XUNTA DE GALICIA

UNIÓN EUROPEA

FEDER - FONDO EUROPEO DE DESENVOLVEMENTO REXIONAL
*"Unha maneira de facer Europa"*

CiQUS Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares

USC

CAMPUS VIDA


# Annual Scientific Report 2018

Cofinanciado pola Unión Europea, Programa Operativo FEDER Galicia 2014-2020
Promover o desenvolvemento tecnolóxico, a innovación e unha investigación de calidade
*Unha maneira de facer Europa*

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## LETTER FROM THE DIRECTOR

CiQUS started with the aim of implementing a new, singular research model within the University, which could allow a more efficient use of human and physical resources and pursue cutting-edge science from a multidisciplinary perspective. Thanks to the excellent managing work of the former commissioner director, and now deputy director, Prof. Dolores Perez Meirás, and the dedication of CiQUS group leaders and students, in just seven years, CiQUS has become a highly recognized, top level research center. The contribution of our managing and technical body has also been key for this progression.

Along the years we have improved in all significant indicators, namely, the average impact factor of our publications, our ability to raise competitive funds, the number of trainees that pursue successful careers and the impact of our technology transfer activities. We do also present better numbers in terms of gender balance and foreign members. Importantly, in seven years we have passed from 1 to 6 ERC grants, which represents a clear indication of success.

In 2018 the tendency has followed a similar path. In addition to obtaining a new ERC proof of concept grant (TRAFFIKGENE), and an international collaborative project (Supraporous) within the highly competitive EIG CONCERT program by Javier Montenegro, a collaborative project by Eduardo Fernández-Megía was also approved for funding by the European Union (ENDOSCAPE, RIA-H2020-SC1-BHC-09-2018). We have also ensured 6 projects from the "Agencia Estatal de Investigación", a number of grants from the Regional Government, and significant contracts with private companies. We have hired two new Ramón y Cajal researchers and one Juan de la Cierva postdoctoral researcher.

As part of our philosophy of having motivated and highly qualified students, we have kept our successful programs for recruiting undergraduate, master, predoctoral and postdoctoral researchers.

I am very proud of PIs and students that are externally recognized with prestigious awards. In this case, up to 6 PIs were awarded with different prizes, medals and recognitions by several scientific societies and institutions. Moreover, former young researchers and PhD students received different awards.

Key to the success of the center is to maintain a competitive but also friendly and collaborative atmosphere. Therefore, we have reinforced our biweekly internal seminar program, in which students have an excellent opportunity to present their work and discuss results.

Importantly, under the coordination of our PI Juan R. Granja, we have worked hard to implement an international master degree program associated to the center, entitled "*Master in Chemistry at the Interface with Biology and Materials Science*", which we expect to launch in the course 2019-2020.

The impact factor of our publications in 2018 reached an average of 7,6 which is quite remarkable in Chemistry and demonstrates the quality of our production. We have also been quite successful in terms of technology transfer, having obtained two IGINICIA

projects from the Galicia Government, and launched new companies, such as Sigillum Knowledge Solutions. We have also been engaged in outreach activities that range from hosting high school students for organized visits (including experimental activities), to the organization of open journeys for general public.

Overall, the combination of our self-demanding model and multidisciplinary approach, with a rigorous external assessment of our outputs, is leading to excellent results. We are significantly contributing to the advancement of science, and to the economic progress of our contour, and increasing the international prestige of our University and the Spanish science. I have no doubt that with the firm commitment of all members of the center, CiQUS will continue to grow and become a main world reference in multidisciplinary science at the boundary between chemistry, biology and materials.

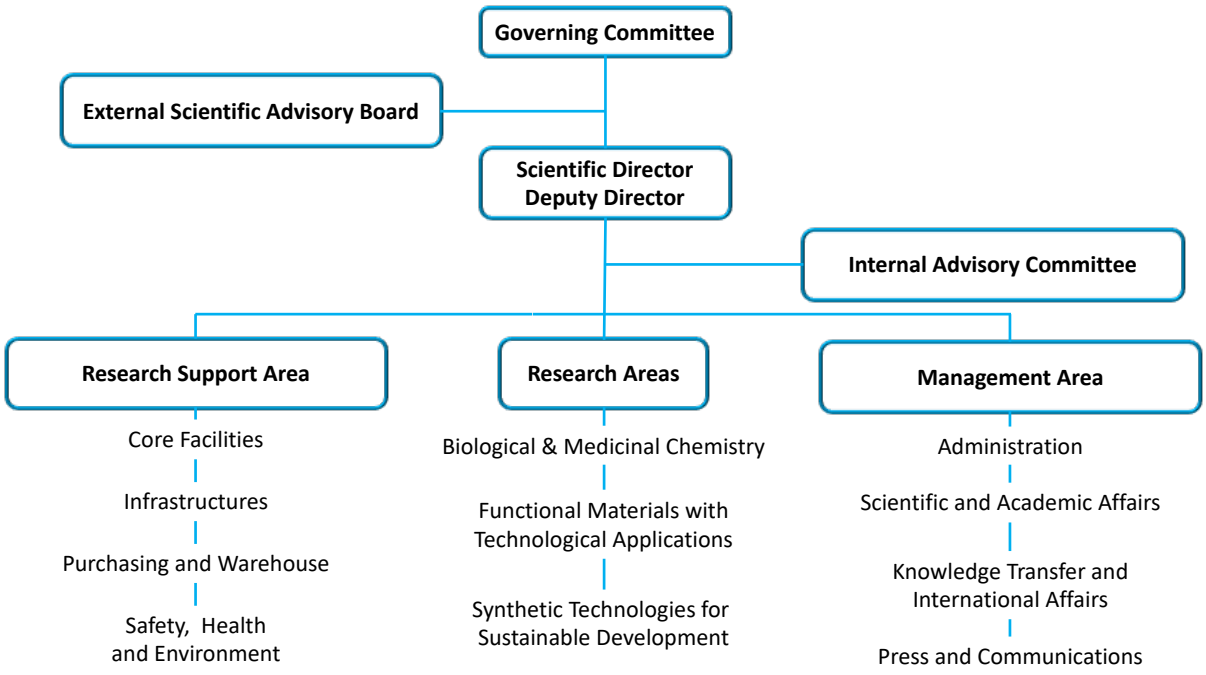
I can only finish thanking all CIQUS members, from the managing and technical staff to the PIs and students, for their dedication and enthusiasm, and their close identification with the spirit of the center.

*José Luis Mascareñas*
CiQUS Scientific Director

# 1. SCIENTIFIC ORGANIZATION

## 1.1. Organization Chart & Team

The organizational model of CiQUS, shared by the other members of the Singular Research Centers Network (CiMUS and CiTIUS), is implemented as per the organization chart shown below.




***Organizational Chart at the CiQUS***

### GOVERNING COMMITTEE (December 31, 2018)

**President**: Antonio López Díaz, Rector, USC

**Vice-president**: Vicente Pérez Muñuzuri, Vice-rector of Research and Innovation, USC

**Members**: Javier Ferreira Fernández, USC Manager

José María Arias Mosquera, President of the Social Council of the USC

José Alberto Díez de Castro, General Secretary for Universities – Xunta de Galicia

Rosa Menéndez López, CSIC President

José Luis Mascareñas Cid, CiQUS Scientific Director

María Dolores Pérez Meirás, CiQUS Deputy Director

**Secretary**: Rogelio Conde-Pumpido Tourón. USC R&D Management and Valorization Director

### DIRECTORS (December 31, 2018)

**Scientific Director**: José Luis Mascareñas Cid

**Deputy Director**: María Dolores Pérez Meirás

## EXTERNAL SCIENTIFIC ADVISORY BOARD (ESAB) (December 31, 2018)

*Prof. Jesús Jiménez-Barbero*
Centre for Research Cooperative in Bioscience (CiCbioGUNE)

*Prof. Miquel Pericás*
Institut Català d'Investigació Química

*Prof. Luis Oro*
Instituto Universitario de Catálisis Homogénea (U. Zaragoza)

*Prof. Avelino Corma*
Instituto de Tecnología Química (ITQ), UPV-CSIC

*Prof. Thomas Carell*
Ludwig-Maximillians-Universitat München

*Prof. Chris Abell*
Department of Chemistry, University of Cambridge

*Prof. Angel Rubio*
Max Planck Institute for the Structure and Dynamics of Matter

Recently, Prof. Jean-Pierre Sauvage (Nobel Laureate in Chemistry 2016, University of Strasbourg) and Prof. Janine Cossy (ESPCI ParisTech) have accepted the invitation to join the CiQUS ESAB. Both of them will be proposed to be appointed as official ESAB members during the next Governing Committee scheduled for March 2019.

### 1.1.1 Directors

- **Scientific Director**: *Prof. Dr. José Luis Mascareñas Cid*, Full Professor of Organic Chemistry (full-time)

Professional profile: José Luis Mascareñas (Allariz, 1961) completed his PhD at the USC in 1988. He was a postdoctoral fellow at Stanford University (USA) under the supervision of Prof. Paul Wender (1989-1990). He became permanent professor in 1993 and full professor in 2005, at the USC.

He has been a visiting scholar in Harvard University (USA) and a visiting scientist in the University of Cambridge and the MIT. As independent researcher, he has published over 175 articles, the majority of them in the most relevant chemistry journals, 7 book chapters, and applied for 19 patents. He supervised 30 PhD theses, delivered more than 100 invited lectures, most of them in international forums, and raised over 5 million euros in competitive grant calls in the last few years. It is important to remark that five PhD students of the group have gained Ramón y Cajal positions. In 2014 he received an **ERC Advanced Grant** for his project METBIOCAT (http://metbiocat.eu/).

His current research focuses on a synthetic program aimed at discovering novel methods based on metal catalysis, and a chemical biology program focused on the development of synthetic tools for biological intervention. The Spanish Royal Society of Chemistry awarded him with the Organic Chemistry Award (2009) and **Gold Medal** (2015). In 2016, he has been appointed as a member of the European Academy of Sciences. He was appointed Scientific Director of the CiQUS in February 2014.

- **Deputy Director**: *Prof. Dr. María Dolores Pérez Meirás*, Full Professor of Organic Chemistry

Professional profile: Dolores Pérez (Ferrol, 1964) completed her graduate studies at the USC with Honors, and obtained her PhD in 1991, under the supervision of Prof. E. Guitián and L. Castedo. She was awarded with a MEC-Fullbright fellowship to conduct postdoctoral training at the University of California Berkeley (1992-1993) in the group of Prof. K. Peter C. Vollhardt, and later she was a visiting scientist in the group of Prof. S. L. Buchwald at the MIT (1996). She joined the faculty of the USC as an

Assistant Professor in 1995, became an Associate Professor of Organic Chemistry in 2000 and Full Professor in January 2019.

She has published over 60 articles in high impact journals, 3 book chapters and supervised 10 PhD thesis. Her current research interests focus on the discovery of new metal-catalyzed reactions of synthetic interest, the further development of aryne chemistry and its application in the synthesis of complex polycyclic aromatic systems and nanographenes. She was the Director of the Organic Chemistry Department (2004-2006), and associate to the Vice-rector of Research an Innovation at the USC (2006-2010). In 2010 she was appointed as Commissioner Director of CiQUS, where she has worked as Deputy Director since 2014. In September 2017 she was appointed as Commissioner for Campus Vida and for the Coordination of the Singular Research Centers Network.

### 1.1.2 Management Structure

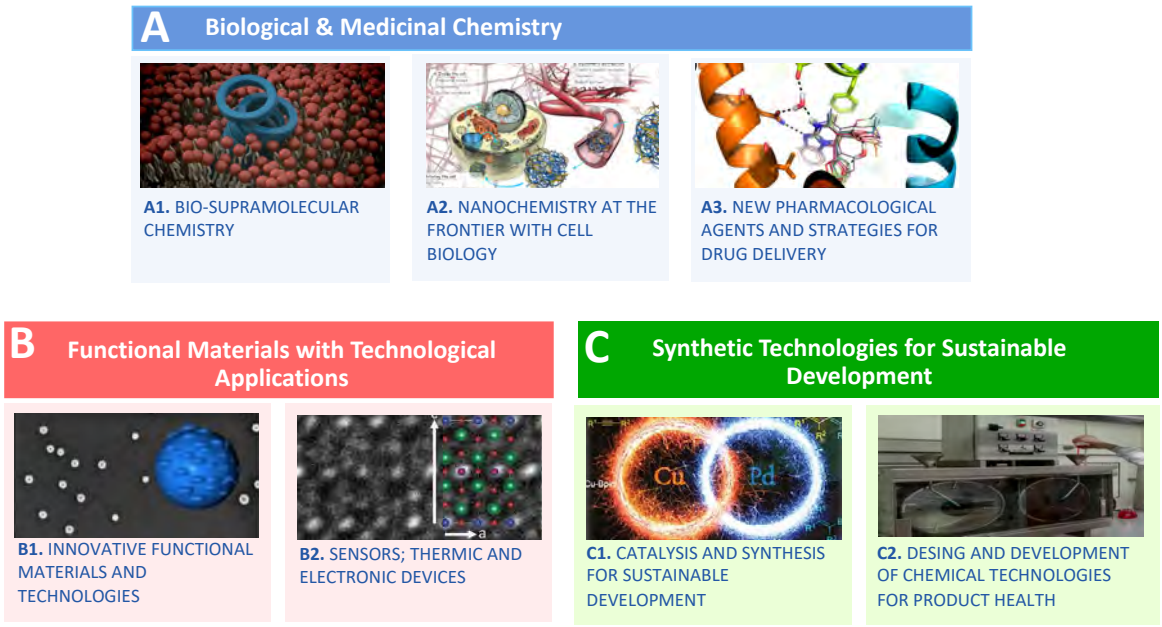
The CiQUS Management Structure is organized in several different units providing support to the scientific and non-scientific activity of the center:

- **Internal Advisory Committee**, which represents the main research areas at the CiQUS. It is responsible for the elaboration and monitoring of the CiQUS Strategic Plan. It is currently formed by CiQUS Research Staff: *Ricardo Riguera, Juan R. Granja, Antonio Fernández, Pablo del Pino, Dolores Pérez and José Luis Mascareñas.*
- **Management Area**: This area includes 4 different units:
  - ✓ Administration Unit: responsible for the financial management of R&D activities, secretarial issues and administrative support (*Elena Veiga* and *Lucía Rodríguez*).
  - ✓ Scientific & Academic Affairs: coordination of the CiQUS Scientific Strategic Project, writing of scientific and activity reports and talent attraction programs (*Dr Almudena García*).
  - ✓ Knowledge Transfer & International Affairs: promotion of international R&D initiatives and identification of technology transfer opportunities (*Fernando Casal).*
  - ✓ Press and Communications Unit: created to develop a joint communication strategy with the CiMUS and the CiTIUS. This unit is responsible of CiQUS' press release and social media networks (*Andrés Ruiz and Elena Mora*).
- **Research Support Area**: responsible for the implementation of the centralized operational model which provides support to the CiQUS' research activity, aiming at the optimization of the available resources and the improvement of the working conditions at the center. This area includes 4 different units:
  - ✓ Core facilities: providing the scientific instrumentation support needed to conduct research at the CiQUS, ensuring the maintenance and correct use of the equipment, developing new applications for the techniques available and providing training in the use of the equipment, sample preparation and data processing (*Dr. Arcadio Guerra, Laura Acevedo*).
  - ✓ Infrastructures: responsible for the management and maintenance of the labs, equipment, furniture and communal spaces at CiQUS (*Laura Acevedo*).
  - ✓ Purchasing and Warehouse: responsible for the negotiation and purchasing of reageants, solvents, disposable laboratory products and management of the CiQUS' warehouse (*Noela Torrente, Pablo Cajaraville*).
  - ✓ Safety, Health and Environment: responsible for the initial training course on safety and risk prevention for all new CiQUS members. Creation and maintenance of the CiQUS' Self-protection Plan, coordination and training of the emergency teams and management of the laboratories' safety (*Noela Torrente, Pablo Cajaraville*).

