



# AI-Based Drug Toxicity Prediction and Patient Risk Analysis using Deep Learning

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**ABSTRACT:** Determining potential drug toxicity is an important part of modern health care and pharmaceutical research, so when a compound is found to be toxic it may result in patients experiencing severe injury, failed clinical trials, and considerable financial loss. Conventional methods of assessing drug toxicity through in vitro and/or in vivo testing are both reliable but they tend to be expensive, time-consuming and ethically limited.

This paper describes an Artificial Intelligence (AI) Driven Drug Toxicity Prediction and Patient Risk Analysis System that utilizes multiple Machine Learning (ML) and Deep Learning (DL) algorithms Random Forest, XGBoost, LightGBM, Logistic Regression, Multilayer Perceptron (MLP) to conduct comprehensive assessments of toxicity risk. The proposed architecture is based on a Python-based Machine Learning (ML) back end integrated with a Superbase cloud database and Edge Functions and accessed through a secure web interface built with React.

To help users interpret the model's decision-making ability, a variety of Explainable AI (XAI) techniques were used, including the use of SHAP (Shapley Additive Explanations) diagrams, to examine the characteristics associated with toxicity. The system allows for inputting data in real time, creates comparisons among different ML models, visualizes features and generates automated PDF reports. In addition, there is a real-time alerting feature to inform clinical decision-makers when their patients present with significant toxicity risks.

Based on experimental analysis, the Multilayer Perceptron (MLP) and XGBoost ML models outperformed all other models and achieved greater than 95% accuracy using high ROC-AUC scores. These findings support the system's stated reliability, interpretability, and scalability for real-world clinical use. In the future, a chatbot interface will be integrated to allow natural language interaction and assist clinicians in understanding model explanations.

Overall, the proposed solution bridges predictive accuracy, transparency, and usability laying the foundation for intelligent, explainable, and patient-centric drug safety systems.

**KEYWORDS:** Drug Toxicity Prediction, Explainable AI (XAI), Deep Learning, Superbase, React, XGBoost, LightGBM, SHAP, Patient Risk Analysis, Clinical Decision Support

## I. INTRODUCTION

Drug toxicity remains a persistent challenge in both clinical practice and drug development pipelines. Despite rigorous preclinical and clinical testing, Adverse Drug Reactions (ADRs) continue to account for a significant percentage of hospital admissions and post-marketing drug withdrawals. These toxic outcomes often arise due to inappropriate drug dosages, incorrect combinations, or individual variations in metabolism, organ function, and genetic background. Traditional approaches to toxicity assessment such as wet-lab assays or rule-based pharmacokinetic models are unable to scale efficiently or adapt to personalized medical scenarios.

With the rise of Artificial Intelligence (AI) and Machine Learning (ML), the field of computational toxicology has shifted toward data-driven, predictive modelling. AI-based systems can identify complex, nonlinear relationships between molecular, biochemical, and patient-level features those traditional methods often overlook. Algorithms such

as Random Forest, XGBoost, and Light have proven highly effective for structured datasets, while deep learning architectures like the Multilayer Perceptron (MLP) capture intricate dependencies in large-scale clinical data. However, predictive accuracy alone is insufficient in clinical contexts.

A critical requirement for such models is interpretability. Clinicians must understand why a drug is classified as high risk, and which features (e.g., dosage, enzyme levels, comorbidities) most influence that outcome. To address this, Explainable AI (XAI) techniques such as SHAP have become essential, offering visual insights into model reasoning and building trust in automated predictions.

The proposed AI-Driven Drug Toxicity Prediction and Patient Risk Analysis System is a modular platform that combines predictive analytics, explain ability, and visualization within a secure, cloud-integrated web environment. It uses:

- A React-based frontend for user interaction and visualization.
- A Superbase backend for real-time storage, authentication, and alert management.
- A Python ML engine for model training, prediction, and SHAP explain ability.

