



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

<u>Presenters</u>		<u>LIST OF ACCEPTED POSTERS</u>	
	Surname	First Name	Poster Title
1	Afriat J	Livnat	The gradual evolution of new enzymes via multi-step loop replacements
2	Andre	Isabelle	Insights into molecular motions of <i>Burkholderia cepacia</i> lipase inferred from mixed molecular modelling and robotic based path planning approaches
3	Awadelkarim	Mohamed	Directed evolution of an existing phenylalanine dehydrogenase, L307V, for enantiopure synthesis of phenylalanine analogues substituted at the 2- and 3-position of the aromatic ring
4	Bar	Hagit	The application of ancestral resurrection for protein engineering – the AChE model case
5	Binay	Baris	Construction of 246Gly and 240Ala mutant for changing the substrate specificity of the <i>Bacillus sterothermophilus</i> lactate dehydrogenase (bs LDH)
6	Brezovsky	Jan	Modulation of enantioselectivity in haloalkane dehalogenase DbjA by engineering of a surface loop
7	Brissos	Vânia	Development of directed evolution assays to improve the redox potential of CotA-laccase
8	Butz	Maren	Tunable protein production system allows directed evolution of highly active enzymes

9	Chadha	Anju	A versatile biocatalyst for deracemisation: Mechanism and scope of <i>Candida parapsilosis</i> ATCC 7330
10	Chaloupkova	Radka	Thermodynamic analysis of enantioselectivity of haloalkane dehalogenase DbjA and its variants DbjA Δ and DbjA Δ +H139A towards brominated esters and β -substituted bromoalkanes
11	Chen	Sihong	Directed evolution of phenylalanine dehydrogenase from <i>Bacillus sphaericus</i> towards activity with an un-saturated non-natural amino acid
12	Chilov	Ghermes	Application of molecular docking methods for modeling enzyme specificity
13	Chovancova	Eva	HotSpot Wizard: Web server for identification of hot spots for mutagenesis experiments
14	Copp	Janine	Identification and improvement of novel bacterial nitroreductases for cancer gene therapy
15	Daroch	Maurycy	Isolation and preliminary characterisation of <i>S. aeruginosa</i> peroxidase with potential industrial relevance
16	Desmet	Tom	Directed evolution of disaccharide phosphorylases
17	Dyguda-Kazimierowicz	Edyta	Phosphotriesterase-catalyzed hydrolysis of sarin: QM/MM simulation of the reaction pathway
18	Fairchild	Steven	Engineering proteins for enhanced activity
19	Feng	Yan	The novel substrate lineages by key motif directed module recombination
20	Ferrario	Valerio	Steered molecular dynamics and GRID for simulation of lipase activation
21	Fuhrmann	Markus	Slonomics – A novel technology for the generation of highly designed gene libraries
22	Gaidukov	Leonid	Directed evolution and mechanistic studies of serum paraoxonases
23	Gatti-Lafranconi	Pietro	(Un)Predictable effects of distant mutations on protein activity and stability
24	Giger	Lars	Illuminating the mechanism of a PLP-dependant aldolase using an <i>in vivo</i> selection system
25	Goedl	Christiane	Molecular mechanisms of glucosyl transfer in retaining disaccharide phosphorylases
26	González	Miguel	QM/MM investigation of the reactions of the hepatitis C virus NS3 protease with its main natural substrates: Reaction mechanism and molecular dynamics simulations
27	Gumulya	Yosephine	Iterative saturation mutagenesis based on B-factors to increase thermostability of <i>Aspergillus niger</i> epoxide hydrolase
28	Heinrichs	Volker	Improvement of protein thermostability, solubility and enzymatic activity by directed evolution
29	Hoebartner	Claudia	Engineering a selective small-molecule substrate binding site into a deoxyribozyme
30	Iranzo	Olga	Designing <i>de novo</i> superoxide dismutases
31	Jesenska	Andrea	Dynamics of water molecules at the tunnel mouths of haloalkane dehalogenases studied by time resolved fluorescence spectroscopy and computer simulations
32	Jochens	Helge	Converting an esterase into an epoxide hydrolase