## 1.2 Scientific Program

The CiQUS research activity is organized in order to optimize efforts and favor collaborations and synergies between the different research groups and disciplines within the center. The CiQUS scientific activity currently focuses on three major areas:

- BIOLOGICAL AND MEDICINAL CHEMISTRY
- FUNCTIONAL MATERIALS WITH TECHNOLOGICAL APPLICATIONS
- SYNTHETIC TECHNOLOGIES FOR SUSTAINABLE DEVELOPMENT




***CiQUS Scientific Organization***

According to this organization, the main research activities in each of the topics, are:

**I. BIOLOGICAL AND MEDICINAL CHEMISTRY**

This area is aimed at developing basic and fundamental research in the fields of supramolecular, biomolecular and cellular chemistry, and exploring applications in medicinal chemistry, especially to address pressing medical issues such as cancer, neurodegenerative diseases and bacterial resistance. Our current organization includes subtopics associated to different PIs:

• BIO-SUPRAMOLECULAR CHEMISTRY: a) Novel supramolecular devices based on peptides and biological applications (PI: J. Granja); b) Metallopeptides for nucleic acid interactions (PI. E. Vazquez). c) Protein, polymer and peptidoglycane folding (PIs: F. Freire, E. Quiñoá; PIs: R.J. Estévez, J.C. Estévez); d) Peptide helicates and oligomeric auto-assembled receptors (PIs: E. Vázquez, M. Vázquez); e) Assembly of supramolecular systems and its influence in chemical reactivity (PI: L. García Río).

• CHEMISTRY AND NANOTECHNOLOGY AT THE INTERFACE WITH CELL BIOLOGY: a) Metal catalysis in biological habitats: New strategies for optical bio-sensing and targeted therapy (PI. J.L. Mascareñas, ERC-AdG-MetBioCat); c) Molecular fluorescent probes to be used in cell biology (PIs. E. Vázquez, M. Vázquez, M. Mosquera); d) Artificial cells: design and synthesis of a fully synthetic self-regulated cytoskeleton (PI. J. Montenegro, HFSP-RGY0066/2017).

• PHARMACOLOGICAL AGENTS AND NEW STRATEGIES FOR DRUG TRANSPORT AND DELIVERY: a) Smart materials for the cellular transport of proteins, nucleic acids and cytotoxic molecules and controlled drug delivery (PI. J. Montenegro, ERC-StG-DYNAP); b) Novel antibiotics for resistant bacteria (PI. C. González-Bello). c) Combinatorial technologies for drug discovery (PI. E. Sotelo); d) Antibiotics as mitochondria-targeted antitumoral agents (PI. E. Vázquez, Spanish Association Against Cancer-AECC); e) Activation strategies of antitumoral prodrugs based on nanoparticles (PI. P. del Pino); f) Biotechnological tools (PI. José Martinez-Costas); g) Nanostructures and dendrimers for conjugation with ligands of biomedical interest with applications in drug delivery or diagnosis (PI. E. Fernández-Megía).

**II. FUNCTIONAL MATERIALS WITH TECHNOLOGICAL APPLICATIONS**

This area is aimed at the discovery of new organic, inorganic and metallo-organic materials with unique properties, as well as their implementation in the development of technological devices for biomedical applications and the design of new molecular electronic and energetic technologies.

• INNOVATIVE MATERIALS AND TECHNOLOGIES: a) Inorganic and metal organic materials with novel thermal, magnetic or reactivity properties (PI. M. Lazzari); b) Nanomaterials with applications in the restoration of works of art. (PI. M. Lazzari); c) Organic semiconductors: synthesis in solution and on surface, and biomedical applications (PIs. D. Pérez, D. Peña and E. Guitián); d) Nanostructures for the control of thermal conductivity based on optical methods (frequency domain thermoreflectance, FDTR) (PI. F. Rivadulla); e) Nanoparticles, MOFs and hybrid nanostructured materials with applications in drug delivery, theranostic or as cell reprogramming agents (PI. P. del Pino); f) Multifunctional metal-carbon hybrid nanostructures for spintronics and energy-related applications (PI: M. Giménez).

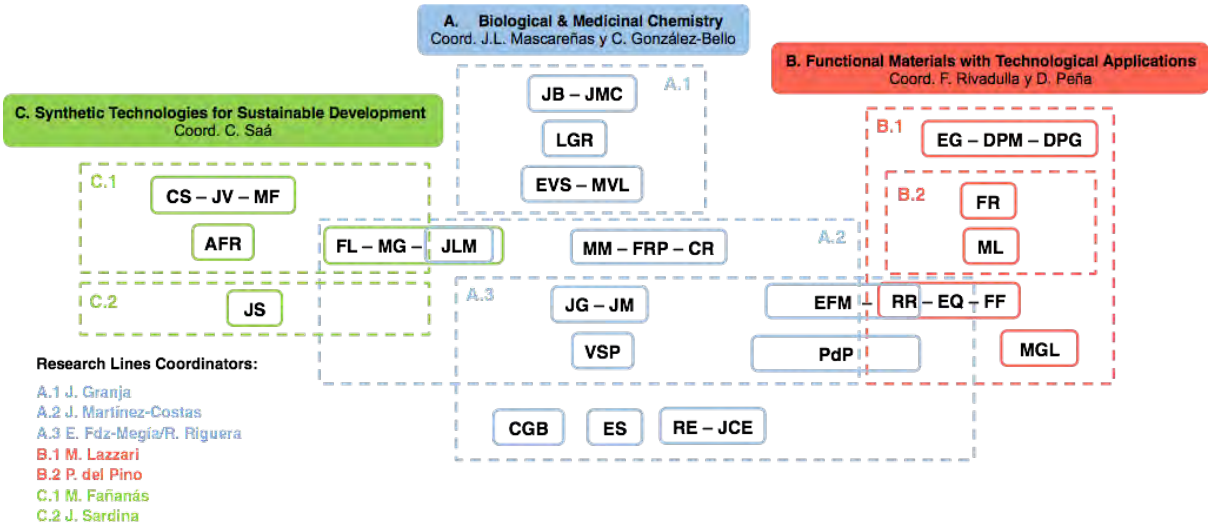
• SENSORS: THERMAL AND ELECTRONIC DEVICES: a) Devices for ultraprecise thermal measurements (PI. F. Rivadulla, ERC-PoC-ANTS); b) Functional polycyclic aromatic hydrocarbons (PAHs) and nanographenes: synthesis and applications (PIs. D. Peña, D. Pérez, E. Guitián); c) Stimuli-responsive dynamic polymers (PIs. R. Riguera, E. Quiñoá and F. Freire).

**III. SYNTHETIC TECHNOLOGIES FOR SUSTAINABLE DEVELOPMENT**

Discovery of effective catalytic processes and sustainable synthetic methods.

• CATALYSIS AND SYNTHESIS FOR A SUSTAINABLE WORLD: a) Metal-based technologies for C-H activation/C-C bond formation (PI. M. Fañanás); b) Catalytic functionalization of “inert” C-H bonds: new tools for synthetic chemistry (PIs. M. Gulías, J.L. Mascareñas); c) Efficient synthetic methods based on metal catalysis for the preparation of enantiopure anticancer agents (PIs. F. López, J.L. Mascareñas); d) New catalytic routes for the preparation of doped PAHs and bioactive heterocycles (PI. C. Saá); e) Theoretical methods and mechanistic studies (PIs. A. Fernández-Ramos and J. Varela).

• CHEMICAL TECHNOLOGIES FOR PRODUCT HEALTH: This line is developed in collaboration with the company INDITEX, S. A. The aim of this collaboration is to lead the application of chemistry technology to the development of sustainable processes for the textile industry (PI. J. Sardina): a) Minimizing the use of toxic substances; b) Developing novel technologies for textile recycling. Although this type of research is somewhat incidental in relation to the main scientific stream of the center, it is very useful from a socioeconomic perspective as it allows social agents to immediately acknowledge the value of chemical research.




***CiQUS Organizational Chart for Scientific Activity***

For a more detailed description of the different research lines of the Strategic Scientific Project, please refer to https://www.usc.es/ciqus/en/research/research-groups.

# 2. TECHNOLOGY RESOURCES

## 2.1 Facilities

The CiQUS building has 5.900 $m^2$ built-up area, with 22 research labs, which have been designed under the criteria of flexibility, safety and sustainability, and are provided with first class laboratory furniture suited to fit the needs of the different research areas. There are also 1.000 $m^2$ of research support facilities, including a Nuclear Magnetic Resonance (NMR) facility, a radioactive facility, a high-pressure laboratory (placed on the roof), culture cell laboratories, a dark room, cold rooms, four rooms for chemical storage, a central purchasing center and a computer cluster. CIQUS researchers also have access to the nearby general research support services of the USC (www.usc.es/gl/investigacion/riaidt/) at the CACTUS building.

Most notably are the **four research support laboratories** which host most of the scientific equipment provided by the research groups or acquired by the center: chromatography SFC, GC, HPLC, MS-GC, MS-HPLC, circular dichroism, lyophilizers, glove box, Thermogravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC), Dynamic Light Scattering (DLS), fluorescence microscopy for live-cell imaging, etc. All these laboratories work on a shared use basis, under the supervision of the technical staff, thus optimizing the resource availability. In addition, there are some highly specialized labs: Live-cell imaging Lab, AFM microscopy, lithography, electrophysiology, PLD, etc.

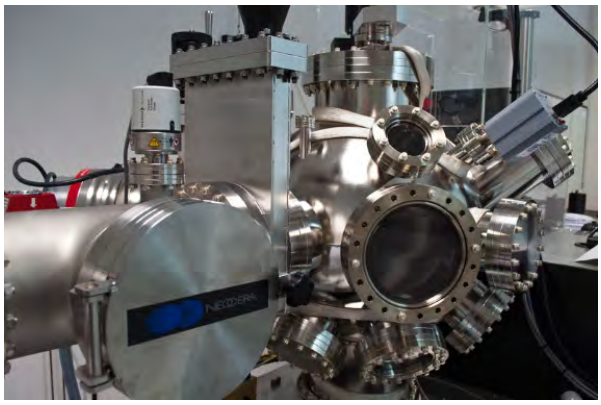
***Representative research support laboratories***

It is highly important to emphasize once again that the management structure of the center allows and encourages the optimization of available resources by promoting the shared use of equipment, both the instruments provided by the different groups and those specifically purchased for the general use of CiQUS researchers. Sharing equipment also allows for expertise exchange in different instrumental techniques and the development of scientific collaborations and interdisciplinary projects. The central purchasing of solvents and other consumables is also critical from the point of view of safety (reduction of stocks of hazardous and flammable materials) and economy.

## 2.2 Singular Laboratories

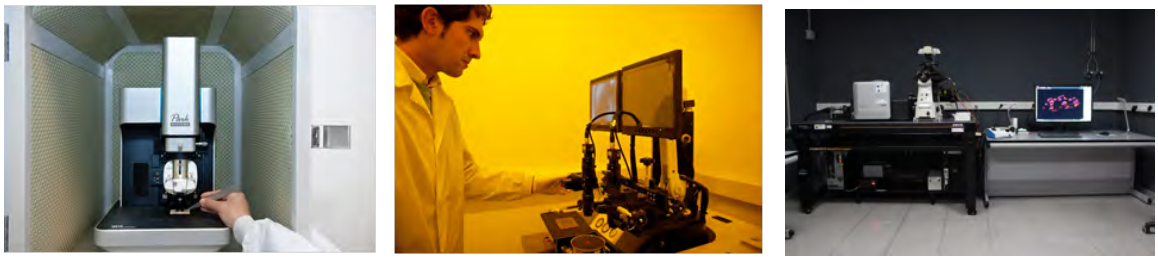
• ***Thin Films Laboratory***: This Lab is committed to the fabrication of thin films and multilayers with different uses, mainly oxide thermoelectrics and ferroic materials. The lab is open to collaborations, includes state-of-the-art nanofabrication tools and techniques for a wide range of applications.

It is equipped with a **PLD** (Pulsed Laser Deposition) for the generation of thin films, acquired by F. Rivadulla (ERC-StG "2DTHERMS" and ERC-PoC "ANTS"). This is an ultrahigh vacuum laser deposition system with a load lock chamber and a 200 mJoule F-Kr (248 nm) laser. It allows substrates to be heated up to 1000 ºC and it is provided with a six-target carrousel. It is also equipped with a **lithography facility** with an etching and coating system, including two deposition guns in the same vacuum chamber. This system is employed for film patterning using stencil masks and subsequent depositions of Au, Ag, etc. (four different targets) or transport measurements, such as Hall effect, magnetoresistance, etc. Finally, the research group of Prof Rivadulla has also developed a **Polymer Assisted Deposition** (PAD) technique, a wet "green" chemical method for large areas, suitable for high quality ultra-thin films of different oxides and nitrides.



***PLD equipment***

• ***AFM microscopy laboratory***. It has a state-of-the-art AFM microscope, NX-10 Park Systems, designed to work in multi-user mode (high degree of automation) and capable of studying surfaces with a resolution in the region of 1 nm, and high-resolution modes for the analysis of structural motifs at submolecular level, and additional modules of electrical conductivity and thermal conductivity. This equipment was purchased jointly by the CiQUS (40% of the cost) and five of its research groups (12% of the cost each), an example of the level of cooperation within the center.

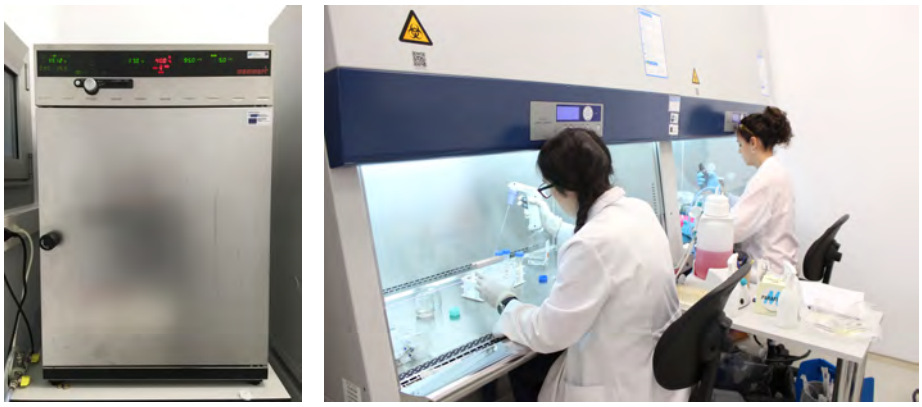


***Rooms for AFM microscopy (left), lithography equipment (center) and living cell microscopy (right)***

• ***Laboratory of living cell microscopy***. In September 2015, through the joint efforts of the CiQUS and several of its groups, and a group of the CiMUS (Mabel Loza), a fluorescence microscope "Nikon Eclipse Ti" for the study of living cells was purchased. In 2017, the CiQUS acquired, through a grant from MINECO for the acquisition of scientific infrastructures (co-funded by ERDF), a confocal microscope with spinning-disk and TIRF modules "Nikon Dragonfly". The confocal spinning disk module allows the

acquisition of images at high speed and is the technique of choice for studies of confocal microscopy in living cells. The TIRF module allows observation on specific sites in the cell. This equipment will be fundamental for the development of several research lines within the area of Biological & Medicinal Chemistry. Additionally, in order to improve the biological area, a new lab has been adapted for culture cell with the installation of two biosafety cabinets and the acquisition of an incubator.

