

Enzyme Engineering XXVI

Dallas/Fort Worth, Texas, USA
22-27 May 2022

ISBN: 978-1-7138-8681-5

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571

Some format issues inherent in the e-media version may also appear in this print version.

Copyright© (2022) by Engineering Conferences International
All rights reserved.

Printed with permission by Curran Associates, Inc. (2025)

For permission requests, please contact Engineering Conferences International
at the address below.

Engineering Conferences International
32 Broadway, Suite 314
New York, NY 10004
USA

Phone: (212) 514-6760
Fax: (212) 514-6030

info@engconfintl.org

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2633
Email: curran@proceedings.com
Web: www.proceedings.com

Sunday, May 22, 2022

14:00 Conference check-in

Opening Session

17:00 – 17:15 Chairs welcome and opening remarks
Andy Bommarius, Georgia Institute of Technology, USA
Vesna Mitchell, Codexis, USA
Doug Fuerst, GSK, USA

17:15 – 18:15 **Plenary Talk**
Using machine learning to improve protein function
Andrew Ellington, The University of Texas at Austin, USA

33

19:00 – 20:30 Dinner

Monday, May 23, 2022

07:00 – 08:30	Breakfast	
	<u>Session 1: Enzyme Engineering in Synthetic Biology</u> (Sponsored by Illumina) Chair: Daniela Grabs, Arzeda, USA	
08:30 – 09:15	Enzyme engineering for metabolic engineering Kristala L.J. Prather, Massachusetts Institute of Technology, USA	
09:15 – 09:45	Exploring constraints of sequence space in search of optimal enzymes Sridhar Govindarajan, ATUM, USA	3
09:45 – 10:05	<i>In silico</i> screening of transaminase using semi-empirical QM/MM approach Marc Hayes, Enzymaster, USA	2
10:05 – 10:45	Coffee Break (Sponsored by the Japanese Society of Enzyme Engineering)	
10:45 – 11:15	Engineering enzymes to produce high purity synthetic DNA Anders Knight, Codexis, USA	1
11:15 – 11:45	A deep learning tool for protein engineering Huimin Zhao, University of Illinois at Urbana-Champaign, USA	4
11:45 – 12:15	Engineering enzymes for green manufacturing of noncanonical amino acids David Romney, Aralez Bio, USA	
12:15 – 13:45	Lunch & Networking	
	<u>Session 2: Computational Tools for Enzyme Engineering</u> Chair: Sridhar Govindarajan, ATUM, USA	
13:45 – 14:30	Evaluation of sequence/activity relationships for more than 50 proteins: Implications for natural and directed evolution, protein engineering and machine learning algorithms David Estell, Genencor International, Inc., USA	
14:30 – 15:00	Advanced database mining integrating sequence and structure bioinformatics with microfluidics challenges enzyme engineering Zbynek Prokop, Masaryk University, Czech Republic	9
15:00 – 15:20	Helix engineering: Combining the power of 3DM with AI to disrupt protein engineering Stephan Heijl, Bio-Product, Netherlands	7
15:20 – 16:00	Coffee Break	

Monday, May 23, 2022 (continued)

16:00 – 16:30	Engineering a C4 fructose epimerase for production of tagatose Kyle Roberts, Arzeda, USA	6
16:30 – 16:50	Powering computational enzyme design with natural evolutionary information Wenjun Xie, University of Southern California, USA	8
16:50 – 17:10	Engineering proteins with 3D convolutional neural networks Daniel Diaz, The University of Texas at Austin, USA	5
17:10 – 17:30	The use of machine learning to navigate the sequence-activity landscape during directed evolution campaigns Oscar Alvizo, Codexis, USA	
18:00 – 19:30	Dinner & Networking	
19:30 – 21:30	Poster Session & Chairs' Reception	

