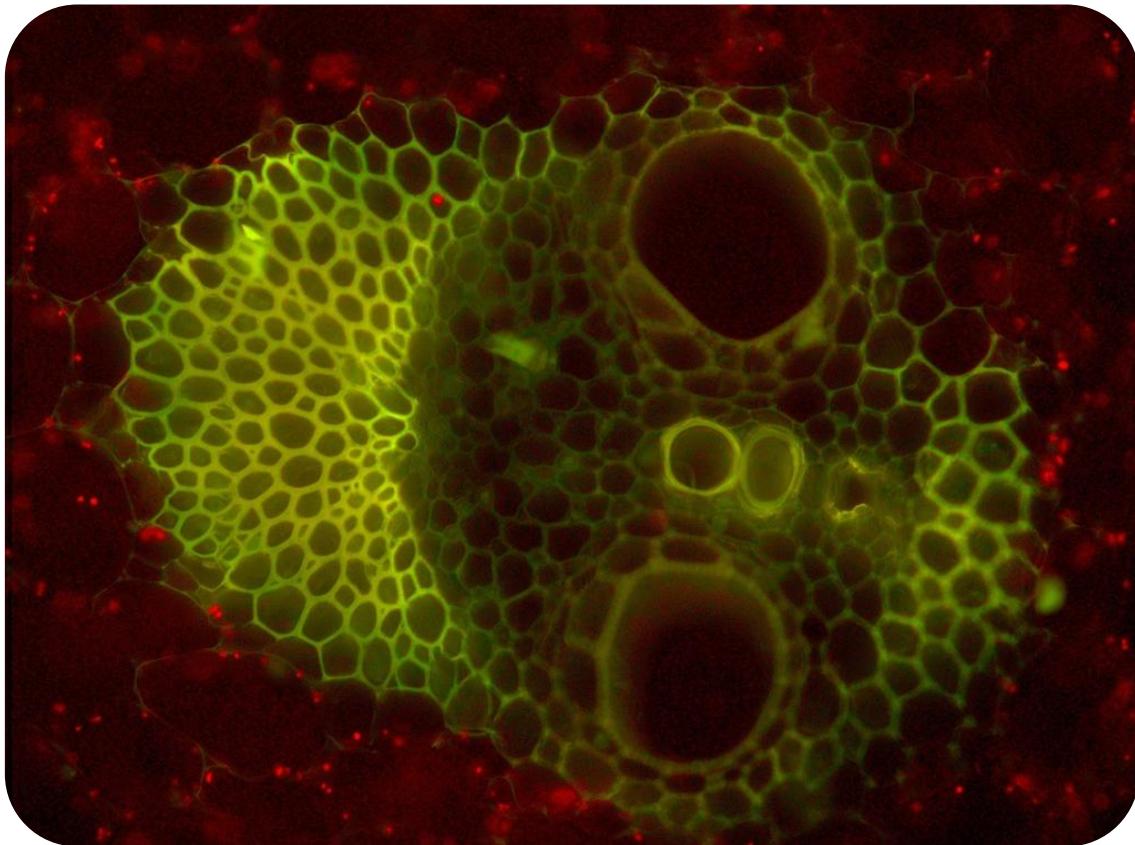


MARCH 9-12 2015 - SÃO PAULO - BRAZIL



Using systems and synthetic biology to  
tailor plant cell walls for a better future

NEWTON FUND AND FAPESP



RESEARCHER  
LINKS



# Using systems and synthetic biology to tailor plant cell walls for a better future

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MARCH 9-12 2015 - SÃO PAULO - BRAZIL



RESEARCHER  
LINKS



Instituto de Biociências – Departamento de Botânica  
Rua do Matão 277, São Paulo, SP, CEP 05508-090

## Program

Day 1*		3/9/2015	G	Day 2*		3/10/2015	G
9:00 - 10:15	Opening <b>José Roberto Krieger</b> , Vice President of Research of the University of São Paulo <b>Camila Morsch</b> , British Council Newton Fund Senior Manager Coordinators Welcome			9:00-9:30	Marcos Buckeridge		
10:15 - 10:45	<b>Coffe Break</b>			9:30-9:45	João Paulo Naldi Silva	3	
10:45-11:15	<b>Simon McQueen-Mason</b>			9:45-10:00	Jonas Weissmann Gaiarsa	3	
11:15-11:30	Fernando Segato	1		10:00-10:15	Ondrej Kosik	4	
11:30-11:45	An Li	1		10:15-10:30	Poliana Cardoso-Gustavson	4	
11:45-12:00	André Rodrigues dos Reis	1					
12:00-12:15	Carlos Driemeier	1					
12:15-12:30	Carolina Feijão	1					
12:30-14:00	<b>Lunch</b>			11:50-14:00	<b>Lunch</b>		
14:00-14:15	Danilo Centeno	1		14:00-14:15	Ricardo da Costa	4	
14:15-14:30	George W. Bassel	2		14:15-14:30	Thiago C.F. Gomes	5	
14:30-15:00	<b>Richard Ward</b>			14:30-14:45	Rosemary Dyson	5	
15:00-15:15	Elisson Romanel	2		14:45-15:00	Eveline Tavares	5	
15:15-15:30	Fabio Squina	2		15:00-15:30	<b>Eric Lam</b>		
15:30-15:45	Jeroen Nieuwland	2		15:30-15:45	Tomas J. Simmons	5	
15:45-16:00	Fernanda Trisltz P. Guedes	2		15:45-16:00	José Pedro Fonseca	5	
16:00-16:30	<b>Coffee Break</b>			16:00-16:30	<b>Coffee Break</b>		
16:30-17:00	<b>Paul Dupree</b>			16:30-16:45	Marco Aurélio Silva Tiné	6	
17:00-17:15	Lenka Frankova	2		16:45-17:00	Valerie Cornuault	6	
17:15-17:30	Igor Cesarino	3		17:00-17:30	<b>Igor Polikarpov</b>		
17:30-17:45	João Renato Carvalho Muniz	3		17:30-17:45	Amanda Rusiska Piovezzani	6	
17:45-18:15	<b>Maurice Bosch</b>			17:45-18:00	Tatiane da França Silva	6	
18:15-18:30	Nicholas Grantham	3		18:00-18:15	Wanderley Dantas dos Santos	6	
				18:15-18:45	<i>Sorting out working groups</i> <i>Explanation of procedure for next day</i>		

\* AG da Botânica

Day 3*		3/11/2015		Day 4*		3/12/2015	
9:00-10:30	Answering questions: <i>What are the main gaps/opportunities in Cell Wall Research?</i>	1		9:00-10:30	Brainstorming for collaboration <i>Discuss possible projects in collaboration using previous day ideas</i>		
10:30-11:00	<b>Coffe Break</b>			10:30-11:00	<b>Coffe Break</b>		
11:00-12:30	<i>How would you approach these gaps scientifically using systems and synthetic biology?</i>	2			<i>Produce a powerpoint presentation of a possible project in collaboration</i>		
12:35-14:00	<b>Lunch</b>			12:35-14:00	<b>Lunch</b>		
14:00-16:00	Discussions continue			14:00-16:00	Groups 10 min. Presentations		
16:00-16:30	<b>Coffee Break</b>			16:00-16:30	<b>Coffee Break</b>		
16:30-18:30	Groups 10 min. presentations			16:30-18:30	General discussions		

\* Sala 132

Group numbers are on the right columns. The arrangement is aleatory

We may resort groups according the affinities or area of research.

Presentations: Mentors: 20min+10 for discussion, Youg Researchers: 10min+5 for discussion

## Coordinators

### Marcos Silveira Buckeridge



Marcos Buckeridge is Associate Professor at the Department of Botany of the University of São Paulo and Director of the National Institute of Science and Technology of Bioethanol (INCT do Bioetanol), that gathers 32 laboratories in 6 states of Brazil with several collaborations in the US and Europe. From 2009 to 2012 he was also Scientific Director of the Brazilian Bioethanol Science and Technology Laboratory (CTBE), in Campinas. He is communicating editor for the international journals *Trees: structure and function* (Springer) and *Bioenergy Research* (Springer). In 2010, Buckeridge was appointed a Lead Authors for the next Intergovernmental Panel of Climatic Changes (IPCC) report (AR5) to be released in 2014.

Buckeridge develops research on *Plant Cell Wall Architecture, Degradation and Bioinformatics* and on the *Physiological and Biochemical Responses of Plants to the Environment*. His research led to discoveries of mechanisms of responses of sugarcane, sorghum and several tropical species to elevated CO<sub>2</sub> and drought. The work on cell walls includes deciphering some mechanisms of degradation and hormonal control of storage cell wall mobilisation of xyloglucans, galactomannans, mixed linkage glucan and arabinogalactan. Recently the sugarcane and miscanthus cell wall structures have been described, with possible impacts on the comprehension of cell wall architecture of grasses. The model systems used for cell wall research are mainly tropical seeds, sugarcane and duckweed. Buckeridge's work has generated 3 edited books and more than 120 publications in plant physiology, biochemistry and molecular biology of plant growth and development and cell wall metabolism.

#### Selected publications:

Buckeridge, M.S., De Souza, A.P. (2014) Breaking the "Glycomic Code" of cell wall polysaccharides may improve second-generation bioenergy production from biomass. *Bioenergy Research* 7:1065-1073.

De Souza, A. P., Leite, D. C. C., Pattathil, S. ; Hahn, M. G. ; Buckeridge, M. S. (2013) Composition and Structure of Sugarcane Cell Wall Polysaccharides: Implications for Second-Generation Bioethanol Production. *Bioenergy Research*, 6: 564-579.

Buckeridge, M.S. (2010). Seed Cell Wall Storage Polysaccharides: models to understand cell wall biosynthesis and degradation. *Plant Physiology*.154:1017-1023.

## Maurice Bosh



Maurice Bosch is a Senior Research Scientist at the Institute of Biological, Environmental & Rural Sciences (IBERS), Aberystwyth University. Before joining IBERS in 2008, he received his PhD at the Radboud University Nijmegen, The Netherlands, followed by postdoctoral studies in the Hepler lab on pectin dynamics in pollen tube growth (University of Massachusetts, USA) and self-incompatibility and associated programmed cell death (PCD) in the Franklin-Tong lab (University of Birmingham, UK). His current research mainly focuses on the identification of the chemical, structural and biological features underpinning cell wall recalcitrance to sugar release, and the genes responsible for this trait in grasses.

A better understanding of these aspects is required before we can rationally breed and design perennial grasses, such as Miscanthus, as commercially viable bioenergy and biorefining feedstocks. Another area of interest is elucidating the changes in cell wall related traits in response to changing environmental conditions, in particular drought and wind stress. For his research Maurice uses i) genetic engineering approaches in maize, Brachypodium and Miscanthus and ii) exploits the genetic and phenotypic diversity of cell wall traits in the Miscanthus and Brachypodium germplasm collections available at IBERS. Besides work on cell wall related projects, Maurice is also increasingly involved in work on self-incompatibility/PCD.

