
The 3rd Aachen Protein Engineering Symposium (AcES) was organised by the EFB Biocatalysis Division, VFL Biotec, and the Aachen Protein Engineering Symposium AcES. The AcES provided an overview on state-of-the-art methodologies in protein engineering with a focus on enzyme discovery, diversity generation and high-throughput screening. Industrially applied enzymes and emerging applications in biomaterials concluded the symposium.

The Scientific Programme included the following sessions:

- Enzyme discovery and production
- Computational and structural biology
- Directed evolution methods
- Protein engineering for biological transformation of industry
- Protein engineering: case studies from industry
- Protein engineering for a circular bioeconomy
- Protein engineering and catalysis: case studies from academia
- Protein Engineering across continents: case studies from intercontinental collaborations


# Programme (all times in CET)

| 1 September 2021 | |
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| **13:00-14:55** | **Session 1: "Enzyme discovery and production"** |
| | **Welcome and introduction to the session**<br>**Ulrich Schwaneberg**, RWTH Aachen University, Germany<br>**Jeffrey Cole**, EFB President, United Kingdom |
| | **Invited lecture**<br>*Novel biocatalysts for biotechnology,* **Karl-Erich Jaeger**, HHU Düsseldorf, Germany |
| | **Invited lecture**<br>*Finding novel plastic degrading enzymes in global metagenomes,* **Wolfgang Streit**, Universität Hamburg, Germany |
| | **Invited lecture**<br>*Applying online monitoring and robotic clone screening for the optimization of protein expression,* **Jochen Büchs**, RWTH Aachen University, Germany |
| | **Invited lecture**<br>*Design and engineering of lanthanide-binding proteins,* **Cathleen Zeymer**, TU München, Germany |
| | **Flash talks**<br>*Identification of novel polyester hydrolases from the North Atlantic Garbage Patch deep sea floor*, **Rebecka Molitor**, Heinrich Heine University Düsseldorf, Germany<br>*Discovery and characterization of biosynthetic pathways for biosurfactant production using Pseudomonas putida*, **Sonja Kubicki**, Heinrich-Heine Universität Düsseldorf, Germany<br>*Enriching the diversity of Polyethylene Terephthalate degrading enzymes from Metagenomes*, **Hongli Zhang**, University of Hamburg, Germany<br>*A biocatalytic route towards a Tyrosine-Derivative*, **Sarah Berger**, University of Graz, Austria<br>*Engineering prebiotics through biocatalysis: cloning and characterization of levansucrase from human milk microbiome*, **Evangelia Chronopoulou**, Agricultural University of Athens, Greece |


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| | **Q & A** |
| **15:05-17:00** | **Session 2: "Computational and structural biology"** |
| | **Introduction to the session**<br>**Jan Marienhagen,** Forschungszentrum Jülich |
| | **Invited lecture**<br>*The structural and functional characterization of mammalian flavin-containing monooxygenases (FMOs) using ancestral sequence,* **Andrea Mattevi**, University of Pavia, Italy |
| | **Invited lecture**<br>*Overcoming the limitations of computational chemistry approaches in industry,* **Maria F. Lucas**, Zymvol, Spain |
| | **Invited lecture**<br>*Radical enzymes - new methods to consider enzyme impact on reaction,* **Anna Croft**, University of Nottingham, United Kingdom |
| | **Invited lecture**<br>*Computer aided enzyme engineering for sustainable detergent applications,* **Mehdi Davari**, Leibniz Institute of Plant Biochemistry, Halle, Germany |
| | **Short talks**<br>*Molecular basis for the endoperoxide formation by Fe(II)/α-KG-dependent oxygenase NvfI*, **Takahiro Mori**, The University of Tokyo, Japan<br>*Engineering of an organic solvent tolerant esterase based on computational predictions*, **Lara Scharbert**, Forschungszentrum Jülich GmbH, Germany<br>*Combining in silico and in vitro methods to discover new aldoxime dehydratases*, **Natalia Kulik**, CNSB, Microbiologicky ustav AV CR, Czech Republic |
| | **Flash talks**<br>*Design and development of acetylcholinesterase (AChE) inhibitor peptides with application in aquaculture: a bioinformatics approach through QSAR*, **Tanya Roman**, PUCV, Chile<br>*Enhancement of laccases thermostability in Betaine - based Natural Deep Eutectic Solvents*, **Simona Varriale**, Biopox, Italy |
| | **Q & A** |


