2013 Snapshots

- Citations in 2013: 9377
- Communications to International Conferences (approx.): 450
- Articles in 2013 (peer-reviewed): 291
- PhD holders: 186
- Ongoing, financed projects: 109
- PhD students: 135
- PhD theses awarded: 38
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What is ITQB

The Instituto de Tecnologia Química e Biológica (ITQB) is an academic research centre of the Universidade Nova de Lisboa. Its mission is to carry out scientific research and post-graduate teaching in Chemistry, Life Sciences, and associated technologies, while also serving the community and performing university extension activities for the promotion of science and technology.

With 53 independent teams in 2013, ITQB hosted over 400 researchers, including 135 PhD students, with different backgrounds and research interests. Researchers benefit from excellent research facilities, equipment, and scientific support services, some of which unique in the country.

ITQB further coordinates the largest Laboratório Associado, a status attributed by the Portuguese Government in recognition of scientific excellence, as determined by international evaluation panels. This consortium includes the Instituto Gulbenkian de Ciência (IGC), the Instituto de Biologia Experimental e Tecnológica (IBET), and the Centro de Estudos de Doenças Crónicas (CEDOC), and has competencies and expertise ranging from the molecule to clinical trials.

Research

ITQB Research Groups are organized into five Research Divisions - Chemistry, Biological Chemistry, Biology, Plant Sciences, and Technology. Collaboration between divisions is strongly encouraged. All scientific matters at ITQB are overseen by the Scientific Council, formed by elected PhD holders, and the Scientific Advisory Board.

Research at ITQB is mainly supported by contracted projects (competitively awarded) with national and international R&D funding agencies such as Fundação para a Ciência e Tecnologia and the European Commission (108 ongoing research projects in 2013). This year, ITQB researchers published 276 WoS papers and were cited 9377 times. Opportunities for industrial applications sometimes arise from research developed at ITQB. Collaboration with industry, patent submissions or the creation of start-up companies are the paths to follow from lab to business. This competence is mainly carried out by ITQB’s association with IBET, the largest private, non-profit biotechnology research organization in Portugal.

Education

ITQB’s highly multidisciplinary nature makes it a leading centre for the advanced training of researchers in Portugal. Education at ITQB is thus strongly embedded in its research activities.

The Pedagogical Council oversees the educational activities at ITQB. High academic standards are ensured by the Teaching Quality Committee.

In 2013, a new PhD Program (Molecular Biosciences) was approved by the national accreditation agency and was selected for funding by the FCT (eleven scholarships per year). The program was scheduled to start in January 2014. ITQB is involved in two additional FCT-funded PhD programs. A new Master Course in Biochemistry for Health in collaboration with FCT-UNL was also accredited in 2013.

ITQB PhD Program in Chemical and Biological Sciences and Engineering

This PhD course ran for the last time in 2013. Built to reflect the highly multidisciplinary nature of the institute, this program aimed to provide a broad perspective of Chemistry, Life Sciences and Bioengineering, and prepare students for their future careers. The strong component of research was complemented by seven curricular units to which students committed a tenth of their time.

Master Research Projects

ITQB welcomes master’s students who wish to develop their research at the institute; students then defend their theses at their host universities.
Master Course in Medical Microbiology
This collaboration with the Instituto de Higiene e Medicina Tropical, the Faculdade de Ciências Médicas, and the Faculdade de Ciências e Tecnologia, aims to train specialists in microbiology skilled in the application of advanced laboratory techniques for diagnoses, for microbiological research, and for quality control and certification of microbiology laboratories.

Master Course in Biochemistry for Health
A collaborative Master with Faculdade de Ciências e Tecnologia and Faculdade de Ciências Médicas, which provides a critical and analytical perspective of Human Health from a Biochemical point of view.

Master Course in Science Communication
A collaborative course with the Faculdade de Ciências Sociais e Humanas, focused on the particularities of communicating science to different audiences, via media, via formal and informal education, or directly from research institutions.

Research Training
Training can take different formats, ranging from a small regular participation in the lab activities to a one-year research project.

Post-Graduation Courses
- Scientific Research Training A - 60 ECTS

University Extension Courses
- Scientific Research Training (Graduates / Masters) - 15 | 30 | 40 ECTS
- Research Integration (Undergraduates) - 16 ECTS

Support Services
Researchers at ITQB are supported by technical and administrative staff in a number of areas (see organizational flowchart). These support services include:

Science Management collaborates with researchers in identifying potential funding sources and in the application process.

Projects Office supports researchers in applying for and managing projects.

Academics Office centralizes information regarding advanced education at ITQB.

Accounting and Treasury offers accounting support to all financed projects, manages all purchases and payroll processing, and is responsible for the inventory and property.

Lab Management coordinates the purchase and maintenance of scientific equipment for the institute and supervises common scientific equipment.

Washing Room conducts washing and sterilization of material and culture media.

Industry Liaison Office offers support in the management of intellectual property and technology transfer, and contracts with industry.

Information Technology (IT) Support offers computational support.

Storages handles the purchase, storage, and supply of materials and reagents.

Maintenance support oversees the maintenance of the building and all infrastructures.

Communication office manages institutional and scientific communication.

Additionally, some scientific support services are also available to outside researchers and companies.

Analytical Services Unit ITQB/IBET analytical development, validation and testing of chemicals and biologicals and studies on candidate pharmaceutical products according to OECD Good Laboratory Practice Principles.

Centro de Ressonância Magnética António Xavier (CERMAX) with several NMR spectrometers (300, 400, 500 and 800 MHz), including the highest field NMR spectrometer in Portugal. It is part of the National NMR Facility.

Library maintains ITQB publication records and manages bibliographic databases.

Teaching Laboratory designed and equipped to support the teaching activities in areas ranging from Biochemistry to Genetics.

Greenhouses manages the cultivation of plants for research purposes.

See full list of staff in the appendix (page 71)
Organization

Institute Council

Scientific Advisory Board

Director

Vice-Directors

Scientific Council

Pedagogical Council

Management Council

Communication Office

Science Management

Industry Liaison Office

Scientific, Tecnological and Teaching Support

Nuclear Magnetic Resonance CERMAX

Analytical Services Unit

Small Molecular X-Ray Crystallography

Fermentation Unit

Library

Lab Management

Teaching Laboratory

Washrooms

Computer Systems Support

Workshop and Maintenance

Research

Chemistry

Biological Chemistry

Biology

Plant Sciences

Technology

Management Support

Administration and Finance

R&D Planning and Management

Health and Safety

Human Resources

Mailing and Archive

Academics

Administrator

Ombudsperson
Research Groups

Chemistry

Biorganic Chemistry
Rita Ventura

Coordination and Supramolecular Chemistry
Rita Delgado

Homogeneous Catalysis
Beatriz Royo Cantabrana

Micro-Heterogeneous Systems
Eurico de Melo

Molecular Thermodynamics
Luís Paulo N. Rebelo

Organic Synthesis
Christopher Maycock

Organometallic Chemistry
Carlos C. Romão

Collaborators
James Yates - Single Molecule Processes

Biological Chemistry

Bacterial Energy Metabolism
Inês Cardoso Pereira

Metalloproteins and Bioenergetics Unit
Manuela M. Pereira

Metalloenzymes and Molecular Bioenergetics
Miguel Teixeira

Biomolecular NMR
Manolis Matzapetakis

Genomics and Stress
Claudina Rodrigues-Pousada

Macromolecular Crystallography Unit
Carlos Maria Franco Frazão

Structural Biology
Pedro Manuel Marques Matias

Membrane Protein Crystallography
Margarida Archer Frazão

Structural Genomics
Maria Arménia Carrondo

Inorganic Biochemistry and NMR
Ricardo Saraiva L. Oliveira Louro

Microbial & Enzyme Technology
Lígia O. Martins

Molecular Genetics of Microbial Resistance
Lígia M. Saraiva

Molecular Interactions and NMR
Patrick Groves

Molecular Simulation
António Baptista

Protein Biochemistry Folding & Stability
Cláudio M. Gomes

Protein Modelling
Cláudio M. Soares

Raman Spectroscopy
Smilja Todorovic

Collaborators
Filipe T. de Oliveira - Mössbauer Spectroscopy

Biology

Bacterial Cell Biology
Mariana G. Pinho

Bacterial Cell Surfaces and Pathogenesis
Sérgio R. Filipe

Bacterial Signaling
Karina B. Xavier

Cell Physiology and NMR
Helena Santos

Cell Signaling in Drosophila
Pedro Domingos

Control of Gene Expression
Cecília M. Arraião

Glycobiology
Julia Costa

Microbial Development
Adriano O. Henriques

Microbiology of Human Pathogens Unit

Molecular Genetics
Hermínia de Lancastre

Molecular Microbiology of Human Pathogens
Raquel Sá-Leão

Bacterial Evolution and Molecular Epidemiology
Maria Miragaia

Plant Sciences

Disease and Stress Biology
Ricardo Boavida Ferreira

Forest Biotech
Célia Miguel

Genomics of Plant Stress
Margarida Oliveira

Plant Biochemistry
Cândido Pinto Ricardo

Plant Cell Biology
Rita Abrantes

Plant Cell Biotechnology
Pedro Fevereiro

Plant Metabolomics
Carla António

Plant Molecular Ecophysiology
Manuela Chaves

Collaborators
Philip Jackson - Plant Cell Wall

Technology

Applied and Environmental Mycology
Cristina Silva Pereira

Biomolecular Diagnostic
Abel Oliva

Animal Cell Technology Unit
Ana Sofia Coroadinha

Cell Bioprocesses
Paula M. Alves

Engineering Cellular Applications
Manuel J.T. Carrondo

Mass Spectrometry
Ana V. Coelho

Microbiology of Man-Made Environments
Teresa Crespo

Nutraceuticals and Delivery
Catarina Duarte

Pharmacokinetics and Biopharmaceutical Analysis
Ana L. Simplício

Systems Biodynamics
Andreas Bohn

Collaborators
Fátima Lopes - Antibiotic Stress and Virulence of Enterococci
Maria do Rosário Bronze - Analytical Chemistry
Cidália Peres - Food Microbial Technology

Invited and Visiting Professors

Alessandro Giuffrè | Fast Kinetics
Alexander A. Konstantinov | Bioenergetics
Alexander Tomasz | Microbiology
David L. Turner | Biology
Hansjörg Hauser | Eukaryotic Molecular Biology
John G. Aunins | Bioprocess Engineering
Jonas Almeida | Biomathematics
José Artur Martins Simões | Chemistry
José Canongia Lopes | Molecular Simulation
Maria Teresa N. Duarte | Crystallography
Kenneth R. Seddon | Ionic Liquids
Otto-Wilhelm Merten | Bioengineering
Peter F. Lindley | Structural Biology
Peter G. Hildebrandt | Raman Spectroscopy
Robert Samson | Mycology
William Frank Martin | Molecular Evolution
Statistics 2013

53 Research Groups
417 Researchers

Average group size 7.9 researchers

Group leaders by gender 30 female / 22 male
Group leaders by nationality 48 Portuguese / 4 other

International PhD Holders 32
EU countries: 18
Bulgaria (1), Germany (1), Greece (1), Ireland (1), Poland (2), Serbia (3), Spain (3), UK (6)
Rest of the world: 4
India (1), Norway (1), Russia (1), Tunisia (1)

38 PhD Theses
291 Research Articles

ISI-WOS journals 277
Other peer-review articles 14
Book chapters 13
Edited Books 2
(see full list in the Research Output Section)
Average number of papers per group 5.4
Citations (2013) 9,377
Total ITQB papers (1990-2013) 3,166
Total ITQB citations (1990-2013) 70,584

Average citations per paper 29
Considering a paper’s maturation time of three years (includes all ITQB papers until 2008 and the corresponding total citations to date)
h-index 98

Communications 450
in International Scientific Meetings

109 Research Projects 6.17 M€

89 Fundação para a Ciência e a Tecnologia | 7 European Commission | 3 European Commission (individual grants)
1 Ministério da Defesa | 4 Pfizer Contract | 1 Sudoe Interreg
1 European Research Council | 2 Ciência Viva | 1 Astellas Pharma Europe Limited

Projects in the last five years

Publications with international teams 115
Countries with more than 20 papers: Usa, Spain, Germany, France
Between 10 and 20 papers: England, Netherlands
Between 3 and 9 papers: Switzerland, Denmark, Scotland, Italy, Brazil, Poland, Canada, Australia, Luxembourg, Ireland, Finland
With two papers or less: South Africa, Russia, Romania, Japan, Czech Republic, Thailand, Sweden, South Korea, Singapore, Philippines, Norway, Kenya, Iran, India, Gambia, Egypt, Ecuador, Croatia, Cambodia, Bulgaria, Belgium, Austria, Argentina

International collaborations within projects 145
Through FCT projects: 25
Argentina (1), Brazil (1), France (4), Germany (6), Spain (5), The Netherlands (2), UK (3), USA (3)

Through EU projects: 120
Argentina (1), Austria (3), Belgium (2), Brazil (1), Bulgaria (3), China (2), Czech Republic (1), Denmark (3), Spain (18), Estonia (1), Ethiopia (1), Philippines (1), Finland (1), France (20), Germany (15), Hungary (4), India (1), Ireland (1), Israel (1), Italy (4), Mali (1), The Netherlands (1), Norway (1), United Kingdom (13), Switzerland (7), Sweden (1), Syria (1), Turkey (1)
Most ITQB PhD students and post-docs are financed directly through FCT fellowships. The chart below depicts ITQB’s budget including this figure (2,12 M€).
Prizes and Awards

Individual distinctions

Cecília M. Arraiano
Elected chair of women in science working group of FEBS

Helena Santos
President of the International Society for Extremophiles (2012-2014)

Paula M. Alves
Nominated Vice-President of the European Society of Animal Cell Technology (ESACT)

Research distinctions

Catarina Duarte
1st Prize for Research Aveleda - White Wine & Health (Research Grant Aveleda - white wine and health)

Margarida Serra
ACTIP (Animal Cell Technology Industrial Platform) Award 2013-2014
Bioengineering approaches for up- and down-stream processing of human stem cells for clinical application.

In scientific meetings

A. R. Oliveira, J. A. Thompson, K. B. Xavier
EMBO / FEBS course on ‘Host-Microbes Interactions’, Inter-species bacterial signaling and gut microbiota.
30 August - 7 September 2013, Spetses, Greece
Best Poster Award

D. Simão, C. Pinto, M Serra, A. Teixeira, G. Schiavo, E. J. Kremer, P. M. Alves e C. Brito
“Modeling human neuronal functionality in vitro: 3D culture for neural differentiation and maturation.”
8th International Meeting of the SPCE-TC, May 2013, Faro, Portugal,
Best Abstract Award

Helena I.M. Veiga, Mário R.C. Soromenho, José M. S. S. Esperança, José N. Canongia Lopes, Luís Paulo N. Rebelo
“Ionic liquids under tension”
COIL-5, Vilamoura, Portugal, 2013
Honourable Mention Poster Award

Nuno Faria
Portuguese Congress of Microbiology and Biotechnology (MicroBiotec’13)
6-8 December 2013, Aveiro, Portugal.
SPM’13 – Best oral presentation (ex aequo)

P. Gomes-Alves, R. Cunha, M. Serra, P. M. Alves
‘Lover’s Proteome’, EuPA OPEN PROTEOMICS 2, 14-20 October 2013, Saint-Malo, France
Third place in Proteomics Photo and Graphic Art Contest

Rute G. Matos
Budapest Biostruct Course on Basics in Protein Crystallization and Crystallography 2013
August 30 – September 3, 2013, Budapest, Hungary
Best oral presentation

Saúl Silva
10º Encontro Nacional de Quimica Orgânica
4-6 September 2013, Lisbon
Best Masters Thesis

V. J. Pereira, B. R. Oliveira, M. J. Benoliel, R. A. Samson, M. T. Barreto Crespo
“Fungiwatch: Benefits and Hurdles Associated with the Presence of Fungi in Water”
MicroBiotec’13, Aveiro, Portugal.
Best Poster in the area Environment

“Characterization of Nanomedicines Uptake and Intracellular Trafficking in Cancer Cells”
VI Symposium on Technology and Health, Instituto Politécnico da Guarda (IPG), 3 May 2013, Guarda, Portugal
Prize for best oral presentation
Events
Main events at ITQB

- **Dia Aberto 2013: Ser Cientista**
  - April 20

- **Biomush Project Meeting**
  - April 12

- **6th CERMAX practical course on basic NMR workshop**
  - June 24-27

- **ITQB PhD Program**
  - Starting session
  - Jan 10

- **“A arte dos fungos filamentosos”**
  - Exhibition by Patricia Noronha
  - 25 May

- **“Planta do Futuro”**
  - Outreach activities in Oeiras Parque
  - International Fascination Plants Day
  - May 18-26

- **Career Development Master Class**
  - Germ Stories - Five Decades in Microbiology with Roberto Kolter (Harvard Medical School)
  - May 6-9
Events

**July**
- ITQB Day
  Celebrating ITQB’s integration in UNL
  July 5
- Best PhD Thesis Prize 2012
  Thesis on biology by Pedro Matos Pereira
  July 5
- Cleanward project meeting
  July 04

**September**
- Awareness Session
  Funding opportunities under HORIZON 2020
  Excellence Science pillar: Marie Curie & ERC
  Sep 13
- European Researchers Night
  Sep 27
- Mini-Symposium
  “Bacterial Cell Surfaces”
  Sep 26
  “Bacterial growth, antibiotic resistance and dormancy”
  Sep 27
  “Analysis of Staphylococcus epidermidis population structure by whole genome sequencing”
  Sep 28
- European Researchers Night
  Sep 27

**October**
- Transbio Workshop | Metabolomics and Molecular Interactions for Biology and Health
  Nov 13-15

**November**
- Course Structure and Function of Membrane Proteins
  Nov 5-8
- Transbio Workshop | Metabolomics and Molecular Interactions for Biology and Health
  Nov 13-15
- “Um cientista vem à escola” Science & Technology Week 2013
  Nov 18-22
- 4th ITQB PhD Students Meeting
  Oct 14-25
Seminars at ITQB

