The phenomenon of structure modulation is relatively well known in small molecule crystallography, however its discovery in macromolecular protein crystals was an unexpected event. The physical manifestation of this phenomenon is observation on diffraction patterns of additional reflections between the main Bragg peaks. As a result of modulation, the translational symmetry of the crystal is disturbed in the three-dimensional space with periodicity restored only in higher-dimensional space. This requires the use of specialized multi-dimensional analysis for correct indexing of the diffraction image and structure description. The modulation of the structure can be related to both periodic changes in the coordinates of atoms from the positions determined by spatial symmetry of the cell, as well as periodic occupancy changes of the given crystallographic position. The existing procedures of solving and refinement of structures routinely used in protein crystallography are not suitable for conducting a complex analysis of modulated structures. Resignation from a multidimensional approach determine commensurateness of modulation, in which the translational order is restored after a certain, total number of elementary cells. The structure should then be considered in the extended supercell, which is a significant increase in the number of parameters in the case of complex protein structures and allows the construction of only an approximate model. The lack of appropriate tools for meticulous analysis of macromolecular modulated structures causes serious problems with proper indexing and processing of diffraction data, and then building a complete, good-quality structure model with satisfactory parameters. For incommensurately modulated structures, existing software limitations allows to use only supercell approach. Scientific significance of this project is connected with development of a new software dedicated to structure analysis of incommensurately modulated macromolecular crystal. Complete rejection of periodicity assumption and description of macromolecular structure in superspace will be innovative and pioneering step for better understanding of modulated protein systems.

So far, it has been possible to perform a full structural analysis for only a few modulated protein crystals. The first successfully solved and refined modulated protein crystal structures belongs to Hyp-1, protein identified in St. John's wort herb, in complex with a fluorescent ligand ANS. Depending on the choice of crystallization conditions, the Hyp-1/ANS protein complexes may form crystals with a seven- or nine-fold modulation of the structure along the c direction of the C2 space group. The aim of the project is a detailed analysis of the diffraction data from Hyp-1 / ANS crystals and methodical description and refinement of the structure in a multidimensional space. The original software implemented in the Matlab environment will be used to refine the structure. The resignation from the simplified assumption of modulation commensurateness as well as introduction of additional corrections taking into account the disorder in the structure will lead to receiving new protein models and improving their discrepancy indices. Prepared package will then be extended with additional modules enabling an innovative approach to the analysis of macromolecular modulated and shared to other users.