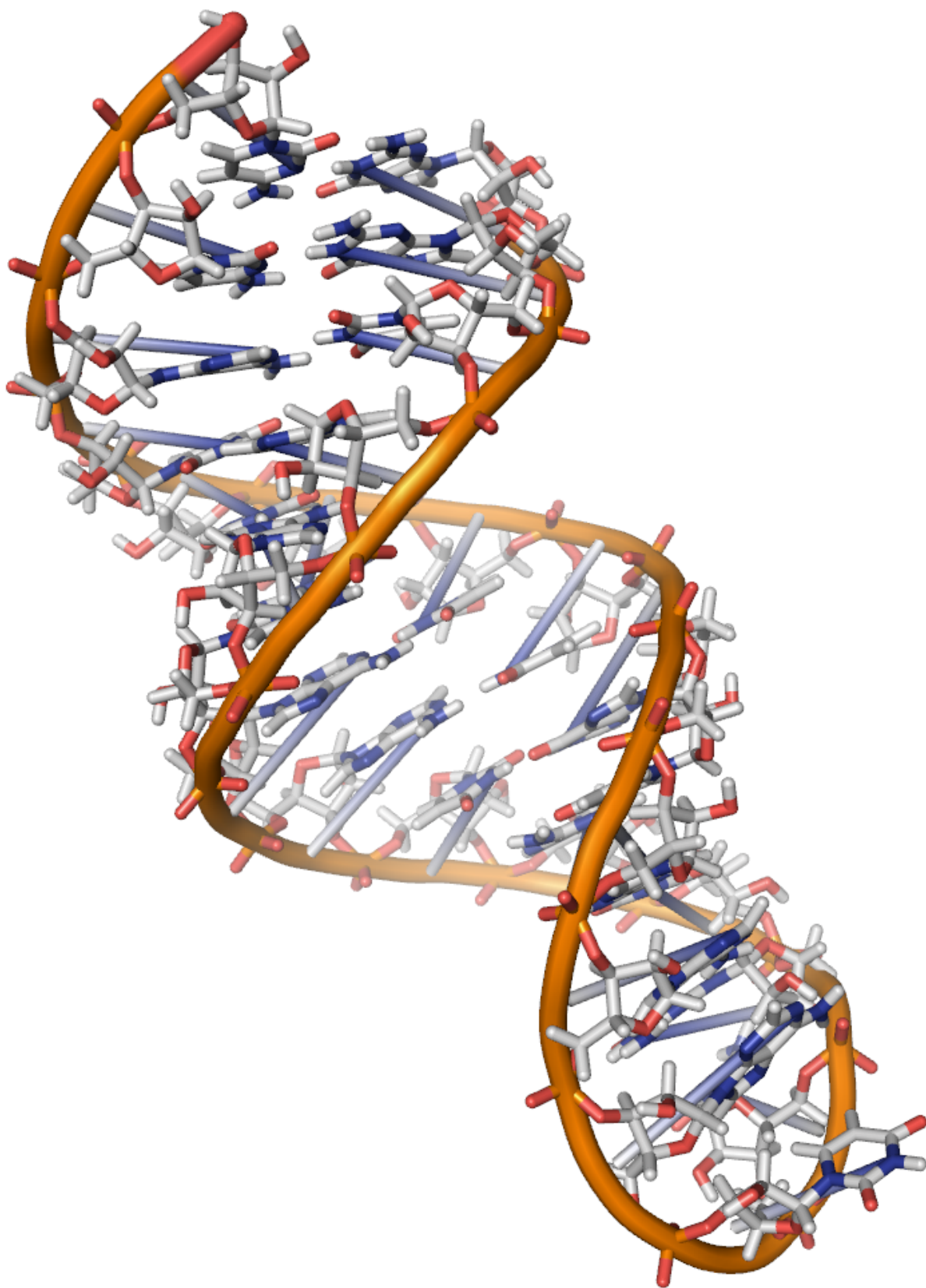


# Researchers develop simplified model of RNA validation

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RNA. Credit: Luuva/Wikimedia Commons

A group from the International School for Advanced Studies (SISSA) in Trieste has developed a faster and simpler method requiring modest resources for validating physical models of RNA used in molecular dynamics. These models are essential for computer simulations of RNA, one of the most important macromolecules of life. The method also helps define areas of improvement for increasing accuracy of the models. The study was published in the *Journal of Physical Chemistry Letters*.

Imagine having to rent a car by choosing from a catalog with nothing but photos: no make or model, no data sheet. You have specific requirements, however. You need a sturdy car suitable for rough terrain and steep inclines. To better understand which car would be most suitable for your needs, you would create a hypothetical model of the vehicle in your mind based on its appearance and your prior knowledge of cars. The hypothesized model would tell you if the image you see corresponds to a small city car, a sports car or an SUV, and this would be the basis of your choice. Driving it would tell you if your assumptions were right or wrong.

Scientists like SISSA Professor Giovanni Bussi are doing something similar in their study of RNA in [molecular dynamics](#). "We study RNA through computer simulations. We start from the structure of the molecule, which is described in a precise way by experimental measurements, kind of like the car photos in the example," says Bussi. "The structure, being the result of experimental observation, is accurate within a good approximation. The real issue is with the physical models."

It is like holding a three-dimensional model of a molecule. In order to experiment, even virtually, you must know how the different parts of the molecule move together, how they interact, how the structure can deform. This information makes up the so-called 'physical' model. "The problem is that the assumptions the model is based on are not always verified or easily verifiable," says Bussi. "There is a risk that the model will eventually prove wrong, that it does not correctly describe the behavior of the molecule, which means results based on these simulations may be unreliable."

## **Smart Strategies**

Molecular dynamics is used for other types of molecules besides RNA. "For example, David Shaw and his group have done a tremendous job of validating physical models of proteins, which has allowed us to do some serious clean-up in the field."

Works like this require a lot of time and powerful computer equipment, however, as it means painstakingly examining each individual model before developing it and testing it in its complete form. This can mean several months of computing time. "Unfortunately, no data exists for RNA at present," notes Bussi. For this reason, he and his team sought a viable solution by developing a "smart" methodology for validating RNA templates.

"We do not do extensive analysis like Shaw did for proteins, but we adopted strategies to reduce complexity and calculation time, while preserving accuracy in our results." How well do the current RNA physical models measure up in these analyses? "Not well, unfortunately. The model we tested, which was supposed to be one of the best in the literature according to tests made by others, does not allow us to make correct predictions on the structure of an RNA molecule." Back to the drawing board? "I would not be so drastic. There is no need to destroy all

that has been done so far. The important thing is to work on improving the current models. The value of our method is that it indicates where and how the model is wrong in order to provide solutions on how to improve it."

**More information:** Sandro Bottaro et al. Free Energy Landscape of GAGA and UUCG RNA Tetraloops, *The Journal of Physical Chemistry Letters* (2016). [DOI: 10.1021/acs.jpcllett.6b01905](https://doi.org/10.1021/acs.jpcllett.6b01905)

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