- ***Laboratory of cell culture***. In line with the emerging research projects based on biological and medicinal chemistry started at our center, the CiQUS has enabled a new laboratory for cell culture. This new facility is located at the CiQUS ground floor and it has been equipped with two biosafety cabinets, a centrifuge and a cell culture incubator among other cell culture common stuff. We are currently in the process of achieving the certification and validation as Biosafety Level 2 (BSL-2) room.



***Cell culture lab equipped with a cell culture incubator (left) and two cell culture biosafety cabinets (right)***

# 3. SCIENTIFIC REPORT 2018

The following chapters describe and summarize the situation of the CiQUS as well as its scientific activity during the year 2018, while more detailed information is available in the Annexes section and the CiQUS website: www.usc.es/ciqus/en.

## 3.1 HUMAN RESOURCES

- 34 Research staff, 37 postdocs, 84 PhD candidates, 25 Master students and 19 Technical and administrative assistants (6 of them support particular CiQUS research groups) (Dec 31, 2018)

In December 2018, over 200 people worked at the CiQUS: 34 Research Staff (4 of them *Ramón y Cajal* associates), 37 postdoctoral researchers (4 of them *Juan de la Cierva* researchers and 3 MSCA-IF), 84 PhD candidates and 25 MSc students, together with 11 technicians in different areas (3 of them are technicians supporting particular groups), 8 people in administration and service tasks (3 people are staff supporting particular groups). Furthermore, around 7 USC faculty members collaborate in the scientific activity of the CiQUS on a daily basis, though they are not officially appointed by the CiQUS. The full list of people (as in December 2018), is included in Annex I.

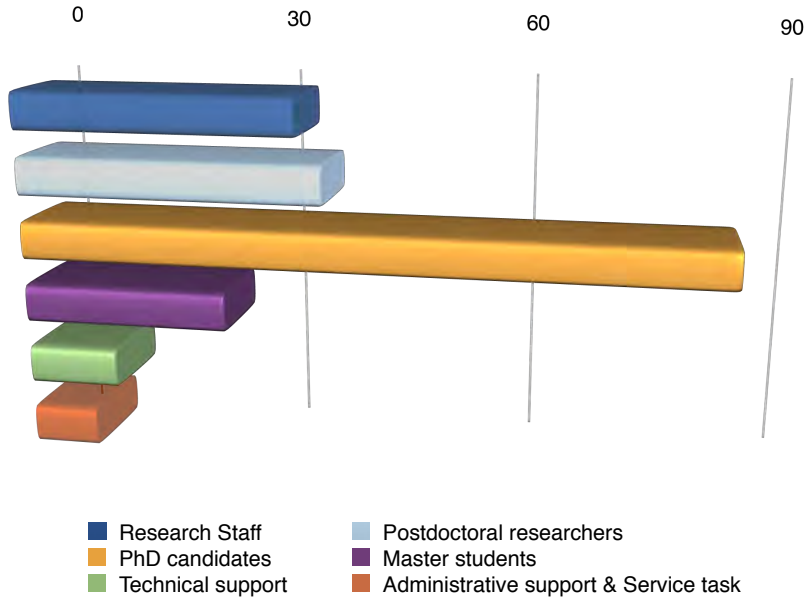



***Chart 1. Distribution of human resources by category***

### 3.1.1 Recruitment Policy

The CiQUS is firmly convinced that the capability to strengthen our capacities and develop our research program in terms of excellent research is deeply reliant on the quality of our group leaders and students.

As a research center that belongs to the University of Santiago de Compostela, the CiQUS recruiting strategy to attract new talent as Research Staff is governed by the legal framework of the access regulation of the University.

Every year, we try to use all available tools to recruit the best researchers. In this sense, the CiQUS has implemented a number of initiatives to attract researchers at different levels. Some of these actions are presented below.

- **Senior and *Ramón y Cajal* researchers:**

Every year the CiQUS offers positions for **Ramón y Cajal** Researchers following the assessment of the External Scientific Advisory Board and the complementary profile required for our ongoing research lines. Along the last 6 years, recruiting excellent researchers through this highly competitive program (four of them with no previous relation with the CiQUS) has been clearly successful.

After the selection of M. Fañanás (2012 call, PhD in Chemistry at the University of Oviedo), J. Montenegro (2013 call) and P. del Pino (2015 call, PhD in Physics, Technische Universität München), the CiQUS recruited Dr. María del Carmen Giménez López and Dr. Rebeca García Fandiño (2016 call) during 2018.

- *Dr. Giménez López*, PhD in Chemistry at the University of Valencia (2006) under the supervision of Prof. E. Coronado and Dr F.M. Romero, 5 years of postdoctoral experience at the University of Nottingham and since 2011 independent researcher as Royal Society Dorothy Hodgking Fellow at the University of Nottingham. Her research activity is currently focused on the development and functional characterization of hybrid metal-carbon nanostructures for spintronics and energy-related applications. She was awarded with an ERC Starting Grant in the year 2015. Dr. Giménez López joined the CiQUS as Research Staff after the approval of the CiQUS External Scientific Advisory Board.

- *Dr Rebeca García Fandiño*, PhD in Chemistry at the University of Santiago (2006) under the supervision of Prof. J.R. Granja, 2 years of postdoctoral experience at IRBB-PCB Barcelona and 2 years of postdoctoral experience at the University of Oxford. Dr García Fandiño joined the CiQUS after a period as FCT Researcher at the Facultade de Ciências, Universidade do Porto (Portugal).

The result of the 2017 Ramón y Cajal call will lead the incorporation of a new RyC researcher in the year 2019:

- *Dr Beatriz Pelaz* (ranked 3rd in the Chemistry panel): European PhD degree from the University of Zaragoza (2012) and over 5 years of postdoctoral experience at the Philipps Universität-Marburg (Germany) (supervisor: Prof. W. J. Parak). Dr Pelaz is an expert on the design of novel nanoparticle materials with biological and medical applications and will strengthen the area of Biological and Medicinal Chemistry at the CiQUS.

It is worth mentioning the CiQUS' commitment to attract young talent and achieve a gender balance as shown by the fact that our three last recruited researchers were female.

- **Postdoctoral researchers and PhD candidates:**

- *Marie Skłodowska-Curie Actions*: Dr Eric Langenberg move to the CiQUS in September 2018 to complete the second step of his MSCA-IF-GB after a two-year period at the Cornell University (Ithaca, USA).

- *The "Juan de la Cierva Incorporación contracts*" led to the recruitment of Dr Julián Bergueiro as postdoctoral research associate (Supervisor: J. Montenegro) in November 2018 (Call 2016).

- *International Postdoctoral Program – Campus Vida*: In coordination with the CiMUS and the CiTIUS, the 3rd edition of this program was launched at the end of the year 2017. This program was partially funded by the Spanish Ministry of Education (singular actions at the Campus of International Excellence) and by the European Regional Development Fund (ERDF) and the Galician Singular Research Centers Network (Centro Singular de Investigación de Galicia accreditation 2016–2019, ED431G/09). Two young postdoctoral researchers were awarded with these contracts at the CiQUS, Dr Fátima García (Supervisor: D. Peña) and Dr Marc Font (Supervisors: J. L. Mascareñas and M. Gulías).

- *CiQUS Predoctoral Contracts: The* CiQUS launched the first call of a new predoctoral contracts program at the end of 2017. This program was designed to provide support to excellent CiQUS

research groups which might be temporarily under funding shortages. This program offers a one-year, non-extendable, full-time employment contract to CiQUS PhD candidates on their first or second year of doctoral studies, in order to keep the scientific production of research groups with no available funding for human resources. Those research groups awarded with one of these contracts must ensure to find the corresponding funding to cover the rest of their doctoral period. The CiQUS internal advisory board assessed the applications received and three PhD candidates were finally hired under this call: David Bouzada (supervisor: Eugenio Vázquez), Tomás Pose (supervisor: Jose Martínez-Costas) and Roi López (supervisor: Eduardo Fernández-Megía). The 2nd call of the program was launched at the end of 2018. This program is funded by the Galician Singular Research Centers Network (Centro singular de investigación de Galicia accreditation 2016-2019, ED431G/09) and the European Regional Development Fund (ERDF).

- **Master students:**

▪ *Research initiation contracts for CiQUS Master Students*: 10 part-time contracts were offered during the year 2018 for the development of a Master Research Project under the supervision of the CiQUS Research Staff. This program aims to help our MSc students at this early stage of research, usually uncovered by state fellowships. Additionally, it also helps to attract young talent with no previous relation with the University of Santiago.

- **Undergraduate students:**

▪ *4th Ed. of the CiQUS Summer Fellowships program*: up to 15 scholarships were awarded to highly motivated undergraduate students with excellent academic records, giving them the opportunity to achieve their first research experience, working with CiQUS research groups in first class labs. The CiQUS received a total number of 89 applications from 31 different universities, where 18% of them were non-Spanish universities from up to 7 different countries. The average mark of the selected candidates was above 8.3 on a scale 0-10. It's worth mentioning that 53% of the fellowships were awarded to women. Furthermore, up to two of the fellowship holders were non-European citizens, coming from the National University of Colombia (Colombia) and the University of La Habana (Cuba), respectively. This program was funded by a special agreement with the Consellería de Educación, Universidade e Formación Profesional of the Xunta de Galicia and by a Contract-Program of the USC. The 5th edition is currently open.


***CiQUS advertising material of the International Postdoctoral Program – Campus Vida 2017/2, Summer Fellowship 2018 and Research Initiation Contracts for CiQUS Master Students (Call 2018)***


***CiQUS Fellowships holders 2018***

**Table 1:** ***List of students awarded with a CiQUS Fellowship 2018***

| Name | Bachelor | University |
|---|---|---|
| *Fernando Bordallo León* | **Chemistry** | La Habana (Cuba) |
| *Iria Esperón Abril* | **Biology & Chemistry** | Santiago de Compostela |
| *Charlene Harriswangler Harriswangler* | **Chemistry** | A Coruña |
| *Jairo Sebastián Martínez Vivas* | **Chemistry** | Nacional de Colombia (Colombia) |
| *Cecilia Ortega Zamora* | **Chemistry** | La Laguna |
| *Marco Pardo Freire* | **Biology & Chemistry** | Santiago de Compostela |
| *Andrea Pérez González* | **Biotechnology & Pharmacy** | Francisco de Vitoria |
| *Rubén Pérez Sevillano* | **Chemistry** | Valladolid |
| *Antía Pintor Lavandeira* | **Biology & Chemistry** | A Coruña |
| *Paula Piñeiro Varela* | **Chemistry** | Vigo |
| *Rubén Prieto Díaz* | **Pharmacy** | Santiago de Compostela |
| *Laura Rodríguez Pérez* | **Chemistry** | Oviedo |
| *Manuel Rodríguez Romero* | **Biology & Chemistry** | Santiago de Compostela |
| *Axel Sarmiento Fuentes* | **Chemistry** | Santiago de Compostela |
| *Lucía Vizcaíno Anaya* | **Chemistry** | Málaga |

In July 19, the 15 summer fellowship holders participated in a mini symposium that took place at the CiQUS seminar room. Everyone gave a 5 min talk to the rest of the CiQUS researchers (directors, Research Staff, postdoctoral researchers, PhD candidates, etc), based on the research project that they were collaborating with during their stay at the CiQUS. It is worth mentioning the high level of the presentations made by the scholarship holders and the good atmosphere of the scientific discussion.

Once the program was finished, a survey was sent to the scholarship holders through the link. https://goo.gl/k17xVOkgJWirCeam1.

The results of the survey showed that the program received an overall score of 8.91 points out of 10 and that 91% of the students gave the maximum score to the CiQUS scientific activity, the training received, the interest of their research project and the support they had received by their corresponding hosting group.

Furthermore, several grants to young **postdoctoral** researchers have been awarded during 2018 to carry out their research activity at the CiQUS:

- 1 New *Ramón y Cajal* researcher (Call 2017): Dr Beatriz Pelaz
- 2 Young talented researchers obtained the very competitive *Juan de la Cierva Incorporación* fellowships (Call 2017): Dr Fátima García Melo (Supervisor: D. Peña) and Dr Marc Font Molins (Supervisor: J. L. Mascareñas).
- 3 Young researchers were awarded with a Juan de la Cierva Formación Contract (Call 2017): Dr Christian Vidal (Supervisor: J.L. Mascareñas), Dr Ignacio Insua (Supervisor: J. Montenegro) and Dr Luis Martínez (Supervisor: M. Fañanás).
- 2 Researchers obtained the Postdoctoral Xunta – "Modalidad B" Fellowships: Lara Villarino Palmaz (Supervisor: J. L. Mascareñas) and Gustavo Rama Martínez (Supervisor: M. Vázquez). Additionally, 2 young researchers were awarded with the Postdoctoral Xunta – "Modalidad A" Fellowships to carry out their research activity at an institution abroad for the following two years and at the CiQUS in the following third year: Noelia Casanova (Mascareñas-López-Gulías Group) and María Maneiro (González-Bello Group).
- *International Postdoctoral Program – Campus Vida*: As result of the 3rd edition of this program, Dr Marc Font (Supervisor: J.L. Mascareñas) and Dr Fátima García (Supervisor: D. Peña) were recruited as postdoctoral researchers in 2018.

