

Protein-ligand binding sites are positions on the protein structure where the protein interacts with other molecules. PrankWeb is a web server developed at MFF UK allowing prediction of such places. These predictions are essential in fields such as bioengineering and computational drug discovery. The goal of this thesis was to update this web server, i.e., replace old and unsupported components with new ones. Another goal was to extend the server architecture to enable the simple addition of modules for the postprocessing of the predicted binding sites. These modules can be implemented either on the client side in case of simple computations, or on the server side in case of complex computations. As part of the thesis, we have implemented a client module for computing the volume of active sites and a server module allowing the docking of small proteins into predicted binding sites. The thesis describes not only the interventions in the architecture but also provides a short introduction to the problem of protein-ligand binding sites and their prediction.