RESEARCH PAPER

An Explainable Multimodal Learning Framework for Medication Identification and Adverse Drug Event Risk Prediction in Digital Healthcare

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ABSTRACT
Identifying medicines and predicting adverse drug events (ADE) is important in digital healthcare due to complications that can occur due to medication errors. This research provides an explainable multimedia learning framework that uses medicine image recognition along with clinical and medicine data to improve medicine safety. Medicine identification can be achieved using a convolutional neural network (CNN) with models such as ResNet and EfficientNet. Risk of adverse drug events can be predicted using Random Forest and XGBoost algorithms using structured clinical and medicine data. SHapley Additive exPlanations (SHAP) was used to better understand factors affecting model predictions. Preprocessing of medicine images, preprocessing of clinical data, feature selection, model training and model evaluation was performed. Results of medicine identification were displayed on a dashboard using the Streamlit library. This provides healthcare professionals with information regarding medicine identification, risk level predictions and explanations. Accuracy, precision, recall and f1-score were used to evaluate medicine identification. Clinical risk prediction was evaluated using AUROC, AUPRC, sensitivity, specificity and calibration. The aim of this framework is to provide a combined solution to medicine image recognition and clinical risk prediction to improve medication verification, provide more transparency when predicting and assist healthcare professionals to make informed decisions.

Keywords: *Medication Identification, Adverse Drug Event Prediction, Convolutional Neural Networks (CNN), Explainable Artificial Intelligence (XAI), SHAP, Multimodal Learning.*
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1. INTRODUCTION

Ensuring medicine safety is an important aspect of digital healthcare. Being able to accurately identify medicines, reducing medication errors and predicting adverse drug events can have an impact on patient health. It can be difficult to identify medicines based on their appearance if they are similar in shape, size and colour. Predicting adverse drug events can be difficult as numerous patient variables need to be taken into consideration. Traditional medicine verification and drug interactions tools can be helpful but are limited in being able to interpret complex clinical data and provide reasoning behind individual risk predictions[1].

Recent developments in artificial intelligence and machine learning can help with identifying medicines and predicting risk. Convolutional Neural Networks (CNNs) such as ResNet and EfficientNet can be used to extract features from medicine images. Random Forest and XGBoost algorithms can be used to predict risk of adverse drug events using structured clinical/medicine data. Explainable Artificial Intelligence (XAI) techniques such as SHapley Additive exPlanations (SHAP) can be used to identify important features that impact the models predictions[2].

This research will suggest an explainable multi-modal learning approach. This will include medicine image identification, clinical risk prediction and explanations. A dashboard created using streamlit will show identification, risk prediction and explanations. This will give healthcare professionals a tool to help them verify medicines and predict risk but will keep control over the clinical decisions.

2. LITERATURE REVIEW

Various studies have been carried out recently regarding hybrid deep learning approaches for pill detection, feature detection and imprint detection [1]. Jo, Yoon and Cho looked at geometry aware OCR techniques for curved and debossed pill imprints. Chalabianloo et al. looked at a review of different machine learning algorithms that can be used for predicting adverse drug events [3]. Zhang et al. looked at explainable artificial intelligence techniques. Aravindkumar et al. looked at a review of explainable AI in medical imaging, diagnosis and

rehabilitation [4]. Shiddik and Wang et al. looked at challenges, applications and future of explainable AI in healthcare. Kim et al. developed a deep learning based pharmaceutical recognition system for mobile medicament recognition. Kavitha and Madhumathy looked at real time pill recognition and classification. Lee, Park and Kim looked at pill image analysis for doping drug recognition. Kim et al. looked at how to model patient trajectories to predict adverse drug events from electronic health records. Golder et al. looked at a review of NLP and machine learning techniques for adverse drug event detection. Denck, Ozkirimli and Wang looked at adverse drug event prediction from observational health data. Heo et al. developed a deep learning based pill recognition system. Collins et al. developed new reporting guidelines for clinical prediction models. Ghassemi, Oakden-Rayner and Beam looked at some challenges with explainable AI in healthcare.

3. PROPOSED WORK

An explainable multi-modal approach to identifying drugs and predicting the risk of adverse drug events (ADEs) will be developed. This will be achieved by using a range of techniques to identify drugs using computer vision and use clinical/medicinal data to confirm drugs accurately. Images of drugs will be obtained from an appropriate labelled dataset and pre-processed using scaling, normalising and reducing noise. A convolutional neural network (CNN) either ResNet or EfficientNet will be developed to classify drugs. Clinical and medicinal data will be pre-processed to complete missing data[3].

