



Astinova AI Platform

Molecular Interaction Transformer

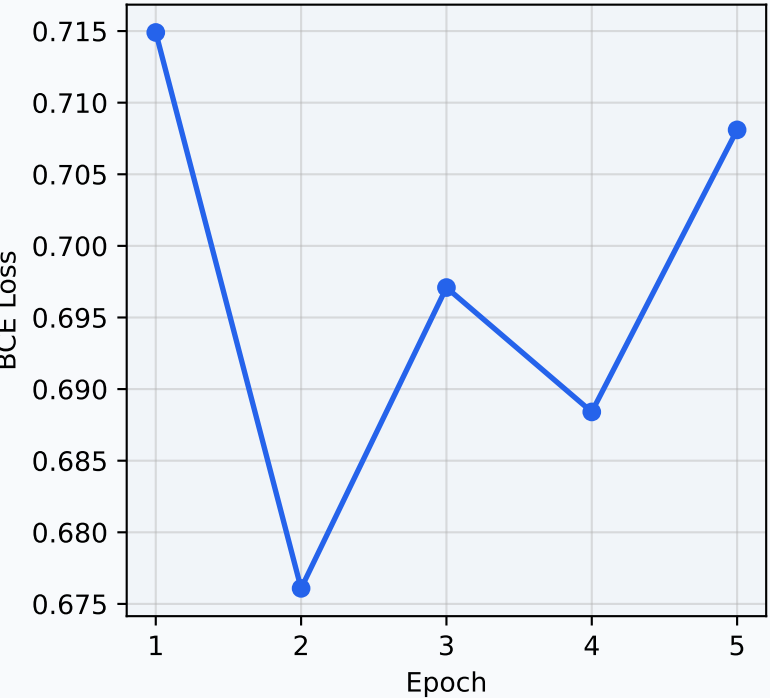
Drug-Target Interaction Prediction

```
Task:          BIOSNAP
  Epochs:       5
  Batch size:   16
Optimizer:  Adam (lr = 1e-4)
  Device:      CPU
```

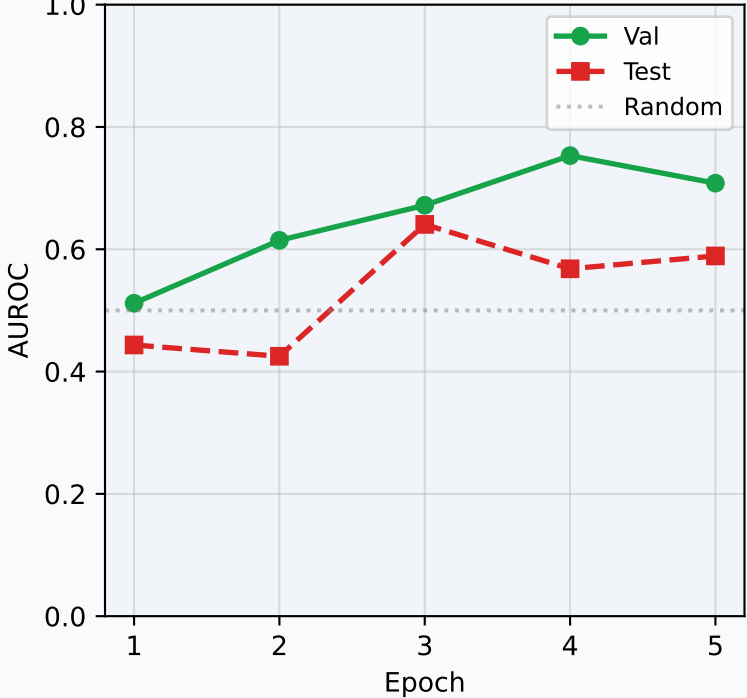
Training Results Summary

— Training Metrics (BIOSNAP)