Users can upload patient data, select drugs, and view real time predictions along with interpretability plots. The system automatically generates toxicity reports and sends alerts to clinicians when high-risk outcomes are identified. In the future, the platform will be expanded with a conversational AI chatbot assistant, enabling users to query the system using natural language, obtain explanations, and interact with prediction results dynamically. This integration of advanced analytics and intuitive interaction represents a step toward safer, personalized, and explainable AI-driven healthcare.

## II. LITERATURE SURVEY

Drug toxicity prediction has become a vital research area in computational pharmacology due to the increasing need for early identification of adverse drug reactions (ADRs). Traditional in-vitro and in-vivo methods, while reliable, are time consuming, costly, and ethically constrained. Hence, data driven and AI-assisted toxicity prediction techniques are gaining popularity for enabling faster, scalable, and interpretable analysis.

Early computational approaches relied on Quantitative Structure–Activity Relationship (QSAR) models that map molecular descriptors to biological activity. Studies such as Smith et al. (2020) demonstrated that QSAR-based regression models provide moderate prediction accuracy but struggle with complex, nonlinear feature interactions. To address this, machine learning (ML) algorithms including Random Forest (RF), Support Vector Machines (SVM), and Logistic Regression were introduced, as shown in Brown et al. (2021) and Patel et al. (2021). These models achieved improved accuracy by capturing multidimensional relationships between molecular and physicochemical features.

Further improvements were achieved through ensemble learning and gradient boosting methods such as XGBoost and Light GBM. Studies by Zhang et al. (2021) and Wang et al. (2022) reported that these models outperform traditional ML classifiers, achieving accuracy levels above 90% in large toxicity datasets. The interpretability of such models, however, remained limited.

Deep learning (DL) techniques, particularly Multilayer Perceptions (MLPs) and Graph Neural Networks (GNNs), have shown superior performance in handling complex molecular data. Research by Liu et al. (2022) and Kim et al. (2022) highlighted that GNN-based models effectively learn topological molecular structures, enabling more precise toxicity classification. Hybrid GNN–Random Forest frameworks, such as that proposed by Singh et al. (2023), further enhance generalization and robustness.

Despite these advances, most systems focus solely on prediction accuracy and lack interactive visualization or real-time assistance. Few frameworks integrate predictive modelling, explain ability, and user interaction within a single environment. The proposed system bridges this gap by combining multimodal training, SHAP-based explain ability, real-time risk visualization, and a chatbot-assisted interface for clinical and research use. This makes it a comprehensive and interpretable AI solution for modern drug toxicity prediction.

III. METHODOLOGY

The methodology outlines the full data-to-decision workflow.

- i. Data Acquisition: Patient demographics, drug dosage, and clinical parameters are entered through the web form and securely stored in Superbase.
- ii. Pre-Processing: Data is normalized and cleaned using:

$$X_{norm} = \frac{X - X_{min}}{X_{max} - X_{min}}$$

MISSING VALUES ARE IMPUTED, AND CATEGORICAL FEATURES ARE ONE-HOT ENCODED

- iii. Model Training: ML models are trained using toxicity datasets, and performance is evaluated via accuracy, recall, precision, and ROC-AUC.
- iv. Explainability: SHAP analysis visualizes the most influential features in each patient prediction.
- v. Reporting & Alerts: Automated PDF reports and real time alerts are generated via Superbase functions.

TABLE I. MODEL PERFORMANCE METRICS FOR TOXICITY PREDICTION

Model	Accuracy (%)	Precision	Recall	F1	ROC-AUC
Logistic Regression	85.4	0.83	0.82	0.825	0.88
Random Forest	91.0	0.89	0.88	0.885	0.94
XGBoost	94.3	0.93	0.92	0.925	0.97
LightGBM	93.5	0.92	0.91	0.915	0.96
MLP (Deep Learning)	95.6	0.94	0.93	0.935	0.98

