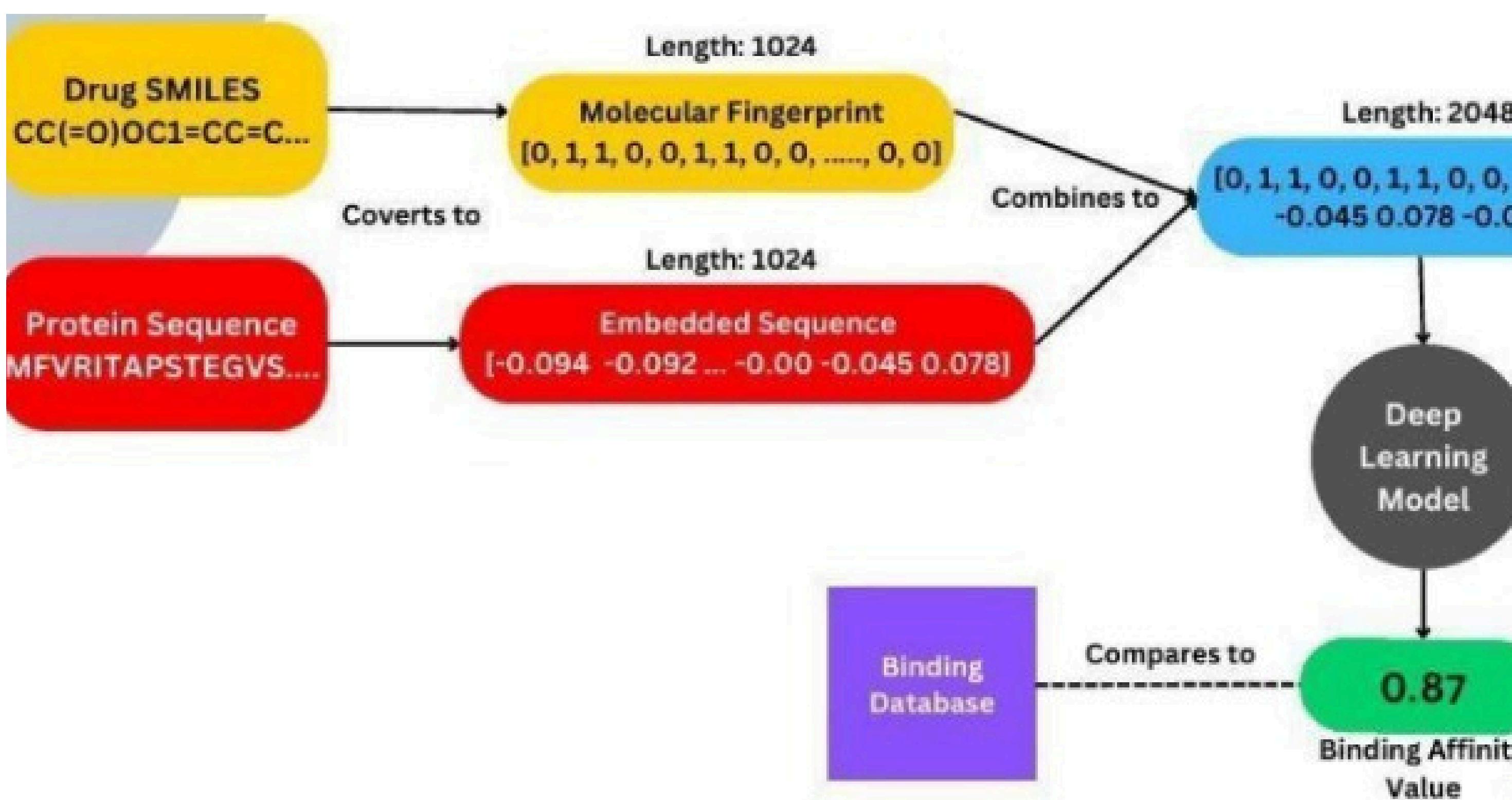


DRUG TARGET INTERACTION PREDICTION

INTRODUCTION

The identification of drug-target interactions is a crucial step in drug discovery and development. Experimental methods for identifying these interactions are often costly, time-consuming, and labour-intensive. By predicting potential drug-target interactions, such models can support the early stages of drug discovery and reduce the reliance on extensive biological testing.

DATA FLOW DIAGRAM



PROBLEM STATEMENT

The project aims to develop a machine learning model to predict drug-target binding affinity using their 1D representations. This involves utilizing SMILES strings for drugs and amino acid sequences for proteins as inputs to train a predictive model, enabling efficient and accurate identification of potential drug-target interactions.

MODEL TRAINING

The training process for the Drug-Target Interaction (DTI) prediction model involved a supervised learning approach with the collected dataset of drug SMILES and protein sequence representations. Training began with an initialized Multi-Layer Perceptron (MLP) model, where the weights were updated iteratively based on the calculated loss function.

CONCLUSION

The project provides a foundation for faster and cost-effective drug discovery but also underscores the potential of integrating machine learning into pharmaceutical research workflows. By leveraging computational tools, researchers can significantly accelerate the identification of promising drug candidates, especially in addressing emerging diseases or optimizing existing drugs.

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