### Selected publications:

Costa RD, Lee SJ, Allison GG, Hazen SP, Winters A, Bosch M (2014) Genotype, development and tissue derived variation of cell wall properties in the lignocellulosic energy crop Miscanthus. *Annals of Botany* 114: 1265-1277

Slavov G, Allison G, Bosch M (2013). Advances in the genetic dissection of plant cell walls: tools and resources available in Miscanthus. *Front Plant Sci.* 4:217

Ings J, Mur LAJ, Robson PRH, Bosch M (2013). Physiological and growth responses to water deficit in the bioenergy crop Miscanthus x giganteus. *Front Plant Sci.* 4: 468

## Mentors

### Igor Polikarpov



Igor Polikarpov is a Full Professor of the Institute of Physics in São Carlos (IFSC), The University of São Paulo (USP) and Deputy Director of the Bioenergy Network of the University. His main scientific interests are centered at Structural Biology and Molecular Biophysics and their applications in Bioenergy and Biotechnology. Igor Polikarpov graduated in Physics from the Byelorussian State University (1983), did his PhD at the same University (1989), and post-docs at the Latvian Academy of Science (1991), Max-Planck Gesselschaft (1993) and the University of Edinburgh (1995). Published over 200 scientific papers, which were cited more than 3.600 times (ISI).

(ISI). Igor Polikarpov coordinates joint scientific projects between Brazil and European Union (FP7) and Brazil and UK (FAPESP-RCUK). He coordinated scientific collaborations with biotechnological and pharmaceutical companies and was responsible for construction, installation and operation of large-scale scientific installations (protein crystallography beamlines MX-1 & MX-2 at the Brazilian National Synchrotron Laboratory/LNLS, Campinas, Brazil). Member of the Editorial Board of *Biotechnology Letters* (Springer). Igor Polikarpov is one of the proponents of the recently approved Integrated PhD Program in Bioenergy (joint graduate course of three São Paulo State Universities: USP, UNESP and UNICAMP). He is a Commander of the Brazilian National Order of Scientific Merit and a Member of São Paulo State Academy of Science.

Polikarpov develops research on structure-activity studies of glycoside hydrolases, enzymatic hydrolysis of plant cell wall and investigate influence of pretreatments on biomass structure, morphology and composition.

#### Selected publications:

Rezende, C.A., Lima, M.A., Maziero, P., deAzevedo, E.R., Garcia, W. and Polikarpov, I. "Chemical and morphological characterization of sugarcane bagasse submitted to a delignification process for enhanced enzymatic digestibility" *Biotechnol Biofuels* (2011) **4**: 54

Marisa A. Lima, Mario Oliveira-Neto, Marco Antonio S. Kadokaki, Flavio R. Rosseto, Erica T. Prates, Fabio M. Squina, Adriana F.P. Leme, Munir S. Skaf and Igor Polikarpov "Aspergillus niger beta-glucosidase has a cellulase-like tadpole molecular shape: insights into GH3 beta-glucosidases structure and function" (2013) *J.Biol.Chem.* **288**:32991-3005

Textor, L.C., Colussi, F., Silveira, R.L., Serpa, V., de Mello, B.L., Squina, F.M., Pereira Jr., N., Skaf, M.S. & Polikarpov, I. "Joint X-ray crystallographic and molecular dynamics study of cellobiohydrolase I from *Trichoderma harzianum*: deciphering the structural features of cellobiohydrolase catalytic activity" *FEBS J.* (2013) **280**(1): 56-69.

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## Paul Dupree



Paul Dupree is a Professor at the Department of Biochemistry, University of Cambridge and has made significant advances in the area of understanding and improving plant lignocellulosic biomass quality and quantity. He directs the Cell Wall Sugars Programme of the BBSRC Sustainable Bioenergy Centre; a virtual centre composed of academic and industrial partners. The programme aims to better understand how sugars are locked into plant cell walls. Dupree is also director of Lignocellulosic Bioenergy Research, Cambridge Bioenergy Initiative and part of the Leverhulme Centre for Natural Material Innovation, aiming to understand and improve wood properties for building construction.

Dupree has taken proteomic and bioinformatic approaches to study plant cell wall polysaccharide synthesis. Recent discoveries (with collaborators) include discovery of some of the genes and enzymes for glucuronoxylan and arabinoxylan backbone synthesis and branching.

His group has demonstrated manipulation of mannan synthesis in plants, a possible target for improved biofuel raw material. His group has developed new methods to enable faster, more effective quantitative studies of plant polysaccharides and polysaccharide depolymerisation enzymes, including PACE for studies of polysaccharides and enzyme activities. The techniques are in use in more than 20 international collaborations. Developed with Kathryn Lilley, the LOPIT and ProCoDeS proteomics techniques have allowed candidate polysaccharide synthesis enzyme prioritisation through high throughput protein localisation and protein complex detection.

Dupree's work has produced more than 100 publications and his ISI h-index is 47.

### Selected publications:

Busse-Wicher M, Gomes TC, Tryfona T, Nikolovski N, Stott K, Grantham NJ, Bolam DN, Skaf MS, Dupree P. (2014) The pattern of xylan acetylation suggests xylan may interact with cellulose microfibrils as a two-fold helical screw in the secondary plant cell wall of *Arabidopsis thaliana*. *Plant J.* 79(3):492-506

Nikolovski N, Rubtsov D, Segura MP, Miles GP, Stevens TJ, Dunkley TP, Munro S, Lilley KS, Dupree P. (2012) Putative glycosyltransferases and other plant Golgi apparatus proteins are revealed by LOPIT proteomics. *Plant Physiol.* Oct;160(2):1037-51

Tryfona T, Liang HC, Kotake T, Tsumuraya Y, Stephens E, Dupree P. (2012) Structural characterisation of *Arabidopsis* leaf arabinogalactan polysaccharides. *Plant Physiol.* Oct;160(2):653-66.

## Richard Ward



Richard Ward undertook postdoctoral studies in Structural Biology at the European Molecular Biology Laboratory (EMBL), Heidelberg (Germany) (1987-1991) and Molecular Biology at the Institut fur Medizinische Mikrobiologie, Universität Mainz (Germany) (1991-1993). He is an Associate Professor III at the Department of Chemistry-FFCLRP, University of São Paulo. Prof. Ward is group leader of the Protein Biochemistry and Biophysics Laboratory (PBBL) DQ-FFCLRP-USP, co-founder and scientific consultant for Verdartis Biotechnology (Ribeirão Preto-SP) and is currently "Joint Appointment" at the CTBE (National Laboratory of Science and Technology for Bioethanol - Campinas). Prof. Ward has been a CNPq research fellow since 1996, and is currently level 1C.

Prof. Ward combines bioinformatics, protein engineering, and spectroscopic approaches to advance the understanding of the relationships between protein 3D-structure, dynamics and catalytic function of enzymes. Many industrial applications require thermostable and/or thermotolerant enzymes, enzymes with altered kinetic characteristics or enzymes that catalyze multiple reactions. Overcoming the protein engineering challenges to create enzymes with interesting and desirable catalytic properties underlies the ongoing research effort in the PBBL. Recent research has focused on engineering multifunctional enzyme chimeras (1), site-directed glycosylation for improved enzyme stability (2), and directed evolution for improving enzyme kinetics (3).

### Selected publications:

Engineering bifunctional Laccase-Xylanase chimeras for improved catalytic performance. (2011) RIBEIRO, L.F., FURTADO, G.P., LOURENZONI, M.R., COSTA-FILHO, A.J., SANTOS, C.R., PEIXOTO NOGUEIRA, S.C., BETINI, J.A., POLIZELI, M.L.T.M., MURAKAMI, M.T., WARD, R.J. *J. Biol. Chem.* 286(50), 43026-43038.

Engineering The Pattern Of Protein Glycosylation Modulates The Themostability Of A GH11 Xylanase. FONSECA-MALDONADO, F., VIEIRA, D.S., ALPONTI, J.S., BONNEIL, E., THIBAULT, P., WARD, R.J. (2013). *Journal of Biological Chemistry.* 286(50), 43026-43038.

Concomitant adaptation of a GH11 xylanase by directed evolution to create an alkalophilic/thermophilic enzyme. RULLER, R., ALPONTI, J., DELIBERTO, L.A., MACHADO-BOTELHO, C., WARD, R.J. (2014). *Prot. Engineering Design and Selection* 27(8):255-262.

## Simon McQueen-Mason



Simon McQueen-Mason left school at 17, and worked in boat yards in Southern California, before returning to the UK as a professional fisherman, eventually owning his own boat. At 26 he returned to education, obtaining a 1<sup>st</sup> class honours degree in Biological Sciences from Portsmouth Polytechnic. He received a PhD in Plant Physiology from the Pennsylvania State University in 1993, and returned to the UK to take up a Royal Society University Research Fellowship at The University of York in 1994. In 2001 he became Chair of Material Biology in the Centre for Novel Agricultural Products (CNPAP), at York, and became CNPAP Director in 2014. His research encompasses understanding the biosynthesis and mechanical properties of plant cell walls, understanding and modifying the digestibility of lignocellulosic biomass, and the discovery of enzymes for lignocellulose digestion. Notable contributions to the field include the discovery and characterisation of expansins and their role in cell wall extension during growth; identifying the roles of arabinans and homogalacturonan in the elastic properties of stomatal guard cell walls, and more recently in identifying a range of mutations that improve the digestibility of plant cell walls.

### Selected publications:

McQueen-Mason, S.J., Durachko, D.M., Cosgrove, D.J. (1992) Two endogenous proteins that induce cell wall extension in plants. *Plant Cell* 4, 1425-1433.

McQueen-Mason, S.J., Cosgrove, D.J. (1994) Disruption of hydrogen bonding between wall polymers by proteins that induce plant wall extension. *Proc. Natl. Acad. Sci USA* 91 (14), 6574-6578.

Jones, L., Milne, J.L., McQueen-Mason, S. (2003) Cell Wall Arabinan is Essential for Guard Cell Function. *Proc. Natl. Acad. Sci. USA* 100:11783-11788.

King AJ, Cragg, S, Li Y, Dymond J, Guille MJ, Bowles DJ, Bruce NC, Graham IA, McQueen-Mason SJ 2010 Molecular insight into lignocellulose digestion by a marine isopod in the absence of gut microbes. *Proc, Natl. Acad. Sci. USA* 107: 5345-5350.

Kern M, McGeehan JE, Streeter SD, Martin RN, Besser K, Elias L, Eborall W, Malyon GP, Payne CM, Himmel ME, Schnorr K, Beckham GT, Cragg SM, Bruce NC, McQueen-Mason SJ. 2013 Structural characterization of a unique marine animal family 7 cellobiohydrolase suggests a mechanism of cellulase salt tolerance. *Proc. Natl. Acad. Sci. USA.* 110; 10189-10194

Marriott P, Sibout R, Lapierre C, Fangel J, Willats W, Hofte H, Gómez L, McQueen-Mason S. 2014 A range of cell wall alterations enhance saccharification in *Brachypodium distachyon* mutants. *Proc. Natl. Acad. Sci. USA* 111(40):14601-6.

