

*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 23<sup>rd</sup> 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 Benozziyo 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	<b>Plenary Lecture</b> <b>Recent methodology developments in directed evolution</b> 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

### **Session 1: de novo Design and the Impact of Structural Biology on Protein Engineering**

***Sponsored by Novozymes A/S***

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  $\beta$ -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
2. **Improvement of thermostability of an alkaline pectate lyase from alkaliphilic *Bacillus* sp. N16-5 by directed evolution**  
Yanfen Xue, Chinese Academy of Sciences, China
3. **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
5. **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 CO<sub>2</sub>-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 >C<sub>5</sub> 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
18. **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, Swisssaustral, USA
21. **A dye-decolorizing peroxidase from *Bacillus subtilis* exhibiting substrate-dependent optimum temperature for dyes and  $\beta$ -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
25. **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

31. **Enzymatic synthesis of cyclic amino acids from diamino acids**  
Ryoma Miyake, Mitsubishi Chemical Group Science and Technology Research Center, Inc., Japan
32. **Efficient 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
36. **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
41. **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
49. **Direct electron transfer from hydrogenases to eliminate oxireductase cofactor requirements**  
Rkia Laamarti, KAUST, Saudi Arabia
50. **Pathway design for biosynthesis of  $\beta$ -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