Title: Graph Neural Networks in Drug Discovery

Section: Methodologies

- GCNs (Graph Convolutional Networks)

- GATs (Graph Attention Networks)

- Message Passing Neural Networks (MPNNs)

Section: Datasets

- ZINC dataset

- MoleculeNet

- PubChem BioAssay

Section: Benchmarks

- ROC-AUC scores

- RMSE on solubility prediction