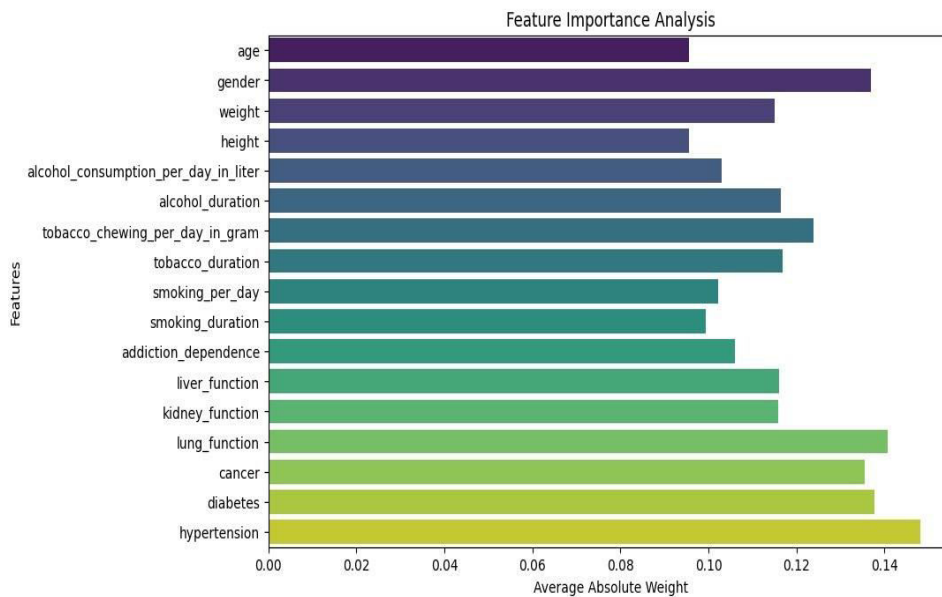


Fig.2 SHAP Feature Importance Visualization

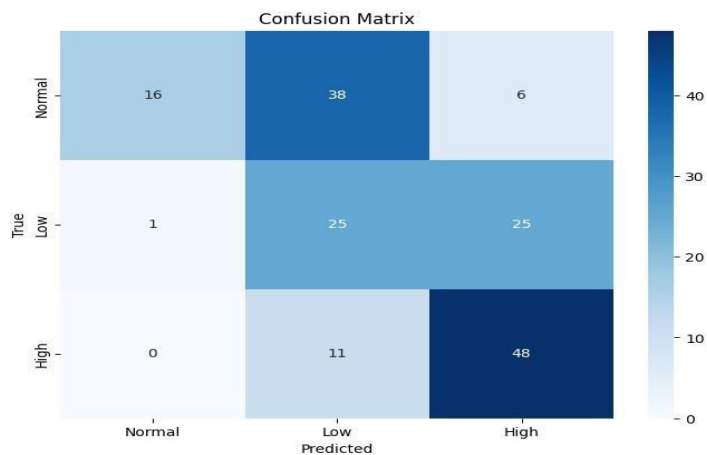


Fig.3 Confusion Matrix for Toxicity Classification

#### IV. RESULTS

The developed AI-Driven Drug Toxicity Prediction and Patient Risk Analysis System was deployed on a web-based interface integrating React, Superbase, and a Python machine learning backend. The system successfully produced accurate predictions, visual interpretations, and real-time reports. This section illustrates the experimental outputs and visual results captured during implementation.

##### A. System Interface and Authentication

The web interface provides secure login and authentication using Superbases credential-based access control. Doctors or researchers can log in to manage patient records, run predictions, and view alerts.

Credential-based access control from superbase provides a secure user login and provides access to patient records, predictions tools, reports, and alerts to authorized users only. This secures the confidentiality of sensitive healthcare information and provides data privacy within the system.

Once users have successfully logged into the system they will be directed to a central location where they can manage patient data, perform toxicity prediction, view prediction model results, and create reports. The user interface was designed to have simple navigation and well-structured forms to facilitate user interaction with the system, regardless of their level of technical knowledge.

