Biocatalysis
22 -24 May 2024
London, UK and online
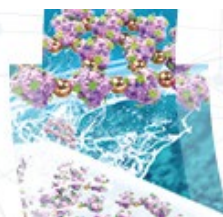
Wednesday 22 May 2024

11:30	Registration with lunch served from 11:45
12:45	**Welcome and introductions** Adrian Mulholland and Nicholas Turner, *Co-Chairs*, *Chair of Scientific Committee*
12:55	**Outline of Discussion format** Robert Hinde and Samuel Oldknow, *Royal Society of Chemistry Publishing Editors*
13:00	**Introductory Lecture – Spiers Memorial Lecture** (Session chair: Nicholas Turner) Donald Hilvert *ETH Zurich, Switzerland*
14:00	Comfort break (no refreshments)
	Session 1: Enzyme evolution, engineering and design: mechanism and dynamics (Session chair: Adrian Mulholland)
14:15	**Indigo production identifies hotspots in cytochrome P450 BM3 for diversifying aromatic hydroxylation** Joelle Pelletier, Douglas J. Fansher, Jonathan N. Besna *University of Montreal, Canada*
14:20	**Tuning the peroxidase activity of artificial P450 peroxygenase by engineering redox-sensitive residues** Zhiqi Cong, Fengjie Jiang, Zihan Wang *Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, China*
14:25	**Exploring the selectivity of cytochrome P450 for enhanced novel anticancer agent synthesis** Jeremy Harvey, Janko Čivić, Neil R. McFarlane, Joleen Masschelein *KU Leuven, Belgium*
14:30	Discussion
15:45	Refreshments
	Session 1 continued: Enzyme evolution, engineering and design: mechanism and dynamics (Session chair: Fraser Armstrong)
16:15	**On synergy between ultrahigh throughput screening and machine learning in biocatalyst engineering** Florian Hollfelder, Maximilian Gantz, Simon V. Mathis, Friederike E. H. Nintzel, Pietro Lio *University of Cambridge, UK*
16:20	**High-throughput selection of (new) enzymes: phage display-mediated isolation of alkylhalide hydrolases from a library of active-site mutated epoxide hydrolases** Mikael Widersten, Marija Blazic, Candice Gautier, Thomas Norberg *Uppsala University, Sweden*
16:25	Discussion
17:15	Lightning presentations – odd numbers (by invitation of the Scientific Committee)
17:30	Poster session (odd numbers)
19:00	Close

Thursday 23 May

	Session 2: Biocatalytic pathways, cascades, cells and systems (Session chair: Uwe Bornscheuer)	
09:00	**Enhancement of essential cofactors for *in vivo* biocatalysis** Pimchai Chaiyen, Pattarawan Intasian, Chalermroj Sutthaphirom, Oliver Bodeit, Duangthip Trisrivirat, Ninlapan Kimprasoot, Juthamas Jaroensuk, Barbara Bakker, Edda Klipp *Vidyasirimedhi Institute of Science and Technology, Thailand*	
09:05	**Developing deprotectase biocatalysts for synthesis** Dominic Campopiano, Lisa Kennedy, Mariyah Sajjad, Michael A. Herrera, Peter Szieber, Natasza Rybacka, Yinan Zhao, Craig Steven, Zainab Alghamdi, Ivan Zlatkov, Julie Hagen, Chloe Lauder, Natalie Rudolfova, Magdalena Abramiuk, Karolina Bolimowska, Daniel Joynt, Angelica Lucero, Gustavo Perez Ortiz, Annamaria Lilienkampf, Alison N. Hulme *University of Edinburgh, UK*	
09:10	Discussion	
10:00	Refreshments	
	Session 2 continued: Biocatalytic pathways, cascades, cells and systems (Session chair: Bruce Lichtenstein)	
10:30	**Retuning the potential of the electrochemical leaf** Clare Megarity, Marta M. Dolinska, Adam J. Kirwan University of Manchester, UK	
10:35	**Surveying the scope of aromatic decarboxylations catalyzed by prenylated-flavin dependent enzymes** Neil Marsh, Anushree Mondal, Pronay Roy, Jaclyn Carrannatto, Prathamesh M. Datar, Daniel J. DiRocco, Katherine Hunter *University of Michigan, USA*	
10:40	**Oxygen-resistant [FeFe]hydrogenases: new biocatalysis tools for clean energy and cascade reactions** Francesca Valetti, Simone Morra, Lisa Barbieri, Sabrina Dezzani, Alessandro Ratto, Gianluca Catucci, Sheila J. Sadeghi and Gianfranco Gilardi *University of Torino, Italy*	
10:45	Discussion	
12:00	Lunch	
	Session 3: Artificial, biomimetic and hybrid enzymes (Session chair: Amanda Jarvis)	
13:30	**Computation-guided engineering of distal mutations in an artificial enzyme** Gerard Roelfes, Fabrizio Casilli, Miquel Canyelles-Niño and Lur Alonso-Cotchico *University of Groningen, Netherlands*	
13:35	**Designing Michaelases: Exploration of novel protein scaffolds for iminium biocatalysis** Ivana Drienovska, Alejandro Gran-Scheuch, Stefanie Hanreich, Iris Keizer, Jaap Harteveld, Eelco Ruijter *VU Amsterdam, Netherlands*	
13:40	**An efficient pyrrolysyl-tRNA synthetase for economical production of MeHis-containing enzymes** Anthony Green, Amy E. Hutton, Jake Foster, James E. J. Sanders, Christopher J. Taylor, Stefan A. Hoffmann, Yizhi Cai, Sarah L. Lovelock *University of Manchester, UK*	
13:45	Discussion	
15:00	Refreshments	
	Session 3 continued: Artificial, biomimetic and hybrid enzymes (Session chair: Jeremy Harvey)	
15:30	**Harnessing conformational dynamics in enzyme catalysis to achieve nature-like catalytic efficiencies: The shortest path map tool for computational enzyme design** Sílvia Osuna, Cristina Duran, Guillem Casadevall *Universitat de Girona & ICREA, Spain*	

