



RESEARCH CONFERENCES

ESF-EMBO Symposium

Protein Design and Evolution for Biocatalysis

Hotel Eden Roc, Sant Feliu de Guixols (Costa Brava) • Spain
25-30 October 2008

Chair: **Jiri Damborsky**, Masaryk University, CZ

www.esf.org/conferences/08255

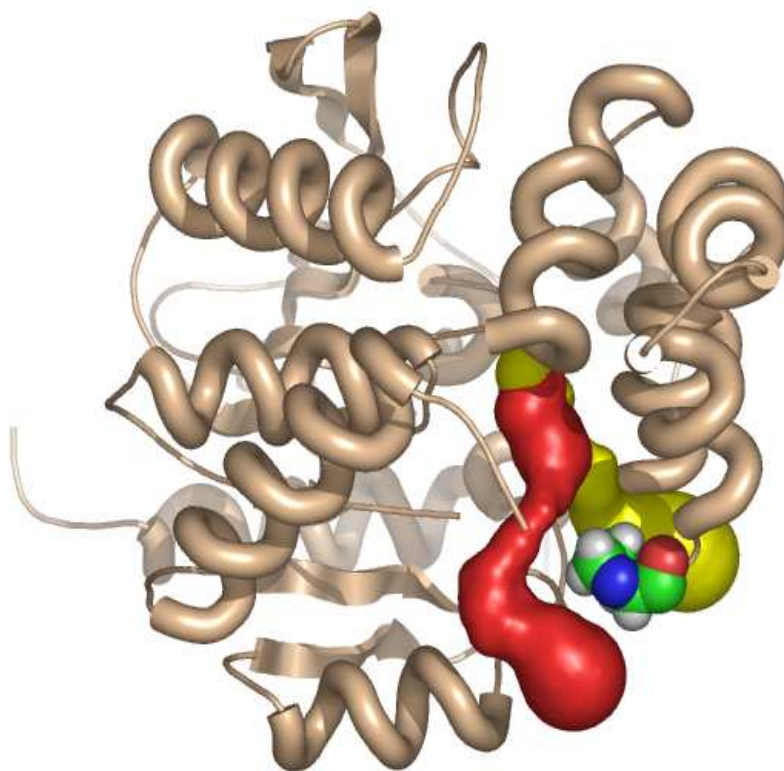
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Final Programme

Saturday 25 October

Late afternoon / early evening	Registration at the ESF-RC desk
19.00	Welcome Drink
20.00	Supper

Sunday 26 October

08.45-09.00	Conference Opening
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Session 1: Fundamentals of enzymatic catalysis

Chairs: Paul Engel, University College Dublin, UK, Peter Neubauer, University of Oulu, FI

09.00-09.35	Stephen Benkovic Pennsylvania State University, US <i>Perspective on Biocatalysis</i>
09.35-09.55	Colin Jackson CSIRO, AU <i>Comparison between Neutral Drift and Classical Evolution in the Development of Insecticide Resistance</i>
09.55-10.30	John Gerlt University of Illinois, US <i>Prediction of Function in the Enolase and RuBisCO Superfamilies</i>
10.30-11.00	Coffee break
11.00-11.35	Gregory Petsko Brandeis University, US <i>What Makes a Binding Site a Binding Site</i>
11.35-12.00	Florian Hollfelder University of Cambridge, UK <i>Multiple Catalytic Promiscuity</i>
12.00	Lunch
15.00-15.30	Coffee break

Session 2: Computer modelling in protein design

Chairs: Volker Heinrichs, Athenix, USA, Anju Chadha, IIT Madras, IN

15.30-16.05	Rebecca Wade EML Research, DE Probing enzyme oligomerization and regulation by protein mutation
16.05-16.30	Emily Mundorff Codexis, USA <i>Development of the Codex Biocatalyst Panels</i>

16.30-17.00	Coffee break
17.00-17.35	Daniela Grabs-Roethlisberger University of Washington, US <i>Computational de novo Design of Protein Catalysts</i>
17.35-18.10	Sven Panke ETH Zurich, CH <i>Engineering Multi-Enzyme Systems</i>
19.00	Dinner
20.00-22.00	Poster session I

Monday 27 October

Session 3: Computer modelling in protein design

Chairs: Miguel Gonzales, University of Barcelona, ES, Pierre Monsan, INSA University of Toulouse, F

09.00-09.35	Arieh Warshel University of Southern California, US <i>Hidden Principles of Enzyme Design</i>
09.35-09.55	Maria Suarez Ecole Polytechnique, F <i>Engineering of a Thioredoxin Protein with Additional Enzyme Function using Computational Design</i>
09.55-10.30	Federico Gago University of Alcala, ES <i>Computer Simulations of Enzyme Activity: Structural Snapshots of the Mechanism of Thioredoxin Reduction by E. coli Thioredoxin Reductase</i>
10.30-11.00	Coffee break
11.00-11.35	Adrian Mulholland University of Bristol, UK <i>Computational Enzymology as a Guide for Catalyst Design</i>
11.35-11.55	Sanja Tomic Rudjer Boskovic Institute, HR <i>Combined 3D QSAR and QM/MM Study of the Burkholderia cepacia Lipase Enantioselectivity</i>
11.55-12.30	Juergen Pleiss University Stuttgart, DE <i>Computational Enzyme Design: Structure, Dynamics and Solvent Effects</i>
12.30	Lunch
15.00-15.30	Coffee break

