The aim of the project is to develop a new, efficient protocol of protein-complex structure prediction, which will enable us to examine both the structure and interactions in protein and peptide complexes, by using algorithms based on global search of the conformational space. For this purpose, the physics-based UNRES (UNited RESidue) force field, which is developed by Professor Adam Liwo group from University of Gdańsk in collaboration with Professor Harold Scheraga group at Cornell University, will be used. The UNRES force field has been recently significantly improved to enable us to examine both the structure of the proteins and their complexes and the mechanism of these processes.

For the purpose of the project, a variety of the cutting-edge methods will be used: methods based on the process of evolution, molecular dynamics (also called virtual microscope, because it enables us to observe movements of the matter on atomic levels) for investigation of the structures of the receptors interacting with ligands (such as drugs) and protein complexes. Proteins, as basic elements of the cells, in most cases need to form bigger aggregates (complexes) with other macromolecules - usually other proteins and nucleic acids, to take part in physiological processes. The presence of abnormal protein complexes, i.e. in form of aggregates is characteristic for many diseases, such as Alzheimer, Huntington and Parkinson disease. For this reason, design of a tool, which allows to perform efficient prediction of the structures of such complexes, is crucial to understand the mechanism of peptide and protein binding.

The UNRES force field is a unique tool, which uses a physics-based approach to protein simulations at a simplified coarse-grained level. UNRES-based approach has been distinguished by the assessors in blind-prediction of protein experiment (CASP) for outstanding prediction of two-domain protein. Moreover, UNRES performs well in the investigations of biological systems and processes, such as molecular chaperones, amyloid formation, signaling, etc. Recent implementation of periodic box to the UNRES enables us to simulate peptide and protein complexes more closely to the real conditions. Furthermore, the advancement of the computational tools and resources enable to perform highly-parallel simulations of large systems. For these reasons, a protocol of the prediction of the protein and peptide complexes, which will be developed in the project, can be used for studying the mechanisms of the diseases caused by abnormal formation of the protein complexes such as, e.g., amyloid formation.