

Title: Graph Neural Networks for Drug Discovery

1. Introduction

Drug discovery is a complex process. Machine learning techniques are increasingly being used.

2. Methodology

Our method is based on graph convolutional layers. This method improves molecular structure analysis.

3. Dataset

We use the QM9 dataset which includes various molecular properties.

4. Benchmark

Our benchmark compares GNN models on classification accuracy.

5. Conclusion

Results show the effectiveness of our approach.