| 2 September 2021 | |
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| **9:00-10:30** | **Session 3: „Directed evolution methods"** |
| | **Introduction to the session**<br>**Lothar Elling**, RWTH Aachen University, Germany |
| | **Invited lecture**<br>*Lessons learned from 20 years directed enzyme evolution and how to recombine beneficial substitutions* **Ulrich Schwaneberg**, RWTH Aachen University, Germany |
| | **Short talks**<br>*cDNA display coupled with next-generation sequencing for rapid activity-based screening: Analysis of transglutaminase substrate preference*, **Jasmina Damnjanovic**, Nagoya University, Japan<br>*Developing a cell-bound detection system for the screening of oxidase activity using the fluorescent peroxide sensor roGFP2-Orp1*, **Clemens Peterbauer**, Universität für Bodenkultur Wien, Austria<br>P*henotypic Selections for Biocatalyst Design and Evolution*, **Rudy Rubini**, University of Groningen, the Netherlands |
| | **Flash talks**<br>*Designing a microfluidics platform to discover enzyme variants for increased fatty acid production*, **Paul Matthay**, KU Leuven, Belgium<br>*Veratrol-O-demethylase - Aromatic and Oxygen-free O-Demethylation*, **Christopher Grimm**, University of Graz, Austria<br>*Biochemical, kinetic, and structural analysis of a BsDyP hit variant with improved activity for phenolic compounds*, **Carolina Rodrigues**, Instituto de Tecnologia Química e Biológica (ITQB), Universidade Nova de Lisboa, Portugal<br>*Stopped-flow kinetic Studies of PQQ-Dependent Coprinopsis cinerea Pyranose Dehydrogenase*, **Georg Schütz**, BOKU University, Austria |
| | **Q & A** |
| **10:40-12:20** | **Session 4: „Protein engineering for biological transformation of industry"** |
| | **Introduction to the session**<br>**Ulrich Schwaneberg**, RWTH Aachen University, Germany |


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| | **Invited lecture**<br>*De novo enzyme cascades for organic synthesis,* **Sabine Flitsch**, University of Manchester, United Kingdom |
| | **Invited lecture**<br>*Functionalization by protein surface coating as an example for biological transformation in production engineering,* **Sebastian Barth**, RWTH Aachen University, Germany |
| | **Invited lecture**<br>*Towards sustainable biocatalyzed synthesis of Rhamnose esters,* **Maria J. Hernaiz**, Universidad Complutense, Spain |
| | **Invited lecture**<br>*Thermostable carbonic anhydrases for enzyme-catalysed capture of $CO_2$,* **Anca Pordea**, University of Nottingham, United Kingdom |
| | **Flash talks**<br>*Rational engineering of D-tagatose 3-epimerase from Pseudomonas cichorii to increase its thermostability and acidic pH stability*, **Debamitra Chakravorty**, Novel Techsciences (OPC) Private Limited, India<br>*Carbon-based nanomaterials for the development of anti-leukemic drugs*, **Rita Barros**, Universidade do Porto - Faculdade de Engenharia, Portugal<br>*Screening and immobilization of commercial lipases for a sustainable and efficient synthesis of sugar esters*, **Pilar Hoyos**, Universidad Complutense de Madrid, Spain<br>*Immobilization of Pseudomonas stutzeri lipase on hydrophobic supports for industrial applications*, **Almudena Perona Requena**, UCM-Faculty of Pharmacy, Spain<br>*Development of a green bioprocess mediated by Pseudomonas stutzeri lipase for the synthesis of sugar-based biosurfactants*, **Cecilia Garcia Oliva**, Universidad Complutense de Madrid, Spain |
| | **Q & A** |
| **13:25-14:50** | **Session 5: „Protein engineering: case studies from industry“** |
| | **Introduction to the session**<br>**Maria J. Hernaiz**, Universidad Complutense, Spain |
| | **Invited lecture** |


