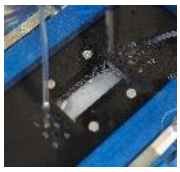

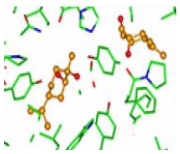
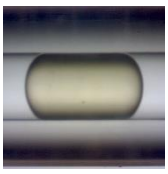

ESAB Webinar

Synthesis planning and data management in biocatalysis

Monday, 22th February 2021 at 14:00 CET

Chairs: Dörte Rother and Torsten Sehl, Institute of Bio- and Geosciences 1: Biotechnology, Research Center Jülich, D

Moderator: Willi Meier, DECHEMA, Frankfurt, D

PROGRAMME

14:00 **Dörte Rother** (IBG-1: Biotechnology, Research Center Jülich, D)

Short introduction.

A motivation, how our community can work together and make use of recent developments in data management and synthesis planning.

14:05 **William Finnigan** (Manchester Institute of Biotechnology, University of Manchester, GB)

RetroBioCat: computer-aided synthesis planning of biocatalytic cascades, and a database for synthetic biotransformations

As the enzyme toolbox for biocatalysis continues to expand, so too does the need for digital tools which capture the potential of enzymes in organic synthesis. Here we present RetroBioCat, a computer aided design tool for the creation of new biocatalytic reactions and cascades [1]. RetroBioCat augments the abilities of scientists by deploying a set of manually curated biocatalysis reaction rules which can be used for computer-aided biocatalytic retrosynthesis. Importantly, RetroBioCat is freely available at https://retrobiocat.com, with a highly accessible user interface. RetroBioCat also leverages its own database of synthetic biotransformations, identifying similar literature reactions where these appear during synthesis planning. The RetroBioCat database is a promising resource in its own right, although data entry remains challenging. To tackle this, we are developing a set tools for community-driven data curation, with automated data extraction from the literature where possible.

1. Finnigan, W., Hepworth, L. J., Flitsch, S. L. & Turner, N. J. RetroBioCat as a computer-aided synthesis planning tool for biocatalytic reactions and cascades. Nat. Catal. (2021) doi:10.1038/s41929-020-00556-z.

14:25 **Jürgen Pleiss** (Institute of Biochemistry and Technical Biochemistry, University of Stuttgart, D)

EnzymeML: F.A.I.R. data management in biocatalysis

Enzyme catalysis provides a powerful toolbox for novel, sustainable synthesis routes and innovative solutions for bio-based chemistry. A comprehensive biochemical characterization of the desired enzyme-catalyzed reaction is essential and provides the basis for enzyme engineering and process development. Standardization of reporting of enzymatic data and metadata is considered as pivotal to accelerating

bioprocess development and reducing costs. Meta-research studies suggest the lack of standardization to report and share experimental protocols, results, and data as one of the causes of the reproducibility crisis in the biomedical sciences. EnzymeML was established as a data exchange format that facilitates interoperability and reusability of enzymatic data by integrating comprehensive information on reaction conditions, time courses of substrate and product concentrations, the selected kinetic model, and the estimated kinetic constants. An Application Programming Interface facilitates the integration of applications such as electronic lab notebooks, modelling platforms, and databases. EnzymeML documents can be stored locally as files or as structured entries on the platform Dataverse, thus making biocatalytic data findable and accessible.

15:45 **Stephan Malzacher** (IBG-1: Biotechnology, Research Center Jülich, D)

BioCatHub – an electronic lab notebook for biocatalysis according to the FAIR data principles

The reproducibility of experiments in biocatalysis is challenging and requires a lot of time and resources. Incomplete or incorrect documentation is one of the main reasons why experiments are not reproducible. To address this challenge, the BioCatHub project was established. The goal of this project is to develop a browser based electronic lab notebook (ELN) in particular for the biocatalysis community. BioCatHub is designed and developed based on the FAIR (Findable, Accessible, Interoperable and Reusable) data principles, using the Strenda (Standards for reporting enzymology data) recommendations as metadata standard and EnzymeML (Enzyme markup language) as exchange format in between researchers, tools and databases. BioCatHub is intended to be a tool, driven by the needs of the biocatalysis community for sustainable research data management.

15:05 **Ulrike Wittig** (HITS gGmbH, Heidelberg Institute for Theoretical Studies, D)

Collecting, curating, interlinking and sharing data with SABIO-RK and FAIRDOM-SEEK

The presentation will focus on two services for collecting, curating, interlinking and sharing data: SABIO-RK and FAIRDOM-SEEK. SABIO-RK (http://sabiork.h-its.org/) is a manually curated database for biochemical reactions and their kinetic properties. Data are mainly extracted from literature and manually curated and annotated to external resources. The database supports experimentalists and modellers in understanding of complex biochemical networks by structuring kinetic data and related information from literature. FAIRDOM-SEEK (https://fairdomseek.org) is a web-based data management platform which supports collaborative and interdisciplinary projects in storing, interlinking and sharing research data. FAIRDOM-SEEK is used in many different national and international research projects and is an integral member of several infrastructure initiatives.

ABOUT THE SPEAKERS

William Finnigan (Manchester Institute of Biotechnology, University of Manchester, GB) received his PhD in 2016, having worked in the groups of Jennifer Littlechild and Nicholas Harmer at the University of Exeter. In Exeter he investigated the use of the thermophile *Thermus thermophilus* as a host organism for whole-cell biocatalysis, and the use of mathematical modelling for the optimization of multi-enzyme systems. Following his PhD, he moved to the University of Manchester where he initially worked on the production of recombinant spider silk as part of the synbiochem center. He now works in the groups of Nicholas Turner and Sabine Flitsch, exploring the potential of digital technologies to speed up research and development in biocatalysis.

Jürgen Pleiss (Institute of Biochemistry and Technical Biochemistry, University of Stuttgart, D) obtained his PhD degree at the Max-Planck-Institute of Biology, Tübingen, under the supervision of Fritz Jähnig. He then joined the company Biostructure S.A., Strasbourg, to develop software for protein modelling. Since 1995, he is head of the bioinformatics group at the Institute of Biochemistry and Technical Biochemistry, where he obtained his habilitation in 2001. His research activities focus on enzyme design by combining bioinformatics and molecular simulation methods, and on the application of computational biology in white and red biotechnology.

Stephan Malzacher (IBG-1: Biotechnology, Research Center Jülich, D) is doing his PhD in the group of Prof. Dörte Rother. He studied biotechnology and focusses in his PhD on the development of BioCatHub, an electronic lab notebook for biocatalysis.

Ulrike Wittig (HITS gGmbH, Heidelberg Institute for Theoretical Studies, D) studied biochemistry at the University of Leipzig and received her PhD in biology at the University of Heidelberg for the experimental work on mechanisms of apoptosis and oxidative stress in mammalian cells. For more than 20 years she is active in the development of biological databases, database curation and data management. She is member of the Systems Biology Service Center of de.NBI /ELIXIR-Germany and the FAIRDOM data management consortium. Ulrike Wittig is getting involved with the Biocuration community and as a member of the STRENDA commission she actively supports the initiative for Standards for Reporting Enzymology Data.

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:

05 March 2021 Novel Enzymes
26 March 2021 Amine Biocatalysis 4.5
April 2021 Sustainable Chemistry, Joint ESAB-SusChem Webinar
May 2021 Biocatalysts from Extremophiles

HOW TO JOIN ESAB

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.