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## Program of the International Summer School “Multiscale Molecular Simulation for Neurological Targets”

June 20, National Institute of Chemistry, Ljubljana, Slovenia  
Organizer: Janez Mavri

20 <sup>th</sup> June Wednesday	Speaker	Topic // Title
9:30-10:00	Registration	
10:00-10:15	Robert Vianello Janez Mavri	Welcome // Introduction
10:15-10:45	Janez Mavri	Statistical Thermodynamics of Binding and Kinetics
10:45-11:30	Robert Vianello	Mechanistic Studies of Monoamine Oxidases
11:30-12:00	Matic Pavlin Andrej Perdih	Rational Ligand Design by Molecular Docking
12:15-14:00	LUNCH	
14:00-14.30	Jernej Stare	Empirical Valence Bond Theory
14.30-17.30	Miha Purg	Practical Aspects of Simulation of Enzyme Catalysis
17:30-17:45	COFFEE BREAK	
17:45-18:15	Nejc Umek Blaž Geršak	Clinical aspects of neural transmission and techniques to disrupt it