## Guest Speakers

### Eric Lam



Eric Lam is currently a Distinguished Professor in the Department of Plant Biology and Pathology at Rutgers University, NJ. He had served as the Director for the Biotechnology Center for Agriculture and the Environment at Rutgers from 2008 to 2010. He also serves on the advisory board for the Rutgers Energy Institute. He is a graduate of UC Berkeley and completed his postdoctoral research at the Rockefeller University on Plant Molecular Biology. His research interests include the study of mechanisms that control programmed cell death and stress tolerance in plants, the regulation of global gene expression via chromatin organization, and more recently, the establishment and promotion of an aquatic agriculture platform with duckweed for sustainable biomass production. Currently, he is leading a team of U.S. researchers to complete a high fidelity reference genome for the Greater Duckweed *Spirodela polyrhiza* using NGS and Genome Feature Mapping technologies. To facilitate the use of duckweeds as novel sources of renewable biomass, he is currently collaborating with the Buckeridge lab at USP to characterize the cell wall composition of these aquatic plants.

His approach emphasizes the use of evolutionary relationships and genomics to identify candidate genes and enzymes for critical metabolic switches in cell wall metabolism. Dr. Lam is author on over 150 publications in journals including *Science* and *Nature* and has been awarded 5 patents relating to biotechnology methods. He is the recipient of the Alexander von Humboldt award in Molecular Biology (2007) and a Fulbright-Brazil Science Fellow (2014-15).

## Leonardo Gomez



Leonardo Gomez is a Senior Research Fellow at the University of York. My area of expertise is the improvement of plant biomass as a renewable feedstock for the production of sustainable biofuels and chemicals. I have worked in the field of plant biology over 25 years of continuous active research.

I specialize in the use of plants as chemical platforms for the production of biorenewable products. I began my career as a research scientist in Argentina, where I obtained a permanent position as a PI funded by the National Research Council. Following a period of three years as a visiting researcher (funded by a Fellowship from the National Research Council of Argentina and the

Royal Society) at Rothamsted Research, I moved to York. Since 2003 I have been working at the Centre for Novel Agricultural Products (CNAP), initially in the group of Prof. Ian Graham and later with Prof Simon McQueen-Mason. My areas of expertise are biomass processing, cell wall metabolism, plant embryo development, transcriptomics, and molecular biology. During the last eight years I have set up, developed and am currently managing a High Throughput Biomass Analytical Facility, which is central to the cutting edge research carried out at the CNAP.

### Selected publications:

Marriott PE, Sibout R, Lapierre C, Fangel JU, Willats WGT, Hofte H, Gómez LD, McQueen-Mason SJ (2014) Range of cell-wall alterations enhance saccharification in *Brachypodium distachyon* mutants. *P.N.A.S.* 111 (40) 14601-6.

Gómez LD, Vanholme R, Bird S, Goeminne G, Trindade LM, Polikarpov I, Simister R, Morreel K, Boerjan W, McQueen-Mason SJ (2014). Side by side comparison of chemical compounds generated by aqueous pretreatments of maize stover, miscanthus and sugarcane bagasse. *Bioenergy Research* (DOI 10.1007/s12155-014-9480-2)

Lima MA, Gomez LD, Steele-King CG, Simister R, Bernardinelli OD, Carvalho MA, Rezende CA, Labate CA, Deazevedo ER, McQueen-Mason SJ, Polikarpov I (2014). Evaluating the composition and processing potential of novel sources of Brazilian biomass for sustainable biorenewables production. *Biotechnol Biofuels*. 7(1):10.

### Young Cell Wall Researchers

#### Amanda Rusiska Piovezani



Amanda Rusiska Piovezani is biologist and PhD student in bioinformatics at Institute of Mathematics and Statistics of University of São Paulo, Brazil. Her thesis addresses plant Systems Biology and is being developed at the Department of Botany at University of São Paulo. She is setting up a computational tool aimed at integrating data from transcriptomics, proteomics and physiology scales arising from experiments focusing on the plant cell wall degradation taking place during aerenchyma formation in the roots of sugarcane. Her skills in bioinformatics include: Linux Programming, Sequence Analysis, Next Generation Sequencing Analysis and Computational Prediction of MicroRNA target sites.

#### Selected publication:

BASTOS, ELEN PEREIRA ; BRENTANI, HELENA ; PASINI, FATIMA SOLANGE ; SILVA, ADERBAL RUY T. ; TORRES, CESAR HENRIQUE ; PUGA, RENATO DAVID ; OLIVIERI, ELOISA HELENA RIBEIRO ; PIOVEZANI, AMANDA RUSISKA ; PEREIRA, CARLOS ALBERTO DE BRAGANÇA ; MACHADO-LIMA, ARIANE ; CARRARO, DIRCE MARIA ; BRENTANI, MARIA MITZI . MicroRNAs Discriminate Familial from Sporadic Non-BRCA1/2 Breast Carcinoma Arising in Patients  $\leq$ 35 Years. *Plos One*, v. 9, p. e101656, 2014.

#### Computer Program Registered:

SIMTar: a tool for prediction of SNPs Interfering on MiRNA Target sites. I.N.P.I./S.P. n°.BR 51 2014 001434-7.

**An Li**



An Li is a second year PhD student at Prof. Paul Dupree's lab at University of Cambridge. She has completed her M.E and B.E. degree at Tsinghua University in China.

An's previous work was focused on using solid-state fermentation on municipal biomass waste (MBW), pig manure and sludge for bio-methane production. She also built a pipeline for fermentation in a metagenomic study. In addition, she developed a method to extract the total DNA of the microbes residing in the fermenter for Roche454/pyrosequencing. Her interest in biomass applications led her to continue her research on biomass-based biofuels.

An's PhD project focuses on the decoration patterns and diversity of xylan across the plant kingdom. In particular, An is interested in 1) characterizing of GH enzyme specificity and using them as tools for detecting of xylan substitutions 2) xylan decoration diversity across the plant kingdom, such as the arrangement of GlcA, Ara and acetyl groups 3) xylan decoration diversity in different tissues of *Arabidopsis*, especially in *Arabidopsis* seed and mucilage.

At present, she is characterizing the decorations of xylan of plants within the Pteridophytes division. To achieve this, she is using Polysaccharide Analysis using Carbohydrate gel Electrophoresis (PACE) and Matrix-assisted Laser Desorption/Ionization Time of Flight Mass Spectrometry (MALDI-TOF MS) with Collision-Induced Dissociation (CID MS/MS).

### Andre Rodrigues dos Reis



Andre Rodrigues dos Reis is Assistant Professor at the Department of Biosystems Engineering of the São Paulo State University (UNESP). He got his PhD in Plant Science from Waseda University, Tokyo – Japan in 2013. From 2011 to 2013 he was Research Associate and Lecture at Waseda University. Reis develops research on *Plant Cell Wall Architecture During Germination of Seeds*, and on the *Physiological and Biochemical Responses of Plants to the Environment*. His research led to discoveries of oxidation mechanism and overall removal rates of endocrine disrupting chemicals by aquatic plants. The work on cell walls includes degradation mechanisms of xenobiotic compounds and histochemical localization of enzymes responsible for oxidize or degrade environmental pollutants. Recently, Reis started research collaboration with George Bassel (University of Birmingham) to study the interdisciplinary approach to understanding stress tolerance and seed quality in soybean. Reis is interested in to evaluate the effects of external nutrients (selenium and nickel) and osmotic stress during germination and growth of soybean seeds and to identify cellular and genetic targets (candidate transcript factors and gene expression related to drought and salt stress) in addition to priming techniques to enhance soybean germination.

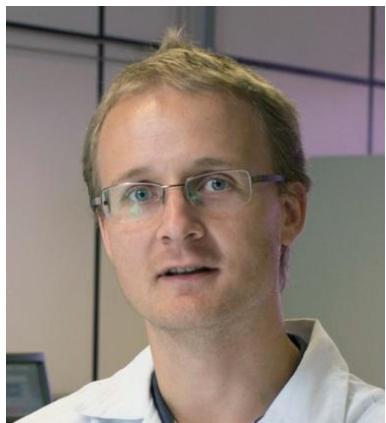
#### Selected publications:

Reis, A.R., Tabei, K., Sakakibara, Y. (2014). Oxidation mechanism and overall removal rates of endocrine disrupting chemicals by aquatic plants. *Journal of Hazardous Materials* 265: 79-88.

Reis, A.R., Sakakibara, Y. (2014). Enzymatic degradation of endocrine disrupting chemicals in aquatic plants and relations to biological Fenton reaction. *Water Science and Technology* 66(4): 775-782.

Reis, A.R., Kyuma, Y., Sakakibara, Y. (2013). Biological Fenton's oxidation of pentachlorophenol by aquatic plants. *Bulletin of Environmental Contamination and Toxicology* 91: 718-723.

## Carlos Driemeier



Carlos Driemeier has graduation (2004) and doctorate (2008) in Physics from Federal University of Rio Grande do Sul, with part of doctorate research at the University of Texas, and post-doctorate (2009) at the Institute of Energy and Environment from University of São Paulo. Has experience in Condensed Matter Physics, working mainly with surfaces, interfaces, physical chemistry of water, and crystallography. Since 2009 is research scientist at the Brazilian Bioethanol Science and Technology Laboratory - CTBE, which integrates the Brazilian Center for Research in Energy and Materials - CNPEM.

CNPEM. His research has been focused on the nanostructure of lignocellulosic biomass, developing characterization methods and applying them to understand nanostructural variability and its role on biomass conversion.

### Selected Publications:

Driemeier C, Bragatto J (2013) Crystallite Width Determines Monolayer Hydration across a Wide Spectrum of Celluloses Isolated from Plants. *J Phys Chem B* 117:415–421

Maziero P, Jong J, Mendes FM, Gonçalves AR, Eder M, Driemeier C (2013) Tissue-Specific Cell Wall Hydration in Sugarcane Stalks. *J Agric Food Chem* 61:5841–5847. doi: 10.1021/jf401243c

Oliveira RP, Driemeier C (2013) CRAFS: a model to analyze two-dimensional X-ray diffraction patterns of plant cellulose. *J Appl Crystallogr* 46:1196–1210.

### Carolina Feijao



Carolina Feijao is a second year PhD student in Professor Paul Dupree's lab at the University of Cambridge. Carolina has previously completed a MSc degree on Quantitative Biology at Imperial College London and a BSc degree on Cellular Biology and Biotechnology at the University of Lisbon.

Carolina is part of the BBSRC Doctoral Training Programme. During the programme's first year, she focused on characterizing rice GT61s that had been overexpressed in *Arabidopsis thaliana* roots and stem, in Professor Paul Dupree's lab. During this year, she also worked on directed evolution of xylanases at Dr Florian Hollfelder's lab.

