

Computational Approaches to Understanding and Engineering Enzyme Catalysis

19–22 October 2021 | Oulu, Finland

Supported by FEBS and the Health and Biosciences Doctoral Programme, University of Oulu Graduate School. An activity of the 3D-BioInfo ELIXIR Community.

University of Oulu, FBMM, Aapistie 7A, Oulu, Finland



All lectures and tutorials will be in the Leena Palotie hall, FBMM, Aapistie 5A. Coffee and tea are provided nearby, in the same place as the poster sessions. Posters can be installed on Tuesday morning and removed on Friday morning. Additionally, the nearby computer room KT285 as well as room L107 are also available for discussions in smaller groups.

This is the current schedule (April 2021). In order to make sure that the remote participation will work smoothly, additional practical details will be added later.

TUESDAY, OCTOBER 19

Day	Time	Lectures	Demonstration/Tutorial	Poster Session
19 October 2021 Tuesday	08:30 Bus departure from the hotel			
	9:00-9:30 REGISTRATION			
	09:30-10:20	Adrian Mulholland General introduction on enzyme engineering and on MD-QM/MM calculations for understanding of enzyme catalyzed reactions		
	10:20-11:10	Rossana Zaru The enzyme portal: a portal for enzyme resources at the European Bioinformatics Institute (EMBL-EBI) and beyond		
	11:10-11:30 Coffee Break and Discussion			
	11:30-12:30		Rossana Zaru The enzyme portal: demonstration	
	12:30-13:30 Lunch Break and Discussion			
	13:30-14:20	Birte Höcker De novo protein design and its experimental validation		
	14:20-14:40	Beata G. Vertessy FEBS-MIC, FEBS opportunities for scientists in molecular life sciences		
	14:40-16:00		Student flash talks (2 minutes each)	
	16:00-16:30 Coffee Break and Discussion			
	16:30-17:30		Rossana Zaru The enzyme portal: tutorial	
	17:30-18:00			Poster session
	18:00-19:00 Dinner and Discussion			
	19:00 Bus back to the hotel			

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WEDNESDAY, OCTOBER 20

Day	Time	Lectures	Demonstration/Tutorial	Poster Session
20 October 2021 Wednesday	08:30 Bus departure from the hotel			
	09:00-09:50	Gerrit Groenhof An introduction into Molecular Dynamics simulations of proteins		
	09:50-11:00		Gerrit Groenhof MD demonstration	
	11:00-11:30 Coffee Break and Discussion			
	11:30-12:30		Gerrit Groenhof MD tutorial	
	12:30-13:30 Lunch Break and Discussion			
	13:30-14:20	Mickel Widersten Pre-steady state and steady-state kinetics of designed enzymes		
	14:20-15:10	Sarel Fleishman (i) Automated design of proteins for high expression and stability; (ii) Automated design of efficient and functionally diverse enzymes		
	15:10-15:40 Coffee Break and Discussion			
	15:40-16:40		Sarel Fleishman PROSS/FuncLib demonstration	
	16:40-17:40		Sarel Fleishman PROSS/FuncLib tutorial	
	17:40-18:30			Poster session
	18:30 departure by bus for Oulu city centre			
	19:00-21:00 social dinner in Oulu city			

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THURSDAY, OCTOBER 21

Day	Time	Lectures	Demonstration/Tutorial	Poster Session
21 October 2021 Thursday	08:30 Bus departure from the hotel			
	09:00-09:50	Jiri Damborsky Engineering ligand access pathways		
	09:50-11:00		Jiri Damborsky CaverWeb demonstration	
	11:00-11:30 Coffee Break and Discussion			
	11:30-12:30		Jiri Damborsky CaverWeb tutorial	
	12:30-13:30 Lunch Break and Discussion			
	13:30-14:20	Aleksandra Marsavelski The EVB method: in silico approach for understanding the mechanism of enzyme catalysis		
	14:20-15:10	Silvia Osuna Conformationally-driven computational enzyme design: development and application of correlation-based tools for distal active site mutation		
	15:10-15:40 Coffee Break and Discussion			
	15:40-16:40		Silvia Osuna DynaComm demonstration	
	16:40-17:40		Silvia Osuna DynaComm tutorial	
	17:40-18:00			Poster session
	18:00-19:00 Dinner and Discussion			
	19:00 Bus back to the hotel			

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FRIDAY, OCTOBER 22

Day	Time	Lectures	Demonstration/Tutorial	Poster Session
22 October 2021 Friday	08:00 Bus departure from the hotel			
	08:30-09:20	James Fraser Ensembles of Ensembles - How multiple conformations exist within and between protein structures		
	09:20-10:10	Reinhard Sterner Analysis of allostery in a multi-enzyme complex by ancestral sequence reconstruction		
	10:10-10:30 Coffee Break and Discussion			
	10:30-12:00		Tutorials	
	12:00-13:00 Final gettogether, handing out of the certificates			
	13:00 Bus to the airport			
	13:00-16:00		ad hoc tutorial sessions	

The meeting will end on Friday, October 22, in time to catch the 14:30 Finnair Oulu-Helsinki flight. For those who attend remotely, we aim to keep the zoom sessions open in the afternoon for further ad hoc discussions.