Frontier Leaders Seminars

Selective Oxidation with Non Heme Iron Complexes that Support High Oxidation States
Miquel Costas, University of Girona, Girona, Spain

Capnocytophaga canimorsus, cave canem!
Guy R. Cornelis University of Basel, Switzerland and University of Namur, Belgium

Integrated molecular circuits for stem cell activity in Arabidopsis roots
Ben Scheres, Wageningen University, Netherlands

Surprising new functions for peptidoglycan maturation enzymes in bacteria
Ivo Gomperts Boneca, INSERM, Institut Pasteur, France

Understanding and exploiting hydrogenases
Kylie A. Vincent, Inorganic Chemistry Lab., Univer. of Oxford, UK

European Research Council: Challenges and Opportunities
Applying for funding within the European Research Council
Teresa Lago, Universidade do Porto, Portugal
Alexandra Velga, ITQB-UNL, Portugal
Maria Arménia Carrondo, ITQB-UNL, Portugal

Relevance of Carbene Bonding Motifs in Enzyme Reactivity
Martin Albrecht, University College, Dublin, Ireland

Starting an electrical conversation between microorganisms and electrodes to achieve bioproduction
Korneel Rabaey, The University of Queensland, Australia

Using exoelectrogenic and electrotrophic microorganisms with different microbial electrochemical technologies for electricity and biofuels production
Bruce Logan, The Pennsylvania State University, USA

Of nature and nurture: connecting gene regulation, metabolism and disease
Matthias Hentze, Eur Molecular Biology Lab., Heidelberg, Germany

AVX Seminars

Computer-driven drug discovery: amyloidosis by transthyretin, a case study
Rui Brito, FCT, Universidade de Coimbra

Medicinal and aromatic plants as sources for bio-based products
Ana Cristina Figueiredo, Faculdade Ciências, Universidade de Lisboa

Advanced fluorescence and microscopy methodologies in membrane biophysics
Manuel Prieto, IST, Universidade de Lisboa

Generating and shaping novel action repertoires
Rui Costa, Fundação Champalimaud

Between commensalism and pathogenicity
Isabel Gordo, Instituto Gulbenkian de Ciência

SCAN

Immune evasion through modulation of Rab and Arf small GTPases expression
Duarte C. Barral, CEDOC

Driving force vs electrostatic interactions - Which plays the main role in collisional electron transfer?
Teresa Catarino, Cell Physiology and NMR

Glycoproteomics in health and disease
Júlia Costa, Head of Glycobiology Laboratory

The translational applications of an Evolutionary Cell Biology
José Pereira Leal, Computational Genomics Laboratory, IGC

Coagulase-negative staphylococci: a tool box for Staphylococcus aureus
Maria Miragaia PhD, Auxiliary Researcher

Tales from the crypt: recognition properties of polyamine cage compounds
Pedro Mateus, Coordination and Supramolecular Chemistry Laboratory

Abiotic stress seen from a plant’s perspective
Margarida Oliveira, Genomics of Plant Stress Laboratory

"Magic mushrooms" The untapped potential of filamentous fungi
Cristina Silva Pereira, Applied and Environmental Mycology

When a gene is worth two: Alternative splicing of an Arabidopsis membrane transporter
Paula Duque, IGC

Impact of the irrigation regime applied to Aragonez (Syn. Tempranillo) grapevines on grape berry flavonoids and ABA biosynthesis and accumulation
Olfa Zarrouk Post-doctoral Fellow

Molecular details of electron transfer in fumarate reduction by flavocytochrome c3
Catarina Paquete, Inorganic Biochemistry and NMR

Prediabetes: what is known and what we would like to know
Maria Paula Macedo, CEDOC

PTMomics – a potpourri of experimental approaches
Ana Varela Coelho, Mass Spectrometry Laboratory
Portuguese public buses as major MRSA reservoirs: a worrisome finding!
Teresa Conceição, Molecular Genetics Lab Laboratory

Novel insights into embryogenesis and secondary growth in forest tree species
Célia Miguel, Forest Biotech Laboratory

Phylogenomics of symbiont-mediated protection to pathogens
Luís Teixeira, Host-microorganism interactions lab, IGC

Design and in vitro Evaluation of Potential CO-Releasing Molecules: a case study
Ana C. Coelho, Organometallic Chemistry Laboratory

Design and Synthesis of new probes for AI-2 quorum-sensing receptors studies
Sofia Miguel, Bioorganic Chemistry Laboratory

Dendritic cells: sugars in the spotlight
Paula Videira, CEDOC

ABCC proteins: molecular and biochemical aspects of their involvement in vacuolar anthocyanin transport
Rita Francisco, Plant Molecular Ecophysiology Lab

Small molecule activation mediated by organometallic complexes
Beatriz Royo, Homogeneous Catalysis Lab, ITQB

Malaria Liver stage infection: A struggle to die
Carlos Penha Gonçalves, IGC

Spore development and toxin production by the human intestinal pathogen Clostridium difficile
Adriano Henriques, Microbial Development Lab, ITQB

Sensing and processing the interspecies quorum sensing signal AI-2
Karina Xavier, Bacterial Signaling Lab, ITQB

UniMS: towards a new operations management for the Mass Spectrometry services
Margarida Oliveira e Paula Alves, ITQB

A Journey into the New RNA World
Cecília Arraiano, Control of Gene Expression Lab, ITQB

Directed evolution for tweaking with protein unfolding pathways
Vânia Brissos, Microbial & Enzyme Technology Lab, ITQB

Mind the gap: linking microbial bioenergetic metabolism to electricity production
Ricardo Louro, Inorganic Biochemistry and NMR Lab, ITQB

Other Seminars

News From Gold Catalysis and Palladium Bioorganometallic Chemistry
Stephen K. Hashmi, University of Heidelberg, Germany

Biophysical Methods in Drug Discovery: Combination is Key
The Project Kinetics for Drug Discovery
Matthias Frech- Merck KGaA, Germany

Design of enzymes: integrating sequence analysis and molecular modelling
Juergen Pleiss University of Stuttgart, Germany

Pathway Engineering in Corynebacterium glutamicum for organic and amino acid production from starch
Bernhard Eikmanns, University of Ulm, Germany

Two Essential Processes in Chloroplast Biology: Protein Complex Assembly and Protein Splicing
David Stern, Boyce Thompson Inst. of Plant Research, Ithaca, New York, USA

LC-MS tools for environmental and food analysis
Teresa Galceran, University of Barcelona, Spain

Evolution and regulation of bacterial growth, morphology, and development
Yves V. Brun, Indiana University, USA

Discovering plant genomes
Michel Delseny- University of Perpignan, France

A molecular insight to the mitochondrial ADP/ATP carrier
Eva Peyer-Peyroula, Institut de Biologie Structurale, Grenoble

A study of Ionic Liquids in the pharmaceutical sector
Robin Rogers, University of Alabama, USA

Mitochondrial diseases – it’s not about energy, after all
Nuno Raimundo - Universitätsmedizin Goettingen, Germany

Metagenomic exploration of Andean mountain microbiomes: who is there and why we care
Maria Mercedes Zambrano, Corpogen Research Center, Colombia

Early bioenergetic evolution
William F. Martin, University of Düsseldorf, Germany

Micro-evolution, transmission and clonal replacement in MRSA
Edward Feil University of Bath, UK

Persistence Pays Off: Understanding the Mechanisms of Antimicrobial Tolerance by Bacterial Pathogens
Gregory Phillips, Iowa State University, USA

Molecular Epidemiology of MRSA in Wisconsin
Sanjay Shukla- Marshfield Clinic Research Foundation, USA
Clostridium difficile ribotypes - interaction with hosts and environments
Maja Rupnik, University of Maribor, Faculty of Medicine, Maribor, Slovenia

The intracellular life of Salmonella
David W. Holden, Imperial College London

Proteoliposomes in nanobiotechnology approaches
Pietro Ciancaglini, Universidade de Sao Paulo, Brazil

Advances in somatic embryogenesis of tropical trees and study of plants transformed with P5CS gene
Marguerite Quoirin, Federal University of Parana, Curitiba, Brazil

Understanding quorum sensing and its impact in the clinic and the environment.
Miguel Cámara, Centre for Biomolecular Sciences, University of Nottingham, UK

Genomic characterization of Enterococcus faecium
Willem van Schaik, University Medical Center Utrecht, The Netherlands

Harnessing pluripotent stem cells for pharmacology
Marc Peschanski, I-STEM, INSERM, Evry, France

Understanding how short-chain lipids help doxorubicin cross membranes
Manuel Nuno Melo, Faculty of Mathematics and Natural Sciences, Groningen, Netherlands

Exploring the complexity of drought and dehydration tolerance in C4 grasses
Melvin J. Oliver, Plant Genetics Research Unit, University of Missouri, Columbia, USA

Trehalose, a sugar for all seasons
Matthew J. Paul, Plant Biology and Crop Science, Rothamsted Research, England

Functional characterization of genes related to abiotic stresses in rice
Márcia Pinheiro Margis, Núcleo de Genômica Funcional de Plantas, Brasil

How does the hydrogenase enzyme work?
Csaba Bagyinka, Institute of Biophysics, Biological Research Center, Szeged, Hungary

COHITEC Program 2014
Presentation Roadshow

What can the sulfur isotope fractionation associated with dissimilatory sulfite reductase tell us about the redox evolution of Earth’s atmosphere?
William D. Leavitt, Harvard University
Science and Society

ITQB Open Day (20 April)
1001 Visitors
Organizing committee
Ana Matias, Eurico Melo, Filipe Almeida, Irina Franco, José Andrade, Marta Alves, Mónica Martins, Pedro Fevereiro

International Fascination Plants Day (18 -28 May)
National Coordinators
Nelson Saibo, Ana Sanchez and Joana Lobo Antunes
Researchers in Oeiras Park
André Cordeiro, Andréia Rodrigues, Carlota Vaz Pato, Célia Miguel, Diana Branco, Diana Macedo, Margarida Rosa, Marta Alves, Natacha Vieira, Inês Chaves, Manuela Veloso, Margarida Oliveira, Nelson Saibo, Pedro Barros, Pinto Ricardo, Rita Abranques

"A minha vida de Planta" (“My Life as a Plant”)
Children's book about Science (Translation from Alan Jones & Jane Ellis, University of North Carolina at Chapel Hill, EUA).
Ana Paula Santos & C. Pinto Ricardo

Open Labs (7, 14, 21, 28 March)
69 Visits / 28 students
Visited Labs
Microbial & Enzyme Technology
Protein Biochemistry Folding & Stability
Molecular Genetics
Bacterial Cell Surfaces and Pathogenesis
Cell Physiology and NMR
Molecular Microbiology of Human Pathogens
Protein Modeling
Plant Cell Biotechnology
Genomics of Plant Stress (GPlantS)
Industry and Medicine Applied Crystallography
Bacterial Cell Biology
Nutraceuticals and Delivery

School Visits
9 Visits / 168 students
Visiting Schools
Agrup. Escolas IBN Mucana
Escola Básica 2,3 com Ensino Secundário de Alvide (Agrupamento de Escolas de Alvide)
Escola Secundária de Camões
Escola Secundária S. João do Estoril
Núcleo de Estudantes de Bioquímica Universidade de Coimbra Universidade Atlântica
Visited Labs
Bacterial Cell Surfaces and Pathogenesis
Bacterial Energy Metabolism
Cell Signaling in Drosophila
Control of Gene Expression
Coordination and Supramolecular Chemistry
Disease and Supramolecular Chemistry
Forest Biotechnology
Genomics and Stress
GPlantS
Mass Spectrometry
Microbiology of Man-made Environments
Molecular Genetics
Molecular Genetics of Microbial Resistance
Plant Biochemistry
Plant Cell Biotechnology
Stress by Antibiotics and Virulence of Enterococci

Summer Training for High School Students (June - July)
Memórias de Stress nas plantas
Ana Paula Santos
Cool plants
J. Miguel Costa
O que escondem os Epigenomas das plantas?
Ana Paula Santos
Técnicas Gerais em Microbiologia e Genética
Adriano Henriques
Espectrometria de massa, proteómica e afins
Ana V. Coelho

Science and Technology Week (18-22 Nov)
Visiting Researchers

Visited Schools
"O Xururuca" em São João do Estoril
Agrupamento de Escolas de Carnaxide
Colégio Oriente (Parque das Nações)
EBI Actor Vale 1º ano, turma A
EBI Moinhos do Restelo
EBI S. José - Agrup. de Escolas Baixa Chiado (Centro de Lisboa)
EBI/JI de Porto Salvo
EBI/JI. S.to António , do Agrupamento de Escolas Rainha D. Leonor, em Lisboa
Escola Básica Conde de Oeiras
Escola Cooperativa “A Torre”
Escola D. Carlos I em Sintra
Escola de Santo António, Parede
Escola Secundária do Forte da casa
Escola Secundária Dr. José Afonso no Seixaal
Escola Secundária Fernando Lopes Graça - Parede - 8ºano turma B
Escola Secundária Quinta do Marquês- Oeiras
St. Julians School Carcavelos
The International Preparatory School (also known as IPS)
Research Highlights

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Bioorganic Chemistry
Rita Ventura  rventura@itqb.unl.pt

The vast majority of biologically active carbohydrates exist as oligo- and polysaccharides and glycoconjugates in which monosaccharide units are linked via glycosidic bonds. The glycosylation reaction is still a major challenge in carbohydrate synthesis, especially the synthesis of 1,2-cis glycosides, where there is not a general method for their efficient stereoselective preparation. Many factors influence the anomeric selectivity, such as the glycosidic donor (choice of protecting groups) and acceptor, the solvent, the anomeric leaving group, the promoter, temperature. Recently, we reported that NIS/TIOH mediated glycosylations of ethyl 6-O-acetyl-2,3,4-O-trinbenzyl-1-O-thioglucoside with several acceptors, ranging from unhindered linear primary alcohols to other sugars, afforded higher alpha-anomeric selectivities when compared with other 6-O-protecting groups.1 The 6-O-acetyl group being electron withdrawing, reduced the reactivity at the anomeric position compared to the tetrabenzyalted thioglucoside and favoured the formation of the alpha-glu- cosides (1,2-cis glycosylation). In the case of galactosides, higher alpha-selectivities were obtained in the glycosylation reactions with phenyl 2,3-O-dibenzy-4,6-O-dichloroacetyl-1-O-thioglactoside as the donor, showing that in this case, a stronger electron withdrawing 4-O-ester group had an influence in the anomeric selectivity favouring the formation of 1,2-cis galactosides.2

During this period the start-up ExtremoChem was created, it employs two post-doctoral researchers and is supported by venture capital.


Coordination and Supramolecular Chemistry
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The search for compounds capable of forming chelates with high thermodynamic stability, fast complexation kinetics, and high inertness toward dissociation for safe use in medicinal applications continues to be a challenging research field. The chelates of some N-functionalized derivatives of cyclen (1,4,7,10-tetraazacyclododecane) are used in these applications.

Two cross-bridged cyclen-based macrocycles with two trans-N-acidic acid arms having a dibenzofuran (H$_2$L1) or a diphenyl ether bridge (H$_2$L2) were studied in our laboratory. Both compounds behave as “proton sponges”, and present high stability constants with Cu$^{2+}$ and Ga$^{3+}$ cations. They exhibit an excellent selectivity for Cu$^{2+}$, ensuring that metal ions largely present in the human body would not interfere. Both [CuL1] and [CuL2] chelates are extremely inert to demetallation, especially [CuL2]. The acid-assisted dissociation of [CuL1] led to half-life time (t$_{1/2}$) of 4.28 h in 5 M HCl at 90 °C, while [CuL2] needed harsher acidic conditions of 12 M HCl at 90 °C with t$_{1/2}$ of 30.8 days. To the best of our knowledge [CuL2] exhibits the highest t$_{1/2}$ value for a complex of Cu$^{2+}$ with a polyaza macrocycle derivative. These features place these copper(II) chelates as good candidates for radiopharmaceuticals using $^{64}$Cu for therapeutic purposes or $^{68}$Cu for positron emission tomography (PET).

Homogeneous Catalysis
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Splitting water to form oxygen and hydrogen by using organometallic catalysts

Nature utilizes solar energy to extract electrons and release protons from water, a process called photosynthetic water oxidation. Inspired by this natural process, chemists are intensely interested in using sunlight to split water and form O_2 and H_2. This process will allow to covert and store solar energy into chemical energy. The critical challenge to practical water splitting schemes is the development of water oxidation catalysts (WOCs).

We have developed an exceptional water oxidation (WO) catalyst, the organometallic iridium Cp*Ir(NHC)Cl_2 complex, which displayed remarkable activity, 17,000 h^{-1} turnover frequencies (TOFs) and turnover numbers (TONs) close to 400,000, the largest ever reported for a metal catalyzed WO reaction, using NaIO_4 as oxidant in water at 40 °C. High turnover numbers were attained by this catalyst system without noticeable degradation of the oxidation activity, even after storage of reaction solutions during several months. Therefore these systems must be susceptible to be incorporated into long-lasting electrochemical cells, operating at low overpotentials to overcome undesirable degradation of the activity in photoelectrocatalytic cells.


