Introducing atomistic details into a base-centered representation of RNA

Simón Poblete[1], Sandro Bottaro[1], and Giovanni Bussi[1]

[1]Scuola Internazionale Superiore di Studi Avanzati, 265, Via Bonomea I-34136 Trieste, Italy

The knowledge of the three-dimensional structure of a given RNA molecule is of fundamental importance for the understanding of its function. Taking into account the complexity of its experimental determination, computational tools appear as a convenient alternative for this aim. Among them, coarse-grained models of RNA are particularly interesting, due to the present limitations of all-atom approaches both in terms of performance and of the accuracy of the current force fields. Nevertheless, the reintroduction of the atomistic details into the coarse-grained predicted structures is not a trivial task.

In the present case, we describe the backmapping procedure employed after folding RNA fragments using the SPlit and conQueR (SPQR) model [1], a nucleobase-centered coarse-grained representation developed in our group. The reintroduction of the atomistic detail makes use of all-atom steered-Molecular Dynamics simulations which minimize the $\mathcal{E}$RMSD[2] distance between the atomistic and target coarse-grained structures. This distance is a function that depends exclusively on the relative positions and orientations of the nucleobases, so it can be defined in both atomistic and coarse-grained representations without ambiguity. In addition, this metric is more accurate than the usual RMSD for the comparison of nucleic acids structures. We also report the results of specific angle conformations involving backbone atoms which are not explicitly enforced during the backmapping procedure, and evaluate if our method is able to recover them without the incorporation of additional restraints.

References

[1] S. Poblete, S. Bottaro and G. Bussi, *submitted.*

[2] S. Bottaro, F. Di Palma and G. Bussi, *Nucleic Acids Res.* **42**, 13306 (2014).