



CiQUS – Annual Scientific Report 2017

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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1. LETTER FROM THE DIRECTOR

CiQUS started with the aim of implementing a new, singular research model within the University. Thanks to the excellent managing work of the former commissioner director and now assistant director Prof. Dolores Perez Meirás, and the dedication of CiQUS group leaders and students, in only six years CiQUS has become a well-recognized, top level research center.

I had the chance of taking over the scientific direction early in 2014, and after these years I can only thank all members, from the managing and technical staff to the PIs and students for their dedication and effort, and their close identification with the spirit of the center.

The steady progression of the center from the beginning in terms of scientific production, fund raising, tech transfer and training success is certainly impressive.

In 2017 the tendency has followed a similar path. In addition to recruiting a new group leader holding a ERC Starting Grant, Maria Giménez, we also ensured the incorporation of a Ramon y Cajal researcher, Rebeca Garcia Fandiño, that will reinforce our research in Computational Chemistry. With Maria Giménez, our research competitiveness in the field of molecular and functional materials will be significantly strengthened. We expect the best from her.

As part of our philosophy of hiring the best students, we have kept our highly successful recruiting undergraduate, master, predoctoral and postdoctoral programs.

In terms of funding, our Starting Grantee Javier Montenegro has gained a highly competitive HFSP-Young Investigator Grant, in which the CiQUS' PI leads an international team with researchers from USA and Japan. We have also ensured 9 projects from MINECO, a number of grants from the Regional Government and significant contracts with private companies.

I am very proud of our PIs and students being externally recognized with prestigious awards. This is the case of Jessica Rodriguez, former PhD student in the center whose thesis has been classified among the ten finalists of the REAXYS international award (out of 500 worldwide).

Key to the success of the center is maintaining an internal highly competitive but also very friendly atmosphere. This is ensured, among other aspects, by combining weekly lectures by highly prestigious scientists with biweekly internal seminar programs that foster collaborations and reinforce the training of our students.

As a consequence of our progress, our scientific productivity continues to grow, achieving an impressive average impact factor average of 7.21 in 2017. We have also progressed in our tech transfer and outreach activities.

Overall, being rigorous with the implementation of a singular model based on a self-demanding, multidisciplinary scientific strategy and a rigorous external assessment of our outputs, we have not only contributed to the advancement of science and the economic progress of the contour, but also to considerably increase the international prestige of our University and Spanish science.

I have not doubt that with the firm commitment of all members of the center, CiQUS will continue to grow and will become a main world reference in multidisciplinary science at the boundary between chemistry, biology and materials,

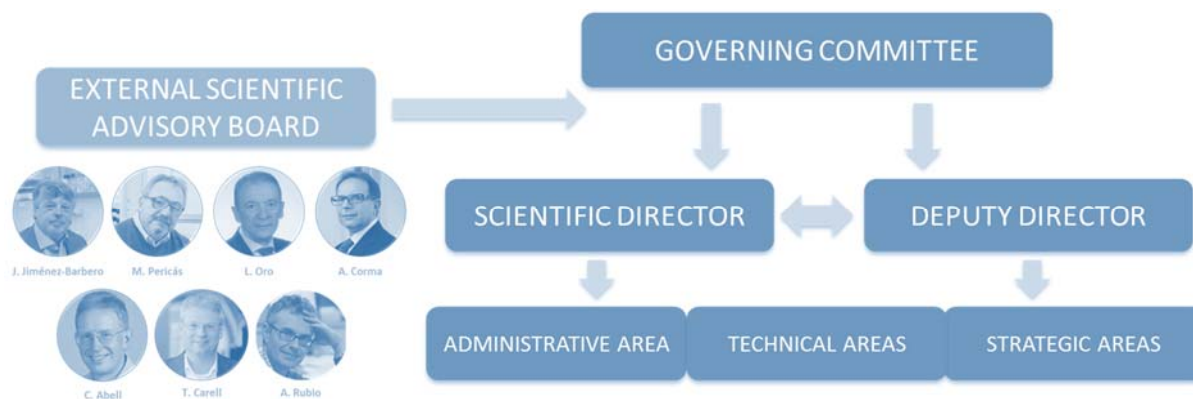


José Luis Mascareñas

2. SCIENTIFIC ORGANIZATION

2.1. 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 CiQUS

GOVERNING COMMITTEE (December 31, 2017)

- President:** Juan Viaño Rey, Rector, USC
- Vice-president:** Isabel Rodríguez-Moldes Rey, Vice-rector of Research and Innovation, USC
- Members:** José María Arias Mosquera, President of the Social Council of the USC
 José Ramón Urquijo Goitia, CSIC representative
 José Manuel Villanueva Prieto, USC Manager
 José Luis Mascareñas Cid, Scientific Director of CiQUS
 M. Dolores Pérez Meirás, Deputy Director of CiQUS
- Secretary:** Rogelio Conde-Pumpido Tourón. Director of R&D Management and Valorization

MANAGEMENT TEAM (December 31, 2017)

- Scientific Director:** José Luis Mascareñas Cid
- Deputy Director:** M. Dolores Pérez Meirás

EXTERNAL SCIENTIFIC ADVISORY BOARD (ESAB) (December 31, 2017)

- Jesús Jiménez Barbero**, CIC bioGUNE
- Miquel Pericás Brondo**, Institut Català d'Investigació Química (ICIQ)
- Luis Oro Giral**, Instituto Universitario de Catálisis Homogénea (Univ. Zaragoza)
- Avelino Corma Canos**, Instituto de Tecnología Química (ITQ; CSIC-UPV)
- Thomas Carrell**, Ludwig-Maximilians-Universität München (DE)
- Christopher Abell**, University of Cambridge (UK)
- Ángel Rubio** (appointed in 2016), Max Planck Institute for the Structure and Dynamics of Matter (DE)

2.1.1 Management Team

- **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 19 patent applications. 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 years. It is important to remark that five PhD students of the group have gained Ramon y Cajal positions. In 2014 he received and **ERC Advanced Grant** for his project METBIOCAT (<http://metbiocat.eu/>).

His current research splits between 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 the Organic Chemistry Award (2009) and **Gold Medal** (2015). In 2016, he has been appointed as 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*, Associate 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 at 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 MIT (1996). She joined the faculty of the USC as Assistant Professor in 1995, became an Associate Professor of Organic Chemistry in 2000 and was habilitated as Full Professor in 2012.

She has published over 60 articles in high impact journals, 3 book chapters and supervised 10 PhD thesis. Her current research interests are focused 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 has been Director of the Organic Chemistry Department (2004-2006), and associate to the Vice-rector of Research and 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.

2.1.2 Management Structure

CiQUS Management Structure is organized in several different units which give support to the scientific and non-scientific center's activity:

- **Internal Advisory Committee**, which is representative of 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*.
- **R&D Management and Knowledge Transfer Office**, responsible for the scientific coordination of CiQUS project, R&D management, talent attraction programmes (*Dr Almudena García*) and the promotion of international R&D initiatives, identification of technology transfer opportunities,

working in full coordination with the staff of the USC Technology Transfer Office (*Fernando Casal*).

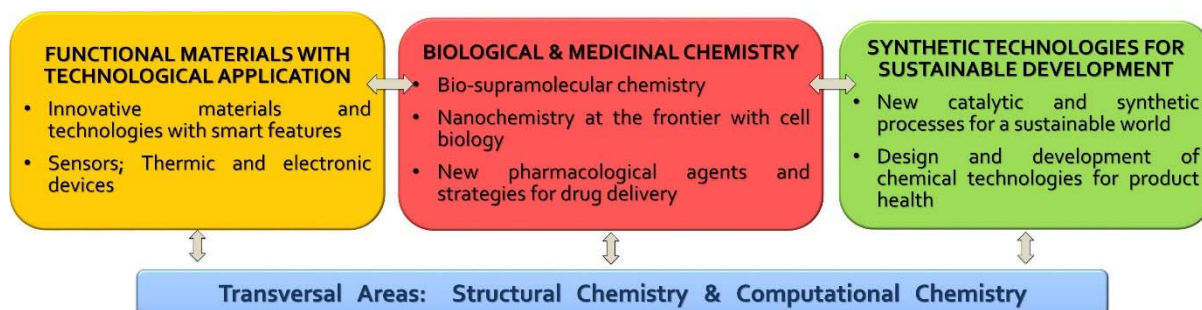
- **Press Office**, created to develop a joint communication strategy with the two other singular research centers (*Andrés Ruiz*, Press Manager).
- **Technical Area**: under the responsibility *Noela Torrente* (chemical storeroom, health and safety office) and *Laura Alicia Acevedo* (scientific facilities and research support area). They are in charge of implementing a centralized operational model, aiming at the optimization of the available resources and the improvement of the working conditions in the center. They are supported by *Dr Arcadio Guerra* (research support management), *Rebeca Menaya* (cell culture) and *Pablo Cajaraville* (chemical storeroom).
- **Administrative Area** (*Elena Veiga*, *Lucía Rodríguez*), among other duties it is responsible for the financial management of R&D activities, secretarial issues and administrative support.

