ABSTRACT

The structure prediction of proteins and their complexes using the UNRES coarse force field utilizing information from databases.

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The aim of my PhD thesis was to develop and refine tools for the structure prediction of proteins and their complexes with the coarse-grained UNRES force field using information from databases and results obtained by experimental methods.

During my research I actively participated in the 11th and 12th edition of the CASP (Critical Assessment of protein Structure Prediction) experiment, which allowed me to determine the prediction capabilities of the UNRES force field, and showed weaknesses in the methodology for protein structure prediction with using information from databases, which could be improved later.

The realization of the assumed goal I continued with the optimization of parameters responsible for the strength of the imposed restraints and investigation of how the restraints affect the process of the simulation and what impact on the results of the simulation has the quality of the utilized models.

Another step in the direction of achieving the aim assumed in this thesis was the development of a method for predicting the protein structure using information obtained from measurements of small-angle X-ray scattering (SAXS) experiment. The SAXS experiment is a method for investigating the structure of proteins in an aqueous environment, thus it is a very helpful tool as a results selection criterion, or as a narrowing of the searched conformational space of the simulated protein.

The final stage of my work was to participate in the creation of a web server to facilitate scientists from around the world carrying out coarse-grained simulations of proteins in the UNRES force field. The server also gives the possibility to use data from the SAXS experiment in simulations.