Kemijski inštitut Ljubljana Slovenija

National Institute of Chemistry Slovenia

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VABILO NA PREDAVANJE / INVITATION TO THE LECTURE

Dr. Gerhard Koenig

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Petek / Friday, 21. 9. 2012, ob / at 11:30

Fegeševa soba na Kemijskem inštitutu / Fegeš Room at the National Institute of Chemistry; Hajdrihova 19, Ljubljana

Predicting ligand binding free energies and protein stability with molecular dynamics simulations

Free energy simulations are considered among the most accurate and general methodologies in the field of computational chemistry. They provide means to study free energy differences associated with diverse processes such as the binding affinities of ligands, enzymatic reactions, the solubility of organic molecules, as well as the effect of point mutations and post-translational modifications in a quantitative way. Thus, free energy calculations represent an interesting option for analyzing systems that are not directly accessible to experimental approaches. In particular, the presentation focuses on the results of ligand binding calculations in the blind SAMPL3 binding prediction competition as well as the effect of point mutations on protein stability in aqueous solution.

Vljudno vabljeni! / Kindly invited!

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