Ribonucleic acid (RNA) molecules are essential ”building blocks” of life at the molecular level and they play key roles in living organisms. RNAs transmit genetic information from DNA to synthesize proteins in cells. They are also capable of catalyzing the chemical reaction as enzymes. It has also been discovered that RNA molecules perform many regulatory functions. They can turn on and off or regulate processes carried out by other biological molecules. RNA molecules are also frequently synthesized for their practical application, for example in medicine as candidates for a new generation of drugs, in biotechnology as biosensors for the detection of chemical molecules, or in nanotechnology for the formation of new nanoparticles and nanomaterials.

While RNA molecules can be isolated and analyzed in test tubes, in cells they do not act alone. In fact, the cellular and biochemical functions of most RNA molecules are critically dependent on their interactions with protein molecules, and on the formation of RNA-protein macromolecular complexes. Thus, the understanding of the molecular basis of RNA functions is incomplete without taking into account their protein partners. In order to understand RNA best, we have to study the structure and dynamics of RNA-protein complexes.

Unfortunately, experimental determination of RNA-protein complex structures is very difficult, mostly because RNA-protein assemblies are often very flexible and switch between different structures. Often we can perform various experiments to obtain a partial view of RNA-protein complex structure (e.g., a rough shape of the whole complex, or detailed information on some of its parts), but it is very difficult to determine the molecular detail of the entire system.

As part of this research project, we propose to develop new computer software for molecular modeling of RNA-protein complexes, which can use fragmentary and “incomplete” experimental data to determine RNA-protein complex structures more accurately than it is possible now. We will start with the existing prototypes of our computer programs SimRNP and PyRy3D and we will develop them to provide a new general-purpose software package to a wide community of users. The project will also involve a series of test to make sure that the new methods perform well (both alone and together). The new programs will be made freely available to the academic community, enabling their broad use.

As a key part of the project, we will carry out extensive experimental analyses to provide data for modeling of new structures, and to test the accuracy of these structural models. The project will be carried out by an interdisciplinary team of researchers, including computer programmers, researchers specializing in computer simulations and data analysis, and biochemists who analyze RNA molecules experimentally.

The expected results of this project will be of great importance for understanding the cellular processes that involve the action of RNA molecules, and in the future, they may find practical use in biotechnology and medicine. Results obtained with the use of the new computational methods will contribute to better understanding of the relationships between sequence, structure, and function of RNA and protein molecules.