Discovering the structure of RNA

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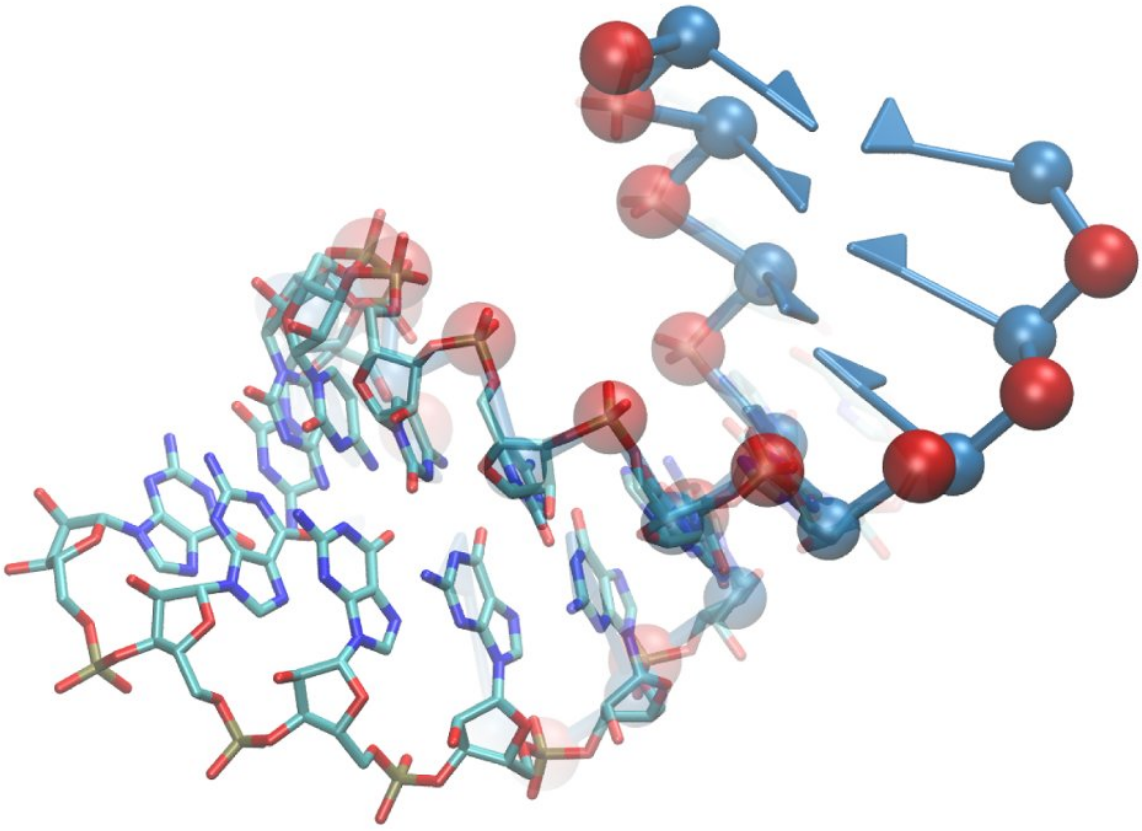

A new study develops an innovative simulation model able to efficiently predict

the conformation of ribonucleic acid molecules, opening up interesting opportunities for application and research Credit: Simon Poblete

RNA, or ribonucleic acid, plays an essential role in many biological processes, not only as messenger molecule with the task of transmitting genetic information from the nucleus to the cytoplasm for protein production, but also as protagonist of different and significantly important cellular mechanisms. In many of these, its structure plays a crucial role. Structure is different and characteristic for each RNA depending on the sequence of specific units, known as nucleotides. A research team at SISSA, led by Professor Giovanni Bussi, has developed a computerised simulation model that effectively predicts the three-dimensional conformation of the RNA filament starting from a sequence of nucleotides. The lead author of the study, just published in the journal *Nucleic Acids Research*, is SISSA researcher Simón Poblete. The work promises to have a significant impact in the research and application field.

"RNA structure is a crucial factor for many of its functions," explains Giovanni Bussi. "The experimental determination of RNA structures may take years, which is why there is great interest in developing methods to predict its structure. Until today, predictive models have concentrated primarily on the study of RNA parts which form double helices. However, the RNA filament can take specific and complex conformations governed by the so-called 'non-canonical' interactions, which are very different from those predicted by Watson-Crick's double helix model for DNA."

Current simulation models, says Bussi, "work very well. Starting from one sequence, they are able to envisage a variety of possible structures. The problem is that they are unable to tell which is the right structure

among many. Our model, which uses a simplified representation of RNA and has been designed explicitly to predict non-canonical interactions, has proven very efficient in this regard." To test its quality, researchers have used it to predict the structure of RNA molecules whose three-dimensional conformation is known, starting from the knowledge of the sequence alone. "Comparing our predictions with known structures, we have understood that our approach really works," confirms Giovanni Bussi.

This could shed light on the relationship between the structure and function of RNA. Bussi says, "RNA is particularly interesting for its practical implications; once an RNA molecule has been identified, as many molecules as desired can be obtained with little effort and identical to the first one by means of a fast and low-cost replication process. If, for example, we were able to find the RNA molecule able to trigger precise processes within the organism with important therapeutic effects due to its specific structure, this would open up truly unheard-of prospects."

More information: Simón Poblete et al, A nucleobase-centered coarse-grained representation for structure prediction of RNA motifs, *Nucleic Acids Research* (2017). DOI: 10.1093/nar/gkx1269

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