

# Graph Neural Networks for Drug Discovery

## 1. Introduction

Graph Neural Networks (GNNs) have emerged as a powerful tool in deep learning for drug discovery.

## 2. Methodologies

Several types of GNN architectures are used including GCN, GAT, and GraphSAGE.

### 2.1 Graph Convolutional Networks (GCN)

GCN applies convolution operations over graph nodes for feature learning.

### 2.2 Graph Attention Networks (GAT)

GAT uses attention mechanisms to assign weights to neighbor nodes.

## 3. Datasets

Common datasets used include PubChem, ChEMBL, and MoleculeNet.

## 4. Performance Benchmarks

We evaluate models based on AUC, accuracy, and RMSE across datasets.

## 5. Applications

Applications include target prediction, toxicity classification, and molecular property prediction.