

Workshop on Multiscale Computational Modeling and Design of Polymer-Degrading Enzymes

Tentative Program

9th march Introduction to Computational Modeling of enzymatic systems

9:30-10:00 registration
10:00-11:00 S. Osuna - Welcome & Overview of Challenges in computational modeling of plastic-degrading enzymes, especial focus on dynamics
11:00-11:30 **TEA BREAK**
11:30-13:30 S. Osuna - Hands-on: Software for proteins visualisation, Artificial Intelligence supported proteins prediction - AlphaFold, Models validation
13:30-14:30 **LUNCH**
14:30-15:30 C. Rovira - QM/MM-MD strategies for enzymatic catalysis
15:30-16:00 **COFFEE BREAK**
16:00-18:00 A. Nin - Hands-on: Intro to QM/MM-MD workflows

10th march Role of protein dynamics and water in enzyme catalysis

9:30-10:30 A. Gora - Role of protein dynamics and water in enzyme catalysis
10:30-11:00 **TEA BREAK**
11:00-13:00 A. Raczyńska - Water network analysis from MD trajectories
13:00-14:00 **LUNCH**
14:00-15:00 V. Moliner - QM/MM strategies for enzymatic catalysis in plastic degradation
15:00-15:30 **COFFEE BREAK**
15:30-17:30 K. Zwiderak - Hands-on: Intro to QM/MM workflows

11th march Computational investigation of protein-ligand interactions and enzyme design tools

9:30-10:30 M. De Vivo - Enhanced sampling & free energy calculations
10:30-11:00 **TEA BREAK**
11:00-13:00 Pietro - Hands-on: Enhanced sampling tutorial and free energy calculations
13:00-14:00 **LUNCH**
14:00-15:00 S. Mazurenko - Stability and design of enzymes: FireProt and beyond.
15:00-15:30 **COFFEE BREAK**
15:30-17:30 P. Kohout: Hands-on: : Enzyme stability prediction using FireProt pipeline
20:00-23:00 **GALA DINNER**

12th march Computational investigation of protein-ligand interactions and enzyme design tools

9:30-10:30 F. Sancho - Strategies for proteins redesign
10:30-11:00 **TEA BREAK**
11:00-13:00 F. Sancho - Hands-on: Strategies for proteins redesign
13:00-14:00 **LUNCH**
14:00-15:00 V. Ferrario - Understanding protein-ligand interactions
15:00-15:30 **COFFEE BREAK**
15:30-17:30 V. Ferrario - Hands-on: Understanding protein-ligand interactions

