

Recently, a new method for ligand based virtual screening was published. It uses pharmacophore fingerprints and statistical methods to create a pharmacophore model which is then used to predict the activity of ligands. In this thesis two possible enhancements of this method were examined. The first one is the removal of correlated pharmacophores, the second one is the utilization of larger pharmacophores (originally only 3-point pharmacophores were used). Both modifications were implemented along with necessary extension of the RDKit cheminformatics toolkit. Finally, both modifications were experimentally evaluated and compared to the original method. Based on the results, combination of the pharmacophore model with the fingerprint similarity was proposed as another modification and evaluated.