2.2 Scientific Program

During the year 2017 CiQUS research activity was reorganized in order to optimize efforts and favour future collaborations and synergies between the different research groups and disciplines within the centre. CiQUS scientific activity is now focused in three major areas:

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

According to the new scientific organization, Structural Chemistry and Theoretical & Computational Chemistry are redefined as transversal areas that should provide support to research in the other three priority thematic areas.



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 problem such as cancer, neurogenerative diseases and bacterial resistance. Our current organization include subtopics associated to different PIs:

- **BIO-SUPRAMOLECULAR CHEMISTRY**: a) Novel supramolecular devices based on peptides and biological applications (J. Granja). b) Metallopeptides for nucleic acid interactions (E. Vázquez). c) Protein, polymer and peptidoglycane folding (F. Freire, E. Quiñoá; R.J. Estévez, J.C. Estévez); c) Peptide helicates and oligomeric auto-assembled receptors (E. Vázquez, M. Vázquez); d) Computational

modeling of noncovalent interactions involving molecular nanostructures (J. Rodríguez Otero); e) Assembly of supramolecular systems and its influence in chemical reactivity (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 (J.L. Mascareñas, ERC-AdG-MetBioCat). c) Molecular fluorescent probes to be used in cell biology (E. Vázquez, M. Vázquez, M. Mosquera). d) Artificial cells: design and synthesis of a fully synthetic self-regulated cytoskeleton (J. Montenegro, HFSP-RGY0066/2017).

- **PHARMACOLOGICAL AGENTS AND NEW STRATEGIES FOR DRUG TRANSPORT AND DELIVERY:** a) Smart for cellular transport of proteins, nucleic acids and cytotoxic molecules and controlled drug delivery. (J. Montenegro, ERC-StG-DYNAP). b) Novel antibiotics for resistant bacteria (C. González-Bello). c) Combinatorial technologies for drug discovery (E. Sotelo). d) Antibiotics as mitochondria-targeted antitumoral agents (E. Vázquez, Spanish Association Against Cancer-AECC). e) Activation strategies of antitumoral prodrugs based on nanoparticles (P. del Pino). f) Biotechnological tools (José Martínez-Costas). d) Nanostructures and dendrimers for conjugation with ligands of biomedical interest with applications in drug delivery or diagnosis (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 (M. Lazzari). b) Nanomaterials with applications in the restoration of works of art. (M. Lazzari). c) Organic semiconductors: synthesis in solution and on surface, and biomedical applications (D. Pérez, D. Peña and E. Guitián). d) Nanostructures for the control of thermal conductivity based on optical methods (frequency domain thermoreflectance, FDTR) (F. Rivadulla). f) Nanoparticles, MOFs and hybrid nanostructured materials with applications in drug delivery, theranostic or as cell reprogramming agents (P. del Pino) g) Multifunctional metal-carbon hybrid nanostructures for spintronics and energy-related applications (M. Giménez).

- **SENSORS: THERMAL AND ELECTRONIC DEVICES:** a) Devices for ultraprecise thermal measurements (F. Rivadulla, ERC-PoC-ANTS). b) Functional polycyclic aromatic hydrocarbons (PAHs) and nanographenes: synthesis and applications (D. Peña, D. Pérez, E. Guitián). c) Stimuli-responsive dynamic polymers (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 (M. Fañanás). b) Catalytic functionalization of "inert" C-H bonds: new tools for synthetic chemistry (M. Gulías, J.L. Mascareñas). c) Efficient synthetic methods based on metal catalysis for the preparation of enantiopure anticancer agents (F. López, J.L. Mascareñas). C) New catalytic routes for the preparation of doped PAHs and bioactive heterocycles (C. Saá).

- **CHEMICAL TECHNOLOGIES FOR PRODUCT HEALTH:** This line is developed in collaboration with the company INDITEX, S. A. The aim of this collaboration lead on the application of chemistry technology to the developing of sustainable processes for the textile industry (J. Sardina): a) Minimize the use of toxic substances. b) Developing of novel technologies for textile recycling. Despite this type of research is somewhat lateral to the main scientific stream of the centre, it is very useful from a socioeconomical

perspective because it allows an immediate recognition by the social agents of the value of chemical research.

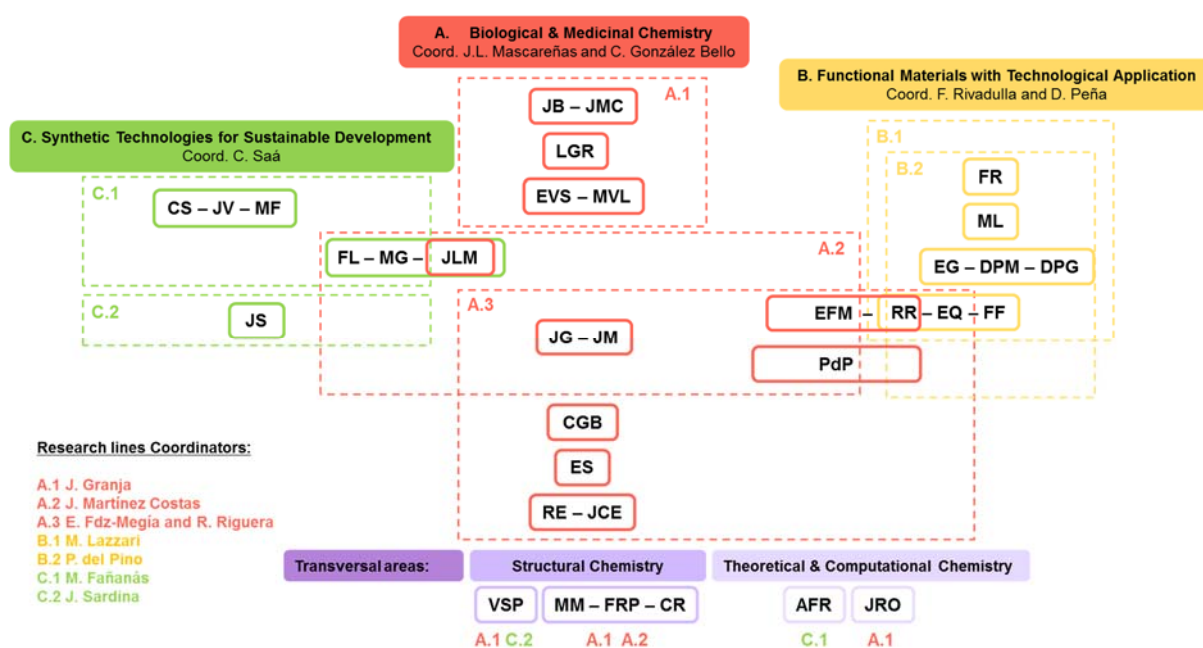
TRANSVERSAL AREAS: STRUCTURAL CHEMISTRY AND THEORETICAL & COMPUTATIONAL CHEMISTRY

This area involves the development of spectroscopic and computational techniques and methods for structural and mechanistic studies and provides support to the whole CiQUS community. a) Fluorescence spectroscopy of individual molecules and resolved in time (M. Mosquera, Flor Rodríguez). b) Theoretical methods and mechanistic studies (A. Fernández-Ramos and J. Varela).

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

Each thematic area involves groups with different expertise and scientific profile in order to favour synergies and collaborative projects. During the year 2017, CiQUS has implemented several actions, such as frequent multidisciplinary meetings, to further increase intramural collaborations of synthetic chemists, materials chemists, physicists and biologists, in order to approach challenging scientific problems and develop ground breaking contributions to the advance of knowledge.

CiQUS Organizational Chart for Scientific Activity



2.3 Recruiting Policy

The fact that CiQUS belongs to the University system largely determines our ability to attract and incorporate talent. This is especially difficult at the level of PIs able to develop new research lines at the center. Thus, today the CiQUS has no capacity to hire research staff itself, not only because of the lack of a specific budget that can be dedicated to a human resources program, but also due to the lack of the proper legal framework at the University.