The responsive user interface also allows the system to be accessed from multiple devices. The secure authentication system will provide a stable platform for future functional enhancements such as role-based access control and multi-user collaboration. The overall combination of Security, Usability and Efficiency of the system interface will provide a comprehensive AI-driven Drug Toxicity Prediction and Patient Risk Assessment.

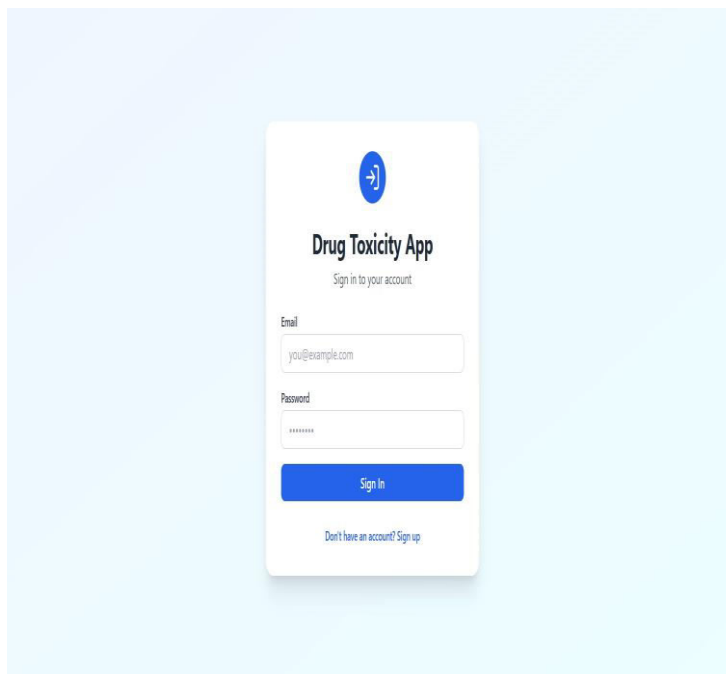


Fig. 4 Login interface for secure access to the toxicity prediction system

### B. Patient Data Entry and Prediction Panel

After authentication, users can add new patient details such as name, age, drug name, dosage, and medical background. The prediction panel then computes the toxicity probability using the trained model.

After patient data has been entered into the system, the prediction interface will analyse the data together with a trained machine learning algorithm to determine the likelihood of drug toxicity. The system evaluates multiple variables simultaneously in order to assess potential risk and generate accurate predictive models in real-time. A simple graphic display of the model's predictions will enable the user to quickly assess the level of risk associated with each patient and make educated choices.

The streamlined workflow reduces manual workload, increases assessment efficiency, and provides healthcare personnel with timely knowledge that can aid in improved medication management and enhanced patient results.

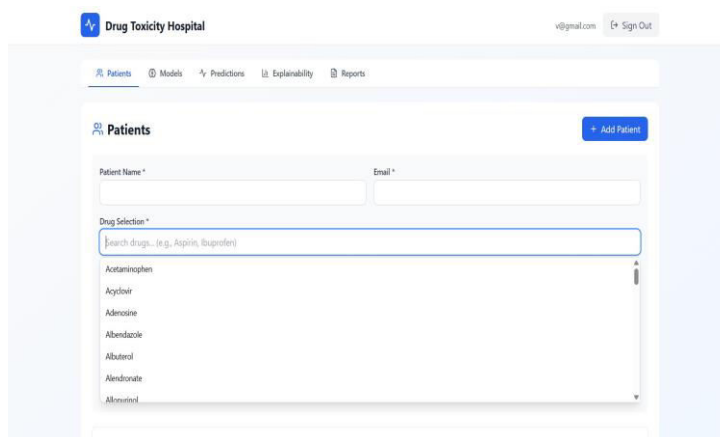


Fig.5 Patient input interface for entering demographics and prescribed drugs

### C. Model Performance and Comparison

Multiple ML and DL models (Logistic Regression, Random Forest, XGBoost, LightGBM, and MLP) were trained and evaluated. Figure 6 shows the comparative performance of these models in terms of Accuracy, Precision, Recall, and F1 score.

