Annual Scientific Report 2021

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 Directors

Dear friends,

In this annual scientific report, you will find a detailed summary regarding CiQUS activity and results along the year 2021. We still had to deal with the COVID struggle, but by the second part of the year we were able to restart many of our activities. 2021 has been a very successful year in terms of reaping fruits of the work carried out in previous years.

As it is detailed in the report, several international, highly relevant projects were initiated in 2021. This is the case of the ERC Synergy Grant MolDAM led by Diego Peña, the ERC Starting Grant SPACING by Beatriz Pelaz, and two ERC Proof of Concept Grants [antiCSC (Mascareñas); ZABCAT (Giménez)]. Overall, up to 10 ERC projects have been awarded to CiQUS PIs since 2014 (1 SyG, 1 AdG, 1 CoG, 3 StG and 4 PoC), which clearly positions CiQUS among the research centres with the highest proportion of ERCs in Spain, even compared with whole Universities. Other international collaborative projects awarded in 2020, such as 2 FET-Open (SWIMMOT, PI. Dr. B. Pelaz; e-Prot, PI. E. Vázquez), 1 H2020-ICT (REAP, PI. B. Pelaz) and 1 EuroNanoMed3 (PI. Dr. E. Polo), also started their journey in 2021. We have also been very successful in national grants, with 10 from the AEI (Retos, Generación de Conocimiento and Prueba de Concepto – including 4 associated predoctoral contracts), among others. Overall, in 2021, CiQUS started 26 new projects and 9 new R&D contracts or Proof of Concept projects for a total amount of 9,6 M €. This figure gains more significance when compared with the same figures from ten years ago, when the fund raising was less than 2 M €. This represents a clear indication of our progress and the success of our science policy.

With regard to our scientific output, we keep up with our philosophy of prioritizing quality over quantity, as we know that this is key for international visibility and impact. Therefore, 83% of CiQUS JCR articles were published in journals indexed in the first quartile (Q1) and, more significantly, 45% in the first decile (D1). In 2021, CiQUS published a total number of 32 papers with IF>9, which represents 34% of CiQUS JCR publications in 2021. Our valorization and tech transfer activities have also been successful, with new patents being granted, some other licensed, and new spin-offs like Celtarys, have started their journey.

In terms of talent attraction, in 2021 the “Distinguished Researchers” Manuel Ortuño and Manuel Nappi started their independent activity as junior scientists, together with four Ramón y Cajal researchers, three from the 2020 call (Ester Polo, Rafael Ramos and Beatriz Orosa), and one from the 2021 call (María Tomás, starting in 2022). The incorporation of these young researchers, and the start of new European projects, has led us to make minor changes in our scientific agenda to include new lines, that anyway are fully integrated in the thematic organization of the center, and should further facilitate synergies and collaborations.

We have also been very successful in competitive postdoctoral calls, including Juan de la Cierva, María Zambrano or Margaritas Salas programs, with more than 10 CiQUS people receiving this type of awards. More than 25 PhD students conducting their work at the center gained either a national or a regional scholarship. Considering all the programs, in 2021, up to 89 researchers were funded via competitive public calls (more than 51% of CiQUS researchers considering postdoctoral researchers and PhD Candidates).

The proportion of female and of foreign members maintains a slow but steady increase, and we expect that after reaching full normality, the application of our current policies will further allow to improve this trend. We feel very proud by the success of our researchers and alumni in competitive awards or in their academic or professional careers after leaving the center.

In 2021 we could also reinforce our infrastructure with the incorporation of new equipment, such as state-of-the-art spectrophotometer and spectrofluorimeter, or new ITCs or DSCs instruments, among others.

Importantly, we have started to renovate laboratory spaces in the neighboring CIBUS building, that have been allocated to CiQYS by the USC, due to occupancy problems in our building.

We keep our firm commitment to society, and we have further increased our outreach and dissemination activities, that after the pandemic outbreak, have been slightly refocused to intensify online actions.