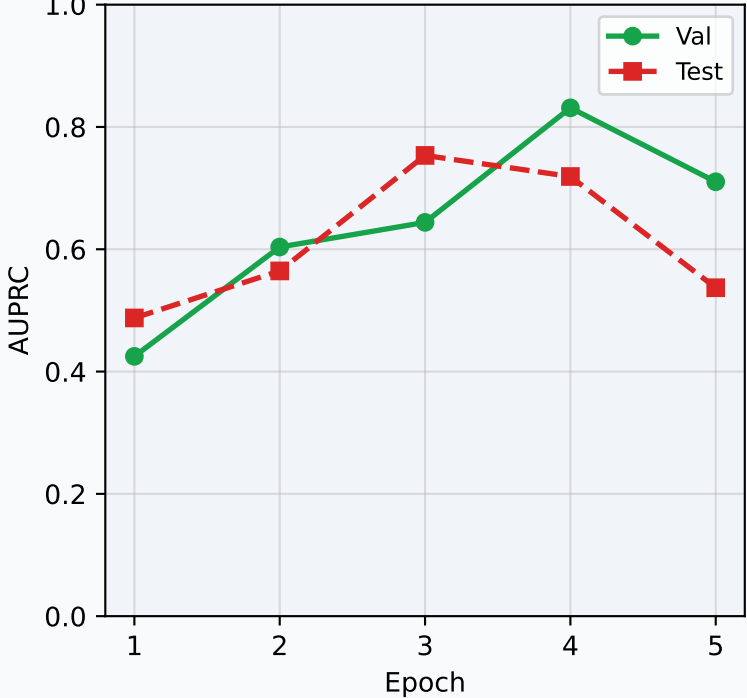
Training Loss



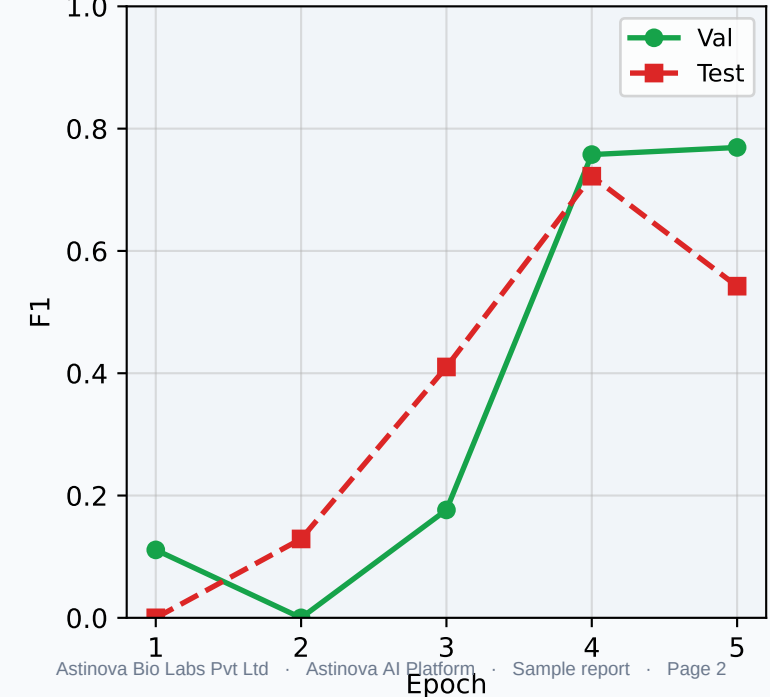
AUROC



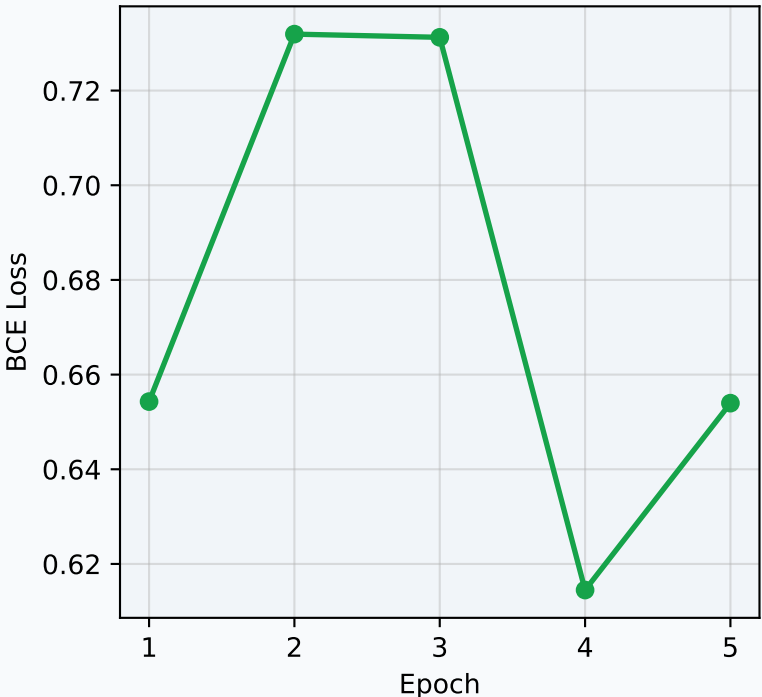
AUPRC



F1 Score



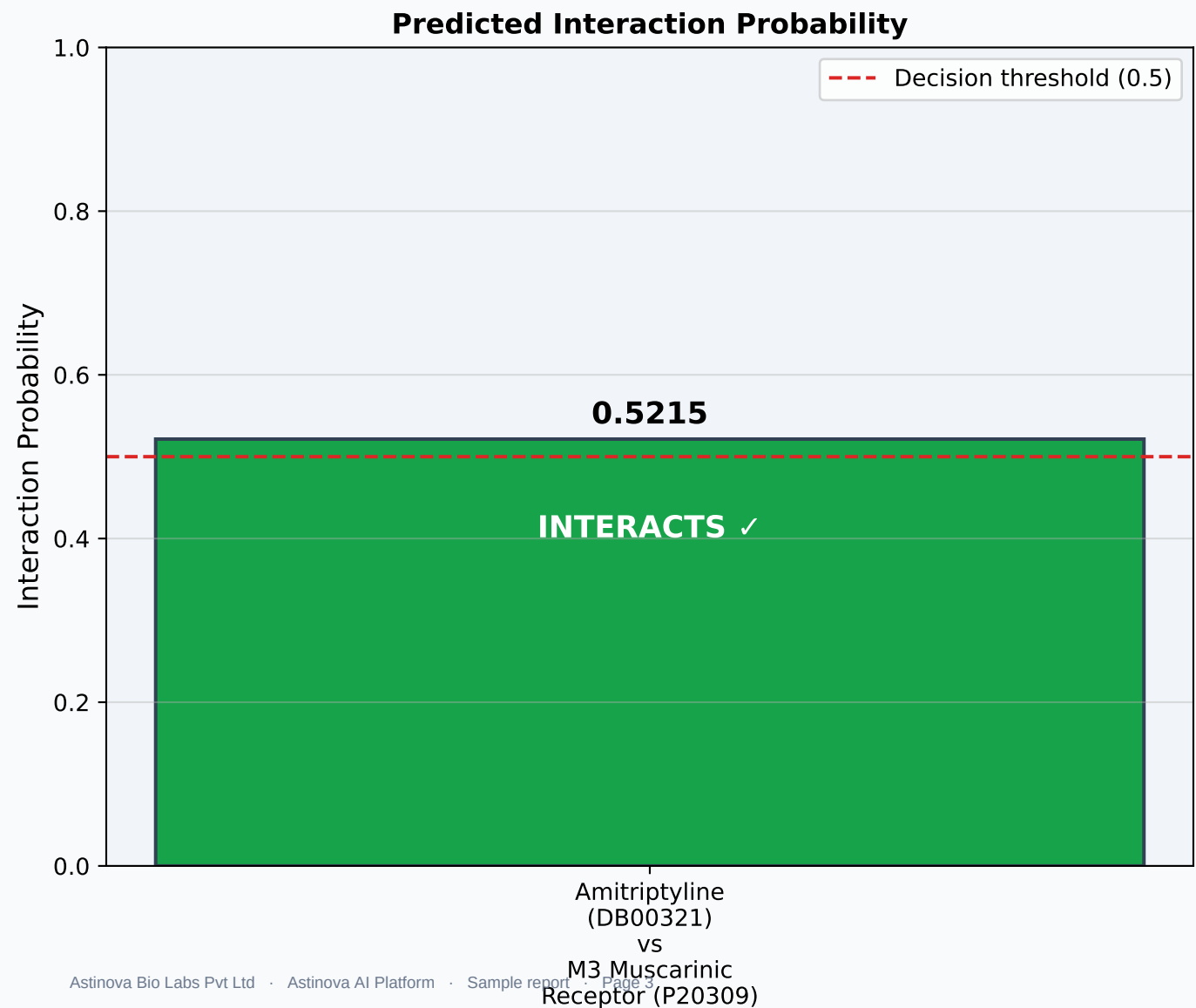
Validation Loss



Best Epoch Summary

Metric	Best Val	Epoch 4
AUROC	0.7531	0.5681
AUPRC	0.8313	0.7190
F1	0.7692	0.7222
Loss	0.6145	—

Drug-Target Interaction — Prediction Example



Example Details

Drug:	Amitriptyline (DB00321)
Drug class:	Tricyclic antidepressant
SMILES:	CN(C)CCC=C1C2=CC=CC=C2CCC2=CC=CC=C12
Target:	M3 Muscarinic Receptor
UniProt:	P20309
True label:	Interacts (1)
Predicted:	Interacts (1)
Probability:	0.5215
Correct:	Yes