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Artificial Intelligence

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# Prediction of Side Effects of Drug Based on Drug-Protein Interaction through Graph Neural Networks

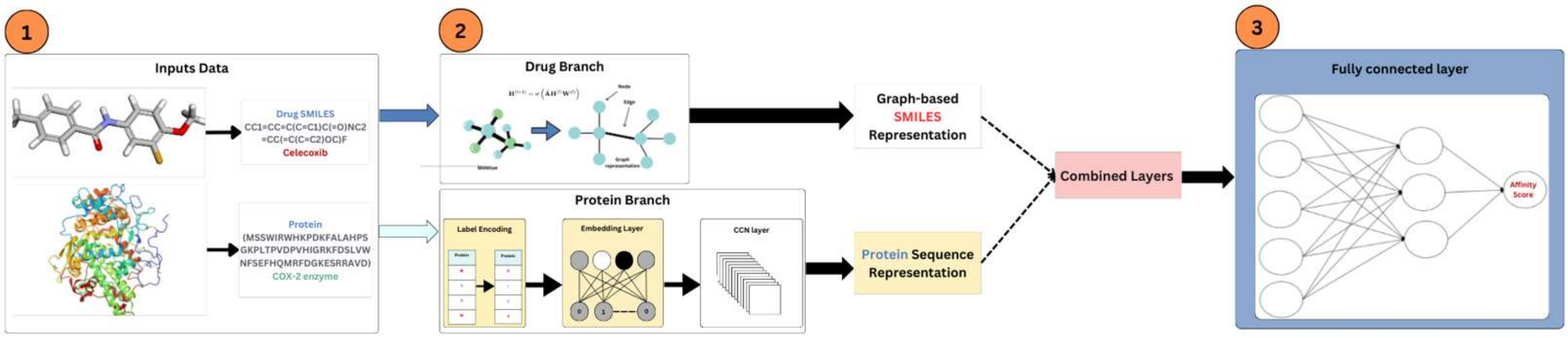
## Project Description:

The Graph DTAx project uses graph mining and deep neural networks, including a graph convolutional network (GCN), to improve the accuracy of drug-protein interaction predictions and identify potential medication side effects. This approach facilitates the efficient repurposing of existing drugs, speeding up treatment discovery and minimizing the need for new drug development.

## Objectives:

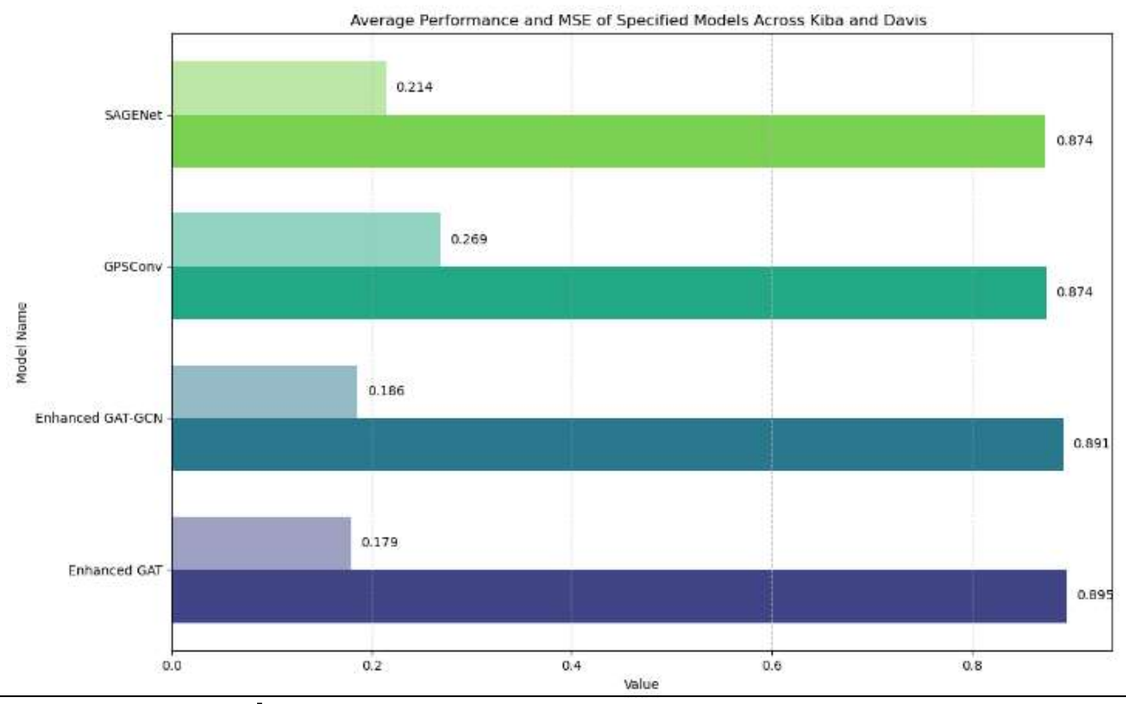
- Developed a larger dataset to ensure robust scalability and improved performance.
- Focused on boosting forecast accuracy through advanced algorithm enhancements.
- Enhanced the GraphDTAx model by integrating richer structural and functional data.
- Identified additional features and potential applications, significantly enhancing the model's utility in drug discovery.

