BISON GUEST LECTURE:

Molecular dynamics as a tool to unravel the atomic basis underlying the physicochemical properties and functioning of bio-macromolecules

CEITEC MU

Kamenice 753/5, Brno
Complex University Campus at Bohunice

Building A4, Room 2.11

START: 14.00

02/08/2016

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Development of novel active compounds for medicine and biotechnologies of new age requires deep understanding of the structure – function relationship and the principles underling the properties of the biological systems. Two isoenzymes of glyceraldehyde-3-phosphate dehydrogenase were studied to reveal the influence of minor mutations on their thermal stability and activity. Combination of static potential energy mapping and MD simulations were applied to construct 3D structure of rhamnogalacturonan I – the most diverse and structurally complicated pectin polysaccharide. Starting from the experimental information of the primary structure of RG-I (i.e. monosaccharides, glycosidic linkage, branching points, etc.) the complete macromolecular 3D structure was generated using the POLYS 2.0 program (Engelsen et al., 2010). The investigation covers the elucidation of the conformational features of each constituting disaccharide segments and proceeds to the whole structure. Analysis of more energetically favorable architectures along the MD trajectories allows us to construct the most likely individual RG-I molecule structures and provides ways to understand functions displayed by RG-I in planta.

More information about the lecture HERE.

This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 692068.