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| | *Enzyme discovery and engineering - two strategies, one goal*, **Alexander Pelzer**, BRAIN Biotech AG, Germany |
| | **Invited lecture**<br>*Rational engineering of industrial biocatalysis,* **Alexandra Teresa Pires Carvalho**, Almac Sciences, United Kingdom |
| | **Invited lecture**<br>*KnowVolution-based engineering of an NADH-dependent Ketol-Acid Reductoisomerase for increased flux efficiency in yeast***, Markus Spiertz**, SeSam-Biotech, Germany |
| | **Short talks**<br>*Efficient BVMO-catalyzed enantioselective sulfoxidation for API production: from assay miniaturization to rationally guided engineering*, **Francesco Falcioni**, AstraZeneca, United Kingdom<br>*Rapid, multiplexed genome editing for improved heterologous protein engineering and expression in E.coli*, **Laura Klitten**, Inscripta Inc., Denmark |
| | **Flash talks**<br>*Anchor peptides: a green and versatile method for polymer and plant surface functionalization***, Abdulkadir Yayci, DWI - Leibniz Institute for Interactive Materials, Germany**<br>*A peptide-based coating toolbox to enable click chemistry on polymers, metals, and silicon through sortagging***, Maximilian Noeth, RWTH Aachen University, Germany** |
| | **Q & A** |
| **15:00-17:00** | **Session 6: „Protein engineering for a circular bioeconomy“** |
| | **Introduction to the session**<br>**Mehdi Davari**, Leibniz Institute of Plant Biochemistry, Halle, Germany |
| | **Invited lecture**<br>*Moving the bioeconomy from mind to market: what drives technology transfer and innovation adoption***, Stefanie Bröring**, Universität Bonn, Germany |
| | **Invited lecture**<br>*Distal mutations shape substrate-binding sites during evolution of a metalle-oxidase into a Laccase,* **Ligia O. Martins**, ITQB NOVA, Portugal |


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| | **Invited lecture**<br>*Engineering of cytochromes P450 as biocatalysts for selective multistep oxidation,* **Vlada Urlacher**, Heinrich Heine University, Germany |
| | **Invited lecture**<br>*Engineering and application of a biosensor with focused ligand specificity*, **Jan Marienhagen**, Forschungszentrum Jülich, Germany |
| | **Short talk**<br>*Enzyme engineering and metabolic engineering for apocarotenoids production*, **Xixian Chen**, Agency for Science, Technology and Research, Singapore |
| | **Flash talks**<br>*Purification and characterization of SeLipC, a novel lipase from Streptomyces exfoliatus with application in sugar ester synthesis*, **Juan Toledo**, Universidad Complutense de Madrid, Spain<br>*Cloning, expression and characterization of novel extracellular lipase A from Streptomyces exfoliatus DSMZ 41693: a useful biotechnological biocatalyst*, **Guillermo Rodriguez**, Universidad Complutense of Madrid, Spain<br>*Exploiting the potential of Photosystem I for in vitro biocatalysis*, **Hitesh Medipally**, Ruhr University Bochum, Germany<br>*Decarboxylation mechanisms to produce drop-in chemicals from fatty acids by P450 peroxygenases,* **Leticia Zanphorlin,** Brazilian Biorenewables National Laboratory, Brazilian Center for Research in Energy and Materials (CNPEM), Brazil<br>*C-terminus influences the thermostability of endoglucanase PvCel5A*, **Francisca Contreras**, Institute of Biotechnology RWTH, Germany |
| | **Q & A** |
| **3 September 2021** | |
| **9:00 – 10:40** | **Session 7: „Protein engineering and catalysis: case studies from academia“** |
| | **Introduction to the session**<br>**Jeffrey Cole**, EFB President, United Kingdom |
| | **Invited lecture**<br>*Enzyme engineering for improved robustness*, **Marco Fraaije**, University of Groningen, the Netherlands |