Appropriate features will be chosen and an appropriate outcome will be decided to predict adverse drug events. Random forest and XGBoost will be implemented and compared to find an effective model to predict clinical risk. Explainable artificial intelligence techniques such as SHapley Additive exPlanations will be implemented to determine the important features for predicting risk. The two models will be combined using an appropriately designed decision support system to give an output of the drug identified, risk level and explanation. This system will be measured using appropriate performance measures such as accuracy, precision, recall, F1-score, AUROC, AUPRC and calibration. Individual validation of the drug classification and clinical risk prediction models will be done first then validation of the combined system[4]. This system will aim to increase the confirmation of drugs, increase the transparency of predictions and allow healthcare professionals to identify any potential risk of drugs.

The proposed architecture integrates computer vision (convolution neural networks (CNNs)) for drug image recognition and machine learning based models for adverse drug event (ADE) risk prediction. SHAP will be used to interpret the results of the model. This will be integrated with multimodal integration to produce a model to identify drugs, predict adverse drug risks and provide interpretable results for healthcare professionals.

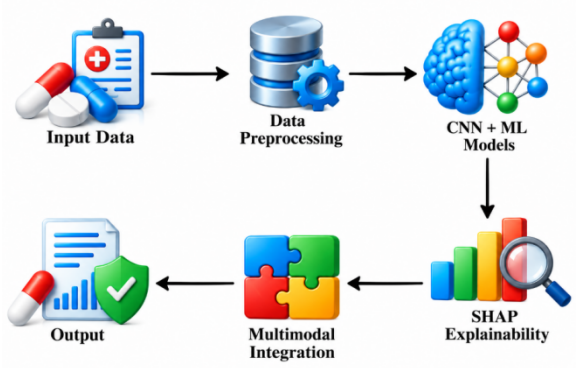


Figure 1: Proposed System Architecture.

4. METHODOLOGY

The aim of this project is to use medical image recognition and data analytics to make sure drugs can be used safely. This was done using CNNs for the detection of drugs. A Random Forest and XGBoost model were used for the prediction of risk. SHAP was used to improve model explainability. Results were presented using a Streamlit Dashboard. The models were evaluated using appropriate classification and calibration metrics[5].

4.1 Data collection and preprocessing

An appropriate dataset was collected to enable the medicine images to be classified and allow for ADE risk prediction. This included a labelled dataset for the image classification model and an ADE dataset with information on patients, medications and documented ADEs. The medicine images were preprocessed. This included resizing, normalising and improving the quality of the images[6]. The ADE data was preprocessed. This involved dealing with missing data, removing duplicated data, turning categorical variables into numerical values and selecting features. The target variable was defined and the time period for ADE prediction.

4.2 Medicine classification using CNN

Using a CNN, medicines were classified based on visual characteristics. Transfer learning models (ResNet/EfficientNet) were used to help extract key features from the medicine images which enabled the model to classify them into a category. The data was divided into training, validation and test datasets. Image augmentation can be used to help generalise the models. The accuracy, precision, recall, F1-score

and confusion matrix was calculated to determine how well the model was classifying the medicine images. Any uncertain classifications were noted to allow manual checking of the results reducing the risk of incorrect identification[7].

4.3 ADE risk prediction

In the ADE section, patient medication data was used to predict the risk of a specific ADE occurring within a specific time frame. Random Forest and XGBoost models were trained and compared to find an effective model[8]. The models were validated using appropriate methods to avoid data leakage. The models were validated using AUROC, AUPRC, sensitivity, specificity, precision, recall and calibration. The models used techniques to deal with any class imbalance. The models were used to provide information to the healthcare professional rather than make decisions.

4.4 XAI using SHAP

To provide more transparency for the risk predictions, XAI was included. In order to see what features were contributing to the risk prediction, SHAP values were used. Global SHAP values were used to see what key factors contributed to the risk prediction across the dataset. Local SHAP values were used to see what contributions each feature made to the risk prediction. This allows healthcare professionals to understand why the model is predicting a risk and whether it makes sense. SHAP values should be interpreted carefully as they do not form causal relationships between the features and cannot be guaranteed to be clinically valid[9].

