

Program

Enzyme Engineering XXV

September 15-19, 2019
Whistler Resort
Whistler, British Columbia, Canada

Conference Co-Chairs

Huimin Zhao
University of Illinois at Urbana-Champaign, USA

John Wong
Pfizer, USA



Engineering Conferences International
32 Broadway, Suite 314 - New York, NY 10004, USA
www.engconfintl.org – info@engconfintl.org

Conference Hotel:

**Hilton Whistler Resort & Spa
4050 Whistler Way
Whistler, BC
V0N 1B4, Canada
Tel: +1-604-932-1982**

Conference Sessions:

**Whistler Conference Centre
4010 Whistler Way
Whistler, BC
V8E 1J2, Canada
Tel: +1 604-932-3928**

Engineering Conferences International (ECI) is a not-for-profit global engineering conferences program, originally established in 1962, that provides opportunities for the exploration of problems and issues of concern to engineers and scientists from many disciplines.

ECI BOARD MEMBERS

Barry C. Buckland, President
Mike Betenbaugh
Joye Bramble
Nick Clesceri
Peter Gray
Michael King
Raymond McCabe
Eugene Schaefer
P. Somasundaran

Chair of ECI Conferences Committee: Nick Clesceri

ECI Technical Liaison for this conference: Jeff Moore

ECI Executive Director: Barbara K. Hickernell

ECI Associate Director: Kevin M. Korpics

Steering Committee

Yasuhisa Asano, Toyama University

Bob DiCosimo, DuPont

Pierre Monsan, Toulouse White Biotechnology

Jeff Moore, Merck

Magali Remaud-Simeon, LISBP-INSA, University of Toulouse

Jon Stewart, University of Florida

John Wong, Pfizer

Huimin Zhao, University of Illinois at Urbana-Champaign

Welcome from the Chairs

It is our great pleasure to welcome you all to Whistler, British Columbia, Canada for Enzyme Engineering XXV. This conference is organized under the auspices of the Engineering Conferences International (ECI). ECI is a not-for-profit global engineering conferences program, originally established in 1962, that provides opportunities for the exploration of problems and issues of concern to engineers and scientists from many disciplines. ECI has held more than 1500 conferences covering a multitude of leading edge topics that are uniquely cross-disciplinary and have served the engineering/scientific community for the past 57 years.

Enzyme Engineering has evolved dramatically over the last 50 years from a primary focus on biocatalysis to applications relevant to human health, design of new materials, and solving energy and environmental problems. This continuing series of conferences has changed to cover emerging areas, but has retained a vital role in defining the field of Enzyme Engineering. Enzyme engineers have always embraced new challenges and modern biology with high energy and enthusiasm. The focus of this year's meeting is to address *Frontiers in Enzyme Engineering* and showcase innovative solutions emerging from the general Enzyme Engineering community in response to these challenges. Sessions in this meeting will cover in breadth and depth a variety of topics such as computational protein design, advanced directed evolution, synthetic biology, and applications of enzyme engineering in biopharmaceutics development, industrial biocatalysis, and food and agriculture industries. The program was developed to engage thoughtful discussion and will feature oral and poster presenters and session chairs from academia and industry with a wide range of experience and from many countries around the world.

We would like to thank the industrial sponsors for their generous support. We also would like to thank all the board members, session chairs, and dedicated ECI staff for putting together a great program. Finally, we would like to thank all the speakers, poster authors, and attendees for providing the superb scientific content and look forward to the interactions that make this meeting so invaluable and productive. We hope you will enjoy the conference and participate to the fullest extent.

Huimin Zhao
University of Illinois
at Urbana-Champaign

John Wong
Pfizer, Inc.

Previous conferences in this series:

Enzyme Engineering

August 9-13, 1971

New England College, Henniker, New Hampshire

Conference Chair:

L.B. Wingard, Jr., SUNY Buffalo

Enzyme Engineering II

August 5-10, 1973

New England College, Henniker, New Hampshire

Conference Chairs:

L. B. Wingard, Jr., University of Pittsburgh

E. K. Pye, University of Pennsylvania

Enzyme Engineering III

August 3-8, 1975

Reed College, Portland, Oregon

Conference Chairs:

E. K. Pye, University of Pennsylvania

Howard H. Weetall, Corning Glass Works

Enzyme Engineering IV

September 25-30, 1977

Bad Neuenahr, W. Germany

Conference Chairs:

G. Manecke, der Freie Universität Berlin

L. B. Wingard, Jr., University of Pittsburgh

Enzyme Engineering V

July 29-August 3, 1979

New England College, Henniker, New Hampshire

Conference Chairs:

Howard H. Weetall, Corning Glass Works

G. P. Royer, University of Delaware

Enzyme Engineering VI

September 20-26, 1981

Kashikojima, Japan

Conference Chairs:

S. Fukui, Kyoto University

I. Chibata, Tanabe Seiyaku Co.

Enzyme Engineering VII

September 25-30, 1983

White Haven, Pennsylvania

Conference Chair:

Allen I. Laskin, Exxon Research & Eng. Co.

