

Molecules of ribonucleic acid (RNA), alongside DNA and proteins, play crucial roles in biochemical processes that are present in living cells of all organisms, and they are essential elements of life at the molecular level. Many RNA molecules are necessary for cells to live. These molecules are used, among many areas, in medicine: e.g. the majority of currently applied antibiotics work in a way that kills bacteria by blocking the function of ribosomal RNA, which is in fact the molecule responsible for the synthesis of bacterial proteins. Studies on RNA create enormous prospects for both a better understanding of how all living organisms operate, as well as for modern medicine.

RNA molecules are chains composed of nucleic residues A, U, C, G, which are the basic "building blocks", similarly as in DNA. Unlike DNA, formed by two very long chains that bind to each other, forming one long helix, RNA molecules are shorter, consisting typically of single chains that are folded into complex shapes that combine relatively short helices and complex structural motifs. In RNA, residues A, U, C, G form not only canonical pairs C-G and A-U (in analogy to pairs C-G and A-T in DNA) but also many other interactions ("non-canonical" contacts).

In order to comprehensively understand the biology of the cell, it is necessary to determine and analyze the structures of RNA molecules and their resulting functions. The experimental determination of RNA structure and its interactions with other compounds is very difficult, time consuming and costly. An alternative is to use computational structure prediction methods. The aim of this project is to develop a new method used for computational modeling of the structure of RNA, in a way better than has been possible until now. Based on the previously created program SimRNA, we propose to introduce innovative ways to model non-canonical interactions between residues A, U, C, G in the RNA, which will allow for much better modeling of RNA structures and thus bring us closer to better prediction of the biological function of these molecules.