## Methodology:

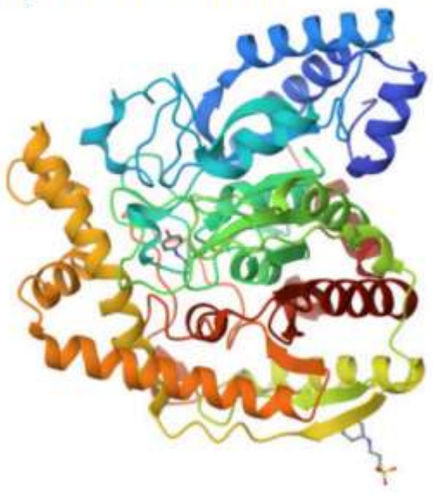



## Results:

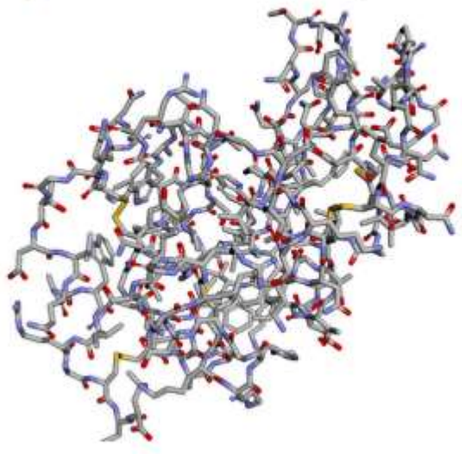
Explore the future of drug discovery with GraphDTAx, where cutting-edge machine learning models like Enhanced GAT, GPSConv, and SAGENet transform predictions of drug-protein interactions, trained on diverse datasets using advanced GPU technology. These models are rigorously evaluated over 1000 epochs with metrics like MSE and Concordance Index, demonstrating high accuracy and providing valuable insights for future advancements.



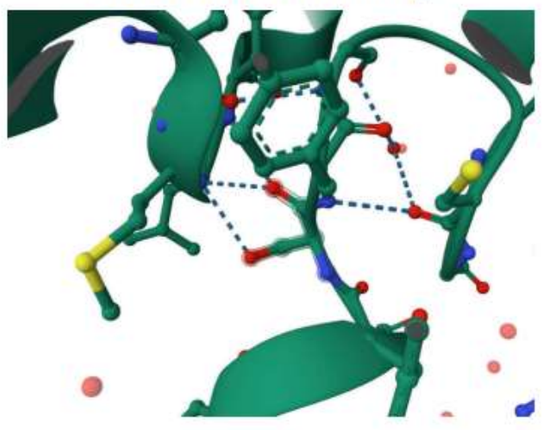

**A) Protein Name: COX-2**



**B) Drug Name: Acetaminophen Tylenol**



**C) Interaction Results: Affinity Score (IC50): 113 µM, binds with low affinity**



## Tools:

jupyter

Bio.PDB

RCSB PDB
PROTEIN DATA BANK