Program

Enzyme Engineering XXIII

September 6 - 11, 2015

St. Petersburg, Florida, USA

Conference Co-Chairs

Jon Dale Stewart University of Florida USA

Robert DiCosimo DuPont Industrial Biosciences USA





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Professor Dan S. Tawfik

Winner of the 2015 Enzyme Engineering Award



Since 1983 the Enzyme Engineering Award has been presented at ECI's biennial International Enzyme Engineering Conference. The 2015 Award will be presented at the 23rd Enzyme Engineering Conference in St Petersburg, Florida. This award recognizes outstanding achievement in the field of enzyme engineering, through basic or applied research in academia or industry.

The 2015 Enzyme Engineering Award, presented in the name of Engineering Conferences International and Genencor, will be awarded to **Professor Dan S. Tawfik**.

Professor Tawfik earned his B.S. degree in Chemistry and Biochemistry from The Hebrew University of Jerusalem (1988) as well as his M.Sc. in Biochemistry (1990). He earned his Ph.D. degree in the investigation of catalytic antibodies from the Weizmann Institute of Science in 1996. Dan then did postdoctoral study at Cambridge University and positions of increasing responsibility at the MRC Center for Protein Engineering in Cambridge. He returned to the Weizmann Institute in 2001 as a Senior Scientist and as Associate Professor in the Department of Biological Chemistry in 2006. In 2010 he became a full professor and was awarded the Nella and Leon Benoziyo Professorial Chair.

Professor Tawfik has made significant contributions to biotechnology. His early work with Andrew Griffiths on the use of emulsion droplets as a means of isolating individual reactions in tiny volumes (in vitro compartmentalization) provided a means of performing billions of parallel biochemical and genetic reactions in femtoliter droplets. This technology has become a leading technology in high-throughput DNA sequencing and in digital droplet PCR. More recently, Prof Tawfik's research has provided insight into mechanisms of protein evolution. His and others identification of the roles of enzyme promiscuity in the evolution of new activities and of the importance of protein stability as a component of evolvability led to his recruitment of 'neutral drift' and chaperone-based approaches to overcome problems of acquired instability, yielding important tools to improve the process of enzyme activity increase. Most recently, in conjunction with David Baker, the development through computational design and evolution of a novel enzyme de novo resulted in the creation of a Kemp eliminase - a reaction for which no natural enzyme is known. His work continues today in several areas, including *de novo* design, enzyme promiscuity and mechanisms of protein evolution, and the enzyme evolution of important enzymatic activities, such as the complete detoxification of lethal nerve agents.

Prof. Tawfik has more than 140 publications.

ENZYME ENGINEERING AWARDEES and LOCATIONS OF ECI ENZYME ENGINEERING CONFERENCES

- 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 DAN TAWFIK

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Sunday, September 6, 2015

16:00 – 17:45	Conference Check-in (Palm Court Foyer)
	Evening Session Session Chair: Robert DiCosimo, DuPont Industrial Biosciences
17:45 – 18:00	Welcome from the Conference Chairs and ECI Liaison Robert DiCosimo, Jon Stewart and Jeff Moore
18:00 – 19:00	Plenary Lecture Recent methodology developments in directed evolution Manfred T. Reetz, Philipp University of Marburg, Germany
19:00 – 19:30	Welcome Reception (Esplanade)
19:30 – 21:00	Dinner (Esplanade)

NOTES

- Technical sessions will be held in the Royal Ballroom.
- Poster Sessions will be in the Majestic Ballroom. Although there are two poster sessions, all posters will
 remain mounted for the entire conference. Authors of odd-numbered posters are asked to stay with their
 presentations on Monday evening, and authors of even-numbered posters are asked to stay with their
 presentations on Tuesday evening.
- All breakfasts and lunches, as well as dinners on Monday and Tuesday, will be in the Mezzanine/Terrace. The conference banquet on Thursday will be in the Vinoy Grand Ballroom.
- Audiotaping, videotaping and photography of presentations are strictly prohibited.
- Speakers Please leave at least 5 minutes for questions and discussion.
- Please do not smoke at any conference functions.
- The ECI office is in the Taylor Room.
- The Thomasson Room is available for small *ad hoc* meetings during the week. Please see ECI staff if you would like to use the room.
- Turn your cellular telephones to vibrate or off during technical sessions.
- Please write your name in the front of this booklet in case it is misplaced.
- Be sure to check the participant list in this booklet to confirm that your listing is correct. If there are changes or updates, please login to the ECI website and update your listing so that the list that ECI will send to all participants after the conference will be correct.

