

ESAB Webinar

PROBLEMS AND TOOLS FOR STANDARDIZED REPORTING OF BIOCATALYSIS EXPERIMENTS

Friday, 03rd September 2021 at 14:00 – 16:00 CET

Welcome Address: Willi Meier, DECHEMA

Chair: Peter Halling, University of Strathclyde, Glasgow, Scotland, UK

PROGRAMME

14.00 Prof. Dr. Zvezdana Findrik Blažević, Faculty of Chemical Engineering and Technology, University of Zagreb, Croatia

Prospects and possibilities of STRENDA DB from a viewpoint of a chemical engineer and applied biocatalysis

Scientific literature contains a significant amount of kinetic data that requires organization and cataloguing to better serve its purpose. Being currently scattered in different publications its full potential is not clearly visible. These data can serve as an immense pool for reaction modelers, as well as other interested parties. It can be used to improve our understanding of the complex enzymatic processes both in vitro and in vivo. Thus, it is the purpose of this talk to stress the need for an active database such as STRENDA DB in applied biocatalysis which is substantiated by practical examples, and to also address the potential of its application. A part of the talk will also be dedicated to other data that could find its place in the database as well, like an important topic of enzyme stability. Additionally, results of a short survey on reporting of process data in selected papers will be addressed.

14.30 Jan Range, Research Software Engineer, Stuttgart Center for Simulation Science, University of Stuttgart, Germany

EnzymeML at work

EnzymeML is an XML-based data exchange format that supports the comprehensive documentation of enzymatic data by describing reaction conditions, time courses of substrate and product concentrations, the kinetic model, and the estimated kinetic constants. An EnzymeML document serves as a container to transfer data between experimental platforms, modelling tools, and databases. The goal of EnzymeML is to support the scientific community by introducing a standardized data exchange format to make enzymatic data findable, accessible, interoperable, and reusable according to the FAIR data principles. However, any data model is only as good as it is served to the community. Application programming interfaces and web services play a key role in delivering FAIR data management to the laboratory. Thus, several tools from simple spreadsheets to web-based applications have been developed and applied to demonstrate a seamless flow of data as well as EnzymeML at work.

15.00 DI Peter Wied, B.Sc., Prof. Dr. Paolo Falcaro, Prof. Dr. Bernd Nidetzky Institute of Biotechnology and Biochemical Engineering, Technical University Graz, Austria

Enzyme immobilization in porous crystalline frameworks: new challenges for standardization in biocatalysis

Porous crystalline frameworks, such as metal-organic frameworks (MOFs) and hydrogen-bonded organic frameworks (HOFs), have recently gained increasing importance in the field of enzyme immobilization. MOFs and HOFs can be constructed in a bottom-up synthesis from nodes and linkers. This modular assembly greatly expands their scope in terms of tuning the material properties and the immobilization strategies applicable (e.g. post-synthetic vs. in situ/one-pot). Use in enzyme immobilization not only increases the potential application of these framework materials but also gives rise to new challenges in respect to the standardized characterization of the immobilized enzymes. Conditions used in different studies of enzyme immobilization within these materials vary in a wide range (e.g., pH, type and concentration of precursors). Careful evaluation of key parameters of enzyme immobilization is thus important and good standards in reporting data are essential. Not only is this essential for comparability and coherence among studies, but it is also required to advance the mechanistic understanding and to identify opportunities and limitations.