Carolina's PhD project focuses on xylan structures and their synthesis. In particular, Carolina is interested in 1) characterizing the sugar side chains present in the xylan backbone of grasses such as rice, 2) assessing if these side chains are arranged in patterns or domains, and 3) determining potential linkages with compounds such as ferulic acid. Regarding xylan biosynthesis, Carolina aims to determine the role and level of functional divergence within the GT61 family. She is currently characterizing several T-DNA knockout mutants for rice GT61s, as well as psyllium GT61s she overexpressed in *Arabidopsis thaliana*. This work includes profiling the cell walls of the mutant plants with Polysaccharide Analysis using Carbohydrate gel Electrophoresis (PACE) and DNA sequencer-Assisted Saccharide analysis in High throughput (DASH).

#### Selected publication:

Tryfona, T., Sorieul, M., Feijao, C. V., Stott, K., Dupree, P. Structural characterization of grass glucuronoarabinoxylan (in preparation).

### Danilo Centeno



Danilo Centeno is Associate Professor at the Centro de Ciências Naturais e Humanas of the Universidade Federal do ABC since 2011. Dr. Centeno works on plant physiology and biochemistry, especially concerning the primary metabolism of plants. Lately he has focused on desiccation tolerant plants, using metabolomics approach to figure out the metabolism during water loss. Some of the organisms he is working on include algae, seeds and resurrection plants. His actual challenge is to have a system biology view, including several levels of organisation, such as metabolism control (based on "omics" analysis), physiological alterations and morphological and anatomical changes in tissues submitted to adversely environment. Dr. Centeno has lately published few articles on this theme.

#### Selected publications :

Suguyama, V.F.; Silva, E.A.; Meirelles, S.T.; Centeno, D.C.; Braga, M.R. (2014) Leaf metabolite profile of the Brazilian resurrection plant *Barbacenia purpurea* Hook. (Velloziaceae) shows two time-dependent responses during desiccation and recovering. *Frontiers in Plant Science* 5: 1-13.

Caccere, R.; Teixeira, S.P.; Centeno, D.C.; Figueiredo-Ribeiro, R.T.L.; Braga, M.R. (2013) Metabolic and structural changes during early maturation of *Inga vera* seeds are consistent with the lack of a desiccation phase. *Journal of Plant Physiology* 170: 791-800.

Mello, J.I.O.; Centeno, D. C.; Barbedo, C. J.; Figueiredo-Ribeiro, R.C.L. (2011) Changes in carbohydrate composition in seeds of three tropical tree species submitted to drying and storage at freezing temperature. *Seed Science and Technology* 39: 465-480.

## Elisson Romanel



Since 2013, Elisson Romanel is Doctor Professor at the Department of Biotechnology of the Escola de Engenharia de Lorena/Universidade de São Paulo (EEL/USP). Romanel develops research on *Bioinformatics and Functional Genomics of Plant* and recently is focusing in *Cell Wall Biosynthesis of hemicellulose and lignin in sugarcane*. His research use sorghum and maize as a model genome species to find sugarcane genes. As a young researcher, his approved two grants (FAPESP and CNPq) to install a basic plant molecular genetics laboratory in EEL/USP. Romanel's has worked seven years with bioinformatics and plant genomics which generated 6 papers in these fields.

### Selected publications:

Vining, K.J.; Romanel, E.; et al., (2014) The floral transcriptome of *Eucalyptus grandis*. New Phytologist, v10.

Myburg et al., (2014). The genome of *Eucalyptus grandis*. Nature, v.510, p356-362.

Paterson, et al., (2012) Repeated polyploidization of *Gossypium* genomes and the evolution of spinnable cotton fibers. Nature, v.492, p423-427.

Romanel et al., (2009) Evolution of the B3 DNA Binding Superfamily: New Insights into REM Family Gene Diversification. Plos One, v4, p.5791.

## Eveline Tavares



Eveline Tavares is a PhD student at the Department of Botany of the University of São Paulo at the Plant Physiological Ecology Laboratory (LAFIECO). From 2008 to 2010 she did her masters at the Molecular Biology Laboratory at the Cell Biology Department of the University of Brasilia.

During her masters she expressed in yeast and characterized a recombinant thermostable endoglucanase which has shown to be active towards several agricultural residues. Currently, her PhD thesis addresses the cell wall degradation underlying aerenchyma formation in the roots of sugarcane. Her ongoing work includes the characterization of the constitutive aerenchyma formation in this plant, the hormone regulation controlling this process and the sequencing of candidate genes among cell wall degradation enzymes and transcription factors. Her main result was the identification of a putative regulator of the first steps of this event, which is the cell expansion and separation, with subsequent pectin hydrolysis. Her skills include molecular cloning, protein purification, heterologous expression in plants, bacteria and yeast, transactivation assays, qPCR and hormone dosage in MS.

### Selected publications :

Tavares EQP, De Souza AP, Buckeridge MS. How Endogenous Plant Cell Wall Degradation Can Help Achieve Higher Efficiency in Saccharification of Biomass. Journal of Experimental Botany (in revision)

Grandis A, De Souza AP, Tavares EQP, Buckeridge MS. 2014. Using Natural Plant Cell Wall Degradation Mechanisms to Improve Second Generation Bioethanol. In: McCann MC, Buckeridge MS, Carpita NC, eds. Plants and BioEnergy. New York: Springer, pp. 211-230.

Tavares EQP, Rubini MR, Mello-de-Sousa TM, Duarte GC, De Faria, FB, Ferreira-Filho EX, Kyaw CM, Silva-Pereira I, Poças-Fonseca MJ. 2013. An Acidic Thermostable Recombinant *Aspergillus nidulans* Endoglucanase Is Active towards Distinct Agriculture Residues. Enzyme Research, Article ID 287343, 1-10

## Fabio Squina



Fabio Squina is Pharmacist from University of São Paulo (USP) with Ph.D in molecular biology from Medical School of Ribeirão Preto of USP. He held two post-doctoral positions in fungal biochemistry and genetics, first at Department of Biochemistry at the same medical school, later at the Department of Microbiology and Molecular Genetics at Oklahoma State University.

Dr Squina's interests combine molecular biology, biochemistry, 'Omics' Sciences and high-throughput screenings. His research is aimed at the development of enzymes and biotechnological routes for plant biomass conversion into bioproducts.

Fabio Squina's work has generated 60 publications in biotechnology, biochemistry and molecular biology of microorganisms and enzymes, along with 7 patents in biofuel research field.

### Selected Publications:

Genomics Review of Holocellulose Deconstruction by Aspergilli. Microbiology and Molecular Biology Reviews, 2014. (IF=15.3) Segato, Fernando ; Damásio, André R. De Lima ; Squina, Fabio Marcio ; Prade, R. A.

Understanding the function of conserved variations in the catalytic loops of fungal glycoside hydrolase family 12. Biotechnology and Bioengineering 2014 (IF=4.2)

Damásio, André R. L. ; Rubio, Marcelo V. ; Oliveira, Leandro C. ; Segato, Fernando ; Dias, Bruno A. ; Citadini, Ana P. ; Paixão, Douglas A. ; Squina, Fabio M. <http://dx.doi.org/10.1016/j.indcrop.2013.12.005>

Development and Biotechnological Application of a Novel Endoxylanase Family GH10 Identified from Sugarcane Soil Metagenome. Plos One, 2013. (IF=3.5) Alvarez, Thabata M. ; Goldbeck, Rosana ; Santos, Camila Ramos; Franco Cairo, João Paulo L.; De Oliveira Neto, Mario ; Murakami, Mário T. ; Squina, Fabio M. <http://dx.doi.org/10.1371/journal.pone.0070014>

High Temperature Enzymatic Cellulose Breakdown. Applied and Environmental Microbiology, 2011 (IF=4.0) Squina F. M.; Wang, H. ; Segato, F. ; Mort, A. ; Lee, D. ; Pappan, K. ; Prade, R. <http://dx.doi.org/10.1128/AEM.00199-11>.

Functional characterization and target discovery of Glycoside Hydrolases from Lower Termite Coptotermes gestroi Digestome. Biotechnol Biofuels, 2011 (IF=6.2) Franco Cairo, Joao Paulo L.; Leonardo, Flavia C. ; Ana Maria; Paes Leme, Adriana F ; Pereira, Goncalo A. G.; Squina, Fabio Marcio. <http://dx.doi.org/10.1186/1754-6834-4-50>.

## Fernanda Guedes



Fernanda Guedes, PhD in plant physiology and molecular biology, Forestry Engineer at Luiz de Queiroz College of Agriculture from University of São Paulo (ESALQ/ USP), specialized on timber production at *Ecole Nationale Du Génie Rural des Eaux et des Forêts* (ENGREF/AgroparisTech) in Nancy, France. From 2005 to 2010 worked on genetic research projects concerning biotic stress and wood quality aspects focusing on strategic results to direct tree breeding programs. Researches on plant cell wall started on 2010 as PhD student at University of Orleans, France in partnership with the *Institut National de la Recherche Agronomique* (INRA). PhD focus was to better understand the ultrastructure of wood cell wall by studying the kinetics of polysaccharides deposition in wood cell wall by using tension wood formed in poplar as a model. Until now, results of that research were presented in six meetings and one article was submitted.

Actually, postdoctoral researcher founded by CAPES at ESALQ she works with the Wood Anatomy & Tree-Ring Laboratory (LAIM) team and is mostly interested in Eucalyptus wood cell wall ultrastructure. Develops research also on physiological and biochemical responses of Eucalyptus to some abiotic stress focusing on its impact on wood structure. However, towards a more integrative study of the tree, participates in two other research projects working closely with Brazilian and French researchers in complementary areas and with forest companies. Her research is expected to provide strategic results on wood structure and possibly direct tree breeding programs according to the industry demand.

### Selected publications:

Guedes F. T. P., Laurans F., Quemener B., Assor C., Boizot N., Vigouroux J., Lessage-Descauses M-C., Leplé J-C., Déjardin A., Pilate G. Modification in non-cellulosic polysaccharide distribution and composition during G-layer formation in poplar tension wood fibers. (submitted)

Guedes, F. T. P.; Laurans, F.; Assor, C.; Takeuchi, M.; Boizot, N.; Vigouroux, J.; Lessage-Descauses, M.; Leple, J. C.; Dejardin, A.; Pilate, G. Biochemical and histochemical characterization of the polysaccharides present in the G-layer of wild type and AGP-modified transgenic poplars. Poster presentation at the XIII Cell Wall Meeting. 2013. Nantes, France.

Guedes, F.; Laurans, F.; Assor, C.; Boizot, N.; Lessage-Descauses, M.; Leple, J. C.; Dejardin, A.; Clair, B.; Pilate, G. Searching for polysaccharides specific to tension wood fibers. Oral presentation at the 7th International Conference on Plant BioMechanics (Plant-BioMech). 2012. Clermont-Ferrand, France

### Fernando Segato



Fernando Segato is an Assistant Professor in the Department of Biotechnology at the Engineering School of Lorena at the University of São Paulo, Brazil. He received his Ph.D. in Molecular Biology and Genetics of Microorganisms from the Ribeirão Preto School of Medicine at the University of São Paulo. From 2011 to 2012 he worked as biotechnology researcher at VTT Technical Research Center of Finland. His research focuses on prospection of hydrolytic and oxidative enzymes applied in lignocellulose depolymerization, exploration of thermophilic fungal genomes, and improvement of fungal cell factories.

