Title: RNAs in silico: what we can learn from metadynamics and steered molecular dynamics

Abstract:
Ribonucleic acid (RNA) is acquiring a larger 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 simulations at atomistic detail, in combination with state-of-the-art free-energy techniques (metadynamics and steered molecular dynamics), can bridge the gap providing an unparalleled perspective on the mechanism and dynamics of RNA folding and conformational transitions. Recent developments of metadynamics [1], steered molecular dynamics [2], and applications to RNA/peptide binding [3] will be discussed.

[1] Branduardi, Bussi, Parrinello, "Metadynamics with adaptive Gaussians" J. Chem. Theory Comput. (2012) 8, 2247.
[2] Colizzi and Bussi, "RNA Unwinding from Reweighted Pulling Simulations" J. Am. Chem. Soc. (2012), 134, 5173.
[3] Do, Carloni, Varani and Bussi, "RNA/peptide binding driven by electrostatics - Insight from bi-directional pulling simulations" J. Chem. Theory Comput. ASAP, doi:10.1021/ct3009914 (2013).