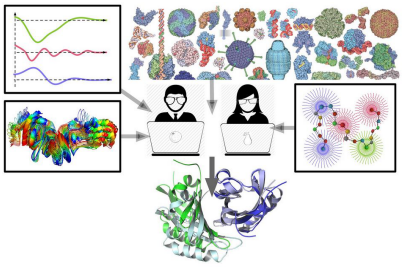

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Fragment-based docking to tackle the ssRNA flexibility

Protein-RNA interactions are involved in many biological processes like the traduction of messenger RNA to protein, and their modelisation is important to understand them. In particular, non-paired regions of the RNA, i.e., single-stranded RNA (ssRNA), are involved in most of these interactions and are essential for their specificity.

However, ssRNAs are highly flexible and their conformational space can not be sampled exhaustively enough for docking by using standard algorithms such as harmonic analysis, template-based modeling or MD simulations.

Here, we present a fragment-based approach for ssRNA/protein docking, developed to address the limitations described above. It includes:

- the building of a conformer library of ssRNA 3-mers;
- the docking of these ssRNA 3-mers on the protein;
- the assembling of the docked solutions on geometric criteria;
- in case of ssRNA loops, the new implementation of distance constraints in order to assemble them in a more efficient way;

We will present the results on several cases and discuss the advantages and the limitations of such an algorithm. Indeed, such a method has the advantage to sample ssRNA flexibility for the docking [Chauvot de Beauchene Isaure et al., PloS 2016] but further optimization is required due to the challenge to sample the enormous size of the ensemble of possible fragment-chains.

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