Institute of Physical Chemistry

ROCASOLANO

Scientific Report 2017-2018

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Rocasolano

Institute of Physical Chemistry

Spanish National Research Council

Editors: **María José Sánchez Barrena, José Emilio Prieto de Castro and Carlos Alberto Cuevas Rodríguez**

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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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Carlos González Ibáñez
Director

Rebeca de Nalda Minguez
Vice-director

Beatriz González Pérez
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

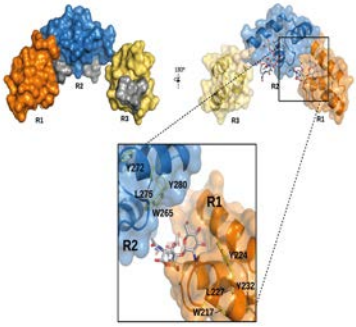
Department of Crystallography and Structural Biology

Armando Albert

Department of Atmospheric Chemistry and Climate

Alfonso Saiz López

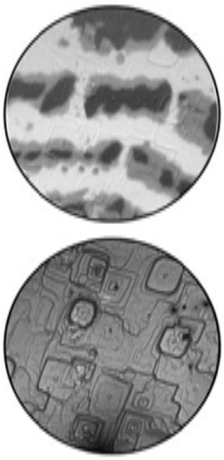
- Energetics, Structure and Molecular Reactions Group (ESMR)
- Photolysis and Chromatography
- Atmospheric Chemistry and Climate



Department of Biological Physical Chemistry

M. Ángeles Jiménez (since 21/9/2017)

- 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

Marta Castillejo

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

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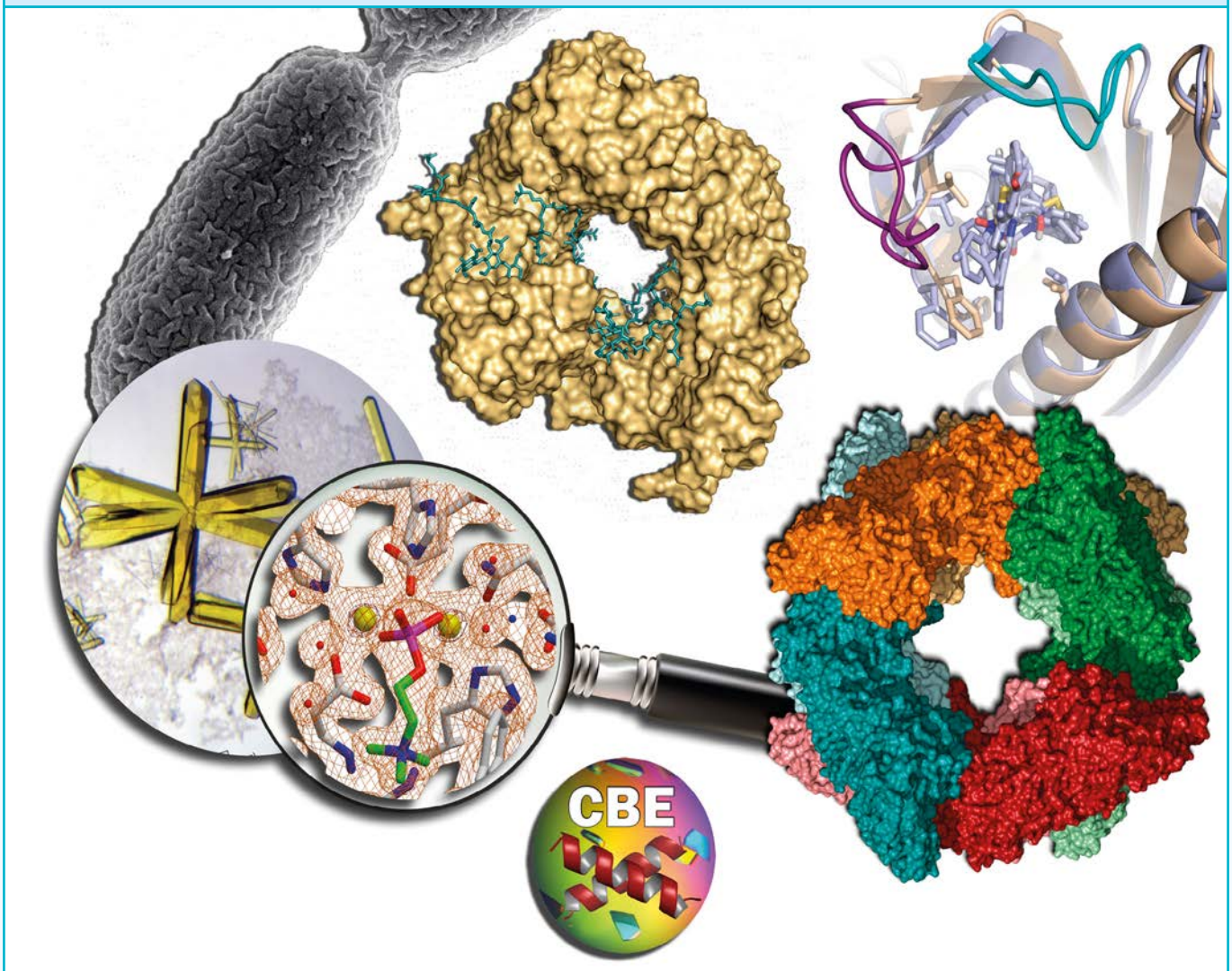
Department of Crystallography and Structural Biology



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Introduction

The members of the Department (http://www.xtal.iqfr.csic.es/) constitute the **Group of Protein crystallography and molecular recognition in biological processes** and focus their research to understand 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 proteins or large stable macromolecular complexes at atomic level. Such knowledge provides the basis for new medical treatments and many biotechnological applications. In addition, our Department is also involved in the development of novel and efficient methods and strategies for phasing structures that make possible the solution of protein structures.

The Department is equipped with the 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. The diffraction laboratory includes a new rotating anode generator equipped with two area detectors and a micro source generator for testing crystals. In addition, we have 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. All these facilities are available for all CSIC researchers and for those coming from other institutions.

Group of Protein Crystallography and Molecular Recognition in Biological Processes

Tenured Staff Scientists

Armando Albert de la Cruz
(Associate Professor) ReID ORCID SCOPUS

Beatriz González Pérez
(Assistant Professor) ReID ORCID SCOPUS

Juan Antonio Hermoso Domínguez
(Professor) ReID

Lourdes Infantes San Mateo
(Assistant Professor) ReID ORCID SCOPUS

José Miguel Mancheño Gómez
(Assistant Professor) ReID ORCID SCOPUS

Martin Martínez Ripoll
(Professor Ad Honorem) ReID ORCID

María José Sánchez-Barrena
(Ramón y Cajal) ReID SCOPUS

Julia Sanz Aparicio
(Associate Professor) ReID ORCID SCOPUS

Non-tenured Scientists

Martín Alcorlo Pages
(Hired)

Concepción Garcia Montañes
(Hired)

Siseth Martinez Caballero
(Hired)

Rafael Molina Monterrubio
(Hired)

Mercedes Ramírez Escudero
(Hired, 01/01/2017-31/10/2017)

Ivanna Rivera Espinosa
(Hired)

Doctoral Students

Mayte Batuecas Mordillo
(Fellowship)

Juan Luis Benavente Fernández
(Hired)

Alejandra Carriles Linares
(Fellowship)

Isabel Cea Rama
(Hired from 01/04/2017)

Elsa Franco Echevarría
(Hired until July 2018)

Elena Jiménez Ortega
(Hired from 15/01/2017)

María Ángeles Márquez Moñino
(Hired from January 2018)

Maria Moreno Alvero
(Hired)

Rogeria Nunes Costa
(i-COOP, COOPA20094, 05/06/2017–01/12/2017)

Laura Plaza Vinuesa
(Hired)

Technical Staff

Juana María González Rubio
(Titulado Grado Medio)

Pablo Fernández Cancelo
(Hired)

Summary

The group seeks to understand the structure, function and interactions of biologically relevant macromolecules at the atomic, molecular and supramolecular level. This provides information on specific molecular recognition events occurring in particular biological environments. The experimental approaches employed include X-ray crystallography, computational studies together with biochemical and molecular biology techniques. Such knowledge provides the basis for new medical treatments and biotechnological applications.

Our research lines frame into the priorities of the H2020:

- Health and wellbeing
  - Virulence and antibiotics resistance
  - Structural Biomedicine: Development of new drugs
  - Design of glyco- and immunosensors
- Food Security and Sustainable Agriculture
  - More efficient harvesting plants
  - Molecular mechanisms of degradation and modification of the vegetal cell-wall
  - Design of biocatalyst
- Teaching Crystallography

Strategic Aims

We intend to extend our objectives towards state-of-the-art topics and close to the demands of society. Overall, we intend to develop challenging projects in the frontier of Structural Biology (large macromolecular complexes and membrane proteins), to incorporate new techniques such as the biophysical characterization of membrane proteins and electron microscopy, and carry out a research closer to translation.

Strategic objectives:

- Structure and regulation of large macromolecular machineries involved in bacterial division, remodeling of the plant and bacterial cell-wall, ionic transport in plants and neuronal function.
- Study of the lipid-protein interaction: Structure and function of membrane proteins.
- Structural characterization of enzymatic and allosteric processes in real-time.
- *In vivo* localization of proteins and molecular machines on the cell surface.
- Assemblage of multienzyme complexes by combination of catalytic domains.
- Multienzyme cascades for second generation prebiotic production and chito-oligosaccharides from biomaterials.
- "On demand" production of bioactive compounds with high added value
- Application of magnetic nanoparticles for the detection of metastases.
- Identification of hot spots in the protein structure and development of new drugs and agrochemicals.
- Development of a tool for the prediction of the formation of multi-component crystals of pharmacological interest.

Remarkable Results

Towards the generation of new agrochemicals to improve the yield of food crops under water limited conditions

Drought is a major threat of crops. Increasing global warming conditions provokes that ordinary seasonal weather variations and other periodical atmospheric phenomena like El Niño have a major influence in crop production areas due to their impact in the decrease of rainfall and the increase of warm periods. Thus, it is required the development of strategies to improve the yield of crops under drought stress. In these situations, the phytohormone Abscisic acid (ABA) plays a central role since it controls plant water loss through the regulation of stomata pores. ABA signaling relies on the family of ABA receptors (PYR/PYL), which upon ABA binding form high-affinity ternary complexes with clade A protein phosphatases type 2C (PP2Cs) and inhibit them. Structural studies performed with *Citrus sinensis* (sweet orange) and *Solanum lycopersicum* (tomato) ABA receptors, we have led to the identification of ABA-bound intermediates that provides novel mechanistic insight on ABA signaling (Figure 1). These intermediates provide the basis for the generation of new chemical compounds agonist of ABA activity. The new synthetized agrochemicals will improve the yield of food crops in water-limited conditions. Spraying crops with the ABA mimicking molecules will exogenously turn on the ABA stress pathway if required, will not require genetic manipulation and the approach is likely to be portable among different plant species including those autochthonous varieties.

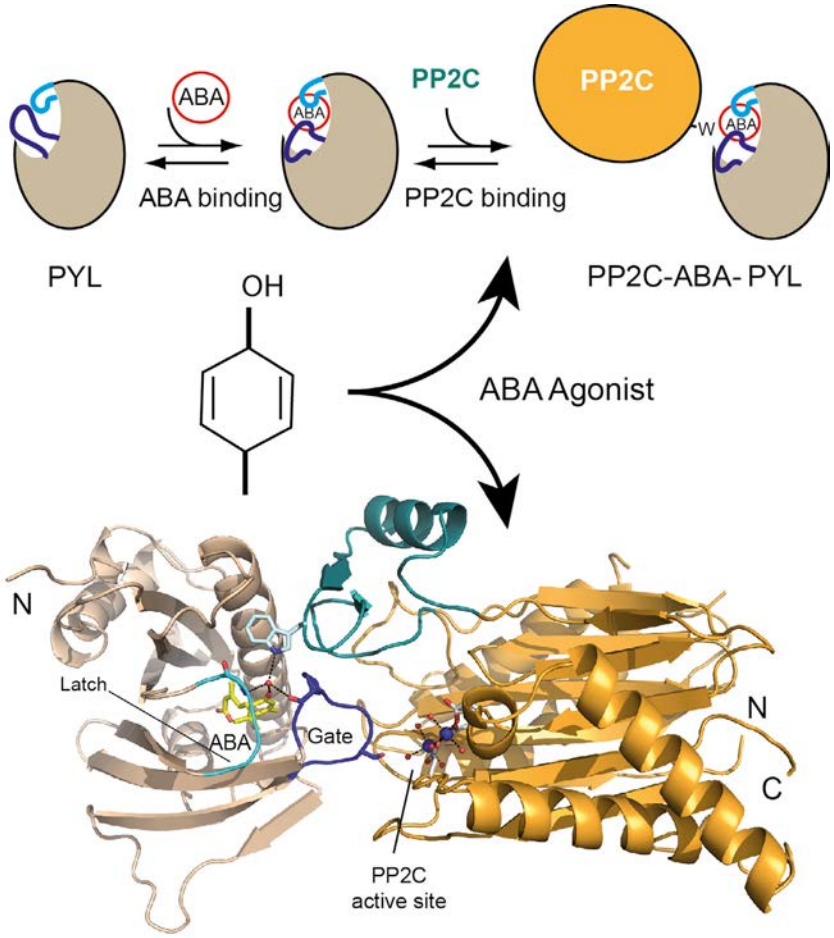

Figure 1: Schematic representation of the ABA signaling mechanism operating in plants

Synthesis of IP6 in mammal cells

Inositol hexakiphosphate (IP6) is a cofactor for proteins involved in mRNA export, DNA editing and it is an anticancer agent. We solved the structure of IP5 2-kinase, the enzyme in charge of IP6 synthesis, by X-ray Crystallography. Inositides are deeply recognized inside IP5 2-K active site. Moreover, IP5 2-K surface exhibits huge basic patches including a large loop crossing over the protein that might be important for protein-protein interactions occurring during mRNA biogenesis (Figure 2).

Non-coding RNAs transcription termination

Nrd1 forms a complex of three proteins involved in transcription termination of non-coding RNAs and specifically recognizes the terminator sequences GUAA/G as well as RNA polymerase II. We solved the crystal structure of Nrd1 RNA binding domain and its complexes with different RNAs. Two domains, a canonical RRM plus a split domain, are involved in RNA binding combining stacking, hydrogen bonds and water mediated specific interactions for GUAA recognition.

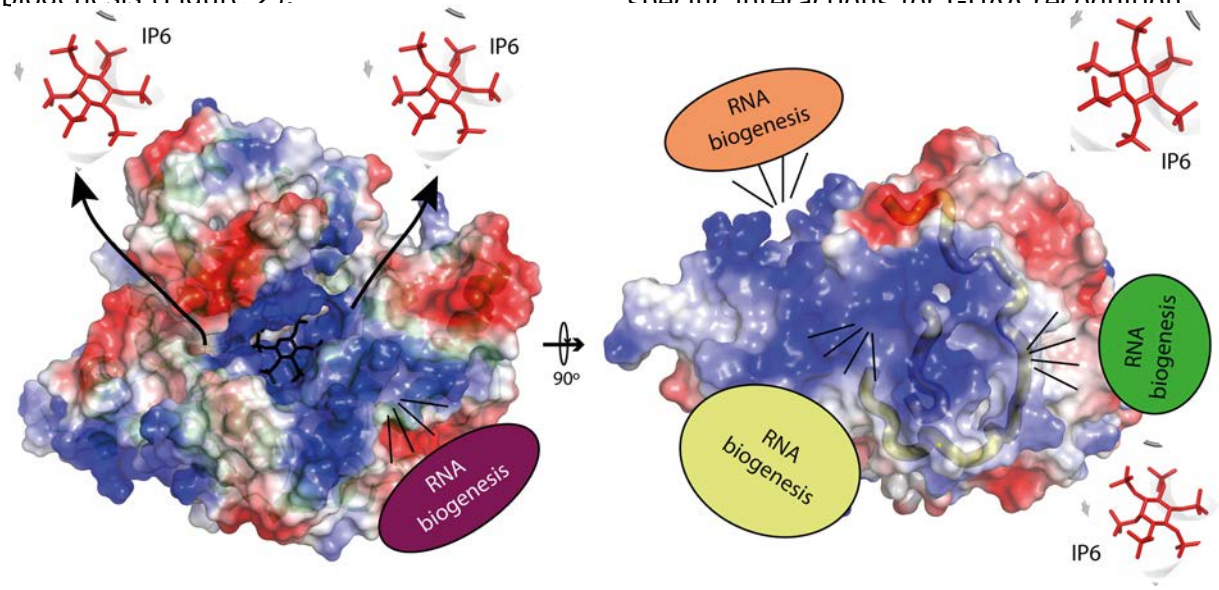

Figure 2: IP5 2-K surface showing its active site and putative interfaces for protein-protein interactions important for RNA biogenesis.

Structural biology of bacterial pathogenesis

β-lactam antibiotics are currently the most used antibiotics. These antibiotics prevent bacterial cell wall formation, critical for bacterial survive. B-lactam antibiotics inhibit the transpeptidation process between peptides promoting the accumulation of aberrant long fragments. Pseudomonas aeruginosa attempts to repair this damage by the lytic transglycosilase Slt. In our work we have managed to solve the structure of the enzyme Slt to carry out the study of its catalytic mechanism getting several complexes with analogous of its natural substrate. Slt is able to degrade the PG through both endolytic (in the middle of chain) and exolytic (in one end) cut. Slt can accommodate the PG thanks to a long catalytic throat with up to 10 positions for NAG/NAM units together with certain key residues that interact with the peptide stems (Figure 3). These results disclose the details of bacterial response to the β-lactam antibiotic challenge.

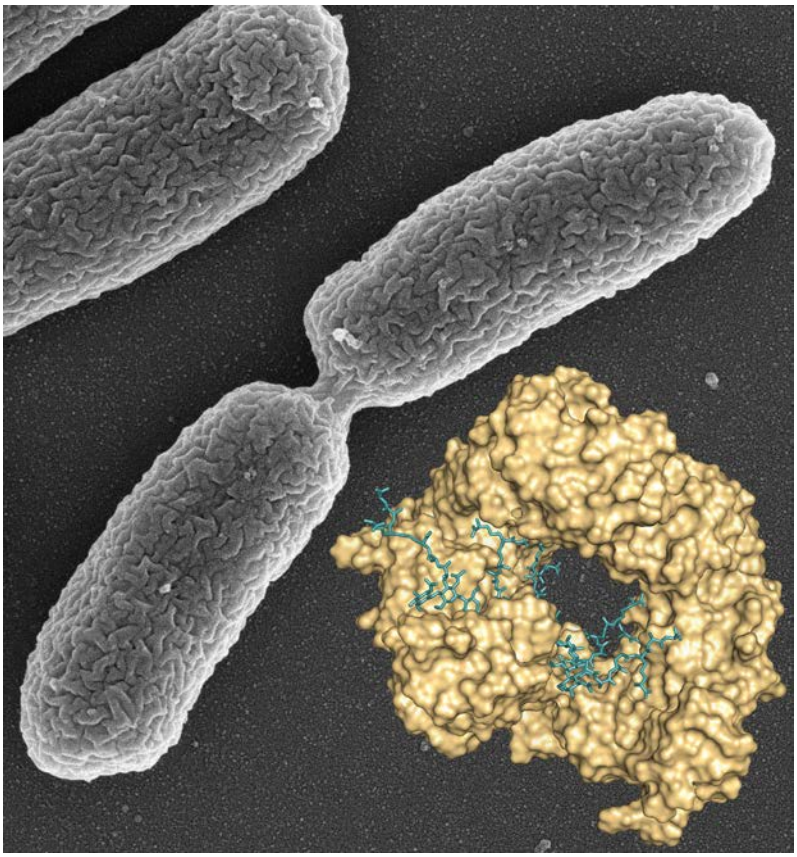

Figure 3: Three-dimensional structure of Slt (in yellow) attached to a fragment of the bacterial wall (green). In the background there is an electron microscopy image of the bacterium Pseudomonas aeruginosa.

Enzymatic synthesis of therapeutic nucleosides

With the aim to synthesize nucleoside derivatives in mild conditions, we looked for enzymatic systems producing such molecules. We found that nucleoside 2´-deoxyribosyltransferases (PDT) from a variety of biological sources are adequate for such a purpose. Hence, we determined the crystal structure of PDT from *Leishmania mexicana* that behave as an efficient biocatalyst for the one-step synthesis of nucleosides from poorly soluble purine bases. The homologue from *Trypanosoma brucei,* with excellent activity and stability in a broad range of experimental conditions, permitted the synthesis of a wide array of therapeutic nucleosides.

Carbohydrate-modifying enzymes from Lactobacillus plantarum WCFS1

Numerous *Lactobacillus* species have been identified in the human gut microbiome with a high catabolic flexibility, in particular, with a high capacity to metabolize carbohydrates. *L. plantarum* is one of these bacterial species, which presents one of the largest genomes in the bacterial strains isolated from mammals and notably a large number of enzymatic systems involved in the hydrolysis, biosynthesis and modification of carbohydrates. The main objective of our research project is to characterize, genetically, functionally and structurally such systems for producing added-value bioactive compounds with interest in the food industry.

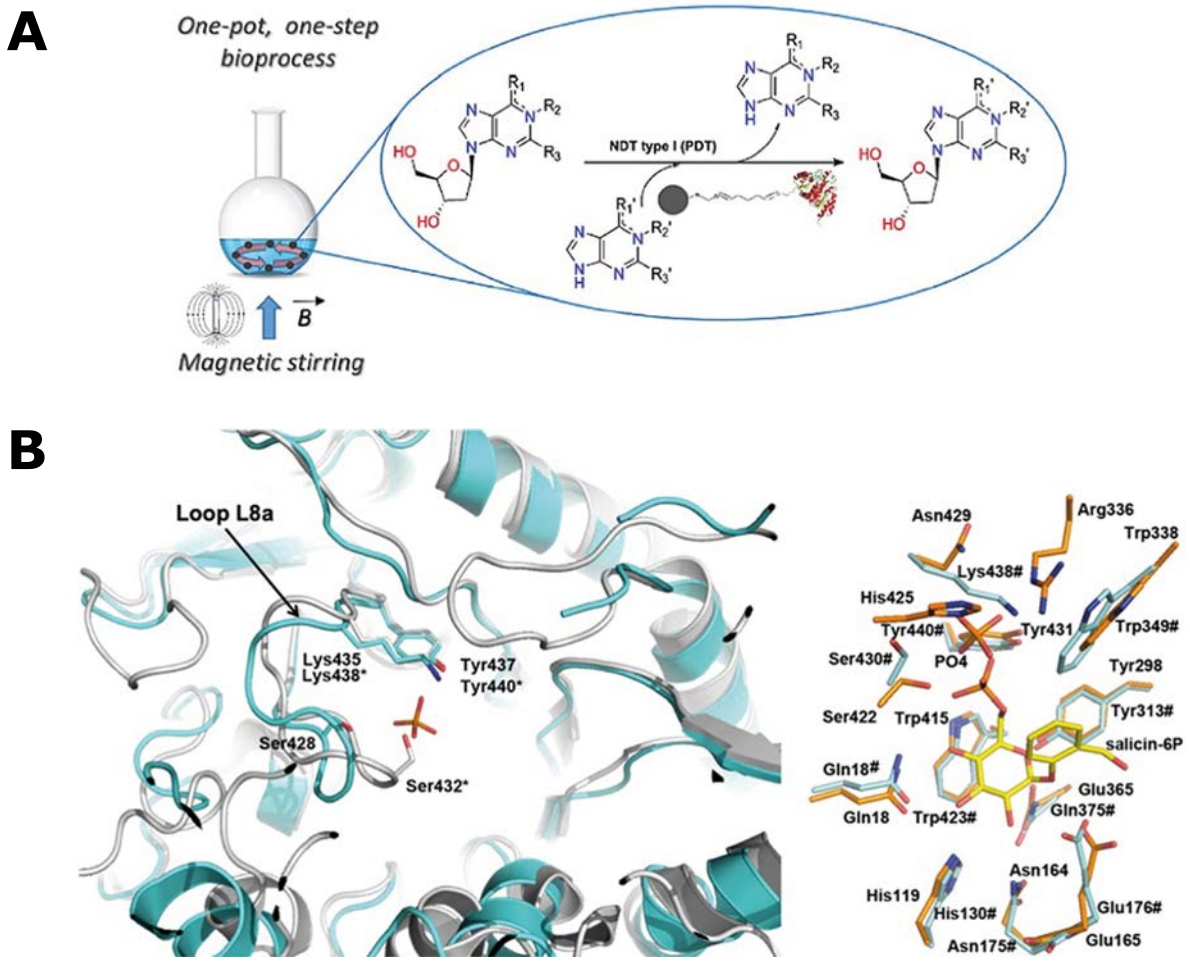

Figure 4: A: Enzymatic synthesis of nucleosides by 2'-deoxyribosyl transferase from T. brucei immobilized on magnetic microspheres. B: Structural analysis of phosphate-binding (left) and substrate-binding (right) modes in 6-phospho-β-glucosidases

Design of new biocatalyst for synthetic biology

We unveiled the exceptional substrate promiscuity of a fungal peroxygenase on the basis of the dynamic trafficking of the substrates through its heme channel, and determined the key residues modulating specificity. This allows the design of variants adapting activity "a la carte"

We have design FFase mutants producing fructosylated-hydroxytirosol, a biophenol with anti-inflamatory, neuroprotective and anti-tumoral properties, the glycosylation improving its bio-availability.

Multidomain enzymes as catalytic nanomachines

Combining X-ray diffraction and crio-EM, we solved the structure of a β-galactosidase degrading lactose, relevant for the population suffering from lactose intolerance, and also in the biosynthesis of prebiotic GOS. This gave the best strategy to design a quimeric enzyme by fusing a carbohydrate-binding domain, which led to a highly efficient biocatalyst easily immobilized in non-expensive cellulose/chitin supports, which is most valuable to produce lactose-free milk-derivatives and GOS.

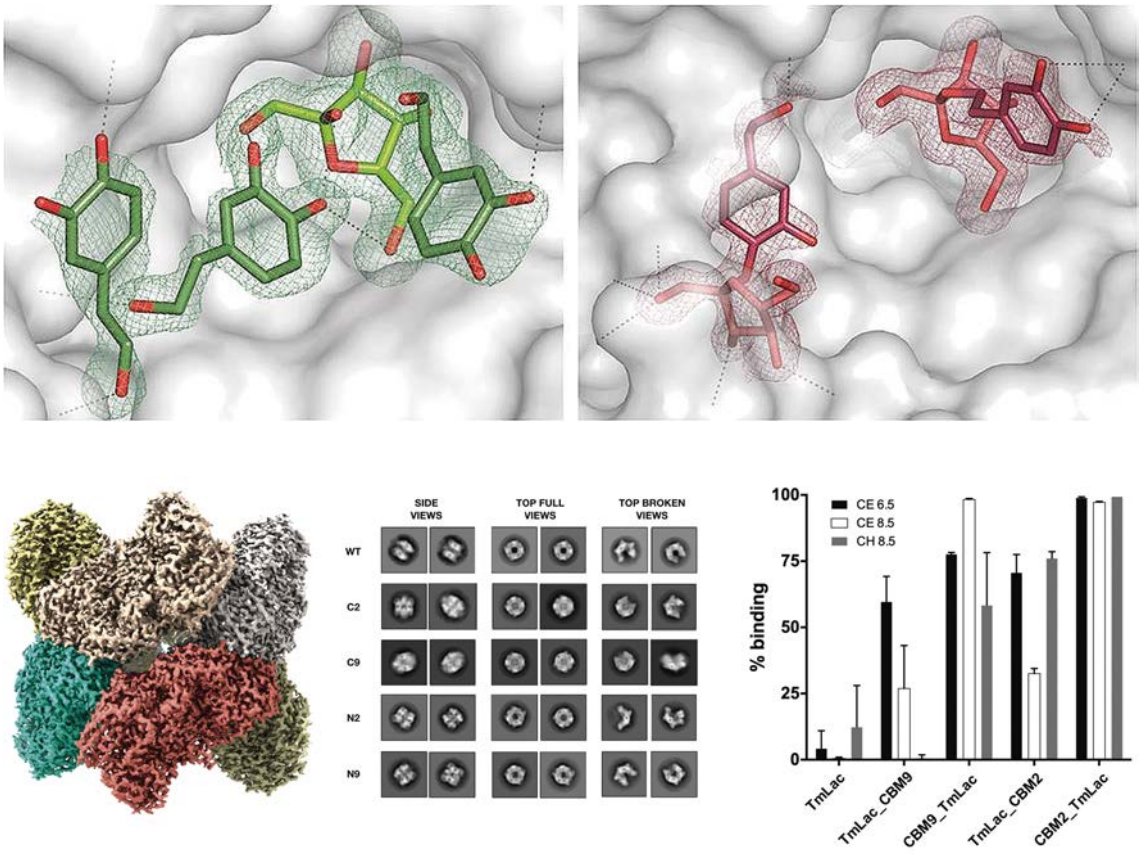

Figure 5: Up:Binding modes of substrates and products to the Ffase active site by crystallography. Down:Structure of TmBgal and cryo-EM analysis of quimeric constructs led to a highly efficiently immobilized biocatalyst

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

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 Fragile X syndrome (FXS), an autistic disorder where neurons show an abnormally high synapse number. In the recent years, we have investigated the structural basis of the NCS-1/Ric8a interaction to find that the formation of this complex is essential to increase synapse number. Interestingly, we have demonstrated that the inhibition of the NCS-1/Ric8a complex with small molecules constitutes a potential strategy for FXS pharmacotherapy, restoring synapse number and improving associative learning. The structural information obtained by X-ray crystallography, together with computational methods has shown the mechanism of action of the compounds and how to improve their drug-like properties (PNAS (2017), J. Med. Chem. (2018)). Since other neuronal disorders show similar synaptic abnormalities, we believe that the compounds would be also useful for diseases such as Rett syndrome or autism.

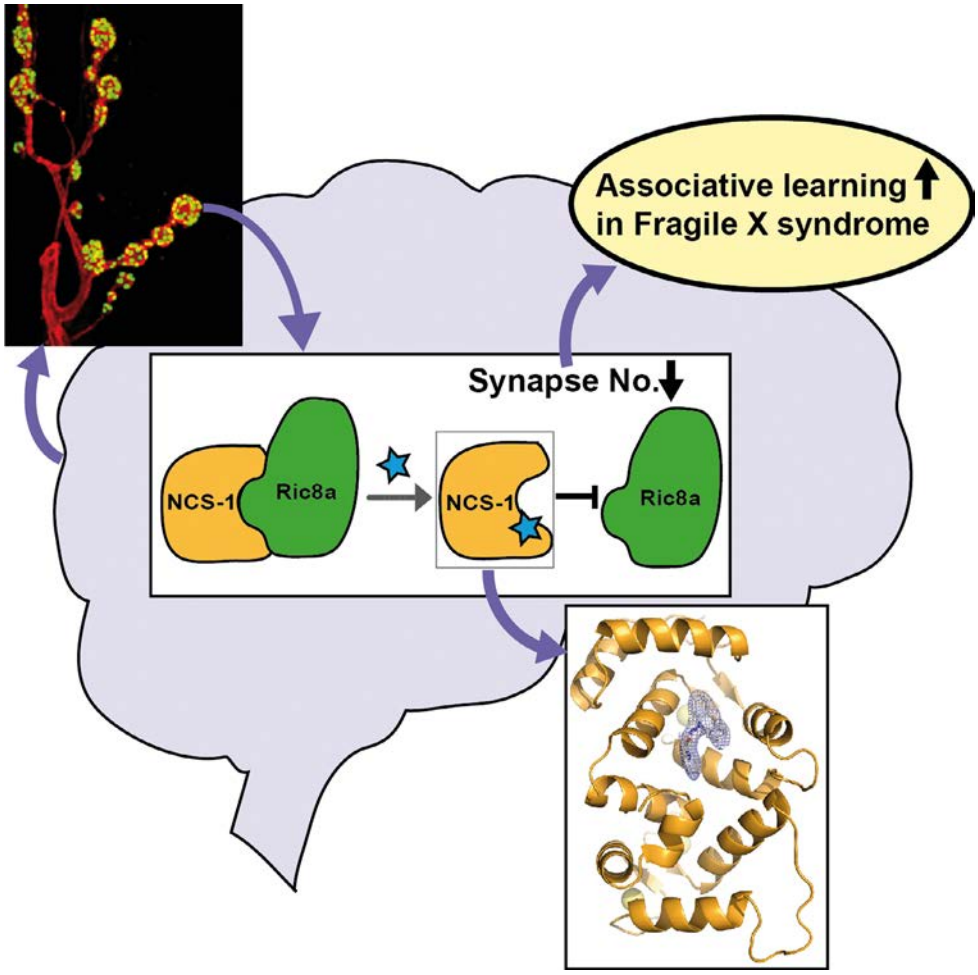

Figure 6: Schematic representation of the activity of the small molecules regulating the NCS-1/Ric8a protein-protein interaction in neurons.

Teaching and diffusion of Crystallography

The Department offers a fully-dedicated website for learning Crystallography (http://www.xtal.iqfr.csic.es/Cristalografia/) written in two languages (Spanish and English). It was announced by the International Union of Crystallography (http://bit.ly/dHj0Q0) and selected by this institution as one of the most interesting sites for learning crystallography (http://bit.ly/1zCsBOX). It was offered as such in the commemorative web for the International Year of Crystallography (http://bit.ly/1BYMGyd), and suggested as the educational website to learn about crystals, diffraction and crystal structure determination in the brochure (http://bit.ly/1DXoqxP) prepared by UNESCO. It is also offered as one of the best learning online tools by several USA universities (see for example: http://bit.ly/guMQax, http://bit.ly/gCLbYk). Google Analytics, and other web counters directly accessible through the web page menu (i.e. http://bit.ly/2bz1qfx), show that this web gets over 1,500 different page visits a day (over 500,000 page visits/year), distributed over 190 countries, but especially from USA, Mexico, India, EU and Latin American countries.

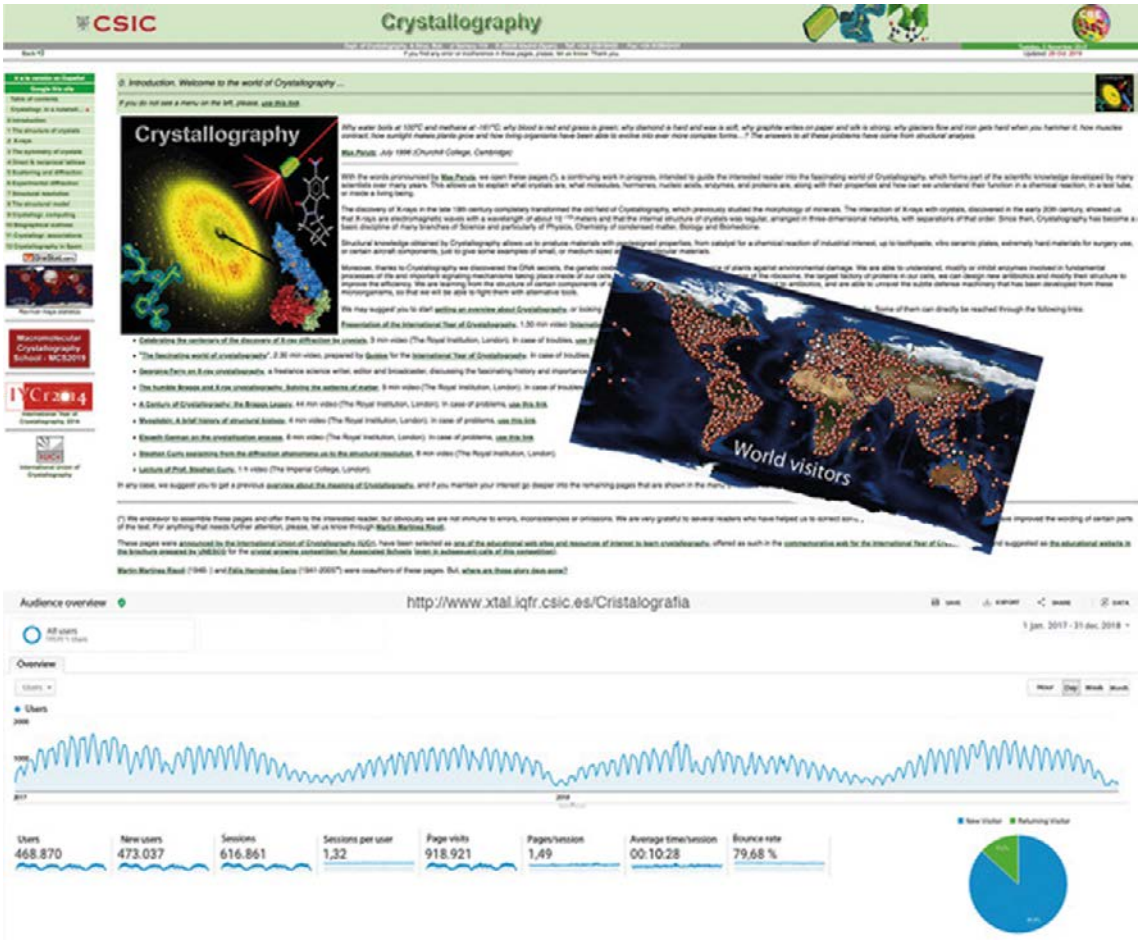

Figure 7: Website for learning Crystallography and analysis of entries.

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2018

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National Grants: individual

Secretaria de Estado de Investigación

Principal Investigator	Title	Reference
Armando Albert de la Cruz	Aproximación estructural a los mecanismos de señalización en membrana que controlan la respuesta al estrés abiótico en plantas	BIO2017-89523-R
Beatriz González Pérez	Desarrollo preclínico de nuevos fármacos para el tratamiento personalizado de cánceres dependientes de RAS	RTC-2017-6478-1
Beatriz González Pérez	Una visión ampliada de la señalización por inositidos: síntesis y dianas en la biogénesis de RNA	BFU2017-89913-P
Beatriz González Pérez	PérezAnálisis estructural y funcional de la señalización mediante inositol fosfatos y su implicación en salud	BFU2014-53762-P
Juan Antonio Hermoso Dominguez	Apuntando a la resistencia a antibióticos: bases estructurales de la regulacion en procesos esenciales de remodelado de la pared celular	BFU2017-90030-P
Juan Antonio Hermoso Dominguez	nanodiscos: una alternativa novedosa para cristalizar proteinas de membrana	BFU2014-61623-EXP
Juliana Sanz Aparicio	Crystallographic analysis and molecular design of glycoenzymes to improve its efficiency for Biotechnology	BIO2016-76601-C3-3-R

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

Secretaria de Estado de Investigación

Principal Investigator	Title	Reference
José Manuel Pardo Prieto	Sistemas de Transporte de Sodio y Potasio en Plantas	BIO2016-81957-REDT
Rosario Muñoz Moreno	Enzimas modificadoras de carbohidratos de Lactobacillus plantarum WCFS1: caracterización genética, funcional y estructural	AGL2017-84614-C2-2-R

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

Spanish National Research Council

Principal Investigator	Title	Reference
Lourdes Infantes San Mateo	Drug design based on the complementarity between molecules to improve their physicochemical properties	COOPA20094

International Grants: coordinated

National Institutes of Health USA

Principal Investigator	Title	Reference
Juan Antonio Hermoso Dominguez	The Quinazolinone Class of Antibacterial Agents	1R01AI116548

Index

Department of Atmospheric Chemistry and Climate

Index

Introduction

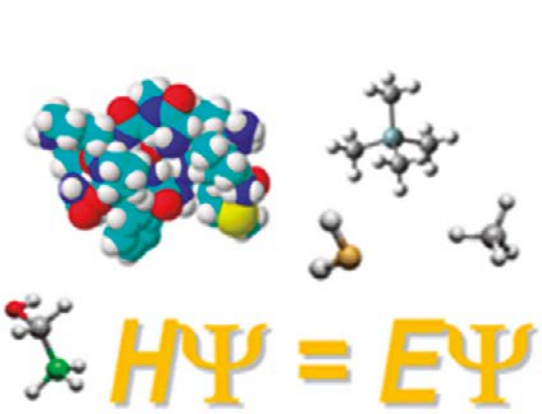
The Department develops different lines of research, which main objectives are:

- 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)



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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.

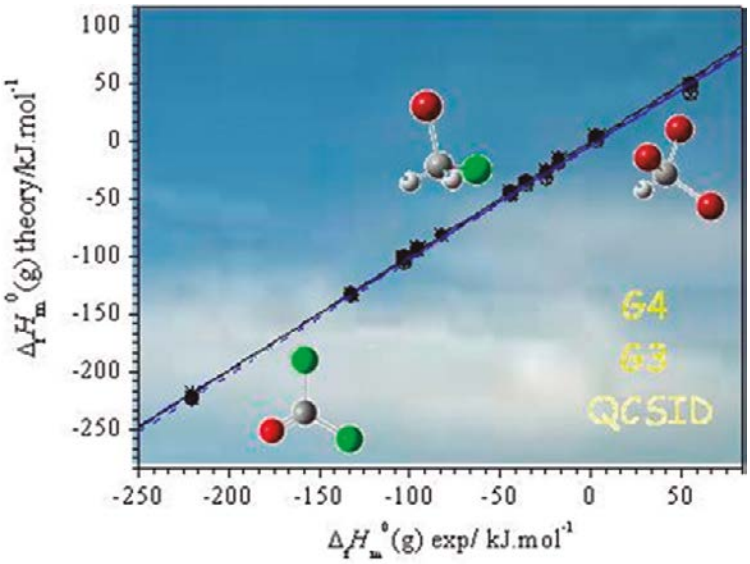
The specific goals pursued are:

- 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

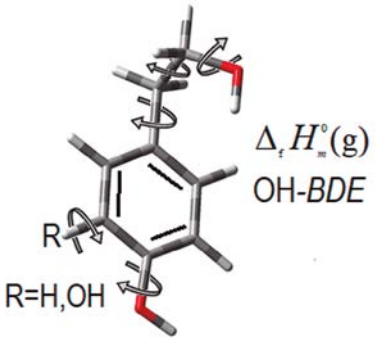
Thermochemistry of halogen-containing organic compounds with influence on atmospheric chemistry

We report a study on the thermochemical properties of a wide variety of halogen-containing organic compounds with relevance on several atmospheric chemical processes, such as catalytic ozone destruction. In particular, we have computationally determined the standard molar enthalpies of formation, (g), and the carbon-halogen bond dissociation enthalpies, *BDE*, in the gas phase at 298.15 K. A reliable estimation of these thermodynamic magnitudes was deduced, using atomization and isodesmic reactions methodologies, from *ab initio* computational methods. The enthalpies of formation of the radicals formed through bond dissociations have also been computed.