Despite the aforementioned limitations, we try to use all available tools to recruit the best researchers. We are firmly convinced that our capability to strengthen our capacities and develop our research program is strictly associated to the quality of our group leaders and students. 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 and, following the assessment of the External Scientific Advisory Board, and the complementary profile required by our ongoing research lines. It is worth mentioning our success in recruiting excellent researchers through this highly competitive system in the past years (two of them without any previous relation with the CiQUS). Thus, after the selection of M. Fañanás (2012 call) and J. Montenegro (2013 call), in 2016 we could recruit P. del Pino (2015 call) - PhD in Physics Technische Universität München (2007) and 8 years of postdoctoral experience in Germany and Spain.

In September 2016, these three RyC researchers (M. Fañanás, J. Montenegro and P. Del Pino) together with F. Freire (RyC 2010) and M. Gulías (Parga Pondal Researcher 2011), were promoted as PIs at CiQUS, after a limited and demanding call supervised and evaluated by the External Scientific Advisory Board.

The result of the Ramón y Cajal 2016 call, will lead the incorporation of 2 new RyC researchers along the year 2018:

- *Dr María Giménez López* (also ERC-Starting grantee), 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 a ERC Starting Grant in the year 2015. Dr Giménez officially joined the CiQUS as Royal Society Fellow in January 2018.
- *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 University of Oxford. During the period 2010-2014, she held a Juan de la Cierva contract at CiQUS. Currently, she works as FCT Researcher at the Faculdade de Ciencias, Universidade do Porto (Portugal).

- **Doctoral and postdoctoral researchers:**

- *Marie Skłodowska-Curie Actions*: 2 postdoctoral researchers were recruited through the competitive MSCA individual fellowships program (2016 call), Dr Alejandro Méndez and Dr Carolina Carrillo-Carrión.
- The 2016 "*Juan de la Cierva Incorporación contracts call*" lead the recruitment of Dr. Ángel Luis Fuentes de Arriba as postdoctoral research associate (Supervisor: J. Granja), Dr. Ester Polo (Supervisor:

P. del Pino, starting date: June 2018) and Dr. Julián Bergueiro (Supervisor: J. Montenegro, starting date: Summer 2018).

- **International Postdoctoral Program – Campus Vida:** In coordination with CiMUS and CiTIUS, the 2nd and 3rd edition of this program were called during the year 2017. A total number of 4 postdoctoral positions were offered at CiQUS. In 2017, this program was partially funded by the Spanish Ministry of Education (singular actions at Campus of International Excellence) and by the European Regional Development Fund (ERDF) and the Galician Regional (Centro singular de investigación de Galicia accreditation 2016–2019, ED431G/09).
- **Research initiation contracts for CiQUS Master Students:** 20 part-time contracts were offered during the year 2017 (Spring call and Fall call) for the development of a Master Research Project under the supervision of a CiQUS PI. 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 without no previous relation with the University of Santiago.

• Undergraduate students:

- **3rd Ed. CiQUS Summer Fellowships program:** 15 scholarships were awarded to highly motivated undergraduate students with excellent academic records, having the opportunity to achieve a first research experience, working with CiQUS research groups in first class labs. CiQUS received around 100 applications from 43 different universities, where 30% of them were non-spanish universities. The average mark of the selected candidates was above 8.4 on a scale 0-10. The 4th edition is currently open.



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

3. TECHNOLOGY RESOURCES

3.1 Facilities

The CiQUS building has 5.900 m² 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 m² 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, dark room, cold rooms, four rooms for the chemical storage, a central purchasing center and a computer cluster. CIQUS researches also have access to the general research support services of the USC (www.usc.es/gl/investigacion/riaidt/), nearby, at the CACTUS building.

It is worth mentioning 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, femtosecond spectroscopy, lithography, electrophysiology, PLD, etc.



Representative research support laboratories

It is very important to emphasize 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.

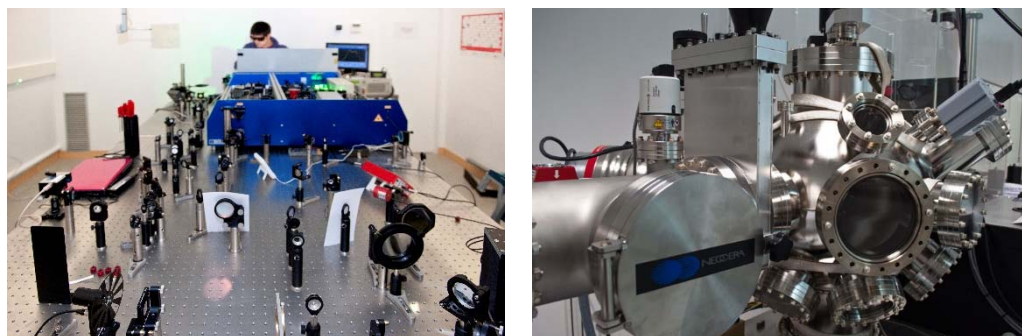
3.2 Singular Laboratories

- **Femtosecond Laboratory.** The laboratory is equipped with an ultrafast laser system Ti:Sa which comprises an oscillator (FEMTOSOURCE Scientific Pro) and a multipass amplifier (FEMTOPOWER Compact Pro), both of FEMTOLASERS. VJ Millennia lasers (Spectra-Physics) and 621-D are used as BMI pumping lasers. The system delivers pulses of 30×10^{-15} s (10^{-15} s = 1 femtosecond, fs) centered at 800 nm with an energy of 1 mJ/ pulse and a repetition rate of 720 Hz.

The fundamental beam is split into four beams destined for: 1) the second harmonic generation (SH, 400 nm); 2) pumping two optical parametric amplifiers femtosecond (fs NOPA, tunable from 480 to 700 nm); and 3) a parametric amplifier pumped picosecond (ps NOPA, tunable from 500 to 700 nm). The combination of the pulses derived from NOPA, processes of sum and difference of frequencies, gives access to the ultraviolet and near infrared respectively.

- **Thin Films Laboratory:** This Lab is committed to the fabrication of thin films and multilayers with different functionalities, 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 “2D THERMS” 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 heating of the substrates up to 1000 °C and it is provided with a six-target carousel. 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 deposition of Au, Ag, etc. (four different targets) or transport measurements, like 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.



Femtosecond spectroscopy laboratory (left) and PLD equipment (right)

- **AFM microscopy laboratory.** It has a state-of-the-art AFM microscopy, NX-10 Park Systems, designed to work in multi-user mode (high degree of automation) and capacity for studying surfaces with resolution about 1 nm, and high-resolution modes for the analysis of structural motifs at sub molecular level, and additional modules of electrical conductivity and thermal conductivity. This equipment was purchased jointly by the CiQUS (40% of the cost) and five research groups of the same (12% of the cost each), which in one 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 CiQUS and several of their groups, and a group of CiMUS (Mabel Loza), a fluorescence microscope “Nikon Eclipse Ti” for the study of living cells was purchased. In 2017, 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, to improve the biological area, a new lab has been adapted for culture cell with the installation of 2 biosafety cabinets and the acquisition of an incubator.

4. SCIENTIFIC REPORT 2017

The following chapters describe and summarize the situation of CiQUS as well as its scientific activity during the year 2017, while more detailed information is available in the CiQUS website: www.usc.es/ciqus/en.

4.1 HUMAN RESOURCES

- 36 Research Staff, 25 postdocs, 90 PhD students, 25 Master students and 13 Technical and administrative assistants (Dec 31, 2017)

In December 2017, over 200 people worked at CiQUS: 36 Research Staff (3 of them *Ramón y Cajal* associates), 25 postdoctoral researchers (3 of them *Juan de la Cierva* researchers and 1 MSCA-IF), 90 PhD students and 25 MSc students, together with 9 technicians in different areas and 4 people in administration and services tasks. Furthermore, around 7 USC faculty members collaborate in the scientific activity of CiQUS on a daily basis, though they are not officially appointed to CiQUS.

