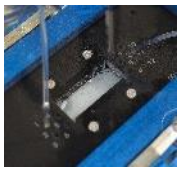

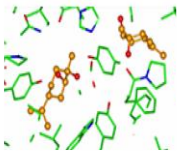
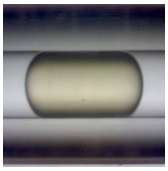

ESAB Webinar

STANDARDIZATION OF BIOCATALYTIC REACTIONS

Thursday, 29th January 2021 at 14:00 CET
Chairs: Roland Wohlgemuth, ESAB Chairman, Lodz University of Technology, Poland
Jennifer Littlechild, ESAB Vice-Chairman, University of Exeter, UK
Moderator: Willi Meier, DECHEMA, Frankfurt, Germany

PROGRAMME

14:00 **Peter Halling** (WestCHEM, Dept Chemistry, University of Strathclyde, Glasgow, Scotland)

Better reporting of biocatalysis experiments: the problem and one contribution to the Solution

Most applied biocatalysis work reported in the literature cannot be repeated. This is not about reproducibility, although that may be problematic. Rather the issue is whether the literature gives all the information needed to repeat the original experiments. This talk will present some examples showing just how widespread the problem is, with an indication of the most common omissions. Our community must solve this problem. One issue (which can cause variation of at least 10% in reported results) is the estimation of initial rate from discontinuous assay data. Methods used are rarely reported, and almost always involve some subjective judgment. By using a simulation approach, I have recently analysed the performance of different methods. This leads to suggestions of the basis for a more objective (and accurate) approach.

Halling, P. J. et al. (2018). "An empirical analysis of enzyme function reporting for experimental reproducibility: Missing/incomplete information in published papers." Biophysical Chemistry 242:22-27. 10.1016/j.bpc.2018.08.004.
Halling, P. J. (2020). "Estimation of initial rate from discontinuous progress data." Biocatalysis and Biotransformation 38(5): 325-342. 10.1080/10242422.2020.1746771.

14:30 **António J. M. Ribeiro** (EMBL-EBI, Hinxton, Cambridge CB10 1SD, United Kingdom)

Enzyme Portal and the M-CSA: two online resources from the EMBL-EBI to explore data related to enzymes

This presentation will be focused on two freely accessible resources developed at the EMBL-EBI (European Bioinformatics Institute) that are dedicated to enzymes: The Enzyme Portal and the M-CSA (Mechanism and Catalytic Site Atlas). I will discuss how existing standards were essential to the creation of these resources, but also how the absence of standards for some types of data (notably the mechanism of enzymes) could impact future research efforts.

The Enzyme Portal integrates publicly available information about enzymes, such as small-molecule chemistry, biochemical pathways, drug compounds, and kinetics. It aims to present this information as a unified user experience – linked to other public data resources. The enzyme portal can be accessed at www.ebi.ac.uk/enzymeportal/.

The M-CSA (Mechanism and Catalytic Site Atlas) is a data-base of enzyme reaction mechanisms with information about the catalytic residues, cofactors, and the mechanism steps of hundreds of enzymes that has been manually curated from the literature and is accessible at www.ebi.ac.uk/thornton-srv/m-csa/ . We are currently developing an algorithm that uses the knowledge stored in M-CSA to predict the mechanism of uncharacterised enzymes using an informatics approach.

15:00 **Carsten Kettner** (Beilstein-Institut, Frankfurt am Main, Germany)

Biocatalysis data flow from the bench to publication platforms

Technical and methodological advances in biocatalysis and enzymology led to enormous amounts of experimental theoretical data which are the basis for the understanding of catalytic mechanisms, enzyme engineering & process development. However, a major challenge for these data and metadata refers to the current practices of sampling and storing of experimental data in academic laboratories which results often in incomplete, irreproducible and even unusable data sets that are not suitable for subsequent research & knowledge generation. Usually, both data acquisition and annotation lacks universally accepted standards for the storage of data and metadata. In addition, even raw data is rarely available in machine-readable format which prevents researchers from analysing, reproducing and reusing it. For the standardized reporting of enzyme function data, the biocatalysis community has established the Standards for Reporting Enzymology Data (STRENDA) Guidelines, which provide the minimum information necessary to describe assay conditions and enzyme activity data. Based on these guidelines the STRENDA Commission has developed a robust web-based validation and storage system for enzymology data – STRENDA DB. As data exchange standards & software support to aid research data management was considered lacking, the community developed the data exchange format EnzymeML. In addition, a first ver-sion of an application programming interface provides Python and Java libraries to be integrated in both applications & databases in order to drive a seamless data flow from the bench to publication platforms. Here, first insights in this EnzymeML landscape are given.

ABOUT THE SPEAKERS

Peter Halling (WestCHEM, Dept Chemistry, University of Strathclyde, Glasgow, Scotland) has researched topics relevant to enzymatic processes since finishing his PhD in 1975, including time in industry. A particular theme for many years was enzyme activity in low water media. Following the closure of his experimental laboratory, he is continuing research using desk studies with meta-analysis of published data, computer simulations and some continuing collaborations with experimentalists. Since his formal retirement at the age of 65 in 2016, Peter Halling is honorary Research Professor at the University of Strathclyde in Glasgow, Scotland.

Antonio Ribeiro (European Molecular Biology Laboratory, European Bioinformatics Institute (EMBL-EBI), Wellcome Trust Genome Campus, Hinxton, Cambridge CB10 1SD, United Kingdom) did his PhD in Porto (Portugal) and Calabria (Italy) where he studied the enzyme mechanisms of several enzymes using computational chemistry methods. After a postdoc in the same group in Porto he then joined the Thornton group at the EBI where Antonio Ribeiro created the M-CSA database by joining two older databases (CSA and MACie). He uses this database to study enzyme evolution and how enzymes work.

Carsten Kettner (Beilstein Institute, Frankfurt, Germany) studied biology at the University of Bonn and obtained his diploma at the University of Göttingen. In 1999, he was awarded his PhD for his work on the biophysical comprehension of the yeast vacuolar ATPase using the patch-clamp tech-niques at the University of Karlsruhe. As a post-doctoral student he continued both the studies on the biophysical properties of both the pump and the plasma membrane potassium channel (TOK1). In 2000 he joined the Beilstein-Institut. Here, he is responsible (a) for the organization of the Beilstein symposia and (b) for the administration and project management of funded research projects. In 2007 he was awarded his certificate of competence as project manager for his studies and thesis from the Studiengemeinschaft Darmstadt (a certified service provider). Since 2004 he coordinates the work of the STRENDA commission and promotes the guidelines for reporting enzyme data along with the commissioners (www.strenda.org). These reporting standards have been adopted by, today, over 55 biochemical journals for their instructions for authors and are incorporated in the electronic data validation and storage tool, STRENDA DB. Since 2011, Carsten co-ordinates the MIRAGE project which aims at establishing uniform reporting and representation of glycomics data in publications and which became an essential hub for the development of glycomics infrastructure (www.beilstein-mirage.org). In 2014, Carsten was appointed the head of the funding and conferences department which is also in charge of the foundation's public relationships. Carsten is very interested in any aspects of open science and open access and thus he is actively engaged in a number of initiatives that are dedicated to make scientific data open and accessible to the wider public including NFDI4Chem, Force11 and RDA (Chemical Data, FAIRsharing).

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 webinars:

22 February 2021 Synthesis Planning and Data Management in Biocatalysis

05 March 2021 Novel Enzymes

26 March 2021 Amine Biocatalysis 4.5

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You are cordially invited to join ESAB online *via* https://esabweb.org/Join+us/Application+form.html

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.