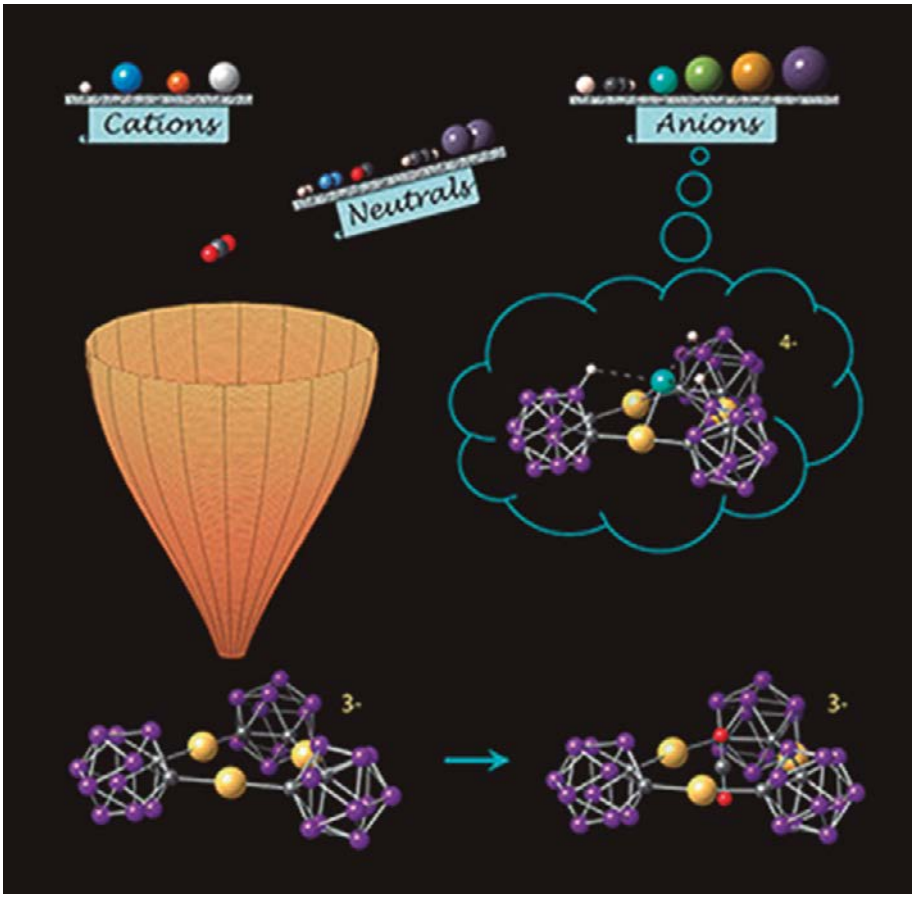
Energetic and Structural Properties of Two Phenolic Antioxidants: Tyrosol and Hydroxytyrosol

Theoretical and experimental studies on the energetic and structural properties of the antioxidant tyrosol and hydroxytyrosol molecules and their corresponding radicals have been reported in this work. The experimental values of the gas-phase enthalpy of formation, (g), in kJ·mol^{-1}, of tyrosol (-302.4 ± 3.4) and hydroxytyrosol (-486.3 ± 4.1) have been determined. Quantum chemical calculations, at DFT (M05-2X) and composite *ab initio* G3 and G4 levels of theory, provided results that served to: i/ confirm the excellent consistency of the experimental measurements performed, ii/ establish that the stabilizing effect of H-bond of hydroxyethyl chain and aromatic ring (OH•••p interaction) is smaller in radicals than in parent molecules, iii/ deduce – combining experimental data in isodesmic reactions – (g) of radicals, iv/ estimate a reliable O-H bond dissociation enthalpy, *BDE* of tyrosol(368.1 ± 5.6 kJ·mol^{-1}) and of hydrixytyrosol (333.7 ± 5.6 kJ·mol^{-1}), corroborating that this is more effective antioxidant than tyrosol.



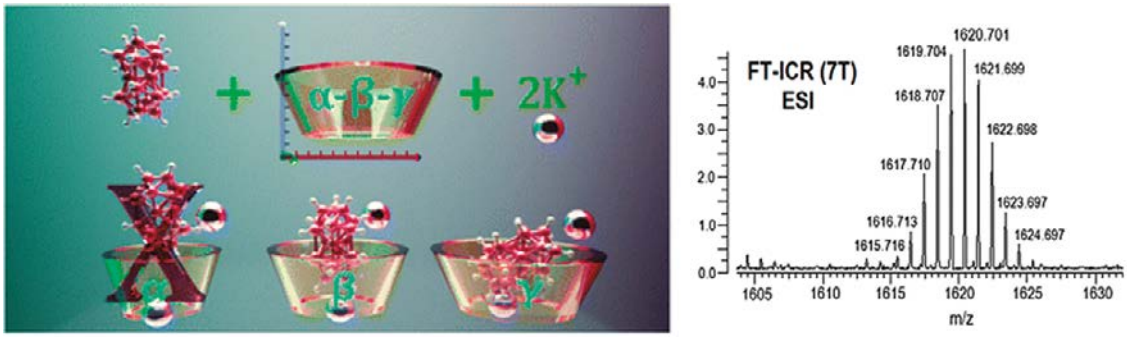
A Trinuclear Gold–Carborane Cluster as a Host Structure Can Trap Anions and Neutral Molecules (CO_2)

The Figure shows the interaction pattern between a triangular gold–carborane cluster trianion (host) and various cations, neutral molecules, and anions (guests). The funnel above the cluster indicates that some of the guests, regardless of their charge or size, can be trapped inside the void of the host. Cations form stable complexes according to the large electrostatic potential that favors attractive host···guest adducts, but some neutral and anionic guests can also be enclosed. Unexpectedly, hydride and fluoride are trapped, forming tetraanionic species, but among neutral molecules, only CO_2 is trapped.



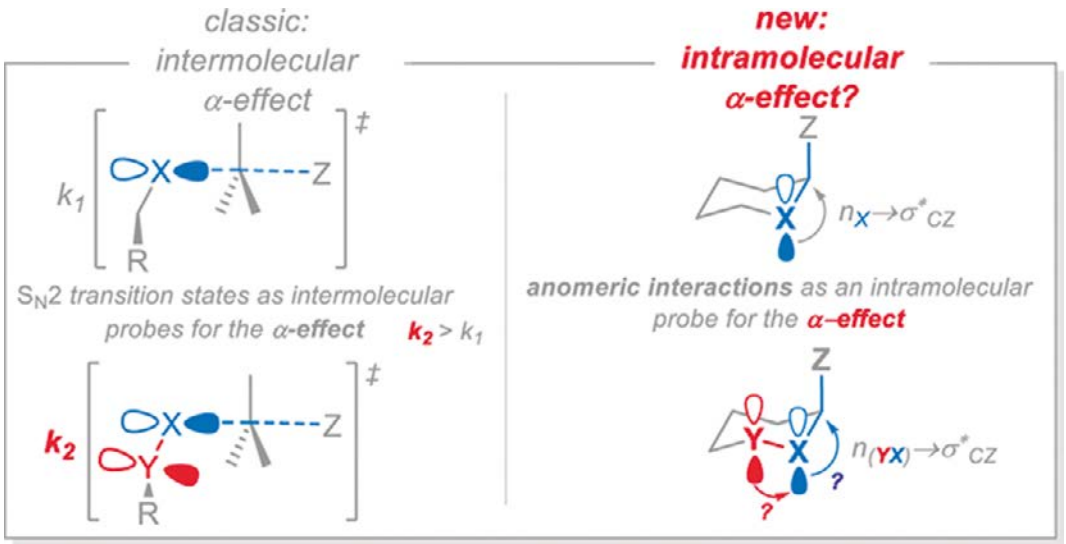
Binary twinned-icosahedral $[B_{21}H_{18}]^-$ interacts with cyclodextrins as a precedent for its complexation with other organic motifs

It has been synthesized the binary macro-polyhedral anion of borane closo type, *closo*-$[B_{21}H_{18}]^-$ (B21**,** symmetry D3h) that can form stable complexes -in gas phase- with sugars b- and g-cyclodextrin (CD) but not with a-CD. This experimental evidence, obtained by high resolution mass spectrometry FT-ICR (7T) with ESI source, has been interpreted by means of quantum mechanical calculations taking into account that b- and g-CD can interact with B21 due to the larger cavities than those of a-CD. The modeling show us that the B-H hydride type vectors of the B21 anion interact with K^+ counterions and with partially charged hydrogens of the CD, by means of dihydrogen bonds. Our studies confirm that macropolyhedral boron hydrides with two counterions can form stable complexes with b- or g-CDs, a result that opens new perspectives in the investigation of these novel anions in areas of supramolecular chemistry and medical chemistry.



Stereoelectronic Interactions as a Probe for the Existence of the Intramolecular α-Effect

The first systematic study of the intramolecular α effect has been carried out, both species in the ground state and in high energy intermediates, using the anomeric effect as an internal stereoelectronic probe. Contrary to what is expected, which is based on a simple model of mixing orbitals, the free pairs in two adjacent heteroatoms do not increase their energy to become strong donors towards adjacent σ and π acceptors. Instead, the key interactions n (X-Y) →σ * (C-F) (X, Y = O, N) in α systems are weaker than interactions nX →σ * (C-F) in "normal" systems.



Publications

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Córdova, B. M. *et al.* Chemical modification of sodium alginate with thiosemicarbazide for the removal of Pb(II) and Cd(II) from aqueous solutions. *Int. J. Biol. Macromol.* **120**, 2259-2270, (2018).

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Perdomo, G. *et al.* Thermochemistry of R-SH group in gaseous phase: Experimental and theoretical studies of three sulfur imidazole derivatives. *The Journal of Chemical Thermodynamics* **122**, 65-72, (2018).

Oliva-Enrich, J. M. *et al.* Predicted Gas-Phase and Liquid-Phase Acidities of Carborane Carboxylic and Dicarboxylic Acids. *Chemistry Select* **3**, 4344-4353, (2018).

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Alcoba, D. R. *et al.* Magnetic Properties of Mononuclear Co(II) Complexes with Carborane Ligands. *Inorg. Chem.* **57**, 7763-7769, (2018).

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Eyrilmez, S. M. *et al.* Binary twinned-icosahedral [B21H18]− interacts with cyclodextrins as a precedent for its complexation with other organic motifs. *Phys. Chem. Chem. Phys.* **19**, 11748-11752, (2017).

Dávalos, J. Z., Notario, R., Cuevas, C. A., Oliva, J. M. & Saiz-Lopez, A. Thermochemistry of halogen-containing organic compounds with influence on atmospheric chemistry. *Computational and Theoretical Chemistry* **1099**, 36-44, (2017).

Londesborough, M. G. S. *et al.* Thermochromic Fluorescence from B18H20(NC5H5)2: An Inorganic–Organic Composite Luminescent Compound with an Unusual Molecular Geometry. *Advanced Optical Materials* **5**, 1600694, (2017).

Oña, O. B. *et al.* Determination of exchange coupling constants in linear polyradicals by means of local spins. *Theor. Chem. Acc.* **136:35**, (2017).

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Juaristi, E., dos Passos Gomes, G., Terent'ev, A. O., Notario, R. & Alabugin, I. V. Stereoelectronic Interactions as a Probe for the Existence of the Intramolecular α-Effect. *J. Am. Chem. Soc.* **139**, 10799-10813, (2017).

National Grants: individual

Organism 1

Principal Investigator	Title	Reference
Josep M. Oliva-Enrich	Novel aspects of the application of VB theory: chemical bonding, excited states and solid-state chemistry of new boron compounds	PRX17/00488

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Summary

The Atmospheric Chemistry and Climate group (AC2) is a newly created research group within CSIC's Institute of Physical Chemistry Rocasolano (IQFR). The group initiated its research activities in August 2009 in Toledo as the former Laboratory for Atmospheric and Climate Science, since December 2012 AC2 is based at IQFR in Madrid.

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 scientific framework, AC2 provides an integrated research approach combining atmospheric measurements (satellite- and ground-based)

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

Production of organic bromine compounds in the sea ice during the Antarctic winter

During polar springtime, active bromine drives ozone, a greenhouse gas, to near-zero levels. Bromine production and emission in the polar regions have so far been assumed to require sunlight. We report measurements of bromocarbons in sea ice, snow, and air during the Antarctic winter that reveal an unexpected new source of organic bromine to the atmosphere during periods of no sunlight. The results show that Antarctic winter sea ice provides 10 times more bromocarbons to the atmosphere than Southern Ocean waters, and substantially more than summer sea ice. Modelling these observationswe show that the emitted bromocarbons will disperse throughout the troposphere in the southern hemisphere and through photochemical degradation to bromine atoms, contribute ~10% to the tropospheric reactive bromine budget. These results suggest that winter sea ice could potentially be an important source of atmospheric bromine with implications for atmospheric chemistry and climate at a hemispheric scale. (*Nature Communications* **9**, Article number: 5291 (2018))

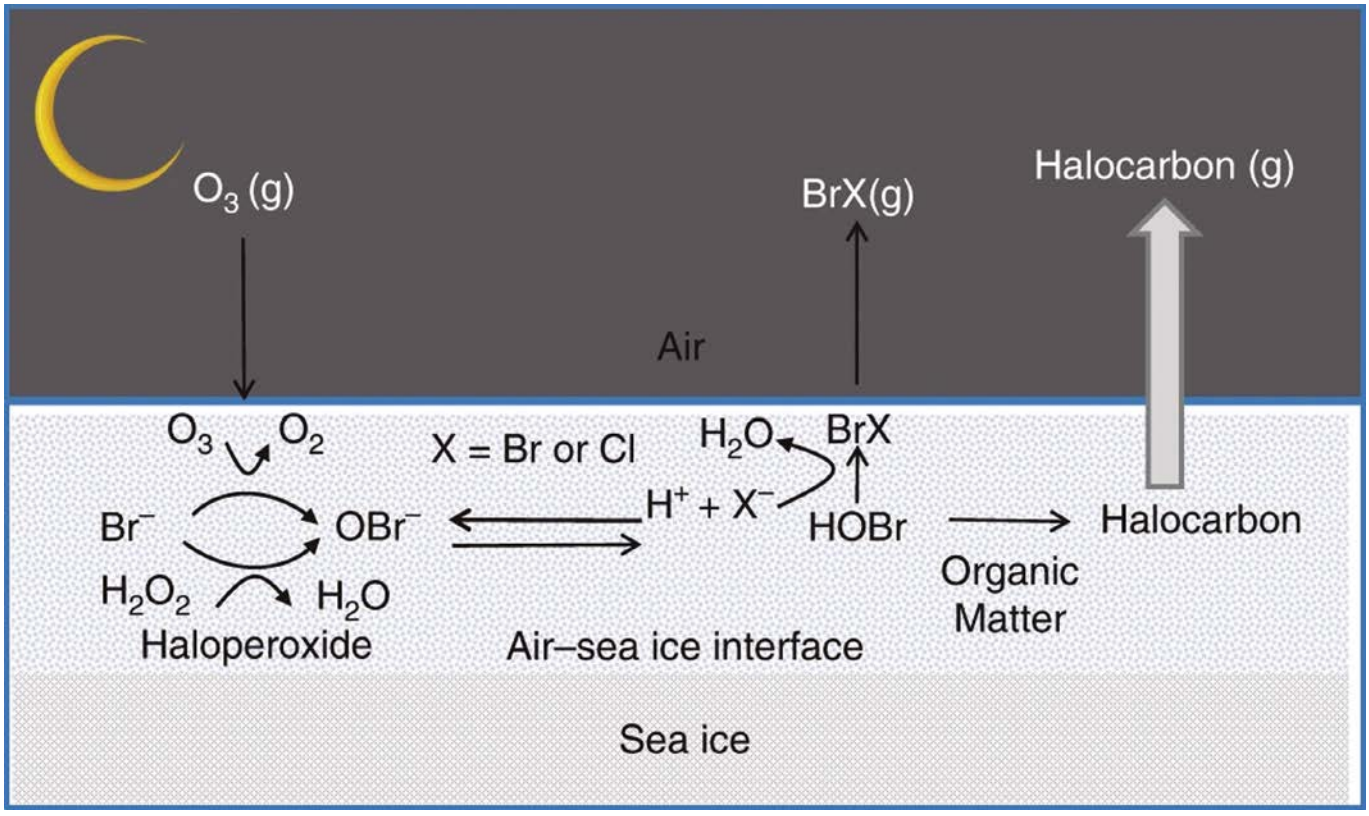

Figure 1: schematic of the possible release mechanisms of bromocarbons from sea ice in the Antarctic winter.

Photoreduction of gaseous oxidized mercury changes global atmospheric mercury speciation, transport and deposition

Anthropogenic mercury (Hg(0)) emissions oxidize to gaseous Hg(II) compounds, before deposition to Earth surface ecosystems. Atmospheric reduction of Hg(II) competes with deposition, thereby modifying the magnitude and pattern of Hg deposition. Global Hg models have postulated that Hg(II) reduction in the atmosphere occurs through aqueous-phase photoreduction that may take place in clouds. We report that experimental rainfall Hg(II) photoreduction rates are much slower than modelled rates. We compute absorption cross sections of Hg(II) compounds and show that fast gas-phase Hg(II) photolysis can dominate atmospheric mercury reduction and lead to a substantial increase in the modelled, global atmospheric Hg lifetime by a factor two. Models with Hg(II) photolysis show enhanced Hg(0) deposition to land, which may prolong recovery of aquatic ecosystems long after Hg emissions are lowered, due to the longer residence time of Hg in soils compared with the ocean. Fast Hg(II) photolysis substantially changes atmospheric Hg dynamics and requires further assessment at regional and local scales. (*Nature Communications* **9**, Article number: 4796 (2018))

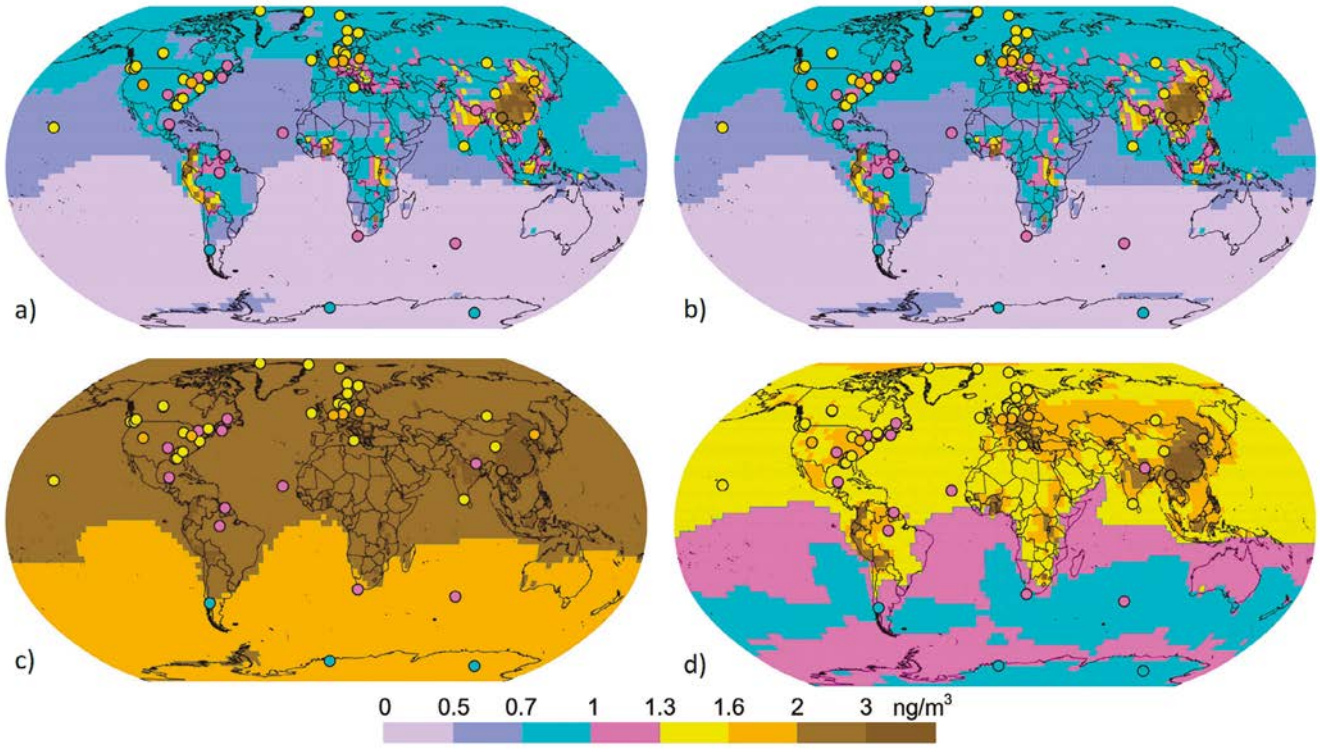

Figure 2: spatial distribution of Hg(0) surface concentration for different atmospheric Hg(II) reduction simulations in the model: a) No Hg(II) reduction, b) Hg(II) reduction in aqueous phase, c) gas phase Hg(II) photoreduction to Hg(0)and d) gas phase Hg(II) photoreduction to HgBr. Circles show observed values in the same colour scale.

Rapid increase in the atmospheric iodine levels in the North Atlantic since the mid-20th century

Atmospheric iodine causes tropospheric ozone depletion and aerosol formation, both of which have significant climate impacts, and is an essential dietary element for humans. However, the evolution of atmospheric iodine levels at decadal and centennial scales is unknown. We report iodine concentrations in the RECAP ice-core (coastal East Greenland) to investigate how atmospheric iodine levels in the North Atlantic have evolved over the past 260 years (1750–2011). The levels of iodine tripled from 1950 to 2010. Our results suggest that this increase is driven by anthropogenic ozone pollution and enhanced sub-ice phytoplankton production associated with the recent thinning of Arctic sea ice. Increasing atmospheric iodine has accelerated ozone loss and has considerably enhanced iodine transport and deposition to the Northern Hemisphere continents. Future climate and anthropogenic forcing may continue to amplify oceanic iodine emissions with potentially significant health and environmental impacts at global scale. (*Nature Communications* **9**, Article number: 1452 (2018))

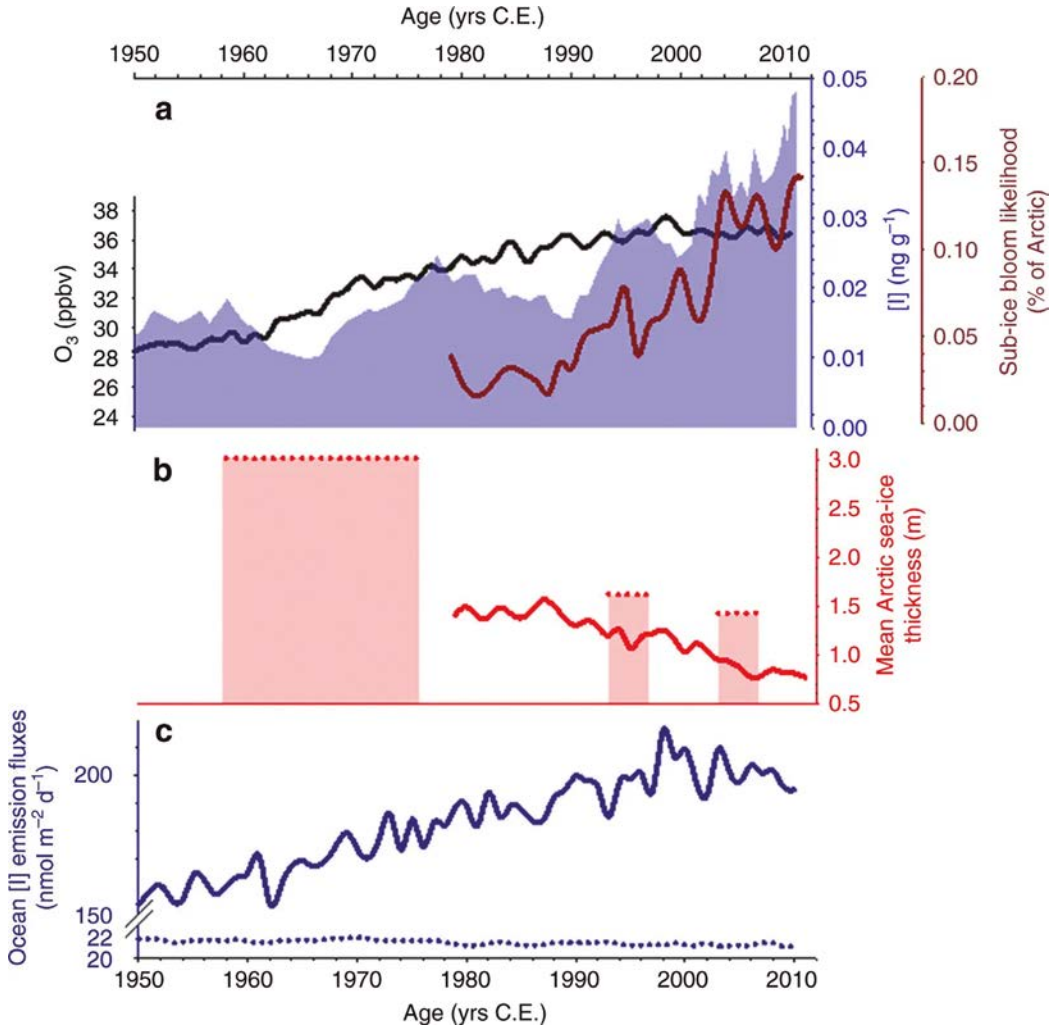

Figure 3: iodine concentration evolution and forcing mechanisms for the period 1950–2011. **a)** Iodine concentration (blue area); ozone annually averaged over the North Atlantic region (dark line) and evolution of the pan-Arctic likelihood of sub-ice blooms in late spring and early summer (May–June–July) over time (red line); **b)** mean Arctic sea ice thickness **c**) modeled ocean emission fluxes of iodine with (solid line) and without (dotted line) the implementation of the ozone-induced iodine emission mechanism

Unexpected increase in the oxidation capacity of the urban atmosphere of Madrid, Spain

Atmospheric oxidants such as ozone (O_3), hydroxyl and nitrate radicals (OH and NO_3) determine the ability of the urban atmosphere to process organic and inorganic pollutants, which have an impact on air quality, environmental health and climate. Madrid city has experienced an increase of 30–40% in ambient air O_3 levels, along with a decrease of 20–40% in NO_2, from 2007 to 2014. Using air pollution observations and a high-resolution air quality model, we find a large concentration increase of up to 70% and 90% in OH and NO_3, respectively, in downtown Madrid (domain-wide average increase of 10% and 32% for OH and NO_3, respectively). The results also show an 11% reduction in the nitric acid concentrations, leading to a remarkable denoxification of this urban atmosphere with implications for lower $PM_{2.5}$ levels and nitrogen input into ecosystems. This study suggests that projected worldwide NO_x emission reductions, following air quality standards, will lead to important changes in the oxidizing capacity of the atmospherein and around large cities. (*Scientific Reports* **volume 7**, Article number: 45956 (2017))

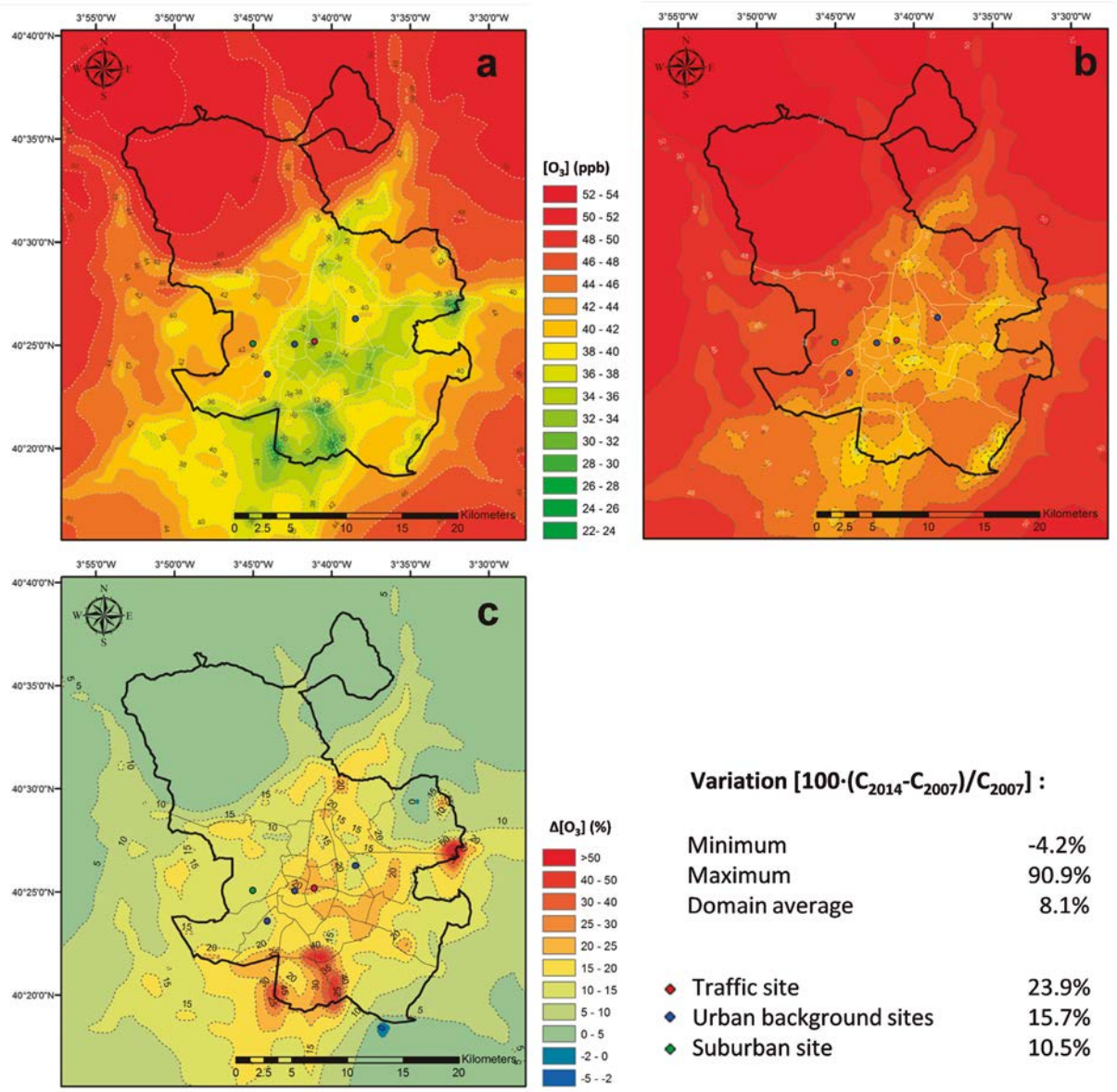

Figure 4: Modelled O_3 annual mean concentration, (**a**) 2007; (**b**) 2014. (**c**) Variation of O_3 annual mean concentration in 2014 with respect to 2007 and resulting statistics.

Measurements of atmospheric HONO vertical distribution and temporal evolution in Madrid (Spain) using the MAX-DOAS technique.

Nitrous acid (HONO) stands as one of the main species in tropospheric chemistry, primarily in polluted, urban regions. Due to its fast photodissociation, it is considered as one the main sources of the hydroxyl radical (OH), the most relevant oxidant in the atmosphere. Therefore, the evaluation of HONO concentration profiles and their temporal evolution is important for urban atmospheric chemistry. In this study, we report a year-round measurement of HONO vertical concentration profiles, as well as their diurnal and seasonal evolution during 2016 in Madrid. Making use of the Multi-AXis Differential Absorption Spectroscopy (MAX-DOAS) technique in addition to inversion algorithms, we retrieved the aerosol extinction and trace gas concentrations. Our results show HONO maximum values of 3.5–4 ppbv in the early morning and late afternoon, and minima around noon, when the lifetime of HONO against photolysis is shortest. On average, there is a pronounced HONO concentration gradient across different seasons, being higher during the autumn and winter months. Finally, we estimate and discuss the production rate of OH radicals from HONO photolysis, along with its variability throughout the year. (Science of the Total Environment 643, 957-966, 2018).

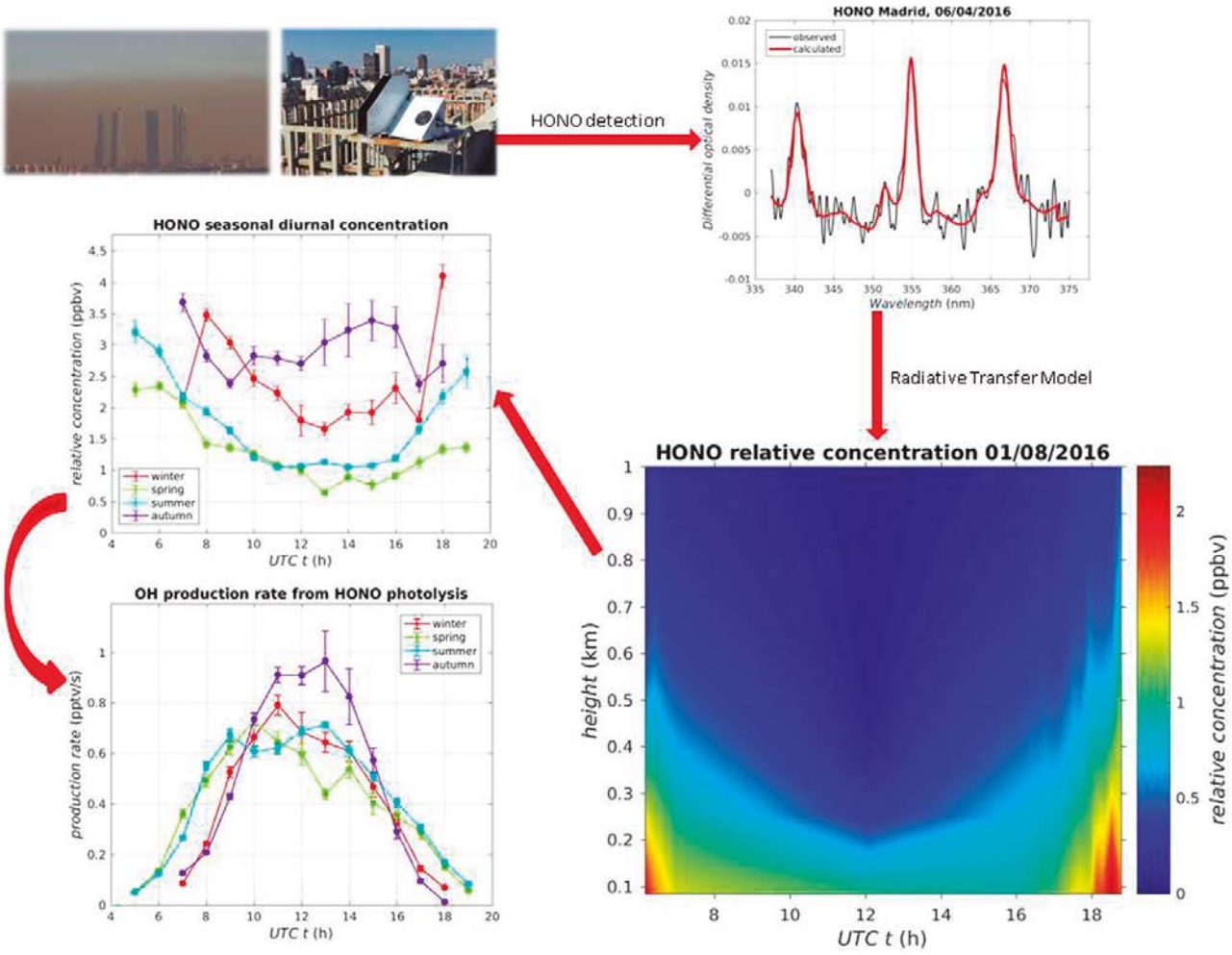

Figure 5: MAX-DOAS instrument employed in this work, HONO spectral fitting, seasonal diurnal variations of HONO relative concentration and vertical column densitites, and vertical profiles of HONO relative concentrations.

The impact of iodine-mediated ozone deposition and halogen chemistry on surface concentrations across the continental United States

The air quality of many large coastal areas in the United States is affected by the confluence of polluted urban and relatively clean marine airmasses, each with distinct atmospheric chemistry. In this context, the role of iodide-mediated ozone (O_3) deposition over seawater and marine halogen chemistry accounted for in both the lateral boundary conditions and coastal waters surrounding the continental U.S. is examined using the Community Multiscale Air Quality (CMAQ) model. Overall, it is the combination of these processes within both the continental U.S. domain and from lateral boundary conditions that lead to the largest reductions in modeled surface O_3 concentrations. Predicted reductions in surface O_3 concentrations occur mainly along the coast where CMAQ typically has large overpredictions. These results suggest that a realistic representation of halogen processes in marine regions can improve model prediction of O_3 concentrations near the coast (*Environ. Sci. Technol.*2017, 51, 3).

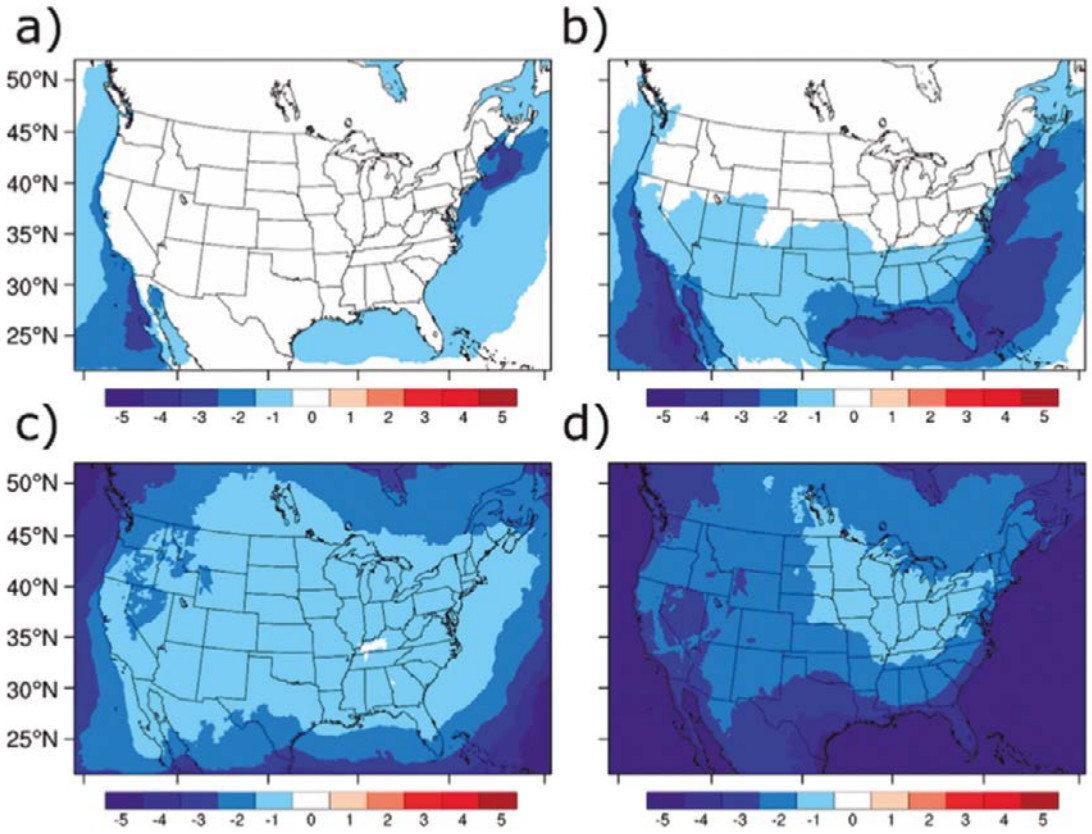

Figure 6: average monthly mean changes in predicted surface O_3 concentrations (in units of ppb) for August 2006 due to (a) iodide-mediated deposition, (b) detailed halogen chemistry, (c) iodide-mediated deposition and detailed halogen chemistry, and (d) the combination of iodide-mediated deposition and detailed halogenchemistry.

Impact of biogenic very short-lived bromine on the Antarctic ozone hole during the 21st century

Active bromine released from the photochemical decomposition of biogenic very short-lived bromocarbons (VSL^{Br}) enhances stratospheric ozone depletion. Our model results show that the maximum Antarctic ozone hole depletion increases by up to 14% when natural VSL^{Br} are considered, in better agreement with ozone observations. We find that the inclusion of VSL^{Br} in the model does not introduce a significant delay of the modelled ozone return date to 1980 October levels, but instead affects the depth and duration of the simulated ozone hole. Our analysis further shows that total bromine-catalysed ozone destruction in the lower stratosphere surpasses that of chlorine by the year 2070 and indicates that natural VSL^{Br} chemistry would dominate Antarctic ozone seasonality before the end of the 21st century. This work suggests a large influence of biogenic bromine on the future Antarctic ozone layer. (Atmos. Chem. Phys., 17, 1673-1688, 2017)

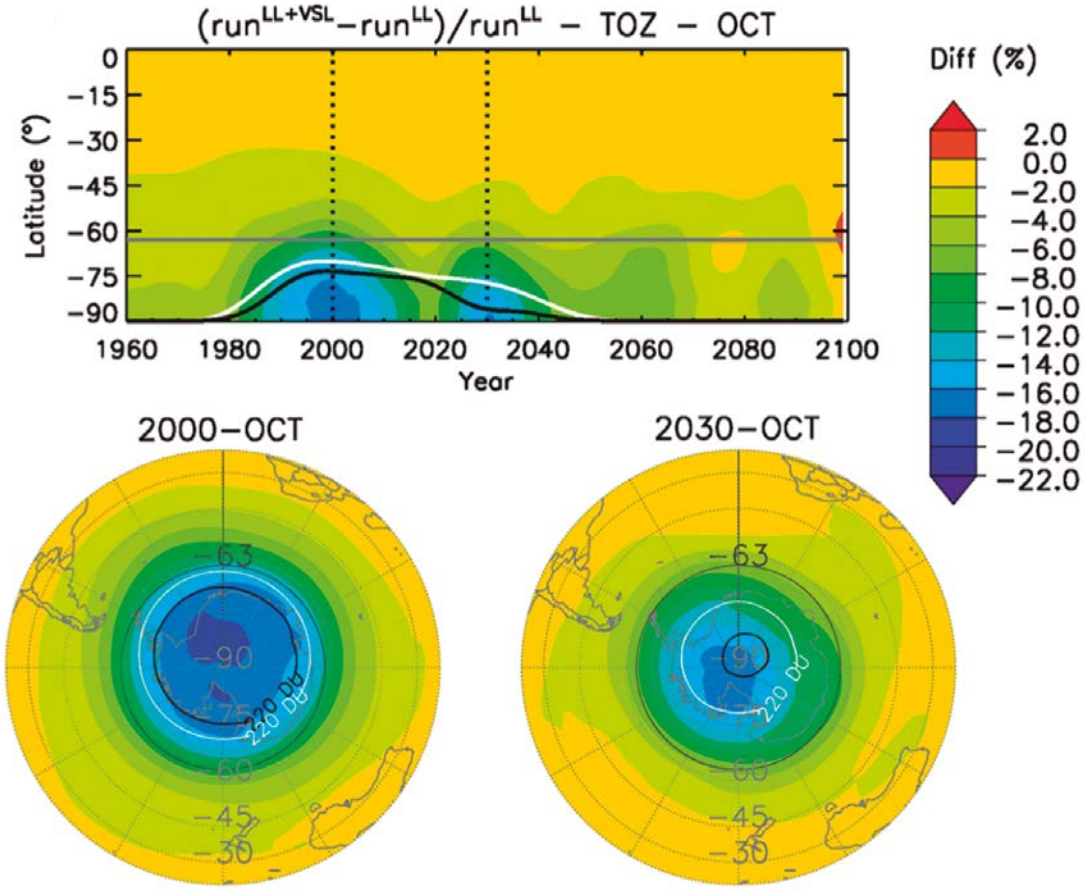

Figure 7: temporal evolution of the southern hemisphere ozone column as a function of latitude. Percentage difference between simulations with and without VSL^{Br}.

