To compare the performance of GNN to conventional neural network, we built multilayer perceptrons (MLPs) using data from HepG2 cell viability assay (mentioned in section 3.1 and 3.2). The table below summarizes the comparison of model performance. We found that GNN outperforms MLP by a large margin. And this is true for all configurations of MLPs we implemented.

|  |  |  |  |
| --- | --- | --- | --- |
| Model name | Number of hidden layers | Number of neurons in each layer | Model AUROC and 95% CI |
| MLP | 1 | 50 | 0.75 ± 0.03 |
| MLP | 1 | 200 | 0.76 ± 0.03 |
| MLP | 1 | 500 | 0.76 ± 0.03 |
| MLP | 2 | 50, 50 | 0.74 ± 0.03 |
| MLP | 2 | 100, 50 | 0.74 ± 0.03 |
| GNN | - | - | 0.85 ± 0.02 |