Title: Drug Interaction Prediction

Abstract:

Drug interactions are a significant concern in pharmacology, as they can lead to adverse effects, reduced efficacy, or even life-threatening consequences. This project proposes a machine learning approach to predicting drug interactions, leveraging a comprehensive dataset of drug properties, target genes, and signaling pathways. The proposed framework integrates multiple heterogeneous data sources to identify potential interactions, taking into account the complex relationships between drugs and their biological targets.

Background: Drug interactions occur when two or more drugs are taken together, resulting in an unintended effect on the body. These interactions can be classified into three categories: pharmacokinetic, pharmacodynamic, and pharmaceutical interactions. Pharmacokinetic interactions involve changes in drug absorption, distribution, metabolism, or excretion, while pharmacodynamic interactions involve changes in drug effects on the body. Pharmaceutical interactions involve changes in drug formulation or delivery.

Methodology: The proposed framework will utilize a machine learning approach to predict drug interactions. The dataset will consist of drug properties, target genes, and signaling pathways, which will be integrated from multiple heterogeneous sources, including:

DrugBank: A comprehensive database of drug information, including chemical structures, target genes, and signaling pathways.

PubChem: A database of chemical compounds, including drugs, with information on their properties and biological activities.

GenBank: A database of genetic sequences, including genes and proteins involved in drug metabolism and response.

The machine learning algorithm will be trained on this dataset to identify patterns and relationships between drugs and their biological targets. The algorithm will be evaluated using metrics such as accuracy, precision, recall, and F1-score.

Expected Outcomes: The proposed framework aims to develop a predictive model that can accurately identify potential drug interactions.