COZYME

Agenda MC and WG meeting

April 24-26, Zagreb, Croatia

Time	Thu / 25.4	Fri / 26.4
9.00-9.30	Registration	
9.30-10.00	Welcome by the Action Chair and LO	WG3
10.00-10.30	WG1	
10.30-11.00		
11.00-11.30	Coffee break	Coffee break
11.30-12.00	WG1	Brainstorming session
12.00-12.30	WG2	
12.30-14.00	Lunch	Lunch
14.00-14.30	WG2	Brainstorming session: conclusions
14.30-15.00		
15.00-15.30		STSM session (research done during STSMs)
15.30-16.00		
16.00-16.30	Poster Session (with coffee/biscuits)	
16.30-17.00		Closure (Action Vice Chair and LO)
17.00-17.30		Social drinks and departure
17:30-19:30		
19.30-22.00	Dinner	

Speaker	Title
WG1 Session	Chair: **Dr. Sérgio Marques** (WG1 leader)
Dr. Giulia Morra (20+10)	*Modelling protein allostery for in silico drug discovery*
Dr. Vladimir Sladek (10+5)	*Fast ranking of residues in (bio)molecular interfaces by topological relevance*
Dr. Mehmet Ozbil (10+5)	*Interpreting the Effect of Mutations on Complexation and Ion Binding in Enzymes*
Dr. Miguel Machuqueiro (20+10)	*Constant-pH MD simulations as a tool to unveil the effects of pH on proteins: the case of DyP-type peroxidases*
WG2 Session	Chair: **Prof. Lucia Gardossi** (WG2 leader)
Prof. Mélanie Hall (20+10)	*Making Enzymes Fit for Process with Enzyme Engineering: Unveiling Challenges and Promises*
Prof. Vincent Eijsink (15+5)	*Recent insights into the catalytic properties of enzymes known as lytic polysaccharide monooxygenases (LPMOs)*
Dr. Gemma Kinsella (15+5)	*Cutinase from Amycolatopsis mediterranei: Modelling, biocatalytic applications and solvent activation.*
Dr. Artur Góra (15+5)	*Water as a key player – investigation of the proteolytic cleavage of TLR8 Z-loop by furin protease, and the impact of water models for water transport inside enzymes.*
WG3 Session	Chair: **Prof. Jürgen Pleiss** (WG3 leader)
Prof. Nur Basak Surmeli (15+5)	*Enhancing Biocatalytic Potential: Engineering CYP119 for Industrial Applications*
Dr. Heather Jameson (15+5)	*The hunt for artifical reactivities in biocatalysis: Metalloproteins as mediators for pericyclic reactions*
Dr. Gábor Tasnádi (15+5)	*Implementation and application of biocatalysis at Servier*
Dr. Emilio Parisini (15+5)	*Engineering of a fructosyl peptide oxidase enzyme for biomedical applications*

Brainstorming Session	Chairs: **Prof. Ligia Martins and Dr. Bettina Nestl**
	Topics: TBA

STSM Session	Chairs: **Dr. Nataša Božić and Prof. Anamaria Todea**
Vsevolod Viliuga (15+5)	*Understanding ProteinMPNN: in-depth analysis of a deep learning-based method for protein design*
Saniye Gul Kaya (15+5)	*Tuning biophysical properties of LOV domains by flavin-fixing*
András Telek (15+5)	*Computational design of KIRED variants for enzymatic reductive aminations*
Nayanika Das (15+5)	*Molecular Dynamics Exploration of the Conformational Landscape of Glutathione Peroxidase 6 (GPX6)*
Konstantinos Grigorakis (15+5)	*Computational design and experimental validation of mutations to stabilize DmPETase, a thermophilic enzyme for PET depolymerization*