Graph Neural Networks for Drug Discovery

Methodologies

This section explores various graph neural network architectures such as GCN, GAT, and MPNN applied to molecular property prediction.

Datasets

Common datasets include QM9, MoleculeNet, and PubChem. These datasets provide labeled molecules for training and evaluation.

Performance Benchmarks

Recent models achieved over 90% accuracy on benchmark tasks such as toxicity prediction and solubility estimation.