Monday, September 7, 2015

07:00 - 08:30	Breakfast
	<u>Session 1: de novo Design and the Impact of Structural Biology on Protein</u> <u>Engineering</u> <i>Sponsored by Novozymes A/S</i> Session Chair: Pratul Agarwal, Oak Ridge National Laboratory
08:30 - 09:10	Effects of point mutations on the stability and activity of enzymes Jens Erik Nielsen, Novozymes A/S, Denmark
09:10 – 09:50	Single molecule mechanics of adenylate kinase Matthias Rief, Technical University of München, Germany
09:50 – 10:30	Imine reductases: Engineering of a novel enzyme for the production of chiral secondary and tertiary amines Oscar Alvizo, Codexis, USA
10:30 – 11:00	Coffee Break Sponsored by Active Enzyme Molecule Conference
11:00 – 11:40	Computation library design for improving enzyme performance Dick Janssen, University of Groningen, The Netherlands
11:40 – 12:20	Enzyme design and evolution: Nearer to nature Don Hilvert, ETH, Switzerland
12:30 – 14:00	Lunch
	Session 2: Biocatalysis Session Chair: Animesh Goswami, Bristol-Myers Squibb
14:00 – 14:40	Engineering biocatalysts in cell-free system: Exploring and exploiting flavoenzymes Stefan Lutz, Emory University, USA
14:40 – 15:20	Engineering substrate binding: Trajectories, mechanisms and dynamics Joelle Pelletier, University of Montreal, Canada
15:20 – 16:00	Discovery and engineering of sucrose-active enzymes for use in chemo- enzymatic synthesis and production of novel glucans Magali Remaud-Simeon, Universite de Toulouse, France
16:00 – 16:30	Coffee Break Sponsored by BASF
16:30 – 17:10	Hints from nature: Tapping the Full potential of functional sequence space Wolfgang Aehle, B.R.A.I.N. AG, Germany
17:10 – 17:50	Exploiting squalene hopene cyclases and their catalytic Brønsted acid for non- natural reactions Bernard Hauer, University of Stuttgart, Germany
18:30 – 20:00	Dinner
20:00 – 21:30	Poster Session / Social Hour (Authors of odd-numbered posters are asked to stay with their presentations)

Tuesday, September 8, 2015

07:00 - 08:30	Breakfast
	Session 3: Biocatalysis Session Chair: Elisabetta Brenna, Polytechnic University of Milan
08:30 – 09:10	Database guided enzyme discovery, protein engineering and applications in biocatalysis Uwe T. Bornscheuer, University of Griefswald, Germany
09:10 – 09:50	D-Threonine aldolase catalyzed synthesis of a 3S-hydroxy-2R-amino acid Animesh Goswami, Bristol-Myers Squibb, USA
09:50 – 10:30	Enzymatic hydroxylations for fine chemicals : p450/ tyrosinase Byung-Gee Kim, Seoul National University, Korea
10:30 – 11:00	Coffee Break Sponsored by the Japanese Society of Enzyme Engineering
11:00 – 11:40	Discovery and engineering of amino acid dehydrogenases for the efficient synthesis of optically Pure D- and β-Amino acids Dunming Zhu, Chinese Academy of Sciences, China
11:40 – 12:20	Chemo-enzymatic cascade reactions Marko Mihovilovic, Vienna University of Technology, Austria
12:30 – 14:00	Lunch
	Session 4: Pathway Engineering Session Chair: Magali Remaud-Simeon, Universite de Toulouse
14:00 – 14:40	Engineering a synthetic metabolic pathway for high level production of isoprenoids Lishan Zhao, Amyris, Inc., USA
14:40 – 15:20	In vitro salvage synthesis of nicotinamide cofactor by thermophilic enzymes Kohsuke Honda, Osaka University, Japan
15:20 – 16:00	Enabling multistep enzyme catalyzed processes via synthetic biology Huimin Zhao, University of Illinois at Urbana-Champaign, USA
16:00 – 16:30	Coffee Break Sponsored by Merck and Co., Inc.
16:30 – 17:10	Tunable systems for bioengineering using machine learning Claes Gustafsson, DNA2.0 Inc., USA
17:10 – 17:50	Use of an enzyme-coupled biosensor to engineer a BIA fermentation pathway from glucose in Saccharomyces cerevisiae John Dueber, University of California, Berkeley, USA
18:30 – 20:00	Dinner
20:00 – 21:30	Poster Session / Social Hour (Authors of even-numbered posters are asked to stay with their presentations)

