USING FREE-ENERGY METHODS TO STUDY RNA CONFORMATIONAL TRANSITIONS

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Ribonucleic acid (RNA) is acquiring a large importance in cell biology, as more functions that it accomplishes are discovered. However, experimental characterization of RNAs dynamical behavior at atomistic level is difficult. Molecular dynamics, in combination with state-of-the-art free-energy techniques and advanced analysis protocols, can bridge the gap providing an unparalleled perspective on the mechanism and dynamics of RNA folding and conformational transitions. Accurate free-energy calculations can be used to explore the conformational space of tetranucleotides [1] and to characterize the role of ligand and divalent cations in the folding of riboswitches [2,3]. Multiple time-stepping techniques help in decreasing the computational cost of collective-variable-based methods [4]. Finally, RNA 3D structure can be described using a coarse-grain representation based on the relative position and orientation of nucleobases that captures RNA structure and dynamics [5].

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