#### Selected publications:

Müller M, Prade RA, Segato F, Atiyeh H, Wilkins M (2015). Continuous xylanase production with *Aspergillus nidulans* under pyridoxine limitation using a trickle bed reactor. *Biotechnology Resource* 41(10): 1563 – 1570.

Segato F, Damásio ARL, de Lucas RC, Prade RA (2014). Genomics review of holocellulose deconstruction by Aspergilli. *Microbiology and Molecular Biology Reviews* 78(4): 588 – 613.

Segato F, Damásio ARL, Gonçalves TA, Murakami MT, Squina FM, Polizeli MLTM, Mort AJ, Prade RA (2012). Two structurally discrete GH7-cellulobiohydrolases compete for the same cellulosic substrate fiber, *Biotechnology for Biofuels* 5:21.

## George Bassel



George Bassel is a Research Fellow at The University of Birmingham. His lab is taking an inter-disciplinary approach to understand two key questions:

- 1) How do plants make the decision to start growing
- 2) How do genes make plants grow

We focus on seed dormancy and post-embryonic growth to address these questions. This biological system provides the opportunity to uncover both the molecular circuitry that underlies a decision making process in plants, and the mechanisms that drive cell shape changes.

Experimental methodologies include the analysis of large-scale -omics datasets to infer regulatory networks, targeted yeast interaction screening, biophysical measurement of plant tissues and the use of quantitative high resolution 3D microscopy with FEM-based models of plant growth. The integration of regulatory networks driving biophysical changes in the cell wall within the context of whole organ growth enables the relationship between cell wall mechanics and plant morphogenesis to be investigated.

George is working closely with multiple industry partners to apply these findings to enhance both seed vigour and seedling establishment using both candidate gene and synthetic biology approaches.

His work has led to the first global gene network model describing a developmental transition in plants, the first full 3D cellular models of plant growth, the establishment of the first online bioinformatics framework for seed biology and the discovery of both oxygen and nitric oxide sensing mechanisms in plants. His lab currently has 2 postdocs, 2 technicians and 2 PhD students and has collaborations across the EU.

### Selected Publications:

Bassel GW, Stamm P, Mosca G, Barbier de Reuille P, Gibbs DJ, Winter R, Janka A, Holdsworth MJ, Smith RS (2014) Mechanical constraints imposed by 3D cellular geometry and arrangement modulate growth patterns in the *Arabidopsis* embryo. *Proc Natl Acad Sci U S A.* 111(23):8685-90

Bassel GW, Gaudinier A, Brady SM, Hennig L, Rhee SY, De Smet I (2012) Systems Analysis of Plant Functional, Transcriptional, Physical Interaction, and Metabolic Networks. *The Plant Cell* 24 (10), 3859-3875

Bassel GW, Lan H, Glaab E, Gibbs DJ, Gerjets T, Krasnogor N, Bonner AJ, Holdsworth MJ, Provart NJ (2011) Genome-wide network model capturing seed germination reveals coordinated regulation of plant cellular phase transitions. *Proc Natl Acad Sci U S A.* 108:9709-14

### Igor Cesarino



Igor Cesarino is a Professor at the Department of Botany of the University of São Paulo since 2014. During his PhD (2009-2012) at the State University of Campinas, he worked on the characterization of peroxidases and laccases potentially involved in the lignification process in sugarcane, and also provided the first in-depth characterization of the phenolic profile of sugarcane stems using a lignomics approach. From 2012 to 2014, he was a postdoctoral fellow in the Bio-Energy lab at the Department of Plant Systems Biology (PSB-VIB/UGent) working on the lignin metabolism and on the engineering of cell wall quality for biofuels in *Arabidopsis* and poplar, under the supervision of Prof. Dr. Wout Boerjan.

Dr. Cesarino's research focuses on *Lignin Metabolism* and *Engineering of Plant Cell Walls* in order to reduce plant biomass recalcitrance for downstream applications. More specifically, his aim is to understand the molecular mechanisms that control secondary cell wall formation in plants, with a major focus on the characterization of the phenolic metabolism and the identification of genes potentially involved in many aspects of lignin deposition. The obtained knowledge might be helpful for future biotechnological strategies to reduce biomass recalcitrance for applications such as papermaking, animal feeding and biofuels production.

#### Selected publications:

CESARINO, I. ; ARAUJO, P. ; SAMPAIO MAYER, J. L. ; VICENTINI, R. ; BERTHET, S. ; DEMEDTS, B. ; VANHOLME, B. ; BOERJAN, W. ; MAZZAFERA, P. . Expression of SofLAC, a new laccase in sugarcane, restores lignin content but not S:G ratio of *Arabidopsis lac17* mutant. *Journal of Experimental Botany*, v. 64, p. 1769-1781, 2013.

VANHOLME, R.\* ; CESARINO, I.\* ; RATAJ, K. ; XIAO, Y. ; SUNDIN, L. ; GOEMINNE, G. ; KIM, H. ; CROSS, J. ; MORREEL, K. ; ARAUJO, P. ; WELSH, L. ; HAUSTRAETE, J. ; MCCLELLAN, C. ; VANHOLME, B. ; RALPH, J. ; SIMPSON, G. G. ; HALPIN, C. ; BOERJAN, W. . Caffeoyl Shikimate Esterase (CSE) Is an Enzyme in the Lignin Biosynthetic Pathway. *Science*, v. 341, p. 1103, 2013.

BOTTCHER, A.\* ; CESARINO, I.\* ; BROMBINI DOS SANTOS, A. ; VICENTINI, R. ; MAYER, J. L. S. ; VANHOLME, R. ; MORREEL, K. ; GOEMINNE, G. ; MOURA, J. C. M. S. ; NOBILE, P. M. ; CARMELLO-GUERREIRO, S. M. ; ANTONIO DOS ANJOS, I. ; CRESTE, S. ; BOERJAN, W. ; LANDELL, M. G. D. A. ; MAZZAFERA, P. . Lignification in Sugarcane: Biochemical Characterization, Gene Discovery, and Expression Analysis in Two Genotypes Contrasting for Lignin Content. *Plant Physiology*, v. 163, p. 1539-1557, 2013.

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## Jeroen Nieuwland



Jeroen Nieuwland is since 2014 Senior Lecturer at the University of South Wales (USW) and member of the Energy and Environment Research Institute at USW. He previously worked with Jim Murray at the University of Cambridge and Cardiff University where he focused on plant cell division and the cell cycle. His research covered the function of positive and negative cell cycle regulators in plant developmental programs, but in particular the root. Jeroen did his PhD with Titti Mariani in Nijmegen, The Netherlands during which he discovered a new type of cell wall loosening protein.

His current interest in plant growth combines the approaches in cell division and cell wall properties. Currently he is using a custom-built extensometer to screen fully sequenced ecotypes of *Arabidopsis* to identify traits involved in cell wall extensibility and plant growth. He will also analyse cell division mutants for cell wall phenotypes to explore the interphase between cell division and elongation.

Furthermore I am using the cellulose-producing prokaryote *Gluconobacter xylinus* as a model system for cell wall characteristics and am planning to develop it further as a synthetic biology platform for the production of cell wall-like substrates.

### Selected publications:

Nieuwland, J., Wen, B., Murray, J.A.H. (2013) The *Arabidopsis* CDK inhibitor ICK3/KRP5 is rate limiting for primary root growth and promotes growth through cell elongation and endoreduplication. *J. Exp. Bot.* **64**, 1-13

Nieuwland, J., Maughan, S.C., Dewitte, W., Scofield, S., Sanz, L., Murray, J.A.H. (2009) The D-type cyclin CYCD4;1 modulates lateral root density in *Arabidopsis* by affecting the basal meristem region. *Proc. Nat. Acad. Science USA* **106**, 22528-22533.

Nieuwland, J., Feron, R., Huisman, B.A., Fasolino, A., Hilbers, C.W., DerkSEN, J., Mariani, C. (2005) Lipid Transfer Proteins enhance cell wall extension. *Plant Cell* **17**, 2009-2019

### Joao Muniz



Joao Muniz is an Assistant Professor at the São Carlos Institute of Physics in São Carlos (IFSC), of the University of São Paulo (USP). His main scientific interests are centered at Structural Biology, Protein Crystallography, Molecular Biophysics and their applications in Bioenergy, Environmentally-friendly Technologies and Health. Joao Muniz graduated in Physics from the São Paulo State University (2000), did his MSc in Physics - Protein Crystallography at the Institute of Physics of São Carlos, University of São Paulo (2003) and PhD in Physics at the Institute of Physics of São Carlos, University of São Paulo (2007) with a doctoral internship in Protein Crystallography and Molecular Modeling in the Department of Biochemistry, University of Cambridge, UK (2006). Joao Muniz did his post-docs in Protein Crystallography at the Institute of Physics of São Carlos (2007-2008) and at the Structural Genomics Consortium, University of Oxford, UK (2008-2012). He has experience in the area of physics, Protein Crystallography, X-ray diffraction, Structural Biology, Structural Biochemistry, Molecular Modeling and crystalline complexes linked to drugs and fragments. The researcher has more than 180 crystal structures already deposited in the Protein Data Bank (PDB).

Joao Muniz develops research on enzymatic hydrolysis such as pretreatment, enzymatic hydrolysis, fermentation of sugars, biochemistry and structural studies of hydrolases, engineering enzymes for enhanced activity and their applications in bioenergy, environmentally-friendly technologies and health.

#### Selected publications:

Bernardes, A.; Textor, L.C., Santos, J.C., Cuadrado, N.H., Kostetsky, E.Y., Roig, M.G., Bavro, V.N., Muniz, J.R.C., Shnyrov, V.L. and Polikarpov, I. Crystal structure analysis of peroxidase from the palm tree *Chamaerops excels*. *Biochimie*, v. 111, p. 58-69, 2015.

Nascimento, A.S.; Muniz, J.R.C.; Aparício, R.; Golubev, A. M.; Polikarpov, I. Insights Into Structure and Function of Fungal beta-mannosidases from Glycoside Hydrolase Family 2 Based on Multiple Crystal Structures of *T. harzianum* Enzyme. *The FEBS Journal (Print)*, v. 281, p. 4165-4178, 2014.

Textor, L.C.; Colussi, F.; Silveira, R.L.; Serpa, V.; De Mello, B.L.; Muniz, J.R.C.; Squina, F.M.; Pereira, N.; Skaf, M.S.; Polikarpov, I. Joint X-ray crystallographic and molecular dynamics study of cellobiohydrolase I from deciphering the structural features of cellobiohydrolase catalytic activity. *The FEBS Journal (Print)*, v. 280, p. 56-69, 2013.