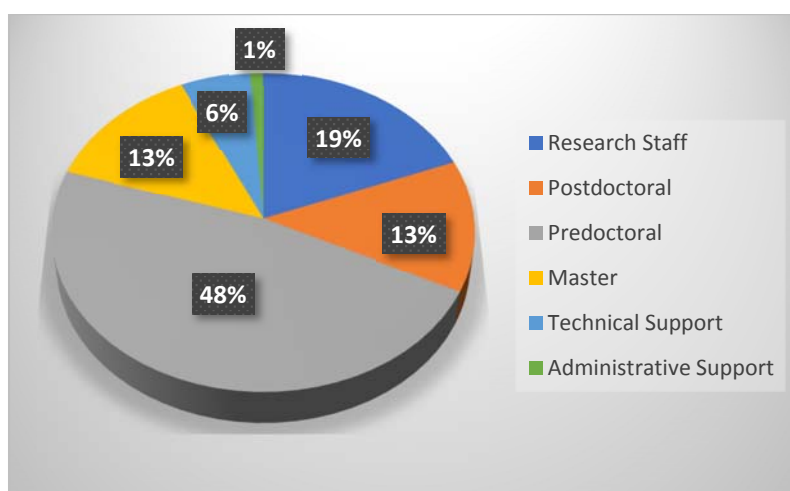


Chart 1. Distribution of human resources by category

Several grants to young **postdoctoral** researchers have been awarded during 2017:

- 2 New *Ramón y Cajal* researchers (Call 2016): Dr. María Giménez (also ERC Grantee) and Dr. Rebeca García will join CiQUS as RyC researchers along the year 2018. M. Giménez has been appointed as Principal Investigator at CiQUS, after positive assessment by our External Scientific Advisory Board.
- 3 Young talented researchers obtained the very competitive *Juan de la Cierva Incorporación* fellowships (Call 2016): Dr. Ángel Luis Fuentes de Arriba (Supervisor: J. Granja), Dr. Ester Polo (Supervisor: P. del Pino) and Dr. Julián Bergueiro (Supervisor: J. Montenegro).
- Dr. Alejandro Méndez (supervisor: J. Montenegro) and Dr. Carolina Carrillo-Carrión (Supervisor: P. Del Pino) were awarded with a highly competitive *Marie Curie Individual Fellowship* (MSCA-IF).
- *International Postdoctoral Program – Campus Vida*: As resulting of the 1st and 2nd edition of this program, Dr. Catalina Rodrigues (Supervisor: J.L. Mascareñas) and Dr. Ester Polo (Supervisor: P. del Pino) were recruited as postdoctoral researchers in 2017.

With regard to **predoctoral** trainees, ten new competitive research contracts have been awarded to CiQUS PhD students in 2017:

- *MECD – FPU Predoctoral fellowships*: Joan Miguel Ávila and Xandro Vidal Pereira (both under supervision of J. L. Mascareñas)

- *MINECO – Predoctoral contracts*: Jacobo Gómez González (supervisor: E. Vázquez) and Manuel Núñez Martínez (supervisor: E. Quiñoá).
- *Xunta de Galicia – Predoctoral contracts*: Héctor Fernández Caro (supervisor: J. Granja), Martín Calvelo Souto (supervisor: J. Granja), Marta Pazo Pascual (supervisor: J. Montenegro), Zulema Fernández Villar (supervisor: F. Freire), Iago Pozo Míguez (supervisor: D. Pérez), David Cagiao Marcote (supervisor: J. L. Mascareñas.)

In addition to these new competitive fellowships, an important number of research contracts have been drawn in 2017 under different funded research projects and contracts.

Overall, CiQUS has maintained an increasing capacity to attract young researchers, especially predoctoral students. The following table and chart demonstrate the evolution since 2011:

Table 1. Young researchers evolution at CiQUS since 2011

Year Type	2011	2012	2013	2014	2015	2016	2017
Postdoctoral	27	28	33	32	28	37	39
Predoectoral	69	71	81	80	86	91	92
Thesis defended	11	9	12	17	10	15	10

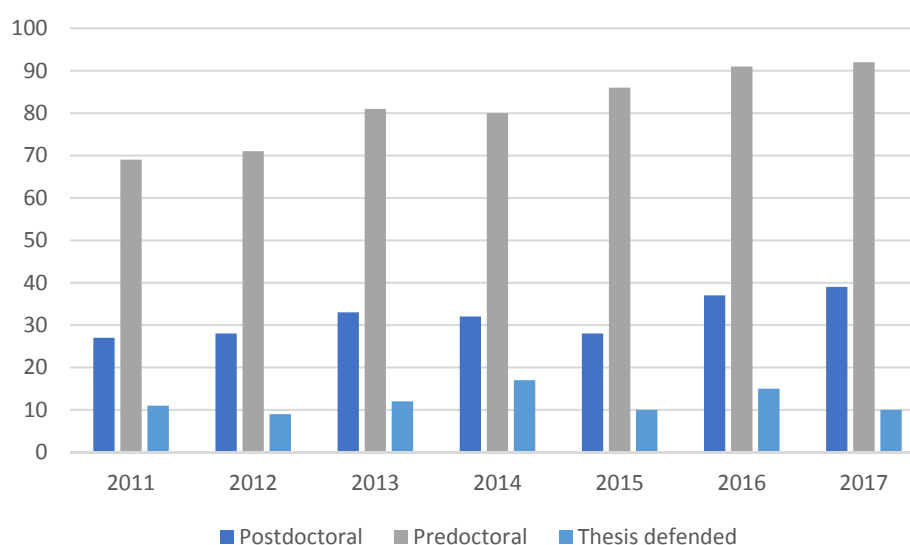


Chart 2. Research trainees and Thesis defended: evolution 2011-2017

4.2 RESEARCH FUNDING

- During 2017 new funding reached 5.6 M € (39% regional, 29% national, 13% international and 19% private)
- 1 ERC-PoC, 1 HFSP – Young Investigator Grant, 2 Marie Curie Individual Fellowships
- In addition to success in the national programs, CiQUS also obtained 7 predoctoral contracts.

CiQUS has demonstrated an excellent fundraising capacity despite the difficult financial environment, increasing not only the regional and national funds but also European funding, as well as that from private sources. Our figures at 31 December 2017 show 50 active projects and 8 contracts, for a total amount of 13.3 M €.

With regard to new funds raised during the 2017th year, CiQUS started 15 new projects and signed 4 new contracts, for a total amount of 5.56 M €. Remarkably there is a significant contribution from private sources, reaching 19% of the total funds. The reason is the strategic long-term partnership with INDITEX (PI J. Sardina), the largest fashion retail group in the world. Next table and chart show the increasing fundraising capacity of CiQUS since its opening in 2011.

Table 2. R&D fundraising evolution at CiQUS since 2011

Year Type	2011	2012	2013	2014	2015	2016	2017
INTERNAT.			553.934	2.356.276	307.391	1.670.215	704.440
NATIONAL	590.890	420.030	143.224	1.400.184	729.620	813.017	1.630.460
REGIONAL	504.000	819.842	1.012.200	1.696.000	850.000	1.085.000	2.165.000
CONTRACTS	172.777	10.000	223.855	513.178	870.545	968.752	1.057.263
TOTAL (€)	1.267.667	1.249.872	1.933.214	5.965.638	2.757.556	4.536.984	5.557.162

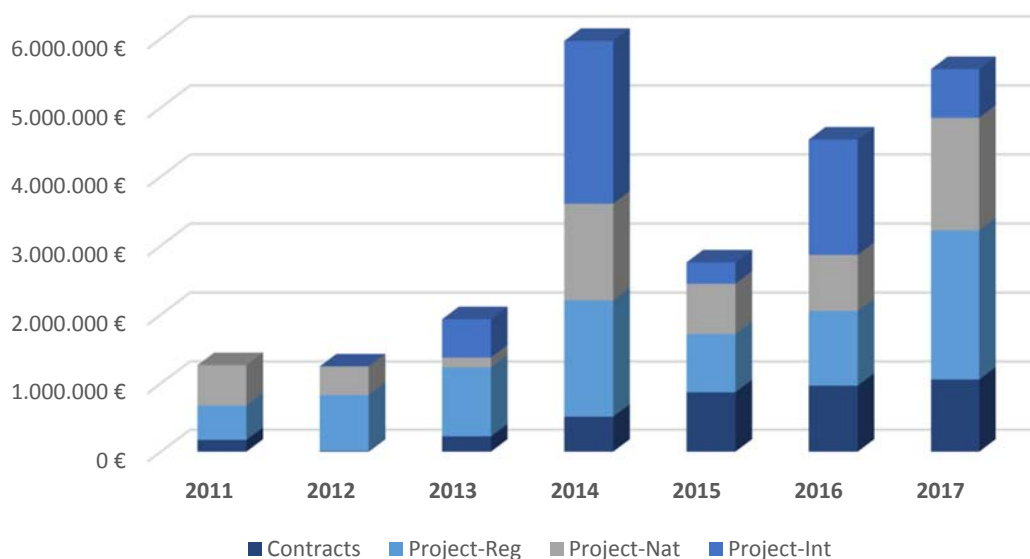


Chart 3. Evolution of the fundraising capacity, 2011-2017

Note: 2014 includes the ERC-AdG of J.L. Mascareñas (2.34 M €), and 2016 ERC-StG of J. Montenegro (1.4 M €)

Regarding the projects awarded in 2017, these are the key facts:

- **Regional Grants: 2.17 M €.** 37% (800 K €) belongs to the support of the Xunta de Galicia to CiQUS as *Singular Research Center* of the Galician University System (SUG), co-funded by the European Regional Development Fund – (ERDF), project ED431G/09.
- **National Projects: 1.63 M €.** CiQUS researchers were really successful competing in the National Research Program (9 projects), which work in a 3 years cycle. In addition to these funds, 7 of these projects were also awarded with one predoctoral fellowship, which also translates as an important landmark.

