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Institut de Biotecnologia
i de Biomedicina

ANNUAL REPORT

2014

UAB
Universitat Autònoma de Barcelona

http://ibb.uab.cat
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Administrative Structure

Director:	Xavier Daura Ribera
Vicedirector:	Laura Masgrau Fontanet
Manager:	Eva Vila Morros
Fundraising Officer:	Margarita Navia de Roux
Administrative Support:	Natividad Infante Cabrera
	Manuela Romero Chávez
	Rosa Calzada Calvo
	María Teresa Jiménez Batista
	Alicia Zorrilla Guinot
Technical Support:	Almudena Merino Palomar
	Francesca Mestres Folch
	Monica Serrano García

Genome Integrity and Instability

Group Leader	Rosa Miró Ametller
Senior Members	Montserrat García Caldés
	Aurora Ruíz-Herrera
	Ignasi Roig
	Immaculada Ponsa
Postdoctoral Fellow	Rosa Ana Sanchez Guillén
PhD Students	Marina Marcet Ortega
	Marta Andrés Nieto
	Guillem Borràs Gas
	Laia Capilla Pérez
	Helena Castillo Ecija
	Jonathan Fernández
	Arià Hernández
	Ana Martínez
	Cristina Pardo Camacho
	Cristina Rojas Torrijos

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

Manteniment i diversificació del banc de línies cel·lulars d'animals provinents de la col·lecció del Zoo de Barcelona. 2014. PI: Aurora Ruiz-Herrera.

Estudio de los mecanismos que regulan la progresion de la profase meiotica en mamiferos. BFU2013-43965-P. MICINN 2013-2015. PI: Ignasi Roig.

Others

MSc Thesis

Marta Andres. Characterization of immortalized mammalian cell lines. Universitat Autònoma de Barcelona (Spain). Advisor Aurora Ruiz-Herrera. 2014

Jonathan Fernández. Title: Recombination rates in Bovidae. Universitat Autònoma de Barcelona (Spain). Advisor Aurora Ruiz-Herrera. 2014

Cristina Rojas Torrijos. Puesta a punto y aplicación de la técnica de cultivo in vitro de fragmentos de testículo de ratón neonatal para el estudio de la meiosis. . Universitat Autònoma de Barcelona (Spain). Advisor Ignasi Roig. 2014

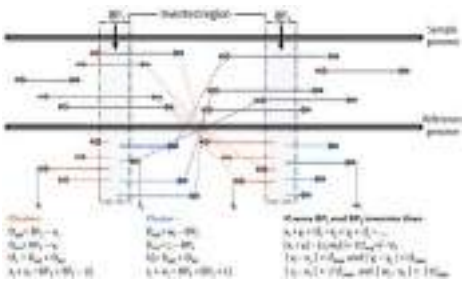
Ana Martínez.: Estudio de la función de CHK2 en ovocitos de ratones perinatales. Universitat Autònoma de Barcelona (Spain). Advisor Ignasi Roig. 2014

Comparative and Functional Genomics

Group Leader	Mario Cáceres Aguilar
Postdoctoral Fellow	Sònia Casillas Viladerrams
	Magdalena Gayà Vidal
	Marta Puig Font
	Lorena Pantano Rubiño
PhD Students	Sarai Pacheco Piñol
	David Vicente Salvador
	David Castellano Esteve
	Carla Giner Delgado
	Esteban Urrea Morales
Lab Technicians	David Izquierdo Fontanils
	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 particualr, 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 INVFEST) UE 2010-2015.

Others

PhD thesis

David Vicente. Análisis, validación y estudio poblacional de las inversiones entre dos genomas humanos. Director: Mario Caceres. 2014

Meritxell Oliva. Functional impact of polymorphic inversions in the human genome. Director: Mario Caceres. 2014

MSc Thesis

Sergi Hervás Fernández. Effects of polymorphic inversions on epigenetic regulation marks in humans. 2014. Mario Cáceres.

Organized meetings

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

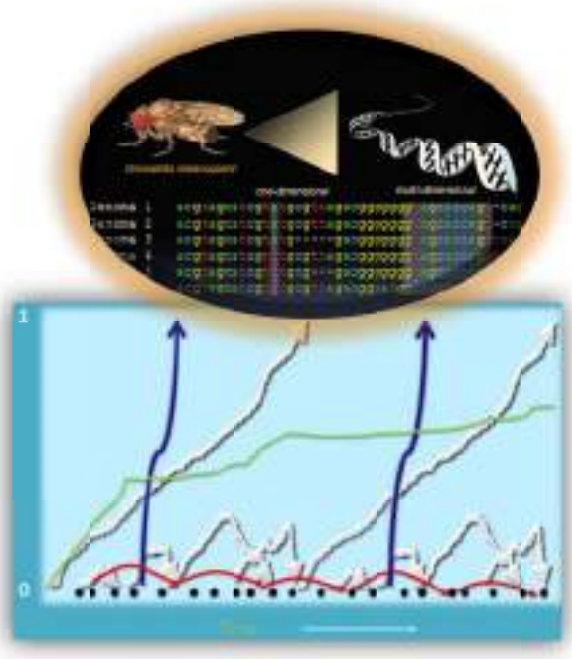
BMC Genomics Associate Editor.

Bioinformatics of Genomics Diversity

Group Leader	Antonio Barbadilla Prados
PhD Students	Sergio González Rodríguez
	Sergio Hervás Fernández
	Maite Garazi Barrón
	Marta Coronado Zamora
	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.

UNAB13-74E-2138. Plataforma Big Data para el análisis bioinformático. IP: Dr. Antonio Barbadilla i Dr. Mario Cáceres. 2013-2015.

