RNApolis – methods and algorithms to model and analyze the RNA structure

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The project aims to solve open problems arising in the area of structural bioinformatics of RNA molecules, connected to computational modelling of RNA structures, their analysis and quality evaluation.

Methods and algorithms created by us will contribute to generate RNA 3D models characterized by high-accuracy and resolution similar to that obtained by experimental methods (like crystallography or NMR). It will also facilitate an assessment of predicted RNA models as well as ranking of these models based on multiple criteria.

Currently used methods for modelling of RNA structures do not apply in the case of modelling large, complicated 3D structures. It remains troublesome to achieve high precision and resolution of models by computational methods as it is the case with the structures determined experimentally. In our research we will develop new methods and algorithms addressing current needs of molecular biologists and bioinformaticians that model RNA 3D structures. The methods will perform drawing upon the knowledge of RNA structures that is already collected in the databases as well as on the information obtained during the latest experimental methods of RNA chemistry and molecular biology.

Our undoubted advantages are: a long-standing experience in this scientific area, awareness of the complexity of this domain as well as our previous works that resulted in a number of already published and well recognized methods and computational tools dedicated to structures of RNA molecules, i.a. RNA FRABASE – a database of RNA structure data (*Nucl Acids Res 2008; BMC Bioinf 2010*), RNAComposer – a system for automated RNA 3D structure prediction (*Nucl Acids Res 2012*), RNApdbee – a system for RNA secondary structure annotation and pseudoknot classification (*Nucl Acids Res 2014*), MCQ4Structures – a torsional angle-based method for RNA structure quality evaluation (*CEJOR 2014*), RNAlyzer i RNAssess – systems for quality evaluation of RNA predicted models based on algebraic representation of structure (*Nucl Acids Res 2013; Nucl Acids Res 2015*). Our team members are experienced in computing science and bioinformatics, and they cooperate with researchers from chemistry and molecular biology of RNA. Such a wide specialization is our unquestionable asset, giving us unique on - a global scale - capabilities in the quality and complementarity of research and proposed solutions. By well constituted cooperation with molecular biology experimentalists, we will be able to process the data derived from enzymatic and chemical probing methods of RNA structures including SHAPE and spectrofluorometry.

Based on the above described experience, we plan to design new combinatorial models and their corresponding algorithms, that will increase the accuracy of predicted RNA structures. Our results will enrich the spectrum of methods that compose RNApolis – computational platform dedicated to RNA structures. Afterwards, selected methods will be integrated into our systems for modelling, analysis, searching and evaluation of RNA structures and RNA structure motifs.

Undoubtedly, the design of novel methods and algorithms to suport modeling of RNA 3D structures with high-accuracy will profoundly influence the structure-function relationship studies in all fields of RNA research. It will particularly concern the design of new methods for RNA-oriented diagnostics and therapy or generation of artificial RNAs for nanotechnology purposes.

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