

## School on molecular computational biochemistry

11 - 14 March 2019

ICSC PAS, Kraków, Poland

### Day 1 (11.03)

Time	Tutor	Topic
9:00–10:30	Łukasz Ćwiklik	MD simulations of biosystems - lipid membranes and transmembrane peptides – part 1
10:30-10:50		break
10:50-12:20	Łukasz Ćwiklik	MD simulations of biosystems - lipid membranes and transmembrane peptides – part 2
12:20-13:20		lunch break
13:20-14:50	Wojciech Płaziński	MD enhanced sampling methods
14:50-15:10		break
15:10-16:40	Fahmi Himo	Modeling Enantioselectivity in Enzymes

### Day 2 (12.03)

Time	Tutor	Topic
9:00–10:30	Artur Góra	Breaking geometry-based methods limits by alternative method for protein tunnels and cavity exploration – part 1
10:30-10:50		break
10:50-12:20	Artur Góra	Breaking geometry-based methods limits by alternative method for protein tunnels and cavity exploration – part 2
12:20-13:20		Lunch break
13:20-14:50	Martin Srnec	Transition State Theory & Concepts in (bio)catalysis: What controls reactivity and selectivity
14:50-15:10		Break
15:10-16:40	Matthias Stein	Electrostatics of molecular interactions

### Day 3 (13.03)

Time	Tutor	Topic
9:00–10:30	Lubomir Rulisek	Solvation models (theory, foundations, principles, implicit and explicit solvation models, polarized continuum models, conductor-like screening model and its statistic-thermodynamic extension)
10:30-10:50		break
10:50-12:20	Andrzej Sokalski	Nonempirical techniques aiding drug and biocatalyst design
12:20-13:20		Lunch break
13:20-14:50	Margareta Blomberg	Reaction mechanisms including electron and proton uptake in Heme-Copper Oxidases – part 1
14:50-15:10		Break

15:10-16:40	Margareta Blomberg	Reaction mechanisms including electron and proton uptake in Heme-Copper Oxidases – part 2
-------------	--------------------	---

#### Day 4 (14.03)

Time	Tutor	Topic
9:00–10:30	Sam de Visser	VB
10:30-10:50		break
10:50-12:20	Sam de Visser	Spin-state reactivity
12:20-13:20		Lunch break
13:20-14:50	Ulf Ryde	QM/MM methods, their application to metalloenzymes and their combination with experimental methods – part 1
14:50-15:10		Break
15:10-16:40	Ulf Ryde	QM/MM methods, their application to metalloenzymes and their combination with experimental methods – part 2