Others

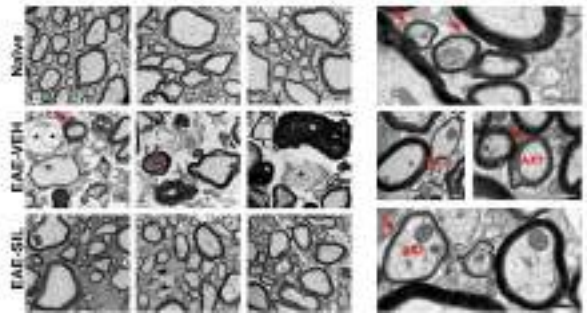
Director of Bioinformatics Platform of campus UAB and UAB sphere Instituts of Health

Promoter of a spin-off of Bioinformatics

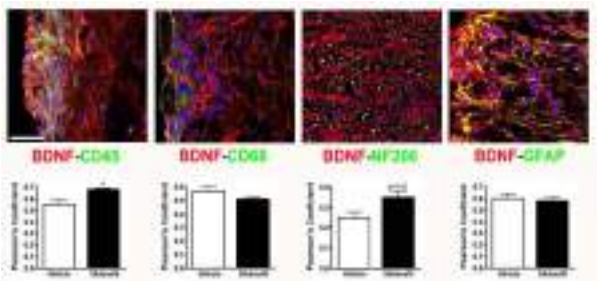
Neuroimmunology

Group Leader	Agustina García Sánchez
Senior Member	Maria Antonia Baltrons Soler
Postdoctoral Fellow	Paula Pifarré
	Maria Gutierrez Mecinas
Predoctoral Fellow	Daniela del Valle Diaz Lucena

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 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 β-amyloid burden reported by other groups in animal models of Alzheimer's disease.

Projects

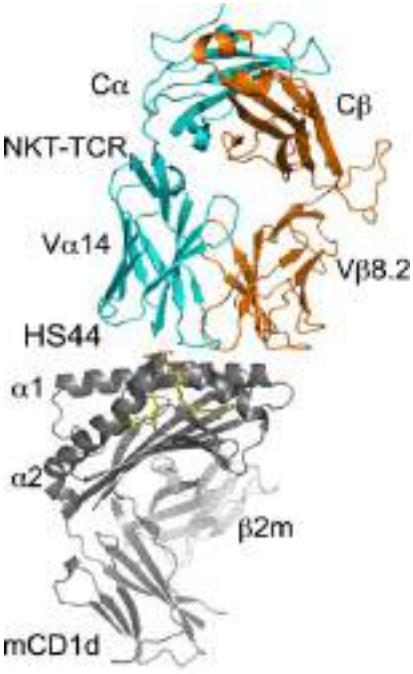
Mecanismos celulares y moleculares del efecto neuroprotector y remielinizante del sildenafilo en la encefalomielitits autoinmune experimental. (SAF2013-44671-P). Ministerio de Ciencia e Innovación. (2014). PI: Agustina García.

Molecular Immunology

Group Leader	Ángel Raúl Castaño
Postdoctoral Fellow	Alari Pahissa, Elisenda
Predoctoral Fellow	Ignasi Esteban
	Noemí Saavedra Ávila

Overview

Activation of iNKT cells by CD1d-ligands is a immunotherapeutic tool under intensive investigation. α-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 α-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 movilization of innate cells from limfoid organs and the chemokines directing such traficking are ongoing efforts in our lab.

Projects

TV32013-130910. Antitumor activity of iNKT activators analogs of the a-GalactosylCeramide: towards immunotherapeutical reagents. IP: Raul Castaño 2014-2016.

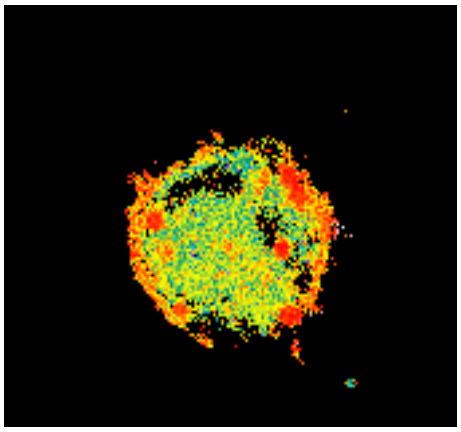
Applied Immunology

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

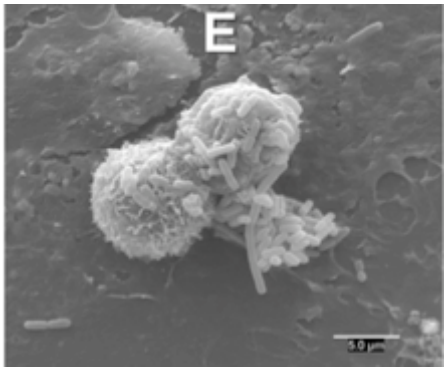
Overview

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 cerevisae* and a new developed prebiotic b-galactomannan, on epithelial intestinal cells and in a porcine model, and their immunomodulation ability in bacterial infections.

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 de1992.

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 Mèdicas de Catalunya i de Baleares des de 1996.

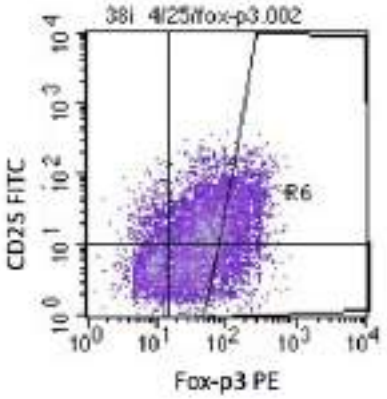
Directora científica del Servicio científico-técnico Cultivos Celulares, Producción de Anticuerpos y Citometría" de la UAB desde Junio de 2009

Celular Immunology

Group Leader	Dolores Jaraquemada
Senior Members	Mercè Martí Ripoll
	Iñaki Alvarez Pérez
	Carme Roura Mir
PhD Students	Teresa Ciudad
	Carolina Guitart
	Erika M. Scholz
	Lorena Usero
	Cristina Xufré
Lab Technician	Annabel Segura
	Anna Mestre Ferrer

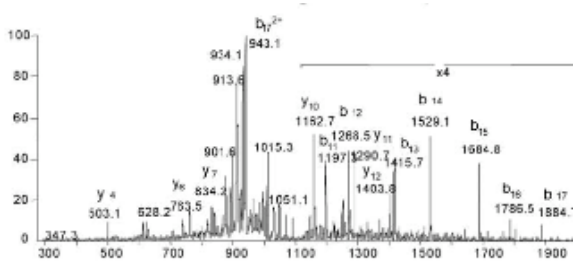
Overview

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.