Tuesday, May 24, 2022

07:00 – 08:30	Breakfast		
	<u>Session 3: New Technologies for Enzyme Engineering</u>		
	Chair: Misha Golynskiy, Illumina, USA		
08:30 – 09:15	Leveraging microfluidics for linking protein sequence to function in high-throughput		
	Polly Fordyce, Standard University, USA		
09:15 – 09:45	Fast evolution of active and/or enantioselective enzymes with a microfluidic enzyme screening platform	14	
	Zhi Li, National University of Singapore, Singapore		
09:45 – 10:15	GENOSCALER™: A Next-Generation high throughput enzyme, pathway, and genome engineering platform		13
	Richard Fox, Infinome, USA		
10:15 – 10:45	Coffee Break (<i>Sponsored by Purolite Ltd</i>)		
10:45 – 11:05	The impact of bioinformatics on industrial enzyme engineering		
	Andreas Vogel, c-LEcta GmbH, Germany		
11:05 – 11:25	High-throughput enzyme engineering for commercial-scale production of natural products		12
	Irina Koryakina, Amyris, Inc., USA		
11:25 – 11:45	A hyperstable glycosyltransferase for blue denim dyeing	11	
	Gonzalo Bidart, Technical University of Denmark, Denmark		
11:45 – 12:05	Immobilized enzymes for green pharmaceutical applications	10	
	Fred Ghanem, Purolite, USA		
12:05 – 13:45	Lunch & Networking		
	<u>Session 4: Novel Enzymes and Enzyme Activity</u>		
	Chair: Ee Lui Ang, Singapore Institute of Food and Biotechnology Innovation, Singapore		
13:45 – 14:30	Photoenzymatic Catalysis - Using light to reveal new enzyme functions		
	Todd Hyster, Cornell University, USA		
14:30 – 15:00	Design and evolution of enzymes with non-canonical catalytic mechanisms		15
	Anthony Green, University of Manchester, United Kingdom		
15:00 – 15:20	Engineering substrates of transglutaminase using the Glutamine-Walk Strategy for specific modification of IgG1 antibodies	17	
	Joelle Pelletier, University of Montreal, Canada		
15:20 – 16:00	Coffee Break		

Tuesday, May 24, 2022 (continued)

16:00 – 16:45	Boosting squalene-hopene cyclase towards an industrial biocatalyst Bernhard Hauer, University of Stuttgart, Germany	
16:45 – 17:15	Carboxyesterase-mediated amidation James Morrison, GSK, USA	16
17:15 – 17:35	New techniques for the production of high-performing industrial enzymes Michael Lischka, BASF Enzymes LLC, USA	18
17:35 – 17:55	Overcoming challenges in organofluorine biosynthesis by engineered fluorinases Pravin Kumar, Kcat Enzymatic Private Limited, India	19
18:00 – 19:30	Dinner & Networking	
19:30 – 21:30	Poster Session	

Wednesday, May 25, 2022

07:00 – 08:30	Breakfast	
	<u>Session 5: Process Modeling in Enzyme Engineering</u>	
	Chair: Huimin Zhao, University of Illinois at Urbana-Champaign, USA	
08:30 – 09:15	Modelling biocatalytic processes to accelerate enzyme and process development	
	John Woodley, Technical University of Denmark, Denmark	
09:15 – 09:45	Benefits of reaction engineering in biocatalysis	21
	Zvezdana Findrik Blažević, University of Zagreb, Croatia	
09:45 – 10:05	Towards engineering an efficient and thermostable α-amino ester hydrolase (AEH): Minimizing substrate inhibition and deactivation for continuous production of cephalexin	20
	Colton Lagerman, Georgia Institute of Technology, USA	
10:05 – 10:45	Coffee Break (<i>Sponsored by Merck & Co., Inc.</i>)	
	<u>Session 6: Enzymes and Nucleic Acids</u>	
	Chair: Sonya Clark, 10xGenomics, USA	
10:45 – 11:30	Biocatalytic synthesis of nucleoside and nucleotide therapeutics	22
	John McIntosh, Merck, USA	
11:30 – 12:00	Biocatalytic oligonucleotide synthesis technology-BOOST	
	Jill Caswell, Almac, USA	
12:00 – 12:20	Biocatalytic approaches to therapeutic oligonucleotide manufacture	24
	Sarah Lovelock, University of Manchester, United Kingdom	
12:20 – 12:40	Optimizing enzyme production to support commercial mRNA manufacturing	23
	Juozas Siurkus, Thermo Fisher Scientific, Lithuania	
12:40	Lunch / Free afternoon for networking & sightseeing	
	Dinner on your own	

