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VABILO NA PREDAVANJE /
INVITATION TO THE LECTURE

Prof. Dr. Marco Klähn

Laboratory for Biomolecular Dynamics, Technische Universität München
Garching, Germany

Četrtek / Thursday, 25. 10. 2012, ob / at 13:00

Velika predavalnica Kemijskega inštituta / Lecture Hall at the
National Institute of Chemistry; Hajdrihova 19, Ljubljana

Proteins Solvated in Ionic Liquids: How the Ionic Constituents Influence Protein Stability

Povzetek / Abstract

The effect of ionic constituents of various ionic liquid (IL) solvents on the enzyme Candida Antarctica lipase B (CAL-B) is investigated. These solutions are analyzed with molecular dynamics (MD) simulations in combination with empirical force fields. Partial unfolding of CAL-B is observed in high-temperature MD simulations. Occurring changes in the solvent accessible protein surface, radius of gyration and secondary structure are monitored and compared across different ILs. Two distinct mechanisms that destabilize the protein are observed: Strong electrostatic interactions of small hydrophilic anions with polar regions of the protein surface destabilize the folded state of the protein. Secondly, hydrophobic cations interact either directly with the hydrophobic core of the protein or induce large conformational changes that expose the protein core to the solvent, thus stabilizing the unfolded protein state. The simulation results outline the underlying molecular mechanisms behind the previously observed relations that connect IL composition and protein stability.

Vljudno vabljeni! / Kindly invited

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