Institute of Physical Chemistry

ROCASOLANO

Scientific Report 2019-2020

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Institute of Physical Chemistry

Spanish National Research Council

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The editors would like to thank all the staff of the Institute who have contributed to the realization of this Scientific Report.

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Vice-director

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Vice-director

Presentation

Carlos González Ibáñez

The "Rocasolano" Institute of Physical Chemistry (Instituto de Química Física "Rocasolano", IQFR) is one of the oldest institutes in CSIC. With the present name, it was founded in 1946. However, its history is much older since it continues the scientific tradition of the old National Institute of Physics and Chemistry (Instituto Nacional de Física y Química), founded in 1932 by the Committee for Advanced Studies (Junta de Ampliación de Estudios, JAE). Our mission in this 87-year history has been to enhance the excellent research in fundamental and applied physical chemistry, contributing to the scientific training of multiple generations of researchers at the highest level. Our vision is to continue being an international reference in multidisciplinary research focused to the resolution of the present challenges of our society in the fields of health, biotechnology, new materials and environment.

The IQFR is located at the so called "Rockefeller" building, constructed and equipped thanks to a donation from the International Education Board of the Rockefeller Jr. Foundation in the 1920s as an acknowledgment of the excellence of the scientific work carried out by Blas Cabrera, Miguel A. Catalán, Enrique Moles, Julio Palacios and others. This was the first "modern" research center in Spain, both in the design of the building, and in terms of its operating standard, comparable to the best modern research centers of that time. The quality of the research and level of international connections can be seen from the number of distinguished visitors such as Arnold Sommerfeld, William Bragg and Marie Curie, among many others. Our guestbook, preserved since the opening day in 1932, is a privileged witness of that period of the history of Spanish science.

This promising start was sadly cut off by the Spanish Civil War. In 1938 the JAE was suppressed and in 1939 the Spanish National Research Council (CSIC) was created. The premises and belongings of the JAE were transferred to the CSIC, and the Rockefeller building became the seat of the institutes "Alonso de Santa Cruz" of Physics (1940-1966) and "Alonso Barba" of Chemistry (1940-1967). Both institutes were the seed of the Institute of Physical Chemistry "Rocasolano", Optics, Organic Chemistry and Plastic and Rubber. Afterwards, the evolution of the "Rocasolano" institute gave rise to the Institute of Catalysis and Petrochemistry (1975), and the Institute for the Structure of Matter (1976). Moreover, the intense training activity performed at the IQFR during the decades from 1950 to 1970 contributed decisively to the creation of multiple university chairs, departments and laboratories of physical chemistry, inorganic, organic and technical chemistry. During all these years, the library of the institute has played an essential role, being an iconic reference in chemistry and physics, and with a good number of historical collections.

Nowadays, the research carried out in the institute can be classified in three main topics: biological physical chemistry, materials and fundamental physical chemistry, and atmospheric chemistry. The application of chemical-physical techniques to problems of biological interest has been a very successful line of research, taking advantage of the top-level instrumentation of the Institute. It has to be highlighted the recent nomination of the "Manuel Rico" High Field Nuclear Magnetic Resonance Laboratory as singular scientific and technical infrastructure (ICTS). The strong activity in biological NMR together with world-wide recognized crystallography group and experts in biophysical techniques make the IQFR an international reference in the field of structural biology. Singular technical capabilities

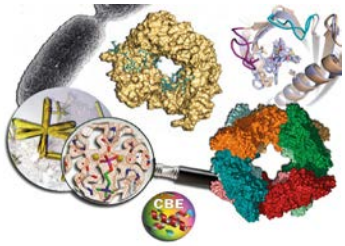
in the institute include a recently installed LEEM (low-energy electron microscopy) and state-of-the art laser techniques. Researchers at the IQFR apply these techniques to multiple fundamental problems in physical chemistry with strong implications in nanoscience and materials technology. The prominent position of the institute in the application of laser technologies to heritage preservation is another strength, which has led researchers from the IQFR to head one of the recently created CSIC Thematic Platforms (PAIS). The activity of the IQFR in atmospheric chemistry is more recent, but very successful. Its excellence was recognized by the awarding of a European Research Council grant (CLIMAHAL) in 2017. Transversal to the different research lines is the position of the IQFR in different aspects of computational methods, which cover fields from theoretical chemistry, phase transitions, bioinformatics, or atmospheric chemistry modeling.

The IQFR has always had a vocation for collaborative research, as shown by the high degree of internationalization of our publications. In this regard, it is also important to mention the intense activity of IQFR's associated units with a number of universities and research centers. All this interdisciplinary research carried out in the institute is clearly linked to some of the United Nation's Sustainable Development Goals. In particular, we expect to contribute to goals like "Good Health and Well-Being", "Industry Innovation and Infrastructure", and "Climate Action".

Finally, it is important to mention the many teaching and science dissemination actions carried out by the personnel of the IQFR. Our privileged location in the center of Madrid certainly facilitates the increasing success of these activities among the general public. Many of these actions are equality-oriented, with a special focus on promoting and visualizing the role of women in Science.

Research and dissemination activity at the IQFR would not be possible without the strong support of specialized units in information technology, electronics and mechanics, as well as a heavy-duty administrative office. The commitment of all the personnel, researchers as well as technical and administrative staff, makes the Rocasolano Institute of Physical Chemistry stay in the frontline of scientific progress.

Departments



Department of Crystallography and Structural Biology

Armando Albert

Department of Atmospheric Chemistry and Climate

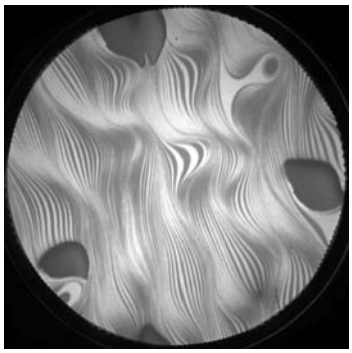
Alfonso Saiz López

- Energetics, Structure and Molecular Reactions Group (ESMR)
- Photolysis and Chromatography
- Atmospheric Chemistry and Climate

Department of Biological Physical Chemistry

M. Ángeles Jiménez

- NMR of Protein Structure, Dynamics and Interactions
- Protein Bioconformatics and Assemblies
- Structural Bioinformatics
- Fluorescence and Molecular Biophysics
- Protein Structure and Thermodynamics
- NMR of Nucleic Acids



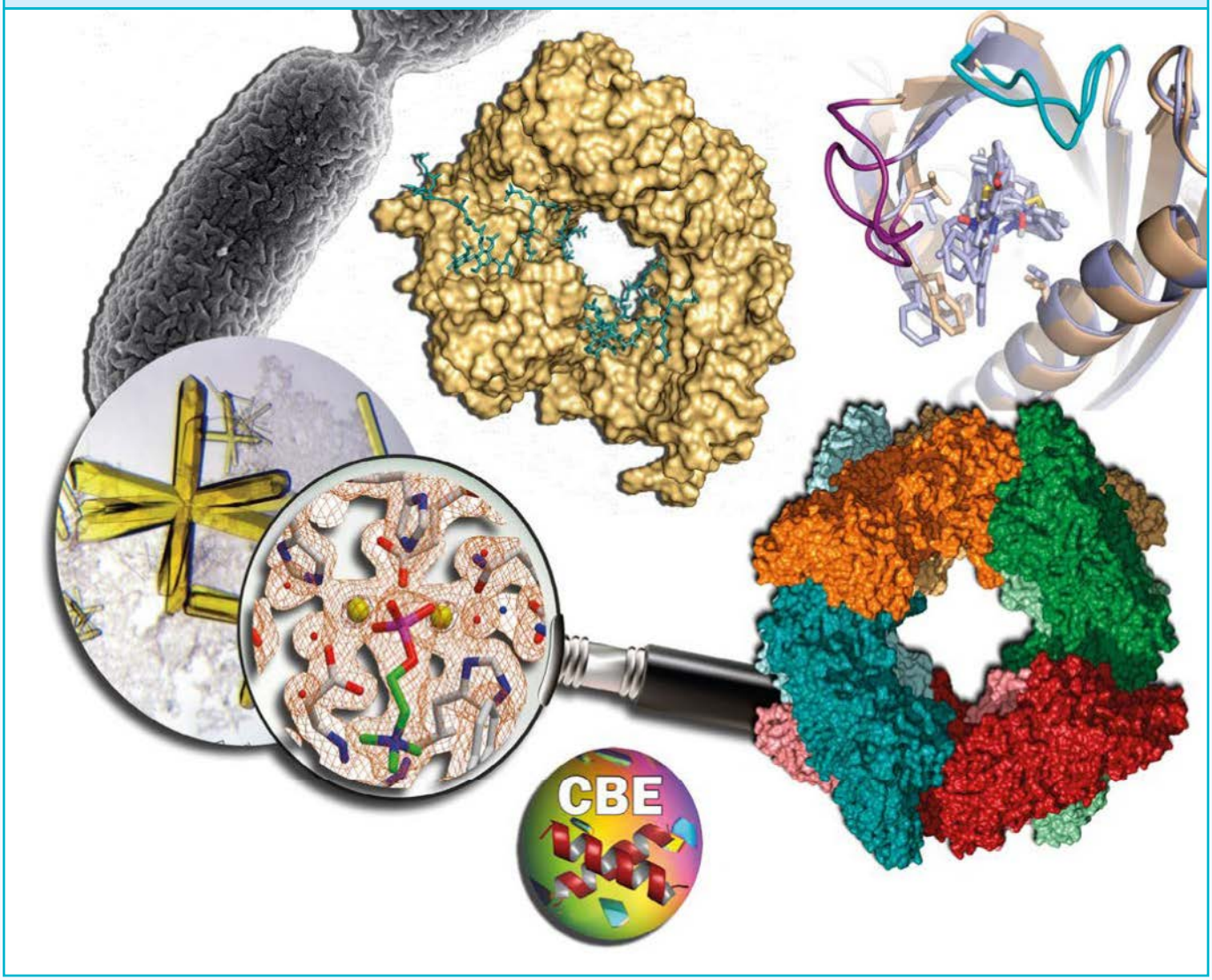
Department of Low Dimensional Systems, Surfaces and Condensed Matter

Eva González Noya (since 23/06/2020)

- Lasers, Nanostructures and Materials Processing
- Laser Materials and Laser-Materials Interaction
- Statistical Mechanics and Condensed Matter
- Surface Analysis and Mössbauer Spectroscopy


CONSEJO SVPERIOR DE INVESTIGACIONES CIENTIFICAS

Department of Crystallography and Structural Biology



Introduction

The research of the Department focuses on understanding the biological functions of macromolecules in terms of their 3D structure at atomic, molecular and supramolecular levels. This provides information on their functionality and ability to recognize other molecular partners or a substrate, or to develop their activity in a particular environment. To achieve these objectives, we combine chemical, physical-chemical and biological techniques. Among them, crystallography occupies a preferential place since it is the most powerful technique to characterize single macromolecules or large stable macromolecular complexes at atomic level. Such knowledge provides the basis for new medical treatments and many biotechnological applications (https://www.xtal.iqfr.csic.es/). In addition, our Department is also involved in the development of novel and efficient phasing methods, and strategies that make possible the solution of protein structures.

The Department is fully equipped with state-of-the-art technologies to develop our research. Our molecular biology laboratory is perfectly set up and equipped with all the modern technologies to produce recombinant proteins at milligram scale with high purity. We have also established an automated crystallization platform, which offers the newest and fastest tools for the screening of crystallization conditions using a minimum amount of protein sample. The platform includes two crystallization robots and a Xe chamber for derivatizing protein crystals. In addition, a diffraction laboratory is equipped with several microscopes and a micro source x-ray generator for assessing protein crystals quality and to accomplish chemical crystallography projects. All these facilities are available for all CSIC researchers and for those coming from other institutions through the "Laboratorio de Difracción de Rayos X para muestras Monocristalinas" (http://www.xtal.iqfr.csic.es/DRXM/).

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(16/03/2019 -31/03/2020)

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(PhD student) (From 25/11/20)

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Paula Sanz Benito
(PEJ)

Summary

The molecular structure contains information related to its function and relationship with the environment. This is key to understand how enzymes recognize and promote the reactivity of a substrate or how complex systems, made up of proteins, interact with others at particular cell place, to transmit a punctual stimulus in a certain time. Crystallography is an essential tool to discover structure, however, its value is increased through the development of new methodological strategies, both for structural resolution and analysis, and through the use of other techniques that establish a multidisciplinary approach that integrates structural information in the biological context.

Strategic Aims

- Membrane delimited signaling pathways involved in plant cell response to abiotic stress.
- Molecular design of highly efficient biocatalysts for synthetic chemistry.
- Multienzyme cascades for the production of second-generation prebiotics from biomaterials.
- Structural characterization of pivotal bacterial cell-wall remodeling processes and implications in antibiotics resistance.
- Identification of new drug targets and development of antimicrobials against multidrug-resistant pathogens.
- Development of new therapeutics and biomedical tools to tackle synaptic dysfunction in neuronal disease.
- Deciphering the molecular basis of major host-pathogen interactions in pathogenic mycobacteria.
- Unravelling the antibiotic resistance mechanisms in bacteria by mix-and-inject serial crystallography techniques at XFELs.

Remarkable Results

Improved plants against climate change

Environmental damage, together with climate change, are driving the water-related crises we see around the world. Stress situations such as drought or the concomitant soil salinity affect crop productivity as they unbalance intracellular ion composition in plants. In these situations, and spontaneously, plants attempt to readjust ion homeostasis for normal growth. We have described the mechanism by which the regulatory protein kinase CIPK23 is specifically assembled to the AKT1 K^+ channel to restore cell ion requirements. This information is central to produce novel crop varieties with improved performance in changing environment.

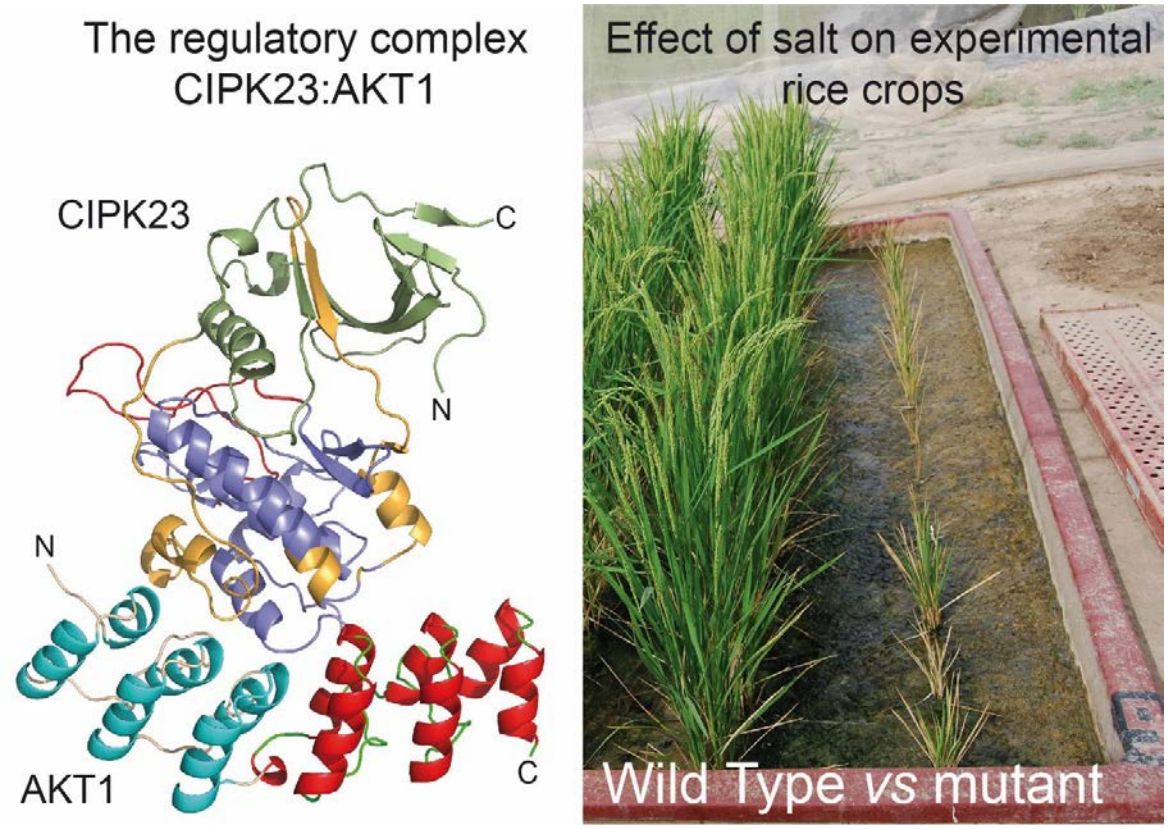

Figure 1: The drawing shows the recognition and activation of the plant AKT1 potassium channel by the kinase CIPK23.Plant Physiology (2020) 182, 2143–2153 (doi:10.1104/pp.19.01084)

Molecular design of highly efficient biocatalysts for synthetic chemistry

Enzymatic engineering allows the generation of highly effective biocatalysts for more sustainable processes and has enormous potential in many other therapeutic and diagnostic applications in biomedicine. In this sense, we have followed two approaches; one has been the *de novo* creation of active sites generating a *plurizyme*, a serine ester hydrolase with two active sites, one natural and one synthetic, in which the catalytic efficiency, specificity and stereoselectivity have been significantly improved. Then, one of the two active sites has been transformed into a metal-complex chemocatalytic site, facilitating synergistic chemo- and biocatalysis in a dual, single protein. The second strategy has been the use of supramolecular engineering of the enzyme nano-environment to create a complex network surrounding the enzyme that transforms substrate promiscuous and non-enantioselective enzymes into highly enantioselective yet promiscuous biocatalysts.

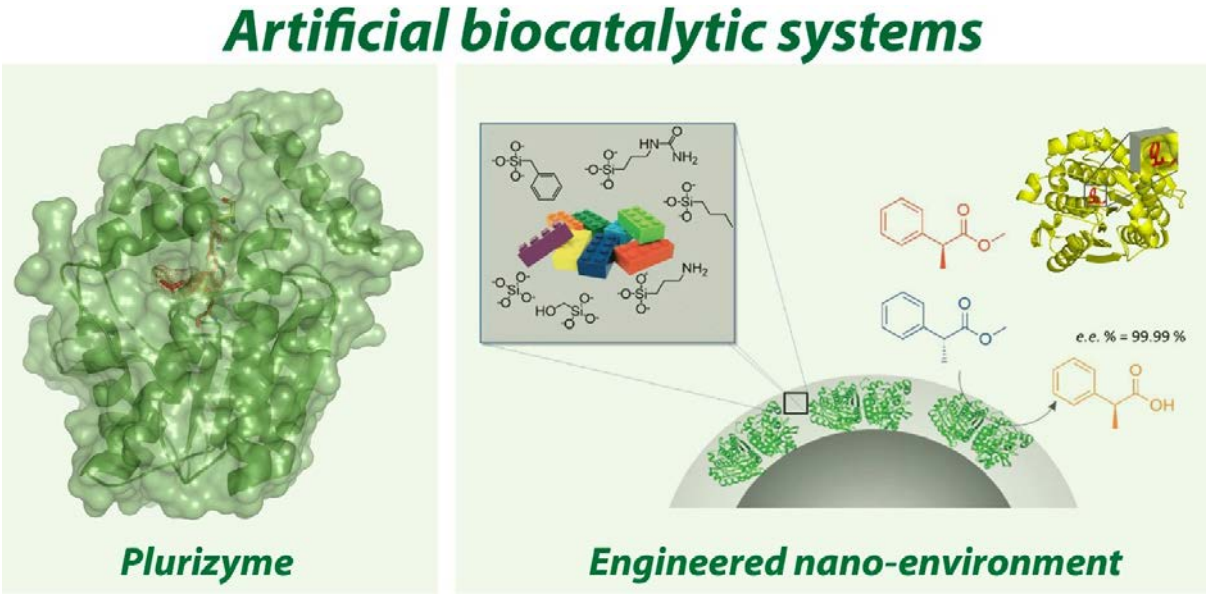

Figure 2: The figure shows a *plurizyme* performing synergistic chemo- and biocatalysis (Nature Catalysis, 2020 3, 319-328), and a highly enantioselective, promiscuous engineered biocatalyst (ACS NANO, 2020, 14, 17652−17664)

Production of prebiotics and bioactive compounds

Our work has focussed in the enzymatic production of bioactive compounds. Among them, prebiotics are functional ingredients stimulating selectively the growth of beneficial bacteria in the digestive tract, contributing to prevent cardiovascular disease, colon cancer and osteoporosis. These compounds show different functional profiles and, therefore, there is a growing interest in the design of new products to manipulate the individual microbiome. Thus, we have studied the molecular mechanisms behind the specificity of several enzymes producing prebiotic galactooligosaccharides (GOS) and xilooligosaccharides (XOS). We have also focused on the glycosylation of polyphenols with anti-inflammatory, neuroprotective and anti-tumoral properties, to improve its biodisponibility profile.

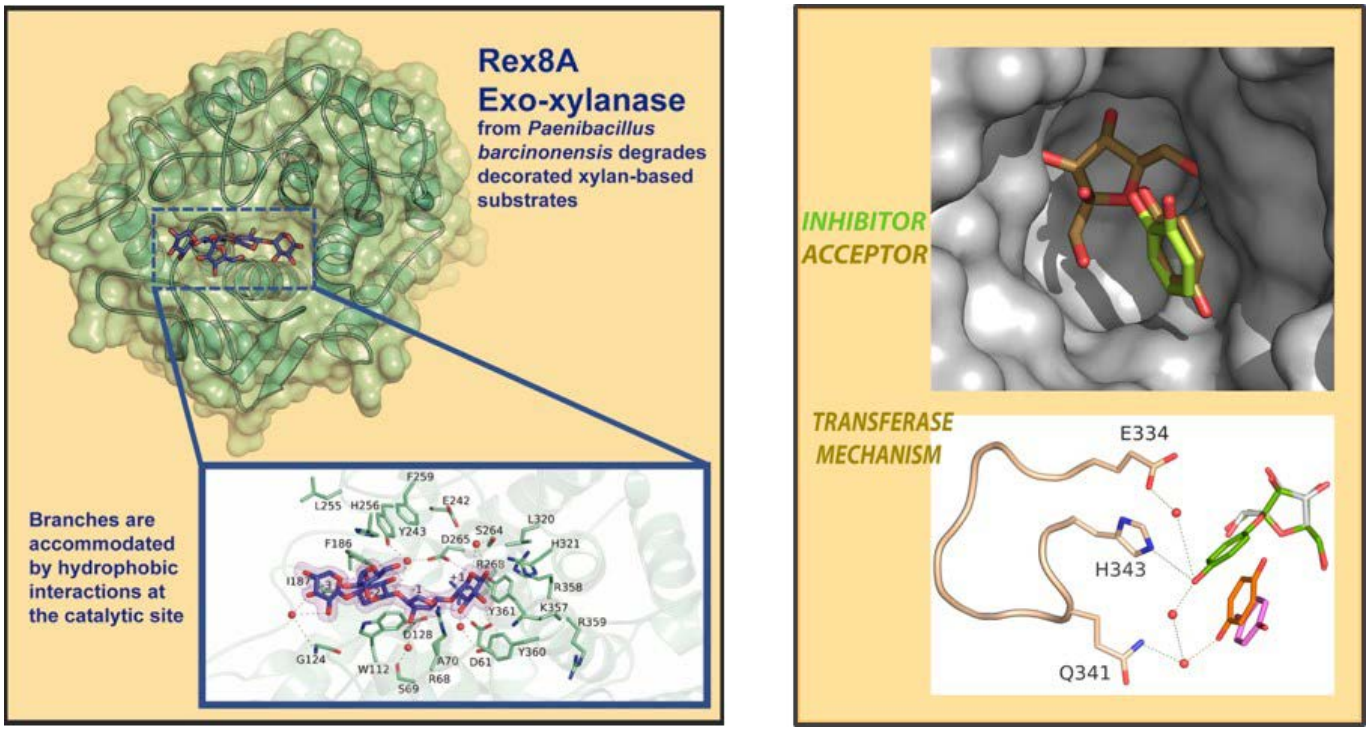

Figure 3: A bacterial xylanase producing XOS by degrading branched xylans (Febs J. 287, 5362-5374 (2020).Molecular basis of the acceptor/inhibitor activity of phenols vs FFase from yeast (Scientific Reports 9:17441 (2019).

Structural characterization of human PAH responsible for phenylketonuria disease

Phenylalanine hydroxylase (PAH) is a key enzyme in the catabolism of phenylalanine, and mutations in this enzyme cause phenylketonuria (PKU), a genetic disorder that leads to brain damage and mental retardation if untreated. Some patients benefit from supplementation with a synthetic formulation of the cofactor tetrahydrobiopterin (BH4) that partly acts as a pharmacological chaperone. Crystal structures, of PAH at 3.18 Å resolution, show the interactions between the cofactor and PAH, explaining the negative regulation exerted by BH4.The crystal structure of phenylalanine hydroxylase (PAH) provided the first and long-awaited 3D-structure of the full-length human PAH, both unbound and complexed with the tetrahydrobiopterin (BH4) cofactor.

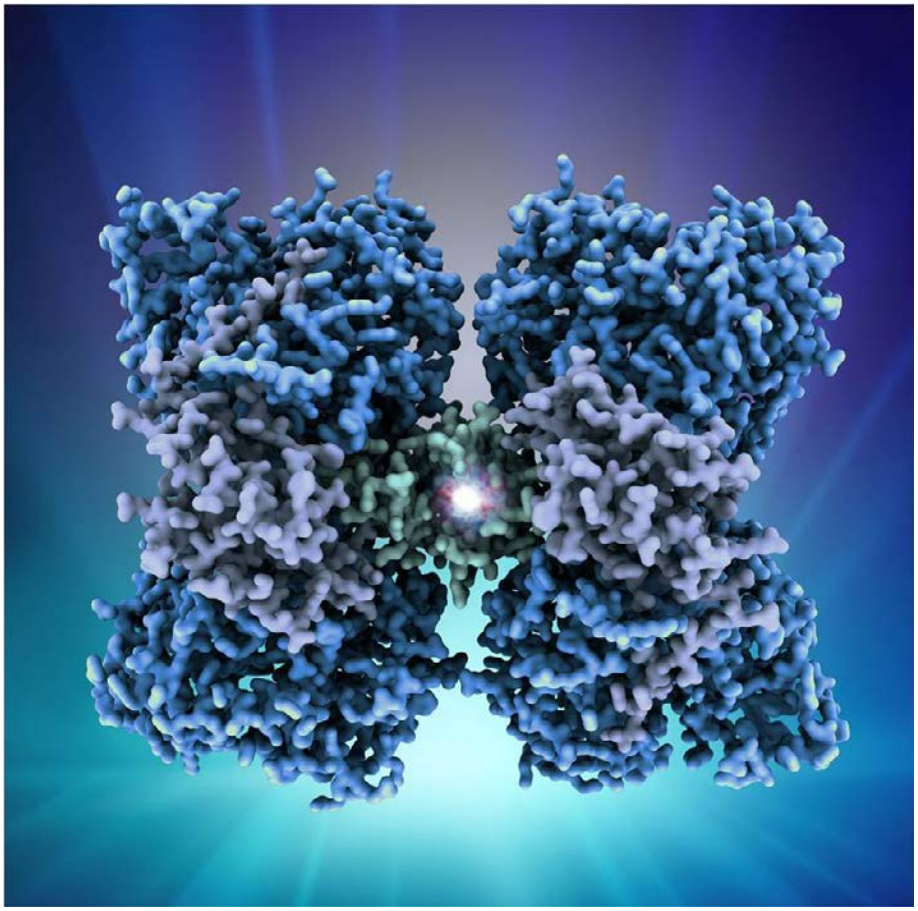

Figure 4: The figure shows the tetrameric arrangement of human PAH as reported in https://www.pnas.org/content/116/23/11229

Structure of a key machinery in the process of bacterial division

A team from the IQFR (CSIC) and the Univ. of Notre Dame (United States) has revealed the structure of a key machinery in the process of bacterial division. The conclusions, published in the journal Nature Communications, open the door to the design of a future drug capable of blocking this precise machinery, without which the bacteria become sensitive to the antibiotic effect.

The crystal structures of the SPOR domain at atomic resolution (1.2 Å), in the apo state and in complex with different synthetic glycans, provided insight into the molecular basis for recognition and delineate a conserved pattern in other SPOR domains. The biological and structural observations presented here are followed up by molecular-dynamics simulations and by exploration of the effect on binding of distinct peptidoglycan modifications. These results provided an explanation to an unresolved question since decades: how the SPOR domains, present in almost all bacteria and with very little sequence homology, can all recognize the same type of cell-wall during bacterial division.

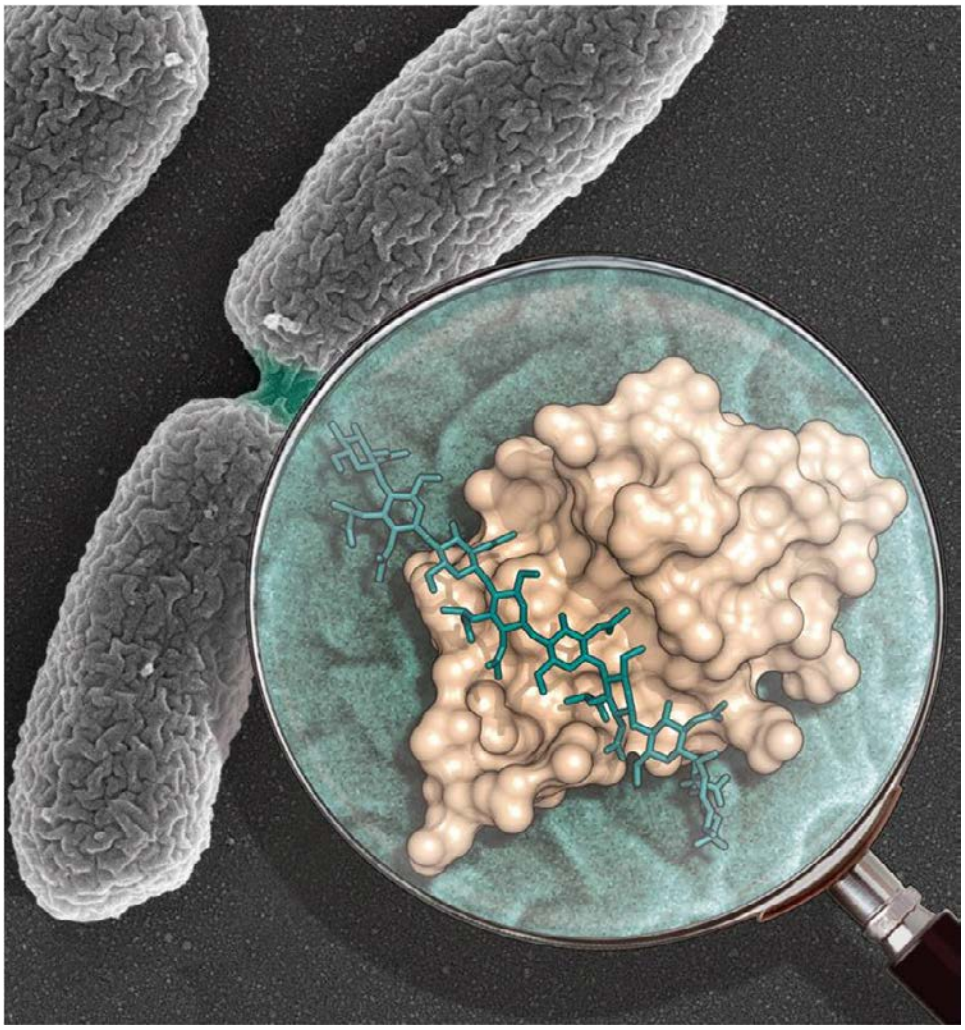

Figure 5: Three-dimensional structure of SPOR domain (light brown surface) in complex with a cell-wall fragment (green sticks). Background electron microscopy picture of the multidrug-resistant bacteria Pseudomonas aeruginosa (https://www.nature.com/articles/s41467-019-13354-4).

Psychrophilic versus mesophilic 2´-deoxyribosyltransferases

The functional and structural characterization of the 2´-deoxyribosyl transferase from the psychrophilic bacteria *Desulfotalea psychrophila* isolated in the arctic marine sediment off the coast of Svalbard and its comparison with the mesophilic homolog from *Enterococcus faecalis* V583 found in the gastrointestinal tracts of healthy mammals is providing important clues about the adaptation of enzymatic activity to conditions of low temperature.

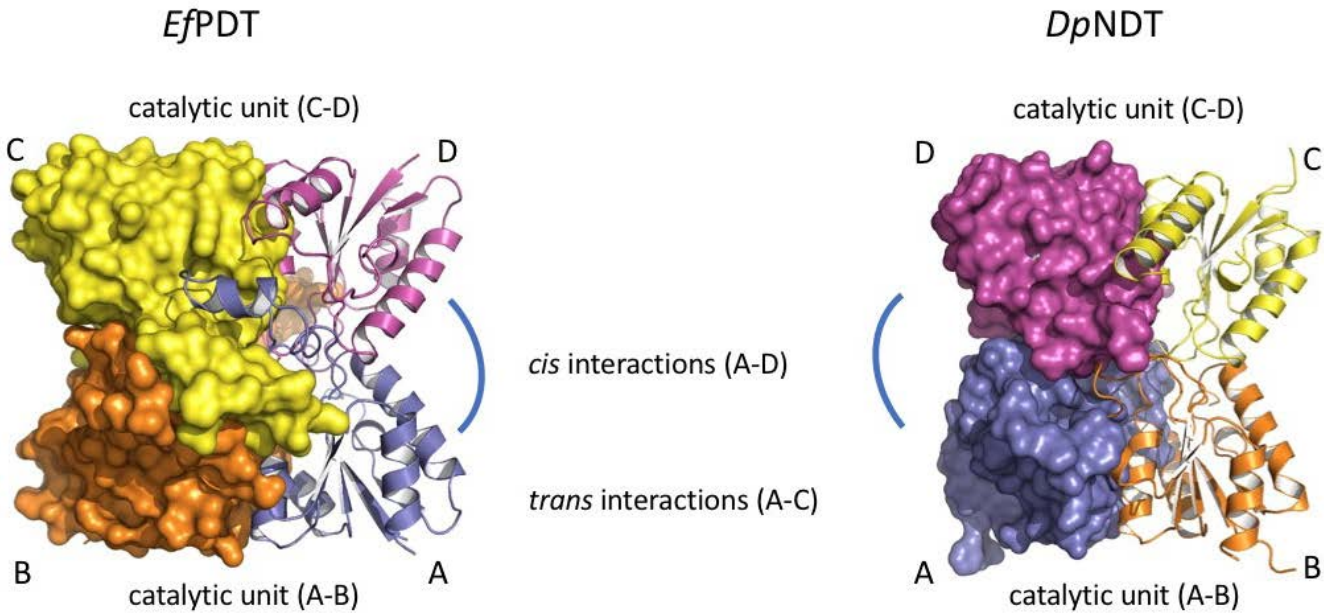

Figure 6: Three-dimensional structures of 2´-deoxyribosyltransferases from *E. faecalis* (*Ef*PDT) and *D. psychrophila* (*Dp*NDT). (Sent for publication).

Tannase from Fusobacterium nucleatum nucleatum

The bacterium *F. nucleatum* is among the most prevalent bacterial species in colorectal cancer tissues. The structure of the hydrolase of gallotannins (tannase) from this bacterium has revealed for the first time the presence of a polyamine-binding site that helps understanding the inhibition of its catalytic activity by these molecules and more importantly the influence of environmental factors of the tumors in the survival of the bacterium.

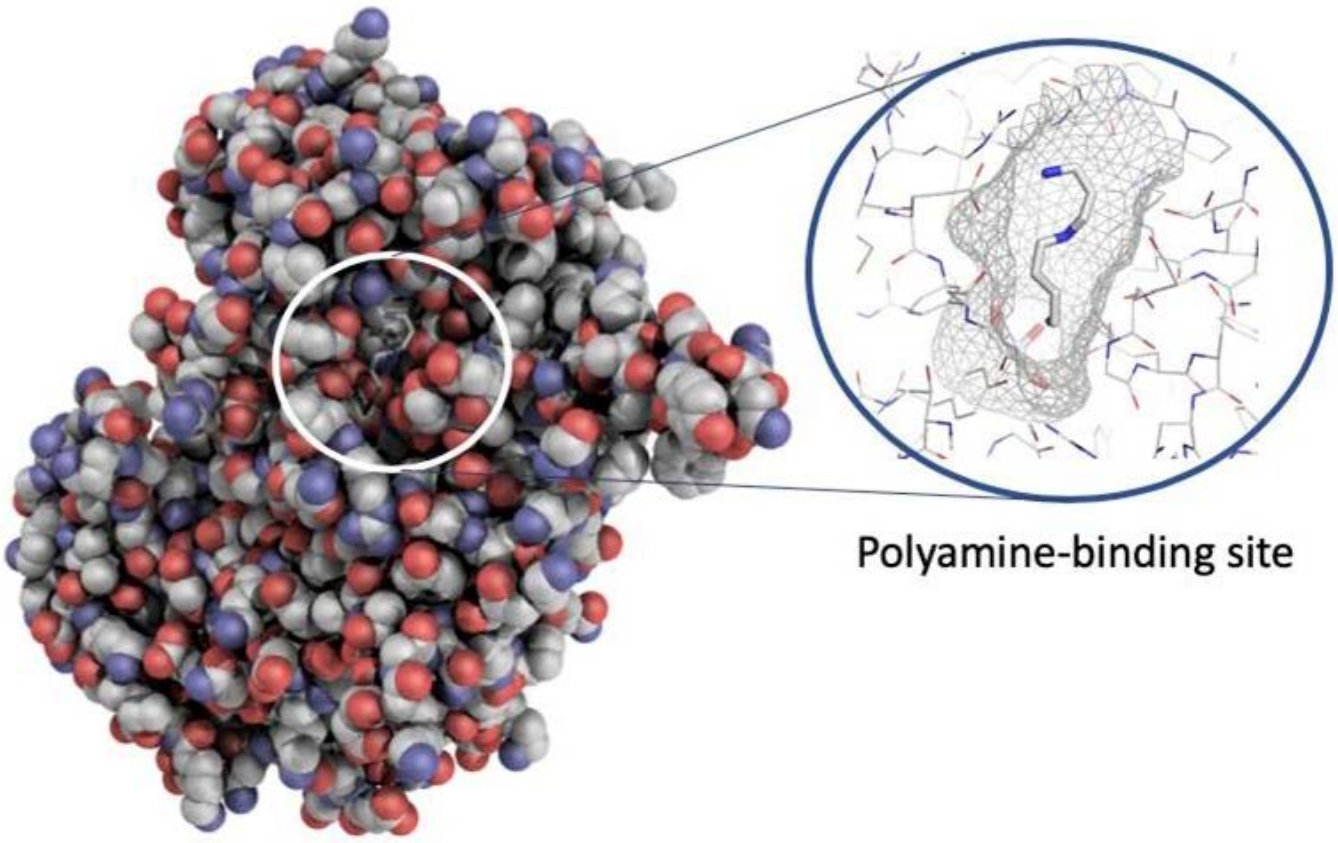

Figure 7: Structure of the tannase enzyme from *F. nucleatum nucleatum* showing a molecule of spermidine within the polyamine-binding site, that connects to the active site. (doi:10.1111/1751-7915.13732).

Inositide signalling and connection with phosphate metabolism

Inositol phosphates (InsPs) are a set of compounds with pleiotropic functions. They are second messengers in signalling, regulators of nucleic acids metabolism etc. Pyrophosphoinositides (PP-InsPs) conform a particular subgroup of InsPs which act as sensors of inorganic phosphate levels in yeasts, and are involved in apoptosis in mammals. InsPs and phosphate metabolisms converge in an enzyme, DDP1, able to degrade PP-InsPs, polyphosphates and dinucleotide phosphates. DDP1 is a NUDIX enzyme with pyrophosphatase activity and unique among its family due to its ability to act on three very different substrates. We have studied the molecular basis of DDP1 function by Crystallography analysing multiple crystal complexes with analogues of its three substrates. Protein-ligand recognitions is produced by phosphate clamping what defines a binding-path in DDP1 active site. As phosphate uptake is essential for fungal metabolism and survival, these findings might be key to treat fungal infections by approaching DDP1 inhibition. (sent for publication).

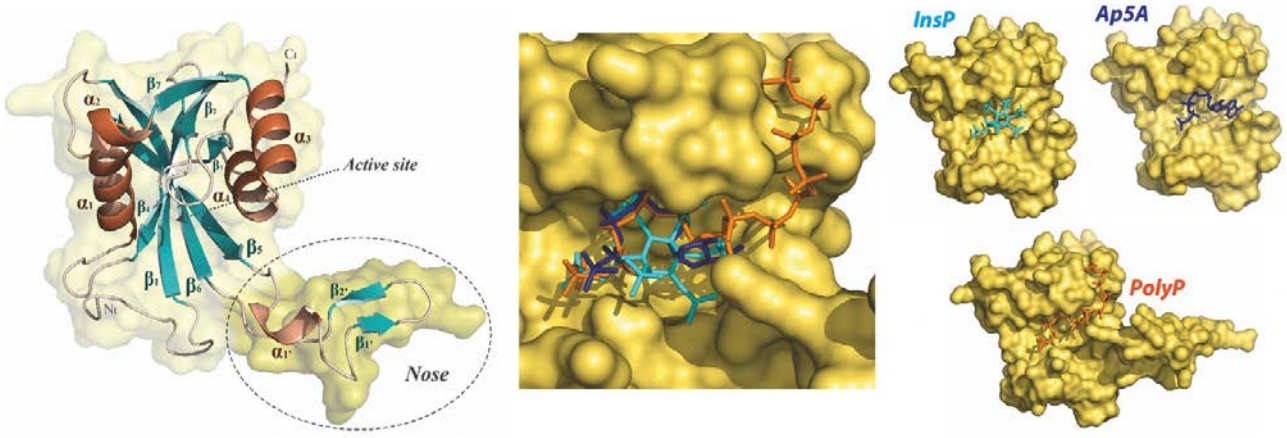

Figure 8: Structure of DDP1 and ligand recognition showing the binding of the three protein substrates in the active site.

Inhibition of RAS family for cancer treatment

In collaboration with the company Allinky Biopharma S.A. we have worked in the crystallization of K-RAS, and other signalling proteins, in complex with different ligands. RAS orchestrate cell signalling leading to responses as cell survival, growth and proliferation, and is the major mutated oncogene found in human cancers. To make its function, RAS acts as a switch on/off by acquiring an active/inactive conformation. RAS conformations depend on the structure of two regions, named switch I and switch II. RAS in active conformation is able to interact with other proteins, as RAS effectors, and in consequence able to transmit the signals received by cells. The aim of our work during this period has been to set up the molecular bases for RAS inhibition to block RAS in its inactive conformation, thus avoiding the survival and proliferation of cancer cells.

Prediction of multicomponent forms

In the pharmaceutical area, it is common screening studies for the development of crystalline modifications of a drug aiming to improve its physicochemical properties. Among all the possible crystalline modifications, multicomponent forms (cocrystals, salts, solvates and eutectic systems) are obtained by including other molecules in the crystalline structure of the drug. However, the screening of multicomponent forms could be expensive in terms of time and money, since there is an infinite number of possible co-former molecules and methodologies that can be employed. Thus, it is necessary a strategy to help scientists in the screening of new multicomponent forms of a target-molecule through the rationalization of co-former selection. In this work, we have developed and validated a new rational strategy to design crystalline modifications and to select co-formers through knowledge-based on supramolecular chemistry, and in the use of statistical tools from the Cambridge Crystallographic Data Centre (CCDC), to prepare and characterize multicomponent solids of a drug.

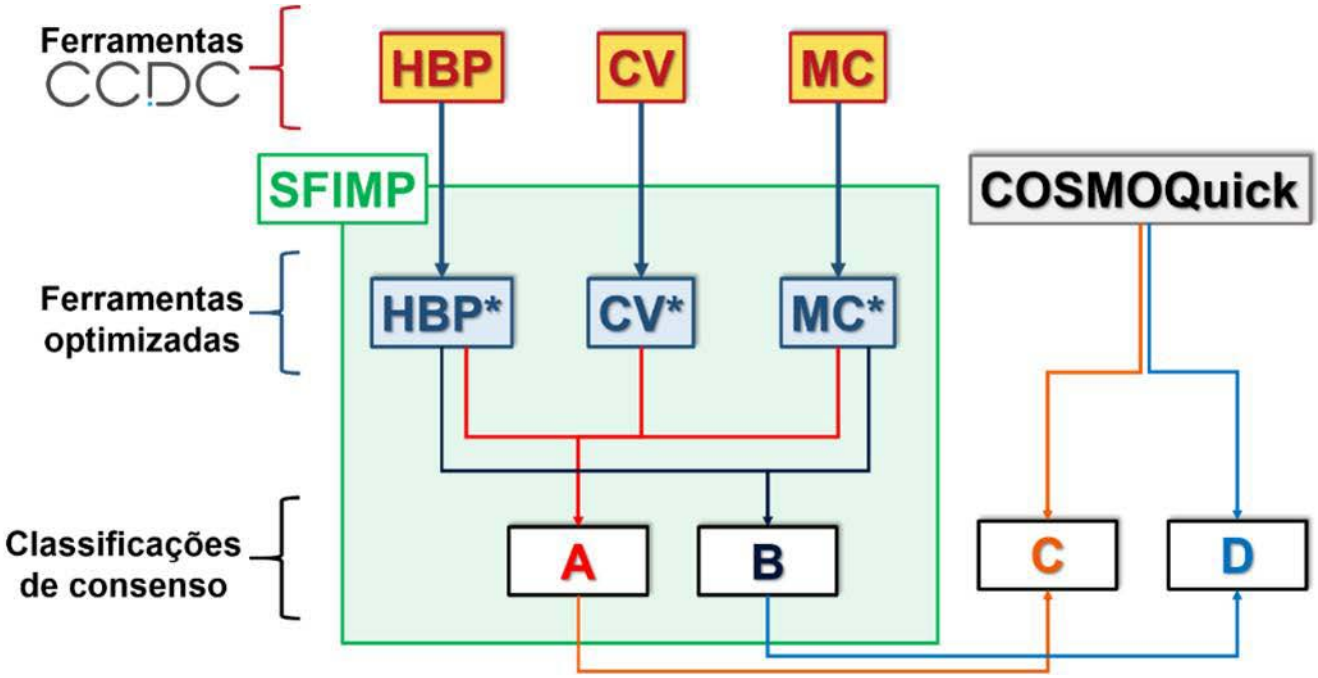

Figure 9: Schematic representation of the methodology developed for the prediction of multicomponent forms.(DOI: 10.1039/D0CE00948B)

New protein-protein interaction modulators for the therapeutic regulation of synapse dysfunction in neurodegeneration

The protein complex formed by the Ca^{2+} sensor NCS-1 and the GEF protein Ric8a co-regulates synapse number and probability of neurotransmitter release, emerging as a potential therapeutic target for synapse dysfunction diseases. Previously, we had demonstrated that the inhibition of this protein-protein interaction with small compounds is a promising therapeutic strategy for Fragile X syndrome, an autistic disorder where neurons show an abnormally high synapse number (Mansilla et al., PNAS (2017), Roca et al, J.Med.Chem. (2018)). Conversely, it would be tempting to speculate that compounds with opposite activity would have potential in neurodegeneration, where patients show a loss of synaptic contacts during the progression of the disease. The combination of protein-driven synthetic chemical methodologies, together with biophysical, crystallographic cellular and physiological approaches have fostered the discovery of a promising hit compound that is able to improve the synaptic function in animal models of Alzheimer´s and Huntington´s disease (Canal-Martín et al, Nat Comms, 2019). The crystal structure of the compound at atomic level bound to NCS-1 will permit to develop new derivatives with improved activity and drug-like properties.

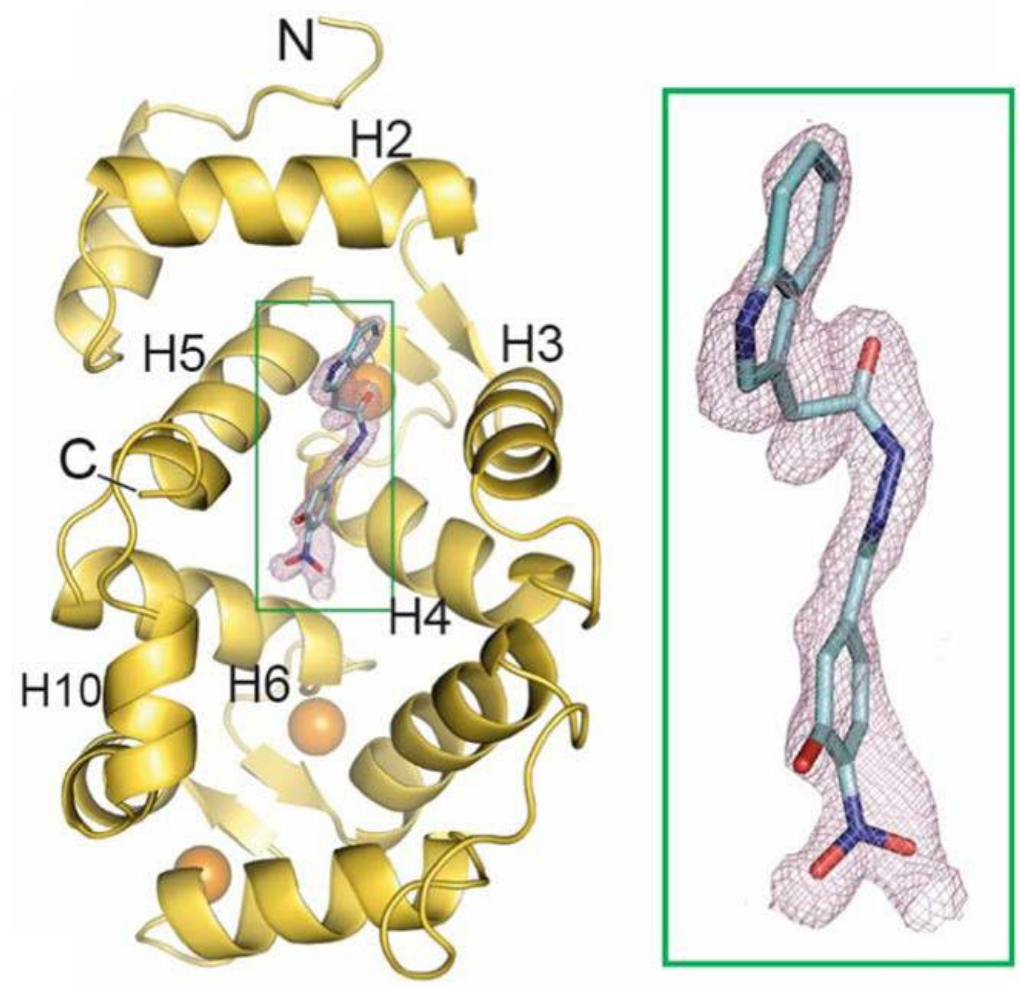

Figure 10: The structure of hNCS-1 bound to the hit compound that improves synapse function in neurodegeneration. An amplified image of the small molecule and its corresponding 2Fo-Fc map is shown on the right.

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National Grants: individual

Agencia Estatal de Investigación (AEI)

Principal Investigator	Title	Reference
Armando Albert	Structural approach to membrane delimited signaling pathways involved in plant cell response to abiotic stress	BIO2017-89523-R
GALCHIMIA SA	Descubrimiento de agroquímicos para mejorar la resistencia a la sequía de plantas de cosecha	RTC-2017-6019-2
Juan A. Hermoso	Apuntando a la resistencia a antibióticos: bases estructurales de la regulación en procesos esenciales de remodelado de la pared celular	BFU2017-90030-P
Beatriz González	Una visión ampliada de la señalización por inositidos: síntesis y dianas en la biogénesis del RNA	BFU2017-89913-P
María José Sánchez Barrena	Descodificación de la especificidad del sensor neuronal de calcio 1 para desarrollar compuestos moduladores de su interacción en aplicaciones biotecnológicas y terapéuticas	PID2019-111737RB-I00
Inmaculada Pérez Dorado	Caracterización del sistema de secreción ESX-5 y factores de virulencia secretados por este transportador en Mycobacterium tuberculosis. Estudio de los mecanismos de patogénesis asociados y su potencial como diana terapéutica	Talento_2019-T1_BMD-14774
José Manuel Martín García	Desentrañar el mecanismo de resistencia alostérico de la proteína de unión a la penicilina (PBP2a) de Staphylococcus aureus por cristalografía en serie de femtosegundo en instalaciones de láseres de electrones libres de rayos X.	2019-T1/BMD-15552

Fundación BBVA

Principal Investigator	Title	Reference
María José Sánchez-Barrena	El sensor de Ca^{2+} NCS-1 como nueva diana para el control de la función sináptica en enfermedades neurodegenerativas	Becas Leonardo a Investigadores y Creadores Culturales 2017. IN[17]_CMA_BIO_0277

National Grants: coordinated

Agencia Estatal de Investigación (AEI)

Principal Investigator	Title	Reference
Julia Sanz Aparicio	Análisis cristalográfico y diseño molecular de glicoenzimas para mejorar su potencial en biología sintética	BIO2016-76601-C3-3-R
Julia Sanz Aparicio	Análisis estructural y diseño molecular de glicoenzimas para la síntesis de compuestos bioactivos de interés farmacológico	PID2019-105838RB-C33
Beatriz González	Desarrollo preclínico de nuevos fármacos para el tratamiento personalizado de cánceres dependientes de RAS	RTC-2017-6478-1

Comunidad de Madrid – Proyectos Sinérgicos I+D

Principal Investigator	Title	Reference
Julia Sanz Aparicio	Química sintética mediante enzimas quiméricas de fusión diseñadas por evolución dirigida y computacional	EVOQUIMERA-CM ref. Y2018/BIO-4738

Fundación La Caixa

Principal Investigator	Title	Reference
Alicia Mansilla Aparicio	Synapse Modulators: small molecules with big impact in nervous system disorders	CaixaImpulse 2018

International Grants: individual

iNEXT from Horizon 2020 programme of the European Union

Principal Investigator	Title	Reference
J.A. Hermoso	Novel Inhibitors Against LD-Transpeptidases In G(-) Multi-Drug Resistant Pathogens	PID: 5834

International Grants: coordinated

SINERGIA Grant from Swiss National Science Foundation

Principal Investigator	Title	Reference
P. Viollier, J.A. Hermoso M. Dal Peraro	Origins Of Broad-Spectrum Beta-Lactam Resistance: Multidimensional Dissection Of Chromosomally Encoded Metallo-Beta-Lactamases	CRSII5_198737/1


CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFICAS

Department of Atmospheric Chemistry and Climate

Introduction

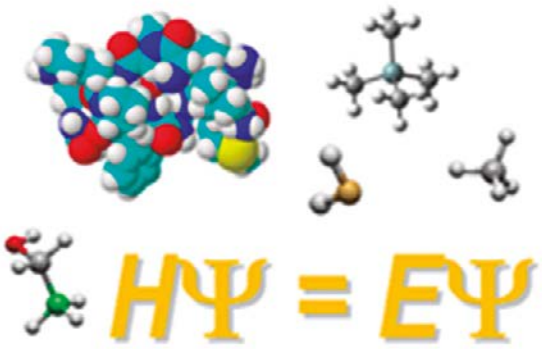
The Department develops different lines of research including:

- Reactivity, structural effects on acidity/ basicity in gas phase and intrinsic thermodynamic stability of species with biological activity and/or technological and environmental interest.
- Photodissociation dynamics and energy of organic species with heteroatoms of N, Cl and S.
- Methodologies with spectrometer of hybrid triple-quadrupole and FT-ICR masses high resolution.
- Heteroborane aggregates chemistry, and their interactions with biomolecules.
- Kinetics of new reactions of Si and Ge carbenes of interest in the industry of the materials.
- Development and characterization of new stationary phases for gas chromatography based on ionic liquids.
- Analysis methods of chromatography and mass spectrometry.
- Interactions between natural and anthropogenic emissions, the climatic, chemical and physical systems and the biosphere, within the context of climate change;

In the Department, several experimental techniques are available to effectively carry out the different lines of research: combustion calorimetry; microcalorimetry combustion (CMRT); differential scanning calorimetry (DSC); high-resolution mass spectrometry FT-ICR (Fourier transform cyclotron resonance) of 4.7 T and 7.0 T; photolysis with pulsed lasers; gas chromatographs for capillary and packed columns with flame ionization detectors; gas chromatograph coupled to a quadrupole mass spectrometer; differential optical absorption spectroscopy (DOAS; resonance and off-resonance fluorescence by lamp excitation (ROFLEX); Incoherent Broadband Cavity Enhanced Absorption Spectroscopy (IBBCEAS).