Projects

SAF2012-35344 (subprogram MED, CICYT, Spanish Science Ministry). From antigens to TCR. A systematic approach to the immune response in type 1 diabetes. IP: Dolores Jaraquemada. 2012 – 2015.

Others

PhD thesis

Carolina Guitart. MHC i malalties autoimmunitàries: contribució específica dels al·lels de susceptibilitat. 2014

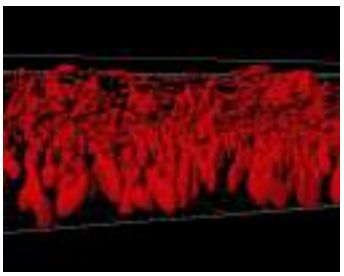
Bacterial Molecular Genetics and Pathogenesis

Group Leader	Isidre Gibert Gonzàlez
Postdoctoral Fellows	Daniel Yero Corona
PhD Students	Celeste Gómez Camacho
	Pol Huedo Moreno
	Sonia Martínez Servat

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

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

Paula Martínez. Caracterització del quorum sensing regulat per les N-acil-L-homoserina lactonas en stenotrophommonas maltophilia. Directors: Isidre Gibert, Daniel Yero, Raquel Planell

MSc Thesis

Pablo Rodríguez Fernández. Stenotrophomonas maltophilia: mecanismos moleculares de resistencia a los antibióticos.2014. Director del treball: Isidre Gibert

Ana Fernandez Carrascal. Utilidad de las técnicas de secuenciación en el estudio de Staphylococcus aureus resistente a la meticil·lina. 2014. Director del treball: Isidre Gibert

Evolutive Immunology

Group Leader	Nerea Roher Armentia
PhD Students	Debora Torrealba Sandoval
	Angels Ruyra Ripoll
	Jie Ji
	Jofre Gasion
	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 (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 INFφ and IL-1b 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

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

Others

PhD thesis

Angels Ruyra. "Liposomes as immunostimulant delivery nanosystems: characterization and application in zebrafish (Danio rerio) and rainbow trout (Oncorhyncus mykiss)". 2014. Directors: N.Roher, D.Maspoch.

Organized meetings

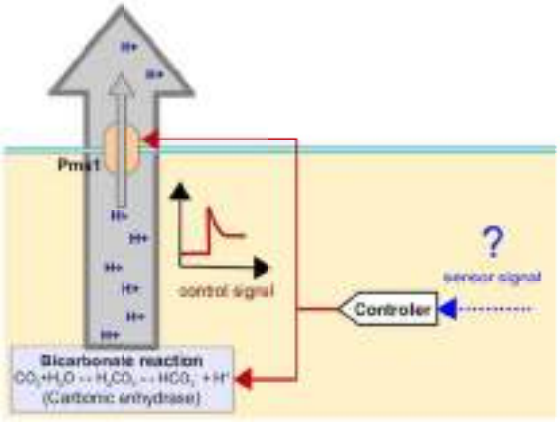
Organization of the workshop: *III Nanomedicine Workshop*; 01/05/ 2014. Universitat Autonoma de Barcelona, Barcelona.

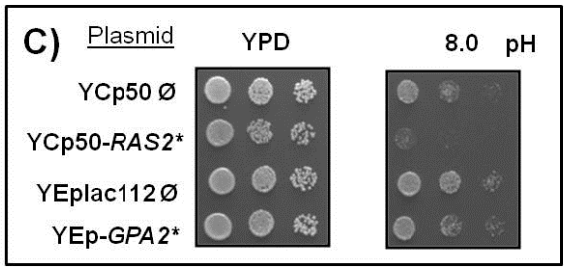
Yeast Molecular Biology

Group Leader	Joaquin Ariño Carmona
Senior Member	Antonio Casamayor Gracia
Postdoctoral Fellows	Silvia Petrezsélyová
	Maria López
PhD Students	Carlos Calafí
	Laura Tatjer Recordà
	Albert Serra Cardona
	Cristina Molero Merinero
	David Canadell i Sala
	Diego Velázquez
	Chun-Yi Zhang
Lab Technician	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 give 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.





Projects

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

Evaluación de la homeostasis ionica y de nutrientes: diferentes estratégias para un objetivo comun (Ref. BFU2011-30197-C03-01) MEC 2011-2014. PI: Joaquin Ariño.

Others

MSc Thesis

Romel Ivan Guevara Guerrero. Análisis de elementos de regulación del promotor de PHO89 de Saccharomyces cerevisiae en respuesta a estrés alcalino. 2014. (Máster oficial en Bioquímica y Biología Molecular). Joaquin Ariño.

Sergio J. García Márquez . Situació actual dels fàrmacs antifúngics i expectatives de futur. 2014. (Máster Oficial de Microbiologia Aplicada, UAB). Joaquin Ariño.

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.

Award to “Excelencia en Investigación 2010”, Universitat Autònoma de Barcelona. (2010-2014)

Computational Biology

Group Leader	Xavier Daura Ribera
PhD Students	Michael Cristòfol Clough
Lab Technician	Oscar Conchillo Solé

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

From genome to antigen: a multidisciplinary approach towards the development of an effective vaccine against Burkholderia pseudomallei, the etiological agent of mieloidosis, Fondazione Cariplo 2011-2014.

