



# ANNUAL REPORT



# 2013

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This has been a year of consolidation for the *Institut de Biotecnologia i de Biomedicina* (IBB) at the *Universitat Autònoma de Barcelona* (UAB). Despite the difficult economic context and its considerable impact on the institute's resources, the scientific production of IBB has remained at a high level, with quality and quantity indicators very similar to those of 2012. To potentiate current priority areas, the research lines of the institute have been reorganised into three research programs focusing on *i*) genomics in evolution and disease, *ii*) response mechanisms to stress and disease and *iii*) applied proteomics and protein engineering. To strengthen these programs further, IBB has signed a collaboration agreement with the Consortium for the Construction, Equipping and Exploitation of the Synchrotron Light Source (CELLS) for research on crystallization and structure determination of proteins. The promotion of scientific discussion in the areas of expertise of the institute has included the co-organisation of the workshop Nanotechnologies in Health: Current Challenges and Future Prospects, together with the International Center for Scientific Debate Barcelona (B-Debate) and the Catalan Institute of Nanoscience and Nanotechnology (ICN2).

I thank every member of the institute for their continued effort and invite you to browse through the coming pages as a way to getting familiar with the research performed at IBB, our people and their results.

IBB Director



<http://ibb.uab.cat>

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Parc de Recerca UAB, Mòdul B – Bellaterra (Cerdanyoladel Vallès) 08193  
ibb@uab.cat

# Administrative Structure

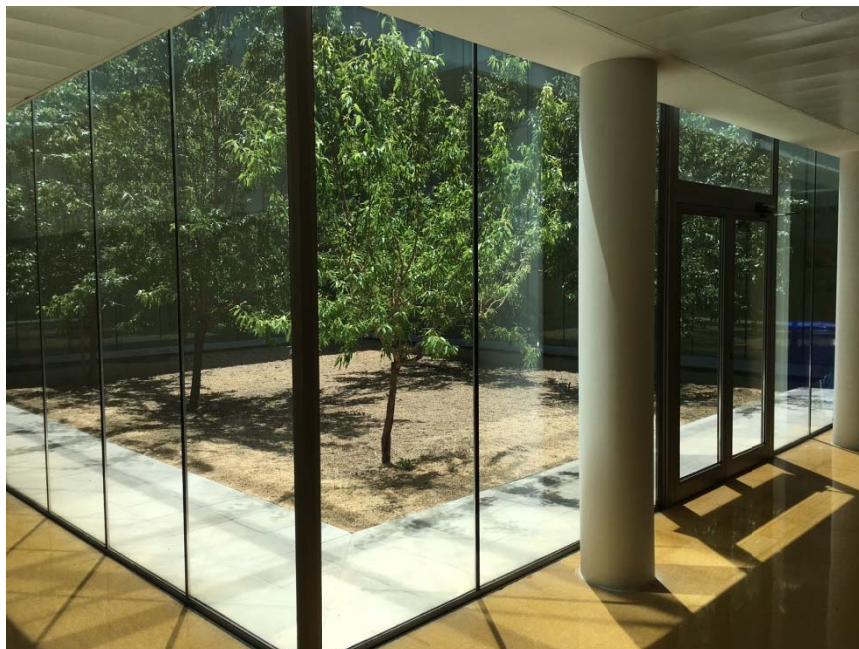


**Director:** Xavier Daura Ribera  
**Vicedirector:** Laura Masgrau Fontanet  
**Manager:** Eva Vila Morros

**Fundraising Officer:** Margarita Navia de Roux

**Administrative Support:** Manuela Romero Chávez  
Rosa Calzada Calvo  
María Teresa Jiménez Batista  
Alicia Zorrilla Guinot  
Vanessa del Pino Pérez

**Technical Support:** Almudena Merino Palomar  
Francesca Mestres Folch  
Monica Serrano García  
Ester Bach Reig



## Genome Integrity and Instability

|                     |  |
|---------------------|--|
| Group Leader        | Rosa Miró Ametller   |
| Senior Members      | Montserrat García Caldés<br>Aurora Ruíz-Herrera<br>Ignasi Roig<br>Immaculada Ponsa |
| Postdoctoral Fellow | Rosa Ana Sanchez Guillén   |
| PhD Students        | Laia Capilla Perez<br>Sarai Pacheco Piñol<br>Marina Marcet Ortega                  |

## Overview

Our group's research focuses on three topics related to genome instability. Firstly, we study the mechanisms implicated in the origin of chromosome instability associated to solid tumors, in particular to colon and bladder cancer. We analyze the mechanisms involved in chromosome reorganizations and aneuploidy origin occurring in tumor cells. Secondly, we explore the implication of chromosome rearrangements as a possible source for the existing mammalian karyotype diversity and the involvement of meiotic recombination in these processes. Finally, we try to understand the mechanisms that control meiotic recombination in mammalian meiosis. Specially, we focus on identifying key players from the pathways that control double strand break repair and genome silencing during meiotic prophase.

## Projects

Estudio de los puntos de rotura evolutivos en la línea germinal y sus implicaciones en el origen de la arquitectura genómica de los mamíferos. MICINN 2011-2013. PI: Aurora Ruiz-Herrera.

El Cryo-Zoo: un repositorio de líneas celulares de individuos de la colección del Zoo de Barcelona. Fundació Barcelona Zoo 2012-2013. PI: Aurora Ruiz-Herrera.

Análisis de los checkpoints existentes en la meiosis de mamíferos. MICINN 2011-2013. PI: Ignasi Roig.

## Others

### PhD thesis

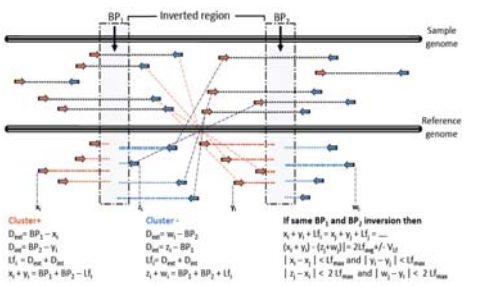
Marta Vila. Thesis title: "Telomerase expression in the mouse germ line". MSc in Cell Biology (UAB). Supervisors: M. Garcia-Caldes and A. Ruiz-Herrera. July 2013.

## Comparative and Functional Genomics

|                     |   |
|---------------------|---|
| Group Leader        | Mario Cáceres Aguilar   |
| Postdoctoral Fellow | Cristina Aguado Esteban<br>Sònia Casillas Viladerrams<br>Magdalena Gayà Vidal<br>Jose Ignacio Lucas Lledó<br>Marta Puig Font<br>Lorena Pantano Rubiño |
| PhD Students        | Alexander Martínez Fundichely<br>Meritxell Oliva Pavia<br>David Vicente Salvador<br>David Castellano Esteve<br>Carla Giner Delgado                    |
| Lab Technicians     | David Izquierdo Fontanils<br>Sergi Villatoro Gómez  |

## Overview

Our laboratory is focused in the study of genome evolution and the genetic changes associated with individual and species differences, applying state of the art techniques and the wealth of available genomic data. In particular, a great degree of structural variation has been described in multiple organisms. In addition, we have information on the variation of expression levels of thousands of genes in different tissues and individuals. However, very little is known about the functional consequences of these changes and their role during evolution. To address these two questions, we use humans as a model and take a multidisciplinary approach that combines experimental and bioinformatic analysis, to generate results of interest in diverse fields.



## Projects

Evolutionary and functional analysis of polymorphic inversions in the human genome (ERC-StG2009 INVVEST) UE 2010-2015.

## Others

### PhD thesis

Alexander Martínez Fundichely. " Bioinformatic characterization and analysis of polymorphic inversions in the human genome".2013 Director: Mario Cáceres..



Raquel Rubio. "Molecular Analysis of the Mecanismos Involved in THBS4 Differential Gene-expression in the Human Brain". 2013. Director: Mario Cáceres

#### **MSc Thesis**

Sergi Sayols Puig Master Thesis. Title: Epigenetic markers for identification of tumor tissue of origin. Universitat Autònoma de Barcelona (Spain). Advisor: Antonio Gómez & Mario Cáceres. September 6, 2013.

Carla Giner Delgado Master Thesis. Title: Evolutionary history of human polymorphic inversions: Bioinformatics approach. Universitat Autònoma de Barcelona (Spain). Advisor: Mario Cáceres and Magda Gayà. September 9, 2013.

Daniel Borrás Morales Master Thesis. Title: Differential expression and enrichment analysis of chronic cadmium exposure effects on MCF-7 breast cancer cell lines. Universitat Autònoma de Barcelona (Spain). Advisor: Zelmina Lubovac & Mario Cáceres. September 9, 2013.

#### **Organized meetings**

Organization of the 9h Workshop on Genomics and Proteomics of the Societat Catalana de Biologia. December 17, 2013. Barcelona, Spain.

Organization of the Seminar Series on Research in Genomics and Evolution at the Universitat Autònoma de Barcelona.

#### **Patent**

M. Cáceres, S. Villatoro, C. Aguado. An in vitro method of genotyping multiple inversions". EU Patent Application EP13382296.5.

#### **Members of:**

Coordinator of the Genomics and Proteomics Section of the Societat Catalana de Biologia.

#### **Editorial work**

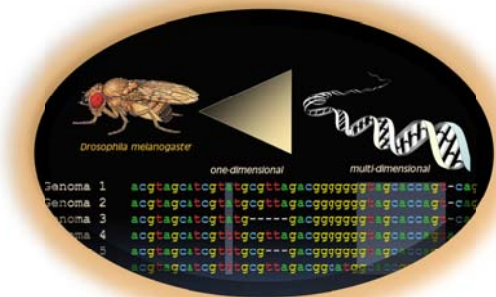
BMC Genomics Associate Editor.