### João Paulo Naldi Silva



João Paulo Naldi Silva is a postdoctoral research associate at the Natural and Human Sciences Center of the Federal University of ABC (Brazil). He has a PhD degree in Botany (2014) from São Paulo State University (UNESP), with sandwich internship at Università Centro Bio-Medico di Roma (Italy - 2013). During PhD, he worked with metabolomics analyzes related to the shutdown of the primary metabolism in desiccation tolerant seeds and the study of the antioxidant system and the accumulation of carbohydrates and lipids in tropical seeds. He conducts research concerning the control mechanisms of desiccation tolerance in plant tissues, focusing on the respiratory metabolism, natural antioxidant compounds

and water relations during plant development. Therefore, he applies techniques to evaluate the primary metabolism, the ascorbate-glutathione antioxidant system, tissue osmotic control provided by soluble carbohydrates and membrane lipid composition during tissue desiccation.

#### Selected publications:

RASCIO, A., PICCHI, V., NALDI, J.P., COLECCHIA, S., GALLO, A., CARLINO, E., DE SANTIS, G., SCALZO, R. L., DE GARA, L. Effects of temperature increase, through spring sowing, on antioxidant power and health-beneficial substances of old and new wheat varieties. *Journal of Cereal Science*, v.61, p.111 - 118, 2015.

LEDUC, S.N.M., SILVA, J.P.N., GASPAR, M., BARBEDO, C.J., FIGUEIREDO-RIBEIRO, R.C.L. Non-structural carbohydrates of immature seeds of *Caesalpinia echinata* (Leguminosae) are involved in the induction of desiccation tolerance. *Australian Journal of Botany*, v.60, p.42 - 48, 2012.

**Jonas Weismann Gaiarsa**



PhD in biotechnology and bioinformatics lead researcher at the Genomics and Transposable Elements Laboratory at the Department of Botany/USP and the Genetics and Molecular Biology of Antioxidants Laboratory at the Department of Genetics/USP.

Research developed and topics of interest:

- Phylogenomics and enzymatic assays of *Xanthomonas* CAZys.
- Genomics, transcriptomics and mobilomics of sugarcane.

- Transcriptomics of *Arabidopsis* enzymatic antioxidant systems.
- Phylogenomics and computational chemistry of prokaryotic enzymatic antioxidants.
- Combinatorial enzyme evolution and gene circuit assembly.
- HPC and cloud computing applied to bioinformatics and computational chemistry.

**Selected publications:**

Gaiarsa, JW & Van Sluys MA. Phytopathogen Plant Polysaccharide Perception (4P): *Xanthomonadaceae* Phylogeny. In preparation.

Vieira AP, Gaiarsa JW, De Jesus EM, De Setta N, Cruz EAO, Van Sluys MA. Thiamine thiazole enzyme (THI1): diversity in plants, molecular and functional analyses of two sugarcane paralogs. In preparation.

Metcalfe CJ, Oliveira SG, Gaiarsa JW, Aitken KS, Carneiro MS, Zatti F, Van Sluys MA. Insight into the evolutionary history of the *Saccharum* genome from retrotransposon-insertion polymorphisms. In submission. Journal of Experimental Botany.

### Jose Pedro Fonseca



Jose Pedro Fonseca is a Postdoc researcher at "Laboratório de Genômica Funcional" in the Genetics Department, Institute of Biology of UFRJ, Rio de Janeiro, Brazil. Jose has experience in plant functional genomics, mainly *Arabidopsis* and worked as a postdoc at Duke University (USA) with plant immunity at Xinnian Dong Laboratory. Recently Jose joined the Laboratory of Functional Genomics at UFRJ to work with expression profiling of monolignol biosynthesis genes in sugarcane for second generation biofuel production. Jose's research interests are: Plant Immunity, Metagenomics, Plant-Microbe interaction, Biofuel and Biotic and Abiotic stress.

### Selected publications:

FONSECA JP, DONG XINNIAN (2014) Functional Characterization of a Nudix Hydrolase AtNUDX8 upon Pathogen Attack Indicates a Positive Role in Plant Immune Responses. Plos One 9: e114119, 20

MUKHTAR K., WANG, W., TADA, Y., OKA, N., TUCKER, C., FONSECA J, Dong, X., (2012) The HSF-like transcription factor TBF1 is a major molecular switch for plant growth-to-defense transition, Current Biology, vol. 22 no. 2, pp. 103 – 112

FONSECA JP, MENOSSI M, THIBAUD-NISSEN F, TOWN CD (2010) Functional analysis of a TGA factor-binding site located in the promoter region controlling salicylic acid-induced *NIMIN-1* expression in *Arabidopsis*. Genet Mol Res. Feb 2;9(1):167-75.

## Lenka Franková



Lenka Franková is a senior postdoctoral researcher in the Institute of Molecular Plant Sciences at the University of Edinburgh. She was awarded her MSc and PharmDr degree from the Faculty of Pharmacy of Comenius University in Bratislava, Slovakia. She completed her PhD in Plant Biochemistry at the Institute of Botany of the Slovak Academy of Sciences, where as a co-investigator and PI, she was focusing on sucrose and starch metabolism, proteolytic process and source-sink relationships in perennial and medicinal plants. Lenka was also involved in numerous projects aimed at plant secondary metabolites, heavy metal stress, photosynthesis and crop improvement. As a PhD student, she received multiple awards for presentations of scientific results at international and domestic conferences.

Lenka has been doing her research in the Edinburgh Cell Wall Group since 2007. She is interested in cell wall glycobiology and biochemistry with emphasis on post-synthetic remodelling, novel transglycosylases, and algal and land-plant biomass-degrading glycosylhydrolases. Her first projects were focused on developing high-throughput screens for wall-modifying enzymes, exploring wall matrix arrangement and novel enzyme activities in algae and ferns, and screening xenobiotics for herbicide effects. She is currently devising new chromogen-coupled detection systems employing unique cell wall-derived enzymes. Her research addresses questions from evolutionary, ecological, pharmaceutical, nutritional and industrial aspects of plant carbohydrates.

Lenka has presented several invited talks at international symposia and well-recognized universities abroad and supervised undergraduate and PhD students at the University of Edinburgh. She has also reviewed several scientific manuscripts and published her research in 17 scientific journals.

### Selected publications:

Franková, L., Fry, S.C. Biochemistry and physiological roles of enzymes that 'cut and paste' plant cell-wall polysaccharides. (Darwin review). *J. Exp. Bot.* 64, 3519-3550, 2013.

Franková, L., Fry, S.C. Trans- $\alpha$ -xylosidase and trans- $\beta$ -galactosidase activities, widespread in plants, modify and stabilize xyloglucan structures. *Plant J.* 71, 45-60, 2012.

Franková, L., Fry, S.C. Phylogenetic variation in glycosidases and glycanases acting on plant cell wall polysaccharides, and the detection of transglycosidase and trans- $\beta$ -xylanase activities. *Plant J.* 67, 662-681, 2011.

## Marco Tiné



Marco Aurélio Silva Tiné is a researcher at the Institute of Botany (São Paulo, Brazil), at the department of Physiology and Biochemistry. From 2011 to 2013, worked at the Brazilian Bioethanol Science and Technology Laboratory (Campinas, Brazil) on the basic science group and collaborated with researchers on cell wall treatment for industry, fermentation, enzyme characterization and high throughput screening.

Marco Tiné focus is on the structure and metabolism of cell wall polysaccharides, particularly on the structure of xyloglucan and arabinoxylan. His research on the structure of a storage xyloglucan with an unique structure showed that the branching pattern of the polysaccharide has a

direct influence on the way the enzymes act on the polymer, hence the importance of knowing the exact structure of the substrate for any technological application. In the case of sugar cane bagasse, approximately 5% of the dry mass is composed of acetyl groups assumed to be linked to hemicelluloses. This acetylation pattern has never been assessed due to the traditional method of analysis based on NaOH fractionation, which remove both the acetylations and the ferulic acid substitutions. To analyze the *in muro* structure of the arabinoxylan, therefore, It is necessary to develop new extraction methods and analysis techniques that preserve the native structure of the cell wall polysaccharides.

### Selected Publications:

Tiné, M.A.S., Silva, C.O., Lima, D.U., Carpita, N., Buckeridge, M.S. (2006). Fine structure of a mixed-oligomer storage xyloglucan from seeds of *Hymenaea courbaril*. Carbohydrate polymers 66 (4), 444-454.

Silva, G.B., Ionashiro, M., Carrara, T.B., Crivellari, A.C., Tiné, M.A.S., Prado, J., Carpita, N.C., Buckeridge, M.S. (2011) Cell wall polysaccharides from fern leaves: evidence for a mannan-rich Type III cell wall in *Adiantum raddianum*. Phytochemistry 72 (18), 2352-2360

Tiné, M.A.S., Lima, D.U., Buckeridge, M.S. (2003) Galactose branching modulates the action of cellulase on seed storage xyloglucans. Carbohydrate polymers 52 (2), 135-141

### Nicholas Grantham



Nick Grantham is a third year PhD student in Prof. Paul Dupree's laboratory in the Department of Biochemistry at the University of Cambridge. In general, this laboratory is dedicated to understanding on how plant cell wall polysaccharides are synthesised prior to deposition into the matrix and what the structural roles of some of the non-cellulosic matrix polysaccharides are.

His PhD has predominantly been focussed on understanding certain stages of xylan synthesis in the Golgi and how this may be a stepwise process. To this end he has investigated the if acetylation may play a role in backbone elongation or polymer length; and in particular how the spacing of acetyl substitutions impacts upon the spacing of glucuronic acid substitutions and the addition of methyl groups to these in the secondary stem cell wall. Observations of alternate residues bearing an acetyl group have helped to develop the hypothesis of a "two-fold" screw of xylan in the wall. This model entails a 180° rotation about the  $\beta$ -glycosidic bond resulting in all the acetyl groups on one side and none on the other. It is proposed that domains of glucuronic acid substitutions and acetyl groups then direct non-covalent bonding, or prevention thereof, of xylan to the cellulose microfibril.

He has used the techniques of PolyAcrylamide Carbohydrate Electrophoresis (PACE), DNA Sequencer Assisted Saccharide Analysis in High Throughput (DASH), Mass Spectrometry (MS), Nuclear Magnetic Resonance (NMR), genetic transformation by floral dip, *Arabidopsis* cross pollination and monosaccharide analysis by HPLC.

#### Selected publications:

Busse-Wicher M, Gomes TC, Tryfona T, Nikolovski N, Stott K, Grantham NJ, Bolam DN, Skaf MS, Dupree P. (2014) The pattern of xylan acetylation suggests xylan may interact with cellulose microfibrils as a two-fold helical screw in the secondary plant cell wall of *Arabidopsis thaliana*. *Plant J.* 79(3):492-506.

Bromley JR, Busse-Wicher M, Tryfona T, Mortimer JC, Zhang Z, Brown D, Dupree P. (2013) GUX1 and GUX2 glucuronyltransferases decorate distinct domains of glucuronoxylan with different substitution patterns. *Plant J.* 74(3):423-434.

