1.3. RNA: Interacciones hidrofóbicas e hidrofílicas de moléculas de RNA con y sin estructura secundaria

RNA: Sensing hydrophobic and hydrophilic interactions of RNA fragments with and without secondary structures

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RNA is a functionally rich biomolecule with multilevel, hierarchical structures whose role in the adsorption to molecular substrates is only beginning to be elucidated. In a recent work [1], we introduced a multiscale simulation approach that combines a tractable coarse-grained RNA structural model with an interaction potential of a structureless flat adsorbing substrate. Within this approach, we study the specific role of stem-hairpin and multibranch RNA secondary structure motifs on its adsorption phenomenology. Our findings identify a dual regime of adsorption for short RNA fragments with and without the secondary structure and underline the adsorption efficiency in both cases as a function of the surface interaction strength. The observed behavior results from an interplay between the number of contacts formed at the surface and the conformational entropy of the RNA molecule.
However, at the coarse-grained level we were not able to reproduce the hydrophobic and hydrophilic interactions of those archetypal RNA fragments.

In this project, the student will help develop a computational approach for calculating the adsorption energies due to hydrophobic and hydrophilic interactions of three archetypical RNA fragments (obtained from a virus sequence), with and without secondary structures. Such endeavor would enable us to evaluate the preferential adsorption structure with high-resolution molecular dynamics simulations, and also the most favorable surface of interaction. We will then evaluate substrates with different polarities, ranging from hydrophobic to hydrophilic, and quantify their adsorption energies. The theoretical methods used in this project involved our in-house developed polarizable surfaces [2]. Moreover, basics of molecular dynamics simulations. Those calculations will be performed at High-Performance-Computing facilities. Prior experience in programming (C, C++ or Python) would be helpful.

[1] S. Poblete, A. Bozic, M. Kanduc, R. Podgornik & **H. V. Guzman**, ACS omega 6, 48 (2021) https://doi.org/10.1021/acsomega.1c04774.
[2] https://tinyurl.com/goCompModeling

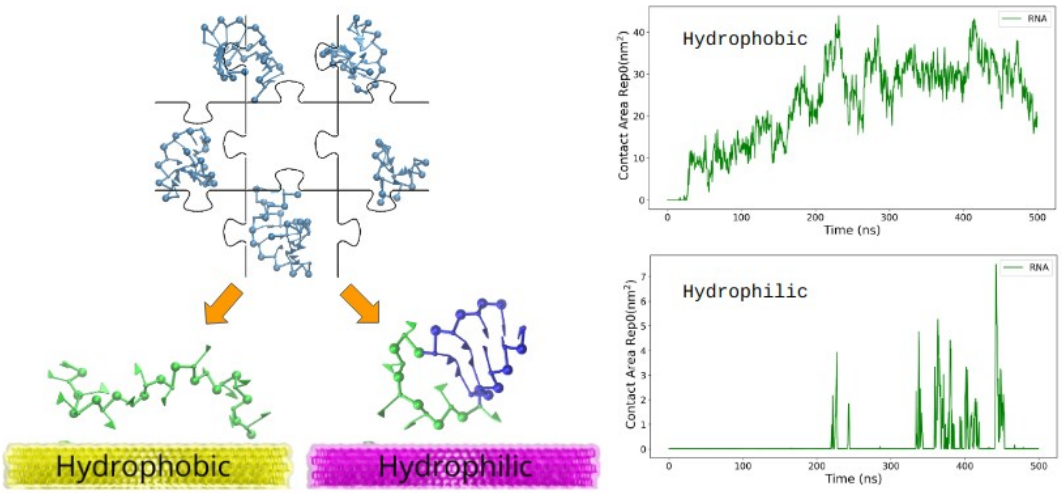

Figure 1:Left: Two different RNA fragments, in green the polymer like ones and in blue the based-paired fragments adsorbing onto hydrophobic and hydrophilic surfaces, respectively. Right, the contact area of those RNA fragments recorded by molecular dynamics simulations of 500 ns.