## Bioinformatics of Genomics Diversity

|                 |  |
|-----------------|--|
| Group Leader    | Antonio Barbadilla Prados  |
| PhD Students    | Sergio González Rodríguez<br>Maite Garazi Barrón<br>Miquel Ràmia Jesús |
| Lab Technicians | David Castellano Esteve  |

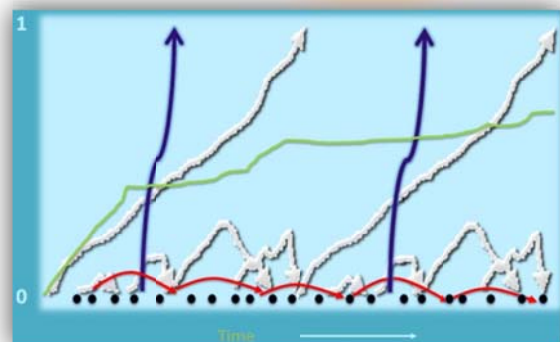
### Overview

In our research we develop and implement population genetics models and estimators to analyze and interpret the pattern of genomic variation. Among the most recent achievements, we have charted the first high resolution map of the trail of natural selection along the genome.



Key words:

- Population Genomics
- Natural selection mapping
- Bioinformatics Genome Variation
- Genome Wide Association ( GWA)
- Genome Variation Browsers



### Projects

BFU2013-42649-P. Understanding genome variation from nucleotides to phenotypes in *Drosophila* and humans. Ministerio de Ecolomía y Competitividad. IP: Dr. Antonio Barbadilla i Dr. Mario Cáceres. 2014-2016. 181.500€. Participación: IP.

BFU2009-09504/BMC. Genomic analysis of polymorphism and divergence in *Drosophila melanogaster*. Ministerio de Ciencia e Innovación (MICINN). IP: Dr. Antonio Barbadilla. 2010-2013. 72.600€. Participación: IP

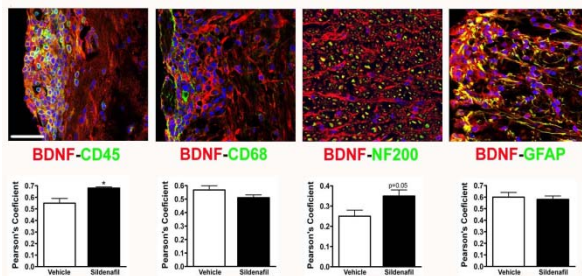
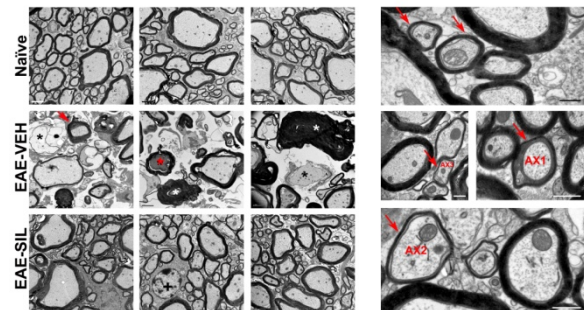


## Neuroimmunology

|                     |                               |
|---------------------|-------------------------------|
| Group Leader        | Agustina García Sánchez       |
| Senior Member       | Maria Antonia Baltrons Soler  |
| Postdoctoral Fellow | Paula Pifarré                 |
|                     | Maria Gutierrez Mecinas       |
| Predocctoral Fellow | Daniela del Valle Diaz Lucena |
| Lab Technicians     | Judith Prado                  |

## Overview

Selective cyclic GMP phosphodiesterase 5 (PDE5) inhibitors, such as sildenafil (Viagra®), widely used for treatment of erectile dysfunction and pulmonary arterial hypertension, have been recently shown to exert neuroprotective actions in animal models of CNS injury and neurodegenerative diseases. Our group has demonstrated beneficial effects of PDE5 inhibitors in animal models of focal brain injury and of multiple sclerosis (MS) that are associated to down-regulation of neuroinflammation. In the later case, we have also shown that PDE5 inhibition can prevent demyelination and promote remyelination.



At present, we are investigating the mechanisms of the anti-inflammatory and remyelinating effects of PDE5 inhibitors in the animal model of MS, experimental autoimmune encephalomyelitis (EAE), as well as in immune cells from humans. Our final goal is to provide evidences that will support the notion of PDE5 as a therapeutic target for MS, taking it to a

preclinical stage. The group is also investigating if regulation of neuroinflammation is involved in the beneficial effects of sildenafil in cognition and  $\beta$ -amyloid burden reported by other groups in animal models of Alzheimer's disease.

## Projects

Papel de las células gliales en el efecto neuroprotector de inhibidores de fosfodiesterasas de cGMP en modelos animales de daño cerebral focal y enfermedades neurodegenerativa (SAF2010-20929). Ministerio de Ciencia e Innovación. (01/01/11 – 28/02/2014). PI: Agustina García.

Mecanismes moleculars de la neurodegeneració associada a la neuropatologia neuroinflammatòria. SGR2009-1322 ( 2009-2013). PI: Agustina García.

## Others

### MSc Thesis

Autor: Norberto Nuñez

Programa: Master Interuniversitari d'Immunologia UB-UAB. Setembre 2013.

Títol: Studies of sildenafil effect on the immune response in an animal model of multiple sclerosis and in human T cells in vitro

Directores: Paula Pifarré, Agustina García

Autora: Diana Blanch Cifré

Programa: Bioquímica, Biologia Molecular i Biomedicina, UAB. Setembre 2013.

Títol: Estudio sobre los mecanismos implicados en la potenciación de la remielinización por el tratamiento con sildenafil en un modelo de esclerosis múltiple

Directores: María Gutierrez-Mecinas, Agustina García

### Organized meetings

Congress: Satellite Meeting of the 2013 International Society for Neurochemistry/American Society for Neurochemistry Joint Meeting "Understanding Glial Cell Functions in the Normal and Injured CNS"

Lloc i data: Mérida, Yucatan, México. Abril 17-19, 2013

Membre comitè organitzador: Agustina García

## Molecular Immunology

Group Leader  
Postdoctoral Fellow  
Predoctoral Fellow

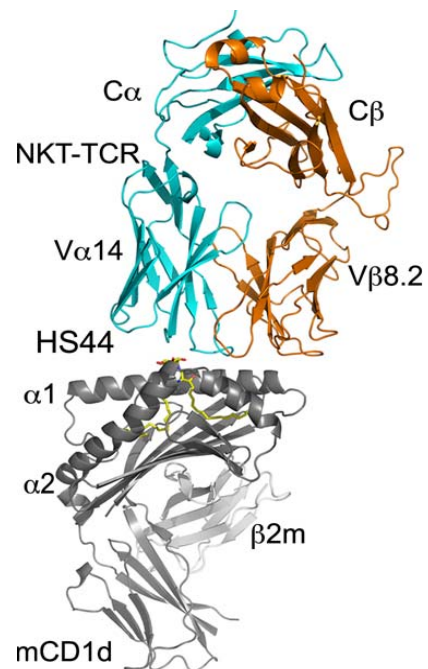
Ángel Raúl Castaño  
Alari Pahissa, Elisenda  
Ignasi Esteban

## Overview

Activation of iNKT cells by CD1d-ligands is a immunotherapeutic tool under intensive investigation.  $\alpha$ -GalCer is the prototypic agonist, but its excessive potency with contradictory activities hampers its potential therapeutic use. In search for novel ligands capable of overcoming these handicaps, we have obtained a series of synthetic analogs aiming for a controlled activation of the immune response

In vitro and in vivo studies demonstrate that some of these analogs are recognized by iNKT activating the immune response. One of them induces a robust IFN-g production, without the characteristic cytokine storm induced by  $\alpha$ -GalCer. Consequently, HS44 induces a very efficient antitumoral response in B16 tumor animal model able to completely avoid the establishment of lung metastasis. On the contrary, it is unable of inducing allergic responses making it suitable as immunotherapeutic reagent for future clinical applications.

New analogs aimed to further increase cellular Th1 response are being assayed as immune stimulants in “in vivo” models. Systemic induction of Th1 responses are being studied by wide spectrum serum cytokine analysis and their expected improved antitumoral capacities tested, and so far proved in one case, in tumor models. Cellular mechanism subjacent to their activation on the immune system, linking iNKT activation and antitumoral effectors, including mobilization of innate cells from limfoid organs and the chemokines directing such trafficking are ongoing efforts in our lab.



## Projects

Design and synthesis of new cyclitol derivatives for the study of the signalling, biosynthesis and metabolism of sphingolipid-mediated processes. Spanish Ministry of Science and Innovation. CTQ2008-01426/BQU.

## Applied Immunology

|                |                      |
|----------------|----------------------|
| Group Leader   | Paz Martínez Ramírez |
| Senior Member  | José Ramón Palacio   |
| PhD Student    | Carlos de la Haba    |
| Lab Technician | Josefa Murillo       |

## Overview

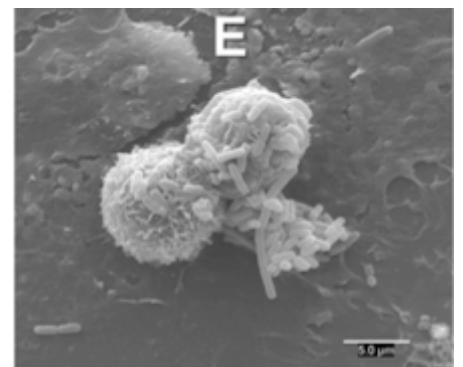
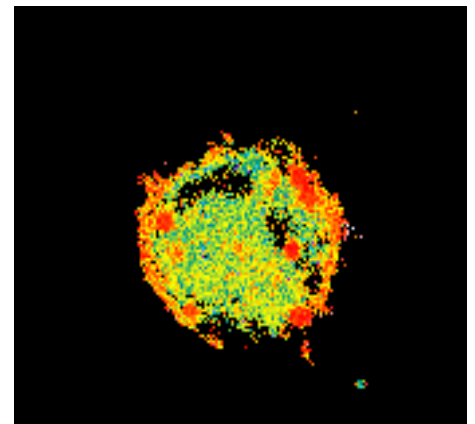
The group follows 3 main research lines:

1.- **Oxidative stress and inflammation in Reproduction.** Chronic inflammation together with oxidative stress modify the molecules which are involved in the materno-fetal dialogue during early embryo implantation. The study of antioxidant and/or anti-inflammatory therapies may contribute to the increase of implantation and pregnancy rates in assisted reproductive techniques.

