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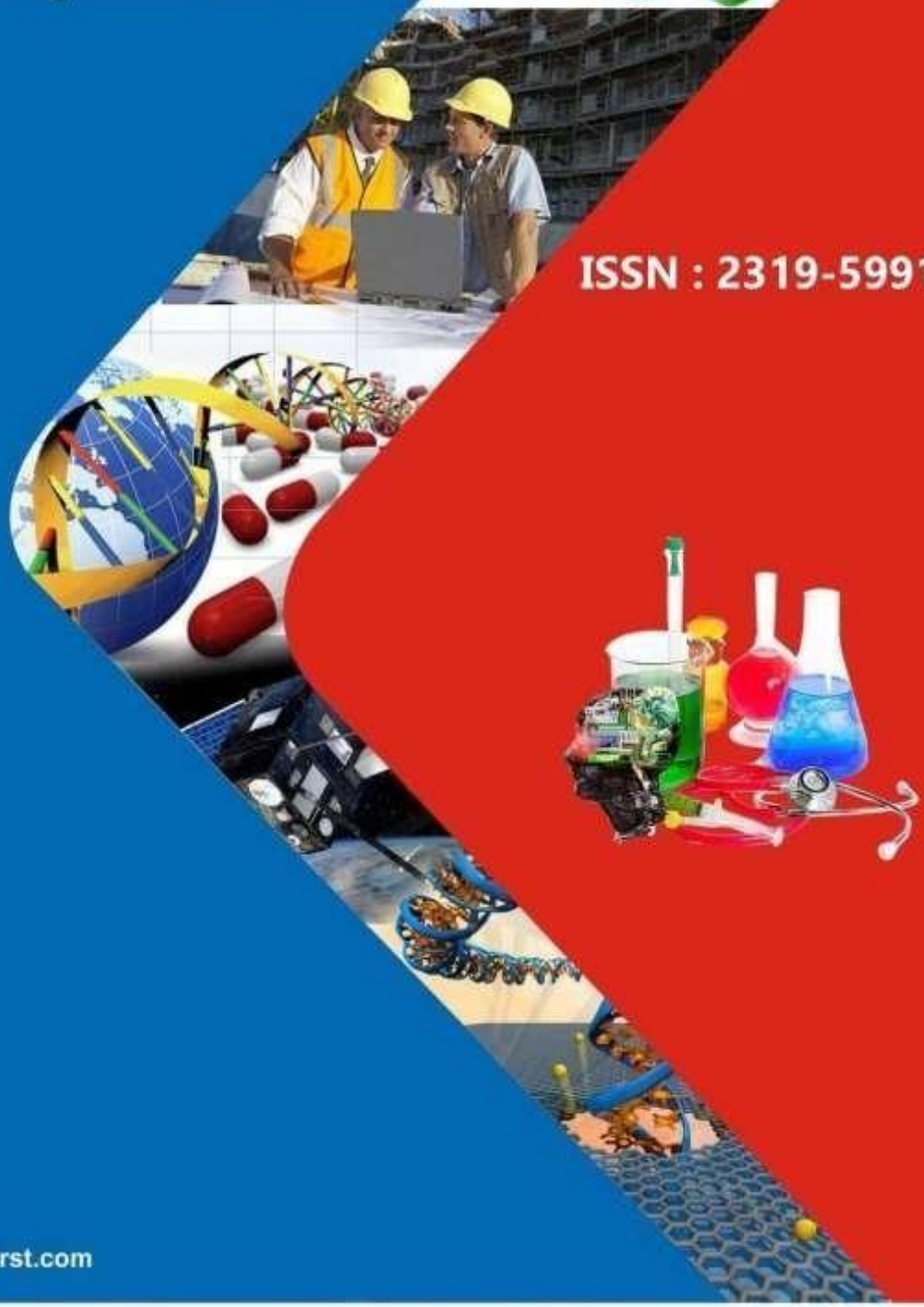

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# DEEP SIDE-A DEEP LEARNING FRAMEWORK FOR DRUG SIDE EFFECT PREDICTION

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## ABSTRACT

Drug failures due to unforeseen adverse effects at clinical trials pose health risks for the participants and lead to substantial financial losses. Side effect prediction algorithms have the potential to guide the drug design process. LINCS L1000 dataset provides a vast resource of cell line gene expression data perturbed by different drugs and creates a knowledge base for context specific features. The state-of-the-art approach that aims at using context specific information relies on only the high quality experiments in LINCS L1000 and discards a large portion of the experiments. In this study, our goal is to boost the prediction performance by utilizing this data to its full extent. We experiment with 5 deep learning architectures. We find that a multi-modal architecture produces the best predictive performance among multi-layer perceptron-based architectures when drug chemical structure (CS), and the full set of drug perturbed gene expression profiles (GEX) are used as modalities. Overall, we observe that the CS is more informative than the GEX. A convolutional neural network-based model that uses only SMILES string representation of the drugs achieves the best results and provides 13:0% macro-AUC and 3:1% micro-AUC improvements over the state-of-the-art. We also show that the model is able to predict side effect-drug pairs that are reported in the literature but was missing in the ground truth side effect dataset.