Micro-heterogeneous Systems
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Barriers isolating cells and cell organelles from each other and the whole body of living organisms from the external environment are molecular constructs whose key components are lipids. In most cases the lipids are organized in bilayer membranes that, besides the barrier function, also have an active role in metabolite trafficking and many other aspects of the biochemical activity of the cell. The physical and chemical properties of these membranes, in particular the primary parameters such as bilayer thickness and area per lipid molecule, are quite well known. However, the measurement of second-order thermodynamic properties such as the variation of the bilayer expansion with temperature was never addressed sufficiently. Along the last year we have developed a new method for the experimental determination of the thermal area expansion coefficient of bilayers, a property that has applications in the study of the interactions between lipid bilayers and proteins, peptides and other amphipathic molecules, and is an input in computer simulations. Based on the data obtained for bilayers with several lipid compositions we proposed a novel molecular mechanism for lipid bilayer thermal expansion.
Organic Synthesis

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The copper oxidation of some suitably substituted tertiary amines in the presence of air is catalytic and only 10% of the copper reagent is required. The mechanism of the reaction, that has been shown to be general for the formation of these Dihydro-1,3-oxazines, is interesting. In many cases the intramolecular cyclisation is stereoselective and while attempting to discover the source of this stereoselectivity we found that the intermediate iminium dissociated to form a pair of molecules that underwent a [4+2] cycloaddition to afford the observed products. This mechanism is unexpected and novel. The aerobic oxidation of the copper species is also of note.


Molecular Thermodynamics

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It’s almost like magic. In their search for better and better solvents, researchers from the Molecular Thermodynamics Lab tested new types of ionic liquids to solve some of the oldest engineering problems in chemistry. Fluorinated Ionic Liquids were developed and characterized, and the formation of three nanosegregated domains was demonstrated. Fluorinated Ionic Liquids can be used as “three in one” solvents, increasing the solubilisation power. Playing with the Van der Waals, coulombic and hydrogen bonding interactions and the size of the fluorous domain will allow the development of solvents designed for each specific application. Unusual LCST-type behaviour - We show for the first time that one of the mechanisms that can lead to systems with LCST phenomena can also be incorporated in binary mixtures using functionalized ionic liquids and ethers. The most remarkable feature is that it is possible to rationalize in a quite straightforward way the diverse fluid phase behavior by simply taking into account the changes at a ionic or molecular level that cause small shifts in the balance between the three types of interaction. Deep eutectic solvents - We were able to create a liquid mixture out of a specific solid salt by adding one of three natural organic acids that are also solids. All these materials are cheap, non-toxic, completely biodegradable, and biocompatible. The results are highly promising liquids, efficient and selective in separations, with the additional benefit of producing a liquid end product that can be recovered and reused.

Research Highlights

Annual Report 2013

The BEM lab is interested in studying Energy Metabolism in environmentally important bacteria to explore their biotechnological applications. We have focused in a widespread group of environmental organisms that respire sulfur compounds. These organisms play a key role in the biogeochemical cycles of sulfur and carbon in anaerobic habitats, and are important players in Environmental Biotechnology.

In 2013 we made an important contribution to expanding the biotechnological application of these organisms by showing that they have a high activity in biological hydrogen production. Using a model organism whose hydrogen metabolism is quite well characterized, we demonstrated a high specific hydrogen production activity from formate, with 100% conversion. This study demonstrates that these organisms can be an attractive option to be used in second stage processes of hydrogen production, as they present higher activity levels than those found for the currently used photosynthetic organisms.

Organometallic Chemistry

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In the late 1970’s the pioneering work of Wolfgang Beck at the Maxi- millian University, Munich, Germany, started populating the chemical space with new entities emerging from two unrelated fields: Biochemistry and Organometallic Chemistry. In 1980, the 18th paper of the series “Metal-Complexes with Biologically Significant Ligands” described the salt [Mo(CO)3(his)]K isolated from the reaction of the natural aminoacid histidine with a reference organometallic species, Mo(CO)6. A typical finding of fundamental research, this compound looked like a mere curiosity because it was made long ahead of its time. When in 2000, carbon monoxide, CO, was recognized as a major cytoprotective, therapeutically useful active principle, such very water soluble, strongly air sensitive complex, non-toxic anion was immediately regarded as a useful prodrug for the controlled delivery of CO. In fact, this anion is one of the most useful experimental CO Releasing Molecules (CORM) known to date. Injected in vivo it behaves like a bolus of “solid CO” providing proof-of-concept for the curative use of CO in many experimental animal models of disease. After almost a decade of regular use of [Mo(CO)3(his)]Na, known as ALF186 at Alfama Inc, ITQB/IBET, its hitherto confidential pharmacological and biochemical properties were published in Dalton Transactions in 2013 thus contributing for the advancement of CO therapy and CORM design.

Bacterial Energy Metabolism

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The BEM lab is interested in studying Energy Metabolism in environmentally important bacteria to explore their biotechnological applications. We have focused in a widespread group of environmental organisms that respire sulfur compounds. These organisms play a key role in the biogeochemical cycles of sulfur and carbon in anaerobic habitats, and are important players in Environmental Biotechnology. In 2013 we made an important contribution to expanding the biotechnological application of these organisms by showing that they have a high activity in biological hydrogen production. Using a model organism whose hydrogen metabolism is quite well characterized, we demonstrated a high specific hydrogen production activity from formate, with 100% conversion. This study demonstrates that these organisms can be an attractive option to be used in second stage processes of hydrogen production, as they present higher activity levels than those found for the currently used photosynthetic organisms.
Respiratory complex I is an energy transducing molecular machine. It converts the redox energy from NADH:Quinone oxidoreduction to membrane potential energy. This potential energy is vital for synthesis of ATP, exchange of solutes/nutrients across the membrane and motility. Most mitochondrial diseases (including neurodegenerative ones such as Parkinson and dystonia disorders), apoptosis (and its resistance in cancer cells) and ageing are associated with the functioning of respiratory complexes, including complex I. We have contributed to the understanding of the structural/functional mechanism of complex I by investigating its constituents and related complexes. We aimed at identify a common denominator, i.e. the conserved structural elements based not the rationale that conservation reflects functional relevance. The identification of such denominator allowed us to put forward an original perspective on the evolution, function and mechanism of respiratory complex I. The coupling mechanism should be based on long range conformational changes, and not on possible conformational changes at the catalytic sites close to the membrane surface.

Ramírez-Gualito et al. (2013) Molecules, 18 5 p. 4929-41
Hydrogenases are enzymes that can potentially be used in bioelectrical devices or for biological hydrogen production, the most studied of which are the [NiFe] type. Most [NiFe] hydrogenases are inactivated by oxygen and the few known O2-tolerant enzymes are hydrogen-uptake enzymes, unsuitable for hydrogen production, due to strong product inhibition. In contrast, the [NiFeSe] hydrogenases, where a selenocysteine is bound to the nickel, are very attractive alternatives because of their high hydrogen production activity and fast reactivation after O2 exposure. In 2013 we reported five high-resolution crystallographic 3D structures of the soluble form of the [NiFeSe] hydrogenase from D. vulgaris Hildenborough in three different redox states (oxidized as-isolated, reduced with H2 and re-oxidized in air), which revealed the structural changes that take place at the active site during enzyme reduction and re-oxidation. We observed the oxidation to sulfinate of the terminal Cys residue bound to the Ni atom in the active site to be irreversible. However, the highly oxidized form of the proximal iron-sulfur cluster found in the oxidized as-isolated structures is fully reversible upon reduction. These results provided new insights into the pathways of O2 inactivation in [NiFe], and in particular, [NiFeSe] hydrogenases. In addition, they suggest that different enzymes may display different oxidized states upon exposure to O2, which are probably determined by the protein structure.
Inorganic Biochemistry and NMR
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Multiheme cytochromes c are ubiquitous proteins in prokaryotes. They play key roles in the bioenergetic metabolism of sediments and soil organisms that are of great interest for biotechnological processes of low environmental footprint, collectively known as bioelectrochemical technologies. These include bioremediation of metal contaminated soils, energy generation from wastewater in microbial fuel cells and the bioelectrosynthesis of fine chemicals. The structures of many of these proteins are organized as domains linked by peptide segments that can have varying levels of flexibility. This flexibility can be essential for their biological activity. NMR spectroscopy is uniquely capable of probing this flexibility in conditions mimicking the physiological context. One of the most powerful NMR probes of molecular flexibility is the phenomenon of Residual Dipolar Couplings. In a collaborative work with the organic synthesis laboratory we measured for the first time the spontaneous RDCs of a multicentre paramagnetic protein. This protein was the small tetraheme cytochrome from Shewanella oneidensis MR-1, a model organism for the study of bioelectrochemical technologies. We showed that the spontaneous RDCs are correlated with the orientation of the ligands coordinating the iron in the hemes. This opens the tantalizing perspective of using known structures of multiheme cytochromes involved in extracellular electron transfer to probe their orientation and dynamics.

Macromolecular Crystallography Unit
Membrane Protein Crystallography
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Our group is interested in the three-dimensional structure determination of proteins by X-ray Crystallography, which will provide insights into their biological function. In the case of enzymes, elucidating their structures allows the visualization at atomic level of the protein global fold and architecture of the active site. If the substrate is bound to the protein, it enables a detailed characterization of the substrate interactions with the protein. This data contributes to a better understanding of the protein function and sheds light into their reaction mechanism.

We have solved the crystal structure of a bacterial α-phosphoglucomutase that has an overall fold similar to eukaryotic phosphomannomutases. It catalyzes the reversible conversion of α-glucose 1-phosphate to glucose 6-phosphate. The crystal structure of α-PGM from Lactococcus lactis (APGM) was determined at 1.5 Å resolution and contains a sulfate and a glycerol bound at the enzyme active site that partially mimics the substrate. The substrate specificity and catalytic mechanism of APGM are discussed based on its structure.
We have established catalytic and spectroscopic fingerprints of two recombinant DyP-type peroxidases (DyPs) from the soil bacteria *Bacillus subtilis* and *Pseudomonas putida* MET 94. DyPs constitute a novel family of heme containing peroxidases that successfully degrade a wide range of substrates, from high redox potential synthetic dyes, iron and manganese ions, aromatic sulphiles to phenolic or nonphenolic lignin compound units and even lignin, using hydrogen peroxide as electron acceptor. DyPs show primary sequence, structural and apparently mechanistic features unrelated to “classical” peroxidases. In particular the H2O2 binding site (i.e. the acid-base catalyst) of DyPs is aspartate, whereas the binding sites in classic peroxidases are found at histidine. They show two domains showing a typical ferrodoxin-like fold distinct from other heme peroxidases that are primarily α-helical proteins. DyPs have been classified into four subfamilies, A-C constituted by bacterial enzymes and class D containing predominantly fungal enzymes. Emerging evidence reveals that DyPs from different subfamilies possibly have different physiological roles and that to a certain extent these enzymes represent the bacterial equivalent of fungal ligninolytic peroxidases. In addition, due to their origin they can be produced in higher yields and genetically engineered for improved performance and therefore they have an utmost importance and potential for White Biotechnology applications.

*Flavo-diiron Proteins (FDPs) are a widespread family of enzymes, present in the three life domains, that reduce directly oxygen to water and/or nitric oxide to nitrous oxide, therefore eliminating the sources of Reactive oxygen or nitrogen species. The molecular determinants for the selectivity of these enzymes towards each of those two putative substrates has been investigated by a thorough comparison of the structures of these enzymes, which led to the construction of single and double site directed mutants of residues close to the active diiron site, using as a model the oxygen-reducing FDP from the anaerobic protozoan *Entamoeba histolytica*. Investigation of the reactivity towards oxygen and nitric oxide, by amperometric and fast kinetics approaches showed that a tyrosine close to the catalytic site plays a determinant role in the enzyme’s reactivity. Its substitution by a serine led to enzymes with enhance NO reductase activity and to a substantial decrease of the kinetic stability of the enzyme under multiple turnover conditions towards oxygen.*
Molecular Genetics of Microbial Resistance

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*Helicobacter pylori* infects over half of the world population causing gastric and duodenal ulcers and ultimately malignant gastric cancer. However, the increasing occurrence of antibiotic-resistant *H. pylori* strains makes treatments more difficult. In Tavares AF, et al. (2013) PLoS One. 8(12):e83157, we showed that CORMs are able to kill different strains of *Helicobacter pylori*, including antibiotic resistant strains, and found two CORMs able to inhibit the growth of the bacteria both in vitro and during infection of mammalian cells in culture. The mode of action seems to involve the release of the carbon monoxide, which in turn interferes with the bacteria respiration and with the activity of an enzyme essential for pathogenesis. This bactericidal effect was stronger when CORMs were used in combination with traditional antibiotics.

Antibiotic resistance is less likely to be developed when using multiple bactericidal agents that affect different pathways. So, the ability of CORMs to kill *Helicobacter pylori* makes them good candidates for fighting antibiotic resistant strains. The benefit of using CORMs might even be double: known for their anti-inflammatory effect, these molecules should help reducing the gastric mucosal inflammation, which is the main cause for the development of malignant lesions.

Molecular Interactions and NMR

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Nucleotides are the building blocks of DNA and our genetic code. They are also important molecules in signaling pathways where changes in their concentrations or binding properties can result in disease or protection from disease. Fluorescent-labeled nucleotides have been developed as very sensitive tools to visualize the location and activity of nucleotides. This is partly because nucleotides have weak properties to be seen by other tools that scientists have in their labs. Unfortunately, the addition of fluorescent groups to the nucleotide can lead to different binding properties compared to the unmodified nucleotide. We showed that NMR spectroscopy can be used to check different fluorescent nucleotide analogs in order to select the most suitable one for a particular study. NMR spectroscopy can also collect information on the unmodified nucleotide for reference.
Protein misfolding and aggregation is a hallmark in several human diseases. In recent years we investigated these processes in models of metabolic disease and neurodegeneration, as well as the pharmacological rescue of misfolded proteins by small molecules. Since amyloid neurodegenerative diseases are mostly sporadic we are now interested in establishing how chemical and biological factors in the cell environment influence aggregation in neurodegenerative diseases such as Amyotrophic Lateral Sclerosis (ALS) and Alzheimer’s disease (AD). This year we highlight two major contributions from our lab towards the goal of understanding how metal ions and interactions between amyloidogenic proteins contribute to disease. In a paper published in the Journal of Biological Chemistry we showed that Ca promotes aggregation of SOD1, which is involved in ALS, into soluble amyloid oligomers rather than into inert fibrils, suggesting a link to toxic effects of the Ca overload observed in patients. We have also uncovered in a PLOS ONE paper the molecular basis of amyloid formation by the calcium-binding S100 glial cytokines, which are highly elevated in AD and ALS, and induce the aggregation of other proteins, namely SOD1. Hopefully this research on disease pathomechanisms will open new avenues towards effective therapies for neurodegeneration.


Peptide dendrimers are synthetic tree-like molecules composed of amino acids, often used as agents for catalysis, binding and drug delivery. Their bio-compatibility and proteolytic resistance makes them promising biomedical agents, but their structural determinants have thus far remained elusive, precluding a truly rational molecular design. Although we previously showed the existence of two distinct levels of compactness, the underlying reasons for such features remained unclear.

We have now conducted a comprehensive study using computational simulations, in order to identify the major structural determinants of dendrimer compactness. Our results clearly show that a trade-off between electrostatic effects and hydrogen bond formation controls structure acquisition in these systems. Moreover, by selectively changing the dendrimers charge we are able to manipulate the exhibited compactness. In contrast, the length of branching residues does not seem to be a major structural determinant.

Our results are in accordance with the most recent experimental evidence and shed some light on the key molecular-level interactions controlling structure acquisition in these systems. Thus, our study provides valuable insights that can contribute to the development of truly tailor-made dendritic systems.

Protein Modeling

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cyc-RKAAAD is a short cyclic peptide known to adopt a remarkably stable single turn $\alpha$-helix in water. We extensively sample the conformational space of cyc-RKAAAD using $\mu$s-long MD simulations. We characterize the peptide conformational preferences in terms of secondary structure propensities and, using Cartesian-coordinate principal component analysis (cPCA), construct its free energy landscape, thus obtaining a detailed weighted discrimination between the helical and non-helical subensembles. The cPCA state discrimination, together with a Markov model built from it, allowed us to estimate the free energy of unfolding ($-0.57$ kJ/mol) and the relaxation time ($0.435$ $\mu$s) at $298.15$ K, which are in excellent agreement with the experimentally reported values ($-0.22$ kJ/mol and $0.42$ $\mu$s). The results obtained attest the suitability of modern simulations methods to explore the conformational behavior of peptide systems with a high level of realism.


Raman Spectroscopy of Metalloproteins

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In the past period we have focused on several metalloenzymes (e.g. cd1 nitrite reductase, DyP peroxidase) and on novel biocompatible electrode materials (SAM modified nanostructured gold/silver and functionalized transparent conducting oxides) which together can provide promising new platforms for bioelectrocatalysis. We have developed a powerful toolbox of analytical approaches, based on confocal surface enhanced (resonance) Raman spectroscopy and spectroelectrochemistry, which allowed us to characterize both, the electrode material and the immobilized enzyme, simultaneously and evaluate the potential of the studied enzymes for biotechnological applications. In addition, we have provided spectroscopic insights into molecular details of active sites of DyPs from two different subfamilies. A comparative study employing resonance Raman (RR) and surface enhanced RR spectroscopies allowed us to correlate the heme coordination patterns of these enzymes in solution, crystal, and immobilized states and understand the parameters that control the spin state distribution and activity in these enzymes. Taken together, the obtained results helped us define structural and mechanistic features of the immobilized DyPs under working conditions of the future bioelectronic constructs that can operate as biosensors or biocatalysts.
Herpesviruses establish life-long latent infections. During latency, gammaherpesviruses, such as Kaposi’s sarcoma-associated herpesvirus (KSHV), persist as multicopy, circularized genomes in the cell nucleus and express a small subset of viral genes. KSHV latency-associated nuclear antigen (LANA) is the predominant gene expressed during latent infection. C-terminal LANA binds KSHV terminal repeat (TR) DNA to mediate DNA replication. TR DNA binding also allows tethering of the viral genome to mitotic chromosomes to mediate DNA segregation to daughter nuclei.

We have identified regions on LANA that are critical for herpesvirus to lie dormant within our bodies, literally tying the virus to our chromosomes. The work funded by the Harvard Medical School-Portugal Program was published in PLoS Pathogens in 2013.