Wednesday, September 9, 2015

07:00 - 08:30	Breakfast
	Session 5: Emerging Technologies Session Chair: Jon Stewart, University of Florida
08:30 – 09:10	A structural perspective on the evolution of protein functions Christine A. Orengo, University College London, United Kingdom
09:10 – 09:50	Designing hyper-catalytic enzymes using conformational modulation Pratul Agarwal, Oak Ridge National Laboratory, USA
09:50 – 10:30	Using fully defined activation protocols and cell-free screening to study [FeFe]hydrogenase maturation and oxygen tolerance James Swartz, Stanford University, USA
10:30 – 11:00	Coffee Break
11:00 – 11:40	Improved illumina sequencing by polymerase engineering Molly He, Illumina Inc., USA
11:40 – 12:40	Plenary Lecture A perspective on biological catalysis Stephen J. Benkovic, Pennsylvania State University, USA
12:40	Box Lunch / Free Time
	Dinner on your own

Thursday, September 10, 2015

07:00 - 08:30	Breakfast
	Session 6: Biocatalysis Session Chair: Joelle Pelletier, University of Montreal
08:30 – 09:10	Applications of ene-reductases in stereoselective organic synthesis Elisabetta Brenna, Polytechnic University of Milan, Italy
09:10 – 09:50	Development of oxidizing enzymes for hair dyeing Yoshihiko Hirose, Amano Enzyme Inc., Japan
09:50 – 10:30	Enzyme engineering of an aminotransferase for use in pharmaceutical process development Michael J. Karmilwicz, Pfizer, USA
10:30 – 11:00	Coffee Break
11:00 – 11:40	Enzymes to the rescue: Battling infectious disease using enzyme technology Jonathan S. Dordick, Rensselaer Polytechnic Institute, USA
11:40 – 12:20	Evolution of cytochrome P450 BM-3 enzymes to improve performance and maintain generality Jeffrey Moore, Merck, USA
12:30 - 14:00	Lunch
	Session 7: Commodity and Industrial Chemicals Session Chair: Jonathan Dordick, Rensselaer Polytechnic Institute
14:00 – 14:40	Engineering nature's enzyme repertoire for food, pharma and biofuels Rene de Jong, DSM Biotechnology Center, The Netherlands
14:40 – 15:20	Engineering laundry enzymes for lower energy use James Kellis, DuPont Industrial Biosciences, USA
15:20 – 16:00	BASF enzymes create chemistry Adrienne Davenport, BASF, USA
16:00 – 16:30	Coffee Break
16:30 – 17:10	Efficient engineering of biocatalysts for industrial needs Andreas Vogel, c-LEcta GmbH, Germany
17:10 – 17:50	Microbial, plant and animal aldoxime-nitrile pathways – discovery of new enzymes, their comparative studies and applications Yasuhisa Asano, Toyama Prefectural University, Japan
19:00 – 20:00	Enzyme Engineering Award presentation and lecture
20:00 – 22:00	Banquet

