Water is the key element of the life on Earth. The human body consists of about 60-70% of water. Dehydration leads to serious consequence to our organisms and may even lead to death. One of the key questions is what role does water play in our organisms. Is it only the milieu for the machinery of life or something more?

Proteins are one the major components of our body. They take part in muscle contraction, movement, transport of compounds in our body, defense against pathogens, and structure our body. Proteins are synthesized in a linear form, which then takes a tridimensional shape in the folding process. The interior of a protein is hydrophobic; however, in some proteins a water molecule can be found inside of the protein. Therefore, the following questions arise: Why does Nature place water inside protein molecules? What is the role of interior water? What function has water in protein folding? This project is an attempt at answering these questions. First we will determine how does water interact with single amino acid residues. Is the binding of water molecules strong? How fast are the water molecules exchanged with another partner? Then studies of the interactions of proteins with water will be carried out. Because it is extremely difficult to study this process experimentally, in this research project we will use computational methods. Additionally, the computational methods enable us to modify water properties and to determine those which are important for protein folding. We will use the simplified (coarse-grained) UNRES model which has been developed for over 20 years. This model has proved to be a powerful tool. We plan to further extend this model to include water molecules interacting with proteins.

Lipids are another important environment of the human body. The lipid molecules do not like to interact with water and they do not mix with water. Lipid molecules form bilayers, which separate cell interior from the outside as well as divide the cell into compartments. To function properly, cells have to communicate with the outer world. In the second part of this research project we will study how do the membrane proteins (immersed in lipid bilayers) function. How is the signal from the outer part of the cell passed to interior? How does a cell decide which substance should be uptaken? How do toxic proteins destroy the lipid bilayer? We will answer those question with use of computational tools and the UNRES model. In the first stage, we will study how do the amino-acid residues interact with lipids, then we will study how is the pore in the lipid bilayer formed. Finally, we will simulate the process of signal transduction through lipid membranes.