By solving the X-ray structure we discovered two functional faces of LANA, “one face binding the viral DNA and the other face linking to the host chromosome”. Studying a human virus is often difficult because of their inability to infect other animals in the same way. With no good animal models it is very hard to test new assumptions on the disease. But for the Kaposi’s sarcoma-associated herpesvirus, we have a mouse virus that acts much in the same way. In this work, it was possible to manipulate mouse LANA and see how virus latency was affected: mutations that prevented DNA binding lead to the loss of virus latency.
**Research Highlights**

**Bacterial Cell Biology**

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*Staphylococcus aureus* is an extremely versatile pathogen capable of causing from minor infections to life threatening ones, such as bacteremia or endocarditis, with high morbidity and mortality rates. Currently it causes more deaths than AIDS and tuberculosis combined in the USA. Besides its virulence, *S. aureus* is well known due to its increasing resistance to antibiotics. Methicillin Resistant *S. aureus* (MRSA) strains are among the most important causes of antibiotic-resistant hospital infections worldwide and have emerged also in the community. An alternative to current antibiotic therapies is the use of two agents that act synergistically to kill bacteria. In the context of various collaborations, we have been involved in elucidating the mechanisms of action of new compounds that resensitize MRSA to beta-lactams. Two examples are murgocil, a staphylococcal-specific inhibitor of the peptidoglycan synthesis enzyme MurG and ticlopidine, an antiplatelet drug which was found to inhibit TarO, the protein that catalyses the first step of wall teichoic acids synthesis. Surprisingly, MRSA lacking teichoic acids become susceptible to beta-lactams, most likely due to disruption of the normal functioning of the penicillin binding proteins (PBPs), enzymes involved in the last stages of peptidoglycan synthesis.

**Bacterial Cell Surfaces and Pathogenesis**

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*Streptococcus pneumoniae* are Gram-positive bacteria often associated with a variety of infections that can range in severity from otitis media to pneumonia or meningitis. We have been interested in the determination of the subcellular localization of enzymes used by this bacterial pathogen to propagate and evade the host immune system. We have recently showed that fluorescent derivatives of key enzymes responsible for the synthesis of capsule, a major virulence factor in *S. pneumoniae*, localize at the division septum of bacteria at a specific time of their cell cycle, to ensure the full encapsulation of bacteria and probably efficient evasion of bacteria from the host immune system. However, we were constrained by the lack of tools that permit efficient protein expression or co-localization of more than two different proteins inside the same *S. pneumoniae* bacteria cell. Therefore we constructed a set of plasmids that allows efficient expression of fluorescent derivatives of pneumococcal proteins. This was achieved by the introduction of a 10 amino acid tag, named i-tag, at the N-terminal end of the fluorescent proteins, which results in an improved translation efficiency and allowed the determination of the subcellular localization of various proteins in pneumococcal bacteria. The availability of the new plasmids described in this work should greatly facilitate studies of protein localization in *S. pneumoniae* and probably in other Gram-positive bacteria.
A solute from (hyper)thermophiles inhibits aggregation of α-synuclein in a model of Parkinson’s disease

Some marine microorganisms thrive at temperatures near 100ºC. They synthesize unique solutes presumably used for protection against heat damage, making them interesting sources of protein stabilizers. While many tests have been performed in vitro, it was important to examine the protecting properties of these compounds in the overcrowded cytoplasm of living cells. We studied the effect of mannosylglycerate in a yeast model of Parkinson’s disease and found that it reduces the formation of α-synuclein (α-Syn) inclusions, a typical marker of Parkinson’s disease. S. cerevisiae cells, expressing α-Syn tagged with a fluorescent protein, were engineered to synthesize mannosylglycerate. Fluorescence microscopy was used to assess the number of cells with fluorescent foci. There was a 3-fold decrease in α-Syn inclusions and this reduction was accompanied by attenuation of the α-Syn-induced cytotoxicity. It is proven that mannosylglycerate acts as a chemical chaperone and the stabilization mechanism involves direct solute/protein interactions. This is the first demonstration that this ionic solute, closely associated with stress adaptation in hyper/thermophiles, acts as a potent chemical chaperone in vivo, preventing protein misfolding/aggregation. The usefulness of these findings to the development of new drugs against protein-misfolding disorders will be assessed.
Cell Signaling in Drosophila

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The highlight of this last year in our laboratory was the publication of our Coelho et al. Cell Reports article. In this work, we show that Ire1 (Inositol requiring enzyme 1) is required for photoreceptor differentiation and rhabdomere morphogenesis in Drosophila. The role of Ire1 in this paradigm occurs by a mechanism that is independent of the most well known mediator of Ire1 signaling, the transcription factor Xbp1. Instead, Ire1 directly degrades several mRNAs, including the one coding for Fatty acid transport protein (Fatp). In Ire1 mutant photoreceptors, the disregulation of Fatp levels causes an increase of phosphatidic acids leading to severe defects in the formation of the rhabdomere, the light sensing organelle of the photoreceptors.


Control of Gene Expression

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The difference was in the tail: A DIStinctively novel exoribonuclease that really likes U

Cells control the expression of their genes at different levels. One strategy is to degrade the molecules that serve as intermediates between the information contained in DNA and the acting proteins, the messenger RNAs. The whole RNA degradation process is highly regulated: mRNA molecules are marked for destruction and ribonucleases (RNases) chop the mRNAs in pieces.

Our lab (Control of Gene Expression Lab) together with collaborators from the IGC Telomere and Genome Stability Lab have identified a new RNA degrading enzyme in fission yeast that constitutes a major player in the 3’-5’ exonucleolytic decay of transcripts. The enzyme has the unprecedented property of preferring RNA molecules with a tail of Us instead of the typical tail of As of messenger RNAs. We have shown that this enzyme represents an alternative pathway of eukaryotic RNA decay that is challenging the models already established.

Subsequent report (in Nature) identified the tumor suppressor micro RNA (miRNA) let-7 as a physiologic substrate of Dis3L2 demonstrating the enzyme association with cancer and stem cell maturation. Moreover, the known association of Dis3L2 gene mutation with Perlman’s syndrome (fetal overgrowth disease) and predisposition to Wilms’ tumors confirms the importance of this protein in maintaining normal cell metabolism and development.

**Research Highlights**

**Microbial Development**  
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*Clostridium difficile* is a strict anaerobic, spore forming bacterium. It is presently the most common cause of hospital-acquired infections associated with antibiotic therapy. The organism relies on the ability to form oxygen-resistant spores to spread and infect new hosts. Despite the importance of spores for the infectious cycle, a detailed characterization of spore differentiation has been lacking. Using a combination of genome-wide approaches with studies of gene expression at the single cell and population levels, researchers at the Microbial Development Laboratory in collaboration with colleagues from the Institut Pasteur in Paris, have published a detailed analysis of the morphological changes that take place during spore differentiation in this organism, in relation to the changes in gene expression during the process. The two articles show that sporulation, a developmental process that emerged some 2.5 billion years ago, is largely conserved in *C. difficile*, but less tightly controlled that in the more recent, aerobic model organism *Bacillus subtilis*. The authors speculate that this feature may be related to the pathogenic nature of *C. difficile*. The two studies further establish a platform for inspecting the function of key sporulation genes, many of which are specific to *C. difficile* and related to host colonization and transmission. Thus, studies of sporulation by *C. difficile* will result in novel strategies for diagnostic and therapy.


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Glycosylation is a common post-translational modification of proteins in eukaryotic cells. In tumor cells alterations in cell surface glycosylation take place and glycans are useful biomarkers in different types of cancer. Exosomes are vehicles of cellular proteins to the outside of the cell. These membrane vesicles are secreted by various cell types, including tumor cells and neurons, and have been associated with the transmission of pathogenicity among cells. Since exosomes are found in biological fluids, such as blood, cerebrospinal fluid, or urine, they are potential diagnostic targets for cancer and other diseases. Exosomes have a unique protein, lipid and glycan composition. We have studied protein glycosylation of exosomes from ovarian carcinoma SKOV3 cells using glycomics techniques (lectin blotting, NP-HPLC and mass spectrometry). The sialoglycoprotein galectin-3-binding protein was identified as an abundant marker of exosomes. Furthermore, exosomes contained specific glycan signatures that consisted predominantly of complex glycans, and high mannose glycans were also detected. Finally, bisecting N-acetylglucosamine containing glycans were also found. The results open novel perspectives to explore the potential roles of glycoproteins and N-glycans in exosome biology and as markers for ovarian cancer.

Escrevente et al. (2013) PLOS One. 8(10): e78631.
Methicillin-resistant Staphylococcus aureus (CA-MRSA) causing infections in healthy persons in the community have increased worldwide and are a major public health concern. CA-MRSA are different from MRSA found in hospitals, having a higher pathogenic potential and distinct clonal types. Portugal is the European country with the highest MRSA prevalence in hospitals (50%), but the frequency of MRSA in the community in our country was unknown.

To understand the extent of dissemination of CA-MRSA in Portugal, we collected MRSA isolates at entrance of 16 hospitals distributed over the country and characterized them using state-of-the-art molecular typing techniques. Surprisingly, we found an extremely high frequency of MRSA in the community, reaching 21%, which is one of the highest described in Europe. However, only a small proportion belonged to typical CA-MRSA epidemic clones; the great majority of the isolates (89%) belonged to epidemic clones highly related to those found in hospitals in Portugal. Our results suggest that the high MRSA frequencies in the community in Portugal result mainly from a spill-over from the hospital.

The high prevalence of MRSA in the community in Portugal is worrisome and should be seen as a warning to the public health providers. Unless strict infection control measures are adopted in the hospital, MRSA will continue to spread from the hospital into the community what will result in an epidemic that will be extremely difficult to control.


Streptococcus pneumoniae (pneumococcus) is an important human pathogen worldwide responsible for systemic diseases such as meningitis, pneumonia, and bacteraemia. It is also frequently carried asymptomatically in the upper respiratory tract. A correct identification of this pathogen is, in most cases, straightforward using methodologies that have been established for several years. However, some pneumococci display atypical properties that hinder their identification. These atypical isolates are most often associated to colonization and non-invasive disease and thus tend to be regarded as less pathogenic. We have analyzed a large collection of invasive and non-invasive disease isolates presumptively identified as atypical pneumococci. This collection was obtained over several years in Spain. We combined the usual phenotypic assays with several DNA-based methodologies. We have found that only one fourth of the isolates were indeed atypical pneumococci. Almost half were S. pseudopneumoniae, a closely-related species described for the first time a decade ago, and the remaining belonged to other streptococcal species. With this study we have shown that: (i) the so-called atypical pneumococci are often misidentified; (ii) S. pseudopneumoniae and non-capsulated pneumococci may cause severe invasive disease.

Forest Biotech

Célia Miguel  cmiguel@itqb.unl.pt

Wood is the result of a differentiation process that ends with the programmed death of specific plant cells - the xylem cells. The correct timing for this cell death is controlled by the molecule thermospermine. We have unveiled how the levels of thermospermine are controlled in wood cells of poplar, the plant model for trees. We tried to assess the effect of increasing thermospermine levels in poplar (by overexpressing the thermospermine synthase gene) and found that this was surprisingly not possible in the xylem. This evidence suggested the existence of a mechanism specific to these tissues to maintain thermospermine homeostasis.

By characterizing the crosstalk between thermospermine and the endogenous hormone auxin, the presence of a negative feedback loop mechanism was established whereby auxin positively influences thermospermine function in delaying death of the wood cells while thermospermine negatively affects endogenous auxin content in order to re-establish the equilibrium in thermospermine levels. This safeguard mechanism ensures the fundamental role of thermospermine during wood formation.

It is proposed that thermospermine is a xylem specific polyamine and should be considered as a novel plant growth regulator essential to ensure proper wood development. These findings are of great interest to the forest tree breeding and biotechnology community as the control of xylem cell death process during wood formation affects tree wood properties and biomass production.


Disease and Stress Biology

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Berry fruits are a good source of phenolic compounds and, thus, potentially beneficial to human health. Polyphenol intake from fresh fruit, and the relative contribution from berries, in the Portuguese population, was assessed by a semi quantitative food frequency questionnaire (1). Berries accounted for 9% of total fresh fruit intake, from which 80% were due to strawberries. Total polyphenol intake from fresh fruits was 783.9 mg ± 31.7 mg of Gallic Acid Equivalents (GAE) per day, from which 14% were from berries. Within berries, strawberries accounted for 11% of total polyphenol intake, with the other consumed berries accounting for 3% of the total polyphenol intake per day. This reflects low consumption of berries in the Portuguese population, the main reasons being low market availability and high prices.

Due to the importance of berries to polyphenol intake, selected varieties of commercial blueberries, raspberries, and blackberries and two wild berries, Portuguese crowberry and strawberry tree fruit, were characterized. Individual phenolic content was determined by liquid chromatography–diode array detection and mass spectrometry (HPLC-DAD-MS) after hydrolysis by a novel combination of the fungal glycosidases, hesperidinase and cellulase (2). This method was able to disclose new sources of dietary phenolic compounds, and highlighted the usefulness of Portuguese crowberry and strawberry tree fruit as a source of polyphenols.

Genomics of Plant Stress (GPlantS)

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In recent years, researchers have realized the importance of other regulatory mechanisms besides transcriptional control, such as the ubiquitin/26S proteasome system (UPS), in the modulation of abiotic stress responses. In the UPS, ubiquitin is covalently bound to target proteins as an ubiquitin chain (polyubiquitination) and often prompts the ubiquitinated target protein for degradation through the 26S proteasome machinery. In this system, the E3-ubiquitin ligases play a crucial role since these proteins confer specificity to target proteins to be ubiquitinated. In our work, we have identified in rice a REALLY INTERESTING NEW GENE (RING) E3-ubiquitin ligase which was named OsHOS1. We have also found that this E3-ubiquitin ligase can target for degradation a master transcription factor in the cold stress response, OsICE1, thus influencing the plant response to cold. We used a RNA interference (RNAi) strategy to down-regulate the expression of OsHOS1 and observed an accumulation of OsICE1 protein in the transgenic rice plants. This accumulation influenced the expression of one of its downstream genes, OsDREB1A, leading to an up-regulation as compared to WT rice plants in response to cold. However, physiological analysis did not reveal an increased tolerance to cold stress in the transgenic plants. These observations suggest that OsHOS1 may have other targets that can influence the rice plants responses to abiotic stress.

Plant Biochemistry

Cândido Pinto Ricardo ricardo@itqb.unl.pt

Coffee is an important commercial product mostly obtained from Coffea arabica. This species is greatly affected by coffee-leaf-rust (CLR), a fungus that causes a major disease and enormous economic loss. “Centro de Investigação das Ferrugenhas do Caffeíno” (CIFC/IICT) has developed expertise in the genetics of coffee resistance to CLR. We have been collaborating with CIFC in studying proteomics of the coffee/CLR interactions, directing attention to the plant extracellular space (or apoplast), which plays a crucial role in initiating and coordinating many defense responses to biotic and abiotic stresses. Coffee is grown in CIFC under greenhouse conditions making it possible to follow the effect of the changing temperature along the year on the patterns of the apoplastic proteins. This information is relevant for the understanding of coffee ecology and, also, for the study of the coffee/CLR interactions. Principal component analysis of the apoplastic protein samples, collected from May to December, revealed the existence of two groups of sampling dates mainly discriminated by the thermal amplitude: higher (group I) and lower (group II). Different proteins are associated with the two groups, indicating that apoplast structural modifications occurred in response to temperature. Our work highlights the dynamics of the apoplast secretome, which acts as the first line of defense against adverse factors.

Plant Cell Biology

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Over the past two decades, plant-based platforms have emerged as valuable systems for the low-cost production of recombinant proteins and as an alternative to established systems such as bacteria or mammalian cell cultures. Our laboratory has been working on the establishment of the legume plant *Medicago truncatula* as a platform for the cost-effective production of recombinant proteins. We work mainly with suspension cell cultures, which offer many advantages, such a controlled environment and the ability to comply with Good Manufacturing Practices. Recently, we showed the successful production of two human proteins, Erythropoietin and Prostaglandin D Synthase. These results strengthen the potential of the *Medicago truncatula* expression platform that we had previously established in our work on feed additives, and pave the way for the synthesis of glycoproteins at a much lower production cost.

Plant Cell Biotechnology

Pedro Fevereiro  psalema@itqb.unl.pt

We show that restriction of plant growth by low temperature or low nitrogen leads to large increases in trehalose-6-phosphate (T6P). While the regulation of the plant sucrose non-fermenting 1 AMP-activated serine/threonine-protein related kinase (SnRK1) in response to endogenous Sucrose levels likely involves factors in addition to T6P, in vitro catalytic data, and now in vivo gene expression data in a physiological context, support the view that T6P regulation of SnRK1 provides an explanation for the control of growth in response to plant tissue sucrose availability providing other factors are not limiting. Evidence presented suggests the mechanism operates above a level of sucrose of 3 μmol g⁻¹ plant fresh weight (FW) and 0.3 to 0.5 nmol T6P g⁻¹ FW likely to indicate a sucrose starvation threshold. This starvation threshold (3–5 μM T6P) is close to the Ki of the T6P/SnRK1 complex. Increases in sucrose above this level through sucrose feeding or through treatments that induce sink-limited growth resulted in a proportionate increase both in T6P content and changes in expression of SnRK1 marker genes. SnRK1 is likely inhibited in vivo by up to 80% or more by T6P under the physiological conditions caused by low temperature. The T6P/SnRK1 signaling pathway is necessary for the acceleration of growth following relief from sink-limited conditions, such as low temperature.
Anthocyanins represent the largest class of flavonoids and constitute one of the most important families of secondary metabolites. They have been shown to be synthesized as protective compounds in response to abiotic stresses, such as UV, cold and drought, but also to attract pollinators. Anthocyanins are synthesized in the cytosol and accumulate in the vacuoles, mostly of the epidermal tissues of fruits, leaves, and flowers. In red grape berries (Vitis vinifera) the accumulation of anthocyanins in the exocarp is one of several events that characterize the onset of fruit ripening. Due to the fact that the vacuolar sequestration of anthocyanins has only been partially characterized, we focused our study on elucidating the role ABC-type transporters on such process. We present biochemical evidence that an ABC protein, ABCC1, localizes to the tonoplast and is involved in the transport of glucosylated anthocyanidins. ABCC1 is expressed in the exocarp throughout berry development and ripening, with a significant increase at véraison (i.e., the onset of ripening). Transport experiments using microsomes isolated from ABCC1-expressing yeast cells showed that ABCC1 transports malvidin 3-O-glucoside. The transport strictly depends on the presence of GSH, which is co-transported with the anthocyanins and is sensitive to inhibitors of ABC proteins. By exposing anthocyanin-producing grapevine root cultures to buthionine sulfoximine, which reduced GSH levels, a decrease in anthocyanin concentration is observed. In conclusion, we provide evidence that ABCC1 acts as an anthocyanin transporter that depends on GSH without the formation of an anthocyanin-GSH conjugate.


