Abstract - Early Drug Discovery using AI

The traditional drug discovery process is often hindered by high costs, extended timelines, and low clinical success rates.

This research proposes a comprehensive, AI-driven framework to enhance early-stage drug discovery by leveraging advanced deep learning techniques.

The framework integrates Protein-Protein Interaction (PPI) networks with Graph Convolutional Networks (GCNs) for accurate target identification.

Hit identification is achieved using 3D-Convolutional Neural Networks (3D-CNNs), while Generative Adversarial Networks (GANs) contribute to de novo compound generation.

Lead optimization is performed using Reinforcement Learning (RL) and Deep-Q Learning to refine efficacy and reduce toxicity.

Additionally, Recurrent Neural Networks (RNNs) are utilized for predicting ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) properties, ensuring pharmacokinetic viability.

A user-friendly interface facilitates seamless interaction with the models, enabling data input, visualization, and analysis.

The proposed system demonstrates significant improvements in scalability, efficiency, and predictive accuracy, offering a promising direction for cost-effective and clinically successful drug development.