DESCRIPTION FOR THE GENERAL PUBLIC

With the birth of science, various scientific areas such as medicine, biology, chemistry, physics and psychology have been developed in the way to better understand, which kind of events within the human organism can influence the health and, therefore, the quality of life. What are the causes of different diseases and how to prevent and/or to cure them – these questions remain central for the broad scientific community also nowadays. Among many health distortions and diseases, wounds and mechanical injuries of different human tissues as skin, bones and muscles make up one of the most common reason for suffering and daily inconvenience for the affected people. That is why there is a strong need in understanding how these distortions can be treated most effectively in terms of time, money and possible side-effects, how a human body or its parts can recovery their normal functions, structure and, last but not least, their physical appearance. The scientific discipline dealing with such questions is called regenerative medicine. However, as most of the modern scientific areas, regenerative medicine cannot be developed alone without establishment of tight interconnections with almost every kind of natural sciences. Rational approaches in the regenerative medicine would be impossible to obtain without the application of biology, chemistry, physics, mathematics and statistics. First, the basics of tissues regeneration at different levels should be understood in order to effectively propose the optimized implementation of particular medical treatment. Tissue regeneration can be studied at several scales: from understanding of cellular behaviour though the processes carried out in cell organelles to gaining the knowledge about interactions of particular single molecules constituting the cells and, therefore, the tissues and organs. There is a huge amount of different biomolecules, each of which plays its own important role in the development of tissues. Revealing the basis of the interactions between them represents the first and one of the most crucial steps required for the creation of the complete picture of the events in regeneration. Which molecules are needed to speed up the regeneration? Which ones are responsible for the inflammation? How one can control all these processes at the molecular level? Answering these questions is the goal of many interdisciplinary studies.

The research project “Computational approaches to study protein-glycosaminoglycan interactions” aims to understand the basis of the events underlying an imporant processes of tissue regeneration by analysis of several particular biomolecular systems involved in such processes at atomic level. Regeneration and cellular behaviour are strongly affected by the events happening in the space between the cells, which is known as extracellular matrix. Two of the most abundant classes of the participants in those processes are proteins and saccharides. One of the especially important classes of the saccharides are glycosaminoglycans (GAGs): long charged and chemically variable molecules interacting with immunologically active proteins and growth factors. There are definitely less computational approaches established for these molecules than for other biomolecular classes, which makes their theoretical analysis quite challenging. Fortunately, in our previous work we demonstrated that molecular docking and molecular dynamics can be very promising tools in analysis of protein-GAG systems. Molecular docking approach allows the prediction of mutual disposition of interacting molecules if their experimentally obtained structures are available. This disposition defines the way the molecules can interact with each other. However, molecular docking gives only a single snapshot of such disposition overlooking the movements in the system. Therefore, the dynamics of the system can be studied by molecular dynamics method, which allows to track the movements of the system in time based on the knowledge of intial coordinates of all atoms in the system and the definition of the forces applied to these atoms. Knowing that, simple Newtonian laws are applied to calculate the evolution of the system. In this project, we are going to use mainly these two methods to characterize interactions between several subsets of proteins and GAGs. The results are going to contribute to the general knowledge on how these system function and how one can more accurately and more effectively model these systems. This knowledge, in turn, could be of a great importance for the development of new approaches in the regenerative medicine, which effects are directly related to the role of protein-GAG interactions in tissue regeneration. In a long term, this project would serve as a basic rationale for medical applications in practice.