Sphingolipids act as structural components of membranes and lipoproteins, and mediate cell-signalling in most eukaryotes. Each of these molecules carry a sphingoid base backbone, but their combinatorial biosynthesis leads to numerous subspecies which vary in their lipid backbones and complex headgroups. Our knowledge on the functional roles of sphingolipids in filamentous fungi is limited when compared to mammals and plants. Through combining gene/protein expression with organic/analytical chemistry, we elucidated how the chemical structure of ionic liquids (i.e. molten salts) affects the toxic response of filamentous fungi. At sub-inhibitory concentrations, ionic liquids alter the fungal metabolic footprint, activate the biosynthesis of osmolytes and uncommon secondary metabolites and increase the expression of genes coding in multidrug transporters, secondary metabolism and cell wall repair, inspiring their use in fungal biology [1,3]. Some ionic liquids activate an uncharacterised alternative pathway of cell wall integrity in Aspergillus nidulans [4], while altering sphingolipid biosynthesis. We are now filling knowledge gaps in this signalling cascade in A. nidulans.

Research highlight I

Human pluripotent stem cells (hPSCs), with their ability for extensive proliferation and multi-lineage differentiation, can serve as a renewable source of cellular material in regenerative medicine, in vitro toxicology and disease modeling applications. A prerequisite for the transition of hPSCs or their progeny to these fields is the establishment of efficient cell culture protocols for large-scale expansion, differentiation, purification, storage and distribution. The major challenges in producing hPSC-derivatives are the scaling up of reproducible pure cell populations of undifferentiated cells without compromising their self-renewal ability and differentiation potential and the directed differentiation to specific cell types with improved differentiation efficiency, high purity and functionality.

The recently published review from the Animal Cell Technology Unit (Serra et al. 2012), has been selected and included in the most recent book from Cell Press Reviews: Stem Cells to Model and Treat Disease. In this chapter, we describe how hPSCs constitute an extremely attractive tool for cell therapy and disease modeling and the latest advances in hPSCs process engineering, underlining why this is one of the main focusing areas of our research group. This book also includes a chapter by Shinya Yamanaka, recipient of the 2012 Nobel Prize for Physiology or Medicine for his work on the reprogramming of mature cells to pluripotency.


Research highlight II

One of the interests of the research group is to further understand the virus host cell interaction. We have been using functional genomics to study the physiological changes imposed in the production of simple and complex retrovirus. This knowledge is being applied by means of reverse metabolic engineering in human cell lines producing retroviral and lentiviral gene therapy vectors. To this end, we have been focusing in: i) understanding the metabolic constraints associated to virus replication, ii) identifying gene targets for manipulation, iii) implementing novel analytical tools to support gene manipulation and clone screening to iv) genetically engineering the phenotype of producer cells towards increased titers, enhanced cell robustness and improved quality of the viral gene therapy bioproduct.

In Rodrigues et al. (2013) functional genomics tools, including microarray transcriptome analysis, metabolite profiling, lipidomics, RNA interference and genetic engineering, were used and inter-crossed for knowledge generation and cell manipulation. Eight metabolic pathways were identified as impacting virus production and within those several gene targets for further study. Through cell engineering titer improvements up to 32-fold were obtained. Additionally to higher productivities, relevant phenotypes – such as reduced toxic by-product secretion, serum independence and increased apoptosis resistance – are being studied.

Omics profiling in echinoderms tissue and organ regeneration

The molecular pathways that trigger and are responsible for the amazing intrinsic regenerative ability that leads to a functional re-growth of echinoderms body-parts are still unknown. In order to approach this subject, several proteomic strategies were used to evaluate the impact of wound healing and tissue re-growth on starfish radial nerve cords, coelomocytes and coelomic fluid upon arm tip amputation. Additionally, a preliminary metabolomic study has been conducted on this fluid, also at different regeneration stages. Our results show that several functional classes of proteins known to be involved in regeneration events in other model organisms, such as chordates, were identified for the first time in echinoderm nervous system regeneration events and interestingly, some were found to be regulated at the post-translational level through proteolytic, phosphorylation or glycosylation pathways. Also, several proteins with no previous association with regeneration events were identified and are considered as interesting molecules for future studies. At the metabolome level, asterosaponins, bioactive secondary metabolites with known immunological, physiological and pharmacological activities, seem to be also promising actors in regeneration. Performance of future studies urge to clarify the importance of the detected molecular profile changes on regeneration and to depict the associated molecular and cellular mechanisms.

Mass Spectrometry

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Biomolecular Diagnostics

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The development of microfabricated structures in polymeric supports allows the miniaturization of channels and reservoir arrangements in micrometer scale, suitable for biological studies of cells. We have been working in the development of microfluidic channels layouts in polydimethylsiloxane (PDMS) blocks for use in cell handling and characterization, namely by the design and construction of an hybrid chip with electrodes and fiber optic next to the flowing channel, which allows an optical and impedimetric interrogation of the passing through cells (e.g. ovine erythrocytes). In a further step we have developed (in collaboration with the CENIMAT/UNL) sealed PDMS structures on glass, that can be used for trapping individual cells in small structures, towards single cell analysis. The different shape and size chips are mounted on top of a inverted microscope and manipulated by pressure, allowing the entrapment of small cells (erythrocytes) or larger cells (Medicago spp in vitro cultured cells) that will be studied in real time assays by challenging with different biomolecules (e.g. antibodies, receptors, ssDNA) conjugated with quantum dots.
Microbiology of Man-made Environments

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Description of Patulibacter medicamentivorans sp. nov.

A Gram-positive, aerobic, non-motile, catalase positive, oxidase negative, non-motile, non-sporulating rods (0.3-0.4x1.0-1.1 μm) with ibuprofen degrading capacity, designated I11T, was isolated from activated sludge from a wastewater treatment plant. Optimum temperature and pH for growth are 32 °C and 6-7.5, respectively. Growth is not observed in media containing more than 1.5 % (w/v) NaCl. The major respiratory quinone was identified, as well the predominant fatty acid and polar lipid, the cell wall contained meso-diaminopimelic acid as the diagnostic diamino acid and the G+C content of the genomic DNA was 74.1 mol%. On the basis of 16S rRNA gene sequence analysis, the closest phylogenetic neighbours of strain I11T were Patulibacter ginsengiterrae, Patulibacter minatonensis, and Patulibacter americanus. The phenotypic characterisation support the inclusion of strain I11T within the genus Patulibacter. However, distinctive features and the 16S rRNA gene sequence analysis suggested the proposal of a new species. Therefore, the name Patulibacter medicamentivorans (me.di.ca.men.ti.vo’rans N.L. n. medicamentus pharmaceutical drug; L. part. adj. vorans devouring, N.L. adj. medicamentivorans eater of pharmaceutical drug) was proposed, and the type strain is I11T.

Nutraceuticals and Delivery

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The project BioNIO “Bioactive Natural Ingredients from Opuntia spp.. Valorisation of plants from Alentejo” (2010-2013), has contributed to expand scientific knowledge and technological solutions pivotal for the development of functional products from Opuntia species. Extracts were obtained with high-yield, using biocompatible procedures; positive bioactivities with relevance for the nutraceuticals, nutricosmetics and cosmeceuticals industries were identified and correlated with metabolites; and conditions to deliver products/formulations with high bioavailability and stability were found. As an example, Opuntia ficus-indica and Opuntia robusta residues from fruit juice production were explored as potential sources of natural chemotherapeutic ingredients towards colon cancer. Hydroalcoholic extraction and adsorption separation processes were used to produce a natural extract that efficiently inhibited cancer cell growth, evaluated in human colon carcinoma HT29 cell line, inducing cell cycle arrest in different checkpoints—G1, G2/M and S. The phytochemical constituents presented in the samples, namely betacyanins, flavonoids (isorhamnetin derivatives) and phenolic acids (ferulic acid) were identified as the main responsible compounds for the cell cycle arrest. Moreover, the extracts that presented the lowest effective dose values in terms of polyphenols showed to increase intracellular ROS accumulation in HT29 cells, suggesting that cancer cell death may be induced by the pro-oxidant effect of these compounds.

Pharmacokinetics and Biopharmaceutical Analysis

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The development of drugs for neurological and oncological brain diseases is strongly limited by difficulties in brain delivery through the Blood Brain Barrier (BBB). The Receptor for Advanced Glycan End-products (RAGE) is overexpressed in biological membranes in diseases such as Alzheimer’s and diabetes, making it a perfect target for transcytosis of drugs in these illnesses.

In our laboratory, we addressed the question of brain permeation of strongly hydrophilic disease modifying peptidomimetic drugs for Alzheimer’s disease, through a strategy based on RAGE receptor mediated transcytosis [1]. The strategy involves the covalent linkage of a small RAGE ligand based on abeta peptide, to the therapeutic agent, a β-Secretase 1 inhibitor. The compound was confirmed to permeate the BBB while maintaining the ability to inhibit of β-Secretase 1 selectively in relation to of β-Secretase 2.

Vila Real H, Simplicio AL et. al., Prov. patent applic. ner 20141000003073 (Portugal). BBB permeable peptidomimetic Beta-secretase 1 inhibitor for the treatment of Alzheimer’s disease

Systems Biodynamics

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The core mission of the Systems Biodynamics (SBD) Group is the creation of systems-level knowledge in environmental life sciences and biotechnology through application of computational and mathematical tools for the simulation of dynamical processes, and for data management and analysis.

In 2013 we provided support in the fields of biostatistics and bioinformatics to various experimental groups at ITQB, IBET, IICT and the Alentejo Biotechnology Center (CEBAL) in Beja. Following a former project on the CorkOak bioinformatics platform CorkOakDB, a focus has been established on analyzing plant gene transcripts in different stages of development and in response to different stress conditions.

For this purpose, bioinformatics workflows - so called pipelines - were deployed in order to detect characteristic patterns in plant gene expression revealing the molecular keys to the response to stresses such as drought, heat or high salinity. Each pipeline was tailor-made for the corresponding project, but as common elements comprised a stage of data management and preprocessing, sequence alignment to already known genomes, and the statistical analysis of the resulting patterns of sequence abundances. These quantitative tools provide the fundament for the thorough biological interpretation of the experiments, leading to new knowledge to be published in the near future.
ITQB Researchers as members of meeting organizing committees

COST Action CM1205 CARISMA
February, Lisbon, Portugal
Beatriz Royo, Member of the Management Committee

COIL 5 - 5th Congress on Ionic Liquids
April 21-25, Vilamoura, Portugal, 2013
Luís Paulo N. Rebelo (chair), José N. Canongia Lopes (co-chair), José M. S.S. Esperança, Isabel M. Marrucho, Cristina Silva Pereira
Executive Committee

IMIL3 - 3rd Iberian Meeting on Ionic Liquids
held as a pre-symposium of COIL-5
Vilamoura, Portugal, 2013
José M. S. S. Esperança, Isabel M. Marrucho (chairs)

Young Scientist Forum
July 6, St. Petersburg, Russia
Claudina Rodrigues-Pousada, Organizer

9th European Biophysics Congress, EBSA 2013
July 13-17, Lisbon, Portugal
Manuela M. Pereira, co-chair
Carlos Frazão, Claudio M. Soares, Ligia Q. Martins, Members of the Organizing Committee

13th Congresso Luso-Espanhol de Fisiologia Vegetal
July 23-27, Lisbon, Portugal
Margarida M. Oliveira, Nelson Saibo and Miguel Costa, Members of the Organizing Committee

3to4 Summer School on Bioinformatics
Nebion workshop in the frame of the 3to4 project
August 27-30, Zurich, Switzerland
Carla Pinheiro Member of the Organizing Committee

COST summer school chemistry of metals in biological systems
September 7-14, Louvain la Neuve, Belgium
Ricardo Louro, Member of the Organizing Committee

Transbio Emergence Forum
September 25-27, Montpelier, France
Ricardo Louro, Member of the Organizing Committee

Concessus/Licor Workshop
practical course/meeting
Miguel Costa, Member of the Organizing Committee

COST Action BM1005 European Network on Gasotransmitters 3rd Workshop
October 24-25, Lisbon, Portugal
Carlos Romão, Member of Organizing Committee

II Colóquio Nacional de Sementes e Viveiros
November 8, APH, Coimbra, Portugal
Miguel Costa, Member of the Organizing Committee

Mini-Symposium
September 26-28, ITQB, Oeiras, Portugal
“Bacterial Cell Surfaces”
M. Gomes de Pinho, A. O. Henriques, co-organizers
“Bacterial growth, antibiotic resistance and dormancy”
Mariana G. Pinho, Adriano O. Henriques, co-organizers
“Analysis of Staphylococcus epidermidis population structure by whole genome sequencing”
Maria Miragaia and Herminia de Lencastre, co-organizers

Course Structure and Function of Membrane Proteins
November 5-8, ITQB, Oeiras, Portugal
Margarida Archer, Carlos Cordeiro, José A. Brito and Ricardo Gomes

Transbio Workshop | Metabolomics and Molecular Interactions for Biology and Health
November 13-15, ITQB, Oeiras, Portugal
Pedro Lamosa, Ricardo Louro, Ana Coelho, Isabel Bento e Margarida Nunes
ITQB Researchers as members of scientific committees

Meeting Scientific Committees

Catarina Duarte
FOOD I&DT - Alimentaria & Horexpo Lisboa 2013, Abril, Lisboa
Member of Scientific Committee

Claudina R. Pousada
38th FEBS Congress, St. Petersburg, Russia Federation
Member of the Scientific Committee

Carlota Vaz Patto

Helena Santos
MicroBiotec’13 - Portuguese Congress in Microbiology and Biotechnology, Aveiro, Portugal. December 6 - 8, 2013.
Member of the Scientific Committee

Herminia de Lencastre
23th European Congress on Clinical Microbiology and Infectious Disease (ECCMID), Berlin, Germany April 27 - 30, 2013. “Streptococcus pneumoniae: evolution, host immunity, prevention and treatment” Chair Oral Session “Is pneumococcal vaccine shifting the serotype distribution?”
Chair Symposium
Member of the Scientific Committee.
MicroBiotec’13 - Portuguese Congress in Microbiology and Biotechnology, Aveiro, Portugal. December 6 - 8, 2013.
Member of the Scientific Committee.

Isabel Bento
BioStruct-X 2nd Annual Meeting, 5 – 6 September 2013, Hamburg, Germany

Luis Paulo N. Rebolo
COIL 5 - 5th Congress on Ionic Liquids
Member of the Scientific Committee

Manuela Chaves
INTERDROUGHT IV, September 2013, Brisbane, Australia.
Member of the Scientific Committee

Manuela Pereira
9th European Biophysics Congress, EBSA2013, Lisbon, Portugal,
Member of the Scientific Committee
VIII IberoAmerican Congress of Biophysics, Valparaiso, Chile,
Member of the Scientific Committee

Manuel J. T. Carrondo
Scale-Up and Manufacturing of Cell-Based Therapies I, January 2013, San Diego, California, USA.
Member of the Scientific Committee

Margarida Oliveira
Member of the Scientific Committee

8th International Symposium on In Vitro Culture and Horticultural Breeding, Coimbra, June 2-7.
Member of the Scientific Committee

Maria Arménia Carrondo
Member of the Science Advisory Committee
SAC ESRF, November 7-8, 2013, Grenoble, France.
Member of the Science Advisory Committee
INSTRUCT Biennial Structural Biology Meeting, 22-24 May 2013, EMBL-Heidelberg, Germany.
Member of the Executive Committee

Nelson Saibo
Member of the Scientific Committee

Paula M. Alves
Scale-Up and Manufacturing of Cell-Based Therapies I, January 2013, San Diego, California, USA.
Member of the Scientific Committee
European Society of Animal Cell Technology, June 2013, Lille, France.
Member of the Scientific Committee
Other scientific committees

Ana Matias
COST Action TD1203, Food Waste Valorisation for Sustainable Chemicals, Materials and Fuels (EUBiS)
Portuguese member of the Managing Committee

Ana V. Coelho
Member of the Management Committee (since 2011)

António M. Baptista
COST Action CM1102, "Multivalent Glycosystems for Nanoscience - MultiGlycoNano"
Portuguese member of the Managing Committee

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Portuguese Centre for Integrated Structural Biology (PCISBIO), an Affliate Centre of Instruct, the European integrated infrastructure for Structural Biology.
Member of the Scientific committee

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Chair of the Portuguese Biophysical Society

Margarida Oliveira
Chair of the Portuguese Society of Plant Physiology

Raquel Sá-Leão
ESGEM (ESCMID Study Group on Epidemiological Markers) for 2011-2013 from the European Society of Clinical Microbiology and Infectious Diseases, Elected member of the Executive Committee

Ricardo Louro
COST action CM 1003 Biological oxidation reduction reactions
Member of the Management Committee

Rita Abranches
COST Action FA0804 (2008-2013) "Molecular farming: plants as a production platform for high value proteins".
National delegate and Management Committee Member

Rita Ventura
COST Action CM0905 (2010-2014) Organocatalysis (ORCA),
Member of the Management Committee

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Raquel Sá-Leão; Member of the Editorial Board