Thursday, May 26, 2022

07:00 – 08:30	Breakfast	
	<u>Session 7: Enzyme Engineering for Environmental Applications</u>	
	Chair: Michael Liszka, BASF Enzymes LLC, USA	
08:30 – 09:15	PET recycling: From enzyme engineering to a first industrial unit Alain Marty, Carbios, France	
09:15 – 09:35	Engineering enzymes for microbial control: Cell-free methods for enhancing antimicrobial efficacy through directed evolution Erika Milczek, Curie Co. Inc., USA	25
09:35 – 09:55	Directed evolution of an efficient and thermostable PET depolymerase Elizabeth Bell, University of Manchester, United Kingdom	
09:55 – 10:15	Engineering of a redox neutral enzyme cascade for production of aliphatic diamines Hannah Valentino, Oak Ridge National Lab, USA	26
10:15 – 11:00	Coffee Break	
	<u>Poster Talks</u>	
	Chairs: Richard Fox, Infinome Biosciences, USA Zhi Li, National University of Singapore	
11:00 – 11:05	Announcement of Winners of the Poster Competition	
11:05 – 11:20	Winner 1	
11:20 – 11:35	Winner 2	
11:35 – 11:50	Winner 3	
12:00 – 13:30	Lunch	
	<u>Session 8: In Memoriam - Hideaki Yamada</u>	
	Chair: Jun Ogawa, Kyoto University, Japan	
13:30 – 14:10	Memories of late professor Hideaki Yamada, a giant in enzyme engineering, and successive activities stemmed from his philosophy Jun Ogawa, Kyoto University, Japan	29
14:10 – 14:50	Continuity and change in screening for industrial enzymes and protein engineering- A tribute to the late Professor Hideaki Yamada Yasuhisa Asano, Toyama Prefectural University; ERATO, JST, Japan	32
14:50 – 15:10	Basics and applications of gut bacterial lipid-metabolizing enzymes- A tribute to the late Professor Hideaki Yamada Shigenobu Kishino, Kyoto University, Japan	31
15:10 – 15:30	Development of P450-BM3 using molecular dynamics simulations- A tribute to the late Professor Hideaki Yamada Satoru Ishihara, Amano Enzyme Inc., Japan	30

Thursday, May 26, 2022 (continued)

15:30 – 16:00 Coffee Break

Session 9: In Memoriam - Dan Tawfik

Chair: David Baker, University of Washington, USA

16:00 – 16:30 **Protein design using deep learning**
David Baker, University of Washington, USA 27

16:30 – 17:00 **Making better proteins: Learning from the best**
Olga Khersonsky, Weizmann Institute of Science, Israel 28

17:00 – 17:30 **Adventures on the routes of enzyme evolution – In memoriam Dan Tawfik**
Nobu Tokuriki, University of British Columbia, Canada

17:30 – 18:00 **Evolutionary-guided cofactor engineering**
Paola Laurino, Okinawa Institute of Science and Technology Graduate University, Japan

Enzyme Engineering Award Presentation and Lecture

18:00 – 18:10 **Introduction and Presentation of the Enzyme Engineering Award**
David Estell, Genencor International, Inc., USA
Jeff Moore, Merck & Co., Inc., USA
Joelle Pelletier, University of Montreal, Canada