With regard to **predoctoral** trainees, fifteen new competitive research contracts have been awarded to CiQUS PhD students in 2018:

- *MECD – FPU Predoctoral fellowships*: Alejandro Guitiérrez (Supervisor: J. L. Mascareñas) and Juan José Tarrío (Supervisor: F. Freire)
- *MINECO – Predoctoral contracts*: Borja Cendón Mariño (Supervisor: M. Gulías) and Berta Álvarez Pérez (Supervisor: D. Pérez), Alejandro Lamas Pérez (Supervisor: J. Granja), Jesús Alfonso Castro Esteban (Supervisor: D. Peña), David Bugallo Ferrón (Supervisor: F. Rivadulla), Ángela Rodríguez Costa (Supervisor: C. González-Bello) and Soraya Learte Aymami (Supervisor: J. L. Mascareñas).
- *Xunta de Galicia – Predoctoral contracts*: Iván Gallego Gómez (Supervisor: J. Granja), Eva Rivera Chao (Supervisor: M. Fañanás), Carlos López Bueno (Supervisor: F. Rivadulla) and Álvaro Velas Rubio (Supervisor: C. Saá).

| Predoctoral Competitive Fellowships and Contracts awarded 2018 | | |
|---|---|---|
| **Program** | **Institution** | **No. grants awarded** |
| Fundación Gil Dávila | Fundación Gil Dávila | 2 |
| Xunta de Galicia – Predoctoral contracts | Xunta de Galicia | 3 |
| MECD – FPU | AEI | 2 |
| MINECO – Predoctoral contracts | AEI | 7 |
| Xunta de Galicia – short stays | Xunta de Galicia | 4 |
| MINECO – short stays | AEI | 2 |
| Fundación Gil Dávila – short stays | Fundación Gil Dávila | 1 |
| **Total** | | **21** |

| Postdoctoral Competitive Contracts awarded 2018 | | |
|---|---|---|
| **Program** | **Institution** | **No. contracts awarded** |
| Ramón y Cajal | AEI | 1 |
| Juan de la Cierva Incorporación | AEI | 2 |
| Juan de la Cierva Formación | AEI | 3 |
| Xunta de Galicia – Mod. A | Xunta de Galicia | 2 |
| Xunta de Galicia – Mod. B | Xunta de Galicia | 2 |
| **Total** | | **10** |

| Ongoing Competitive Contracts 2018 | | |
|---|---|---|
| **Program** | **Institution** | **No. contracts awarded** |
| Ramón y Cajal | AEI | 5 |
| Juan de la Cierva Incorporación | AEI | 4 |
| Juan de la Cierva Formación | AEI | 1 |
| Marie Curie Individual Fellowships- Marie Sklodowska-Curie Actions | European Union | 3 |
| Xunta de Galicia – Mod. A | Xunta de Galicia | 4 |
| Xunta de Galicia – Mod. B | Xunta de Galicia | 3 |
| MECD - FPU | AEI | 8 |
| MINECO - Predoctoral contracts | AEI | 15 |
| Xunta de Galicia - Predoctoral Contracts | Xunta de Galicia | 17 |
| Fundación Gil Dávila | Fundación Gil Dávila | 3 |
| **Total** | | **61** |

In addition to these new competitive fellowships, an important number of research contracts have been drawn in 2018 under different funded research projects and contracts.

Overall, the CiQUS has maintained an increasing capacity to attract young researchers, especially predoctoral students.

## 3.2 RESEARCH FUNDING

- During 2018 new funding reached 4.3 M € (37% international projects, 27% regional projects, 17% national projects and 20% contracts)
- 1 ERC-StG
- In addition to its success in the national programs, the CiQUS also obtained 2 predoctoral contracts.

The CiQUS has proved to have an excellent fundraising capacity despite the difficult financial environment, increasing not only the regional and national funds but also European funding, as well as funds from private sources. Our figures as on 31 December 2018 show 57 active projects and 9 contracts for a total amount of 14.5 M €.

With regard to new funds raised during the year 2018, the CiQUS started 15 new projects and signed 7 new contracts for a total amount of 4.34 M €. Remarkably, there is a significant contribution from private sources, reaching 20% of the total funds. The reason for this is the strategic long-term partnership with INDITEX (PI J. Sardina), the largest fashion retail group in the world. The following table and chart show the increasing fundraising capacity of the CiQUS since its opening in 2011. More detailed information regarding 2018 is shown in Annex II and Annex III.

**Table 5.** R&D fundraising evolution at the CiQUS since 2011

| | 2011 | 2012 | 2013 | 2014 | 2015 | 2016 | 2017 | 2018 |
|---|---|---|---|---|---|---|---|---|
| International Projects | 0 € | 0 € | 553.934 € | 2.356.276 € | 307.391 € | 1.670.215 € | 799.596 € | 1.571.692 € |
| National Projects | 494.890 € | 420.030 € | 1.503.409 € | 1.503.409 € | 689.620 € | 1.018.717 € | 1.404.760 € | 715.488 € |
| Regional Grants | 504.000 € | 1.069.842 € | 1.112.200 € | 1.281.000 € | 850.000 € | 1.085.000 € | 2.195.000 € | 1.172.000 € |
| Contracts | 268.777 € | 10.000 € | 223.855 € | 513.178 € | 895.545 € | 1.084.724 € | 1.188.752 € | 885.310 € |
| TOTAL (€) | 1.267.667 € | 1.499.872 € | 3.393.398 € | 5.653.862 € | 2.742.556 € | 4.858.656 € | 5.588.108 € | 4.344.490 € |

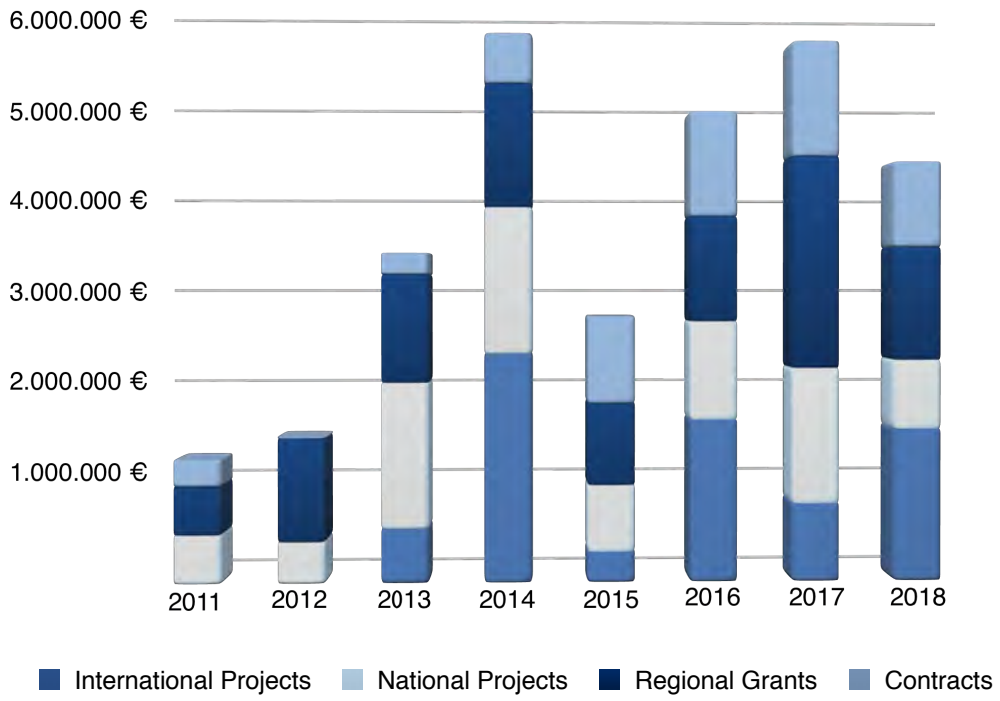
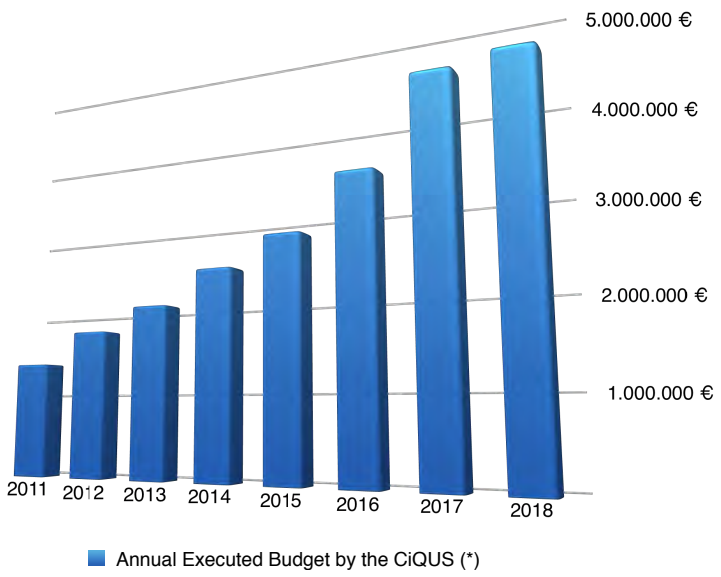



***Chart 3. Evolution of the fundraising capacity, 2011-2018***

Additionally, it is also worth mentioning the CiQUS fundraising capacity in terms of annual implemented budget.




(*) HR Programs and Overheads are not included in this chart.

***Chart 4. Evolution of the annual implemented budget, 2011-2018***

Since its creation in 2011, the CiQUS annual implemented budget has continuously increased from 1.3 M € up to 4.5 M €, which represents an increase of 246% since 2011.

Regarding the projects awarded in 2018, these are the key facts:

- **International Projects: 1.57 M €**. Dr. M. Giménez-López was awarded an ERC-StG in 2016 (NANOCOMP: Complex Dynamics of Clusters in High-Aspect Ratio Hollow Nanostructures). After an initial period at the University of Nottingham, she decided to move her research group to the CiQUS, where she is currently developing the ERC project. Dr Giménez-López officially joined the CiQUS as Research Staff, Ramón y Cajal researcher and ERC grantee in February 2018.

Thanks to international funding, a collaborative project of Prof E. Fernández-Megía with colleagues from many different countries has been approved with funding by the European Union in August 2018 (ENDOSCAPE: a clinically applicable non-viral gene delivery technology. RIA-H2020-SC1-BHC-09-2018). The grant agreement was signed at the end 2018 and the project is due to start in January 2019. In addition, Dr J. Montenegro was awarded an ERC-PoC in December 2018 (the grant agreement being still under negotiation) and an international collaborative project within the highly competitive EIG CONCERT program.

Prof. Rivadulla participates in SPICOLOST, a research exchange network (MSCA-RISE) and supervised a Marie Curie Individual Fellowship (MSCA-IF-GB). Additionally, Dr. Montenegro and Dr. del Pino supervise 2 Marie Curie Individual Fellowships (MSCA-IF-EF) at the CiQUS.

Finally, a number of highly competitive projects have been submitted to different international calls and are still under evaluation (3 ERC-CoG, ERC-CH2020-MSCA-ITN-2018…) which is a clear sign of the increasing implication of the CiQUS Research Staff in international initiatives.

- **National Projects: 0.72 M €**. CiQUS researchers successful competed in the National Research Program (6 projects: 4 of them associated with the RETOS (societal challenges) call and 2 of them

associated to the EXCELENCIA call, both of which work in a 3- or 4-year cycle. In addition to these funds, 2 of these projects were also awarded with one predoctoral fellowship.

The national funding also included the young talent incorporation programs Ramón y Cajal (awarded to Dr Giménez-López and Dr García-Fandiño) and Juan de la Cierva (awarded to Dr Polo and Dr Bergueiro).

- **Regional Funding: 1.18 M €**. 68% (800 K €) accounts for the support of the Xunta de Galicia to the CiQUS as a *Singular Research Center* of the Galician University System (SUG), co-funded by the European Regional Development Fund – (ERDF), project ED431G/09. It is worth noting there was a delay in the regional competitive public calls for funding of research groups during 2018. By the end of 2018, project proposals were still under evaluation and the regional government approved advance funding for those proposals and the CiQUS received a total of 76.000 €. The rest of the regional funding belongs to different signed agreements with the Xunta de Galicia.

- **Research contracts: 0.89 M €.** In 2018, the CiQUS attracted a significant income from contracts with the private sector, mainly due to the strategic alliance of Prof. J. Sardina with INDITEX (0.60 M €). Moreover, it is worth mentioning the signed contracts of Prof. E. Sotelo with the Biotech startups ONCOSTELLAE and Landsteiner Genmed S.L. (0.15 M €) for the development of synthetic methodologies and the preparation of organic molecules libraries.

- **Scientific and Technical Equipment**: **0.11 M €**. In 2018, the CiQUS received funding for the acquisition of GC-MS equipment through the competitive public call launched by the Spanish Government. It is expected that the new equipment will be installed at the CiQUS during fall 2019.

Finally, it is also worth noting the income associated with the contracts of some of the CiQUS researchers (e.g. RyC researchers, JdC, postdoctoral and predoctoral researchers from regional and national calls) awarded by Human Resources Competitive public calls (Chart 5), which reached a peak of 2.4 M € in 2018. Unfortunately, we do not have any data available before the year 2014.

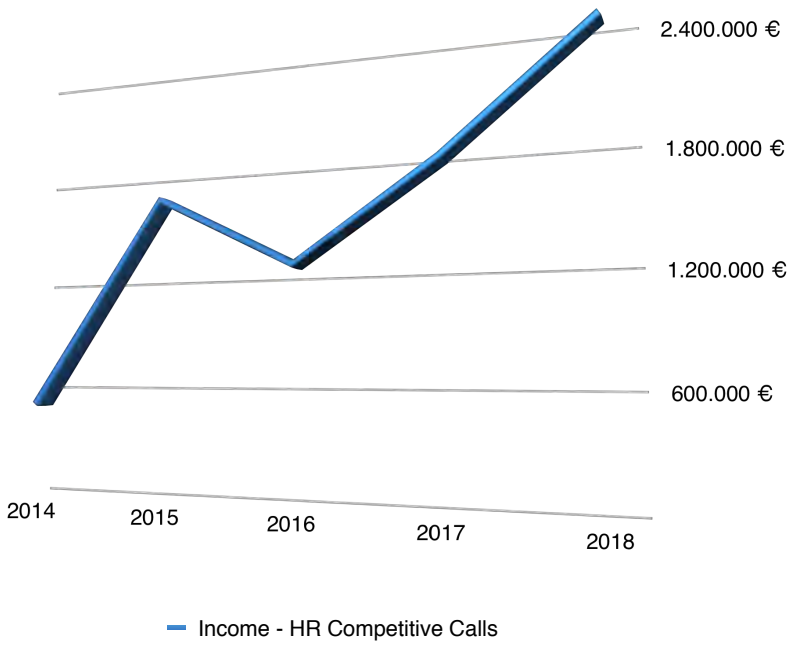



***Chart 5. Evolution of the income from Human Resources Competitive Calls, 2014-2018***

# 3.3 RESEARCH OUTPUT

## 3.3.1 Scientific publications

The CiQUS maintained an excellent record of scientific contributions in 2018, with **101 articles,** 97 of which were published in JCR Journals (96% of the total of the CiQUS publications). **84% of CiQUS JCR articles were published in journals indexed in the first quartile (Q1)** and, more significantly, **44% in the first decile (D1)** of their respective thematic areas of the Web of Science data base (WoS) (see Annex IV). In 2018 the **average impact factor of CiQUS JCR articles was 7,591, t**hus keeping the remarkable rising trend from the last 5 years.

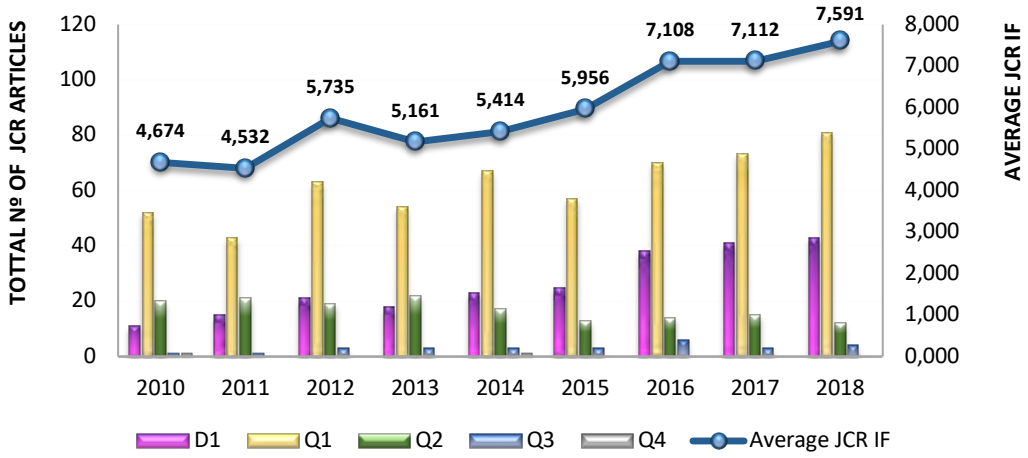



***Chart 6. Evolution of the number of publications and average impact factor (*) 2010-2018.***

(*) Journal Impact factor values for the year 2018 are based on *2018 Journal Citation Reports (2017 data)*. 2018 data have not yet been published.