Groups Structure

Energetics, Structure and Molecular Reaction Group (ESMR)



Staff

Juan Z. Dávalos Prado (Assistant Professor) ORCID ReID

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Summary

We study energetic, chemical reactivity, electronic and structural properties of neutral and ionic species – in the gas phase- of fundamental, technological and environmental relevance. For this purpose, we use a variety of experimental (Mass Spectrometry; Calorimetry of Combustion; Knudsen's effusion; Photoelectron-Photoion Coincidence Spectroscopy-PEPICO) and theoretical techniques. The combination of the experimental results with those obtained by means of quantum-mechanic calculations (*ab-initio*, DFT) allow us to:

i) obtain quantitative information on thermodynamics and kinetics of a variety of chemical reactions in the phase gas,

ii) determine interesting and novel relationship of reactivity-chemical structure,

iii) determine the thermodynamic stability of neutral and ionic species.

Strategic Aims

Our research lines focus on the theoretical/experimental study of the energetics, chemical reactivity, structure, electronic properties and interactions of neutral and ionic species in the absence of the disturbing effect of the solvent.

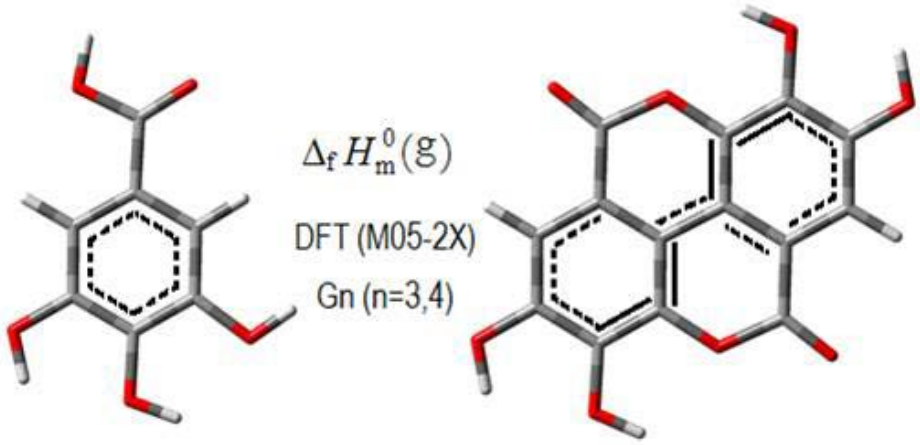
The specific goals pursued are:

- Thermodynamic stability, reactivity (by proton-interchange processes), structural effects and electronic properties of species with fundamental, technological and environmental relevance.
- Electronic structure of heteroborane clusters (HBC) in their ground and excited states.

Remarkable Results

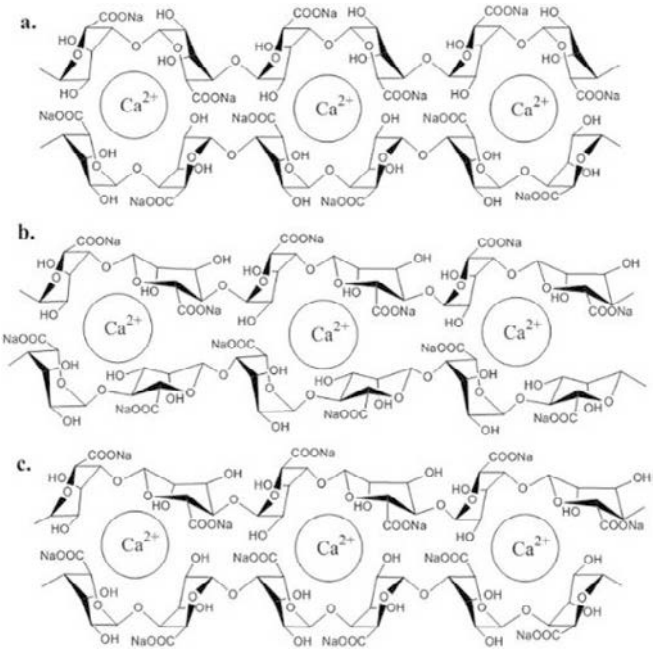
Thermochemical and structural studies of gallic and ellagic acids

We report a study on the energetics and structural properties of gallic (**1**) and ellagic (**2**) acids. The experimental values of standard enthalpy of formation in solid state at 298.15 K, $\Delta_f H_m^0$ (cd) of **1** as (-985.0 ± 2.9 kJ·mol^{-1}) and **2** as (-1377.9 ± 4.7 kJ·mol^{-1}) have been determined. The vapor pressure of **1** has been measured by Knudsen effusion methodology and the derived enthalpy of sublimation, $\Delta_{cd}^{g} H_m^0$, was combined with the $\Delta_f H_m^0$(cd) in order to derive its gas-phase enthalpy of formation, $\Delta_f H_m^0$(**1**,g) = -835.7 ± 4.0 kJ·mol^{-1}. Quantum chemical calculations, at DFT (M05-2X) and composite *ab initio* Gn (n = 3,4) levels of theory, provided the consistency of the experimental results and a plausible estimation of $\Delta_f H_m^0$(g) of **2** as (-1128.6 ± 6.4 kJ·mol^{-1}), which was deduced from the isodesmic-reactions methodology.



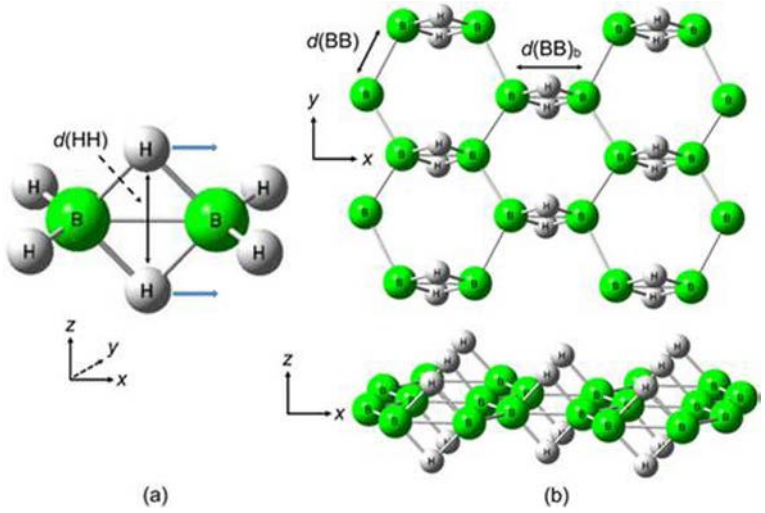
Chemical modification of alginate with cysteine and its application for the removal of Pb(II) from aqueous solutions

It has been synthesized, characterized and tested a new biomaterial AlgS (sodium alginate functionalized with cysteine) to remove Pb(II) in a queous media. The maximum Pb(II)-sorption capacity of AlgS (Q_{max} =770 mg·g^{-1}) is between almost two and nine times higher than other alginate-materials reported in the literature. Techniques, such as TGA/DSC, SEM/EDS, BET, FTIR, UV–Vis, XRD and ^{13}C solid state-NMR have been used to study the chemical-modification of alginate at oxidation and aminofication stages. The Δ*H*° and Δ*G*° negative values for Pb(II) sorption indicate that it is an exothermic process and occurs spontaneously. Finally, it was found that the Pb(II) sorption on AlgS is significantly affected by the presence of cationic (Na^+, Mg^{2+} and Al^{3+}) and anionic (Cl^-, NO_3^-) co-ions.



Diborane Concatenation Leads to New Planar Boron Chemistry

Diborane has long been realized to be analogous to ethylene in terms of its bonding MOs, both as to symmetries and splitting patterns. This naturally suggests an investigation to see whether other similar conjugated hydrocarbons manifest a similar boron-substituted and H_2 supplemented borane. That is, for a conjugated hydrocarbon structure with a neighbor-paired resonance pattern, we propose to look at boranes where each carbon atom is replaced by a boron atom, and an H-atom pair is added to each double bond of the resonance structure, with one H above the molecular plane and one below. This construction of concatenated diboranes is uniformly different than that for the previously known stable boranes of 4 or more B atoms. We find from quantum-chemical computations that our so constructed polyboranes are stable.

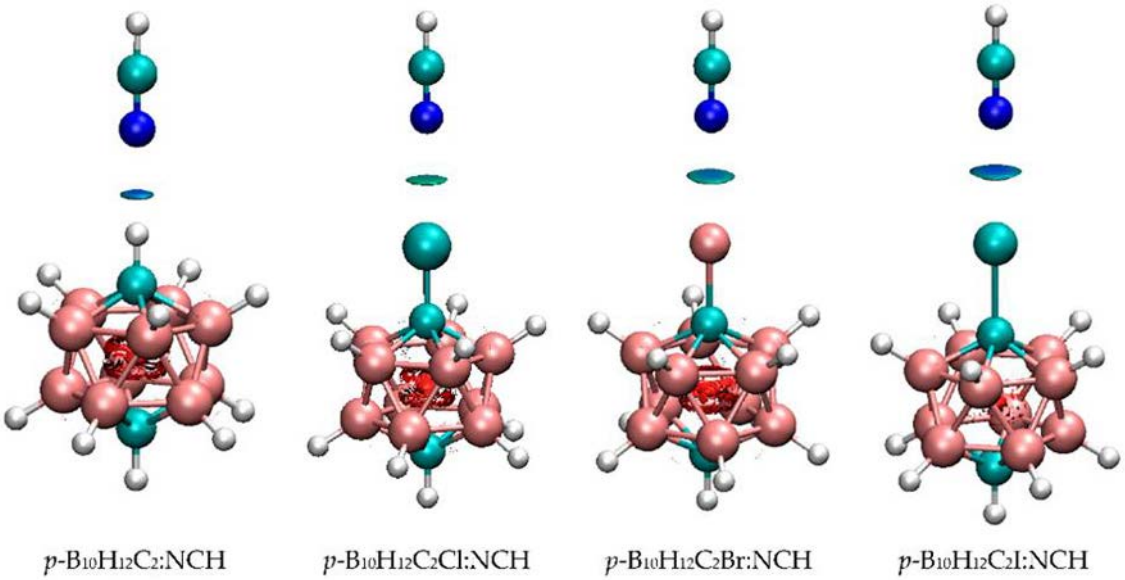


Magnetic Properties of Co(II) Complexes with Polyhedral Carborane Ligands

We present a computational analysis of a new family of magnetic Co(II) single-ion complexes with large magnetic anisotropy based on icosahedral and octahedral carborane ligands. In particular, we extend our previous computational work on mononuclear Co(II) complexes with 1,2-$(HS)_2$-1,2-$C_2B_{10}H_{10}$ and 9,12-$(HS)_2$-1,2-$C_2B_{10}H_{10}$ icosahedral *o*-carborane ligands to a larger set of complexes where the Co(II) ion is doubly chelated by those ligands and by other two positional isomers belonging to the 1,2-dicarba-*closo*-dodecaborane family. We also describe Co(II) complexes with octahedral ligands derived from 1,2-dicarba-*closo*-hexaborane and study the effects of replacing a thiol group by a hydroxy group in both polyhedral geometries, as well as the influence of the position of the carbon atoms. On analysis of the results for a total of 20 complexes, our results show that carborane-based Co(II) single-ion compounds present a distorted-tetrahedral geometry, high-spin ground states, and high values for the magnetic anisotropy parameters.

Hydrogen vs. Halogen Bonds in 1-Halo-Closo-Carboranes

A theoretical study of the hydrogen bond (HB) and halogen bond (XB) complexes between 1-halo-closo-carboranes and hydrogen cyanide (NCH) as HB and XB probe has been carried out at the MP2 computational level. The energy results show that the HB complexes are more stable than the XBs for the same system, with the exception of the *isoenergetic* iodine derivatives. The analysis of the electron density QTAIM shows the presence of a unique intermolecular bond critical point with the typical features of weak noncovalent interactions. The natural energy decomposition analysis (NEDA) of the complexes shows that the HB and XB complexes are dominated by the charge-transfer and polarization terms, respectively. The work has been complemented with a search in the CSD database of analogous complexes and the comparison of the results, with those of the 1-halobenzene:NCH complexes showing smaller binding energies and larger intermolecular distances as compared to the 1-halo-closo-carboranes:NCH complexes.



p-$B_{10}H_{12}C_2$:NCH *p*-$B_{10}H_{12}C_2Cl$:NCH *p*-$B_{10}H_{12}C_2Br$:NCH *p*-$B_{10}H_{12}C_2I$:NCH

Publications

Dávalos, J. Z., Lima, C. F. R. A. C., Santos, L. M. N. B. F., Romero, V. L. and Liebman, J. F. Thermochemical and structural studies of gallic and ellagic acids. *J. Chem. Thermodyn.* **129**, 108-113 (2019).

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COMPETITIVE FUNDING

National Grants: individual

Agencia Estatal de Investigación (AEI)

Principal Investigator	Title	Reference
Carlos Cuevas Rodríguez/ Alfonso Saiz-López	El ciclo atmosférico del azufre en un clima cambiante (SULCLIM)	PID2019-111677RB-I00
Juan de la Figuera Bayón/ José Fco. Marco Sanz	Nuevos materiales y dispositivos para el procesado de señales ultra-rápido y/o de baja disipación	RTI2018-095303-B-C51

National Grants: coordinated

Agencia Estatal de Investigación (AEI)

Principal Investigator	Title	Reference
Ibon Alkorta/ Manuel Yañez	Diseño y caracterización de nuevos materiales moleculares y optimización de fármacos: sinergia experimento y teoría	CTQ2018-094644-B-C22/ CTQ2018-094644-B-C21

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Summary

The Atmospheric Chemistry and Climate group (AC2) is a research group based at IQFR since 2012. AC2 research efforts are directed at studying the role of atmospheric composition and chemistry in the climate system. The goals are to explore the interactions between anthropogenic and natural emissions, the chemical and physical climate system, and the biosphere, within a changing climate context. Within this broad scientific framework, AC2 provides an integrated research approach combining atmospheric measurements (satellite- and ground-based), laboratory experiments, theoretical and global chemistry-climate modelling.

Strategic Aims

- The goals are to explore the interactions between anthropogenic and natural emissions, the chemical and physical climate system, and the biosphere, within a changing climate context.

Remarkable Results

Natural halogens buffer tropospheric ozone in a changing climate

Reactive atmospheric halogens destroy tropospheric ozone (O_3), an air pollutant and greenhouse gas. The primary source of natural halogens is emissions from marine phytoplankton and algae, as well as abiotic sources from ocean and tropospheric chemistry, but how their fluxes will change under climate warming, and the resulting impacts on O_3, are not well known. Here, we use an Earth system model to estimate that natural halogens deplete approximately 13% of tropospheric O_3 in the present-day climate. Despite increased levels of natural halogens through the twenty-first century, this fraction remains stable due to compensation from hemispheric, regional and vertical heterogeneity in tropospheric O_3 loss. Notably, this halogen-driven O_3 buffering is projected to be greatest over polluted and populated regions, due mainly to iodine chemistry, with important implications for air quality.

Nat. Clim. Chang., https://doi.org/10.1038/s41558-019-0675-6, 2020

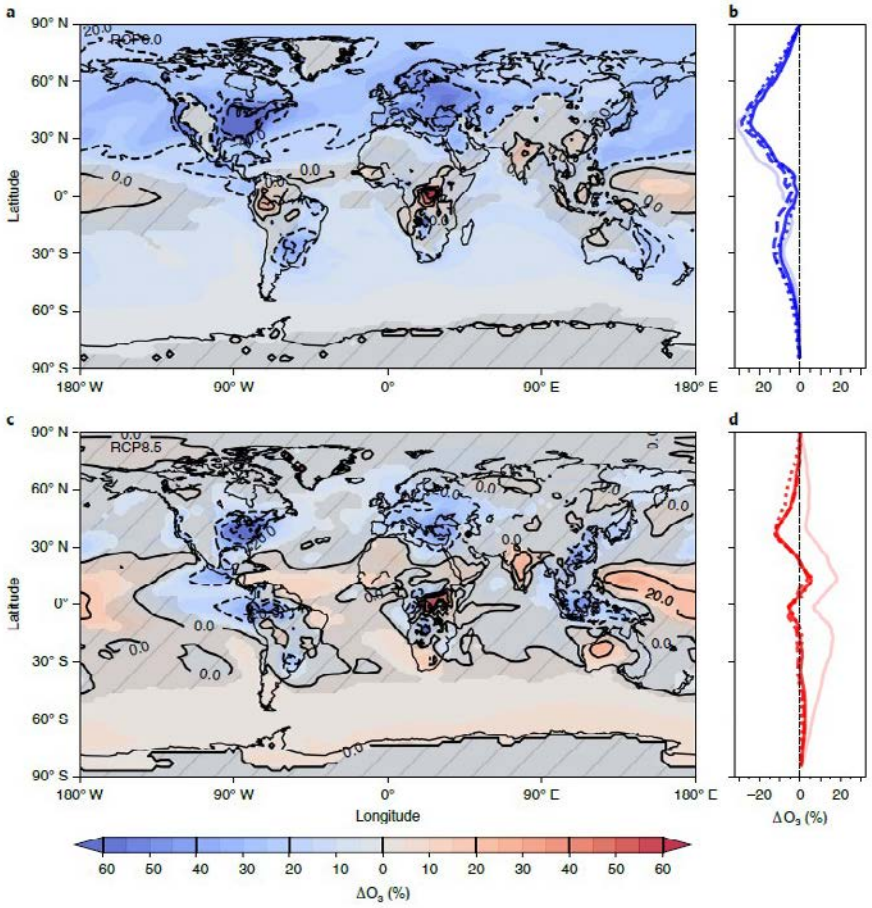

Figure 1: Maps of halogen-driven near-surface O_3 loss change between the present (1990–2009) and the end of the century (2080–2099). a,c, Maps for emission scenarios RCP 6.0 (a) and RCP 8.5 (c).b,d, Zonal mean O_3 loss changes for the RCP 6.0 (b) and RCP 8.5 (d) emission scenarios. Zonal mean O_3 loss changes are latitudinally weighted (using latitudinal cosines).

A gas-to-particle conversion mechanism helps to explain atmospheric particle formation through clustering of iodine oxides

Emitted from the oceans, iodine-bearing molecules are ubiquitous in the atmosphere and a source of new atmospheric aerosol particles of potentially global significance. However, its inclusion in atmospheric models is hindered by a lack of understanding of the first steps of the photochemical gas-to-particle conversion mechanism. Our laboratory results show that under a high humidity and low HO_x regime, the recently proposed nucleating molecule (iodic acid, $HOIO_2$) does not form rapidly enough, and gas-to-particle conversion proceeds by clustering of iodine oxides (I_xO_y), albeit at slower rates than under dryer conditions. Moreover, we show experimentally that gas-phase $HOIO_2$ is not necessary for the formation of $HOIO_2$-containing particles. These insights help to explain new particle formation in the relatively dry polar regions and, more generally, provide for the first time a thermochemically feasible molecular mechanism from ocean iodine emissions to atmospheric particles that is currently missing in model calculations of aerosol radiative forcing.

Nature Communications volume 11, Article number: 4521 (2020), https://doi.org/10.1038/s41467-020-18252-8

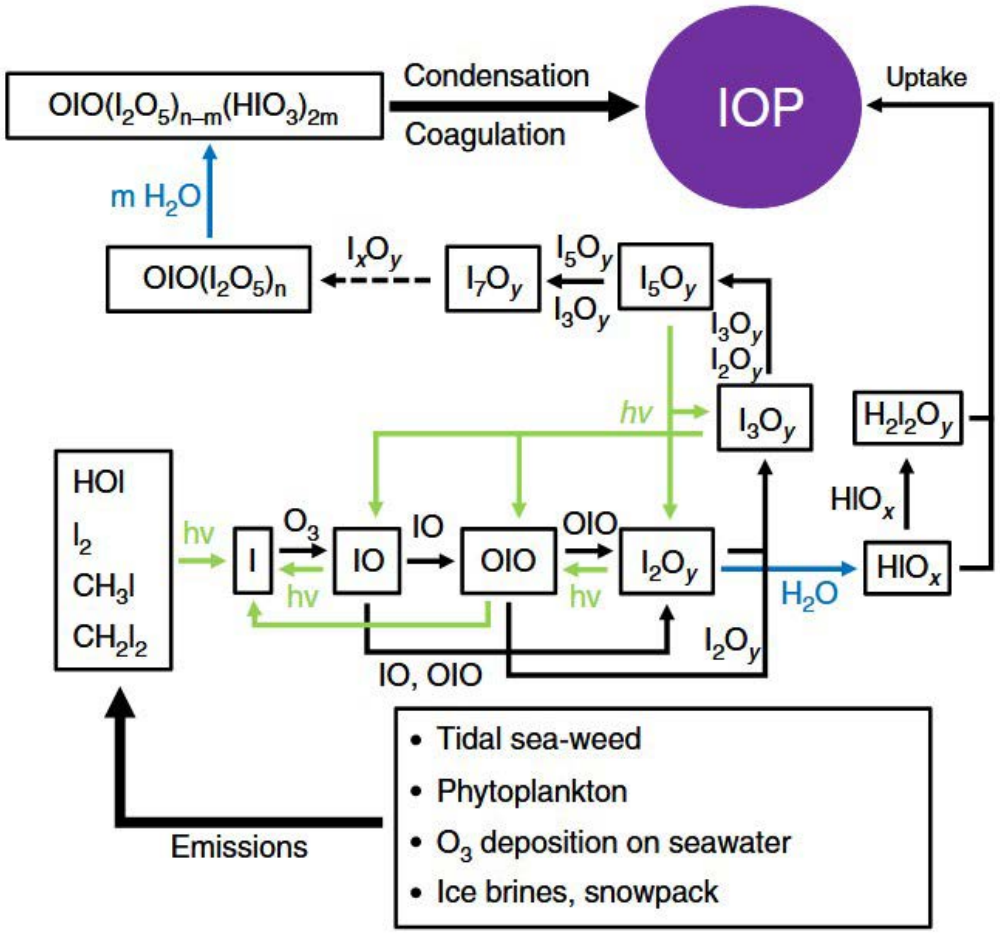

Figure 2: Proposed mechanism of iodine oxide new particles (IOPs) formation

Photochemistry of oxidized Hg(I) and Hg(II) species suggests missing mercury oxidation in the troposphere

The atmospheric chemistry of mercury, a global priority pollutant, is key to its transport and deposition to the surface environment. Assessments of its risks to humans and ecosystems rely on an accurate understanding of global mercury cycling. This work shows that the chemical reactions and rates currently employed to interpret Hg chemistry in the atmosphere fails to explain observed atmospheric mercury concentrations and deposition. We report that model simulations incorporating recent developments in the photoreduction mechanisms of the oxidized forms of mercury (Hg^{I} and Hg^{II}) lead to a significant model underestimation of global observations of these oxidized species in the troposphere and their surface wet deposition. This implies that there must be currently unidentified mercury oxidation processes in the troposphere.

PNAS November 23, 2020; https://doi.org/10.1073/pnas.1922486117

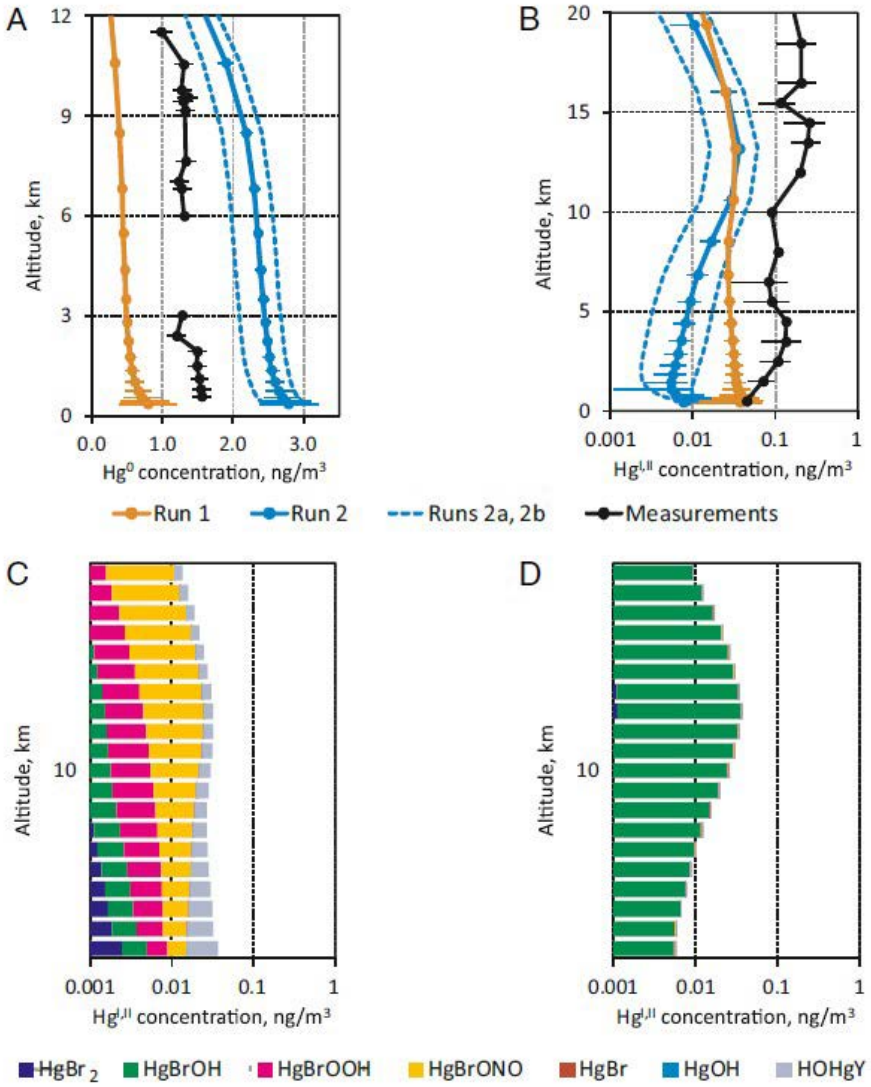

Figure 3:Modeled and observed vertical profiles of atmospheric concentration of Hg^0 (A) and $Hg^{I,II}$ (B) over northern midlatitudes; and contribution of various species to $Hg^{I,II}$ concentration for run 1 (C, no photolysis) and run 2 (D, $Hg^{I,II}$ photolysis).

Potential Effect of Halogens on Atmospheric Oxidation and Air Quality in China

Air pollution is a hazard in China threatening the health of half a billion people. Mitigation of air pollution in China has led to a significant reduction in primary pollutants emissions from 2013 to 2017, while a continuously worsening trend of surface ozone was observed over the same period. Atmospheric oxidation, dominated by daytime reactions involving hydroxyl radicals (OH), is the critical process to convert freshly-emitted compounds into secondary pollutants, and is underestimated in current models of China's air pollution. Halogens are known to profoundly influence oxidation chemistry in the marine environment; In the present study, we report for the first time that halogens enhance the total atmospheric oxidation capacity in polluted areas of China, typically 10% to 20% (up to 87% in winter) and mainly by significantly increasing OH level. Enhanced oxidation along the coast is driven by oceanic emissions, and that over the inland areas by anthropogenic emission.

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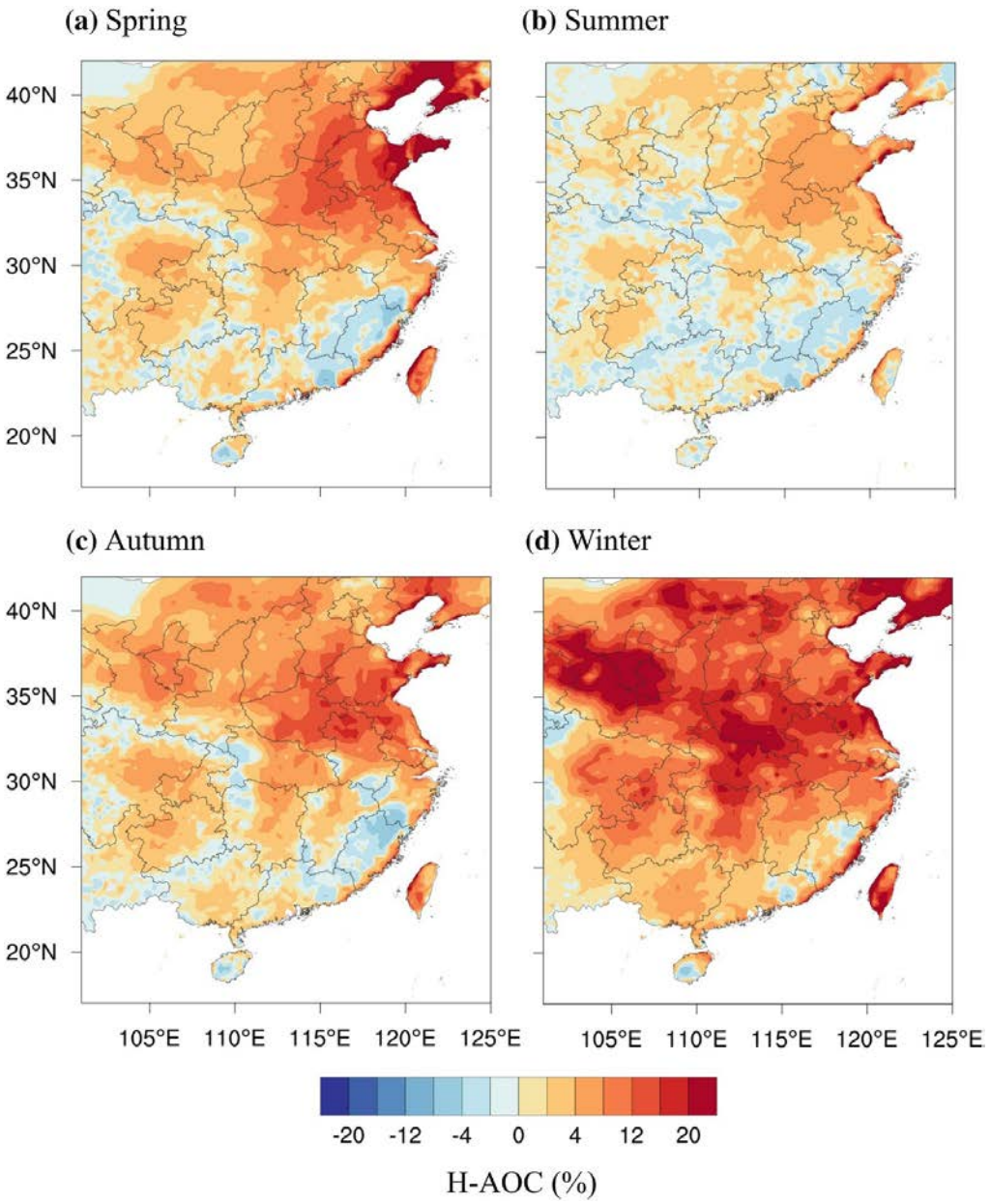

Figure 4: Impact of halogen chemistry on the atmospheric oxidation capacity (H-AOC) at the surface in China in Spring, Summer, Autumn and Winter.

MAX-DOAS measurements and vertical profiles of glyoxal and formaldehyde in Madrid, Spain

Glyoxal (CHOCHO) and formaldehyde (HCHO) are organic trace gases that play an important role in tropospheric chemistry as oxidation products of a number of volatile organic compounds (VOCs). We report year-round daytime measurements of glyoxal and formaldehyde in the urban atmosphere of Madrid, Spain. Their vertical concentration profiles were retrieved using the Multi AXis Differential Optical Absorption Spectroscopy (MAX-DOAS). The diurnal variations of HCHO show two peaks during the day, in the early morning and late afternoon in spring and summer, while the second peak is shifted towards noon in autumn and winter, due to lower photolysis rates and more effective boundary layer accumulation of HCHO in those seasons. The ratio between glyoxal and formaldehyde (R_{GF}) surface mixing ratios, as an indicator of the nature of VOCs precursors, was also correlated with the measured NO_2, which represents a direct signal of anthropogenic emissions.

Atmospheric Environment Volume 199, 15 February 2019, Pages 357-367

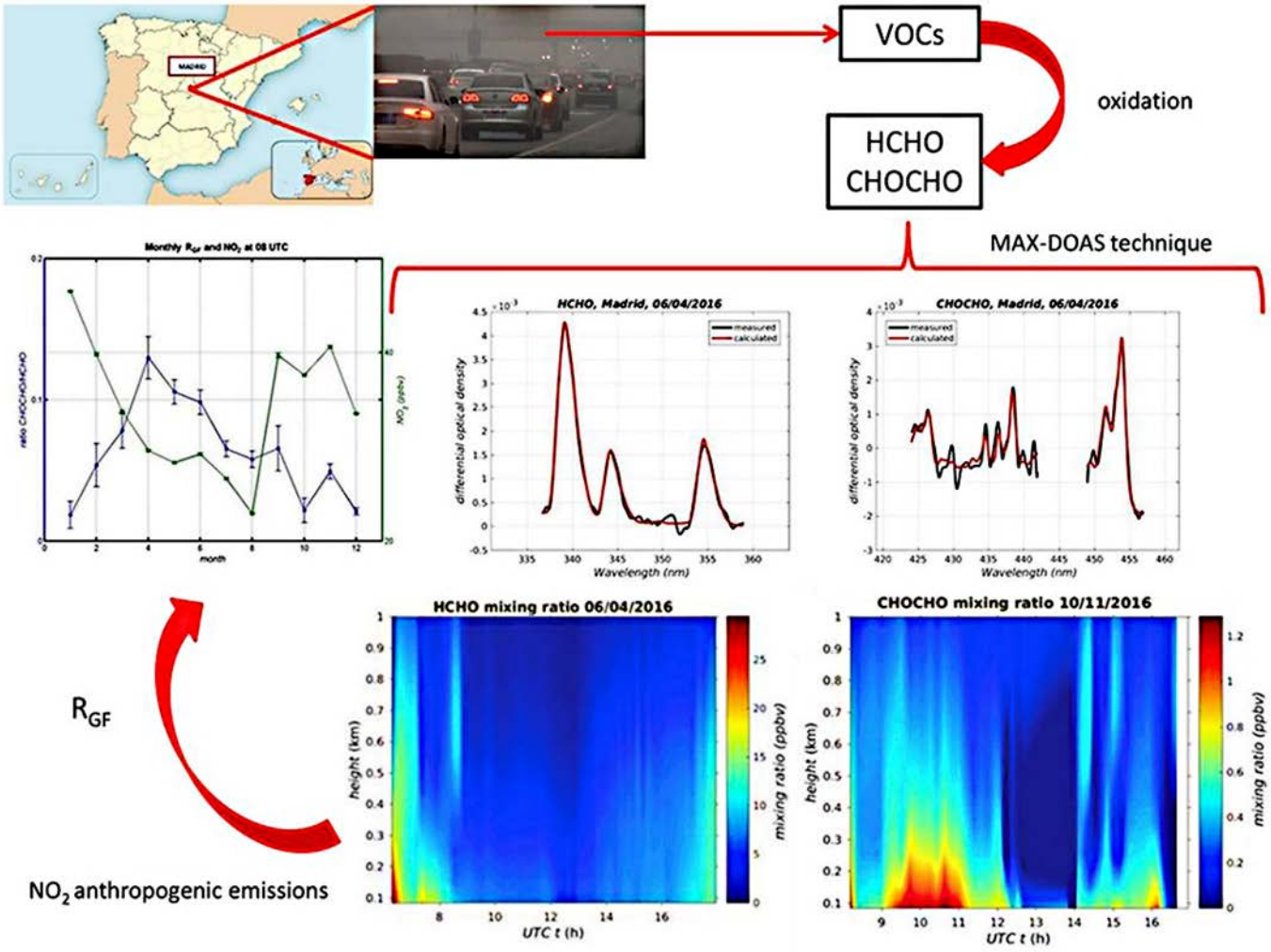

Figure 5: Monthly variation of R_{GF} and NO_2 at 8 UTC time, together with examples of formaldehyde and glyoxal spectral fitting and vertical profile mixing ratios.

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COMPETITIVE FUNDING

National Grants: individual

Agencia Estatal de Investigación (AEI)

Principal Investigator	Title	Reference
Carlos A. Cuevas Rodríguez / Alfonso Saiz-López (SULCLIM)	El ciclo atmosférico del azufre en un clima cambiante	PID2019-111677RB-I00

National Grants: coordinated

Comunidad de Madrid

Principal Investigator	Title	Reference
Alfonso Saiz López	Tecnologías de vanguardia para Investigación en Aerosoles y Gases Atmosféricos (TIGAS-CM)	Y2018/EMT-5177
Alfonso Saiz López	Evaluación Integral de la Calidad del Aire Urbano y Cambio Climático (AIRTEC-CM)	P2018/EMT-4329

CSIC

Principal Investigator	Title	Reference
Alfonso Saiz López	Estudio de la química de halógenos VSLs a partir del acoplamiento entre un modelo atmosférico global (CAM-Chem) y uno regional(WRF/Chem)	COOPB20331

International Grants: individual

EU

Principal Investigator	Title	Reference
Alfonso Saiz López	Climate dimension of natural halogens in the Earth system: past, present, future (CLIMAHAL)	ERC-2016-COG 726349

International Grants: coordinated

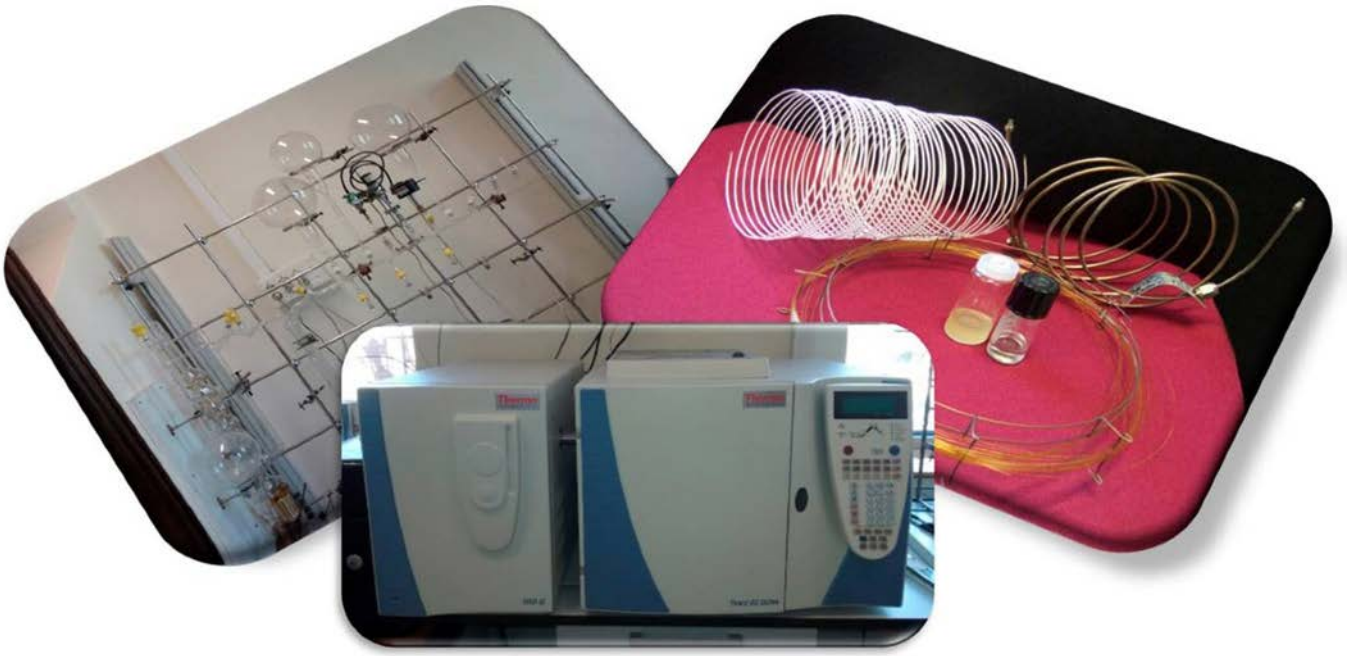
Aarhus University

Principal Investigator	Title	Reference
Alfonso Saiz López	DOAS measurements of Halogen oxides at Station Nord (Greenland)	DOASGREEN

Korea Polar Research Institute

Principal Investigator	Title	Reference
Alfonso Saiz López	Study on the fate of halogen species in Antarctica using MAX-DOAS	KOPRI

Group of Photolysis and Chromatography



Tenured Staff Scientists

María Rosa Becerra Arias (*Associate Professor*) ReID

Rosa Lebrón Aguilar (*Assistant Professor*) ReID SCOPUS ORCID

Technical Staff

Plácido Galindo Iranzo (*Superior Specialized Technician*) ReID SCOPUS ORCID

Jesús Eduardo Quintanilla López (*Superior Specialized Technician*) ReID SCOPUS ORCID

Summary

The Photolysis and Chromatography group (https://fyc.iqfr.csic.es/) is focused on the development of sustainable and innovative analytical methodologies for the determination of compounds of interest in the food, environmental, materials, and atmospheric fields, as well as on the study of their reactivity. The main goals are to understand and improve chromatographic separation processes, and the application of advanced chemometric procedures to maximize the efficiency of analytical methods.

The Group also manages the IQFR Chromatography and Mass Spectrometry laboratory (https://serviciomasas.iqfr.csic.es/), which since 2002 has been providing research support for the different departments of the IQFR, as well as to external users of other Research Public Institutions, Universities and private companies.

Strategic Aims

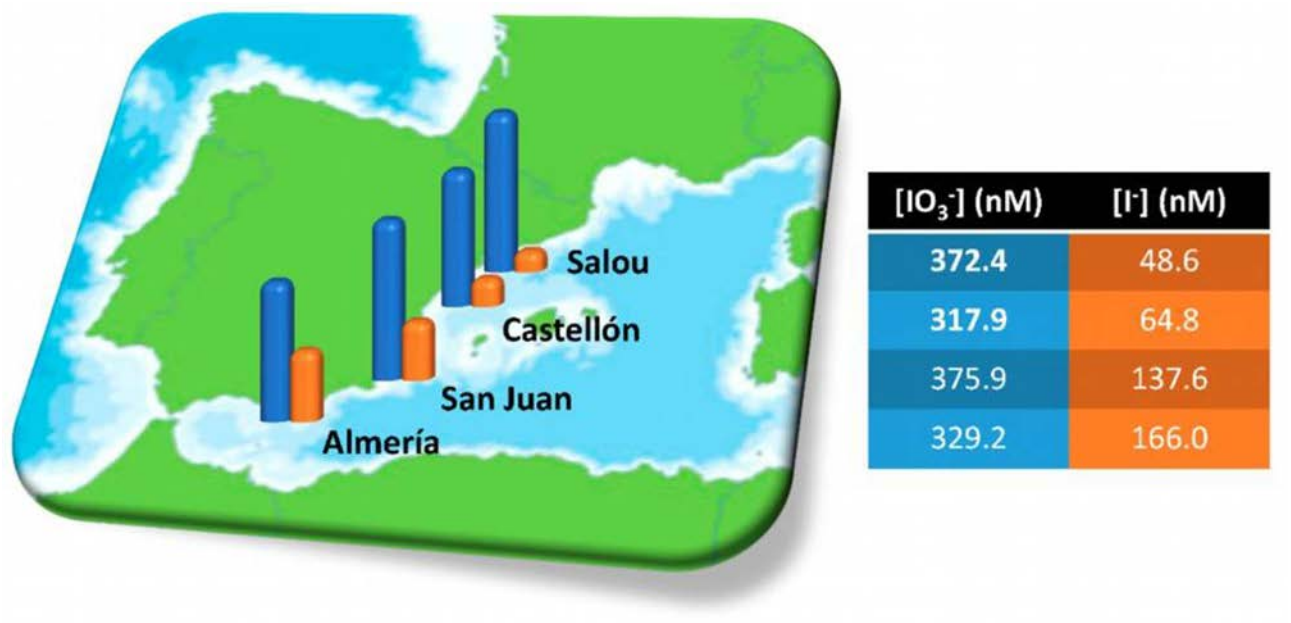
- Synthesis and characterization of new polymers based on ionic liquids for gas chromatography and solid phase microextraction.
- Development of advanced chromatography-mass spectrometry methods to solve complex analytical problems of environmental, food and atmospheric interest.
- Determination of chromatographic and thermodynamic parameters by inverse gas chromatography.
- Application of supervised and unsupervised chemometric techniques to the characterization and classification of different plant extracts.
- New reaction kinetic studies of Si, Ge and Sn containing heavy carbenes of interest in the materials industry.

Remarkable Results

Iodide and iodate in seawater

Atmospheric iodine plays a relevant role in climate change. Most of the iodine comes from the oceans, so analytical methods capable of detecting and quantifying iodine in seawater are necessary. However, this is a challenging matrix because the concentration of predominant iodine species (iodide and iodate) extends over several orders of magnitude and huge amounts of other anions and cations are also present.

Last biennium, we have faced this problem developing a methodology based on a preliminary clean-up step followed by LC-MS analysis. Now, we have improved this methodology by avoiding the time-consuming clean-up step: iodide is quantified by dilution and direct injection of filtered samples, and iodate is determined as iodide after its reduction with ascorbic acid at low pH. The new method is rapid, easy to apply and to automate, minimizes sample treatment and requires just a few microliters of sample.



$[IO_3^-]$ (nM)	$[I^-]$ (nM)
372.4	48.6
317.9	64.8
375.9	137.6
329.2	166.0

Figure 1: Concentrations of iodate and iodide in seawater samples collected from different locations along the Spanish Mediterranean coast, obtained by the LC-ESI-MS method developed.

Determination of atmospheric amines

Volatile amines have attracted increasing attention in recent years because they play an important role in the formation and transformation of atmospheric aerosols. The most common and abundant amines in the atmosphere are the low-molecular weight aliphatic amines with carbon numbers from 1 to 6. They are emitted from a wide range of sources such as ocean, vegetation, industry, etc. The growing interest on atmospheric amines implies the necessity for advanced analytical methods for its determination both in gaseous and particulate phases.

We have improved and implemented one of the most commonly GC-MS methods used for the analysis of primary and secondary volatile amines. Due to the difficulty of separating and quantifying the different amines at the low levels found in the atmosphere, the corresponding standard mixtures were used to optimize every step of the analytical method:derivatization, extraction, preconcentration, and finally, detection and quantification.

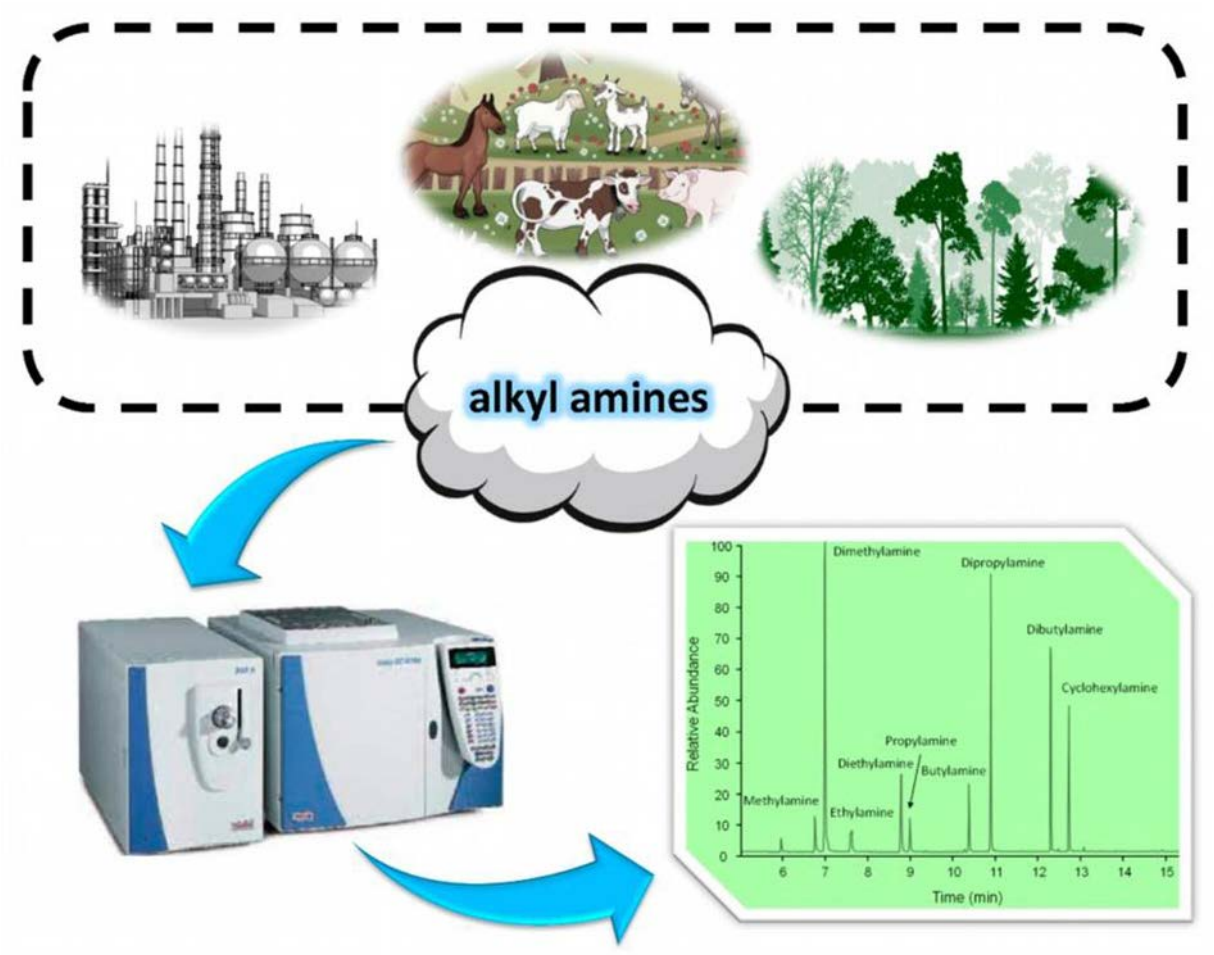


Figure 2: Sources of atmospheric amines and its determination by GC-MS.

Comprehensive mass spectrometric characterization of the transglucosylation of a Stevia extract

The consumption of high-intensity sweeteners (HIS) in the place of free sugars is in constant growth, due to the incidence of obesity worldwide. Stevioside and rebaudioside A, two of the most used HIS, are obtained from the leaves of the *Stevia rebaudiana* plant, but its lingering bitterness limits their applications as a sweetener in low-calorie foods and beverages formulations.

We have carried out, in collaboration with Drs. F.J. Moreno and O. Hernández-Hernández (CIAL, CSIC-UAM), a comprehensive mass spectrometric approach using LC-ESI-MS and MALDI-TOF MS to reveal the structural modifications of the transglucosylation of a *Stevia* extract. The chemical modifications carried out with a cyclodextrin glucosyltransferase from *Geobacillus* sp., led to the addition of up to 11 glucose units to the steviol aglycone, which meant the achievement of enhanced sensory profiles due to a diminution of bitterness and licorice appreciations.

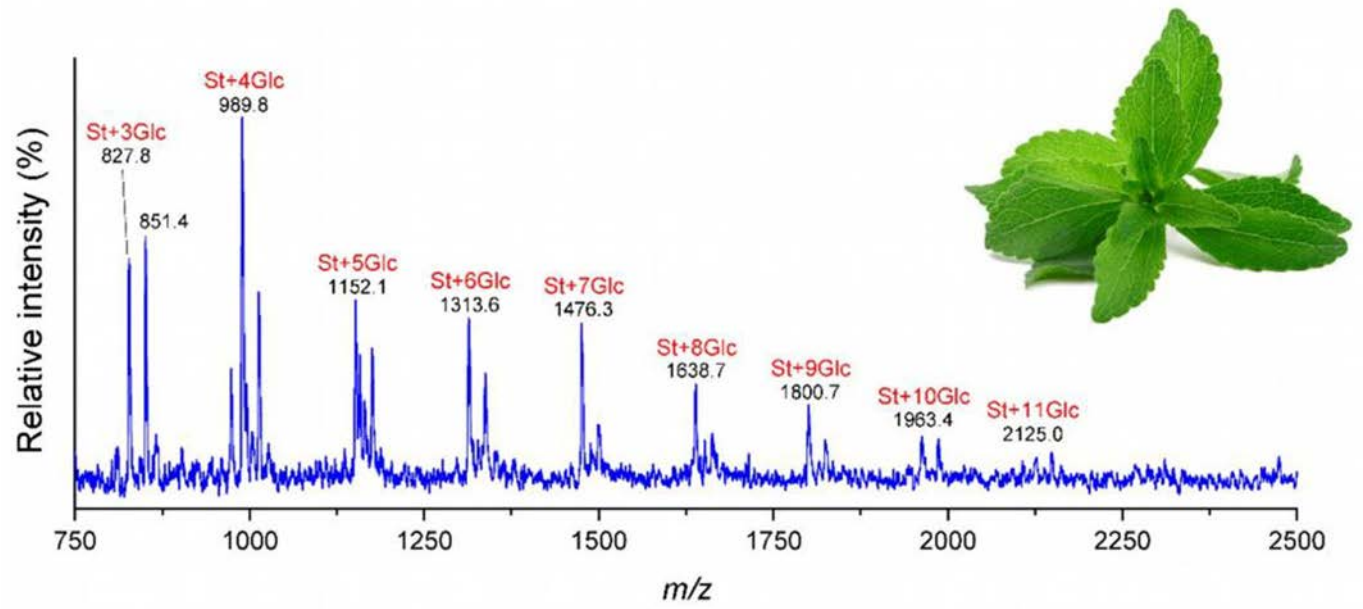


Figure 3: MALDI-TOF MS profile of glucosylated steviol glycosides using the CGTase from *Geobacillus* sp. (St: steviol; Glc: glucose).

