International Summer School
"Multiscale Molecular Simulation for Neurological Targets"

Background
Monoaminergic neurotransmitters such as dopamine and serotonin play a central role in the pathophysiology of major neuropsychiatric illnesses. Neurotransmitter-binding proteins such as receptors, transporters and common metabolic enzymes are the starting points for development of tools to diagnose and drugs to treat specific clusters of symptoms.
The aim of the summer school is to give an overview of some of the *in silico* tools that are applicable to neurological targets. We will learn how to perform molecular dynamics simulation of proteins in complex environments, how to calculate binding free energy of an enzyme inhibitor by molecular docking and how to calculate the rate constant of an enzymatic reaction by multiscale molecular simulation.

Time: June 20, 2015, starting at 10am

Venue: National Institute of Chemistry, Ljubljana, Slovenia, (large lecture room)

Organizer: Janez Mavri, e-mail janez.mavri@ki.si

Participants: MS Students, PhD Students, Postdoctoral Fellows, researchers, interested in neuroscience, biophysics, drug design and computational (bio)chemistry

Organization scheme: Before lunch will be mainly *ex cathedra* lectures for those who would like to get an overview. In the afternoon practical work in groups will follow for those who would like to obtain practical experience with the enzyme reaction simulation. It is desirable that the participants bring their laptops. **Summer School is Free of Charge.**

Additional information - https://bit.ly/2t1Gk3w

Registration - https://bit.ly/2JKYgJK

Speakers/instructors: Robert Vianello, Miha Purg, Matic Pavlin, Nejc Umek, Blaž Geršak, Andrej Perdih, Jernej Stare, Janez Mavri