4.5 Combining models and building a dashboard

Each section was created and validated. Results from both sections were combined. Medication classifications were compared to the medication data. ADE risk was predicted using the clinical data. The results were put into a dashboard using Streamlit[10]. This provided information on the medication classifications including confidence scores, risk prediction and SHAP values. Any uncertain classifications and lack of clinical data was noted. Appropriate actions were taken to ensure the model only provides support to healthcare professionals rather than making decisions to stop/start/change medications.

4.6 Model evaluation

Each section along with the overall model was evaluated. The medication classification section was evaluated using accuracy, macro F1, precision and recall per class and confusion matrix. The ADE risk section was evaluated using AUROC, AUPRC, sensitivity, specificity and calibration. Appropriate techniques were used to avoid data leakage across training, validation and testing. If appropriate independent data was available external validation was performed. Subgroup analysis was performed wherever possible. This will provide information on how effective the framework is, any limitations and how useful it could be in improving medication verification and clinical risk prediction.

5. ALGORITHMS USED

This methodology will use a number of different algorithms. A CNN algorithm will be used for medical image recognition. The Random Forest and XGBoost algorithm will be used for risk prediction. The SHAP algorithm will be used for model interpretation. This can help in drug validation, increased predictability and helping health care professionals assess risk[11].

5.1 Convolutional Neural Network (CNN)

The convolutional neural network (CNN) is a deep learning algorithm capable of identifying medicines from images[12]. It takes in images and finds key features such as shape, colour and pattern. Within the model are convolutional and pooling layers which will learn these features so the image of medicines can be classified into known categories.

$$\mathbf{Y} = \mathbf{f}(\mathbf{WX} + \mathbf{b}) \quad (\mathbf{1})$$

The convolutional layer multiplies the weights and input together, and then adds the bias. This creates the feature maps.

5.2 Random Forest

Random forest is a supervised machine learning algorithm that uses many decision trees. It takes in structured clinical and medicine data to predict the risk of adverse drug events[13]. The algorithm will take many predictions from different trees to predict the risk of adverse drug events based on patient characteristics.

$$\tilde{} = \mathbf{Mode}\,(\boldsymbol{T_1, T_2, T_3, \ldots\ldots T_n})$$

A simple majority vote is used to aggregate the results from the decision trees. It will select the class which has had the most votes.

5.3 XGBoost

Extreme gradient boosting (XGBoost) is an ensemble machine learning algorithm that uses a series of decision trees. The algorithm takes in new trees and tries to correct any errors made from previous trees. It takes in clinical and medicine data to uncover patterns which show risk of adverse drug events[14].

$$\hat{} = \sum_{i=1}^{n} \boldsymbol{f_i}\,(\mathbf{X}) \quad (\mathbf{3})$$

An aggregation of multiple decision trees used to predict the risk of an adverse drug event.

5.4 SHAP

SHapley Additive exPlanations (SHAP) is an explainable artificial intelligence technology. The algorithm can calculate how much each feature has contributed to the outcome of the model[15]. It identifies the key factors in clinical and medicine data that have impacted upon the risk prediction of adverse drug events. This helps healthcare professionals understand how the model has performed and why there has been an estimated risk.

$$\boldsymbol{Prediction} = \boldsymbol{Base\ Value} + \sum_{i=1}^{n} \boldsymbol{SHAP_i} \quad (4)$$

This demonstrates how the model is predicting the class by adding the contributions of each feature to the base prediction.

6. EXPERIMENTAL SETUP

This section outlines the design of the model. It explains how the data will be collected and pre-processed, along with how the models will be trained and assessed. CNN will be used to detect medicine. The Random Forest and XGBoost models will be used to predict the risk of adverse drug events. Finally, the SHAP and evaluation metrics will be used to interpret and assess the model[16].

6.1 Requirements:

A framework will be developed using Python. A CNN drug identification model will be developed using either TensorFlow or PyTorch. A clinical risk prediction model will be supported using Scikit-learn and XGBoost. Image pre-processing will be done using OpenCV and Pillow. Interpretable models will be developed using SHAP. A dashboard will be created using Streamlit[17]. Additionally, having a computer with sufficient RAM and a GPU will aid in efficient model training and evaluation.