Advances in structure elucidation of low molecular weight carbohydrates

Oligosaccharides are gaining importance because of their beneficial properties in human health; then, a detailed characterization of their chemical structures is demanding.However, its structural characterization is not a straightforward task considering the low availability of commercial standards, the similarity of their structures, their presence in complex mixtures and their different abundances.

In collaboration with the laboratories of Drs. M.L. Sanz (IQOG-CSIC) and F.J. Moreno (CIAL, CSIC-UAM), we have faced the problem by two ways:

- by GC-MS, using new ionic liquid columns with different selectivity. Among these columns, only SLB™-IL82 allowed the elution of all the carbohydrates studied.
- by LC-MS^n, combining chromatographic data and MS^2 spectra of 23 disaccharides with different linkages and monomeric units. MS^2 diagnostic fragment ions selected by stepwise linear discriminant analysis for each structural feature, in combination with the chromatographic data, allowed a rapid tentative structural characterization of trisaccharides in complex mixtures.

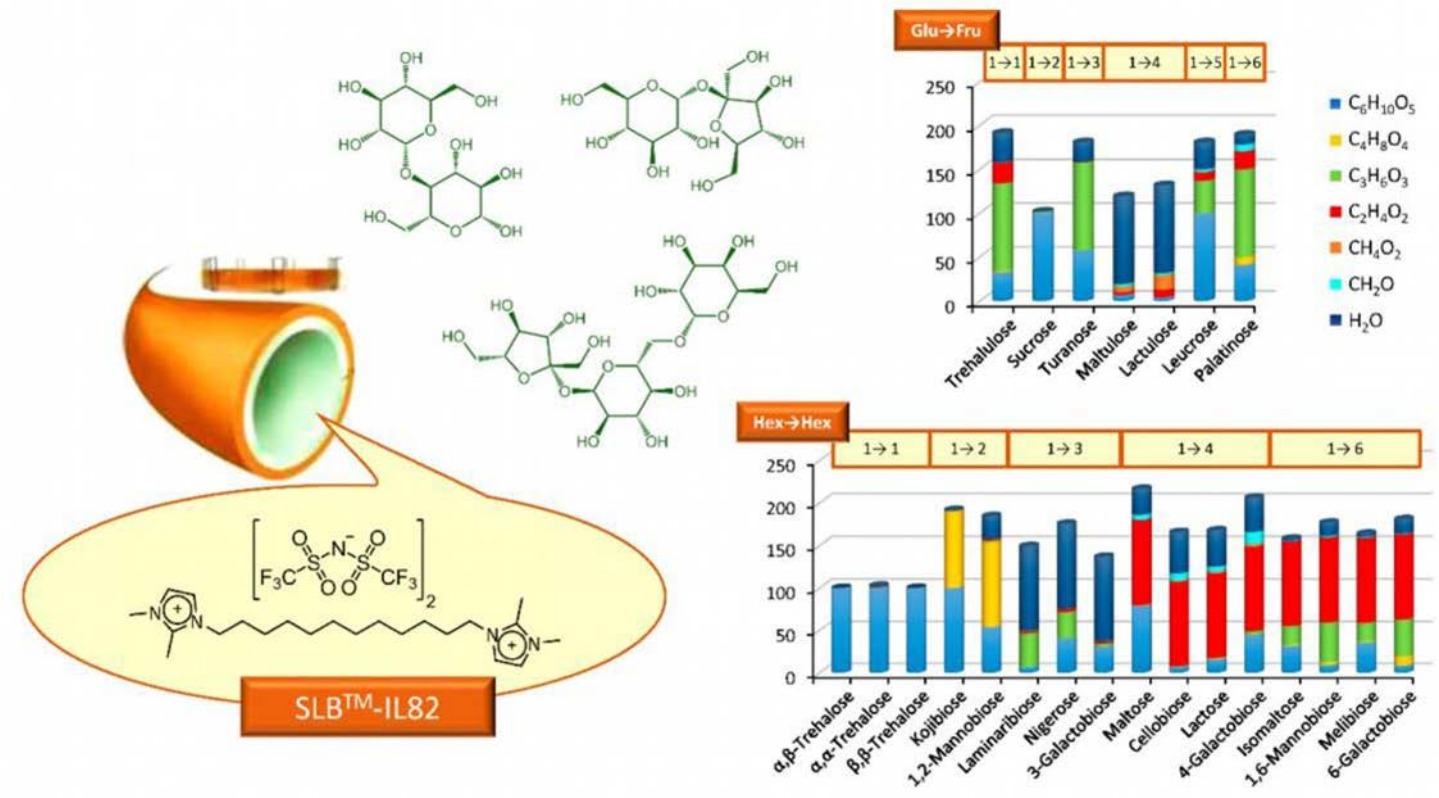


Figure 4: Chemical structure of the GC stationary phase used for the separation of low molecular weight carbohydrates and relative abundances of characteristic neutral losses from MS^2 of disaccharides.

Metabolites of polychlorinated biphenyls in human serum

Polychlorinated biphenyls (PCBs) are toxic and persistent pollutants that are metabolized into their corresponding hydroxylated metabolites (OH-PCBs) in living organisms. Therefore, it is key to determine not only parent PCBs but also OH-PCB metabolites.

LC is usually the technique of choice, but the common C_{18} and phenyl columns lead to the coelution of isobaric compounds. Some years ago, we have studied in depth the retention mechanism of hydroxylated compounds on a polar embedded amide-type column, and found that the separation process is driven by a mixed hydrophobic/hydrophilic mechanism whose nature can be modulated modifying the eluent composition. On this basis, a sensitive LC-ESI-MS^2 method for the congener specific separation and determination of relevant OH-PCBs using a polar-embedded LC column was developed in collaboration with Dr. B. Gómara (IQOG-CSIC), and applied to human serum samples with excellent results.

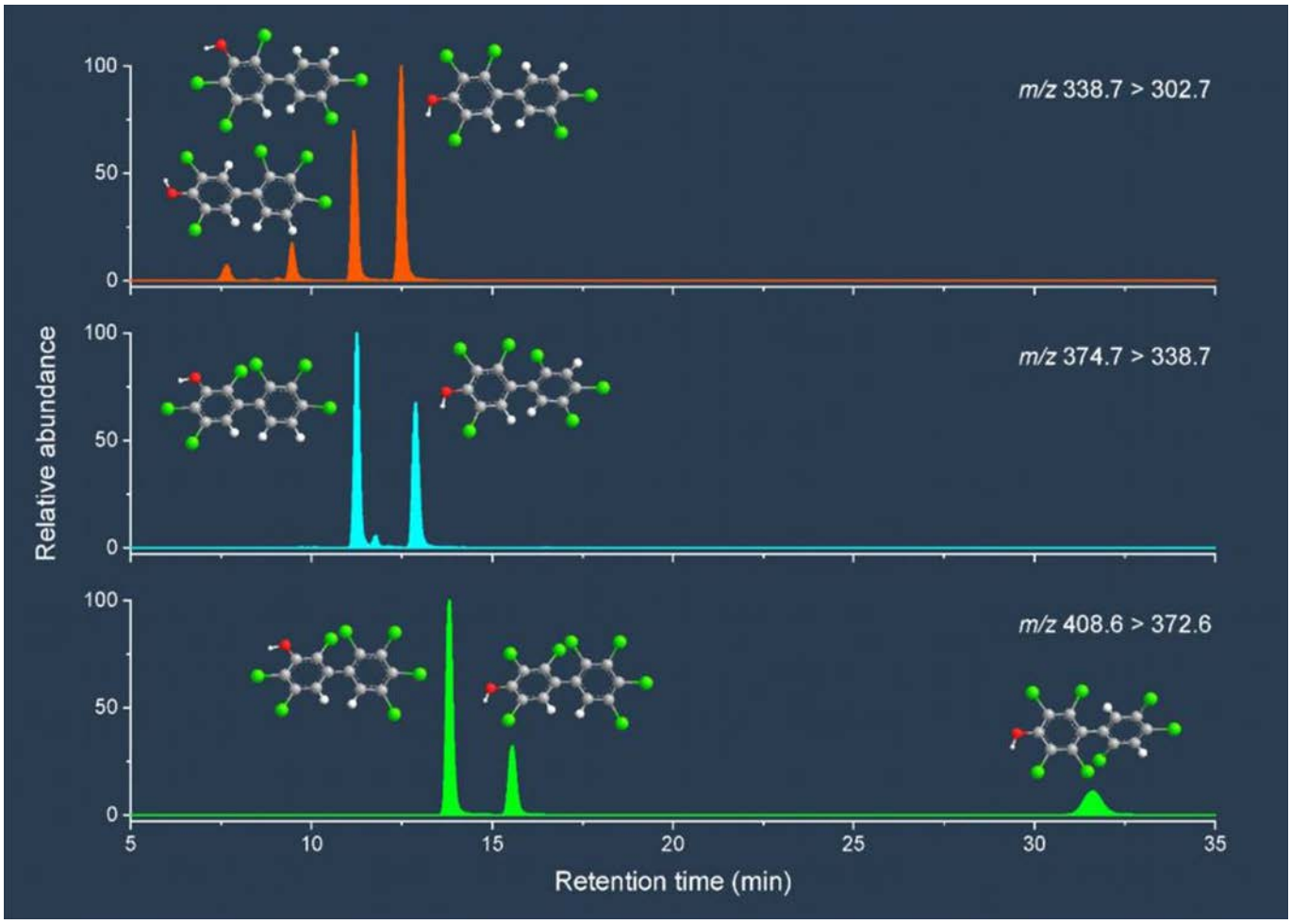


Figure 5: Chromatographic separation, in a polar-embedded amide-type LC column, of a blank-serum sample spiked with the eight OH-PCBs studied.

Si, Ge and Sn compounds

We carried out a study of the gas phase reactions of Me_2E (E=Si, Ge, Sn) with SO_2, combining kinetics measurements with quantum mechanical calculations (*ab initio*) and RRKM calculations. SO_2 is a molecule of atmospheric interest.

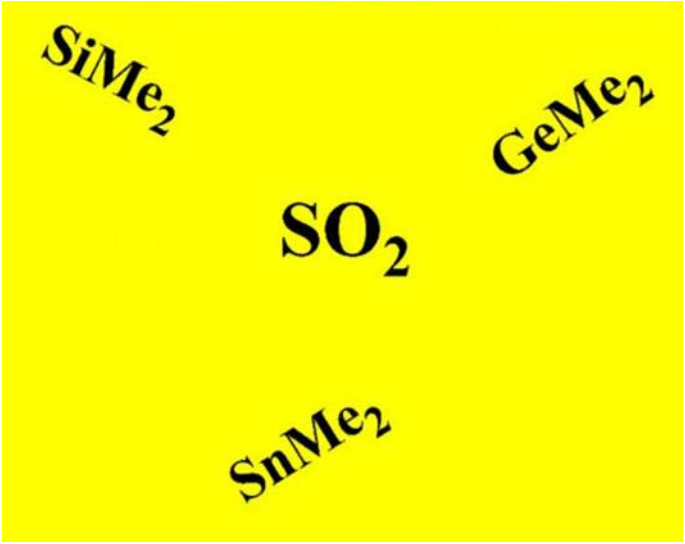


Figure 6: Reactions studied in this project.

Thermochemistry of Germanium and Organogermanium compounds

Germanium is a semiconductor and is a component of many electronic devices. It is similar in its chemical behavior to silicon although it is less abundant in nature. Thermochemistry is the basis of understanding the stabilities of chemical compounds in general. We have already written a review of the Thermochemistry of Organosilicon compounds, we extend this idea to the same thing for Germanium. The emphasis is on data from experimental measurements, results of quantum chemical (*ab initio*) calculations are also included. The review provides a set of current best values for tetravalent (GeX_4) compounds covering both inorganic (X = H, F, Cl, Br, I) compounds and organic (X = Me) well as mixed GeX_nY_{4-n} compounds. In addition to the stable tetravalent compounds, data is included for less stable (more reactive) species such as GeX_3 (free radicals), GeX_2 (germylenes) and π-bonded molecules which play prominent roles as intermediates in many thermal and photochemical reactions of germanium compounds.

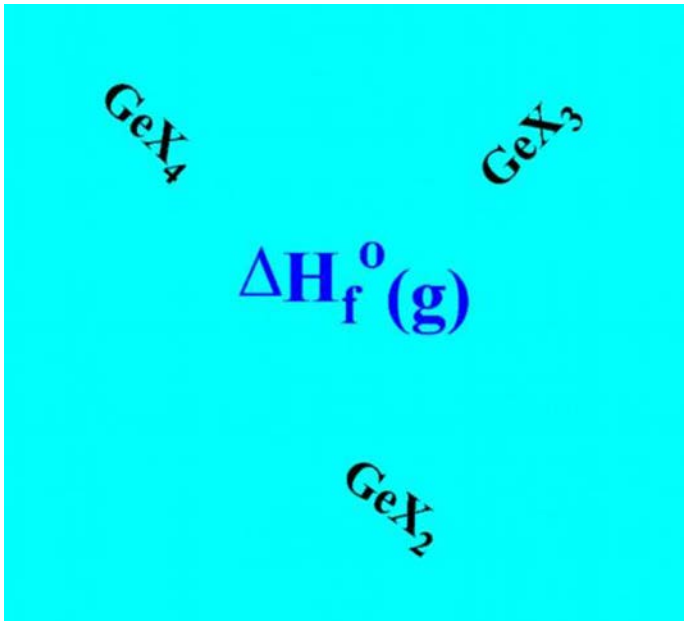


Figure 7: Schematic representation of the topics covered in this research.

Publications

Hernáiz-Izquierdo, M., Galindo-Iranzo, P., García-Armada, M.P., Saiz-López, A., Gómara, B., Quintanilla-López, J.E. and Lebrón-Aguilar, R. Direct quantification of inorganic iodine in seawater by mixed-mode liquid chromatography-electrospray ionization-mass spectrometry. *J. Chromatogr. A* **1588**, 99-107 (2019).

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Muñoz-Labrador, A., Azcarate, S., Lebrón-Aguilar, R., Quintanilla-López, J.E., Galindo-Iranzo, P., Kolida, S., Methven, L., Rastall, R. A., Moreno, F. J. and Hernandez-Hernandez, O. Transglycosylation of steviolglycosides and rebaudioside A: Synthesis optimization, structural analysis and sensory profiles. *Foods* **9**, 1753 (2020).

National Grants:individual

Agencia Estatal de Investigación (AEI)

Principal Investigator	Title	Reference
L. Ramos and B. Gómara	Procesos analíticos más sostenibles mediante el uso de disolventes modulables	PID2019-106405GB-I00

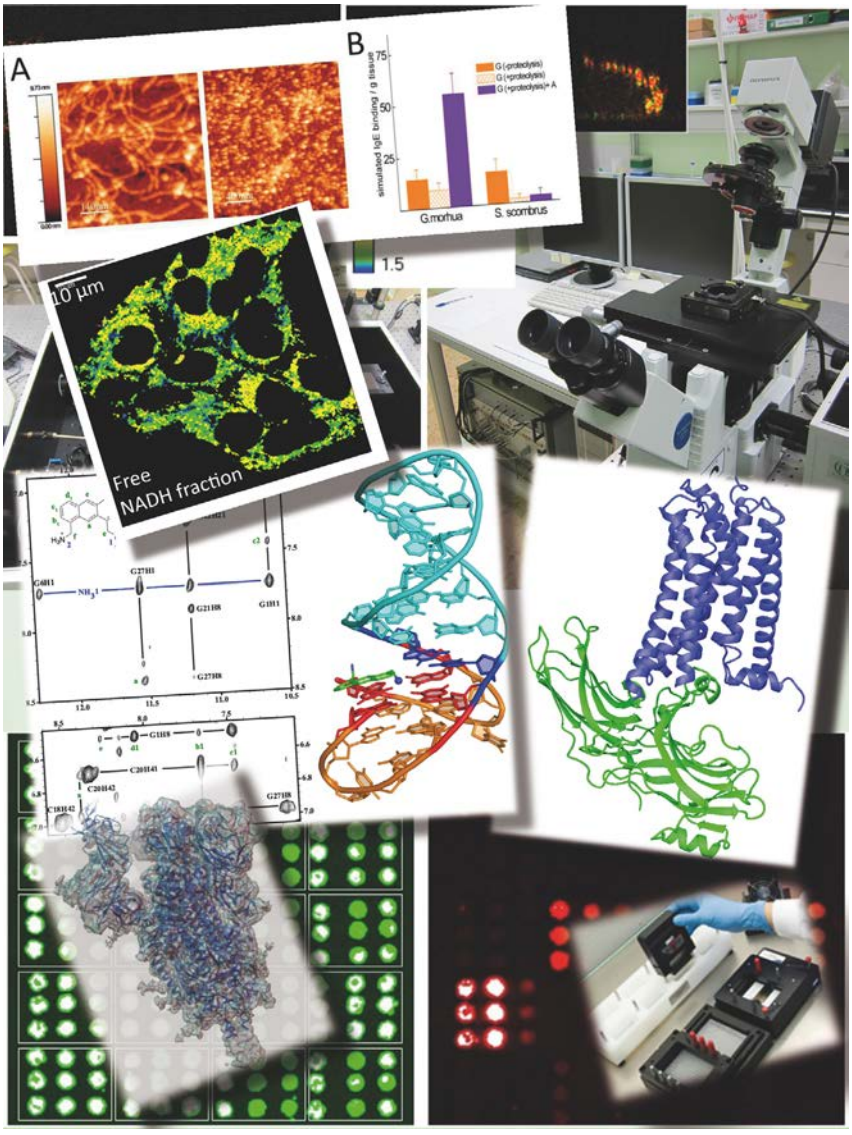
National Grants: coordinated

Comunidad de Madrid

Principal Investigator	Title	Reference
Alfonso Saiz López/ (Rafael Borge García, Coordinator of the program)	Evaluación integral de la calidad del aire urbano y cambio climático	P2018/EMT4329, AIRTEC-CM


CONSEJO SVPERIOR DE INVESTIGACIONES CIENTIFICAS

Department of Biological Physical Chemistry



Introduction

The research of our Department (http://qfbio.iqfr.csic.es) includes the fields of Biochemistry, Molecular Biology, Structural Biology, Biophysics, Glycobiology, Bioinformatics and Bio-thermodynamics. Our main goal is to understand the physical-chemical bases governing the structure, stability, dynamics and interactions of biological molecules, i.e. peptides, proteins, nucleic acids and carbohydrates. We tackle systems with different levels of complexity, ranging from isolated molecules to macromolecular assemblies, membrane mimetics, cells and tissues. Many of these systems have biomedical, pharmacological or biotechnological importance.

Our Department has all the necessary instrumentation for in depth experimental studies of biological samples: basic techniques for isolating, cloning, expressing, and purifying proteins and nucleic acids; diverse methods for biochemical and biophysical characterization: immuno chemical analysis, high-performance liquid chromatography, analytical ultracentrifugation, light scattering (MALLS), spectropolarimetry (CD), UV-visible and fluorescence spectroscopies, isothermal titration calorimetries (ITC), and specific advanced methodologies: i) microarray platform for molecular recognition studies, ii) fluorescence methods with high-temporal (ps-to-ms) and spatial (mm-sub mm) resolution, iii) solution NMR spectroscopy for determination of structure, dynamics and molecular recognition of biomolecules (Manuel Rico high field NMR laboratory, LMR; http://lmr.csic.es). Besides, we develop novel methods for simulation, analysis and modelling of large biomolecular systems.

Group Structure

Group of Fluorescence and Molecular Biophysics

Tenured Staff scientists

A. Ulises Acuña Fernández (*Profesor Ad honorem*)

Mª Pilar Lillo Villalobos (*Assistant Professor*) ReID ORCID SCOPUS

Technical Staff

Carolina García Rodríguez (TSE) ReID ORCID SCOPUS

Victor Manuel Orejuela Sánchez (Research contract, from 7/10/2019 to 30/09/2020)

Summary

The overall objective of the Group is to understand the molecular and cellular basis of diseases to improve both, their diagnosis and treatment, using non-invasive quantitative methods that discriminate and characterize supramolecular structures in different subcellular locations, in very heterogeneous media, with single molecule resolution, in time scales ranging from picoseconds to second-hours.

Techniques: Fluorescence lifetime (FLIM, FLIM-phasors), energy transfer (FLIM-FRET, FLIM-FRET-phasors), polarization fluorescence (TRAIM and homo-FRET), and second harmonic generation (SHG) imaging, in different regions of the emission spectrum, with One- and Two-photon excitation.

In vitro samples, living cells and tissues.

Strategic Aims

- Quantitative characterization of molecular species and their interactions, mainly in cellular membranes, subcellular compartments: *in vitro* and living cell studies.

Remarkable results

Bioenergetics deficiency caused by the dysfunction of any of the five complexes that comprise the oxidative phosphorylation process (OXPHOS) constitutes the main genetic cause of the inborn errors of energy metabolism. We have developed a set of micro-spectroscopy methods based on time-resolved fluorescence, that allow to quantify absolute concentrations of different metabolites associated with OXPHOS (free and bound NADH, FAD, redox index and membrane potential) in living cells. Our approach is part of an interdisciplinary study to comparatively detect biochemical and biophysical hallmarks on deficient mitochondria as compared with their healthy counterparts.

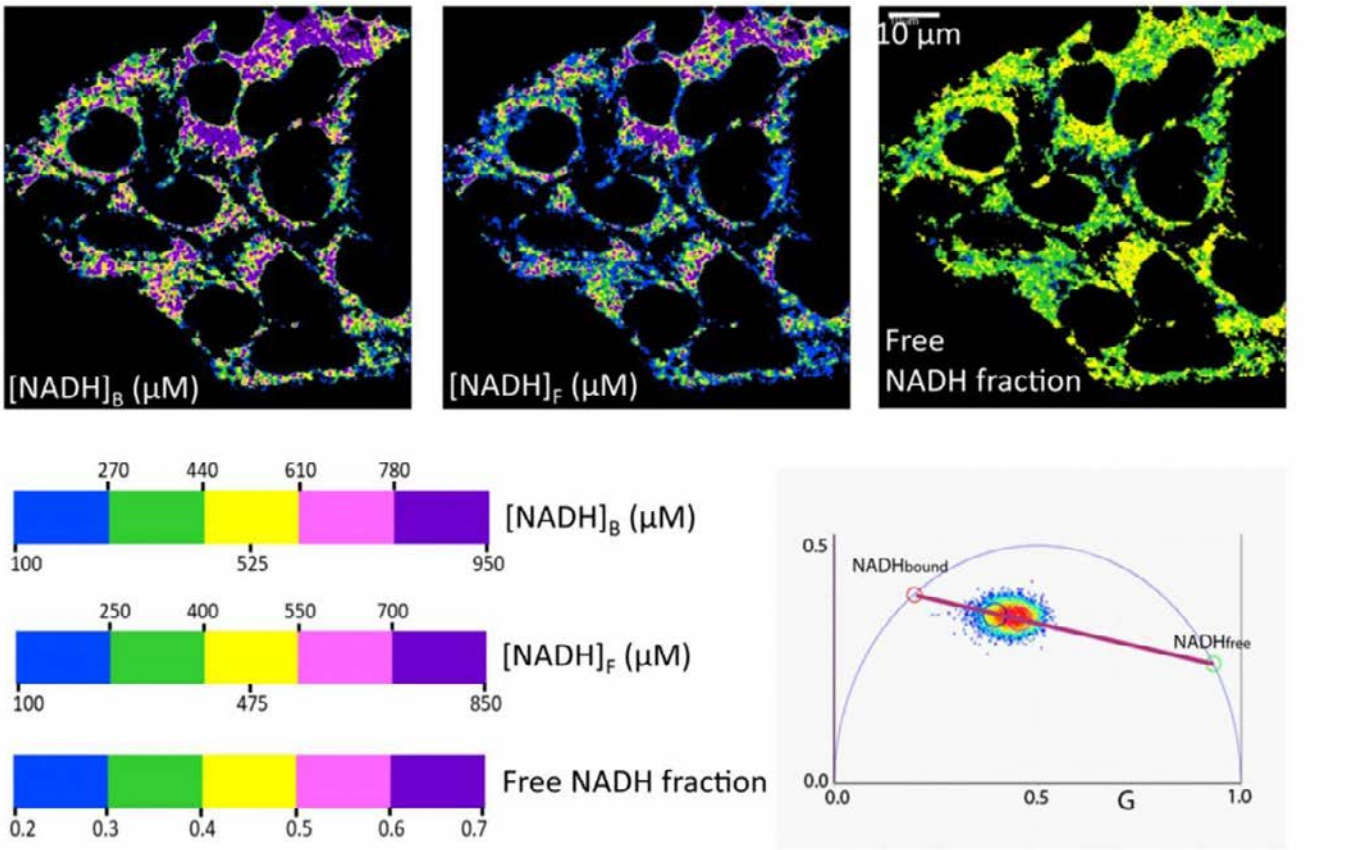


Figure 1: Illustrative example of live cell images of absolute concentration of bound and free NADH, free NADH fraction, and the corresponding phasor plot (FLIM-phasor approach). The color scale of concentration images is in μM units. The pink and green circles in the phasor plot indicate the phasor position for free and bound NADH, respectively. Along the purple line, every point would represent a different linear combination of free and bound NADH. The phasor cluster on this line corresponds to the experimentally determined phasors for these representative cells.

Publications

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COMPETITIVE FUNDING

National Grants:individual

Ministerio de Ciencia, Innovación y Universidades

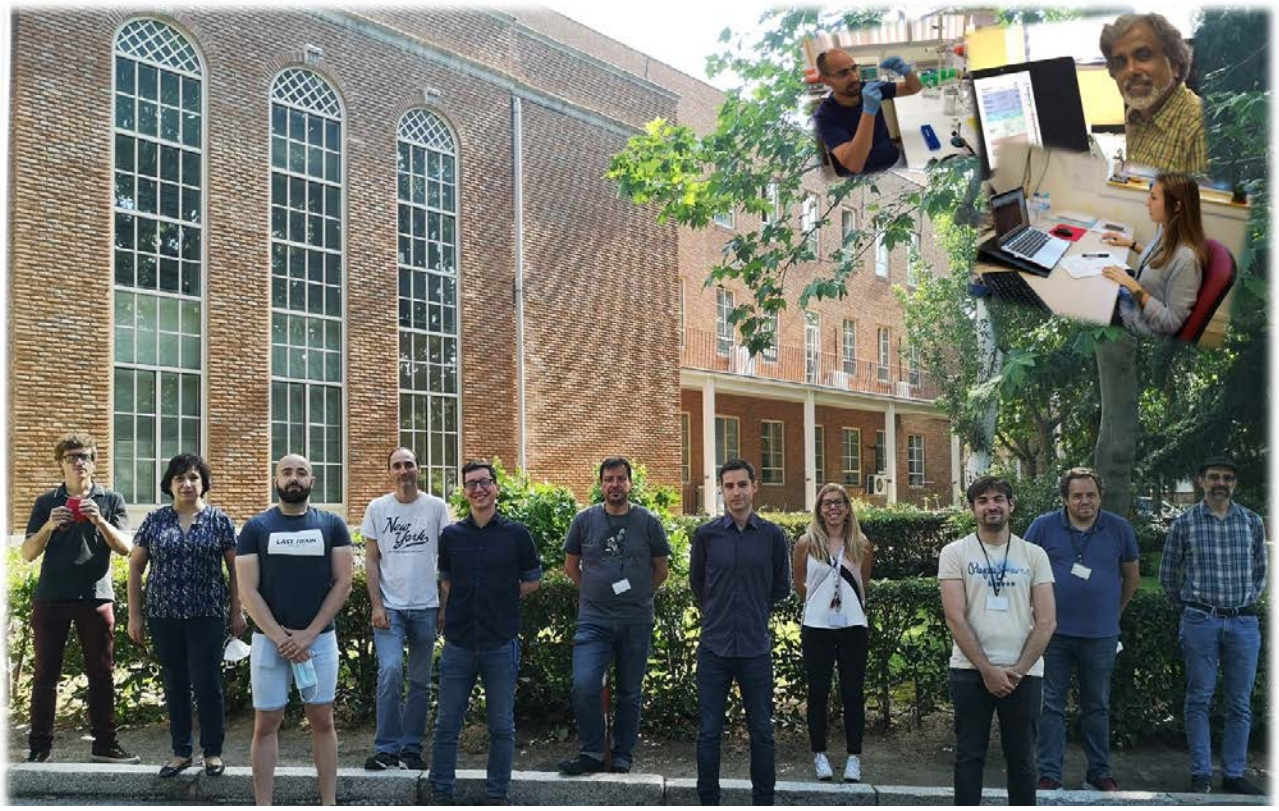
Principal Investigator	Title	Reference
I. López Montero M.P. Lillo	Propiedades emergentes de nanorotores biológicos en medios viscoelásticos.	PGC2018-097903-B-I00

National Grants: coordinated

Comunidad de Madrid

Principal Investigator	Title	Reference
I. López Montero	Soluciones interdisciplinares con control de edición génica al déficit bioenergético OXPHOS	SINOXPHOS-CM P2018/BAA-4403

Group of NMR of Protein Structure, Dynamics and Interactions



Tenured Staff scientists

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(*Professor*)

María Ángeles Jiménez López
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Douglas V. Laurents
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José Manuel Pérez Cañadillas
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Paula Morales
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Miguel Mompeán
(LaCaixa Banking Foundation - Junior Leader "Retaining" prog., since 1/06/2019)

Sergio Camero Gigante
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Rubén López Sánchez
(since 16/12/2020)

Technical Staff

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Miguel Ángel Treviño (TSE)

Daniel Calvo Marco (PTA; since 16/12/2019)

Summary

The main goal of our group (https://rmnpro.iqfr.csic.es/en/) is understanding the structural bases of life. We aim to elucidate the physicochemical principles that determine the structure, dynamics, stability, folding and recognition of peptides, proteins, and nucleic acids, with a particular focus in disease-related biomolecules. This knowledge is crucial for a detailed description of their biological function. To that end, we use mainly high resolution multidimensional nuclear magnetic resonance (NMR) spectroscopy and get additional data from various biophysical techniques as well as from computational methods.

Strategic Aims

- To understand the structure-activity relationships in peptides of biomedical relevance: applications in cancer, infections, and analgesia.
- To study protein structure, dynamics, stability and recognition, mainly directed to understand the molecular basis of disease, such as, amyloid proteins, proteins involved in rare diseases (PHOX2B responsible for CCHS), and host-pathogen interactions.
- Characterization of intrinsically disordered proteins (IDPs) and phase transitions (monomer-to-condensate and monomer-to-amyloid), such as the intrinsically disordered domains from coronavirus SARS-CoV-2, functional and pathological amyloids, and polyproline II helices.
- To understand photosensory regulation and signal transduction in bacteria.
- Development and implementation of novel NMR methodologies to study biomolecules; currently, the focus is on those applicable to intrinsically disordered proteins (IDPs).
- Optimization of protocols for expression and purification of uniformly and specifically labeled proteins.

Remarkable Results

Relevant molecular processes upon memory consolidation

We have characterized structural transitions in Orb2, a functional prion which is key for memory consolidation in *Drosophila*. Recently, Science published the structural characterization of the mature amyloid fibrils formed by Orb2 in drosophila brain, which yielded transcendental insights into the structural basis of memory consolidation. However, knowledge on structural transitions involved in Orb2 mediated memory consolidation was still lacking. In collaboration with scientists from Nova University of Lisboa scientists, we have characterized the structural and dynamic properties of the prion-like domain of Orb2 revealing structural plasticity. In particular, Orb2 acquires alpha-helical structure in a His-rich region at neutral pH, while at acidic pH Orb2 is fully disordered. Orb2 binds RNA at acidic pH. At neutral pH, it is unable to bind RNA or Ca^{+2} but binds $Zn^{+2}$and starts to oligomerize. Finally, a model of the regulation of the functional amyloidogenesis of Orb2 was proposed. See *J Biol Chem*. **295** (52), 18122-18133 (2020). doi: 10.1074/jbc.RA120.015211

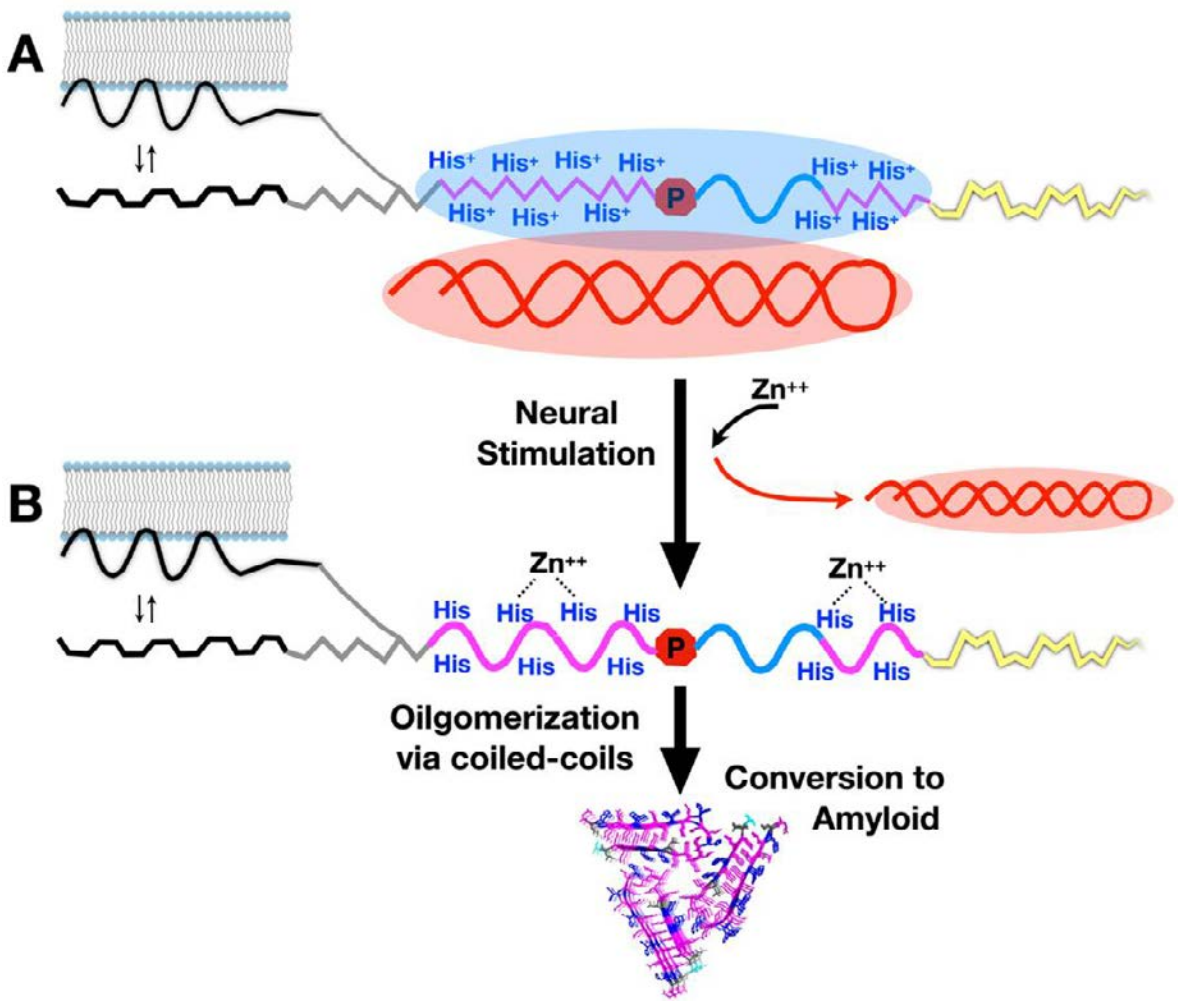


Figure 1: Model for Orb2 conformational changes triggered by Zn^{++} binding and the release of mRNA (**A**), leading to functional amyloid formation (**B**).

Two proteins can co-assemble to form hetero-polymeric hybrid amyloids in necrosome complexes

We have obtained for the first time atomic-level evidence that co-assembly of two proteins to form hetero-polymeric, hybrid amyloids in necrosome complexes. These co-polymers adopt a 1:1 alternating assembly (grey and gold representing such alternating molecules) and constitute a family of protein complexes named necrosomes that participate in the activation of necroptosis. See Mompeán et al., EMBO Rep. 2019 Feb; 20 (2): e47433. doi: 10.15252/embr.201847433

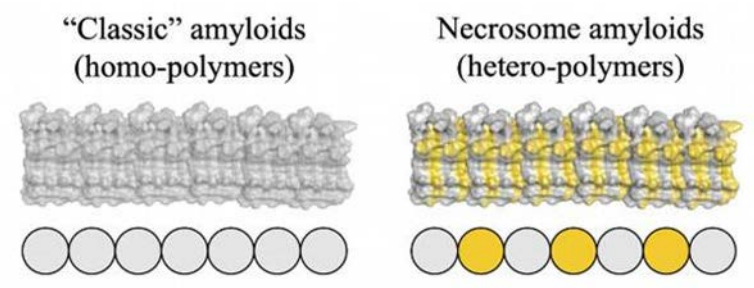


Figure 2: Conventional or "classical" amyloids were regarded homo-polymers that built on copies of a same protein (represented in grey).

Structural properties of phosphorylation motifs in the intrinsically disordered C-terminal domain of Histone H1.0

H1 linker histones bind to DNA at the nucleosome and play a regulatory role in transcription. The C-terminal of the eukaryotic Histone H1.0 is intrinsically disordered and comprises three phosphorylation motifs. Phosphorylation of these motifs affect DNA binding. The conformational behavior of model peptides containing the phosphorylation motifs TPKK and TPVK has been examined by NMR. The NMR data obtained provides evidence that the two motifs, both non- and phosphorylated, present the same backbone conformations, but differ in side chain interactions. Besides, the pK_a value of the phospho-threonine (pT) residue in the TPKK motif is much lower than the intrinsic one, but only slightly lower in the case of the TPVK motif. This can be explained by positively charged Lys side chains stabilizing the anionic form of the phosphate group in the two motifs and by the non-polar valine compensating this effect in the case of the pTPVK motif. See *Chem. Eur. J.* **26** (27), 5970-5981 (2020). doi: 10.1002/chem.201905496

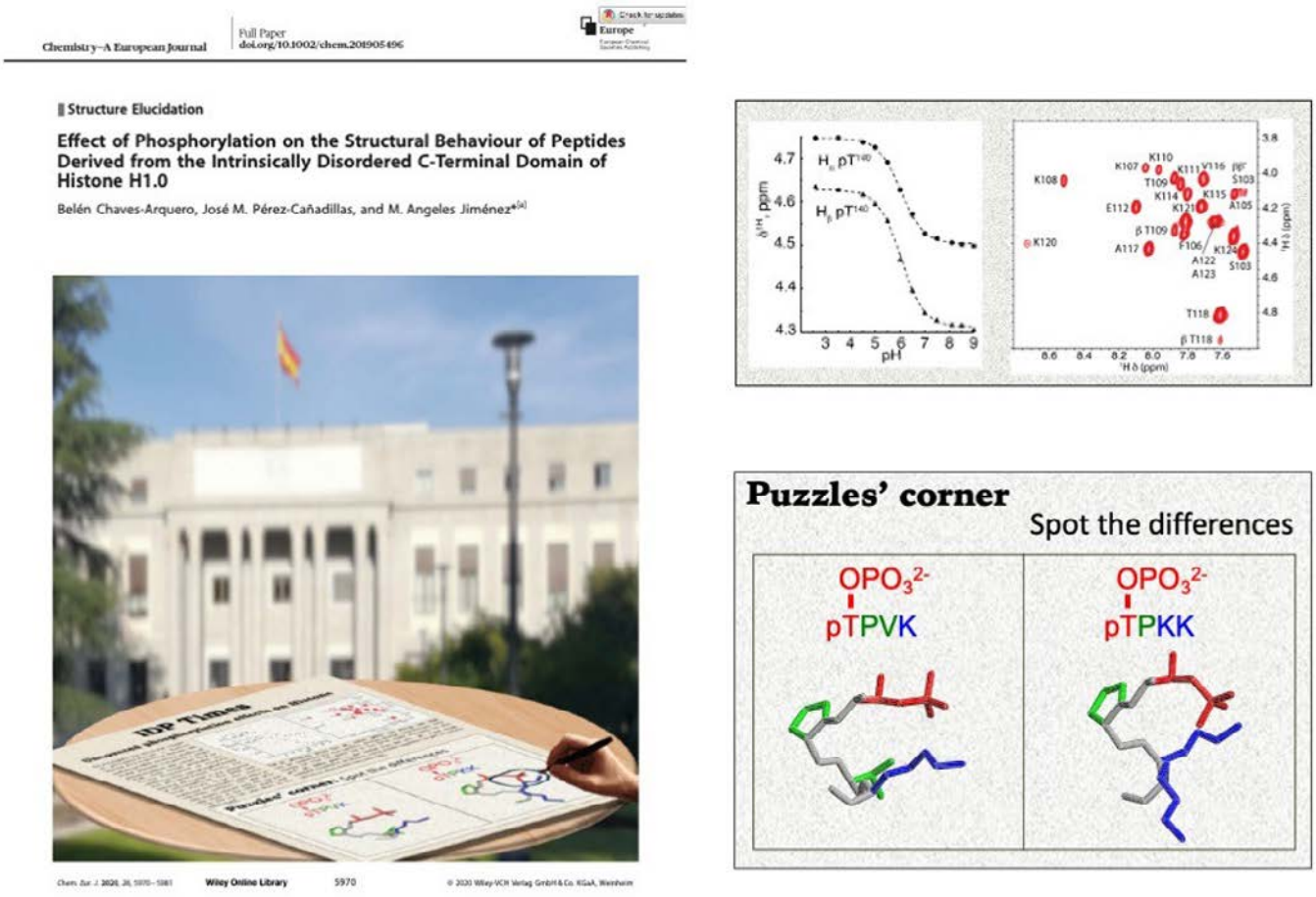


Figure 3: (Left) Frontispiece in which a fictional newspaper dedicated to IDPs highlights the results on the conformational similitudes and differences of two phosphorylation motifs present in the intrinsically disordered C-terminal domain of Histone H1.0. (Right) Expansions of the newspaper's pictures. The pH dependence of the chemical shifts of two protons of a phosphorylated threonine (pT) and a 2D TOCSY spectral region of a peptide containing the TPKK motif are shown at the top; and structures of the phosphorylated pTPVK and pTPKK motifs at the bottom.

Peptide models provide insights into the interaction between the cannabinoid receptor CB1 and the beta-arrestin 1protein

The cannabinoid receptor type 1 (CB1) is the most abundant G protein coupled receptor (GPCR) in the central nervous system and participates in the regulation of numerous physio-pathological processes. Diverse signalling pathways are initiated upon its activation by different effector proteins, such as G-protein and β-arrestins. To gain insight into the poorly understood CB1/β-arrestin interaction, we designed peptides that mimic the motifs putatively involved in the interaction: the transmembrane helix 7-helix 8 (TMH7-Hx8) elbow located at the intracellular side of the CB1 receptor and the β-arrestin1 finger loop. Based on CD and NMR data, these peptides adopt helical conformations and interact with each other in several solvent conditions (water, mixed trifluoroethanol/water, and zwitterionic detergent micelles). Our results provide us details on the binding mode of β-arrestin and CB1 receptor and validate minimalist approaches to structurally understand complex protein systems. See Int J Mol Sci. 21(21), 8111 (2020). doi: 10.3390/ijms21218111.

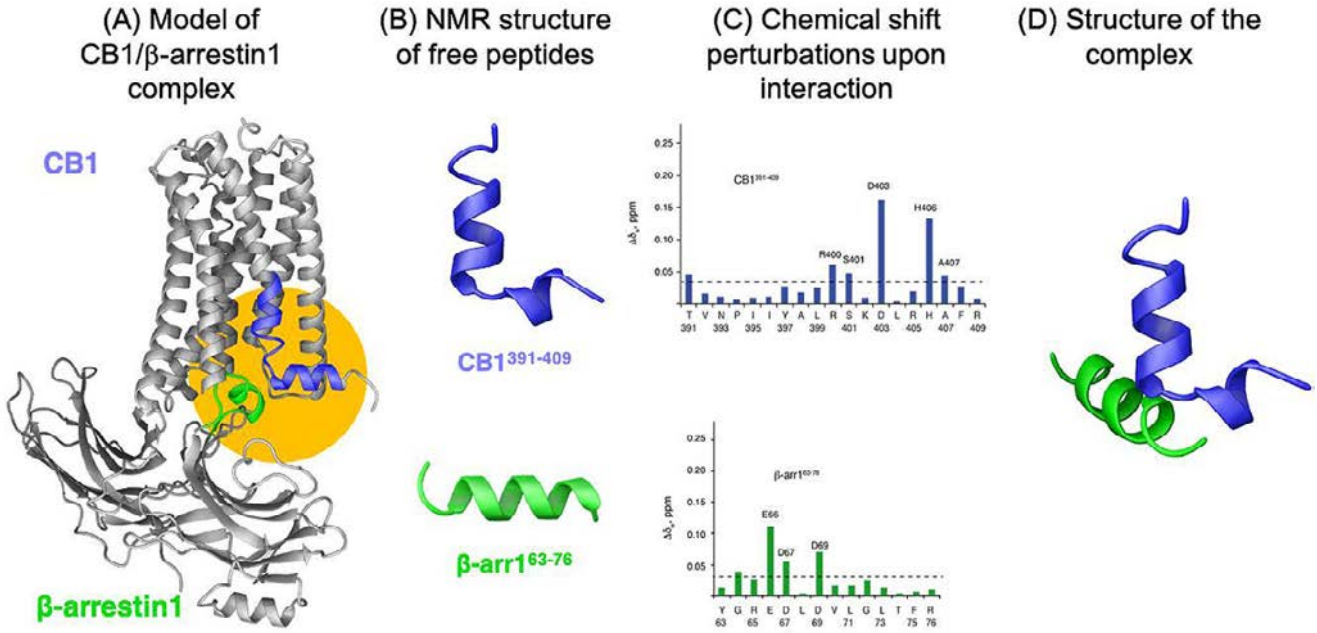
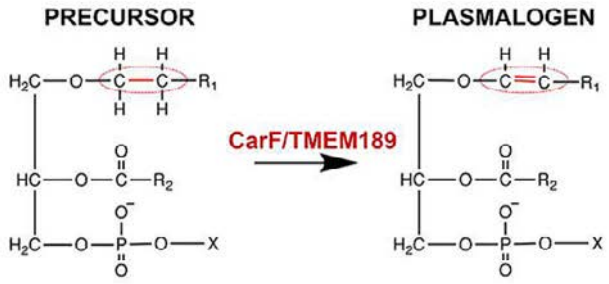


Figure 4: (A) Homology model of the cannabinoid receptor CB1/ β-arrestin1 complex. The putative interacting region is highlighted. (B) Ribbon representation of the structures peptides $CB1^{391-409}$ and $\beta\text{-arr1}^{63-76}$ in free state. (C) Bar plots of the chemical shift perturbations of peptides $CB1^{391-409}$ and $\beta\text{-arr1}^{63-76}$ upon interaction. (D) Ribbon representation of the $CB1^{391-409}$ / $\beta\text{-arr1}^{63-76}$ complex.

A bacterial light response reveals an orphan desaturase for human plasmalogen synthesis

Plasmalogens are glycerophospholipids with a hallmark sn-1 vinyl ether bond found in animals and some anaerobic bacteria but not plants, fungi, or most aerobic bacteria. In mammals, they occur in most subcellular membranes and are abundant in the brain and heart. They have proposed membrane organization, signaling, and antioxidant roles, and their deficiency correlates with many human disorders, including cancer and Alzheimer's disease. A vital enzyme for plasmalogen biosynthesis remained unknown for five decades until we discovered that it was CarF, a protein we had established was essential in how the soil bacterium *Myxococcus xanthus* senses and responds to light. We uncovered this CarF activity in homologs in worms, flies, fish, mice, and human (where it was called TMEM189) but not plants, which lack plasmalogens, and that plasmalogens participate in sensing photooxidative stress. Our discovery will spur studies of plasmalogen biogenesis, functions, and roles in disease. See *Science* 366,128-132 (2019).



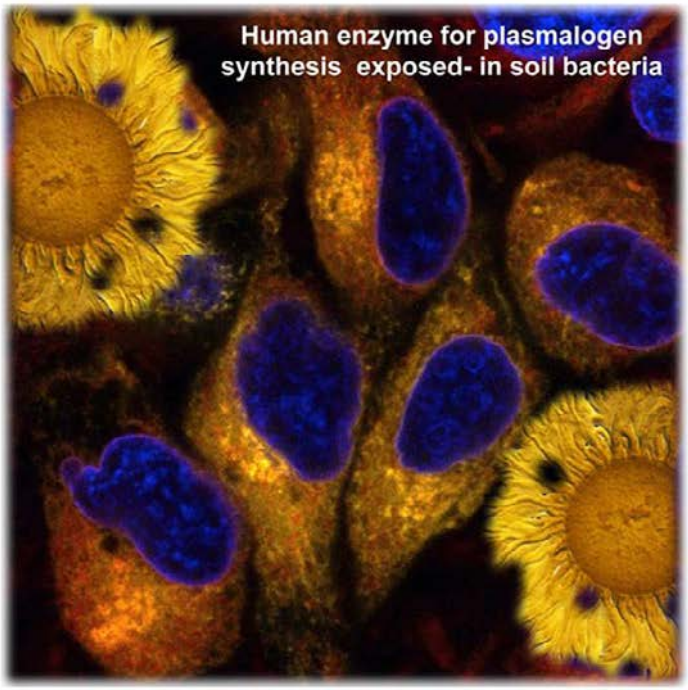


Figure 5: (Left) Precursor to plasmalogen reaction catalysed by CarF. (Right) Human HeLa cells with enzyme TMEM189 localized in the endoplasmic reticulum. Top left and bottom right: Two colonies of the soil bacterium *Myxococcus xanthus.* Courtesy: "Genética Molecular" group, Univ. Murcia (Associated Unit IQFR-CSIC)

Conformational Priming of RepA-WH1 for Functional Amyloid Conversion Detected by NMR Spectroscopy

How proteins with a stable globular fold acquire the amyloid state is still largely unknown. RepA, a versatile plasmidic DNA binding protein from *Pseudomonas savastanoi*, is functional as a transcriptional repressor or as an initiator or inhibitor of DNA replication, the latter via assembly of an amyloidogenic oligomer. Its N-terminal domain (WH1) is responsible for discrimination between these functional abilities by undergoing insufficiently understood structural changes. RepA-WH1 is a stable dimer whose conformational dynamics had not been explored. Here, we have studied it through NMR $\{^{1}H\}$-^{15}N relaxation and H/D exchange kinetics measurements. The N- and the C-terminal α-helices, and the internal amyloidogenic loop, are partially unfolded in solution. S4-indigo, a small inhibitor of RepA-WH1 amyloidogenesis, binds to and tethers the N-terminal α-helix to a β-hairpin that is involved in dimerization, thus providing evidence for a priming role of fraying ends and dimerization switches in the amyloidogenesis of folded proteins. See Structure 28, 336-347.e4 (2020).

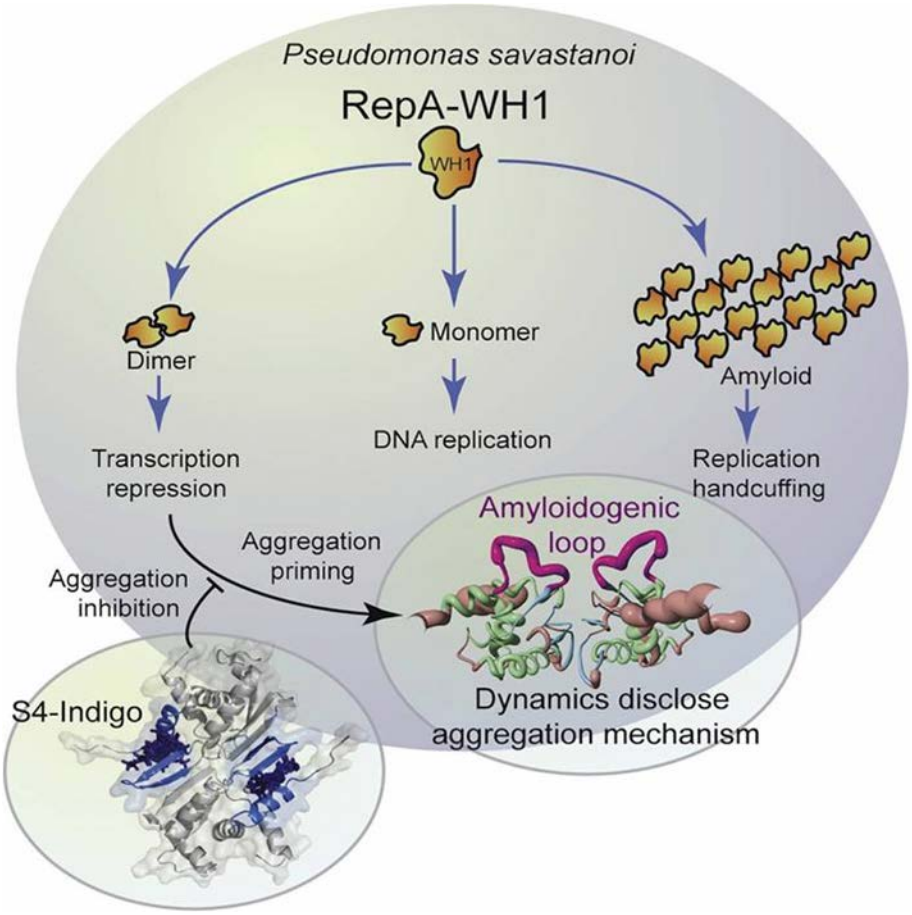


Figure 6: Diverse oligomeric forms of RepA-WH1 play contrasting roles in transcription repression, DNA replication and plasmid replication inhibition. Our NMR studies provide insight into the mechanisms of oligomerization regulation by ligand binding.

