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Drug Target Interaction Prediction

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Abstract: *Drug–target interaction (DTI) prediction is vital to drug discovery, assisting in the identification of drug- target protein interactions more efficiently than usual methods of experimentation, which are frequently costly and time-consuming. To In order to tackle these issues, this piece presents a web-based application that predicts DTIs and illustrates molecular information. The system takes drug samples and protein sequences as input and outputs molecular formula, predicted activity status with probabilities, and molecular structure visualization. Including ML and DL models, the application enables comparative evaluation of different algorithms, highlighting their strengths and limitations in order to identify most effective approach for DTI prediction. This project's primary purpose is to create reliable models for DL and ML that can precisely determine whether a medication and protein combination is active or inert. Because of this, it is feasible to forecast drug-target interactions with accuracy. Data on drug-protein interactions was acquired from ChEMBL then was pre- processed and represented using SMILES, molecular fingerprints, and ProtBERT embeddings. Multiple ML and DL models (RF, SVM, KNN, Decision Trees, Logistic Regression, Naïve Bayes, CNN, RNN) were trained, and their performance was reviewed using accuracy, precision, recall, and ROC-AUC to determine the most effective approach. Logistic Regression achieved highest performance with the highest accuracy of 96% which outperformed several deep learning approaches on this dataset, however deep learning retains advantage of automatic feature learning and may surpass machine learning when larger and more dataset available. This dual evaluation confirms our hypothesis on both sides in a much more robust way. This comparison provides hands-on experience on benefits and drawbacks of the two approaches.*

Keywords: DTI, Machine Learning, Deep Learning, Molecular Fingerprints Protein Sequence Embedding Feature Extraction Random Forest(RF) Recurrent Neural Network(RNN) Convolutional Neural Network (CNN).