers patients to make more informed choices about their medications. However, it is essential to ensure the continuous improvement and validation of such systems to minimize false positives and negatives. With ongoing research and refinement, AI-driven drug interaction prediction systems hold the promise of creating a safer and more efficient healthcare landscape for all.

Drug–Drug interaction prediction can help to screen out unsuitable compounds and is an important step in the development of new drugs. In this review, we describe the importance of drug–drug interaction prediction system.A drug prediction interaction system aims to predict and assess potential drug-drug interactions to enhance patient safety and optimize medication management. It involves the integration of computational methods, data analysis, clinical knowledge, and regulatory compliance to provide actionable insights for healthcare professionals and patients.