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COMPETITIVE FUNDING

National Grants: individual

MICINN

Principal Investigator	Title	Reference
Alfonso Saiz López	Fases finales (C2/D/E1) del instrumento Ultraviolet and Visible Atmospheric Sounder (UVAS) en SEOSAT/INGENIO	ESP2014-60774-R
Alfonso Saiz López	Fases de desarrollo final y ensayos (C2/D) del instrumento Ultraviolet and Visible Atmospheric Sounder (UVAS) en SEOSAT/INGENIO	ESP2015-71299-R

National Grants: coordinated

Comunidad de Madrid

Principal Investigator	Title	Reference
Alfonso Saiz López	Tecnologías innovadoras para la evaluación y mejora de la calidad del aire urbano (TECNAIRE-CM)	S2013/MAE2972

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 halogen sintheearth system: past, present, future (CLIMAHAL)	ERC-2016-COG 726349

International Grants: coordinated

EU

Principal Investigator	Title	Reference
Alfonso Saiz López	Quality Assurance for Essential Climate Variables	EU-FP7 QA4ECV

Aarhus University

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

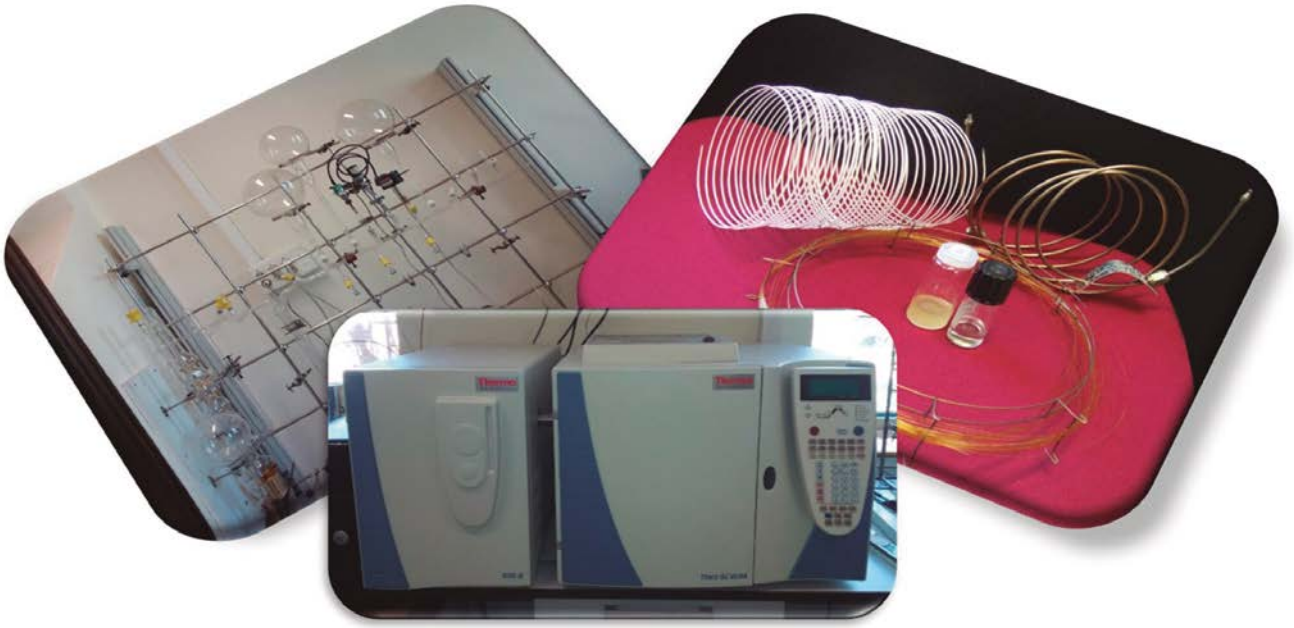
Royal Belgian Institute for Space Aeronomy

Principal Investigator	Title	Reference
Alfonso Saiz López	2ND Cabauw Intercomparison of Nitrogen Dioxide Measuring Instruments	CINDY-2

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



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María Hernáiz Izquierdo (hired technician, 1/7/2017-31/12/2017)

Summary

The main objectives of the Photolysis and Chromatography group are the study of chemical reactivity and molecular interactions. Specifically, we study the reactivity and reaction mechanisms of the intermediate species of Si, Ge, and Sn known as heavy carbenes. These heavy carbenes have high technological, industrial and theoretical interest. Absolute rates of the reactions of heavy carbenes are obtained by direct, time-resolved kinetic experiments using laser flash photolysis. The analysis of reaction products and stable intermediates is carried out by gas chromatography coupled to mass spectrometry (GC-MS).

In our studies of molecular interactions, we use the inverse gas chromatography (IGC) to characterize substances capable of being employed as GC stationary phases. This technique allows us to ascertain not only the type and intensity of the solute-stationary phase interactions, but also the solvation properties of the latter. We use this information both to improve the separation capacity of GC by the synthesis of stationary phases with new selectivities, and to develop methodologies suitable for solving complex analytical problems of interest in different areas (food, environment, etc.).

The Group manages the Mass Spectrometry laboratory of the IQFR (http://serviciomasas.iqfr.csic.es/), which has a MALDI-TOF mass spectrometer and an ion trap LC-MS system with electrospray and APCI sources. Since 2002, the laboratory provides 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

- New reaction kinetic studies of silicon and germanium containing heavy carbenes of interest in the materials industry.
- Development and characterization of new stationary phases for gas chromatography (polysiloxanes and ionic liquids).
- Determination of chromatographic and thermodynamic parameters by inverse gas chromatography.
- Development and application of innovative methodologies for the analysis of environmental, food and biological compounds of relevance by chromatography and mass spectrometry.

Remarkable Results

Silicon Compounds

We carried out a review of the state of thermochemistry (enthalpies of formation) of silicon and organosilicon compounds, focusing mainly on post-1998 results. While the emphasis is on data from experimental measurements, results of quantum chemical (*ab initio*) calculations are also included. We provide a set of current best values for SiX_4 compounds (X = H, Me, F, Cl, Br, I) as well as mixed SiX_nY_{4-n} compounds. Also included are Si/C/H/, Si/C/H/O, Si/C/H/N compounds and Si_2 and Si_3 containing molecules. Further inclusions are data for species such as SiX_3 (free radicals), SiX_2 (silylenes) and π-bonded molecules which *play prominent roles as intermediates in many thermal and photochemical reactions of silicon and organosilicon compounds.* Bond dissociation enthalpies are derived for most commonly encountered Si-X bonds. The evaluation of preferred values is further assisted by exploiting relationships (increments, substituent effects) within specific series and between series. In particular, we have developed a procedure of "experimentally adjusted theory" for SiX_nY_{4-n} compounds.

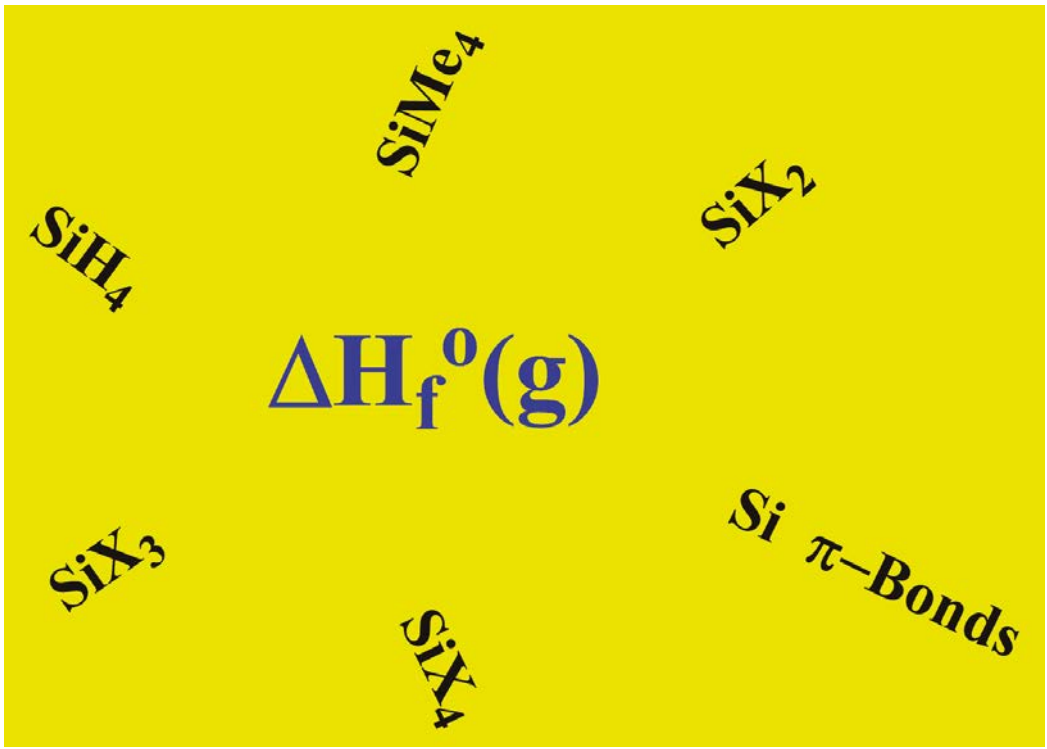

Figure 1: Schematic representation of the topics covers in this research.

Synthesis and characterization of new ionic liquids as stationary phases for Gas Chromatography

The advent of ionic liquids (ILs) in chromatography has had a strong impact on the development of new stationary phases, especially due to the possibility of modulating ILs properties just combining different cations and anions. With the aim of merging the high thermal stability and good wettability of poly(siloxanes) with the different selectivity of ILs, our research group has synthetized hybrid stationary phases by inserting an IL into the siloxane chain. In particular, we have obtained two hybrid polymers based on a poly(dimethylsiloxane) with a 5% and 19% of substitution of 1-propyl-3-methylimidazolium bistriflimide, respectively.

The chromatographic columns prepared with both polymers have shown a high efficiency and a selectivity very different from the columns commercially available. In addition, they have been used successfully for the separation of volatile constituents in spirits and the control of purity of common organic solvents.

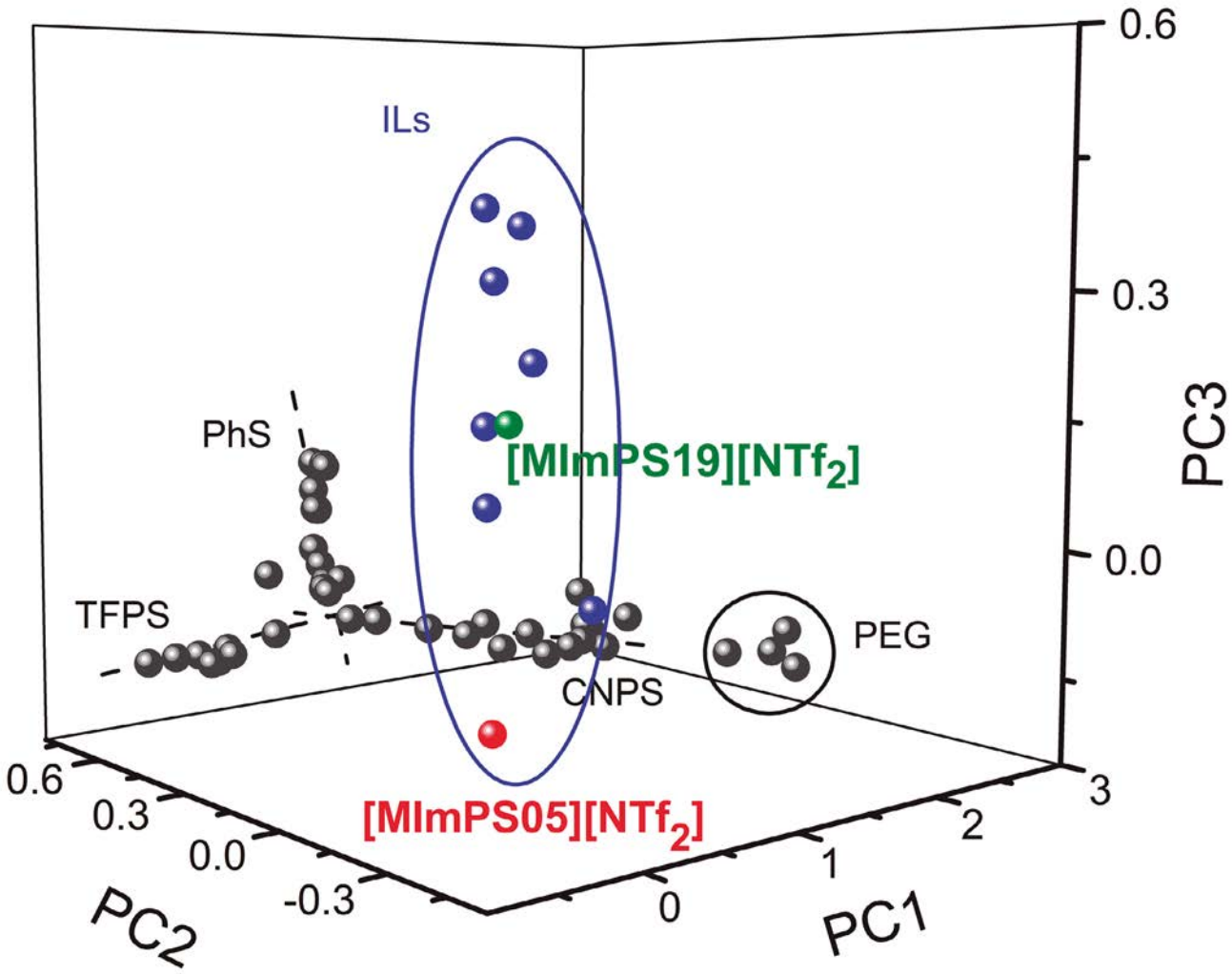

Figure 2: Selectivity of GC stationary phases. Red and green names correspond to the two new hybrid siloxane-ILs stationary phases.

Analysis of iodide and iodate in seawater

Atmospheric iodine comes mainly from oceans, and plays a relevant role in climate change. Therefore, analytical methods capable of determining iodine in seawater are necessary. However, this is a challenging task because iodine species (mainly iodide and iodate) can be found at very low concentrations, while many other interfering ions are present in huge quantities. We have faced this problem developing a liquid chromatography-mass spectrometry (LC-MS) method capable of quantifying iodide and iodate at subnanomolar level, using a mixed-mode stationary phase.

The preliminary studies produced very good results, because the developed LC-MS method is able to resolve iodide and iodate from their interferents. Furthermore, the optimized clean-up procedure, based on weak anion exchange solid phase cartridges, allows a significant increase in sensitivity.

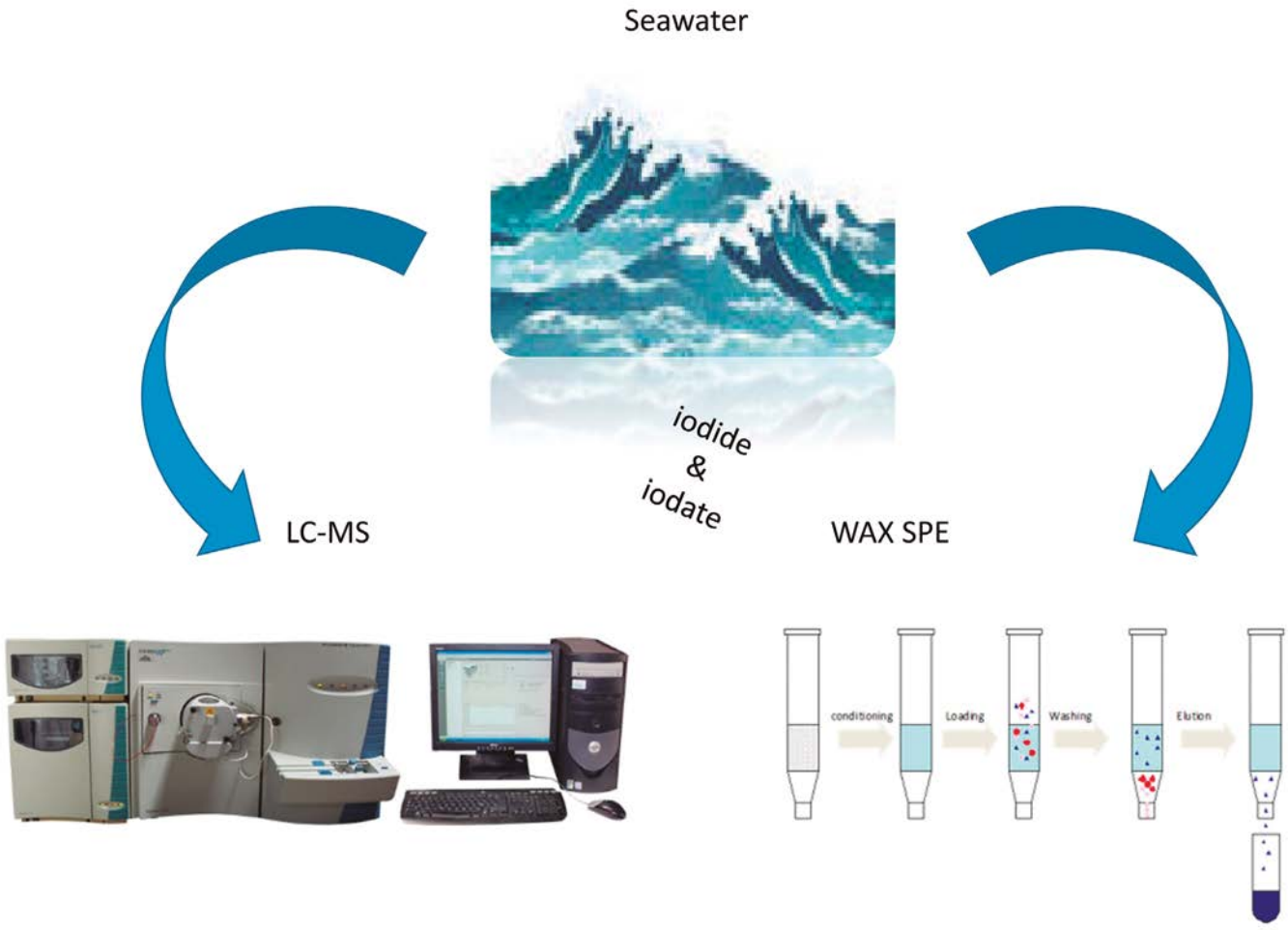

Figure 3: Determination of iodide and iodate in seawater.

Qualitative and quantitative study of sulfatides in myelin

Sulfatides are sulfoglycolipids found in the myelin sheath. The composition ratio of sulfatide molecular species changes with age, and it has also been associated with the pathogenesis of various human central nervous system diseases. However, profiling sulfatides in biological samples is difficult, due to the great variety of molecular species. Our group have developed a new, easy and reliable liquid chromatography-mass spectrometry (LC-MS) method to profile sulfatide content in biological samples of myelin.

A 'wrong-way-round' ionization effect has been described for this type of molecules for the first time, making it possible to identify as many as 37 different sulfatides, including molecules with different fatty acid chain lengths and varying degrees of unsaturation and hydroxylation. A chemometric analysis of their relative abundances showed that the main difference among individuals of different ages was the content of sulfatides with odd-numbered fatty acid chains, in addition to hydroxylated species.

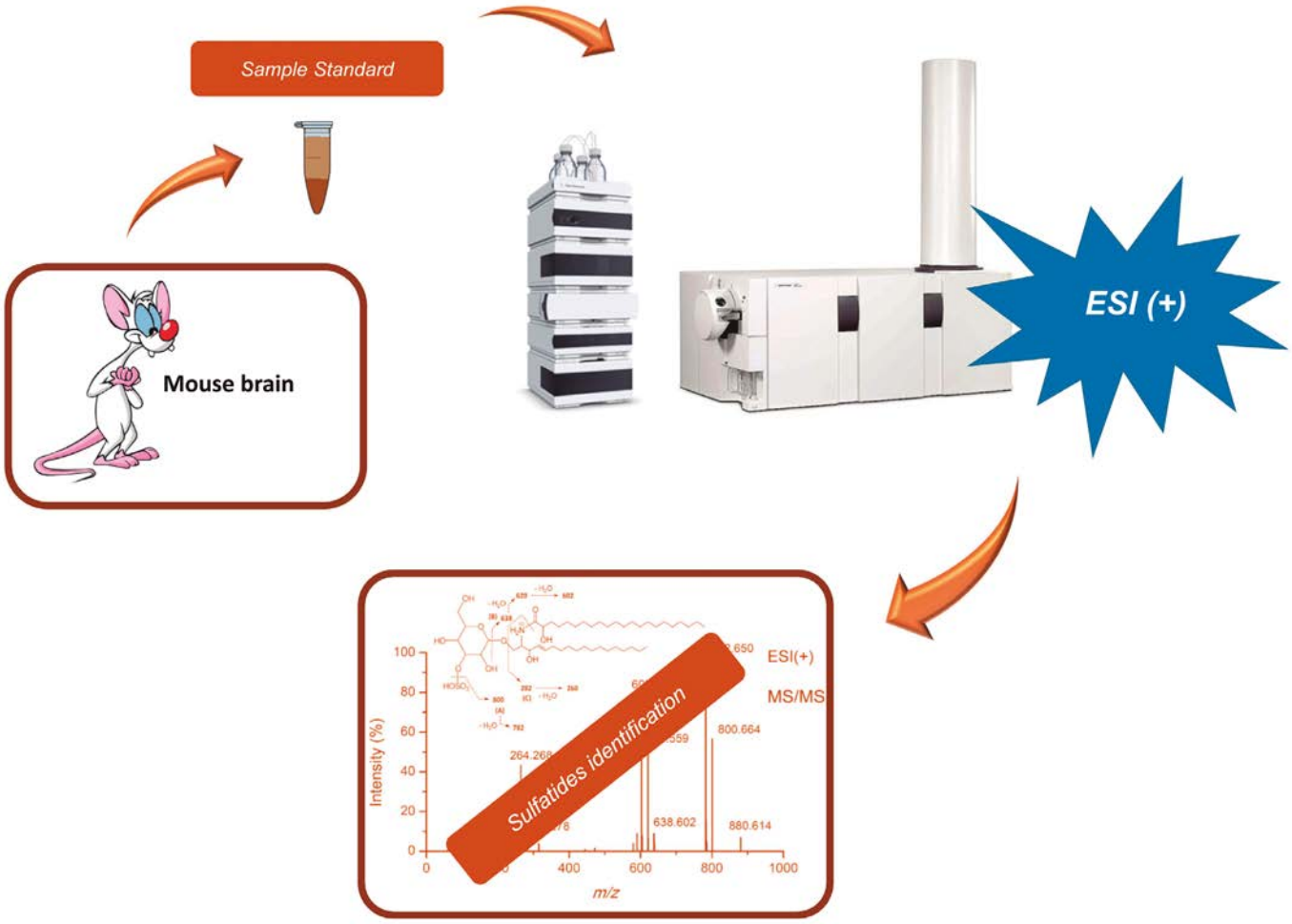

Figure 4: Analytical process to profile the sulfatides content in myelin from mouse brain.

Proanthocyanidin characterization of extracts from *Uncaria tomentosa L.*

Uncaria tomentosa L., also known as cat's claw, is a plant from South and Central America that is used in traditional medicine due to its anti-inflammatory properties. Bioactive properties have been attributed mainly to its alkaloid contents, however its antioxidant effect could be related to its phenolic contents. Although there are some reports concerning low-molecular-weight polyphenols in *U. tomentosa*, its polymeric phenolic composition has been scarcely studied. Thus, we studied the phenolic-rich extracts from leaves, stems, bark and wood of *Uncaria tomentosa* plants from several regions of Costa Rica in respect to their proanthocyanidin profile using a quadrupole-time-of-flight mass analyzer.

Main structural characteristics found for *U. tomentosa* proanthocyanidins were: (a) monomer composition, including pure procyanidins, pure propelargonidins and mixed proanthocyanidins; and (b) degree of polymerization, from 3 up to 11 units. These particularities of *U. tomentosa* proanthocyanidins suggest the potential value of these extracts with prospective use as functional ingredients.

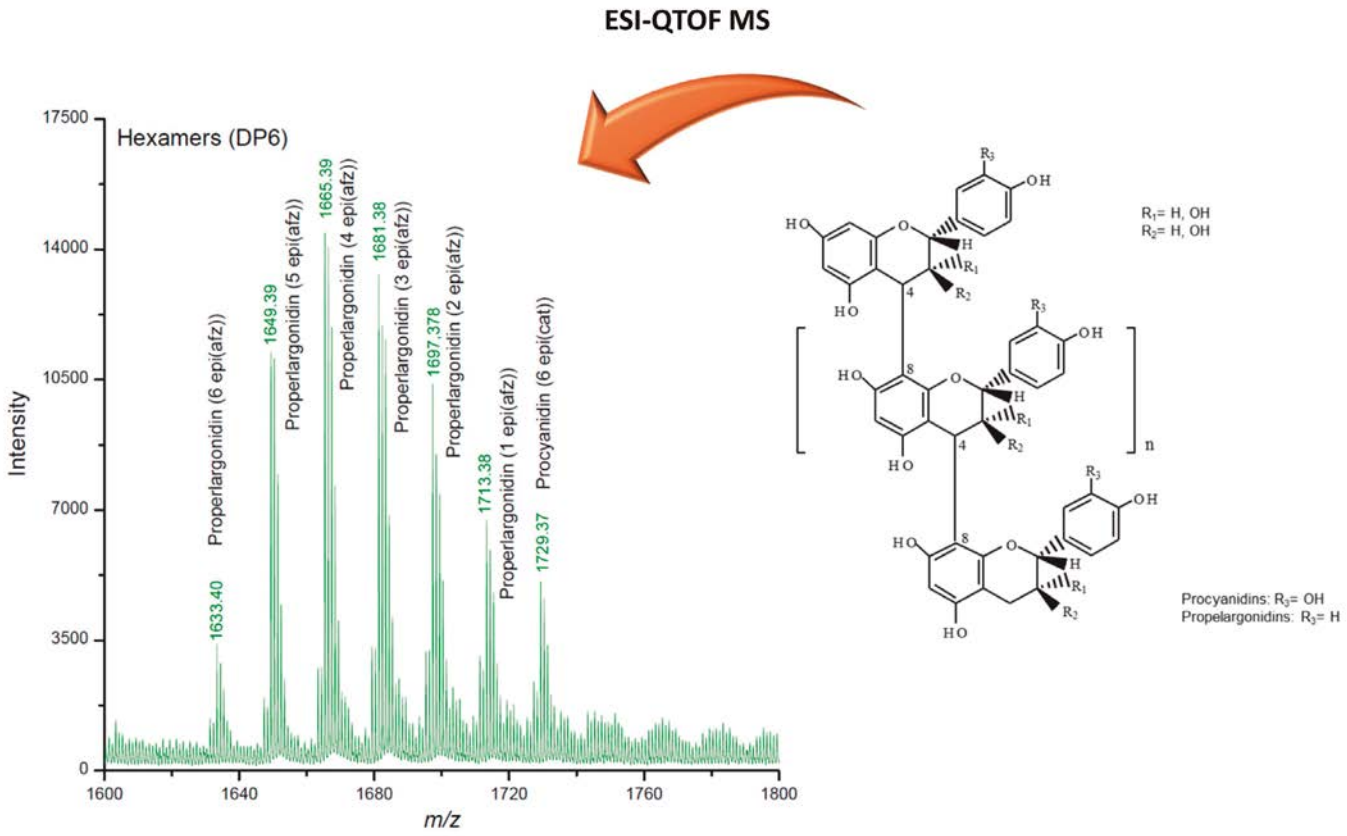

Figure 5: Mass spectrum of proanthocyanidins with DP=6 from a sample of *U. tomentosa* leaves.

Publications

Báez, J. E., Marcos-Fernández, Á., Martínez-Richa, A. & Galindo-Iranzo, P. Poly(ε-caprolactone) Diols (HOPCLOH) and Their Poly(ester-urethanes) (PEUs): The Effect of Linear Aliphatic Diols [HO–(CH2)m–OH] as Initiators. *Polym.-Plast. Technol. Eng.* **56**, 889-898, (2017).

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National Grants: coordinated

Comunidad Autónoma de Madrid

Principal Investigator	Title	Reference
Mª Luisa Marina Alegre	Estrategias avanzadas para la mejora y el control de la calidad y la seguridad de los alimentos	S2013/ABI-3028

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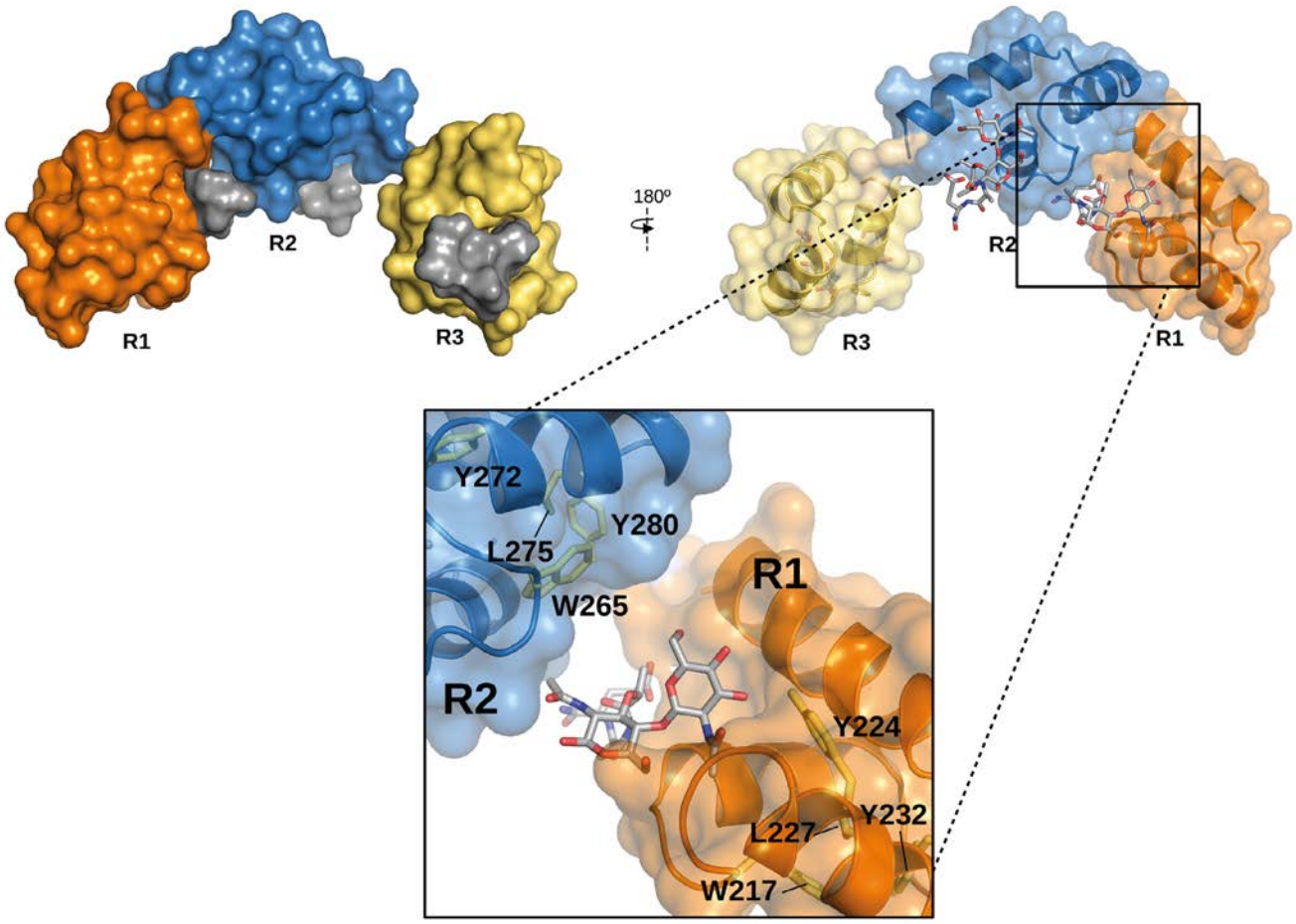
Department of Biological Physical Chemistry



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Introduction http://qfbio.iqfr.csic.es

Our research covers the fields of Biochemistry, Molecular Biology, Structural Biology, Biophysics, Glycobiology, Bioinformatics and Bio-thermodynamics. The objective of our on-going work is to understand the physical-chemical bases governing the structure, stability, dynamics and interactions of different biological molecules, such as peptides, proteins, nucleic acids and carbohydrates. This investigation is conducted on 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 characterisation: immunochemical 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-ms) and spatial (mm-sub mm) resolution, iii) solution NMR spectroscopy for determination of structure, dynamics and molecular recognition of biomolecules (two high-field NMR spectrometers, 600 MHz & 800 MHz, and the software required for multidimensional NMR spectra analysis, structure calculations and docking studies). Also, we develop novel methods for simulation, analysis and modelling of large biomolecular systems.

Group Structure

Group of NMR of Protein Structure, Dynamics and Interactions

http://rmnpro.iqfr.csic.es

Tenured Staff scientists

Marta Bruix Bayés
(Profesor de investigación/Professor)

Subramanian Padmanabhan Iyer
(Profesor de investigación/Professor)

María Ángeles Jiménez López
(Investigador científico/Associate Professor)
ORCID code: 0000-0001-6835-5850;
Researcher ID: C-7193-2008

Douglas V. Laurents
(Investigador científico/Associate Professor),
Orcid code: 0000-0002-4187-165X Researcher ID E-7527-2015, Research Gate: https://www.researchgate.net/profile/Douglas_Laurents

José Manuel Pérez Cañadillas
(Científico titular/Assistant Professor)

Non-tenured scientists

Paula Morales
(JdC, 1/3/2018 to 15/2/2019)

Javier Oroz Garde
(Postdoc)

Jesús Fernández Zapata
(Predoctoral: FPI 01/01/2014 to 31/12/2017 and research contract 01/02/2018 to 31/12/2018)

Diego Bernal Bernal
(Research contract 01/01/2018 to 31/12/2018)

Belén Chaves Arquero
(Predoctoral FPI)

Angélica Partida Hanon
(Until 31/08/2018)

Technical Staff

David Pantoja Uceda (TSE)

Miguel Ángel Treviño (TSE)

Sergio Camero Gigante

Strategic Aims

- New NMR methods to study IDPs (intrinsically disordered proteins) and detection of structural tendencies.
- Design of model peptides to understand solvent-driven structural transitions.
- Structure-activity relationships in peptides and proteins of biomedical relevance: applications in cancer, infections and allergy.
- Structural study of protein-nucleic acid complexes: applications in the control and regulation of gene expression.
- Characterization of the conformation and dynamics of amyloidogenic proteins.
- Protein-RNA structures relevant to understand mechanism in RNA biology
- Structural biology of disease-related RNA binding proteins
- Understanding the molecular mechanisms of cellular responses to light, discovery, biology, design and applications of photoreceptors in optogenetics and synthetic biology.

Remarkable Results

A novel CON-based NMR assignment strategy for disordered proteins with low signal dispersión was proposed and applied to the C-terminal domain of histone H1.0

Characterisation of intrinsically disordered proteins (IDPs), which are very abundant in eukaryotic organisms, is difficult sed. NMR is the best technique to get insights into the conformational and dynamics properties of IDPs. However, assignment methods commonly applied in globular proteins failed in the case of IDPs because of their repetitive sequences and low signal dispersion. We have proposed a novel strategy to assign NMR spectra of these proteins and have demonstrated its usefulness by applying it to the C-terminal of histone H1.0.

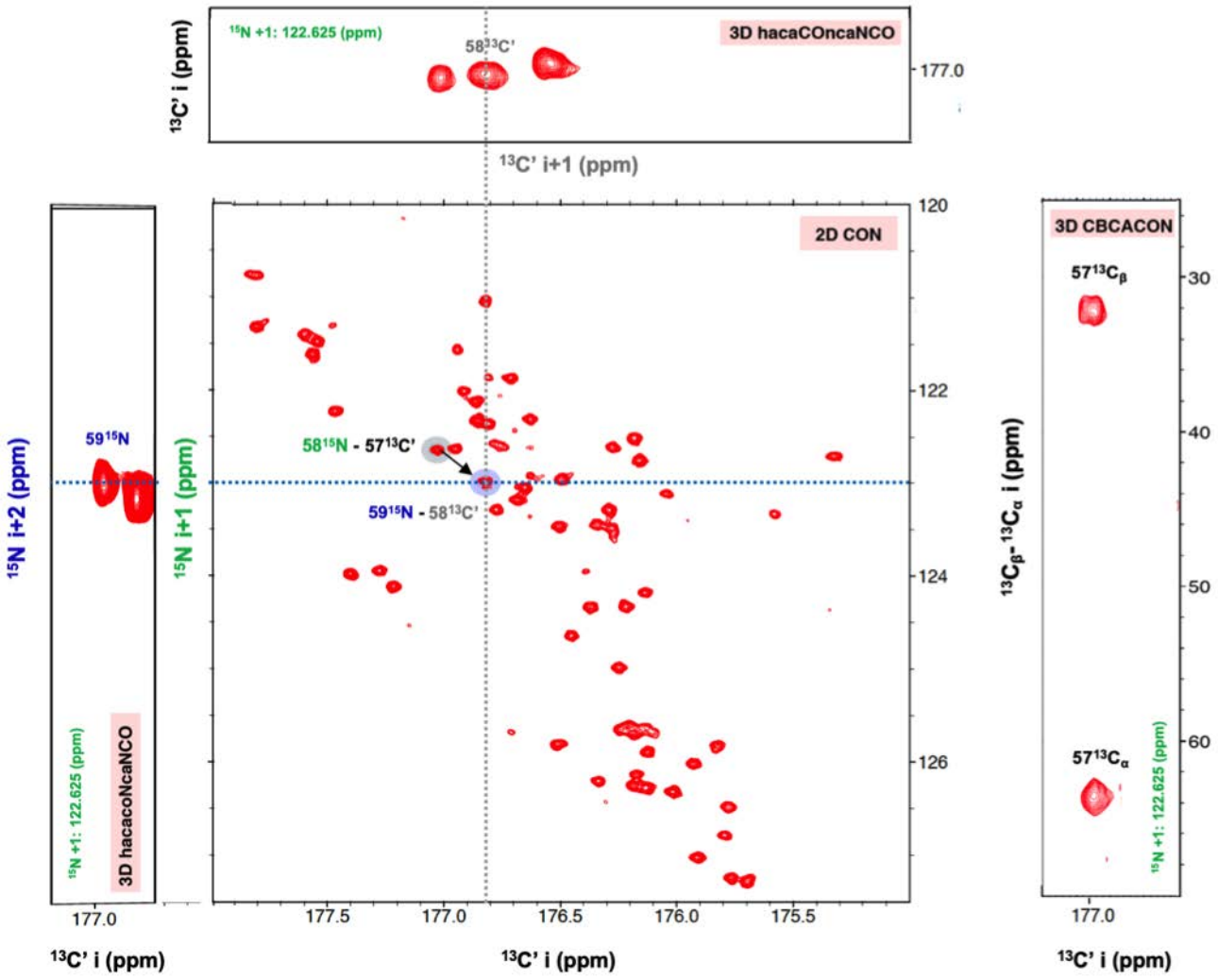

Figure 1: Selected spectral regions showing the novel ^{13}C-detected CON-based assignment strategy.

Hydrophobicity and amphipathicity as driving forces for helix stability in a chameleonic peptide

The structure of a 14-mer peptide switches between two ordered conformations: a β-hairpin in aqueous solution, and an α-helix in micelles. To understand the factors responsible for this unusual transition we designed a series of peptide variants. Based on their structural characterisation by NMR, CD and fluorescence, we found that, when the turn sequence is not optimal, side chain interactions will be essential for β-hairpin stability, and that both hydrophobicity (<H>) and amphipathicity (<μ_H>) are important for helix stabilisation in micelle media in a way unpredictable by current theoretical methods.

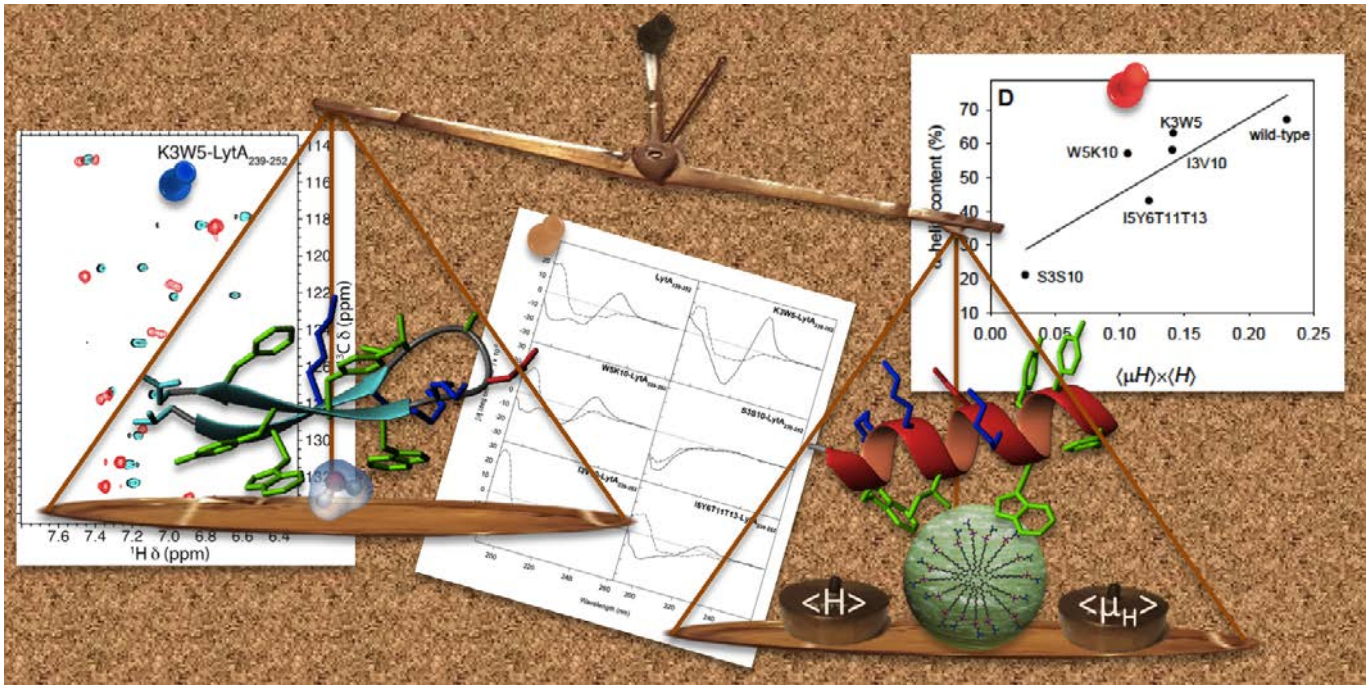

Figure 2: NMR & CD data of a series of peptides show that they form β-hairpins in aqueous solution, and α-helices in micelle media. Helix stability depends on the balance of hydrophobicity and amphipathicity.

Cool H-bonds Help Polyproline II Antifreeze Protein Corral Snowflakes

We have performed the first NMR characterization of a protein formed exclusively of polyproline II helices and is. Polyproline II (PPII) helices form collagen and transient PPII helices are believed to be present in intrinsically disordered proteins (IDPs) and may be key for amyloid formation, yet the bases of their stability are poorly understood. The snow flea antifreeze protein (sfAFP), which consists of a bundle of six PPII helices, is an attractive model system. Whereas attempts in other laboratories have hitherto failed, our successful production of recombinant sfAFP labeled with ^{13}C and ^{15}N has enabled its thorough characterization by NMR spectroscopy. Our results provide key insight to understand PPII helical bundle stability, revealing crucial contributions from Cα-H|||O=C H-bonds, and to detect these structures in IDPs.

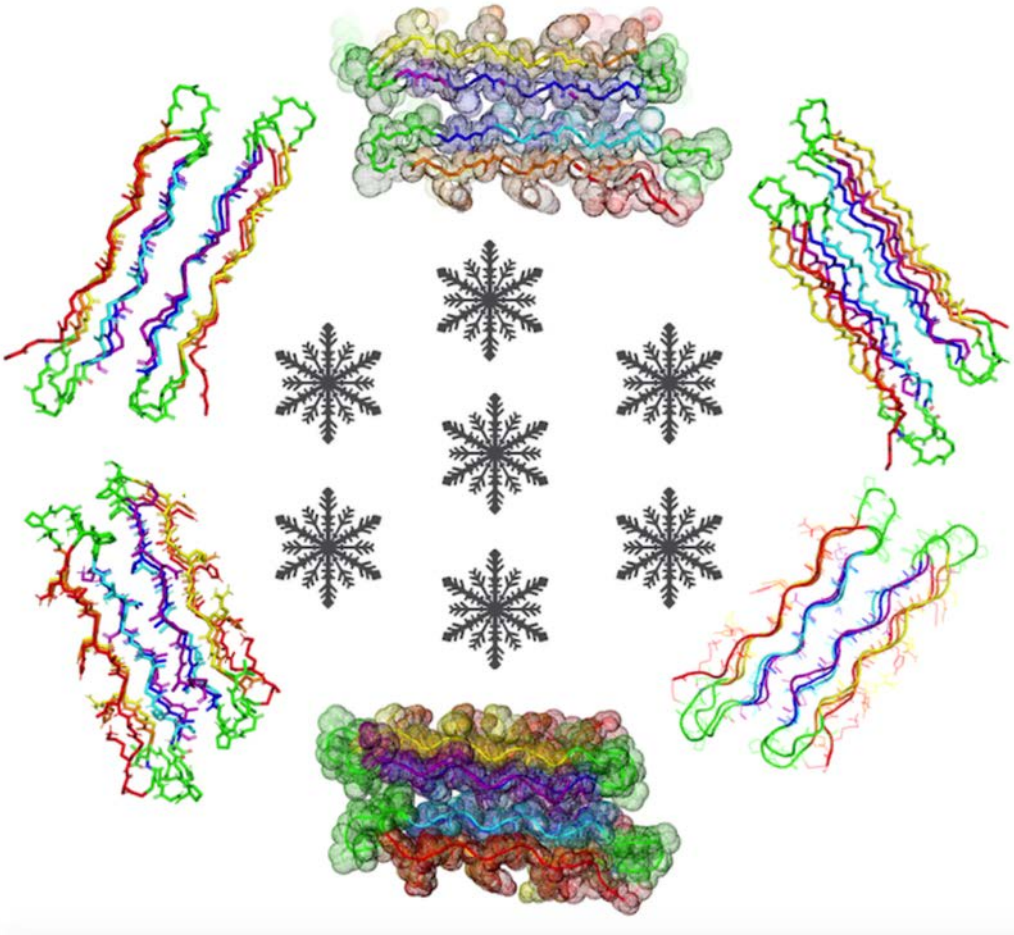

Figure 3: Six ribbon and shape filling structural models of the snow flea antifreeze protein dimer, which is formed exclusively of polyproline II helices and is crucially stabilized by Cα-H ||| O=C H-bonds.