Remarkably, another 0.52 M € have been already granted for 5 projects starting in 2018, most of them associated to the *RETOS* (societal challenges) call-2017.

The national incomes also include a project funded by the Spanish Association against Cancer Foundation (AECC) awarded to Prof. E. Vázquez (Title: Repurposing antibiotics as mitochondria-targeted antitumoral agents), 1 RETOS-Jóvenes awarded to Dr. Beatriz Pelaz and a 1 IJCI-Talento awarded to Dr. María Tomás.

- **International Projects: 0.70 M €.** Among these projects the HFSP-Young Investigator Grant awarded to Dr. Montenegro, the ERC-PoC and the Marie Curie-RISE both awarded to Prof. Rivadulla. The other projects are the highly competitive Marie Curie Individual Fellowship (MSCA-IF-EF) awarded to Dr. Alejandro Méndez (Supervisor: J. Montenegro) and Dr. Carolina Carrillo-Carrión (Supervisor: P. del Pino):

- ✓ **HFSP-Young Investigator Grant:** *Fully synthetic self-regulated cytoskeleton*, Dr. J. Montenegro leads a collaborative project with the participation of Neal Devaraj (University of California, San Diego-USA) and Toshihide Takeuchi (University of Osaka, Suita-Japan). The Human Frontiers Science Program (HFSP) support novel collaborations among teams of scientists working in different countries. It is a three-year funding project (total funding support 0.4 M €).
- ✓ **ERC-PoC:** *A new technology of microthermal sensing for application in microcalorimetry (ANTS)*, based on patented results obtained within the ERC-StG-2DTHERMS, awarded to Prof. Rivadulla (0.15 M €).

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

A number of highly competitive projects have been submitted to different international calls, some of them still under evaluation (ERC-StG, ERC-CoG, ERC-CH2020-MSCA-ITN-2018, H2020-SC1-BHC-09-2018, etc). This is a clear sign of the increasing implication of CiQUS PIs in international initiatives.

- **Research contracts: 1.06 M €.** In 2017, CiQUS raised a record income from contracts in the private sector, mainly due to the strategic alliance of Prof. J. Sardina with INDITEX (0.94 M €).

4.3 RESEARCH OUTPUT

4.3.1 Scientific publications

The CiQUS maintained an excellent record of scientific contributions in 2017, with **88 articles** where 84 articles were published in JCR Journals, **85% of them in the first quartile (Q1)** and, more significantly, **50% in the first decile (D1)** of their respective thematic areas of the Web of Science data base (WoS) (see <https://www.usc.es/ciqus/en/research/publications>). In 2017 the **average impact factor was 7.211**.

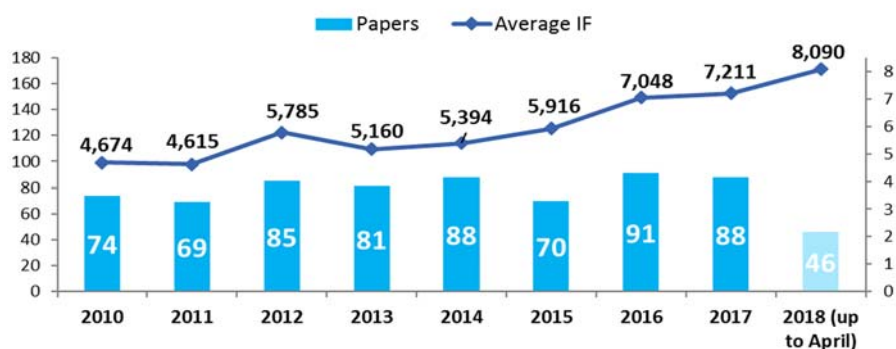


Chart 4. Evolution of the number of publications and average impact factor, 2010-2018 (April)

The increasing impact of the research output is clearly demonstrated by the evolution of the average impact factor (JCR) of the publication journals along the years. Furthermore, CiQUS has achieved a sharp increase in the number of publications in top-ranked journals. During 2017, CiQUS published 20 papers with IF>10 (1 Chem. Rev., 3 ACS Nano, 3 J. Am. Chem. Soc., 1 Nano Energy, 1 Adv. Funct. Mater., 1 Nat. Commun., 4 Angew. Chem. Int. Ed., 5 ACS Catal., 1 Nat. Protoc.).

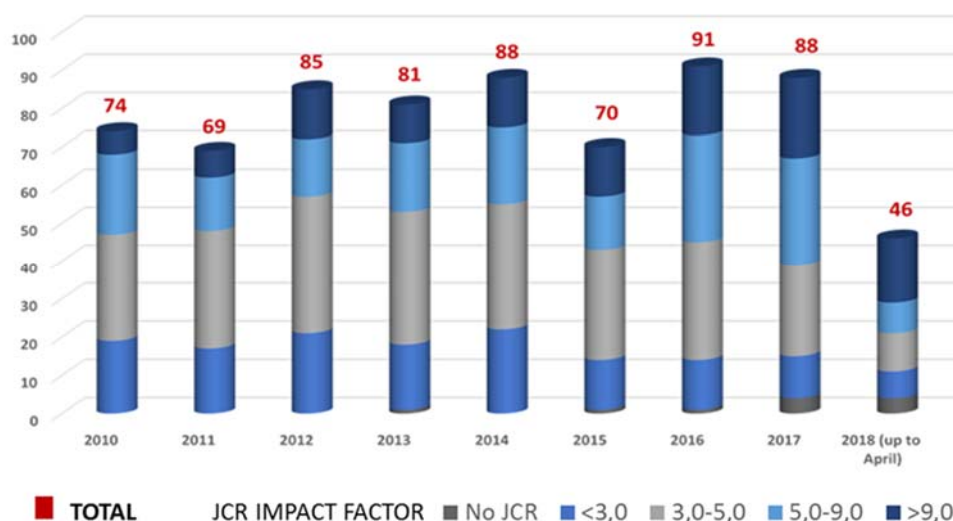


Chart 5. Evolution of the % of publications aggregated by IF sections, 2010-2018 (up to April)

Our compromise and ambition to generate top-level science is demonstrated by the ability of producing high impact factors in a variety of topics which also confirms the quality and interdisciplinary nature of CiQUS as research center. **Tables 3 and 4** show the list of scientific journals in which CiQUS articles were published in 2017. These journals are listed by impact factor order and quartile. Additionally, the total number of articles published in each journal during 2017 it is also shown.

Table 3. Scientific Journals in which CiQUS articles, ordered by Impact Factor and Quartil, were published during 2017 and total number of articles per Journal.

Full Journal Title	Impact Factor	Quartile	Nº of articles
Chemical Reviews	47.928	1	1
ACS Nano	13.942	1	3
Journal of the American Chemical Society	13.858	1	3
Nano Energy	12.343	1	1
Advanced Functional Materials	12.124	1	1
Nature Communications	12.124	1	1
Angewandte Chemie-International Edition	11.994	1	4
ACS Catalysis	10.614	1	5
Nature Protocols	10.032	1	1
Chemistry of Materials	9.466	1	1
Chemical Science	8.668	1	4
Small	8.643	1	2
Particle and Fibre Toxicology	8.577	1	1
ACS Applied Materials & Interfaces	7.504	1	1
Nanoscale	7.367	1	2
Organic Letters	6.579	1	3
Chemical Communications	6.319	1	6
Journal of Medicinal Chemistry	6.259	1	2
Current Opinion in Colloid & Interface Science	6.136	1	1
Polymer Chemistry	5.375	1	3
Chemistry-A European Journal	5.317	1	2
Journal of Chemical Theory and Computation	5.245	1	1
Organic Chemistry Frontiers	4.955	1	1
Journal of Materials Chemistry B	4.543	1	3
Journal of Physical Chemistry C	4.536	1	2
Biochimica et Biophysica Acta-Molecular Cell Research	4.521	1	1
Applied Catalysis A-General	4.339	1	1
Antimicrobial Agents and Chemotherapy	4,302	1	1
Antiviral Research	4.271	1	1
Scientific Reports	4.259	1	2
Journal of Cheminformatics	4.220	1	1
Physical Chemistry Chemical Physics	4.123	1	3
Computer Physics Communications	3,936	1	1
Physical Review B	3.836	2	1
Langmuir	3.833	1	1
Organic & Biomolecular Chemistry	3.564	1	2
ChemMedChem	3.225	2	1
ACS Combinatorial Science	3.168	1	1
Energy & Fuels	3.091	1	1
Current Topics in Medicinal Chemistry	2.864	2	1

Table 4. Scientific Journals in which CiQUS articles, ordered by Impact Factor and Quartile, were published during 2017 and total number of articles per Journal (continuation from the previous table 4).

