Title: ***Graph Neural Networks for Drug Discovery***

Section 1: Introduction

Graph Neural Networks (GNNs) have emerged as powerful tools for learning on graph-structured data. In recent years, their application to drug discovery has accelerated due to their ability to model molecular interactions effectively.

Section 2: Methodologies

Several GNN architectures have been developed for molecular property prediction:

- Graph Convolutional Networks (GCNs)
- Graph Attention Networks (GATs)
- Message Passing Neural Networks (MPNNs)

Each has unique strengths in capturing local vs. global chemical patterns.

Section 3: Datasets Used

Popular benchmark datasets for drug-related GNN research include:

- MoleculeNet (e.g., Tox21, HIV)
- ZINC dataset
- QM9 dataset for quantum property prediction

Section 4: Performance Metrics

Evaluation is often done using AUC-ROC, RMSE, or MAE depending on the task. GATs have shown strong performance on classification tasks, while MPNNs perform well on regression tasks.

Section 5: Conclusion

GNNs offer a promising future for AI-assisted drug discovery, especially when combined with domain-specific priors and 3D structural data.