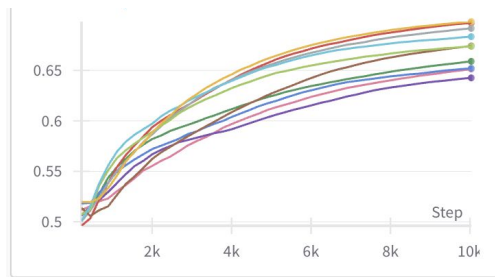


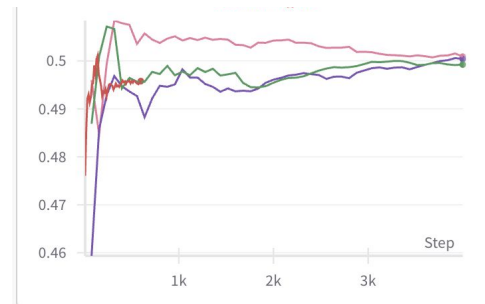
Past 2 Weeks

- Training models
 - Simple SMILES Transformer
 - Molformer (pretrained on PubChem & Zinc 1bil)
- Data
 - Mouse LD50 (35,000)
 - hERG IC50 (1,500)
- Type
 - Regression
 - Classification
 - Binary Classification

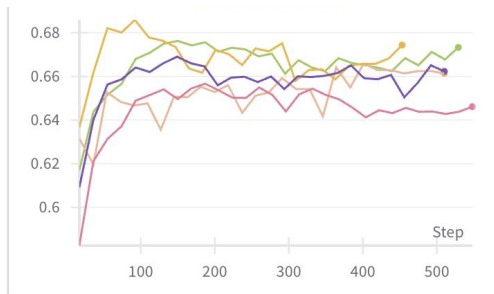
SST Mouse Classification (~0.66)



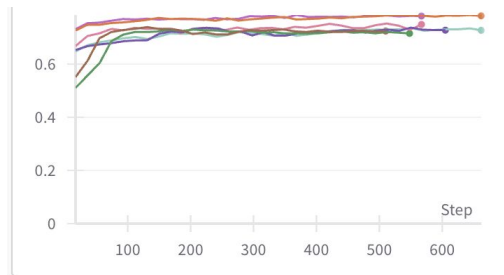
SST hERG Classification (~0.50)



MolForm hERG Classification (~0.66)



MolForm hERG Binary (~0.75)



Next 2 Weeks

- Keep trying other models
 - Multitask models
 - GNNs
- ConPlex
 - Predicts drug-target interactions
 - Check if predicted binding lines up with IC50 values

ConPlex