Structural understanding of control and regulation of gene expression: The case of the N-terminal domain of eIF4G and the RNA binding proteins Pab1 and Pub1

eIF4G1 is a critical factor in the regulation of translation. Its interaction with Poly(A) binding protein Pab1 is key for translation initiation. At the same time it also interacts with other proteins like Pub1 involved in the Stress Granule response. We have led an exhaustive study of the N-terminal domain of eIF4G1 by NMR, SAXS and confocal microscopy. This multidisciplinary study was presented on the PhD thesis of Belén Chaves-Arquero. The eIF4G11-249 is an important regulatory domain of the protein and is majorly unstructured, but with some crucial long-range interactions that have been characterized by Paramagnetic Resonance Enhancements. The work describes one of the few full-atoms models of an IDP, generated by an innovative approach and that that simultaneously fulfill SAXS and NMR data. The study has been done in collaboration with groups of Centre de Biochimie Structurale in Montpellier (France) and the Centro de Investigaciones Biológicas (CSIC). See bioRxiv 2020.08.07.234443 (2020).

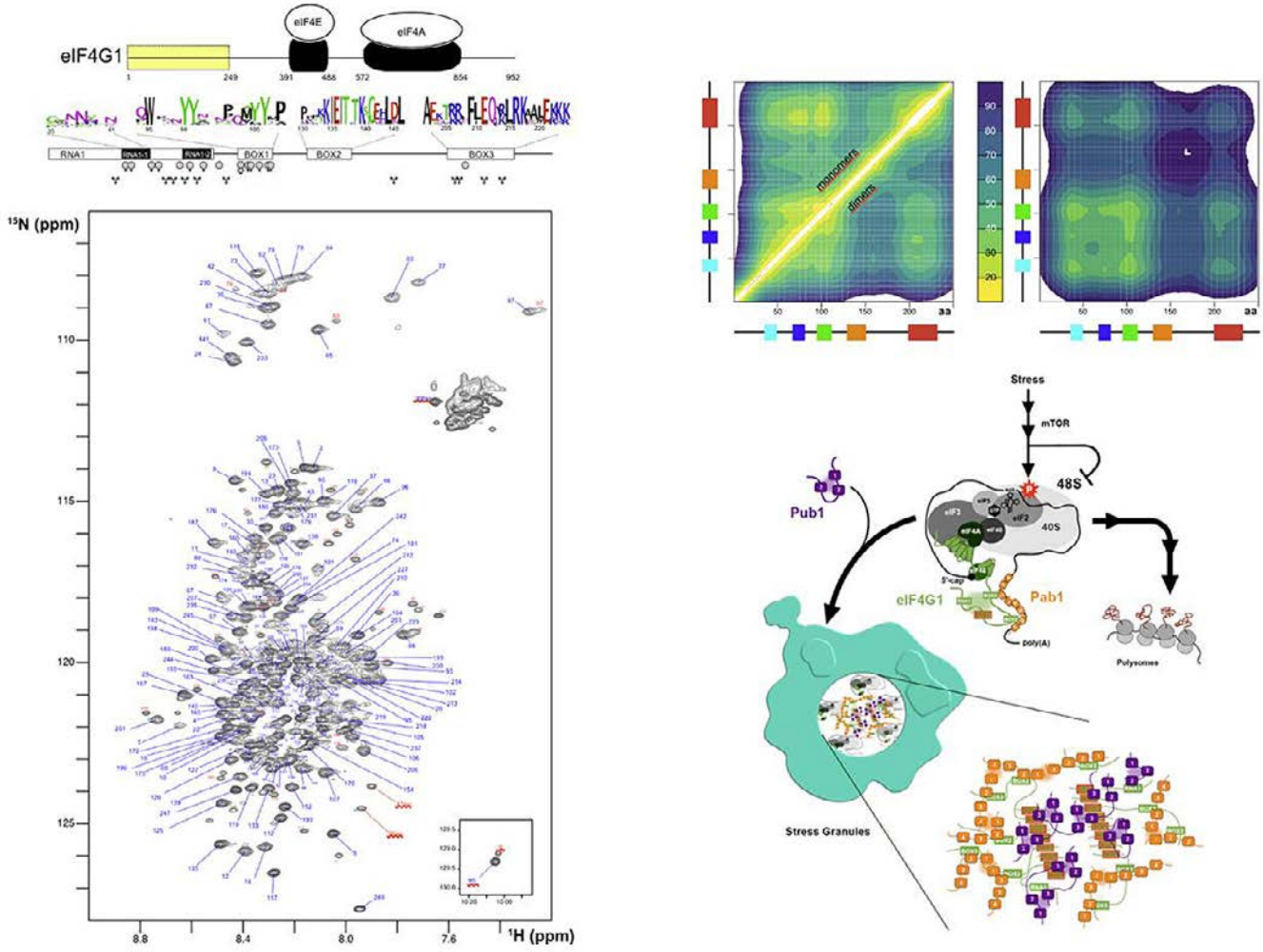


Figure 7: Schematic representation of eIF4G1. The yellow-shaded area corresponds to the N-terminal IDR that have conserved sequence elements (weblogo below). The ^{1}H-^{15}N HSQC spectra corresponds to the eIF4G1$_{1-249}$ construct. The upper right panels show the intramolecular (on the left) and intermolecular (on the right) contact maps for assemble of IDR structures. The all-atom ensembles have been calculated using a new computational method and integrate NMR and SAXS data. The down-right biological model represents the proposed mechanism of nucleation of stress-granules that incorporates the findings in this work. See bioRxiv 2020.08.07.234443 (2020), for further details.

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National Grants:individual

MICINN/AEI

Principal Investigator	Title	Reference
M. Angeles Jiménez	Transiciones orden/desorden en reconocimiento molecular de proteínas: Estudio estructural por RMN	CTQ2017-84371-P
Douglas V. Laurents	Polyproline II Helices in Biomolecular Condensates and for Biotech Applications	PID 2019-109306RB-I00
F. Javier Oroz Garde	Bases estructurales de la toxicidad de ensamblados tempranos de proteínas en proteinopatias degenerativas	PID2019-109276RA-I00

Instituto de Salud Carlos III y CSIC

Principal Investigator	Title	Reference
Douglas V. Laurents, Miguel A. Mompeán	Structural and dynamic characteristics of intrinsically disordered proteins in the virus SARS-CoV-2	COV 20·100764

La Caixa Banking Foundation

Principal Investigator	Title	Reference
Miguel A. Mompeán	Structural Elucidation of Hybrid Amyloids involved in ALS	LCF/BQ/PR19/11700003

BBVA Foundation

Principal Investigator	Title	Reference
F. Javier Oroz Garde	Las chaperonas moleculares en el inicio de la ELA	BBM_TRA_0203

Asociación Ondine España

Principal Investigator	Title	Reference
F. Javier Oroz Garde	Bases Estructurales de la Agregación Patogénica de Mutantes de PHOX2B en el Síndrome de Hipoventilación Central Congénita (CCHS)	

National Grants: coordinated

MICINN/AEI

Principal Investigator	Title	Reference
Subramanian Padmanabhan Iyer	Stress signaling at the cell envelope and associated gene regulatory mechanisms in *Myxococcus xanthus*: structural studies	PGC2018-094635-B-C22

Comunidad de Madrid. Programa de Biomedicina 2017

Principal Investigator	Title	Reference
José M. Pérez Cañadillas (Coordinator: Encarna Martínez-Salas)	RNA y Proteínas de unión a RNA: Implicaciones en Salud y Enfermedad	B2017/BMD-3370
M. Ángeles Jiménez (Coordinator: José M. Carazo)	TomoXLiver: Estudio de la disfunción del hepatocito desde un abordaje multidisciplinar	B2017/BMD-3817

International Grants: individual

Síndrome de Ondine AC (México)

Principal Investigator	Title	Reference
F. Javier Oroz Garde	The Structural Basis of Mutated PHOX2B Pathogenic Aggregation in Congenital Central Hypoventilation Syndrome (CCHS)	

Group of NMR of Nucleic Acids

Tenured Staff scientists

Carlos González Ibáñez (Professor) ORCID ReID

Non-tenured Scientists

Miguel Garavís Cabello (Marie Courie Global Fellowship MSCA-G)

Doctoral Students

Israel Serrano Chacón (FPI)

Cristina Cabrero Fernández (FPI; since 01/07/2019)

Technical Staff

Irene Gómez Pinto

Summary

The general goal of our research is to understand molecular recognition events involving nucleic acids. Such events are of key importance in a myriad of processes in Biology and Nanoscience. Increasing our knowledge of molecular recognition by nucleic acids will have an impact in the development of new therapeutical agents.

To fully understand these recognition processes, knowing the three dimensional structure of nucleic acids (DNA, RNA, and their derivatives) is essential. For this reason our group is devoted to the structural determination of nucleic acids, both alone and in complexes with proteins and small ligands.

With this aim, we use several spectroscopic techniques, especially, Nuclear Magnetic Resonance Spectroscopy (NMR).

In the last few years, we have focused on the study of non-canonical DNA structures, as well as chemically modified DNAs.

Strategic Aims

- To study non-canonical nucleic acids structural motifs.
- To understand molecular recognition between nucleic and proteins and small ligands.
- To study artificial nucleic acids.

Remarkable Results

Non-canonical nucleic acids structural and molecular recognition studies

We have continued our efforts to understand the role of non-canonical nucleic acids structures in the cell, and how they are recognized by proteins and small ligands. In collaboration with international groups in Australia and New Zealand, we have contributed to understand how one particular G-quadruplex fold, the so-called parallel G-quadruplex, is recognized by telomerase; or how other proteins, like the histone HP1a, are involved in telomeric and centromeric heterochromatine formation by recognizing specific DNA and RNA G-quadruplex structures.

In addition, we have progressed in our search of new specific ligands for non-canonical DNA and RNA structures, paying particular attention to the recognition of interphases between different DNA secondary structures, such as G-quadruplex/duplex or i-motif/duplex junctions.

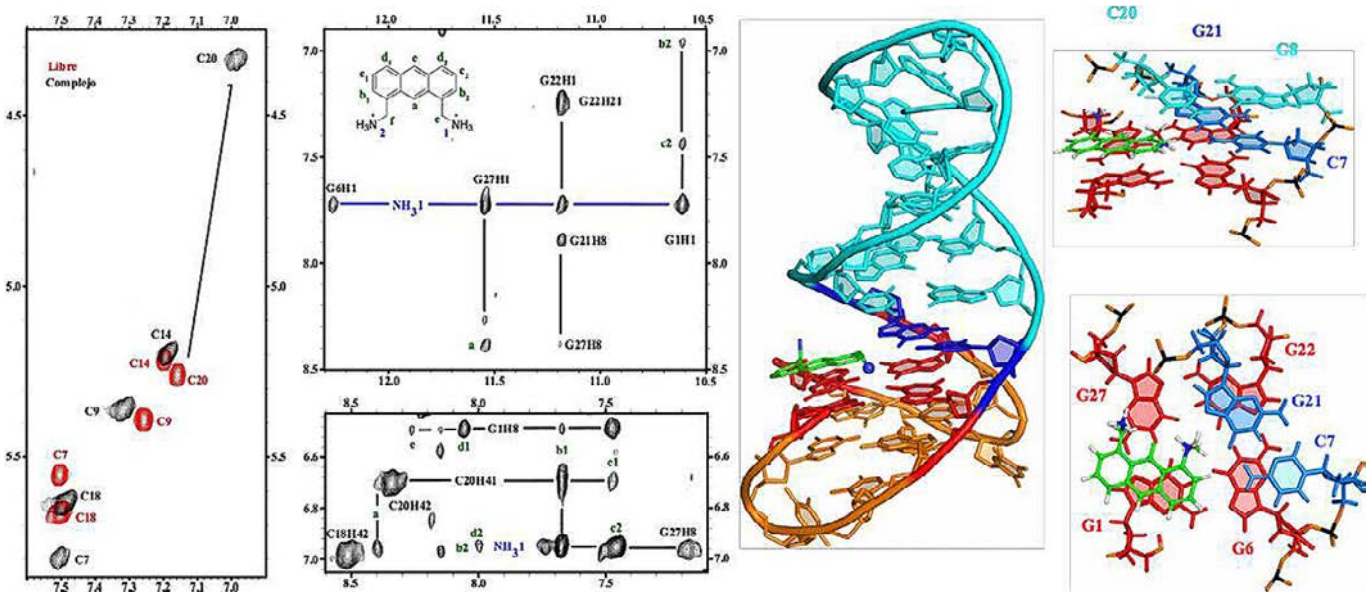

Figure 1: Molecular recognition of a G-quadruplex/duplex junction by a small ligand.

Nucleic acids structures involved in diseases

A growing body of evidence indicates that non-canonical nucleic acids structures are involved in a number of human diseases. Of particular interest is the Amyotrophic Lateral Sclerosis (ALS). This fatal disease produces progressive neurodegeneration. The most frequent genetic cause of ALS is a mutation in the *C9ORF72* gene. This gene contains a sequence of six nucleotides (5′-GGGGCC-3′/3′-CCCCGG-5′) which appears massively repeated in a high proportion of ALS patients. It has been proposed that this defect in *C9ORF72* gene contributes to the disease through the toxicity mediated by transcription of RNA containing the expansion of the repeated motif.

Our Combat_ALS action aims to develop molecules to counteract the deleterious effects produced by the presence of RNAs containing the repeat expansion of *C9ORF72*. To that end, two kinds of molecules are being developed: (I) antisense oligonucleotides (ASO) and (II) small organic compounds with affinity for the RNAs.

Part of this project has been done in collaboration with Prof. Masad J. Damha (McGill University, Canada).

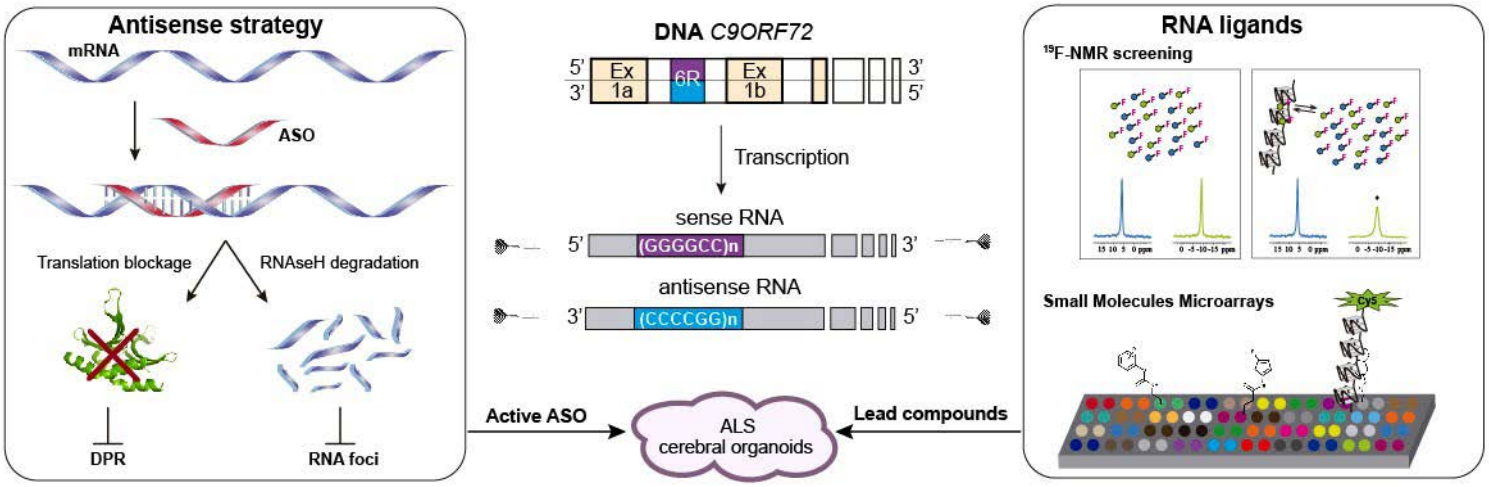

Figure 2: Illustration of the two different strategies to target RNAs involved in ALS.

Publications

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COMPETITIVE FUNDING

National Grants: individual

MICINN-AEI

Principal Investigator	Title	Reference
Carlos González Ibáñez	Estructuras cuádruplex como diana farmacológica. Nuevas oportunidades terapéuticas en Biomedicina	BFU2017-89707-P

International Grants: individual

MSCA-IF-GF. Global Fellowships

Principal Investigator	Title	Reference
Carlos González Ibáñez	Combat-ALS	EU-799693

Group of Protein Bioconformatics and Assemblies

Tenured Staff scientists

Maria Gasset Vega (*Associate Professor)*

Technical Staff

Raquel Pérez Tavarez (*TSE y similares, 1 January 2019-30 March 2020*)

Summary

The common thread to an increasing group of pathologies and of hidden functions of proteins is the formation of aggregates that can be used either that can be exploited as interventions targets or as biotechnological tools, respectively. Our short-range aims are:

1. to determine the role of amyloids in food allergies.
2. to search for hidden switches dictating protein conformational changes.
3. to use de novo and template-generated sequences for the production of functional materials.

Strategic Aims

- unveiling the role played by amyloids in food allergies and provide evidence-guided recommendations for food security.
- developing novel assemblies for the production of bioinspired materials with added value.

Remarkable Results

1. Fish isoallergens differ in their amyloid formation trait under gastric and intestinal conditions (Fig1A).
2. Fish allergenicity can be reconstructed considering the content, structural and stability features of the component allergen isoforms (Fig1B).
3. Gaining insights the effects of fish muscle processing on the allergen burden (Fig1C).
4. Extending the knowledge acquired on fish allergens to shellfish allergy. (Fig1D).
5. Metal guided assembly properties of de novo design peptide sequences (Fig1E).

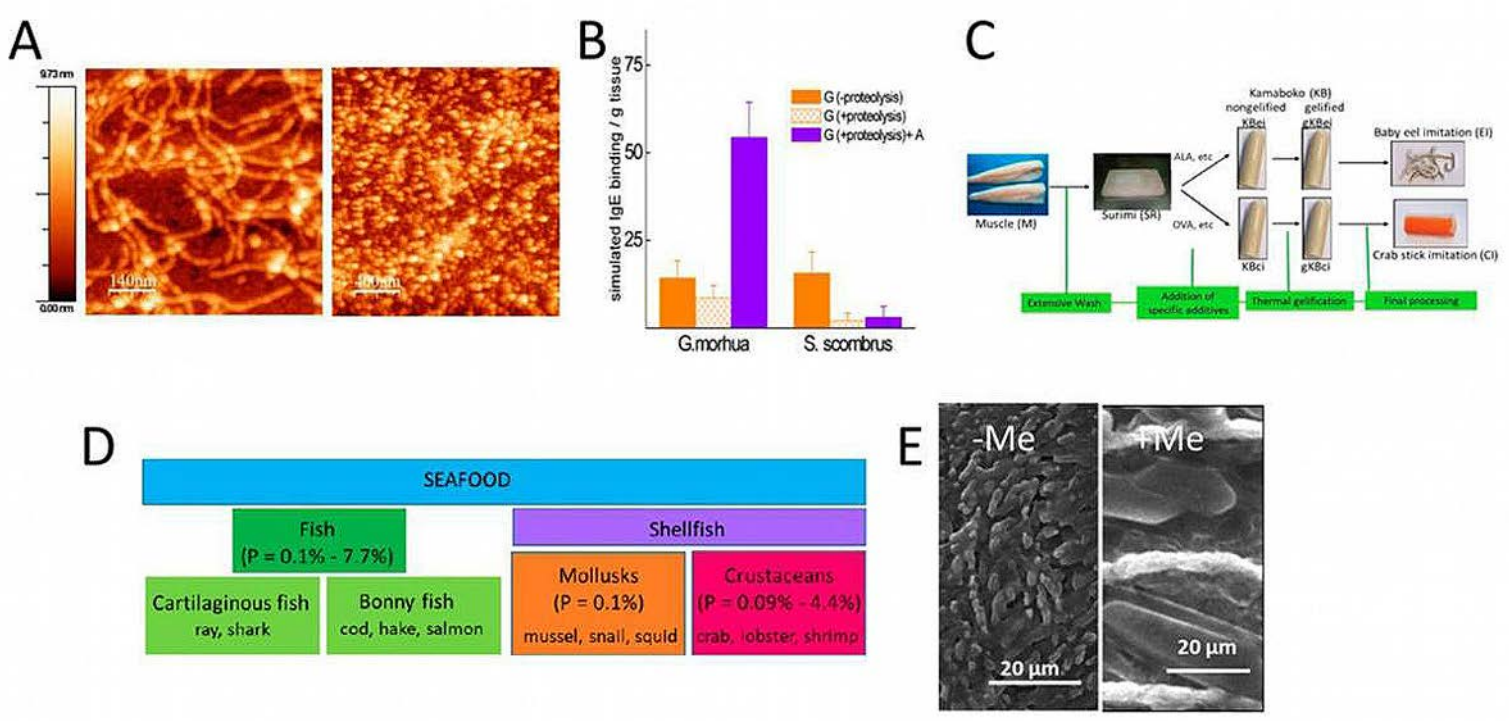


Figure 1: (A) AFM images of the aggregates formed by different β-parvalbumin isoforms. (B) Simulation of *Gadus morua* and *Scomber scombrus*muscle allergenicity. Abbreviations: G (-proteolysis), globular folds under proteolysis inhibition; G (+proteolysis), globular folds with proteolysis; G (+proteolysis)+A, globular folds with proteolysis and amyloids. (C) The transformations used in the Alaska pollock muscles valorization chain to seafood products impacts its allergenic properties. (D) Prevalence of shellfish allergy deserves the deep study of the allergens causing it. (E) Repetitive dipeptides undergo selfassembly conversion when chelated by metal cations.

Publications

Pérez-Tavarez, R., Carrera, M., Pedrosa, M., Quirce, S., Rodríguez-Pérez, R. and Gasset, M. Reconstruction of fish allergenicity from the content and structural traits of the component β-parvalbumin isoforms. *Sci Rep*. **9**, 16298 (2019).

Rey-Campos, M., Moreira, R., Romero, A., Medina-Gali, R.M., Novoa, B., Gasset, M. and Figueras, A. Transcriptomic Analysis Reveals the Wound Healing Activity of Mussel Myticin C. *Biomolecules* **10**, 133 (2020).

Carrera, M., Pazos, M. and Gasset M. Proteomics-Based Methodologies for the Detection and Quantification of Seafood Allergens. *Foods* **9**, 1134 (2020).

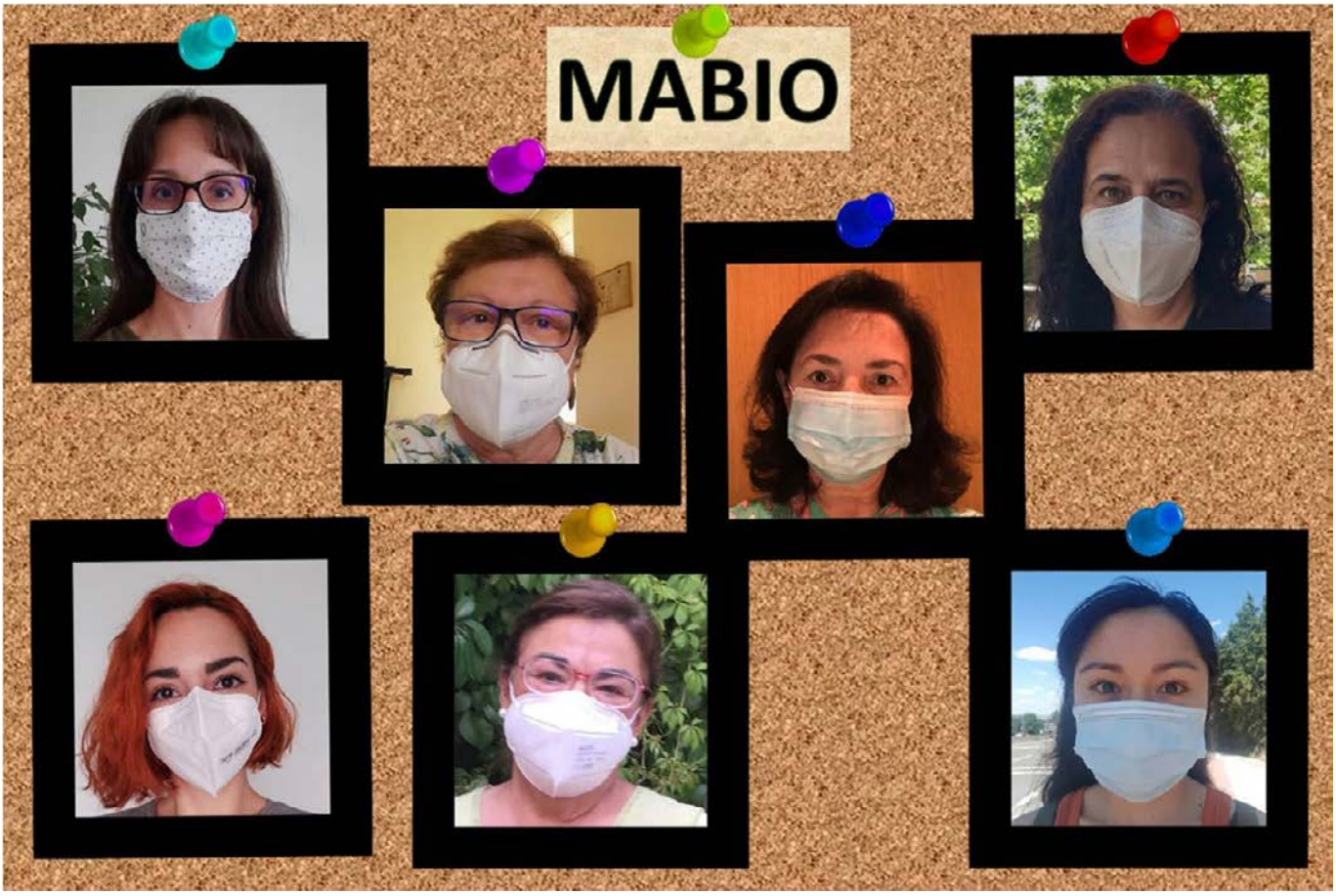
COMPETITIVE FUNDING

National Grants: individual

MINECO, MICCIN-AEI

Principal Investigator	Title	Reference
M. Gasset	Sistemas pregenéticos basados en peptidos GVAD	BFU2015-72271-EXP
M. Gasset	Análisis de la presencia y de las propiedades de ingredientes alergénicos en los productos de procesado de pescado	FCIEN-CDTI: Tolera 20177024
M. Carrera	Biología de sistemas basada en proteomica y biologia estructural en la alergia al pescado en productos pesqueros frescos y procesados	PID2019-103845RB-C21

Group of Protein Structure and Thermodynamics



Tenured Staff scientists

Margarita Menéndez Fernández
(*Associate Professor*) ORCID SCOPUS

Mª Dolores Solís Sánchez
(*Associate Professor*) ORCID ReID

Non-tenured scientists

Noemí Bustamante Spuch
(CIBERES contract; until 18/01/19)

Mª Asunción Campanero Rhodes
(Non-tenured staff scientist) ORCID

Technical Staff

Noelia Hernández Ortiz
(Specialized Technician (MINECO Project), until 30/06/19, since 16/09/19)

Mª Victoria López Moyano
(Specialized Technician, until 04/02/2019)

Zarina Méndez Onoc
("Garantía juvenil" contract (CAM), until 31/03/2019)

Summary

Elucidation of the structural and thermodynamic aspects that govern biomolecular interactions is essential to understand, and when possible modulate, such interactions. This information is particularly important for biomedically relevant systems, as it facilitates a rational design of new bioactive compounds (e.g. drugs or vaccines) and the development of novel diagnostic or therapeutic approaches, which are main final goals of the research carried out by the group (http://mabio.iqfr.csic.es/en/). During the last two years, the work has principally focused on host–pathogen interactions and potential antimicrobial agents. The list of molecules targeted includes, among others, bacterial glycans, lectins of the innate immune system as well as glycan-specific antibodies, cell wall hydrolases with antibacterial capacity, and small synthetic molecules with potential antimicrobial activity, also pursuing elucidation of the mechanism of action of active compounds.

Strategic Aims

- Study of protein–carbohydrate interactions of relevance to health and disease.
- Analysis of bacterial glycosylation and identification of receptors involved in carbohydrate-mediated bacteria–host interactions.
- Development of novel microarray approaches for molecular recognition studies.
- Identification, development and characterization of novel antimicrobials.
- Structural, thermo(dynamic), and functional characterization of biomedically relevant proteins and their complexes with other biomolecules.

Remarkable Results

The most remarkable results of the group include:

i) Comprehensive review of microarray strategies used to examine carbohydrate structures displayed on bacterial surfaces and their recognition by diverse glycan-binding proteins, including description of applications in different areas, from basic science to the clinical, food safety, or environmental fields.

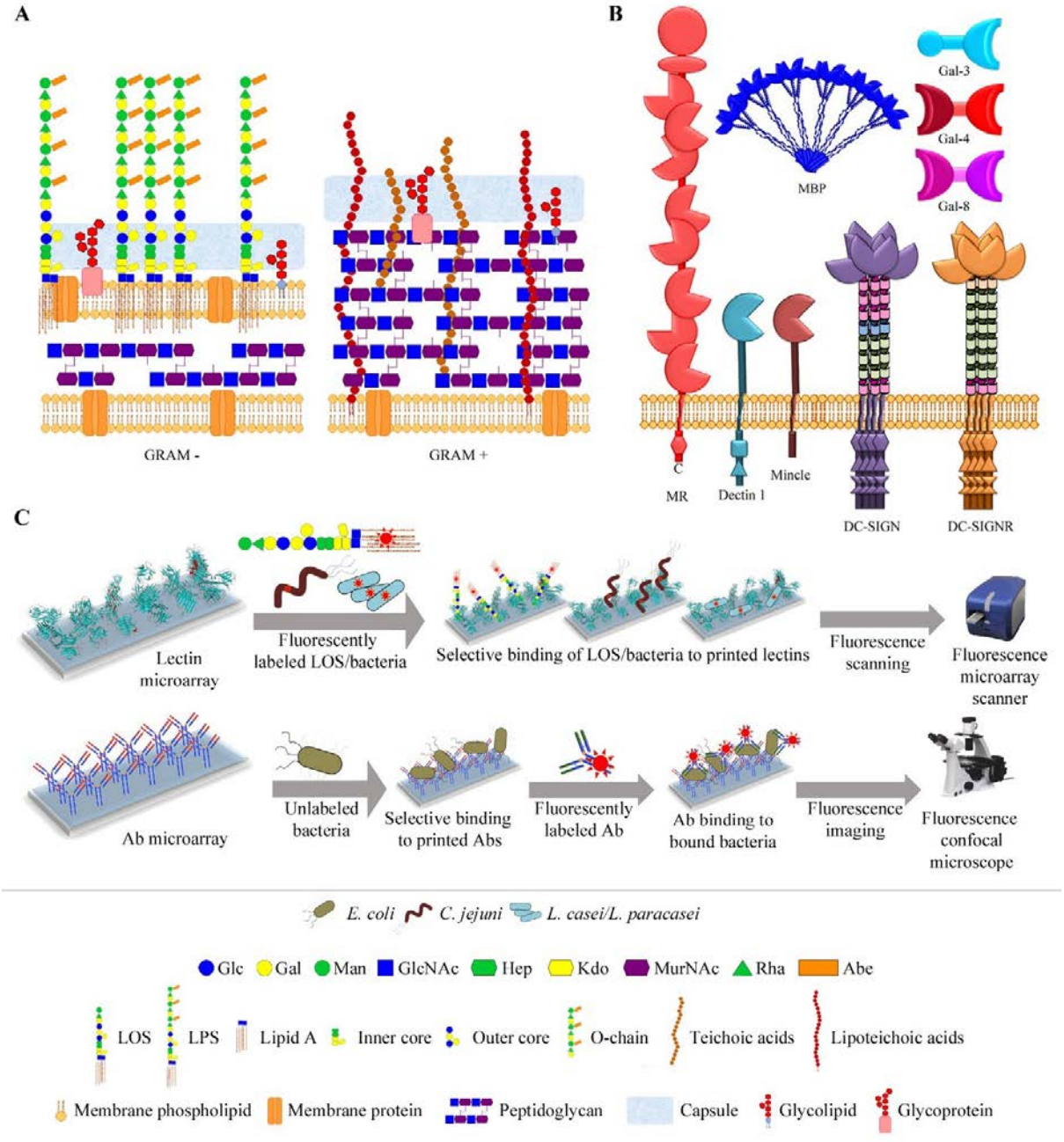


Figure 1: Illustration of some of the issues covered by the review. A) Architecture of the cell wall of Gram- and Gram+ bacteria; B) Several lectins of the innate immune system examined using bacterial glycan microarrays; C) Illustration of different lectin and antibody microarray approaches used for glycophenotyping, differentiation, and detection of bacteria.

ii) Establishment of a microarray set-up for detection in human serum of antibodies against specific serotypes of *Streptococcus pneumoniae*, using array-printed capsular polysaccharides.

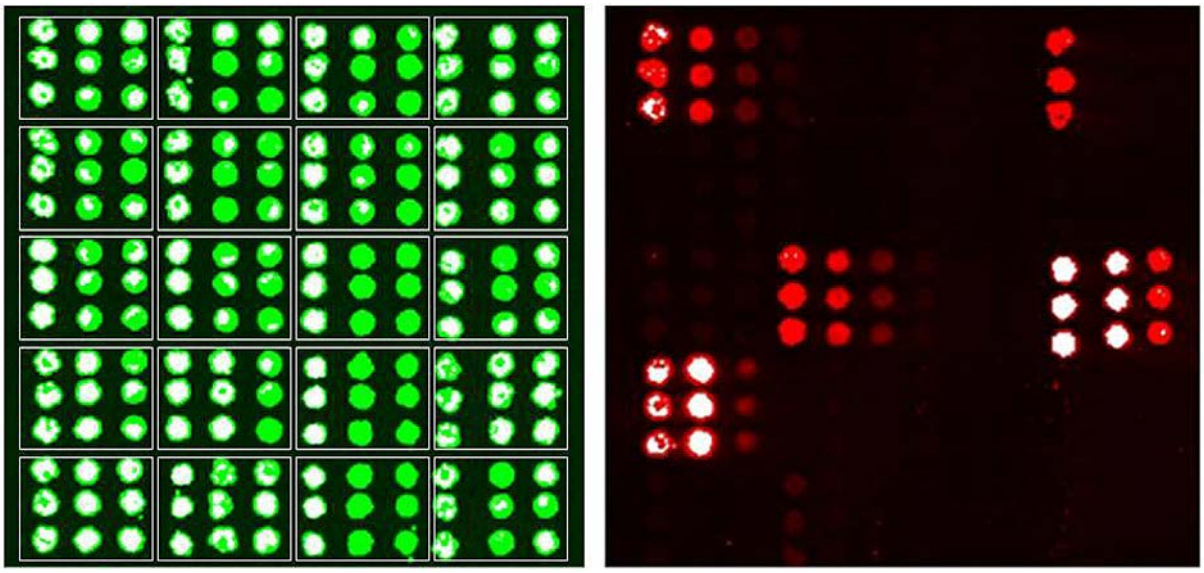


Figure 2: Representative results of the binding of serum samples to array-printed *S. pneumoniae* capsular polysaccharides. Left panel, collection of capsular polysaccharides printed in the arrays at three different concentrations in triplicate. Right panel, selective binding of serum IgG antibodies to the printed polysaccharides.

iii) Demonstration of the versatility of galectins in the selective recognition of Gram-negative bacteria displaying different cell surface architectures.

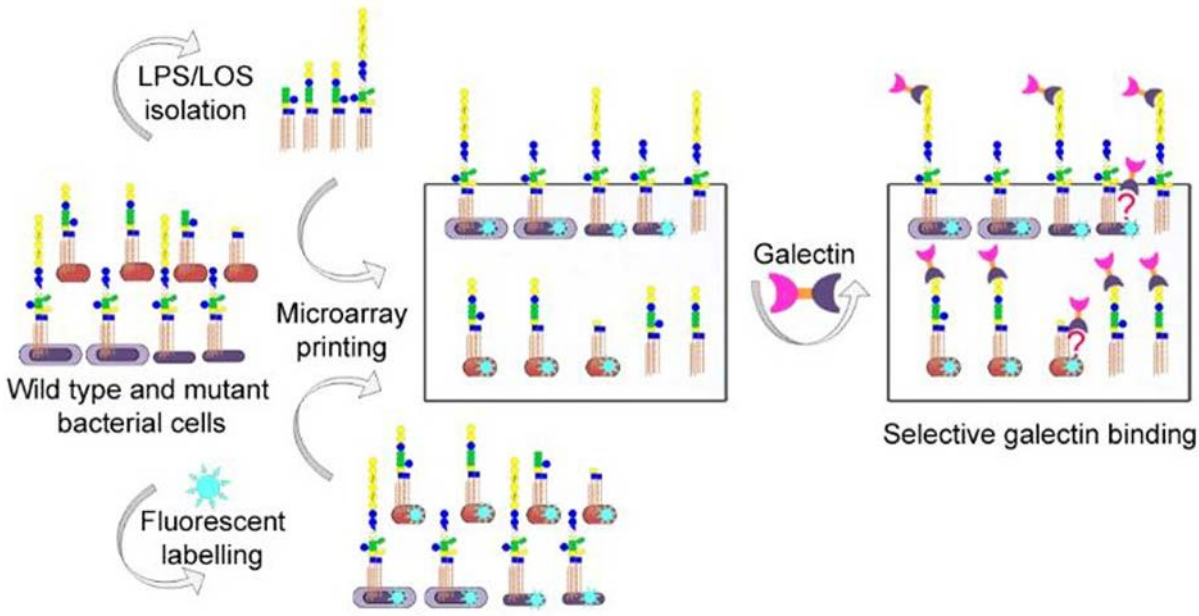


Figure 3: Illustration of the microarray approach used for exploring recognition by galectins of *Klebsiella pneumoniae* (capsulated) and nontypeable (non-capsulated) *Haemophilus influenzae* wild type and mutant cells and of their isolated lipopolysaccharides (LPS) and lipooligosaccharides (LOS).

iv) Elucidation of the structural and thermodynamic basis for selective recognition of teichoic acids by the pseudo-symmetric SH3b-like repeats of the Ply500 endolysin, an anti-*Listeria* agent, from both ligand and protein perspectives (collaborative project).

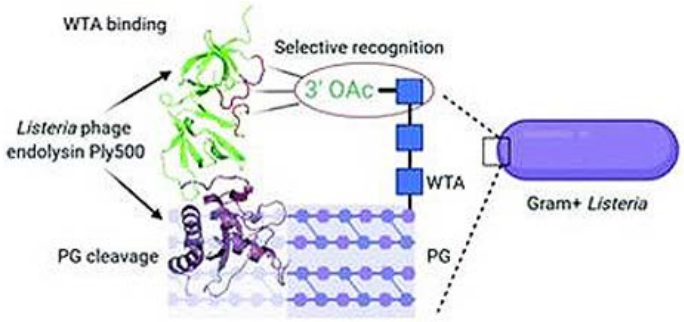


Figura 4: Scheme illustrating the attachment of Ply500 endolysin to the cell wall of *Listeria* spp. through specific recognition of the *O*-acetylated GlcNAc residues integrated into the peptidoglycan(PG)-attached teichoic acid chains (WTA) by a cavity located at the interface of the two pseudo symmetric SH3b-like repeats comprised in the Ply500 cell wall binding domain. The catalytic domain of Ply500 cleaves covalent bonds of the PG.

v) Characterization of nonviral vectors for gene therapy, based on cationic niosomes and minicircle DNA technology (collaborative project).

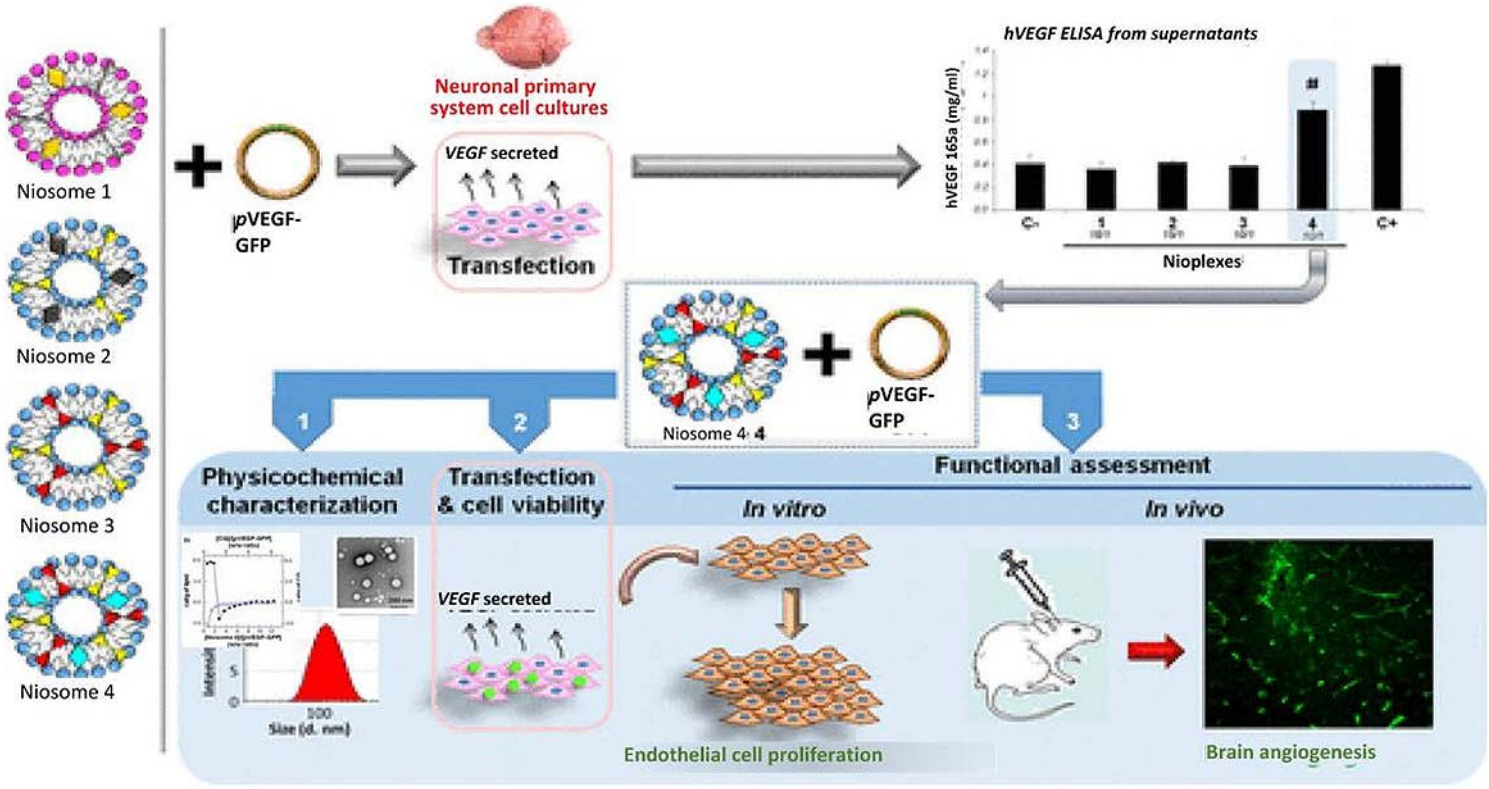


Figure 5: Comprehensive scheme of the broad approach used to characterize nioplexes as nonviral nanocarriers for gene therapy. Application of nioplexes based on cationic niosomal formulations in combination with the pVEGF-GFP plasmid carrying the VEFG (vascular endothelial growth factor) and the GFP (green fluorescent protein) genes to achieve angiogenesis in the brain.

Publications

Fernández-Calvet, A., Euba, B., Caballero, L., Díez-Martínez, R., Menéndez, M., Ortiz de Solórzano, C., Leiva, J., Micol, V., Barrajón-Catalán, E. and Garmendia, J. Preclinical evaluation of the antimicrobial-immunomodulatory dual action of xenohormetic molecules against *Haemophilus influenzae* respiratory infection. *Biomolecules* **9**, 891 (2019).

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Campanero-Rhodes, M.A., Palma, A.S., Menéndez, M. and Solís, D. Microarray strategies for exploring bacterial surface glycans and their interactions with glycan-binding proteins. *Front Microbiol.* **10**, 2909 (2020).

Hernando-Pérez, M., Martín-González, N., Pérez-Illana, M., Suomalainen, M., Condezo, G.N., Ostapchuk, P., Gallardo, J., Menéndez, M., Greber, U.F., Hearing, P., de Pablo, P.J. and San Martín, C. Dynamic competition for hexon binding between core protein VII and lytic protein VI promotes adenovirus maturation and entry. *Proc Natl Acad Sci U S A.* **117**, 13699-13707 (2020).

Gallego, I., Villate-Beitia, I., Soto-Sánchez, C., Menéndez, M., Grijalvo, S., Eritja, R., Martínez-Navarrete, G., Humphreys, L., López-Méndez, T., Puras, P., Fernández, E. and Pedraz, J.L. Brain angiogenesis induced by nonviral gene therapy with potential therapeutic benefits for central nervous system diseases. *Mol Pharm.* **17**, 1848-1858 (2020).

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Shen, Y., Kalograiaki, I., Prunotto, A, Dunne, M., Boulos, S., Taylor, N.M.I., Sumrall, E.T., Eugster, M.R., Martin, R., Julian-Rodero, A., Gerber, B., Leiman, P.G., Menéndez, M., Peraro, M.D., Cañada, F.J. and Loessner, M.J. Structural basis for recognition of bacterial cell wall teichoic acid by pseudo-symmetric SH3b-like repeats of a viral peptidoglycan hydrolase. *Chem Sci* (E-published 2020).

National Grants:individual

Ministerio de Ciencia e Innovación

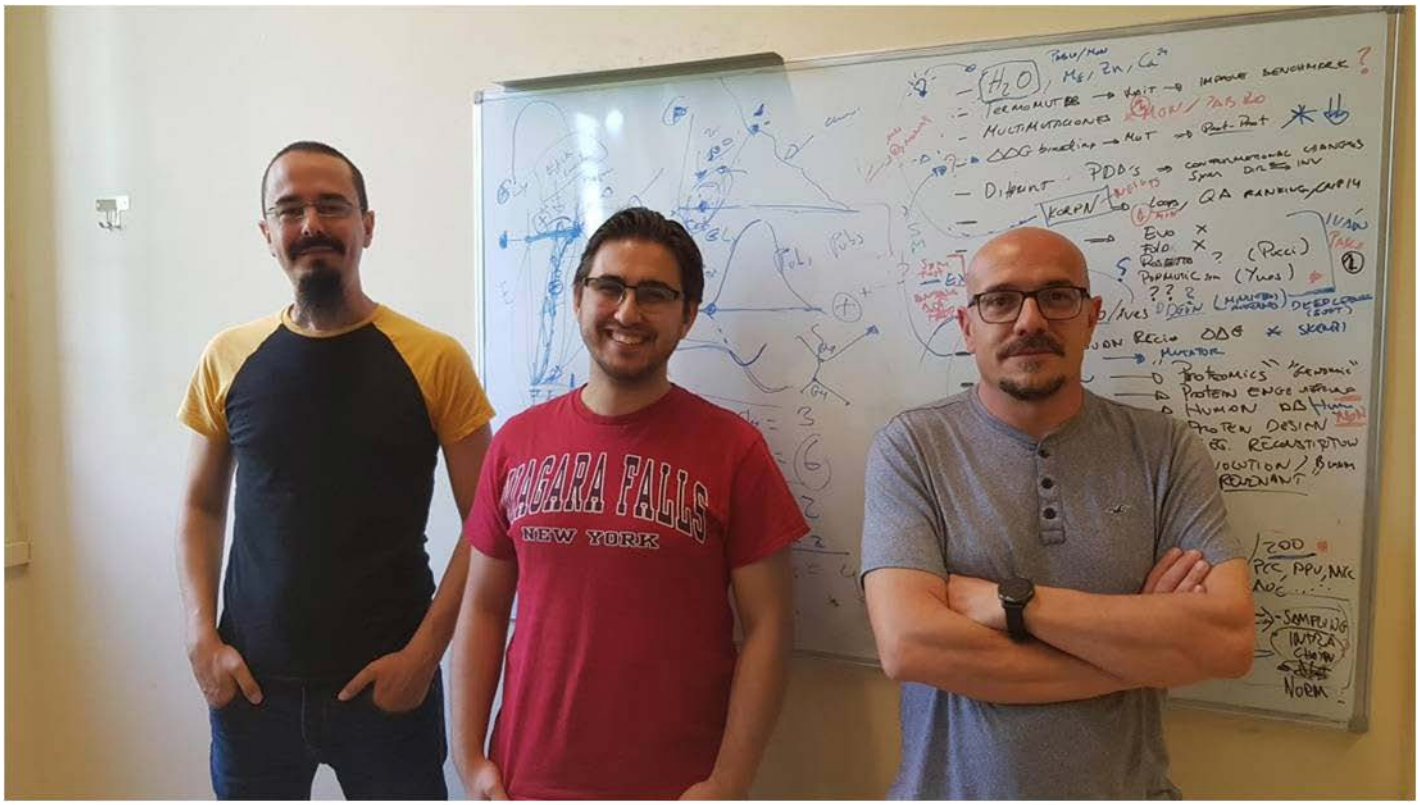
Principal Investigator	Title	Reference
Mª Dolores Solís	Exploring surface glycans of circulating exosomes and bacteria in respiratory infection and susceptibility to lectin recognition and antimicrobial lipopeptides	RTI2018-099985-B-I00
Margarita Menéndez & Mª Dolores Solís	Search and development of new preventive and therapeutic approaches for fighting infections caused by *Streptococcus pneumoniae*	BFU2015-70052-R

National Grants: coordinated

ISCIII

Principal Investigator	Title	Reference
Margarita Menéndez	CIBERES	CB06/06/1102

Group of Structural Bioinformatics



Tenured Staff scientists

Pablo Chacon Montes
(Associate Professor) ORCID

Non-tenured scientists

José Ramón López-Blanco

Technical Staff

Iván Martín Hernández

Summary

The Structural Bioinformatics Group (http://chaconlab.org) is focused on developing innovative techniques for the modelling, analysis and simulation of molecular structures in close contact with experimental labs. We are particularly interested in large macromolecules of dynamic composition and conformation whose actions and interactions are essential for cellular function. Our research lines include efforts to integrate structural information at different resolutions, analysis of molecular flexibility, loop modelling and the prediction of protein-protein and protein-ligand interactions. The developed methodologies are available via software distributions and web servers.

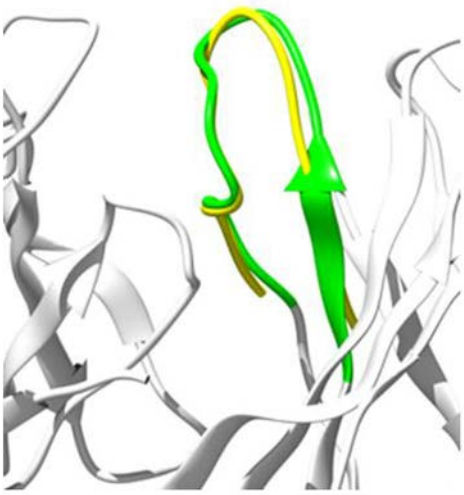
Strategic Aims

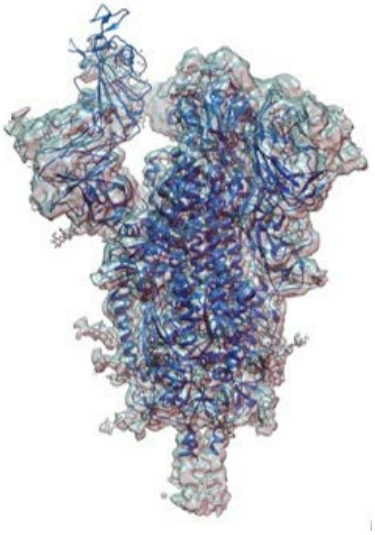
- **Bridging the resolution gap with hybrid methods**. We develop and apply new hybrid methods for combining multiresolution structural information in collaboration with several experimental labs.
- **Multiscale dynamics of macromolecular biomachines**. We address the study and simulation of the dynamics of large biomolecular systems Normal-Mode Analysis (NMA), geometric algebra and other multiscale approximations.
- **Protein modeling**. We develop tools for modeling protein structures and their interactions. This includes novel methods for protein docking and loop modeling problems.

Remarkable Results

In the last two years we have developed a novel knowledge-based pairwise potential which takes into account information of the relative position and orientation of the protein residues. This side-chain-independent potential, termed KORP, derived from known protein structures by classical Boltzmann inversion has been successfully used in protein and loop modeling, in protein-ligand and more recently to predict stability upon mutation.

We continue to work on integrative structural biology, in collaboration with Prof. Carazo (CNB) and J. McLellan (UTEXAS) we characterize the flexibility and conformational dynamics of the SARS-CoV-2 spike in the prefusion state.





Publications

López-Blanco J.R. and Chacón P. KORP: Knowledge-based 6D potential for fast protein and loop modeling. *Bioinformatics* **35** (17) 3013–3019 (2019).

Melero, R., Sorzano, C., Foster, B., Vilas, J. L., Martínez, M., Marabini, R., Ramírez-Aportela, E., Sanchez-Garcia, R., Herreros, D., Del Caño, L., Losana, P., Fonseca-Reyna, Y. C., Conesa, P., Wrapp, D. Chacon, P., McLellan, J. S., Tagare, H. D. and Carazo, J. M. Continuous flexibility analysis of SARS-CoV-2 Spike prefusion structures. *IUCrJ* **7** (6) 1059-1069 (2020).

Kadukova, M., dos Santos Machado, K., Chacón, P. and Grudinin, S. KORP-PL: a coarse-grained knowledge-based scoring function for protein-ligand interactions. *Bioinformatics* **37** (7), 943–950 (2020).

