## Utilizing Self-Supervised Graph Neural Networks in De Novo Drug Discovery

Introduction and Background
Overview of Graph Neural Networks
Drug Discovery Challenges
Model Architecture and Self• Supervised Learning
GNN Architectures
Self• Supervised Learning Techniques
Property Prediction and Binding Affinity Estimation
Enhanced Prediction Techniques
Binding Affinity Estimation
Uncertainty Quantification
Incorporating Uncertainty Measures
Impact on Decision• Making

Active Learning Frameworks

Integration with GNNs

Prioritization Strategies

Case Studies and Future Directions

Successful Applications

Future Research Directions