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Universitat de Barcelona

Gary Pielak, Ph.D.
Distinguished Term Professor of Chemistry, Biochemistry and Biophysics
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THANK YOU

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electrophysiology will be used to study the metabolic components of neurodegeneration in aging and in diseases such as epilepsy and Parkinson's.

POST 03-250

Structural Analysis And Molecular Dynamics Of The Self-Sufficient P450 CYP102A5 And CYP102A1: A Combined Computational/Experimental Approach To Increase The Efficiency Of Biocatalyst Engineering

Maximilian Ebert[4, 1], Brahm Yachnin[2], Guillaume Lamoureux[3, 1], Albert Berghuis[2, 1], Joelle Pelletier[4, 1]
[1]PROTEO, Montreal, Quebec, Canada, [2]McGill University, Montreal, Quebec, Canada, [3]Concordia University, Montreal, Quebec, Canada, [4]Université de Montréal, Montreal, Quebec, Canada

P450s catalyze the oxidation of non-activated carbon atoms, which is chemically demanding. Members of the CYP102 family are termed "self-sufficient P450s", meaning that they contain all the machinery necessary to ensure the electron transfer and active site regeneration in one single protein. However, the macromolecular assembly remains unknown. Here we report results of SAXS analysis that bring new insights into the formation of the active complex. The recently reported new member CYP102A5 is highly interesting due to its sequence similarity to the intensively studied member CYP102A1, accompanied by a significant increase in electron transfer rate and improved regioselectivity. Homology models were generated, compared and used to identify the structural basis for these differences in catalytic activity. Based on this result we identified residues that may be involved in the gating and substrate capturing mechanism in CYP102A5. Predictions of differences in substrate incorporation and product release from the active site were computed using the adaptive biasing force (ABF) method. With this pioneering application of ABF in enzyme engineering, we were able to predict all known important residues for fatty acid substrate binding in CYP102A1, as well as two additional residues which were identified and analyzed *in vitro* to support the *in silico* finding. This newly developed computational biology approach, in addition to conformational studies, will help to guide directed evolution efforts towards the oxidation of non-native substrates.

POST 03-251

Isolation And Characterization Of Proline Specific Dipeptidyl Peptidase IV From The Tenebrio Molitor Larval Midgut

Valeriya F. Sharikova[1], Irina Goptar[1], Yulia Smirnova[2], Brenda Oppert[3], Irina Filippova[1], Elena Elpidina[2]
[1]Chemistry, Lomonosov Moscow State University, Moscow, Moscow, Russian Federation, [2]A.N. Belozersky Institute of Physico-Chemical Biology, Lomonosov Moscow State University, Moscow, Russian Federation, [3]Center for Grain and Animal Health Research, Stored Product Insect Research Unit, Manhattan, Kansas, US

The yellow mealworm *Tenebrio molitor* (Coleoptera: Tenebrionidae) is a stored product pest and a biochemical model organism of the family Tenebrionidae. The main food proteins of this insect are storage seed proteins - prolamins, which are also present in the diet of most people. Prolamins contain 10 - 30% proline and 30 - 50% glutamine residues. Several proline- and glutamine-rich prolamin peptides, which are resistant to proteolysis by human digestive enzymes, cause autoimmune Celiac Disease in 1% of the susceptible human population. In this regard, proline specific peptidases (PSP) are urgently needed for therapeutics, capable of hydrolyzing peptide bonds formed by proline residues that are resistant to proteolysis by peptidases of broad substrate specificity. We have carried out a bioinformatic search for PSP in the *T. molitor* larvae gut transcriptome and found 12 sequences similar to human PSP. Two predicted dipeptidyl peptidase IV (DPP IV) sequences were found, one with the highest mRNA expression level among all PSPs in the larval transcriptome. These enzymes are serine exopeptidases from the S9 family, which cleave Xaa-Pro dipeptides from the N-terminus of polypeptides. The major DPP IV-like

enzyme was purified from the *T. molitor* larvae midgut and analyzed by mass-spectrometry analysis. The amino acid sequence of the enzyme coincided with that of the highly-expressed DPP IV found in *T. molitor* gut transcriptome. The isolated enzyme was characterized by substrate specificity, pH-dependence, pH stability, and inhibitor sensitivity. The importance of DPP IV in insect digestion as well as the potential for new treatments of Celiac Disease will be discussed. This work was supported by ISTC grant 3455 and RFBR grants 12-03-01057-a, 14-04-91167-NSFC_a.

POST 03-252

Characterization Of Hydrolytic Enzyme-Producing Bacteria Isolated From Paper Mill

Manel Ghribi[5, 2], Fatma Meddeb-Mouelhi[2, 3], Marc Beauregard[1, 2, 4]

[1]biologie médicale, Université de Québec à Trois Rivieres, Trois-Rivieres, Quebec, Canada, [2]CRML, Trois-Rivieres, Quebec, Canada, [3]Buckman North America, Vaudreuil-Dorion, Quebec, Canada, [4]PROTÉO, Laval, Quebec, Canada, [5]physique,chimie et biochimie, Université de Québec à Trois-Rivières, Trois-Rivieres, Quebec, Canada

Enzymes act as biocatalyst in many industries, such as textiles, detergent, food, animal feed, bio-fuel, paper and pulp, pharmaceutical, to name a few. Cellulases and hemicellulases are efficient hydrolytic enzymes used in the pulp and paper industry to reduce the cost of production. In addition, industrial enzymes reduce the environmental impact by replacing harmful chemicals. The leading industrial enzyme suppliers (Novozymes, Genencor) offer a limited library of enzymes. Thoses enzymes are poorly adapted to the need of the paper industry. Therefore, our partner, Buckman North America, wants to expand his enzymes portfolio by characterizing new enzymes-producing bacteria. Pulp and paper mills offer untapped biodiversity for microorganisms that use cellulose-based substrates as nutriments. In this project, we will isolate and characterize cellulose and hemicellulose degrading microorganisms from paper mill sludges. To conserve microorganism's biodiversity, we used two temperatures (37 °C and 50 °C) for the isolation step. Detection of extracellular enzymatic activities was carried out on minimum agar plate medium supplemented with either cellulose (carboxylmethylcellulose or Avicel) or beechwood xylans. Bacteria strains showing extracellular cellulase and/or xylanase activities were isolated from various sludges (primary, secondary, presses and machines) found in a paper mill. These bacteria were identified based on their morphology, biochemical characterization and DNA 16s sequencing. The biorefining potential of these enzymes will be evaluated.

POST 03-253

Isolation of NRPS and PKS Gene Clusters from Soil Microbes

Danielle N. O'Hara, Connor P. Craig

University of Richmond, Richmond, Virginia, US

Greater than 90% of microbes living in soil are unculturable due to their complex nutrient and temperature requirements for growth. These microorganisms present a potential source of natural products that could be developed for biotechnological and pharmaceutical uses. Microorganisms with phosphopantetheinyl transferase (PPTase) activity are of high interest due to the role PPTase plays in activating non-ribosomal peptide synthetase (NRPS) and polyketide synthetase (PKS) gene cluster products. The proteins expressed by these gene clusters synthesize complex natural products that are utilized by the microorganism or its host for selective advantages. We screened for NRPS and PKS gene clusters in microbes isolated from soil on the University of Richmond campus. Genomic DNA was isolated from each of these samples and was used to construct metagenomic libraries. We will continue to screen the libraries for PPTase activity in order to identify positive clones. We extended this study to include a library of pigmented microbes previously isolated from Chesapeake Bay sponges, *Clathria*