15:35	**Computational study of the Mechanism of a polyurethane esterase A (PueA) from *Pseudomonas chlororaphis*** <u>Vincent Moliner</u>, Katarzyna Świderek, Sergio Martí, Kemel Arafet *Universitat Jaume I, Spain*
15:40	**Friends and relatives: insight into conformational regulation from orthologues and evolutionary lineages using KIF and KIN** <u>Lynn Kamerlin</u>**, Dariia Yehorova, Rory M. Crean, Peter M. Kasson *Georgia Institute of Technology, USA*
15:45	Discussion
17:00	Lightning presentations – even numbers (by invitation of the Scientific Committee)
17:15	Poster session – (even numbers)
18:45	Conference dinner – Library, Burlington House

Friday 24 May

	Session 4: Biocatalysis for industry, medicine and the circular economy (Session chair: Meilan Huang)
09:00	**Degradation of PET microplastic particles to monomers in human serum by PETase** Per-Olof Syrén, Ximena Lopez-Lorenzo, David Hueting, Eliott Bosshard *KTH Royal Institute of Technology, Sweden*
09:05	**Towards controlling activity of a peptide asparaginyl Ligase (PAL) by lumazine synthetase compartmentalization** Louis Luk and T.M Simon Tang *Cardiff School of Chemistry, UK*
09:10	**On the biocatalytic synthesis of silicone polymers** Lu Shin Wong and Yuqing Lu *University of Manchester, UK*
09:15	Discussion
10:30	Refreshments
	Session 4: Biocatalysis for industry, medicine and the circular economy (Session chair: Dominic Campopiano)
11:00	**An engineered T7 RNA Polymerase for efficient co-transcriptional capping with reduced dsRNA byproducts in mRNA synthesis** Stefan Lutz *Codexis, USA*
11:05	**Application of rational enzyme engineering in a new route to Etonogestrel and Levonorgestrel: Carbonyl reductase bioreduction of ethyl secodione** Daniel Dourado, Andrew S. Rowan, Sergej Maciuk, Gareth Brown, Darren Gray, Jenny Spratt, Alexandra T. P. Carvalho, Dražen Pavlović, Fernando Tur, Jill Caswell, Derek J. Quinn, Thomas S. Moody and Stefan Mix *Almac Sciences, UK*
11:10	**Investigating the effect of fusion partners on the enzymatic activity and thermodynamic stability of poly(ethylene terephthalate) degrading enzymes** Bruce Lichtenstein, Liliana Oliveira, Alex Cahill, Len Wuscher, Kerry R. Green, Victoria Bemmer *University of Portsmouth, UK*
11:15	Discussion
12:30	**Concluding remarks lecture** (Session chair: Adrian Mulholland) Uwe Bornscheuer *University of Greifswald, Germany*
13:00	**Acknowledgements and presentation of poster prizes**
13:15	**Close of meeting and lunch**

All timings are in BST
** presenting online
Please note that this is a draft programme and timings may change.