Advances in Graph Neural Networks for Drug Discovery

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3. Methodology

In this section, we describe our proposed GNN architecture which is based on Graph Attention Networks (GAT).

We evaluated the performance using datasets such as PubChem BioAssay and DrugBank.

Our model achieved 87% ROC-AUC on the test set, outperforming previous baselines.

The training was done on standard drug-target interaction benchmarks.