During the period 2016-2018, the distribution of CiQUS articles per scientific area, according with our scientific organization, shows that the percentage of scientific publications with respect to the total CiQUS production is directly related to the total number of groups with active research lines in each area. Remarkably, all areas present a scientific production higher than 75% in JCR publications indexed in the first quartile (75% Biological and Medicinal Chemistry, 92% Functional Materials with Technological Applications and 89% Synthetic Methodologies for Sustainable Development). As for JCR publications published in journals of the first decile of their category, the respective percentages per area are also outstanding: 38% Biological and Medicinal Chemistry, 45% Functional Materials with Technological Applications and 78% Synthetic Methodologies for Sustainable Development, respectively.

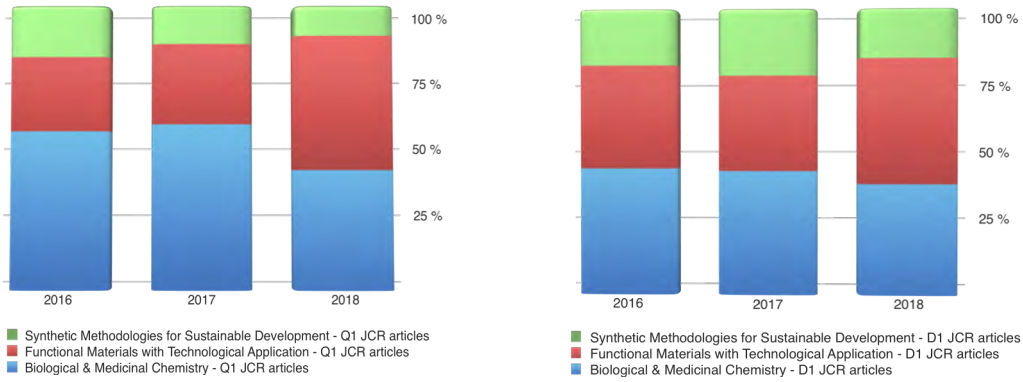



***Chart 7. Distribution of %D1 and %Q1 among CiQUS scientific areas 2016-2018***

Furthermore, the CiQUS has achieved a sharp increase in the number of publications in top-ranked journals. During 2018, the CiQUS published a total number of **35 papers with IF>9**, which represents 36% of CiQUS JCR publications in 2018.

**Table 6.** Scientific Journals with IF > 9, in which CiQUS articles were published during 2018 and total number of articles per Journal

| Full Journal Title | Impact Factor(*) | Nº of articles |
|---|---|---|
| Science | 41,058 | 1 |
| Nano Today | 17,753 | 1 |
| Coordination Chemistry Reviews | 14,499 | 1 |
| Journal of the American Chemical Society | 14,357 | 7 |
| ACS Nano | 13,709 | 1 |
| Advanced Functional Materials | 13,325 | 1 |
| Nature Communications | 12,353 | 2 |
| Trend in Pharmacological Sciences | 12,108 | 1 |
| Angewandte Chemie International Edition | 12,102 | 5 |
| Nano Letters | 12,080 | 1 |
| Science Advances | 11,511 | 1 |
| ACS Catalysis | 11,384 | 6 |
| Annals of Neurology | 10,244 | 1 |
| Chemistry of Materials | 9,890 | 2 |
| Nanoscale Horizons | 9,391 | 1 |
| Chemical Science | 9,063 | 3 |

(*) Journal Impact factor values for the year 2018 are based on *2018 Journal Citation Reports (2017 data)*. 2018 data have not yet been published.

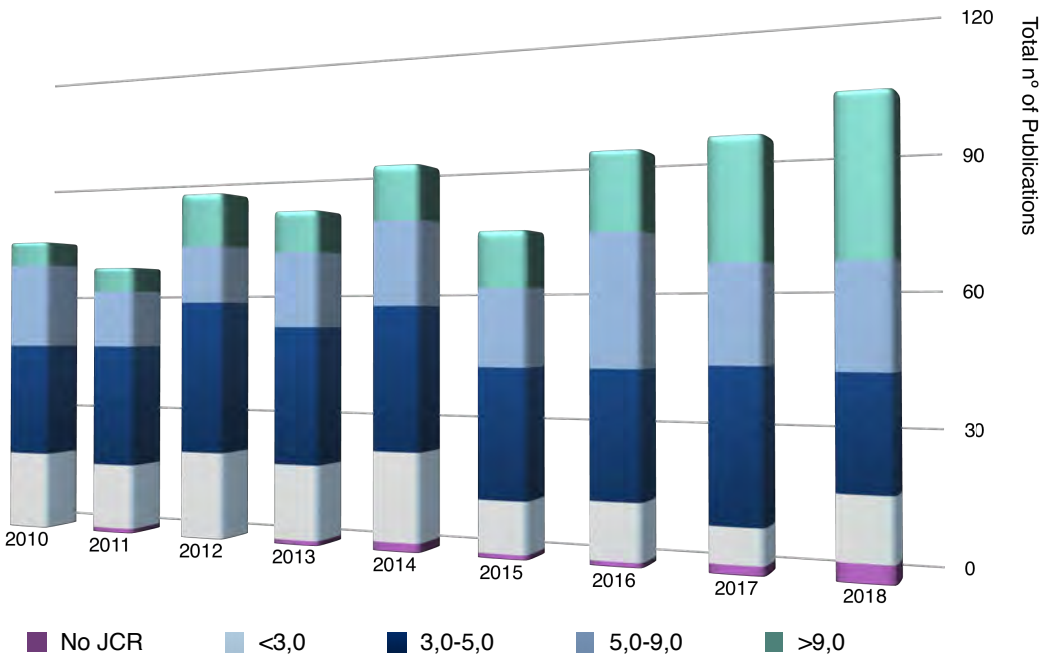



***Chart 7. Evolution of the % of publications aggregated by IF sections, 2010-2018***

Our commitment and ambition to generate top-level science is demonstrated by the ability of producing high impact factors in a variety of topics which is also consistent with the quality and interdisciplinary nature of the CiQUS as ra esearch center. **Table 7** shows the list of scientific journals in which CiQUS articles were published in 2018. These journals are listed according to the total number of CiQUS articles published in each journal during 2018 and the corresponding journal impact factor order.

**Table 7.** Scientific Journals in which CiQUS articles were published during 2018 and total number of articles per Journal.

| Full Journal Title | Journal Impact Factor (*) | Quartile | nº of articles |
|---|---|---|---|
| *Journal of the American Chemical Society* | 14,357 | Q1 | 7 |
| *Chemical Communications* | 6,290 | Q1 | 7 |
| *Chemistry - A European Journal* | 5,160 | Q1 | 7 |
| *ACS Catalysis* | 11,384 | Q1 | 6 |
| *Angewandte Chemie-International Edition* | 12,102 | Q1 | 5 |
| *Physical Chemistry Chemical Physics* | 3,906 | Q1 | 4 |
| *ACS Omega* | No JCR | N/A | 3 |
| *Chemical Science* | 9,063 | Q1 | 3 |
| *Journal of Organic Chemistry* | 4,805 | Q1 | 3 |
| *Nature Communications* | 12,353 | Q1 | 2 |
| *Chemistry of Materials* | 9,890 | Q1 | 2 |
| *Journal of Physical Chemistry Letters* | 8,709 | Q1 | 2 |
| *Journal of Physical Chemistry C* | 4,484 | Q1 | 2 |
| *Scientific Reports* | 4,122 | Q1 | 2 |
| *Organic and Biomolecular Chemistry* | 3,423 | Q2 | 2 |
| *Synthesis-Stuttgart* | 2,722 | Q2 | 2 |
| *Nature Reviews Chemistry* | No JCR | N/A | 1 |
| *Science* | 41,058 | Q1 | 1 |
| *Nano Today* | 17,753 | Q1 | 1 |
| *Coordination Chemistry Reviews* | 14,499 | Q1 | 1 |
| *ACS Nano* | 13,709 | Q1 | 1 |
| *Advanced Functional Materials* | 13,325 | Q1 | 1 |
| *Trends in Pharmacological Sciences* | 12,180 | Q1 | 1 |
| *Nano Letters* | 12,080 | Q1 | 1 |
| *Science Advances* | 11,511 | Q1 | 1 |
| *Annals of Neurology* | 10,244 | Q1 | 1 |
| *Nanoscale Horizons* | 9,391 | Q1 | 1 |
| *Physical Review Letters* | 8,839 | Q1 | 1 |
| *ACS Applied Materials & Interfaces* | 8,097 | Q1 | 1 |
| *Nanoscale* | 7,233 | Q1 | 1 |
| *Journal of Materials Chemistry C* | 5,976 | Q1 | 1 |
| *Biomacromolecules* | 5,738 | Q1 | 1 |
| *Journal of Chemical Theory and Computation* | 5,399 | Q1 | 1 |
| *Journal of Nanobiotechnology* | 5,297 | Q1 | 1 |
| *Inorganic Chemistry* | 4,700 | Q1 | 1 |
| *ChemCatChem* | 4,674 | Q1 | 1 |
| *Contact Dermatitis* | 4,275 | Q1 | 1 |
| *Frontiers in Chemistry* | 4,155 | Q2 | 1 |
| *APL Materials* | 4,127 | Q1 | 1 |
| *Dalton Transactions* | 4,099 | Q1 | 1 |
| *Langmuir* | 3,789 | Q1 | 1 |
| *Journal of Biophotonics* | 3,768 | Q1 | 1 |
| *Computer Physics Communications* | 3,748 | Q1 | 1 |
| *Applied Physics Letters* | 3,495 | Q1 | 1 |
| *Optics Express* | 3,356 | Q1 | 1 |
| *Journal of Computational Chemistry* | 3,221 | Q2 | 1 |
| *Polymers* | 2,935 | Q1 | 1 |
| *European Journal of Organic Chemistry* | 2,882 | Q2 | 1 |
| *Spectrochimica Acta Part A-Molecular and Biomolecular Spectroscopy* | 2,880 | Q1 | 1 |
| *Journal of Chemical Physics* | 2,843 | Q2 | 1 |
| *Journal of Physical Chemistry A* | 2,836 | Q2 | 1 |
| *Israel Journal of Chemistry* | 2,607 | Q2 | 1 |
| *Synthetic Metals* | 2,526 | Q2 | 1 |
| *Materials* | 2,467 | Q2 | 1 |
| *Surface Science* | 1,997 | Q3 | 1 |
| *Magnetic Resonance in Chemistry* | 1,776 | Q3 | 1 |
| *ChemistrySelect* | 1,505 | Q3 | 1 |
| *Chimia* | 1,245 | Q3 | 1 |

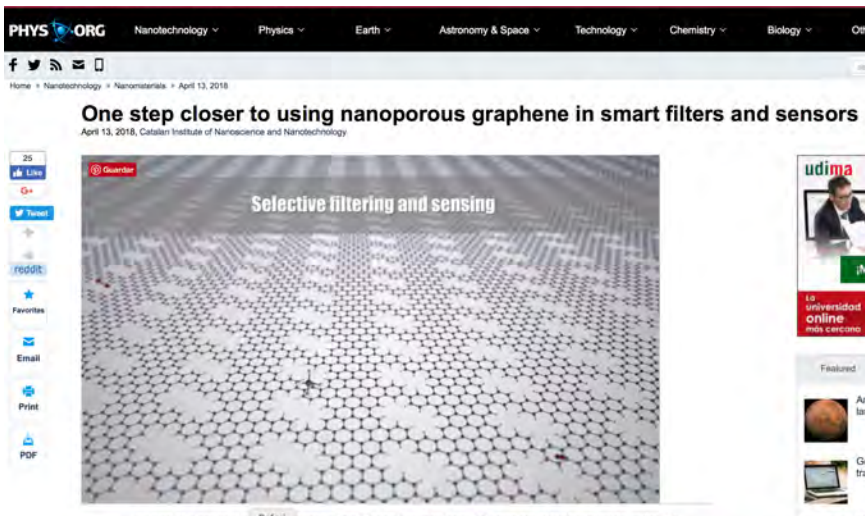
(*) Journal Impact factor values for the year 2018 are based on *2018 Journal Citation Reports (2017 data)*. 2018 Data have not yet been published.

It is also worth mentioning that 49% of the contributions during the period of reference are the result of international collaborations, many of them from prestigious research centers. Also, 7 articles (8%) result from active collaborations between different CiQUS research groups and also with groups from the CiMUS, which confirms the emerging cooperative research lines within the *singular research centers network*. **Annex IV** shows a full listing of the scientific articles in JCR journals published by CiQUS researchers in 2018.

### 3.3.2 CiQUS Scientific highlights

Among the most outstanding scientific findings in the year 2018, there are contributions from the three priority areas of the CiQUS scientific organization. Many of them have been featured in special theme collections or highlighted in different ways. Thus, the article "*Intracellular Deprotection Reactions Mediated by Palladium Complexes Equipped with Designed Phosphine Ligands*" published in ACS Catalysis journal by Prof J. L. Mascareñas was selected as ACS Editors' Choice (the selection of these articles is based on the recommendations by the scientific editors of ACS journals from around the world); the article "*Magnetically Recyclable Catalytic Carbon Nanoreactors*" published in Adv. Funct. Mat. by Dr M. Giménez-López was selected for the Hot Topic: Magnetic Materials; "*Stereoselective Synthesis of Borylated 1,3-Dienes by Synergistic Cu/Pd Catalysis*" by Dr M. Fañanás-Mastral and published in ChemCatChem was selected for the special issue "Young Researchers Series"; "*Oligoalanine Helical Callipers for Cell Penetration*" published in Chem. Commun. by Dr. J. Montenegro was included in the special collection 2018 Emerging Investigators; the Chem. Eur. J. article "*Tunable Performance of Manganese Oxide Nanostructures as MRI Contrast Agents*" by Prof. F. Rivadulla was selected as Hot paper; another Chem. Eur. J. article "*Supramolecular Recognition and Selective Protein Uptake by Peptide Hybrids*" by Dr J. Montenegro was included in the Hot Topic: Membrane issue and a Phys. Chem. article "*Site-selective Reversible Diels–Alder Reaction between a Biphenylene-based Polyarene and a Semiconductor Surface*" published by Prof E. Guitián, Prof. D. Pérez and Prof. D. Peña was selected for the theme collection: 2018 PCCP Hot articles.