In summary, 2021 has been an extremely successful year in terms of quality of our scientific production, fundraising in competitive calls, incorporation of new talent, and impact of our technology transfer activities, among others, and we firmly expect that once the consequences of the pandemic are fully overcome, we will reach a new cruising speed that will further boost a new leap in our outcomes.

Ten years have passed since the opening of CiQUS, and we could not feel more proude of the achievements and commitment of CiQUs members, from PIs and researchers to our technical and management team, which have undoubtedly allowed to position the center as an European reference in Chemistry, Chemical Biology and Molecular Materials.

With kind regards,

Santiago de Compostela, June 2022

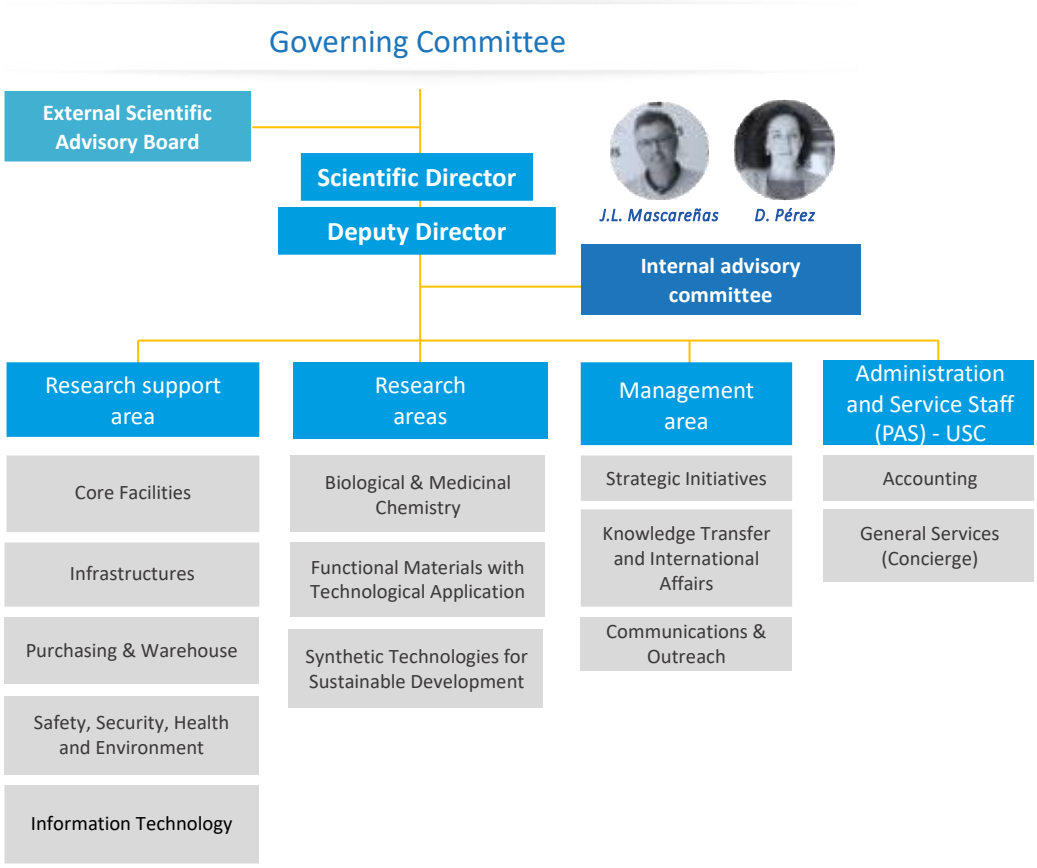
José Luis Mascareñas
CiQUS Scientific Director

Dolores Pérez
CiQUS Deputy Direct

1. ORGANIZATION

1.1. Organizational Chart & Team

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



Organizational Chart at CiQUS

GOVERNING COMMITTEE (December 31, 2021)