33	Jones	Aubrey	Directed evolution of two key cellulases for the conversion of biomass to ethanol
34	Joosten	Henk-Jan	3DM: A tool for optimal use of superfamily data for enzyme engineering
35	Khersonsky	Olga	Directed evolution of <i>in silico</i> designed enzymes
36	Klvana	Martin	Pathways and mechanisms for product release in engineered haloalkane dehalogenase DhaA explored using classical and random acceleration molecular dynamics simulations
37	Knapic	Lorena	3D-QSAR model for the quantitative prediction of enantioselectivity of lipase B from <i>Candida antarctica</i>
38	Konrad	Manfred	Cellular delivery of catalytically improved nucleoside kinases to enhance metabolic activation of prodrugs and improve anticancer and antiviral therapy
39	Kotik	Michael	Modification of activity and enantioselectivity of an epoxide hydrolase by saturation mutagenesis and novel epoxide hydrolases from environmental DNA
40	Koudelakova	Tana	Analysis of substrate specificities of wild-type haloalkane dehalogenases and their mutants by multivariate statistics
41	Krol	Marcin	Protein engineering of the cancer drug: L-Asparaginase
42	Kufka	Julia	Mechanistic studies and modification of prenylating enzymes
43	Lafaquière	Vincent	A structure-controlled lipase enantioselectivity investigated by a path planning approach
44	Leitner	Christian	Improving the activity of pyranose 2-oxidase via site directed mutagenesis of the active site loop
45	Leow	Thean Chor	Structural implication of T1 lipase through rational design
46	Mansfeld	Johanna	Approaching the function of the C2 domain in plant phospholipases D by semi-rational design approaches
47	Martins	Ligia	Development of directed evolution assays to improve the redox potential of CotA-laccase
48	Mazura	Pavel	Rational design and directed evolution of the maize beta-glucosidase Zm.p60.1
49	Mitchell	Vesna	Combining shuffling, ProSAR and biocatalyst panels to develop enzymes for chemical synthesis
50	Muellegger	Johannes	ZymeCAD, a versatile and comprehensive molecular simulation platform. Application in the study of antigen-antibody complexes
51	Munawar	Nayla	<i>In-vitro</i> reactivation of inclusion bodies and homologous expression of recombinant glutamate dehydrogenases from <i>Halobacterium salinarum</i>
52	Narayanan	Rajesh	Kinetic studies of phenylalanine dehydrogenase from <i>Bacillus sphaericus</i> and derived mutants with a variety of substrates
53	Nerinckx	Wim	An upside-down substrate flip within the active site of evolutionary related beta and alpha glycopyranoside hydrolases explains their mechanistic relationship
54	Neubauer	Antje	EnBase - high density cell cultivation for high throughput screening
55	Neubauer	Peter	TIM-based biocatalyst platform for chiral synthesis of chemical compounds
56	Ochoa-Leyva	Adrian	Protein design for new activities through catalytic loop exchange in the ($\beta\alpha$) ₈ -fold