Previous conferences in this series:

Enzyme Engineering VIII

September 22-27, 1985

Elsinor, Denmark

Conference Chair:

Klaus Mosbach, University of Lund

Enzyme Engineering IX

October 4-9, 1987

Santa Barbara, California

Conference Chairs:

Harvey W. Blanch, University of California, Berkeley

Alexander M. Klibanov, Massachusetts Institute of Technology

Enzyme Engineering X

September 24-29, 1989

Kashikojima, Japan

Conference Chair:

H. Okada, University of Osaka

Enzyme Engineering XI

September 22-27, 1991

Kona, Hawaii

Conference Chairs:

David A. Estell, Genencor

Douglas S. Clark, University of California, Berkeley

Enzyme Engineering XII

September 19-24, 1993

Deauville, France

Conference Chairs:

Daniel Thomas, University of Technology of Compiègne

Marie Dominique Legoy, University of Technology of Compiègne

Enzyme Engineering XIII

October 15-20, 1995

San Diego, California

Conference Chairs:

Jon Dordick, University of Iowa

Alan Russell, University of Pittsburgh

Enzyme Engineering XIV

October 12-17, 1997

Beijing, China

Conference Chairs:

Yao-Ting Yu, Nankai University

Gao-Xiang Li, Academia Sinica

Previous conferences in this series:

Enzyme Engineering XV

October 10-15, 1999

Kailua-Kona, Hawaii

Conference Chairs:

David Anton, DuPont

Frances H. Arnold, California Institute of Technology

Robert Kelly, North Carolina State University

Enzyme Engineering XVI

October 7-12, 2001

Potsdam, Germany

Conference Chairs:

Frieder W. Scheller, University of Potsdam

Christian Wandrey, Research Center Jülich

Oreste Ghisalba, Novartis Pharma AG

Enzyme Engineering XVII

November 9-14, 2003

Santa Fe, New Mexico

Conference Chairs:

Stephen Benkovic, Pennsylvania State University

Chi-Huey Wong, Scripps Research Institute

Jeffrey Moore, Merck & Co., Inc.

Birgit Kosjek, Merck & Co., Inc.

Enzyme Engineering XVIII

October 9-14, 2005

Gyeong-ju, Korea

Conference Chairs:

Hak-Sung Kim, KAIST, Korea

Ji-Yong Song, LG Life Sciences, Ltd, Korea

Tae-Kwang Oh, Korea Research Inst.of Biosciences & Biotech, Korea

Moon-Hee Sung, Kookmin University, Korea

Enzyme Engineering XIX

September 23-28, 2007

British Columbia, Canada

Conference Chairs:

Romas Kazlauskas, University of Minnesota

Stefan Lutz, Emory University

David Estell, Danisco/Genencor

Enzyme Engineering XX

September 20-24, 2009

Groningen, the Netherlands

Conference Chairs:

Dick Janssen, University of Groningen

Oliver May, DSM Pharmaceutical Products

Andreas Bommarius, Georgia Institute of Technology

Previous conferences in this series:

Enzyme Engineering XXI

September 18-22, 2011

Vail, Colorado

Conference Chairs:

Lori Giver, Codexis

Steve Withers, University of British Columbia

Enzyme Engineering XXII

September 22-26, 2013

Toyama, Japan

Conference Chairs:

Yasuhisa Asano, Toyama Prefectural University

Jun Ogawa, Kyoto University

Yoshihiko Yasohara, Keneka Corp.

Enzyme Engineering XXIII

September 6-11, 2015

St. Petersburg, Florida, USA

Conference Chairs:

Jon Dale Stewart, University of Florida

Robert DiCosimo, DuPont Industrial Biosciences

Enzyme Engineering XXIV

September 24-28, 2017

Toulouse, France

Conference Chairs:

Pierre Monsan, Toulouse White Biotechnology, France

Magali Remaud-Simeon, LISBP-INSA, University of Toulouse, France

2019 Enzyme Engineering Award



Dr. Huimin Zhao

Dr. Huimin Zhao is the Steven L. Miller Chair of chemical and biomolecular engineering, and professor of chemistry, biochemistry, biophysics, and bioengineering at the University of Illinois at Urbana-Champaign (UIUC). He received his B.S. degree in Biology from the University of Science and Technology of China in 1992 and his Ph.D. degree in Chemistry from the California Institute of Technology in 1998 under the guidance of Nobel Laureate Frances Arnold. Prior to joining UIUC in 2000, he was a project leader at the Industrial Biotechnology Laboratory of the Dow Chemical Company. He was promoted to full professor in 2008. Dr. Zhao has authored and co-authored over 300 research articles and over 25 issued and pending patent applications with several being licensed by industry. In addition, he has given plenary, keynote or invited lectures in over 370 international meetings, universities, industries, and research institutes. Twenty-six (26) of his former graduate students and postdocs became professors or principal investigators in the United States (10), China (11), Korea (2), Singapore (2), and Egypt (1).

Dr. Zhao has made profound contributions to enzyme engineering. He pioneered the development of many directed evolution methods for engineering enzymes for industrial applications. For example, he invented the staggered extension process (StEP) in vitro recombination method which was licensed by Maxygen and used by many academic laboratories around the world. He also invented the targeted site saturation mutagenesis method which has been widely used for engineering enzyme specificity and selectivity (enantio-, regio-, and chemo-). Moreover, the in vitro co-evolution method he invented was adopted by Merck and Codexis to create a transaminase mutant with novel substrate specificity for commercial synthesis of the blockbuster anti-diabetes drug sitagliptin. By using directed evolution, he developed a novel phosphite dehydrogenase based enzymatic system to

regenerate cofactors NAD(P)H, which made many oxidoreductases useful for preparative synthetic applications. Notably, five of his publications (he was the first author on four of them) were cited in the scientific background document prepared by the Nobel Prize committee for the 2018 Nobel Prize in Chemistry. In recent years, Dr. Zhao pioneered the development of directed evolution methods for engineering biochemical pathways and whole genomes, and has made foundational contributions to multiple research areas including synthetic biology, metabolic engineering, and natural product discovery.

