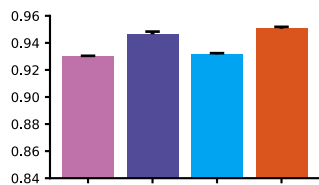


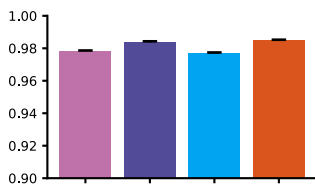
AUROC

A



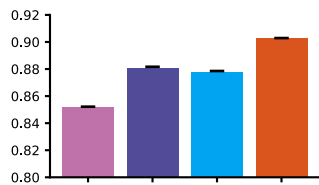
AUPRC

B

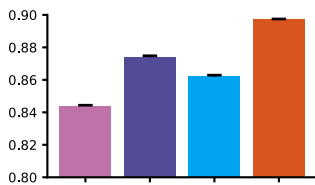


Training: 20% randomly selected pairs from ChEMBL
Test: The remaining pairs from ChEMBL

C

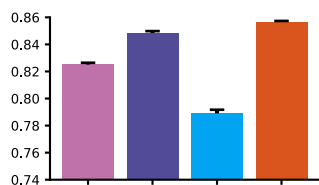


D

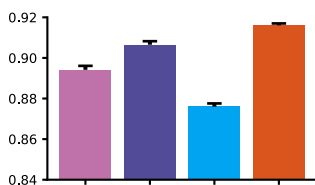


Training: Non-unique pairs from ChEMBL
Test: Unique pairs from ChEMBL

E



F



Training: ChEMBL
Test: BindingDB (overlaps with training data were removed)

SLNN

Random forest

DNN with conventional features

DeepCPI