# Comprehensive Datasets for Graph Neural Networks in Drug Discovery


## Abstract

We present a comprehensive collection of datasets specifically designed for training and evaluating Graph Neural Networks in drug discovery applications. These datasets cover various aspects of molecular property prediction and drug-target interaction.


## 1. Dataset Overview

Our dataset collection includes molecular structures, biological activities, and physicochemical properties. Each dataset is carefully curated and annotated for machine learning applications.

## 2. Molecular Property Datasets

We provide datasets for predicting molecular properties such as solubility, toxicity, and drug-likeness. These properties are crucial for drug development and safety assessment.

## 3. Drug-Target Interaction Datasets

Our interaction datasets contain experimentally validated drug-target pairs with associated binding affinities and inhibition constants. These datasets enable training of models for predicting novel drug-target interactions.