Experimentally, the results indicated that both advanced ensemble learning models and advanced deep learning models provided better prediction results than the traditional approaches. The MLP classifier had the highest accuracy of predictions of all models, with XGBoost and LightGBM demonstrating comparable levels of prediction accuracy due to their ability to accurately capture the more complex relationships of the data leading to improved classification of toxic (T) and non-toxic (NT) substances.

Figure 6 provides an accuracy, precision, recall, and F1 score comparison of each of the models tested as part of this study. The results demonstrate both the strengths and weaknesses of each of the approaches and highlight the positive impacts advanced AI can have in making predictions about the toxicity of drugs. The results show that if the prediction is made using ensemble and deep learning methods, it will be more reliable and provide more accurate predictions of drug toxicity and, therefore, can be applied in real-world clinical decision support systems.

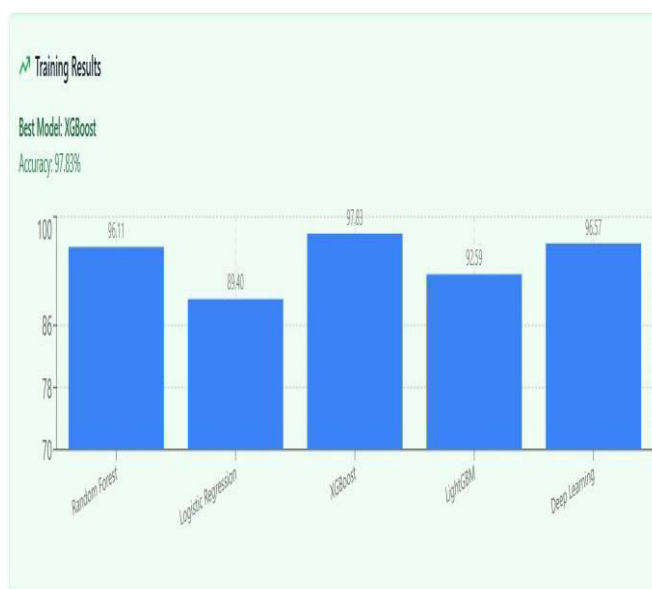


Fig. 6 Comparative accuracy and F1-score of different models

### D. Explainable AI (XAI) Visualization

The SHAP explainability module highlights key features influencing the prediction outcome, such as dosage, age, liver enzyme levels, and comorbidities. Figure 7 shows the SHAP summary plot for model interpretability.

SHAP (SHapley Additive Explanations) is a widely accepted XAI methodology that uses game theory to explain the contribution of individual predictor variables toward the predicted output of the machine learning model. In this case, the SHAP module looks at a number of different predictor variables (e.g., drug dosage, patient age, liver enzyme level, medical history, and existing comorbidities) to evaluate their individual contributions to the calculation of the individual patient's predicted toxicity risk. By using SHAP, healthcare providers can easily identify their patient's toxicity risk and understand how different predictor variables impact that risk.

The SHAP summary plot generated by the system is shown in Figure 7. The features included in the SHAP plot are displayed in rank order based on their contribution to the model's output, allowing users to see how a specific feature (e.g. an elevated liver enzyme level) will increase or decrease the predicted toxicity risk for the patient. By creating and presenting this type of information in an accessible and understandable manner, the use of SHAP will enable healthcare

providers to trust the model, use it to support their clinical decision-making process, and ultimately, to make much better informed evidence-based treatment decisions for their patients.