Molecular basis of recognition of terminitation signals GUAA has been unravelled

We have determined the NMR and X-ray structures in collaboration with B. Gonzalez (X-ray Department) of Nrd1 RNA Binding Domain. The protein shows a novel fold of an RRM domain fused to a split-domain. The X-ray structure of various protein-RNA complexes unravel the molecular basis of recognition of termination signals GUAA. Structural water molecules are fundamental to determine base specificity at each of the four positions. The study is completed with cell biology and biophysics data.

Novel mechanisms for bacterial photosensory regulation and activation of CRISPR-Cas systems

1. In-depth review of the new and large family of B_{12}-dependent photoreceptors, their discovery, distribution and mode of action, and the structural and photochemical basis of how they orchestrate signal transduction and control gene expression. [*Annu. Rev. Biochem.* 86, 485-514 (2017)].
2. Discovery of a new multifactorial mechanism for regulated expression of a CRISPR-Cas system in the soil bacterium *Myxococcus xanthus*, which relies on an alternative σ factor of the ECF ("extracytoplasmic function") family, its anti-σ factor, and a global regulatory complex. The findings represent yet another aspect in the multifaceted biology of these intriguing prokaryotic immune systems. [*Nucleic Acids Res.* 46, 6726-6745 (2018)].

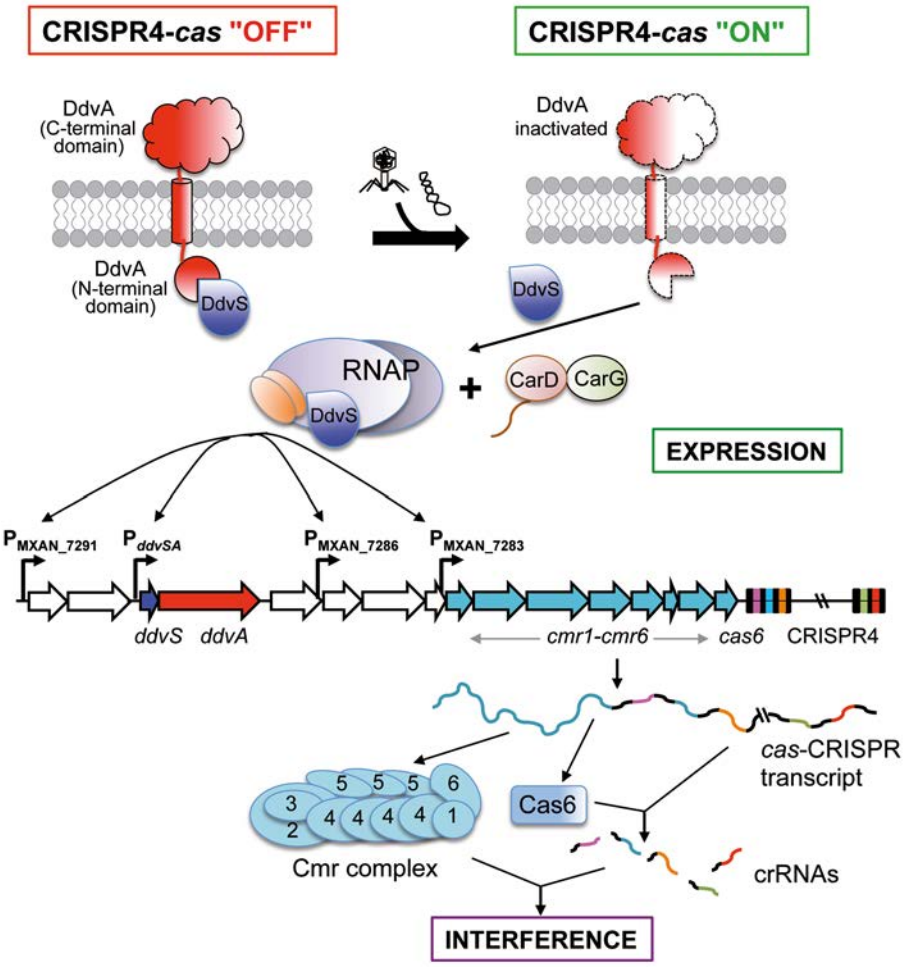

Figure 4: A novel mechanism controlling CRISPR-Cas expression, mediated by an extracytoplasmic function (ECF) σ factor (DdvS), its membrane-bound anti-σ (DdvA) and a global regulatory complex (CarD-CarG).

3. Demonstration of a remarkable plasticity in the mode of action of B_{12}-based CarH photoreceptors, which is important for their biological functions and development as optogenetic tools. [*J. Biol. Chem.* 293, 17888-17905 (2018)].

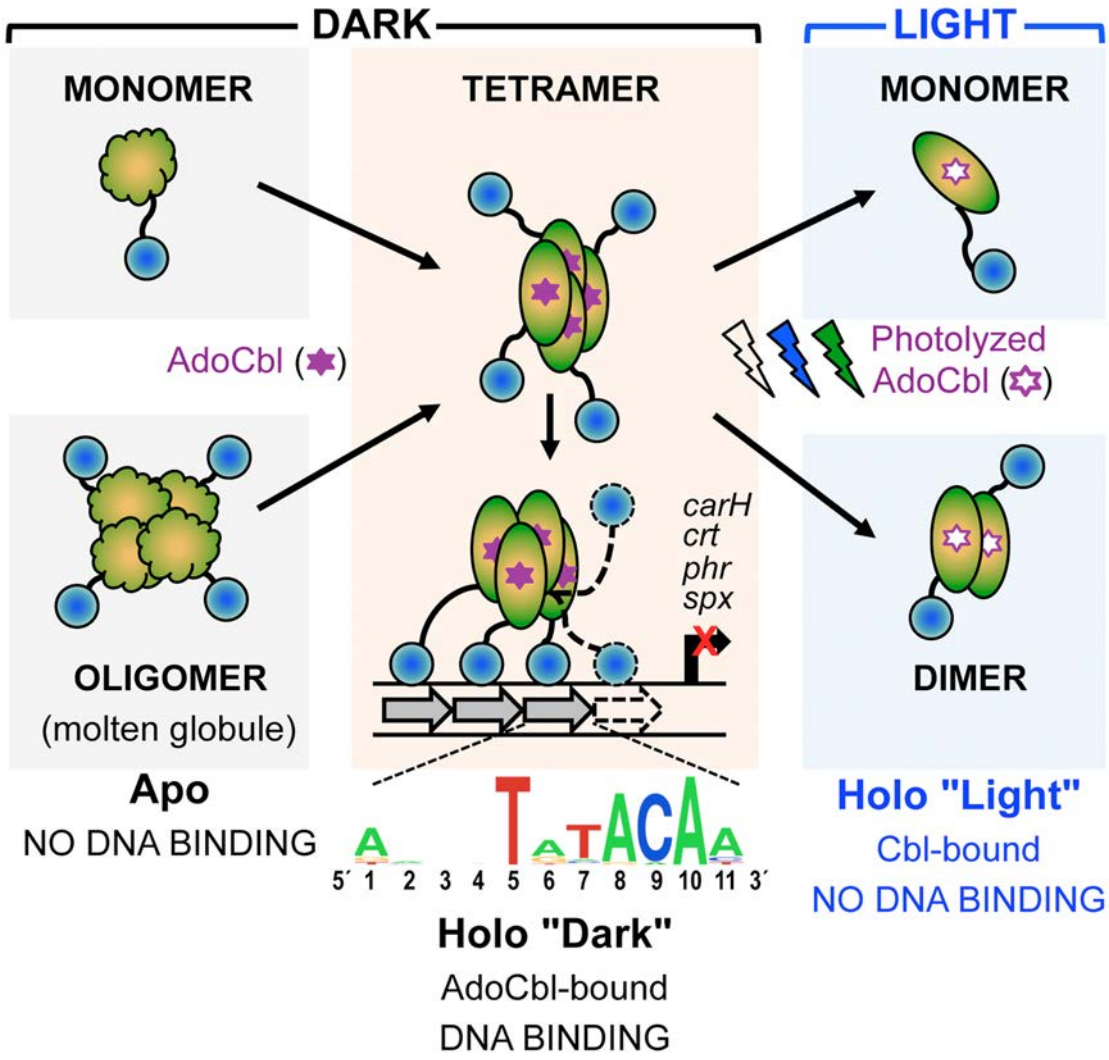

Figure 5: Plasticity in oligomerization, operator architecture, and DNA binding in the mode of action of B_{12}-based photoreceptors.

Publications

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COMPETITIVE FUNDING

National Grants: individual

Ministerio de Economía y Competitividad

Principal Investigator	Title	Reference
M. Ángeles Jiménez	Transiciones orden/desorden en reconocimiento molecular de proteínas: Estudio estructural por RMN	CTQ2017-84371-P
Marta Bruix & M. Ángeles Jiménez	Reconocimiento en sistemas complejos de biomoléculas mediante RMN: metodología, interacciones multimoleculares e IDPs	CTQ2014-52633P

National Grants: coordinated

MINECO

Principal Investigator	Title	Reference
Douglas Laurents	Determinants moleculares de dominios prionoides de amiloides funcionales versus patologicos: Hacia el desarrollo de nuevos inhibidores con aplicaciones terapeúticas	SAF2016-76678-C2-2-R
Subramanian Padmanabhan Iyer	Nuevos aspectos moleculares de la red fotorreguladora en la bacteria *Myxococcus xanthus* y su conservación evolutiva: análisis estructurales	BFU2015-67968-C2-2-P
Douglas Laurents	Estructura, estabilidad y optimización de complejos QBP1 + dominio prión de CPEB implicados en la inhibición de la consolidación de la memoría	SAF2013-49179-C2-2-R

Comunidad de Madrid. Programa de Biomedicina 2017

Principal Investigator	Title	Reference
José M. Perez Cañadillas. Encarna Martínez-Salas (Coordinator)	RNA y Proteínas de unión a RNA: Implicaciones en Salud y Enfermedad	B2017/BMD-3770
M. Ángeles Jiménez José M. Carazo (coordinator)	TomoXLiver: Estudio de la disfunción del hepatocito desde un abordaje multidisciplinar	B2017/BMD-3817

International Grants: coordinated

European Joint Programme in Neurodegenerative Diseases

Principal Investigator	Title	Reference
Douglas V. Laurents	Mising Link	EU JPND AC14/00037

Group of Protein Bioconformatics and Assembly

Tenured Staff scientists

María Gasset Vega (Investigador científico/Associate professor)

Technicians

Rosa Sánchez Herreros (1-01-2017, 20-09-2018)
Laura Montoya González (1-11-2017, 31-12-2018)
Raquel Pérez Tavarez (1-10-2018,31-12-2018)

Summary

The common thread to an increasing group of physiological and pathological functions is the formation of amyloid aggregates that can be used either as targets for intervention or as biotechnological tools for functional designs. Our main aims at LIFE-MATER intersection are:

1. to identify novel amyloids with relevance in food security.
2. to use both de novo generated and bioinspired sequences for the production of eco-friendly materials.

Strategic Aims

1. To determine the role played by amyloids in type-I food allergy for the enhancement of food security.
2. To develop novel amyloids for the production of bioinspired materials with added value.

Remarkable Results

1) Exploiting the gastric compartment as an amyloid-forming factory (Figure 1).

2) Biomaterial-unrelated protein amyloids efficiently seed calcite formation under novel shapes (Figure 1).

3) Amyloid spines are sequence selective RNA traps allowing its transport (Figure 1)

4) Mapping the MytC *in vitro* and *in vivo* wound healing activity in a short fragment (Figure 1).

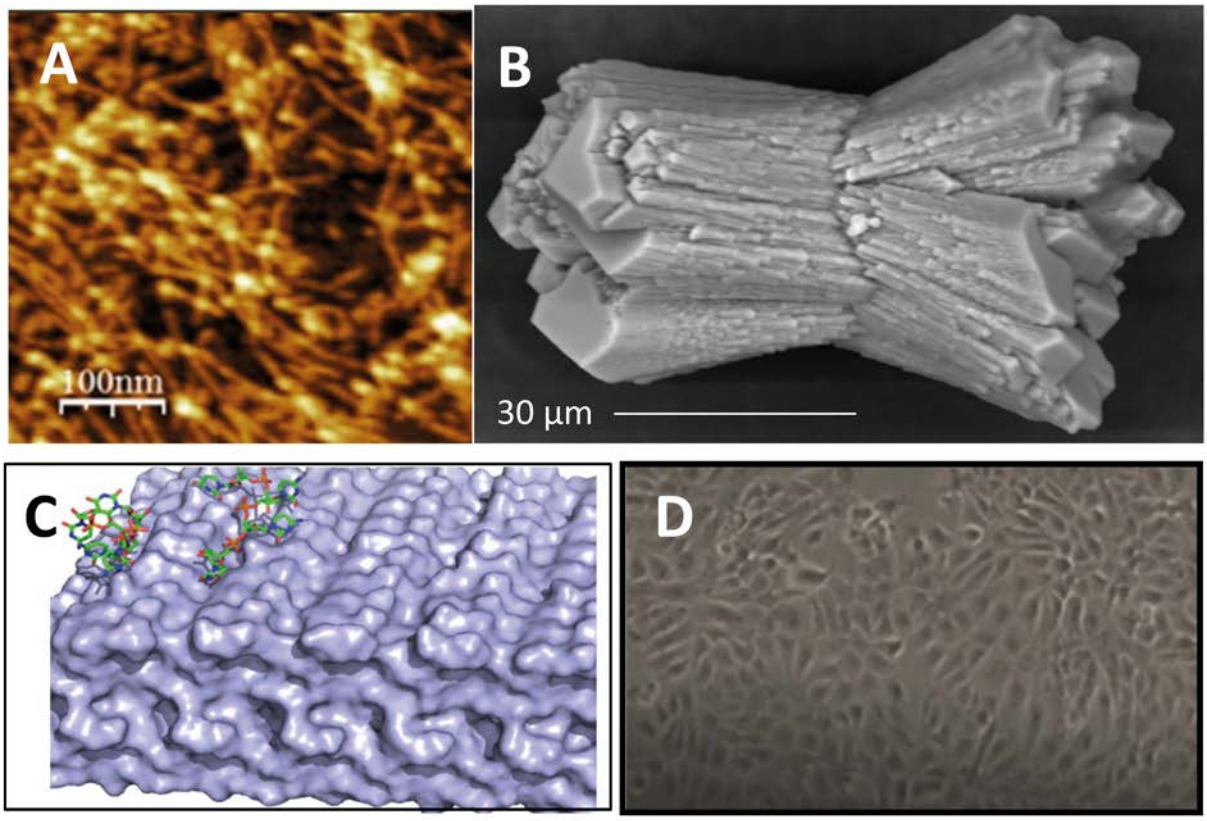

Figure 1: (A) Amyloid fibrils formed by Gad m 1, the major allergen from cod, under gastric conditions. (B) Gad m 1 amyloids seed calcite formation (B) Surface interaction of UCCU molecules with SNQNNF steric zipper. (D) Injured HaCaT-monolayer after treatment with Myt-C fragments.

Publications

Meli, M., Gasset, M.,& Colombo, G. Are Amyloid Fibrils RNA-Traps? A Molecular Dynamics Perspective. *Front Mol Biosci*. doi: 10.3389/fmolb.2018.00053 (2018).

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Castellanos, M., Torres-Pardo, A., Rodríguez-Pérez, R., & Gasset, M. Amyloid Assembly Endows Gad m 1 with Biomineralization Properties. *Biomolecules* doi: 10.3390/biom8010013 (2018).

National Grants: individual

MINECO

Principal Investigator	Title	Reference
Maria Gasset	GAVD-based pregenetic systems	BFU2015-72271-EXP
Maria Gasset	Amyloids in fish processed products	Angulas Aguinaga Contract (Tolera-CDTI)

Structural Bioinformatics Group

Tenured Staff scientists

Pablo Chacon Montes (Investigador científico/Associate professor)
SCOPUS 7005148641

Non-tenured scientists

José Ramón López-Blanco
Erney Ramírez-Aportela (Until 1-1-2018)

Summary

The Structural Bioinformatics Group (http://chaconlab.org) is focused on developing innovative techniques for the modeling, 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. To better understand such systems, we work on new bioinformatics tools for bridging the resolution gap between atomic structures with low to medium resolution experimental data from different biophysical techniques (e.g. X-ray crystallography, Electron microscopy, SAXS, etc). Our research lines include efforts to deal with the analysis and prediction of molecular flexibility with Normal-Mode Analysis (NMA), geometric algebra and other multiscale approximations. We also expand our interest to predict protein-protein and loop modeling. The developed methodologies are available via software distributions and web servers.

Strategic Aims

- Bridging the resolution gap with hybrid methods. We develop 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 with NMA and other multiscale approximations.
- Protein modeling. We develop tools for modeling protein structures and their interactions. This includes novel methods for protein-protein docking and loop modeling problems.

Remarkable Results

The structural characterization of large biomolecular complexes can be only tackled with coordinated application of complementary biophysical approaches. Computational hybrid methods bridge the gap between such experimental techniques. We develop several approaches to solve this problem that are accessible from our web. In collaboration with Prof. E. Nogales (U.C Berkeley) we have tested their usefulness in the interpretation of the inflammasome bound to flagelling (Tenthorey et al., 2017).

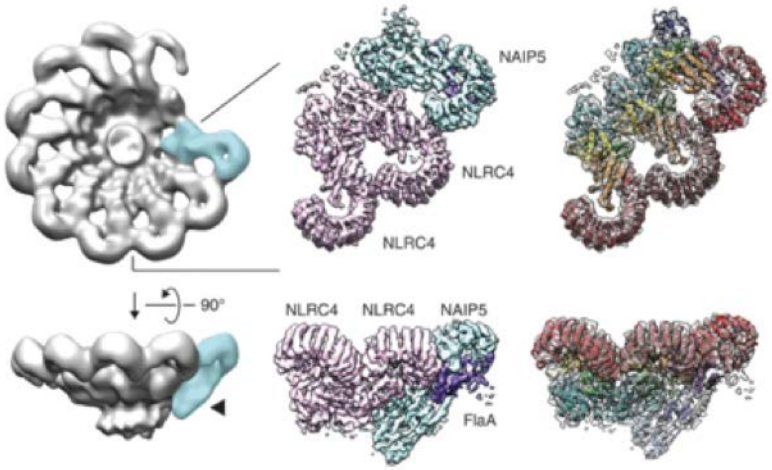

Figure 1: Modeling of the NAIPS inflamasomebound to flagelling from a 5.2 cryo-EM reconstruction.

Continuing our bioinformatics tools development, we have improved our servers for protein-protein prediction (http://frodock.chaconlab.org), for loop prediction (http://rcd.chaconlab.org), and for structural flexibility prediction (http://imods.chaconlab.org). In this context, we have recently developed KORP, a 6D knowledge-based pairwise coarse-grained potential for proteins. This state-of-the-art potential depends only on the relative position and orientation between residues (López-Blanco and Chacón, 2019).

Publications

Artola, M., Ruíz-Avila, L.B., Ramírez-Aportela, E., Martínez, R.F., Araujo-Bazán, L., Vázquez-Villa, H., Martín-Fontecha, M., Oliva, M.A., Martín-Galiano, A.J., and Chacón, P. (2017). The structural assembly switch of cell division protein FtsZ probed with fluorescent allosteric inhibitors. *Chem Sci* 8, 1525-1534.

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COMPETITIVE FUNDING

National Grants: individual

MINECO

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

Group of Fluorescence and Molecular Biophysics

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Technical Staff

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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.

The multi-disciplinary nature of these studies often requires a very close collaboration between different laboratories, institutions, and pharmaceuticals companies.

Methodology. We develop and implement both theoretical and experimental "tailored" methods based on ps-resolved fluorescence spectroscopy and two-photon excitation microscopy (micro-spectroscopic imaging), to provide the required temporal (ps-s) and spatial (subμm-nm) resolution *in vitro*, in living cells and tissues:

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.

Strategic Aims

Quantitative characterization of molecular interactions, mainly in cellular membranes, subcellular compartments, and hybrid materials: in vitro and living cell studies.

Results

The most relevant results for this period cover the following three topics:

1. Dynamic cellular maps of molecular species: Application to drug-target interactions.

We were able to follow, in real time, the formation and relative distribution of two sets of drug (Plitidepsin, APL)- target (elongation factor eEF1A2) complexes in living cells, revealing two distinct patterns of behavior for HeLa-wt and APL resistant HeLa-APL-R cells. These findings opened new avenues of study to decipher the mechanism of action of the antitumor drug APL.

Methodology: Generalized Polarization (GP) imaging, Phasor approach and fluorescence lifetime imaging microscopy (FLIM-phasor) (García et al. 2018).

2. Dynamics and 3D organization of active hydrogels actuated by biological living FtsZ polymers.

We were able to characterize simultaneously the structure of collagen hydrated gels and the fluorescently labeled FtsZ filaments (Figure 1).

Methodology: Second harmonic generation (SHG) imaging and FLIM-phasor approach.

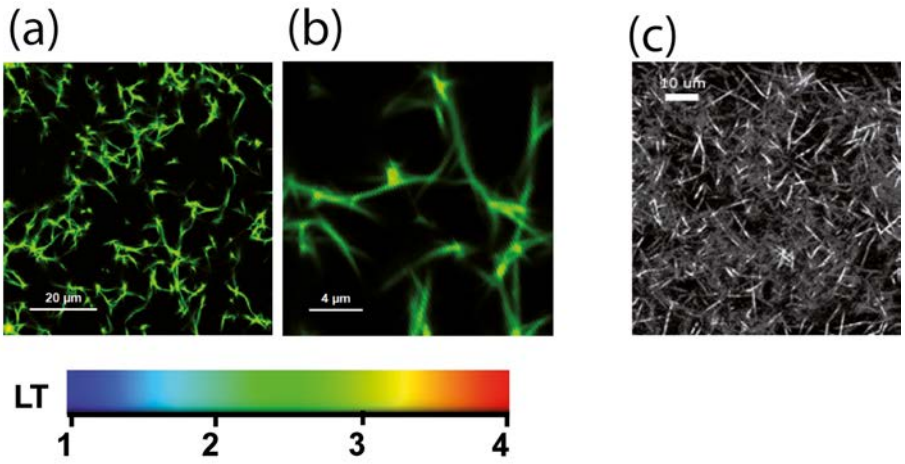

Figure 1: FtsZ /collagen hybrid material in buffer solution. T=20ºC. (**a**) FAST FLIM XY section of Alexa 488 (A488) fluorescent labelled FtsZ polymers. λ_{exc} =780nm; λ_{em}=520/35nm. Lifetime LT scale 1-4ns. (**b**) FAST FLIM zoom of a representative region of the previous image (**a**). (**c**) SHG XY imaging of collagen type I fibers.

3. Membrane adhesion induced by NAO stacking accounts for the supramolecular basis of its cytotoxicity.

In this work, we have revealed the mechanism by which the fluorescent dye 10-nonyl acridine orange (NAO) exhibits cytotoxicity when used at high micromolar concentrations (Almendro-Vedia et al. 2018).

Methodology: FLIM-phasor approach. Living and model membrane GUVs studies

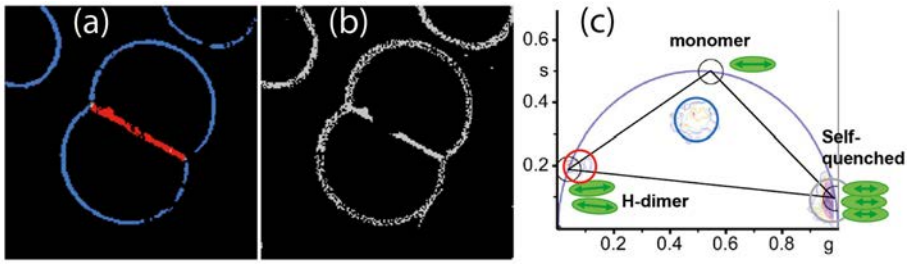

Figure 2: Spatial distribution of NAO molecular species in E-coli polar lipid extract (PLE) vesicles. Lifetime color maps of NAO molecular species at two emission regions, the red channel (**a**) and green channel (**b**). Pixels corresponding to the cluster of phasors enclosed by the colored circles are highlighted on the intensity image using the same color. (**c**) Phasor plot showing the phasor cluster locations corresponding to regions enriched in long-lifetime NAO antiparallel H-dimers (red cursor), intermediate-lifetime NAO monomers (blue cursor), and short-lifetime self-quenched NAO aggregates (grey cursor). Black cursors on the phasor plot represent 100% pure NAO species: NAO antiparallel H-dimers, monomeric NAO, and self-quenched NAO aggregates (Almendro-Vedia et al., 2018).

Publications

de la Fuente-Herreruela, D., González-Charro, V., Almendro-Vedia, V.G., Morán, M., Martín, M.A., Lillo, M.P., Natale, P & López-Montero, I. Rhodamine-based sensor for real-time imaging of mitochondrial ATP in living fibroblasts. *BBA - Bioenergetics* 1858, 999-1006 (2017). doi: 10.1016/jbbabio.2017.09.004

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COMPETITIVE FUNDING

National Grants: coordinated

Ministerio de Economía y Competitividad
Universidad Complutense de Madrid

Principal Investigator	Title	Reference
F. Monroy, I.López-Montero	Materia activa accionada mediante polímeros vivos biológicos: de la estocasticidad a la mecánica macroscópica a través de la hidrodinámica	FIS2015-70339-C2-1-R

CSIC.ICP-IQFR

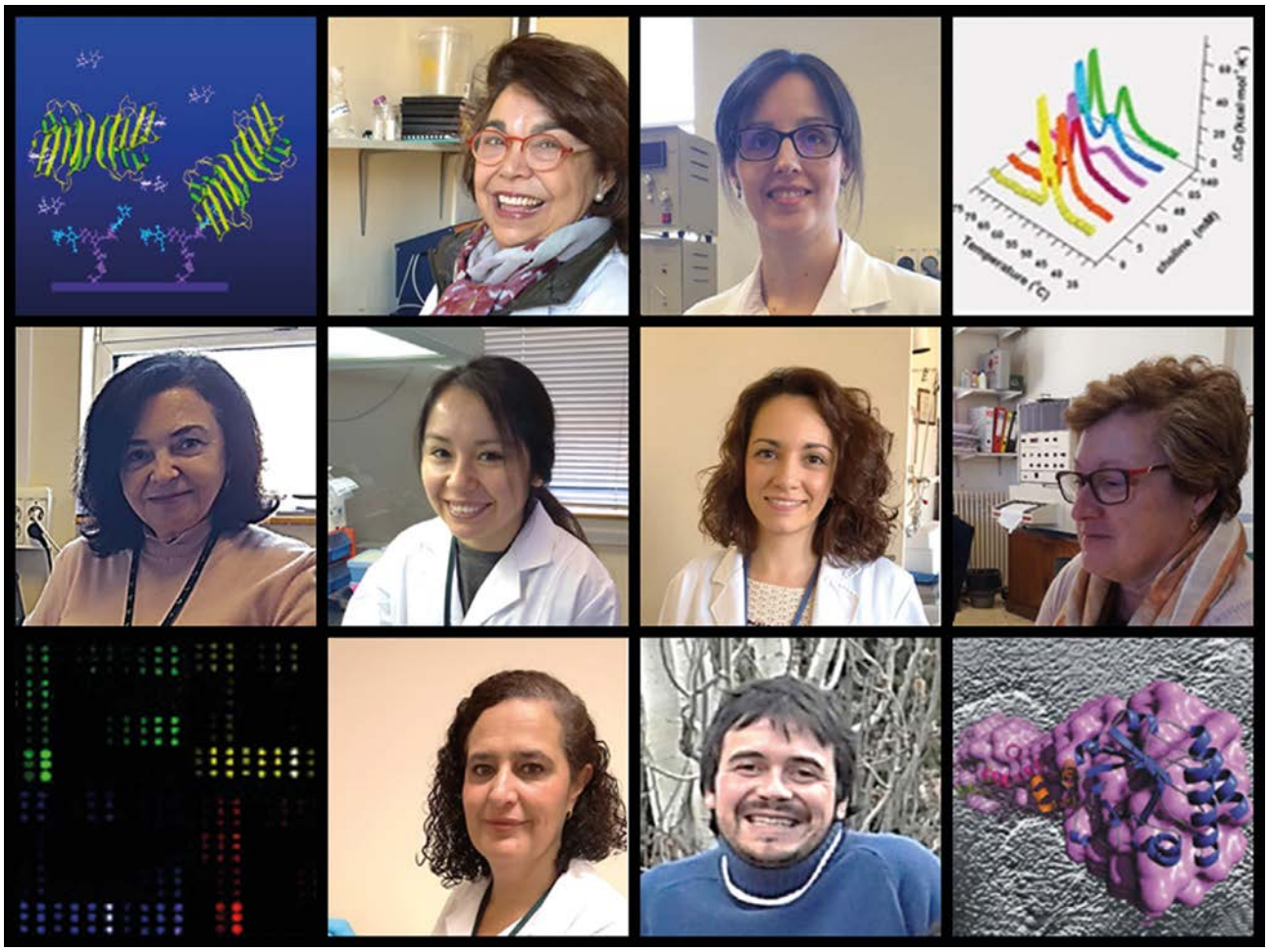
Principal Investigator	Title	Reference
M. Vélez, M.P.Lillo	Hidrogeles activos actuados por polímeros biológicos vivos: mecánica y dinámica de las proteínas fuera y dentro del hidrogel	FIS2015-70339-C2-2-R

Contracts and Agreements with Companies

Contrato I+D CSIC-PharmaMar S.A.

Principal Investigator	Title	Reference
Lillo, M.P.	Estudio de las interacciones de Aplidina e Irvalec con la membrana celular	20131162

Group of Protein Structure and Thermodynamics



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(National project contract)

Manuel Iglesias Bexiga
(CIBERES contract; until 09/09/2017)

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(Specialized Technician)

Noelia Hernández Ortiz
(Contrato garantía juvenil (CAM), until 30/06/2018; Specialized Technician (MINECO Project), since 01/08/2018)

Zarina Méndez Onoc
(Contrato garantía juvenil (CAM), since 01/04/2017)
* Para aquel personal sin vinculación durante todo el periodo indicar fechas de alta y baja.

Summary

Breve descripción del grupo. IMPORTANTE: incluir hipervínculos a la página web del grupo o servicios gestionados por el mismo (bases de datos, etc.). No aplica a los departamentos monogrupo

Knowledge of the structure and energetics of proteins in solution provides information on the nature of forces governing structural stability or ligand recognition, among other properties. This information is particularly relevant for proteins of biomedical or technological interest, since it facilitates a rational design of bioactive compounds (drugs, vaccines, etc.), or the stabilization of proteins themselves, what is in line with the objectives of the group (http://mabio.iqfr.csic.es/en/). During the last two years we have studied, among other systems, different lectins, cell wall hydrolases with antibacterial capacity, either natural or *de novo* designed, and other proteins of biomedical or biotechnological interest. In addition, we have investigated the recognition of carbohydrates and other compounds by these and other proteins, with the final aim of elucidating their role in numerous processes of biomedical relevance, as host–pathogen interactions or virulence, and developing new diagnostic and/or therapeutic strategies. In parallel, the glycosylation patterns of bacterial surfaces and cell-derived exosomes have also been examined in the search of distinctive signatures and new biomarkers.

Strategic Aims

- Study of carbohydrates as biological recognition signals and of protein carbohydrate interactions of relevance to health and disease.
- Bacteria glycophenotyping and identification of receptors involved in carbohydrate-mediated bacteria–host interactions.
- Development of novel microarray approaches for molecular recognition studies.
- Identification and development 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) Set-up of a microarray approach for evaluation of uropathogenic *Escherichia coli* adhesion and efficiency of mannose-specific FimH-targeted antiadhesive compounds.

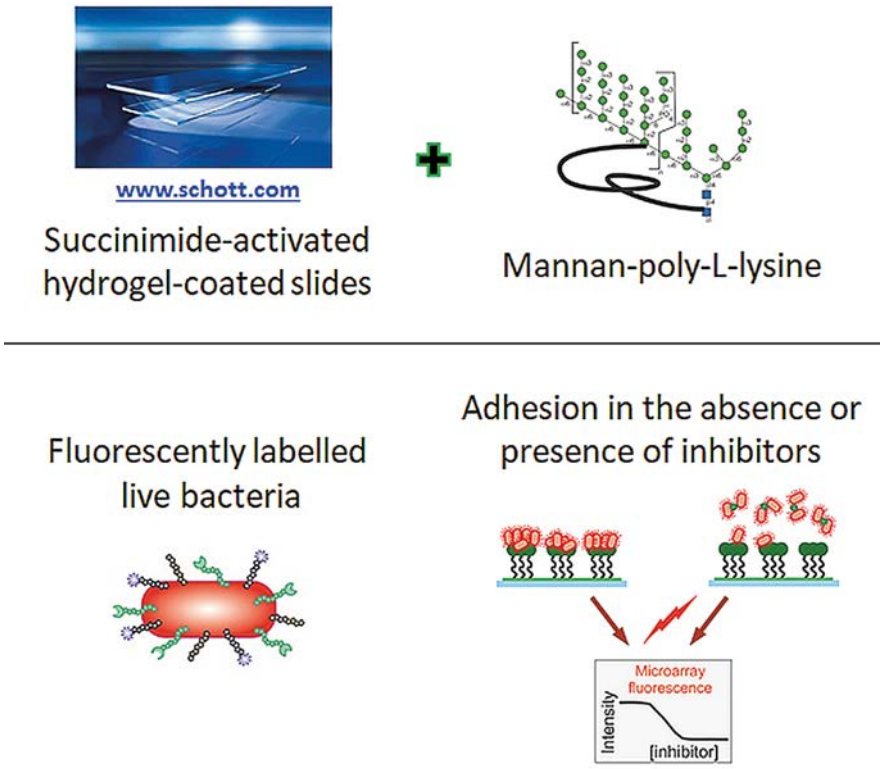

Figure 1: Microarray approach developed for evaluation of *Escherichia coli* UTI89 adhesion and efficiency of anti-adhesive compounds, using mannan-poly-L-lysine covalently printed onto succinimide-activated hydrogel-coated slides and binding assays of fluorescently labelled live bacteria in the absence or presence of inhibitors.

ii) Uncovery of a differential recognition of nontypeable *Haemophilus influenzae* cells and isolated lipooligosaccharides by the galactose-specific agglutinins from *Viscum album* and *Ricinus communis*.

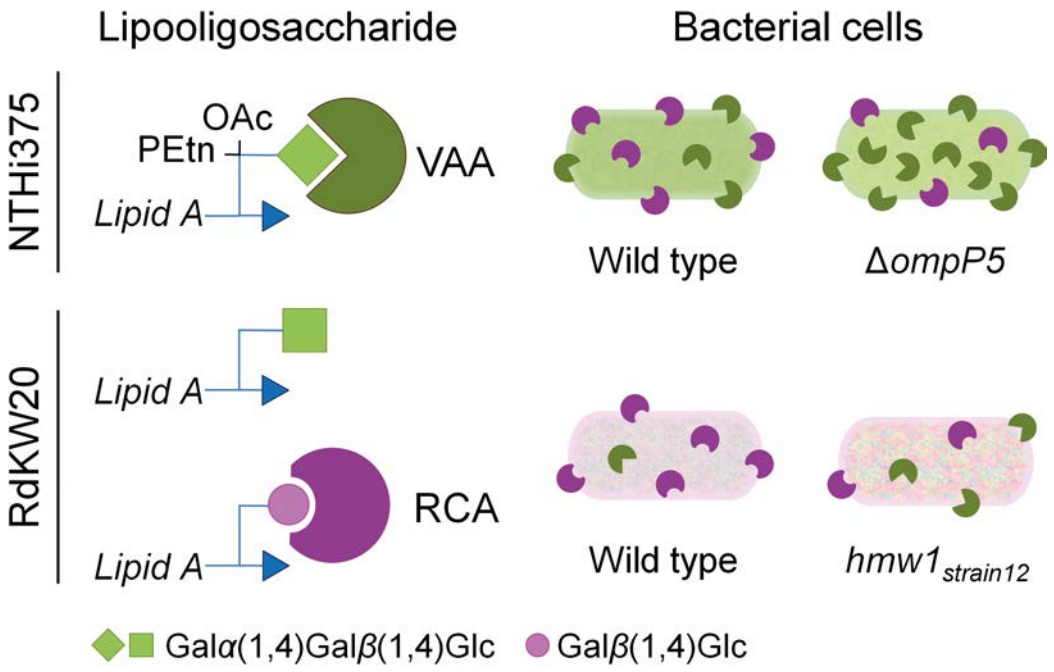

Figure 2: Illustration of the differential recognition by VAA and RCA of isolated LOSs and whole cells of *H. influenzae* strains NTHi375 and RdKW20, and of their mutants NTHi375Δ*ompP5*, which overexpresses the LOS, and RdKW20*hmw1*$_{strain12}$, which expresses the HMW1 glycoprotein that is absent in the wild type strain.

iii) Glycoprofiling of *Klebsiella pneumoniae* clinical isolates, unveiling a specific glycotope present in hypervirulent strains with hypermucoviscous phenotype.

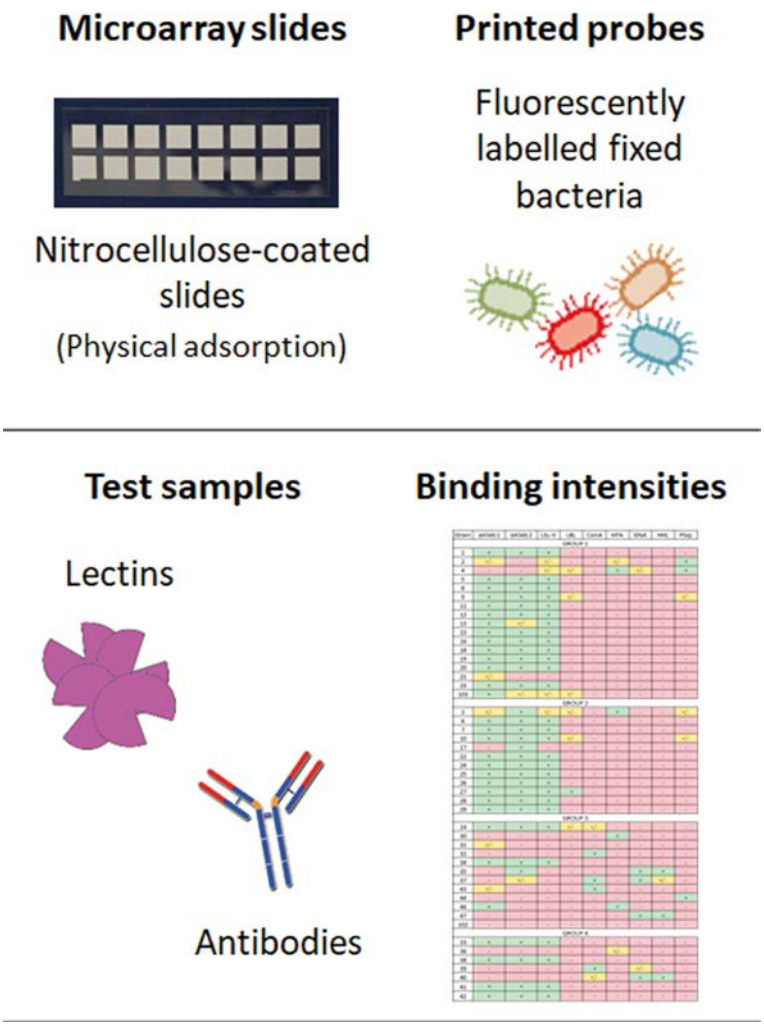

Figura 3: Microarray approach used for glycophenotyping of Hmv/non-Hmv *K. pneumoniae* clinical isolates, using fluorescently labelled fixed bacteria printed on nitrocellulose-coated slides and a panel of anti-*K. pneumoniae* antibodies and lectins with various binding specificities.

iv) Development of a new microarray set-up for high throughput screening of the glycosylation of exosomes, as potential biomarkers.

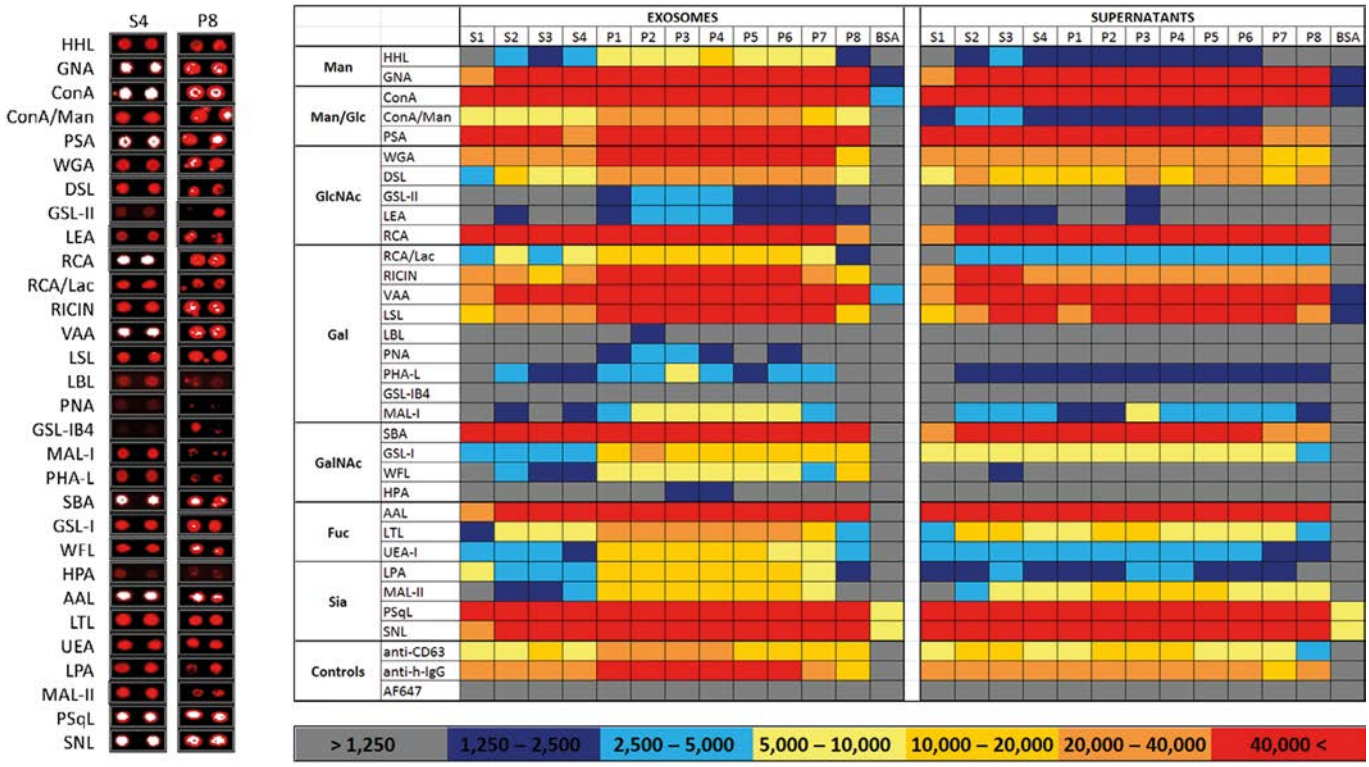

Figura 4: Lectin binding fingerprints of exosomes isolated from sera of healthy controls (S1-S4) and from patients with chronic obstructive pulmonary disease (P1-P8), in comparison with the supernatants of exosome isolation. The colour code corresponds to the fluorescence intensities (relative fluorescence units) specified at the bottom. Representative microarray images for lectin binding to two exosome samples are shown on the left.

v) Elucidation of the mechanism of recognition of the bacterial peptidoglycan by the cell wall binding repeats of the Cpl-7 enzybiotic.

