**Abstract**

Understanding the biological functions of proteins is a basal knowledge that contributes to advances in medicine, pharmaceutics, but also agriculture and even energy sectors. The ultimate goal of proteomic research is to describe functions of all protein complexes in cellular space and life time. Protein interaction patterns are, however, very complex and revealing these is a challenging and time-consuming scientific process. Studying interaction between proteins is related to the identification of an appropriate spatial conformation in which these proteins are interacting. These studies span from investigating interactions between two proteins up to exploring large multi-molecular complexes. Then the complexity becomes enormous and suitable visualization technology, which could aid the analytic workflow, does not exist to this date.

In our project we propose to investigate novel visualization techniques in order to fill this gap. These techniques will focus on effective visual explorations, comparisons and ranking of data obtained from algorithms for predicting 3D spatial conformations and protein-protein docking. Moreover, we extend the solutions for protein-protein docking to more general molecular complexes, where many molecules are mutually interacting – this process is called multidocking. Further we will integrate the proposed techniques into the visual analysis environment and based on the features of the highly structured input data, we will design a formalization of visual analysis systems in order to provide a systematic exploration of the visualization design space with respect to user tasks.

All proposed techniques will be designed in tight cooperation with the proteomic domain experts involved in the project. The techniques will be then tested on data from their currently ongoing research on SMC complexes.

All proposed techniques will be integrated into the CAVER Analyst software tool. This visualization tool will serve also for fast prototyping of new ideas.