**Invited lecture**

*Photobiocatalytic decarboxylation reactions,* **Frank Hollmann**, TU Delft, the Netherlands

**Invited lecture**

*Enzyme cascades for the synthesis of hyaluronic acid*, **Lothar Elling**, RWTH Aachen University, Germany

**Invited lecture**

*Wild-type & engineered aldoxime dehydratases as biocatalysts for an alternative nitrile synthesis*, **Harald Gröger**, Universität Bielefeld, Germany

**Short talk**

*Characterization and improvement of a nicotine degrading flavoenzyme*, **Mark Dulchavsky**, University of Michigan, USA

**Flash talks**

*Enzymatic phosphorus mobilization from deoiled seeds,* **Anna Joelle Ruff**, RWTH Aachen University - Lehrstuhl für Biotechnologie, Germany

*Anchor peptide-mediated enhancement of synthetic polymer degradation,* **Yi Lu**, Institute of Biotechnology RWTH, Germany

*Biofilm systems as tools in the production of recombinant proteins and other added-value compounds*, **Luciana Gomes**, LEPABE - Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculty of Engineering, University of Porto, Portugal

*Engineering lactate oxidase by ancestral sequence reconstruction*, **Leander Suetzl**, University of Natural Resources and Life Sciences - BOKU, Austria

*Immobilization as a protective strategy for plasma-driven biocatalysis*, **Tim Dirks**, Ruhr-Universität Bochum, Germany

*Exploring the evolutionary trajectory of a bacterial pyranose-2-oxidase*, **André Taborda**, ITQB NOVA, Portugal

*Immobilization of Thermostabilized Enzymes in Flow Reactors*, **Martin Peng**, Karlsruhe Institute of Technology, Institute for Biological Interfaces, Germany

**Q & A**


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| **10:50-12:55** | **Session 8: "Protein Engineering across continents: case studies from intercontinental collaborations"** |
| | **Introduction and signing ceremony for the cooperation agreement on TIB-IB RWTH Joint Center of Biotechnology**<br>**Qinhong Wang,** Tianjin Institute of Industrial Biotechnology, China<br>**Ulrich Schwaneberg**, RWTH Aachen University, Germany |
| | **Invited lecture**<br>*Valorization of formaldehyde and protein engineering of the key enzyme,* **Leilei Zhu**, Tianjin Institute of Industrial Biotechnology, China |
| | **Short talks**<br>*Semi-rational engineering for asymmetric synthesis,* **Jinhui Feng**, Tianjin Institute of Industrial Biotechnology, China<br>*Protein engineering of glycosyltransferase and phosphorylase to improve their activity and thermostability,* **Jiangang Yang**, Tianjin Institute of Industrial Biotechnology, China<br>*Droplet-based microfluidics for high-throughput screening and industrial application*, **Ran Tu**, Tianjin Institute of Industrial Biotechnology, China<br>*Rational design of industrial enzymes*, **Ge Qu**, Tianjin Institute of Industrial Biotechnology, China |
| | **Invited lecture**<br>*Rational design of hydrolytic enzymes for industrial applications,* **Anna Dotsenko**, FRC "Fundamentals of Biotechnology" of the Russian Academy of Sciences, Russia |
| | **Invited lecture**<br>***Protein engineering for asymmetric synthesis of L-Phosphinothricin,*** **Feng Cheng**, Zhejiang University of Technology, China |
| | **Q & A and closing remarks** |
| **13:00-14:00** | **Poster session** |