

BImBS 2019 - Bioinformatics meets BioSimulations in protein and DNA studies: from theory to practice

Università della Svizzera italiana, Via G. Buffi 13, 6900 Lugano, Switzerland

October 5, 2019 – October 12, 2019

School Program

Saturday, 5th October - Day 1

Opening

- 09:00 to 09:15 - Welcome and Introduction

Bioinformatics for Sequence Analysis and Structure Prediction

- 09:15 to 10:45 - Andrei N. Lupas (*Max Planck Institute Tübingen, Germany*): From Sequence to Structure – Deducing Structural Features of Proteins from Their Sequences
- 10:45 to 11:15 - *Coffee Break*
- 11:15 to 12:45 - Gianni Cesareni (*University of Rome "Tor Vergata", Italy*): Disnor and CancerGeneNET: Two Open Resources to Infer Affected Pathways and Phenotypes from Disease Associated Protein Variants
- 12:45 to 14:00 - *Lunch*
- 14:00 to 16:00 - Exercises
- 16:00 to 16:30 - *Coffee Break*
- 16:30 to 18:30 - Exercises
- 18:30 - *Social Aperitif*

Sunday, 6th October - Day 2

Bioinformatics for Sequence Analysis and Structure Prediction

- 09:00 to 10:30 - Rita Casadio (*University of Bologna, Italy*): Transfer of Knowledge for Structural and Functional Annotation of Protein Sequence
- 10:30 to 11:00 - *Coffee Break*

Ligand-Protein Docking

- 11:00 to 12:30 - Ruben Abagyan (*University of California San Diego, USA*): Discovering, Designing or Screening for a Specific Multi-Target Profile of a Drug or Drug Candidate
- 12:30 to 14:00 - *Lunch*
- 14:00 to 16:00 - Exercises
- 16:00 to 16:30 - *Coffee Break*
- 16:30 to 18:30 - Exercises

Monday, 7th October - Day 3

Bioinformatics for Personalised Medicine

- 09:00 to 10:30 - Alfonso Valencia (*Barcelona Supercomputing Center, Spain*): Cell Level Simulations
- 10:30 to 11:00 - *Coffee Break*

Protein-Protein Docking

- 11:00 to 12:30 - Alexandre Bonvin (*Utrecht University, The Netherlands*): Integrative Modelling of Biomolecular Complexes
- 12:30 to 14:00 - *Lunch*
- 14:00 to 16:00 - Exercises
- 16:00 to 16:30 - *Coffee Break*
- 16:30 to 18:30 - Exercises

Tuesday, 8th October - Day 4

Atomistic Molecular Dynamics (MD) Simulations

- 09:00 to 10:30 - Modesto Orozco (*University of Barcelona, Spain*): Multiscale Simulations of DNA
- 10:30 to 11:00 - *Coffee Break*
- 11:00 to 12:30 - Bert L. de Groot (*Max Planck Institute Göttingen, Germany*): Alchemical Free Energy Calculations
- 12:30 to 14:00 - *Lunch*
- 14:00 to 16:00 - Exercises
- 16:00 to 16:30 - *Coffee Break*
- 16:30 to 18:30 - Exercises

Wednesday, 9th October - Day 5

Free Energy Calculations

- 09:00 to 10:30 - David Wales (*University of Cambridge, UK*): Exploring Energy Landscapes: From Molecules to Nanodevices
- 10:30 to 11:00 - *Coffee Break*
- 12:00 to 12:30 - Vittorio Limongelli (*University of Lugano USI, Switzerland*): FMAP: the Funnel-Metadynamics Automated Protocol for Ligand Binding Free-Energy Calculations
- 12:30 to 14:00 - *Lunch*
- 14:00 to 16:00 - Exercises
- 16:00 to 16:30 - *Coffee Break*
- 16:30 to 18:30 - Exercises

Thursday, 10th October - Day 6

- 09:00 to 09:45 - Stefano Alcaro (*University "Magna Graecia" of Catanzaro, Italy*): The MTDD Approach and the Chemotheca Tool in the MuTaLig COST Action
- 09:45 to 10:30 - Jiangning Song (*Monash University, Australia*): Harnessing the Power of Machine-Learning Techniques to Address Biomedical Classification Problems
- 10:30 to 11:00 - *Coffee Break*
- 11:00 to 11:30 - *CSCS Swiss National Supercomputing Centre* - Victor Holanda Rusu
- 11:30 to 12:30 - Poster Presentation
- 12:30 to 14:00 - *Lunch*
- 14:00 to 16:00 - Poster Session
- 16:30 to 18.30 - Visit @ CSCS
- 20:00 to 23:00 - *Social Dinner*

Friday, 11th October - Day 7

Free Energy Calculations

- 09:00 to 10:30 - Helmut Grubmüller (*Max Planck Institute Göttingen, Germany*): Atomistic Simulation of Biomolecular Function
- 10:30 to 11:00 - *Coffee Break*

Coarse-grained Simulations

- 11:00 to 12:30 - Luca Monticelli (*CNRS Lyon, France*): The MARTINI Coarse-Grained Force Field: Principles and Applications
- 12:30 to 14:00 - *Lunch*
- 14:00 to 16:30 - Exercises
- 16:00 to 16:30 - *Coffee Break*
- 16:30 to 18:30 - Exercises

Saturday, 12th October - Day 8

Coarse-grained Simulations

- 09:00 to 10:30 - Gregory A. Voth (*University of Chicago, USA*): Systematic Coarse-graining: Fundamentals and Applications
- 10:30 to 11:00 - *Coffee Break*
- 11:00 to 12:30 - Exercises
- 12:30 to 13:00 - Concluding remarks