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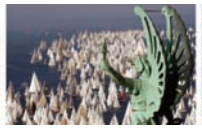
http://www.irene-fp7.eu/


Dipartimento di Scienze Chimiche e Farmaceutiche

FEDERCHIMICA
ASSOBIOTEC
Italian Association for the Development of Biotechnology

ESAB
Section on Applied Biocatalysis

ESTECO

BIOPOX

novozymes
Rethink Tomorrow

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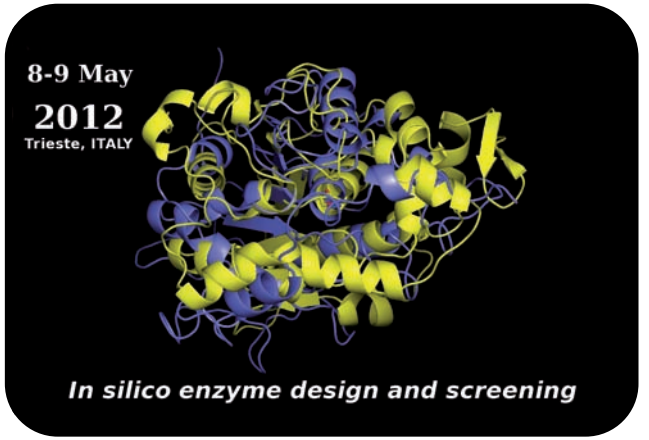

ICTP
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

Adriatico Guesthouse - Giambiagi Lecture Hall

The three-year work of FP7 IRENE project made possible the convergence of different expertise for developing computational methods and strategies for rationally design and produce the next generation of efficient biocatalysts for industrial applications. Now, we intend to present the final results of IRENE's project and to stimulate the dialogue between academic and industrial excellence in the field of computational enzymology. The objective is to explore new horizons for a novel, integrated and effective study of enzyme characteristics.

irene
in silico rational engineering of novel enzymes

SEVENTH FRAMEWORK PROGRAMME

Conference Agenda

MONDAY, May 7, 2012

17:30 - 19:00 Registration (ICTP Adriatico Guesthouse)

19:30 Welcome Reception at the ICTP Adriatico Guesthouse

TUESDAY, May 8, 2012

8:00 - 8:45 Registration (ICTP Adriatico Guesthouse)

9:00 - 09:10 Welcome and Opening (Giambiagi Lecture Hall)
Fabio Benedetti - Deputy Rector for Research
Università degli Studi di Trieste

09:10 - 10:00 OPENING LECTURE: ENZYME FUNCTION
Chair: Lucia Gardossi

Karl Hult - Royal Institute of Technology,
KTH Stockholm, Sweden
Knowledge-based rebuilding of Candida antarctica lipase B

Session: BIOINFORMATICS AND STRUCTURE BASED IN SILICO DESIGN PART A
Chair: Vytas Svedas

10:00 - 10:50 **Arieh Warshel -** University of Southern California,
Los Angeles, U.S.A.
Advances in Quantitative Computer Aided Enzyme Design

10:50 - 11:20 Coffee-break

Session: BIOINFORMATICS AND STRUCTURE BASED IN SILICO DESIGN PART B
Chair: Janez Mavri

11:20 - 12:05 **Jan H. Jensen -** University of Copenhagen,
Copenhagen, Denmark
Industrial Strength QM/MM: Computational high throughput screening of enzyme activity in enzyme mutants

12:05 - 12:40 **Hein J. Wijma -** University of Groningen,
Groningen, the Netherlands
In silico design of enzyme thermostability

12:40 - 13:05 **Dmitry Suplatov -** Lomonosov Moscow State
University, Moscow, Russian Federation
Bioinformatic selection of subfamily-specific positions as hotspots for rational enzyme engineering

13:05 - 14:30 Lunch

14:30 - 16:00 POSTER SESSION

16:00 - 16:20 Coffee-break

Session: DATA DRIVEN DIVERSITY SCREENING AND DESIGN
Chair: Allan Svendsen

16:20 - 17:10 **Andreas Bommarius -** Georgia Institute
of Technology, Atlanta, U.S.A
Activity and selectivity enhancements with restricted libraries

17:10 - 18:00 **Gabriele Cruciani** - University of Perugia,
Perugia, Italy
A common reference framework for Structure-based screening. Fingerprints for Ligands and Proteins (FLAP): theory and application

18:00 - 18:25 **Valerio Ferrario -** Università degli Studi di Trieste,
Trieste, Italy
3D analysis of catalytic differences of hydrolases by integrating modeling and multivariate statistics

18:25 - 18:50 **Oleg Stroganov -** MolTech Ltd.
and N.D.Zelinsky Institute of Organic Chemistry,
Moscow, Russian Federation
TSAR: a new graph-theoretical approach for protein modeling and in silico protein engineering

20:30 **Conference Dinner at the Hotel Riviera & Maximilian's**

WEDNESDAY, May 9, 2012

Session: ENZYME FUNCTIONALITY BY IN SILICO METHODS PART A
Chair: Karl Hult

09:00 - 09:50 **Claudio Soares** - Universidade Nova de Lisboa,
Oeiras, Portugal
Simulating the unusual properties of enzymes in nonaqueous media: basic knowledge approaching rational engineering

09:50 - 10:40 **Jürgen Pleiss** - University of Stuttgart,
Stuttgart, Germany
Simulation of proteins in organic solvents

10:40 - 11:05 **Tomić Sanja** - Ruđer Bošković
Institute, Zagreb, Croatia
Molecular dynamics based studies on human DPP III revealed determinants for its broad substrate selectivity

11:05 - 11:40 Coffee-break

Session: ENZYME FUNCTIONALITY BY IN SILICO METHODS PART B
Chair: Ulf Hanefeld

11:40 - 12:05 **Per-Olof Syrèn** - University of Stuttgart,
Stuttgart, Germany
Amidases have a hydrogen bond that facilitates nitrogen inversion but esterases have not

12:05 - 12:30 **Janez Mavri** - EN-FIST, National Institute
of Chemistry, Ljubljana, Slovenia
Nuclear Quantum Effects in Small Hydrogen Bonded Systems, Enzymes and Receptors

12:30 - 14:15 Lunch

Session: ENZYME FUNCTIONALITY BY IN SILICO METHODS PART C
Chair: Jan H. Jensen

14:15 - 15:05 **Jung-Hsin Lin** - Academia Sinica & National Taiwan
University, Taipei, Taiwan
Development of Scoring Functions for Protein-Ligand Interactions based on Quantum Chemical Charge Models and Robust Regression Analysis

15:05 - 15:30 **Adeline Ranoux** - TU Delft, the Netherlands
Transketolase: Enhancement of the Substrate Scope

15:30 - 15:55 **Robert Vianello** - Ruđer Bošković Institute, Zagreb,
Croatia & National Inst. of Chemistry,
Ljubljana, Slovenia
Computational Insight into the Catalytic Activity and Inhibition of Monoamine Oxidase B

16:00 CLOSING REMARKS

16:15 Coffee-break