National Grants: individual

MINECO

Principal Investigator	Title	Reference
Pablo Chacón	Function and dynamics of macromolecular complexes explored by integrative structural and computational biology	BFU2016-76220-P

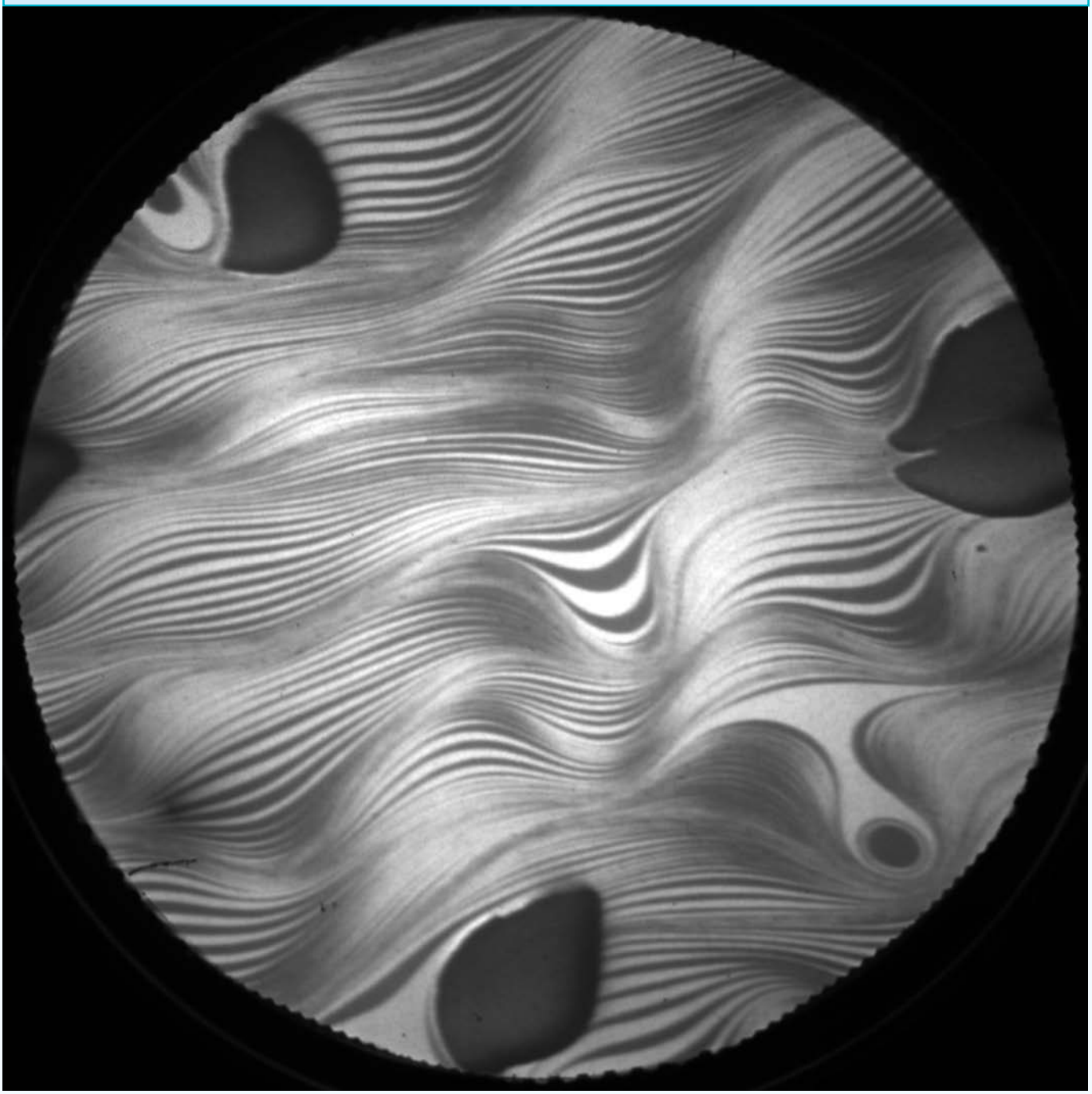
National Grants: coordinated

MICCIN-AEI

Principal Investigator	Title	Reference
Pablo Chacón	Advances on computational tools for Integrative structural biology with new methodologies for protein loop modeling and Prediction	PID2019-109041GB-C21


CONSEJO SVPERIOR DE INVESTIGACIONES CIENTIFICAS

Department of Low Dimensional Systems, Surfaces and Condensed Matter



Introduction

The Department of Low Dimensional Systems, Surfaces and Condensed Matter https://www.iqfr.csic.es/es/investigacion/departamentos/16-cabeceraweb/estructura-investigacion/departamentos/37-sbdsmc is constituted by four groups that develop their research in a multidisciplinar environment that covers physico-chemical aspects of Materials Science and Nanoscience. Research in the present period includes the investigation of the physicochemical processes involved in the micro- and nanofabrication of materials by laser ablation and irradiation, design and development of new photonic systems based on photosensitized and nanostructured materials for optoelectronic and biophotonic applications, the study of various types of materials with sensitivity to the surface region and of the preparation of thin films using microscopy and spectroscopy techniques, some of them in ultra high vacuum, as well as Mössbauer spectroscopy. On the theoretical side, investigations are aimed at applying statistical mechanics and condensed matter theory tools, in conjunction with simulation approaches, in order to analyze problems of physico-chemical interest. The activity of the Groups pursues its practical application in areas of optoelectronics, biophotonics, biomedicine, magnetism and preservation and conservation of cultural heritage. In this Department, the scientific exchanges with other groups of CSIC, Universities and other international partners are frequent and provide the right framework for generating new knowledge and for training of young researchers.

Group Structure

Group of Lasers, Nanostructures and Materials Processing

Tenured Staff Scientists

Marta Castillejo Striano
(Associate Professor) ReID ORCID SCOPUS

Rebeca de Nalda Mínguez
(Assistant Professor) ReID ORCID

Esther Rebollar González
(Ramón y Cajal, until 31/05/2019) ReID ORCID SCOPUS

Non-tenured Scientists

Mohamed Oujja Ayoubi SCOPUS ReID ORCID Google Scholar

Mikel Sanz Monasterio (Research contract, Until 30/09/2020) SCOPUS

Esther Rebollar González
(research contract, since 15/06/2019) ReID ORCID SCOPUS

Doctoral Students

Ana Carolina Alcántara Sánchez
(Comunidad de Madrid YEI Predoctoral fellow, April 2019-March 2020)

Marina Gabriela Martínez Weinbaum
(JAE Intro, from 01/10/2020)

Technical staff

Álvaro Alonso Mazadiego
(Comunidad de Madrid YEI Research technician, May 2019-March 2020)

Summary

The activity of the Group is focused on the investigation of the physicochemical processes involved in the micro- and nanofabrication of materials by laser ablation and irradiation in the nano- and femtosecond temporal domains and in the ultraviolet to infrared spectral range and in the development of laser-based analytical methods. Our interest is the understanding and description of the mechanisms that govern the laser-material interaction from a fundamental perspective, in the ablative and sub-ablative regimes, and the development of laser control strategies by application of advanced methods of manipulation of the pulsed laser radiation. We apply the understanding of these phenomena to the conservation of Cultural Heritage, the development of low-cost, flexible electronic devices, data storage devices and sensors and others. In 2019 CSIC approved the creation of the CSIC Interdisciplinary Thematic Platform Open Heritage: Research and Society, PTI-PAIS under the coordination of Marta Castillejo. This Platform brings together 16 CSIC research groups and up to 39 associated entities, including cultural and research institutions, educational centres and private companies, collaborating synergistically to develop joint capacities, acquire new knowledge and adopt innovative solutions focused on a better understanding of CH and its conservation in a sustainable way.

The activities and the results of our research are described in the continuously updated web pages http://lanamap.iqfr.csic.es/ and (https://pti-pais.csic.es/).

Strategic Aims

- Understanding of the laser-material interaction processes for guiding the selection of controlled fabrication of nanomaterials with specific properties (thin, nanostructured films, colloids, etc.).
- Laser nanostructuring of soft matter and polymers by applying advanced processing techniques.
- Development of new methodologies for *in situ* determination of growth and self-assembly of nanomaterials generated in controlled deposition processes.
- Development and application of advanced laser methodologies for the analysis, valorisation and conservation of substrates and objects of Cultural Heritage (CH).
- Implementation and application of nonlinear optical microscopy for non-invasive structural and chemical characterization of CH objects.
- Understanding and control of ultrafast molecular dynamics using femtosecond pulses.

Remarkable Results

Laser nanostructuring of soft matter

Nanostructuring is one promising alternative to modify the functionalities of polymers aiming at applications in, for instance, organic electronics and medical devices. Nowadays, there is an increasing interest in alternative ways of nanostructuring more economic, quicker and reproducible, avoiding the necessity of stringent environmental conditions like clean rooms, high vacuum or complex mask fabrication. We prove that laser nanostructuring, and in particular the formation of laser induced periodic surface structures (LIPSS) is a promising approach. We have fabricated LIPSS using nanosecond and femtosecond laser pulses and we study, from the fundamental point of view, LIPSS on different polymeric materials, both synthetic and fully bio-based, on polymer based nanocomposites and on fullerene derivatives.

We systematically study the effect of relevant experimental parameters such as substrate thickness, polymer properties in terms of crystallinity, optical absorption, thermal properties, and laser properties in terms of wavelength and pulse duration.

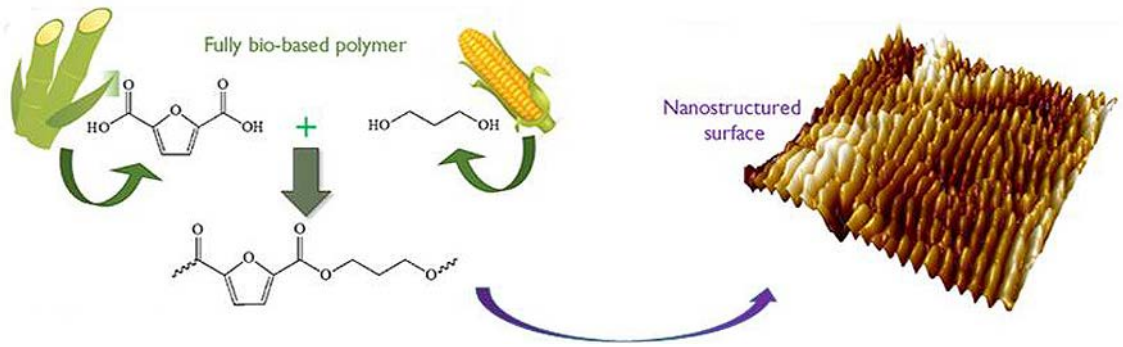


Figure 1: Polymer nanostructures were developed on fully bio-based poly(trimethylene furanoate) (PTF) films, by using the technique of Laser Induced Periodic Surface Structures (LIPSS)

Functional nanostructured surfaces

Polymer nanostructured were characterized in terms of their functional properties paying special attention to the mechanical properties, which were found to be improved, as evidenced by force spectroscopy measurements. We have also explored the tribological properties of the nanostructured systems at the nanoscale.

Additionally, the combination of LIPSS with the deposition of Pd NPs by sputtering at different deposition incidence angles resulted in the formation of an array of NP ribbons and the planar arrays were studied as candidates for both flexible, transparent conductor and hydrogen sensors.

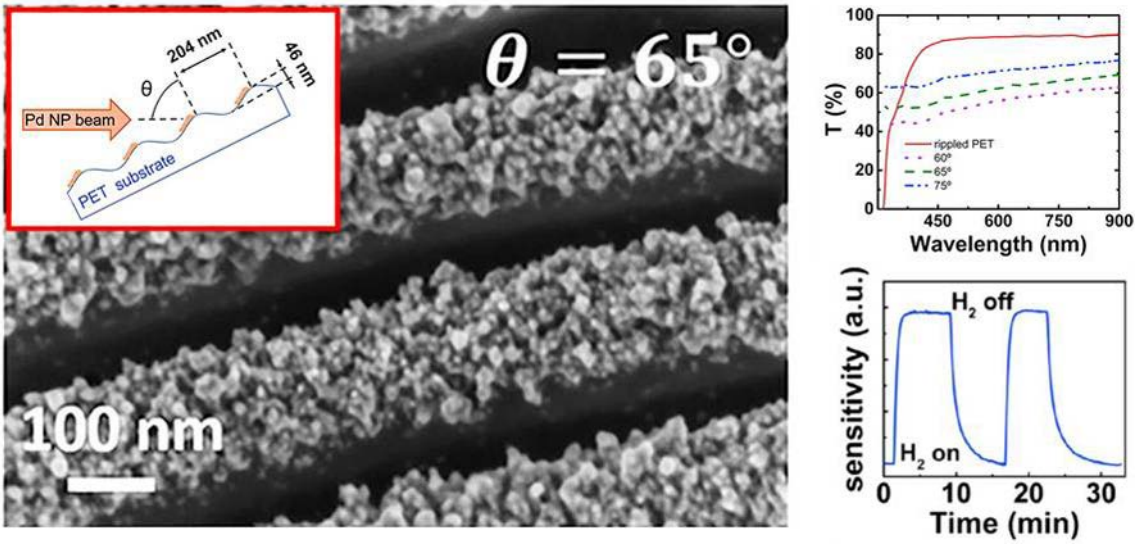


Figure 2: Left: SEM image of Pd nanoribbon arrays at incidence angle of 65°, as indicated in the inset. Right: (Upper graph) Optical transmittance of nanoribbon arrays made on LIPSS for different incidence angles and (bottom graph) time evolution of the resistance in the Pd nanoribbon array for two hydrogen cycles up to the same static pressure (10^5 Pa).

Coulomb explosion visualization of a molecular conical intersection

In this work, Coulomb explosion imaging of the fragments in a molecular dissociation process is demonstrated as a method to map the presence of conical intersections encountered by the propagating wave packet as it proceeds to dissociation. The case of choice is the methyl iodide molecule, where the nonadiabatic coupling between two dissociative surfaces is probed by Coulomb explosion with short, intense near-infrared pulses causing multiple ionization. On-the-fly multidimensional trajectory calculations with surface hopping using perturbation theory and including spin−orbit coupling are performed to visualize the dynamics through the conical intersection and compare with experimental results. The work shows that Coulomb explosion imaging can be applied as a powerful tool for the visualization of wave packet branching in molecular nonadiabatic dynamical processes, with the advantage of its quasi-direct energy real space mapping. The possibilities and limitations of the technique are examined and discussed.

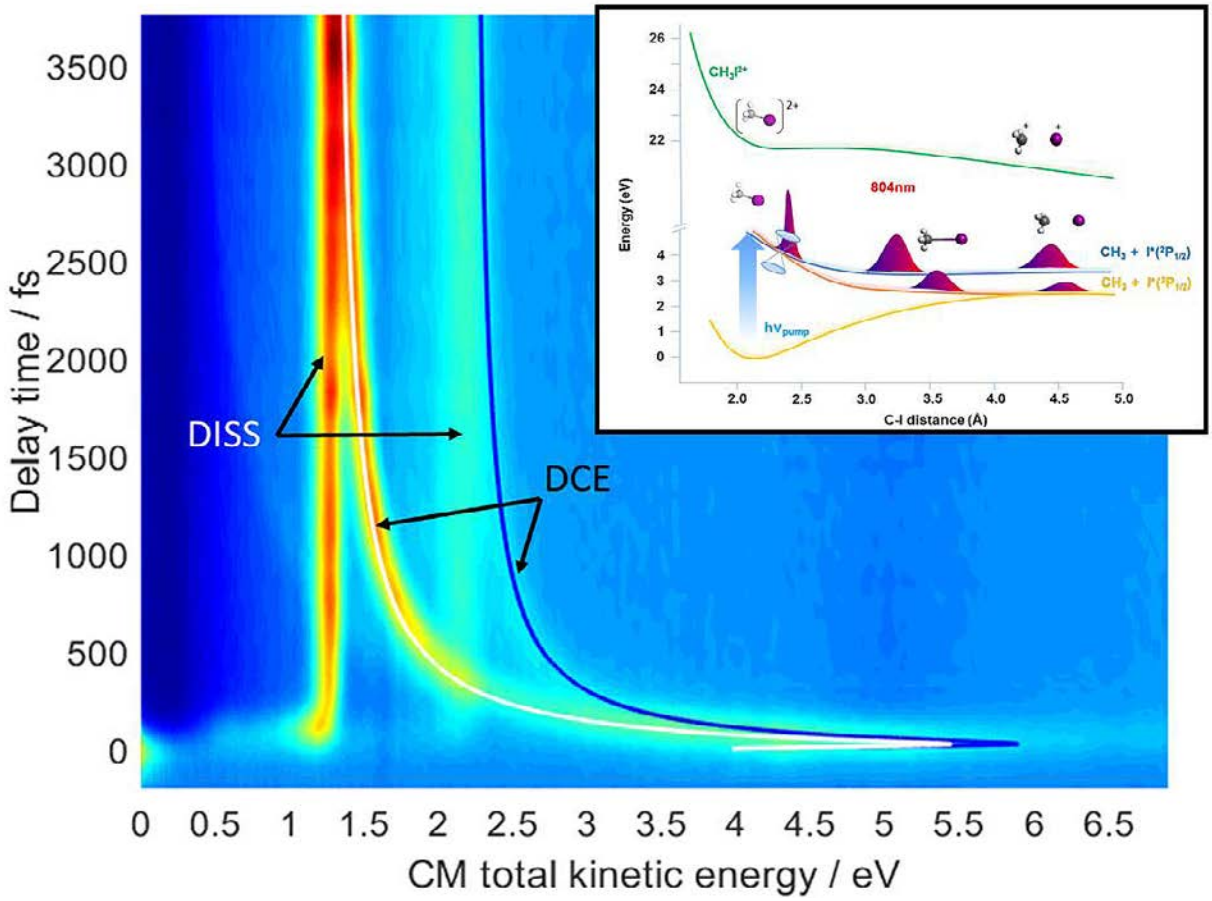


Figure 3: False-color map with the center-of-mass total kinetic energy released in the fragmentation process, as a function of time delay. The channels labeled DISS correspond to one-photon dissociation; those labeled DCE correspond to dynamic Coulomb explosion. The inset contains the diagram of potential energy surfaces involved in the process.

Detailed assessment of laser-generated metal plasmas and their behavior as nonlinear optical media

Nobel metal plasmas (Cu, Ag, Au) generated through laser ablation with nanosecond near-infrared pulses at 1064 nm have been spatially and temporally characterized by optical emission spectroscopy. Brehmsstrahlung emission, together with discrete emissions from neutral and ionized species were studied both as a function of the location from the target surface and of the time delay from the laser pulse arrival. A detailed analysis of the features of the metal plasmas has been used to assess critical plasma parameters such as temperature, electron density, and abundance of metal atoms in different ionization stages. In the case of Cu, laser-induced ablation plasmas were examined as media for third harmonic generation of a nanosecond driving pulse, and a narrow optimization window was found for fluence and spatiotemporal region of the plasma, which could be correlated with local plasma conditions.

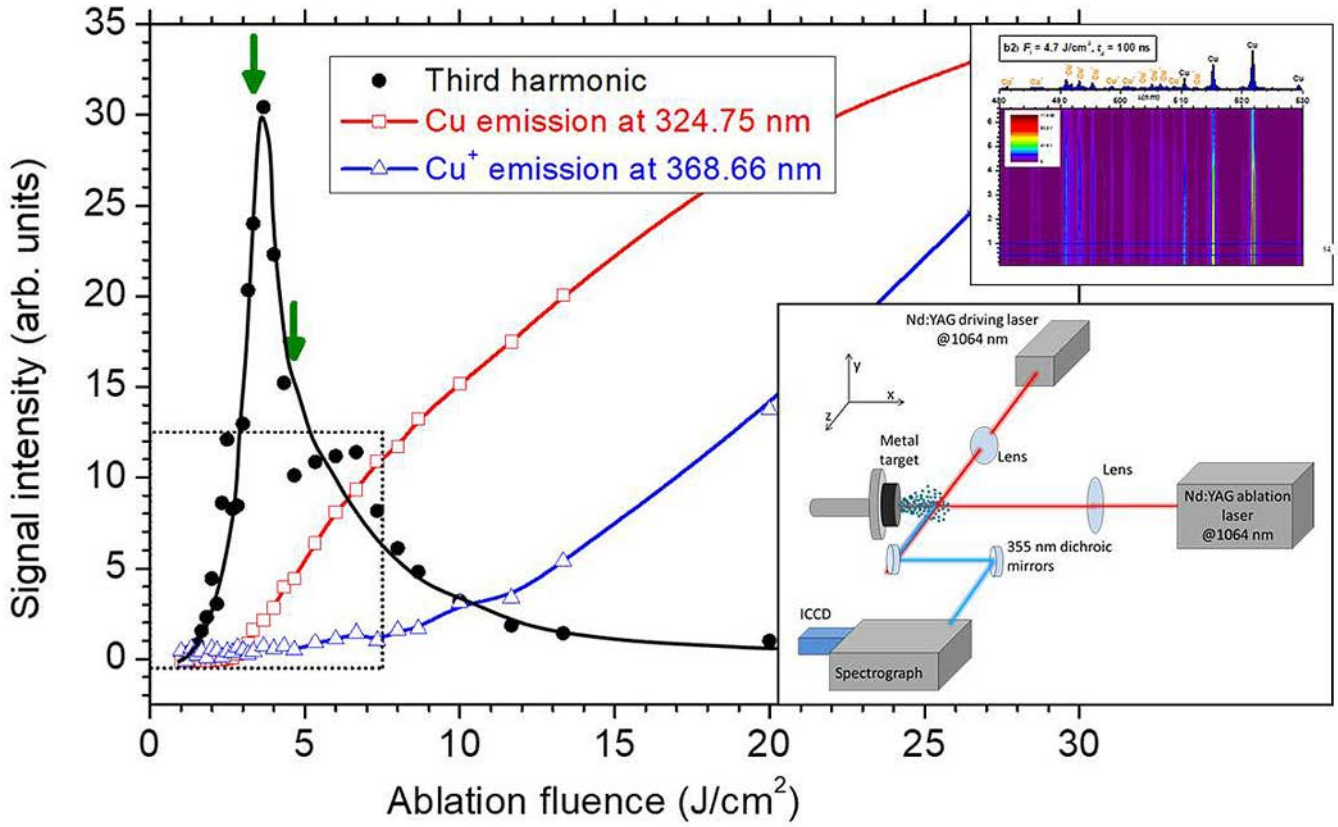


Figure 4: Simultaneous measurement of optical emissions and nonlinear response of a laser-induced Cu plasma. In the upper insets, spatially resolved emission spectra in the 500 nm region. In the lower inset the experimental scheme is shown.

Femtosecond and Nanosecond pulsed laser deposition of thin films

Nanostructured thin films were synthetized through femtosecond and nanosecond laser pulsed deposition (PLD). Femtosecond pulses at 800 nm were used for the synthesis of nanostructured thin films of Co-doped zinc sulfide. The scheme involved ablation of physically mixed Co and ZnS with pairs of ultrashort pulses separated in time in the 0-300 ps range. *In situ* monitorization of the deposition process was carried out through a simultaneous reflectivity measurement. The crystallinity of generated nanoparticles and the inclusion of Co in the ZnS lattice is demonstrated by transmission electron microscopy and energy dispersive X-ray microanalysis (TEM-EDX) characterization. Surface morphology, Raman response and photoluminescence of the films have also been assessed. The role of interpulse temporal separation is most visible in the thickness of the films obtained at the same total fluence, with much thicker films deposited with short delays than with individual uncoupled pulses. The proportion of Co in the synthesized doped ZnS nanoparticles is found to be substantially lower than the original proportion, and practically independent on interpulse delay.

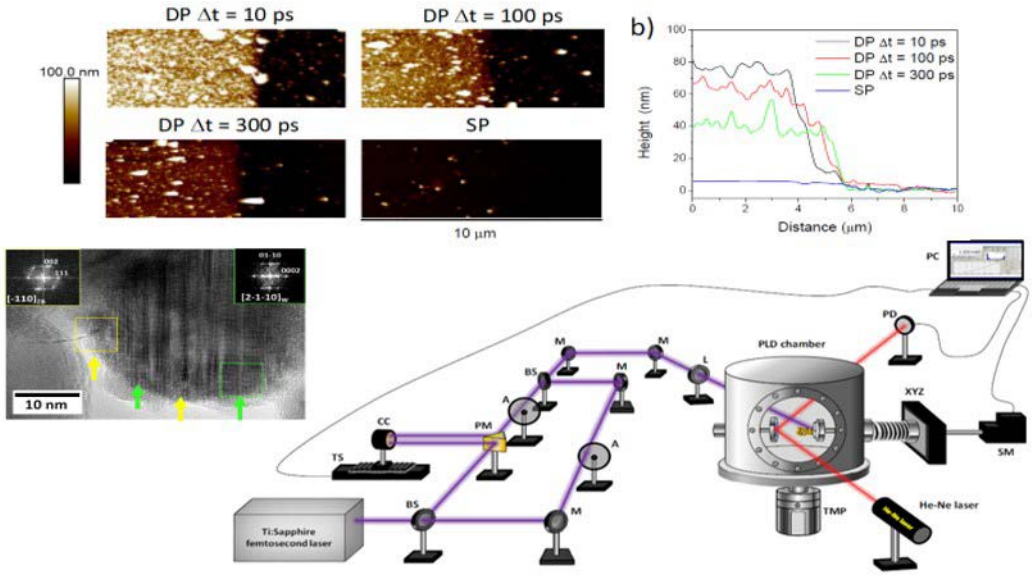


Figure 5: Double-femtosecond pulse scheme employed for pulsed laser deposition of Co:ZnS thin films, with in situ diagnostic through laser reflectivity. In the upper part of the figure we show the atomic force microscopy images of the samples grown for different pulse delays, demostrating control of the deposit through control of the global pulse envelope. The coexistence between wurtzite and zincblende phases is shown in the TEM image.

We have also studied micrometer-thick cobalt ferrite films deposited on Si (1 0 0) single crystal substrates by nanosecond pulsed laser deposition at 1064 nm. The thickness of the deposited films was monitored by AFM while the chemical and structural characterisation of the films was carried out by Raman spectroscopy and transmission Mössbauer spectroscopy at 300 and 26 K. For comparison purposes, transmission Mössbauer data at these two temperatures were also recorded from a commercial cobalt ferrite powder and the home-made target used to grow the films. The surface characterisation was performed by X-ray Photoelectron Spectroscopy (XPS) and Integral Low Energy Electron Spectroscopy (ILEEMS). XPS showed Co and Fe to be present as Co^{2+} and Fe^{3+}, as expected for cobalt ferrite. The Raman spectra showed the lines characteristic of cobalt ferrite. The Mössbauer spectra, both in the transmission and backscattering modes, were fitted to two sextets whose hyperfine parameters are in good agreement with those expected from Fe^{3+} cations occupying the tetrahedral and octahedral sites in the spinel-related structure. No significant differences were observed in the relative areas of the two sextets in the transmission and ILEEMS spectra, suggesting that the cation distribution at the surface and the bulk are not too different. However, the relative areas of the two components changed drastically with temperature both in the spectra of the films as in those recorded from the cobalt ferrite standards. We discuss the possible origin of the evolution with temperature of those relative areas.

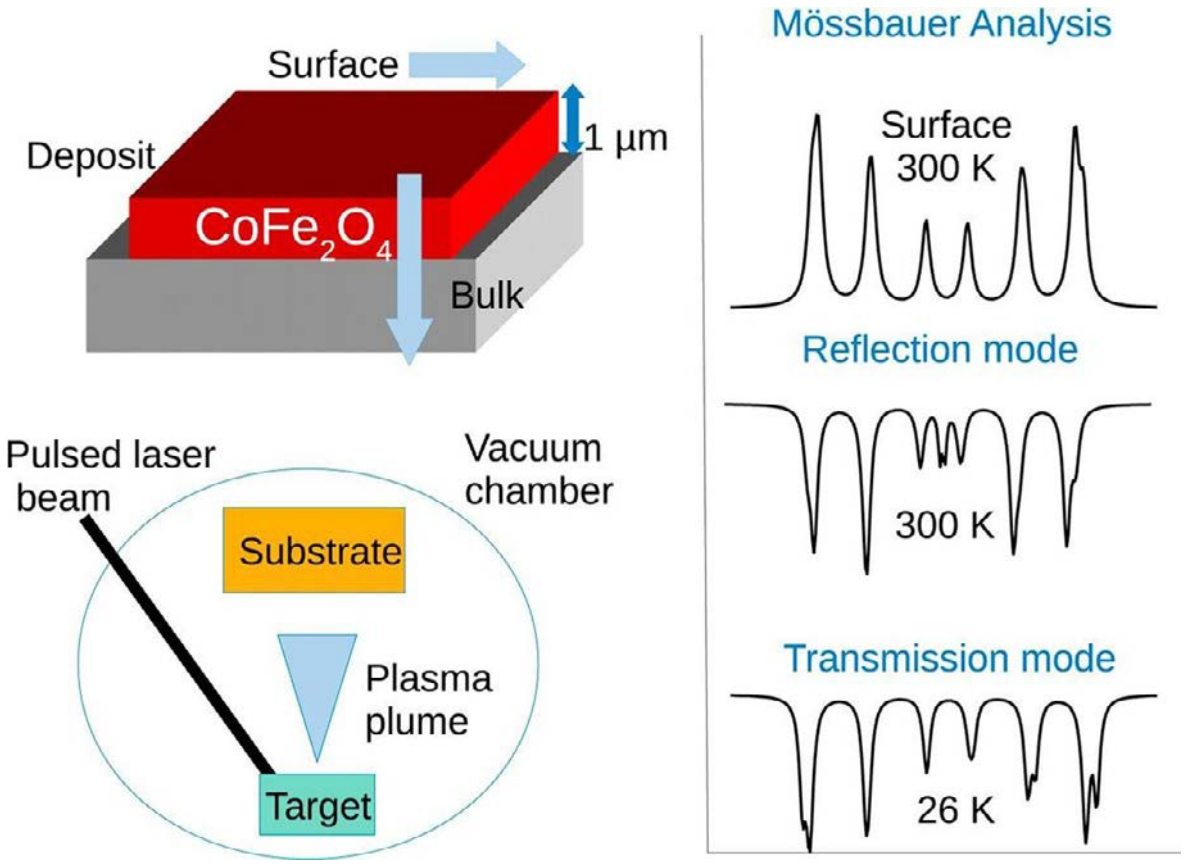


Figure 6: Mössbauer spectra of the cobalt ferrite film prepared by nanosecond near-infrared pulsed laser beam at 1064 nm. Right column: Mössbauer spectra acquired in the transmission and reflection modes at different temperatures.

Non-invasive laser based non-linear microscopy and spectroscopy for chemical and structural analysis of cultural heritage materials

The non-invasive depth-resolved imaging by means of linear optical techniques represents a challenge in the field of Cultural Heritage. The presence of opaque and/or highly-scattering materials may obstruct the penetration of the radiation probe, thus impeding the visualization of the stratigraphy of multilayer structures. Nonlinear Optical Microscopy (NLOM), which makes use of tightly-focused femtosecond pulsed lasers as illumination sources, is an emerging technique for the analysis of CH objects enabling micrometric three-dimensional (3D) resolution with good penetration capability in semi-transparent materials. We evaluated the potential of NLOM, specifically in the modality of Multi-Photon Excitation Fluorescence (MPEF), to probe the stratigraphy of egg-tempera mock-up paintings. A multi-analytical non-invasive approach, involving ultraviolet-visible-near infrared (UV-Vis-NIR) Fiber Optics Reflectance Spectroscopy, Vis-NIR photoluminescence, and Laser Induced Fluorescence, yielded key-information for the characterization of the constituting materials and for the interpretation of the nonlinear results. Furthermore, the use of three different nonlinear optical systems allowed evaluation of the response of the analyzed paints to different excitation wavelengths and photon doses, which proved useful for the definition of the most suitable measurement conditions. The micrometric thickness of the paint layers, which was not measurable by means of Optical Coherence Tomography (OCT), was instead assessed by MPEF, thus demonstrating the effectiveness of this nonlinear modality in probing highly-scattering media,while ensuring the minimal photochemical disturbance to the examined materials.

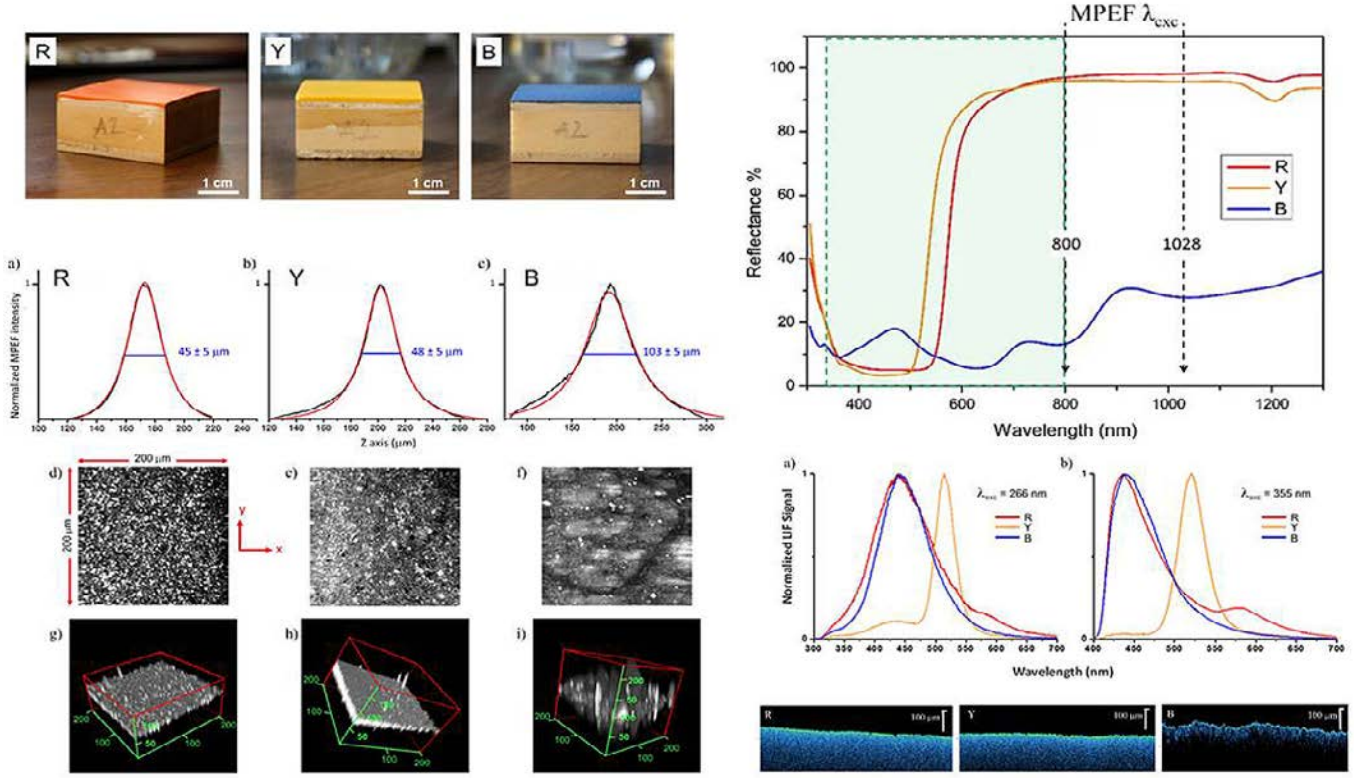


Figure 7: Left up: Red, yellow, and blue (R, Y, and B) samples simulating egg-tempera painting on wooden support. Left down: MPEF imaging results: (a–c) z-scans of the MPEF signals of R, Y, B (in black), fits by Lorentzian functions (in red), and full width at half maximum (FWHM) values after refractive index correction, corresponding to the paint thickness (indicated in blue); (d–f) fluorescence intensity xy images (200 × 200 µm, 256 × 256 pixels) extracted from the MPEF stacks at a depth corresponding to the maximum signal intensity; (g–i) Three-dimensional (3D) fluorescence reconstructions showing the thickness of each paint layer. Right up: Reflectance spectra of red (R), yellow (Y), and blue (B) tempera paint samples. The excitation wavelengths (800 and 1028 nm) and the spectral range for detection used for Multi-Photon Excitation Fluorescence (MPEF) measurements (335–800 nm, dashed green rectangle) are highlighted in the reflectance spectra. Right middle: Laser Induced Fluorescence (LIF) spectra acquired by laser excitation at 266 nm (a) and 355 nm (b) of red, yellow, and blue tempera samples. Right down: Optical Coherence Tomography (OCT) tomograms of red, yellow, and blue samples with vertical scale bars (in white).

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National Grants: individual

Agencia Estatal de Investigación

Principal Investigator	Title	Reference
Rebeca de Nalda and Esther Rebollar.	Control y modificación de la materia en la nanoescala con tecnologías avanzadas basadas en luz	PID2019-106125GB-I00/ AEI / 10.13039/501100011033.
Marta Castillejo and Mohamed Oujja	Estudio y conservación del patrimonio cultural con láseres	PID2019-104124RB-I00/ AEI /10.13039/501100011033.

Ministerio de Economía y Competitividad

Principal Investigator	Title	Reference
Rebeca de Nalda and Esther Rebollar.	Procesado avanzado por láser para síntesis y modificación de materiales en la micro-y nanoescala	CTQ2016-75880-P.

Ministerio de Educación Cultura y Deporte

Principal Investigator	Title	Reference
Marta Castillejo	Desarrollo y aplicación de la microscopía óptica no-lineal para el análisis de materiales	Movilidad de Profesores e Investigadores Senior en Centros Extranjeros, Programa "Salvador De Madariaga" (PRX18/00029)

National Grants: coordinated

Consejería de Educación – Comunidad Autónoma de Madrid

Principal Investigator	Title	Reference
Marta Castillejo Striano, Emilio Cano (CENIM)	Red de Ciencia y Tecnología para la Conservación del Patrimonio Cultural. Technoheritage	HAR2016-81748-REDT/AEI.
Marta Castillejo, Rafael Fort (Instituto de Geociencias)	Tecnologías en Ciencias del Patrimonio. TOP HERITAGE-CM	S2018/NMT-4372.

International Grants: coordinated

European Commission, H2020

Principal Investigator	Title	Reference
Marta Castillejo, Luca Pezatti, INO-CNR	Integrated Platform for the European Research Infrastructure ON Heritage Science, IPERION HS.	H2020-INFRAIA-2018-2020.
Marta Castillejo, Luca Pezatti, INO-CNR	The European Research Infrastructure for Heritage Science Preparatory Phase (E-RIHS PP)	(N. 739503). H2020-INFRADEV-2016-2.
Marta Castillejo, Luca Pezatti, INO-CNR	Integrated Platform for the European Research Infrastructure ON Cultural Heritage, IPERION CH	H2020-INFRAIA-2014-2015.
Marta Castillejo, Franco Niccolucci, Universita di Firenze, Italy	Pooling Activities, Resources and Tools for Heritage E-research Networking, Optimization and Synergies, PARTHENOS	H2020. 01/05/2015-31/10/2019.

Group of Laser Materials and Interaction Laser-Materials

Tenured Staff Scientists

Inmaculada García-Moreno Gonzalo
(*Professor*) ReID ORCID

Clara Gómez Hernández
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Summary

The research of the group centers in the design and development of new photonic systems based on photosensitized and nanostructured materials for optoelectronic and biophotonic applications. For this, the processes that regulate their preparation, behavior and properties in relation to their structure and nanostructure are studied. We also study the modulation of the optical properties of materials based on dye-doped multifunctional photonic nanostructures, be they ordered or disordered, organic or inorganic, rigid or flexible, 1D or 3D as well as mono- or multi-chromophoric for photonic (laser and waveguides) and biophotonic (imaging) applications. In the field of biomedicine we continue our studies on the interaction of laser radiation with biological tissues and applications to Photodynamic Therapy.

Strategic Aims

- General objective: obtaining new advanced nanomaterials with defined optoelectronic and biophotonic applications.
- Design, synthesis and characterization of new molecular dyes, including chiral dyes, based on the BODIPY chromophore, with efficient and stable emission in the blue, red, and near infrared spectral regions, low synthetic cost, and with improved photonic and structural properties.
- Development of organic dyes in the red and near IR spectral regions for applications in photodynamic therapy.
- Study of the photophysical properties of the new materials and their relationship to structure, microstructure and composition.
- Characterization of the new materials as laser systems, micro- and nano-lasers, photonic coatings, and saturable absorbers with improved laser action by non-resonant feedback lasing induced by nanometric sized scatters.
- Evaluation of the new photoactive materials in biophotonic applications allowing the development of easy-to-access, minimally invasive and cost-effective methods for improved diagnosis (bioimaging).
- Use of computational strategies for the design of new materials with optimized properties for application in the various proposed uses.
- Study of the laser radiation-biological tissue interaction to maximize the applications of the laser tool in Dermatology.

Remarkable Results

Synthesis of COO-BODIPY laser dyes with high efficiency and outstanding photostability

During the two years covered by this report, we have continued with the design, synthesis and characterization of new organic dyes with emission covering the spectral range from the blue to the near infrared, using BODIPYs as base chromophores. A general and straightforward method for the synthesis of COO-BODIPYs from F-BODIPYs and carboxylic acids is established. The method is based on the use of boron trichloride to activate the involved substitution of fluorine, which leads to high yields through rapid reactions under soft conditions. This mild method opens the way to unprecedented laser dyes with outstanding efficiencies and photostabilities, which are difficult to obtain by the current methods.

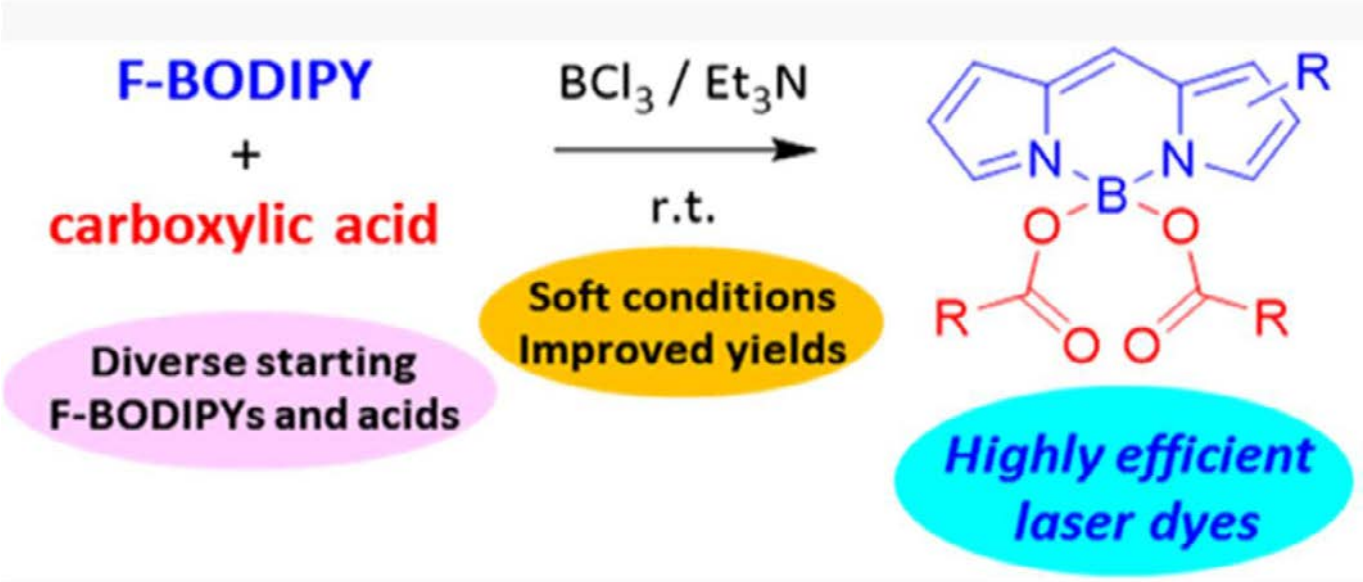

Figure 1: Schematic drawing of the synthesis of COO-BODIPYS.

Multichromophoric COO-BODIPYS

Molecular multichromophoric arrays (MMAs) allow the development of dyes with optical and optoelectronic properties which are not available from a single chromophore, expanding their capabilities to a specific photonic field, from advanced biomedicine to clean energy. COO-BODIPYs are highlighted as cutting edge scaffolds for easy access to a new generation of multichromophoric architectures with enhanced (photo)chemical stability, showing either boosted capability for excitation energy transfer, glow fluorescence and laser emission, or photoinduced electron transfer. The new finding paves the way for the rapid development of smarter organic dyes for advancing photonics and optoelectronics.

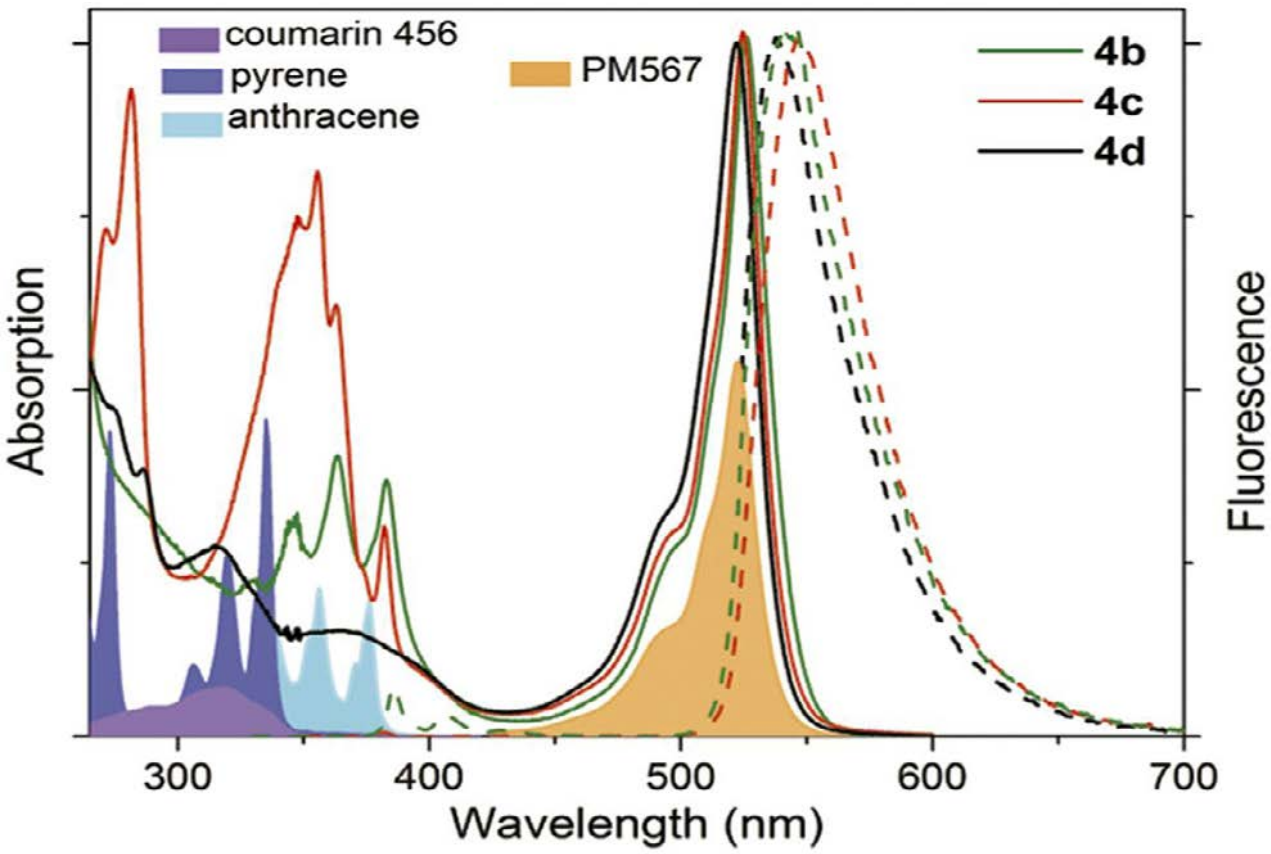

Figure 2: Normalized UV-vis absorption spectra (bold lines) and fluorescence spectra upon UV-excitation of the donor units (dashed lines) of PM567-based 4b–d in cyclohexane (tetrahydrofuran was used for 4d due to insolubility in cyclohexane), as well as the UV-vis absorption spectra of monochromophoric PM567, coumarin 456 (7-hydroxy-4-methylcoumarin), pyrene and anthracene (filled spectra).

BODIPYs revealing lipid droplets as valuable targets for photodynamic theragnosis

Endowing BODIPY PDT agents with the ability to probe lipid droplets is demonstrated to boost their phototoxicity, allowing the efficient use of highly fluorescent dyes (poor ROS sensitizers) as phototoxic agents. Conversely, this fact opens the way to the development of highly bright ROS photosensitizers for performing photodynamic theragnosis (fluorescence bioimaging and photodynamic therapy) from a single simple agent. On the other hand, the noticeable capability of some of the reported dyes to probe lipid droplets in different cell lines under different conditions reveals their use as privileged probes for advancing the study of interesting lipid droplets by fluorescence microscopy.

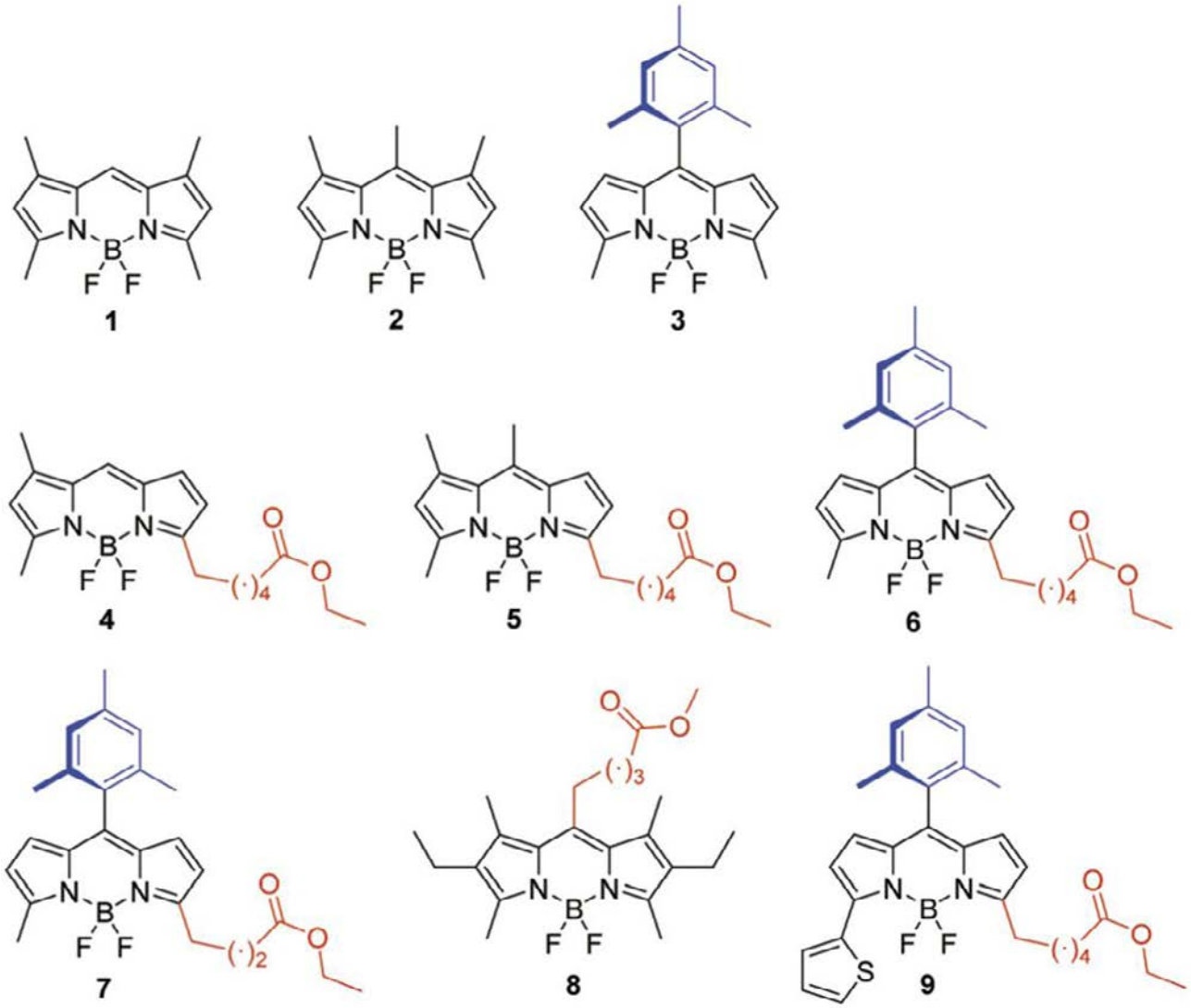

Figure 3: Studied BODIPYS. Key mesityl and long-ester moieties in blue and red, respectively.

New functional probes (BCT) based on BODIPY chromophore and carnitine as biotargeting element

The first fluorescent probes that are actively channeled into the mitochondrial matrix by a specific mitochondrial membrane transporter in living cells have been developed. The new functional probes (BCT) have a minimalist structural design based on BODIPY chromophore and carnitine as a biotargeting element. Both units are orthogonally bonded through the common boron atom, thus avoiding the use of complex polyatomic connectors. In contrast to known mitochondria-specific dyes, BCTs selectively label these organelles regardless of their transmembrane potential and in an enantioselective way. The obtained experimental evidence supports carnitine–acylcarnitine translocase (CACT) as the key transporter protein for BCTs, which behave therefore as acylcarnitine biomimetics. This simple structural design can be readily extended to other structurally diverse starting F-BODIPYs to obtain BCTs with varied emission wavelengths along the visible and NIR spectral regions and with multifunctional capabilities. BCTs are the first fluorescent derivatives of carnitine to be used in cell microscopy.

