

INVESTICE DO ROZVOJE VZDELÁVÁNÍ

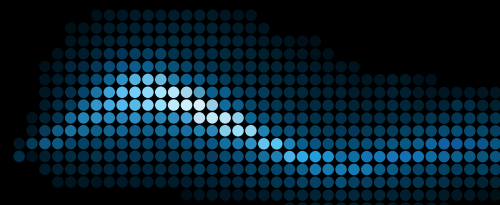
Zapojení regionálního centra pokročilých technologií a materiálů do mezinárodních sítí nanotechnologického a optického výzkumu.
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REGIONÁLNÍ CENTRUM POKROČILÝCH TECHNOLOGIÍ A MATERIÁLŮ - ODBORNÝ SEMINÁŘ

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Enhanced sampling for RNA

Abstract: 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 simulations at atomistic detail, in combination with state-of-the-art free-energy techniques, can bridge the gap providing an unparalleled perspective on the mechanism and dynamics of RNA folding and conformational transitions. Our recent results on the zipping and unzipping mechanisms for double stranded RNA and on the role of ligand and divalent counterions in the folding of riboswitches will be discussed. Moreover, a recently developed variant of Hamiltonian replica exchange will be outlined which allows a the conformational space of a tetranucleotide to be efficiently sampled.