Dr. Zhao received numerous awards such as Marvin Johnson Award (2018), Biotechnology Progress Award for Excellence in Biological Engineering Publication (2017), Charles Thom Award (2016), Elmer Gaden Award (2014), Guggenheim Fellowship (2012), the American Chemical Society (ACS) Division of Biochemical Technology Young Investigator Award (2008), DuPont Young Professor Award (2005), and National Science Foundation CAREER Award (2004). He is an elected Fellow of the Association for the Advancement of Science and the American Institute of Medical and Biological Engineers. He served as a consultant for over 10 companies and a Scientific Advisory Board member of Gevo, Myriant Technologies, Toulouse White Biotechnology, and AgriMetis.

ENZYME ENGINEERING AWARDEES

with

a list of conference sites

1971 - Henniker, New Hampshire, USA

1973 - Henniker, New Hampshire, USA

1975 - Portland, Oregon, USA

1977 - Bad Neuenahr, Germany

1979 – Henniker, New Hampshire, USA

1981 – Kashikojima, Japan

1983 – White Haven, Pennsylvania, USA - **ICHIRO CHIBATA**

1985 – Helsingor, Denmark - **KLAUS MOSBACH**

1987 – Santa Barbara, California, USA - **EPHRIAM KATCHALSKI-KATZIR**

1989 – Kashikojima, Japan - **SABURO FUKUI**

1991 – Kona, Hawaii, USA - **ALEX KLIBANOV**

1993 – Deauville, France - **MALCOLM LILLY**

1995 – San Diego, California, USA - **MARIA-REGINA KULA** and **CHRISTIAN WANDREY**

1997 – Beijing, China - **HARVEY BLANCH**

1999 – Kona, Hawaii, USA - **CHI HUEY WONG**

2001 – Potsdam, Germany - **HIDEAKI YAMADA**

2003 – Santa Fe, New Mexico, USA - **JON DORDICK** and **DOUG CLARK**

2005 – Gyeongju, Korea - **DEWEY RYU**

2007 - Harrison Hot Springs, British Columbia, Canada - **FRANCES H. ARNOLD**

2009 – Groningen, The Netherlands - **SAKAYU SHIMIZU**

2011 – Vail, Colorado, USA – **DAVID ESTELL**

2013 – Toyama, Japan – **YASUHISA ASANO**

2015 – St. Petersburg, Florida, USA – **DAN TAWFIK**

2017 – Toulouse, France – **PIERRE MONSAN**

Conference Sponsors

ACS Catalysis

Almac

Amano Enzyme Inc.

Arzeda

ATUM

BASF

c-LEcta GmbH

Codexis

DuPont

Japanese Society of Enzyme Engineering

KCAT ENZYMATIC PRIVATE LIMITED

Merck and Co., Inc.

Nature Catalysis

Novartis

Novozymes

Pfizer

**PROTEO, the Québec Network for Research on Protein Function,
Engineering and Applications**

Protéus

Purolite Life Sciences

Quantumzyme

Roquette

Zymvol Biomodeling, S.L.

Sunday, September 15, 2019

16:30 – 18:45	Conference check-in (Whistler Conference Center Foyer)
18:45 – 19:00	Opening Remarks – Conference chairs and ECI liaison
19:00 – 21:00	Dinner

Room locations and notes

- General Sessions will be held in Sea to Sky Ballroom A.
- Poster Sessions will be in Sea to Sky Ballrooms B and C.
- Meals will be in the Whistler Conference Center Foyer.
- The ECI office is the Soo Valley Room on the lower level.
- Audio, still photo and video recording by any device (e.g., cameras, cell phones, laptops, PDAs, watches) is strictly prohibited during the technical sessions, unless the author and ECI have granted prior permission.
- Speakers – Please have your presentation loaded onto the conference computer prior to the session start (preferably the day before).
- Speakers – Please leave discussion time as previously directed by your session chair.
- Please do not smoke at any conference functions.
- Turn your mobile telephones to vibrate or off during technical sessions.
- Please write your name on your program so that it can be returned to you if lost or misplaced.
- After the conference, ECI will send an updated participant list to all participants. Please check your listing now and if it needs updating, you may correct it at any time by logging into your ECI account.
- Emergency Contact Information: Because of privacy concerns, ECI does not collect or maintain emergency contact information for conference participants. If you would like to have this information available in case of emergency, please use the reverse side of your name badge.

