5th Hands-on Computational **Enzyme Design**

12–14 February 2024, ONLINE



Introduction

Computational tools can dramatically accelerate the discovery and design of improved enzymes. This course will introduce a number of user-friendly software tools for predicting and redesigning enzyme properties, and will provide intensive practical training. The developers of those tools will run this interactive course. In the end the participants will be able to use the tools independently. Prior experience in molecular modelling or bioinformatics is not required and experimentalists are welcome.



Registration fees

| | Academia | Industry |
|--------------------------------|----------|----------|
| Early (30 Nov. 2023) | 400€ | 700€ |
| Late (15 Dec. 2023) | 550€ | 850€ |

Fees include: theoretical materials, protocols, tips and tricks, advanced exercises, personalized hands-on sessions, troubleshooting, certificate

★ Limited number of participants ★



Program

Main topics

- ☑ Mining of novel enzymes
- ☑ Design of protein stability and solubility
- ☑ Design of enzyme activity and specificity
- ☑ Machine learning in biochemistry

Software and databases covered

- ☑ EnzymeMiner
- ☑ Hotspot Wizard
- ☑ FireProt, FireProt^{ASR}, FireProt^{DB}
- ☑ Caver, Caver Web, CaverDock,
- ☑ LoopGrafter
- ☑ SoluProt, SolubiS, SoluProtMut^{DB}, AggreProt
- AlphaFold, ProteinMPNN, RF Diffusion

Workshop format

- ☑ Theoretical lectures
- ☑ Hands-on practical sessions
- ☑ User-personalized sessions



- Loschmidt Laboratories, RECETOX, Faculty of Science, Masaryk University
- Enantis Ltd., FNUSA-ICRC
- ELIXIR.CZ; COST-COZYME

Contact: nevolova.sarka@gmail.com