2.- **Oxidative stress and biomembranes.** Lipid peroxidation may influence plasma membrane fluidity in cells from the innate and adaptative immune system (macrophages, lymphocytes). By using two-photon microscopy, a high resolution technique which allows the study of lipid dynamics *in vivo*, in individual cells, we detect how oxidative stress induces membrane changes so that the binding efficiency of ligand-receptor decreases, raft formation is prevented and cell activation may be inhibited.

A preliminary study on the relationship between oxidative stress, the biological age and quality of life in elderly people was performed. The influence of oxidative stress on membrane fluidity of immune cells, and how oxidative damage can modify the immune response is of great interest in the evaluation of disability in aging.

3.- **Nutrition and Immunology.** Probiotic and prebiotics have a protective role on several bacterial infections, so that they have been proposed as an alternative to the use of antibiotics and they are used in animal feeding to prevent neonatal diarrhea. We have investigated the protective effect of the probiotic *Saccharomyces cerevisiae* and a new developed prebiotic b-galactomannan, on epithelial intestinal cells and in a porcine model, and their immunomodulation ability in bacterial infections.



## Projects

2009 SGR 165. Inflamació, resposta i regulació en autoimmunitat. Generalitat de Catalunya (2009-2013).

## Others

### Members of:

Soci ordinari de la Sociedad Española de Bioquímica, desde 1984.

Membre ordinari de la "European Society of Human Reproduction and Embryology", des de 1987.

Membre de la "International Society for Immunology of Reproduction" (I.S.I.R.) des de 1988.

Membre de la "American Society for Immunology of Reproduction" (A.S.I.R.) des de 1992.

Soci numerari de la Sociedad Española de Inmunología des de 1992.

Membre fundador de la European Society of Reproductive & Developmental Immunology (ESRADI)

Soci numerari de la Acadèmia de Ciències Mèdiques de Catalunya i de Balears des de 1996.

Directora científica del Servicio científico-técnico Cultivos Celulares, Producción de Anticuerpos y Citometría” de la UAB desde Junio de 2009

# Response Mechanisms to Stress and Disease



## Celular Immunology

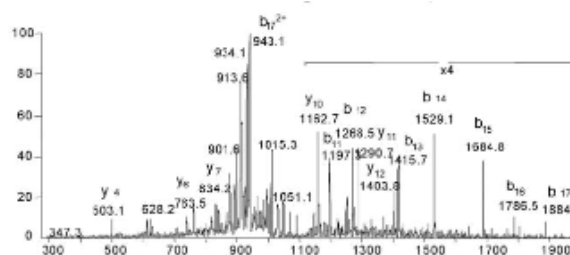
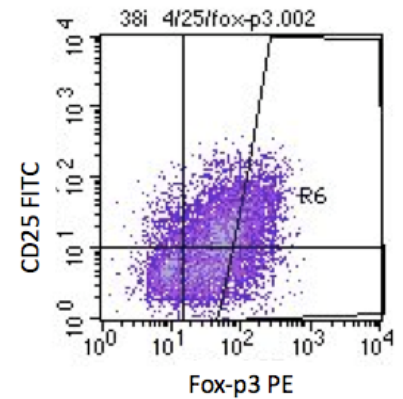
|                |   |
|----------------|---|
| Group Leader   | Dolores Jaraquemada   |
| Senior Members | Mercè Martí Ripoll<br>Iñaki Alvarez Pérez<br>Carme Roura Mir  |
| PhD Students   | Teresa Ciudad<br>Javier Collado Miguens<br>Carolina Guitart<br>Erika M. Scholz<br>Lorena Usero<br>Cristina Xufré<br>Soledad Carinelli |
| Lab Technician | Annabel Segura<br>Anna Mestre Ferrer  |

## Overview

The group's research interests are centered in the study of central tolerance, antigen processing, auto-antigen presentation and recognition in autoimmune diseases.

Specific lines include:

- Auto-antigen presentation in target organs.
- Autoreactive and regulatory T cells in autoimmunity.
- NKT Cells in Autoimmunity.
- Antigen processing in tolerance and autoimmunity.



# Response Mechanisms to Stress and Disease



## *Projects*

2009 SGR 165. Inflamació, resposta i regulació en autoimmunitat. Generalitat de Catalunya (2009-2013).

2011 – 2015: SAF2012-35344 (subprogram MED, CICYT, Spanish Science Ministry). From antigens to TCR. A systematic approach to the immune response in type 1 diabetes

## *Others*

### **PhD thesis**

Caracterización de los repertorios peptídicos asociados a HLA-DR en tejido linfoide humano: Homeostasis y tolerància. Javier A. Collado, Juliol 2013



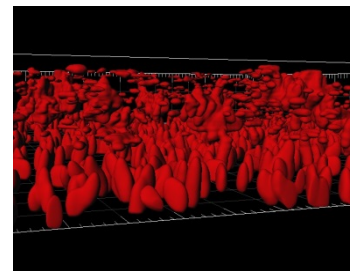
## Bacterial Molecular Genetics and Pathogenesis

|                      |                         |
|----------------------|-------------------------|
| Group Leader         | Isidre Gibert González  |
| Postdoctoral Fellows | Daniel Yero Corona      |
| PhD Students         | A.Celeste Gómez Camacho |
|                      | Pol Huedo Moreno        |
|                      | Paula Martínez Alcalá   |

### Overview

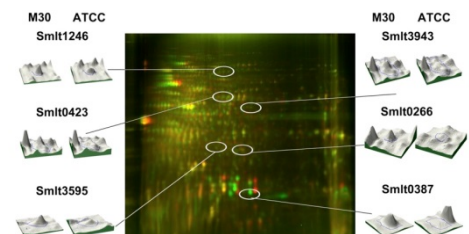
The main research interests of our group are:

- The molecular basis of bacterial pathogenesis and antimicrobial resistance.
- The identification and validation of new antimicrobial targets for Gram-negative pathogens.



Other research interest:

- Host-pathogen interactions and infection models: mouse, *C. elegans* and Zebrafish
- Bioinformatic approach to identify new potential candidates for vaccine and/or drug targets.



### Keywords

Bacterial Pathogenesis, Virulence, Host-Pathogen Interactions Molecular Genetics, Genomics, Proteomics, Gene Expression, Antimicrobial Resistance, Antimicrobial Drug

### Projects

Ajuts de Suport als Grups de Recerca Consolidats. Departament d'Universitats, Recerca i Societat de la Informació (Generalitat de Catalunya) (Ref.: 2009 SGR 108). 2009-2013. PI: A. Vilaverde.

Identification and validation of novel drug targets in Gram-negative bacteria by global search: a trans-system approach (Contract no. HEALTH-F3-2009-223101). UE 2009-2013. PI: Xavier Daura.



# Response Mechanisms to Stress and Disease



Aproximación proteómica para la determinación y análisis de factores de virulencia en *Stenotrophomonas maltophilia* (Ref. BFU2010-17199). MICIN 2011-2013. PI: I. Gibert.

From Genome to Antigen: a Multidisciplinary Approach towards the Development of an Effective Vaccine Against *Burkholderia pseudomallei*, the Etiological Agent of Melioidosis. Investigador responsable: Xavier Daura. Participació: Investigador. Entitat financiadora: Fondazione CARIPOLO. Data d'inici: 01/11/2010 (3 anys). Quantia total: 175.000

Participació: Investigador. Entitat financiadora: VII EU FP7 (7 th Framework Programme for Research and Technological Development). Data d'inci: 01/02/2009 (4 anys). Quantia total: 921.912

Convenis de transferència i prestació de serveis en relació a programes de qualitat microbiològica amb Sociedad Española de Bioquímica Clínica y Patología Molecular i Fundació pel control de qualitat dels laboratoris clínics

## Others

### PhD thesis

Andromeda Celeste Gomez. Estudio de la implicación de los genes Rv1686c-Rv1687c y Rv3161c de *Mycobacterium tuberculosis* en la resistencia a fármacos. Directores: Isidre Gibert i Núria Andreu



## Evolutionary Immunology

|                   |  |
|-------------------|--|
| Group Leader      | Nerea Roher Armentia   |
| PhD Students      | Debora Torrealba Sandoval<br>Angels Ruyra Ripoll<br>Jie Ji<br>Jofre Gasion |
| Visiting students | Agnes Callol<br>Eva Vallejos   |

---

## Overview

### ➤ Development of nanovaccines for fish species of commercial interest

It's been a central focus of our work. We are searching for non-toxic, non-stressful and effective systems to protect commercial fish from diverse pathogenic challenges. Taking into account the particularities of the fish immune system, we have recently completed a nanoformulation (Ruyra et al., 2013) able to increase the survival of bacterial challenged fish (Ruyra et al, manuscript in preparation). The development of sustainable aquaculture, a strategic sector to feed the ever-increasing human population (Khan et al, 2011), relies on disease prevention through the implementation of preventive immunostimulation and effective vaccination strategies (Evensen et al., 2009). In particular, fish immunologists face now a major challenge trying to prevent the massive economic losses caused by viral diseases. Development of novel vaccines to protect fish from viral diseases such as Spring Viremia Carp Virus, SVCV or Viral haemorrhagic septicemia viruses, VHSV (Gomez-Casado et al., 2011) will be a major goal of our research efforts during the next years. In collaboration with a fish virologist (Dr. A. Estepa) we aim to encapsulate plasmids coding for antigenic viral proteins into nanoliposomes and characterise them in zebrafish to finally, test the formulations in the real host. A hallmark of our work in the next five years would be to design and develop new nanovaccines against SVCV and VHSV.