Monday, September 16, 2019

- 07:00 – 08:25 Breakfast
- Session 1: Biocatalysis and Enzymology**
Chairs: Scott France, Pfizer, USA
- 08:25 – 09:10 **The development of new biocatalytic reactions for organic synthesis**
Nicholas Turner, University of Manchester, UK
- 09:10 – 09:40 **Functional dynamics of proteins on catalysis from combined QM/MM and experimental studies**
Jiali Gao, University of Minnesota, USA
- 09:40 – 09:55 **Structural insight into enantioselective inversion of an alcohol dehydrogenase reveals a “Polar Gate” in stereo-recognition of diaryl ketones**
Ye Ni, Jiangnan University, China
- 09:55 – 10:10 **Surpassing thermodynamic, kinetic, and stability barriers to isomerization catalysis for tagatose biosynthesis**
Nikhil Nair, Tufts University, USA
- 10:10 – 10:40 Coffee/ Tea Break
- 10:40 – 11:10 **Revisiting alcohol dehydrogenases: Self-sufficient regio- and enantio-selective formation of bi- and tri-cyclic lactones**
Mélanie Hall, University of Graz, Austria
- 11:10 – 11:40 **Exploring marine carbohydrates: P450-catalyzed demethylation and identification of a complete "PUL" for polysaccharide degradation**
Uwe Bornscheuer, Greifswald University, Germany
- 11:40 – 11:55 **Multi-engineering of Microbial Cytochrome P450 Enzymes**
Shengying Li, Shandong University, China
- 11:55– 12:10 **Dissecting polyunsaturated fatty acid synthases for product profile control**
Tohru Dairi, Hokkaido University, Japan
- 12:10 – 13:25 Lunch
- Session 2: Enzyme Promiscuity, Evolution and Dynamics**
Chairs: Yan Feng, Shanghai Jiao Tong University, China
- 13:25 – 14:10 **Promiscuity, serendipity and metabolic innovation**
Shelley Copley, University of Colorado, USA
- 14:10 – 14:40 **Where do we find new enzymes? – Rules and tools**
Florian Hollfelder, University of Cambridge, UK
- 14:40 – 15:10 **Strategies and software tools for engineering protein tunnels and dynamical gates**
Jiri Damborsky, Masaryk University, Czech Republic
- 15:10 – 15:40 Coffee/Tea Break

Monday, September 16, 2019 (continued)

- 15:40 – 16:10 **Exploring sequence-function space in the Old Yellow Enzyme superfamily**
Stefan Lutz, Emory University, USA
- 16:10 – 16:40 **Understanding promiscuity in class II pyruvate aldolases**
Ulf Hanefeld, Technische Universiteit Delft, Netherlands
- 16:40 – 16:55 **Thrice upon a time: The repeated emergence of a novel enzymatic function from an evolvable protein scaffold**
Janine Copp, University of British Columbia, Canada
- 16:55 – 17:10 **Reconstruction of ancestral L-amino acid oxidases to broaden substrate selectivity**
Shogo Nakano, University of Shizuoka, Japan
- 17:30 – 18:45 Dinner
- 19:00 – 20:00 **Plenary Lecture**
The coming of age of de novo protein design
David Baker, University of Washington at Seattle, USA
- 20:00 – 22:00 **Poster Session A**
(Authors of even-numbered posters are asked to stay with their posters)

Tuesday, September 17, 2019

07:00 – 08:25 Breakfast

Session 3: New Tools for Enzyme Engineering

Chairs: Daniela Grabs, Arzeda Corporation, USA

08:25 – 09:10 **Mechanism, inhibition and recent evolution of an unusual, promiscuous reductase**

Joelle Pelletier, University of Montreal, Canada

09:10 – 09:40 **Mass-activated sorting of nanoliter droplets for label free screening of enzyme libraries**

Jeff Moore, Merck and Co., Inc., USA

09:40 – 10:10 **Computational enzyme design for industrially relevant reactions**

Bian Wu, Institute of Microbiology, Chinese Academy of Sciences, China

10:10 – 10:40 Coffee/Tea Break

10:40 – 11:10 **The PEN CSR, using external molecular programs to control directed evolution of enzymes**

Adèle Dramé-Maigné, ESPCI, France

11:10 – 11:25 **I_{PRO}+/-: a computational protein design tool allowing not only for amino acid changes but also insertions and deletions**

Ratul Chowdhury, Penn State University, USA

11:25 – 11:40 **7D QSAR based grid maps generated using quantum mechanic probes to identify hotspots and predict activity of mutated enzymes for enzyme engineering**

Pravin Kumar, Kcat Enzymatic Pvt Ltd, India

11:40 – 11:55 **New technologies for enzyme engineering: Combining computational predictions and automated experimental feedback**

Uwe Jandt, Hamburg University of Technology, Germany

11:55 – 12:10 ***In Silico* enzyme engineering – The importance of fast and accurate algorithms**

Maria F. Lucas, Zymvol, Spain

12:10 – 13:25 Lunch

Session 4: Enzyme Engineering for Biomedical Applications

Chairs: Stefan Lutz, Emory University, USA

13:25 – 14:10 **New engineered peptide ligases and substrate phage libraries for understanding cellular proteolysis**

James Wells, University of California San Francisco, USA

14:10 – 14:40 **Reconstruction of the active site of a bacterial phosphotriesterase for the catalytic hydrolysis and detoxification of organophosphate nerve agents**

Frank Raushel, Texas A&M, USA

Tuesday, September 17, 2019 (continued)

- 14:40 – 15:10 **Validation and stabilization of a prophage lysin of *Clostridium perfringens* by yeast surface display and co-evolutionary models**
Ben Hackel, University of Minnesota, USA
- 15:10 – 15:40 Coffee/Tea break
- 15:40 – 16:10 **High-level expression, high-throughput screening and direct recovery of nitroreductase enzymes from metagenome libraries**
David F. Ackerley, Victoria University of Wellington, New Zealand
- 16:10 – 16:25 **Enzymatic transformation of antibodies to obtain single glycoforms**
Michael Butler, National Institute for Bioprocessing Research and Training, Ireland
- 16:25 – 16:55 **New enzymes for cell surface modification: Towards universal blood and improved organ transplants**
Stephen Withers, University of British Columbia, Canada
- 16:55 – 17:10 **A facile scheme for biosynthesis of peptides with no length constraints**
Zhanglin Lin, South China University of Technology, China
- 18:00 – 19:30 Dinner
- 19:30 – 21:30 **Poster Session B**
(Authors of odd-numbered posters are asked to stay with their posters)

