

Virtually all processes in living organisms are conducted by proteins. Proteins perform their function by binding to other proteins (protein-protein interactions) or small molecules – so called ligands (protein-ligand interactions). Active sites for protein-ligand interactions are pockets in protein structure where ligand can bind. Predicting of ligand binding sites is the first step to study and predict protein functions and structure based drug-design. In this thesis we reviewed current approaches for binding site prediction and proposed our own improvement. We have developed a novel pocket ranking function based on prediction model that predicts ligandability (ability to bind a ligand) of a given point inside of a pocket. Prediction is done considering only a local physicochemical and geometric properties derived from neighbourhood.