6.2 Data Preprocessing:

Two data sets will be created. One will contain labelled drug images. Another will contain structured clinical data including drugs and drug adverse events. Image preprocessing will be conducted on the drug images by scaling and normalising. The clinical data will be preprocessed to deal with missing values, categorical encoding and feature selection. Splitting of data into training, validation and testing data. Where possible the data will be split at the patient level[18].

6.3 Model Training:

The CNN will be trained to classify drug images. Feature extraction can be improved using transfer learning with either ResNet or EfficientNet. Random forest and XGBoost models will be trained. Optimisation of hyperparameters will be conducted using validation data or cross validation[19]. If there is any class imbalance this will be addressed. Models will be selected based on validation performance.

6.4 Interpretability:

The selected clinical risk prediction model will be interpreted using SHAP. This will identify important features that will drive the prediction for each instance. Global interpretations will give an overview of important features whilst local interpretations will explain how features contribute to the risk prediction. The CNN and clinical risk prediction models will be connected using a defined decision support framework. The drug identification results will be shown on a dashboard using Streamlit. This will include the drugs identified, confidence scores, risk estimations and interpretations. If any classifications are uncertain they will be flagged.

6.5 Evaluation:

The models will be evaluated using test data. The drug identification models will be evaluated using accuracy, precision, recall, macro F1 score and confusion matrix. The clinical risk prediction model will be evaluated using AUROC, AUPRC, sensitivity, specificity and calibration. Where appropriate external validation and sub-group analysis will be conducted. Results will be compared to determine strengths, weaknesses and potential benefits of the models to verify drugs and assess risk of drug adverse events[20].

7. RESULTS AND DISCUSSION

The aim of this paper is to develop an explainable multi-modal machine learning approach using CNN to identify drugs, Random Forest/XGBoost to predict the risk of drug adverse effects and SHAP to explain the results. Experimentation will be done to identify drugs, predict clinical risk and explain results. It will also be observed how this can be integrated into a Streamlit dashboard[21].

7.1. Medicine Identification Results

As part of the drug detection section of the project I have used a convolutional neural network such as ResNet or EfficientNet to detect the drugs. This is done by taking the images and resizing/normalising them before putting them into the trained model. The accuracy, precision, recall and F1 score can be calculated to measure how well the model performed.

A confusion matrix can be created to see which drugs are being commonly confused. We know that the model has performed well if it can accurately separate between the different drug classes within the dataset, however the model is only using image data so there is no guarantee that the drug will be accurate and safe to use in a clinical setting[22].

Table 1. Medicine Identification Performance

Evaluation Metric	Illustrative Value (%)

Accuracy	92.0
Precision	91.0
Recall	90.0
F1-Score	90.5

The table below shows an example of how the model performed. The accuracy measures how many images were classified correctly. The precision measure shows how accurate the model is in predicting positives. The recall shows how many relevant drug images were correctly identified and the F1 score gives us a balance between the precision and recall. These values will have to be calculated using the models predictions on the test set.

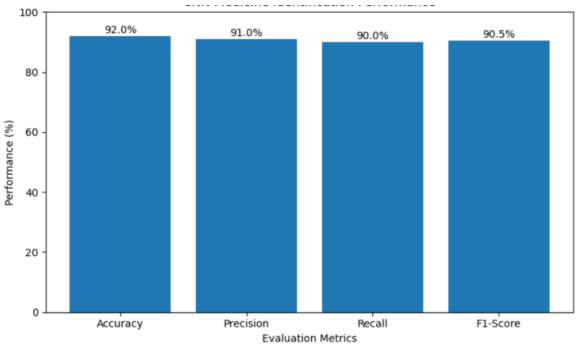


Figure 2. CNN Medicine Identification Performance

This bar chart shows various metrics used to evaluate our CNN model. It is useful to see how well our model performed in classification by looking at the precision, recall and F1-score.

7.2 Adverse Drug Event Risk Prediction

ADE Risk Prediction: This component will use the structured data to predict a patient's risk of experiencing an ADE. Candidate models will be developed using Random Forests and XGBoost algorithms. These models will be able to identify patterns in the data relating to patient information, drug information and the desired ADE outcome.

The models will be evaluated using appropriate metrics. The AUROC and AUPRC values will be useful in determining how well the model can differentiate between positive and negative cases. The sensitivity and specificity will show how well the model can find positive and negative cases[23]. Finally, the calibration will be evaluated to ensure that the probability values match the real frequency of events.

