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RNA Nanostructures and Their Properties: A Modelling Perspective

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Ribonucleic acid (RNA) has been proposed as a promising alternative to DNA and proteins for the design of the artificial self-assembled materials at nanoscale (see [1] and references therein). As compared to DNA and some other bio-molecules, RNA offers not only a much greater variety of interactions but also great conformational flexibility of RNA structures, making RNA a very promising functional nano-material for the design of the man-made molecular devices and systems. We first present a model based on all-atom Molecular Dynamics, demonstrating the stability and conformational dynamics of several simple RNA nanostructures. We explain the effect of the counterions and solvent, that are both known to modify strongly the stability and dynamics of RNA nanostructures, on the behaviour of the "kissing loops". This effect is very important due to the fact that the "kissing loop" motif can be used as a basic constructional element to join the simplest building blocks into a symmetric structures with their spatial dimensions lying in the range of 10-20 nm. Then, we present several promising multiscale methodologies for simulation of biomolecular systems such as RNA nanostructures, focusing on our recent efforts in the development of a hierarchy of simplified coarse-grained mesoscopic models suitable for the description of these complex systems [2].

[1] M. Paliy, R. Melnik, B.A. Shapiro, *Physical Biology*, **6 (4)**, 046003, 2009.
[2] M. Paliy, R. Melnik, B.A. Shapiro, *Physical Biology* **7 (3)**, 036001, 2010.