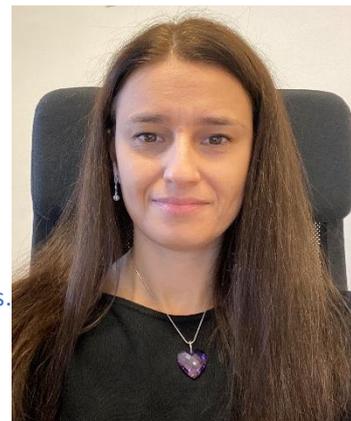
15.30 Discussion and Feedback: All Speakers and Webinar Organizer Prof. Dr. Peter Halling

Breakout Rooms

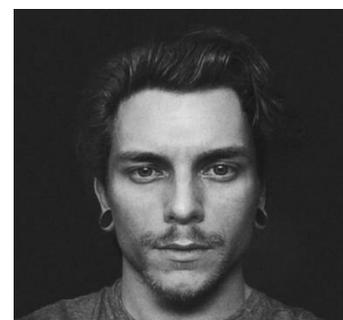
One objective of this webinar is to seek feedback from the applied biocatalysis community on what is needed in effective tools for collection and transfer of data and metadata from experiments. This feedback can include specific points about the tools STREND A DB and EnzymeML and more general comments. To aid such feedback, after the presentations and discussions are over, we will open Zoom Breakout Rooms – one for each speaker and one for general points. Participants will be able to move freely between these rooms, using the Breakout Rooms tools in Zoom. That will give the opportunity for informal discussion and feedback to each speaker. The webinar organiser Peter Halling will be in the general Breakout Room to receive appropriate comments.

ABOUT THE SPEAKERS

Zvezdana Findrik Blažević is a full professor of Chemical Engineering at the Faculty of Chemical Engineering and Technology of the University of Zagreb from 2018. She finished her PhD in Chemical Engineering in 2006 on the topic in applied biocatalysis. During and after her PhD study she spent some time abroad for research stays at the Research Center Jülich in Germany, Department of Technical Chemistry at the University of Rostock, Institute of the Advanced Chemistry at the CSIC in Barcelona, University of Pannonia in Veszprem, Hungary, and University of Maribor, Slovenia. Her research involves the application of Chemical Engineering methodology on the development and optimization of single and multi-enzymatic reactions and on that topic, she published around 50 publications in peer-reviewed journals and several book chapters. For her scientific work she received several awards. She was a partner in the H2020 project Carbazymes, and is currently a partner in H2020 project RadicalZ, and a beneficiary in an ITN C-C Top. She currently supervises 4 PhD students, has supervised 2 finished PhDs, and around 60 undergraduate and graduate student works. She is the Croatian representative of ESAB.



Jan Range is a Research Software Engineer at the Cluster of Excellence EXC 2075 „Data-Integrated Simulation Science“ in Stuttgart and main developer of the data exchange format EnzymeML. Originally trained in the field of technical biology, Jan Range specialized in research data management and software engineering in biocatalysis and simulation sciences. His aim is to provide bottom-up solutions for data management in close collaboration with researchers to facilitate seamless workflows and intuitive web applications from the beginning to the end of an experiment.



Peter Wied is a PhD candidate within the Lead Project “Porous Materials at Work” under the joint supervision of Prof. Paolo Falcaro and Prof. Bernd Nidetzky at Graz University of Technology. He completed his BSc in Biomedical Science at F. H. Joanneum (University of Applied Sciences, Austria). After which he completed his MSc in Biotechnology in the group of Prof. Robert Kourist at the Institute of Molecular Biotechnology (Graz University of Technology), working in photobiocatalysis. In 2019 he started his PhD where his focus is on the application of Metal–Organic Frameworks in enzyme immobilization.



NEXT ESAB WEBINARS

ESAB aims to promote the development of Applied Biocatalysis and takes initiatives in areas of growing scientific and industrial interest in the field.

Schedule and Topics of next ESAB webinar:

22 Oct. 2021, Synthetic Biology and Metabolic
14.00-16.00 Engineering Tools & Methodologies
CET organized by Frangiskos Kolis and
Roland Wohlgemuth

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Personal membership is free. ESAB, founded in 1980, has the mission of promoting the development of Applied Biocatalysis throughout Europe. The aims of ESAB are to promote initiatives in areas of growing scientific and industrial interest of importance within the field of Applied Biocatalysis. Further information can be found on the ESAB website www.esabweb.org
[ESAB - European Society of Applied Biocatalysis \(esabweb.org\)](http://www.esabweb.org)