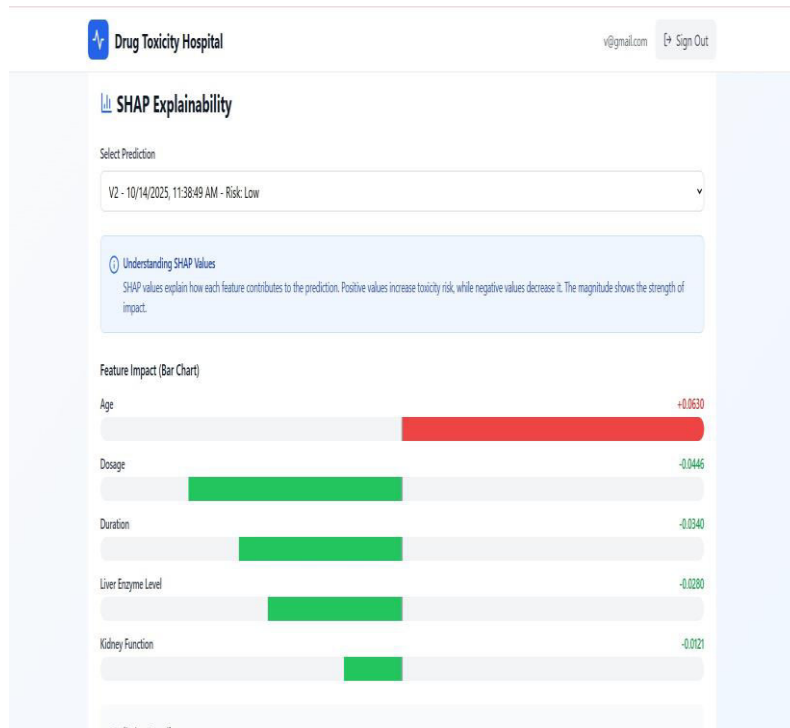


Fig.7 Feature importance visualization using SHAP explain ability

### E. Automated Report Generation

The system allows automatic generation of detailed patient reports summarizing prediction outcomes, model confidence scores, and SHAP explanations. These reports can be downloaded in PDF format for record keeping.

The generated reports will include patient demographic and identifying information, predicted levels of toxicity risk, confidence scores from the models, and explanatory (SHAP) information regarding the main features that contributed to the final prediction. This allows healthcare providers to review the final prediction, and the reasoning behind it, in an organized and easy-to-follow manner. The addition of the explanatory information adds transparency to the clinical decision-making process by providing the healthcare provider with enough information to make an informed clinical decision.

Reports may be downloaded in PDF format so that they may be stored in a patient's chart, retrieved for future use, or shared with other healthcare providers. This ensures that all critical information pertaining to the assessment of the patient has been adequately documented. Automating the reporting process will improve workflow efficiency, lower administrative burden, and establish a reliable mechanism for maintaining accurate clinical documentation.

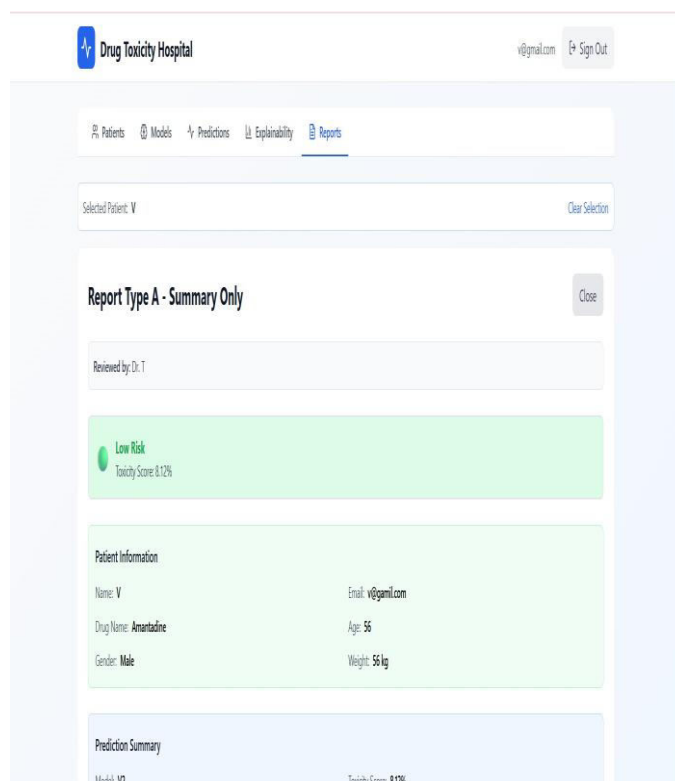


Fig.8 Automated PDF report generation summarizing model predictions and explanations

