



Kemijski inštitut
Ljubljana
Slovenija

National
Institute of Chemistry
Slovenia

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vabilo na predavanje / invitation to the lecture

Prof. Alessandra Magistrato

CNR IOM and International School for Advanced Studies, Trieste. Italy

ponedeljek / Monday, 9. 5. 2016, ob / at 13:00

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

Computational Studies of Biological Systems Related to Human Diseases

Computational biology is playing an ever increasing important role in understanding at atomistic level of detail the complex mechanisms of biological processes, complementing experimental data and predicting novel aspects of those processes, which are inaccessible to experiments. In this talk multi scale simulations ranging from force field based molecular dynamics to hybrid quantum classical (QM/MM) simulations, in combination with state of the art advanced sampling techniques, will be used to understand the molecular mechanisms of biological processes related to human diseases. In particular, I will focus on enzymes metabolizing hormones, on self splicing ribozymes, on DNA repair enzymes, and finally, on membrane proteins, which transport nutrients across the cellular membranes.

Vljudno vabljeni! / Kindly invited!

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