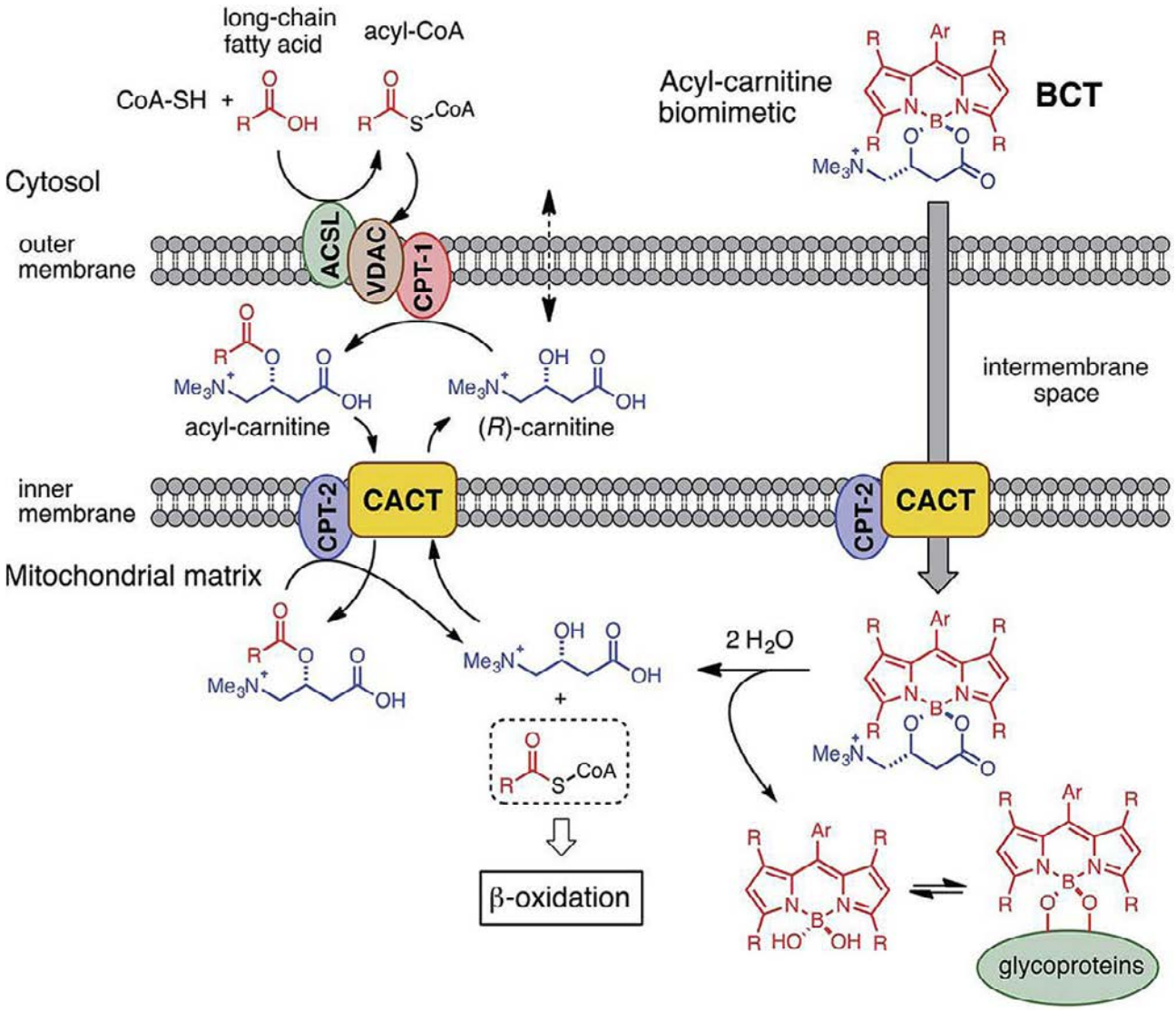

Figure 4: Mechanistic hypothesis for the transport (and fate) of BCT probes into the mitochondrial matrix via the carnitine shuttle system.

Photodynamic therapy (PDT) in Dermatology:

Antimicrobial PDT for treatment of Pityriasis versicolor

In collaboration with the dermatologist Dr. Enrique Alberdi, we have evaluated for first time the effect of PDT mediated by methylene blue (MB) for Pityriasis versicolor (PV). Five women with PV disseminated on the back and shoulder diagnosed by fresh microscopic analysis were treated with six sessions of MB/PDT with a 2-week interval in between (Figure 5). Complete cure (clinical and mycological cure) was observed in the five women at the 4 weeks post-treatment follow-up, without appearance of side effects. At this point, dermoscopic images did not show any of the proper characteristic of PV such as diffuse hypopigmented blotches (fairy demarcated) with fine scales, as the same time that microscopic analysis by KOH was negative. Fluorescence images from PV lesions by Wood´s lamp allowed to evaluate whether the lesions were healed or not at each time point. No patient showed relapse at the 6-month follow-up.

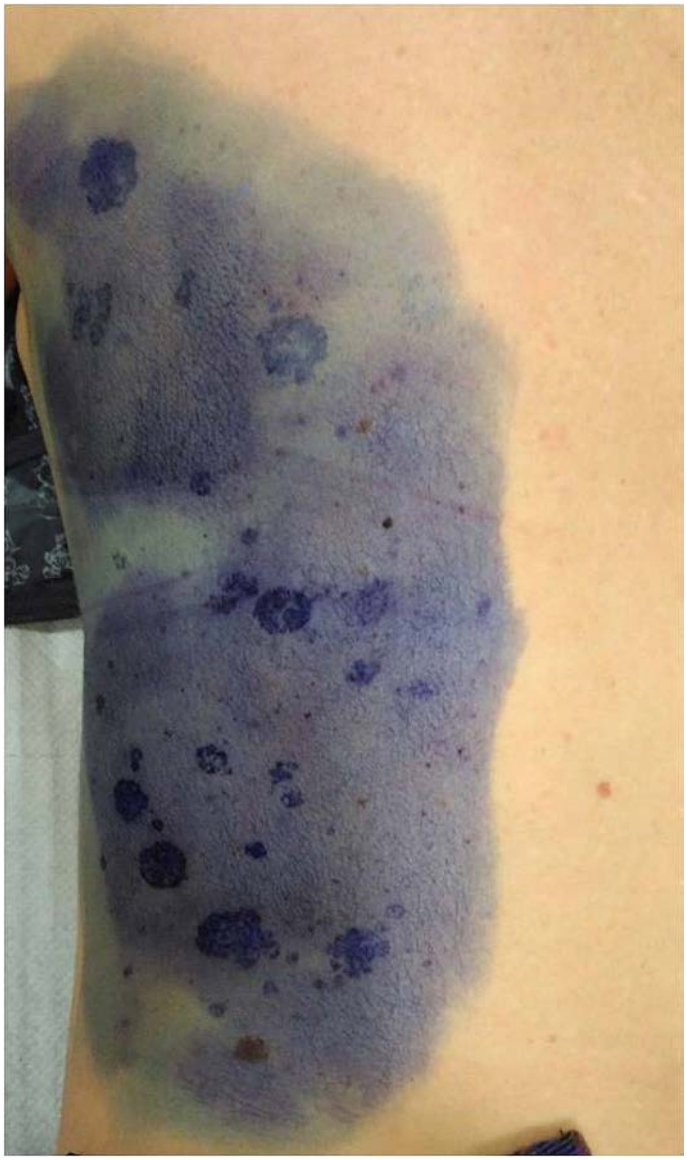

Figure 5: Application and incubation of MB aqueous solution.

Antifungal PDT for treatment of moderate onychomycosis

We have compared the impact of methylene blue (MB) *vs* methyl aminolevulinate (MAL) for the treatment of mild-to-moderate onychomycosis. A controlled trial of 40-week duration was designed. Twenty patients were randomly allocated into two different treatment groups: MB/ PDT or MAL/ PDT, to receive 9 sessions of PDT distributed over 16 weeks. MB application resulted in temporary discoloration of the nail. Onychomycosis severity index (OSI) scores decreased significantly along the study, from 12.1±5.4 to 3.6±3.2 (MB/PDT group) and from 14.8±6.0 to 5.4±4.4 (MAL/PDT group). At 16-week follow-up, only 20% of the patients in the MB/PDT group reached complete cure and none in the group of MAL/PDT. At 40-week follow-up, complete cure rates were 70% and 40% in the MB/PDT group and MAL/PDT group respectively. Both modalities showed good outcomes. MB/ PDT showed a faster action but with relapse rates slightly higher than MAL/PDT.

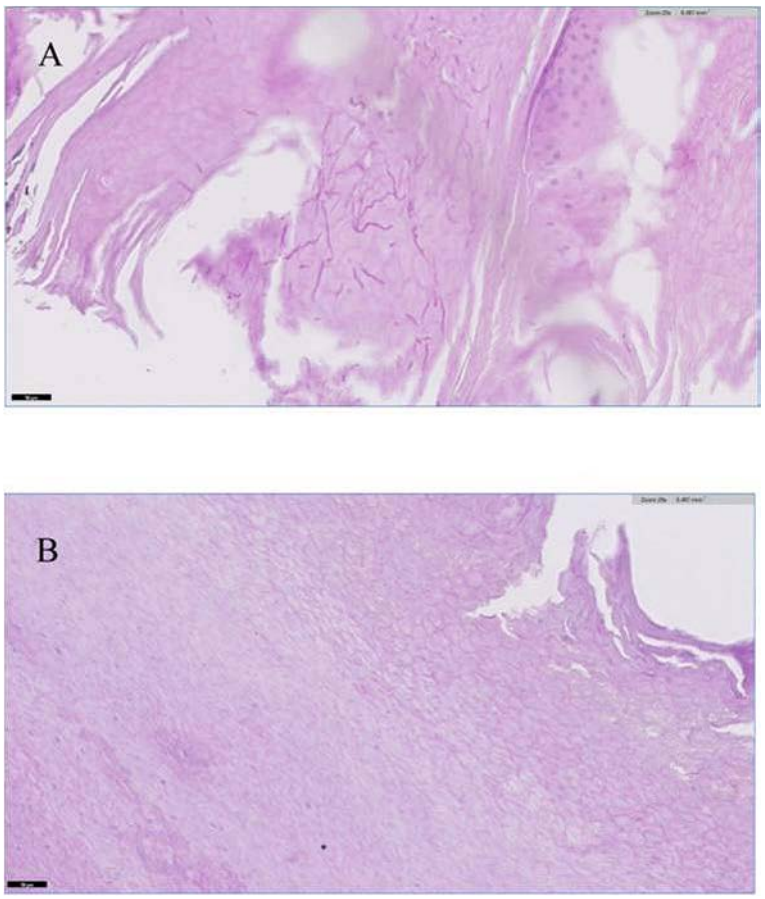

Figure 6: Histological analysis of a nail of one patient through PAS stain: (A) before the study, where the presence of fungal elements can be seen; (B) after the study, without presence of fungal elements.

Antifungal PDT for treatment of severe onychomycosis

We have compared the efficacy of combined therapies based on oral terbinafine (TN) plus adjunctive PDT mediated by methylene blue (MB) or methyl aminolevulinate (MAL) in the treatment of severe onychomycosis. Twenty patients received oral TN for 12 weeks and concomitantly were randomly allocated to receive 9 sessions, separated by 2-week intervals, of urea (40%) plus a PDT protocol mediated by MB (TN+MB/PDT) or MAL (TN+MAL/PDT). Clinical and mycological efficacy was evaluated at 16, 40 and 52- week follow-up. Mycological cure rates were significantly higher during the last third of the evaluated period of time, reaching 100% and 90% in TN+MB/PDT group and TN+MAL/PDT group, respectively, at the 52-week follow-up. In both modalities, complete cure was achieved in 70% of the patients at the 52-week follow-up. TN+MB/PDT and TN+MAL/PDT show similar outcomes in the treatment of toenails with severe onychomycosis. PDT is an effective method to accelerate the TN-mediated healing process.

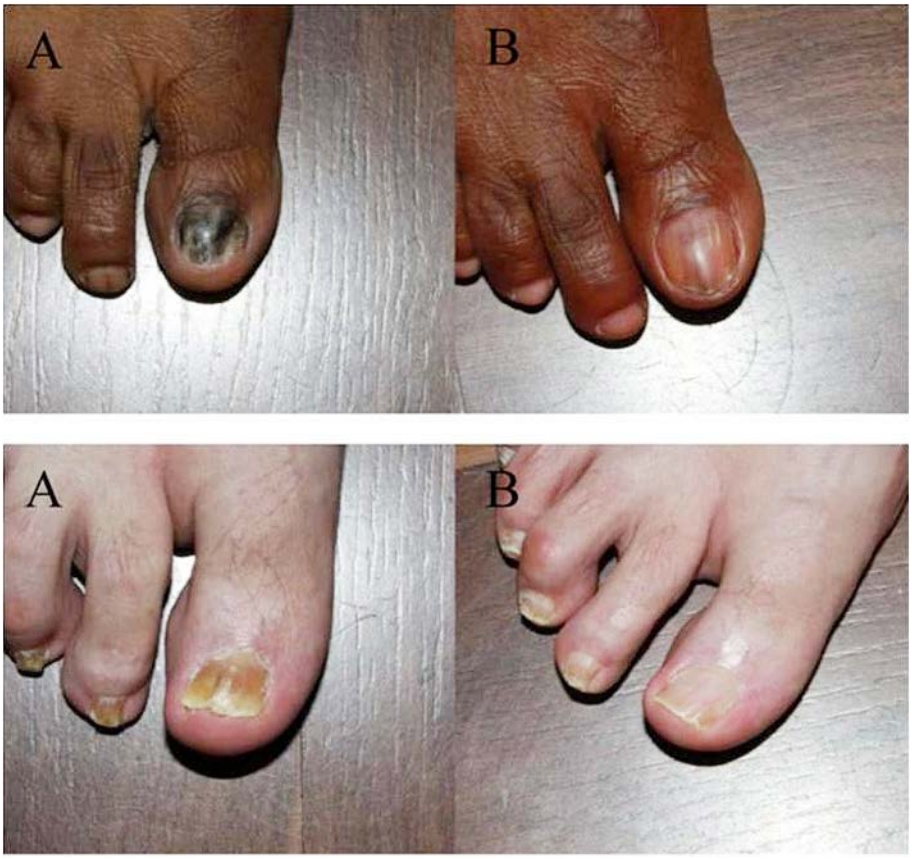

Figure 7: Clinical evolution of two toenail treated by TN + MAL/PDT assessed by photographs: (A) baseline; (B) 52-wk follow-up.

Antineoplastic PDT for Bowen disease

Surgical excision is the gold standard therapy for non-melanoma skin cancer (NMSC). A type of superficial NMSC is the Bowen´s disease (BD). There are cases in which by age, comorbidities, use of anticoagulants, location, cosmetic result, or size, it is preferable to use other treatments such as PDT. This study aimed to evaluate the long term effectiveness of MAL/PDT on a wide range of Bowen lesions in different locations and sizes. Patients diagnosed with BD received 3 MAL/PDT sessions with a 4-week interval in between. Clinical response and tumour characteristics were analyzed during the first year after start of the PDT sessions. In total, 21 BD lesions in 18 patients were included in the study. Complete regression after 3rd PDT session was 87.5% and 100% at the 6-month follow-up. Treatment was well tolerated with scarce side effects and very good cosmetic outcomes. No recurrence was observed at 12-month follow-up.

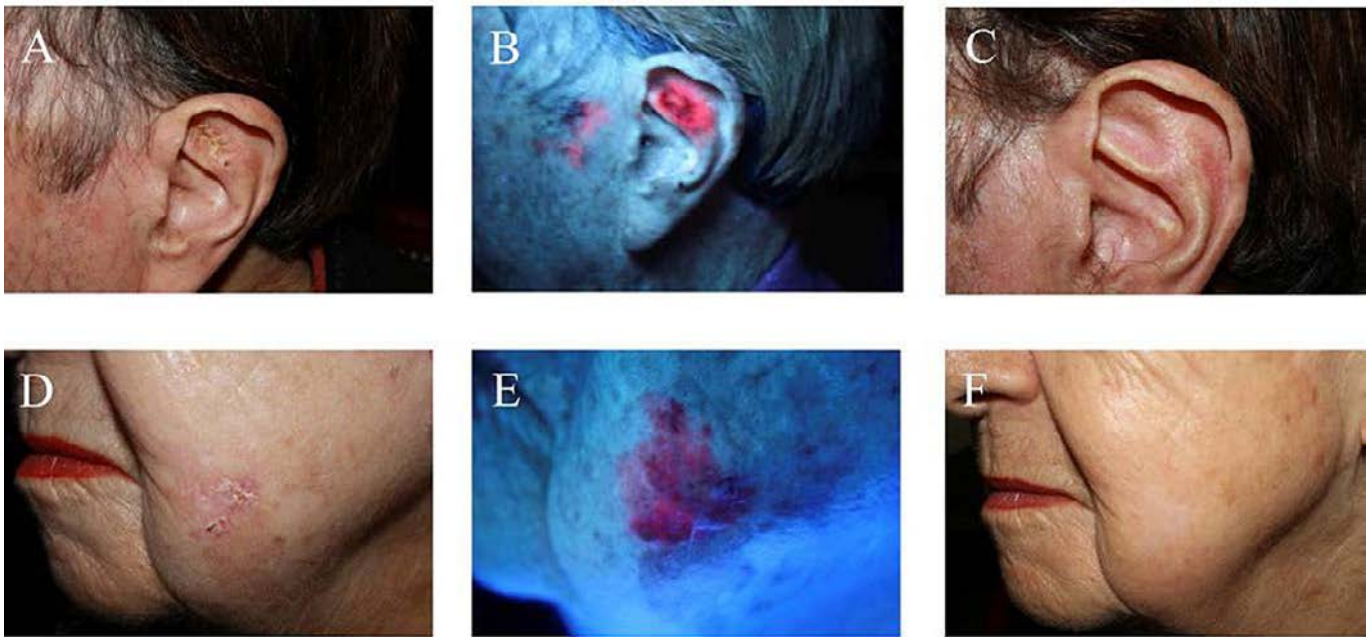

Figure 8: BD in the ear (A), delineated lesion by Wood´s lamp before PDT (B), complete regression four months after 3rd PDT (C); BD in the cheek (D), delineated lesion by Wood´s lamp before PDT (E), complete regression four months after 3rd PDT session (F).

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National Grants: individual

Fundación Eugenio Rodríguez Pascual

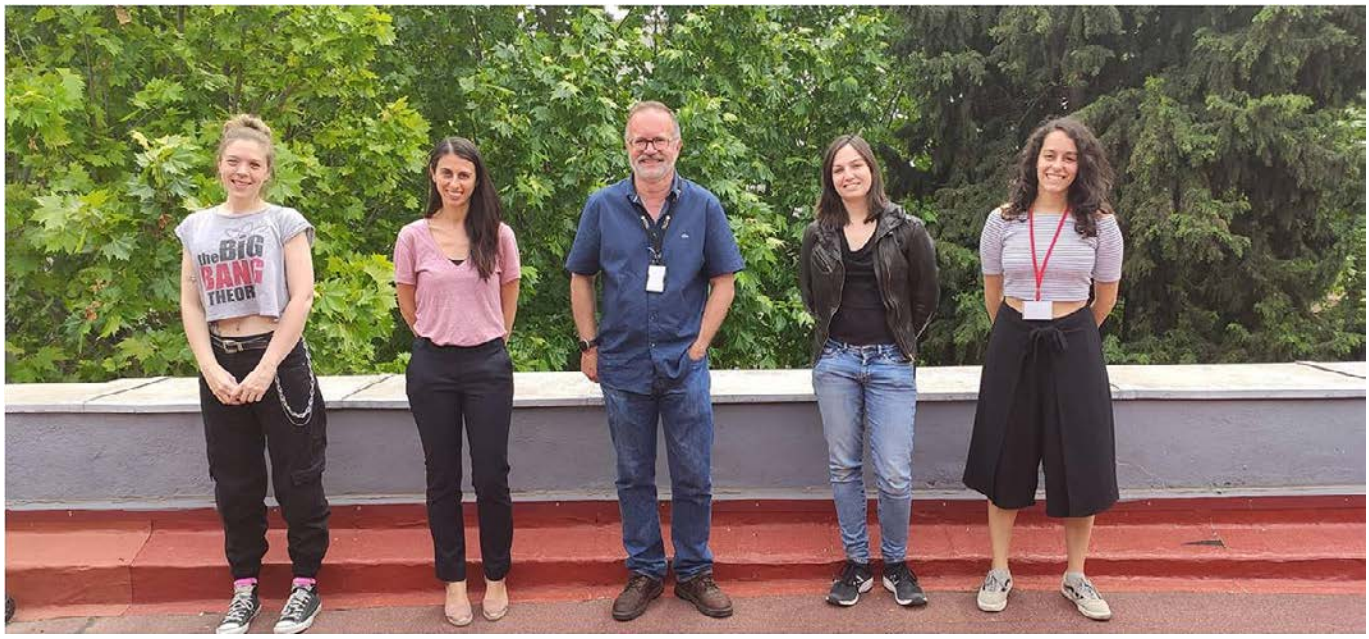
Principal Investigator	Title	Reference
Clara Gómez Hernández	Cuantificación de la capacidad antibacteriana, antifúngica e inmunomoduladora de la Terapia Fotodinámica en infecciones odontológicas y dermatológicas.	

National Grants: coordinated

Ministerio de Ciencia e Innovación (MICINN)

Principal Investigator	Title	Reference
Inmaculada García-Moreno Gonzalo	Materiales fotónicos "diseñados a medida" como marcadores avanzados para bioimagen	MAT 2017-83856-C3-1-P

Group of Statistical Mechanics and Condensed Matter



(May 2021, on the picture, from left to right: Luciana Luque (UNLP), Eva G. Noya, Enrique Lomba, Lucía Fernandez (UCM), Cintia Pulido)

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Enrique Lomba García
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Eva González Noya
(Assistant Professor) ORCID

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Leandro Guisández
(RISE exchange visiting researcher from UNLP, January 1st-July 1st 2019)

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(*CoFund, codirection with the Polish Academy of Sciences*)

Carolina Cruz
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Murilo Sodré Marques
(CAPES, Brasil, Exchange student of UFRGS at Porto Alegre, November 2019-May 2020)

Cintia Pulido Lamas
(JAEIntro February-May 2019)

Summary

The research carried out by the Group of Statistical Mechanics and Condensed Matter focuses on the application of statistical mechanics and condensed matter theory tools in conjunction with simulation approaches to analyse problems of physico-chemical interest, basically in connection to phase transitions in bulk and under confinement, self-association in colloids and nanoparticles as a tool for the design of novel materials, and the study of disordered hyper-uniform materials, as well as adsorption processes in nanostructured porous materials. Our main contributions can be cast into three main complementary lines: methodology, systems of fundamental interest, and systems of experimental interest.

Strategic Aims

- Development of new methodologies for the use of GPUs in computer simulation.
- Study of phase transitions and anomalous behaviour in complex fluids (water, liquid crystals, anomalous liquids).
- Design of simple models that assemble into complex ordered structures.
- Study of disordered hyper-uniform materials as candidates for stealth materials and optical.

Remarkable Results

Design of simple anisotropic models to assemble into complex structures

Anisotropic colloids and nanoparticles can be used to build new materials with improved functionalities for technological applications. Understanding the structures that emerge from a given model system and, inversely, providing recipes to build model systems that form a given target structure are two major milestones to optimize this process. Our group tries to address both questions. One of our major findings is that even the simplest particles geometries can form complex, unexpected structures. In particular, in collaboration with the University of La Sapienza, we found that tetrahedral particles designed to form a diamond crystal assemble into complex clathrate structures if the interactions are very directional. Regarding the second question, in collaboration with the University of Oxford, we have proposed a recipe to design model systems that form a given crystal structure based on their Wyckoff positions, which we are currently extending to the more complex case of quasi-crystals.

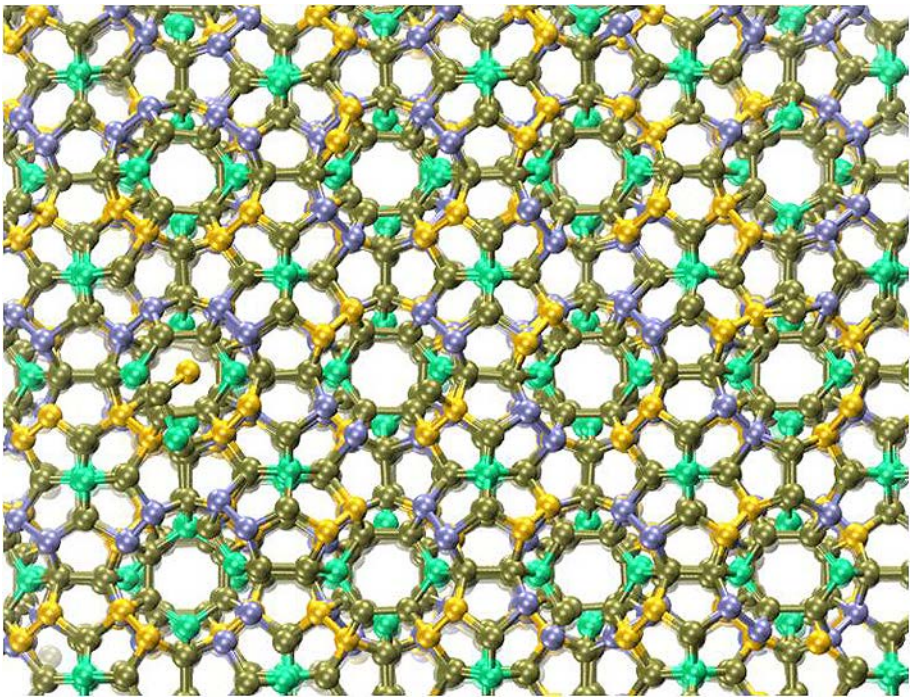

Figure 1: Clathrate crystal assembled from a model system with four particles.

Novel hyperuniform materials and hyperuniform states of nature

This work is the product of a collaboration with the group of Prof. Salvatore Torquato at Princeton University, who introduced the concept of disordered hyperuniformity in a joint work with Prof. Frank Stillinger back in 2003. Disordered hyperuniform materials are a class of systems in which long wavelength density or concentration fluctuation are strongly attenuated. As a consequence, these systems tend to have share some properties with ordered materials (such as crystals) while keeping the variability of disordered materials. In a series of works, we have managed to introduce a recipe to manufacture two-dimensional hyperuniform materials from a combination of suitable magnetic colloidal particles confined within a plan (Ma et al., 2020). On the other hand, we have devised an artificial model that mimics the hyperuniform distribution of photoreceptors in avian retina. We have shown what essential features must display the interparticle interaction to attain the proper multi-hyperuniform distribution, which is thought to be responsible for the extreme accuracy of the visual systems in birds. Avian retina is formed by five types of photoreceptors that follow a spatially disordered multi-hyperuniform distribution. In contrast, arthropods display crystalline-like patterns, which are not compatible with the different sizes of every type of photoreceptor in birds (Lomba et al., 2020).

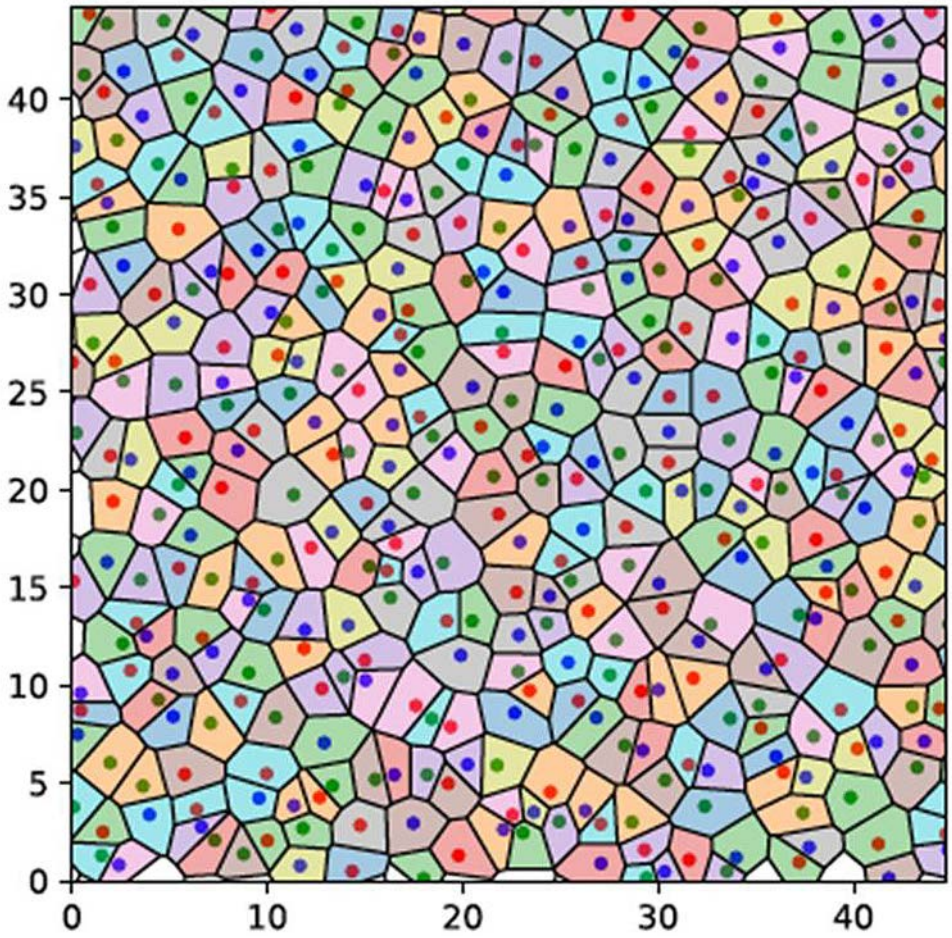

Figure 2: Spatial distributions of photoreceptors in an artificial model of bird retina.

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COMPETITIVE FUNDING

National Grants: individual

Agencia Estatal de Investigación (AEI)

Principal Investigator	Title	Reference
Eva González Noya	Network formation in colloids, aqueous solutions and interfaces	FIS2017-89361-C3-2-P
Eva González Noya	Quasicrystal design using colloidal particles	FIS2015-72946-EXP

International Grants: coordinated

MSCA Rise (EU)

Principal Investigator	Title	Reference
Eva González Noya	Effects of confinement on inhomogeneous systems	CONIN 734276

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Juan de la Figuera Bayón
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(until 31/2/2020)

Guiomar Delgado Soria

Eduardo García Martín
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Maria Sánchez Arenillas
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Eva María Trapero Díaz
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Summary

The scientific activity of this research group focuses on the study of various types of materials with sensitivity to the surface region and to the preparation of thin films. To do this, we use microscopy and spectroscopy techniques, some of them in ultra high vacuum (including nanospectroscopy techniques based on synchrotron radiation), as well as Mössbauer spectroscopy.

In this period we have devoted most of our time to the study of oxides of transition metals, with special emphasis on oxides with the spinel structure. We have performed a detailed chemical, structural and magnetic characterization of several of such oxides, and we have studied the growth of oxide thin films on different substrates. An aspect of our activity that should be remarked is the construction of instrumentation for surface analysis. More information can be found on the website, http://surfmoss.iqfr.csic.es.

Also the group offers some of its equipment to the scientific community through the Laboratorio de Caracterización "Ramón Gancedo", https://labrg.iqfr.csic.es.

Strategic Aims

- To understand and control the growth of transition metal oxide thin films from a few atomic layers to thicknesses of hundreds of nanometers.
- To determine the structural and magnetic properties of these films, taking advantage of the possibilities of specific techniques of growth to obtain new or improved properties.
- To build and implement new instrumentation for surface analysis and Mössbauer spectroscopy.

Remarkable Results

Growth of complex oxides followed by photoemission microscopy

In mixed metal oxides we find, using maps of their composition acquired while growth takes place, that the nucleation of a new phase can trigger a compositional change in the previously present phase.

The growth of mixed cobalt-iron oxides on Ru(0001) by high-temperature oxygen-assisted molecular beam epitaxy has been monitored in real time and real space by x-ray absorption photoemission microscopy. The initial composition is a mixed Fe-Co (II) oxide wetting layer reflecting the ratio of the deposited materials. However, as subsequent growth of three dimensional spinel islands nucleating on this wetting layer takes place, the composition of the oxide in the wetting layer changes as iron is transferred into the spinel islands. The composition of the islands themselves also changes during growth.

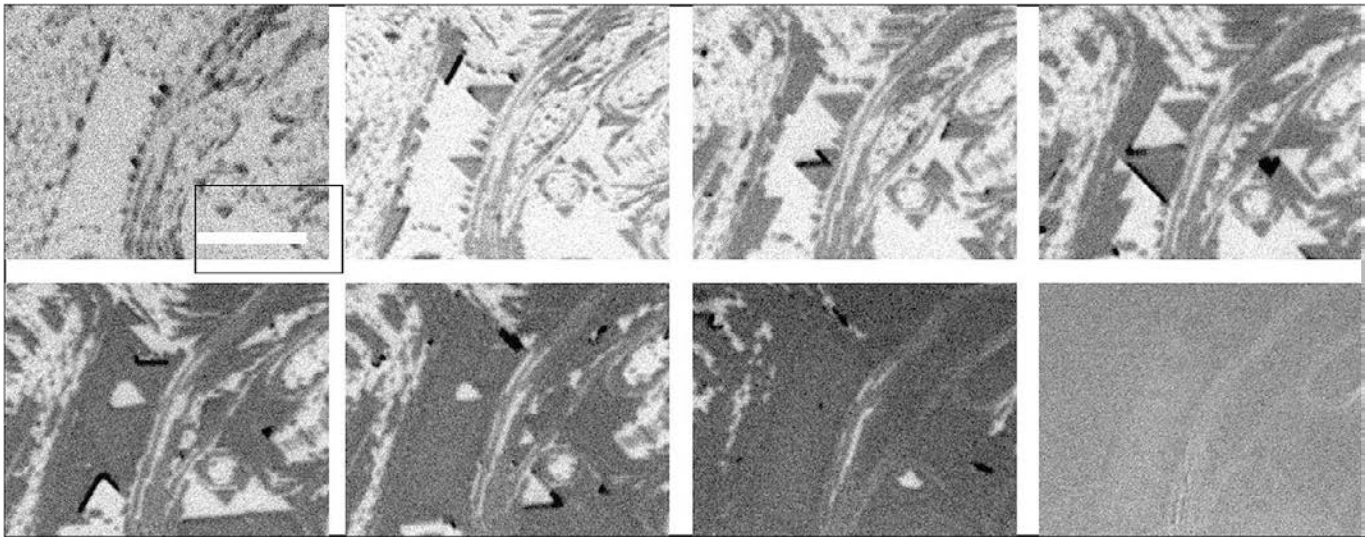

Figure 1: correspond to a mixed Co-Fe oxide growing on the Ru substrate.
S. Ruiz-Gómez, A. Mandziak, J. E. Prieto, M. Aristu, E. M. Trapero, G. D. Soria, A. Quesada, M. Foerster, L. Aballe, J. de la Figuera, "A Real Time XAS PEEM Study of the Growth of Cobalt Iron Oxide on Ru(0001)", *J. Chem. Phys*. 152 (2020) 074704 , DOI: 10.1063/1.5140886

Determination of spin direction in antiferromagnetic domains

We present a spatially resolved X-ray magnetic dichroism study of high-quality, in situ grown nickel oxide films. NiO thin films were deposited on a Ru(0001) substrate by high temperature oxygen-assisted molecular beam epitaxy. We found that by adding a small amount of Fe, the growth mode can be modified in order to promote the formation of micron-sized, triangular islands. The morphology, shape, crystal structure and composition are determined by low-energy electron microscopy and diffraction, and synchrotron based X-ray absorption spectromicroscopy. The element specific XMLD measurements reveal strong antiferromagnetic contrast at room temperature and domains with up to micron sizes, reflecting the high structural quality of the islands. By means of vectorial magnetometry, the spin axis orientation was determined with nanometer spatial resolution, and found to depend on the relative orientation of the film and substrate lattices.

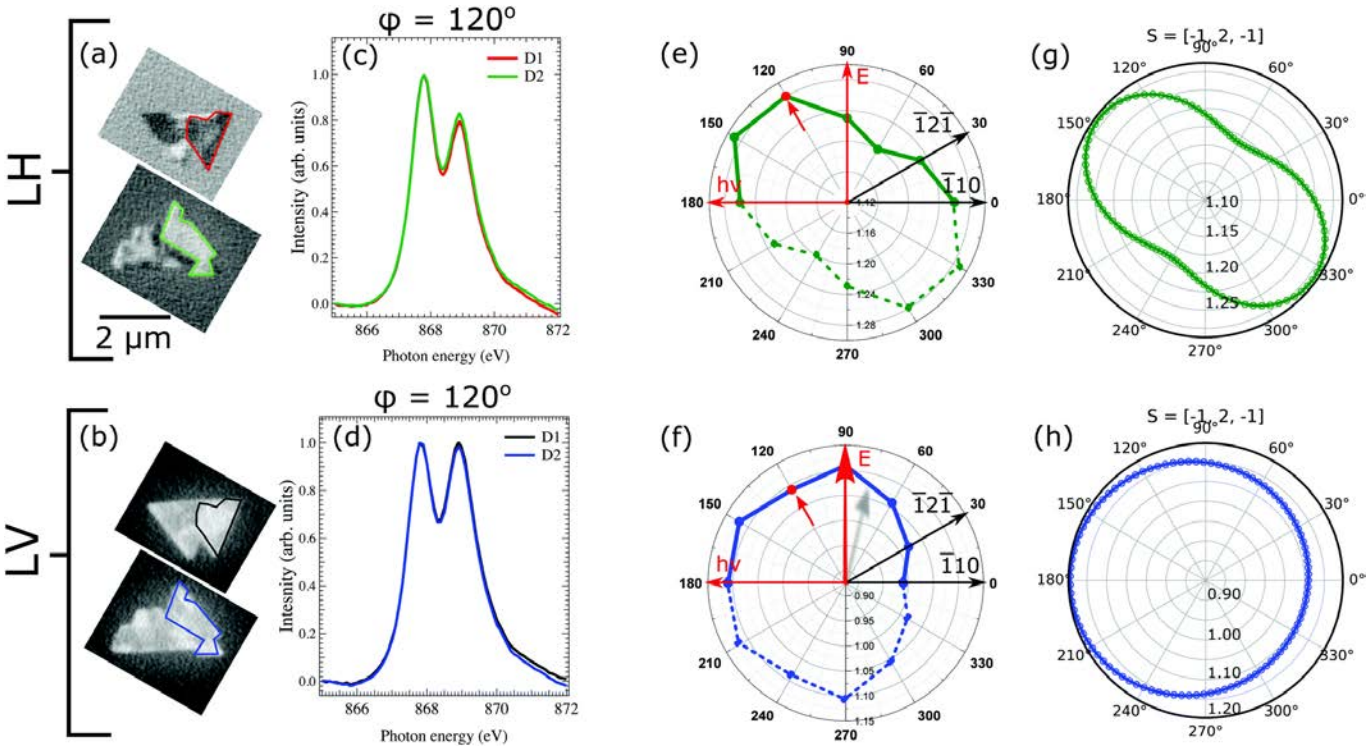

Figure 2: Antiferromagnetic domains are imaging by acquiring images of x-ray linear dichroism. The experimental dependence of the dichroism with the azimuthal angle of the incoming rays is compared with simulations assuming a given spin direction in a magnetic domain. A. Mandziak, G.D. Soria, J.E. Prieto, M. Foerster, J. de la Figuerab, L. Aballe, "Different spin axis orientation and large antiferromagnetic domains in Fe-doped NiO/Ru(0001) epitaxial films", *Nanoscale* 12 (2020) 21225, DOI: 10.1039/D0NR05756H.

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National Grants: coordinated

Agencia Estatal de Investigación (AEI)

Principal Investigator	Title	Reference
Juan de la Figuera and Jose F. Marco	Nuevos materiales y dispositivos para el procesado de señales ultra-rápido y/o de baja disipación	RTI2018-095303-B-C51

Comunidad de Madrid

Principal Investigator	Title	Reference
Rodolfo Miranda Soriano (UAM)	Soluciones del Nanomagnetismo a los retos sociales	S2018/NMT-4321

Research Support Services


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4000

Library

Dorotea Barnés Chemical Physics Library

The Dorotea Barnés Library of Chemical Physics is a specialized library within the areas of physical sciences and technologies and chemical sciences and technologies. The library belongs to the CSIC Library and Archives Network.

It was born in 2020 as a result of the unification of the libraries of the Rocasolano Institute of Physical Chemistry (IQFR) and the Miguel A. Catalán Physics Center, which includes the Structure of Matter Institute (IEM), Daza de Valdés Optical Institute (IO) and the Fundamental Physics Institute (IFF).

The library is physically located in the Rocasolano Physical Chemistry Institute, a unique building founded in 1946 and also known as the Rockefeller Building, since part of the funds contributed for its construction were paid for by this foundation.

Brief history of the origins of the Dorotea Barnés Library

The physical unification of the library became a reality in 2020, although the planning of the transfer, merging of the collections and changes in the computer configuration began in 2019. The irruption of the COVID-19 pandemic disrupted its inauguration, scheduled for the day March 11, 2020. This was suspended and postponed sine die.

Dorotea Barnés's name was chosen as a tribute to pioneering scientists. Several names were contemplated, being finally chosen the one of Dorotea by means of a vote between the members of the implied institutes.

Dorotea Barnés had a brilliant but short research career. He graduated in Chemical Sciences in 1929 from the Central University of Madrid.

Library space: designed by the architects M. Sánchez Arcas and L. Lacasa (1932), innovators at the time.

Collection: Old collections-unique in Spain holds a valuable holding, mainly journals.

The aim of the library is to provide the necessary support to the research process, facilitating access to digital information resources, open dissemination of scientific production, obtaining documents and managing physical collections as well as existing archival funds.

Library

Library Manager

Esperanza Iglesias Fernández
(until April 2020)

Flora Granizo Barrena

Technicians

Victoria Garrido Martínez
(until November 2019)

Laura Romera Guereca

Lourdes Moreno Gutiérrez
(since July 2019)

Strategic Aims

- Provide the necessary support to the research process.
- Facilitating access to digital information resources.
- Open dissemintion of scientific production.
- Obtaining documents and managing physical collections.
- Management of the archival funds.

Bibliographic and Authorities holdings: CSIC catalogs

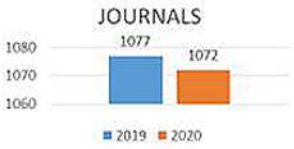
Physical collection:

Books / Researh Journals / Thesis

The library's collection of books and scientific journals has increased significantly due to the sum of the IQFR and CFMAC libraries.

PHYSICAL COLLECTION

	2019	2020
Total Physical Books /News	23365/302	23640/406
Journals/Vivas	1077/67	1072/60
Thesis/News	198	221/23

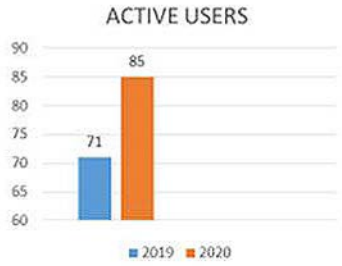


Circulation and Interlibrary Loan (ILL):

The extraordinary collection of books and scientific journals that our library has, makes us a supplier of documents both to other CSIC libraries and to universities and external research centers.

ORIGINAL BOOKS CIRCULATION

	PERSONAL LOANS	ACTIVE USERS
2019	260	71
2020	127	85



INTERBIBLIOTECARY CIRCULATION

	TOTAL	RECUESTED SOLICITADAS	calc	Nles.	Ext.	RECEIVED RECIBIDAS	calc	Nles.	Ext.
2019	436	113	80	22	11	323	255	65	3
FOT/ORIG.	395/41	88/25	59/21	19/3	10/1	307/16	242/13	62/3	3/0
2020	360	33	20	5	8	327	264	53	10
FOT/ORIG.	340/20	21/12	8/12	5/0	8/0	319/8	256/8	53/0	10/0

Institutional Repository:

This line of work has been reinforced in the repository, becoming a priority when implementing deposit strategies and growth of scientific production due to the multiplication of mandates from funding agencies, that require researchers to make their research results freely available.

INSTITUTIONAL REPOSITORY DIGITAL CSIC

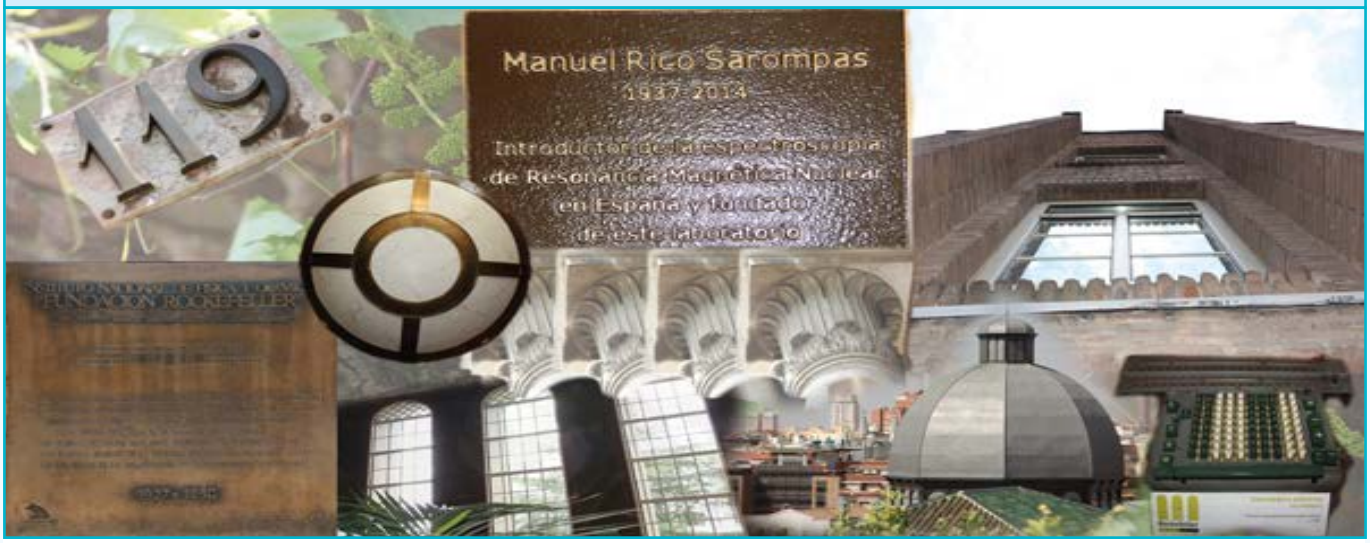
TOTAL RECORDS		RECORDS DEPOSITED
IQFR+CFMAC	2019	280
10561	2020	1420

Bibliometric study:

SCIENTIFIC PRODUCTION 2019-2020 / Q1 / D1*					
		IQFR (Rocasolano Institute of Physical Chemistry)	**IEM** (Structure of Matter Institute)	**IFF** (Fundamental Physics Institute)	**IO** (Daza de Valdes Optical Institute)
2019	**PUBS.**	**194**	**170**	**122**	**91**
	Q1	**117**	**72**	**66**	**41**
	D1	**41**	**25**	**16**	**10**
2020	**PUBS.**	**171**	**157**	**111**	**90**


CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFICAS

Administration-Stockroom-Reception



Management and administration Manager

Marta María Granja Perdices

Administration

Gloria Alonso Gómez

Gloria Pinillos Pérez
(until 10/04/2020)

Mar de la Torre Tante

Nuria Raboso Pérez
(from 05/11/2019)

Susana Fernández García
(from 16/03/2020)

Mónica Adelina Rivera Campos
(from 16/12/2020)

Stockroom

Consuelo Martín de Loeches
(Stockroom Manager) (until 05/05/2019)

Eva María Carpintero Vázquez

Héctor Caño Alonso (from 20/07/2020)

Reception

José Luis Rodríguez Garro

María Carmen Arcas Cañizares
(since October 2019)


CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFICAS

Technical Support Units

Electronics Workshop

Ángel Guirao Elías
(until April 2019)

Manuel Pérez García
(from April 2019)

Mechanics Workshop

Jose Antonio Serna Ferrero

Ignacio Sanz Gómez

Computer Support

Antonio Diaz Pozuelo

Building Maintenance

Jesús López Mascaraque

Juan Luis Martínez García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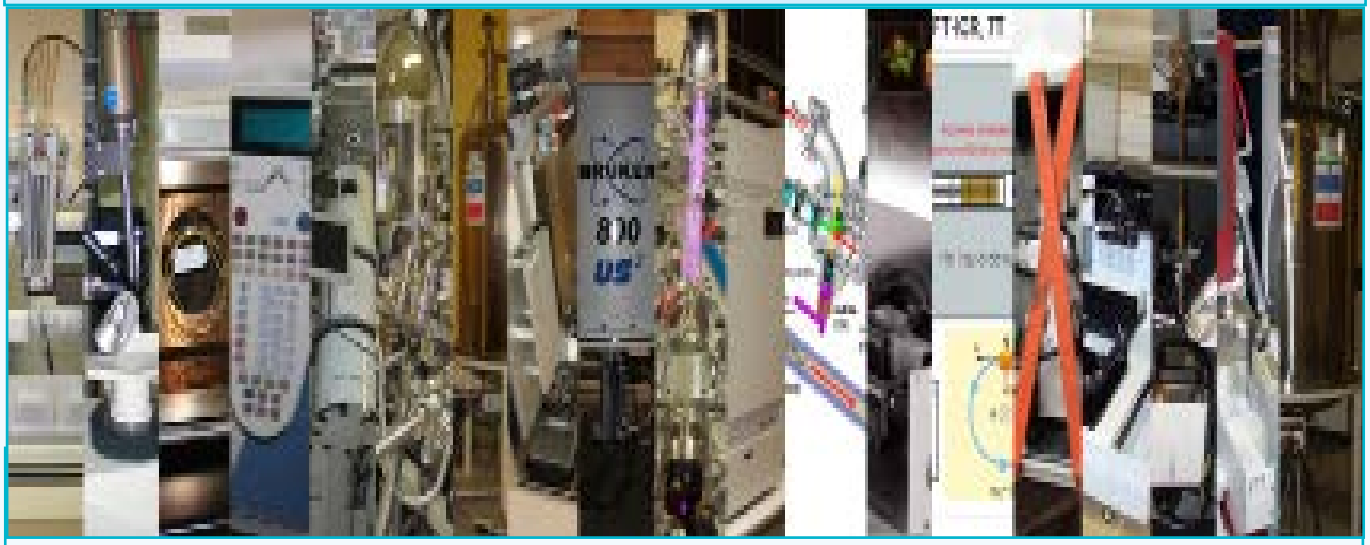
Singular Instrumentation



Laboratory for single crystal X-ray diffraction (DRXM)

The services offered by the laboratory are aimed at obtaining:

a) single crystals,

b) X-ray diffraction patterns of single crystals from samples of any nature: inorganic, organic, organometallic, macromolecular (proteins, enzymes) and polymer fibers

c) if required, the three-dimensional structure of the sample.

The laboratory has the latest equipment and facilities suitable for crystallization, observation, sample selection and mounting as well as for applying controlled temperature during the diffraction experiment, between 350 and 100 K, including a cryoprotected environment.

Crystallization robots

Liquid handlers for crystallization purposes, Oryx, Glison and Innovadine, for scaling from mililiters to nanoliters. Setup for 96 or 192 crystallization experiments per plate.

X-ray diffractometer #1

- Rotating anode X-ray source (2,7 kW, MicroStar, Bruker), 100 µ micro-focus, brilliance 3 times higher than conventional rotating anodes. CuKα radiation through Helios mirrors (Bruker).
- Four-circle Kappa goniometer and CCD detector (Bruker).
- Cryoprotecting system (Oxford Cryosystems) with N2 stream in the range 350-100 K.

X-ray diffractometer #2

- This equipment shares the X-ray source with diffractometer #1
- Imaging plate Mar345dtb (MarResearch).
- Cryoprotecting system (Oxford Cryosystems) with N2 stream in the range 350-100 K.

X-ray diffractometer #3

- X-ray micro-source IµS (Bruker) for CuKα X-ray radiation. Multilayer optics Elm3 (Bruker).
- Four-circle goniometer with APEX II detector (Bruker).
- Cryoprotecting system (Oxford Cryosystems) with N2 stream in the range 350-100 K.

Responsible/contact person: Armando Albert

X-ray diffractometers. From left to right: #1, #2, #3

Microarray Platform

Brief description: The microarray platform of the Department of Biological Physical Chemistry enables the preparation of "designer" microarrays of use in molecular recognition studies. The platform features:

- A non-contact microarray robot (Sprint, Arrayjet Ltd.) and a manual contact-system for microarray printing (V & P Scientific). A wide variety of samples, including proteins, glycoconjugates, polysaccharides, bacteria, cell extracts, etc., can be printed onto any kind of conventional microarray slide. The format of the arrays can be adapted in term of number of samples, doses, strains, replicates, etc, according to the requirements of the assay.
- A microarray scanner (GenePix 200-AL, Axon, Molecular Devices) with four different lasers (red, green, yellow, blue), compatible with all conventional microarray slides.

Responsible/contact person: Dolores Solís/ María Asunción Campanero-Rhodes

Microarray platform. From left to right, manual contact-system for microarray printing, non-contact microarray robot, and microarray scanner.

Two-photon laser microspectrometer with ps-s time resolution

Brief description: We have all the necessary fluorescence micro-spectroscopy tools to study, at the single molecule level, the global structure, 3-D organization, conformational changes, biomolecular interactions and dynamics of multicomponent complexes. Applications include: Structure, dynamics and biomolecular interaction studies; Conformational changes and 3-D organization (FRET and fluorescence anisotropy) of multi-component complexes; Nanostructure characterization; Molecular bio-sensor studies; Protein folding; and Cell biology. Diluted solutions, protein crowded solutions mimicking physiological media, cellular extracts, and live or fixed cells can be analyzed.

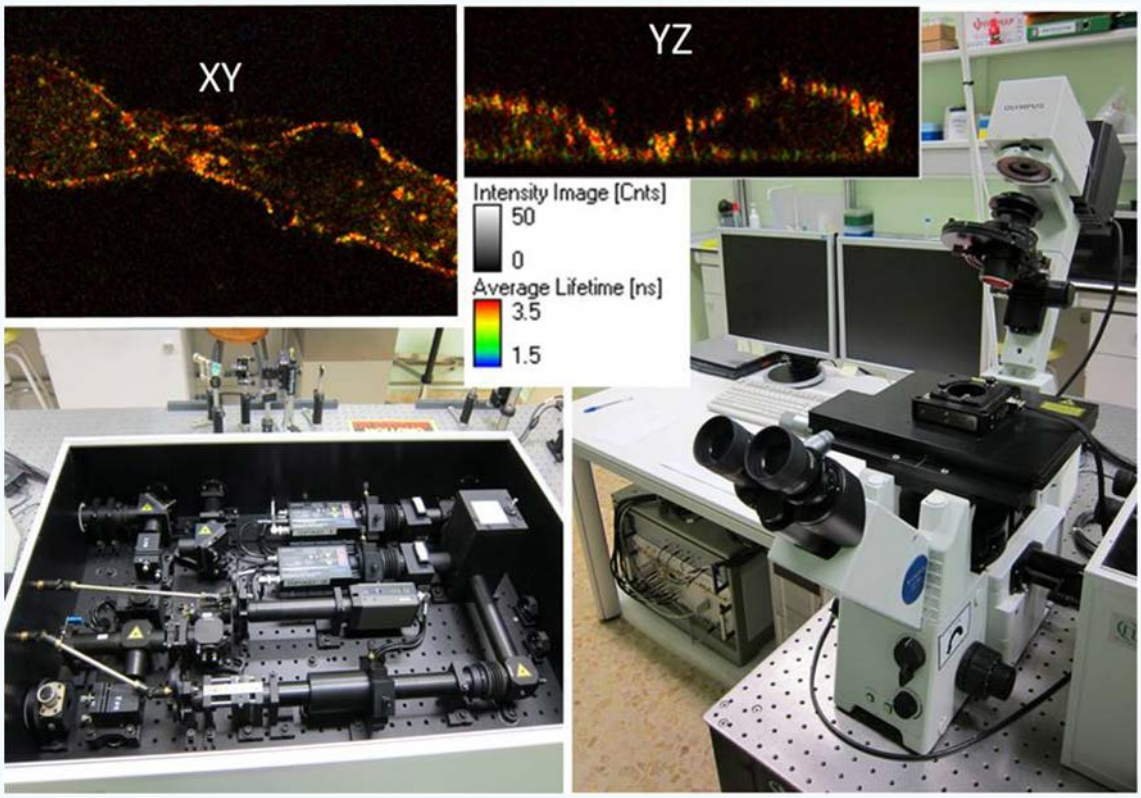
Technical information:

Multiphoton excitation (Ti: Za 750-850 nm, 80 MHz, 100fs) and Time-Tagged Time-Resolved (TTTR) detection.