57	Otten	Linda G.	New nitrile hydratases for biocatalysis
58	Pawlak	Sebastian	Rational design of restriction endonuclease specificity through computational analysis and subunit rearrangement
59	Rannes	Julie	Directed evolution of new galactose oxidase variants for glycan labelling
60	Remaud-Simeon	Magali	Tailoring alpha-transglucosidase specificity for programmed chemo-enzymatic synthesis of complex bacterial oligosaccharides
61	Robin	Aelig	Fused cytochrome P450 enzymes for more effective biohydroxylations
62	Sawayama	Andrew	A Panel of cytochrome P450 BM3 variants to produce drug metabolites and diversify lead compounds
63	Schaerli	Yolanda	Isothermal DNA amplification in microdroplets
64	Schneider	Sarah	Changing the substrate scope of transaldolase B <i>E. coli</i> towards non-phosphorylated compounds
65	Schneider	Manfred	Carba analogues of PAF: Enzyme assisted syntheses and biological activities
66	Schreier	Bettina	Engineering the enolase active site pocket: Is the second magnesium ion essential for enolase activity?
67	Schuermann	Martin	Directed evolution and specific engineering of industrial biocatalysts for enantioselective C-C-bond formation
68	Shubina	Tatyana	New cage compounds as potential influenza A inhibitors: Synthesis and docking/QSAR study
69	Skowronek	Krzysztof	Engineering of the NlaIV restriction endonuclease sequence specificity
70	Smith	Thomas John	Mutagenesis and directed evolution of key bacterial monooxygenases toward improved biocatalysis
71	Snajdrova	Radka	Towards biocatalysts for organosilane biotransformations
72	Soni	Pankaj	B factor iterative test (B-FIT) for enhancing enzyme stability in organic solvents
73	Soumillion	Patrice	Engineering a beta-lactamase allosterically regulated by kanamycin
74	Soumillion	Patrice	Everything is there but it is not a beta-lactamase
75	Spadiut	Oliver	Improving pyranose 2-oxidase from <i>Trametes multicolor</i> for biocatalytic applications by genetic engineering
76	Spelberg	Jeffrey Lutje	Biocatalyst panels: Using tunable biocatalysts to accelerate process development
77	Strerath	Michael	Evolution of screening assays during the extensive phenotypic remodeling of an unspecific human serine protease towards higher activity, high selectivity and blood serum inhibitor insensitivity
78	Stroganov	Oleg	Molecular modeling of substrates recognition by penicillin acylase
79	Suarez	Maria	Construction of a library of orthogonal transcription factors with their corresponding promoters based on design of synthetic zinc-finger proteins
80	Suplatov	Dimitry	Bioinformatic analysis of penicillin acylase family reveals key residues essential for enzyme stability

81	Svedas	Vytas	Molecular modeling of nucleophile binding and reactivity in penicillin acylase-catalyzed acyl transfer
82	Syrén Vallin	Per-Olof Michaela	Rational design of <i>Candida antarctica</i> lipase B for kinetic resolution of bulky sec-alcohols
83	Takwa	Mohamad	Rational design of <i>Candida antarctica</i> lipase B for the ring opening polymerization of lactides
84	Tengku Abdul Hamid	Tengku Haziyaamin	Protein solvent interaction study of recombinant thermostable and solvent stable lipase from <i>Bacillus</i> sp., strain 42, by molecular dynamic simulation
85	Tkaczuk	Karolina L.	Comprehensive evolutionary analysis, comparison of active sites and re-classification of the SPOUT superfamily of methyltransferases
86	Valentini	Maria	Characterization of site-specific interactions of the MTGase enzyme with G-CSF: Why is Q134 PEGylated and Q131 is not?
87	Van Loo	Bert	A Most promiscuous enzyme: Six reactions catalyzed by one active site
88	Villiers	Benoit	Substrate promiscuity and directed evolution of a nonribosomal peptide synthetase adenylation domain (TycA)
89	Thomas	Veena	Stability and activity constrain evolution of an antibiotic resistance enzyme
90	Weignerova	Lenka	The alpha-galactosidase type A gene from <i>Aspergillus niger</i> encodes a fully functional alpha-N-acetylgalactosaminidase
91	Whitehead	Sarah	Novel tandem reactions and the directed evolution of a promiscuous bifunctional enzyme
92	Yamabhai	Montarop	Improvement of endochitinase activity by directed evolution
93	Yelboga	Emrah	Site saturation mutagenesis of crucial residues in NAD/NADP specificity of formate dehydrogenase from <i>Candida methylca</i>
94	Yuan	Bo	Selective oxidation of primary and secondary alcohols using variants of galactose oxidase
95	Yun	Chul-Ho	Oxidation of human cytochrome P450 1A2 substrates by <i>Bacillus megaterium</i> cytochrome P450 BM3: Humanized bacterial monooxygenase system
96	Zhang	Guirong	Directed evolution of a hyperthermophilic esterase from the archaeon <i>Aeropyrum pernix</i> K1 to improve the hydrolysis efficiency towards plant cell wall
97	Carballeira Rodriguez	Jose Daniel	Changing DNA specificity of TrwC, a DNA strand transferase

IMPORTANT

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**.

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** (Poster Session II) and keep their posters on display until the end of the conference.