### ➤ The evolution of pathogen recognition in vertebrates

In the last 7 years we have been investigating the molecular basis of the fish immune system, and we have been trying to decipher the particularities of its innate immune response. Most fish species lack the TLR4 receptor that senses the LPS presented in the outer membrane of bacterial cells. We are interested to tackle the characterization of the molecule responsible for LPS sensing and why fish are less sensitive to the toxic and pro-inflammatory effects of LPS. Genomic tools have been of great importance for the fish research field during the last years. Fish genomes such as fugu, puffer fish, medaka, cod or salmon among others start to be available to the scientific community. A major achievement in fish biology has been the completion of the zebrafish reference genome sequence, with publication of the Zv9 assembly. The Sanger Institute provides the research community with a high-quality zebrafish genome sequence. The number of identified protein-coding genes in the zebrafish genome now stands at around 24000 and fish supplied by the Zebrafish Mutation Resource

# Response Mechanisms to Stress and Disease



(Sanger Institute) can be used to study a wide range of biological processes such as response to pathogens, cancer, diabetes etc. Our lab will be provided with INF $\gamma$  and IL-1 $\beta$  mutant fish that will be used to investigate the anti-viral and the inflammatory response respectively. Our fish facility is open to house other mutants of interest for the research of groups in the IBB-MRB.

## ➤ Defense mechanisms in *Branchiostoma lanceolatum*

Lastly, besides the above mentioned research lines, we will have an additional long-term research line aimed to explore the defense mechanisms in a non-vertebrate marine organism, the amphioxus (*Branchiostoma lanceolatum*) that would allow us for a better understanding of the vertebrate immune system. From an evolutionary point of view the amphioxus is an excellent living organism to study what was going on before vertebrates arose. The amphioxus is a cephalochordate with a small genome and simple body architecture that makes it very suitable for evolutionary studies. In collaboration with Dr. Bayes (IIB, Hospital de Sant Pau) we will study different aspects of amphioxus biology such as nervous system architecture, defense mechanisms or tolerance and biodistribution of nanoliposomes.

## Projects

Uso de nanoesferas como vehículo para la administración de inmunoestimulantes en especies de interés para la acuicultura (NANOQUA). Fundació Ramon Areces 2010-2013.

Estudio in vivo de la biodistribución y efecto inmunológico de compuestos activos encapsulados en nanoliposomas marcados con quantum dots. Universitat Autònoma de Barcelona APOSTA2011-01).

Desarrollo de nanoliposomas como vehículos de inmunoestimulantes/vacunas en especies de interés para la acuicultura. AGL2012-33877 (01/01/2013 – 31/12/2015).

Establish the distribution of proactive and reactive coping styles in an outbred Tilapia (*Oreochromis niloticus*) population. Head(s) researcher(s): Nerea Roher Armentia Funding body: Aquaexcel, European Commission

## Others

### PhD thesis

**Reynaldo Elías Vargas.** “Contribución de la personalidad en la variación fenotípica y su impacto sobre la biología del pez cebra (*Danio rerio*)”. 2013. Directors: Simon Mackenzie i Sònia Rey Planellas.

### Organized meetings

Organization of the international meeting I: *Nanotechnologies in Health: Current challenges and future prospects*; 9-11 October 2013. CosmoCaixa, Barcelona

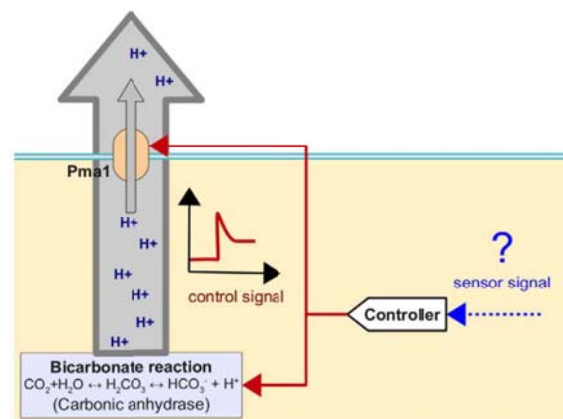
Organització del workshop: *II Nanomedicine Workshop*; 8 october 2013. Universitat Autònoma de Barcelona, Barcelona.

## Yeast Molecular Biology

|                      |  |
|----------------------|--|
| Group Leader         | Joaquin Ariño Carmona  |
| Senior Member        | Antonio Casamayor Gracia   |
| Postdoctoral Fellows | Lina Patricia Barreto<br>Carlos Casado Vázquez<br>Silvia Petrežsélyová<br>Boris Rodriguez                    |
| PhD Students         | Jofre Ferrer-Dalmau<br>Laura Tatjer Recordà<br>Albert Serra Cardona<br>Anna Bahí<br>Cristina Molero Merinero |
| Lab Technician       | David Canadell i Sala<br>Montse Robledo Costas   |

## Overview

Our group is interested in different aspects of the biochemistry, molecular biology and genomics of the yeast *Saccharomyces cerevisiae*, particularly in those involving cell signaling via phospho-dephosphorylation processes. This includes research on ion homeostasis, response to various forms of stress or cell cycle regulation. Particular emphasis is given to the interaction between ion and nutrient homeostases. The ultimate goal is to obtain a comprehensive view of the yeast response to perturbations in their environment that may lead to a deeper insight into the biology of this organism, as well as to new biotechnological applications. As an example, we are carrying out a project to develop new strains tolerant to acetic acid, to improve the fermentative processes involved in the generation of bio-alcohol from plant debris.



| C) Plasmid  | YPD | 8.0 pH |
|-------------|-----|--------|
| YCp50 Ø     |     |        |
| YCp50-RAS2* |     |        |
| YEplac112 Ø |     |        |
| YEp-GPA2*   |     |        |

## Projects

Modelado de redes génicas y de proteínas relevantes en la homeostasis de cationes en levadura (ERA-SysMo2, EUI2009-4147) EU 2010-2013. PI: Joaquín Ariño.

Diseño integral de levaduras tolerantes a ácido acético (INTACT) – (ERA-IB, Industrial Biotechnology, PIM2010EEI-00610). 2011-2014. PI: Joaquín Ariño.

Evaluación de la homeostasis iónica y de nutrientes: diferentes estrategias para un objetivo común (Ref. BFU2011-30197-C03-01) MEC 2011-2014. PI: Joaquín Ariño.

## Others

### PhD thesis

Anna Bahí Salavedra(15/11/2013) Identificació de noves funcions de les proteïnes cinases Pkh en el llevat *Saccharomyces cerevisiae*. Director: A. Casamayor.

### Members of:

Joaquín Ariño ha sido nombrado miembro del Editorial Board de la nueva revista Microbial Cell (<http://microbialcell.com/>), editada por Shared Science Publishers OG.Editorial work

# Applied Proteomics and Protein Engineering



## Computational Biology

|                      |  |
|----------------------|--|
| Group Leader         | Xavier Daura Ribera  |
| Postdoctoral Fellows | Lionel Costenaro<br>Mario Ferrer Navarro<br>Martin Indarte |
| PhD Students         | Alejandro Panjkovich                                       |
| Lab Technician       | Oscar Conchillo Solé                                       |

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## Overview

The group's trajectory has been, until recent years, largely based on the use of molecular-dynamics simulation methods to study biomolecular systems at atomic resolution, mostly in connection with the process of polypeptide folding. Since 2007, however, the group has expanded its scope towards the proteomic analysis of pathogenic bacteria for the identification of antigens and putative drug targets. This expansion has been enabled by the incorporation of new members with expertise on additional computational and experimental techniques, and by teaming up with IBB's Bacterial Molecular Genetics group. Currently, the group has active projects, often intertwined, in the following topics:

- Study of biophysical properties of peptides and proteins by molecular-dynamics simulation methods.
- Computational compound screening and redesign for drug discovery.
- Bioinformatic and experimental identification and characterization of proteins of pathogenic bacteria for vaccine and antibacterial-drug development.

In general each of these topics is being developed within the context of a collaborative project.

## Projects

Identification and validation of novel drug targets in Gram-negative bacteria by global search: a trans-system approach (Contract no. HEALTH-F3-2009-223101), EU 2009-2013.

From genome to antigen: a multidisciplinary approach towards the development of an effective vaccine against *Burkholderia pseudomallei*, the etiological agent of melioidosis, Fondazione Cariplo 2010-2013.

# Applied Proteomics and Protein Engineering



Aproximación proteómica para la determinación y análisis de factores de virulencia en *Stenotrophomonas maltophilia* (Ref. BFU2010-17199). MICINN 2011-2013.

## Others

### PhD thesis

Alejandro Panjkovich. Structure and evolution of protein allosteric sites. Universitat Autònoma de Barcelona, November 7, 2013

### Invited address

*A bioinformatics approach to the identification of vaccine candidates in the genome of Burkholderia pseudomallei.* The 50th Khon Kaen University and 36th Faculty of Associated Medical Sciences Anniversary Celebration Conference. 2013 Infection & Immunity: From Basic to Translational Research, Hua Hin, Thailand (September 21-23, 2013).