Microbial Cell
Cláudia R. Pousada, Editorial Advisor

Microbial Drug Resistance and European Journal of Clinical Microbiology & Infectious Diseases
Herminia de Lencastre, Member of Editorial Board

Microbiologia
journal of the Portuguese Society of Microbiology
Sérgio Filipe Member of Editorial Board

MicrobiologyOpen
Ligia O. Martins, Member of the Editorial Board

PeerJ
Maria Miragaia, Member of Editorial Board
Manuela Chaves, Member of Editorial Board (since 2012)

Plant Cell Tissue and Organ Culture
Journal of Plant Biotechnology", Springer Associate
Margarida Oliveira, editor

PLoS ONE
Cláudio Gomes, Member of Editorial Board
Herminia de Lencastre, Member of Editorial Board
Cláudio M. Soares, Member of Editorial Board
Inês Cardoso Pereira, Member of Editorial Board
Ligia O. Martins, Member of Editorial Board
Ligia M. Saraiva, Member of Editorial Board

Scientific Reports
Cláudio Gomes, Member of Editorial Board
Cláudio M. Soares, Member of Editorial Board

Oxidative Medicine and Cellular Longevity
Special issue “Neurodegeneration, Neurogenesis, and Oxidative Stress”
Cláudio Gomes, Guest Editor

The Open Micology Journal
Cláudia R. Pousada, Member of Editorial Board

The Scientific World Journal
Ana Sofia Coroadinha, Member of Editorial Board – Biotechnology Panel

Tree Physiology Journal
Célia Miguel Member of the Editorial Review Board

WIREs RNA Journal (Wiley Interdisciplinary Reviews)
Cecília Arraiano, Member of Editorial Board

Yeast Journal
Cláudia R. Pousada, Member of Editorial Board
Research Output

Project Coordination, Publications (WoS) and PhD Theses by Group

please refer to full list of publications (p. 55), full list of PhD Theses (p. 68), and projects (p. 49) / (projects submitted via IBET - p. 53)

Chemistry

Bioorganic Chemistry
Head: Rita Ventura
Project Refs: 25; 96
Publication Refs: 127; 135; 161
PhD Theses Refs: 36

Coordination and Supramolecular Chemistry
Head: Rita Delgado
Project Refs: 85
Publication Refs: 75; 76; 96; 97; 147; 213

Homogeneous Catalysis
Head: Beatriz Royo
Project Refs: 17; 70
Publication Refs: 47; 134; 275
Book Chapter 9

Microheterogeneous Systems
Head: Eurico Melo
Project Refs: 37

Molecular Thermodynamics
Head: Luis Paulo N. Rebele
Project Refs: 7; 29; 45; 54; 57; 58; 79; 87; 93
Publication Refs: 11; 15; 16; 53; 57; 88; 92; 109; 121; 131; 144; 145; 165; 177; 190; 197; 182; 183; 207; 208; 233;
245; 246; 247; 248; 249; 258; 259; 260; 261
PhD Theses Refs: 6; 34; 37

Organic Synthesis
Head: Christopher Maycock
Publication Refs: 22; 58; 70; 127; 161; 222

Organometallic Chemistry
Head: Carlos C. Romão
Project Refs: 60
Publication Refs: 106; 228; 229
Book Chapter 8

Collaborators
James Yates
Publication Refs: 34; 35

Others
Olga Iranzo
Project Refs: 18; 84; 94
Publication Refs: 93; 96; 97
António Lopes
Publication Refs: 9
Yann Astier
Project Refs: 107
Publication Refs: 38
Mª José Calhorda
Publication Refs: 133

Biological Chemistry

Bacterial Energy Metabolism
Head: Inês A. Cardoso Pereira
Project Refs: 71
Publication Refs: 61; 111; 114; 115; 142; 146; 155; 240; 267; 273; other articles 7
PhD Theses Refs: 5

Biological Energy Transduction
Metalloproteins and Bioenergetics Unit
Head: Manuela M. Pereira
Project Refs: 11; 55; 81
Publication Refs: 25; 143; 203

Biomolecular NMR Laboratory
Head: Manolis Matzapetakis
Project Refs: 59
Publication Refs: 13; 163; 199; 244

Genomics and Stress
Head: Claudina R. Pousada
Publication Refs: 13; 26; 28; 103; 155; 204; 264
PhD Theses Refs: 5

Industry and Medicine Applied Crystallography
Macromolecular Crystallography Unit
Head: Pedro Matias
Project Refs: 72; 25; 26; 27
Publication Refs: 142; 164; 215

Inorganic Biochemistry and NMR
Head: Ricardo O. Louro
Project Refs: 12; 46; 48
Publication Refs: 23; 94; 105; other articles 10;
Book edited 2; Book Chapters 5, 6
PhD Theses Refs: 2

Membrane Protein Crystallography
Macromolecular Crystallography Unit
Head: Margarida Archer
Project Refs: 53
Publication Refs: 138; 234
PhD Theses Refs: 11

Metalloenzymes and Molecular Bioenergetics
Metalloproteins and Bioenergetics Unit
Head: Miguel Teixeira
Project Refs: 11; 32; 33; 36
Publication Refs: 241; 242; 243
PhD Theses Refs: 7; 9

Microbial and Enzyme Technology
Head: Ligia O. Martins
Publication Refs: 108; 128; 232; 239

Molecular Genetics of Microbial Resistance
Head: Ligia M. Saraiva
Annual Report 2013
Research Output

Molecular Interactions and NMR
Head: Patrick Groves
Project Refs: 28; 44
Publication Refs: 112
Book Chapter: 7

Molecular Simulation
Head: António M. Baptista
Project Refs: 78
Publication Refs: 39; 62; 91; 137
PhD Theses Refs: 4

Protein Biochemistry Folding and Stability
Head: Cláudio M. Gomes
Project Refs: 50; 51; 65
Publication Refs: 42; 58; 80; 107; 129; other articles 11
Book Chapter 1
PhD Theses Refs: 12

Protein Modelling Laboratory
Head: Cláudio M. Soares
Project Refs: 23; 26
Publication Refs: 62; 94; 115; 137; 274
PhD Theses Refs: 4

Raman spectroscopy of Metalloproteins
Head: Smilja Todorovic
Publication Refs: 168; 232

Structural Biology
Macromolecular Crystallography Unit
Head: Carlos Frazão
Project Refs: 34
Publication Refs: 19; 20

Structural Genomics
Macromolecular Crystallography Unit
Head: Maria Arménia Carrondo
Project Refs: 4; 10; 22; 36; 39
Publication Refs: 36; 51; 67; 70; 108; other articles 8
PhD Theses Refs: 3

PhD Theses Refs: 13; 73
Publication Refs: 90; 162; 251; 267
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Molecular Interactions and NMR
Head: Patrick Groves
Project Refs: 28; 44
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Molecular Simulation
Head: António M. Baptista
Project Refs: 78
Publication Refs: 39; 62; 91; 137
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Head: Smilja Todorovic
Publication Refs: 168; 232

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Head: Carlos Frazão
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Structural Genomics
Macromolecular Crystallography Unit
Head: Maria Arménia Carrondo
Project Refs: 4; 10; 22; 36; 39
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PhD Theses Refs: 3

Collaborators
Filipe Tiago de Oliveira
Project Refs: 14

Biology

Bacterial Cell Biology
Head: Mariana G. Pinho
Project Refs: 8; 68
Publication Refs: 52; 77; 87; 141; 175; 187; 212; other articles 9
PhD Theses Refs: 28

Bacterial Cell Surfaces and Pathogenesis
Head: Sérgio R. Filipe
Project Refs: 20; 21; 89; 100
Publication Refs: 119; 257

Bacterial Signalling
Head: Karina Xavier
Publication Refs: 31; 176

Cell Physiology & NMR
Head: Helena Santos
Project Refs: 27; 69; 77; 83; 98
Publication Refs: 40; 46; 59; 60; 75; 76; 78; 95; 97; 104; 127; 161; 164; 194; 195; 221; 262
Book Chapter 4
PhD Theses Refs: 10; 36

Cell Signaling in Drosophila
Head: Pedro Domingos
Project Refs: 9; 75
Publication Refs: 49

Control of Gene Expression Laboratory
Head: Cecília M. Arraiano
Project Refs: 3; 40; 90; (17)
Publication Refs: 13; 14; 18; 20; 21; 27; 66; 71; 117; 124; 140; 205; 206; 216; 236; 271
PhD Theses Refs: 14

Glycobiology
Head: Júlia Costa
Project Refs: 42
Publication Refs: 73
Book Chapter: 3

Microbial Development
Head: Adriano O. Henriques
Project Refs: 102
Publication Refs: 1; 122; 177; 227; other articles 12
PhD Theses Refs: 17; 24; 27

Molecular Genetics
Microbiology of Human Pathogens Unit
Head: Hermínia de Lencastre
Project Refs: 47; 63; 88
Publication Refs: 10; 24; 45; 50; 74; 79; 101; 120; 125; 214; 250; 263; 277;
other articles 4; 5

Molecular Microbiology of Human Pathogens
Microbiology of Human Pathogens Unit
Head: Raquel Sa-Leão
Project Refs: 103; 104; 105; 106
Publication Refs: 10; 81; 101; 184; 192; 214; 217; 226; 263; 269

Others
Ana Rute Neves
Project Refs: 24
Publication Refs: 43; 44; 110; 268

Jaime Mota
Project Refs: 41; 43; 86
Publication Refs: 172

Ana Rute Neves
Project Refs: 24
Publication Refs: 43; 44; 110; 268

Jaime Mota
Project Refs: 41; 43; 86
Publication Refs: 172
Plant Sciences

Disease and Stress Biology
Head: Ricardo Ferreira
Project Refs: 18; (4, 5)
Publication Refs: 29; 32; 185; 186; 223; 252; 253; 254; other articles 3; 6

Forest Biotechnology
Head: Célia Miguel
Project Refs: (3, 18, 19)
Publication Refs: 68; 69; 152; 153; other articles 3
PhD Theses Refs: 13

Genomics of Plant Stress Lab (GPlantS Lab)
Head: Margarida Oliveira
Project Refs: 19; 52; 74; 97; (6)
Publication Refs: 3; 136; 151; 158; 191; 225; 231; other articles 1; 11

Plant Biochemistry
Head: Cândido Pinto Ricardo
Project Refs: 30; 91
Publication Refs: 186

Plant Cell Biology
Head: Rita Abranches
Project Refs: 38; 66; 83

Plant Cell Biotechnology
Head: Pedro Fevereiro
Project Refs: 1; 31; 61; 92; (16, 22)
Publication Refs: 12; 17; 33; 85; 86; 100; 132; 165; 173; 222; 276; other articles 13
Book chapter: 2; 13

Plant Molecular Ecophysiology Laboratory (LEM)
Head: Manuela Chaves
Project Refs: 5; 6; 15
Publication Refs: 54; 64; 65, 99; 190; 204; 225; 237

Collaborators
Jorge Almeida
Publication Refs: 197

Technology

Applied and Environmental Mycology
Head: Cristina Silva Pereira
Project Refs: 56; (20)
Publication Refs: 41; 88; 89; 102; 118; 145; 149; 272
PhD Theses Refs: 8; 8; 34; 37

Animal Cell Technology Unit
Head: Paula M. Alves
(Cell Bioprocesses + Cell Line Development and Molecular Biotechnology + Engineering Cellular Applications)
Project Refs: (8; 9; 10; 11; 12; 13; 21; 22; 28; 30; 31; 32; 33; 34; 35; 36; 37; 38)
Publication Refs: 37; 48; 82; 83; 84; 95; 126; 210; 252; 270; other articles 2; 14
Book chapters 10; 11; 12

Biomolecular diagnostic
Head: Abel Gonzalez Oliva
Project Refs: 76; 95; (2)
Publication Refs: 116; 222
PhD Theses Refs: 33

Mass Spectrometry
Head: Ana V. Coelho
Project Refs: 25; 62; 67; 80; 99; 101
Publication Refs: 33; 49; 100; 150; 171; 198; 224; other articles 13;
Book Chapters: 4; Book edited: 1

Microbiology of Man-made Environments
Head: Teresa Crespo
Project Refs: (1, 15)
Publication Refs: 4; 6; 7; 8; 168; 179; 180; 218; 219; 220; 266
PhD Theses Refs: 16; 35; 38

Nutraceuticals and Delivery
Head: Catarina Duarte
Project Refs: (7, 23, 24)
Publication Refs: 72; 98; 113; 154; 181; 211; 230; 265; 266

Pharmacokinetics and Biopharmaceutical Analysis
Head: Ana Luisa Simplicio
Project Refs: (14)
Publication Refs: 5; 98; 126; book chapter 11

Systems Biodynamics
Head: Andreas Bohn
Project Refs: 64

Collaborators
Maria de Fatima Silva Lopes
Publication Refs: 2; 30; 148; 200; 201; 256
PhD Theses Refs: 30
Maria Rosário Bronze - Analytical Chemistry
Publication Refs: 193; 209

Others
Cidalia Peres
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Jonas Almeida
Publication Refs: 167
Francisco Malcata
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<td>3 Standarization and orthogonalization of teh gene expression flow</td>
<td>FP7-KBBE-289326</td>
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<td>7 Innovative ionic polymers from natural sources for energy &amp;</td>
<td>PIRSES-GA-2012-318873</td>
<td>Isabel M. Marrucho</td>
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<td>8 Finding new mechanisms for protein localization in Bacteria</td>
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<td>9 ER Stress and Photoreceptor Degeneration in Drosophila (DROSOERSTRESS)</td>
<td>PIRG03-GA-2008-230935</td>
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<td>10 The role of Base Excision Repair (BER) for extreme radiation and</td>
<td>PIEF-GA-2011-301202</td>
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<td>11 Ion Transport at atomic level (Itrans)</td>
<td>PCIG11-GA-2012-322346</td>
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<td>12 Biocluster Transnational de l'Espace Sud-Ouest Européen (TRANSBIO</td>
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<td>13 Unraveling the mechanisms of nitrosative stress resistance of</td>
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<td>Marta Justino</td>
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<td>Helicobacter pylori: relevance for immune subversion and</td>
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<td>14 Mössbauer spectroscopy and density functional theory studies of</td>
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<td>Filipe Oliveira</td>
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<td>NO and O2 reductases</td>
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<td>15 Phenotypic plasticity of maritime pine to climate change</td>
<td>PTDC/AGR-CFL/099614/2008</td>
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<td>16 Engineered biomimetics for large-scale enrichment of</td>
<td>PTDC/EBB-BIO/102163/2008</td>
<td>Olga Iranzo</td>
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<td>17 Sustainable catalysis based on N-heterocyclic carbene metal</td>
<td>PTDC/QUI-JUI/110349/2009</td>
<td>Beatriz Royo</td>
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<td>18 Polyphenols as protective agents in cellular models of alpha-</td>
<td>PTDC/BIA-BCM/111617/2009</td>
<td>Ricardo B. Ferreira</td>
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<td>synucleinopathies, in particular Parkinson's diseases.</td>
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<td>19 Effect of environmental stresses on rice epigenome.</td>
<td>PTDC/BIA-BCM/111645/2009</td>
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<td>20 Small immunoactive peptidoglycan (siPGN) derivates to modulate an</td>
<td>PTDC/SAU-IMU/11806/2009</td>
<td>Sérgio Filipe</td>
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<td>21 Synthesis of peptidoglycan in Streptococcus pneumoniae - where and</td>
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<td>why is it necessary to branch?</td>
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<td>22 GRIM-19, a novel protein involved in cell apoptosis: struture-</td>
<td>PTDC/BIA-PRO/113064/2009</td>
<td>Isabel Bento</td>
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<td>23 Proton transfer and proton pumping in haem-copper oxides. Methodological developments and their application to unravel the molecular mechanism.</td>
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<td>PTDC/QUI-BIQ/113446/2009 Cláudio Soares</td>
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<td>24 PhytoLac- Engineered Lactococcus lactics for the optimizes production of nutraceutical plant-derived polyphenols</td>
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<td>PTDC/EBB-EBI/113727/2009 Ana Rute Neves</td>
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<td>25 Studies on the structure/activity relationship of Al-2, a bacterial signalling molecule for inter-species communication.</td>
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<td>PTDC/QUI-BIQ/113880/2009 Rita Ventura</td>
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<td>26 Membrane fusion mechanism of Influenza Hemagglutinin: a simulation and biophysical approach.</td>
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<td>PTDC/QUI-BIQ/114774/2009 Cláudio Soares</td>
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<td>27 Solution structure and mode of action of the dimeric bacteriocin Lon972</td>
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<td>PTDC/QUI-BIQ/114904/2009 David Turner</td>
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<td>28 Identification of plants extracts with protective action against bacterial enterotoxins belonging to ABS group: cholera toxin, heat labile toxin from Escherichia coli and Shiga toxin (dysentery).</td>
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<td>PTDC/QUI-BIQ/115298/2009 Malgorzata Palczewsk</td>
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<td>29 Playing with the ionic character of ionic liquids</td>
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<td>PTDC/QUI-BIQ/116015/2009 Luís Paulo N. Rebelo</td>
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<td>30 Search for candidate protein biomarkers of Coffea arabica resistance to Hemileia vastatrix (leaf rust)</td>
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<td>PTDC/AIR-GPL/109990/2009 Cândido Pinto Ricardo</td>
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<td>31 Deciphering grain filling mechanisms in Phaseolus vulgaris L. under water deficit.</td>
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<td>PTDC/AIR-GPL/110244/2009 Pedro Fevereiro</td>
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<td>32 Detoxification of nitric oxide and/or oxygen in pathogenic (anaerobic) microbes: exploring the molecular determinants of substrate selectivity</td>
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<td>PTDC/QUI-BIQ/111080/2009 Miguel Teixeira</td>
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<td>33 Response to oxidative and nitrosative stress by Entamoeba histolytica: searching for new virulence factors.</td>
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<td>PTDC/SAU-MIC/111447/2009 Miguel Teixeira</td>
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<td>34 hCE- expression and characterization in in vitro and in silico models.</td>
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<td>PTDC/EBB-BIO/111530/2009 Carlos Frazão</td>
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<td>35 Hepatic toxicity in HIV-infected individuals exposed to nevirapine.</td>
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<td>PTDC/SAU-TOX/111663/2009 Ana Coelho</td>
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<td>36 Structural determinants of superoxide reduction- A detoxification system essential for life.</td>
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<td>PTDC/BIA-MIC/111940/2010 Célia Romao</td>
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<td>37 On characterization polarity within phospholipid/cholesterol lipid bilayers and its effects in membrane enzymology.</td>
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<td>PTDC/QUI-BIQ/112943/2009 Eurico de Melo</td>
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<td>38 The pathogen’s perspective of molecular plant-microbe-interactions: genes expressed during the infection process of coffee leaf rust- Hemileia vastarix.</td>
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<td>PTDC/AGR-GPL/114949/2010 Rita Abranches</td>
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<td>39 Patogenia da protína LANA do herpesvírus do sarcoma de Kaposi</td>
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<td>40 Global analysis of antisense regulatory mechanisms in Staphylococcus aureus: ARMS</td>
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<td>ERA-PTG/0002/2010 Susana Domingues</td>
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<td>41 Characterisation of host cell pathways altered by effectors of Brucella, Chlamydia, and Coxiella: identification of novel therapeutic targets”</td>
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**Project funded by Ministry of National Defence**