Full Journal Title	Impact factor	Quartile	Nº of articles
Molecules	2.861	2	3
European Journal of Organic Chemistry	2.834	2	1
Synthesis-Stuttgart	2.650	2	1
Pure and Applied Chemistry	2.626	2	1
Journal of Photochemistry and Photobiology A-Chemistry	2.625	2	1
Bioorganic & Medicinal Chemistry Letters	2.454	2	1
Synlett	2.151	2	1
Chemistry of Heterocyclic Compounds	0.865	3	1
ChemistrySelect	No IF	N/A	2
Physical Review Materials	No IF	N/A	1
SynOpen	No IF	N/A	1

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 CiMUS, which confirms the emerging cooperative research lines within the *singular research centers network*.

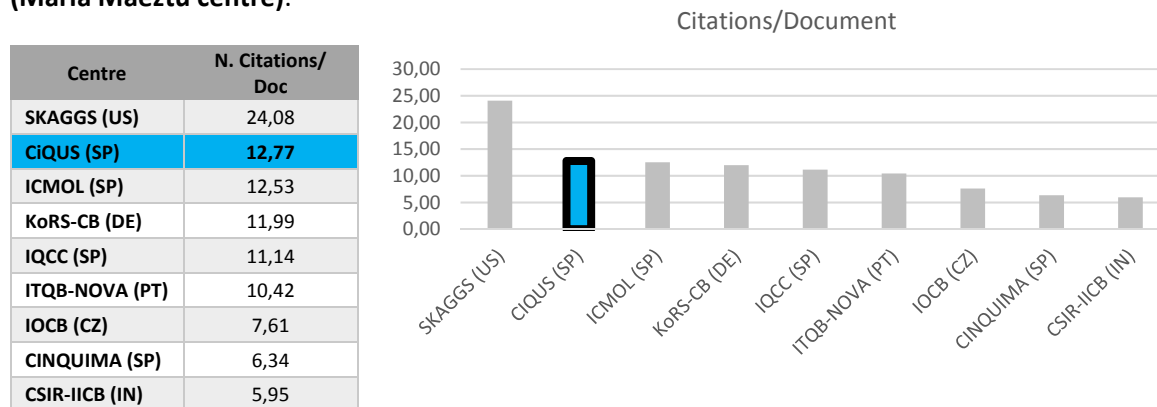
This comprehensive list of articles, with links to the respective journal websites, can also be found in the [CiQUS web page](#). Additional information about selected articles, considered as significant scientific contributions of the period, can be found in the *News* section of the website (<https://www.usc.es/ciqus/en/news>).

▪ **Benchmarking analysis**

A benchmarking of the Scientific Production of CiQUS during the period 2013-2017 (up to June 30th) was conducted by the “Research Institute for Higher Education and Science (INAECU). This study was carried out based on the analysis of the scientific production in the Web of Science (WoS) database of CiQUS and 8 different research centers in order to compare their scientific activity. Some of the results are shown below:

▪ **Impact normalized with respect to the number of citations per WoS document**

With a relative impact of 12,77 citations per document, CiQUS is in **second position in relation to all the analysed centres and, importantly, the first in relation to the national centres, including ICMOL (Maria Maeztu centre).**

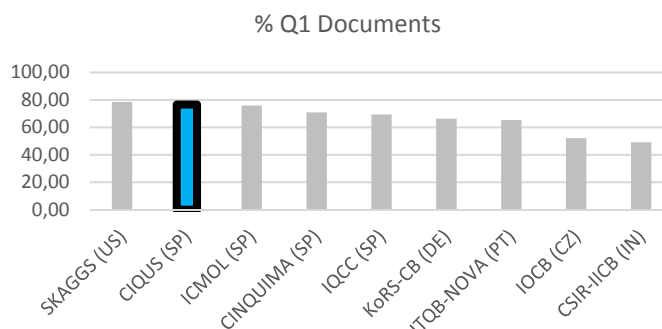


▪ Visibility of research

- Percentage of documents in journals of the first quartile (2013-2016)

The average quality of the scientific production of CiQUS is very high, with **76,62% of its production in journals of the first quartile**. CiQUS is in second position, just behind the internationally top SKAGGS, which has 78,46% of its production published in journals of maximum visibility, and **on top of all national centres**.

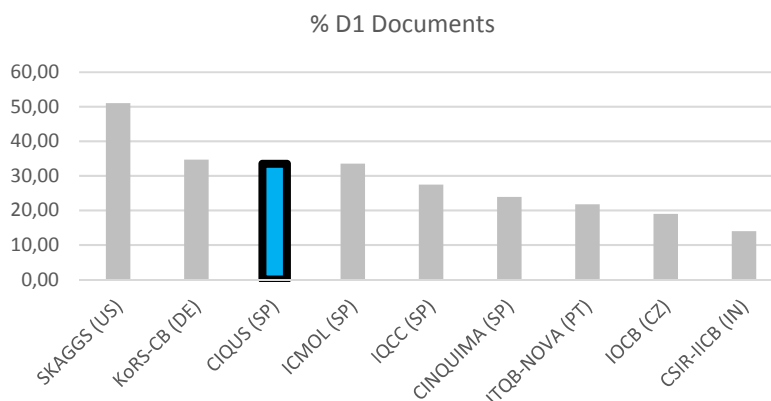
Centre	% Q1 Doc.
SKAGGS (US)	78,46
CiQUS (SP)	76,62
ICMOL (SP)	75,85
CINQUIMA (SP)	70,80
IQCC (SP)	69,36
KoRS-CB (DE)	66,33
ITQB-NOVA (PT)	65,22
IOCB (CZ)	52,03
CSIR-IICB (IN)	49,00



- Percentage of documents in journals of the first decile (2013-2016)

With **33,51% of its production in journals of the first decile**, CiQUS is in third position in relation to the rest of national and International centres, and **on top of all national centres**.

Centre	% D1 Doc.
SKAGGS (US)	51,05
KoRS-CB (DE)	34,67
CiQUS (SP)	33,51
ICMOL (SP)	33,54
IQCC (SP)	27,46
CINQUIMA (SP)	23,89
ITQB-NOVA (PT)	21,74
IOCB (CZ)	18,96
CSIR-IICB (IN)	13,99



Additionally, a **comparative with the NATURE INDEX** of CiQUS with the Centers included in the Benchmarking study and 14 additional centers already accredited as SO - Severo Ochoa Centres (8) or MM - María de Maeztu Units (6) in similar fields (chemistry - bio - materials); and other four relevant Spanish centres is shown below. The main conclusions are:

- Article Count (AC). CiQUS has a better value than 4 SO Centres and 3 MM Units.
- Fractional Count (FC). CiQUS value is also better than 4 SO Centres and 3 MM Units, but very close to another 3 SO Centres, strongly reducing the existing gap in the AC value.

It is important to note that these are absolute values (personnel are not considered), and several Centres with better indexes than CiQUS are considerable larger than us, e.g., according their websites: IRB (450), ICIQ (339), ITQ (258), IBEC (245).