## Theoretical Molecular Biology

|                     |   |
|---------------------|---|
| Group Leader        | Josep M. Lluch  |
| Senior Members      | Àngels González Lafont<br>Mireia García Viloca<br>Laura Masgrau |
| Postdoctoral Fellow | Reynier Suárez Díaz   |
| PhD Students        | Hansel Gómez<br>Ayax Pérez Gallego<br>Maria Fernanda Mendoza    |

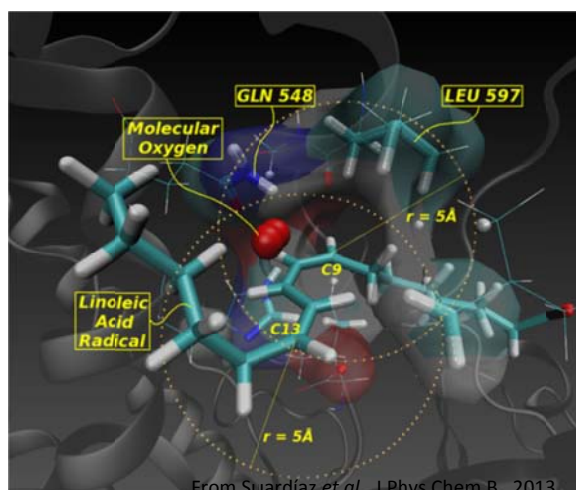
## Overview

In the Theoretical Molecular Biology group we are interested in understanding how enzymes work at the atomic/molecular level. We are particularly specialized on the theoretical study of the chemical reactions taking place inside enzymes and in identifying the main actors that make possible these exquisite catalytic processes. Among other mechanistic aspects, for example, we analyse how the high regio and stereospecificity of this biological catalysis is achieved. Our final aim is to use all that knowledge to force conveniently modified enzymes to work in the way we need to achieve outstanding biomedical and biotechnological applications.

To do this, we apply and develop Theoretical and Computational Chemistry methods, including hybrid quantum mechanics/molecular mechanics methods on the solvated enzyme-substrate(s) system, molecular dynamics simulations, free energy calculations, the EA-VTST/MT scheme and protein-ligand dockings.

Our current main lines of research focus on:

- **Mammalian lipoxygenases (LOs)**: LOs are implicated in the pathogenesis of inflammatory and hyperproliferative diseases. Moreover, some isoforms like the 15S-LO, are highly regio and stereospecific in the hydroperoxidation reaction they catalyse; specificity required for its correct physiological function. We have been analysing the possible causes of this regiospecificity in the oxygen attack step catalysed by rabbit 15S-LO. Our results conclude that, among the different possibilities proposed in the literature, the steric-shielding hypothesis seems to be the operating one in this enzyme. On another hand, we have started the study of the hydrogen abstraction step.

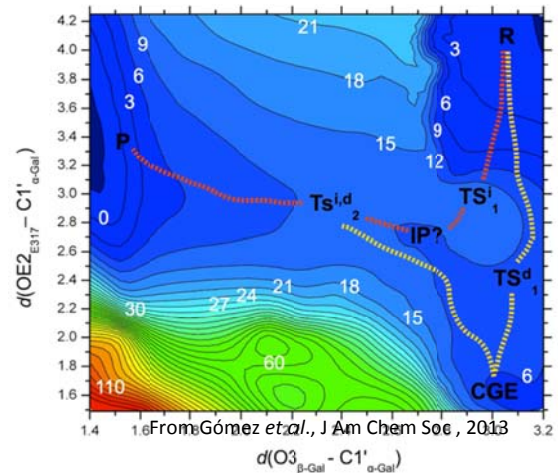




# Applied Proteomics and Protein Engineering

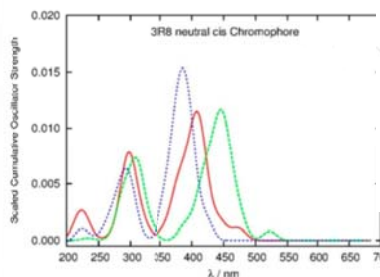
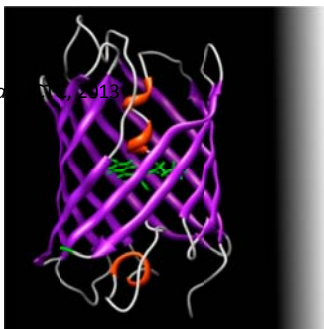
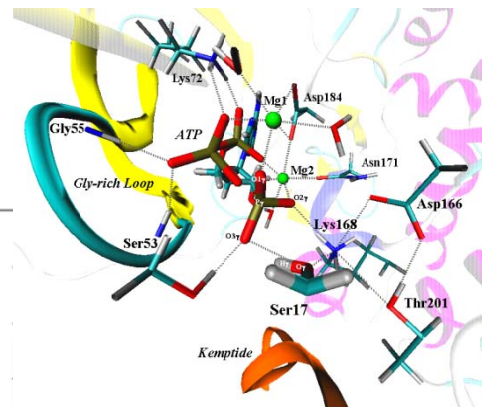


- **Computational chemical glycobio**logy: the biosynthesis of glycans has been the focus of this research line. In particular, we are providing computational evidences that are helping clarify the catalytic mechanism used by retaining glycosyltransferases, a matter that has been under debate for the last decades and has remained as one of the unanswered fundamental questions in glycosciences. We have studied *in silico* several of these enzymes, some of these works being compiled in the PhD thesis of H. Gómez, defended in October 2013.



- **Serine-threonine kinases**: The cAMP-dependent protein kinase A (PKA) is a prototypical kinase that plays pivotal roles in numerous signaling pathways. During this period, important progress has been done on the study of the reaction mechanisms (dissociative and associative) of the phosphoryl transfer catalyzed by PKA and the Asp166Ala mutant. As Asp166 has a fundamental role in the dissociative mechanism, the only way to explain the experimental activity observed for the mutant enzyme is via an associative process never taken into account by other modeling studies of this important catalytic process. The energetic and structural analysis of the catalytic reaction pathway performed in our laboratory is shedding some light on the origin of transition state stabilization within the kinase family.

- **Fluorescent Proteins**: Part of our group has a strong background in the study of chemical reactivity in excited states. In the last years, this experience is also being



applied to investigate several aspects related to the fluorescence phenomena in fluorescent proteins,

which have many applications in biomedicine as *in vivo* biomarkers. The Green Fluorescence Protein (GFP) and many members of the Red Fluorescence Protein (RFP) family are being the focus of our research. Especially we are working on the design of RFP variants that excite and emit in the optical window in which mammalian tissues are relatively transparent to light. This new fluorescent proteins for imaging in mammals should be useful for following biological processes “in vivo”.

From Nadal-Ferret et al., 2013

## Projects

Adscribed at the Department of Chemistry of the UAB.

## Others

### PhD thesis

Hansel Gomez. "Theoretical Study of the Catalytic Mechanism of Retaining Glycosyltransferases". 2013. Directors: Josep Maria Lluch López i Laura Masgrau Fontanet

### MSc Thesis

"Theoretical study of glycosidic bond formation by EXTL2", M. F. Mendoza. September 2013. Supervisors: L. Masgrau, J.M. Lluch.

"Estudio teórico de la abstracción de hidrógeno de ácido araquidónico catalizada por lipoxigenasa-15 de mamífero: regioespecificidad de los canales de abstracción", P. Saura. September 2013. Supervisors: À. González-Lafont, J.M. Lluch.

"Theoretical study of the hydrogen abstraction process catalized by 15-lipoxygenase", D. Garcia, September 2013. Supervisors: À. González-Lafont, L. Masgrau.

### Talks in international Congresses.

"Theoretical study of the mechanism of the hydride transfer between ferredoxin NADP+ reductase and NADP+. The role of Tyr303", À. González-Lafont, invited conference in "Theoretical Chemistry in Spain told by women. A symposium in Honour of Rosa Caballol", Tarragona, 2013.

"Substrate vs. nucleophilically assisted catalysis in retaining glycosyltransferases. Insights from QM/MM calculations", L. Masgrau, H. Gómez and J.M. Lluch. Flash presentation and poster in "10th Carbohydrate Bioengineering Meeting", Prague, 2013.

"Mechanism of glycosidic bond formation by retaining glycosyltransferases. Insights from QM/MM calculations", L. Masgrau, oral communication in "Chemistry for Life Sciences. 5th European Conference", Barcelona, 2013.

# Applied Proteomics and Protein Engineering



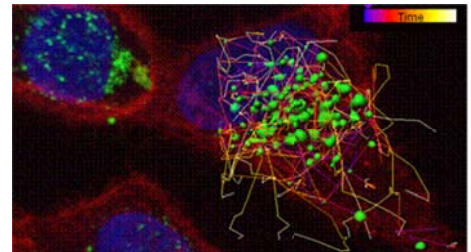
## Nanobiotechnology

|                |  |
|----------------|--|
| Group Leader   | Antonio P. Villaverde  |
| Senior Members | Neus Ferrer<br>Esther Vazquez<br>José Luis Corchero<br>Elena Garcia Fruitós<br>Joaquin Seras |
| PhD Students   | Olivia Cano<br>Mireia Pesarrodonna<br>Paolo Saccardo<br>Ugutzu Unzueta<br>Xu Zhikun          |
| Lab Technician | Fabián L. Rueda<br>Rosa Mendoza  |



## Overview

- Development of self-assembling protein nanoparticles for non-viral gene therapy.
- Development of new bacterial nanomaterials for tissue engineering.
- Design and production of enzymes and antibodies for cell therapy.
- Design of processes for production of recombinant proteins of therapeutic interest in bacteria, insect cells and mammal cells.
- Study of cell stress responses to the production of proteins of pharmacological interest.
- Study of the physiology and genetics of protein aggregation in recombinant bacteria.
- Generation and engineering of virus-like-particles of biomedical interest.
- Design of functionalized proteins for targeted drug delivery, endosomal escape and blood-brain barrier crossing.



## Projects

Ajuts de Suport als Grups de Recerca Consolidats. Departament d'Universitats, Recerca i Societat de la Informació (Generalitat de Catalunya) (Ref.: 2009 SGR 108). 2009-2013. PI: A. Vilaverde.