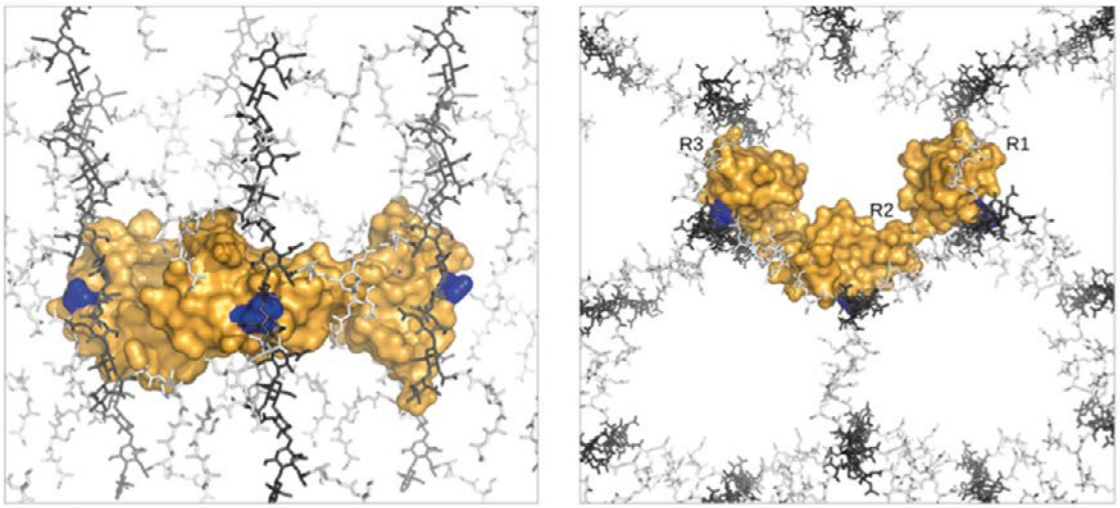

Figura 5: Lateral (left) and apical (right) view of the SAXS-based model of C-Cpl-7 superimposed into a pore of the NMR-based model structure of the bacterial cell wall. Glycan strands (black) and peptide stems (grey) are shown in stick representation. C-Cpl-7 surface is shown in orange, with the N-acetyl-D-glucosaminyl-(β1,4)-N-acetylmuramyl-L-alanyl-D-isoglutamine" binding site of each repeat (R1, R2 and R3) highlighted in blue. Site disposition is compatible with a 1:3 C-Cpl-7-to-GMDP stoichiometry involving three different glycan chains.

vi) Design, production, and evaluation of Csl2, a novel chimeric enzybiotic to fight infections caused by *Streptococcus suis.*

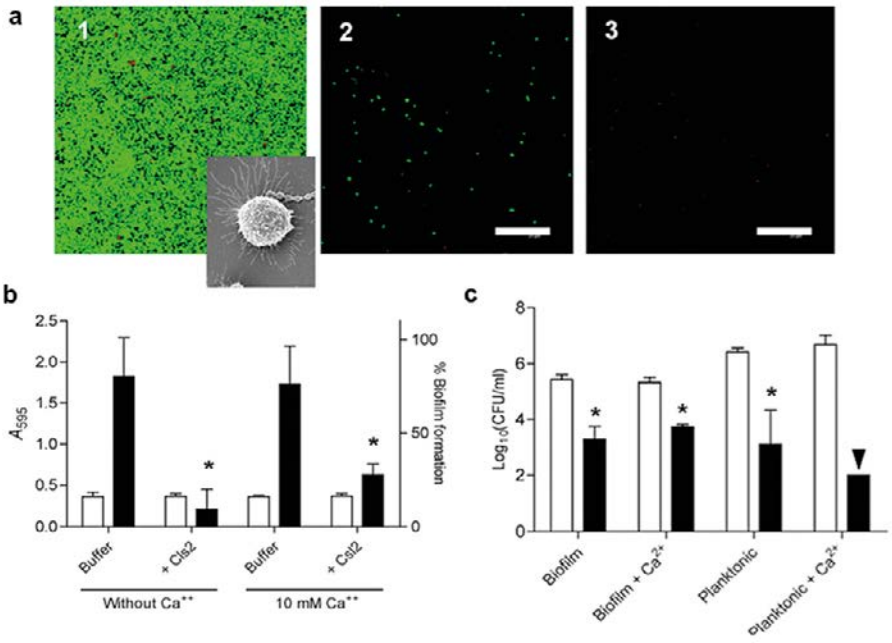

Figure 6: (**a**) CLSM image of the viability of biofilm-grown *S. suis* DB101 untreated (Buffer; panel 1a) or treated with 15 μg/ml (2a) and 30 μg/ml (3) Csl2 for 1h (scale bars, 25 μm). Biofilms were stained with BacLight LIVE/DEAD kit to reveal viable (green fluorescence) or nonviable (red fluorescence) bacteria. (**b**) Antibiofilm activity quantification by crystal violet staining of untreated (buffer) and treated biofilms (30 μg/ml Csl2; 1h at 37 ºC). White and black bars represent the growth of adherent plus non-adherent cells, and the percentage of biofilm remaining with respect to maximum biofilm formation, respectively. (**c**) Viable counting from samples of biofilms and planktonic of the biofilms treated (black bars) or not (white bars) with 30 μg/ml Csl2. The arrowhead means a value below detection. Asterisks denote statistical significance of data with relation to controls (P<0.0001).

vii) Characterization of the DNA substrate preferences of the *Leishmania infantum* endonuclease EndoG, associated with programmed cell death.

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Singh, A.K., Nguyen, T.H., Vidovszky, M.Z., Harrach, B., Benk, M., Kirwan, A., Joshi, L., Kilcoyne, M., Berbis, M.A., Cañada, F.J., Jiménez-Barbero, J., Menéndez, M., Wilson, S.S., Bromme, B.A., Smith, J.G., van Raaij, M.J (2018). Structure and N-acetylglucosamine binding of the distal domain of mouse adenovirus 2 fibre. *J. General Virol.* 99: 1494. doi: 10.1099/jgv.0.001145. PMID:30277856.

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COMPETITIVE FUNDING

National Grants: individual

MINECO

Principal Investigator	Title	Reference
Margarita Menéndez & 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 NMR of Nucleic Acids

http://rmnac.iqfr.csic.es/en

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Non-tenured scientists

Miguel Garavís Cabello (Juan de la Cierva)

Israel Serrano Chacón (predoctoral, FPI)

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 acids and proteins and small ligands.
- To study artificial nucleic acids.

Remarkable Results

Non-canonical DNA structural studies

We have observed that some i-motif can be formed at physiological pH provided the stack of C:C+ base pairs are flanked by minor groove tetrads.These tetrads result from the association of two G:C or G:T base pairs through their minor groove side, forming G:T:G:T, G:C:G:T or G:C:G:C tetrads. We have called these structures "mini i-motif" and we have found that they are prevalent in the human genome, being particularly common in regulatory regions.

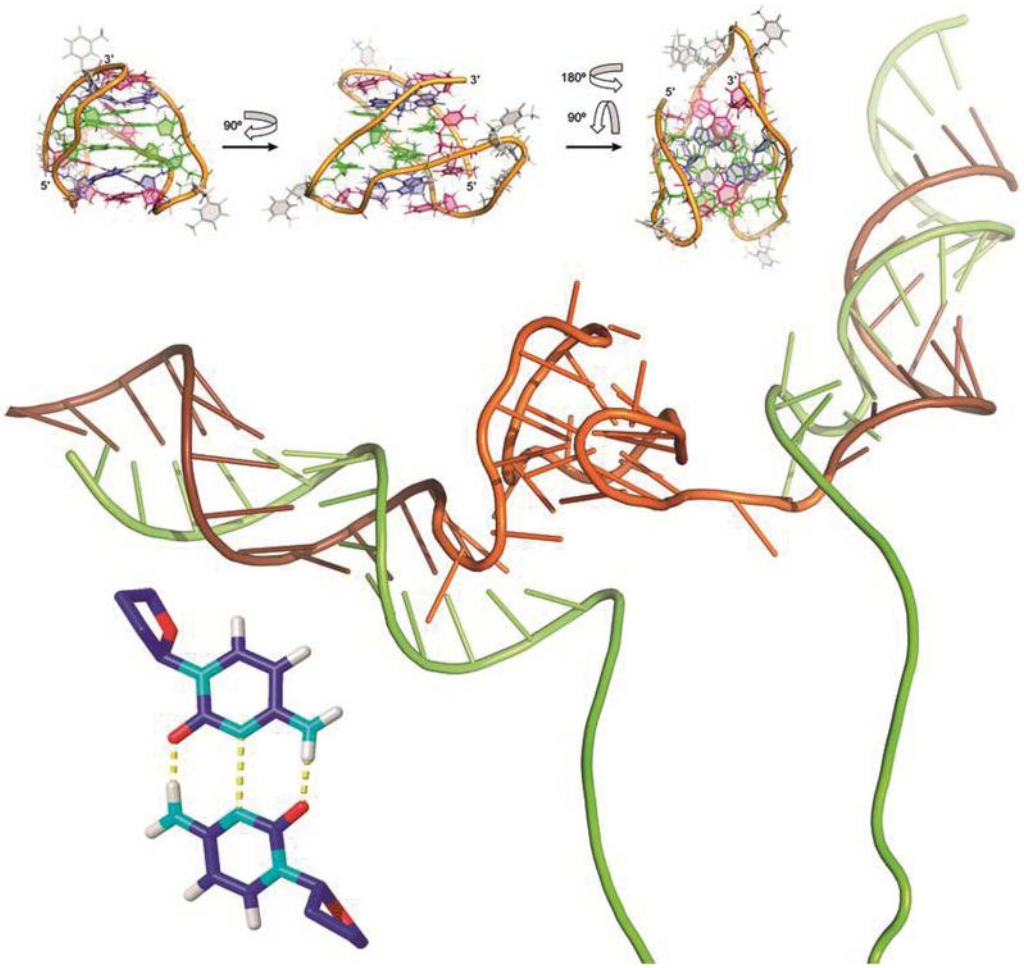

Figure 1: Structure of a minimal i-motif and illustrative representation of its formation in genomic DNA

Nucleic acids with chemical modifications

We have explored the effect of several chemical modifications in the stability of i-motif structures. Most of them have a destabilizing effect, or are barely tolerated. However, 2´-fluoro-arabino-cytidines (2'F-araC) provoke a dramatic stabilization in different conditions, including neutral pH. Moreover, combination of 2´-fluoro-arabino-cytidines with 5-Met-cytidines provokes an extreme stabilization at neutral pH.

Of particular importance, it is our recent observation that 2'F-araC substitutions in G-quadruplexes and i-motifs are able to trap these structures, slowing done the hybridation of the complementary strands in human telomeric DNA.

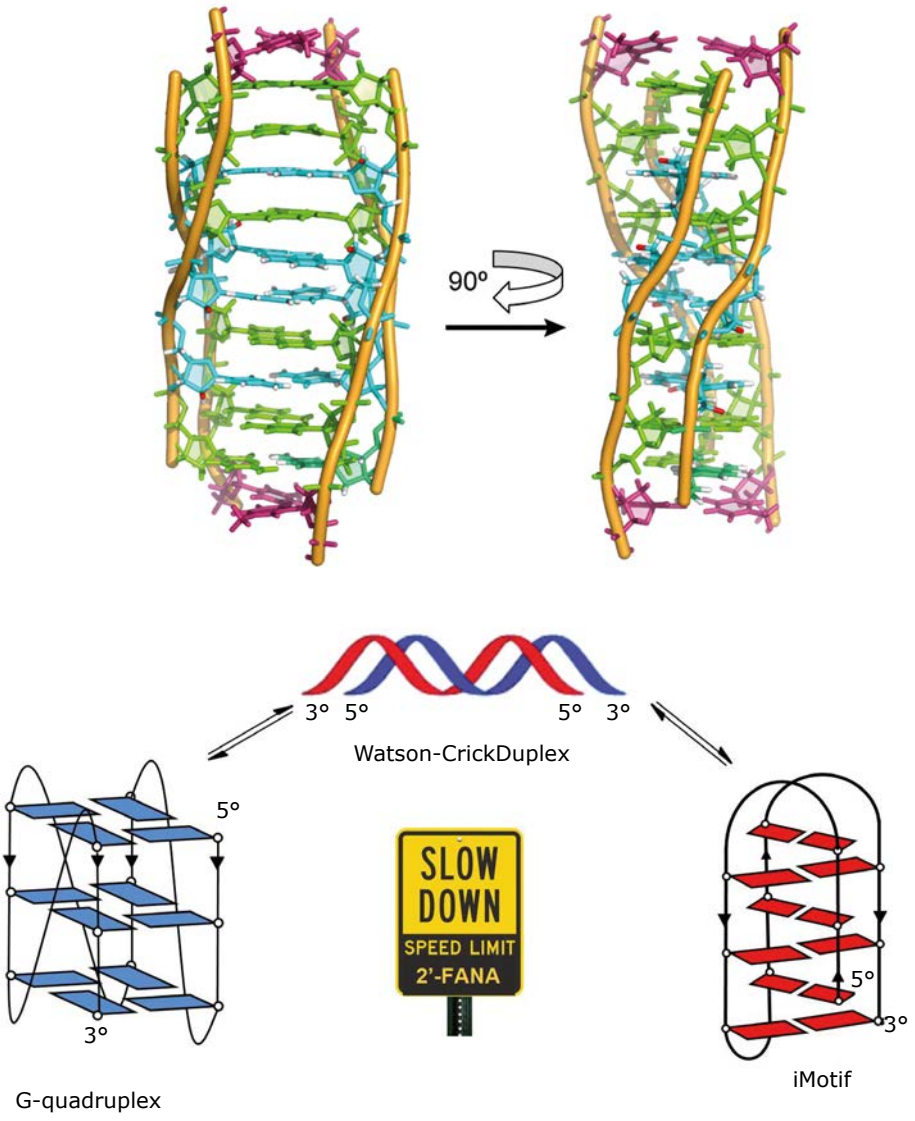

Figure 2: Structure of a 2'F-araC modified i-motif and representation of the effect of this substitution on the hybridization of two complementary strands.

Publications

Dans, P.D., Ivani, I., Hospital, A., Portella, G., González*, C. & Orozco*, M.How Accurate Are Accurate Dorece-Fields for DNA?. Nucleic Acids Res. 45, 4217-4230 (2017).

Lietard, J., Abou-Assi, H., Gómez-Pinto, I., González, C., Somoza, M.M. & Damha, M.J.Mapping the Affinity Landscape of Thrombin-binding Aptamers on 2'F-ANA/DNA Chimeric G-Quadruplex Microarrays. Nucleic Acids Res.45, 1619-1632 (2017).

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Abou-Assi, H., Garavís, M., González, C.*& Damha, M.J.*i-Motif DNA – Structural Features and Significance to Cell Biology. Nucleic Acids Res.,46, 8038-8056 (2018).

National Grants: individual

MINECO

Principal Investigator	Title	Reference
Carlos González Ibáñez	Más allá de la doble hélice de Watson y Crick. Estructuras no-canónicas de ácidos nucleicos y sus posibles aplicaciones en biomedicina	MINECO BFU2014-52864-R
Carlos González Ibáñez	Estructuras cuádruplex como diana farmacológica. Nuevas oportunidades terapéuticas en Biomedicina	MINECO BFU2017-89707-P

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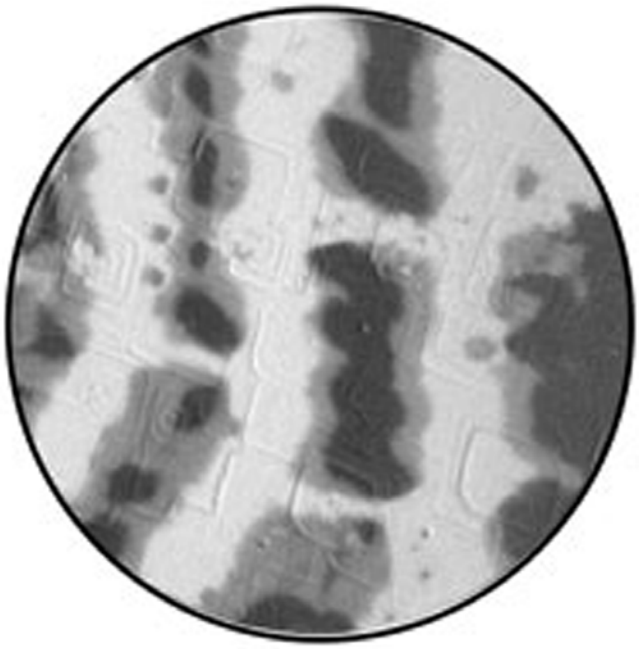
Department of Low Dimensional Systems, Surfaces and Condensed Matter



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 includesthe 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

Científicos en plantilla

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Científicos contratados

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Becarios pre-doctorales

Adela González Jiménez
Becaria JAE Intro 2018. 01/10/2018-31/12/2018

Técnicos

Alejandro Martínez Hernández
(Técnico de Garantía Juvenil, 01/05/2016-30/04/2018)

Summary

The activity of the Group is focused in 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. 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 pay special attention to those phenomena that are susceptible of application in areas such as the development of low-cost, flexible electronic devices, data storage devices and sensors and in the conservation of Cultural Heritage. The activities and the results of our research are described in the continuously updated web page http://lanamap.iqfr.csic.es/.

Strategic Aims

The main goal of the research carried out in the Group is the understanding of the laser-material interaction processes that allow guiding the selection of control strategies for the laser fabrication of nanomaterials. The specific objectives are:

- Laser nanostructuring of soft matter and polymers by applying advanced processing techniques.
- Controlled laser synthesis of materials with specific properties, prepared as thin or nanostructured films.
- Development of new methodologies for in situ determination of growth and self-assembly of nanomaterials generated by pulsed laser deposition.
- Application of nonlinear optical microscopy for material analysis.
- Understanding and follow-up of ultrafast molecular dynamics using femtosecond pulses.
- Development and application of advanced laser methodologies for the analysis, valorisation and conservation of Cultural Heritage.

Remarkable Results

Laser induced periodic surface structures on thin polymer films

We have continued our studies on the generation of laser induced periodic Surface structures (LIPSS) by irradiation with nanosecond pulses in thin films of polymers. From the fundamental point of view, the influence of the film thickness and of the substrate on LIPSS formation have been investigated and it was found out that the number of pulses needed for LIPSS formation depends on polymer thickness while the thermal conductivity and diffusivity and the optical properties of the supporting substrate affect the onset for LIPSS formation and their quality.

Regarding the materials, we have paid special attention to semiconducting polymers and to polymer-based nanocomposites with expanded graphite and carbon nanotubes and we have focused on the physicochemical modifications accompanying the formation of nanostructures, especially wettability, surface energy and adhesion.

Part of the work here reported has taken place in collaboration with the group of Prof. T. Ezquerra, Instituto de Estructura de la Materia, CSIC.

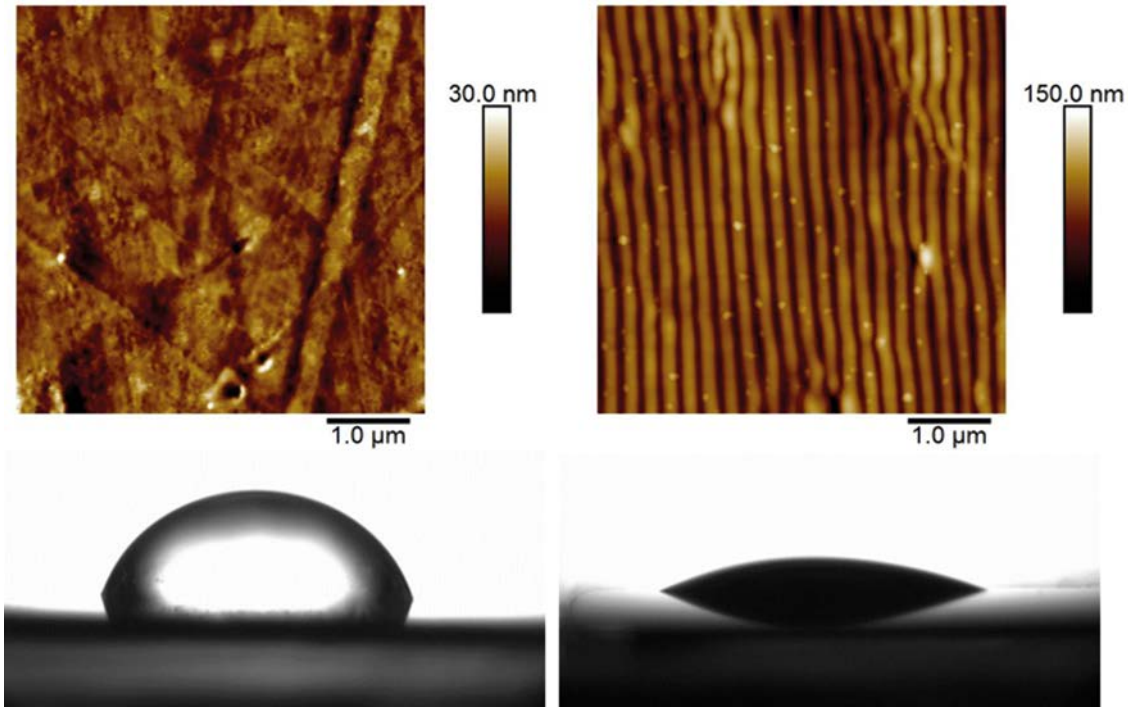

Figure 1: AFM images of poly(trimethyleneterephthatalate) (PTT) reinforced with single wall carbon nanotubes SWCNT, and the corresponding optical images of a water drop on top of their surfaces (left) before irradiation (right) after laser irradiation at 266 nm with 3000 pulses and a fluence of 11 mJ/cm^2.

Demonstration of laser control of the stereochemistry of a chemical reaction. Nat. Comm. 8, 1345 (2017)

The notion that strong laser light can intervene and modify the dynamical processes of matter has been demonstrated and exploited both in gas and condensed phases. The central objective of laser control schemes has been the modification of branching ratios in chemical processes, under the philosophy that conveniently tailored light can steer the dynamics of a chemical mechanism towards desired targets. Less explored is the role that strong laser control can play on chemical stereodynamics, i.e. the angular distribution of the products of a chemical reaction in space. This work demonstrates for the case of methyl iodide that when a molecular bond breaking process takes place in the presence of an intense infrared laser field, its stereodynamics is profoundly affected, and that the intensity of this laser field can be used as an external knob to control it.

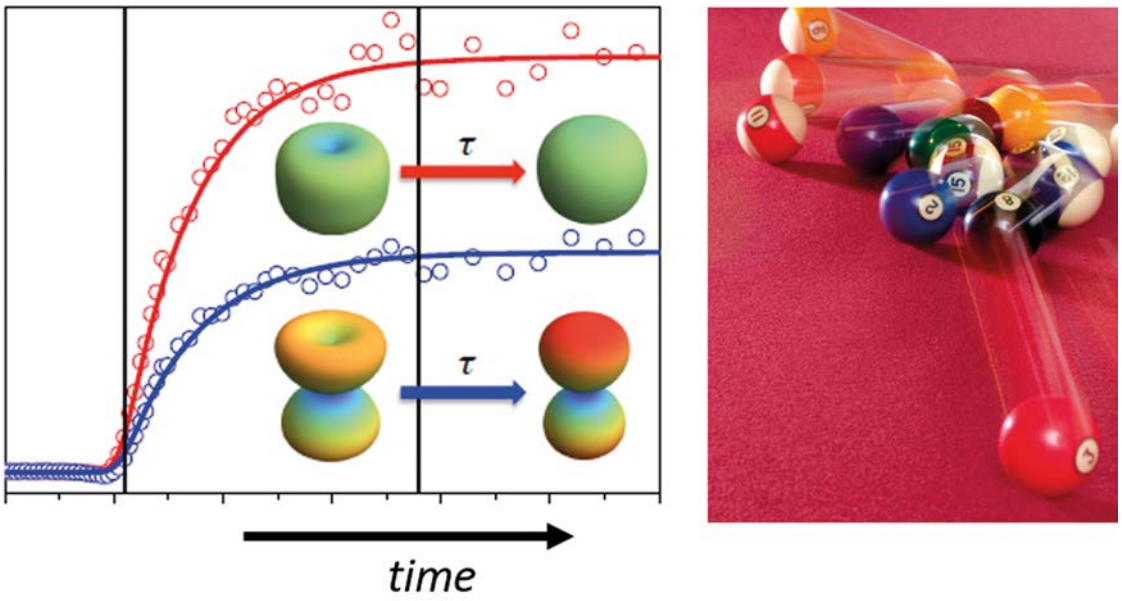

Figure 2: Global intensity pump-probe temporal behaviour of the signal corresponding to two fragmentation channels. 3D insets are polar plots of the angular distributions of each channel at two different delays (left). Schematic representation of the chemical reaction event.

Nonlinear optics for the elusive detection of clusters in laser ablation plasmas. Phys. Chem. Chem. Phys. 20, 16956 (2018)

Femtosecond laser ablation of solids is known to produce ejection of material to a large extent composed of particles of nanometer dimensions for a broad variety of targets. This work explores the ultrashort laser ablation of metal targets (Ag, Cu, Al, Mn) through non-conventional diagnostics based on the nonlinear response of the transient medium created upon ablation. The full temporal mapping of the nonlinear response constitutes a useful flag that signals the abundance of clusters and nanoparticles in the plume. The use of this method for diagnosis has allowed us to perform direct observation of middle-sized aggregates that are extremely elusive with other techniques. Additionally, one crucial and seldom explored parameter in this context has been identified: the ablation laser spot size. Optimum conditions for overall nanoparticle generation as well as relative nanoparticle/cluster/atom ratios have been found.

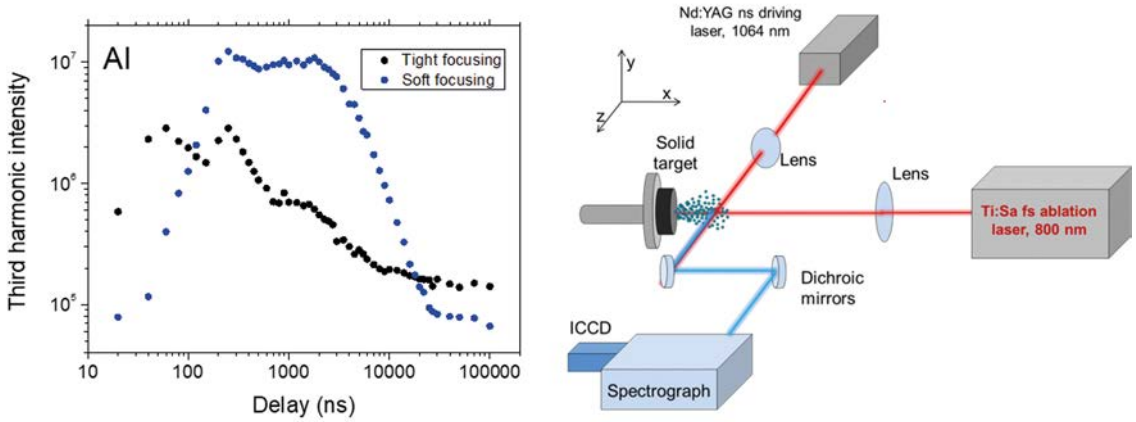

Figure 3: Example of dependence of third harmonic signal in a laser ablation plume of a metal target (left) and experimental setup (right).

Nonlinear Optical Microscopy for material analysis

Nonlinear optical microscopy (NLOM) is a technique initially developed in the field of biomedical optics that relies in ultrafast (femtosecond) laser excitation to exploit several nonlinear optical effects of materials. In order to extend the use of the technique for analysis of materials, and particularly those of cultural heritage. In this period, we have built and set up a nonlinear optical microscope working in the imaging mode of Multi-Photon Excitation Fluorescence (MPEF) and applied it for the non-destructive accurate determination of thickness within multi-layer samples. In the framework of the EU Project IPERION CH we have worked in the determination of thickness of transparent or partly transparent copper-phthalocyanine acrylic paint layers and for the assessment of modifications following laser removal of varnish (results published in Phys. Chem. Chem. Phys. 19 (2017) 22836).

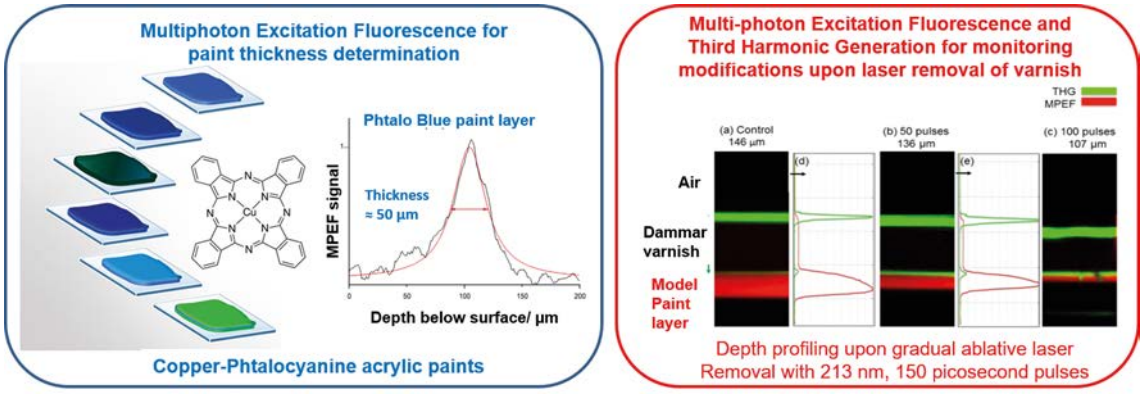

Figure 4: Non-Linear Optical Microscopy in painting analysis.

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Pena-Poza, J., Ascaso, C., Sanz, M., Pérez-Ortega, S., Oujja, M., Wierzchos, J., Souza-Egipsy, V., Cañamares, M.V., Urizal, M., Castillejo, M. & García-Heras, M. Effect of biological colonization on ceramic roofing tiles by lichens and a combined laser and biocide procedure for its removal. *Int. Biodeterior. Biodegr.* **126**, 86-94 (2018).

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COMPETITIVE FUNDING

National Grants: individual

Ministerio de Educación Cultura y Deporte

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

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. 30/12/2016-29/12/2019

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. 01/07/2017-30/06/2019
Marta Castillejo, Rafael Fort (Instituto de Geociencias)	Tecnologías y Conservación de Geomateriales del Patrimonio (GEOMATERIALES)	S2013/MIT-2914 01/10/2014 - 31/12/2018
Rebeca de Nalda Mínguez. M. R.: María Teresa Pérez-Prado (Fundación IMDEA Materiales, Madrid)	Diseño multiescala de materiales avanzados (DIMMAT)	S2013/MIT-2775 1/10/2014 - 30/09/2018

International Grants: coordinated

European Commission, H2020

Principal Investigator	Title	Reference
Marta Castillejo, Luca Pezatti, INO-CNR	The European Research Infrastructure for Heritage Science Preparatory Phase (E-RIHS PP)	(N. 739503). H2020-INFRADEV-2016-2. 01/02/2017-31/01/2020
Marta Castillejo, Luca Pezatti, INO-CNR	Integrated Platform for the European Research Infrastructure ON Cultural Heritage, IPERION CH	H2020-INFRAIA-2014-2015. 01/05/2015-31/10/2019
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

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Inmaculada García-Moreno Gonzalo (Profesor de Investigación)
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Clara Gómez Hernández (Científico Titular)
Researcher ID: J-8997-2015

Científicos contratados

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Post-Doctoral Researcher with Project Contract (until 31/12/2017)
ResearcherID: E-8612-2011

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.
- Functionalization of nanoscaffolds of different nature and geometries (organic and inorganic nanoparticles, fullerenes, nanocrystalline cellulose, and polyhedral oligosilsesquioxanes), with a variable number of dye molecules and chemically- and biologically-active groups.
- Encapsulation and anchorage of laser dyes in nanoparticles, polymers, and porous systems (hybrid and inorganic).
- 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 Orthodontics.

Remarkable Results

Photosensitized and nanostructured materials for optoelectronic and biophotonicapplications (Part I)

We have carried out 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. By covalent linkage of coumarins to BODIPYs to create hybrid compounds or the incorporation of stabilized C nucleophiles to the *meso* position of BODIPYs, dyes are obtained with increased absorption in the UV region and tunable laser emission, highly efficient and stable, over the spectral region from the green to the red.

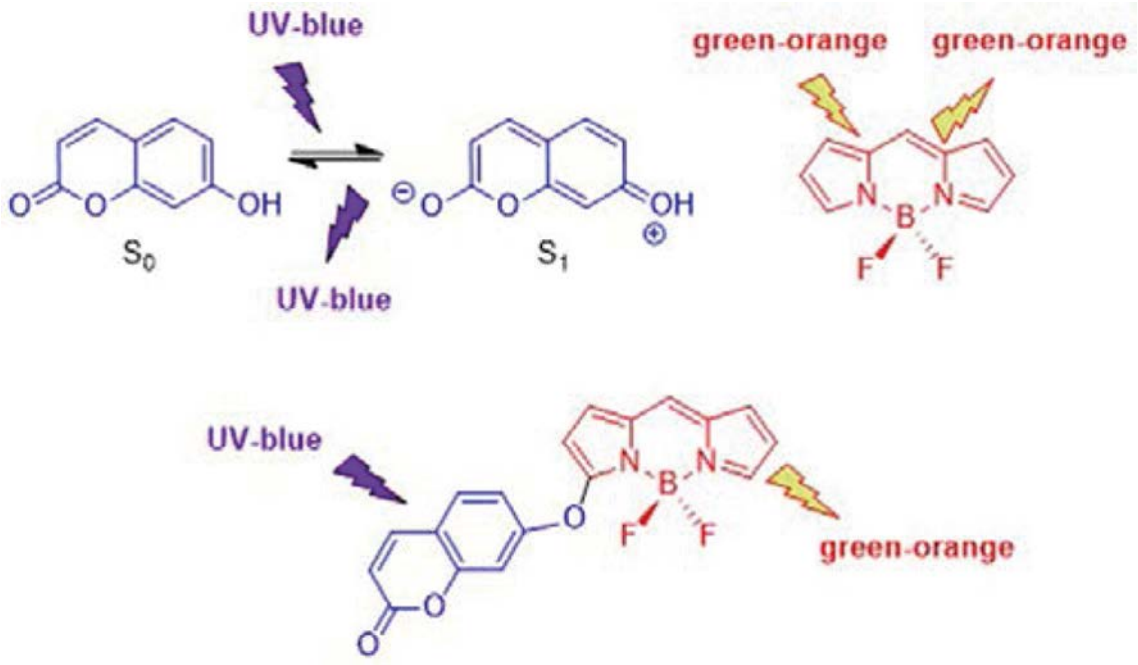

Figure 1: Simple 7-hydroxycoumarin (blue) and BODIPY (red) chromophores, and a hybrid system based on them, indicating the absorption and emission regions of each compound.

Photosensitized and nanostructured materials for optoelectronic and biophotonicapplications (Part II)

The design and development asymmetric cassette triads based entirely on BODIPY chromophores provides panchromatic absorption, with efficient light harvesting capacity over the UV-visible spectral region *via* very efficient energy-transfer processes. The programmed functionalization of polyfunctional BODIPY building blocks allows the versatile preparation of complex BODIPY derivatives, resulting in a new library of compounds with tailored photophysical properties for advanced photonic and biophotonic applications. In particular, it was possible to shift the BODIPY emission deep into the near-infrared spectral region while retaining high fluorescence quantum yields as well as efficient and stable laser action.

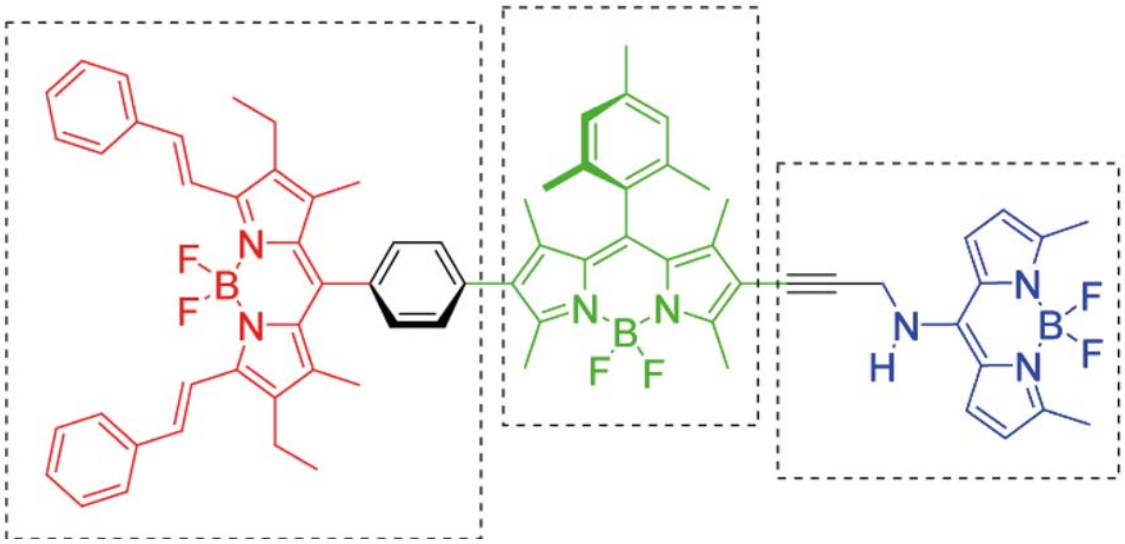

Figure 2: Cassette constituted by a triad of BODIPY compounds.

Photosensitized and nanostructured materials for optoelectronic and biophotonicapplications (Part III)

Blue-emitting lasers are tools of uppermost importance to many applications, ranging from spectroscopy and material processing to biotechnology and medicine. So far, blue-emitting laser materials are based on organic compounds or semiconductor nanocrystals that have significant limitations, such as low solubility in common solvents and polymers, low chemical- and/or photo-stability and/or lengthy and costly synthetic procedures which result in uncompetitive prices. We have demonstrated a novel and competitive alternative to these existing laser materials with emission in the blue that is based on boron hydrides (boranes), inorganic cluster compounds with a rich and diverse chemistry. In particular, we have demonstrated that solutions of the borane *anti*-$B_{18}H_{22}$ show, under pulsed excitation, blue laser emission at 406 nm with an efficiency of 9.5% and a photostability superior to many of the commercially available state-of-the-art blue laser dyes.

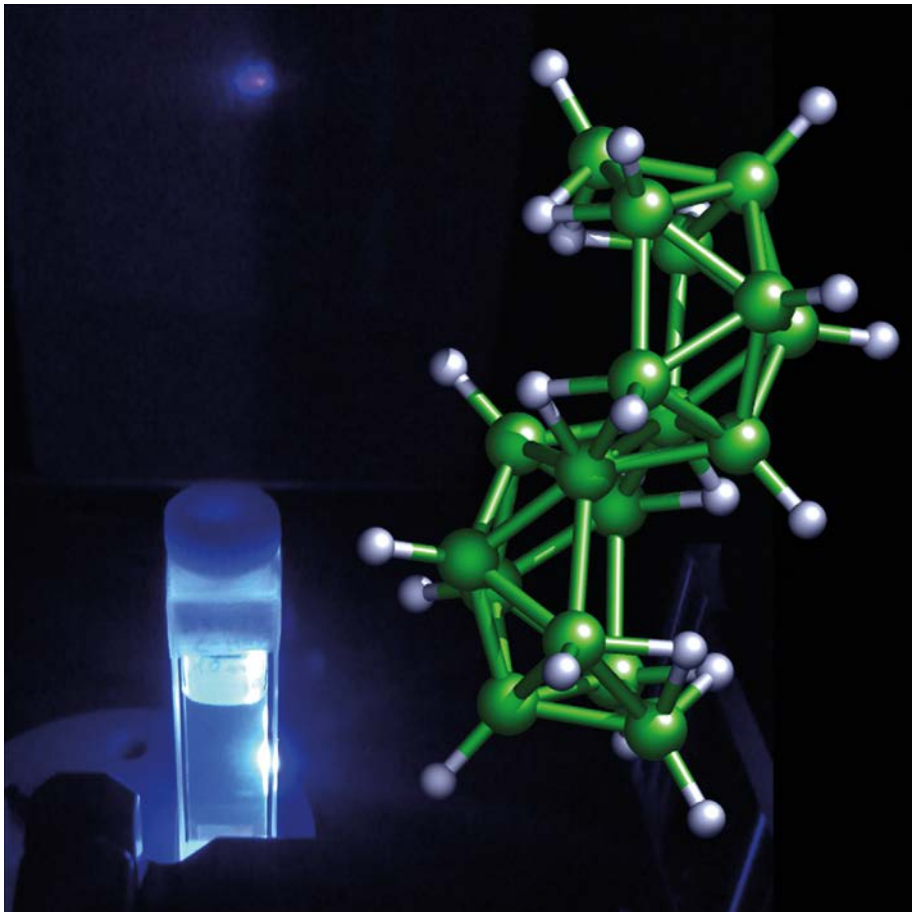

Figure 3: *Anti*-$B_{18}H_{22}$ borane structure and laser emission in cyclohexane solution.

Photosensitized and nanostructured materials for optoelectronic and biophotonicapplications (Part IV)

Finally, we have recently started systematic studies on the generation of circularly polarized laser emission (CP), induced in achiral and isotropic dye laser systems without the use of extracavity polarizing elements. We demonstrated that it is possible to generate and modulate CP laser light from efficient and photostable conventional laser dyes.

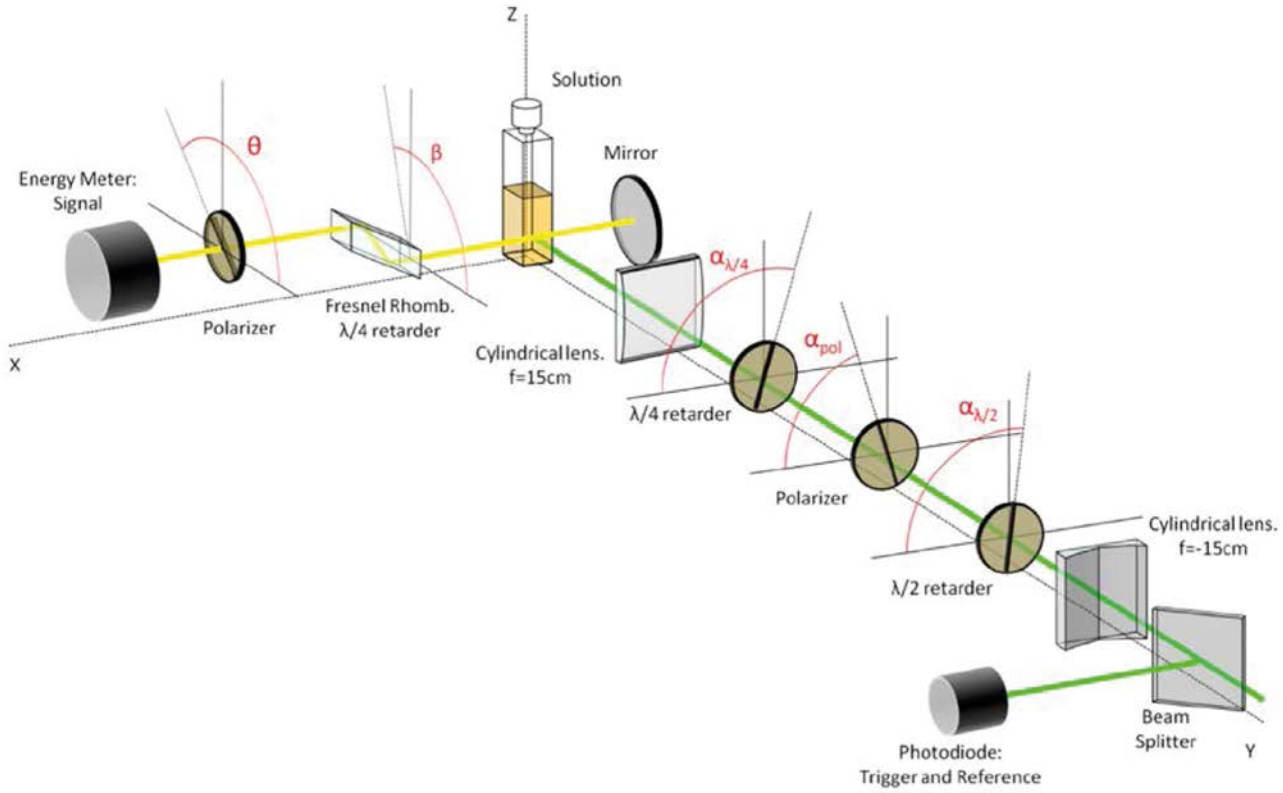

Figure 4: Generation of CP laser emission in achiral laser systems: experimental set-up used to determine the polarization state of a dye laser emission as a function of the pump polarization state.