Nature Excellence Index (data obtained 18-Dec-2017)			PERIOD: Oct 2016 - Sep 2017	
Name of the Centres / Units	Nature Index link	SO / MM	AC	FC
Center for Research in Biological Chemistry and Molecular Materials (CIQUS)	CIQUS		22	7,91
Centers included in the Bechmarking				
Skaggs Institute for Chemical Biology, TSRI (USA)	TSRI-Skaggs		36	6,91
Institute of Organic Chemistry and Biochemistry - IOCB, ASCR (Czech Republic)	IOCB		36	15,16
Institute for Molecular Science (ICMol), UV, Spain	ICMol	MM 2015	32	10,76
Institute of Computational Chemistry and Catalysis (IQCC), UdG, Spain	IQCC		24	6,13
Indian Institute of Chemical Biology (IICB), CSIR (India)	CSIR-IICB		7	4,02
Konstanz Research School Chemical Biology (KoRS-CB), University of Konstanz	KoRS-CB		5	1,28
Instituto de Tecnologia Química e Biológica (ITQB NOVA), UNL (Portugal)	ITQB NOVA		4	0,57
Institut de Ciència i Tecnologia Ambientals (ICTA), UAB, Spain	ICTA	MM 2015	3	0,51
CINQUIMA, UVA, Spain	Cinquima		1	0,50
Selection of Centers/Units Severo Ochoa / Maria de Maeztu				
Institute of Chemical Research of Catalonia (ICIQ)	ICIQ	SO 2013	46	28,01
Institute for Research in Biomedicine (IRB Barcelona)	IRB	SO 2011	39	10,23
Cooperative Research Center nanoGUNE Consolider (CIC nanoGUNE)	nanoGUNE	MM 2016	38	13,66
IMDEA Nanoscience	Imdea Nano	SO 2016	36	9,97
Institute of Materials Science of Barcelona (ICMAB), CSIC	ICMAB	SO 2015	34	8,82
Center for Cooperative Research in Biosciences (CIC bioGUNE)	bioGUNE	SO 2016	18	4,8
Institut de Bioenginyeria de Catalunya (IBEC)	IBEC	SO 2014	16	3,65
Department of Experimental and Health Sciences (DCEXS), UPF	DCEXS	MM 2014	15	3,83
Instituto de Tecnología Química (ITQ)	ITQ	SO 2016	13	6,31
Institute of Nanoscience and Nanotechnology (IN2UB), UB	IN2 UB	SO 2013	12	2,43
Molecular Biology Institute of Barcelona (IBMB), CSIC (data from the whole center, but only the "Structural Biology Unit" is accredited as Maria de Maeztu)	CSIC-IBMB	MM 2015	10	3,14
Andalusian Centre for Developmental Biology (CABD) (data from the whole center, but one of their Departments is accredited as Maria de Maeztu)	CABD	MM 2016	4	0,32
Other Spanish reference centres in the field				
Centre for Cooperative Research in Biomaterials (CIC biomaGUNE)	biomaGUNE		12	4,17
Institute of Chemical Synthesis and Homogenous Catalysis (ISQCH) (CSIC-U.Zaragoza)	ISQCH		14	5,75
Institute of Physical Chemistry "Rocasolano" (IQFR), CSIC	IQFR		20	5,02
Institute for Chemical Research (IIQ) (CSIC-U. Sevilla)	IIQ		22	2,76

4.3.2 Other research outputs

- **Patent applications**

During 2017 CiQUS researchers applied for 8 patents (i.e. 1 PCT and national phases EU (x2), USA (x2), JP, CN and KR).

- **PhD Theses**

During 2017 up to 10 CiQUS graduate students presented their PhD dissertations. All of them obtained the qualification of *Sobresaliente cum laude* and two 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 the [CiQUS website](#). These graduate students had external financial support either from competitive research fellowships (1 FPU, 2 FPI and 1 Gil Dávila fellowships) or through contracts linked to their advisor's research grants.

Currently, 99 PhD students are developing their thesis work at CiQUS. As a sign of the internationalization of CiQUS in this level, 12% of students came from other countries.

- **Contributions to scientific congresses**

CiQUS PIs gave over 59 lectures during the year 2017, 47 of them as Plenary, Keynote or Invited speaker at universities and congresses from 16 different countries. Furthermore, it is particularly remarkable the number of CiQUS PIs participations at international congresses (31).

- **Research Mobility**

During 2017, seven CiQUS members made short stays at prestigious international research institutions, either for scientific collaborations (as invited visiting professors) or as a part of their PhD training program (predoctoral secondments). Host institutions including the University of Cambridge (UK), Institute Curie (France), University Carnegie Mellon (USA, 2 cases), University of Leeds (UK), University of Zurich (Switzerland) and ICMA-B-CSIC (Spain).

4.3.3 Awards

Prof. **José L. Mascareñas** was elected as a member of the European Academy of Sciences. CiQUS Scientific Director becomes one of the four Spanish chemists within this Academy.

Regarding the awards achieved by PhD students, we should highlight:

- The "*Lilly Research Award for Doctoral Students*" awarded by the European Committee for Academic Relations (EUACC) of Lilly Spain to Noelia Casanova (Supervisors: J.L. Mascareñas and M. Gullías).
- Jéssica Rodríguez (Supervisors: J.L. Mascareñas and E. Vázquez) was awarded with "*the Best Thesis in Biological Chemistry Award*", given by the Group in Biological Chemistry (GEQB) of the Spanish Royal Society of Chemistry (RSEQ) and the *Honorific Mention of Ernesto Viéitez Prize* from the Royal Academy of Galician Sciences.
- Jéssica Rodríguez was also selected between the 10 finalists of the international "*Reaxy PhD Prize 2017*" (Shangai).
- Esteban Suárez received the *best Poster award at the 29th Chirality International Symposium* (Tokyo).
- Iván Gallego received the *best Poster Presentation award at the Bienal RSEQ 2017* (Sitges).

- Antonio Sánchez (Supervisor: E. Sotelo) received the *best Predoctoral Poster award at the bioMAPP17* (Santiago de Compostela)
- Leticia Suárez (Supervisor: J. Montenegro) received the *best Poster Presentation award at the Máster Universitario de Química Orgánica Symposium (MASTERQO)* (Madrid).

4.4 TRAINING

4.4.1 Master

Most of the CiQUS PIs are involved in the Master in Investigation Chemistry and Industrial Chemistry (with the University of Vigo and the University of A Coruña) and the Masters in Organic Chemistry (with the UCM and the UAM). It is also relevant their participation in the Master of Theoretical Chemistry and Computational Modelling (Erasmus Mundus) and the Research and Development of Medicines. CiQUS offers between 25 and 30 vacancies for the Final Degree Project annually. Approximately 60-65% of the Master students in Chemistry are trained at the CiQUS.

Outstandingly, the Master in Organic Chemistry was ranked 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 Theoretical Chemistry and Computational Modelling was ranked again as the 3rd best option within the category of “Experimental and Technological Sciences”.

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

4.4.2 Doctoral programs

One of the major strengths at CiQUS is the successful activity in the training of researchers, both at doctoral and post-doctoral level. In the year 2017 the number of doctoral students supervised by CiQUS' PIs did nothing but increase, since 2011 to 2017 the evolution of PhD students is: 69, 71, 81, 80, 86, 91, 102.

Most of the 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 40% of doctoral students are women. Moreover, it is noteworthy that more than 11% of doctoral students come from abroad, highlighting the presence of students from EU countries (Italy, France, Greece, UK), South America (Chile,) and Asia (Jordan).

10 Theses were defended by CiQUS students in 2017, all of them granted with top marks *cum laude*. A complete list of theses presented yearly can be found in <https://www.usc.es/ciqus/en/research/phd-theses>.

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 <https://www.usc.es/ciqus/en/news/events> for the complete list of speakers in 2017)

The success of the training activity is evident in 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.

4.4.3 Postdoctoral programs

During 2017, 44 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,

Iran and Romania). Regarding the gender distribution, 30% of the postdoctoral researchers at CiQUS during 2017 were women.

Two excellent young researchers joined the CiQUS after been awarded with the highly competitive Marie Curie Individual Fellowship (MSCA-IF-EF, Call2016), Dr Alejandro Méndez (started 2017) and Dr Carolina Carrillo-Carrión (starting 2018).

The success in attracting postdoctoral researchers through national and regional competitive calls is also considerable. In particular, the Juan de la Cierva Program allowed the recruitment of three investigators in the 2016 Call [Angel Luis Fuentes de Arriba (started 2017), Ester Polo and Julián Bergueiro (both starting in 2018)], while the postdoctoral grants of Xunta de Galicia resulted in the recruiting of Andrés Seoane as postdoctoral researcher (currently at University of California – outgoing phase).

Even more remarkable was the success in the program Ramón y Cajal (RyC) that allowed the recruitment of Dr. María Giménez (ERC Grantee) and Dr. Rebeca García, both will join the CiQUS along 2018.

Additionally, CiQUS launched the 2nd and 3rd edition of the International Postdoctoral Program – Campus Vida in 2017 (Spring and Fall Call). Resulting of these competitive calls, 3 brilliant young researchers joined the CiQUS (1 of them already started in 2017 and the other 2 will join the CiQUS along 2018) as postdoctoral associates. This program is partially funded by the 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).

4.4.4 Funding for training (grants and contracts)

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

Regarding the doctoral stage, 26 PhD students are currently developing their theses supported by competitive national grants and contracts (8 FPI, 3 FPU, 13 Predoc by Xunta de Galicia, 1 by private foundations and 1 by international programs). Most of the remaining doctoral students have contracts linked 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, they all have contracts linked 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).