Measurements:

- Whole-cell fluorescence analysis.
- Picosecond time-resolved fluorescence intensity and polarization.
- Förster-resonance energy transfer (FRET) efficiencies.
- Fluorescence correlation and cross-correlation spectroscopy.
- Fluorescence lifetime and anisotropy imaging.

Responsible/contact person: M. Pilar Lillo



Manuel Rico high field NMR laboratory (LMR) (http://rmn.iqfr.csic.es)

Brief description: The LMR lab (http://lmr.csic.es) has the most advanced techniques in the field of NMR spectroscopy required to address problems involving biomacromolecular structures and interactions. LMR is a node of the Spanish Biomolecular Nuclear Magnetic Resonance Laboratory Network or Red de Laboratorios de RMN de Biomoléculas (R-LRB), a distributed Unique Scientific and Technical Infrastructure (ICTS) in the health sciences field. Our high field spectrometers are the main research tools utilized by the groups of Structure, Dynamics and Interactions of Proteins by NMR (http://rmnpro.iqfr.csic.es) and NMR Spectroscopy of Nucleic acids (http://rmnac.iqfr.csic.es) to address the questions posed by their research projects. Moreover, the lab operates as a service to external users, from both Spain and Europe, providing the instrumentation, support and the expertise of the specialized staff to resolve their problems in the most efficient manner.

The LMR provides access to two NMR spectrometers:

- Spectrometer Bruker AVNEO60:

- Magnet Oxford 14.1T
- Console AVANCE NEO
- Cryoprobe TXI (1H,13C,15N)/Z gradients
- Probe TXI (1H,13C,15N)/5 mm
- Probe TBI (1H,13C, BB)/5 mm/gradient
- Probe TXI (1H,13C,15N)/8 mm/Z gradients
- Probe (1H-BB reverse)/10 mm

- Spectrometer Bruker AVNEO800

- Magnet Bruker US2 18.8T
- Console AVANCE NEO
- Cryoprobe TCI (1H,13C,15N)/ Z gradients
- Probe TXI (1H,13C,15N)/5mm/ Z gradients
- Probe QXI (1H, 13C, 15N, 31P)/5mm/ Z gradients

Laboratory director:

Carlos González

Technical director:

David Pantoja-Uceda

Technical staff:

Miguel Treviño, Irene Gómez Pinto, Daniel Calvo

Scientific committee:

M. Angeles Jiménez, Douglas V. Laurents, José M. Pérez, S. Padmanabhan.

LMR lab. From left to right, the work stations, the Magnet Oxford 14.1T of the 600 MHz NMR spectrometer, the AVANCE NEO consoles of the two NMR spectrometers, and the Magnet Bruker US2 18.8T of the 800 MHz NMR spectrometer.

Nonlinear Optical Microscope

The homemade nonlinear optical microscope uses a mode-locked Ti:Sapphire femtosecond laser oscillator as excitation source. The laser emits at 800 nm, with an average power of 680 mW, delivering 70 fs pulses at a repetition rate of 80 MHz. Nonlinear optical signals corresponding to multiphoton excitation fluorescence (MPEF) originated from the focal volume in the sample plane are collected in reflection mode. A variable neutral density filter serves to control the laser power reaching the sample. The laser beam is modulated using a chopper at a frequency of 130 Hz and conducted to the sample through the aperture of a microscope objective lens by using a dichroic beam splitter with a high reflection at 800 nm. The focal plane of the laser is selected with motorized translation XYZ stages. The lateral and axial resolutions achieved are of 1 and 2 µm, respectively.

Responsible/contact person: Marta Castillejo

Instrument: Mössbauer spectrometers.

Description: Mössbauer spectroscopy, based on the recoilless resonant nuclear absorption of gamma quanta or Mössbauer effect, is a technique which provides information on the chemical state, coordination geometry and magnetic state of a particular Mössbauer active isotope in a solid. In our case we focus on Fe-57 Mössbauer spectroscopy. In the transmission mode we obtain information from the materials in bulk while in the scattering mode (detection of conversion, Auger and low energy electrons) we obtain surface information. This surface information ranges from a fraction of monolayer, if the sample is enriched in Fe-57, to a depth of 300 nm. We have two transmission spectrometers, one for room temperature measurements and a second equipped with a He-closed cycle cryostat which allows measurements between 8.5 and 300 K. We have a third spectrometer for electron detection mode which can be operated either at room temperature with a parallel plate avalanche counter or between 100K and 300K by using a channeltron in ultra high vacuum conditions.

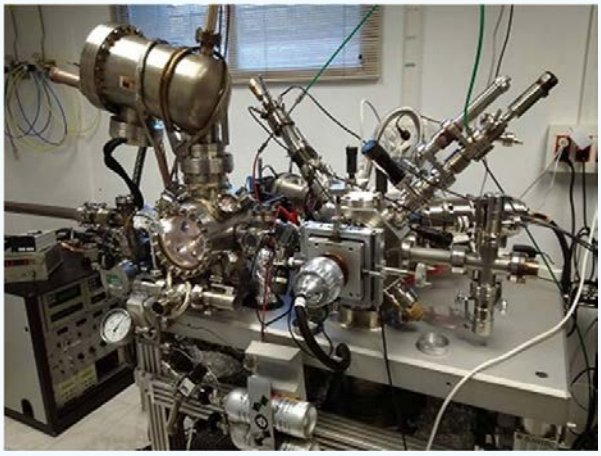
Responsible/contact person: José F. Marco

Instrument: Low Energy Electron Microscope

Description: Low-energy electron microscopy (LEEM) is a technique devoted to the observation of the surfaces of a crystalline materials in ultra-high vacuum conditions with an spatial resolution of a few nanometers and temporal resolution of fractions of a second using a beam of electrons with energies between a few eV and a few hundred eV. LEEM is used to observe in real time the growth of materials by molecular beam epitaxy, and to follow dynamic processes of surfaces such as phase transitions or the evolution with temperature of nanometric structures. The instrument available to us is the LEEM III from Elmitec GmbH and has been purchased with funding from the ERDF (European Regional Development Fund). In Spain there are two instruments of this type. The other one is at the Alba synchrotron.

Our system includes a load lock entry system, and a preparation chamber with an ion gun for cleaning and an XPS spectrometer (CLAM2) for chemical analysis.

Responsible/contact person: Juan de la Figuera/José E. Prieto.




CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFICAS

IQFR Facts and Figures

Academic Training:

Technology Transfer and Socio-Economic Impact:

Academic Training

PhD awardees

Name	Department	Date	University	Thesis title
Bélen Chaves Arquero	Biological Physical Chemistry (M.Ángeles Jiménez, J.M. Pérez-Cañadillas)	21/11/2019	Univ. Alcalá de Hénares (UAH)	Reconocimiento molecular en ribonucleoproteínas e histonas mediante RMN
Daniel Ramírez de Mingo	Inst. Cajal & Biological Physical Chemistry (Mariano Carrión-Vázquez, Douglas V. Laurents)	20/11/2020	Universidad Autónoma de Madrid	Relación estructura-función del prioniode humano CPEB3 en la consolidación de la memoria.
Edgar Gutiérrez Fernández	Sistemas de baja dimensionalidad, superficies y materia condensada (Aurora Nogales, Mari Cruz García Gutiérrez, Esther Rebollar)	21/10/2019	Universidad Complutense de Madrid	Nanostructuring of soft matter for organic electronics/Nanoestructurado de materia condensada blanda con aplicaciones en electrónica orgánica
Alberto Blazquez	Sistemas de baja dimensionalidad, superficies y materia condensada (José Luis Chiara, Inmaculada García-Moreno)	21/10/2020	Universidad Complutense de Madrid	Posfuncionalización de colorantes BODIPY para aplicaciones fotónicas y biofotónicas
Pablo Llombart González	Sistemas de baja dimensionalidad, superficies y materia condensada (Luis G. MacDowell, Eva G. Noya)	18/10/2019	Universidad Complutense de Madrid	Estructura molecular y hábitos cristalinos en interfases sólidas complejas: un estudio mediante simulación por ordenador
Anna Mandziak	Sistemas de baja dimensionalidad, superficies y materia condensada (Juan de la Figuera, Lucia Aballe)	9/10/2020	Universidad Complutense de Madrid	Growth and characterization of high-quality functional (Ni-Co-Fe) oxides on Ru (0001)

PhD fellowship/contract holders

Department of Crystallography and Structural Biology

Name	Funding body	Date	Supervisor
Juan Luis Benavente Fernández	Agencia Estatal de Investigación	2016	Armando Albert
Miguel Daniel Mozo	Agencia Estatal de Investigación (FPI program)	2018	Armando Albert
Elena Jiménez Ortega	Agencia Estatal de Investigación	2017	Julia Sanz
Isabel Cea Rama	Agencia Estatal de Investigación	2017	Julia Sanz
Angela Fernández García	Comunidad de Madrid	2020	Julia Sanz
Alejandra Carriles Linares	Agencia Estatal de Investigación (FPU program)	2016	J.A. Hermoso
Mayte Batuecas Mordillo	Agencia Estatal de Investigación (FPI program)	2016	J.A. Hermoso
Vega Miguel Ruano	Agencia Estatal de Investigación (FPI program)	2019	J.A. Hermoso
Plaza Vinuesa, Laura	Proyecto AGL2017-84614-C2-2-R	2017	J.M. Mancheño
Márquez Moñino, María Ángles	BFU2017-89913-P	2017	Beatriz González
Daniel Muñoz Reyes	PID2019-111737RB-I00	2020	M.J. Sánchez Barrena

Department of Atmospheric Chemistry and Climate

Name	Funding body	Date	Supervisor
Maxime Ferrer	MICINN	15/10/2020	Ibon Alkorta (IQM-CSIC) Josep M. Oliva-Enrich (IQFR-CSIC)

Department of Biological Chemical-Physics

Name	Funding body	Date	Supervisor
Israel Serrano Chacón	FPI/project contract	01/12/2015 -30/11/2019	Carlos González Ibáñez
Cristina Cabrero Fernández	FPI	01/07/2019	Carlos González Ibáñez
Bélen Chaves Arquero	FPI reference BES-2015-073383 (Project CTQ2014-52633-P)	01/01/2016 -30/09/2019	M. Ángeles Jiménez / José M. Pérez Cañadillas
Daniel Ramírez de Mingo	SAF 2016-76678	01/10/2015 - 20/11/2019	Mariano Carrión Vázquez/ Douglas V. Laurents
Sara S. Félix	U. Nova de Lisbon (joint PhD student with IQFR)	15/02/2019	Eurico Cabrita/F. Javier Oroz/ Douglas V. Laurents
Iván Martín Hernández	PID2019-109041GB-C21	2020	P. Chacon

Department of Low Dimensional Systems, Surfaces and Condensed Matter

Name	Funding body	Date	Supervisor
Javier Prada Rodrigo	FPU Program	2018	Esther Rebollar and Pablo Moreno
Eduardo García Martín	AEI (FPI)	1/8/2020-	Jose Emilio Prieto/ Pilar Prieto
Guiomar Delgado Soria	AEI (proyecto)	1/6/2020-	Juan de la Figuera/ Adrian Quesada

Post-doctoral fellowship/contract holders

Name	Funding body	Starting date	Supervisor
Iván Acebrón Avalos	Agencia Estatal de Investigación	2018	J.A. Hermoso
Martín Alcorlo Pages	Agencia Estatal de Investigación	2016	J.A. Hermoso
Carol Siseth Martínez Caballero	Agencia Estatal de Investigación	2016	J.A. Hermoso

Name	Funding body	Starting date	Supervisor
Mayte Batuecas Mordillo	Agencia Estatal de Investigación	2019	J.A. Hermoso
Juan Pablo Corella Aznar	MICINN	March 2015-March 2019	Alfonso Saiz-Lopez
F. Javier Oroz	SAF2016	01/04/2018 -30/06/2019	D.V. Laurents
F. Javier Oroz	Contracted with Explorer Project	01/07/2019-31/12/2019	J.M. Pérez Cañadillas, M. Gasset, R. Giraldo
F. Javier Oroz	Ramón y Cajal Fellow	01/01/2020	D.V. Laurents
Miguel A. Mompeán	Caixa Foundation Junior Group Leader	01/07/2019	D.V. Laurents
Miguel Garavís Cabello	Marie Sklodowska Curie global individual fellowship (MSCA-g)	01/03/2019	C. González Ibáñez
J.R. López-Blanco	Contrato Proyecto BFU2016-76220-P	01/01/2016 -31/12/2019	P. Chacón

TFG/TFM students

Name	Department	Date	University	Thesis title
Alvaro Gutiérrez Sánchez	Crystallography and Structural Biology (TFM, Super visor: A. Albert)	2019	Universidad Politécnica de Madrid	Structural characterization of ABA agonists
Ana Púa Bocos	Crystallography and Structural Biology (TFM, Supervisor: A. Albert)	2019	Universidad Autónoma de Madrid	Structural basis of the interaction with membrane of the tandem C2 domains of the extended synaptotagmin of Arabidopsis thaliana
Elena Nieves Jiménez	Crystallography and Structural Biology (TFM, Supervisor: J.A. Hermoso)	2019	Universidad Complutense de Madrid	Biología estructural de maquinarias de remodelado de la pared bacteriana
Laura López de Oro	Crystallography and Structural Biology (TFM, Supervisor: J.A. Hermoso)	2019	Universidad Complutense de Madrid	Caracterización estructural y funcional de lipoproteínas transportadoras de oligopéptidos en Streptococcus pneumoniae. Implicaciones en virulencia
Alejandra Alba	Crystallography and Structural Biology (TFM, Supervisor: J.A. Hermoso)	2020	Universidad Complutense de Madrid	Caracterización estructural de maquinarias de biosíntesis de la pared bacteriana
Nerea Pardo Cundís	Crystallography and Structural Biology (TFM, Supervisor: J.M. Mancheño)	2019	Universidad Complutense de Madrid	Producción heteróloga de la L-arabinosa isomerasa recombinante de Lactobacillus plantarum WCFS1
Laura Pérez Durango	Crystallography and Structural Biology (TFG, Supervisor: M.J. Sánchez Barrena)	2020	Universidad Politécnica de Madrid	Estructura del complejo NCS1/ Ric8a, diana terapéutica para enfermedades neurodegenerativas y del neurodesarrollo
Julio Barrios Llacuachaqui	Atmospheric Chemistry and Climate	02/06/2019	Universidad Nacional de Ingeniería, Lima-Perú	Estudio teórico/ experimental de las propiedades estructurales y energéticas del tirosol e hidroxitirosol

Name	Department	Date	University	Thesis title
Carlos del Burgo Olivares	Atmospheric Chemistry and Climate	From July to September 2019	Universidad Complutense	Estudio estructural, termodinámico y cinético de la reacción de HOI + NO3
Iván Martín Hernández	Biological Physical Chemistry (Supervisor P. Chacon)	2019		
Aarón Teran More	Biological Physical Chemistry (supervisors: J.M. Pérez-Cañadillas/ S. Herrero Domingo)	2019	Univ. Complutense de Madrid (UCM), Madrid	Master en Bioquímica, Biología Molecular y Biomedicina
Karima Tabakouht	Sistemas de baja dimensionalidad, superficies y materia condensada (TFG, Supervisor: Mohamed Oujja)	2019	Universidad Rey Juan Carlos.	Fabricación de materiales nanoestructurados por deposición por láser pulsado (PLD)
Elena Santamarina Ortiz	Sistemas de baja dimensionalidad, superficies y materia condensada (TFM, Supervisors: Esther Rebollar, Pablo Moreno)	2019	Universidad de Salamanca	Fabricación de sistemas compuestos con base polimérica mediante ablación láser en líquidos
Vladimir Zamorano Álvarez	Sistemas de baja dimensionalidad, superficies y materia condensada (TFM, Supervisor: Eva G Noya)	16/12/2020	Universidad de Huelva	Cristalización de partículas coloidales tetraédricas: competición entre diamante y clatratos
Francisco Javier Franco Carmona	Sistemas de baja dimensionalidad, superficies y materia condensada (TFM, Supervisor: Eva G Noya)	13/12/2019	Universidad Internacional de Andalucía	Diseño de nuevos materiales a partir de partículas anisótropas
Cintia Pulido Lamas	Departamento de Química-Física (TFM, Supervisors: Eva G Noya and Eduardo Sanz)	03/07/2019	Universidad Complutense de Madrid	Estudio del inicio de las transiciones de fase de primer orden por simulación
Julia Gómez Juan	Sistemas de baja dimensionalidad, superficies y materia condensada (TFM, Supervisor: Eva G Noya)	13/12/2019	Universidad Internacional de Andalucía	Simulación de nucleación de cristales de moléculas diatómicas

Scientist exchange

Name	Home institution	Destination institution	Dates
Irene García Maquilón	Instituto de Biologia Molecular y Celular de Plantas CSIC	IQFR-CSIC	September-December 2019
Jonathan Trapala Reina	Fac. de Química UNAM (Mexico)	IQFR-CSIC	September-December 2019
Sven Hammerschmidt	Dept. of Molecular Genetics and Infection Biology Center for Functional Genomics of Microbes Universität Greifswald (Germany)	IQFR-CSIC	November 2019
Leiv Sigve Håvarstein	Faculty of Chemistry, Consejo Nacional de Biotechnology and Food Science, Norwegian University of Life Sciences, Norway	IQFR-CSIC	February-March 2020
Rafael Pedro Fernández Cullen	Investigaciones Científicas y Técnicas (CONICET) FCEN-UNCuyo, UNT-FRM	IQFR-CSIC	01/02-2019
Rafael Pedro Fernández Cullen	Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) FCEN-UN Cuyo, UNT-FRM	IQFR-CSIC	11/12-2019
Juan Carlos Gómez Martín	Instituto de Astrofísica de Andalucia (IAA-CSIC)	IQFR-CSIC	09-10/2019
Xucheng He	Universidad de Helsinki	IQFR-CSIC	03-05/2020
Ana Isabel López Loreña	Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) FCEN-UNCuyo, UNT-FRM	IQFR-CSIC	05-07/2019
Alfonso Saiz López	IQFR-CSIC	Fudan University – Shanghai	07/2019
M. Garavís	IQFR-CSIC	MacGill University, Canada	01/03/2019 – 28/02/2021

Name	Home institution	Destination institution	Dates
Li Li Xu	College of Food Science and Engineering, Ocean University of China, Qingdao, Shandong China	IQFR-CSIC	1-12-2020/ 30-11/2021
Gustavo A. Titaux-Delgado	National Autonomous University of Mexico, Mexico	IQFR-CSIC	20/03/2019-07/11/2019
Marta Castillejo	IQFR-CSIC	Istituto Nazionale di Ottica, Consiglio Nazionale delle Ricerche, Florence, Italy	01/10/2018-31/03/2019
Miguel Angel Gonzalez Barrio	Universidad Complutense de Madrid	IQFR-CSIC	1/7/2019-31/1/2020
Andreas K. Schmid	Lawrence Berkeley National Laboratory	IQFR-CSIC	1/9/2019-31/9/2019
Leonardo Morales de la Garza	Universidad Nacional Autónoma de México	IQFR-CSIC	1/1/2020-31/3/2021
Guiomar Delgado Soria	IQFR-CSIC	Jerzy Haber Institute of Catalysis and Surface Chemistry, Poland	16/9/2019-18/10/2019

Courses and scientific meeting organization and participation

Researcher	Event	Organizer	Title	Date	Place
Beatriz Gonzalez	Master in Molecular and Cellular Integrative Biology MCIB	UIMP-CSIC		2018-2019 2019-2020	CIB/IQFR
María José Sánchez Barrena					
Douglas Laurents			Coordinator of Module on Structural Biology	October 2019	
Pilar Lillo			Métodos Avanzados MCIB. Advanced Fluorescence Microspectroscopy	January 2019 and January 2020	
Douglas Laurents			Protein Folding and Unfolding and Intrinsically Disordered Proteins	October 2019	
F. Javier Oroz			Protein Structure and Dynamics	18/10/2019 and 09/10/2020	
Maria Gasset			Protein diversity: Proteoforms	24/10/2019	
David Pantoja Uceda			Practical NMR session @LMR	15/11/2019 and 21/11/2020	
Lourdes Infantes	Master in Biomolecules and Cell dynamics	UAM		2018-2019	IQFR
M. Ángeles Jiménez			Nuclear Magnetic Resonance spectroscopy: Basic concepts	18/11/2019 and 16/11/2020	
			Determination of biomolecule structures from NMR parameters	19/11/2019 and 17/11/2020	

Researcher	Event	Organizer	Title	Date	Place
Douglas Laurents			Biomolecular Complexes Studied by NMR Spectroscopy	20/11/2019 and 18/11/2020	UAM, Cantoblanco, Madrid
F. Javier Oroz			Protein Dynamics and Intrinsically Disordered Proteins Studies by Nuclear Magnetic Resonance	25/11/2019 and 23/11/2020	
Armando Albert and Juan A. Hermoso	Macromolecular Crystallography School - MCS2019	Armando Albert and Juan A. Hermoso		22-28 April 2019	IQFR
Jose Miguel Mancheño and Esther Rebollar	IQFR Seminars	Jose Miguel Mancheño and Esther Rebollar		2019-2020	IQFR
Jose Miguel Mancheño and Rebeca de Nalda	Colloquium Marie S. Curie-CSIC	Jose Miguel Mancheño and Rebeca de Nalda		2019-2020	CSIC (central) IQFR
Douglas Laurents	BIFI IX National Conference 2019	BIFI / U Zaragoza	Poster: Unmasking the bases of a polyproline II helical bundle's folding and stability by NMR spectroscopy	31/01/2019	Zaragoza, Spain
María Gasset	International Congress BIOMATSEN 2019	Gebze Technical University (GTU)	Amyloids as biomineralizing tools	10/05/2019	Oludeniz (TR)
M.Á. Jiménez, D. V. Laurents	XIII Manuel Rico NMR Summer School	M.Á. Jiménez, D. V. Laurents (GERMN-RSEQ)		June 16-21, 2019	Jaca, Huesca, Spain
M. A. Jiménez			2D Homonuclear NMR Spectroscopy via Scalar Coupling		
Douglas Laurents			Intrinsically Disordered Proteins		

Researcher	Event	Organizer	Title	Date	Place
Douglas Laurents	Joint 12th EBSA European Biophysics Society/ Spanish Biophysical Society	Spanish Biophysical Society	Poster: Amyloid proteins as synthetic devices for biotechnological purposes. D. Laurents & others. Poster: "Nucleotide and osmolyte induced folding of FtsZ from S. aureus. " D. Laurents & others Poster: "NMR studies on intrinsically disordered domains of Histone H1.0 and eIFG1: Effect of phosphorylation ans multivalent protein-nucleic acid recognition "	20/07/2019	Madrid, Spain
B. Chaves, J.M. Pérez-Cañadillas, & M.A. Jiménez					
Douglas Laurents	Nova Biophysica Masters Class	Requimte/ UCIBIO Applied Molecular Bioscience Unit, University Nova Lisbon, Portugal	Characterization of Intrinsically Disordered Proteins as a Via Towards Drug Development.	04/09/2019	Lisbon, Portugal
David Pantoja Uceda	ICTS NMR Course		Curso avanzado de RMN	23-25/10/2019	CIPF, Valencia, Spain
Pilar Lillo	Grado en Biotecnología: Experto en metodología en investigación biotecnológica	UFV	Técnicas Instrumentales Avanzadas: Fluorescencia	09/2019 and September 2020	UFV, Madrid
M.A. Campanero Rhodes	Seminar	Glycosciences Laboratory, ICL (UK)	Bacteria microarrays for examining bacterial surface glycans and their recognition by glycan-binding proteins	14/05/2020	Online webinar

Researcher	Event	Organizer	Title	Date	Place
M. A. Jiménez, D. Pantoja	17th Iberian Peptide Meeting (EPI 2020; http://epi2020.iqfr.csic.es/)	M. A. Jiménez, D. Pantoja (IQFR, IQM)			
Douglas Laurents			Oral communication: Structure and application off antifreeze polypeptides	5-7/02/2020	IQFR, Madrid
Miguel Mompeán			Oral communication: The homo- and hetero-oligomeric foldomes of functional and pathological amyloids		
Douglas Laurents	COVID19 NMR Consortium Global Meeting	COVID19-RMN Consortium	Short Talk: "Characterization of some putatively disordered regions of SARS-CoV-2 by NMR spectroscopy"	22/09/2020	on-line
Miguel Mompeán	Exploring the Druggability of SARS-CoV2	COVID19-RMN Consortium	Oral communication: Partial structure and dampened mobility in SARS- CoV-2 Nsp2 C-terminal region revealed by NMR spectroscopy	9-10/11/2020	on-line
J.M. Pérez-Cañadillas	"Prácticas de empresa"	Biological Physical Chemistry, Univ. Complutense de Madrid (UCM)	Prácticas en empresa de Beatriz Fernández del Rio Prácticas en empresa de Andrés Arribas Delgado	2019	IQFR
Marta Castillejo	I Encuentro transferencia Patrimonio Cultural (PTI-PAIS)	Marta Castillejo		October 8th-9th 2020	Virtual
Marta Castillejo	E- ED-ARCHMAT H2020-MSCA-ITN-EJD Winter School, RIHS PP, PTI		Invited lecture	20/01/2020	Universidad de Évora (Évora, Portugal)

Researcher	Event	Organizer	Title	Date	Place
Mohamed Oujja	Summer School organized by Universidad Internacional Menéndez Pelayo – CSIC. "Nuevos retos en la caracterización y conservación de los bienes del Patrimonio Cultural"	UIMP-CSIC (Marta Castillejo)	Invited Conference: Laser induced plasma spectroscopy for analysis of cultural heritage materials		
Marta Castillejo			Invited Conference: Espectroscopias y microscopias láser para la caracterización de materiales y objetos del patrimonio cultural	July 2019	Palacio de la Magdalena, Santander, Spain.
Mikel Sanz			Invited Conference: Metodologías avanzadas de limpieza láser en patrimonio cultural		
Mohamed Oujja	Máster Interuniversitario en Ingeniería Química	Universidad Rey Juan Carlos	Prácticas en Máster	2019	IQFR
Mohamed Oujja	Course "Últimas tecnologías aplicadas a la conservación del patrimonio cultural: problemática y soluciones"	Universidad de Zaragoza	"Últimas tecnologías aplicadas a la conservación del patrimonio cultural: problemática y soluciones"	November 2019	Universidad de Zaragoza
Marta Castillejo	Feria Bienal Ibérica de Patrimonio Cultural AR&PA – Resiliencia del Patrimonio Cultural	Marta Castillejo (co-organizer)		November 2020	Virtual
Eva G. Noya	Master in Molecular Simulation	Universidad Internacional de Andalucía	Advanced Monte Carlo course	2018/2019 2019/2020 2020/2021	Master on-line

Researcher	Event	Organizer	Title	Date	Place
J.F. Marco	Postgraduate Course	CEDENNA, Universidad de Santiago de Chile (Chile)	Teoría y práctica en la evaluación de espectros XPS (X-ray Photoelectron Sectroscopy)	25-28/03/2019	Facultad de Química y Biología, Universidad de Santiago de Chile, Chile
		Universidad Católica del Norte, Antofagasta (Chile)	Taller de Espectroscopía de Fotoelectrones generados por Rayos X (XPS)	26-28/06/2019	Unidad de Equipamiento Científico-MAINI de la Universidad Católica del Norte, Antofagasta (Chile)
	International School: IV Escuela Colombiana de Espectroscopía Mössbauer	Universidad de Tolima	Mössbauer Spectroscopy and Surface Analysis Mössbauer Spectroscopy Applied to Corrosion Research	10-12/07/2019	Universidad del Tolima, Ibagué, Colombia
	Postgraduate Course: Sensores electroquímicos: Caracterización superficial y aplicaciones	Universidad de Chile	Caracterización de superficies mediante técnicas espectroscópicas	03/12/2019	Facultad de Ciencias Químicas y Farmaceúticas de la Universidad de Chile, Santiago de Chile (Chile)
Josep M. Oliva Enrich (Julio Palacios Chair)	Conference	Josep M. Oliva Enrich (Julio Palacios Chair)	Conference by Prof. Eluvathingal D. Jemmis: 2019 Año internacional de la Tabla Periódica Conference by Prof. Jesús Martínez-Frías	20/06/2019 10/12/2020	Fundación Ramón Areces

Researcher	Event	Organizer	Title	Date	Place
Juan Z. Dávalos	XXII International Conference on Chemical Thermodynamics in Russia	Juan Z. Dávalos (Member of the Scientific Committee)		19/07/2019-23/07/2019	San Petersburgo (Federación Rusa)
	Specialization virtual course	MSc Emma J. Urrunaga / Innovación y Transferencia-Vicerrectorado de Investigación-UNSAAC	Métodos de Cálculo (Semi-Empíricos, DFT, ab-initio) para determinar la Estructura y Reactividad de Especies Neutras e Ionizadas	05/06/2020-03/07/2020	Cusco-Perú Universidad Nacional San Antonino de Abad, UNSAAC
	Invited Conference	Universidad Nacional San Antonio de Abad del Cusco (UNSAAC)	Ciencia y Tecnología: simbiosis perfecta del conocimiento humano	27/06/2020	UNSAAC-Cusco-Perú
	Ciclo Conferencias Virtuales-Escuela Profesional de Química-UNI	Universidad Nacional de Ingeniería (UNI)	Invited Conference: Antioxidantes y la Química Computacional	23/09/2020	Lima- Perú
	XIX Meeting of Physics	Universidad Nacional de Ingeniería (UNI)	Invited conference: Molecular reactivity of the atmospheric gas-trace	25/09/2020	Lima- Perú,
	I Simposio Internacional-Perspectivas de la Investigación y Seguridad Alimentaria	UNSCH	Invited conference: Propiedades energéticas de las harinas de pseudocereales andinos con alto valor nutricional	25/09/2020	Ayacucho-Perú,
	IX Semana de la investigación científica del I Congreso Internacional en investigación, innovación y emprendimiento en tiempos de COVID-19	EPCFM -UNSAAC	Invited conference: Influencia de los gases traza en la naturaleza oxidativa de la atmósfera	07/10/2020	Cusco-Perú

Researcher	Event	Organizer	Title	Date	Place
Rosa Lebrón Aguilar	Specialization course: Cromatografía de Líquidos acoplada a la Espectrometría de Masas. 2019. (26 h)	Rosa Lebrón Aguilar		21-24/10/2019	IQFR

Technology Transfer And Socio-Economic Impact

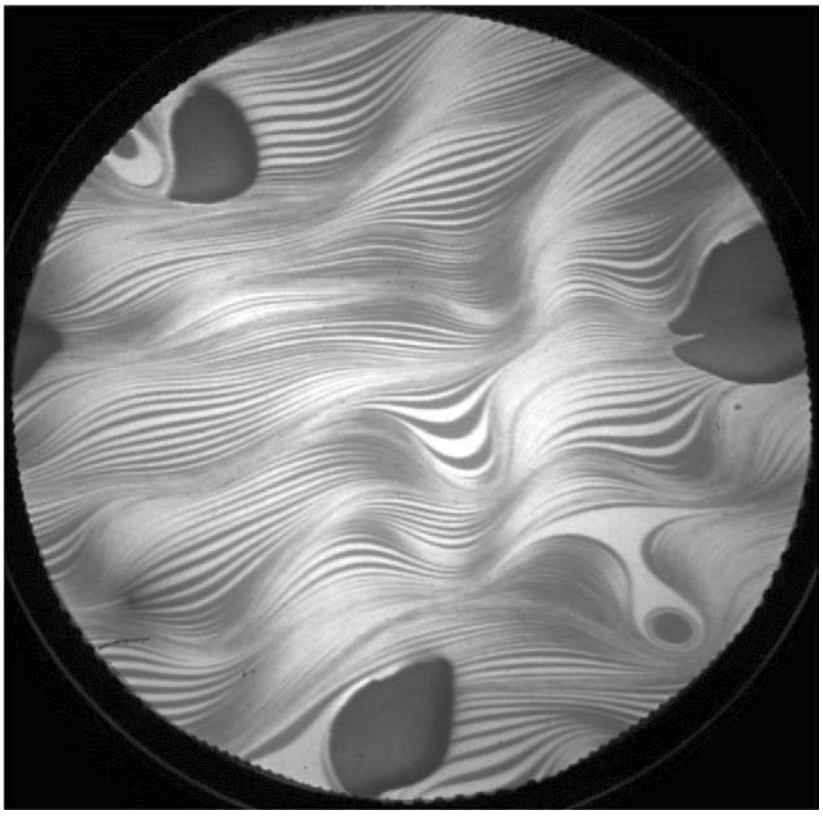
Patents

Authors	Title	Year	Code
Héctor Rodríguez, José M. Mancheño, Juan Anguita, Gonzalo Jiménez-Osés	Compounds for the treatment of diseases associated with oral pathobionts	2020	P19323EP00
Ruth Pérez Fernández, Andrea Canal Martín, Mª José Sánchez Barrena and Alicia Mansilla Aparicio	Acylhydrazones as synaptic function modulators	2019	PCT/ES2019/070649
Novoa, B., Mallavia, R., Figueras, A., Gasset, M., Rey-Campos, M.	Péptido de miticina y su uso en regeneracion celular	2019	PCT/ES19/070815

Awards and distinctions

Name	Award	Link
Guiomar Delgado	Prize to the Best Poster: "Study of the magnetic coupling in soft-hard bilayer systems" 23.05.2019	Conference MECAME - GFSM2019; https://mecame-gfsm2019.irb.hr/
José Emilio Prieto, Juan de la Figuera, Guiomar Delgado	Image selected for the catalogue and exhibition of scientific photography FOTCIENCIA17 (itinerant, 2020) Low-energy electron microscopy (LEEM)	https://www.fotciencia.es https://www.ivoox.com/m11-veo-todo-el-cristal-blanco-y-audios-mp3_rf_58267196_1.html
Francisco Javier Oroz	III Ayudas a la Investigación "Muévete por los que no pueden"	https://mueveteporlosquenopueden.org/2020/01/06/resolucion-iii-convocatoria-ayudas/

Guiomar Delgado receiving the prize for the best poster of MECAME-GFSM 2019, Montpellier, France.



LEEM image selected for the catalogue and exhibition FOTCIENCIA17. Field of view is 20 micrometers and it shows a Ru(0001) surface imaged in dark-field mode. It contains three regions of epitaxial graphene. Atomic terraces are separated by monoatomic steps and present an alternating black-white contrast.

Editorial and scientific committees

Participant	Committee/Journal	Role
Juan A. Hermoso	Editorial Advisory Board Member of Encyclopedia of Life Sciences in Structural Biology. John Wiley & Sons, Ltd	Editor
Juan Z. Dávalos	Revista de la Sociedad Química del Perú	Consulting Commitee Member
Juan Z. Dávalos	REVCIUNI (Fac. Ciencias, UNI-Perú)	Editorial Board Member
Juan Z. Dávalos	J Phys Chem, J Chem Thermodyn, J Phys Org Chem, J Therm Anal Calorim, React Kinet, Mech Cat, J Colloid Interf Sci; Heterocyclic Comm.; J Fluorine Chem. Letters;Appl. Surf. Sci.; Chem. Data Coll.; Polycyclic Aromatic Comp.; European J. Mass Spectrom.; J. Mol. Graph & Model.; Arabian J. Chem.; Molecules.	Reviewer
Josep M. Oliva-Enrich	Second Julio Palacios International Symposium	Organizing and Scientific Committees
Josep M. Oliva-Enrich	Theor Chem Acc, Phys Chem Chem Phys, J Phys Chem, J Molec Model, Chem Commun, J Solid State Chem	Reviewer
M. Gasset	PLosOne	Academic Editor
M. Gasset	Biomolecules	Academic Editor
M. Gasset	Allergies	Academic Editor
M. Gasset	Alzheimer's Association Research Grant Program (AARG and AARG-D)	Peer Reviewer
M. A. Jiménez	Archives in Biochemistry and Biophysics, Elsevier	Guest Editor, Special Issue
Marta Castillejo	International Conference on Laser Ablation (COLA), 2019.	Member of Scientific Committee
Marta Castillejo	Plataforma Temática Interdisciplinar del CSIC "Patrimonio Abierto, Investigación y Sociedad"	Coordinator
Marta Castillejo	European Research Infrastructure for Heritage Science (E-RIHS), preparatory phase.	Integration Director
Marta Castillejo	Laser Research Infrastructure HiLASE, Institute of Physics, Czeck Republic.	Member of the Scientific Advisory Board.
Esther Rebollar	"Materials Processing with Lasers", in X Iberoamerican Optics Meeting / XIII Latinamerican Meeting on Optics, Lasers and Applications/Mexican Optics and Photonics Meeting, RIAO-OPTILAS-MOPM 2019	Co-chair

Participant	Committee/Journal	Role
Esther Rebollar	Applied Surface Science	Co-editor of the special issue "Photon-assisted synthesis and processing of materials in nano-microscale"
Esther Rebollar	Polymers	Editor of the special issue "Laser processing of polymer materials"
Esther Rebollar	Polymers	Editor of the special issue "Laser processing of polymer materials II"
Rebeca de Nalda and Esther Rebollar	Nanomaterials	Editors of the special issue "Laser Synthesis and Modification of Materials at the Nanoscale"
Esther Rebollar	Materials	Editor of the special issue "Laser Applications in Polymers"
Juan de la Figuera	Executive Committee of the Spanish Vacuum Society (ASEVA)	Member
Juan de la Figuera	International Review Panel of the Solaris Synchrotron (Poland)	Member
Juan de la Figuera	J. Phys. D: Applied Physics	Surface Science Section Editor
Juan de la Figuera	International Board of the European Conference on Surface Crystallography and Dynamics	Member
Juan de la Figuera	Organizing Committee of the LEEM-PEEM 2020 conference	Member
José Emilio Prieto	Organizing Committee of the LEEM-PEEM 2020 conference	Member
José F. Marco	Scientific Executive Committee of the International Symposium on the Industrial Applications of the Mössbauer Effect	Permanent Member

Media coverage

Name	Media y date	Link
Juan A. Hermoso	Madri+d (30/05/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/2019-madridmasd-2.pdf
Juan A. Hermoso	Univadis (31/05/2019)	https://www.univadis.es/viewarticle/avances-en-la-comprension-de-la-fenilcetonuria-pnas-673414
Juan A. Hermoso	AS.com (31/05/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/AS.com.pdf
Juan A. Hermoso	WebConsultas (31/05/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/WebConsultas.pdf
Juan A. Hermoso	Diario de León (25/05/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/diario-de-leon-2019.pdf
Juan A. Hermoso	CSIC (24/05/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/CSIC-PNAS-mayo2019.pdf
Juan A. Hermoso	Madri+d (11/12/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/2019-madrimasd.pdf
Juan A. Hermoso	Diario de León (3) (08/12/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/2019-Diario-Leon.pdf
Juan A. Hermoso	Diario de León (1) (08/12/2019) + Diario de León (2) (08/12/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/2019-diario-de-leon.pdf https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/2019-diario-de-leon-2.pdf
Juan A. Hermoso	Córdoba Buenas Noticias (07/12/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/2019-cordobabn.pdf
Juan A. Hermoso	65yMás (06/12/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/2019-65ymas.pdf
Juan A. Hermoso	Salud a Diario (06/12/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/2019-saludadiario.pdf
Juan A. Hermoso	Bolsamanía (05/12/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/2019-bolsamania.pdf
Juan A. Hermoso	El Médico Interactivo (05/12/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/2019-medico-interactivo.pdf

Name	Media y date	Link
Juan A. Hermoso	ALBA Synchrotron Facility (05/12/2019)	https://www.cells.es/en/media/news/researchers-unveil-the-mechanism-in-bacterial-division
Juan A. Hermoso	CSIC (05/12/2019)	https://www.xtal.iqfr.csic.es/grupo/xjuan/CHBP_archivos/press-notes/2019-csic-bacterias_spor.pdf
María José Sánchez Barrena	NIUS Diario (09/12/2020)	https://www.niusdiario.es/sociedad/sanidad/frio-nanobolsa-grasa-escudos-protectores-vacuna-arn-coronavirus_18_3053670165.html
Miguel Mompeán	Interview published on El Mundo, January 2020	https://www.elmundo.es/madrid/2020/01/20/5e2497e6fc6c83530a8b4644.html
Grupo de RMN de Proteínas	Press note on the CSIC headquarters' webpage, 13/06/2020 on our characterization of coronavirus proteins	https://www.csic.es/en/node/1252608
Miguel Mompeán	Interview on TVE (24 hours), October 2020	https://www.rtve.es/alacarta/videos/diario-24/diario-24-19-10-20-1/5687758/ (prog1-1h14m) https://twitter.com/ma_mompean/status/1318263106380943362?s=20
Miguel Mompeán	Interview on 7TV, October 2020	http://webtv.7tvregiondemurcia.es/informativos/informativos-mediodia/2020/miercoles-21-de-octubre/ (52m30s)
Grupo de RMN de Proteínas	Press note on the CSIC headquarters' webpage, 13/10/2020 on our participation in the International Consortium COVID19-NMR	https://www.csic.es/en/node/1258591
Miguel Mompeán	Interview on 7TV, November 2020	http://webtv.7tvregiondemurcia.es/informativos/informativos-manana/2020/lunes-16-de-noviembre-ii/ (18min16s)

Associated units

Genética Molecular (Universidad de Murcia, GM-UMU)

- https://myxoum.blogspot.com/; https://www.um.es/mucorgen/en/index.html
- Responsible persons: Carlos González Ibañez, IQFR (CSIC) and Montserrat Elías, Universidad de Murcia.

This Associated Unit, continually active since its establishment in 2006, complements and enhances the research lines of both GM-UMU and the Department of Biological Physical Chemistry of the IQFR. It is focused on elucidating the molecular mechanisms of cellular responses to light as well as to other environmental and/or stress signals using markedly multidisciplinary approaches that combine biomolecular structure determination (X-ray diffraction, nuclear magnetic resonance or electron microscopy methods) to genetics, molecular biology, protein/ nucleic acid chemistry, biophysics, and bioinformatics. The very fruitful association has yielded excellent results amply reflected in: (a) joint publications in renowned journals such as *Science*, *Nature*, *PNAS, Nature Communications*, *Nucleic Acids Research*, *Journal of Biological Chemistry* etc.; (b) invited reviews of the work in the very prestigious *Annual Review of Biochemistry* and *Current Opinion in Structural Biology*; (c) presentation of the work in meetings of high international stature such as various *Gordon Research Conferences* on a wide range of topics from microbial stress response to photosensory signal transduction mechanisms, the chemistry and biology of tetrapyrroles such as heme, chlorophyll and vitamin B_{12}, and the cell biology of metals; (d) continuous research funding in coordinated projects between members of the unit; (e) shared mentoring of doctoral students.

Group of stability, folding and interactions of proteins, BIFI, Universidad de Zaragoza

Responsible persons: M. Ángeles Jiménez, IQFR-CSIC, and Javier Sancho, BiFi, Universidad de Zaragoza.

Description: This associated unit aims to facilitate to all its members the use of the most suitable methodology to face the challenges of their projects in the Structural Biology field. Researchers from the Department of Crystallography and Structural Biology, and the Department of Biological Physical Chemistry participate in this associated unit. The main objectives of this associated unit are: Increase and promote the scientific collaborations between IQFR-CSIC and BiFi-UZ, and share instrumentation facilities, particularly those which are available only in one of the centers.

Associated unit for the Biophysical and Structural Study of Nucleic Acids (BioEstrAN); Department of Organic Chemistry of the University of Barcelona (UB)

Responsible persons: Carlos González, IQFR-CSIC, and Nuria Escaja, UB.

Web: https://www.iqfr.csic.es/es/investigacion/unidades-asociadas/56-cabeceraweb/estructura-investigacion/unidades-asociadas/368-estudio-biofisico-y-estructural-de-acidos-nucleicos-bioestran

The aim of this Unit is the study of nucleic acids structural motifs involved in biological processes with potential application to Biomedicine, Nanotechnology and Synthetic Biology. The Unit brings together the expertise in NMR spectroscopy from the IQFR with the high capabilities of the UB in synthetic chemistry and different analytical techniques.

Associated unit "Química Física Molecular": Departamento de Química Física I, Facultad de Ciencias Químicas, Universidad Complutense de Madrid

https://www.iqfr.csic.es/es/investigacion/unidades-asociadas/56-cabeceraweb/estructura-investigacion/unidades-asociadas/98-unidad-asociada-quimica-fisica-molecular

Responsible person at IQFR: Rebeca de Nalda Mínguez

Description: The associated unit "Química Física Molecular" facilitates the collaboration between groups with experience in investigating the structure and dynamics

of molecular systems. The combined set of advanced theoretical and experimental tools allows a better understanding of phenomena under study than that resulting from individual efforts.

- Dynamics and kinetics of physicochemical processes
- Study of structures of molecules and condensed phases (ice) of atmospheric and astrophysical interest
- Interaction of laser radiation with solid molecules and substrates

Surface Science and Magnetism of Low Dimensional Systems

Responsible: Juan de la Figuera

https://www.iqfr.csic.es/es/investigacion/unidades-asociadas/56-cabeceraweb/estructura-investigacion/unidades-asociadas/38-superficies-y-magnetismo

The Associated Unit "Fisicoquímica de Superficies" is formed by the team of the Surface Laboratory of the Faculty of Physical Sciences of the Complutense University of Madrid and the IQFR and was established in 2014. From a scientific point of view, the Associated Unit works in the following lines of research:

1. Magnetic nanostructures and nanowires: magnetic and chemical characterization.
2. Influence of surfaces on magnetic properties.
3. Manipulation of magnetism in low dimensional systems.

These central themes are supported by instrumental objectives. These include the transfer of knowledge between the members of the consortium.

Scientific Cloister

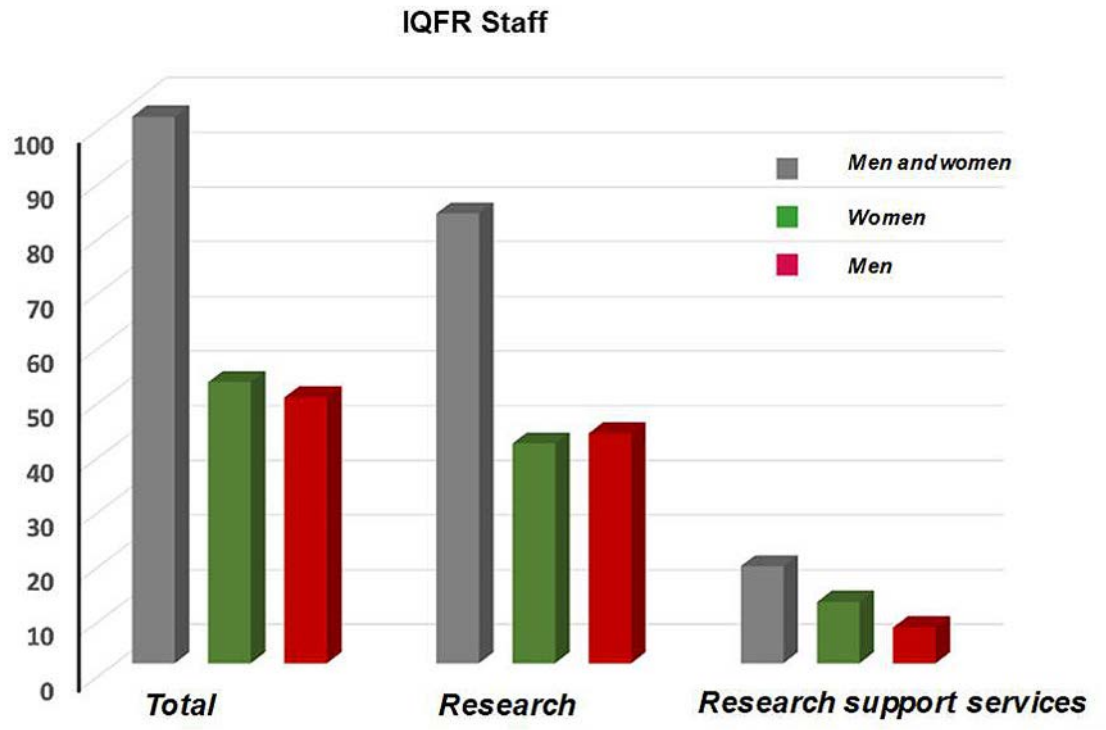
President:	Carlos González Ibañez	**Professor**
Secretary:	Beatriz González Pérez	**Associate Professor**
Members:	A. Ulises Acuña Fernández	**Professor ad Honorem**
	Martín Martínez Ripoll	**Professor ad Honorem**
	Inmaculada García-Moreno Gonzalo	**Professor**
	Carlos González Ibañez	**Professor**
	Juan Antonio Hermoso Domínguez	**Professor**
	Enrique Lomba García	**Professor**
	Subramanian Padmanabhan	**Professor**
	Alfonso Sáiz López	**Professor**
	Armando Albert de la Cruz	**Associate Professor**
	Rosa Becerra Arias	**Associate Professor**
	Marta Castillejo Striano	**Associate Professor**
	Pablo Chacón Montes	**Associate Professor**
	Juan de la Figuera Bayón	**Associate Professor**
	Maria A. Gasset Vega	**Associate Professor**
	Beatriz González Pérez	**Associate Professor**
	Maria Angeles Jiménez López	**Associate Professor**
	Douglas V. Laurents	**Associate Professor**
	José Francisco Marco Sanz	**Associate Professor**
	Margarita Menéndez Fernández	**Associate Professor**
	Juliana Sanz Aparicio	**Associate Professor**
	Maria Dolores Solís Sánchez	**Associate Professor**
	Juan Z. Dávalos Prado	**Assistant Professor**
	Clara Gómez Hernández	**Assistant Professor**
	Eva González Noya	**Assistant Professor**
	Lourdes Infantes San Mateo	**Assistant Professor**
	Rosa Lebrón Aguilar	**Assistant Professor**
	Maria Pilar Lillo Villalobos	**Assistant Professor**
	José Miguel Mancheño Gómez	**Assistant Professor**
	Rebeca de Nalda Mínguez	**Assistant Professor**
	José Maria Oliva Enrich	**Assistant Professor**
	José Manuel Pérez Cañadillas	**Assistant Professor**
	José Emilio Prieto de Castro	**Assistant Professor**
	Maria José Sánchez Barrena	**Assistant professor since 16/07/2020**
	Carlos Alberto Cuevas Rodríguez	**Investigador Distinguido**
	Francisco Javier Oroz Garde	**Ramón y Cajal Contract**
	Esther Rebollar González	**Ramón y Cajal Contract, until 31/05/2019**
	J. Inmaculada Pérez Dorado	**Programa de Atracción de Talento-CAM, since 01/09/2020**
	José M. Martín García	**Programa de Atracción de Talento-CAM, since 01/09/2020**

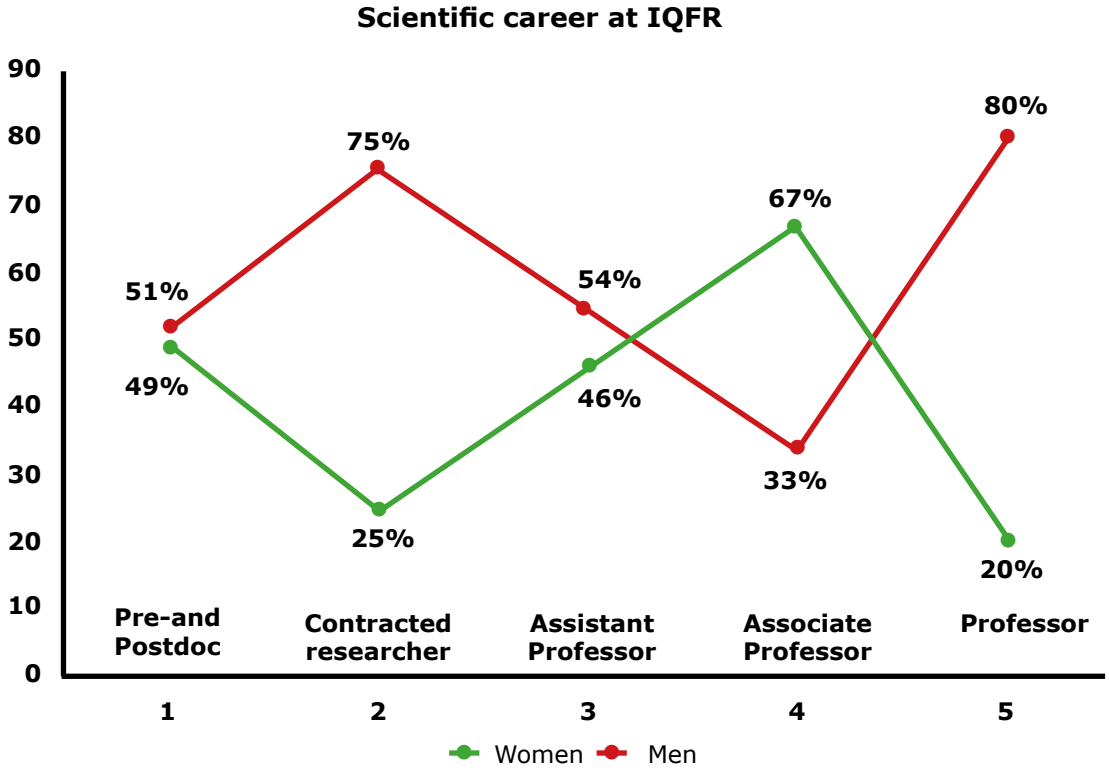
Board of Institute

President:	**Carlos González Ibáñez**	
Secretary:	**Marta María Granja Perdices**	
Members:	**Beatriz González Pérez**	
	Rebeca de Nalda Mínguez	
	Armando Albert de la Cruz	(Head of Department of Crystallography and Structural Biology)
	Alfonso Sáiz López	(Head of Department of Atmospheric Chemistry and Climate)
	M. Ángeles Jimenez	(Head of Department of Biological Physical Chemistry)
	Marta Castillejo Striano	(Head of Department of Low Dimensional Systems, Surfaces and condensed Matter, until 22/06/2020)
	Eva González Noya	Head of Department of Low Dimensional Systems, Surfaces and condensed Matter, (since 23/06/2020)
	Plácido Galindo Iranzo	(Personnel Representative)
	Carolina García Rodriguez	(Personnel Representative)
	Mohamed Oujja Ayoubi	(Personnel Representative, since 04/06/2019)
	Jesús López Mascaraque	(Personnel Representative, since 04/06/2019)

Gender distribution of scientific staff according to professional category

At IQFR there is a Gender Equality Commission which was constituted by agreement of the Board in 2020. They have performed an analysis of the gender distribution at IQFR and the data are as follows:





There are a total of 35 researchers divided into 50% men and 50% women. The staff in the rest of professional categories (pre-and postdoctoral, technical staff, management and general services) overall also presents the same parity.