Others

Institutional responsibilities

Director of the Institute of Biotechnology and Biomedicine (IBB) of UAB

Commissions of trust

Member of Three Delegate Commissions of UAB's Governing Council: Research (since 2011), Knowledge Transfer and Strategic Projects (since 2012) and Doctorate (since 2013).

Project evaluation for EU's H2020, since 2014.

Project evaluation for the Italian Association for Cancer Research (AIRC), Italy, since 2011.

Project evaluation for the Partnership for Advanced Computing in Europe (PRACE), EU, since 2012.

Peer rewiew for several journals, including Journal of the american Chemical society, Andgewandte Chemie International Edition, PLoS Computational Biology, Journal of Chemical Theory and Computational, Bioinformatics, etc.

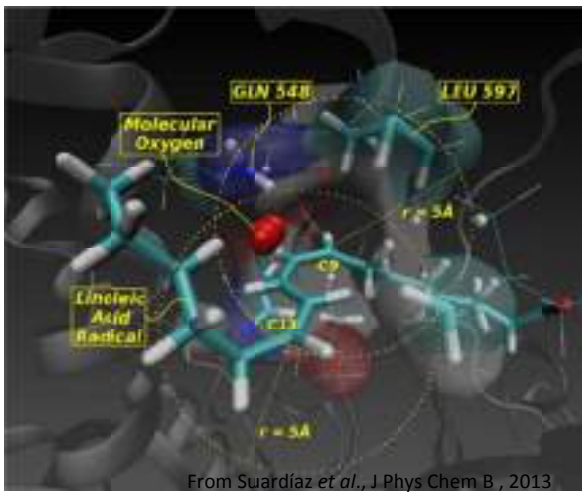
Theoretical Molecular Biology

Group Leader	Josep M. Lluch
Senior Members	Àngels González Lafont
	Mireia García Viloca
	Laura Masgrau
Postdoctoral Fellow	Reynier Suárez Díaz
	Patricia Saura Martínez
PhD Students	Ayax Pérez Gallego
	Maria Fernanda Mendoza
	Chun-Yi Zhang

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 anb 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.



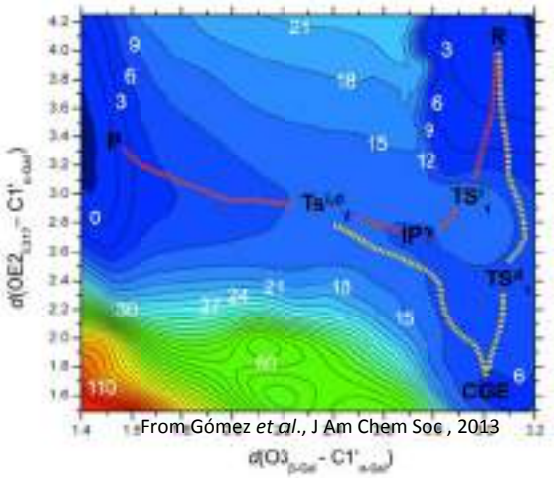
From Suardíaz *et al.*, J Phys Chem B , 2013

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 stereosecific 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

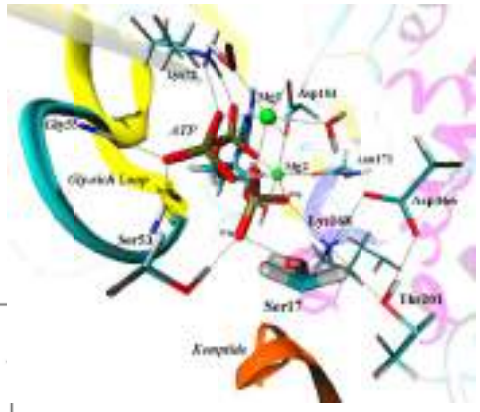
hypothesis seems to be the operating one in this enzyme. On another hand, we have started the study of the hydrogen abstraction step.

- **Computational chemical glycobiology:** 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.

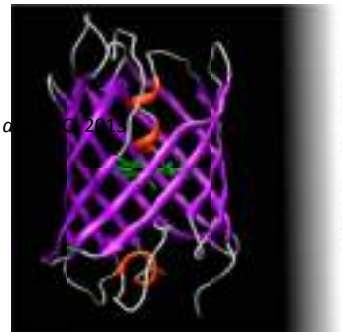


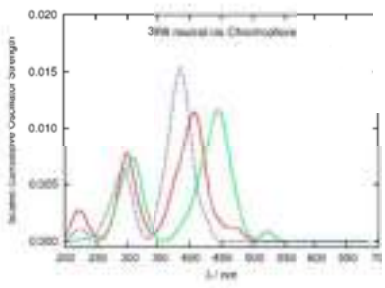
From Gómez *et al*., J Am Chem Soc , 2013

- **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 applyied 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*., JPC 2013



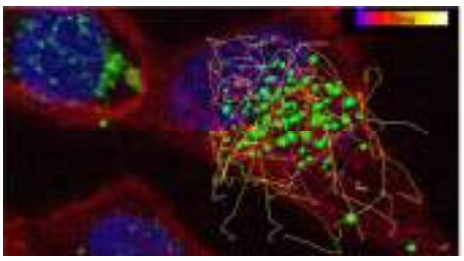
Projects

Adscribed at the Department of Chemistry of the UAB.

Nanobiotechnology

Group Leader	Antonio P. Villaverde
Senior Members	Neus Ferrer
	Esther Vazquez
	José Luis Corchero
	Elena Garcia Fruitós
	Joaquin Seras
PhD Students	Olivia Cano
	Mireia Pesarrodona
	Paolo Saccardo
	Ugutz Unzueta
	Xu Zhikun
	Naroa Serna
	Laura Sanchez
	Fabián L. Rueda
Lab Technician	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

Provision of operational and technical expertise in relation to chemical and biochemical processes and advanced product development. INNOTUNE BVBA. IP Antoni Villaverde

Genotoxic nanoparticles targeting colorectal cancer stem cells. TV32013-132031. IP Antoni Villaverde

Ingenieria de nanoparticulas proteicas para la entrega dirigida de proteinas terapeuticas y de acidos nucleicos. BIO2013-41019-P. IP Antoni Villaverde.