4.5 INTERNATIONALIZATION

- 2017: 49% of the 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-PoC, 1 HFSP-Young Investigator Grant, 1 MSCA-RISE, 2 MSCA-Individual Fellowships

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

- Over **43 papers (49%) resulting from international collaborations** (35% in 2011-2014), **81% of them in the first quartile (Q1)** and **44% in the first decile (D1)**. Up to 67% of these works have at least one corresponding author from CiQUS. Among the collaborators there are a number of research groups from prestigious research centers, such as the University of Cambridge (UK), CNRS (FR), University of Groningen (ND) or IBM Research (CH).
- With regards to **international projects**, in 2017 CiQUS PI, Dr. J. Montenegro, was awarded with the HFSP-Young investigator Grant with a total budget of 0,4 M € and 2 International partners, Dr. Devaraj (University of California, USA) and Dr. Takeuchi (University of Osaka, Japan), while Prof. Rivadulla launched the ERC-PoC project ANTS. Even though this is not strictly a collaborative Project, the prestige and relevance of the ERC grants are an extraordinary contribution to the international prestige and visibility of the CiQUS.
- In 2017, 2 young researchers were awarded with the highly competitive Marie Curie Individual Fellowships (MSCA-IF-EF) to perform their postdoctoral research at CiQUS.
- **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 offering of our research results and technology platforms but also the public presentation of project ideas for H2020.
- Since 2015 CiQUS also belongs to the **ETP Nanomedicine** and to the **European Cluster on Catalysis**.
- **COST Actions**. CiQUS research groups are also participating in over 8 of these networking projects, as a tool for boosting their networks and set up new collaborations (see 6.5). Since 2015 3 PIs are participating in 2 COST actions and in both of them, after a competitive process managed by the Spanish Ministry, being part of their Management Committees.
- **CiQUS Seminars**. During the year 2017 up to 24 top level international scientists including the Príncipe de Asturias Laurate Avelino Corma and world leader scientists as Prof. Barry Trost and Prof. Hayashi among others, were invited to give a talk on their own research fields at CiQUS.
- Finally, 17% CiQUS personnel came from foreign countries during 2017 (Italy, Uk, The Netherlands, France, Greek, Chile, Jordan, South Korea, Indonesia, Cuba, Venezuela, Brazil).

4.6 TECHNOLOGY TRANSFER AND VALORIZATION

4.6.1 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**, PI at 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.

CiQUS leads the 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) and 940.000 € (2017)**.

Designed and supported by 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 investments coming from this relationship.

4.6.2 R&D projects with other companies and entities

The following paragraphs summarize the relevant information about the new contracts during 2017.

- **INDITEX** (multinational, A Coruña). Since 2013 the overall value of the contracts exceeds 2 million €, reaching a peak of 940.000 € in 2017.
- **zLabels GmbH**. A company focused on the creation of contemporary fashion brands which sold online via Zalando and other global retail platforms. 3 Contracts were signed during 2017 with CiQUS (around 35.000 €).
- **Oncostellae S.L.** (Spin-off, Ourense). A new contract of 30.000 € was signed in 2017. 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.
- **GalChimia S.A.** (Spin-off, O Pino). Continuing a steady partnership from the very foundation of the company in 2001, in 2017 a contract over 32.000 €. It is focused on the development of complementary therapies-cancer treatments.
- **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 PI, has signed a contract with this company in 2017 (15.500 €). Prof. Sardina will give scientific, technical and commercial advice regarding new analytical techniques in the field quality control for product health.

Other small contracts were also signed during 2017 with Concello de Vigo and ABCR GmbH.

In summary, during 2017 CiQUS researchers had 15 active contracts with up to 9 different companies/institutions adding up to 2.05 M €. Despite the fact that this is not a big 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).

4.6.3 Patents, Licensing and Valorization

During 2017 CiQUS researchers applied for 8 patents (i.e. 1 PCT and national phases EU (x2), USA (x2), JP, CN and KR).

- **ERC - Proof of Concept.** Lead by Prof. F. Rivadulla (ERC-Starting Grantee). This project aims to develop a new sensing element for a High-Throughput Calorimetry going beyond the current capabilities on Isothermal Titration Calorimetry. (ITC, company: Malvern).
- **MATPRINT.** This project (0.25 M €), co-lead by CiQUS IP Prof. Eddy Sotelo with the Galician Institute of Ceramics (also from USC), has been approved by the Regional program for technology valorization - IGNICIA (only 7 projects were approved), after a competitive evaluation by experts from Oxford University Innovation. The project is focused on bioceramics and 3D Printing in Catalysis.
- **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, there was signed a first agreement for developing 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 frame 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.

Since 2012 CiQUS has been a member of SusChem Spain, part of the European Technology Platform for Sustainable Chemistry, ETP SusChem. CiQUS has been also actively participating in many national and European networking events, including the presentation of project ideas and institutional posters.

Thus, during 2017 CiQUS assisted to a number of international events: Nanotechnologies and Advanced Materials - NMBP H2020 (Cambridge); EuroNanoforum 2017 (Malta); Industrial Innovation Matchmaking Event (Brussels); SusChem 2017 Brokerage Event (Brussels); Brokerage Event on Nanotechnology and Advanced Materials (Munich).

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

4.7 OUTREACH

4.7.1 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 with social networks: Facebook (2011), LinkedIn (2012), YouTube (2013), Twitter (2014) and Google+ (2014).

Nowadays, **CiQUS website** has an 28% of international traffic over the total visits (45% when considering only new visits): 5% USA; 3,2% UK; 2,2% Germany.

YouTube. Since December 2013, CiQUS started to broadcast a serie of divulgation videos made by our Press Manager. Currently, CiQUS YouTube channel has reached over 18.800 visualizations and a total of 300 hours, 48% from outside Spain, e.g. 8% from USA and 4% from 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. 1303 followers. Currently, around 26% of the post had over 3.000 impressions according to Facebook statistics, and the top 10% reach more than 5.000 impressions. Considering that CiQUS is only 6 years old, our average impact is comparable to the best excellent Spanish research centers, according the comparative 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 566 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 private sector.

Twitter. 818 followers, which means a 60-70% increase in the number of followers every year: 150 (2015), 388 (2016) and 662 (2017). Nowadays, it has 1.500 visits and over 20.000 impressions per month.

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

It is worth mentioning the presence of CiQUS PIs in several National Newspapers (El País, La Razón, El Mundo,...), such as the interviews to Dr. Pablo del Pino (awarded with a Leonardo Fellowship – BBVA Foundation) and Dr. J. Montenegro (awarded with a HFSP – Young Investigators' Grant). 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, regularly cover press release about CiQUS members and CiQUS activity.

An outstanding impact was achieved in January 2017, Chemistry World chose the joint work of CiQUS PI D. Peña with IBM Research (Nature Chem, 2016) **among the ten best articles of 2016 worldwide**. Furthermore, ChemistryViews and PHYS.ORG also issued 3 news by CiQUS researchers during 2017.

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

4.7.2 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 2017, CiQUS organized, in collaboration with the Faculty of Chemistry of the Universidade de Santiago, the 5th Edition of this program with the participation of over 550 high school students from 16 different centers all around Galicia.

Apart from this program, during the whole year, CiQUS regularly organizes the visit of groups of students from different school and high school classes at the center. Particularly, in May 2017, CiQUS hosted a reception to the winners of the Galician Chemistry Olympiad 2017.

In November 2017, CiQUS collaborated with the Faculty of Chemistry of the University of Santiago in the organization of "**the Day of the Chemistry 2017**", which was hosted at the Faculty of Chemistry.

Last December, 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, CiQUS organized the "**Ciencia Singular**" - **Open Doors Day**, addressed to the general public (adults, families, teenagers, ...). Over 500 people (300 adults and 200 kids) visited the center on December 2nd, attended to the lectures and participated in the chemical games and experiments.

In May 2017, we organized a very successful round table meeting of enthusiastic students and young researchers with the **Príncipe de Asturias Laureate Avelino Corma**. In addition to our commitment with education and our interest in stimulating young people's scientific vocations, the aim of this meeting was to raise public awareness about the contributions of chemistry to the progress of humankind, the current challenges in chemical research and the future perspectives in terms of job offers.

CiQUS also participated in external divulgation workshops, as the scientific divulgation event *A Pint of Science* (with José Luis Mascareñas as one of the speakers at the Event in Santiago de Compostela), 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 for helping high school students to choose their future university studies).

Finally, 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.

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



Some CiQUS pictures from outreach activities: “CienciaSingular Open Doors 2017”, “Research in Chemistry: creative science for a better world”, “CiQUS Reception to the winners of the Galician Chemistry Olympiad 2017”, “A woman scientist in every school”.