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. The cellular and molecular functions of RNA molecules depend on their spatial structures, which in turn is encoded in RNA sequence. Interestingly - it often happens that the same RNA molecule can take two or more shapes and it can “switch” between different structures depending on the situation. This is how RNA molecules are adapted to function as “molecular switches”.

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. Therefore, computer-aided design of new RNA molecules with defined structure and function is crucial not only for understanding the molecular basis of biological processes but also to use this knowledge in practice.

Unfortunately, so far no accurate method has been developed for computer-aided design of RNA molecules in the context of 3D structures, which could take into account the ability of RNAs to fold into alternative structures and their ability to bind to each other in various ways. As part of the OPUS project, we propose to develop a new computational method, in which we intend to combine our existing software: SimRNA for RNA molecular modeling with the possibility of introducing "mutation" into the modeled sequence, and DesiRNA for designing RNA molecules of a given secondary structure, which allows RNA molecules to take alternative shapes and to bind to each other.

The project will include the development of computer software, its practical application, and the experimental testing of the results obtained. It will be implemented 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 basic biological processes that govern the action of RNA molecules, and in the future they may find practical use in biotechnology and medicine. The new computational method will contribute to better understanding of the relationships between sequence, structure, and function in RNA molecules; for instance we plan to use it to predict functions for newly discovered RNAs. New designed RNA molecules will be constructed and analyzed and will be made available for future applications. The new computer program will be made widely available to the academic community, with broad possibilities for its future use.