Mortimer JC, Miles GP, Brown DM, Zhang Z, Segura MP, Weimar T, Yu X, Seffen KA, Stephens E, Turner SR, Dupree P. (2010) Absence of branches from xylan in *Arabidopsis* gux mutants reveals potential for simplification of lignocellulosic biomass. *Proc Natl Acad Sci U S A.* Oct 5;107(40):17409-14.

## Ondrej Kosik



Ondrej Kosik is Postdoctoral Research Associate at Department of Plant Biology and Crop Science of Rothamsted Research UK. Rothamsted is the longest running agricultural research station in the world which mission is to increase crop productivity and quality and develop sustainable solutions for food and energy production.

Ondrej is interested in plant cell wall architecture; particularly cell wall structure, sugar polymer composition and their interaction and remodelling during cell wall biosynthesis and development.

His current research is focusing on modifications in primary composition of xylans and beta-glucans in cereals, their ferulate decoration and spatial confirmation in the plant cell wall and their utilization for nutritional use from food production waste. His other projects are focusing on role and importance of spatial confirmation of polysaccharides in plant cell walls, and their responses to *in situ* physicochemical changes in the gastro-intestinal (GI) tract and their influence on human health.

### Selected publications:

Derba-Maceluch M, Awano T, Takahashi J, Lucenius J, Ratke C, Kontro I, Busse-Wicher M, Kosik O, Tanaka R, Winzell A, Kallas A, Lesniewska J, Berthold F, Immerzeel P, Teeri TT, Ezcurra I, Dupree P, Serimaa R and Mellerowicz EJ (2015). Suppression of xylan endotransglycosylase *PtxtXyn10A* affects cellulose microfibril angle in secondary wall in aspen wood. *New Phytol.* 205, 666-681.

Kosik O, Bromley JR, Busse-Wicher M, Zhang Z and Dupree P (2012). Studies of enzymatic cleavage of cellulose using Polysaccharide Analysis by Carbohydrate gel Electrophoresis (PACE). *Methods Enzymol.* 510, 51-67.

Kosik O, Auburn RP, Russell S, Stratilova E, Garajova S, Hrmova M and Farkas V (2010). Polysaccharide microarrays for high-throughput screening of transglycosylase activities in plant extracts. *Glycoconjugate J* 27, 79-87.

### Poliana Cardoso-Gustavson



Poliana Cardoso-Gustavson is Postdoctoral Research Associate at the Centro de Ciências Naturais e Humanas of the Universidade Federal do ABC and visiting researcher at Instituto de Botânica de São Paulo. She has degree in Biological Sciences at Universidade Estadual de Campinas (2007), master's degree in Plant Biology at the same institution (2010), and PhD degree at Instituto de Botânica de São Paulo (2014), with internship periods at The New York Botanical Garden, USA (2012) and the University of Saskatchewan, Canada (2013). Her scientific production is linked to plant anatomy (external/internal morphology, cell biology), whose primary interest refers to the structural aspects/cellular processes related to the development of healthy plants and how different stresses (ozone, UV light and herbivory), alone or together, reflect structural changes locally and along the development of the plant. She also aims to comprehend the role of secretory structures as constitutive and induced defenses in these different scenarios. Her skills involve several techniques of plant imaging (light, scanning and transmission electron, and confocal microscopies) to describe tissue and subcellular structures, and to detect metabolites and indicatives of stress tolerance and oxidative damages (NO, ascorbic acid, glutathione, reactive oxygen species, hydrogen peroxide, phenolic compounds, terpenoids).

#### Selected publications:

Cardoso-Gustavson P, Bolsoni VP, Oliveira DP, Guarantini MTG, Aidar MPM, Marabesi MA, Alves ES, Souza SR (2014) Ozone-induced responses in *Croton floribundus* Spreng. (Euphorbiaceae): metabolic cross-talk between volatile organic compounds and calcium oxalate Crystal formation. Plos One 9: e105072.

Cardoso-Gustavson P, Aguiar JRBV, Pansarin ER, Barros F (2013) A light in the shadow: the use of Lucifer Yellow technique to demonstrate nectar reabsorption. Plant Methods 9: 20.

### Rakesh Bhatia



Rakesh Bhatia is an Energy Crop Biology and Bioconversion PhD student at the Institute of Environmental, Biological and Rural Sciences of Aberystwyth University. From 2010 to 2012, he graduated with a MRes degree in Molecular Plant Biology and Biotechnology from Imperial College London, and was a research assistant in the European Commission funded ENERGYPOLAR project where he assessed various poplar clones from SweTree Technologies, INRA and CRA for altered cell wall traits and biofuel potential. He was also a research consultant at the Imperial College London spin-off company Mycologix Ltd where he investigated natural pre-treatment solutions for next generation biofuels including from Eucalyptus, Wheat straw, Sugarcane bagasse, Miscanthus, Poplar, Cassava stalk & Municipal solid waste for Suzano, CTBE, BioGasol, TMO Renewables and Direvo.

Rakesh, currently in his 3<sup>rd</sup> PhD year of his 4-year BBSRC research funding scheme and member of the Integrated Bio-refining Research and Technology Club (IBTI), has been focusing on the gene regulatory networks controlling secondary cell wall (SCW) formation in grasses in order to help overcome the challenges of modifying biomass yield and recalcitrance for rational breeding and sustainable bio-energy production and bio-refining activities. His research aims to characterise several candidate SCW biosynthesis related transcription factors and a glycosyltransferase via transgenic over-expression in the grass model species maize and examining their effects on cell wall composition and digestibility, so as to reconstruct and comprehend the SCW biosynthesis, deposition and transcriptional regulatory network in grasses for targeted manipulation of cell wall architecture.

#### Selected publications:

Bhatia R and Bosch M (2014) Transcriptional regulators of *Arabidopsis* secondary cell wall formation: tools to re-program and improve cell wall traits. *Front. Plant Sci.* 5:192.

## Ricardo da Costa



Ricardo da Costa is a final year PhD candidate at the Institute of Biological, Environmental & Rural Sciences (IBERS) of Aberystwyth University. Since he joined IBERS in late 2011, he has been actively involved in studying how cell wall composition and structure impact the efficiency of producing economically relevant materials derived from *Miscanthus* spp. biomass; an environmentally versatile perennial grass with high potential for lignocellulosic biorefining. In particular, his research addresses one of the major factors limiting the optimal use of energy crops: cell wall recalcitrance to enzymatic deconstruction.

To tackle this problem, a multilevel and multidisciplinary approach has been employed, which combines cell biological, biochemical, molecular, and spectroscopic methods (briefly: *in situ* immunolabelling of glycan epitopes, HPAEC-PAD analysis of acid and enzymatic hydrolysis products, and the assessment of biomass amenability to *Clostridium phytofermentans*-mediated fermentation). Most notably, the largest dataset of *Miscanthus* spp. cell wall glycome profiling reported to date has been collected, and is planned to be ready for publication later this year. Currently, Ricardo is preparing his PhD dissertation (to be submitted by mid-2015), and developing models for the integration of the complex yet highly informative dataset collected during his project.

### Selected publications:

da Costa RMF, Lee SJ, Allison GG, Hazen SP, Winters A, Bosch M. 2014. Genotype, development and tissue-derived variation of cell-wall properties in the lignocellulosic energy crop *Miscanthus*. *Annals of Botany*, 114: 1265-77.

da Costa RMF, Allison G, Bosch M. 2015. Cell wall biomass preparation and Fourier transform mid-infrared (FTIR) spectroscopy to study cell wall composition. *Bio-protocol*, [currently being reviewed].

da Costa RMF, Lee SJ, Hazen SP, Winters A, Avci U, Sivakumar P, Hahn M and Bosch M. 2015. Glycan comparative analysis and determination of lignocellulosic quality for a comprehensive characterisation of the *Miscanthus* cell wall. [currently being prepared]

da Costa RMF, Winters A, Avci U, Sivakumar P, Hahn M and Bosch M. 2015. *Miscanthus* cell wall features and their potential for saccharification prediction. [currently being prepared]

### Rodrigo L. Silveira



Rodrigo L. Silveira is a Postdoctoral Research Fellow in the Prof. Munir Skaf's group (Institute of Chemistry - University of Campinas). He obtained his PhD in Chemistry in 2014 for applying modern computational chemistry techniques to understand molecular aspects of plant cell walls and mechanisms of carbohydrate-modifying enzymes.

Currently, he develops research on thermodynamic forces in plant cell walls, exploring effects of hemicellulose/lignin chemical composition and extreme thermodynamic conditions commonly present in thermochemical treatments. Also, he applies computational simulations to study the dynamics of glycoside hydrolases and accessory proteins as well as their interactions with both crystalline and soluble substrates, aimed at a detailed picture of biophysical processes such as enzyme-substrate complexation, product release and inhibition. Most of these works are performed in close collaboration with experimental groups.

### Selected publications

Silveira, R. L., Skaf, M. S. (2015) Molecular Dynamics Simulations of Family 7 Cellobiohydrolase Mutants Aimed at Reducing Product Inhibition. *J. Phys. Chem. B* (In press. DOI: 10.1021/jp509911m)

Silveira, R. L., Stoyanov, S. R., Gusarov, S., Skaf, M. S., Kovalenko, A. (2015) Supramolecular Interactions in Secondary Plant Cell Walls: Effect of Lignin Chemical Composition Revealed with the Molecular Theory of Solvation. *J. Phys. Chem. Lett.* **6**, 206-211.

Silveira, R. L., Stoyanov, S. R., Gusarov, S., Skaf, M. S., Kovalenko, A. (2013) Plant Biomass Recalcitrance: Effect of Hemicellulose Composition on Nanoscale Forces that Control Cell Wall Strength. *J. Am. Chem. Soc.* **135**, 19048-19051.

## Rosemary Dyson



Rosemary Dyson is a Lecturer in Applied Mathematics at the University of Birmingham where she has been since 2011. From 2007-2011 she was a Postdoctoral Research Fellow at the Centre for Plant Integrative Biology at the University of Nottingham.

Rosemary applies mathematical modelling techniques to mechanical problems found in biological contexts, generating novel insight and predictions into the system's governing mechanisms. A major area of my research looks at the mechanics of plant growth, with a particular focus on modelling the mechanical properties of the cell wall and how those affect (and are affected by) growth. In particular, recent work has

investigated root growth dynamics across multiple spatial scales and identified the key mechanical and geometrical features which govern growth. This includes research on how the evolving microstructure of the cell wall (taking into account oriented networks of cellulose and hemicellulose embedded within a pectin ground matrix) can produce the observable macroscale mechanical properties, and how these properties are affected by enzymes such as XTH which rearrange the microstructure.

### Selected Publications:

R.J. Dyson et al. (2014) Mechanical modelling quantifies the functional importance of outer tissue layers during root elongation and bending. *New Phyt.* 202 (4), 1212-1222

RJ Dyson, LR Band and OE Jensen (2012). A model of crosslink kinetics in the expanding plant cell wall: yield stress and enzyme action. *J. Theor. Biol.* 10.1016/j.jtbi.2012.04.035.