Wednesday, September 18, 2019

- 07:00 – 08:25 Breakfast
- Session 5: Industrial Applications of Enzyme Engineering**
Chairs: Vesna Mitchell, Codexis, Inc., USA
- 08:25 – 09:10 **Protein and process engineering towards biocatalysts useful in industrial processes**
Andreas Bommarius, Georgia Institute of Technology, USA
- 09:10 – 09:40 **Enzyme engineering for industrial applications at BASF**
Adrienne Davenport, BASF, USA
- 09:40 – 10:10 **Engineering of industrial biocatalysts**
Daniel Dourado, Almac Group, UK
- 10:10 – 10:40 Coffee/Tea break
- 10:40 – 10:55 ***In Silico* engineered SmSDR enzyme for the preparation of enantiopure R-phenylephrine**
Sindriila Dutta Banik, Quantumzyme, India
- 10:55 – 11:10 **Addressing the problem of plastic waste: Development of an enzymatic process for PET recycling**
Alain Marty, Carbios, France
- 11:10 – 11:25 **Engineering enzymes to control the chain-length selectivity of biosynthesized oleochemicals**
Brian Pfleger, University of Wisconsin-Madison, USA
- 11:25 – 11:55 **High-throughput enzyme engineering for commercial-scale production of natural products**
Yue Yang, Amyris, Inc, USA
- 11:55 – 12:10 **Multidimensional engineering of Chymosin for efficient cheese production by machine learning guided directed evolution**
Christian Jäckel, Chr. Hansen, Denmark
- 12:10 Free afternoon, boxed lunch provided

Thursday, September 19, 2019

07:00 – 08:25 Breakfast

Session 6: Design and Engineering of Artificial Enzymes

Chairs: Ulrich Schwaneberg, RWTH Aachen, Germany
Mélanie Hall, University of Graz, Austria

08:25 – 09:10 **Artificial metalloenzymes for *in vivo* catalysis: Challenges and opportunities**
Thomas Ward, University of Basel, Switzerland

09:10 – 09:40 **Designing artificial metalloenzymes with high activity through engineering secondary coordination sphere interactions**
Yi Lu, University of Illinois, USA

09:40 – 10:10 **From natural to artificial metalloproteins – Challenges and opportunities**
Johannes Schiffels, RWTH Aachen University, Germany

10:10 – 10:40 Coffee/Tea break

10:40 – 11:10 **Engineered myoglobin catalysts for selective carbene transfer reactions**
Rudi Fasan, University of Rochester, USA

11:10 – 11:40 **Artificial (beta / alpha)₈ barrel enzymes by *in vitro* evolution**
Burckhard Seelig, University of Minnesota, USA

11:40 – 11:55 **An artificial metalloenzyme for a bimolecular Diels–Alder reaction**
Sophie Basler, ETH Zurich, Switzerland

11:55 – 12:10 **Guiding transition-metal catalyst selectivity using proteins**
Amanda Jarvis, University of Edinburgh, UK

12:10 – 13:25 Lunch

Session 7: Enzyme Engineering and Synthetic Biology

Chairs: Doug Fuerst, GlaxoSmithKline, USA

13:25 – 14:10 **Construction of novel metabolic pathways with artificial enzymes**
Akihiko Kondo, Kobe University, Japan

14:10 – 14:40 **Engineering decarboxylases for consolidated bioprocessing and more**
Volker Sieber, TU München, Germany

14:40 – 15:10 **Engineered enzymes, pathways, and tools for the biosynthesis of non-natural polyketides and terpenes**
Gavin Williams, NC State University, USA

15:10 – 15:40 Coffee/Tea Break

15:40 – 16:10 **Nanomachine biocatalysts: Tools for cell-free artificial metabolic networks**
Carol Hartley, CSIRO, Australia

16:10 – 16:20 **A data-driven approach for exploiting enzyme promiscuity as a means to predict novel biochemical reactions**
Sanjan TP Gupta, University of Wisconsin Madison, USA

Thursday, September 19, 2019 (continued)

- 16:20 – 16:30 **Enzyme Engineering towards a Fully Biocatalytic Manufacturing Route for MK-8591**
Hao Yang, Merck & Co., Inc., USA
- 16:30 – 16:40 **Engineering PET-degrading enzymes for biorecycling and bioremediation**
En Ze Linda Zhong, Massachusetts Institute of Technology, USA
- 16:40 – 16:50 **Newly discovered enzymes and cascades for the determination of amino acids**
Yasuhisa Asano, Toyama Prefectural University, Japan
- 16:50 – 17:00 **Protein dynamics at slow timescales in engineered β -lactamases does not limit evolvability**
Lorea Alejaldre, Universite de Montreal, Canada
- 17:00 – 17:30 **Enzyme evolution in synthetic biology: A key role from proof-of-concept towards precision function**
Yan Feng, Shanghai Jiao Tong University, China
- 18:00 – 19:00 **2019 Enzyme Engineering Award**
Enzyme Design by Directed Evolution
Huimin Zhao, University of Illinois at Urbana-Champaign, USA
- 19:00 – 19:30 Reception
- 19:30 – 21:00 Gala Dinner
- 21:00 – 21:30 Entertainment