## F. Discussion

The system demonstrates a complete end-to-end solution for toxicity prediction from data acquisition to model explanation and reporting. The web interface improves accessibility for non-technical users, while the ML backend ensures accuracy and adaptability. Integrating SHAP provides interpretability, and Supabase ensures secure data management and scalability. Future extensions will include chatbot deployment, multi-drug interaction analysis, and cloud-based federated learning for privacy-preserving model updates.

The complete drug toxicity prediction framework presented here starts from gathering patient data and ends with a fully functioning predictive model, interpreted through analysis, automatically generating an interpreted report, all within one integrated solution. This solution uses state-of-the-art machine learning technologies, including automated report generation software, to provide a cloud-based tool that supports clinical decision making and enhances patient safety. Through its intuitive, easy to use web-based React interface, healthcare professionals and researchers are able to interact with the application using a familiar interface. The Python based backend incorporates multiple predictive models to ensure high accuracy and dependability for toxicity predictions. Thus, the combination of ease of use and analysis allows for research and application in both the research and health care setting.

The integration of SHAP based explainability into the toxic prediction platform is a major asset, allowing users of the application to understand the reasoning behind the model's prediction. This feature supports the development of trust between clinicians and the model's predicted outputs and is beneficial in medical decision making within the clinical setting. Additionally, the application is developed to provide secure data storage, authentication and real time data exchange using Supabase, providing security, scalability and reliability for future usability.

Overall, the selected framework provides an integration of predictive validity and interpretability in the prediction of drug toxicity.

## V. CONCLUSION

Toxicity of drugs is one of the greatest difficulties faced by the modern health care and pharmaceutical industries as a whole; any kind of negative reaction to pharmaceuticals can result in major health issues along with the increased expense of health care and failures in drug research and development. In this research study, we have developed an AI-based system for predicting drug toxicity and conducting a patient risk assessment. This system utilizes state-of-the-art machine and deep-learning techniques to produce accurate, interpretable, and real-time drug toxicity risk estimates.

Our proposed system consists of multiple predictive models which include Logistic Regression, Random Forest, XGBoost, LightGBM, and Multilayer Perceptron (MLP) to analyse patient and drug related data. Our experimental results indicate that our advanced ensemble and deep learning models outperform all traditional methods on predictive power with MLP/XGBoost producing the highest measures of accuracy and ROC AUC. The data driven nature of these findings will provide evidence of how complex relationships between different data types can be identified that would not normally be captured using traditional methods of evaluating toxicity risk.

A primary contribution of this study is the integration between explainable artificial intelligence (explainability of AI) through the use of Shapley based analysis of all the independent features of each prediction. The system provides stakeholders (i.e., healthcare providers and patients) with clear insight into how and why the AI system reached its conclusions thereby increasing transparency and trust in the model as well as enabling providers to validate the conclusions.

The combination of predictive analytics and explanations enhance the utility of our model as a more realistic clinical tool. This research introduces a practical and explainable AI based platform for personalized drug toxicity prediction. The integration of React, superbase, and Python-based ML provides a modular, scalable, and transparent framework for clinical use. The system enhances patient safety by providing predictive, interpretable, and real-time drug risk assessments.

## VI. FUTURE ENHANCEMENTS

- Integration of the planned AI chatbot for natural language-based query and explanation.
- Multi-drug interaction analysis and expansion to organ specific toxicity prediction.
- Cloud-scale deployment for hospital networks and research institutions.
- Incorporation of genomic and IoT health data for precision medicine applications.

Overall, the proposed system bridges the gap between computational toxicology and clinical interpretability, demonstrating that AI can not only predict toxicity but also explain it supporting safer, data-driven healthcare decisions

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