At present the commission is formed by:

Supervision: Inmaculada Garcia-Moreno Gonzalo

Coordination: Eva González Noya

Members: Javier Oroz, Irene Gómez Pinto, Manuel Perez, Miguel Daniel and Cristina Cabrero

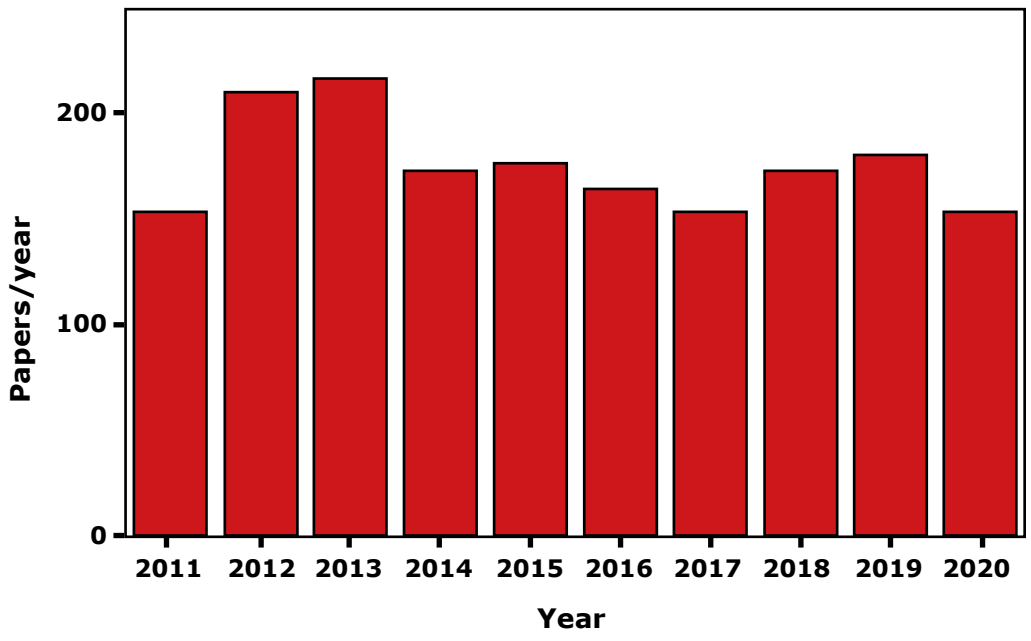
Summary of scientific output

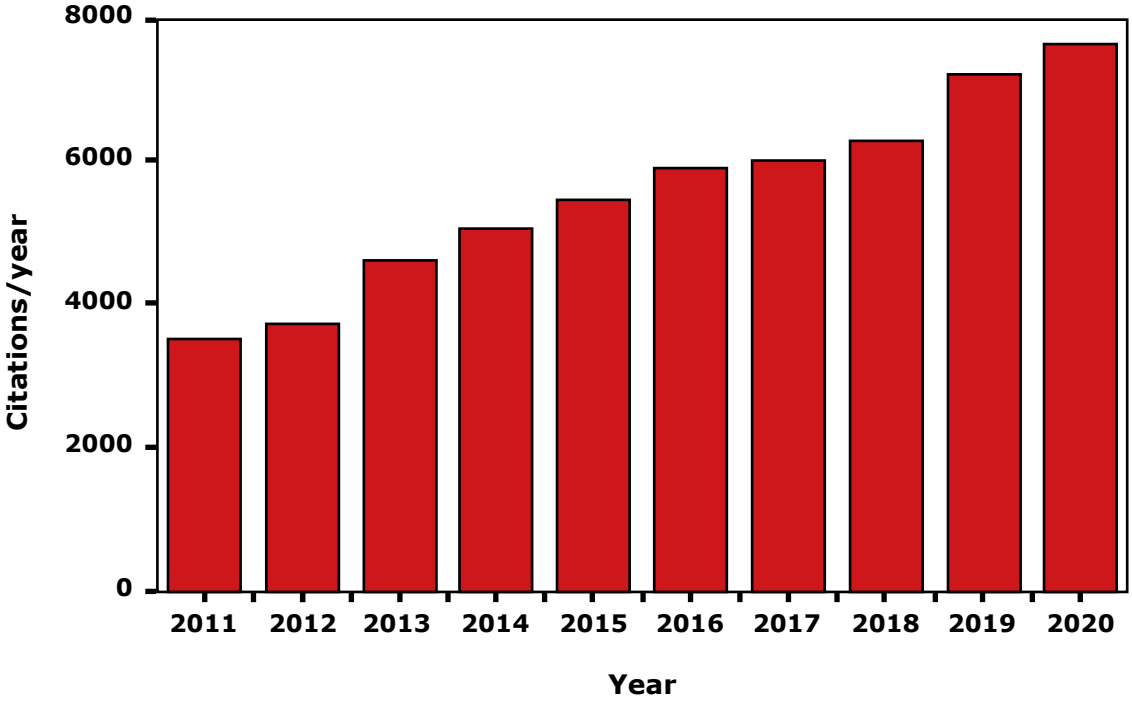
2019-2020	
Total number of publications in Web of Knowledge (WoK):	335
Total number of citations:	2015
Average citations/publication:	6

(06-09-2021)

Data since the foundation of IQFR in 1946	
Total number of publications in WoK:	4791
Total number of citations:	98472
Average citations/publication:	20.6
h-index:	105

(06-09-2021)




8000
6000
4000
2000
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Citations/year
2011
2012
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2015
2016
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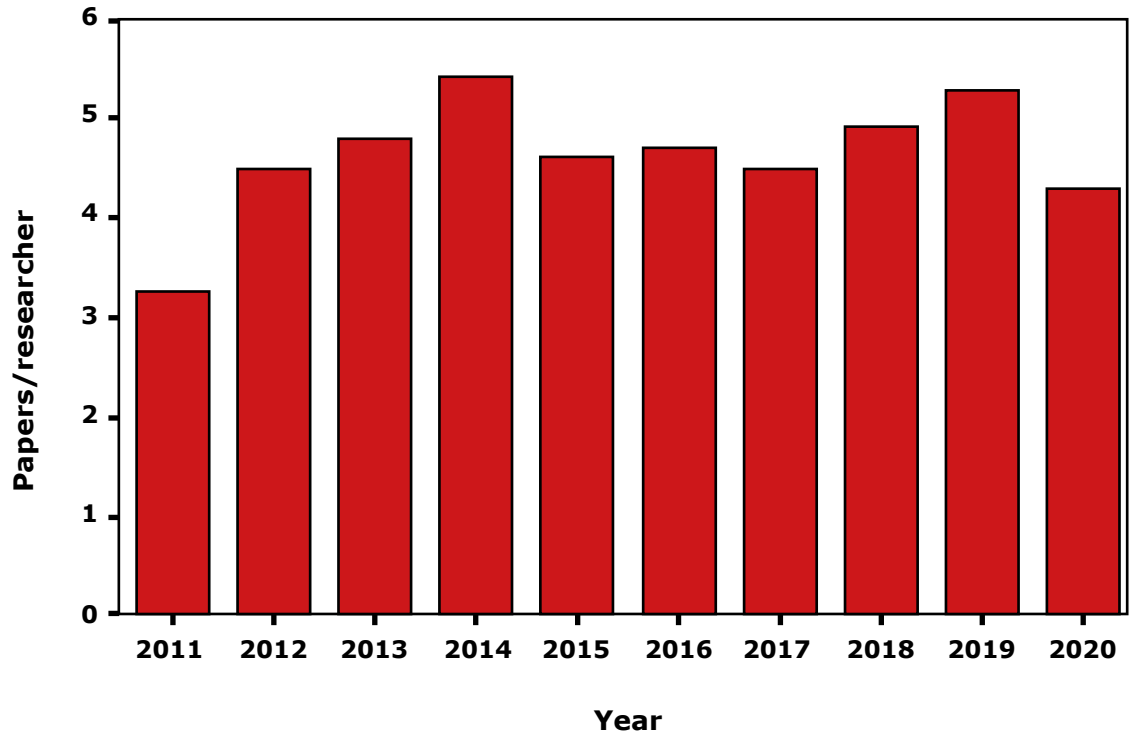
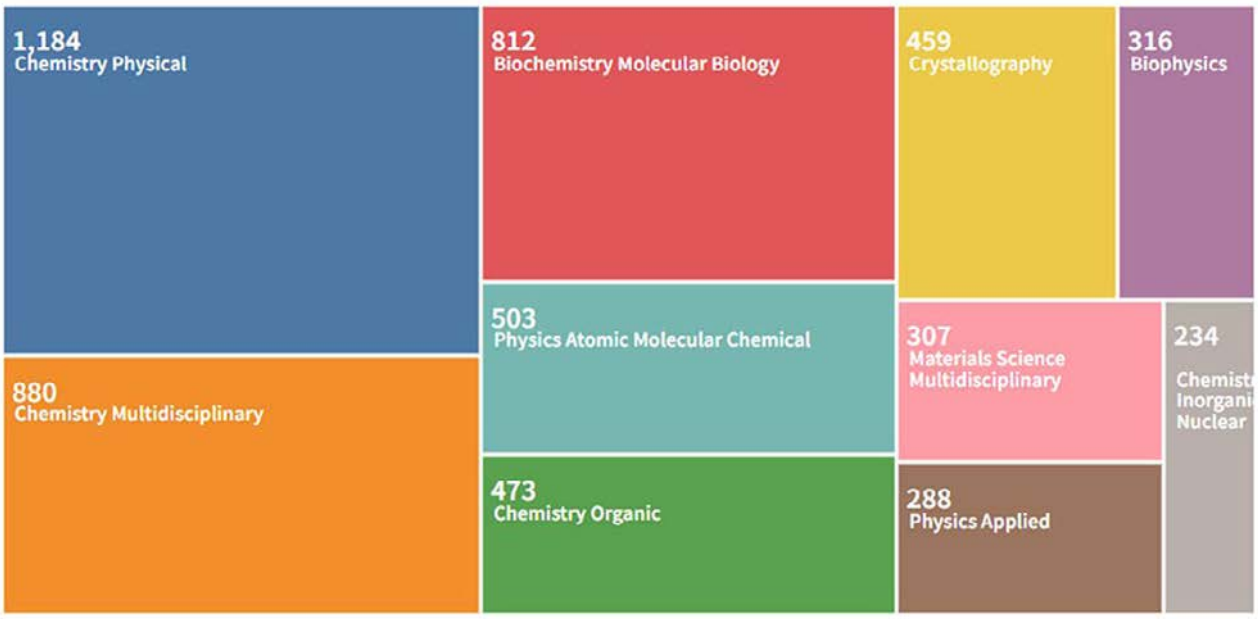
2018
2019
2020
Year


6
5
4
3
2
1
0
Papers/researcher
2011
2012
2013
2014
2015
2016
2017
2018
2019
2020
Year

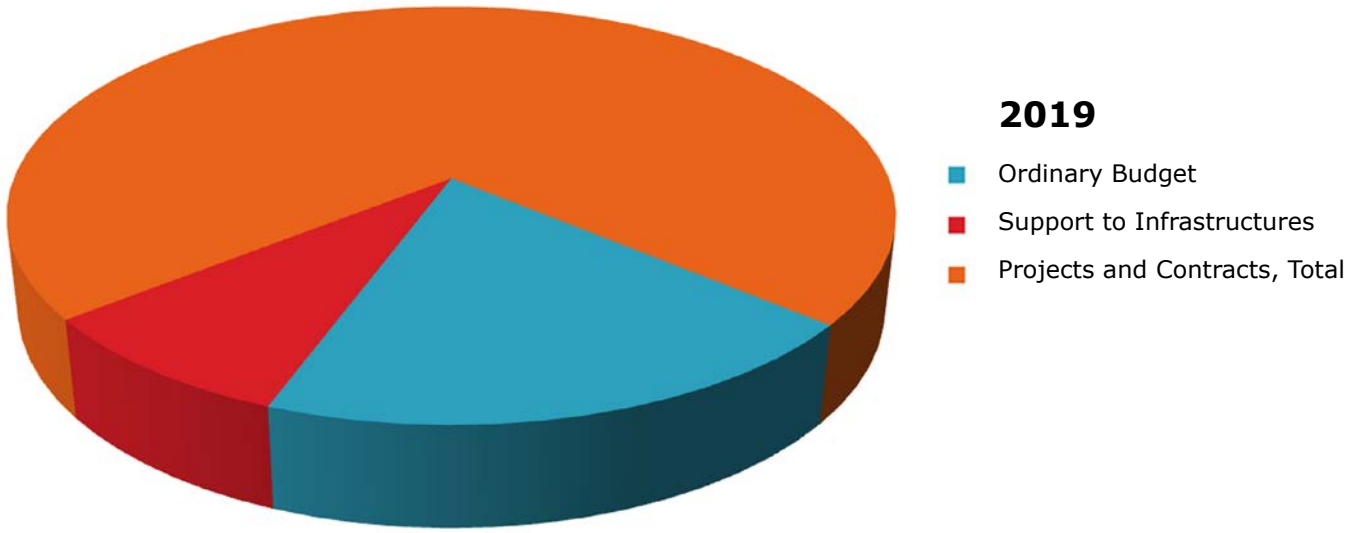
Areas distribution 2019-2020

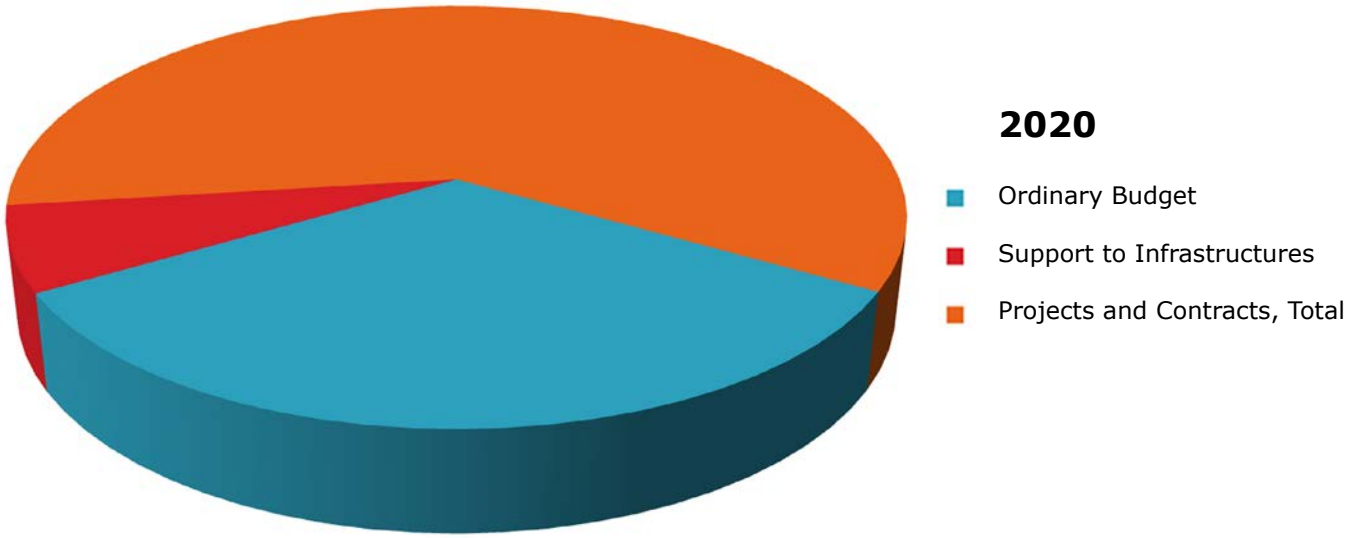
Since the foundation of IQFR in 1946



Summary of economic data

Concept	2019	2020
Ordinary Budget	523.148,61	1.337.506,32
Support to Infrastructures	231.637,04	262.006,21
Projects and Contracts, Total	1.920.183,39	2.428.989,29
Total	**2.676.988,04**	**4.030.521,82**






CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFICAS

Outreach

IQFR seminar series

During 2019-2020, 17 leading scientist from different fields of Science participated in the IQFR seminar series, which were organized by Esther Rebollar, and José Miguel Mancheño.

Speaker	Title	Date
Jordi García Ojalvo	Self-organization of bacterial biofilms	06/02/2019
Ugo Bastolla	Structural and dynamical constraints on the evolution of proteins	27/02/2019
Daniel Jaque	Nanotermómetros luminiscentes: Nuevos elementos de diagnosis en biomedicina	06/03/2019
Mauricio García Mateu	Los virus entre la Física, la Química y la Biología: autoensamblaje y propiedades mecánica	13/03/2019
José Cernicharo	El medio interestelar y circunestelar: Un laboratorio de química-física fundamental	20/03/2019
Ignacio Solá	Quantum all the way up	03/04/2019
Andrés Castellanos-Gómez	Strain engineering in 2D materials: towards strain tunable optoelectronic devices	23/04/2019
Fernando Moreno Herrero	Molecular Biophysics of Protein Machines	08/05/2019
Emilio Cano	Aplicaciones de la electroquímica para el estudio y conservación del patrimonio cultural metálico	16/05/2019
Rafael Delgado	Enhanced cell-binding and infectivity through DC-SIGN in the West African Ebola virus	22/05/2019
Nunilo Cremades	Protein amyloid aggregation and its role in the development of neurodegenerative disorders	06/11/2019
Fernando T. Maestre	Siguiendo los pasos de Humboldt: comprendiendo la ecología de nuestro planeta	11/12/2019

Speaker	Title	Date
Pere Roca-Cusachs	Sensing the matrix: transducing mechanical signals from integrins to the nucleus	15/01/2020
Maria Cruz Moreno-Bondi	Advances in the quest for new selective recognition elements for optical biosensors using phage display techniques	22/01/2020
Juan José García Ripoll	Métodos cuánticos y "quantum inspired" para análisis numérico	05/02/2020
Paloma Fernández Sánchez	Gracias y desgracias de los óxidos metálicos en el siglo XXI	19/02/2020
María del Puerto Morales	Magnetic Nanoreactors for Health, Environmental and Catalytic applications	04/03/2020

Conferences of the Marie Sklodowska Curie Colloquium

The Institute of Physical Chemistry "Rocasolano", together with the Institute for the Structure of Matter, the Institute of Optics "Daza de Valdés" and the Institute of Fundamental Physics promote and organize the series of conferences "Colloquium Marie Sklodowska Curie", that are directed to the general audience and are presented by leading personalities from the fields of Science and Culture. The IQFR representatives at the organizing committee are José Miguel Mancheño and Rebeca de Nalda.

Speaker	Title	Date
Jon Marangos	Ultrafast X-ray Science: Measuring the very fast and the very small	19/02/2019
María García Parajo	New eyes to the nano-world of living cells	14/06/2019
Mariano Barbacid	Las nuevas terapias oncológicas del siglo XXI. Medicina de precision e inmunoterapia	11/10/2019
Pilar Goya	La tabla periódica de los elementos químicos: otra mirada	17/12/2019
José María Bermúdez de Castro	Claves de la evolución Humana	14/02/2020

Science Week

The Institute organizes the activity "Science at the Library". This initiative allows the wide audience to visit the Rocasolano Library, a historical place at CSIC, and also know about the research it is conducted in the Institute. A workshop on laser cleaning is also organized. Finally, there are two open doors days and visits to the different laboratories are organized.

These activities were coordinated by Rebeca de Nalda.

Science at the Library 2019

Speaker	Title	Date
Armando Albert	¿Qué dicen las proteínas sobre los transgénicos y los compuestos agroquímicos?	04/11/2019
Carlos González Ibañez	La estructura del ADN: El poder de la hélice	11/11/2019
Juan de la Figuera	Haciendo películas con electrones	12/11/2019
Science at the Library 2020		
Douglas Vinson Laurents	Proteínas desordenadas en la patología molecular del SARS-Cov-2	05/11/2020
Armando Albert	Medicinas para las plantas. Nuevas estrategias en la mejora de cultivos frente al cambio climático	10/11/2020
Carlos González Ibañez	La estructura del ADN: El poder de la hélice	11/11/2020
Juan de la Figuera	Haciendo películas con electrones	12/11/2020

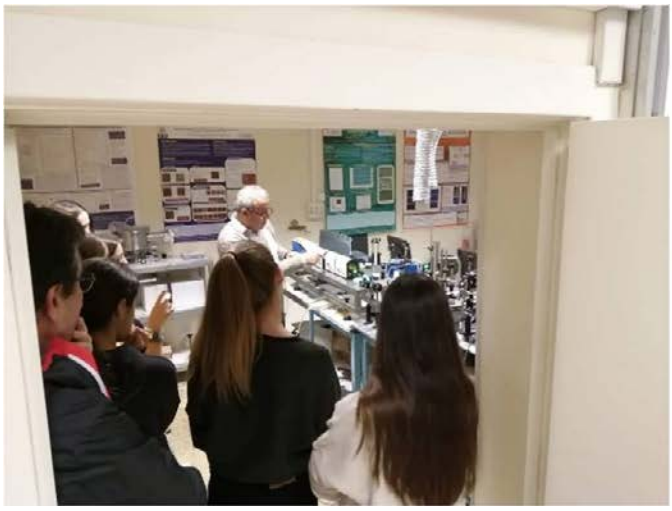
Laser Cleaning Workshop 2019

This activity was organized and coordinated by Mohamed Oujja. The workshop consisted in:

Talk about "¿Qué es investigar?" by Esther Rebollar

Talk about "Introducción al laser y aplicaciones en limpieza de materiales" by Mohamed Oujja.

Guided visit to the laser laboratories and demonstration of laser cleaning by Mohamed Oujja and Mikel Sanz.



Open Day 2019

Laboratories	Researcher	Activity	Visitors	Degree
Biological Physical Chemistry, Crystallography and Structural Biology (13/11/2019)	Carlos González Ibañez	Talk "Espectroscopía de Resonancia Magnética Nuclear: la Mata Hari de las moléculas"	Fundación Colegio Bérriz, Las Rozas, Colegio Sámer Calasanz, Valdemoro	1º, 2º Bachillerato
	Javier Oroz/ Douglas Laurents	Divulgation talk with participative experiment "La magia de las proteínas (y cómo entenderla)"		
	Iván Acebrón	Talk "Cristalografía: la vida a escala atómica"		
	M. Asunción Campanero Rhodes	Guided visit and divulgation talk at Microarrays Facility		
	David Pantoja Uceda	Guided visit to LMR lab		
	Julia Sanz/ Armando Albert/ José Miguel Mancheño	Guided visit to the Crystallography and Structural Biology labs		
Lasers, Surfaces, Nanomaterials and Chromatography (12/11/2019)	Esther Rebollar	Short talk about "Ciencia en el Rocasolano"	IES Francisco Giner de los Ríos, Alcobendas	2º Bachillerato
	José Emilio Prieto	Talk about "Nanociencia y ciencia de superficies"		
	Nuria Benavent Oltra, David García Nieto	Short talk about MAX-DOAS measurements and instruments and guided visit to atmospheric chemistry and climate lab		
	Rosa Lebrón Aguilar, Jesús Eduardo Quintanilla López	Short talk about Gas Chromatography and guided visit to the Chromatography lab		
	Mohamed Oujja Ayoubi/ Mikel Sanz	Guided visit to laser labs, experiments of optics, and demonstration of laser cleaning and laser processing of materials		
	José Emilio Prieto/ Guiomar Delgado/ María Sánchez	Guided visit to the Surface Analysis and Mössbauer Spectroscopy Group		

Young IQFR Researchers Simposium

An internal symposium dedicated to young researchers was organised in 2019.

Speaker	Title
María Ángeles Márquez Moñino	Purification and crystallization of an inositol polyphosphate phosphatase
Israel Serrano	Explorando nuevos motivos estructurales de ADN: la interfase i-motif/duplex
Sandra Salillas	Alternative treatments for *Helicobacter pylori* infection in an era of an increasing antibiotic resistance
Gustavo Titaux	Biosíntesis y caracterización estructural por RMN de Magi3, una toxina de araña rica en enlaces disulfuro
Fernando Iglesias-Suarez	Halogen-driven ozone response to El Nino-Southern Oscillation
Qinyi Li	Impact of halogen chemistry on surface ozone in Europe and China
Alba Badia	Future tropospheric O3 budget and its drivers under changes in climate and emissions
Marta Murillo Sánchez	Dinámica de predisociación en tiempo real del yoduro de etilo en la banda B
Julio R. Barrios	Propiedades Estructurales y Energéticas de Antioxidantes Fenólicos
Cintia Pulido Lamas	Fluid-solid direct coexistence simulations to determine a binary phase diagram

Programa 4º ESO + Empresa

This CSIC activity focuses in bridging academia with the professional world and is directed to students with the aim of helping them in their future academic and professional decisions. In 2019, the institute welcomed 9 students from: IES Ramiro de Maeztu (2), Colegio Nuestra Señora de la Merced (1), Colegio Gamo Diana (2), C.C. Villa de Navalcarnero (1), IES Margarita Salas (1), Colegio Montserrat (1), IES José Saramago (1).

This activity was coordinated by Beatriz González and the following IQFR researchers participated:

José Manuel Pérez Cañadillas

Juan de la Figuera

José Miguel Mancheño

Armando Albert

Lourdes Infantes

Beatriz González

International Day of Women and Girls in Science

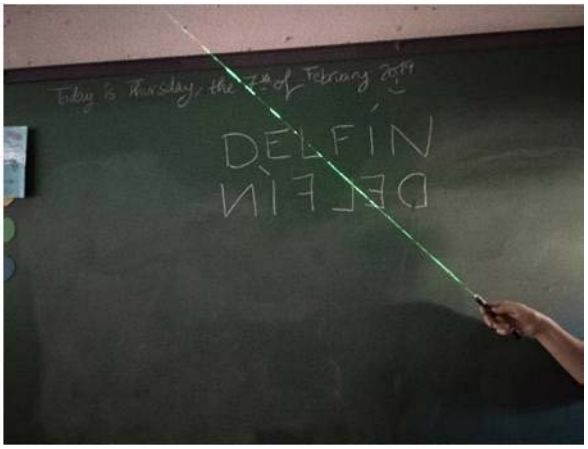
In 2019 and 2020, researchers from IQFR have participated in activities organized on the occasion of February 11th, the International Day of Women and Girls in Science. The objective of these activities is to make visible the role of women in science and promote that scientific research is one of the aspirations of our children, regardless of their gender. In particular, researchers have organized and participated in several workshops, talks and presentations at schools.

- **Charla "Una divertida excursión con la ciencia" y taller "Bienvenid@s al mundo atómico"**
  Lourdes Infantes y Beatriz González
  Alumnos 4º Primaria del CEIP Ramiro de Maeztu, Madrid, 5,6 y 7 de febrero
- **Taller científico "Jugamos con la luz"**
  Rebeca de Nalda y Esther Rebollar
  Alumnos 3º de Primaria del CEIP Ramiro de Maeztu, Madrid, 5, 6 y 7 de febrero
- **Taller científico "Química para los más pequeños"**
  María José Sánchez Barrena
  Alumnos 1º de Educación Infantil del Colegio Ángel León, Colmenar Viejo, 8 de febrero
- **Charla "Experiencia investigadora en el Ártico"**
  Nuria Benavent
  Alumnos 3º de Educación Infantil y Primaria del CP Rafael Altamira, Quatretonda (València), 8 de febrero
- **Charla "Experiencias de científicos en los polos"**
  Nuria Benavent
  Alumnos 3º y 4º de Primaria del CP Beata Inés, Benigànim (València), 11 de febrero
- **Taller científico "Ciencia en el aula"**
  Irene Gómez Pinto y Paula Morales
  Alumnos 2º de Primaria del CEIP Ramiro de Maeztu, Madrid, 11 de febrero
- **Charla "Un viaje al micromundo con la ciencia"**
  Lourdes Infantes y Beatriz González
  Alumnos 1º y 2º de ESO, Colegio San Ramón y San Antonio, Madrid, 13 de febrero
- **Charla "La luz como herramienta"**
  Esther Rebollar
  Alumnos 2º de Bachillerato, Centro Cultural Elfo Nuestra Señora de Fátima, Madrid, 15 de febrero

- **Presentación "Grandes mujeres científicas en la historia: Rosalind Franklin" y "Las mujeres científicas de hoy"**
  Irene Gómez (IQFR) y Sagrario Martínez (IEM)
  Alumnos 4º ESO IES Satafi, Getafe, 20 de enero
- **Taller científico "Taller de Cristalización. Recordando a Rosalind Franklin y Dorothy Crawford Hodgkin"**
  María José Sánchez
  Alumnos 1º y 6º primaria CPB Ángel León. Colmenar Viejo, Madrid, 7 de febrero.
- **Taller "Ciencia y Cocina con Nitrógeno Líquido"**
  Lourdes Infantes
  Alumnos 1º ESO IES Manuel Elkin Patarroyo de Parla, Madrid, 10 de Febrero.
- **Presentación "Grandes mujeres científicas en la historia: Rita Levi-Montalcini, Rosalind Franklin, Madame Lavoisier, Mildred Dresselhaus" y "Las mujeres científicas de hoy y en tu barrio"; Debate: "¿Qué dicen las encuestas sobre las carreras que escogen chicos y chicas? ¿Te atreves a ser científica?"**
  Irene Gómez (IQFR), Marta Hernández (IFF), Aixa Morales (I. Cajal), Sagrario Martínez y Aurora Nogales (IEM)
  Alumnos 2º y 3º ESO IES Ramiro de Maeztu, Madrid, 11 de febrero
- **Taller científico "La magia del agua"**
  María Asunción Campanero
  Alumnos 2º de Infantil y 2º Primaria CEIP Pinar de San José, Madrid, 11, 12 y 13 de febrero.
- **Charla "Una divertida excursión con la ciencia" y taller "Bienvenid@s al mundo atómico"**
  Lourdes Infantes y Beatriz González
  Alumnos 4º Primaria CEIP Ramiro de Maeztu, Madrid, 3, 4 y 5 de marzo.
- **Taller científico "Jugamos con la luz"**
  Rebeca de Nalda y Esther Rebollar
  Alumnos 3º Primaria CEIP Ramiro de Maeztu, Madrid, 3, 5 y 6 de marzo.
- **Inauguración de la biblioteca Dorotea Barnés: un homenaje a las científicas pioneras en la Colina de los Chopos**
  Proyección del documental "Las mujeres de la herencia del 98: la primera oportunidad" e intervenciones de Carmen Sarasúa y Carmen Magallón.
  Salón de Actos del IQFR-CSIC, 11 de marzo

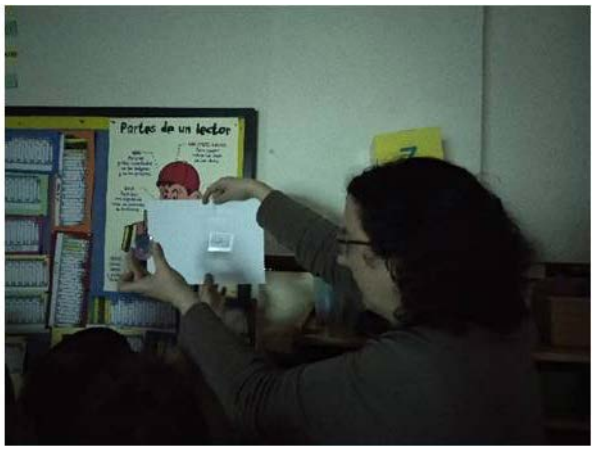
11F 2019

Researcher	Title	Type of activity
Lourdes Infantes/ Beatriz González	Un viaje al micromundo con la ciencia	Talk in Colegio San Ramón y San Antonio for high School students
Lourdes Infantes/ Beatriz González	Una divertida excursión con la ciencia	Talk in Colegio Ramiro de Maeztu for primary strudents
María José Sánchez Barrena	Taller de Química para alumnos de 1º y 4º de Primaria	Talk in C.E.I.P. Ángel León, Colmenar Viejo
María José Sánchez Barrena	Cristalografía: los ojos de la Química para el desarrollo de aplicaciones en biomedicina y biotecnología	Talk in Colegio de Secundaria "Ruta de la Plata", Almendralejo
Rebeca de Nalda and Esther Rebollar	Jugamos con la luz	Scientific workshop for 3rd year Primary school students in the CEIP Ramiro de Maeztu
Esther Rebollar	La luz como herramienta	Talk for 2nd Bachillerato students at the Centro Cultural Elfo Nuestra Señora de Fátima



11F 2020

Researcher	Title	Type of activity
Lourdes Infantes/ Beatriz González	Una divertida excursión con la ciencia	Talk in Colegio Ramiro de Maeztu for primary strudents
Lourdes Infantes	Ciencia y cocina con nitrógeno líquido	Talk in I.E.S. Patarroyo-Parla
Lourdes Infantes/ Beatriz González	Un viaje al micromundo con la ciencia	Talk in I.E.S. Gredos San Diego
María José Sánchez Barrena	Taller de Cristalografía	Talk in C.E.I.P. Ángel León, Colmenar Viejo
M. Asunción Campanero Rhodes	Themagic of water	Workshop for pre-school and primary school students, CEIP Pinar de San José, Madrid
Rebeca de Nalda and Esther Rebollar	Jugamos con la luz	Scientific workshop for 3rd year Primary school students



Festival of Nanoscience and Nanotechnology

The IQFR participated in the 4th and 5th editions of the festival, which were held in 2019 and 2020, respectively. The purpose of this initiative, co-organized by several institutions at the national level, was to disseminate the impact of nanoscience and nanotechnology in our lives. The activities organized at IQFR included visits to the laboratories and several talks at secondary schools.

These activities were coordinated by Dr. Rebeca de la Nalda.

Actividades IQFR

Nanoinmersión en el Rocasolano: 2 de abril de 2019 de 10 a 14 h. Para estudiantes de Enseñanza Secundaria o Bachillerato. Necesaria reserva.

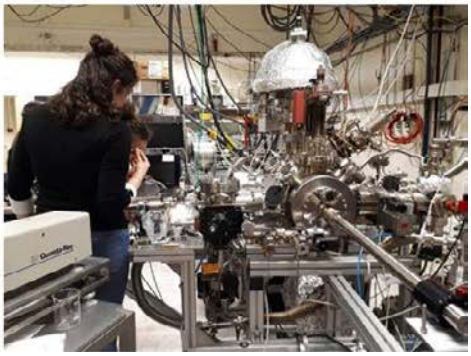
Conferencias en centros educativos:

Centro Cultural Elfo-Nuestra Señora de Fátima: Esther Rebollar
Colegio Concertado Retiro: Eva González Noya
Colegio Nuestra Señora del Buen Consejo: Eva González Noya
Colegio Nuestra Señora del Pilar Fundación Trilema: José Emilio Prieto
IES Cardenal Cisneros: Mikel Sanz
IES Ciudad de Jaén: José Emilio Prieto
IES Don Pelayo: María Sánchez Arenillas
IES Gregorio Peces Barba: Rebeca de Nalda
IES Las Musas: Esther Rebollar
IES Lope de Vega: Juan de la Figuera
IES María de Molina: Enrique Lomba
IES Pacífico: Juan de la Figuera
IES Palomeras-Vallecas: Mohamed Oujja
IES Rey Pastor: Enrique Lomba
IES San Mateo: Mikel Sanz
IES Santa Teresa de Jesús: María Sánchez Arenillas

Más información en:
https://www.iqfr.csic.es/es/info/publico-en-general/nanofestival-2019

Nanofestival 2019

Researcher	Title	Type of activity
Mohamed Oujja Ayoubi	Nanotecnología	Talk about Nanotechnology and its use and effects in our daily life at IES Palomeras-Vallecas
Esther Rebollar	Nanociencia y nanotecnología: Una visión general	Talk about Nanotechnology and its use and effects in our daily life at Centro Cultural Elfo-Nuestra Señora de Fátima
Rebeca de Nalda	Nanoscience and nanotechnology	Nanoscience and nanotechnology talk for Secondary school students in IES Gregorio Peces Barba.
Eva González Noya	Nanotecnología	Talk about Nanotechnology at Colegio Concertado Retiro
Eva González Noya	Nanotecnología	Talk about Nanotechnology at Colegio Nuestra Señora del Buen Consejo
José Emilio Prieto	Introduccción a la Nanociencia	Talk at Colegio Nuestra Señora del Pilar
José Emilio Prieto	Introducción a la Nanociencia	Talk at IES Ciudad de Jaén
Juan de la Figuera	Introducción a la Nanociencia	Talk at IES Lope de Vega
Mikel Sanz	La nanociencia llega al instituto	Talk at IES Cardenal Cisneros
Mikel Sanz	La nanociencia llega al instituto	Talk at IES San Mateo
Esther Rebollar	Jornadas de puertas abiertas "Nanoinmersión en el Rocasolano" IES José Luis Sampredro, Tres Cantos (2º Bachillerato)	Talk: "Introducción a la Nanociencia"
José Emilio Prieto		Talk: "Haciendo películas con electrones"
Enrique Lomba		Talk: "Diseño asistido por ordenador en Nanotecnología"
Mohamed Oujja Ayoubi/ Mikel Sanz		Guided visit to laser labs, experiments of optics, and demonstration of laser processing of materials
José Emilio Prieto/ José F. Marco/ Guiomar Delgado/María Sánchez Arenillas		Guided visit to the Laboratory of Low Energy Electron Microscopy



Nanofestival 2020

Researcher	Title	Type of activity
Eva González Noya	Nanotecnología	Talk at Colegio público Blas de Otero
José Emilio Prieto	Introducción a la (nano)ciencia	Talk at IES Joaquín Rodrigo
Juan de la Figuera	Introducción a la nanociencia	Talk at IES Santa Francisca Javier Cabrini

Cuenta la ciencia

Cuenta la Ciencia is a program funded by Fundación General CSIC whose objective is to transfer the research carried out at CSIC to society through the realization of activities aimed at promoting scientific, technological and innovation culture.

In 2020, the project 1er RAP conCIENCIA leaded by Lourdes Infantes and Beatriz González was funded. The objective of this project is to bring the scientific world closer to students through RAP.

https://youtu.be/dSc8RJaf0E4

Catalogue of CSIC Scientific Conferences

Since 2015 the Institutional Delegation of the CSIC in the Community of Madrid publishes the "Catalogue of CSIC Scientific Conferences aimed at the Educational System of the Community of Madrid". These conferences are offered by researchers that carry out their activity in the different centers and institutes of CSIC located in the Community of Madrid. The catalogue is distributed in various entities related to the Educational System of the Community of Madrid and in 2019 and 2020 researchers from Rocasolano gave the conferences listed below.

2019

Researcher	Title	Place
Lourdes Infantes/ Beatriz González	Lo que nos dice la forma 3D de las moléculas	Colegio Alpajés for high School students
Lourdes Infantes	Ciencia y cocina con nitrógeno líquido	I.E.S. Joaquín Rodrigo
Lourdes Infantes	Ciencia y cocina con nitrógeno líquido	I.E.S. Lope de Vega
Lourdes Infantes	Ciencia y cocina con nitrógeno líquido	I.E.S. La Serna
Lourdes Infantes/ Beatriz González	Un viaje al micromundo con la ciencia	I.E.S. Isaac Albéniz
Lourdes Infantes/ Beatriz González	Ciencia y cocina con nitrógeno líquido	I.E.S. Santa Teresa de Jesús
Lourdes Infantes	Ciencia y cocina con nitrógeno líquido	I.E.S. Herrera Oria
Lourdes Infantes	Ciencia y cocina con nitrógeno líquido	Colegio Virgen del Remedio

2020

Researcher	Title	Place
Lourdes Infantes/ Beatriz González	Ciencia y cocina con nitrógeno líquido	I.E.S. Santa Teresa de Jesús
Lourdes Infantes	Ciencia y cocina con nitrógeno líquido	I.E.S. Herrera Oria
Lourdes Infantes	Ciencia y cocina con nitrógeno líquido	Colegio Virgen del Remedio

Left "Un viaje al micromundo con la ciencia" I.E.S. Isaac Albéniz. Right "Ciencia y cocina con nitrógeno líquido" I.E.S. Santa Teresa de Jesús

Other activities

Researcher	Activity	Title	Date	Description
Rebeca de Nalda	Ciencia en Primera Persona, MUNCYT	Pulsos de luz que congelan el tiempo	13/01/2019	General audience talk in the National Museum of Science and Technology
Douglas Laurents	Divulgation talk	Los amiloides y su papel en enfermedades neurodegenerativas	17/01/2019	Divulgation talk in "Ciclos formativos de la familia de profesiones de sanidad"
David Pantoja-Uceda	Visit	Guided visit to LMR lab	15/02/-2019	Guided visit of secondary students (2º Bachillerato), IES Rusiñol (Toledo)
Juan de la Figuera	Scientific Seminar	Growth and Magnetism of iron oxides	12/03/2019	Scientific Seminar organized by Universidad Católica Pontificia de Chile, open to all the Academic Community
Juan de la Figuera	Scientific Seminar	Tweaking magnetic anisotropy beyond the monolayer limit: low energy electron microscopy studies on spin-reorientation transitions on Cu/Ru	29/03/2019	Scientific Seminar organized by CEDENNA, Universidad de Santiago de Chile, open to all the Academic Community
David Pantoja-Uceda	Visit	Guided visit to LMR lab	09/04/2019	Guided visit of Prevention and Laboral Health Service of CSIC
Mikel Sanz Monasterio	Paseo científico por Toledo dentro del Programa Entre Lunas 2019	El uso de los láseres en la conservación del patrimonio	04/2019	Divulgation talk about the use of lasers in Cultural Heritage
M.A. Campanero Rhodes	Scientific workshop	Themagic of water	29-31/05/ 2019	Workshop for pre-school students, CEIP Ramiro de Maeztu, Madrid
David Pantoja-Uceda	Video recording	Making of CSIC corporative video in NMR lab	30/05/2019	Making of CSIC corporative video in NMR lab
José F. Marco	Scientific Seminar	Espectroscopía de absorción de Rayos X: XANES y EXAFS: Principios básicos y aplicaciones en Ciencia de Materiales	01/07/2019	Scientific Seminar organized by CEDENNA, Universidad de Santiago de Chile, open to all the Academic Community
Mikel Sanz Monasterio	Noche del Patrimonio en Toledo	Edificios de luz: láseres y patrimonio	09/2019	Divulgation talk about the use of lasers in Cultural Heritage

Researcher	Activity	Title	Date	Description
David Pantoja-Uceda	Visit	Guided visit to LMR lab	20/12/2019	Visit of Dr Mario Torrado del Rey, University of Sidney
M. Mompeán	Dissemination paper	Colaboraciones en Química: La expansión del mundo amiloide: nuevas oportunidades terapéuticas.	12/2019	Revista 100cias@ uned 12, 56-63 (https://app.uned.es/biblioteca/revista100cias.aspx) *UNED yearly Journal Con100Ciencia*
David Pantoja-Uceda	Visit	Journalist and photographer of the newspaper "EL MUNDO" @LMR	08/01/2020	Journalist and photographer of the newspaper "EL MUNDO" @LMR
David Pantoja-Uceda	Visit	Guided visit to LMR lab	05-07/02/2020	Attendants at the 17th Iberian Peptide Meeting
Douglas Laurents	Divulgation talk	"Proteínas desordenadas en la patología molecular de SARS-CoV-2"	05/11/2020	Charla de Divulgación con Experimento Participativo
C. González, D. Pantoja, I. Gómez, D. Laurents M. Mompeán	Prime Minister's visit	Visit to LMR lab	06/11/2020	Visit of D. Pedro Sánchez, Prime Minister of Spain, D. Pedro Duque, Minister of Science and Innovation and Prof. Rosa Menéndez, CSIC president
Marta Castillejo	Presentation	Plataforma Temática Interdisciplinar Patrimonio Abierto: Investigación y Sociedad (PTI-PAIS)	26-28/11/2020	AR&PA Virtual Fair, Bienal Ibérica de Patrimonio Cultural,
María José Sánchez Barrena	I Jornadas de responsabilidad social. Enfermedades poco frecuentes: Síndrome del Cromosoma X Frágil	New approaches to discover protein-protein interaction modulators for Fragile X syndrome pharmacotherapy: the case of NCS-1/Ric8a complex as a regulator of synaptic function	2020	Universidad Europea de Madrid

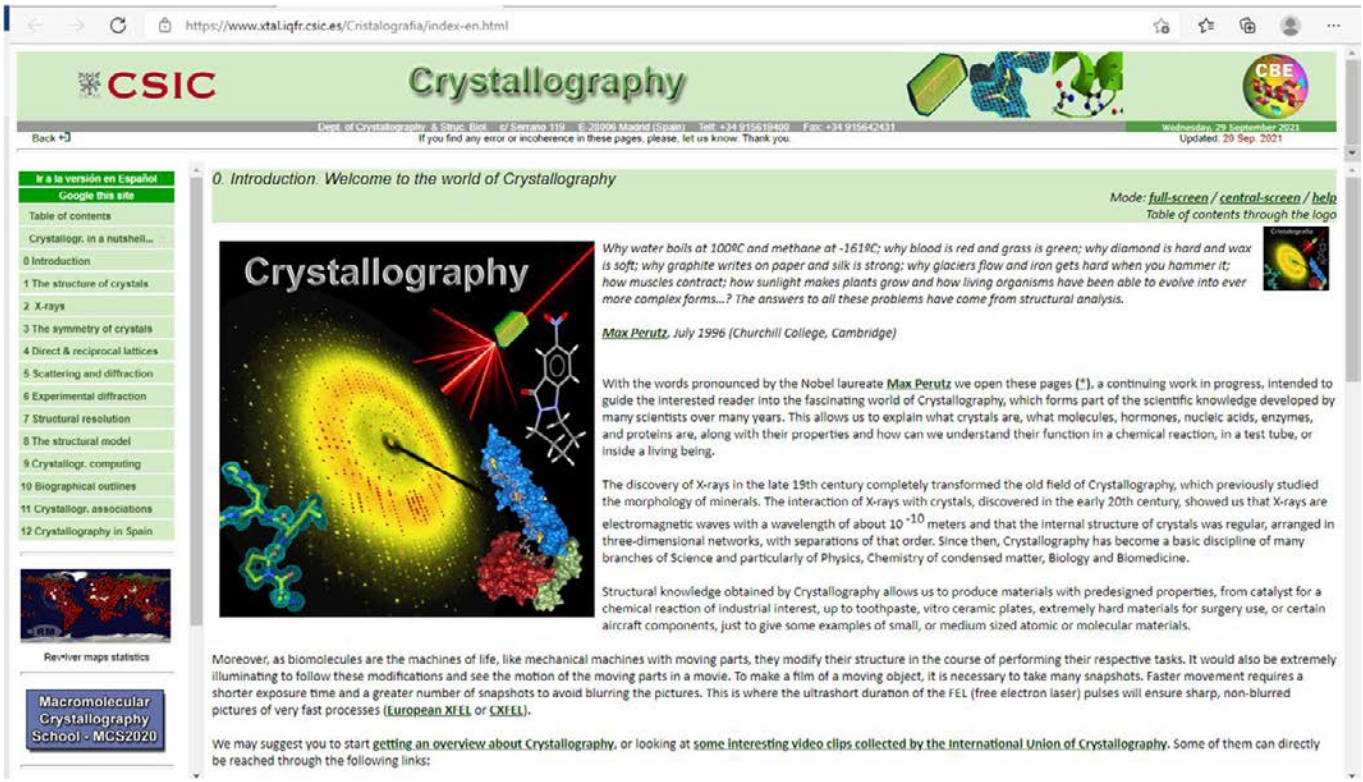

CONFERENCIA:
ESPECTROSCOPIA DE ABSORCIÓN DE RAYOS-X: XANES Y EXAFS
PRINCIPIOS BÁSICOS Y APLICACIONES EN CIENCIA DE MATERIALES.
Jose Francisco Marco Sanza. Doctor en Ciencias Físicas.
Investigador Científico de CSIC, en Instituto de Química Física Rocasolano. Madrid, España.
"En esta charla se describirán brevemente los principios físicos básicos de esta espectroscopía, se mencionarán algunos aspectos instrumentales y se comentará el modo en que se puede extraer la información de los espectros".
La espectroscopía de absorción de rayos X se ha convertido en una de las técnicas más populares y demandadas en las instalaciones de radiación sincrotrón, debido a la rica información química y estructural que entrega. Así, la estructura de un borde de absorción (XANES=X-Ray Absorption Near Edge Structure) de un elemento informa el estado de oxidación y la coordinación de ese elemento en el sólido al que pertenece. Mientras que del análisis de la estructura oscilatoria del espectro más allá del borde de absorción (EXAFS=Extended X-Ray Absorption Fine Structure) se pueden derivar parámetros estructurales como números de coordinación y distancias interatómicas. Es claro, entonces que esta técnica desempeña un papel fundamental como herramienta de caracterización en la Física y la Química del Estado Sólido y en la Ciencia de Materiales.
01 DE JULIO DE 2019 I 16:00 HRS.
Auditorio Facultad de Química y Biología / Universidad de Santiago de Chile.
CEDENNA | Centro para el Desarrollo de la Nanociencia y la Nanotecnología

Websites

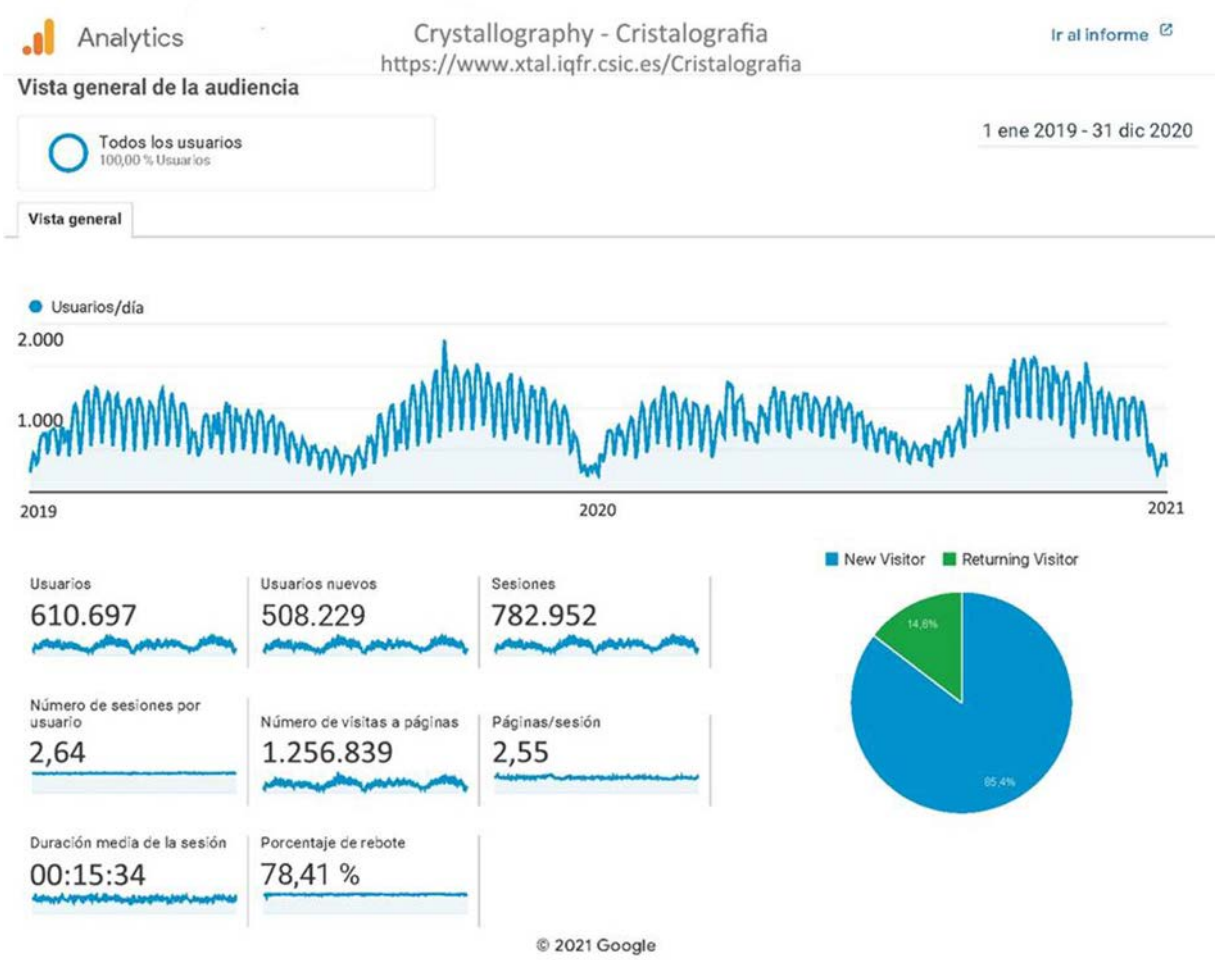
Crystallography-Cristalografía, by Martín-Martínez Ripoll

Website for learning Crystallography:

https://bit.ly/3hhuLzU



An educational website collecting over 1.200.000 visits during the period 2019-2020



Statistics about the use of the educational website for learning Crystallography (https://www.xtal.iqfr.csic.es/Cristalografia). Data extracted yearly from Google Analytics.

Social Networks

Since October 2017 all the news of the institute –publications, seminars, events, offers, awards- are published in IQFR Twitter (@iqfr_csic) and Facebook (@rocasolano.csic) sites. In 2020 Youtube channel (InstitutodeQuímicaFísicaRocasolanoIQFRCSIC) and Instagram (@iqfr_csic) sites were launched.

At the moment the IQFR Twitter account has 1097 followers, Facebook account, 293, Instagram account, 503, and Youtube channel 131 subscribers.

The social networks of the IQFR are managed by Esther Rebollar.

Additionally, other social networks from some of the IQFR groupsin this period are:

Group of Lasers, Nanostructures and Materials Processing twitter: @lanamap-iqfr (283 followers)

Group of Surface Analysis and Mössbauer Spectroscopy twitter: @surfmoss_iqfr (16 followers)

Group of NMR of Protein Structure, Dynamics and Interactions twitter: @RMNPro_IQFR (82 followers)

CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

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28006 MADRID