Posters

Enzyme Engineering XXV

September 15-19, 2019

Whistler Resort
Whistler, British Columbia, Canada



ECI 
Engineering Conferences International

Poster Presentations

Monday, September 16, 2019, 20:00 – 22:00 Poster Session A - Authors of even-numbered posters are asked to stay with their posters

Tuesday, September 17, 2019, 19:30 – 21:30 Poster Session B - Authors of odd-numbered posters are asked to stay with their posters

- 1 **Engineering bacterial nitroreductases for anticancer gene therapy and targeted cell ablation**
Abigail V. Sharrock, Victoria University of Wellington, New Zealand
- 2 **QM/MM MD studies of polyester synthesis/hydrolysis**
Alexandra T. P. Carvalho, CNC, Coimbra University, Portugal
- 3 **Directed evolution of the non-ribosomal peptide synthetase BpsA to enable recognition by the human Sfp-like PPTase**
Alistair Sinclair Brown, Victoria University of Wellington, New Zealand
- 4 **Broadening substrate specificity across short-chain dehydrogenase reductases (SDRs)**
Andreas Bommarius, Georgia Institute of Technology, USA
- 5 **Enzymatic biotransformation of adipic acid to 6-aminocaproic acid and 1,6-hexamethylenediamine using engineered carboxylic acid reductases and aminotransferases**
Anna Khusnutdinova, University of Toronto, Canada
- 6 **Design and evolution of enzymes with non-canonical catalytic mechanisms**
Anthony Green, University of Manchester, United Kingdom
- 7 **New pathways for sustainable terpene materials from wood**
Arne Stamm, KTH Royal Institute of Technology, Sweden
- 8 **Highly oxygen-stable CO₂ reductase-catalyzed bioconversion of carbon dioxide into formate in electrochemical reactor**
Byoung Wook Jeon, Ulsan National Institute of Science and Technology, South Korea
- 9 **Cobalamin dependent methylation and demethylation by veratrol O-demethylase**
Christopher Grimm, University of Graz, Austria
- 10 **Light-driven kinetic resolution of α -functionalized acids enabled by engineered Fatty Acid Photodecarboxylase**
Danyang Li, Zhejiang University, China
- 11 **High-throughput enzyme discovery and engineering for bioprocess optimization**
Doug Hattendorf, Zymergen, USA
- 12 **Engineering PET-degrading enzymes for biorecycling and bioremediation**
En Ze Linda Zhong, Massachusetts Institute of Technology, USA
- 13 **Genetic biosensor enables in vivo glycosyltransferase screening**
Evan K. Chaberski, DTU Biosustain, Denmark

- 14 **Cofactor switch: Development of A Nad⁺-dependent cascade for the production of ursodeoxycholic acid (UDCA)**
Fabio Tonin, TU Delft, Netherlands
- 15 **CaverDock: Software tool for fast screening of un/binding of ligands in protein engineering**
Gaspar Pinto, Masaryk University, Czech Republic
- 16 **Prenylated Flavin-dependent decarboxylases: Structure-guided engineering and synthetic applicability**
Godwin Aleku, Manchester Institute of Biotechnology, University of Manchester, United Kingdom
- 17 **The role of cavity residue leucine 95 and channel residues glutamine 204, aspartic acid 211, and phenylalanine 269 on toluene o-xylene monooxygenase activity and regiospecificity**
Gonul Vardar-Schara, California State University Stanislaus, USA
- 18 **Rational engineering of a hyperstable glycosyltransferase for blue denim dyeing**
Gonzalo Bidart, The Novo Nordisk Foundation Center for Biosustainability - Technical University of Denmark, Denmark
- 19 **Directed evolution of glycosyltransferase for the artificial biosynthesis of natural product glycosides**
Guangyu Yang, Shanghai Jiao Tong University, China
- 20 **Access tunnel engineering to optimize the catalytic cycle of carbohydrate hydrolases with buried active site**
Guimin Zhang, Hubei University, China
- 21 **Sustainable biocatalytic synthesis of β -hydroxyl- α -amino acids on an industrial scale**
Haibin Chen, Enzymaster (Ningbo) Bio-Engineering Co., Ltd., China
- 22 **Smart engineering of various enzymes for asymmetric synthesis of chiral molecules on industrial scale**
Haibin Chen, Enzymaster (Ningbo) Bio-Engineering Co., Ltd., China
- 23 **Structural synthetic biology strategy for the design of a new metabolic pathway**
Hak-Sung Kim, KAIST, South Korea
- 24 **Enzyme Engineering towards a Fully Biocatalytic Manufacturing Route for MK-8591**
Hao Yang, Merck & Co., Inc., USA
- 25 **Identification of the residues that are responsible for improving the activities of cyanobacterial enzymes for hydrocarbon biosynthesis**
Hisashi Kudo, University of Tokyo, Japan
- 26 **A coupled chlorinase-fluorinase system with high efficiency of trans-halogenation and a shared substrate tolerance**
Huihua Sun, Agency for Science, Technology, and Research, Singapore
- 27 **A naked-eye detection of cholesterol using enzyme cascade reactions on chitosan beads**
Hyunbeom Lee, Korea Institute of Science and Technology, South Korea