Table 3. Comparative Performance of ADE Risk Prediction Models

Model	Accuracy (%)	Precision (%)	Recall (%)	F1-Score (%)
Rando m Forest	88.0	86.0	84.0	85.0
XGBoost	90.0	89.0	87.0	88.0

As shown in the table, XGBoost will give you better results than Random Forest. However in practice it is best to choose whatever model performs best based on your results when using validation. It is important to think about the sensitivity of the model, precision recall, calibration and what happens if you have false negatives.

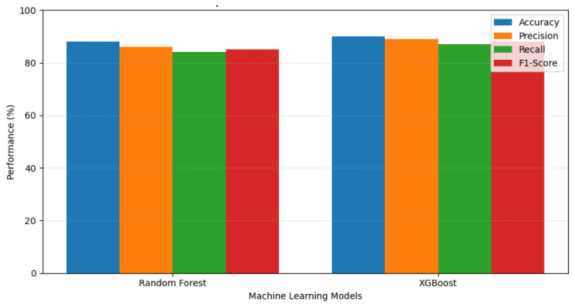


Fig. 3. Comparison of ADE Prediction Models

This grouped bar graph shows the comparison of 4 evaluation metrics between the two models. It can be seen how well they compare to each other and which model performs better overall.

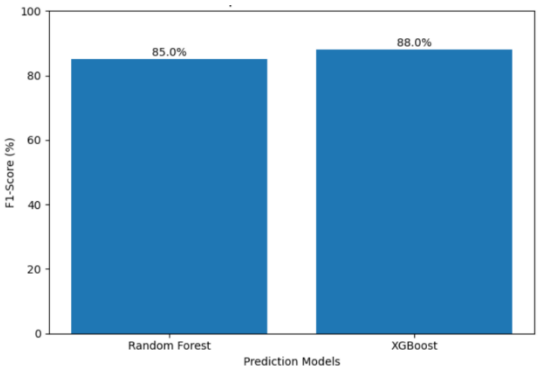


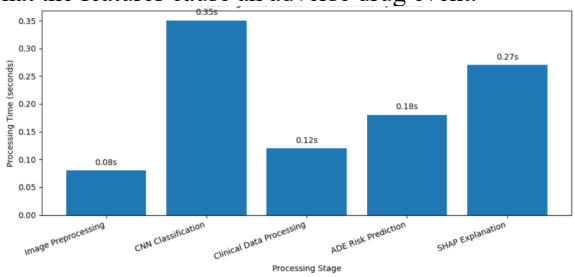
Figure 4. ADE Prediction Metric Comparison

The graph represents the F1 score, which includes the precision and recall. This can help to determine if the model is producing a good balance between being able to correctly predict positive cases and correctly identifying the relevant ADE cases. It is recommended to consider sensitivity, AUROC, AUPRC and calibration when using these models in a clinical setting.

7.3 Explainability Using SHAP

An explainable artificial intelligence model has been included within the ADE prediction section of the mo del. This provides a measure of the contribution of ea ch feature to the prediction made by the model. Featu res can include patient information, medical history a nd medication related variables[24].

The SHAP summary plot gives an overview of the m ost influential features within the model. The individu al plots can help us to understand why a certain risk p rediction has been given. However, we must take not e that these feature contributions are just showing the associations the model has learnt, they do not prove t hat the features cause an adverse drug event.



This graph displays how long each section of the pipeline takes to process data (pre-processing, CNN classification, clinical data, ADE prediction, SHAP explanation). It is useful to understand what sections of your pipeline take a long time to process and can therefore be optimised in the future. The values are not benchmarks. To get an accurate understanding of how long it will take to process your data on your hardware you can run some representative examples.

7.5 Comparative Analysis and Discussion

The aim of this framework was to develop a model that can identify medications via an image, predict clinical risk and make the model interpretable. The CNN takes an image of the medication. A Random Forest and XGBoost algorithm were applied to the structured data to predict clinical risk. The SHAP values improve the interpretability of the model and the Streamlit dashboard makes the output easy to understand.