Furthermore, it is worth mentioning the article published by Prof. Diego Peña in collaboration with the Catalan Institute of Nanoscience and Nanotechnology (ICN2) and the Donostia International Physics Center (DIPC) in ***Science*** - "Bottom-up Synthesis of Multifunctional Nanoporous Graphene" (DOI: 10.1126/science.aar2009). In this work, researchers successfully synthesized a graphene membrane with pores, whose size, shape and density can be modified at a nanoscale with atomic precision, thus developing new material with promising and potential applications in electronics, filters and sensors. These findings resulted in a patent and were collected by numerous national and



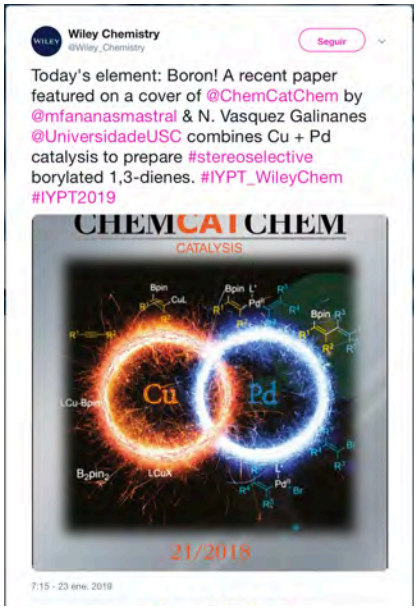

international media and scientific blogs (Phys.Org, Nanowerk, SINC Agency, EFE Futuro, La Vanguardia, El Periódico, Radio Cable, La Voz de Galicia, etc).

In January 2019, the molecule of **nanoporous graphene** was selected by the readers of C&EN-Chemical & Engineering News as the **molecule of the year 2018**.

Within the area of Biological and Medicinal Chemistry, the work published by the group of Prof. Mascareñas in the journal ***Nature Communications*** - "Concurrent and Orthogonal Gold (I) and Ruthenium (II) catalysis inside living cells" (DOI: 10.1038/s41467-018-04314-5) focuses on the development of orthogonal organometallic catalysis in living cells, which constitutes a pioneer contribution to the development of metabolic networks based on artificial enzymes.



Regarding the area of Synthetic Methodologies for Sustainable Development, Wiley Chemistry selected a ChemCatChem article published by CiQUS Research Staff M. Fañanás- Mastral with the featured “Boron” as the element of the day, within the celebration of the International Year of the Periodic Table 2019.



Finally, it is also worth mentioning that up to 9 CiQUS research articles were featured as Journals Covers during 2018.


**Stereoselective Synthesis of Borylated 1,3-Dienes by Synergistic Cu/Pd Catalysis**

*ChemCatChem* **2018**, *7*, 4817


**Microwave-induced covalent functionalization of few-layer graphene with arynes under solvent-free conditions**

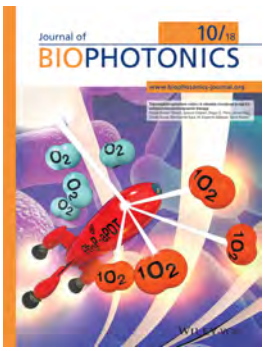
*Chem. Commun.* **2018**, 54, 2086


**On-surface synthesis of superlattice arrays of ultra-long graphene nanoribbons**

*Chem. Commun.* **2018**, 54, 9402


**Unravelling the spin-state of solvated $[Fe(bpp)_2]^{2+}$ spin-crossover complexes: structure–function relationship**

*Chem. Eur. J.*, **2018**, *24*, 1295




**Triphenylphosphonium cation: A valuable functional group for antimicrobial photodynamic therapy**

*J. Biophotonics,* **2018**, 11, e201800054


**A valuable functional group for antimicrobial photodynamic therapy**

*Dalton Trans.*, **2018**, 47, 10453


**pH-Triggered Self-assembly and Hydrogelation of Cyclic Peptide Nanotubes Confined in Water Micro-droplets**

*Nanoscale Horizons,* **2018**, 3, 391


**QM/MM Simulations Identify the Determinants of Catalytic Activity Differences Between Type II Dehydroquinase Enzymes**

*Org. Biomol. Chem.*, **2018**, *16*, 4443


**Synthetic materials at the forefront of gene delivery**

*Nat. Rev. Chem.*, **2018**, *2*, 258

A complete list of articles, with links to their respective journal websites, can also be found in the CiQUS web page. Additional information about the selected articles, considered as significant scientific contributions of the period, can be found in the *News* section of the website (https://www.usc.es/ciqus/en/news).

### 3.3.3 Other research outputs

• ***Patent applications***

During 2018 CiQUS researchers applied for 5 new patents: *Iron oxide nanotubes* (PI Juan Granja, in collaboration with an Italian research group), *Cell penetrating peptides* (PI. Javier Montenegro), *G6 fosfatasa* (PI. Jose Martínez-Costas), *Stable polymer composites* (PI Massimo Lazzari in collaboration with Prof Arturo López Quintela) and *A nanoporous graphene structure and method for preparation thereof* [PI. Diego Peña in collaboration with César Moreno and Aitor Mugarza (ICN2, Spain)]. Furthermore, the patent "Applications of the protein muns and the derivates" from the Martínez-Costas group has been approved in the USA – US10059745 (see Annex VIII for the details of these patents).

• ***PhD Theses***

During 2018 up to 13 CiQUS graduate students presented their PhD theses. All of them obtained the qualification of *Sobresaliente cum laude* and five of them had a mention as *European doctorate/International Mention*. Detailed information about the CiQUS PhD theses presented in this period can be found in Annex V and on the CiQUS website. These graduate students had external financial support either from competitive research fellowships or through contracts attached to their advisor's research grants.

Currently, 84 PhD students are developing their thesis work at CiQUS. 7% of students came from other countries and 41% are female.

• ***Contributions to scientific congresses***

***The*** CiQUS Research Staff gave up to 55 lectures during the year 2018. **7 of them as Plenary, 2 as Keynote and 46 as Invited speaker** at international conferences and meetings from 13 different countries (USA, UK, Germany, Denmark, Italy, France, Spain, Portugal, Taiwan, Japan, Turkey, Mexico and Colombia). Some examples were: Chirality 2018 (USA), 10 èmes Recontres de Chimie Organique de Marseille (France), 12$^{th}$ Spanish-Italian Simposium on Organic Chemistry (Italy), 10$^{th}$ Asian-European Symposium on Metal-Mediated efficient Organic Synthesis (Taiwan) and 10$^{th}$ EUCHEMS Young Investigator Workshop 2018 (UK). Furthermore, it is particularly remarkable the total number of CiQUS scientific contributions at congresses (220).

• ***Organization of scientific congresses and symposiums***

Prof. Concepción González-Bello organized with Scientists from Merck the Symposium "Antibiotic Resistance: Recent Advances in Drug Discovery and Development" at 256th ACS National Meeting (Boston, MA, August 19-23, 2018). In addition, several CiQUS Research Staff (Prof. Carlos Saá, Dr. Martín Fañanás-Mastral, Prof. Eugenio Vázquez, Prof. Eduardo Fernández-Megía, Prof. Félix Freire, Prof. Concepción González-Bello, Dr. Fernando López, Dr. Javier Montenegro, Prof. Diego Peña and Prof. Jesús Varela), all of them members of the Organic Chemistry Group (GEQOR) of the Spanish Royal Society, organized the XXVII Biennial Meeting in Santiago de Compostela (Spain), from 20 to 22 June 2018.

• ***Research Mobility***

During 2018, up to 20 CiQUS members had short stays at prestigious international research institutions from 12 different countries, either for scientific collaborations (as invited visiting professors) or as a part of their PhD training program (predoctoral secondments). Host institutions included Trinity College Dublin (Ireland), the National Institute of Chemistry - Kemijski inštitut (Slovenia), the University of Minnesota (USA), the University of Manchester (UK), New College-University of Oxford (UK), the University of Zurich (Switzerland), Technische Universiteit Eindhoven

(The Netherlands), the University of Nantes (France), the University of Angers (France), Max-Planck-Institut für Kohlenforschung (Germany), CIC nanoGUNE (Spain), the Universidade de Lisboa (Portugal), the University of Toronto (Canada), Northwestern University (USA), the Universidad de Málaga (Spain), the Universidad Complutense de Madrid (Spain), the University of Oxford (UK), the Universidad de Málaga (Spain), the University of Cambridge (UK) and Univ. G. D'Annunzio - CNR-SPIN (Italy).

### 3.3.4 Awards

Regarding the awards achieved by CiQUS researchers, we should highlight that 2018 has been specially remarkable in this area. Thus, the CiQUS Principal Investigators received the following recognitions:

- *Prof José Luis Mascareñas*: Galician Critic Prize in research 2018
- *Prof Ricardo Riguera*: GERMN Bruker Award 2018
- *Prof Francisco Rivadulla*: Technology Transfer Award: Best work on Applied Research 2018
- *Prof Diego Peña: RSEQ* – Ignacio Ribas Medal 2018
- *Dr Martín Fañanás*: 2018 Lilly-RSEQ Young Investigator Award
- *Dr Javier Montenegro*: 2018 RSEQ-Sigma Aldrich Young Investigator Award


***Awarded CiQUS Research Staff in 2018***

Regarding CiQUS young researchers, several postdoctoral researchers and PhD candidates have also been awarded during 2018:

- Dr Sandra Arias (supervisors: Emilio Quiñoá and F. Freire) received "the second-best thesis award" by the Polymers Group of the RSEQ.
- Dr Jéssica Rodríguez (supervisors: J.L. Mascareñas and E. Vázquez) was selected as finalist at the European Young Chemist Award (EYCA), Liverpool-UK 2018.
- Dr Cristian Vidal has received the Best Oral Communication Award at the XV Young Researchers Symposium RSEQ-Sigma Aldrich (Toledo, November 2018).
- Dr María Tomás Gamasa was awarded with Best Oral Communication at the XI School of Organometallic Chemistry – Marcia Moreno Mañas (Oviedo, June 2018)

- Andrea Álvarez Pérez (supervisors: C. Saá and J. Varela) and Iván Gómez Gallego (supervisors: J. Granja and J. Montenegro) received the Poster's Prizes at the Bienal de Química Orgánica – RSEQ (Santiago de Compostela, June 2018).

### 3.3.5 Benchmarking analysis

In January 2019, CiQUS has submitted a new application to be accredited as Unit of Excellence María de Maeztu within the Severo Ochoa & María de Maeztu call 2018. In this context, a benchmarking analysis has been elaborated with respect to previous accredited units. A summary of this benchmarking study is shown below.

Based on public available information (Nature Index, WoS database, as well as the Activity Reports of the Units and information on their own websites), we have conducted a benchmark exercise with the accredited units "Maria de Maeztu" since the first call launched in 2014. This study relies on 3 key objectively verifiable indicators, associated to the evaluation criteria and some of them expressly specified in the text of this Call:

A) NATURE INDEX - FRACTIONAL COUNT (FC). The Nature Index is a database of author affiliation information collated from research articles published in an independently selected group of 68 high-quality science journals (www.natureindex.com/faq#journals). The database is compiled by Nature Research. The Nature Index provides a close to real-time proxy for high-quality research output at the institutional, national and regional level. The Nature Index is updated monthly, and a 12-month rolling window of data is openly available at www.natureindex.com. The Fractional Count (FC) index takes into account the percentage of authors from that institution and the number of affiliated institutions per article. For calculation of the FC, all authors are considered to have contributed equally to the article. The maximum combined FC for any article is 1.0.

B) ERC GRANTEES. It is well known that the quality of the ERC projects and researchers are the sole selection criteria for these grants. Thus, the number of granted researchers is considered a good indicator of the level of scientific excellence and international leadership of an institution, as stated in the text of this call. We have included all the ERC grantees of each unit, even if their projects have already finished.

C) CITES PER PAPER. This indicator is related to the impact of the scientific production of the Unit, independently from the total number of papers, during the period of the scientific report, 2014-2018, and thus independent of the size of the unit.

***Comparison of CiQUS and accredited María de Maeztu Units:***

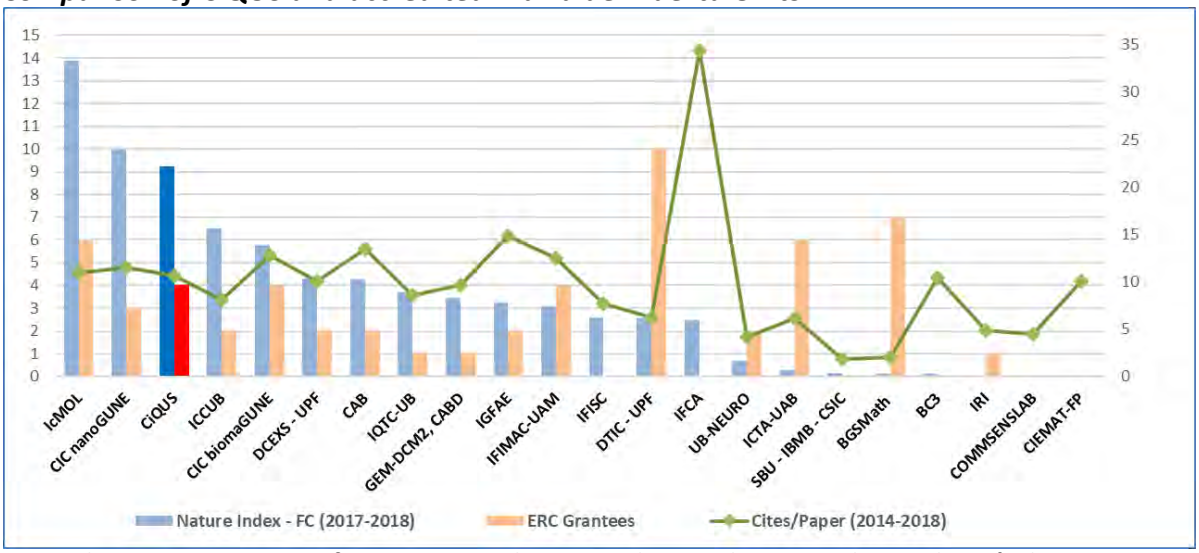



***Chart 8. Comparaison of some CiQUS indicators with several Severo Ochoa and María de Maeztu accreditated centers.***

**NOTES:**

1. Due to their very different profile, we have not included the two Units devoted to the fields of Economics and Finance (Social Sciences and Humanities Panel).

2. Missed data in Nature Index – FC: some Units have not been found in the Nature Index database. In two cases (CEM-DCM2-CABD and the SBU–IBMB-CSIC we have indicated the value of the whole Center which includes the Maria de Maeztu Unit.

3. A zero value in ERC Grantees means that the Unit has (had) no ERC, according their own websites and public reports.

4. We have included the Units working on Astrophysics, Nuclear Physics or High Energy Physics (see IGFAE, IFCA and CIEMAT-FP), even though the special features of these thematic areas with regard to scientific production metrics (participation in large experiments and consortia, high number of papers with hundreds of authors and citations, etc.).

5. Missed data in Cites/Paper are due: 1) Lack of information on the websites; 2) Poor results when searching (WoS) the scientific production of some new Units by using the official names/acronymous.

From these data, it is clear for us that CiQUS' indicators can only be compared to the best research units previously funded by the María de Maeztu Program. In fact, it would be in 3rd position according to the Nature Index metrics, 4th in number of ERC Grantees [1 ERC-AdvG and 3 ERC-StG (two of them holding ERC-PoC, not included)] and 6th-7th in cites/article for the currently evaluated period.