107 Chemical and Biological Single Molecule Detection Roaming Robot (SENTINEL) | Yann Astier |

**Projects funded by Ciência Viva (outreach)**

108 Da escola à Universidade | PEC245 | Ana Sanchez |
| 109 Hoje, um Cientista vem à nossa escola | PEC243 | Ana Sanchez |

**Projects involving ITQB researchers where IBET is the host institution**

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<td>36 Estratégias integradas para descifrar o receptoma de células estaminais cardíacas humanas e o seu papel no processo de regeneração cardíaca</td>
<td>PTDC/BBB-BIO/1414/2012</td>
<td>Patricia Alves</td>
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<td>37 A arquitetura da vida: a estrutura quartenária de cápsulas virais por espectrometria de massa nativa</td>
<td>REC/BBB-BEP/0104/2012</td>
<td>Patricia Alves</td>
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<td>38 Integração de tecnologias de sirma e AAV no desenvolvimento de terapias dirigidas a cancro da mama basal: do desenvolvimento de vetores a avaliação anti-tumoral</td>
<td>PTDC/BBB-BIO/1240/2012</td>
<td>Paula Alves</td>
</tr>
</tbody>
</table>

Additionally, a number of projects with national and international companies involving ITQB researchers were established by IBET. These are not listed here.
Publications 2013

Articles indexed in Web of Science


Ribeiro, B. D., Coelho, M. A. Z., Rebelo, L. P. N., & Marrucho, I. M. (2013). Ionic Liquids as Additives for Extraction of Saponins and Polyphenols from Mate (Ilex paraguariensis) and Tea (Camellia sinensis). Industrial & Engineering Chemistry Research, 52(34), 12148-12153. doi:10.1021/ie400529h


Research Output


**Book Chapters**


**Books (edited)**


Education Output

PhD Theses

Bioquímica

1. Ana Filipa Nogueira Tavares
   “Novel insights into the action of antimicrobial agents against human pathogens”
   Supervisor: Lígia Saraiva

2. Bruno Miguel Oliveira Maia da Fonseca
   “Mind the gap: characterization of periplasmic cytochromes from Shewanella oneidensis involved in extracellular electron transfer”
   Supervisor: Ricardo Louro

3. Catarina Isabel Simões Pires da Silva
   “Structure-function analysis of Multicopper oxidases”
   Supervisor: Isabel Maria Bento; Mª Arménia Carrondo

4. Diana Andreia Pereira Louisa
   “Molecular determinants of nonaqueous biocatalysis: A computational analysis”
   Supervisor: Cláudio Soares; António Baptista

5. Fábio de Oliveira Morais e Silva
   “Deciphering the genome of Desulfovibrio gigas: the role of the hydrogenases”
   Supervisor: Claudia Rodrigues-Pousada; Inês Cardoso Pereira

6. Isabel Tavares Lima Martins
   “On the way towards the understanding of suberin degradation by Aspergillus nidulans”
   Supervisor: Cristina Silva Pereira; Luis Paulo N. Rebelo

7. Mafalda Cristina de Oliveira Figueiredo
   “Desulfovibrio vulgaris defenses against oxidative and nitrosative stresses”
   Supervisor: Lígia Saraiva; Miguel Teixeira Pereira

8. Mariana Boavida Lopes Carvalho
   “The biotransformation of pentachlorophenol by Mucor plumbeus: Mechanistic insights”
   Supervisor: Cristina S. Pereira/Andrew Hursthouse

9. Pedro Miguel Ferreira Assis de Sousa
   “Supercomplexes of Prokaryotic Aerobic Respiratory Chains – Escherichia coli and Bacillus subtilis supramolecular assemblies”
   Supervisor: Ana Margarida Melo; Miguel Teixeira Pereira

10. Pedro Oliveira Quintas
    “Electron Transfer and Ligand Binding Properties of Cytochromes”
    Supervisor: David L. Turner; Teresa M. Catarino

11. Przemysław Michal Nogły
    “Crystallographic studies on membrane and cytoplasmic enzymes: Bifunctional cytidylytransferase /CDP-alcohol phosphatidyltransferase and α-phosphoglucomutase”
    Supervisor: Margarida Archer

12. Vesna Prosinecki
    “Protein stability in a proteomic perspective”
    Supervisor: Cláudio Gomes

Biologia

13. Ana Filipa Gonçalves Milhinhos
    “Novel insights into plant vascular development: disclosing a mechanism to maintain thermospermine homeostasis in the xylem”
    Supervisor: Célia Miguel

14. Ana Margarida Teixeira Saramago
    “The relevance of Ribonuclease III in several pathogenic bacteria”
    Supervisor: Cecília Araíal; Susana Domingues

15. Arnon Dias Jurberg
    “Extension and patterning of the vertebrate body: roles of Gdf11 and Wnt3a signaling in the axial progenitors”
    Supervisor: Moises Mallo

16. Bárbara Fonseca de Almeida
    “Micropollutant bioremoval in wastewater treatment systems: from microbial population structure to function”
    Supervisor: Maria Teresa Crespo; Gilda Carvalho

17. Cláudia Alexandra dos Reis Serra
    “Biology and applications of an undomesticated gut strain of Bacillus subtilis”
    Supervisor: Adriano Henriques; Ghislain Schyns

18. Cláudia Sofia dos Santos Martinho
    “Regulation of gene expression by SnRK1 kinases and miRNAs during the plant stress response”
    Supervisor: Elena Baena González

19. Elizabeth Ann Ball
    “Uncovering the role of IFNAR1 in Experimental Cerebral Malaria”
    Supervisor: Carlos Penha Gonçalves

20. Hugo Liberal Fernandes
    “Uncertainty, generalization, and neural representation of relevant variables for decision making”
    Supervisor: Zachary Mainen; Konrad Kording

21. Hugo Ricardo Noronha de Almeida
    “Measuring chromosome-end fusions in fission yeast”
    Supervisor: Miguel Godinho Ferreira

22. Iris Margarida Donga Vilares
    “Uncertainty and decision-making in the human brain”
    Supervisor: Rui Costa; Konrad Kording

23. José Joaquim Fonseca Ribas Fernandes
    “Hierarchical Reinforcement Learning in Behavior and the Brain”
    Supervisor: Joseph J. Paton; Matthew Botvinick

24. Maria Luisa Gouveia e Freitas Cárte
    “Dissecting the function of the SpoIIIJ and YqjG membrane protein insertases during bacterial spore development”
    Supervisor: Adriano Henriques

25. Mariluz Gómez Rodríguez
    “Inheritance of histone H3 variants across mitotic cell divisions”
    Supervisor: Lars E. T. Jansen

26. Miłąś Miskińyte
    “Role of biotic interactions in generating and maintaining biodiversity”
    Supervisor: Isabel Gordo

27. Patricia Irene da Silva Inácio
    “The Liver Endoplasmic Reticulum in Malaria liver infection – a functional study of the Unfolded Protein Response”
    Supervisor: Maria Manuel Mota; Adriano Henriques

28. Pedro Matos Pereira
    “Peptidoglycan assembly machines: The Staphylococcus aureus Penicillin-Binding Proteins”
    Supervisor: Mariana Gomes Pinho
<table>
<thead>
<tr>
<th>Number</th>
<th>Name</th>
<th>Title</th>
<th>Supervisor(s)</th>
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<tr>
<td>29</td>
<td>Thiago dos Santos Guzella</td>
<td>“Analysis of Stochastic Fluctuations in the Dynamics of Signaling and Transcriptional Regulation”</td>
<td>Vasco Barreto, Jorge Carneiro</td>
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<td>30</td>
<td>Renata Filipa Cruz de Matos</td>
<td>“Enterococcus faecalis V583 prophages: dynamic interactions and contribution to bacterial pathogenic traits”</td>
<td>Maria de Fátima Silva Lopes; Pascale Serror</td>
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<td>31</td>
<td>Ricardo de Sousa e Paiva</td>
<td>“T cell Maturation and Regulatoty T Cell Differentiation: From the Thymus to the Periphery”</td>
<td>Jocelyne Demengeot</td>
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<td>32</td>
<td>Vivian Leite de Oliveira</td>
<td>“Impact of viral immunomodulatory proteins at the level of the cell and the whole animal”</td>
<td>Michael Parkhouse</td>
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<td>33</td>
<td>Elisa Regina Figueiras</td>
<td>“A nanopore-based stochastic detection method: Single molecule characterisation of nanoparticles using α-hemolysin”</td>
<td>Abel OlivaYann Astier</td>
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<td>34</td>
<td>Helga Margarida Correia</td>
<td>“Development of suberin films driven by an ionic liquid-based depolymerisation process”</td>
<td>Cristina Silva Pereira; Luís Paulo N. Rebelo</td>
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<td>Ferreira Garcia</td>
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<td>35</td>
<td>Ana Filipa Correia da Silva</td>
<td>“Microbiology of membrane bioreactors for wastewater treatment: a molecular approach”</td>
<td>Maria Teresa Crespo; Gilda Carvalho</td>
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<tr>
<td>36</td>
<td>Eva Correia Lourenço</td>
<td>“New enzyme stabilisers inspired by compatible solutes of hyperthermophilic microorganisms”</td>
<td>Rita Ventura; Helena Santos</td>
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<td>37</td>
<td>Rui Manuel Cordeiro Ferreira</td>
<td>“Creating greater value for biomass residues – extraction of suberin and betulin using alternative solvents”</td>
<td>Cristina Silva Pereira; Luís Paulo N. Rebelo</td>
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<tr>
<td>38</td>
<td>Sandra Marisa Lourenço Sanches</td>
<td>“Integration of membrane filtration and photolysis processes for drinking water treatment”</td>
<td>Teresa Crespo; Vanessa Pereira</td>
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**Masters in Science Communication**

Collaboration with FCSH

<table>
<thead>
<tr>
<th>Name</th>
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<tbody>
<tr>
<td>Silvio Mendes</td>
<td>“Os Sons da Ciência” (project)</td>
<td>Sílvio Mendes</td>
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<td>Carmo Nunes</td>
<td>“A Nuclipédia” (project)</td>
<td>Carmo Nunes</td>
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<tr>
<td>Fátima Guerra</td>
<td>“Conceção de um Website para Acompanhamento de um Projeto Científico em Contexto Escolar” (project)</td>
<td>Fátima Guerra</td>
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<tr>
<td>Idalina Lourenço</td>
<td>“Ferramentas para Melhorar a Relação entre um Centro de Ciência e o Público Escolar” (project)</td>
<td>Idalina Lourenço</td>
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<tr>
<td>Ana Isabel Pinheiro</td>
<td>“Desenvolvimento e Implementação de Diferentes Estratégias de Comunicação e Divulgação Científica - um projeto para a Escola de Ciências da Universidade do Minho” (project)</td>
<td>Ana Isabel Pinheiro</td>
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<td>Silvana Araújo Cunha</td>
<td>“O recurso a exposições na divulgação de astronomia: o caso Um Universo Deslumbrante” (project)</td>
<td>Silvana Araújo Cunha</td>
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<td>Adalberto Fernandes</td>
<td>“Comunicação de Ciência no Observatório Astronómico de Lisboa e no Centro de Astronomia e Astrofísica da Universidade de Lisboa” (project)</td>
<td>Adalberto Fernandes</td>
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<td>Lúcia Vinheira Alves</td>
<td>“Agência de Noticias de Ciência” (project)</td>
<td>Lúcia Vinheira Alves</td>
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**Ciências da Engenharia e Tecnologia**

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<tr>
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<td>Jana Kracmarova</td>
<td>Research Integration</td>
<td>Pedro Fevereiro; Ana Sofia Duque</td>
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<td>Sofia Baptista de Carvalho</td>
<td>Scientific Research Training A</td>
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**University Extension Courses**

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<td>Margarida Oliveira</td>
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Cristiana Magalhães Sousa  
Scientific Research Training A  
Supervisor: Tiago Bandeiras

Joana Isabel Filipe Maricato  
Scientific Research Training C  
Supervisor: Cidália Peres

Carlos Fernandez Rodríguez  
Scientific Research Training C  
Supervisor: Cláudio Soares

Ana Margarida Lameiras Nunes  
Scientific Research Training C  
Supervisor: Cláudio Gomes

Laura Calvo Barreiro  
Scientific Research Training C  
Supervisor: Ana Teixeira

Andreia Filipa Campos Tavares  
Scientific Research Training C  
Supervisor: Mariana Gomes de Pinho

Daniela Filipa Policarpo Sequeira  
Scientific Research Training D  
Supervisor: Catarina Paquete

Mafalda de Arrábida Farelo  
Scientific Research Training D  
Supervisor: Rita Abranches

André Catarino Guerra  
Scientific Research Training D  
Supervisor: Ana Varela Coelho

Olga de Jesus Alves Cortes  
Scientific Research Training D  
Supervisor: Ana B. Pereiro

João Nuno de Sousa Machado  
Scientific Research Training D  
Supervisor: Helena Santos

Raisa Costa Paes Oliveira  
Scientific Research Training D  
Supervisor: Rita Delgado
Full List of Staff
as per December 31st 2013

Director
Cláudio M. Soares

Vice-Directors
M. Margarida Oliveira

Administrator
Teresa Venda

Secretariat to the Direction
Rosina Gadit

Management Support

Administration and Finance
Head: Fernando Jorge Tavares

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Ana Cristina Afonso Silva
Mónica Adriano Vieira
Helena Cordeiro
Isabel Mestre
Nuno Lopes
Sónia Ermida

Treasury Section
Ana Freire
Anabela Bernardo Costa

Storages
Ana Isabel Santos
Bruno Gouveia
Carlos Martins
João Rodrigues
Ricardo Pinto

Human Resources
Head: Maria Cristina Pinto
Ana Luísa Cruz
Goretti Rocha
Maria Madalena Pereira

Mailing and Archives
Artur Freitas

R&D Planning and Management
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Cristina Amaral
Cristina Lopes
Cristina Oliveira
Isabel Murtta

Legal Advisor
Anabela Simões

Academics
Ana Portocarrero
Fátima Madeira

Ombudsperson
Manuela Chaves

Science Management
Alexandra Veiga

Industry Liaison Office
Francisco Pereira do Valle

Communication Office
Head: Ana M. Sanchez
Cláudia Lopes Pinheiro
Isaura Santos
Margarida M. Nunes
Luís Morgado
Scientific, Technological and Teaching Support

Scientific Services

Nuclear Magnetic Resonance CERMAX
Coordinator: Helena Santos
Manager: Pedro Miguel Lamosa
Helena Pereira Matias
João Pires

Analytical Services Unit
Coordinator: Teresa Crespo
Vice-coordinator: Rosário Bronze
Quality Assurance: Ana Luisa Simplicio
Quality Control: António Ferreira
Qualified Person: Eduardo Correia

Analytical Team
Sandra Silva
Cláudia Duarte
Cláudio Almeida
Paula Chicau
Ana Silva
Maria Conceição Almeida
Cristina Pereira
Paula Isabel Alves
Ana Fulgêncio
Susana Tenedório

Archive
Paula Neves
Isabel Ribeiro

UniMS
Joint commision
Margarida Oliveira
Paula Alves

Users direction
Ana Luísa Simplicio
Isabel Abreu
Patrícia Alves
Susana Araújo

Technicians
Elisabete Pires
Conceição Almeida
Renata Soares
Catarina Correia

Small Molecule X-Ray Crystallography
Isabel Bento

Fermentation Unit
Coordinator: Miguel S. Teixeira
João Carita

Lab Manager
Cláudia Almeida

Teaching Laboratory
Coordinator: Adriano O. Henriques
Teresa Baptista da Silva

Library
Librarian: Isabel Murta
Susana Lopes (until May 2013)

Washrooms
Coordinator: Teresa B. da Silva
Ana Cristina Barreiros
Carmen Fernandes
Helena Vilaranda
Lúcia David
Maria Alice Ferreira
Maria Eugénia Santos
Pilar Campos
Sónia Serrano
Sónia Moita

Workshop and Maintenance
Head: Henrique Campas Nunes
Alexandre Maia
Aníbal Ribeiro
António Ramalho
Miguel Rodrigues
João Carlos Zanão Simões
José Luís Liberato
Luís Gonçalves
Nuno Soares
Nuno Monteiro
Tiago Escóbar

Computer Systems Support
Coordinator: Carlos Frazão
Executive coord.: Daniel F. Branco
Carlos Manuel Cordeiro
Hugo Gonçalo Cordeiro
Hugo Luiten
José Miguel Loureiro
Maria Manuel Rato
Research Divisions