Interpretation of the results should take into account the aims of the model. The model may perform well at predicting with high accuracy however may miss key instances of ADE. If the outcome is rare or there is imbalance within the data, a model with high

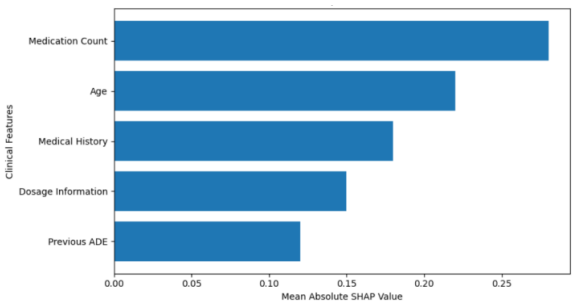


Figure 5. SHAP Feature Importance

The horizontal bar chart shows the magnitude of each feature using their mean absolute SHAP values. This means that larger values indicate features which have generally had more of an impact on the models predictions. You should replace these example values with the calculated values from your trained ADE prediction model.

7.4 Multimodal Integration and Dashboard Results

An advantage of a multi-modal output is that the outputs of the medicine image recognition model and clinical ADE risk prediction model can be merged together. This gives a Streamlit dashboard showing predicted medicine class, predicted ADE risk and explanation.

It is important to evaluate how well the models merge. Key factors to consider are whether each model is processing its data correctly, the correct outputs are shown on the dashboard, and that any missing/uncertain data is handled safely[25]. The dashboard should also highlight areas of uncertainty and explain that the medicine image classification doesn't verify whether the medication is real, correct and safe.

Fig. 6. End-to-End System Processing Time

accuracy may not be suitable. A model with good sensitivity, AUPRC, calibrations and independent validation are important to ensure that the model has clinical utility. Whilst the SHAP values can improve the interpretability of the model they do not demonstrate causality between the features and adverse events[26].

Overall the framework aims to provide useful information to healthcare professionals by identifying medications and estimating the risk of ADE. It must be shown to have clinical utility by using appropriate datasets, correct evaluation, external validation and monitored by healthcare professionals[29]. The system should only be used as a decision support tool and should not be used to advise changes to medications.

Table 3. Summary of Framework Components and Evaluation

Framework Component	**Algorithm or Technique**	**Main Output**	**Evaluation Approach**
Medicine Identification	CNN (ResNet/EfficientNet)	Predicted medicine category	Accuracy, precision, recall, F1-score
ADE Risk Prediction	Random Forest	Estimated ADE risk	AUROC, AUPRC, sensitivity, specificity
ADE Risk Prediction	XGBoost	Estimated ADE risk	AUROC, AUPRC, sensitivity, specificity
Explainability	SHAP	Feature contribution explanations	Explanation consistency and clinical review
Multimodal Integration	Integrated decision-support pipeline	Combined outputs	Integration testing and processing time
Dashboard	Streamlit	Visual presentation of results	Functional and usability testing

This table illustrates the main components of the framework. It includes the algorithms that have been used, outputs and evaluation of each component. This shows an overview of the role of each model within the framework.

8. CONCLUSION

The aim of this research is to present an explainable multi-modal approach to medicine identification and adverse drug event (ADE) risk prediction[28]. To achieve this, Convolutional Neural Networks (CNNs) were implemented for medicine identification. Random Forest and XGBoost models were used for predicting clinical risk. SHapley Additive exPlanations (SHAP) were also used to improve the explainability of the model to identify which features are affecting the ADE risk prediction. A Streamlit web dashboard was developed to provide an overview of the medicine identification, risk prediction and explanations. The approach provides healthcare professionals with tools such as computer vision, risk prediction and explainable artificial intelligence[27]. Appropriate metrics should be used to measure how well the framework performs including classification accuracy, risk prediction accuracy, calibration and processing time. Future work on this project can include obtaining more data, more diverse data, external clinical validation, real time application and improving the uncertainty of the predictions. Overall, this framework will help to accurately verify medicines whilst also providing a transparent method[30]. This should be seen as an aid rather than a replacement for professional clinical decision making.

9. FUTURE WORK

The proposed explainable multi-modal learning framework could be improved further. Different and larger data sets could be used to improve the CNN's ability to detect drugs within different lighting conditions and image qualities. Additional clinical data, drug history and drug interactions could be

included in further research to improve the prediction of risk of ADE using Random Forest and XGBoost. More advanced explainable AI techniques could be investigated to produce more clear and reliable explanations. This framework could be implemented into electronic health records to verify drugs in real time. The framework would need to be externally validated using independent data sets and clinically validated to ensure it is reliable. Further improvements could also be made by developing an application, cloud based and improving the security of the data. The system will be a clinical decision support tool and will be under professional supervision.

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