Efficacy of photodynamic therapy *vs* ultrasonic scaler for preventing white spot lesions during orthodontic treatment

In collaboration with the Department of Dental Specialties of the Faculty of Dentistry of the UCM (Madrid), we have evaluated the effectiveness of Photodynamic Therapy (PDT) in the maintenance of a healthy mouth during a prolonged orthodontic treatment with fixed devices.

Twenty orthodontic adolescents, with slight signs of gingival inflammation and low caries risk, were randomly assigned to receive either PDT or ultrasonic scaler (US), applied in repeated doses (4 times at intervals of 2 weeks at the beginning of the study), and booster doses in the re-evaluations (3, 6 and 9 months). Clinical periodontal parameters (PI, GI, PD) were scored to evaluate gingival inflammation and the ICDAS index was measured to evaluate the degree of enamel demineralization. Clinical assessments [PI, GI and PD] yielded no differences ($p>0.05$) between groups, which showed a major decrease at the start of the trial. ICDAS started to increase after the 6-month re-evaluation, without observing intergroup differences ($p> 0.05$) (Figure 5).

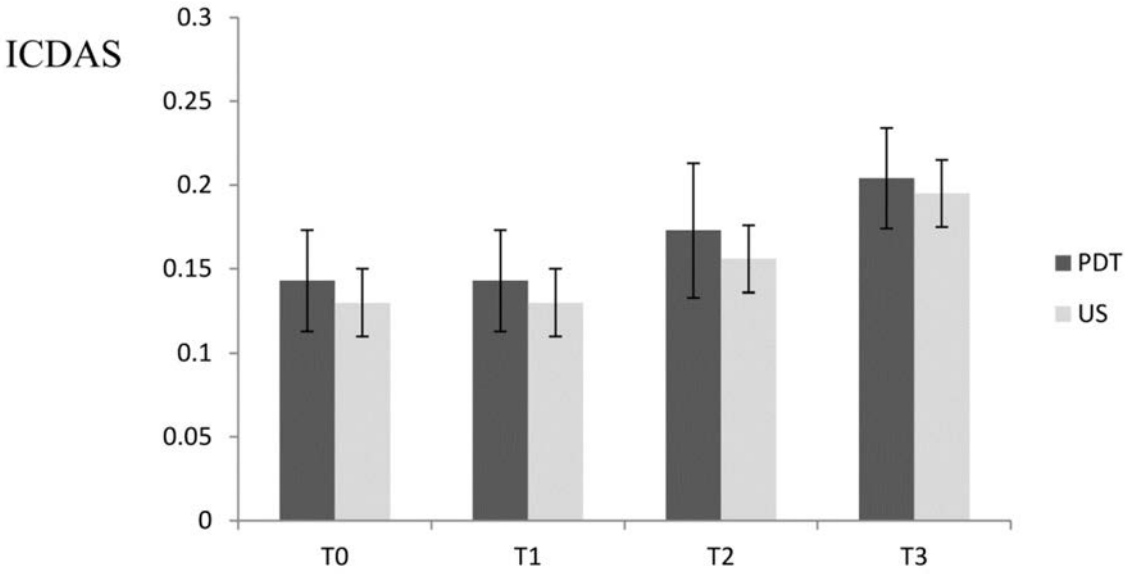

Figure 5: International Caries Detection and Assessment System (ICDAS index): Mean Scores (±SD), (n=10 patients/group) at baseline (T0), and at follow-ups of 3, 6 and at 9 months (T1, T2, T3, respectively).

Efficacy of photodynamic therapy *vs* ultrasonic scaler for preventing gingival inflammation during orthodontic treatment

In the same population reported in the above study, samples of subgingival plaque, saliva and gingival crevicular fluid (FGC) were taken for the determination of 10 periodontopatopathogens, Streptococcus mutans and 6 pro-inflammatory cytokines, respectively. The records were made before the preventive treatments were carried out and in the re-evaluations.

Similar reductions in total colony forming units (log CFU reduction) were observed with both treatments for total periodontopathogenic flora (Figure 6) and salivary S. mutans (mainly at 3 months), but with no differences between groups (p>0.05). The two groups also showed similar trends for inflammatory mediators with no differences (p>0.05) among them. PDT and US presented a similar efficacy in the prevention of the processes triggered by fixed orthodontic appliances. TFD is a valid and novel method for oral decontamination during fixed orthodontic treatment.

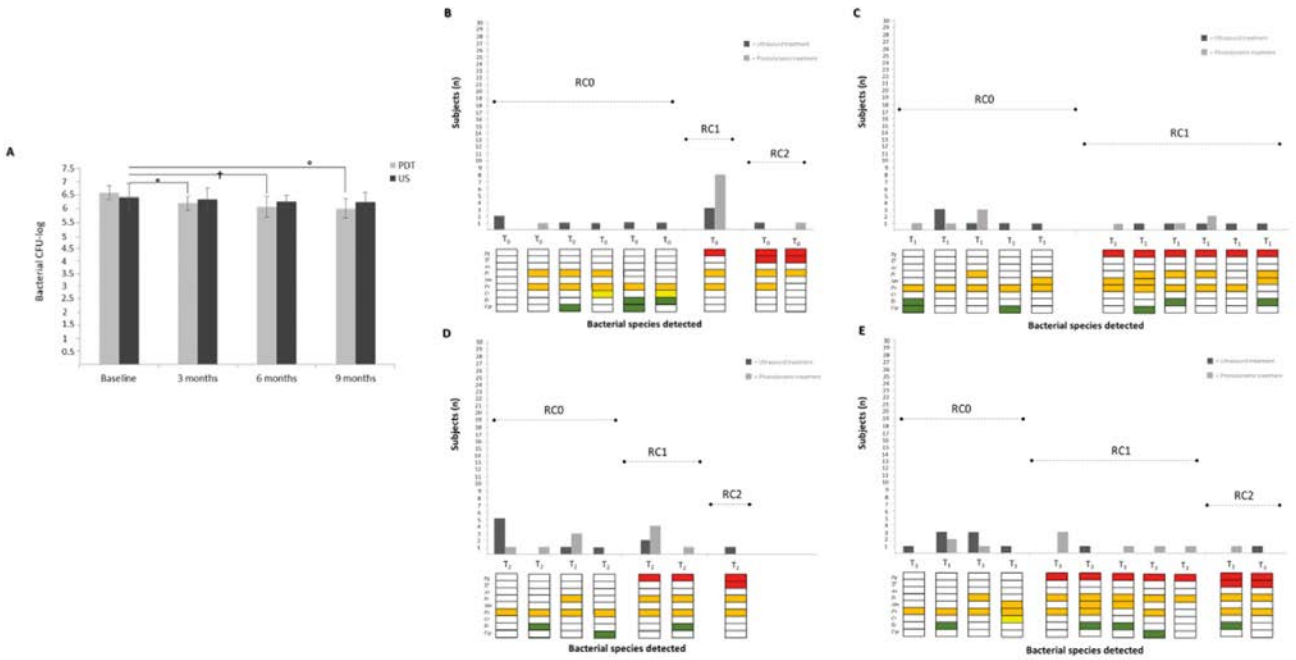

Figure 6: Graphical representation of oral microbiota progression in both experimental groups. A) Decimal logarithm-transformed colony-forming units (log CFU) of total periodontopathogenic flora. Mean Scores (±SD), (n=10 patients/group) at baseline, and at 3-, 6-, and 9-month follow-ups; (*) Significance of *intragroup* differences compared to baseline at 3-month follow-up; (†) Significance of *intragroup* differences compared to baseline at 6-month follow-up; (°) Significance of *intragroup* differences compared to baseline at 9-month follow-up. No statistically significant differences were detected for any bacteria counts between PDT and US groups at any of the evaluation times. B) Distribution of microbiological complexes within both treatment groups, PDT and US, at baseline, and at 3-, 6-, and 9-month follow-ups. The color represents the different complexes described by Socransky et al., (1998). RC0: none of the pathogens of the 'red complex' present; RC1: one of the pathogens of the 'red complex' present; RC2: two of the pathogens of the 'red complex' present.

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Contributions to books

Cerdán, L. "State of the art active materials for organic lasers", in Organic lasers - fundamentals, developments, and applications. Eds. Anni, M & Lattante, S. (Pan Stanford Publishing). ISBN: 978-98-14774-46-8

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COMPETITIVE FUNDING

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.	

International 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
Inmaculada García-Moreno Gonzalo	Photonic materials as bioimaging markers	MAT2015-68837-REDT

Group of Statistical Mechanics and Condensed Matter

Científicos en plantilla

Eva González Noya
(Científica Titular)

Enrique Lomba García
(Profesor de Investigación)

Científicos contratados

Ariel Meyra
(1.03.2018-28.02.2019, científico de intercambio RISE)

Leandro Guisández
(27.05.2018-24.05.2019, científico de intercambio RISE)

Becarios pre-doctorales

Pablo Llombart González
(1.12.2017-30.11.2018)

Técnicos

Itziar Zubieta Urzainqui
(1.10.2017-30.9.2018)

Summary

The research carried out by the Group of Statistical Mechanics and Condensed Matter for the last two year focuses on the application of statistical mechanics and condensed matter theory tools in conjunction with simulation approaches in order to analyze problems of physico-chemical interest, basically in connection to phase transitions in bulk and under confinement, self-association in colloids as a tool for the design of novel materials, and the study of disordered hyper-uniform materials as potential a 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 behavior in complex fluids (water, liquid crystals, anomalous liquids)
- Self-assembly phenomena in simple models.
- Study of disordered hyper-uniform materials as candidates for stealth materials and optical
- Adsorption of complex fluids (e.g. alcohols and alcohol/water mixtures) in disordered and regular porous media (disordered carbons, zeolites, graphite slits)

Remarkable Results

Disordered hyper-uniform systems: conditions for multi-hyperuniformity and potential design routes

In collaboration with S. Torquato (Princeton University) we have devised an strategy to determine the conditions to be fulfilled by interparticle interactions so as to guarantee the presence of hyperuniformity (i.e. the cancellation of long wavelength density fluctuations). This property is connected to the acute sense of vision of birds due since it is reflected in the spatial distribution ofphotoreceptors in their retina. Our analysis opens the path to a rational design of these materials using colloidal particles.

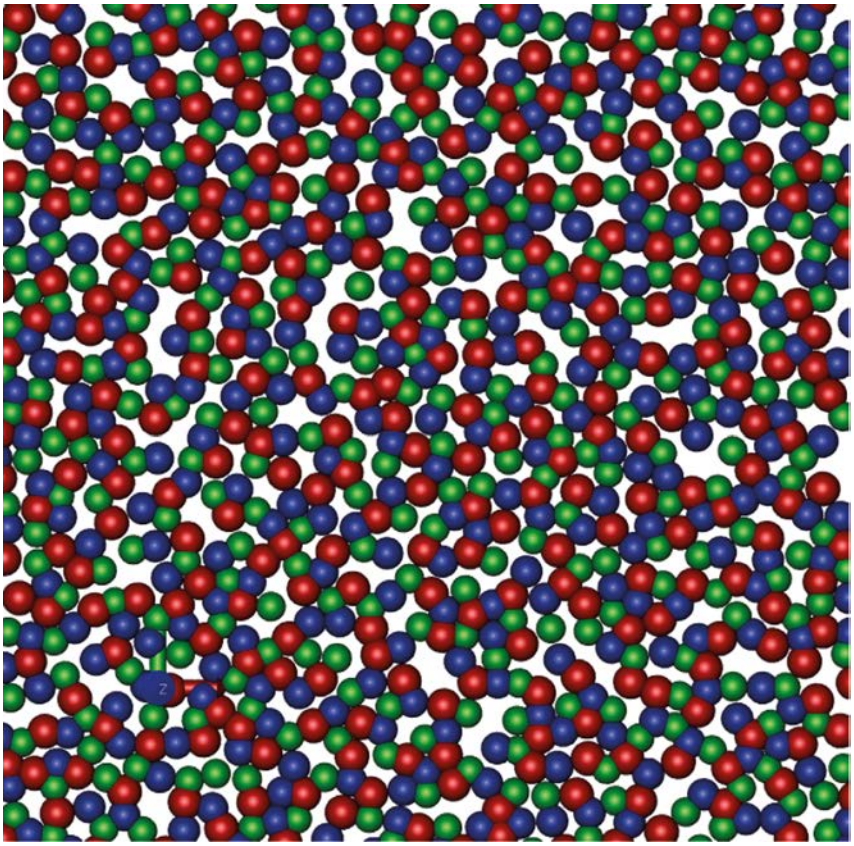

Figure 1: A simple model of photoreceptor (rgb) configuration designed with simple interactions that lead to a multi-hyperuniform structure

Selective adsorption of alcohols in water/alcohol mixtures on zeolites and carbon slits

With the general aim of improving process of alcohol purification in bio-alcohol synthesis we have studied the effect of pore geometry and slit with in the adsorption of methanol in zeolites and graphite pores. Our results, when compared with experimental adsorption experiments evidence the ability of well-designed computer simulations "experiments" to aid in the design of novel adsorbents.

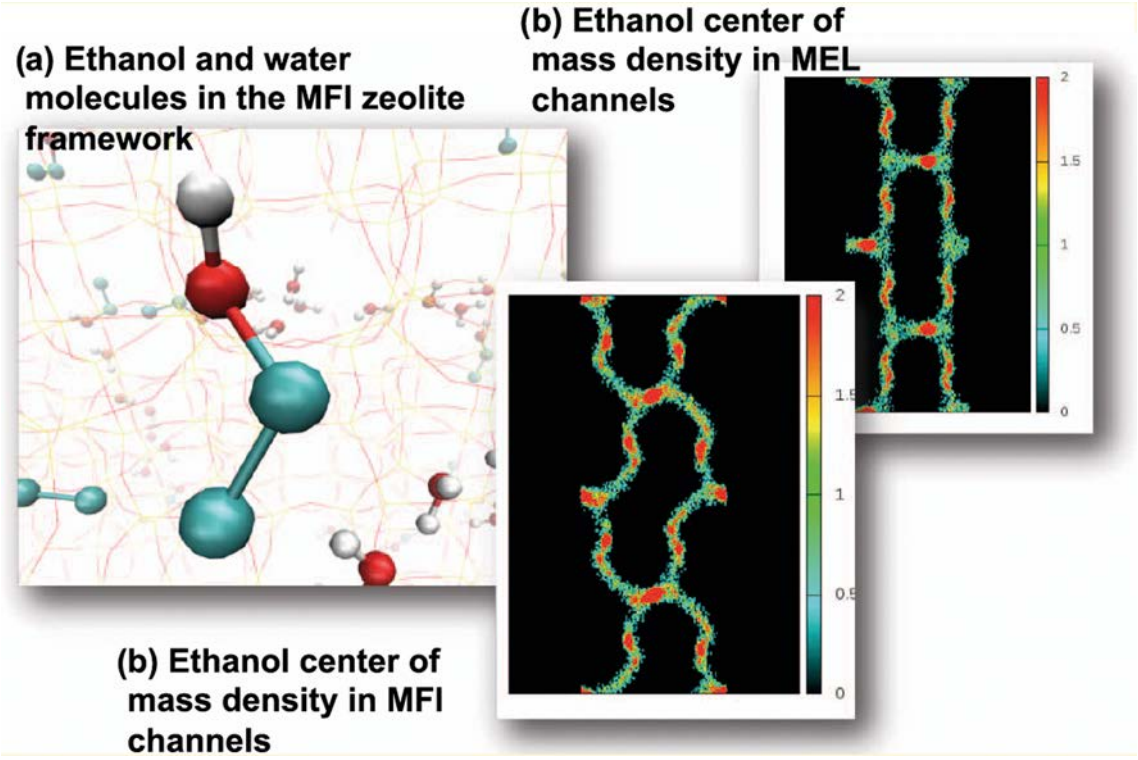

Figure 2: A simple model of photoreceptor (rgb) configuration designed with simple interactions that lead to a multi-hyperuniform structure

Phase diagrams and self-assembly in anisotropic colloids

Anisotropic colloidal particles are a potential route to the fabrication of new materials designed with specific properties in mind. The core of the question implies first to fully understand the complex relation between their mutual interactions and the process of self-assembly. In the context, it is essential to answer two key questions: 1) Given a certain particle geometry, how can one determine the material structures compatibles with it? 2) If we aim at building a particular material microscopic structure, which properties should display the constituent particles? Our research has focused on providing answers to these two questions using molecular simulations. One of our most relevant results was the determination of the phase diagram of trivalent colloidal particles confined to a plane. Our simulations have shown that this system exhibits an unusual solid phase with a honeycomb lattice, in which the interstitial holes are filled in a continuous fashion, which opens an interesting avenue to tune its properties, depending on the nature of the guest particles.

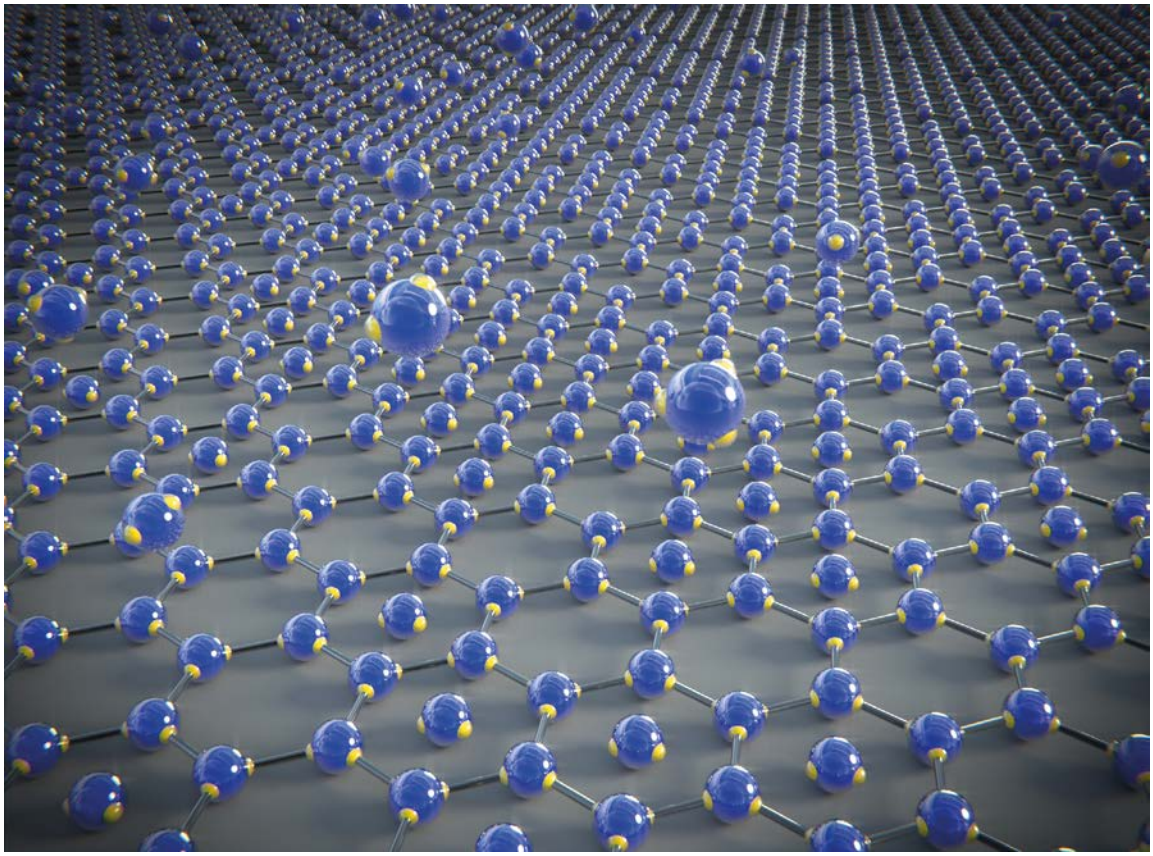

Figure 3: Honeycomb lattice in a system of trivalent colloidal particles.

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Lomba, E., Weis, J. J. & Torquato, S. Disordered hyperuniformity in two-component non-additive hard disk plasmas. *Phys. Rev. E* **96**, 062126 (2017).

COMPETITIVE FUNDING

National Grants: individual

Agencia Estatal de Investigación

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
Enrique Lomba García	Theory and simulation of complex	FIS2013-47350-C5-4-R

National Grants: coordinated

European Comission

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

Group of Surface Analysis and Mössbauer Spectroscopy

Científicos en plantilla

Científicos en plantilla

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José Emilio Prieto de Castro (Científico Titular) ORCID: https://orcid.org/0000-0003-2092-6364, ResearcherID: L-3120-2013, Google Scholar: luF_KkYAAAAJ.

Científicos contratados

Fernando Moutinho (investigador contratado FC3, 06/2018-3/2019)

Becarios pre-doctorales

Laura Martín García (01/01/2014-13/07/2017)

Anna Mandziak (01/02/2017-)

Guiomar Delgado Soria (16/04/2017-)

Técnicos

Carlos Alonso (Titulado Superior)

Maria Sánchez Arenillas (Ayudante de laboratorio contratado a través del programa de Técnicos de Apoyo del MINECO, 15/02/2017-)

Guillermo Lobato (Técnico de laboratorio contratado a través del programa de la CAM del Fondo de Garantía Juvenil, 03/2018-)

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 ultrahigh 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 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 thin films from a few atomic layers to thicknesses of hundreds of nanometers.

- To determinate 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

Geometrically defined spin structures in ultrathin Fe_3O_4

We have grown high quality magnetite microcrystals free from antiphase boundaries on Ru(0001) by reactive molecular beam epitaxy, conserving bulk magnetic properties below 20 nm thickness. Magnetization vector maps were obtained by X-ray spectromicroscopy and compared with micromagnetic simulations. The observed domain configurations are dictated purely by shape anisotropy, overcoming the possible influences of (magneto) crystalline anisotropy and defects, thus demonstrating the possibility of designing spin structures in ultrathin, magnetically soft magnetite at will.

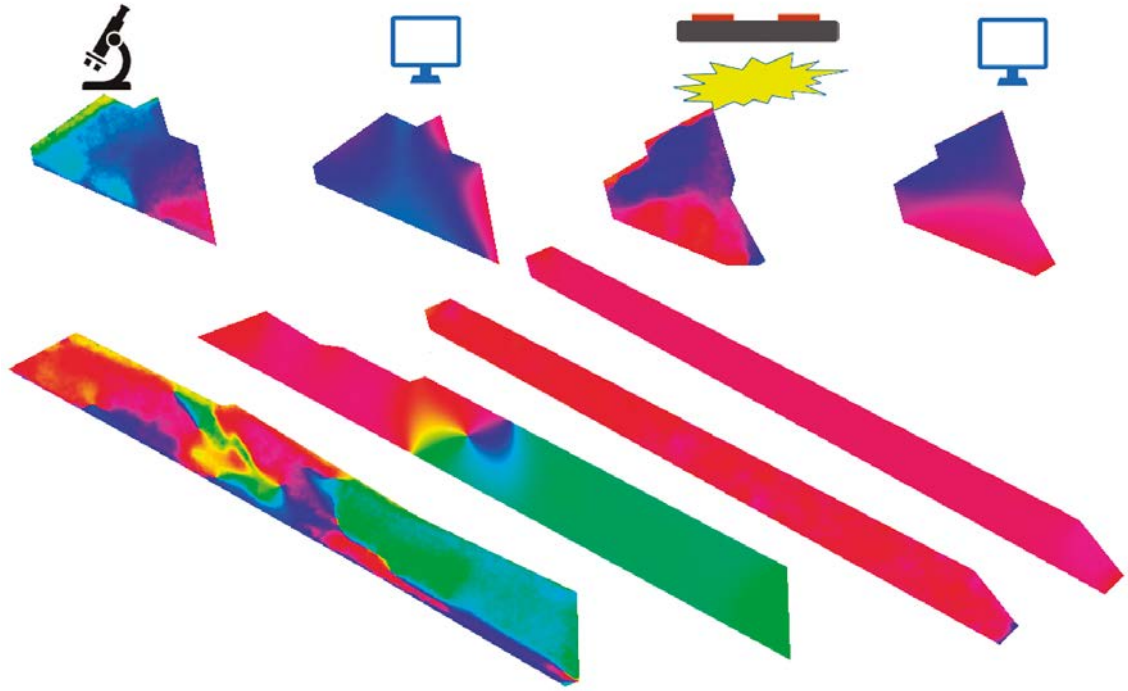

Figure 1: Experimental (left) and computer simulated (right) patterns are shown for several magnetite crystals, both as grown (left side) and after annealing the film (right side). The agreement between experiment and simulation proves that the material properties of the crystals are close to those of bulk magnetite.

Epitaxial highly perfect Ni-Fe ferrites

We have demonstrated the preparation of ultrathin Fe-rich nickel ferrite (NFO) islands on a metal substrate. Their nucleation and growth have been followed in situ by low-energy electron microscopy (LEEM) and a comprehensive characterization was performed combining LEEM for structural characterization and PEEM (Photo Emission Electron Microscopy) with synchrotron radiation for chemical and magnetic analysis via X-ray Absorption Spectroscopy and X-ray Magnetic Circular Dichroism (XAS-PEEM and XMCD-PEEM, respectively). The growth by oxygen-assisted molecular beam epitaxy takes place in two stages. First, islands with the rocksalt structure nucleate and grow until they completely cover the substrate surface. Later three-dimensional islands of spinel phase grow on top of the wetting layer. Only the spinel islands show ferromagnetic contrast, with the same domains being observed in the Fe and Ni XMCD images. A significant out-of-plane magnetization component was detected by means of XMCD-PEEM vector maps.

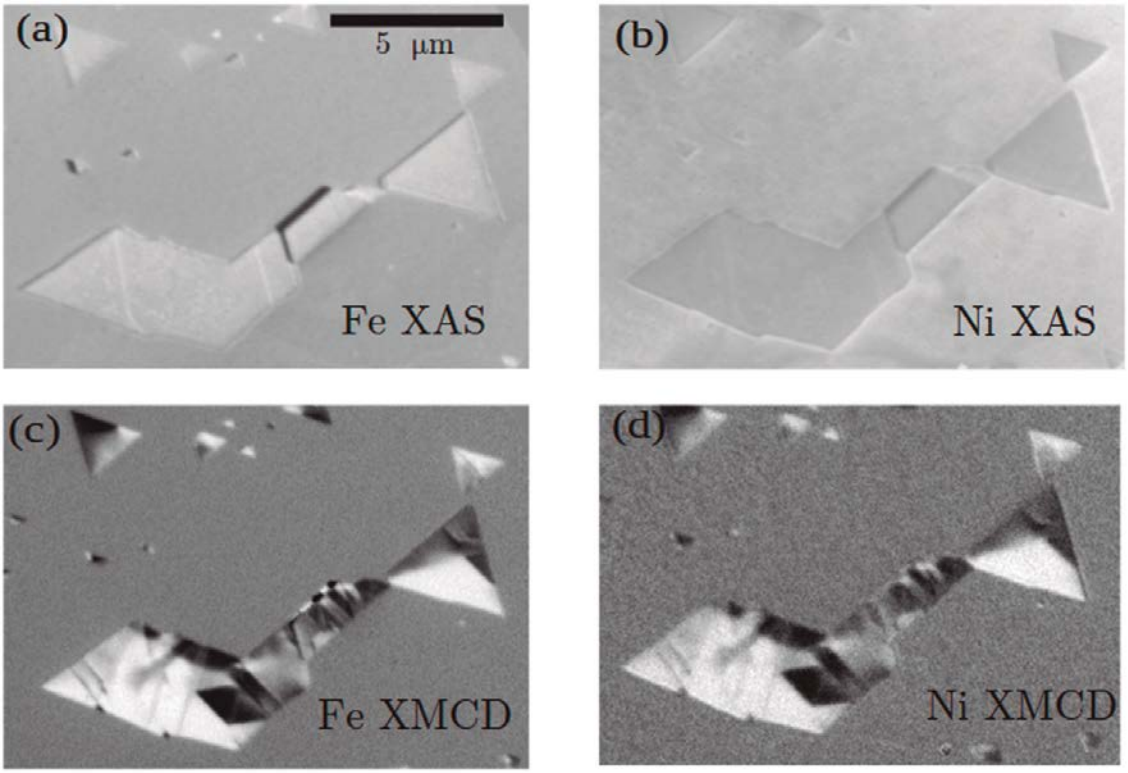

Figure 2: a) and b) X-ray absortion spectroscopy images of Fe and Ni respectively acquired at the L3 edge of each element. c) and d) x-ray magnetic circular dichroism images of the same area for Fe and Ni respectively showing ferrimagnetic domains in the spinel crystals.

Strontium Hexaferrite: a path towards rare-earth free magnets

We have performed a characterization of strontium hexaferrite platelets to be used in mixtures with high-saturation magnetization metals in order to improve their performance for building magnets. The highly crystalline platelets of strontium hexaferrite (SFO) have been grown by an hydrothermal method. The platelets are up to several micrometers in width, and tens to a hundred nanometers thick. They have been studied by a combination of structural and magnetic techniques, with emphasis on x-ray absorption techniques including spectroscopy and microscopy on the iron L edges and the oxygen K edge. In remanence, both the dichroic spectrum and the domain pattern can be determined from a single platelet.

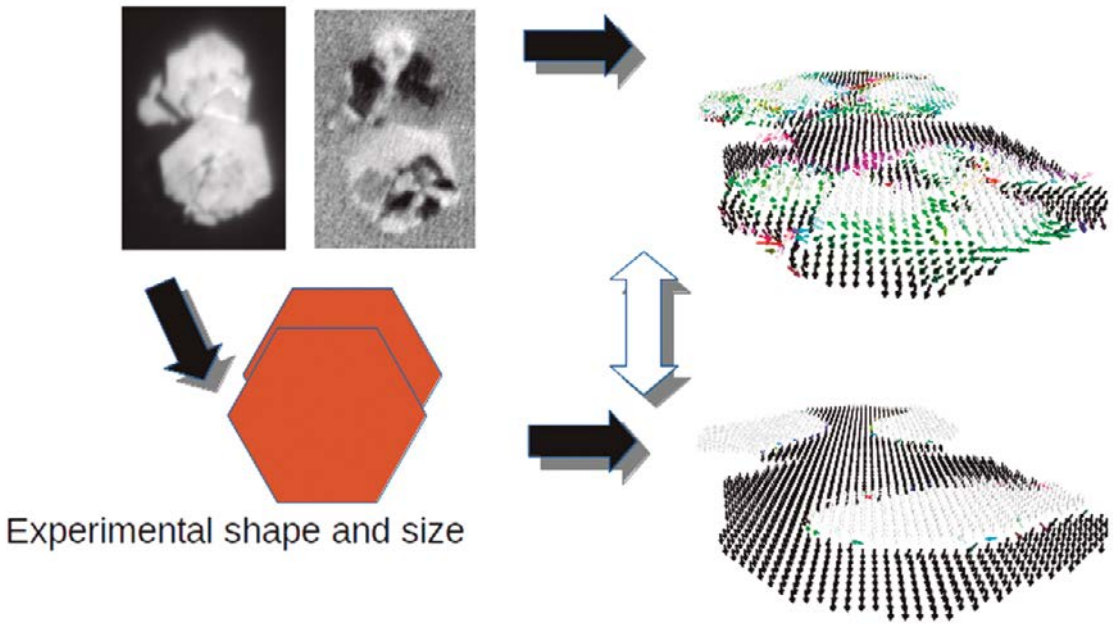

Figure 3: X-ray absorption and dichroism images of platelets of strontium hexaferrite are shown on the top left, indicating their morphology and magnetization respectively. By measuring along different azimuthal angles, each component of the magnetization can be determined, giving the vector magnetization represented on the right top image. This is compared with the result from micromagnetic simulations using the experimental shape and magnetization (right bottom).

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COMPETITIVE FUNDING

National Grants: individual

MINECO

Principal Investigator	Title	Reference
Juan de la Figuera	Microscopio de electrones de baja energía para dinámica y crecimiento en superficies	CSIC15-EE-3056

National Grants: coordinated

MINECO

Principal Investigator	Title	Reference
Juan de la Figuera (coordinador)	Structural and chemical control at the atomic level of spinel oxide thin films and surfaces	MAT2015-64110-C2-1-P

International Grants: coordinated

H2020

Principal Investigator	Title	Reference
Adrian Quesada Michelena (ICV)	Anisometric Permanent Hybrid Magnets based on Inexpensive and Non-critical Materials	H2020-NMBP-2016-720853

Research Support Services

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Library “BIQFR”

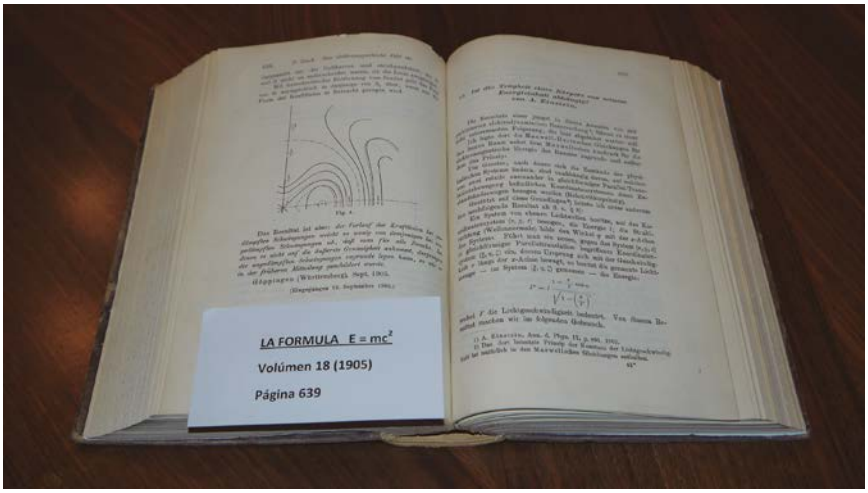
Introduction

The Rocasolano Institute of Physical Chemistry was set up in 1946 at same time as the Biqfr. Its holdings come from the "National Institute of Physics and Chemistry" created in 1932. Commonly known as the Rockefeller Institute, it was the cradle of all the research teams in the different disciplines of Chemistry, not only in Madrid, but throughout Spain. Three elements characterize the Biqfr: its Collection, Space and Management.

Collection: old collections-unique in Spain-can The Biqfr holds a valuable holding, mainly journals, of which 113 are complete starting from the first issue, 11 date from the 19th century to our days, and 16 start prior to 1920.

Space: Designed by the architects M. Sánchez Arcas and L. Lacasa (1932), innovators at the time. Because of its singular interest the library is the subject of visits by architects from various universities.

Management: At its genesis, the Biqfr was organized in a way that was revolutionary for those days, free access was permitted, and display stands facilitated access to the latest and the previous year's issues of the journals.The Biqfr is considered by the scientific community as the Reference Scientific Periodical Library, a historical landmark in the service of innovation



Einstein, A. (1905). Ist die Trägheit eines Körpers von seinem Energieinhalt abhängig? *Ann. Phys.* 18, 639-641. *(The equation $E=mc^2$).*

Library "Biqfr"

Library Manager

Esperanza Iglesias Fernández

Technicians

Victoria Garrido Martínez

Mª Felipa Arroyo Villa
(until 26/11/2018)

Strategic Aims

- New technologies.
- Visibility and Dissemination: The Blog & Social Networks
- Access to knowledge.
- Supply Documents.
- The Historic Documents Collection of the Institute of Physical Chemitry "Rocasolano"

Highlights

New technologies

In recent years, the concept value has been the mainstay of technical work to ensure that the library is competitive, proactive and even co-creative. By knowing the researchers' perception of the library in relation to the alternatives offered by its competitors (eg. Google), the Biqfr has developed links with scientists, to help researchers achieve their goals. Because of this, the Biqfr has an edge on its competitors.

Visibility and Dissemination: The Blog & Social Networks

The blog is the key tool for Biqfr dissemination and visibility. The Blog posts news from all areas of science and innovation. Always with the same purpose: trying to democratize "Science" and bring it to the public in a fun and an entertaining way.

In 2016-2017, on the blog 396 news items were posted. During this biennium, we achieved 172,883 visits to reach a total of 1,737,590 visits. The activity of our followers on the social networks Twitter and Facebook is constant and stable, as is the case with the Blog.

The Biqfr Blog is not only considered a scientific dissemination source in America (United States, Mexico, Colombia and Argentina, Peru, Chile) and Germany, but we have also detected that it begins to attract followers from other European countries (Russia, Ucrania) and Japon.

Access to knowledge: iLumina

iLumina is a smart tool to accelerate the search for scientific information, providing a competitive advantage to Biqfr over Google, while saving the user time and mouse clicks. Through a single search box, with one-click access to PDF or HTML, the user can access full-text content directly through the detailed record or from the result list preview pane.

During 2017-2018, observing the results of the statistics, we find that many searches have been made with few queries, in addition, the returned results were analyzed carefully by consulting the abstracts, and then the most relevant and applicable search results were downloaded.

In 2018, the online holds managed through iLunima were 76,559 journals & books. The Biqfr current subscriptions are available online.

iLumina is available from the CSIC's site to the whole Institution, and ubiquitously through the VPN to Biqfr users. Technology for mobile devices is offered.

Years	Sessions	Searches	Abstracts	Downloads
2017	18,875	33,265	812	1459
2018	14,326	30,107	803	644

Document supply: Inter librarian loan (ILL)

The wealth of the Biqfr's holdings satisfies the needs of its direct users, which is verified by the small number of documents requested to other centers and the significant number documents supplied to external centers such as universities, laboratories, and other CSIC centers.

In 2017-2018, as expected from modern science, 97.5 of document transactions were journal articles and only 2.5 were book loans.

Remarkably, the Biqfr supplied 7% of all the shared journal articles within the whole CSIC Library Network.

In the last 2 years, the average Biqfr ratio of the supplied documents to requested documents is eight. That is to say, the Biqfr supplied 8.16 times more documents than we requested from other centers. In contrast, on the whole, the CSIC Library Network is slightly beneficiary as it shares 1.2 documents for every document that it requests.

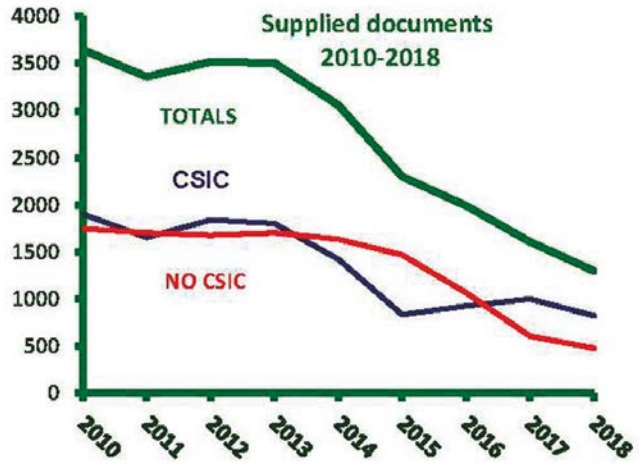


Figure 3

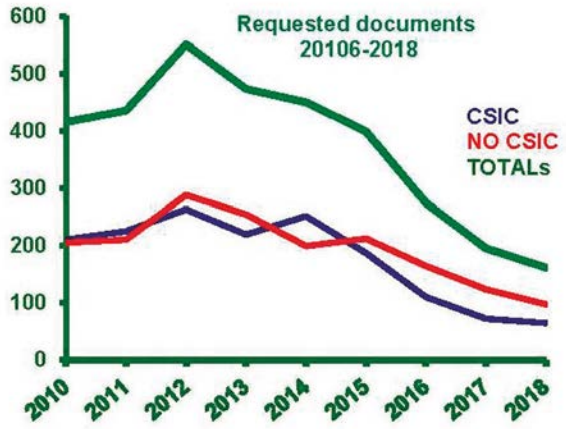


Figure 4

Over the last years, the flow of transactions among libraries has dropped, due to the advance of new technologies. And a putative decrease of the CSIC's scientific activity and the closing of libraries at some CSIC centers.

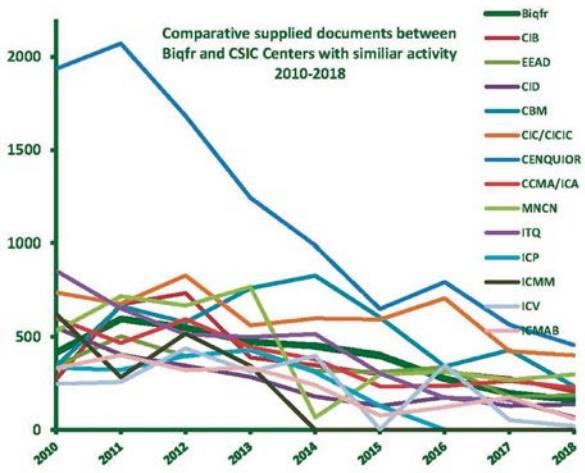


Figure 5

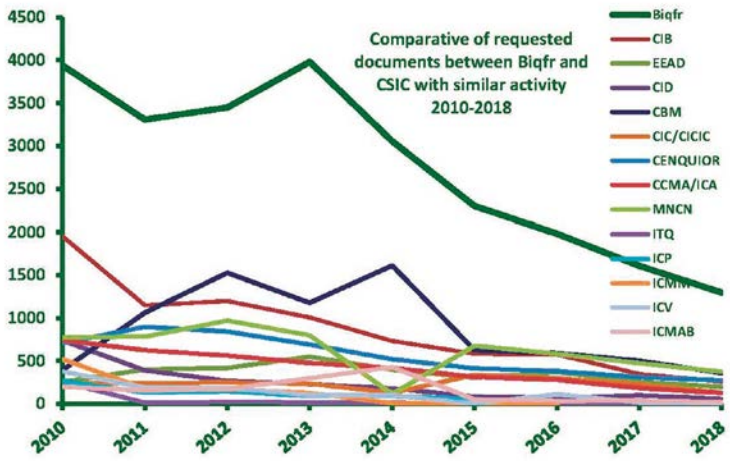


Figure 6

During 2017-18, the total number of document transactions was 3,260 (both supplied and requested.) Of these, 2.904 documents were delivered (-32.3% lower than 2015-15) Regarding our requests, 356 documents (-10.9% lower than); 19.1% documents requested from other libraries were supplied by Subito. Of these 2,904 documents supplied, 2,826 came from journal articles and 78 were book loans.

The number of book loaned to users was 25 in 2017 and 20 in 2018.

The Historic Documents Collection of the Institute of Physical Chemitry "Rocasolano"

This Institute was created in 1946 and, at that time, the Library took responsibility for preserving the unique scientific documental legacy that was formerly assembled and curated by the Instituto Nacional de Física y Química, a research facility implemented in 1932 by the Junta para la Ampliación de Estudios. Although this legacy mainly consisted in a collection of Physics and Chemistry books and journals, there was also a large number of written documents, memories, photographs and even films which are of great historical interest. To better preserve and popularize this part of the BIQR funds the Library opened a new section at the web page of the Institute, named Rockefeller Building https://www.biblioteca.iqfr.csic.es/en/rockefeller-building in which the digitized version of these written and graphic documents of historic interest would be made easily available to the interested reader.

Historic documentation of the Julio Palacios Chair (CSIC)

In 2015 the CSIC funded the Julio Palacios Chair, with the specific purpose of contributing to the general knowledge of the life and works of the Spanish scientist Prof. Julio Palacios Martínez (1891-1970). The BIQFR actively collaborated with this project in different ways from its inception. On one side the Library carried out an extensive compilation of scientific and historic documents relevant to the aims of the Chair. This search was performed in close connection with Prof. Palacios family, which provided a large number of very interesting manuscripts, press articles, photographs, etc. In addition, the Library designed a section on "Documentación" within the web page associated to Prof. Palacios Chair, www.jpalacios.iqfr.csic.es, that contains the digitized results of the compilation mentioned above. Later on, the Library also included within that web page an additional section, named "Galeria", specifically dedicated to graphic documents. More than 350 items were analyzed and digitized for both sections, that included journal papers, books, biographies, letters, press notes, etc.

Standard management

The Biqfr has continued the work of technical process, collections control, organization of the holding and signaling, maintaining the reading room service, etc.