- 28 **Towards the de novo design of metallohydrolases**
Indrek Kalvet, University of Washington, USA
- 29 **Therapeutic protein expression platform of microbial system**
Jen-Wei Chang, Development Center for Biotechnology/Institute of Biologics, Taiwan
- 30 **Functional assessment of hydrophilic domains of lea proteins from distant organisms**
Jin Wang, Biotechnology Research Institute, Chinese Academy of Agricultural Sciences, China
- 31 **In-silico based redesign of CO-dehydrogenase catalyzing the oxidation of toxic waste CO gas for improved O₂ resistance and mediator affinity**
Jinhee Lee, UNIST, South Korea
- 32 **Kinetics of glycosyl hydrolase family 2 beta-glucuronidases**
John J. Tomashek, Integrated Micro-Chromatography Systems, USA
- 33 **Variants of glycosyl hydrolase family 2 beta-glucuronidases**
Caleb Schlachter, Integrated Micro-Chromatography Systems, USA
- 34 **The growing need to assess the kinetic stability of enzymes**
Rowan Lindeque, Technical University of Denmark, Denmark
- 35 **Molecular dynamics provides insights into an engineered oxidoreductase with altered cofactor specificity**
Josef M. Sperl, Technical University of Munich, Germany
- 36 **Engineering substrate specificity into a promiscuous ancestral diterpene synthase**
Karen Schriever, KTH, Royal Institute of Technology, Sweden
- 37 **TreasureDrop – enzyme engineering for applied biocatalysis using microfluidics**
Katharina Neufeld, Johnson Matthey, United Kingdom
- 38 **Active-site structure of D-threonine aldolase from a green alga Chlamydomonas reinhardtii**
Katsushi Nishimura, Nihon University, Japan
- 39 **Construction of thermostable enzymes**
Kazuhiko Ishikawa, National Institute of Advanced Industrial Science and Technology (AIST), Japan
- 40 **Using E. coli NfsA as a model to improve our understanding of enzyme engineering**
Kelsi R. Hall, Victoria University of Wellington, New Zealand
- 41 **In vivo and in vitro FMN prenylation and (de)carboxylase activation under aerobic conditions**
Khorcheska Batyrova, University of Toronto, Canada
- 42 **Protein dynamics at slow timescales in engineered β -lactamases does not limit evolvability**
Lorea Alejaldre, Universite de Montreal, Canada
- 43 **Controlling the fatty acid hydroxylation regioselectivity of CYP152A1 (P450Bsb) by active site engineering**
Lucas Hammerer, ACIB, University of Graz, Austria

- 44 **Computational study of the structure-function relationship of an artificial Friedel-Crafts alkylase**
Lur Alonso-Cotchico, University of Groningen, Netherlands
- 45 **Understanding enzymes specificities as a tool for cofactor engineering**
Madhuri Gade, OIST Okinawa Japan, Japan
- 46 **A structure-based approach to control the size and linkage-type of sucrose derived alpha-glucans**
Magali Remaud-Simeon, LISBP/INSA Toulouse, University of Toulouse, France
- 47 **Engineering the biosynthesis of non-ribosomal peptides**
Mark Jonathan Calcott, Victoria University of Wellington, New Zealand
- 48 **Identification and engineering of a Dye-Decolorizing Peroxidase (DyP) for C—C-bond forming carbene-transfer reactions**
Martin Weissenborn, Leibniz-Institut für Pflanzenbiochemie & MLU Halle Wittenberg, Germany
- 49 **Purification and pressure dependence of alanine racemase from the psychropiezophilic bacterium shewanella violacea DSS 12**
Minoru Tanigawa, Nihon University, Japan
- 50 **Cloning and expression of a serine racemase gene homologue of the green alga Chlamydomonas reinhardtii and characterization of the gene product**
Miya Koike, Nihon University, Japan
- 51 **Exploring the potential of ancestral phenylalanine/tyrosine ammonia-lyases for therapeutic applications**
Natalie Marie Hendrikse, KTH Royal Institute of Technology, Sweden
- 52 **Molecular packaging of biocatalysts using a robust protein cage**
Nikola Loncar, University of Groningen, Netherlands
- 53 **Preparation of pectate lyase/Cu₃(PO₄)₂ hybrid nanoflower and its catalytic performance as an immobilized enzyme**
Pan Wu, Hubei University, China
- 54 **Fungal peroxygenase chimera identified by sub-domain shuffling and split-gfp reveal retained activity and altered specificity**
Pascal Püllmann, Leibniz IPB Halle, Germany
- 55 **WITHDRAWN**
- 56 **A retrobiosynthetic approach to generate terpene-derived polymers**
Per-Olof Syrén, KTH Royal Institute of Technology, Sweden
- 57 **Engineering of a specific CYP450 for an industrial process shows 700-fold increase in activity with K_{cat} of 6.2 s⁻¹ - Residues causing Hydrogen Migration and Double Hydrogen Abstraction at Δx Carbon identified by Quantum Mechanics revealed to be the game**
Lalitha Roopa, Kcat Enzymatic Private Limited, India
- 58 **Enabling medium-chain fatty acid production in yeast via high-throughput MALDI MS-based enzyme engineering**
Pu Xue, University of Illinois at Urbana-Champaign, USA