## I.INTRODUCTION

project represents a pivotal advancement in pharmaceutical research and healthcare. Predicting potential side effects of drugs is a critical aspect of drug development and patient safety.

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Traditional methods often lack accuracy and efficiency in identifying adverse reactions early in the drug discovery process. In response to this challenge, DeepSide proposes a state-of-the-art deep learning framework that leverages large-scale drug data to predict drug side effects with remarkable precision. By harnessing the power of deep learning algorithms, DeepSide aims to revolutionize drug safety assessment, facilitating the identification of potential side effects at an early stage and enabling proactive measures to mitigate risks for patients.

## II.EXISTING SYSTEM

A drug-drug interaction (DDI) is defined as an association between two drugs where the pharmacological effects of a drug are influenced by another drug. Positive DDIs can usually improve the therapeutic effects of patients, but negative DDIs cause the major cause of adverse drug reactions and even result in the drug withdrawal from the market and the patient death. Therefore, identifying DDIs has become a key component of the drug development and disease treatment.

In this study, an existing system, develops a method to predict DDIs based on the integrated similarity and semi-supervised learning (DDI-IS-SL). DDI-IS-SL integrates the drug chemical, biological and phenotype data to calculate the feature similarity of drugs with the cosine similarity method. The Gaussian Interaction Profile kernel similarity of drugs is also calculated based on known DDIs. A semi-supervised learning method (the Regularized Least Squares classifier) is used to calculate the interaction possibility scores of drug-drug pairs. In terms of the 5-fold cross validation, 10-fold cross validation and de novo drug validation, DDI-IS-SL can achieve the better prediction performance than other comparative methods. In addition, the average computation time of DDI-IS-SL is shorter than that of other comparative methods. Finally, case studies further demonstrate the performance of DDI-IS-SL in practical applications.

### Disadvantages

• The complexity of data: Most of the existing machine learning models must be able to accurately interpret large and complex datasets to detect an accurate Drug Side Effect.

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• Data availability: Most machine learning models require large amounts of data to create accurate predictions. If data is unavailable in sufficient quantities, then model accuracy may suffer.

• Incorrect labeling: The existing machine learning models are only as accurate as the data trained using the input dataset. If the data has been incorrectly labeled, the model cannot make accurate predictions.

## III.PROPOSED SYSTEM

Multi-layer perceptron (MLP) Our MLP [22] model takes the concatenation of all input vectors and applies a series of fully-connected (FC) layers. Each FC layer is followed by a batch normalization layer [10]. We use ReLU activation [16], and dropout regularization [27] with a drop probability of 0:2. The sigmoid activation function is applied to the final layer outputs, which yields the ADR prediction probabilities. The loss function is defined as the sum of negative log- probabilities over ADR classes, i.e. the multi-label binary cross-entropy loss (BCE). An illustration of the architecture for CS and GEX features is given in this system.

Residual multi-layer perceptron (ResMLP) The residual multi-layer perceptron (ResMLP) architecture is very similar to MLP, except that it uses residual-connections across the fully-connected layers. More specifically, the input of each intermediate layer is element-wise added to its output, before getting processed by the next layer. Such residual connections have been shown to reduce the vanishing gradient problem to a large extend [7].

This effectively allows deeper architectures, therefore, potentially learning more complex and parameter-efficient feature extractors. Multi-modal neural networks (MMNN) The multi-modal neural network approach contains distinct MLP sub-networks where each one extract features from one data modality only. The outputs of these sub-networks are then fused and fed to the classification block. For feature fusion, we consider two strategies: concatenation and summation. While the former one concatenates the domain-specific feature vectors to a larger one, the latter one performs element-wise summation. By definition, for summation based fusion, the domain-specific feature extraction sub-networks have to be designed to produce vectors

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of equivalent sizes. We refer to the concatenation and summation based MMNN networks as MMNN.Concat and MMNN.Sum, respectively.

Multi-task neural network (MTNN) our multitask learning (MTL) based architecture aims to take the side effect groups obtained from the taxonomy of ADReCS into account. For this purpose, the approach defines shared and task-specific MLP sub-network blocks. The shared block takes the concatenation of GEX and CS features as input and outputs a joint embedding. Each task-specific sub-network then converts the joint embedding into a vector of binary prediction scores for a set of inter-related side-effect classes.

**Advantages**

- The proposed system implemented many ml classifies for testing and training on datasets.
- The proposed system developed Convolutional neural networks (CNN) which are known to provide a powerful way of automatically learning complex features in vision tasks to find an accurate accuracy on the datasets.