Ingeniería del vehículo y el cargo en la terapia génica no vírica del cáncer colorrectal metastásico. PI12/00327. IP Esther Vazquez Gomez.

Personalized nanomedicine for triple negative breast cancer stem cells. TV32013-133930. IP Esther Vazquez Gomez.

Others

MSc Thesis

Naroa Serna. Design, production and characterization of neurotropic self assembling protein nanoparticles. 2014. Neus Ferrer-Miralles

Patent

Marco Colás, María Pilar; Pascual Durán, Nuria; Pastells Díez, Carme; Sanchez Baeza, Francisco; Villaverde Corrales, Antonio Pedro; Rodríguez Carmona, Escarlata. Haptenos y conjugados derivados de piocianina, anticuerpos de los mismos, y método inmunoquímico para la detección de infecciones provocadas por pseudomonas aeruginosa. WO2014135730 A. US20160033489. 2014

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.

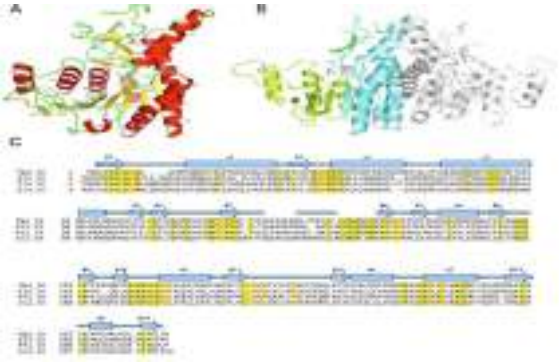
Editor de Medical Sciences (ISSN 2076-3271) desde 2012.

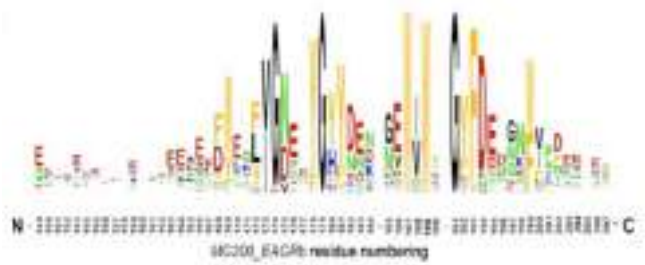
Molecular Biology

Group Leader	Enrique Querol Murillo
Senior Members	Jaume Piñol Ribas
	Josep A. Perez Pons
Postdoctoral Fellow	Ángel Mozo
	Xavier Serra Hartmann
	Oscar Quijada
	Merçe Ratera
PhD Students	Isaac Amela Abellán
	Luis González González
	Luis Franco Serrano
	Ana María, Martínez
	Luis García Morales
	Mario Huerta Casado
	Marta Hernández Solans
	Cristian Ponce Basco
	Sergi Torres Puis

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

¿Son la mayoria de las proteinas multifunionales (MOONLIGHTING)?. BFU2013-50176-EXP. IP Enrique Querol.

Coordinació i dinamització Grups Tecnio UAB-CSIC a l'entorn del PRUAB. TECCIT12-1-0007-08. IP Enrique Querol.

Analisis de los mecanismos de virulencia y patogenicidad en micoplasmas: diseño de vacunas contra algunas especies de interes clinico. BIO2013-48704-R. IP Jaume Piñol.

Others

PhD thesis

Alicia Broto. Anàlisi Funcional de Dominis de Proteïnes Implicades en la Motilitat de Mycoplasma genitalium.2014. Directors: E.Querol, J.Piñol

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* straints, and use thereof ”EP 2 684959 A1”.

Inventors Gonzalez Luis Gonzalez, RIBAS Jaume PIÑOL, Giralt Jordi Montane, Malet Maria Camats, Murillo Enrique Querol, ARNAU Marta SITJA. WO2014135730 A1. Haptenos y conjugados derivados de piocianina, anticuerpos de los mismos, y método inmunoquímico para la detección de infecciones provocadas por pseudomonas aeruginosa. US20160033489

RIBAS Jaume PIÑOL, Virgili Sergi Bru, SOLER Laura FERRER, ARNAU Marta SITJA, Murillo Enrique Querol. WO2014009586 A3. Cepa viva atenuada de actinobacillus pleuropneumoniae. US20150306200

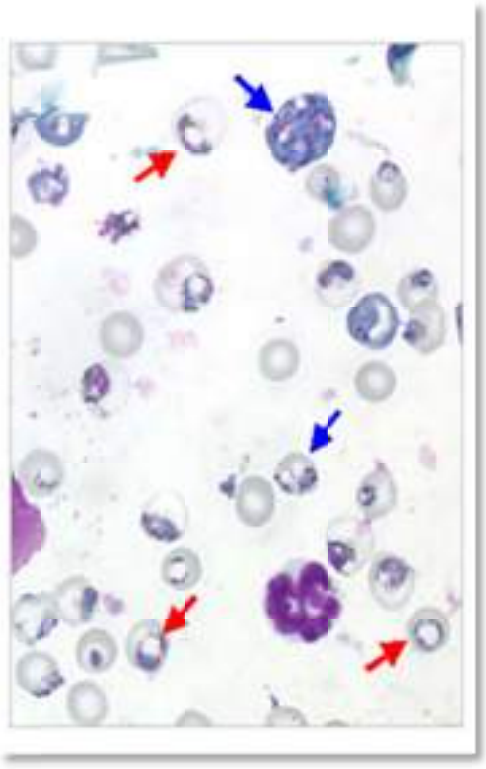
Protein Engineering and Proteomics

Group Leader	Francesc X. Avilés Puigvert
Senior Members	Josep Vendrell Roca
	Julia Lorenzo Rivera
PhD Students	Giovanny Covaleda
	Olivia Tort Regas
	Anabel Otero
	Javier Garcia Pardo
	Esther Berenguer de la Cuesta
	Marc Fernández Méndez
	María del Carmen García Guerrero
	Carla Granados Colomina
	Sergi Montané Bel
	David Montpeyó García-Moreno
	Anabel Otero Bilbao
	Irantzu Pallarés Goitiz
	Alejandra Rodríguez Morales

Overview

Our group's interests lie in protein engineering, focusing on the study of protease precursors and inhibitors in general, and on metallocarboxipeptidases 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 Cataluña 2014SGR1658. 2014. IP: F. X. Avilés.