The Organization of Courses and Events

We have also involve with several holdings in exhibitions

El Cosmo

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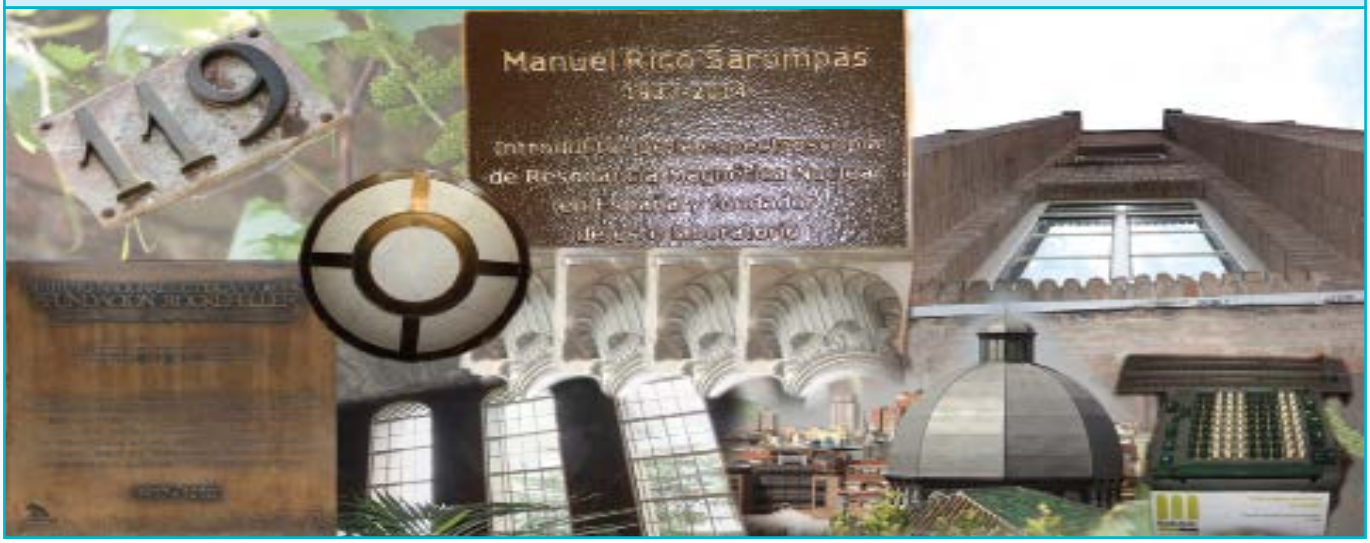
Administration-Stockroom-Reception



Management and administration Manager

Antonio Rubinos Pérez (until 06/09/2018)

Marta María Granja Perdices
(from 25/09/2018)

Administration

Julia Cano Garcia
(Paymaster until 04/06/2018/)

Gloria Alonso Gómez

Jose Enrique García Ortega
(until 15/03/2017)

Gloria Pinillos Pérez

Pilar Ruiz Lafita (until 21/01/2018)

Sagrario Salado Rey (until 15/12/2018)

Mar de la Torre Tante

Stockroom

Consuelo Martín de Loeches
(Stockroom Manager)

Eva María Carpintero Vázquez

Reception

José Luis Rodríguez Garro

Tomasa Grande Alonso
(until 31/03/2017)

Francisco González García
(from 29/12/2017 until 28/04/2018)

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Technical Support Units

Electronics Workshop

Angel Guirao Elias (from 01/03/2017)

Mechanics Workshop

Jose Antonio Serna Ferrero

Ignacio Sanz Gómez

Computer Support

Antonio Diaz Pozuelo

Building Maintenance

Jesús López Mascaraque

Juan Luis Martínez García

José Antonio Mulero Bravo
(until 31/01/2018)

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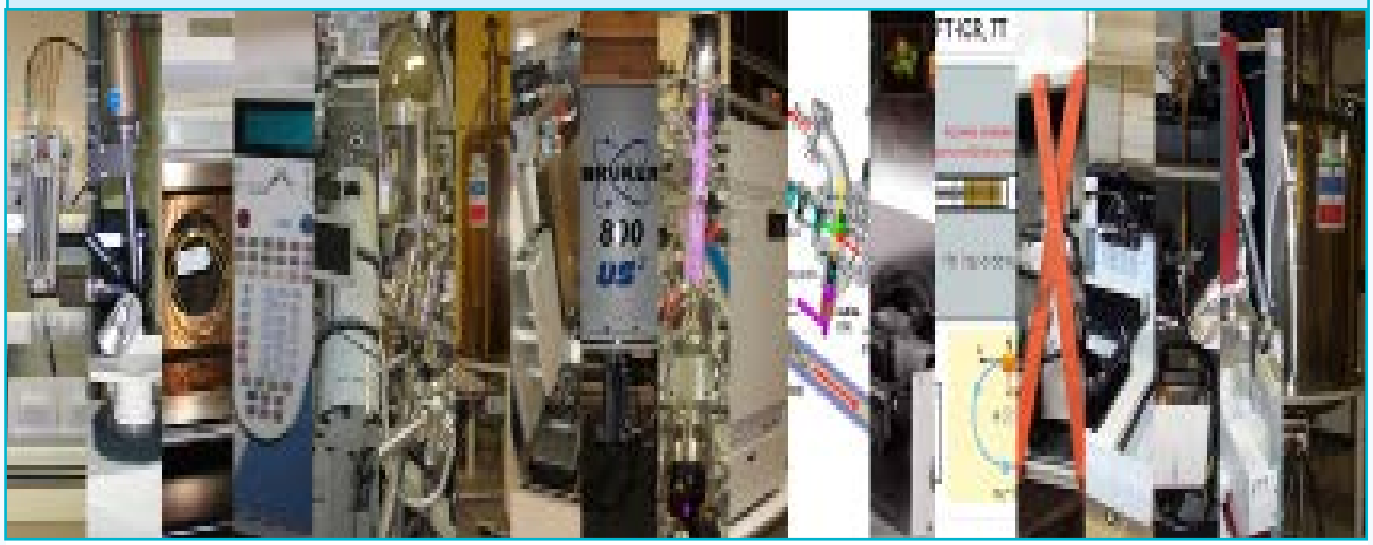
Singular Instrumentation

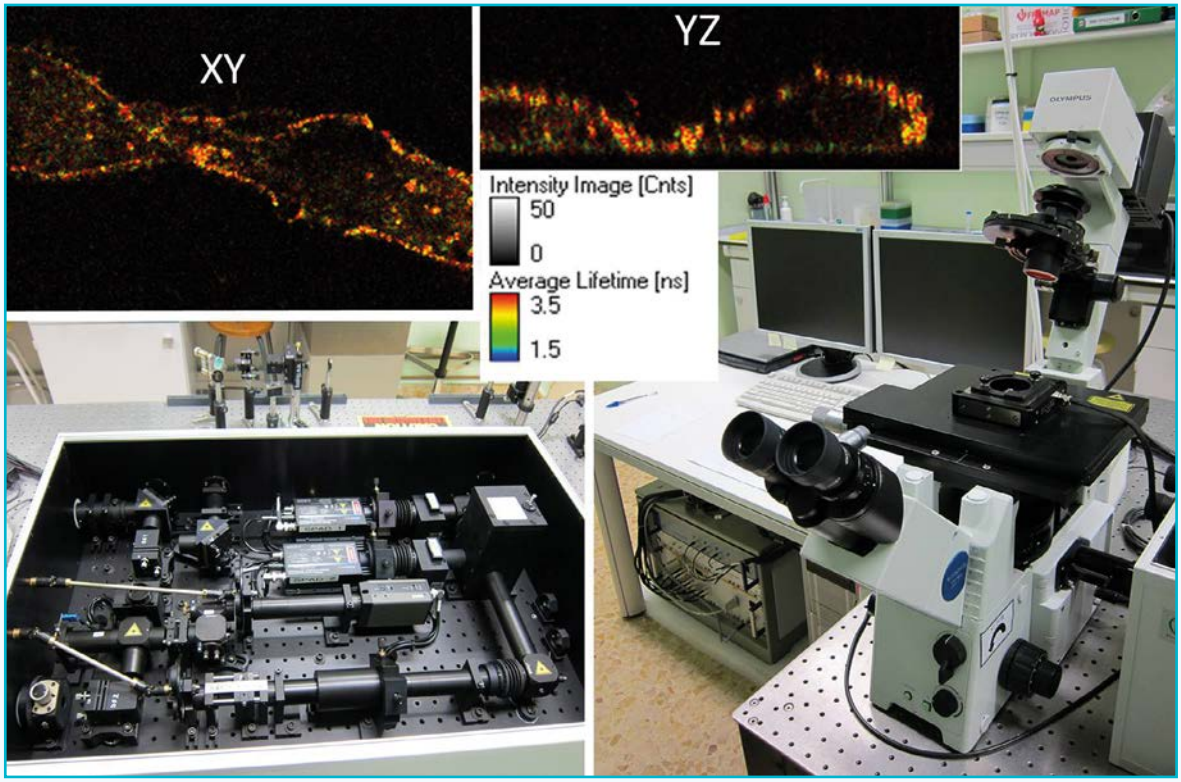


One- and Two-photon laser micro-spectrometer with ps-s time resolution

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.

Diluted solutions, crowded solutions mimicking physiological media, cellular extracts and living cells.

Contact person: M. Pilar Lillo



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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.

Applications:

- 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
- Cell biology

Diluted solutions, protein crowded solutions mimicking physiological media, cellular extracts, and live or fixed cells.

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.

Contact person: Dolores Solis/Maria Asunción Campanero-Rhodes

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

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

Brief description:The LMR lab hasthe most advanced techniques in the fieldof NMR spectroscopy required to addressproblems involving macromolecularstructures and interactions. Our high fieldspectrometers are the main researchtools utilized by the groups of Structure,Dynamics and Interactions of Proteins byNMR (http://rmnpro.iqfr.csic.es) and NMR Spectroscopy of Nucleic acids (http://rmnac.iqfr.csic.es/index.php/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.

Laboratory director:
Marta Bruix (until 15/08/2018)/ Carlos González (since 16/08/2018)

Technical director:
David Pantoja Uceda

Technical staff:
Miguel Treviño, Irene Gómez Pinto, Sergio Camero

Scientific committee:
M. Angeles Jiménez, Douglas V. Laurents, José M. Pérez, S.Padmanabhan.
Spectrometer

Spectrometer Bruker AV-600

- 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 AV-800 US2

- Cryoprobe TCI (1H,13C,15N)/ Z gradients
- Probe TXI (1H,13C,15N)/5mm/ Z gradients
- Probe QXI (1H, 13C, 15N, 31P)/5mm/ Z gradients

GC-MS system

Gas chromatograph coupled to a quadrupolar mass spectrometer, fitted with sample introduction systems for liquids and gases.

(Contact: Rosa Becerra Arias)

Gas chromatographs

Gas chromatographs for capillary and packed columns, with flame ionization detectors.

(Contact: Rosa Lebrón Aguilar)

MALDI-TOF mass spectrometer

Matrix assisted laser desorption/ionization-time of flight mass spectrometer, with a mass range in low resolution up to 300.000 u (linear mode) and in high resolution up to 10.000 u (reflector mode).

(**Contact**: Rosa Lebrón Aguilar)

LC-MS system

Liquid chromatograph with a quaternary gradient pump coupled to an ion trap mass spectrometer, with electrospray (ESI) and atmospheric pressure chemical ionization (APCI) interfaces, and with the possibility of tandem mass experiments (MS^n).

(**Contact**: Rosa Lebrón Aguilar)

Mössbauer spectrometers
José F. Marco

Spectrometer for 57Fe transmission Mössbauer spectroscopy in the temperature range 20-300 K (bulk analysis)

Spectrometer for room temperature Integral Conversion Electron Mössbauer Spectroscopy, ICEMS (surface analysis)

Ultra High Vacuum spectrometer for Integral Low Energy Electron Mössbauer spectroscopy, ILEEMS, in the temperature range 100-300 K (surface analysis)

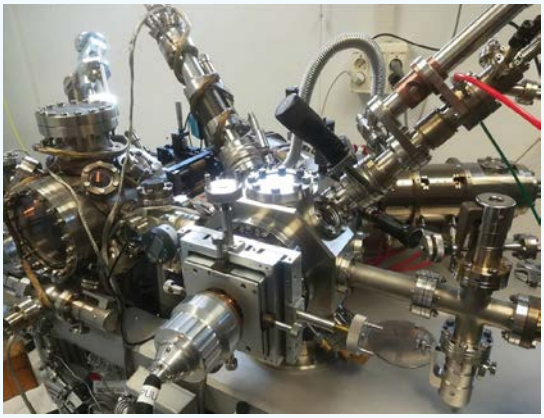
Nonlinear Optical Microscope
Marta Castillejo

The setup has been developed at IQFR-CSIC to operate in the modalities of multi-photon excited fluorescence, second- and third -harmonic generation, for the point wise collection of signals in epi-detection and transmission modes. The excitation source is a mode-locked Ti: Sapphire femtosecond laser emitting at 800 nm, with average power of 680 mW, releasing 70 fs pulses at a repetition rate of 80 MHz. The system allows retrieving morphological, structural and compositional information in 3D with micrometric resolution of thin films of different materials.

Low Energy Electron Microscope
Juan de la Figuera

Low Energy Electron Microscope mounted inside a Ultra High Vacuum chamber equipped with facilities for thin film deposition. The microscope allows to image surfaces with a lateral resolution of about 10 nm and to monitor in real time surface dynamical processes.

Different operation modes: diffraction contrast, phase contrast, (selected area) Low Energy Electron Diffraction, bright field and dark field imaging, etc. It is attached to an auxiliary UHV chamber with different facilities for surface preparation and characterization by XPS and a load lock system for fast sample exchange.



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IQFR Facts and Figures

Academic Training:

Technology Transfer and Socio-Economic Impact:

Academic Training

PhD awardees Exclusively during 2017-2018 period

Name	Department	Date	University	Thesis title
Elsa Franco Echevarría	Crystallography and Structural Biology (Beatriz González Pérez)	Jan 2018	Universidad Complutense de Madrid	Estudio Cristalográfico de las Inositol Quinasas de Mamífero y su Relación con RNA
María Moreno Alvero	Crystallography and Structural Biology (Armando Albert)	Jan 2017	Universidad Internacional Menéndez Pelayo	Bases estructurales de la percepción del ácido abscísico en plantas de cosecha
Mercedes Ramírez Escudero	Crystallography and Structural Biology (Julia Sanz Aparicio)	Jan 2017	Universidad Complutense de Madrid	Structural basis of the specificity in enzymes producing prebiotics
Ioanna Kalograiaki	Biological Chemical-Physics	05/06/2017	Universidad Complutense of Madrid	Patrones de glicosilación y reconocimiento por lectinas / Glycosylation patterns and recognition by lectins
Cristina Gallego Páramo	Biological Chemical-Physics	19/12/2017	Universidad Autónoma de Madrid	Nuevos Antibacterianos Basados en Enzimas Líticas de la Pared Celular de *Streptococcus mitis* y *Streptococcus pneumoniae*
Angélica Partida Hanon	Biological Chemical-Physics	26/10/2018	UCM	Design and structural characterization of minimized systems to study biomolecular interactions thorugh NMR
Jesús Fernández Zapata	Biological Chemical-Physics	30/11/2018	Universidad de Murcia	Modo de acción molecular de CarH, el prototipo de una nueva familia de fotorreceptores dependientes de la vitamina B12:plasticidad en su oligomerización, unión al DNA y diseño de su operador
Diego Bernal Bernal	Biological Chemical-Physics	27/11/2018	Universidad de Murcia	El complejo CarD-CarG y su implicación en un nuevo mecanismo de regulación de la expresión de un sistema CRISPR-Cas

Name	Department	Date	University	Thesis title
Álvaro Rodríguez Rodríguez	Sistemas de baja dimensionalidad, superficies y material condensada (Mari Cruz García Gutiérrez, Tiberio Ezquerra, Esther Rebollar)	22/09/2017	Universidad Complutense de Madrid	Propiedades físico-químicas de polímeros conjugados nanoestructurados y sus aplicaciones en células solares orgánicas/ Physicochemical properties of nanostructured conjugated polymers and their applications in organic photovoltaics
René Israel Rodríguez Beltrán)	Sistemas de baja dimensionalidad, superficies y material condensada (Pablo Moreno, Esther Rebollar)	13/03/2018	Universidad de Salamanca	Micro- y nanoestructurado de superficies de materiales avanzados con láseres pulsados de nano- y femtosegundos
Laura Martín García	BSDM	13/july/2017	Universidad Complutense de Madrid	Characterization of oxide surfaces and films: real-time growth, interface effects and magnetism

PhD fellowship/contract holders

Department of Crystallography and Structural Biology

Name	Funding body	Starting date	Supervisor
Elsa Franco Echevarría	Ministerio de Economía y Competitividad	Jan 2017-July 2018	Beatriz González Pérez
María Ángeles Márquez Moñino	Ministerio de Economía y Competitividad	Jan 2018-present	Beatriz González Pérez
Elena Jimenez Ortega	Ministerio de Economía y Competitividad	July 2018-present	Julia Sanz Aparicio

Department of Low Dimensional Systems, Surfaces and Condensed Matter

Name	Funding body	Starting date	Supervisor
Anna Mandziak	CSIC/Alba synchrotron	01/02/2017	Juan de la Figuera (IQFR) and Lucía Aballe (Alba)
Guiomar Delgado Soria	YEI/MINECO	16/04/2017	Juan de la Figuera (IQFR) and Adrian Quesada (ICV)

Department of Biological Chemical-Physics

Name	Funding body	Starting date	Supervisor
Jesús Fernández Zapata	Ministerio de Economía, Competividad	30/11/2018	Subramanian Padmanabhan Iyer and Montserrat Elías Arnanz
Diego Bernal Bernal	Ministerio de Economía, Competividad	27/11/2018	Subramanian Padmanabhan Iyer and Montserrat Elías Arnanz
Angélica Partida Hanon	CONACYT	01/09/2015-31/08/2018	Marta Bruix & M. Ángeles Jiménez
Belén Chaves Arquero	MINECO	01/01/2016-31/12/2019	M. Ángeles Jiménez and José M. Pérez Cañadillas
Israel Serrano Chacón	MINECO	01/12/2015-30/11/2019	Carlos González Ibáñez

Post-doctoral fellowship/contract holders

Name	Funding body	Starting date	Supervisor
Andrea Faganini	Fondo Gianesini Med	01/09/2017-31/08/2018	Douglas Laurents
Noemí Bustamante Spuch	CIBERES		Margarita Menéndez
Mª Asunción Campanero Rhodes	MINECO		Dolores Solís
Manuel Iglesias Bexiga	CIBERES	until 09/09/2017	Margarita Menéndez
Paula Morales	Juan de la Cierva-Formación	01/03/2018-15/02/2019	Marta Bruix and M. Ángeles Jiménez
Héctor Zamora Carreras	MINECO	01/01/2017-31/12/2017	Marta Bruix and M. Ángeles Jiménez
Miguel Garavís Cabello	Juan de la Cierva-Formación	xxx	Carlos González Ibáñez
Juan Pablo Corella Aznar	Juan de la Cierva (MICINN)	03/2015	Alfonso Saiz López
Luis Cerdán Pedraza	Project Contract	Finished: 31/12/2017	Inmaculada García-Moreno Gonzalo

TFG/TFM students Exclusively during 2017-2018 period

Name	Department	Date	University	Thesis title
Ester Sánchez Sánchez (TFG)	Crystallography and Structural Biology (M.J. Sánchez-Barrena)	June 2018	Universidad Politécnica de Madrid	Información estructural de la interacción entre el factor intercambiador de guaninas Ric8a y el sensor neuronal de calcio NCS-1
Patricia Blanco Gabella (TFG)	Crystallography and Structural Biology (M.J. Sánchez-Barrena)	June 2018	Universidad Politécnica de Madrid	Estudio estructural de la interacción de NCS-1 con moléculas reguladoras del complejo NCS-1/Ric8a
Miguel Daniel Mozo (TFG)	Crystallography and Structural Biology (M.J. Sánchez-Barrena)	June 2017	Universidad Politécnica de Madrid	Regulación de la función sináptica con pequeñas moléculas inhibidoras del complejo NCS-1/Ric8a
Elena Molina López (TFG)	Crystallography and Structural Biology (M.J. Sánchez-Barrena)	June 2017	Universidad Politécnica de Madrid	Determinantes estructurales de la tolerancia salina en plantas
Carla Berenguer Serrano	Biological Chemical-Physics (M. Gasset)	September 2017	Universidad Complutense de Madrid	Structural studies of the amyloids of the Atlantic Cod and ChubMackerel β-parvalbumins
Beatriz Escudero Lago	Biological Chemical-Physics (M. Gasset)	June 2017	Universidad Complutense de Madrid	Allergen extraction from fish: Atlantic Cod and Chub Mackerel
Celia Gil Campillo	Biological Chemical-Physics (Margarita Menéndez)	18/09/2017	Universidad Complutense de Madrid	Identificación y Caracterización de Nuevos Antibacterianos a Partir del Cribado de Quimiotecas
Alicia Plaza Sanz (TFG)	Biological Chemical-Physics (J.M. Pérez-Cañadillas)	2018-09-24	Universidad Complutense de Madrid	Estudio por resonancia magnética nuclear de GEMIN5
Alejandro Rubio Elías (TFG)	Biological Chemical-Physics (J.M. Pérez-Cañadillas)	2018-09-24	Universidad Complutense de Madrid	Estudio por Resonancia Magnética Nuclear de la proteína Hrp1

Name	Department	Date	University	Thesis title
Rocío Pliego Magán	Atmospheric Chemistry and Climate	20/06/2017-10/09/2017	Universidad de Castilla- La Mancha	Detección de especies traza relevantes en procesos atmosféricos y de la calidad del aire mediante espectroscopía de absorción óptica
Francisco Miguel Martín Ruz	Atmospheric Chemistry and Climate	03/02/2017-22/05/2017	Universidad Rey Juan Carlos	Análisis geoquímicos elementales e isotópicos, interpretación de resultados, búsqueda bibliográfica de aspectos relacionados con la temática a estudiar y análisis de retrotrayectorias atmosféricas
Paula Melero Abad	Química Atmosférica y Clima	01/02/2017-02/03/2018	Universidad Politécnica de Madrid	Poli(dimetilsiloxano) funcionalizado con un bajo porcentaje de 1-propil-3-metilimidazolio como nueva fase estacionaria para cromatografía de gases
Jesús Huamán Cjuno	Facultad de Ciencias-Escuela de Pos-grado	18/08/2018	Universidad Nacional de Ingeniería, Lima-Perú	Interacción de especies halogenadas en la atmósfera (Tesis de Maestría)
Jhonatan Eliel Martínez Oré	Facultad de Ciencias-Escuela de Pos-grado	03/07/2018	Universidad Nacional de Ingeniería, Lima-Perú	Energética olecular de M especies Orgánicas e Inorgánicas con impacto Ambiental (Tesis de Maestría)
Luis Roberto Carlos Ochoa	Facultad de Ciencias-Escuela de Pos-grado	03/07/2018	Universidad Nacional de Ingeniería, Lima-Perú	Procesos de protonación y su influencia en la fragmentación de isómeros orgánicos. Caso hidroxibenzofenonas (Tesis de Maestría)

Name	Department	Date	University	Thesis title
Adriano José García Martín (TFG)	Sistemas de baja dimensionalidad, superficies y materia condensada (Esther Rebollar)	19/07/2017	Universidad Politécnica de Madrid	Fabricación de sistemas poliméricos nanocompuestos mediante técnicas láser
Edgar Gutiérrez Fernández (TFM)	Sistemas de baja dimensionalidad, superficies y materia condensada (Aurora Nogales, Mari Cruz García Gutiérrez, Esther Rebollar)	15/06/2017	Universidad Internacional Menéndez Pelayo	Nanopartículas y nanocompuestos poliméricos
Javier Prada Rodrigo (TFM)	Sistemas de baja dimensionalidad, superficies y materia condensada (Esther Rebollar, Pablo Moreno)	29/06/2018	Universidad de Salamanca	Funcionalización de superficies de nanocompuestos poliméricos mediante LIPSS (Laser inducedperiodic Surface structures)
Farouk Ben Naamia	Sistemas de baja dimensionalidad, superficies y materia condensada	12/07/17	Ecole Nationald Ingenieurs de Gafse	Performing Intensive Molecular dynamics of mixtures of water/methanol
Antonio Díaz Pozuelo	Sistemas de baja dimensionalidad, superficies y materia condensada	23/07/18	Universitat Rovira I Virgili	Serial and parallel (CUDA) general purpose Monte Carlo code for atomistic simulations
Miguel Vázquez del Saz	Sistemas de baja dimensionalidad, superficies y materia condensada	11/07/18	Universidad Complutense de Madrid	Simulación de nuevos materiales por ordenador: sistemas coloidales
Paulina Prslja	Sistemas de baja dimensionalidad, superficies y materia condensada	25/09/17	University of Ljubljana	Properties of bulk and confined water-alcohol mixture

Scientist exchange

Se incluirán estancias pre-doctorales y sabáticos hacia o desde el IQFR

Name	Home institution	Destination institution	Dates
Rogeria Nunes Costa	Univ. Federal de São Paulo (Brasil)	IQFR/CSIC	05/06/2017–01/12/2017
Lourdes Infantes	IQFR, CSIC	UK	11/08/2017–27/08/2017 12/08/2018–27/08/2018
Andrea Martín Canal	CIB, CSIC	IQFR, CSIC	2017-2018
Belén Chaves Arquero	IQFR, CSIC	CBS, Montpellier, France	19/01/2018-13/04/2018
Federico Scoto	Ca' Foscari University of Venice	IQFR-CSIC	15/03/2018-31/07/2018
Diego Ricardo Alcoba Dabini	Universidad de Buenos Aires/Instituto de Física de Buenos Aires-CONICET	IQFR/CSIC	29/09/2017-14/10/2017
Julio Barrios	Univ. Nac. Ingeniería (Perú)	IQFR/CSIC	01/10/2017-30/10/2017
Ofelia Beatriz Oña	Universidad Nacional de la Plata/CONICET	IQFR/CSIC	23/05/2018-03/o6/2018
Alexsandre Lago	Universidade ABC-Sao Paulo	IQFR/CSIC	01/09/2018-07/09/2018
Josep M. Oliva-Enrich	IQFR, CSIC	Universidad de París Sur	01/09/2017-28/02/2018
J.Z. Dávalos	IQFR, CSIC	Univ. Nac. Ingeniería (Perú)	30/10/2017-03/11/2017
J.Z. Dávalos	IQFR, CSIC	Univ. Nac. San Cristóbal de Huamanga (Perú)	06/11/2017-10/11/2017
J.Z. Dávalos	IQFR, CSIC	Univ. Nac. San Cristóbal de Huamanga (Perú)	09/07/2018-13/07/2018
J.Z. Dávalos	IQFR, CSIC	Univ. Nac. San Cristóbal de Huamanga (Perú)	26/11/2018-28/11/2018
Enrique Lomba	IQFR, CSIC	Princeton University	01/07/17-30/10/17
Ariel Meyra	UNLP	IQFR	1/03/18-27/02/19

Name	Home institution	Destination institution	Dates
Leandro Guisández	UNLP	IQFR	27/05/18-25/05/19
Adela Reyes Contreras	Universidad Autónoma de México	IQFR	23/01/2017-18/07/2017
Marta Castillejo	IQFR, CSIC	Istituto Nazionale di Ottica, CNR	01/10/2018-31/03/2019

Courses and scientific meeting organization and participation

Organizer	Class	Title	Date	Place
UIMP-CSIC	Master in Molecular and Cellular Integrative Biology	Recognition by lectins (D. Solís)	11/10/2017	IQFR
		Calorimetric techniques (M. Menéndez)	04/10/2017	IQFR
		Laboratory rotations (D. Solís M. Menéndez)	27/11/2017 to 1/12/2017	IQFR
		Peptide structural characterization by solution NMR (M. Á. Jiménez)	10/2017	IQFR
		Prácticas de Cristalización (Beatriz González)	2018	IQFR-CSIC
		Protein production and purification (Beatriz González and M.J. Sanchez Barrena)	2018	CIB and IQFR-CSIC
		PPIs as drug target (M.J. Sánchez Barrena)	Jan 2018	IQFR-CSIC
		Structure of carbohydrate-active enzymes (Julia Sanz Aparicio)	Jan 2018	IQFR-CSIC
Universidad Autónoma de Madrid	Master in Molecular Biosciences-Biotechnology	Microbial and Enzymatic Biotechnology (Julia Sanz Aparicio)	Jan 2018	Dept de Bioquímica y Biología Molecular-UAM
Armando Albert & J.A. Hermoso	Macromolecular Crystallography School		May 2017 and 2018	IQFR-CSIC
Lourdes Infantes & Martín Martínez Ripoll	Organization of the Meeting "40 años de Cristalografía en el Rocasolano… ¿Y ahora qué?"		Jan 2017	IQFR-CSIC
Douglas V. Laurents		IV Simposio de Jóvenes Investigadores del IQFR	15/03/2017 15/03/2017	IQFR

Organizer	Class	Title	Date	Place
		Peptide structural characterization by solution NMR (M. Á. Jiménez)	10/2018	IQFR
		Advanced Fluorescence Microspectroscopy (P. Lillo)	01/2018	IQFR
		Title C. González	10/2017	IQFR
UAH	Master on Therapeutic Targets and Cellular Signalling: Design and Selection of Biologically Active Molecules	Biophysical approaches to characterize drug-target interactions (M. Menéndez)	09/02/2017	Faculty of Pharmacy (UAH)
UAH	Máster en Biomoléculas y Dinámica Celular	Estructura de macromoléculas y complejos macromoleculares: NMR		
		(M. Á Jiménez)	11/2017 and 2018	UAM
		(D. V. Laurents)	11/2017 and 2018	UAM
		(D. Pantoja-Uceda)	11/2017 and 2018	IQFR
Universidad Francisco de Vitoria	Grado en Biotecnología -Título propio: Experto en metodología en investigación biotecnológica	Técnicas Instrumentales Avanzadas – Fluorescencia (P. Lillo)	09/2017 09/2018	
		Técnicas instrumentales avanzadas (Armando Albert)	2017 and 2018	Universidad Francisco de Vitoria
Dept. Genetics, Univ. Murcia	Masters in Molecular Biology and Biotechnology expression"	"Prokaryotic transcription factors" in the seminars on "Regulation of gene	06-08/03/2017 and 26-28/02/2018	Univ. Murcia, Murcia
GERMN	XII Manuel Rico NMR summer school	(M. Á. Jiménez)	06/2017	Jaca, Huesca
		(D. V. Laurents)	06/2017	Jaca, Huesca

Organizer	Class	Title	Date	Place
XIª Reunión de Nucleótidos, Nucleósidos y Ácidos Nucleicos (RANN-XI)	Member of the Organising Committee	(C. González)	June 2017	Madrid
VIII Ribored	Member of the Organising Committee	(C. González)	June 2018	Madrid
Rosa Lebrón Aguilar	Curso de especialización	Cromatografía de Líquidos acoplada a la Espectrometría de Masas. 2017	13-16/11/ 2017	Instituto de Química-Física "Rocasolano" (Madrid)
Rosa Lebrón Aguilar	Curso de especialización	Cromatografía de Líquidos acoplada a la Espectrometría de Masas. 2018	22-25/10 /2018	Instituto de Química-Física "Rocasolano" (Madrid)
J.Z Dávalos Prado	Specialization-course	Técnicas (nano) espectroscópicas y microscópicas para el estudio de láminas delgadas y nanoestructuras	03/12/2018 07/12/2018	Fac. Ciencias, Univ. Nac. Ingeniería (Perú)
J.Z Dávalos Prado	Specialization course	Estructura y energética molecular de antioxidantes polifenólicos	26/11/2018 28/12/2018	UNSCH-Ayacucho-Perú
J.Z Dávalos Prado	Specialization course	Introducción a la Modelización Estructural de especies con efectos atmosféricos: Química Computacional	09/07/2018 13/07/2018	UNSCH-Ayacucho-Perú
J.Z Dávalos Prado	Specialization course	Identificación y Análisis estructural de especies mediante Espectrometrías de última generación	06/11/2017 10/11/2017	UNSCH-Ayacucho-Perú
J.Z Dávalos Prado	Specialization course	Espectroscopía de absorción de Rayos X (XAS)	30/10/2017 03/11/2017	Fac. Ciencias, Univ. Nac. Ingeniería (Perú)
XXVI-Aniversario EPCFM-UNSCH	Invited conference (JZ Dávalos)	Ciencia y tecnología, ¿dualidad clave para el desarrollo de la sociedad?	30/11/2018	UNSCH-Ayacucho-Perú
SINAPSIS-2018	Master Conference (JZ Dávalos)	Papel crucial de los gases traza en la química atmosférica	25/10/2018	Barcelona-España

Organizer	Class	Title	Date	Place
ECITEC 2017	Invited conference (JZ Dávalos)	Energética molecular y reactividad química de contaminantes-traza atmosféricos	2-3/11/2017	Fac. Ciencias, Univ. Nac. Ingeniería (Perú)
XVI Encuentro de Física	Invited conference (JZ Dávalos)	Reactividad molecular de contaminantes atmosféricos	02/08/2017	Univ. Nac. Ingeniería (Perú)
Josep M. Oliva-Enrich	Organizer	II Julio Palacios International Symposium	11-12/08/2018	A Coruña
II Workshop on Chemistry of Group 11 Elements	Poster (JM Oliva-Enrich)	Gold-Carboranes as a Host Structure	26-27/01/2017	Univ. Barcelona
CECAM Workshop on ab initio Valence Bond and Non-Orthogonal CI approaches	Invited Conference (JM Oliva-Enrich)	Valence-Bond Theory for Solids? (A Wishful Thinking)	27-30/03/2017	Institut Henri Poincaré, París, Francia
XXXVI Reunión BIENAL de la RSEQ	Oral Presentation+Poster (JM Oliva-Enrich)	Heteroborane Chemistry Beyond Frontiers: Designing Properties from Electronic Structure Computations	25-29/06/ 2017	Sitges, Barcelona
Seminario de Química Teórica, INIFTA-CONICET	Comunicación oral (JM Oliva-Enrich)	Anisotropía Magnética en Complejos de Co(II)	09/11/2017	Buenos Aires, Argentina
II Simposio Internacional Julio Palacios	Poster (JM Oliva-Enrich)	Magnetic properties in mononuclear Co (II) complexes with polyhedral carborane ligands	11-12/07/2018	A Coruña
II Simposio Internacional Julio Palacios	Poster (JM Oliva-Enrich)	Theoretical calculation of acidity constants of carbaborane dicarboxylic acids in aqueous solution	11-12/07/2018	A Coruña
XI ESPA Congress	Attendance (JM Oliva-Enrich)		16/07/2018	Toledo
Congreso de la Asociación Física Argentina	Poster (JM Oliva -Enrich)	Propiedades Magnéticas en Complejos Mononucleares de Co(Ii) con Ligandos Carborano Poliédricos	17-21/09/2018	Buenos Aires, Argentina

Organizer	Class	Title	Date	Place
Mohamed Oujja in Universidad Internacional Menéndez Pelayo – CSIC	Conferencia invitada en el marco del Curso Taller: Metodologías destructivas: análisis de patrimonio (MetAnD)	Laser Induced Breakdown Spectroscopy	31-5-2017	Instituto de Tecnología Físicas y de la Información avanzadas no "Leonardo Torres Quevedo" (CSIC), Madrid, España
Mohamed Oujja in Fundación Arquitectura COAM, Madrid	Ciclo conferencias: Patrimonio y nuevas tecnologías: Sistemas y tecnologías innovadoras en la conservación del Patrimonio Cultural	El láser para limpieza de sustratos pétreos del patrimonio cultural	24-10-2017	Sede de la Fundación Arquitectura COAM, Madrid
Mohamed Oujja in Centro de Investigaciones Energéticas, Medioambientales y tecnológicas, CIEMAT, CSIC, Madrid	Conferencia invitada en el marco del Curso técnicas espectroscópicas para la caracterización de materiales naturales y Sintéticos	Espectroscopia de ruptura inducida por láser (LIBS) y fluorescencia nducida por iláser (LIF) para análisis de materiales	29-11-2017	Centro de Investigaciones Energéticas, Medioambientales y tecnológicas, CIEMAT, CSIC, Madrid
Mohamed Oujja in Biblioteca Nacional, Madrid	Conferencia invitada en el marco del Curso *"La codicología Cientifica y los Manuscritos Iluminados"*	Técnicas aplicadas III. Espectrometrías: LIBS y LIF. Microscopía óptica no-lineal	25-11-2018	Biblioteca Nacional, Madrid
Esther Rebollar	Member of organizing local committee of congress	VIII AUSE Congress	9-11/10/2017	CSIC, Madrid
Esther Rebollar	Co-organizer of symposium	"Photon-Assisted Synthesis and Processing of Materials in Nano-Microscale" at E-MRS 2018	18-22/06/2018	Strasbourg, France
Rebeca de Nalda	Simposium	5th IQFR Young Researchers' Simposium	29-5-2018	IQFR-CSIC Madrid
Rebeca de Nalda	IQFR seminarcycle 2016-2017	7 scientific seminars organized in 2017	January to June 2017	IQFR-CSIC Madrid
Rebeca de Nalda (member of the scientific committee)	Curie Colloquiumseminar series	2 seminars organized in 2017; 5 seminars organized in 2018	October 2017 to December 2018	CSIC Madrid

Organizer	Class	Title	Date	Place
Rebeca de Nalda (member of the advisory committee)	National scientific conference	Ultrafast Science and Technology – Spain 2017	November 2017	Salamanca
Coordination	Rebeca de Nalda	Semana de la Ciencia IQFR 2017	November 2017	Coordination of activities of Semana de la Ciencia IQFR 2017
Coordination	Rebeca de Nalda	Semana de la Ciencia IQFR 2018	November 2018	Coordination of activities of Semana de la Ciencia IQFR 2018
Coordination	Rebeca de Nalda	Nanofestival 2018	March-April 2018	Coordination of activities of Nanofestival 2018 in IQFR
Universidad de Santiago de Chile	J.F. Marco	Curso de caracterización de Materiales (15 h)	August 2018	Santiago de Chile (Chile)
Pontificia Universidad Católica de	J.F. Marco and J. De la Figuera	Curso de Caracterización de Materiales mediante electrones (15 h)	November 2018	Santiago de Chile (Chile) Chile
Universidad Nacional de Ingeniería (Lima, Perú)	J. F. Marco and J. De la Figuera	Curso de Caracterización de Materiales mediante electrones (15 h)	December 2018	Lima (Peru)

Scientific Outreach

Activity	Researcher	Title	Date	Description
International Day of Women and Girls in Science	Lourdes Infantes San Mateo/Beatriz González Pérez		Feb 2017 y 2018	Talleres para alumnos de 4º primaria del Colegio Ramiro de Maeztu
	MJ Sánchez-Barrena	I am a scientist	March 2018	Activity for 5 year old kids to promote science and research. C.E.I.P. Ángel León (Colmenar Viejo)
	MJ Sánchez-Barrena	My research on autistic disorders	Feb 2018	Activity in C.E.I.P. Santa Marina (Badajoz) with 9 year old pupils (4º Primaria)
	MJ Sánchez-Barrena	Cristalografía: los ojos de la Química para el desarrollo de aplicaciones en biomedicina y biotecnología	2018	Activity in I.E.S. Albarregas (Mérida) with 16 and 17-year-old kids on the power of Crystallography and the participation of women
	Mª Asunción Campanero Rhodes	Deciphering the sugar code	12/02/2018	Divulgation talk to students of 4º of ESO. San Ramón and San Antonio School
	Mª Asunción Campanero Rhodes	Deciphering the sugar code	14/02/2018	Divulgation talk to Corazón Inmaculado High School students
	Mª Asunción Campanero Rhodes	Deciphering the sugar code	08/02/2018	Divulgation talk to Blanca de Castilla 4º of ESO and High School students
	Irene Gómez Pinto	Grandes mujeres científicas en la historia: *Rita Levi-Montalcini* (Neurobióloga) y *Rosalind Franklin* (Química cristalógrafa). -Las mujeres científicas de hoy y en tu barrio.	09/02/2018	Trata de llevar a cabo un debate sobre ¿Qué dicen las encuestas sobre las carreras que escogen chicos y chicas?. Y ¿Porque hay menos chicas que deciden estudiar as carreras llamadas STEM?

Activity	Researcher	Title	Date	Description
XVII Science week at CSIC: Ciencia en la biblioteca	Douglas Laurents	Los amiloides y su papel en enfermedades neurodegenerativas como la esclerosis lateral amiotrófica	06/11/2017	Divulgation talk about proteins, amiloids and their role in diseases
	Carlos González Ibáñez	La estructura del ADN: El poder de la hélice	07/11/2017	Divulgation talk about the DNA structure, how our view of DNA sructure is changing, and how thischange of view will affectfuture medicine.
	Douglas Laurents	Los amiloides y su papel en enfermedades neurodegenerativas como la esclerosis lateral amiotrófica	13/11/2018	Divulgation talk about proteins, amiloids and their role in diseases
	Carlos González Ibáñez	La estructura del ADN: El poder de la hélice	12/11/2018	Divulgation talk about the DNA structure, how our view of DNA sructure is changing, and how this change of view will affect future medicine
XVII Science week at CSIC. Open doors day at the IQFR	Margarita Menéndez Noelia Hernández & Noemí Bustamante	Heat exchange: a tool to follow chemical and physical processes or the interactions between molecules	15/11/2017	Divulgation talk and guided visit to ESO and High School students
	Douglas Laurents & David Pantoja Laboratorios Title	Jornada de Puertas Abiertas y Visitas Guiadas a los	15/11/2017	Short talk about proteins and guided visit to NMR lab
	Israel Serrano Chacón & Belén Chaves Arquero	Visita guiada por los laboratorios	15/11/2017	Guided visit to IQFR labs
	Mohamed OujjaAyoubi	Procesado láser de materiales	November 2017 - 2018	Demostración en laboratorio sobre el procesado láser de materiales

Activity	Researcher	Title	Date	Description
XVIII Science week at CSIC. Open doors day at the IQFR	Margarita Menéndez Fernández	Heat exchange: a tool to follow chemical and physical processes or the interactions between molecules	14/11/2018	Divulgation talk and guided visit to ESO and High School students
	Douglas Laurents & David Pantoja	Jornada de Puertas Abiertas y Visitas Guiadas a los Laboratorios	14/11/2018	Short talk about proteins and guided visit to NMR lab
	Israel Serrano Chacón, Cristina Cabrero Fernández & Belén Chaves Arquero	Visita guiada por los laboratorios	14/11/2018	Guided visit to IQFR labs
XVIII Science week 2018	Mohamed OujjaAyoubi	Taller de limpiezaláser	November 2017 - 2018	Charla introductoria sobre láseres para procesado de materiales y demostración en laboratorio sobre la limpieza láser de materiales
	José Emilio Prieto	Nanociencia y Ciencia de Superficies	13-11-2018	Charla de presentación de la investigación del IQFR. Día de puertas abiertas IQFR
	José Emilio Prieto	Presentación de la investigación del IQFR	13-11-2018	Visita guiada a los laboratorios de XPS, Mössbauer y LEEM
	Guiomar Delgado Soria	Presentación de la investigación del IQFR	13-11-2018	Visita guiada a los laboratorios de XPS, Mössbauer y LEEM
	María Sánchez-Arenillas	Presentación de la investigación del IQFR	13-11-2018	Visita guiada a los laboratorios de XPS, Mössbauer y LEEM
	Fernando Moutinho	Presentación de la investigación del IQFR	13-11-2018	Visita guiada a los laboratorios de XPS, Mössbauer y LEEM
	Mikel Sanz	Fundamentos y aplicaciones del láser	16-11-2017	Conference

Activity	Researcher	Title	Date	Description
	Mikel Sanz	Limpiezaláser	13-11-2017	Workshop
	Mikel Sanz	Open Doors Day	16-11-2017	Visit to the laboratories
	Mikel Sanz	Limpiezaláser	07-11-2018	Workshop
	Mikel Sanz	Open Doors Day	13-11-2018	Visit to the laboratories
Scientific Conferences of CSIC for the Education System of the Community of Madrid	Mª Asunción Campanero Rhodes	Deciphering the sugar code	17/10/2018	Divulgation talk to I.E.S. "Alpajés" High School students
III Festival de la Nanociencia y de la Nanotecnología "10ALAMENOS9"	Mohamed OujjaAyoubi	Nanotecnología	10-4-2018	Charla sobre la nanotecnología y su presencia y efectos en nuestro día a día.
Jornadas de puertas abiertas "Nanoinmersión en el Rocasolano"	Mohamed OujjaAyoubi	Visita guiada a los laboratorios de Láseres, Nanoestructuras y Procesado de Materiales	12-4-2018	Demostración en laboratorio sobre el procesado láser de materiales
Festival de la Nanociencia y la Nanotecnología	Mikel Sanz	La nanotecnología en nuestras vidas	06-04-2017	Conference
Ciencia a la carta	Mikel Sanz	Edificios de luz	11-02-2018	Radio programme
Festival de la Nanociencia y la Nanotecnología	Mikel Sanz	La nanotecnología en nuestras vidas	20-04-2018	Conference
Ciencia a la carta	Mikel Sanz	Edificios de luz	03-05-2018	Conference
Ciencia a la	Mikel Sanz	Edificios de luz	18-11-2018	Scientific tour
Workshop	Luis Cerdán	Workshops in Physics and Chemistry for Gifted and Talented Kids	02/12/2017-01/12/2018	Madrid
Workshop	Luis Cerdán	Finde Científico	27/05/2017	FECYT, Alcobendas

Activity	Researcher	Title	Date	Description
Workshop within CSIC Science Week	Luis Cerdán	Open Lab Day	16/11/2017	IQFR
Talk	Rebeca de Nalda	Pulsos de luz que congelan el tiempo	23/02/2017	Talk in IES (Bachillerato de Excelencia)
Talk	Rebeca de Nalda	¿Qué es investigar?	13/11/2017	Talk in IQFR – Semana de la Ciencia 2017
Workshop	Rebeca de Nalda y Esther Rebollar	Descubriendo la luz	5, 7, 9, 20 February 2018	Workshop with 7 and 8 year old kids, 11-F activity
Talk	Rebeca de Nalda	Nanociencia y Nanotecnología	09/03/2018	Talk in IES – Nanofestival 2018
Talk	Rebeca de Nalda	¿Qué es investigar?	07/11/2018	Talk in IQFR – Semana de la Ciencia 2018

Technology Transfer And Socio-Economic Impact

Patents

Authors	Title	Year	Code
Ruth Pérez Fernández, Andrea Canal Martín, Mª José Sánchez Barrena and Alicia Mansilla Aparicio	Acilhidrazonas para el tratamiento de enfermedades neurológicas	2018	P201830933
Novoa, B., Figueras, A., Gasset, M., Rey, M., Mallavia, R., Medina, R., Martínez, A.	Myticin-based peptide and its use in cell regeneration	2018	P201831154
J L Chiara, I García-Moreno, A Blázquez, MD Chiara, I Saíz de Santamaría	Derivados de BODIPY carnitina: compuestos y sus usos como sondas fluorescentes	2017	P201730885

Awards and distinctions

- 2017 "Jose Tormo" prize on Structural Biology to Dr. Antonio Chaves-Sanjuán to give recognition to the work performed at the Department of Crystallography and Structural Biology, on the development of therapeutic molecules for Fragile X syndrome, which was published in PNAS in 2017.
- The NMR specialized group (GERMN) from RSEQ has awarded Héctor Zamora-Carreras, who was supervised by Marta Bruix and M. Ángeles Jiménez, the prize to the "best NMR thesis" defended in the 2016/2017 academic year.
- Belén Chaves Arquero was awarded the3rd prize to poster communication presented in GERMN Biennal, June 2018, hold in Lisbon, Portugal
- Enrique Lomba, Americal Physical Society Outstanding Referee Award, 2018.
- Enrique Lomba, HPC AdminTech 2018 Award to a career in HPC.

