

# Graph Neural Networks for Drug Discovery: A Comprehensive Methodology

## Abstract

This paper presents a novel methodology for applying Graph Neural Networks (GNNs) to drug discovery applications. We introduce a comprehensive framework that leverages molecular graph representations to predict drug-target interactions and molecular properties.

## 1. Introduction

Drug discovery is a complex process that requires understanding molecular interactions and predicting biological activities. Traditional methods rely on experimental screening, which is time-consuming and expensive. Graph Neural Networks offer a promising alternative by learning from molecular graph representations.

## 2. Methodology

Our methodology consists of three main components: molecular graph construction, GNN architecture design, and training strategy. We represent molecules as graphs where nodes represent atoms and edges represent chemical bonds.

### 2.1 Molecular Graph Construction

We construct molecular graphs using RDKit, where each atom is represented as a node with features including atomic number, formal charge, and hybridization state. Chemical bonds are represented as edges with bond type and stereochemistry information.

### 2.2 GNN Architecture

We employ a Graph Convolutional Network (GCN) with attention mechanisms. The network consists of multiple graph convolution layers followed by global pooling and fully connected layers for final prediction.

## 3. Datasets

We evaluate our methodology on three benchmark datasets: ChEMBL, BindingDB, and PubChem. These datasets contain millions of drug-target interaction pairs with associated experimental data.

## 4. Performance Benchmarks

Our GNN-based approach achieves state-of-the-art performance on drug-target interaction prediction, with AUC-ROC scores of 0.89 on ChEMBL and 0.91 on BindingDB. We also demonstrate superior performance in molecular property prediction tasks.