Interactomica diseño de sondas e imagen de carboxipeptidasas. en transito de la funcion a la aplicabilidad. BIO2013-44973-R.2014. IP: F. X. Avilés

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 (2007-2014)

Coordinator of the Network on "Genomics and Proteomics", at the Catalunya level (Xarxa Generalitat) (an. 2001- 2014).

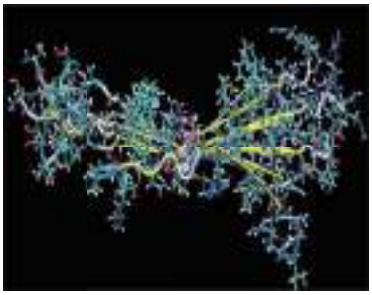
Protein Folding and Conformational Diseases

Group Leader	Salvador Ventura Zamora
	Susana Navarro Cantero
PhD Students	Ricardo Graña-Montes
	Patrizia Marinelli
	Anita Carija
	Marta Díaz Caballero
	Sebastián Andrés Esperante Bedani
	Francisca Pinheiro
	Ricardo Sant'Anna Oliveira

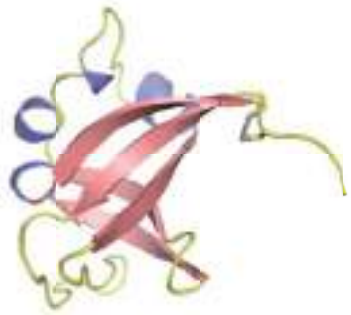
Overview

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.

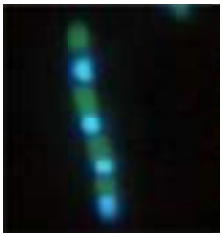
Among other achievements, in the present year:



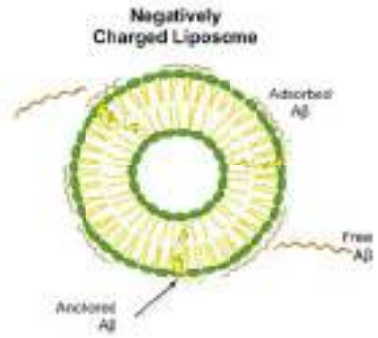
1.- Using atomic force microscopy, single molecule force spectroscopy and molecular dynamics we have addressed the inner forces that stabilize amyloid fibrillar structures (Valle-Delgado JJ. et al. 2012)



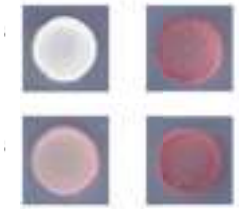
2.- We have deciphered the role played by disulfide bonds on the thermodynamic stability of proteins, folding kinetics and specially on the their aggregation into amyloid fibrils. They act as key molecular elements promoting the formation of stable functional forms and precluding the population of aggregating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



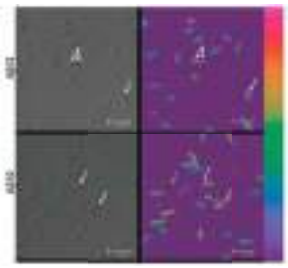
3.- The formation of aggregates by misfolding polypeptides is inherently toxic for the cell, decreasing cellular fitness. Using bacteria as a model organism we have developed a robust system to model and quantify the impact of protein aggregation in cell homeostasis. (Villar-Pique et al., 2012a)



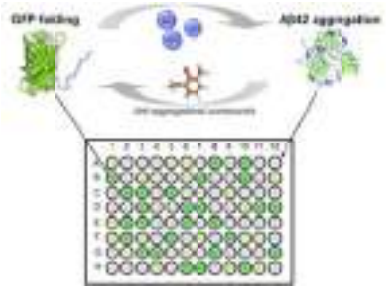
4- The neurotoxicity of the amyloid peptide Abeta is exerted through interactions with neuronal membranes. Using liposomes as model membranes, we have shown that it is the balance between peptide insertion and adsortion in the membrane that modulates its aggregation and toxicity (Sabate et al 2012a).



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

Grup d'estudis de proteïnes autoagregatives (**2014SGR 938**) 2014. Generalitat de Catalunya.

ICREA-ACADEMIA Award 2009 in Life and Medical Sciences. 2010-2015. Generalitat de Catalunya. IP: Salvador Ventura

Descubrimiento, caracterizacion y diseño de nuevos amiloides funcionales auto-replicativos. BFU2013-44763-P. IP: Salvador Ventura.

Desarrollo de un medicamento para el tratamiento de la amiloidosis por transtiretina. Empresa: SOM INNOVATION BIOTECH SLU. RTC-2014-1931-1. IP: Salvador Ventura.

Others

PhD thesis

Ricardo Graña. Analysis of different evolutionary strategies to prevent protein aggregation. 2014. Director: Salvador Ventura.