With regard to one of the indicators, Nature Index-FC, which we consider particularly relevant as a proof of the high quality/excellent scientific outcome of a unit or center, we provide a list with the values of CiQUS, the whole current list of Maria de Maeztu units and Severo Ochoa centers, and other national and international chemistry/chemical biology centers. In this context, it is especially remarkable the Nature Index values reached by CiQUS if we take into account the fact that, in our particular case, the calculated numbers for our center are the result of dividing our articles by a factor of 2 due to the double affiliation of our CiQUS Research Staff (e.g. CiQUS and the corresponding University Department).

| Nature Excellence INDEX | | | 01 October 2017 - 30 September 2018 | | |
|---|---|---|---|---|---|
| **Cat.** | **Year** | **Name of the Centres / Units** | **Link** | **FC** | **AC** |
| SO | 2013 | Institute of Chemical Research of Catalonia (ICIQ) | ICIQ | 28,5 | 49 |
| SO | 2016 | Institute for Theoretical Physics (IFT) | IFT | 25,5 | 69 |
| SO | 2015 | Institute of Materials Science of Barcelona (ICMAB), CSIC | ICMAB | 15,5 | 39 |
| Internat. | | Institute of Organic Chemistry and Biochemistry - IOCB, ASCR (Czech Republic) | IOCB | 14,2 | 38 |
| **MM** | 2015 | Institute for Molecular Science (ICMol), UV, Spain | IcMol | 13,9 | 43 |
| SO | 2011 | Institute for Research in Biomedicine (IRB Barcelona) | IRB | 13,1 | 51 |
| SO | 2016 | Centre for Genomic Regulation (CRG), BIST | CRG | 13,0 | 70 |
| SO | 2017 | Catalan Institute of Nanoscience and Nanotechnology (ICN2) | ICN2 | 11,4 | 41 |
| SO | 2016 | IMDEA Nanoscience | Imdea Nano | 11,0 | 51 |
| **MM** | 2016 | Cooperative Research Center nanoGUNE Consolider (CIC nanoGUNE) | nanoGune | 10,0 | 26 |
| SO | 2016 | Instituto de Tecnología Química (ITQ) | ITQ | 9,3 | 18 |
| | | Center for Research in Biological Chemistry and Molecular Materials (CIQUS) | CiQUS | **9,2** | 30 |
| Internat. | | National Institute of Chemistry, Slovenia | KI | 7,4 | 16 |
| SO | 2014 | Institut de Bioenginyeria de Catalunya (IBEC) | IBEC | 7,3 | 27 |
| SO | 2016 | Center for Cooperative Research in Biosciences (CIC bioGUNE) | bioGUNE | 6,9 | 24 |
| **MM** | 2014 | Molecular Biology Institute of Barcelona (IBMB), CSIC<br>(data from the whole center, but ONLY "Structural Biology Unit" is accredited as Maria de Maeztu) | IBMB-CSIC | 6,9 | 13 |
| **MM** | 2014 | Institute of Cosmos Sciences of the University of Barcelona (ICCUB) | ICC-UB | 6,5 | 97 |
| **MM** | 2017 | Center for Cooperative Research in Biomaterials (CIC biomaGUNE) | biomaGUNE | 5,8 | 31 |
| Internat. | | Instituto de Tecnologia Química e Biológica (ITQB NOVA), UNL (Portugal) | ITQB NOVA | 4,6 | 15 |
| Internat. | | Indian Institute of Chemical Biology (IICB), CSIR (India) | CSIR-IICB | 4,3 | 8 |
| **MM** | 2014 | Department of Experimental and Health Sciences (DCEXS), UPF | DCEXS | 4,3 | 18 |
| **MM** | 2017 | Centro de Astrobiología (CAB) | CAB | 4,3 | 30 |
| Internat. | | Skaggs Institute for Chemical Biology, TSRI (USA) | TRSI-Skaggs | 4,2 | 41 |
| **MM** | 2017 | Institute of Theoretical and Computational Chemistry (U. of Barcelona) (IQTC-UB) | IQTC-UB | 3,7 | 18 |
| SO | 2016 | Institute for High Energy Physics (IFAE), BIST | IFAE | 3,6 | 74 |
| **MM** | 2016 | Gene Regulation and Morphogenesis GEM-DCM2 (CABD)<br>(data from the whole CABD, but only GEM-DCM2 is accredited as María de Maeztu) | CABD | 3,5 | 13 |
| **MM** | 2016 | USC Galician Institute of High Energy Physics (IGFAE) | IGFAE | 3,2 | 29 |
| **MM** | 2014 | Condensed Matter Physics Center (IFIMAC), UAM | IFIMAC | 3,1 | 35 |
| **MM** | 2017 | Institute for Cross-Disciplinary Physics and Complex Systems (IFISC) | IFISC | 2,6 | 7 |
| **MM** | 2015 | Department of Information and Communication Technologies Engineering (ETIC) UPF, (DT | DTIC-UPF | 2,6 | 9 |
| **MM** | 2017 | Instituto de Física de Cantabria (IFCA) | IFCA | 2,5 | 79 |
| SO | 2016 | Centre for Plant Biotechnology and Genomics (CBGP) | CBGP | 2,2 | 8 |
| SO | 2013 | Institute of Nanoscience and Nanotechnology (IN2UB), UB | IN2 UB | 2,1 | 15 |
| Internat. | | Konstanz Research School Chemical Biology (KoRS-CB), University of Konstanz | KorS-CB | 1,8 | 6 |
| **MM** | 2017 | Institut de Neurociéncies de la Universidad de Barcelona (UBNEURO) | UBNEURO | 0,7 | 7 |
| **MM** | 2015 | Institut de Ciència i Tecnologia Ambientals (ICTA), UAB | ICTA | 0,3 | 5 |
| **MM** | 2014 | Barcelona Graduate School of Mathematics (BGSMath) | BGSMath | 0,1 | 1 |
| **MM** | 2017 | Basque Centre for Climate Change (BC3) | BC3 | 0,1 | 2 |
| **MM** | 2014 | Universidad Carlos III de Madrid - Departamento de Economía (ECO-UC3M) | - | - | - |
| **MM** | 2016 | Department of Signal Theory and Communications (TSC), UPC | TSC-UPC | - | - |
| **MM** | 2015 | Particle Physics Unit at CIEMAT, (CIEMAT-FP) | | - | - |

# 3.4 TRAINING

## 3.4.1 Master

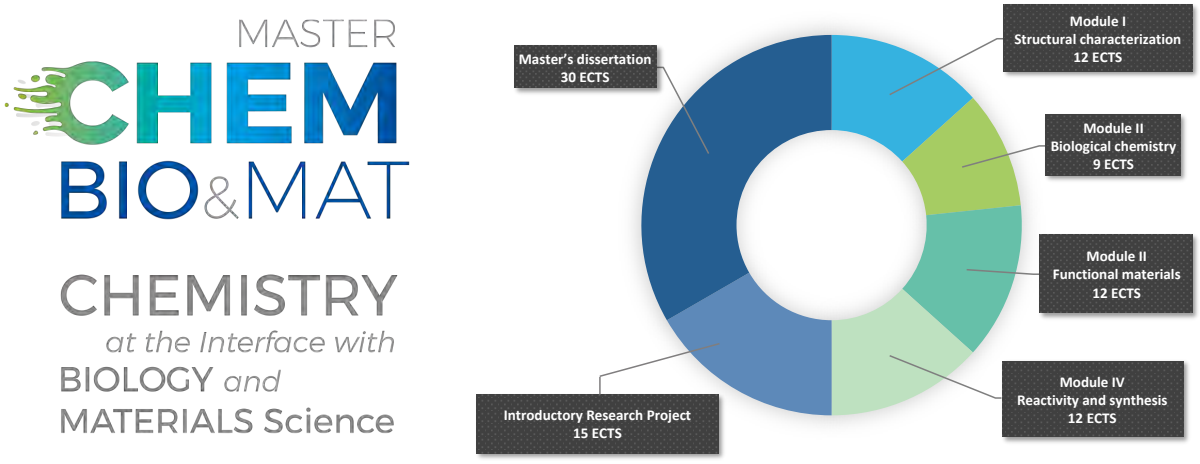
Most of the CiQUS Research Staff are involved in the Master in Chemical Research and Industrial Chemistry (with the University of Vigo and the University of A Coruña) and the Master in Organic Chemistry (with the UCM and the UAM). Also relevant is their participation in the Master of Theoretical Chemistry and Computational Modelling (Erasmus Mundus) and the Research and Development of Medicines. Every year the CiQUS offers between 25 and 30 vacancies for the Master Project. Approximately 60-65% of the Master students in Chemistry are trained at the CiQUS.

Outstandingly, the Master in Organic Chemistry was ranked for the second time as the second-best Master in Spain, within the category of "Experimental and Technological Sciences", and the best master in chemistry, according to the ranking annually published by "El Mundo" newspaper.

The Master in Drug Research and Development was also ranked as the 3rd best option within the category of "*Pharmacy*".

It is also worth mentioning that during the year 2018, a new master's degree program "*Master in Chemistry at the Interface with Biology and Materials Science*" has been designed and written by an academic board of CiQUS Research Staff from all scientific areas of the center. The proposed Master's program has the approval of the USC, the SXU and the ACSUG, and is currently under the evaluation of the Council of the Universities, the last step before being launched by CiQUS, the Faculty of Chemistry and the USC for the academic course 2019/2020.

The new master's degree, which will be coordinated by CiQUS Research Staff Prof. Juan Granja, is a 1.5-year program (90 ECTS) aiming to provide first-class multidisciplinary training at the frontier of chemistry, biomedicine and materials sciences, from a molecular approach, so as to give students the necessary practical skills and knowledge to undertake a professional or a research career.




***Official master's logo and ECTS distribution by thematic modules of the study program***

## 3.4.2 Doctoral programs

One of the major strengths of the CiQUS is the successful activity in the training of researchers, both at doctoral and post-doctoral level.

Most students (85%) are enrolled in the PhD program in Science and Chemical Technology (Mention of Excellence). Other doctoral programs are Research and Development of Drugs, Materials Science or Biology. Regarding the gender distribution, currently 41% of doctoral students are women.

Moreover, it is noteworthy that more than 7% of doctoral students come from abroad, especially from EU countries (Italy), South America (Chile) and Asia (Jordan).

13 Theses were defended by CiQUS students in 2018, all of them granted with top marks *cum laude*. A complete list of theses presented yearly can be found in Annex V.

The excellent training received by our PhD students is remarkable, not only due to the scientific level of most of the research groups of the center, but also the stimulating and competitive environment of the CiQUS, the biweekly interdisciplinary seminars program or the training in transferable skills. Additionally, our MSc and PhD students, together with the rest of the CiQUS members, have the opportunity to attend to the CiQUS Lectures Program, with top level international speakers from many different scientific disciplines (see Annex IX for the complete list of speakers in 2018).

The success of the training activity is evident judging by the awards and recognitions received by our PhD students (see section 4.3.3) and their success in accessing the best international centers: www.usc.es/ciqus/en/research/docs.

## 3.4.3 Postdoctoral programs

During 2018, over 40 researchers developed their postdoctoral training at the CiQUS, 18% of them from foreign countries (UK, Italy, The Netherlands, South Korea, Portugal, Brazil, Venezuela, Cuba, Chile). Regarding the gender distribution, 23% of the postdoctoral researchers at CiQUS during 2018 were female.

The success in attracting postdoctoral researchers through national and regional competitive calls is also considerable. In particular, in 2018 the Juan de la Cierva Program made it possible to recruit a total of 4 investigators in the 2017 Call (2 of them as Juan de la Cierva Formación – Cristian Vidal and Ignacio Insua and another 2 as Juan de la Cierva Incorporación – Fátima García and Marc Font, all of them starting in 2019), while the postdoctoral grants of Xunta de Galicia resulted in the recruitment of María Maneiro and Noelia Casanova as postdoctoral researchers (Mod. A-outgoing phase, currently at Imperial College-London and the University of Cambridge, respectively), Lara Villarino and Gustavo Rama (Mod. B).

Even more remarkable was the success in the program Ramón y Cajal (RyC) that made it possible to recruit Dr Beatriz Pelaz.

Additionally, the CiQUS launched the 3$^{rd}$ edition of the International Postdoctoral Program – Campus Vida (Fall Call). As a result of this competitive call, 2 brilliant young researchers joined the CiQUS as postdoctoral associates. This program is partially funded by the Consellería de Cultura, Educación e Ordenación Universitaria of the Galician Government (Centros Singulares de Investigación de Galicia e Agrupacións estratéxicas consolidadas, 2016-2019) and the European Regional Development Fund (ERDF).

## 3.4.4 Funding for training (grants and contracts)

As previously mentioned, every year the CiQUS offers part-time contracts to support the best MSc students, prioritizing those who work in collaborations or strategic lines.

Regarding the doctoral stage, 43 PhD students were developing their theses supported by competitive national grants and contracts during 2018 (15 FPI, 8 FPU, 17 Predoc by Xunta de Galicia and 3 by private foundations). Most of the remaining doctoral students have contracts attached to research projects.

In relation to postdoctoral researchers, in addition to those hired through national competitive programs (see 4.4.3) and international exchange programs, all of them have contracts attached to research projects.

It is worth mentioning the recent success in applying for the Individual Fellowships of the Marie Curie Program (H2020-MSCA-IF). Currently, 3 postdoctoral researchers hold a MSCA fellowship at CiQUS: Dr Eric Langenberg (outgoing phase – GF (USA), F. Rivadulla Group), Dr Alejandro Méndez (EF-ST, J. Montenegro Group) and Dr Carolina Carrillo-Carrión (EF-ST, P. del Pino Group).

### 3.4.5 Other training and courses

Throughout the year, the CiQUS organizes several technical courses to implement scientific skills on the use of different equipment. During 2018, the CiQUS hosted specialized training for the use of spectrometers of fluorescence and DLS equipment. In addition, CiQUS members had the opportunity to attend different courses organized by other research centers at the USC (e.g. statistical methods, scientific writing and scientific presentations, patents and IP, etc).

It is worth mentioning that the CiQUS, in collaboration with the USC library, hosted an Open Access seminar to raise awareness of how important it is for our researchers to archive their scientific publication in online repositories to meet the commitments of the National and European R&D funded projects. Nowadays, over 60% of CiQUS publications are archived in Minerva, the USC online repository.

## 3.5 INTERNATIONALIZATION

- 2018: 49% of papers include some international collaboration (50% D1, 85% Q1) (WoS database)
- 67% of the international collaborations have at least one CiQUS corresponding author
- 1 ERC-StG

CiQUS researchers have proved their commitment with internationalization, both in funding and publications. This section describes the most relevant facts and efforts.

- **41 papers (41%) resulting from international collaborations** (35% in 2011-2014), **80% of them in the first quartile (Q1)** and **37% in the first decile (D1)**. Up to 61% of these works have at least one corresponding author from the CiQUS. Among the collaborators there are a number of research groups from prestigious research centers, such as the Philipps Univeristat Marburg (DE), the University of Cambridge (EN), or IBM Research (CH).

- With regard to **international projects**, in 2018 CiQUS Research Staff, Dr. M. Giménez López, launched the ERC-StG project NANOCOMP at our center. The European Collaborative Project "ENDOSCAPE", of which Prof E. Fernández-Megía is a member, was selected for funding and Dr. J. Montenegro was awarded with an ERC-PoC at the end of 2018.

- **European Technology Platforms (ETP).** Since 2012 CiQUS is a member of SusChem Spain, which is part of the **ETP for Sustainable Chemistry (SusChem)**, and a CiQUS representative has attended almost all their European brokerage events and stakeholder meetings. This participation has not only included the offer of our research results and technology platforms but also the public presentation of project ideas for H2020.

- Since 2015 the CiQUS also belongs to the **ETP Nanomedicine** and the **European Cluster on Catalysis**.