18:10 – 19:10 **Enzyme Engineering Award Lecture**
Biocatalysis and enzyme engineering – a personal view on the last three decades
Uwe Bornscheuer, Greifswald University, Germany

19:30 – 22:00 Reception and Banquet

Friday, May 27, 2022

07:00 Breakfast & Departure

Poster Presentations

1. **Design and evolution of enzymes for the Morita-Baylis-Hillman reaction** 34
Amy Crossley, University of Manchester, United Kingdom
2. **An engineered cytidine deaminase for biocatalytic production of a key intermediate of the COVID-19 antiviral Molnupiravir** 35
Ashleigh Burke, University of Manchester, United Kingdom
3. **Galectin-Anchored indoleamine 2,3-dioxygenase tissue-targeted therapeutic enzyme suppresses local inflammation in multiple animal models** 36
Benjamin Keselowsky, University of Florida, USA
4. **Biocatalytical access to amides** 37
Erna Zukic, acib, University of Graz, Austria
5. **Engineering of styrene oxide isomerase for enhanced production of (S)-2-arylpropionaldehydes** 38
Joel Choo Ping Syong, National University of Singapore, Singapore
6. **Assessment of C-type halohydrin dehalogenase stability** 39
Nevena Milčić, University of Zagreb, Croatia
7. **Screening millions of droplet-compartmentalized single cells with Xdrop®** 40
Peter Mouritzen, Samplix Aps, Denmark
8. **Determination of the rate limiting step during zearalenone hydrolysis by ZenA** 41
Sebastian Fruhauf, DSM - BIOMIN Research Center, Austria
9. **Efficient enzyme discovery from complex environmental microbiota using microbial single-cell sequencing** 42
Soichiro Tsuda, bitBiome Inc., Japan
10. **A cell-free platform for the directed evolution of toxic enzymes and proteins** 43
Will Shindel, Curie Co, USA
11. **FireProt ASR: Automated design of ancestral proteins** 44
Zbynek Prokop, Masaryk University, Czech Republic
12. **EnzymeMiner: Exploration of sequence space of enzymes** 45
Zbynek Prokop, Masaryk University, Czech Republic
13. **Unlocking the key to successful commercialization by coupling the power of biocatalysis, strain engineering, and application studies** 46
Khin Oo, Fornia BioSolutions, Inc., USA
14. **Ketoreductase immobilization for batch and flow processes** 47
Fred Ghanem, Purolite, USA
15. **In silico screening of transaminase using semi-empirical QM/MM approach** 48
Marc Hayes, Enzymaster, USA

16. **Toward engineering an efficient and thermostable α -Amino Ester Hydrolase (AEH): Minimizing substrate inhibition and deactivation for continuous production of cephalixin** 49
Colton Lagerman, Georgia Institute of Technology, USA
17. **Engineering of a redox neutral enzyme cascade for production of aliphatic diamines** 50
Hannah Valentino, Oak Ridge National Lab, USA
18. **Overcoming challenges in organofluorine biosynthesis by engineered fluorinases** 51
Pravin Kumar, KCAT Enzymatic Private Limited, India
19. **7D-Grid-AI-Technology: A technology that translates enzymes from a computer to business with limited lab experiments** 52
Pravin Kumar, KCAT Enzymatic Private Limited, India
20. **In silico guided CRISPR-Cas driven enzyme engineering framework: An automated and efficient enzyme engineering method** 53
Pravin Kumar, KCAT Enzymatic Private Limited, India
21. **QM/MM Studies of The phenylalanine ammonia-lyase variants helped to understand the mechanistic role of the mutations** 54
Pravin Kumar, KCAT Enzymatic Private Limited, India
22. **discovery of CDX-6512, a gastrointestinal-stable methionine-gamma-lyase as a potential orally-administered enzyme therapy for homocystinuria**
Leann Teadt, Codexis, Inc., USA