Chemistry

Bioorganic Chemistry

Rita Ventura, Investigador Auxiliar
Ana Sofia Miguel
Eva Correia Lourenço
Osvaldo Ascenso
Vanessa Miranda
Lara Fidalgo
Gustavo Fonseca
Jessica Pereira
Marlinda Fernandes

Coordination and Supramolecular Chemistry

Rita Delgado, Professor Associado com Agregação Jubilada IST
Luís M. P. Lima
Pedro Mateus
Catarina Alexandra Veríssimo Esteves
Lígia Mesquita
Rui Fernandes

Homogeneous Catalysis

Beatriz Royo Cantabrana, Investigador Auxiliar
Lorena Postigo Galindo
João M.S. Cardoso
Rita Isabel Lourenço da Silva Lopes
María Pinto
Ana Fernandes
Rui Lopes

Micro-Heterogeneous Systems

Eurico de Melo, Professor Auxiliar IST
Joana Rita Ripado Valério

Organic Synthesis

Chris Maycok, Professor Associado FCUL
Mohit Lal Deb
Saul Silva
Paula Rodrigues

Molecular Thermodynamics

Luís Paulo N. Rebelo, Professor Catedrático
Isabel M. Marrucho
José M. S. S. Esperança
Ana B. Pereira
Helena I. M. Veiga
João M. M. Araújo
Magdalena Kowacz
Mara G. Freire
Mohammad Tariq
Patricia Reis
Marjia Petkovic (cosup. Cristina S. Pereira)
Ana Lobo Ferreira
Anabela Costa
Diana Ruivo
Filipe Oliveira
Helga Garcia (cosup. Cristina Silva Pereira)
Isabel Martins (cosup. Cristina Silva Pereira)
Liliana Tomé
Mário Soromenho
Paulina Papis
Rui Ferreira (cosup. Cristina Silva Pereira)
Rita Leones
Sowmiah Subbiah
André Mão de Ferro
Catarina Florindo
David Patinha
Susana Martinho
Karen João
Olga Cortes
Fabiana Teixeira
Filipa Cristina Alves
Marita Cardoso
Nicole Vieira
Pedro Bastos

Organometallic Chemistry

Carlos C. Romão, Professor Catedrático
Ana Catarina Martins Coelho
Hélia Jeremias

Collaborators

James Yates, Single Molecule Process
Biological Chemistry

Bacterial Energy Metabolism
Inês Cardoso Pereira, Investigador Principal
Sofia Venceslau  
Mónica Martins  
Américo Duarte  
Ana Raquel Ramos  
Marta Marques (cosup. Pedro Matias)  
André Santos  
Fábio Silva (cosup. C. Rodrigues-Pousada)  
Cláudia Mourato  
Gonçalo Oliveira  
Sónia Zacarias (cosup. Pedro Matias)  
André Rocha  
Joana Silva Pinto

Metalloproteins and Bioenergetics Unit

Biological Energy Transduction
Manuela M. Pereira, Investigador Auxiliar
Ana Patricia Refojo (cosup. Miguel Teixeira)  
Ana Paula Batista (cosup. Miguel Teixeira)  
Afonso M. Duarte  
Bruno Marreiros  
Filipa Sena  
Filipa Calisto  
Joana Sousa  
Paulo Castro

Biomolecular NMR
Manolis Matzapetakis, Investigador Auxiliar
Ivo Saraiva  
Meire Coelho de Almeida  
Mariana Palma  
Ana Catarina Silva Pereira

Genomics and Stress
Claudina Rodrigues-Pousada, Prof. Catedrático Convidado
Regina Andrade Menezes  
Catarina Isabel Ribeiro Pimentel  
Catarina Sá Almeida Amaral  
Sofia Isabel Marques da Silva  
Fábio de Oliveira  
Ana Rita Tomé Ferreira  
Soraia Caetano  
Cátia Inês Baptista Santos

Genomics and Stress

Macromolecular Crystallography Unit

Bacterial Energy Metabolism
Marina Oliveira  
Carolina Rodrigues  
Daniela Santos

Metalloproteins and Bioenergetics Unit

Inorganic Biochemistry and NMR
Ricardo Louro, Investigador Auxiliar
Catarina Morais Vaz Paquete  
Bruno Miguel Oliveira Maia da Fonseca  
Maria Alexandra Alves  
Diego Hartman (shared Applied Env. Micology)  
Nazua Lima Costa  
Sónia Estêvão Neto  
Mónica Alves  
Tiago Mestre  
Afonso Carrelo  
Isabel Pacheco (shared Bac. Energy Metabolism)  
Technician

Metalloproteins and Bioenergetics Unit

Metalloenzymes and Molecular Bioenergetics
Miguel Teixeira, Professor Catedrático
Vera Lúcia Gonçalves  
Sandra Santos  
Miguel Ribeiro  
Joana Carrilho
**Molecular Genetics of Microbial Resistance**

**Lígia M. Saraiva**, Investigador Principal

- Marta Justino, Post Doc
- Susana Lobo, Post Doc
- Lígia Nobre, PhD Student
- Adelina Parente, PhD Student
- Joana Baptista, PhD Student
- Ana Filipa Tavares, PhD Student
- Sara Sousa, BI
- Inês Santos, Trainee
- Ana Antão, Trainee
- Inês Ladeira, Trainee

**Molecular Interactions and NMR**

**Patrick Groves**, Investigador Auxiliar

- Malgorzata Palczewska-Groves, Post Doc
- Magdalena Komiazyk, BI

**Molecular Simulation**

**António M. Baptista**, Investigador Auxiliar

- Dragana Popovic de Barros, Post Doc
- Sara R. R. Campos, Post Doc
- Pedro Magalhães, PhD Student
- Luís C. S. Filipe, PhD Student
- Catarina A.C. dos Santos, BI

**Protein Biochemistry Folding & Stability**

**Cláudio M. Gomes**, Investigador Auxiliar

- Sónia Leal, Post Doc
- Bárbara Henriques, Post Doc
- Tânia Gomes Lucas, PhD Student
- Joana Margarida Cristovão, BI
- Sofia Baptista de Carvalho, BI
- Ana M. Nunes, BI
- Sara Francisco, BI

**Protein Modelling**

**Cláudio M. Soares**, Professor Associado

- Bruno Lourenço da Silva Victor, Post Doc
- Ana Sofia Fernandes de Oliveira, Post Doc
- Diana Andreia Pereira Louza, PhD Student
- João Miguel Marques Martins Damas, PhD Student
- Carla Baltazar, PhD Student
- Davide Cruz, PhD Student
- Jorge Miguel Antunes, PhD Student
- Helia Jeremias, BI
- Carlos Fernández Rodríguez, Eramus Student
- Luis Dflammhuber, Eramus Student
- Emanuel Lopes, Summer Student

**Raman Spectroscopy**

**Smilja Todorovic**, Investigador Auxiliar

- Célia Silveira, Post Doc
- Zélia Licínio Ferreira Gouveia, PhD Student
- Daniela Presa, BI

**Macromolecular Crystallography Unit**

**Structural Biology**

**Carlos Maria Franco Frazão**, Investigador Principal

- Patrícia Alexandra Teixeira Borges, PhD Student

**Structural Genomics**

**Maria Arménia Carrondo**, Professor Catedrático

- Isabel Bento, Investigador Auxiliar
- Colin Edward McVey, Investigador Auxiliar
- Célia Romão (colab. Miguel Teixeira), Marie Curie Fellow
- Elie Moe, Post Doc
- Rajesh Ponnusamy, Post Doc
- Ana Maria Gonçalves, PhD Student
- Alexandra Marques (colab. Isabel Abreu), PhD Student
- Ana Teresa da Silva Gonçalves, PhD Student
- Bruno Correia, PhD Student
- Patrícia Borges (colab. Carlos Frazão), MSc Student
- Cecilia Miranda (colab. Miguel Teixeira), MSc Student
- Daniela Moutinho, BI
- Pedro Castro, BI
- Sara Brandão, BI
- Cristina Sousa (colab. Tiago Bandeiras), BI
- Samarpita Lahiri (colab. Isabel Bento), Technician
- Ricardo Coelho, Technician

**Collaborators**

**Filipe Tiago de Oliveira**, Mössbauer Spectroscopy
Biology

Bacterial Cell Biology

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Patrícia Reed
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Andrea Tavares
Gabriela Henriques
Pedro Escada Fernandes

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Ana Raquel Ramos Pereira
Andrea Tavares
Gabriela Henriques
Pedro Escada Fernandes

Bacterial Cell Surfaces and Pathogenesis

Sérgio R. Filipe, Investigador Auxiliar
Maria João Catalão
Mafalda Henriques
Filipa Vaz
Vânia Dias
Gonçalo Covas
Ana Rita Narciso
Joana Silva Figueiredo
Sara Ramalhete

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Filipa Vaz
Vânia Dias
Gonçalo Covas
Ana Rita Narciso
Joana Silva Figueiredo
Sara Ramalhete

Bacterial Signaling

Karina B. Xavier, Investigador Auxiliar
Jessica Thompson
Pol Nadal
Rita Valente
Ozhan Ozkaya
Ana Rita Oliveira
Jorge André Pereira
Filipe Vieira

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Pol Nadal
Rita Valente
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Ana Rita Oliveira
Jorge André Pereira
Filipe Vieira

Cell Physiology and NMR

Helena Santos, Professor Catedrático
David Turner
Teresa Catarino
Nuno Borges
Pedro Lamosa
Luís Pedro Gafeira Gonçalves
Carla Jorge
Marta Rodrigues
Ana Lúcia Carvalho
Gonçalo Graça

Helena Santos
Professor Catedrático
David Turner
Teresa Catarino
Nuno Borges
Pedro Lamosa
Luís Pedro Gafeira Gonçalves
Carla Jorge
Marta Rodrigues
Ana Lúcia Carvalho
Gonçalo Graça

Control of Gene Expression

Cecília M. Arraiano, Investigador Principal com Agregação
Lisete Galego
Sandra Viegas
Susana Domingues
José Andrade
Ricardo Moreira
Michal Malecki
Rute Margarida Gonçalves Matos
Ana Filipa Reis
Inês Silva
Vânia Pobre
Ana Margarida Saramago
Andreia Aires
Cátia Bárria
Teresa Pinto
Ricardo Santos
Susana Barahona
Patrícia Apura

Cecília M. Arraiano
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Lisete Galego
Sandra Viegas
Susana Domingues
José Andrade
Ricardo Moreira
Michal Malecki
Rute Margarida Gonçalves Matos
Ana Filipa Reis
Inês Silva
Vânia Pobre
Ana Margarida Saramago
Andreia Aires
Cátia Bárria
Teresa Pinto
Ricardo Santos
Susana Barahona
Patrícia Apura

Glycobiology

Júlia Costa, Investigador Principal
Joana Batista
Susana Jorge

Júlia Costa
Investigador Principal
Joana Batista
Susana Jorge
Microbial Development

Adriano O. Henriques, Professor Associado
Mónica Serrano
Catarina Fernandes
Patricia Amaral
Fátima Pereira
Wilson David Antunes
Filipa Nunes
Ana Paiva
Rita Tomé
Carolina Freitas

Microbiology of Human Pathogens Unit

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Catarina Fernandes
Patricia Amaral
Fátima Pereira
Wilson David Antunes
Filipa Nunes
Ana Paiva
Rita Tomé
Carolina Freitas

Microbiology of Human Pathogens Unit

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Maria Miragaia
Catarina Isabel Catarino Milheiriço
Nuno Alexandre Gomes Faria
Nelson Emanuel da Silva Frazão
Teresa Margarida Gomes da Conceição
Ons Bouchami
Ana Lopes Tavares
Teresa Carla de Almeida Figueiredo
Joana Rita Gonçalves Araújo Rolo
Inês Grilo
Diana Espadinha
Céline Catherine Coelho
Isílida Gueifão
Manuela Nogueira

Plant Sciences

Disease and Stress Biology

Ricardo Boavida Ferreira, Professor Catedrático ISA-UTL
Cláudia Nunes Santos
Paula Marinho Pinto
Lucélia Rodrigues Tavares
Regina Menezes
Rui Pimpão
Diana Macedo
Inês Figueira
Andrea Filipa Gomes
Carolina Emanuel Jardim
Inês Costa
Gonçalo Garcia
Vítor Gonçalves
Tânia Silva

Forest Biotech

Célia Miguel, Investigador Auxiliar
Sofía Leal
José de Vega-Bartol
Inês Chaves
Nuno Mendes
Andrea Miguel
Ana Milhinhos
Andrea Rodrigues
Andrea Matos
Ilanit Salmoski
Inês Modesto

Plant Biochemistry

Cândido Pinto Ricardo, Prof. Catedrático Jubilado ISA-UTL
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José António Pires Passarinho
Isa Catarina Monteiro Brás Ribeiro
Adelaide João Machado

Plant Cell Biology

Rita Abranches, Investigador Auxiliar
Ana Sofia Pires
Ana Rita Basílio Santos
Ana Cláudia Nogueira
Sara Ramalhete
Plant Cell Biotechnology

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Carlota Vaz Patto
Jorge Paiva
André Almeida
Susana Araújo
Susana Neves
Ana Maria Ferreira
Jorge Cunha
Sofia Amaral Duque
Cátia Nunes
Diana Branco
Mara Alves
Matilde Cordeiro
Nuno Almeida
Pedro Mendes Moreira
Susana Leitão
Victor Carocha
Rita Severino
Priscila Pereira
Sara Costa
Letice Gonçalves
Ana Catarina Afonso
Clara Graça
José Salvado
Maria Assunção
Susana Pera
Susana Leitão
Diana Tomás
Olivia Costa
Marco Dinis

Investigator Auxiliar
Invited Researcher
Invited Researcher
Invited Researcher
Invited Researcher
Post Doc
Post Doc
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PhD Student
PhD Student
PhD Student
PhD Student
PhD Student
PhD Student
PhD Student
MSc Student
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MSc Student
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Genomics of Plant Stress

Margarida Oliveira, Professor Associado com Agregação
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Nelson José Madeira Saibo
Ana Paula Santos
Ana Paula Farinha
Sónia Negrão
Tiago Lourenço
Pedro Barros
Bruno Alexandre
Tânia Serra
Alexandra Marques
Inês Silva Pires
Cecília Pina
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Ana Ferro
Mafalda Rodrigues
Nuno Gonçalves
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Margarida Rosa
Alicia Marta Góvska
Ana Rita Leal
Natacha Vieira
Rita Borba
Vanessa Azevedo
Sofia Rodrigues
Graiciela Castilhos
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Collaborators

Phil Jackson, Plant Cell Wall

Plant Molecular Ecophysiology

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Maria Catarina Bicho

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BI MSc
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Technology

Applied and Environmental Mycology

Cristina Silva Pereira, Investigador Auxiliar
Tiago Lopes Martins
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Mariana Carvalho (cosup. Andrew Hursthouse)
Isabel Martins (cosup. Luís Paulo N. Rebelo)
Adélia Varela Castro
Helga Garcia (cosup. Luís Paulo N. Rebelo)
Rui Ferreira (cosup. Luís Paulo N. Rebelo)
Paula Cristina de Azevedo Alves
Diego de Oliveira Hartmann
Marina Guerreiro
Celso Martins
Dina Mestre

Biomolecular Diagnostic

Abel Oliveira, Investigador Auxiliar
Carmo Barreto
Sara Horta Iaracema Martinho
Rita Morgado

Animal Cell Technology Unit

Cell Bioprocesses

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Catarina Brito
Margarida Serra
Gonçalo Real
Marco Patrone
Patrícia Isabel Alves
Vitor Espírito Santo
Carina Silva
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Francisca Monteiro
Paulo Fernandes (cosup. Ana S. Coroadinha)
Sofia Rebelo (cosup. Catarina Brito)
Daniel Simão (cosup. Catarina Brito)
Cláudia Correia (cosup. Margarida Serra)
Tiago Duarte (cosup. Ana Teixeira)
Barbara Cunha (cosup. Margarida Serra)
Mafalda Dias (cosup. Ana Teixeira)
Marcos Sousa
Marta Estrada
Marta Silva

Animal Cell Technology Unit

Cell Line Development and Molecular Biology

Raquel Cunha
Rita Costa
Ana Terrasso
Ana Pinto
Nuno Espinha
Carolina Pinto Ricardo
Aniz Hamdis
Susana Veloso (sup Catarina Brito)
Carina Vieira Brilha

Animal Cell Technology Unit

Engineering Cellular Applications

Manuel J. T. Carrondo, Professor Catedrático FCT-UNL
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Cristina Peixoto
Ana Barbas
Gonçalo Real
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Ricardo Silva
Ricardo Perdigão
Piergiuseppe Nestola
João Vidigal (cosup. Ana Teixeira)
João Sá
Duarte Martins
Daniel Pais
Ana Raposo
Mass Spectrometry

Ana V. Coelho, Professor Auxiliar Convidado
Renata Soares
Isabel Marcelino
Catarina de Matos Ferraz Franco
Natacha Couto
Ilídio Magalhães
Miguel Ventosa
Rita Laires
Pedro Alves
Joana Martins
André Guerra
Filipa Lopes
Bruno Pedras
Ana Oliveira
Conceição Almeida
Elisabete Andrade Alves Pires
S Mercúrio
A Moumenne
V Uliana

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BI
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Trainee
Trainee
Trainee
Trainee
Technician
Technician
Visiting PhD Student
Visiting PhD Student
Visiting Trainee

Nutraceuticals and Delivery

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Ana Teresa Serra
Vanessa Gonçalves
Cátia Carmo
Sara Nunes
Mário Bordalo
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Pharmacokinetics and Biopharmaceutical Analysis

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Hugo Serra
Catarina Correia
Helena Coelho
Márcia Alves
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Collaborators

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Maria Rosário Bronze, Analytical Chemistry
Maria de Fatima Silva Lopes, Food Microbial Technology

Microbiology of Man-Made Environments

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Joana Lamego
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2013 Curiosities

- Research groups: 53
- Invited speakers: 45
- % articles with international teams: 44%
- % Foreign PhD holders: 22%
- M€ in Research Projects: 6.2