The polysaccharides are fundamental components for many different biomaterials. Polysaccharides commonly exist in in microorganisms, as well as plant tissue and animal organisms. They are – together with proteins and polynucleotides – essential (bio)macromolecules what play important roles in cell–cell communication, cell adhesion, and molecular recognition in the immune system etc. Polysaccharides reveal many different biological functions affected by different chemical structures. For example the immunostimulatory activity of arabinogalactans extracted from *Chlorella pyrenoidosa* cells depends on their molecular weights. The antitumor activities of polysaccharides may be also related to their chain conformations, e.g., the triple helical conformation of the (1 → 3)-*β*-D-glucan backbone chain for some polysaccharides, such as lentinan and schphylizophyllan.

The structural changes in the polysaccharides have been widely investigated by the Atomic Force Microscopy (AFM) method. The polysaccharides reveal a particular wealth of conformational changes that could be controlled by external forces. The force-induced conformational transitions in the pyranose ring in saccharides depend generally on the presence of axially oriented terminal groups. Despite many studies in this area there are still many questions about the potential physiological significance of such force-induced transitions. The enforced conformational transitions can moderate the interaction of polysaccharides with a variety of other molecules in vivo. The studies of the force-induced conformational changes that occur in the sugar rings of the anionic glycosaminoglycans family (AGAG), i.e., the dermochondans suggest that the nanomechanics of that conformational transitions may play a role in directly controlling macroscopic tissue properties. Understanding of such functions may allow polysaccharides to be used in many nanotechnology applications including sensors and advanced materials. However, polysaccharides may have also the complicated hyper branched structure and are usually composed of various types of monosaccharides linked with different glycosidic bonds. In consequence, the precise characterization of the chemical structures and chain conformations of polysaccharides is not an easy task. Similarly, for the same reasons the proper interpretation of the AFM experimental results is quite difficult, especially for hetero polysaccharides. In this case, different conformational transitions can take place under the same external force and it can be manifested on the force-extension curve in different ways. Molecular insights on the origins of mechanical responses can be inferred from simulations based on theoretical methods. The theoretical simulations of AFM experiments provide the qualitative and quantitative information about the mechanical properties of biological and/or synthetic macromolecules.

In this project we will use the recently proposed EGO (Enforced Geometry Optimization) approach as well as the commonly used CGO (Constrained Geometry Optimization) method and the molecular dynamics to simulate the effect of the external forces acting on the single oligosaccharide chains. We will investigate the mechanism of the enforced conformational changes in the selected bio oligosaccharides. The crucial goal of this project is to understand the relationships between structural and mechanical properties of biopoly/(oligo)mers at an atomic level. The knowledge gained from proposed research in future can be used for elucidating basic phenomena such as: molecular recognition that mediates interactions between proteins and sugars, what is fundamental to all biology.