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Dmitrii V Shalashilin, J Proteomics Bioinform 2017, 10:8(Suppl)
DOI: 10.4172/0974-276X-C1-0100

9th International Conference on

STRUCTURAL BIOLOGY

September 18-20, 2017 Zurich, Switzerland

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New applications of boxed molecular dynamics: Atomistic simulations of atomic force microscopy experiments and peptide cyclization

New applications of Boxed Dynamics (BXD), an efficient technique to extend the time scale of molecular dynamics and simulate rare events, will be presented. BXD allows analysis of thermodynamics and kinetics in complicated molecular systems. It is a fully atomistic multiscale technique, in which thermodynamics and long-time dynamics are recovered from a set of short-time molecular dynamics simulations. BXD is many orders of magnitude faster than standard MD and can produce well converged results. Previously BXD has been applied to peptide cyclization, solution-phase organic reaction dynamics, and desorption of ions from self-assembled monolayers (SAMs). Here two new applications of BXD will be reported. First atomistic simulations of protein pulling with Atomic Force Microscope AFM) will be presented, where BXD is able to reproduce correctly the Potential of Mean Force (PMF) of a protein pulled in AFM experiments, the experimentally observed force profile and its relationship with the protein structure. Second, an application of BXD to enzymatic peptide cyclization will also be presented, where BXD predicts correctly the cyclizable peptide sequences. All such sequences have a conformation with their C and N termini close to each other. In both applications calculations were done with standard force field without any adjustment of the force field parameters. Thus, BXD proves to be a good predictive tool. It is implemented in CHARMM molecular dynamics code and can be used for many other applications.

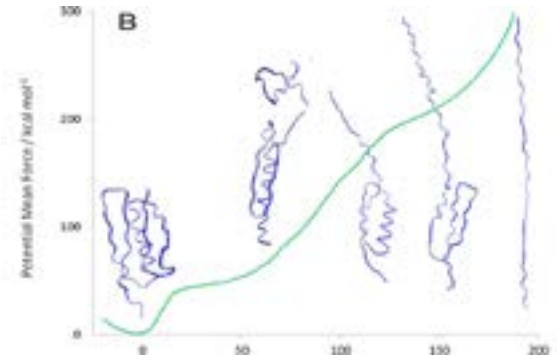

Figure1: Potential of mean force as a function of end-to-end distance calculated with BXD correlates with the structures of the unfolding protein.

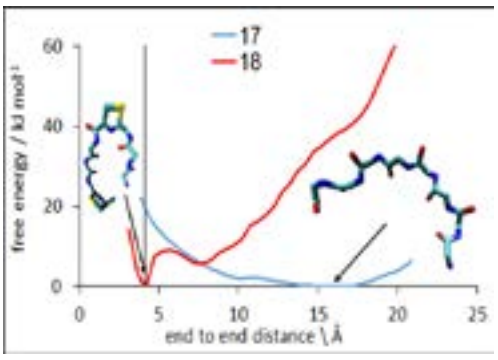

Figure2: PMF as a function of end-to-end distance for two peptides P18 and P17. Only P18, which has a stable conformation with C and N termini close to each other, is cyclizable.

Biography

Dmitrii V Shalashilin is a Professor of Computational Chemistry at the University of Leeds. His research is focused on the development of efficient computational techniques for quantum and classical simulations in chemistry and their applications.

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