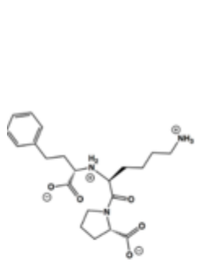
a

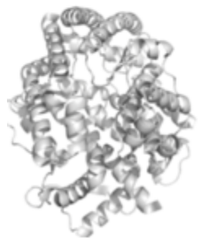


Drugs from DrugBank

Natural Compounds from NCFD

Pre-trained Chemical Embeddings

e.g., Mol2vec, VAE embedding
Siamese embedding



Novel Protein Targets

Pre-trained Protein Embeddings

e.g., ProtVec, Siamese embedding

Neural Network trained on Network-Derived Negatives

e.g., VecNet, VAENet, SiameseNet

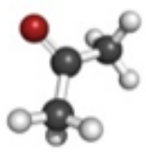
Select top-N pairs

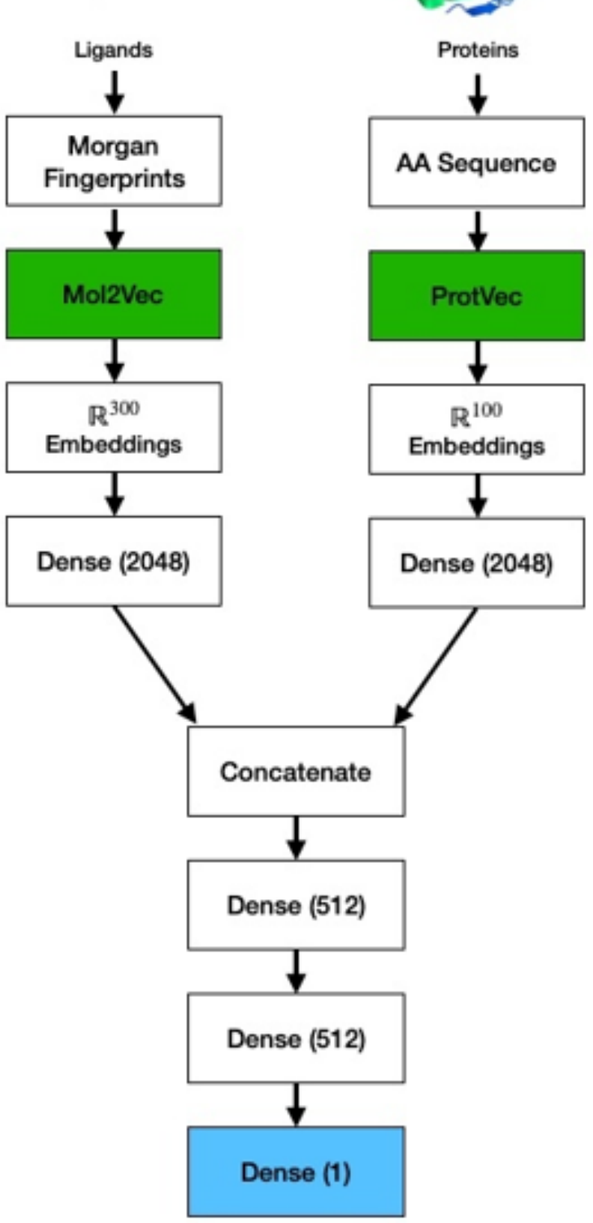
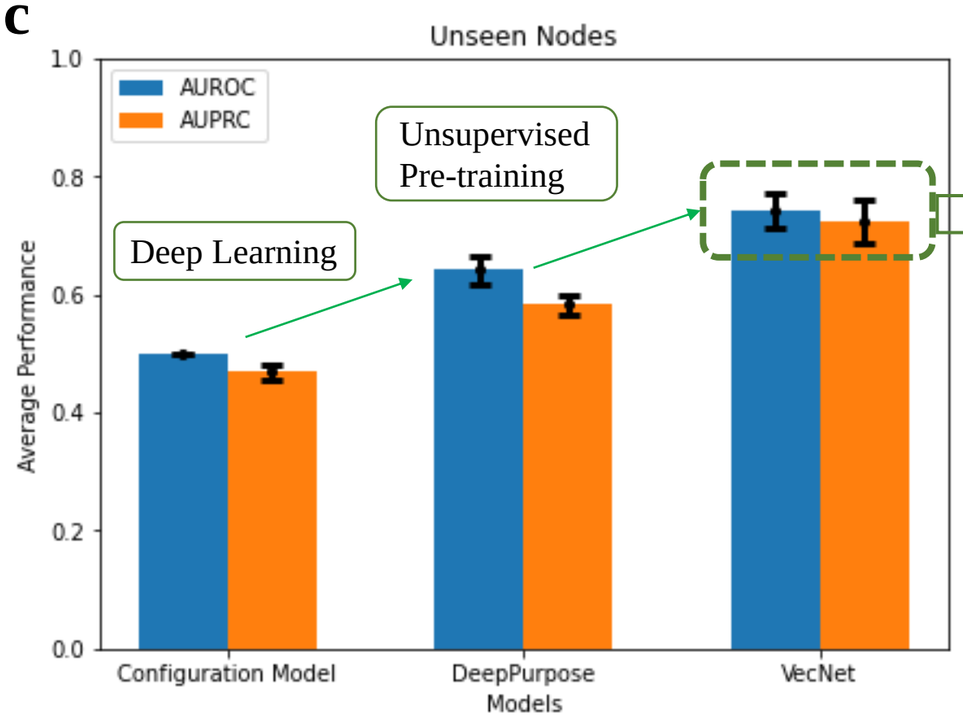
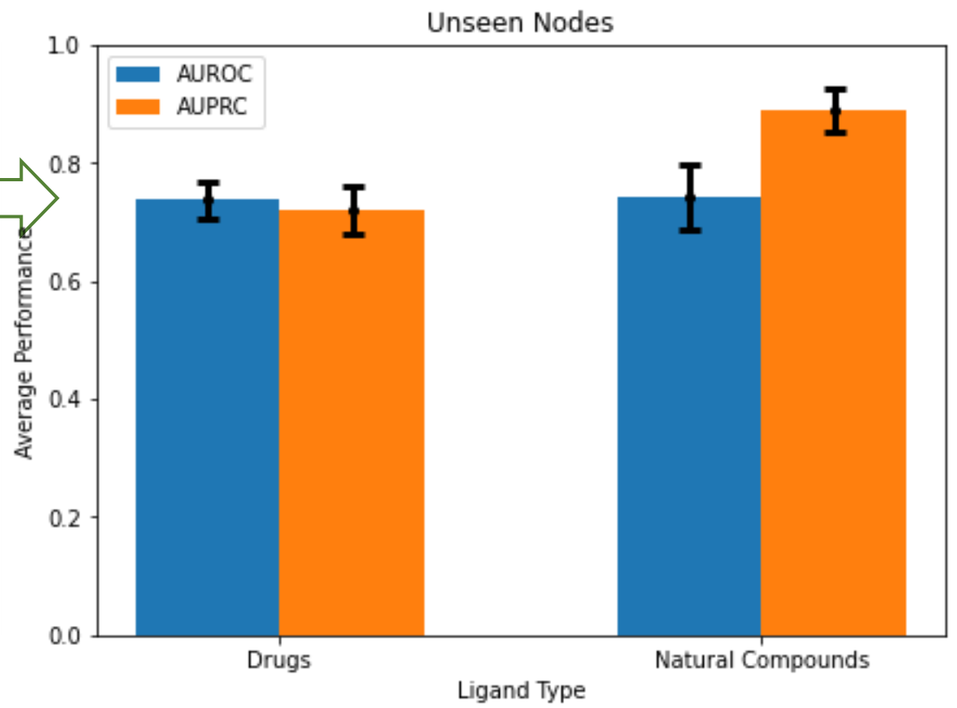