Protein Structure

Group Leader	David Reverter Cendrós
Postdoctoral Fellow	Nathalia Varejáo 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

PhD thesis

Pablo Gallego. Structural studies of Protein-Protein interactions: Analysis of the regulation of the DYNLL/LC8 binding to Nek9 and characterization of the enzymes composing the arginine deiminase pathway inMycoplasma penetrans. 2014. Director: D. Reverter

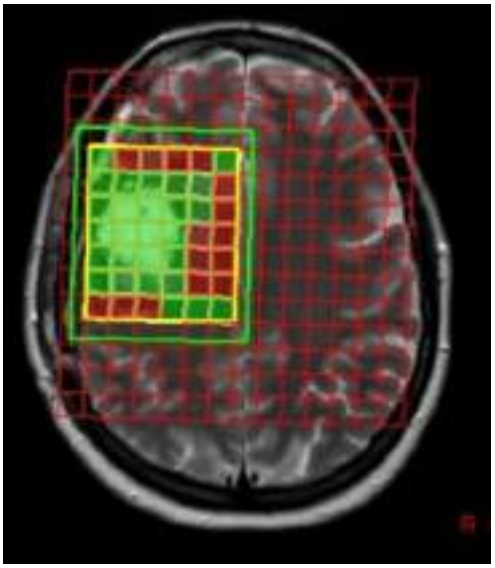
Zhen Yang. Structural and funcional studies on the regulation of the USP28 de-ubiquitinase and the SENP5 de-SUMOylase. 2014. Director: D. Reverter

NMR Applications in Biomedicine (GABRMN)

Group Leader	Carles Arús Caraltó
Senior Members	Margarida Julià Sapé
	Ana Paula Candiota
PhD Students	Magdalena Ciezka
	Victor Mocioiu
	Laura Ferrer Font
	Xavier Serra Mocioiu
Lab Technician	Alina García Chacón

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 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.

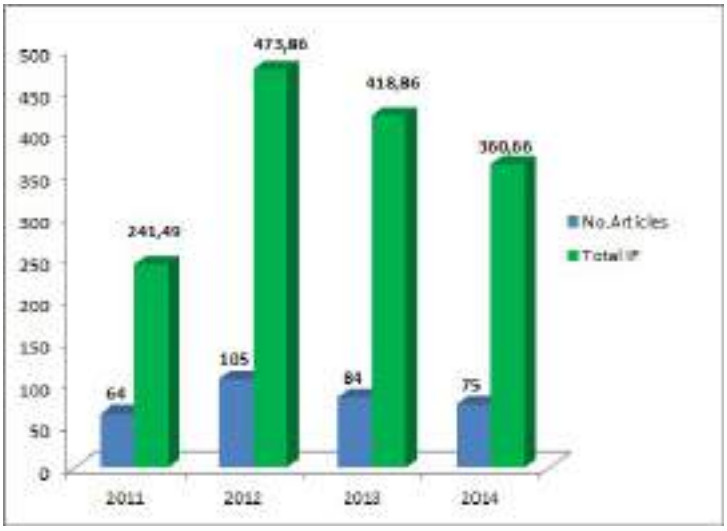
Others

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	241,49	3,77
2012	105	473,86	4,51
2013	84	418,86	4,99
2014	75	360,66	4,81



Huang, Wen, Andreas Massouras, Yutaka Inoue, Jason Peiffer, Miquel Ramia, Aaron M. Tarone, Lavanya Turlapati, Thomas Zichner, Dianhui Zhu, Richard F. Lyman, Michael M. Magwire, Kerstin Blankenburg, Mary Anna Carbone, Kyle Chang, Lisa L. Ellis, Sonia Fernandez, Yi Han, Gareth Highnam, Carl E. Hjelmen, John R. Jack, Mehwish Javaid, Joy Jayaseelan, Divya Kalra, Sandy Lee, Lora Lewis, Mala Munidasa, Fiona Ongeri, Shohba Patel, Lora Perales, Agapito Perez, LingLing Pu, Stephanie M. Rollmann, Robert Ruth, Nehad Saada, Crystal Warner, Aneisa Williams, Yuan-Qing Wu, Akihiko Yamamoto, Yiqing Zhang, Yiming Zhu, Robert R. H. Anholt, Jan O. Korbel, David Mittelman, Donna M. Muzny, Richard A. Gibbs, Antonio Barbadilla, J. Spencer Johnston, Eric A. Stone, Stephen Richards, Bart Deplancke, and Trudy F. C. Mackay. 2014. "Natural variation in genome architecture among 205 Drosophila melanogaster Genetic Reference Panel lines." *Genome Research* 24 (7): 1193-1208.

Aguado, C., M. Gaya-Vidal, S. Villatoro, M. Oliva, D. Izquierdo, C. Giner-Delgado, V. Montalvo, J. Garcia-Gonzalez, A. Martinez-Fundichely, L. Capilla, A. Ruiz-Herrera, X. Estivill, M. Puig, and M. Caceres. 2014. "Validation and Genotyping of Multiple Human Polymorphic Inversions Mediated by Inverted Repeats Reveals a High Degree of Recurrence." *Plos Genetics* 10 (3).

Alamo, P., A. Gallardo, M. A. Pavon, I. Casanova, M. Trias, M. A. Mangues, E. Vazquez, A. Villaverde, R. Mangues, and M. V. Cespedes. 2014. "Subcutaneous preconditioning increases invasion and metastatic dissemination in mouse colorectal cancer models." *Disease Models & Mechanisms* 7 (3): 387-396.

Alegre, K. O., and D. Reverter. 2014. "Structural insights into the SENP6 Loop1 structure in complex with SUMO2." *Protein Science* 23 (4): 433-441.

Angarica, V. E., A. Angulo, A. Giner, G. Losilla, S. Ventura, and J. Sancho. 2014. "PrionScan: an online database of predicted prion domains in complete proteomes." *Bmc Genomics* 15(14):1194-1203.

Arino, J., E. Aydar, S. Drulhe, D. Ganser, J. Jorrin, M. Kahm, F. Krause, S. Petrezselyova, L. Yenush, O. Zimmermannova, G. P. H. van Heusden, M. Kschischo, J. Ludwig, C. Palmer, J. Ramos, and H. Sychrova. 2014. "Systems Biology of Monovalent Cation Homeostasis in Yeast: The Translucent Contribution." In *Advances in Microbial Systems Biology*. Ed. R. K. Poole, 1-63.