RJ Dyson & OE Jensen (2010). A fibre-reinforced fluid model of anisotropic plant root cell growth. *J. Fluid Mech.* 655:472-503.

**Tatiane da Franca Silva**



Since 2014, Tatiane da Franca Silva is Doctor Professor at the Department of Biotechnology of the Escola de Engenharia de Lorena/Universidade de São Paulo (EEL/USP). Tatiane has experience in Plant Molecular Genetics and Plant-Pathogen interaction. Recently she is focusing her research on study of genes associated the cellulose microfibrill structure and morphogenesis in sugarcane cell wall, project with CNPq financial support.

**Selected publications:**

Silva, TF, Romanel, EAC, Corrêa, RL, Farinelli, L, Hawkins, JS., Schrago, CEG, Vaslin, MFS (2012). Global alteration of microRNAs and transposon-derived small RNAs in cotton (*Gossypium hirsutum*) during Cotton leafroll dwarf polerovirus (CLRDV) infection. *Plant Molecular Biology.*, v.80, p.443 - 460.

Silva, TF; Romanel, EAC; Andrade, RRS; Deluen, C; Corrêa, RL; Schrago, C G; Vaslin, MFS. (2011). Profile of small interfering RNAs from cotton plants infected with the polerovirus Cotton leafroll dwarf virus. *BMC Molecular Biology.*, v.12, p.1 - 12.

### Thiago C. F. Gomes



Thiago C. F. Gomes concluded his Ph.D in 2013 and since February 2014 holds a tenure-track position as an Assistant Professor of Chemistry at ITA (Instituto Tecnológico de Aeronáutica), located at São José dos Campos, São Paulo state, Brazil. Thiago Gomes specializes in computational chemistry, and during his Ph.D. his focus has been on studying glycoside hydrolases and plant cell wall architecture at the molecular level, using computational chemistry methods. He currently uses computational chemistry methods, mainly molecular dynamics simulations, to investigate, at the molecular level, fundamental problems about plant cell wall structure, and also enzymes with potential applications in biorefineries. He is particularly interested in elucidating how different cell wall constituents interact among them at the molecular level and how the detailed molecular structure of glycans which constitute cell walls affect such interactions and, consequently, cell wall properties. He is also interested in studying glycoside hydrolases, especially in what manner mutations in such enzymes can enhance their properties for potential application in biorefining processes.

His most relevant publications, in chronological order, are: [dx.doi.org/10.1021/jp200330z](https://dx.doi.org/10.1021/jp200330z) , [dx.doi.org/10.1002/jcc.22959](https://dx.doi.org/10.1002/jcc.22959) and [dx.doi.org/10.1111/tpj.12575](https://dx.doi.org/10.1111/tpj.12575) . The first publication mentioned consists of a joint experimental and computational study on the thermostability and thermophilicity of laminarinases (members of glycoside hydrolase family 16). The second paper describes a computer program Thiago Gomes developed which saves a lot of time and effort for computational chemists interested in studying, by means of molecular dynamics simulations or other computational methods, systems containing crystalline cellulose domains. The third aforementioned paper, which has been produced in collaboration with British researchers, reports remarkable findings on the molecular structure of acetylated xylan in *Arabidopsis thaliana*, and their possible implications for cellulose-xylan interactions in plant cell walls.

#### Selected publications:

Molecular Basis of the Thermostability and Thermophilicity of Laminarinases: X-ray Structure of the Hyperthermostable Laminarinase from *Rhodothermus marinus* and Molecular Dynamics Simulations Lucas Bleicher, Erica T. Prates, Thiago C. F. Gomes, Rodrigo L. Silveira, Alessandro S. Nascimento, Adriana L. Rojas, Alexander Golubev, Leandro Martínez, Munir S. Skaf, and Igor Polikarpov *The Journal of Physical Chemistry B* **2011** *115* (24), 7940-7949

Cellulose-Builder: A toolkit for building crystalline structures of cellulose Thiago C. F. Gomes, Munir S. Skaf *Journal of Computational Chemistry* 2012 *33* (14), 1338-1346

The pattern of xylan acetylation suggests xylan may interact with cellulose microfibrils as a twofold helical screw in the secondary plant cell wall of *Arabidopsis thaliana* Marta Busse-Wicher, Thiago C. F. Gomes, Theodora Tryfona, Nino Nikolovski, Katherine Stott, Nicholas J. Grantham, David N. Bolam, Munir S. Skaf, Paul Dupree *The Plant Journal* 2014 *79* (3), 492-506

### Tomas J. Simmons



Tom did his undergraduate research project in Paul Knox's lab at the University of Leeds and completed his PhD in Steve Fry's lab at the University of Edinburgh. He has since 2013 been a postdoctoral researcher in Paul Dupree's lab at the University of Cambridge.

Tom has a broad research experience on cell walls. During his undergraduate research he employed immunochemical methods to analyse xylanase activity on extracted polysaccharides and lignocelluloses. During his PhD he used a diverse array of methods to perform a collection of related research projects. Among other things, he purified the novel cell wall enzyme MXE, identified its gene using transcriptomics, recombinantly expressed the gene in yeast and biochemically characterised the native and recombinant enzyme's catalytic repertoire [1] and its polysaccharide substrates [2].

His present postdoctoral work is split between the characterisation of lytic polysaccharide mono-oxygenase (LPMO) enzymes and characterisation of lignocellulose structure using solid-state NMR (ssNMR) spectroscopy. His analysis of LPMOs involves the identification and biochemical analysis of novel LPMOs [3] and the investigation of LPMOs substrate specificity toward different lignocellulosic architecture; thereby investigating the nature of lignocellulosic architectures. This enzymological exploration of lignocellulosic architectures complements the other strand of Tom's present research: the ssNMR project is developing strategies to analyse the native architecture of intact, un-modified, lignocelluloses. Notably, this work has led to novel understandings of the nature of xylan in *Arabidopsis* cell walls.

#### Selected publications:

Mohler et al. (2013) Mixed-linkage glucan:xyloglucan endotransglucosylase (MXE) re-models hemicelluloses in *Equisetum* shoots but not in barley shoots or *Equisetum* callus. *New Phytol.* 197(1):111-22.

Simmons et al. (2013) An unexpectedly lichenase-stable hexasaccharide from cereal, horsetail and lichen mixed-linkage  $\beta$ -glucans (MLGs): implications for MLG subunit distribution. *Phytochemistry.* 95:322-32.

Lo Leggio et al. (2015) Structure and boosting activity of a starch-degrading lytic polysaccharide monooxygenase. *Nat Commun.* 6:5961.

## Valérie Cornuault



Valérie Cornuault is a postdoctoral research fellow at the Centre for Plant Sciences at the University of Leeds. She has been a member of the Paul Knox Cell Wall Biology lab since 2011. She completed her PhD as part of the WallTraC network, a European Marie Curie Initial Training Network. During her PhD, she worked in collaboration with several European laboratories and companies, particularly with INRA Nantes (Institut de Recherche Agronomique) in France and Bayer in Belgium. During her PhD she developed the Epitope Detection Chromatography technique by which epitope containing polysaccharides can be studied depending on their charges. In addition she is generating new monoclonal antibodies targeting various hemicellulosic and pectic epitopes. She is now particularly interested in cell wall assembly and polysaccharide interlinkages particularly regarding biosynthesis, cell wall remodelling and mechanical properties. Her current research focuses on the modulation of polysaccharides occurrence in *Arabidopsis thaliana* cell walls and the repercussions on global cell wall architecture as well as the study of pectic supramolecules particularly regarding the occurrence and distribution of pectic galactan and arabinan.

### Selected publications:

Cornuault, V., Manfield, I., Ralet, M.C., Knox, J.P., Epitope Detection Chromatography (EDC): a method to dissect the structural heterogeneity and interconnections of plant cell wall matrix glycans. *Plant J.* (2014) 78: 715-722.

Lee, K., Cornuault, V., Manfield, I., Ralet, M.C., Knox, J.P., Multi-scale spatial heterogeneity of pectic rhamnogalacturonan I (RG-I) structural features in tobacco seed endosperm cell walls. *Plant J.* (2013) 75: 1018-1027.

Cornuault, V., Buffetto, F., Rydahl, MG., Marcus, SE., Torode, TA., Xue, X., Crépeau, MJ., Faria-Blanc, N., Willats, W., Ralet, MC., Dupree, P., Knox, JP., Monoclonal antibodies indicate low-abundance links between heteroxylan and other glycans of plant cell walls. *Submitted*

## Wanderley Dantas dos Santos



Wanderley Dantas dos Santos is Professor of Biochemistry at the Department of Biochemistry of the State University of Maringá (UEM). He is coordinator of the Central Laboratory of Bioenergy of UEM and member of the National Institute of Science and Technology of Bioethanol. From 2009 to 2010, he was Plant Biologist at the Brazilian Bioethanol Science and Technology Laboratory (CTBE), in Campinas. Dedicated to lignin metabolism, he and his group investigate the impact of phenylpropanoids in digestibility of lignocellulosic biomass and in the nitrogen use efficiency. Using techniques of virtual screening and enzyme kinetics the group have been developing new enzyme inhibitors for specific enzymes of the phenylpropanoid pathway. In vivo assays – in growth room, greenhouse and field – they have assessed the ability of the inhibitor to reduce the recalcitrance of lignocellulosic biomass to enzyme saccharification. The assays have proven the application potential of these compounds in livestock and agro-energy. His group also investigates the role of feruloylated arabinoxylans in higher nitrogen use efficiency of commelinaceae. This research line may provide information about the evolution of type II cell wall architecture and ground the development of treatments and plants with lower requirement of nitrogen.

### Selected publications:

Oliveira, D.M., Finger-Teixeira, A., Mota, T.R., Salvador, V.H., Moreira-Vilar, F.C., Molinari, H.B.C., Mitchell, R.A.C., Marchiosi, R., Ferrarese-Filho, O., dos Santos, W.D. 2014. Ferulic acid: a key component in grass lignocellulose recalcitrance to hydrolysis. *Plant Biotechnology Journal*, doi: 10.1111/pbi.12292.

Moreira-Vilar F.C., Siqueira-Soares, R.C., Finger-Teixeira, A., Oliveira, D.M., Ferro, A.P., Rocha, G.J., Ferrarese, M.L.L., dos Santos, W.D., Ferrarese-Filho, O. The Acetyl Bromide Method Is Faster, Simpler and Presents Best Recovery of Lignin in Different Herbaceous Tissues than Klason and Thioglycolic Acid Methods. *PLoS One*, DOI: 10.1371/journal.pone.0110000.

dos Santos, W.D., Marchiosi, R., Moreira-Vilar, F.C., Lima, R.B., Soares A.R., Parizotto, A.V., Oliveira, D.M., Ferrarese-Filho, O. 2014. Polyvalent lignin: Recent approaches in determination and applications. In Lignin: Structural Analysis, Applications in Biomaterials and Ecological Significance. Eds. Fachang, L. pp. 1-25. Nova Science Publishers, Hauppauge, NY.

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