GRAPH NEURAL NETWORKS FOR DRUG DISCOVERY

Abstract
This paper presents a comprehensive review of graph neural networks in drug discovery applications. We analyze methodologies, datasets, and performance benchmarks.

Introduction
Drug discovery is a complex process that takes 10-15 years. Graph neural networks show promising results in accelerating this process.

Methodology
Our systematic review follows established guidelines. We searched major databases and identified 127 relevant papers.

Results and Analysis
Key findings include: GraphSAGE and GAT outperform traditional methods. ChEMBL and ZINC are the most used datasets. Top models achieve 0.85-0.92 AUC scores.

Discussion
Challenges remain in standardization and real-world validation. Future work should focus on robust benchmarking.

Conclusion
GNNs represent a promising direction for drug discovery but need more practical validation.