Multiscale modelling of RNA and DNA structural motifs

Filip Lankas*[1]

[1]Department of Informatics and Chemistry, University of Chemistry and Technology Prague – Czech Republic

Abstract

Natural and artificial RNA structures could be understood as assemblies of recurrent building blocks - the structural motifs. Non-helical motifs often play a key role. These include internal loops such as C-loops or kink-turns, terminal loops, or junctions where three or more helices meet. In the DNA world, non-helical motifs such as the DX motif serve as helix connectors in nanostructures. We set out to model these motifs at various levels of detail. To this end we adopt a consistent bottom-up approach where large-scale atomistic MD simulations with explicit inclusion of water and ions are a source of data to parametrize models with reduced number of degrees of freedom. We employ models where bases or base pairs are considered rigid objects, and those where groups of bases are represented as effective rigid bodies. The coarse-grained coordinates are computed for each snapshot of the atomistic MD trajectory, resulting in a statistical ensemble from which the model paramers describing its structure and stiffness are deduced. In this way, the mechanical properties of the motif as a whole are captured, which enables one to assemble the motifs into larger structures inaccessible to atomistic simulations.

Keywords: RNA, DNA, structural motifs, molecular dynamics, coarse, grained models, mechanical properties

*Speaker