Session 4: Bioinformatics in protein design

Chairs: Yan Feng, Jilin University, CN, Patrice Soumillon, Université Catholique de Louvain, BE

15.30-16.05	Janet Thornton European Bioinformatics Institute, UK <i>The Evolution of Enzyme Specificity in Large Protein Families</i>
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16.05-16.25	Paul Alan Bates Cancer Research, UK <i>Protein Engineering of the Cancer Drug: L-Asparaginase</i>
16.25-17.00	Brian Shoichet University of California - San Francisco, US <i>Forward and Reverse Chemical Information in Biology</i>
17.00-17.30	Coffee break
17.30-18.05	Janusz Bujnicki International Institute of Molecular and Cellular Biology, PL <i>Protein Structure Prediction for Protein Engineering</i>
18.05-18.40	Jan Kmunicek CESNET and Masaryk University, CZ <i>Enabling Grids for E-SciencE - Infrastructure for In Silico Experiments</i>
19.00	Dinner
20.30-21.30	Forward Look Plenary Discussion Chairs: Stephen Benkovic, Uwe Bornscheuer, Dick Janssen, Romas Kazlauskas, Manfred Reetz, Daniel Tawfik

Tuesday 28 October

Session 5: Directed evolution of biocatalysts

Chairs: Manfred Konrad, Max-Planck-Institute for Biophysical Chemistry, DE, Montarop Yamabhai, Suranaree University of Technology, TH

09.00-09.35	Dan Tawfik Weizmann Institute of Science, IL <i>The Makings of New Biocatalysts</i>
09.35-09.55	Ulrich Schwaneberg Jacobs University Bremen, UK <i>Steering Directed Protein Evolution</i>
09.55-10.30	Manfred Reetz Max-Planck-Institut für Kohlenforschung, DE <i>Methodology Development for Fast Directed Evolution</i>
10.30-11.00	Coffee break
11.00-11.35	Philipp Holliger MRC Cambridge, UK <i>Evolving Polymerases by Compartmentalized Self-Replication</i>
11.35-11.55	Aurelio Hidalgo Universidad Autónoma de Madrid, ES <i>Expanding the short-chain selectivity of Pseudomonas fluorescens esterase I by focused directed evolution and rational design</i>
11.55-12.30	Burckhard Seelig Harvard Medical School, US <i>De novo Enzyme Creation and Evolution using mRNA Display</i>
12.30	Lunch
Afternoon	Half-day excursion to Girona
19.00	Dinner
20.00-22.00	Poster session II

Wednesday 29 October

Session 6: Directed evolution and engineering of biocatalysts

Chairs: Manfred Schneider, Bergische Universitaet, DE, Vytas Svedas, Lomonosov Moscow State University, RU

- 09.00-09.35 **Romas Kazlauskas**
University of Minnesota, US
Teaching Enzymes to Catalyze New Reactions
- 09.35-09.55 **Amir Aharoni**
Ben Gurion University, IL
Directed Evolution of Cytosolic Sulfotransferases for Enhanced Thermostability and Specificity
- 09.55-10.30 **Karl-Erich Jaeger**
Heinrich-Heine-University Duesseldorf, DE
Production and Design of Novel Biocatalysts
- 10.30-11.00 Coffee break
- 11.00-11.35 **Karl Hult**
Royal Institute of Technology, SE
Protein Engineering of Candida antarctica Lipase B for New Substrate and Reaction Specificities
- 11.35-11.55 **Nobuhiko Tokuriki**
Weizmann Institute of Science, IL
GroEL/ES Chaperones Promote Genetic Variation and Accelerate Enzyme Evolution
- 11.55-12.30 **Stefan Lutz**
Emory University, US
Engineering Enzymes by Circular Permutation: Beyond CALB
- 12.30 Lunch
- 15.00-15.30 Coffee break

Session 7: Directed evolution and engineering for biocatalysis

Chairs: Magali Remaud-Simeon, University of Toulouse, F, Thomas John Smith, Sheffield Hallam University, UK

- 15.30-16.05 **Uwe Bornscheuer**
University Greifswald, DE
Rational Protein Design vs. Directed Evolution: Examples to Improve Enantioselectivity of Biocatalysts
- 16.05-16.25 **Zbynek Prokop**
Masaryk University, CZ
Two Independent Enantioselective Elements Confined to a Single Active Site of Haloalkane Dehalogenase
- 16.25-17.00 **Dick Janssen**
University of Groningen, NL
Engineered Enzymes for Enantioselective Epoxide Ring Opening
- 17.00-17.30 Coffee break

17.30-18.05

Nick Turner

University of Manchester, UK

Directed Evolution of Enzymes for Applications in Organic Synthesis

18.05-18.25

Marc Creus

University of Neuchatel, CH

Artificial Metalloenzymes are Versatile Systems for Enantioselective Biocatalysis

20.00

Get-together & Conference Dinner

Thursday 30 October

Breakfast & Departure

Posters

For authors presenting posters, panels measuring 140 cm high x 100 cm wide will be available at the conference site.

Poster sessions will be held on Sunday and Tuesday: 20.00 to 22.00.

Numbers will be allocated a few weeks before the conference.

Authors with odd poster numbers should be available at their posters during the session on Sunday (*Poster Session I*), keeping their posters on display until Tuesday morning.

Authors with even numbers will present on Tuesday evening (*Poster Session II*) and keep their posters on display until the end of the conference.

A list with poster numbers will be made available on the website a few weeks before the conference