- 59 **Engineering alcohol oxidases for substrate scope and their application in flow and cascade biocatalysis**
Rachel Heath, University of Manchester, United Kingdom
- 60 **Using protein engineering to accelerate implementation of continuous biocatalysis for API synthesis**
Rowan Lindeque, Technical University of Denmark, Denmark
- 61 **Innov'SAR: A new approach for protein engineering and screening**
Rudy Pandjaitan, PEACCEL, France
- 62 **A data-driven approach for exploiting enzyme promiscuity as a means to predict novel biochemical reactions**
Sanjan TP Gupta, University of Wisconsin Madison, USA
- 63 **Engineering enzymes with non-canonical active site functionality**
Sarah L. Lovelock, University of Manchester, United Kingdom
- 64 **Enzyme engineering of fungal-derived FAD-GDH by circular permutation**
Satoru Ishihara, Amano Enzyme Inc., Japan
- 65 **Application of directed divergent evolution strategy in natural product biosynthesis**
Shuang-Yan Tang, Institute of Microbiology, Chinese Academy of Sciences, China
- 66 **A technology platform for in vitro transcription and translation of enzymes in micro compartments**
Silvia Calabrese, Hahn-Schickard, Germany
- 67 **Design strategy for creating catalytically active metal binding proteins**
Stacey Gerben, University of Washington, Baker Group, USA
- 68 **Evolution of the ThDP dependent pyruvate dehydrogenase E1 subunit for the conversion of long chain aliphatic ketoacids**
Stefan R. Marsden, Delft University of Technology, Netherlands
- 69 **Engineering of halohydrin hydrogen-halide-lyase (H-lyase) for efficient L-carnitine production**
Takanori Akiyama, Mitsubishi Chemical Corporation, Japan
- 70 **Improved biomass conversion with Trichoderma reesei beta-glucosidase Cel3A engineered for broader substrate specificity**
Thijs Kaper, DuPont, USA
- 71 **Substrate promiscuity in evolved Alcohol Dehydrogenase A (ADH-A)**
Thilak Reddy Enugala, Uppsala University, Sweden
- 72 **Unravelling the relationship between substrate selectivity and primary sequence of UDP-glycosyltransferases**
Tiia Kittilä, Novo Nordisk Foundation Center for Biosustainability, Denmark
- 73 **Oligopeptides production by a method involving an enzymatic reaction and a subsequent chemical reaction**
Tomoko Abe, Tokyo Denki University, Japan
- 74 **A non-natural Nicotinamide cofactor for biotransformation at extreme conditions**
Volker Sieber, TU München, Germany

- 75 **WITHDRAWN**
- 76 **Designing de novo retroaldolase catalysts**
Yakov Kipnis, University of Washington, USA
- 77 **Tailored biosynthesis of pseudosugars against diabetes by repurposing the promiscuous microbial enzymes**
Yan Feng, Shanghai Jiao Tong University, China
- 78 **Genetically encoded biosensor for engineering branched-chain higher alcohol production pathway in *saccharomyces cerevisiae***
Yanfei Zhang, Princeton University, USA
- 79 **Newly discovered enzymes and cascades for the determination of amino acids**
Yasuhisa Asano, Toyama Prefectural University, Japan
- 80 **Engineering an aldehyde dehydrogenase via structure based directed evolution for enhancement of 3-hydroxypropionic acid production**
Ye Seop Park, Ajou University, South Korea
- 81 **A novel C-terminal protein degron identified in bacterial aldehyde decarbonylases using directed enzyme evolution**
Yilan Liu, University of Toronto, Canada
- 82 **Enantiocomplementary synthesis of chiral alcohols combining photocatalysis and whole-cell biocatalysis in a one-pot cascade process**
Yongzhen Peng, Zhejiang University, China
- 83 **Substrate specificity of tRNA-dependent amide bond-forming enzyme**
Yoshimitsu Hamano, Fukui Prefectural University, Japan
- 84 **Engineering of penicillin G acylases for the production of β -lactam antibiotics on an industrial scale**
Young Sung Yun, Amicogen, Inc., South Korea
- 85 **Fusing enzymes to transcription activator LuxR for the rapid creation of metabolite sensors**
Yuki Kimura, Chiba University, Japan
- 86 **Expression and characterization of keratinase from *Deinococcus gobiensis* I-0**
Zhengfu Zhou, Biotechnology Research Institute, CAAS, China
- 87 **Engineering T1 lipase for degradation of poly-(R)-3-hydroxybutyrate**
Normi Mohd Yahaya, Universiti Putra Malaysia, Malaysia
- 88 **Development and application of novel engineered transaminase panels assisted by in-silico rational design for the production of chiral amines**
Daniel F.A.R. Dourado, Almac Sciences, United Kingdom
- 89 **WITHDRAWN**
- 90 **Purification and characterization of a novel alginate lyase from the marine bacterium *bacillus* sp. Alg07**
Peng Chen, Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, China

- 91 **In silico approach to better understand the role of active site residue**
Sindrila Dutta Banik, Quantumzyme LLP, India
- 92 **WITHDRAWN**
- 93 **Deletion studies for elucidating the role of Streptomyces griseus ChiC non-catalytic residues**
Normi Mohd Yahaya, Universiti Putra Malaysia, Malaysia
- 94 **Improving the catalytic activity of isopentenyl phosphate kinase through protein coevolution analysis**
Xuerong Xing, Tianjin Institute of Industrial Biotechnology, China
- 95 **Improving the thermostability of glutamate decarboxylase by consensus mutagenesis**
Jun Huang, Zhejiang university of Science and Technology, China