# Applied Proteomics and Protein Engineering



Desarrollo de vehículos recombinantes no víricos para la terapia génica del cáncer colorrectal, PS09/00165, Instituto de Salud Carlos III, FIS, Proyectos de Investigación en Salud. Acción estratégica en Salud, 2010-2012. IP Esther Vazquez Gomez

Desarrollo de sistemas eficientes de purificación de biomoléculas basados en la separación magnetoforética. Ministerio de Ciencia e Innovación (Subprograma Innpacto). Grupo Microbiología Aplicada (IBB-UAB, CIBER BBN), Sepmag Technologies, y ICMAB, (2010/2013)

Diseño y producción de partículas proteicas para la ingeniería de micro y nano entornos en proliferación celular y medicina regenerativa. BFU2010-17450. 1/1/2011-31/12/2013. IP. A. Villaverde.

Insights into Gla-rich Protein (GRP) function and molecular mechanism of action in vascular calcification (BioGlaGRP). Carla Alexandra São Bento Viegas (coordinadora) Centro de Ciências do Mar (CCMar/CIMAR) Portugal. Fundação para a ciência e a tecnologia. Ministerio da educação e Ciencia (PTDC/SAU-ORG/117266/2010; 2012-2015). 159.755 €. Partners: C. Vermeer-VitaK BV, Alemania y N. Ferrer Miralles-Universidad Autónoma de Barcelona

## Others

### PhD thesis

Joan Domingo. "Development and characterization of artificial viruses for gene therapy". 2013. Director: Dra. Neus Ferrer i Dra. Esther Vázquez

Ugutzu Unzueta. "De novo design of self-assembling protein nanoparticles towards the gene therapy of colorectal cancer". 2013. Directors: Dr. Antonio Villaverde Corrales, Dra. Esther Vázquez Gómez i Dra. Neus Ferrer Miralles

### Organized meetings

Chairman y miembro del comité científico del B-DEBATE on "Nanotechnology in human and animal health". Barcelona, Spain, 2013.

Chairman y miembro del comité científico del 2st Workshop on Nanomedicine UAB-CEI. Barcelona, Spain, 2013.

Miembro del International Advisory Board del Asian Congress on Biotechnology (Acb2013).

### Patent

Marco Colás, María Pilar; Pascual Durán, Nuria; Pastells Díez, Carme; Sanchez Baeza, Francisco; Villaverde Corrales, Antonio Pedro; Rodríguez Carmona, Escarlata. Haptens y conjugados derivados

# Applied Proteomics and Protein Engineering



de pirocianina, anticuerpos de los mismos, y método inmunoquímico para la detección de infecciones provocadas por pseudomonas aeruginosa. P201330312. 5 Marzo 2013.

## **Members of:**

Member of CIBER en Biomateriales, Bioingeniería y Nanomedicina (ISCIII) since 2006.

Member of the Spanish Platform on Nanomedicine since 2007.

Member of the European technological Platform in Nanomedicine since 2008 and UAB representative.

Chairman B-DEBATE on "Nanotechnology in human and animal health". Barcelona, Spain, 2013.

Chairman 2st Workshop on Nanomedicine UAB-CEI. Barcelona, Spain, 2013.

Asian Congress on Biotechnology (Acb2013). India. 2013.

Scientific advisor of the la TWAS, The academy of sciences for the developing world, since 2013

## **Editorial work:**

BMC Genomics Associate Editor.

Editor-in-Chief de Microbial Cell Factories (ISSN: 1475-2859).

Editor de Microorganisms (ISSN 2076-2607) desde 2012.

Editor de Medical Sciences (ISSN 2076-3271) desde 2012.

# Applied Proteomics and Protein Engineering

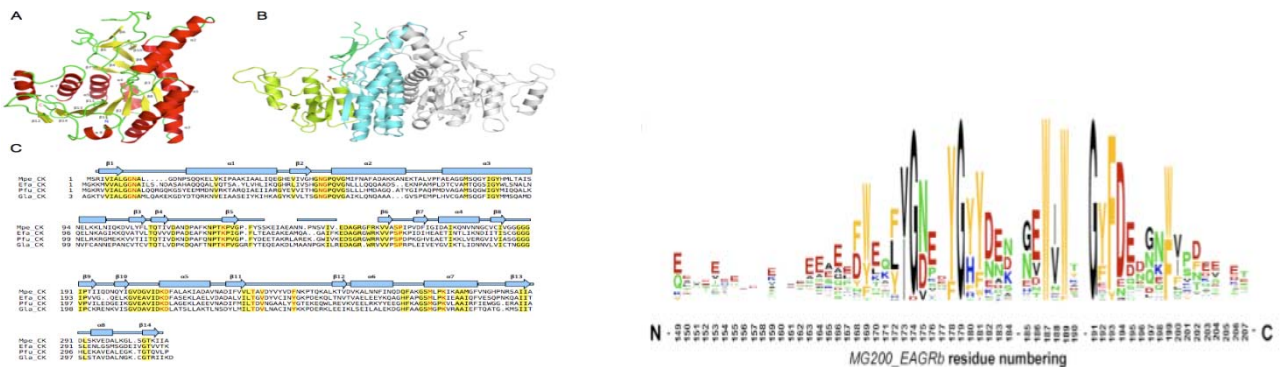


## Molecular Biology

|                     |  |
|---------------------|--|
| Group Leader        | Enrique Querol Murillo   |
| Senior Members      | Jaume Piñol Ribas<br>Josep A. Perez Pons   |
| Postdoctoral Fellow | Ángel Mozo<br>María Camats<br>Xavier Serra Hartmann<br>Oscar Quijada<br>Merçe Ratera   |
| PhD Students        | Alicia Broto Hernandez<br>Isaac Amela Abellán<br>Luis González González<br>Ana María, Martínez<br>Luis García Morales<br>Mario Huerta Casado |

## Overview

- *Mycoplasma genitalium* as a model of minimal cell and genome. Functional proteomics, adhesion and gliding mechanism, pathogenicity.
- Bioinformatics: Analysis of protein structure and function. Gene expression algorithms. Vaccine and drug target identification.
- Biotechnology: vaccine and diagnostic kits design.



## Projects

Friedreich Ataxia Integrative Research Consortium: a Pathophysiological and Therapeutic Approach (FAIR). Projecte Marató TV3 2009 – 2013

Mecanismos moleculares de patogenicidad en *Mycoplasma genitalium* y validación de nuevas dianas terapéuticas. Proyecto MCINN **BFU2010-22209-C02-01**. Proyecto Coordinado UAB-IQS (Inst. Químico Sarriá de Barcelona, Dr. A. Planas). Años 2011-2013. Investigador responsable: E. Querol. Investigadores participantes: 9 (en el subproyecto 1). Importe: 290.400 € (subproyecto 1).

## Others

### PhD thesis

**Isaac Amela.** “Bioinformatics Approaches to Protein Interaction and Complexes: Application to Pathogen-Host Epitope Mimicry and to Fe-S Cluster Biogenesis Model”. 2013. Directors: Enrique Querol i Juan A. Cedano

### MSc Thesis

Mining databases: The IEDB for biomedical and biotechnological applications Óscar Marin Sala. Septiembre 2013. Codirigida Dr. I. Amela.

Naia Cartañá Gamboa. Análisis de expresión diferencial del fenotipo proliferativo dependiente de origen embrionario del tejido. Septiembre 2013. Codirigida M. Huerta.

### Patent

- Inventores: L. González, J. Piñol, J. Montane, M. Camats, E. Querol, M. Sitja. “Cepas mutantes de *Mycoplasma hyopneumoniae*” WO2014/009586 A2. “Vectors for transforming *Mycoplasma hyopneumoniae*, transformed *M. hyopneumoniae* strains, and use thereof” EP 2 684959 A1”.

## Protein Engineering and Proteomics

|                     |  |
|---------------------|--|
| Group Leader        | Francesc X. Avilés Puigvert  |
| Senior Members      | Josep Vendrell Roca<br>Julia Lorenzo Rivera  |
| Postdoctoral Fellow | Hugo M. Baptista   |
| PhD Students        | Giovanny Covaleda<br>Sebastian Tanco<br>Olivia Tort Regas<br>Anabel Otero<br>Javier Garcia Pardo |
| Lab Technician      | Erica Serrano Barbero<br>Mónica Rodríguez de la Vega   |

## Overview

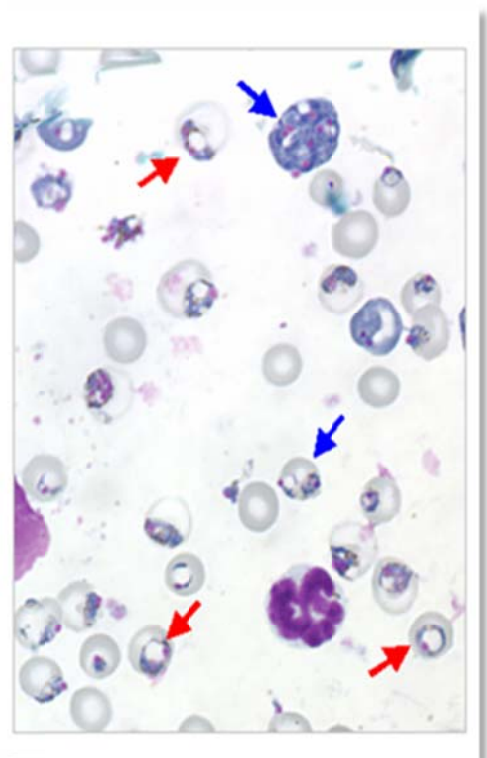
Our group's interests lie in protein engineering, focusing on the study of protease precursors and inhibitors in general, and on metalloproteases in particular. Among this lines we work in redesigning proteins or organoproteic molecules capable of keeping these enzymes inactive, and in such way finding out determinant factors for their activation and inactivation.

We also develop methodologies for high-throughput proteomics as well as for the classification, structural prediction / simulation and modeling of proteins, ligand design, drug design and protein engineering in general.