Editorial and scientific committees

Participant	Committee/Journal	Role
Maria Gasset	PLOS ONE	Academic Editor
María Gasset	Biomolecules	Academic Editor
Maria Gasset	American Alzheimer´s Association	Research Grant Reviewer
M. Ángeles Jiménez	NMR Group (GERMN) of the RSEQ	Treasurer (until 26/6/2018)
David Pantoja Uceda	NMR Group (GERMN) of the RSEQ	Treasurer (since 27/6/2018)
Rebeca de Nalda	Conference Ultrafast Science and Technology Spain - USTS2017. Salamanca, November 2017	Member of the international scientific committee
Marta Castillejo	Simposium "Light-Matter Interactions and Materials" Internacional Conference CLEO Europe, Munich, Germany, June 2017	Member of the international scientific committee
Marta Castillejo	International Conference on Laser Ablation, COLA, Marseilles, France, September 2017	Member of the international scientific committee
Marta Castillejo	International Conference on Lasers in the Conservation of Artworks (LACONA), Paris, France September 2018	Member of the international scientific committee
Marta Castillejo	Technart Bilbao, May 2017	Member ofthe international scientific committee
Marta Castillejo	International Review Panel of the Hilase Laser facccility, Czech Republic	Member of the review panel
Esther Rebollar	Applied Surface Science	Co-editor of special issue "Photon-assisted synthesis and processing of materials in nano-microscale"
Juan de la Figuera	International Board of the European Conference on Surface Crystallography and Dynamics	Member
Juan de la Figuera	Journal of Physics d: Applied Physics	Member of the Editorial Board
Juan de la Figuera	International Review Panel of the Solaris Synchrotron (Poland)	Member of the review panel

Media coverage

Name	Media y date	Link
MJ Sanchez-Barrena	Diario Hoy de Extremadura	http://www.hoy.es/extremadura/201703/06/reto-madre-cientifica-20170306001358-v.html
MJ Sánchez-Barrena	"Te doy mi palabra", Ondacero. April 2017	http://www.ondacero.es/programas/te-doy-mi-palabra/audios-podcast/entrevistas/maria-jose-sanchez-barrena-hemos-conseguido-regular-el-numero-de-contactos-sinapticos-en-el-autismo_2017040158df61f30cf2f2c8754f3bd1.html
MJ Sánchez-Barrena	Diario ABC. August 2017	https://www.abc.es/ciencia/abci-estos-leonardos-siglo-investigan-espana-201708290839_noticia.html
MJ Sánchez-Barrena	Madri+d. January 2017	http://www.madrimasd.org/noticias/hallada-una-nueva-molecula-capaz-de-modificar-el-numero-de-contactos-sinapticos-entre-neuronas/68226
MJ Sánchez-Barrena	Instruct ERIC. February 2017	https://www.structuralbiology.eu/news/interference-of-the-complex-between-ncs-1-and-ric8a-with-phenothiazines-regulates-synaptic-function-/
MJ Sánchez-Barrena	SEBBM. January 2017	http://www.sebbm.es/web/es/noticias-en-portada/sala-prensa/1916-hallada-una-nueva-molecula-capaz-de-modificar-el-numero-de-contactos-sinapticos-entre-neuronas
MJ Sánchez-Barrena	Agencia EFE. January 2017	https://www.efefuturo.com/noticia/molecula-mejora-aprendizaje-autismo-severo/
MJ Sánchez-Barrena	Cataluña Vanguardista. January 2017	https://www.catalunyavanguardista.com/tag/maria-jose-sanchez-barrena/
MJ Sánchez-Barrena	Asociación para vencer el Autismo y T.G.D. January 2017	http://www.autismoava.org/noticias/maria-jos%C3%A9-s%C3%A1nchez-cient%C3%ADfica-qu%C3%ADmica-en-el-csic-maria-jos%C3%A9-s%C3%A1nchez-cient%C3%ADfica-qu%C3%ADmica-en

Name	Media y date	Link
MJ Sánchez-Barrena	Asociación Frágil X	http://www.xfragil.net/investigacion-autismo/
¿Profesiones de chicos?	El Pais, 23 de Mayo 2018	https://elpais.com/economia/2018/05/22/actualidad/1527002625_327491.html?id_externo_rsoc=FB_CM
Rebeca de Nalda, Luz láser ultracorta para cambiar la dirección de los productos de reacciones químicas	Nota de Prensa CSIC, 7 noviembre 2017	http://documenta.wi.csic.es/alfresco/downloadpublic/direct/workspace/SpacesStore/5462e0a2-35d1-4473-ac2d-e97a6e4473fe/07noviembre17estereoquimica.pdf

Associated units

1. **Química Física Molecular**: Departamento de Química Física I, Facultad de Ciencias Químicas, Universidad Complutense de Madrid

In this Associated Unit CSIC participates with three Institutes: IEM, IFF and IQFR. Permanent staff members at IQFR participating in the Associated Unit are: Enrique Lomba García, Eva González Noya, Marta Castillejo Striano and Rebeca de Nalda Mínguez (Unit manager at IQFR).

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.

Research topics:

- Dynamics and kinetics of photochemical processes.
- Study of structures of molecules and condensed phases (ices) with interest in atmosphere and astrophysical science.
- Interaction of laser radiation with molecules and solid substrates.

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

2. Genética Molecular (Universidad de Murcia)

The responsible persons are Carlos González from the IQFR-CSIC and Montserrat Elías from the Universidad de Murcia.

Description:

Scientific research in the current (and future) Genomics era has a marked multidisciplinary character that requires and is reinforced by the exchange of ideas and information. This multidisciplinarity is especially relevant in the areas of Structural and Functional Genomics nourished by combining disciplines that span from biomacromolecular structure determination (by X-ray diffraction, nuclear magnetic resonance or electron microscopy methods) to Genetics, Molecular Biology, Protein and Nucleic Acid Chemistry, Biophysics, and Bioinformatics. This Associated Unit between the Molecular Genetics group at the University of Murcia and the Institute of Chemistry-Physics "Rocasolano" (IQFR) has been continually active since its establishment in 2006. It complements and enhances the research lines of both GM-UMU and the Department of Biological Physical Chemistry of the IQFR, and is focussed on elucidating the molecular mechanisms of cellular responses to light. The association has yielded excellent results amply reflected in progress reports submitted every three years as part of the renewal process of the Associated Unit. Its success is evident in: (a) joint publications in renowned journals such as Nature, 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; (d) continuous research funding in coordinated projects between members of the unit; (e) shared mentoring of doctoral students.

3. Estabilidad, Plegamiento y Estructura de Proteínas (BIFI, Universidad de Zaragoza).

The responsible persons are M. Ángeles Jiménez at the IQFR-CSIC, and Javier Sancho from the BiFi, Universidad de Zaragoza.

Description:

This associated unit aims to facilitate to all its members the use of the most suitable methodology to face thechallenges of theirprojects in the Structural Biology field. Researchers from the Deparmentof Cristallography 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.

4. Estudio Biofísico y Estructural de Ácidos Nucleicos (Universidad de Barcelona)

The responsible persons are Carlos González, on the side of IQFR-CSIC, and Nuria Escaja from the UB side.

Description:

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 form the IQFR with the high capabilities of the UB in synthetic chemistry and different analytical techniques.

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

5. **Fisicoquímica de Superficies** (Laboratorio de Superficies, Facultad de Ciencias Físicas, Universidad Complutense de Madrid).

The responsible persons are Juan de la Figuera (IQFR-CSIC) and Arantzazu Mascaraque (UCM).

Description:

This associated unit is devoted to the study of low-dimensional magnetic systems as well as surfaces.

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

Scientific Cloister

President:	**Juan de la Figuera Bayón**	**Associate Professor** (Director until 03/07/2017)
	Carlos González Ibañez	**Professor** (Director from 04/07/2017)
Secretary:	**Beatriz González Pérez**	**Assistant Professor**
Members:	**A.Ulises Acuña Fernández**	**Professor ad Honorem**
	Martín Martínez Ripoll	**Professor ad Honorem**
	Marta Bruix Vallés	**Professor** (until 15/08/2018)
	Angel Costela González	**Professor** (until 09/06/2017)
	Inmaculada García-Moreno Gonzalo	**Professor**
	Carlos González Ibañez	**Professor**
	Juan Antonio Hermoso Domínguez	**Professor**
	Enrique Lomba García	**Professor**
	Rafael Notario Bueno	**Professor** (until 03/09/2018)
	Subramanian Padmanabhan	**Professor** (from 09/01/2018)
	Armando Albert de la Cruz	**Associate Professor**
	Rosa Becerra Arias	**Associate Professor**
	Marta Castillejo Striano	**Associate Professor**
	Pablo Chacón Montes	**Associate Professor** (from 01/08/2018)
	Juan de la Figuera Bayón	**Associate Professor**
	Maria A. Gasset Vega	**Associate Professor**
	Maria Angeles Jiménez López	**Associate Professor**
	Douglas V. Laurents	**Associate Professor** (from 19/12/2017)
	Jose Francisco Marco Sanz	**Associate Professor**
	Margarita Menéndez Fernández	**Associate Professor**
	Alfonso Saíz López	**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**
	Beatriz González Pérez	**Assistant Professor**
	Lourdes Infantes San Mateo	**Assistant Professor**
	Rosa Lebrón Aguilar	**Assistant Professor**
	Maria Pilar Lillo Villalobos	**Assistant Professor**

Members:	**Jose Miguel Mancheño Gómez**	**Assistant Professor**
	Rebeca de Nalda Mínguez	**Assistant Professor**
	Jose Maria Oliva Enrich	**Assistant Professor**
	Jose Manuel Pérez Cañadillas	**Assistant Professor**
	Jose Emilio Prieto de Castro	**Assistant Professor** (from 23/07/2018)
	Esther Rebollar González	**Ramon y Cajal Contract**
	Maria José Sánchez Barrena	**Contracted Dr.** (from 21/10/2016)
	Carlos Alberto Cuevas Rodríguez	**Contracted Dr.** (from 01/10/2018)

Board of Institute

President: **Juan de la Figuera Bayón** (until 03/07/2017)
Carlos González Ibáñez (from 04/07/2017)

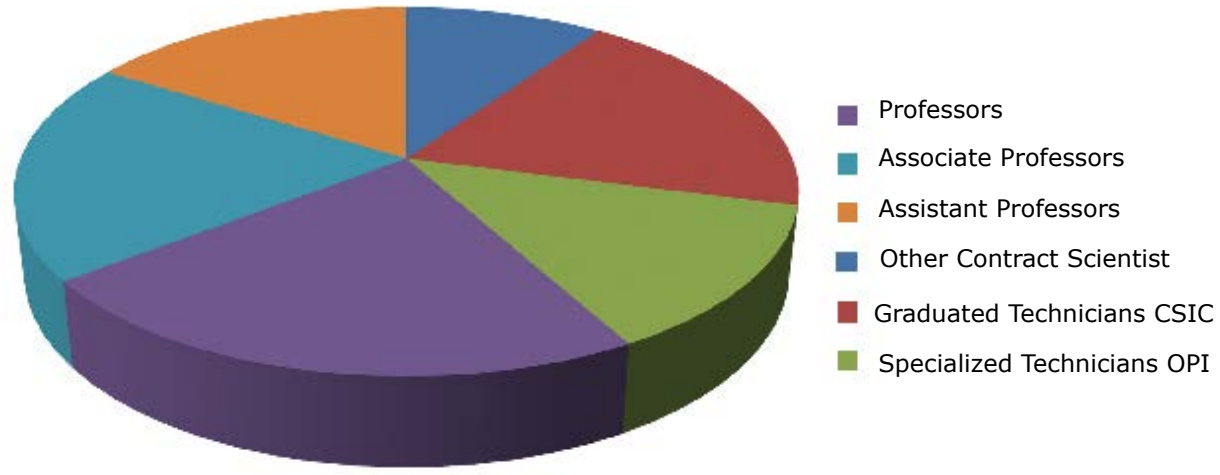
Secretary: **Antonio Rubinos Pérez** (until 06/09/2018)
Marta María Granja Perdices (from 25/09/2018)

Members:
Juan Dávalos Prados (Vice Director until 03/07/2017)
Beatriz González Pérez (Vice Director from 05/07/2017)
Douglas V. Laurents (Vice Director until 03/07/2017)
Rebeca de Nalda Mínguez (Vice Director from 05/07/2017)
Armando Albert de la Cruz
(Head of Department of Crystallography and Structural Biology)
Alfonso Sáiz López
(Head of Department of Atmospheric Chemistry and Climate)
Carlos González Ibañez (Head of Department of Biological Physical Chemistry, until 21/09/2017)
M. Ángeles Jimenez (since 21/09/2017)
Marta Castillejo Striano
(Head of Department of Low Dimensional Systems, Surfaces and condensed Matter)
Plácido Galindo Iranzo (Personnel Representative)
Eva González Noya (Personnel Representative
Carolina García Rodriguez (Personnel Representative from 04/10/2017)
Rebeca de Nalda Minguez (Personnel Representative until 05/07/2017)
Sagrario Salado Rey (Personnel Representative until 15/12/2018)

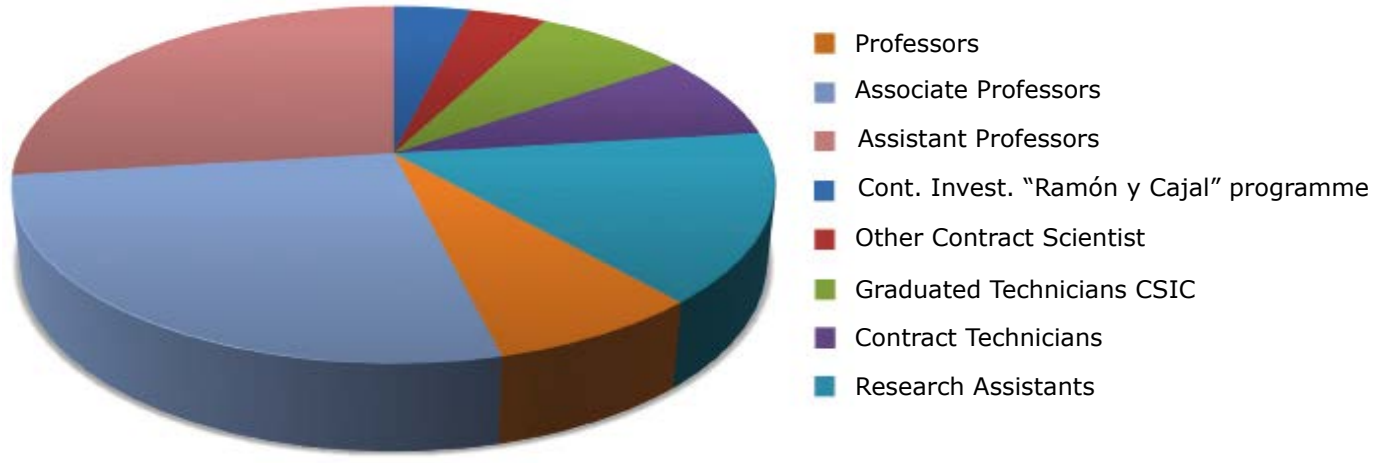
Gender distribution of scientific staff according to professional category

Category	Women	Men
Professors	2	7
Associate Professors	7	6
Assistant Professors	7	5
Scientific Investigators OPI	0	0
Contract Investigators "Ramón y Cajal" programme	1	0
Other Contract Scientists	1	3
Graduated Technicians CSIC	2	6
Contract Technicians	2	0
Specialized Technicians OPI	0	4
Research Assistants	4	0
Total	**26**	**31**

Men



Women



Summary of scientific output

2017-18

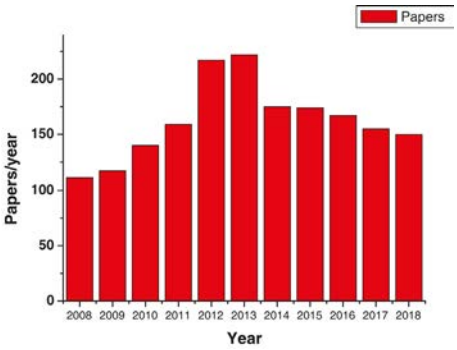
Total number of publications in Web of Knowledge (WoK):	305
Total number of citations:	1546
Average citations/publication:	5

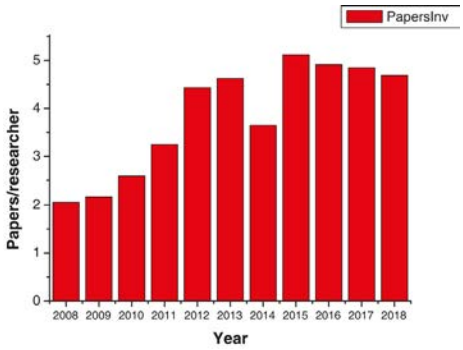
(01-10-2019 data)

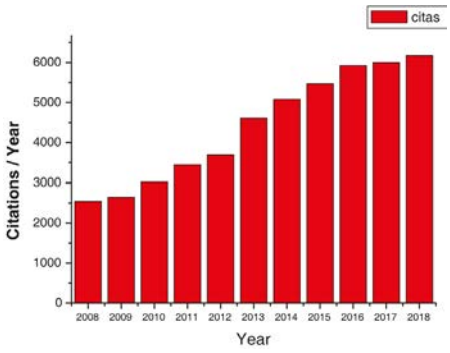
Data since the foundation of IQFR in 1946

Total number of publications in WoK:	4484
Total number of citations:	82605
Average citations/publication:	18.4
h-index:	95

(01-10-2019 data)





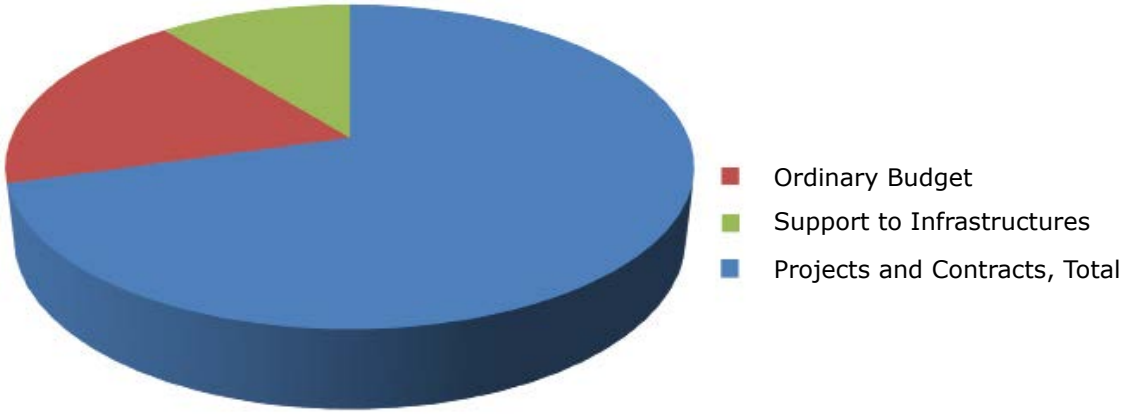


Areas distribution:

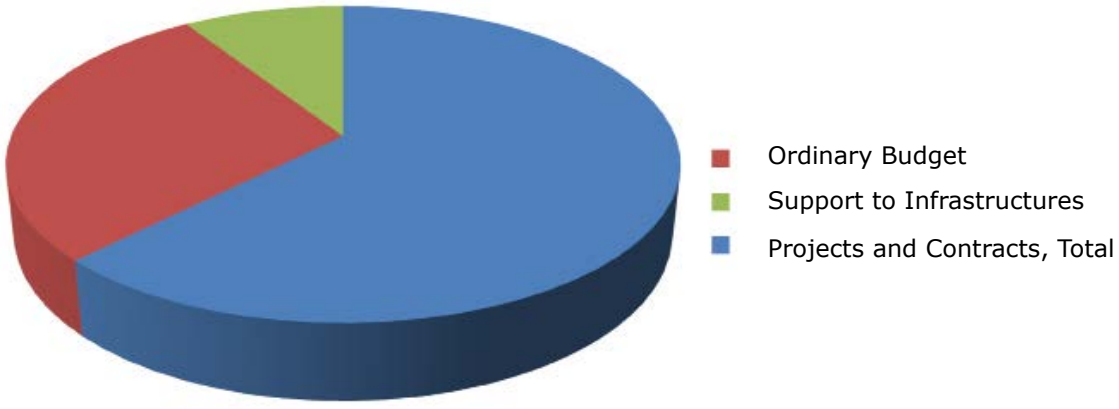
Summary of economic data

Concept	2017	2018
Ordinary Budget	607.456,42	424.509,74
Support to Infrastructures	349.071,12	136.581,35
Projects and Contracts, Total	2.289.910,17	932.488,33
Total	**3.246.437,71**	**1.493579,42**

2017



2018



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Outreach

IQFR seminar series

During 2017-2018, 33 leading scientist form different fields of Science participated in the IQFR seminar series, which were organized by Dr. Esther Rebollar, Dr. Rebeca de Nalda and Dr. José Miguel Mancheño.

Speaker	Title	Date
Germán Sierra (Instituto de Física Teórica UAM-CSIC)	El Premio Nobel en Física 2016: Materia Topológica	11/01/2017
José Manuel Sánchez Ron (Universidad Autónoma de Madrid)	Rayos cósmicos, Arturo Duperier y Patrick Blackett	25/01/2017
Manuel Serrano (Centro Nacional de Investigaciones Oncológicas. Madrid)	Reprogramación celular	1/02/2017
Alfonso Valencia (Centro Nacional de Investigaciones Oncológicas, Madrid)	Genomas, Proteínas y Redes: dónde estamos y dónde podemos llegar	15/02/2017
Juan Parrondo (Universidad Complutense de Madrid)	El demonio de Maxwell y la termodinámica de la información	22/03/2017
José L. Carrascosa (Centro Nacional de Biotecnología. Madrid)	"Nanotomografía con rayos X blandos: Un enfoque correlativo para explorar la estructura celular y la caracterización química a nivel nanométrico"	29/03/2017
Ricardo García (Instituto de Ciencia de Materiales de Madrid, CSIC)	A force microscopy perspective of atoms, cells and beyond	05/04/2017
Óscar Millet (Unidad de Biología Estructural. Programa de Metabolismo y Enfermedad CIC bioGUNE. San Sebastián)	Chaperonas farmacológicas y proteínas: una pareja estable	20/04/2017
Alec Talin (Sandia National Laboratory, Livermore, CA, USA)	The Non-Volatile Redox Transistor for Neuromorphic Computing	10/05/2017
Juan Rojo (Instituto IMDEA-Nanociencia)	La vida es difícil sin superficies	24/05/2017
Mariano Barbacid (Centro Nacional de Investigaciones Oncológicas. Madrid)	The Future of Precision Medicine in Cancer Treatment	31/05/2017
Javier García de Abajo (ICFO-Institut de Ciencies Fotoniques (Barcelona))	Resonancias de plasmón a escala atómica: desde materiales 2D hasta moléculas pequeñas	12/06/2017
Francisco J. Blanco (StructuralBiologyUnit. CIC biomagune. San Sebastián)	Reconocimiento molecular de PCNA, la pinza de deslizamiento sobre el ADN	24/11/2017

Speaker	Title	Date
Nazario Martín (Universidad Complutense de Madrid)	Efficient Hole Transporting Materials for Perovskite Solar Cells	29/11/2017
María García Parajo (ICFO-Institute of PhotonicSciences&ICREA-Institució Catalana de Recerca i EstudisAvançats. Barcelona, Spain)	Membrane receptor nanoclustering as functional unit of immune cells: from nanoscopy to single molecule dynamics	13/12/2017
Guillermo Montoya (Integrative Structural Biology Cluster. University of Copenhagen; ISBUC)	Structural Biology of Genome Editing: How RNA-guided endonucleases cut specific regions of the Genome?	20/12/2017
María Vallet Regí (Departamento de Química en Ciencias Farmacéuticas, Universidad Complutense de Madrid, Instituto de Investigación Sanitaria Hospital 12 de Octubre i+12 y Centro de Investigación Biomédica en Red de Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN))	Implantes y portadoras de fármacos	10/01/2018
José Manuel Sánchez Ruiz (Department of Physical Chemistry. Faculty of Sciences. University of Granada. Spain)	Biotechnological Applications of Resurrected Ancestral Proteins"	17/01/2018
Fernando Martín (Departamento de Química de la Universidad Autónoma de Madrid)	Attosecond science: the superslow-motion camera of physics, chemistry and … biology?	24/01/2018
Óscar Fernández Capetillo (Grupo de Inestabilidad Genómica. CNIO, España.CancerTherapy, KarolinskaInstitute, Sweden)	Investigando en cáncer, envejecimiento y desarrollo de fármacos"	31/01/2018
Montserrat Calleja, del (Instituto de Micro y Nanotecnología, CSIC, Madrid)	Nanomechanics foe the life science	07/02/2018
Víctor de Lorenzo (Systems Biology Program, National Center of Biotechnology-CSIC, Cantoblanco-Madrid, Spain)	"How environmental bacteria conquest new chemical landscapes	14/02/2018
Luis Plaja (Universidad de Salamanca, Spain)	Attoaventuras: escenarios exóticos para la generación de pulsos de attosegundo	21/02/2018
Salvador Ferrer (Sincrotrón ALBA, Spain)	La radiación sincrotrón y su utilidad en ciencia de materiales	07/03/2018
Marcelo Guerín (StructuralBiologyUnit. CIC biomagune. San Sebastián)	Membrane enzymes: working at the water-lipid interface	14/03/2018

Speaker	Title	Date
Maria A. H. Vozmediano (Instituto de Ciencia de Materiales de Madrid, CSIC)	Graphene and novel Dirac materials	21/03/2018
Claudio Aroca (Instituto de Sistemas Optoelectrónicos y Microtecnología (ISOM) de la Universidad Politécnica de Madrid)	El ISOM y su magnetismo	04/04/2018
Luis Serrano (Design of Biological Systems, Centre for Genomic Regulation, Spain)	Quantitative understanding of a bacteria and its engineering to treat human lung disease	10/04/2018
Isabel Usón Finkenzeller (Structural Biology Unit, Institute of Molecular Biology of Barcelona (IBMB-CSIC), 08028 Barcelona, Spain)	The eyes of chemistry: methods in crystallography	18/04/2018
Aitziber L. Cortajarena (CIC biomagune. San Sebastián)	Proteins as tools for engineering functional structures and materials	24/04/2018
Abderrazzak Douhal (Departamento de Química Física de la Facultad de Ciencias Ambientales y Bioquímica, y del INAMOL, Universidad de Castilla-La Mancha, Toledo)	Recent Advances in the Photodynamics of Luminescent Zr-Based MOFs for Lighting and Sensing Applications	16/05/2018
Rodolfo Miranda (IMDEA Nanociencia, Madrid)	Magnetism in 2D: From Long Range Order to Chiral Structures	30/05/2018
John Plane (School of Chemistry, University of Leeds, United Kingdom)	Impacts of Cosmic Dust in the Earth's Atmosphere	12/06/2018

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 were Dr. José Miguel Mancheño and Dr. Rebeca de Nalda.

Speaker	Title	Date
Federico Mayor Zaragoza (Presidente de la Fundación Cultura de Paz)	Marie S. Curie, destello pionero hacia la igualdad de género y la sociedad del conocimiento	20/10/2017
J. Ignacio Cirac Sasturain (Max-Planck-Institut für Quantenoptik)	Ciencia y Tecnologías Cuánticas de la Información	12/12/2017
Eero P. Simoncelli (Howard Hughes Medical Institute and New York University)	Representation of visual information in the brain, and its implications for engineering and perception	23/02/2018
María A. Blasco (Centro Nacional de Investigaciones Oncológicas)	Papel de los telómeros en cáncer y envejecimiento	27/04/2018
Gabriela González (Lousiana State University, Colaboración LIGO)	Astronomía de ondas gravitacionales	09/07/2018
Margarita Salas (Centro de Biología Molecular Severo Ochoa)	Mi experiencia investigadora	17/10/2018
Modesto Orozco (Instituto de Investigación Biomédica, Barcelona)	Deciphering the 3D structure of the genome	14/12/2018

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 is an open day and a visits to the different laboratories are organized.

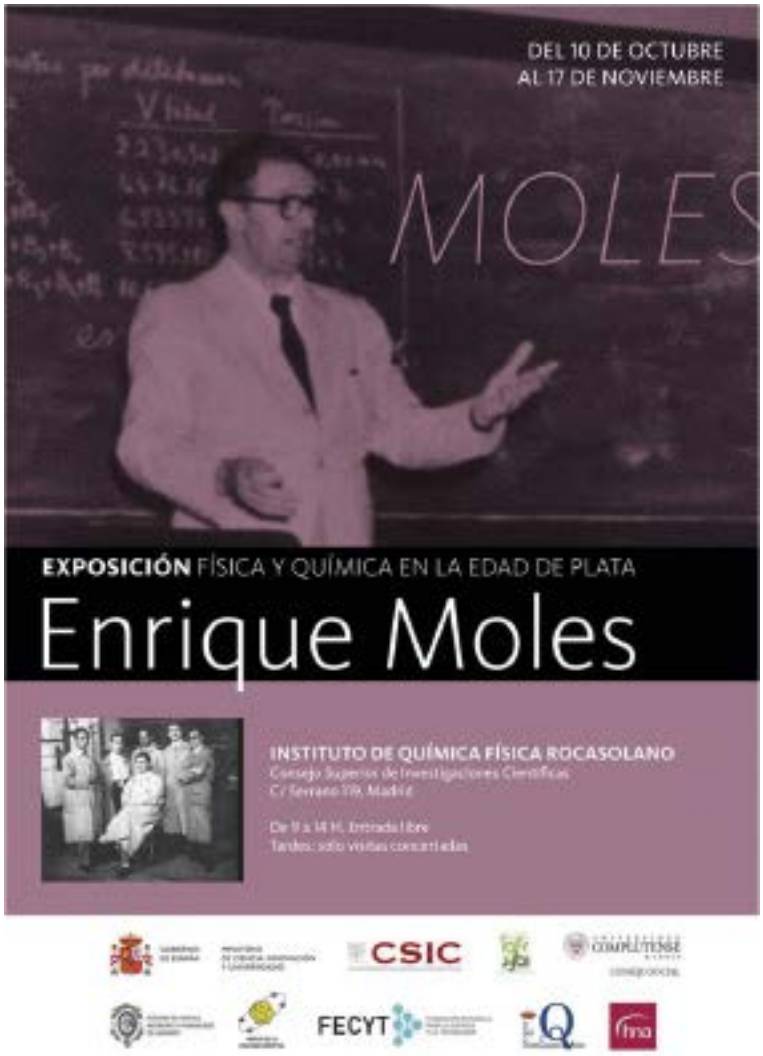
2017 Open day

Laboratories	Visitors	Degree
Biological Physical Chemistry, Crystallography and Structural Biology	IES Valle Inclán (Torrejón de Ardoz) IES Ramiro de Maeztu (Madrid) Colegio Bérriz (Madrid)	1º Bachillerato 2º Bachillerato 1º Bachillerato
Lasers, Surfaces, Nanomaterials and Chromatography	IES Rafael Frübeck de Burgos (Madrid) Colegio Hispano-Alemán (Madrid) IES Gregorio Peces Barba (Colmenarejo)	1º Bachillerato 1-2º Bachill. 1º Bachillerato

2018 Open day

Biological Physical Chemistry, Crystallography and Structural Biology	IES Maestro Juan Calero (Monesterios, Badajoz) IES Mirasierra (Madrid) IES Santa María de los Apóstoles (Madrid)	1º Bachillerato 1º Bachillerato 1º Bachillerato
Atmospheric Chemistry, Lasers, Surfaces, Nanomaterials and Chromatography	IES Giner de los Ríos (Alcobendas) IES María Zambrano (El Espinar, Segovia)	2º Bachillerato 1º Bachillerato

Additionally, an **exhibition on Prof. Enrique Moles** was organized in 2018. Enrique Moles was a prominent scientist of the so-called Silver Age of Spanish Science and Literature (first third of XXth Century) who worked in this Institute.



Young and Senior IQFR Researchers Simposium

Two different internal simposia are organized during the year, one is dedicated to young researchers and the other to principal investigators.

Speakers at 2017 Young Researchers Simposium

Elsa Franco Echevarría. *Estructura de una proteína involucrada en la terminación de la transcripción en hongos.*

Juan Luis Benavente Fernández. *Structural bases of the main determinants of plant ionic homeostasis: Progress in the discovery of the regulatory mechanism of the K^+ channel AKT1.*

Mayte Batuecas. *Estudio estructural de proteínas de remodelado de la pared bacteriana implicadas en virulencia y resistencia a antibióticos.*

Ioanna Kalograiaki. *Exploring recognition of bacterial ligands: from isolated molecules to the entire pathogen surface.*

Cristina Gallego-Páramo. *Diseño y caracterización de QSLA2, una nueva lisina quimérica activa contra neumococo.*

María Sanchez-Arenillas. *Spectroscopic studies of sulfur amino acids and alanine adsorption on Pyrite (100) surface.*

Antía Carmona. *Estudio y modelado de química de halógenosen la atmósfera polar.*

David García. *Estudio de la composición atmosférica mediante el empleo de la técnica espectroscópica DOAS.*

Ernest Anoz-Carbonell. *Characterization of antimicrobial compounds against an unexploited prokaryotic target, the FAD synthetase.*

Jorge Castro-López. *Deciphering the differences between serine and threonine O-glycosylation sites in biological systems.*

Jesús Fernández Zapata. *Reprogramación molecular en el diseño de un nuevo tipo de fotorreceptor bacteriano dependiente de B_{12}.*

Speakers at 2018 Young Researchers Principal Investigators Simposium

Anna Mandziak. *Structural and magnetic properties of ultrathin epitaxial transition metal oxides on Ru(0001).*

Beatriz Loreto Rodilla González. *Nanotecnology for neural activity measurement and stimulation.*

Antía Carmona-Balea. *Halógenos en las regiones polares, variaciones en el ozono troposférico.*

Nuria Benavent. *Estudio de la composición atmosférica utilizando la técnica MAX-DOAS.*

Belén Chaves Arquero. *Reconocimiento molecular en ribonucleoproteínas e histonas mediante Resonancia Magnética Nuclear.*

Alejandro Mahía Moros. *Díseño y síntesis de derivados más solubles de potenciales fármacos para el tratamiento de la infección causada por Helicobacter pylori.*

Silvia Romero Tamayo. *Functional characterization of hAIF (and its mutants) and molecular basis of the interactions with its proteins partners.*

Pablo Llombart González. *Transiciones morfológicas de agregados de CTAB.*

María Eugenia Corrales Castellanos. *Control de la estereodinámica de predisociación del CH3I en la banda B mediante la aplicación de campos intensos.*

Edgar Gutiérrez Fernández. *Nanostructuring of PEDOT:PSS thin films by laser and its influence on its electrical properties.*

Elsa Franco Echevarría. En las últimas batallas para la cristalización de una inositol kinasa.

Mayte Batuecas. La degradación del peptidoglicano a través de la transglicosilasa lítica Slt en Pseudomonas Aeruginosa.

Carol Siseth Martínez. Combined use of allosteric effectors and obsolete ß-lactams against MRSA as a new strategy.

Diego Bernal. Control multifactorial de la expresión de un sistema CRISPR-Cas por una pareja σ/anti-σ y un complejo regulador de acción global.

Speakers at 2017 Principal Investigators Symposium

Rafael Notario
Margarita Menéndez
Juan Antonio Hermoso Domínguez
Enrique Lomba

Speakers at 2018 Principal Investigators Symposium

Carlos González. *Estudios estructurales de DNA: Más allá de la doble hélice*.

Carlos Cuevas. *Ultraviolet and Visible Atmospheric Sounder (UVAS): concepto de misión y estado de desarrollo.*

Maria José Sánchez Barrena. *Diseño de moléculas terapéuticas basado en la estructura para enfermedades neuronales*

Enrique Lomba *A simple modelling of hyperuniform states of matter: from chicken retina to stealth materials*

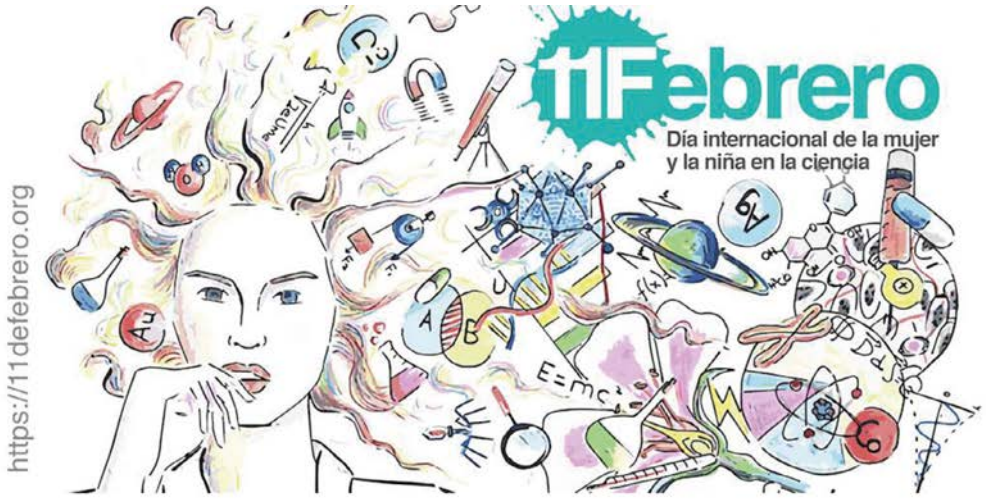
Programa 4º ESO + Empresa

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 2018, the Institute welcomed students from Colegio San Luis Bonzaga, CEPSO El Cantizal Las Rozas, Colegio Nuestra Señora de las Nieves, IES Gómez Moreno and Colegio Gamo Diana from Madrid.

International Day of Women and Girls in Science

In 2018, 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.

Furthermore, the Institute has collaborated with "El País" and "Inspiring Girls" initiative to record the following video: https://elpais.com/economia/2018/05/22/actualidad/1527002625_327491.html



- **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, 5,7,9 febrero

- **Taller científico: Descubriendo la luz**
  Rebeca de Nalda, Esther Rebollar y Conchi Pulido
  Alumnos 2º y 3º de Primaria del CEIP Ramiro de Maeztu, 5, 7, 9, 20 febrero

- **Charla: Descifrando el código de los azúcares**
  Maria Asunción Campanero
  Alumnos de 4º ESO y 1º Bachillerato Colegio Blanca de Castilla, 8 febrero
  Alumnos de 4º ESO del Colegio Ramón y San Antonio, 12 febrero
  Alumnos de Bachillerato del Colegio Corazón Inmaculado, 14 febrero

- **Presentación: Grandes científicas en la historia y Debate: qué dicen las encuestas sobre las carreras que eligen chicos y chicas? Te atreves a ser científica?**
  Mar Fernández (ICTP), Irene Gómez (IQFR), Marta Hernández (IFF), Sagrario Martínez (IEM), Aixa Morales (I. Cajal), Aurora Nogales (IEM)
  Alumnos de 2º y 3º de ESO del I.E.S. Ramiro de Maeztu, 9 febrero

- **Charla: Mujeres científicas de ayer de hoy y de mañana**
  Marta Bruix
  Alumnos de Primaria del CEIP Miguel Delibes, San Sebastián de los Reyes, 9 febrero

Festival of Nanoscience and Nanotechnology

The IQFR participated in the third edition of the festival, which was held in April 2018. 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 an exhibition, visits to the laboratories and several talks at secondary schools.

Actividades IQFR

Nanoinmersión en el Rocasolano: 12 de abril de 2018 de 10 a 14 h. Para estudiantes de Enseñanza Secundaria o Bachillerato. Necesaria reserva.

Exposición: un paseo por el nanomundo: del 4 al 12 de abril de 10 a 18 h. Días laborables.

Conferencias en centros educativos:
Colegio Cultural Elfo-Nuestra Señora de Fátima: Esther Rebollar
IES Duque de Rivas: José Francisco Marco
IES Fortuny: Mikel Sanz
IES Gómez Moreno: Enrique Lomba
IES Juan de Mairena: Juan de la Figuera
IES Nuestra Señora de la Almudena: Juan de la Figuera
IES Santa Teresa de Jesús: Enrique Lomba
IES Santamarca: Mikel Sanz
IES Vallecas: Mohamed Oujja
Colegio Fundación Santamarca: Esther Rebollar
Ponce de León: Rebeca de Nalda

Más información en:
https://www.iqfr.csic.es/es/info/publico-en-general/nanofestival-2018

Social Networks

In October 2017 IQFR social networks were launched, in particular Twitter (@iqfr_csic) and Facebook (@rocasolano.csic). All the news of the institute –publications, seminars, events, offers, awards- are published, as well as other information of interest to fans of the Institute social media sites. At the moment the IQFR Twitter account has 593 followers while Facebook account, 184. The social networks of the IQFR are managed by Esther Rebollar.

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