## IV.MODULES

- **Service provider**

In this module, the service provider has to login by using valid user name and password.


After login successful he can do some operations such as browse datasets and train & test data sets,


view trained and tested accuracy in bar chart,

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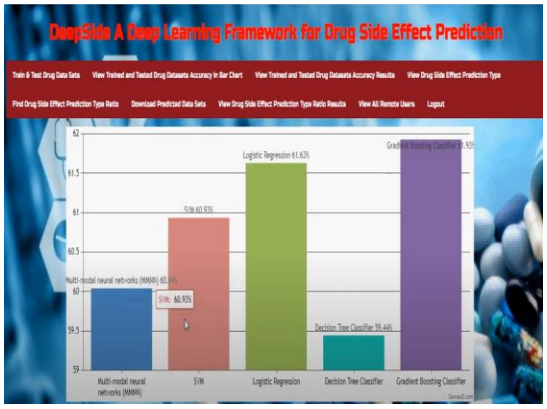



view trained and tested accuracy results, view predicted type,

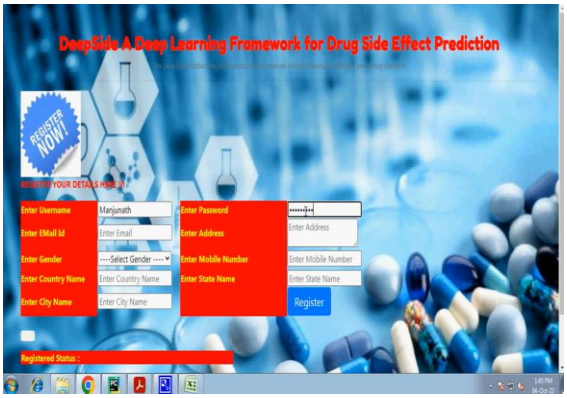

view type ratio, download predicted data sets, view type ratio results, view all remote users.

### ➢ View and authorize users

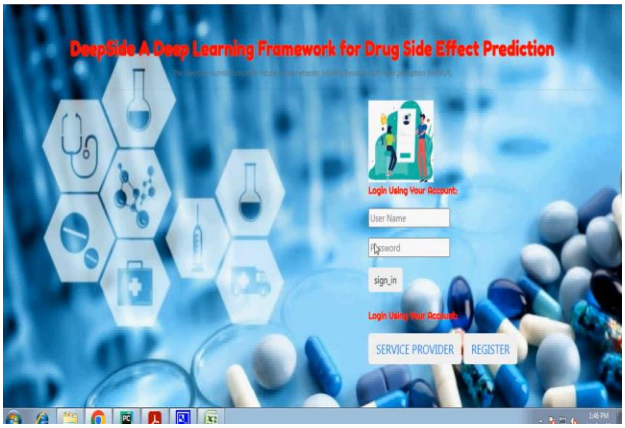
In this module, the admin can view the list of users who all registered. In this, the admin can view the user's details such as, user name, email, address and admin authorizes the users.

### ➢ Remote user

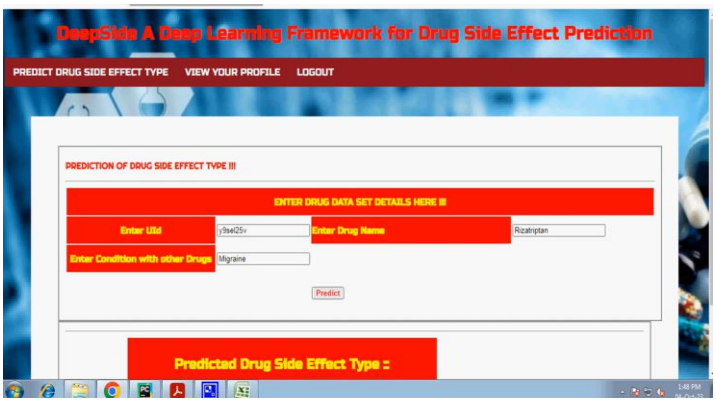
In this module, . User should register before doing any operations.




Once user registers, their details will be stored to the database. After registration successful, he has to login by using authorized user name and password.




Once login is successful user will do some operations like register and login, after login we have to predict type, view your profile.



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## V.CONCLUSION

In conclusion, the "DeepSide: A Deep Learning Framework for Drug Side Effect Prediction" project holds immense promise for advancing drug safety assessment and patient care. By developing an innovative deep learning framework, DeepSide aims to enhance the accuracy and efficiency of drug side effect prediction, thereby improving ies.

patient safety and reducing adverse drug reactions. Through the integration of large-scale drug data and cutting-edge deep learning algorithms, DeepSide offers a transformative approach to drug safety assessment, empowering pharmaceutical researchers and healthcare providers with valuable insights to optimize drug development and patient treatment strateg

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