## Projects

Grup consolidat de la Generalitat de Catalunya 2009SGR218. Durada, des de: 2009-2013. Subvenció: 50.960 euros. Investigador responsable: F. X. Avilés.

"Light-based functional in vivo monitoring of diseases related enzymes" (LIVIMODE). Research (strep) Project granted by the European Commission (EC) within FP7-HEALTH-2009-single-stage. (Ref. 241919). Coordinador: B. Turk + other 8 European research groups, academic and industrial (Sanofi-Aventis). Period 2010-2013. 319.000,00 eur (to the F.X. Aviles Group as IP).





# Applied Proteomics and Protein Engineering



"Proteómica, Búsqueda de Fármacos e Imagen de Enzimas Proteolíticos" (S1) (Ref. BIO2010-22321-C02-01) Proyecto de Investigación coordinado (Coordinador, F.X. Aviles, dos grupos de investigación) dentro de la convocatoria del 2009 del Plan Nacional de Biotecnología (MICINN). Periodo 2010-2013. 190.000 euros + 1 becario (para grupo con F.X. Aviles como IP).

"Proteómica y quimiogenómica de inhibidores de proteasas de origen natural con potencial terapéutico en Malaria". Research Project of CYTED, with the participation of 9 partners from different iberian and latin america locations (UAB- & UCM- Spain, Portugal, Argentina, Cuba ....etc). ref. P210RT0398. IP researchers of the spanish team : Francesc Xavier Aviles & Josep Vendrell. From 1/05/2010 -30/04/2013. Financing 36.000 €/year

## Others

### Members of:

Evaluator/referee of different scientific journals and, particularly, of Eur. J. Biochem./ FEBS J./ Proteomics / J Biol Chem...etc... etc (1985-2015), and member of the Editorial Board of J. Protein Chem & The Protein Journal (2001- to now), Microbial Cell Factories (2004-2014) and J Biol Chem (1990-1995 & 2009-2014).

Member of the Executive Board of the Spanish Society for Biophysics-SBE (1993-96; & 2003-2008) and of the Spanish Society for Biochemistry and Molecular Biology-SEBBM (1998-2002). Coordinator of the Section for Genomics and Proteomics of SEBBM (2001-2005); the same for the Catalan Society for Biology-SCB (2007-2013)

Coordinator of the Network on "Genomics and Proteomics", at the Catalunya level (Xarxa Generalitat) (an. 2001- 2013).

## Protein Folding and Conformational Diseases

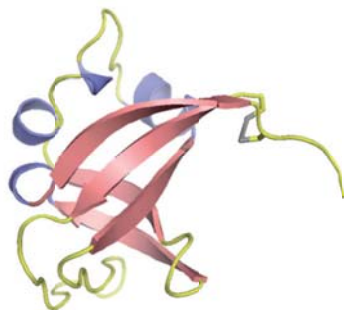
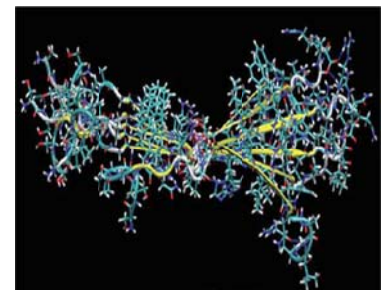
|                     |  |
|---------------------|--|
| Group Leader        | Salvador Ventura Zamora  |
| Postdoctoral Fellow | Hugo Fraga Duarte<br>Susana Navarro Cantero  |
| PhD Students        | Virginia Castillo Cano<br>Alba Esparagró Colomé<br>Anna Villar Piqué<br>Ricardo Graña-Montes<br>Patrizia Marinelli |

### Overview

We aim to understand the chemistry and biology of protein folding and how this reaction is competed in the cell by misfolding and aggregation processes, leading to the onset of a variety of human conformational diseases.

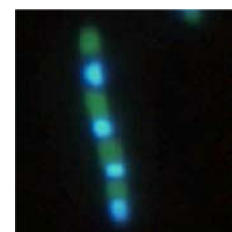
Among other achievements, in the present year:

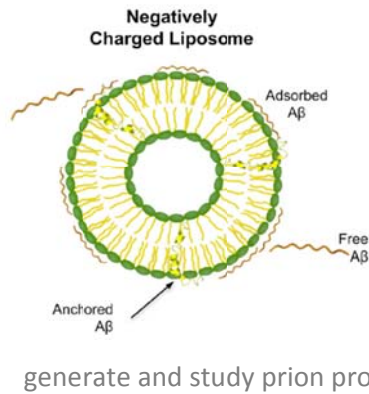
1.- Using atomic force microscopy, single molecule force spectroscopy and molecular dynamics we have addressed the inner forces that stabilize amyloid fibrillar structures (Valle-Delgado JJ. et al. 2012)



2.- We have deciphered the role played by disulfide bonds on the thermodynamic stability of proteins, folding kinetics and specially on the their aggregation into amyloid fibrils. They act as key molecular elements promoting the formation of stable functional forms and precluding the population of aggregating species that might trigger pathological processes. (Grana-Montes R, et al. 2012)

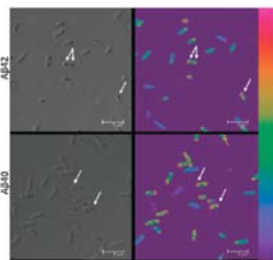
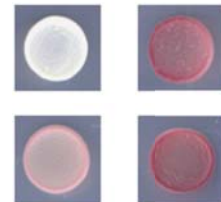
3.- The formation of aggregates by misfolding polypeptides is inherently toxic for the cell, decreasing cellular fitness. Using bacteria as a model organism we have developed a robust system to model and quantify the impact of protein aggregation in cell homeostasis. (Villar-Pique et al., 2012a)





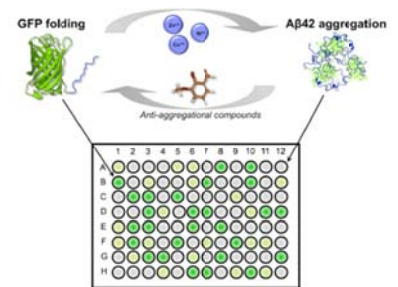
4- The neurotoxicity of the amyloid peptide Aβ is exerted through interactions with neuronal membranes. Using liposomes as model membranes, we have shown that it is the balance between peptide insertion and adsorption in the membrane that modulates its aggregation and toxicity (Sabate et al 2012a).

5- We have shown that bacterial cells might form infective amyloid structures and therefore that they can be used to generate and study prion proteins (Espargaro et al 2012a).



6- We have developed a method that exploits flow-cytometry to screen the impact of genetic mutations or chemical compounds in the aggregation of proteins involved in different pathologies (Espargaro et al 2012b).

7- We have developed a method based on GFP refolding to identify chemical compounds that promote or avoid the aggregation of biotechnological/biomedical relevant proteins (Villar-Pique et al., 2012a).



## Projects

Una visió integrada de la agregació proteica: anàlisi in silico, in vitro, celular, transcriptòmic y proteòmic (INTAG) (BFU2010-14901) Ministerio de Ciencia e Innovación. 2011-2013.

Grup d'estudis de proteïnes autoagregatives (2009 SGR 760) 2009-2013. Generalitat de Catalunya.

ICREA-Academia 2010-2015. Generalitat de Catalunya.

## Others

### PhD thesis

Title: Characterization of intracellular protein aggregates

PhD Student: Anna Villar-Pique

Program: Biochemistry, Universitat Autònoma de Barcelona.

Direction: Salvador Ventura

Year: 2013.

Qualification: Suma Cum Laude

### MSc Thesis

Anna Tarruella. Determinacion y caracterización del principal inductor de fibras amiloides en biofilms de *Staphylococcus aureus* (2013). Universitat Autònoma de Barcelona.

Ricard Illa. AGGRESKAN-3D. A tool to predict aggregation propensity in protein surfaces (2013). Universitat Autònoma de Barcelona.

# Applied Proteomics and Protein Engineering



## Protein Structure

|                     |                                  |
|---------------------|----------------------------------|
| Group Leader        | David Reverter Cendrós           |
| Postdoctoral Fellow | Nathalia Varejão Nogueira da Paz |
| PhD Students        | Pablo Gallego Alonso             |
|                     | Zhen Yang                        |
|                     | Bing Liu                         |

## Overview

- Structural characterization of the activation cascade by the mitotic kinases NEK6, NEK7 and NEK9.
- Structural and functional studies of the de-ubiquitin proteases USP25 and USP28 regulated by SUMO modification.
- Structural characterization of the complex SMC5/SMC6 and its roles as a SUMO E3 ligase.

## Projects

Estudio funcional y estructural de las modificaciones post-traduccionales por la familia ubiquitin/ubiquitinlike (Ref. BFU2012-37116). MEC 2013-2015.

## Others

### *PRESS Communications*

El sincrotró ALBA s'estrena com a microscopi per determinar l'estructura de proteïnes. Noticies UAB. INVESTIGAR. <http://www.uab.es/servlet/Satellite/noticies/detall-d-una-noticia/el-sincrotró-alba-s-estrena-com-a-microscopi-per-determinar-l-estructura-de-prote-nes-1090226434100.html?noticiaid=1345654932646&rendermode=1203663828107%3Fparam1%3D1195026080648%3Fparam1%3D1195026073071>

El sincrotró Alba ajuda a obrir vies en la investigació contra el càncer. <http://www.regio7.cat/gent/2013/04/11/sincrotró-alba-ajuda-obrir-vies-investigació-contra-càncer/229933.html>

# Applied Proteomics and Protein Engineering



El sincrotró Alba detalla per primera vegada l'estructura tridimensional de dues proteïnes.  
<http://www.europapress.cat/societat/noticia-sincrotró-alba-detalla-per-primera-vegada-lestructura-tridimensional-dues-proteines-20130410115618.html>

Descobreixen l'estructura de dues proteïnes que organitzen divisió cel·lular.  
<http://www.324.cat/noticia/2093459/societat/Descobreixen-lestructura-de-dues-proteines-que-organitzen-divisio-cellular>

La luz del sincrotrón ALBA 'ilumina' su primera estructura proteica.  
<http://www.agenciasinc.es/Noticias/La-luz-del-sincrotron-ALBA-ilumina-su-primera-estructura-proteica>

Resolució de les primeres estructures aconseguides amb el sincrotró ALBA.  
<http://www.irbbarcelona.org/index.php/cat/news/irb-news/scientific/irb-barcelona-participates-in-the-resolution-of-the-first-structures-achieved-with-the-alba-synchrotron>

Troben un nou mecanisme d'inhibició enzimàtica, que actua "cap per avall". / Reverter, David (Dpt. Bioquímica i Biologia Mol., Institut de Biotecnologia i de Biomedicina (IBB)).UAB divulga, juny 2013.