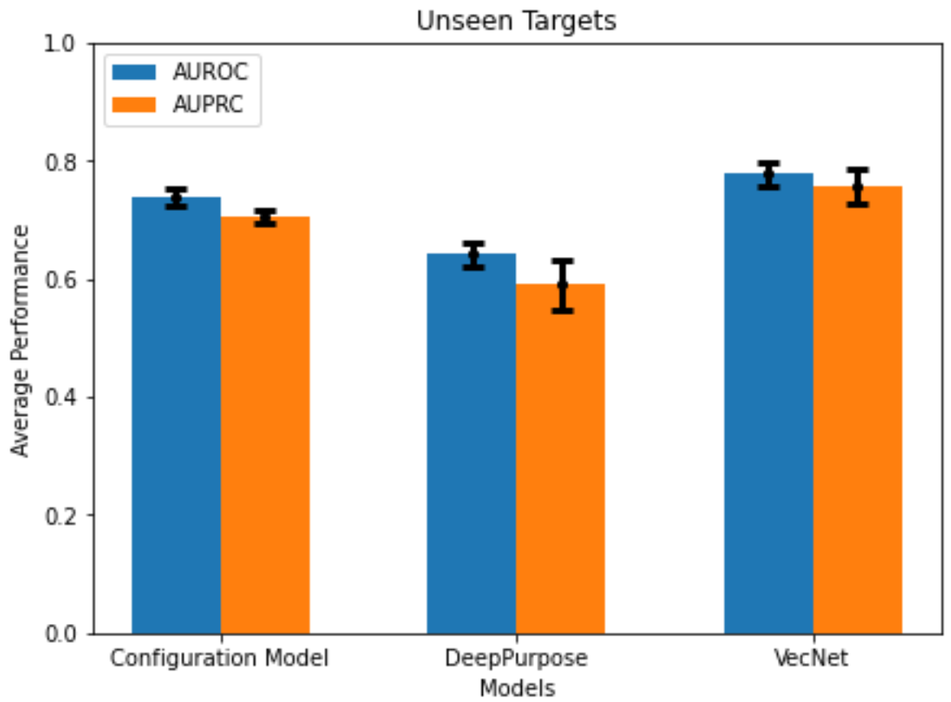
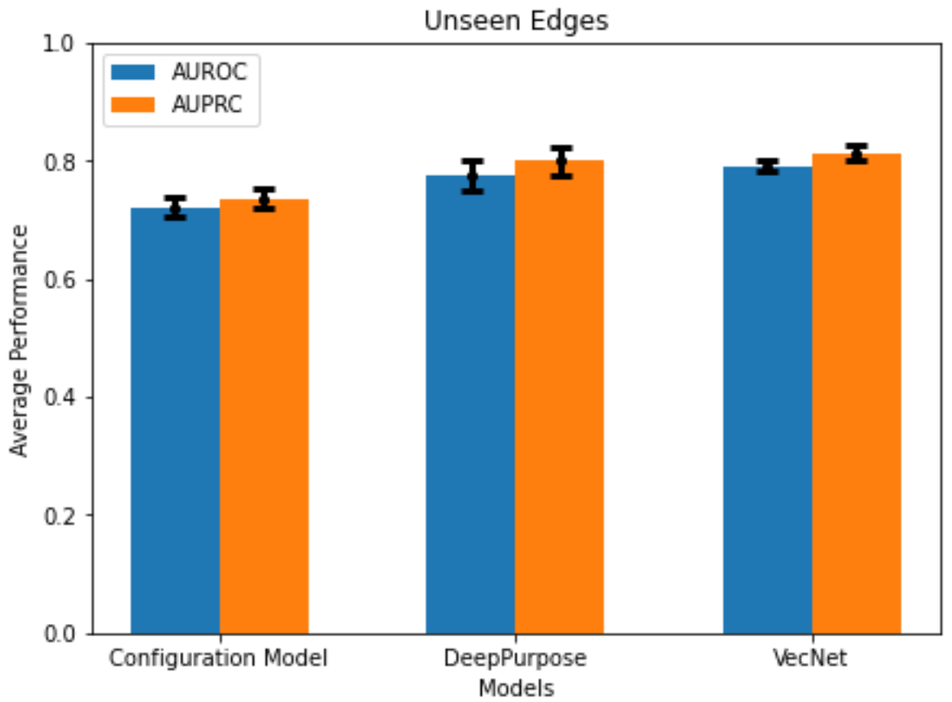
Blind Auto Docking and Thresholding

Pairs with binding affinity less than -1.75 kcal/mole are selected

Potential Ligands

b

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