- **COST Actions.** Prof. E. Fernández-Megía was selected as member of the management committee of COST Action CA17410 "Cancer Nanomedicine – from the Bench to the Bedside".

- **CiQUS Lectures Program.** During the year 2018 up to 32 top level international scientists including Prof Mathias Beller (Leibniz-Institut für Katalyse and the University of Rostock, Germany), Prof Eijimi Yashima (Nagoya University, Japan) and Prof Janine Cossy (ESPCI-CNRS, France) among others, where invited to give a talk on their own research fields at the CiQUS.

- Finally, 17% CiQUS personnel came from foreign countries during 2018 (Italy, UK, The Netherlands, France, Greece, Chile, Jordan, South Korea, Indonesia, Cuba, Venezuela, Colombia).

# 3.6 TECHNOLOGY TRANSFER AND VALORIZATION

## 3.6.1 Research and innovation projects with other agents

Dating back to 2008, we have been holding a strategic partnership with **INDITEX**, the biggest fashion group in the world. It is coordinated by **Prof. Javier Sardina**, Research Staff at the CiQUS and a member of the INDITEX's Social Council since December 2013. Additionally, other research groups, not only from the CiQUS but also from the USC, are joining this partnership under his coordination.

The CiQUS leads R&D about chemical safety standards (Clear to Wear and Safe to Wear) in the production of safe products, including the auxiliary chemical industry and its suppliers. It is expected that the new knowledge and tools could lead to synergies with the health area within the CiQUS. This partnership received **715.000 € (2015), 860.000 € (2016), 940.000 € (2017) and 600.000 € (2018)**.

Designed and supported by the CiQUS, INDITEX has also launched a cooperation project (EUREKA Project), with EKOTEKS (Turkey): "Scientific Advice for the Development of R&D Programs in the Field of Textile Manufacturing and Cosmetics". We are further exploring new collaborations and investment from this relationship.

## 3.6.2 R&D projects with other companies and entities

The following paragraphs summarize the relevant information about the new contracts during 2018. The complete list is available in Annex III.

• **INDITEX** (multinational, A Coruña). Since 2013 the overall value of the contracts exceeds 2.5 million €. A new contract of 600.000 was signed in 2018.

• **zLabels GmbH.** A company focused on the creation of contemporary fashion brands which sells online via Zalando and other global retail platforms. In 2018, four Contracts were signed with the CiQUS (around 14.000 €).

• **Oncostellae S.L.** (Spin-off, Ourense). Two new contracts of 25.000 € and 60.000 € were signed in 2018. This cooperation aims to develop new complementary therapies for the treatment of oncological diseases. In fact, two molecules developed in this project are already finishing its characterization prior to its possible entry in the preclinical phase.

• **Landsteiner Genmed S.L.** (Spin-off, Sevilla). Prof. E. Sotelo has signed a contract of 65.000 € with this company to develop new organic molecules libraries.

• **AMSLab, S.L.** (Spin-off, Lugo). A leader company in the quality control sector with a high level of specialization in matrices or highly complex components for developing and improving determination and quantification analytic techniques. Prof. J. Sardina, CiQUS Research Staff, has signed two new contracts with this company in 2018 (18.000 € and 50.000 €, respectively). Prof. Sardina will give scientific, technical and commercial advice regarding new analytical techniques in the field quality control for product health.

• **MestreLab Research:** Prof J. Sardina has signed a contract of 45.000 € with this company to provide support for the development of chemical software.

Other small contracts were also signed during 2018 with Ekoteks Laboratuvar Goztim Hizmetleri Limited and Artegal Restauraciones.

In summary, during 2018 CiQUS researchers have signed 13 new contracts with up to 8 different companies/institutions adding up to 0.89 M €. Despite the fact that this is not a large figure, these projects are important because they demonstrate our commitment and support to the most

innovative local industry, providing highly specialized advice to technology-based companies (see 4.6. Advisory & Technology services).

### 3.6.3 Patents, Licensing and Valorization

During 2018 CiQUS researchers applied for 5 new patents: *Iron oxide nanotubes* (PI Juan Granja, in collaboration with an Italian research group), *Cell penetrating peptides* (PI. Javier Montenegro), *G6 fosfatasa* (PI. Jose Martínez-Costas), *Stable polymer composites* (PI Massimo Lazzari in collaboration with Prof Arturo López Quintela) and *A nanoporous graphene structure and method for preparation thereof* [PI. Diego Peña in collaboration with César Moreno and Aitor Mugarza (ICN2, Spain)]. Furthermore, the patent "Applications of the Protein Muns and the Derivates" from Martínez-Costas group has been approved in USA – US10059745 (see Annex VIII for the details of these patents).

Additionally, a number of MTA and NDA agreements were signed with different partners, as the leading company SYNGENTA AG or other institutions as INIA (National Institute for Agronomic Research, Spain).

- **SIGILLUM KNOWLEDGE SOLUTIONS** (http://sigillumks.com). A start-up company created by Prof. J. Sardina. This represents the third company founded by CiQUS Research Staff. It was created with the aim of responding to the growing need of fashion companies to comply with the diverse and dynamic international regulations as well as evaluating in a cost and time-efficient manner the health, safety, quality and sustainability of their products.

- **MATPRINT**. New 3D Printing Materials (2017, 0.25 M €), granted to a collaborative initiative of CiQUS Research Staff E. Sotelo with the Institute of Ceramics (USC), which focuses on bioceramics and 3D printing in catalysis. Before setting up a new spin-off, the industrial validation of the IP has been addressed during 2018 supported by the IGNICIA program.

- **FLUOROTOOLS**. This project (0.38 M € of initial funding), co-led by CiQUS Research Staff Prof Eddy Sotelo with Prof Mabel Loza (CiMUS PI) and Prof Javier Sardina, has been approved by the Regional program for technology valorization - IGNICIA (only 6 projects were approved), after a competitive evaluation by experts from the Oxford University Innovation.

- **RuCSC**. An IGNICIA project (0.25 M € of initial funding) led by Prof José Luis Mascareñas for the development of new antitumor products bases on targeting stem cells.

- **IC-tagging Technology Platform** (Group Benavente - Martínez Costas). This platform allows for: the tagging of proteins, their directed relocation into dense cytoplasmic inclusions (either in the nucleus or in the cytoplasm), detection of protein-protein interactions (either in the nucleus or in the cytoplasm of living cells), production of in vivo micro/nanoparticles containing different proteins for their use as polyantigenic vaccines, therapeutic proteins and immobilized enzymes for industrial use. The two related patents have been already licensed (non-exclusive) to the company VIRBAC. Additionally, a first agreement was signed to develop the corresponding proof of concept.

- **ComBioMed - Chemical Library** (Group E. Sotelo). A proprietary multicomponent-based drug discovery platform (identification and optimization of drug candidates). Compounds generated by this platform in the context of diverse synthetic and medicinal chemistry programs were grouped in the ComBioMed Exploratory Library, a large, diverse and exclusive collection containing more than 4000 drug-like small-molecules. Remarkably, an A2B antagonist drug (ISAM-140) developed in this group has been recognized in 2017 as one of the most potent and selective drugs from this family. Leading commercial suppliers in chemistry (Sigma-Aldrich, Tocris Bioscience) already market this compound.

- **ERC-PoC ANTS**. Several networking actions and meetings took place both at a national and an international level, aiming to set up a new collaborative project during 2018.

Since 2012 the CiQUS has been a member of SusChem Spain, part of the European Technology Platform for Sustainable Chemistry, ETP SusChem. The CIQUS has also been actively participating in many national and European networking and stakeholder events, including the presentation of project ideas and institutional posters. Furthermore, CiQUS researchers regularly collaborate in the revision of technology priorities covered under the new SusChem Strategic Innovation and Research Agenda (SIRA).

Thus, during 2018 CiQUS attended a number of international events: the Brokerage event for Nano and Advanced Materials (Cambridge), the Nano-Carbon Enhanced Materials Consortium (NCEM) Meeting (Cambridge), the UltraWire Workshop (Cambridge), the SusChem Brokerage Event (Brussels), the INDustrial TECHnologies 2018 (Viena), the H2020 Brokerage Event on Nanotechnology and the Advanced Materials & Manufacturing (Birmingham).

Finally, it is worth mentioning that the CiQUS website provides detailed and accessible information about all the activities of the center, including its scientific production and the patents generated, as well as a specific section with the technology transfer offers (www.usc.es/ciqus/en/technology-transfer).

## 3.7 OUTREACH

### 3.7.1 CiQUS website and presence in the media

The CiQUS website (www.usc.es/ciqus/es) is a fully trilingual web page with updated information about research areas, scientific production, research groups, facilities, job offers, training programs and comprehensive information about the center's activities and research outputs. It is currently complemented by social networks: Facebook (2011), LinkedIn (2012), YouTube (2013), Twitter (2014) and Google+ (2014).

The **CiQUS website** had 136.113 visits during 2018 (44% were new visitors), with 23% of international traffic over the total visits: 2.3% UK; 2.3 % India; 2,1% USA; 1.9% Germany.

**YouTube**. Since December 2013, the CiQUS started to broadcast a serie of dissemination videos made by our Press Manager. Currently, the CiQUS YouTube channel has reached over 18,800 visualizations and a total of 300 hours, 48% from outside Spain, e.g. 8% from the USA and 4% from the UK. We must highlight the outstanding impact achieved by two videos (2015, 2016) by IBM Research (Zurich) with the participation of CiQUS researchers. The second one has over 566,000 views (12,000 during the first 3 weeks) in the **IBM YouTube Channel** (www.youtube.com/watch?v=OOkbt16M3Mg), being among its 40 most watched videos. Obviously, this visibility is an invaluable asset for the CiQUS.

**Facebook**. 1515 followers. Currently, around 26% of the posts had over 3,000 impressions according to Facebook statistics, and a 10% reach with more than 5,000 impressions. Considering that the CiQUS is only 7 years old, our average impact is comparable to the best excellent Spanish research centers, according the comparative analytics provided by Facebook.

**LinkedIn**. The CiQUS followers in LinkedIn has had a moderate but steady growth since this profile was created in 2013. It currently has 731 followers. However, the most interesting impact is being achieved through posts in the specialized groups, which are used to target specific professional groups, both from the academia and the private sector.

**Twitter**. 1180 followers, which means a 60-70% increase in the number of followers every year: 150 (2014), 388 (2015), 662 (2016) and 818 (2017). Nowadays, it has 1,500 visits and over 20,000 impressions per month.

Since 2013, the incorporation of a **Press manager** (shared with the CiMUS and the CiTIUS) boosted the impact of the CiQUS dissemination, including frequent press releases, which are commonly posted on several international scientific dissemination websites (Nanowerk, Nanotech-Now, TG Techno…) and LinkedIn, as well as the most important national scientific divulgation channels and other dissemination websites, as Agencia SINC, Madrimasd or Noticias de la Ciencia-NCYT and SusChem Spain Newsletter. Thus, the CiQUS has significantly increased its presence and impact in the media.

It is worth mentioning the presence of CiQUS Research Staff in several National Newspapers (La Vanguardia, El Periódico,…) and Regional media such as the general newspapers La Voz de Galicia and El Correo Gallego and specialists webpages as GCiencia-O Portal da Ciencia Galega or Agencia SINC, Fundación Madri+d and SusChem España Newsletter which regularly cover press releases about CiQUS members and CiQUS activity.

An outstanding impact was achieved in January 2019, C&EN News awarded the title of "Molecule of the year 2018) to the porous nanographene ("Bottom-up Synthesis of Multifunctional Nanoporous Graphene", Science 2018) jointly synthetized by CiQUS Research Staff D. Peña and colleagues from the Catalan Institute of Nanoscience and Nanotechnology (ICN2) and the Donostia's International Physics Center (DIPC). Furthermore, PHYS.ORG, Nanowerk, EFE Futuro also highlighted this Science article.

Additionally, CiQUS scientific Director, José Luis Mascareñas, and CiQUS Deputy Director, Dolores Pérez are regularly interviewed on the occasion of special events or announcements (Cadena Ser Radio, Radio Galega and regional newspapers).

### 3.7.2 Outreach and promotion of scientific vocations aimed at students and the general public

The Management and CiQUS members are strongly committed to education and popularization of science. In every academic course there is a considerable collective effort to organize the CiQUS Open Days Program "***Research in Chemistry: creative science for a better world***", aimed at high-school students. These actions have the objective of explaining the importance of chemistry in the economic development and welfare of society.

Attendee students had the opportunity to visit the center, participate in scientific demonstrations, and perform simple experiments such as the preparation of well-known drugs (aspirin, paracetamol), and through these experiments they also learn the most common structural characterization techniques. In 2018, the CiQUS organized the 6$^{th}$ Edition of this program with the participation of over 500 high school students from 16 different centers all around Galicia.

Apart from this program, during the whole year, the CiQUS regularly organizes the visit of groups of students from different school and high school classes at the center. Particularly, in May 2018, the CiQUS hosted for the second time a reception to the winners of the Galician Chemistry Olympiad 2018.

In November 2018, the CiQUS with the other Singular Research Centers of the USC (CiMUS and CiTIUS), and co-funded by the Consellería de Cultura, Educación e Ordenación Universitaria through a signed agreement with the USC, the CiQUS organized the second edition of the **"Ciencia Singular" - Open Doors Day**, addressed to the general public (adults, families, teenagers, …). Over 250 people (36% kids) visited the center on November 10$^{th}$, attended the lectures and participated in the chemical games and experiments.

The CiQUS also participated in external dissemination workshops, such as the *Feira da Innovación Abanca-USC*, the Galicia Maker Faire, the "Recuncho Científico"- San Pedro's neighborhood, the local program *Una científica en cada cole* (*A woman scientist in every school)* and the Program *"A Ponte entre o Ensino Medio e a USC* (a program from the USC to help high school students to choose their future university studies). It is worth mentioning that the "Sociedade Xuvenil Galega de Química (SXGQ)", a student' association mainly formed by CiQUS PhD candidates was awarded with the first prize in Outreach at the last Maker Faire Galicia (November 2019).

Furthermore, CiQUS researchers regularly visit regional public and private schools to give lectures, they also participate in other outreach activities organized by public libraries and civil organizations.

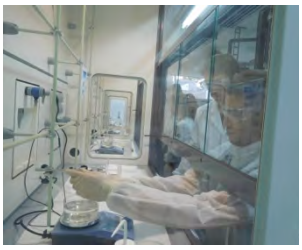
Finally, CiQUS Research Staff Prof Flor Rodríguez Prieto collaborated in a special section published in El País, one the major national newspapers, answering scientific questions previously sent by the general public. The main goals of this initiative are the outreach of science among the general public and the promotion and visibility of scientific women.

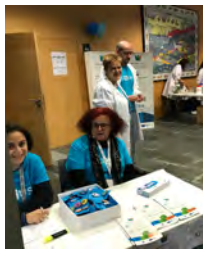
https://elpais.com/elpais/2018/07/11/ciencia/1531310604_993034.html

This program was organized by El País and the AMIT (an association of female researchers and technologists).

Our efforts significantly contribute to increase the demand of Chemistry studies at the USC and, last but not least, to turn the public view about chemistry and chemicals into a more positive opinion.





***Some CiQUS pictures from outreach activities:*** *"Ciencia Singular Open Doors 2018", "Research in Chemistry: creative science for a better world", visits of students at the CiQUS, visit at schools, etc.*