<http://www.uab.es/servlet/Satellite?cid=1096481466568&pagename=UABDivulga%2FPage%2FTemplatePageDetallArticleInvestigar&param1=1345657406790>

## NMR Applications in Biomedicine (GABRMN)

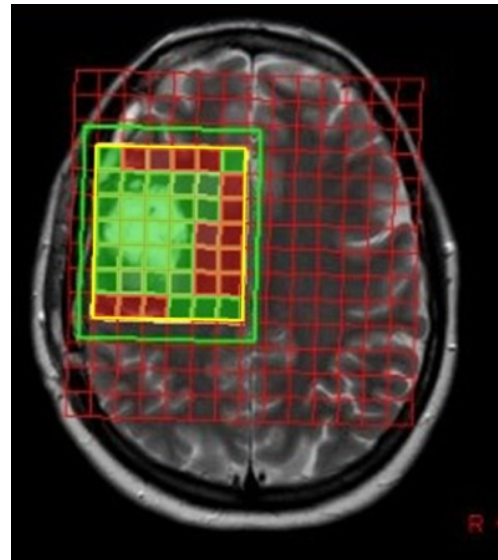
|                |  |
|----------------|--|
| Group Leader   | Carles Arús Caraltó  |
| Senior Members | Margarida Julià Sapé<br>Ana Paula Candiota                 |
| PhD Students   | Myriam Dávila Huerta<br>Magdalena Ciezka<br>Victor Mocioiu |
| Lab Technician | Sandra Ortega Martorell<br>Alina García Chacon             |

### Overview

GABRMN stands for "Grup d'Aplicacions Biomèdiques de la Ressonància Magnètica Nuclear".

Our research group is located jointly at the IBB and at the Unitat de Biociències of the Departament de Bioquímica i Biologia Molecular, located at the Faculty of Biosciences of the Universitat Autònoma de Barcelona, UAB.

The GABRMN@IBB hosts all infrastructure and personnel related to bioinformatics developments needed to fulfil our research lines. The GABRMN@IBB hosts, jointly with the Servei de Ressonància Magnètica (Nuclear Magnetic Resonance Facility) (SeRMN) (<http://sermn.uab.cat/>) of the UAB, one of the CIBER-BBN platform units, the Platform of Biomedical Applications of Nuclear Magnetic Resonance at the Universitat Autònoma de Barcelona.



The bioinformatics platform @IBB, with a total storage capacity of 12TB, is accessible through the UAB network ([agarcia@gabrmn.uab.es](mailto:agarcia@gabrmn.uab.es) for access). It hosts two multicentre databases (INTERPRET and eTUMOUR), with NMR and clinical data for more than 1000 human brain tumour patients and provides consultancy in processing and mathematical analysis of MRSI data, preclinical and clinical.

The platform also distributes GABRMN software packages such as the INTERPRET decision-support system for human brain tumour diagnosis based on MRS and SpectraClassifier, for pattern recognition of in vivo MRS data.

## Others

### PhD thesis

Elena Jiménez Xarrié . Caracterización de la proliferación celular en las zonas subventriculares y de la evolución del infarto mediante espectroscopía de resonancia magnética en un modelo preclínico de isquemia cerebral. Data de lectura: 30/10/2013. Directors: Carles Arús Caralto.

Juana Martín Sitjar de Togores. Contribución al fenotipado molecular de tumores cerebrales preclínicos mediante estudios in vitro e in vivo. Data de lectura: 04/11/2013. Directors: Carles Arús Caralto i Margarida Julià Sapé.

Milena Acosta González. Mejora de los modelos preclínicos de tumores cerebrales. aplicación a la caracterización ex vivo e in vivo de agentes de contraste nanoparticulados para imagen de resonancia magnética. Data de lectura: 03/12/2013. Directors: Carles Arús Caralto i Ana Paula Candiota Silveira.

### Members of:

Carles Arús was awarded the “Certificate of MR Excellence in Basic Science 2013”. Awarded by the ESMRMB society.

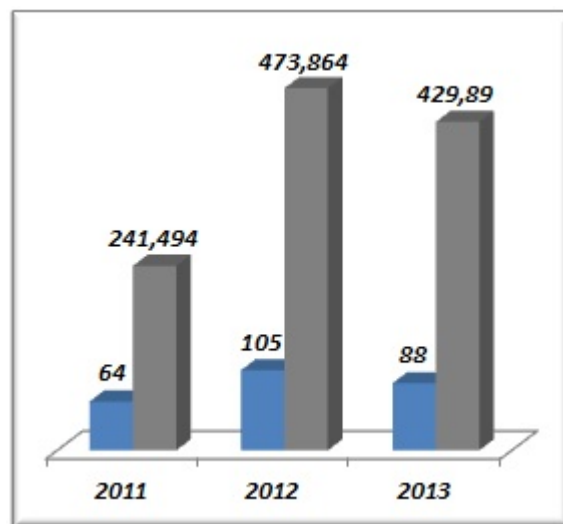
### Editorial work

Carles Arús is member of the editorial board of “MAGMA Magnetic Resonance Materials in Physics, Biology and Medicine”.



## Publications

| Year | No.Articles | Total IF | Average IF |
|------|-------------|----------|------------|
| 2011 | 64          | 241,494  | 3,77       |
| 2012 | 105         | 473,864  | 4,51       |
| 2013 | 88          | 429,89   | 4,89       |



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Aznar, R., A. Grabulosa, A. Mannu, G. Muller, D. Sainz, V. Moreno, M. Font-Bardia, T. Calvet, and J. Lorenzo. 2013. "RuCl<sub>2</sub>(eta(6)-p-cymene)(P\*) and RuCl<sub>2</sub>(kappa-P\*-eta(6)-arene) Complexes Containing P-Stereogenic Phosphines. Activity in Transfer Hydrogenation and Interactions with DNA." *Organometallics* 32 (8): 2344-2362.

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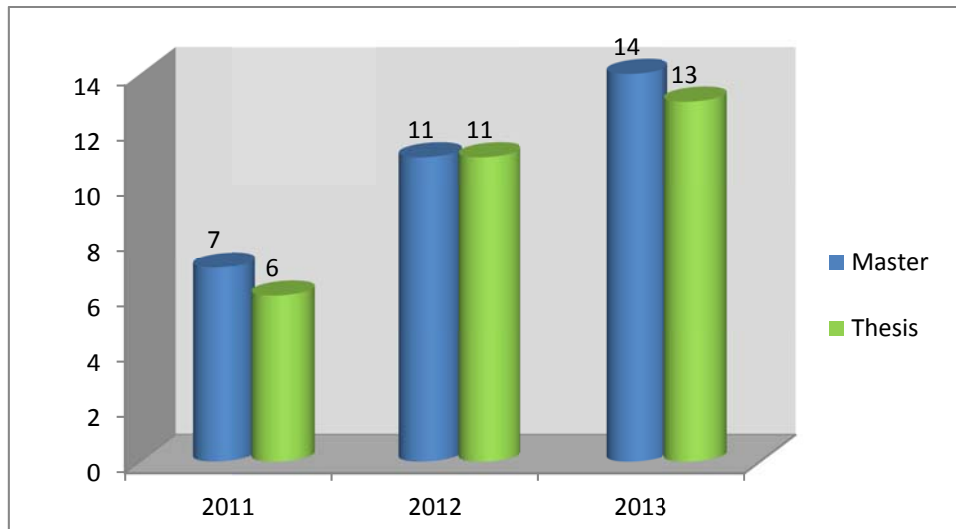
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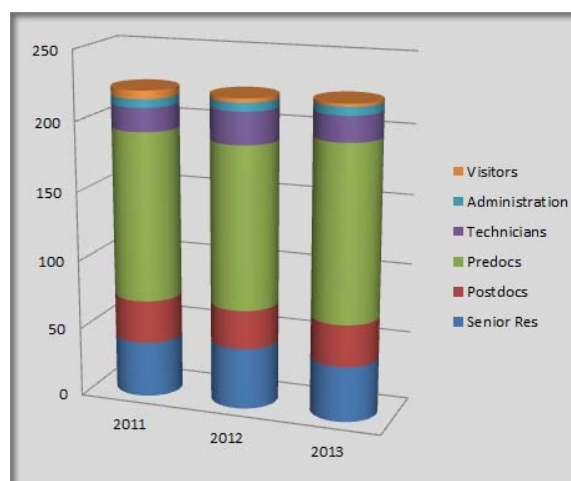
# Key figures

## Thesis



## Human Resources

|      | Senior Res | Postdocs | Predocs | Technicians | Administration | Visitors | Total |
|------|------------|----------|---------|-------------|----------------|----------|-------|
| 2011 | 40         | 31       | 122     | 17          | 6              | 6        | 222   |
| 2012 | 44         | 28       | 117     | 23          | 6              | 3        | 221   |
| 2013 | 40         | 30       | 126     | 18          | 6              | 2        | 222   |



## Funding

