Ranking model

A

1 (more active) or 0 (less active)

Classification model

Difference fingerprint
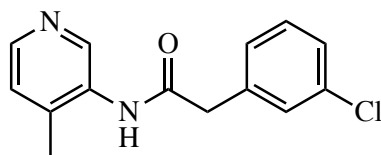
(-1 0 0 0 1 0 0 ...)

Pharmacophore fingerprint
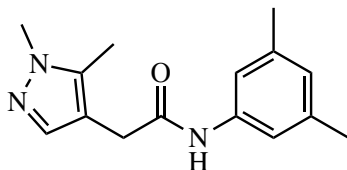
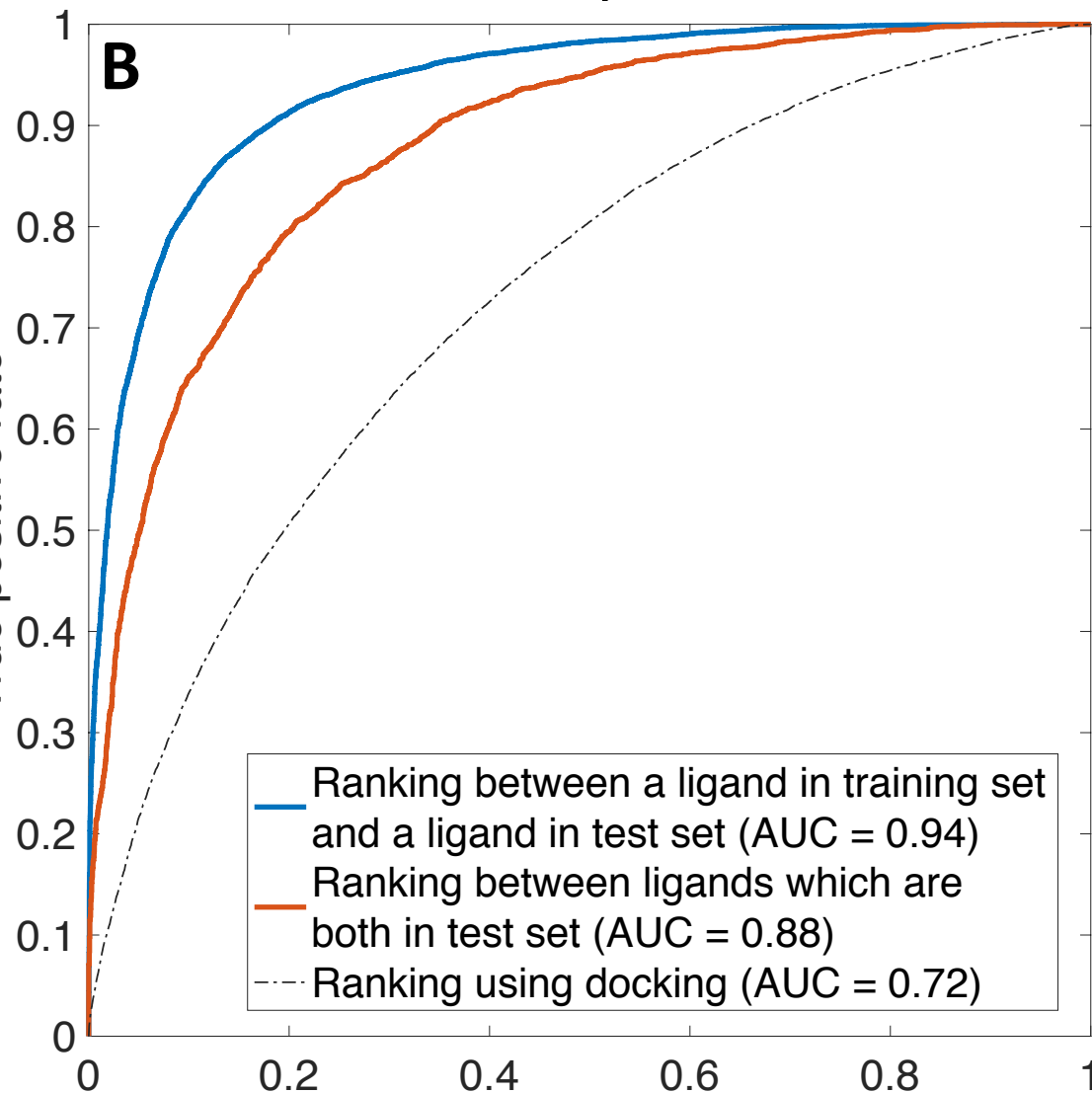(0 0 1 0 1 0 1 ...) - (1 0 1 0 0 0 1 ...)

Molecular structure

IC_{50} = 24.6 μM   Inactive

ROC model performance

B

Ranking between a ligand in training set and a ligand in test set (AUC = 0.94)
Ranking between ligands which are both in test set (AUC = 0.88)
Ranking using docking (AUC = 0.72)