Friday, September 11, 2015

06:30 – 08:30 Breakfast and departures

Enzyme Engineering XXIII

Poster Presentation List

- 1. Selective oxidation of lignin model compounds by the laccase-mediator system Joseph O. Rich, US Department of Agriculture, USA
- Improvement of thermostability of an alkaline pectate lyase from alkaliphilic Bacillus sp. N16-5 by directed evolution Yanfen Xue, Chinese Academy of Sciences, China
- Engineering of bacterial (R)-selective hydroxynitrile lyases for broadened substrate scope Kerstin Steiner, ACIB, Austria
- 4. Engineering of ketoreductase enzymes for chiral synthesis on industrial scale Pramod P. Wangikar, Indian Institute of Technology Bombay, India
- Exploring evolutionary diversity to identify putative alcohol dehydrogenase enzymes as starting point for directed evolution
 Priyanka Dalal, Indian Institute of Technology Bombay, India
- 6. Smart peptides: Immobilization of enzymes and antibodies on inexpensive mineral matrices for biocatalysis and cell capture Peter L. Bergquist, Macquarie University, Australia
- 7. Characterizing broad specificity proteases by in vitro selection Michael D. Lane, University of Minnesota, USA
- 8. **Reaction simulation of sarcosine oxidase by using FMO and QM/MM method** Yukihiro Abe, Toyobo Co. Ltd., Japan
- 9. **Quantitative analysis reveals great potential of CO2-fixation in** *Escherichia coli* Zhen Cai, Chinese Academy of Sciences, China
- 10. **Directed evolution of alcohol dehydrogenase** Emil Hamnevik, Uppsala University, Sweden
- 11. Engineering of *E. coli* isopropylmalate dehydrogenase (LeuB) to improve the efficiency of the "+1" pathway for the production of >C5 alcohols Paresh C. Sanghani, Dow AgroSciences LLC, USA
- 12. Fermentative production of 1-propanol from glycerol using metabolically engineered *Escherichia coli* Michihiko Kataoka, Osaka Prefecture University, Japan
- 13. Alteration of the substrate specificity of alanine dehydrogenase Emily C. Mundorff, Hofstra University, USA
- 14. A comparative analysis of biosensors for fast detection of toxic compounds Ruchi Singla, Chandigarh Engineering College, Mohali, India

- 15. NADH-dependent reductions in baker's yeast: Flow-cytometry-driven strain and process engineering for improved whole-cell biocatalysis Magnus Carlquist, Lund University, Sweden
- 16. Engineering of access tunnel as strategy to balance activity-stability trade-off in haloalkane dehalogenase Radka Chaloupkova, Masaryk University, Czech Republic
- 17. Engineering of a plant cytochrome P450 for improved light-driven biosynthesis Silas B. Mellor, University of Copenhagen, Denmark
- Cloning, expression and characterization of novel omega-transaminases from hot terrestrial environments
 Erica E. Ferrandi, University of Copenhagen, Denmark
- 19. Rational directed evolution of an esterase for improved enantioselectivity towards a diester substrate used in the production of dehydrocoronamic acid Toni Fleming, Dr Reddy's, United Kingdom
- 20. Extremozymes development for industrial biocatalysis Felipe Sarmiento, Swissaustral, USA
- A dye-decolorizing peroxidase from *Bacillus subtilis* exhibiting substrate-dependent optimum temperature for dyes and β-ether lignin dimer Kyoungseon Min, Kwangwoon University, South Korea
- 22. A novel NAD-independent thermophilic D-lactate dehydrogenase from Acidobacter aceti and Acidocella species MX-AZ02 Young Joo Yeon, Seoul National University, South Korea
- 23. Genetically encoded biosensors for polyketide synthetic biology and directed evolution Christian M. Kasey, North Carolina State University, USA
- 24. Vibrio vulnificus glycogen branching enzyme preferentially transfers very short chains: N1 domain determines the chain length transferred Jong-Tae Park, Chungnam National University, South Korea
- Production of tailor-made bacterial polysaccharides from a novel Escherichia coli mutant Jong-Tae Park, Chungnam National University, South Korea
- 26. Engineering of artificial enzymes toward the construction of a new metabolic pathway for 2,4-dihydroxybutyric acid production Yannick Malbert, Institut National De La Recherche Agronomique, France
- 27. Engineering of biocatalysts at Johnson Matthey Ahir Pushpanath, Johnson Matthey, United Kingdom
- 28. **Development of the amine dehydrogenase towards production of chiral amines** Samantha K. Au, Georgia Institute of Technology, USA
- 29. The nitroreductase superfamily; complexity, diversity and redundancy Janine N. Copp, University of British Columbia, Canada
- 30. A biomimetic approach to coelenterazine-type luciferins Richard Metzner, Toyama Prefectural University, Japan