Armengol, P., R. Gelabert, M. Moreno, and J. M. Lluch. 2014. "New insights into the structure-spectrum relationship in S65T/H148D and E222Q/H148D green fluorescent protein mutants: a theoretical assessment." *Organic & Biomolecular Chemistry* 12 (48): 9845-9852.

Boltana, S., R. Tridico, M. Teles, S. Mackenzie, and L. Tort. 2014. "Lipopolysaccharides isolated from Aeromonas salmonicida and Vibrio anguillarum show quantitative but not qualitative differences in inflammatory outcome in Sparus aurata (Gilthead seabream)." *Fish & Shellfish Immunology* 39 (2): 475-482.

Bomati-Miguel, O., N. Miguel-Sancho, I. Abasolo, A. P. Candiota, A. G. Roca, M. Acosta, S. Schwartz, C. Arus, C. Marquina, G. Martinez, and J. Santamaria. 2014. "Ex vivo assessment of polyol coated-iron oxide nanoparticles for MRI diagnosis applications: toxicological and MRI contrast enhancement effects." *Journal of Nanoparticle Research* 16 (3): 1-13.

Candiota, A. P., M. Acosta, R. V. Simoes, T. Delgado-Goni, S. Lope-Piedrafita, A. Irure, M. Marradi, O. Bomati-Miguel, N. Miguel-Sancho, I. Abasolo, S. Schwartz, J. Santamaria, S. Penades, and C. Arus. 2014. "A new ex vivo method to evaluate the performance of candidate MRI contrast agents: a proof-of-concept study." *Journal of Nanobiotechnology* 12.

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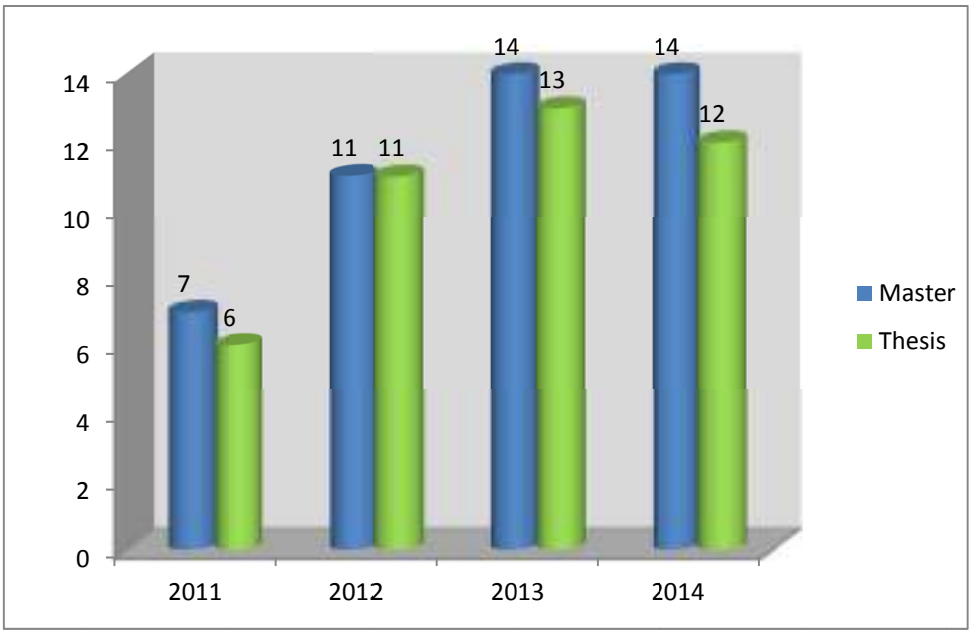
Thesis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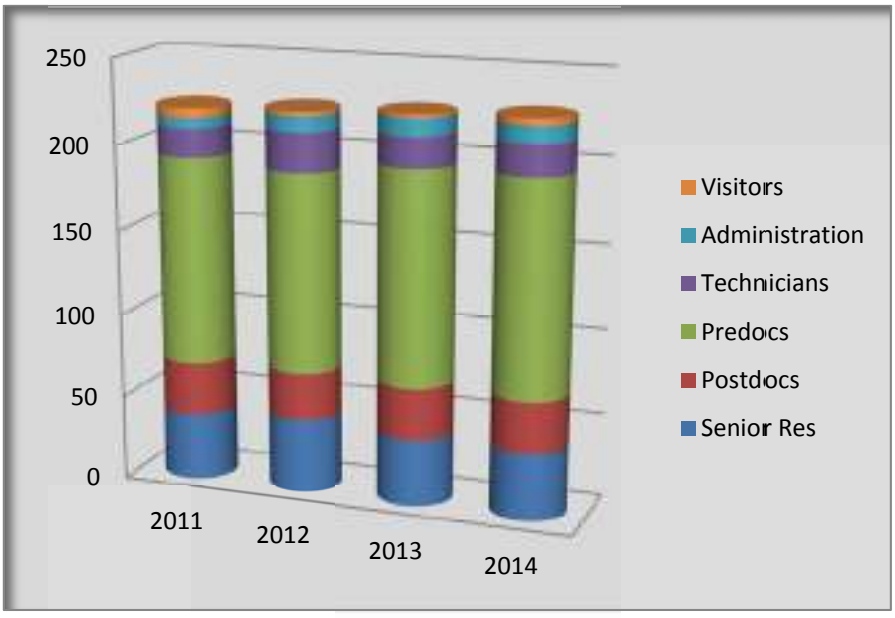
Human Resources

	Senior Res	Postdocs	Predocs	Technicians	Administration	Visitors	Total
2011	40	31	122	17	6	6	222
2012	44	28	117	23	9	3	224
2013	40	30	126	18	10	2	226
2014	40	30	126	18	10	4	228



Funding


Competitive Funds
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918.839,58 €
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