- Enzymatic synthesis of cyclic amino acids from diamino acids Ryoma Miyake, Mitsubishi Chemical Group Science and Technology Research Center, Inc., Japan
- 32. Efficent production of (S)-equol by recombinant Escherichia coli expressing stereospecific dihydrodaidzein reductase mutant Pyung-Gang Lee, Seoul National University, South Korea
- 33. Engineering enzyme enantioselectivity by computational library design and screening Hesam Arabnejad, University of Groningen, Netherlands
- 34. General strategy for enzymatic O-alpha-glycosylation of natural products using engineered alpha-glycosidases Young-Wan Kim, Korea University, South Korea
- 35. Enhancing nitroreductase substrate selectivity using simultaneous positive and negative directed evolution selection pressures Rory Little, Victoria University of Wellington, New Zealand
- Towards preparative scale thymol bromination with vanadium chloroperoxidase from Curvularia inaequalis
 Elena Fernández-Fueyo, Delft University of Technology, Netherlands
- 37. Functional analysis of hydroxy fatty acid dehydrogenase in polyunsaturated fatty acid saturation metabolism in *Lactobacillus plantarum* AKU 1009a Michiki Takeuchi, Kyoto University, Japan
- 38. **New concepts and software tools for rational design of enzymes** Radka Chaloupkova, Masaryk University, Czech Republic
- 39. **Process considerations for use of galactose oxidase as an industrial biocatalyst** Asbjørn Toftgaard Pedersen, Technical University of Denmark, Denmark
- 40. Development of positive selection methods to improve nitroreductase activity by directed evolution Michelle Rich, Victoria University of Wellington, New Zealand
- Characterization of functionally important binding sites of enzymes by bioinformatic analysis of diverse protein families
 Vytas Svedas, Lomonosov Moscow State University, Russia
- 42. **BASIC a novel DNA assembly method for pathway & genetic circuit optimization** Marko Storch, Imperial College London, United Kingdom
- 43. Mutagenesis and screening of bacterial nitroreductases to develop cell ablation tools for developmental and regenerative studies in zebrafish Elsie Williams, Victoria University of Wellington, New Zealand
- 44. Development of activity-based ultra-high-throughput screening system of peroxidase by using microbead display
 Bo Zhu, Nagoya University, Japan
- 45. **Designing highly robust yet promiscuous monooxygenase enzymes: Combinatorial libraries of ancestor reconstruction and directed evolution (clade)** Yosephine Gumulya, The University of Queensland, Australia

- 46. **Protein engineering of alpha-glucosidase results in altered substrate specificity** Satoru Ishihara, Amano Enzyme USA Co., Ltd., USA
- 47. Ancestral enzymes as a platform for generating new biocatalysts Bryan J. Jones, University of Minnesota, USA
- 48. **Engineering enzyme cofactor specificity improves fermentation for chemical production** Cara A. Tracewell, Genomatica, USA
- Direct electron transfer from hydrogenases to eliminate oxireductase cofactor requirements Rkia Laamarti, KAUST, Saudi Arabia
- 50. **Pathway design for biosynthesis of β-valienamine in** *Streptomyces hygroscopicus* Yan Feng, Shanghai Jiao Tong University, China
- 51. Sphingolipid ceramide N-deacylase as a useful tool for the enzymatic assembly of glycosphingolipids Guangyu Yang, Shanghai Jiao Tong University, China
- 52. Engineering transaminase to expand its substrate scope towards bulky ketones using a novel *in silico* high throughput screening framework Uwe Bornscheuer, Greifswald University, Germany