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

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

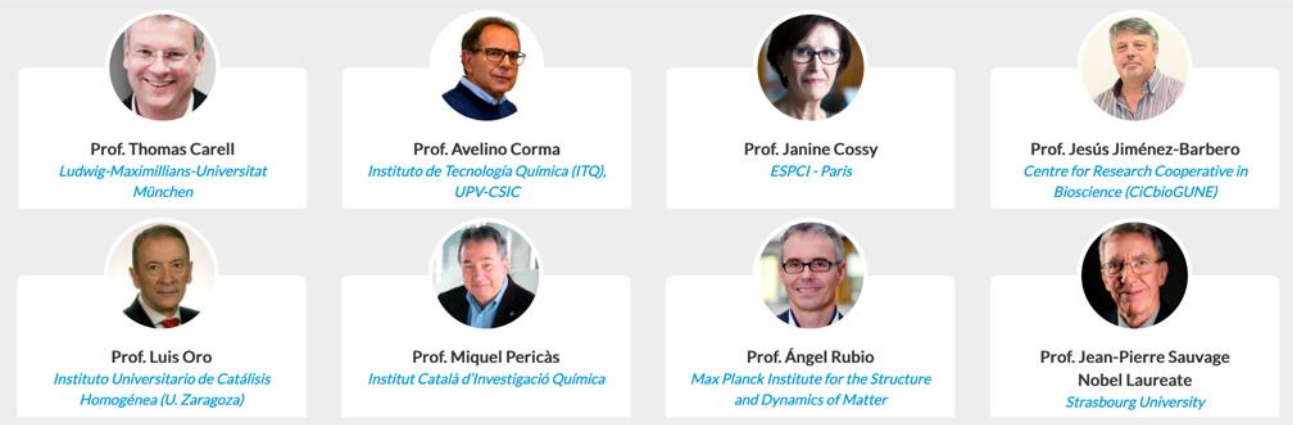
Members: Javier Ferreira Fernández, *USC Manager*
Cecilia Sierra Rey, *USC Social Council President*
José Alberto Díez de Castro, *General Secretary for Universities | Xunta de Galicia*
Rosina López-Alonso Fandiño, *CSIC Vice-President for Organization and Institutional Affairs*
José Luis Mascareñas Cid, *CiQUS Scientific Director*
María Dolores Pérez Meirás, *CiQUS Deputy Director*

DIRECTORS (December 31, 2021)

Scientific Director: José Luis Mascareñas Cid

Deputy Director: María Dolores Pérez Meirás

EXTERNAL SCIENTIFIC ADVISORY BOARD (ESAB) (December 31, 2021)



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, oct 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 at Harvard University (USA) and a visiting scientist at the University of Cambridge and the MIT. As independent researcher, he has published over 210 articles, the majority of them in the most relevant chemistry journals, 10 book chapters, and 23 patent applications. He has supervised 39 PhD theses, delivered more than 160 invited lectures, most of them in international forums, and raised over 5 million Euros in competitive grant calls in the last 5 years. Many students from the group have received relevant awards, and many of them have started relevant academic careers. Thus, Dr. Elena Pazos, now professor in the University of Coruña, has gained a prestigious ERC starting grant in 2019. In 2014, Prof. Mascareñas received and **ERC Advanced Grant** for his project METBIOCAT (http://metbiocat.eu/) and, more recently, an **ERC Proof of Concept** (antiCSC, 2020).

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 was appointed as member of the European Academy of Sciences. He was appointed Scientific Director of CiQUS in February 2014. the CiQUS Governing meeting held on September 25, 2019 approved the renewal of Prof. Mascareñas as CiQUS Scientific Director for 4 years.

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

Professional profile: Dolores Pérez (Ferrol, 1964) completed her graduate studies at the USC with Honours and obtained her PhD in 1991, under the supervision of Prof. E. Guitián and L. Castedo. She was awarded 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 Full Professor in January 2019.

She has published over 80 articles in high impact journals, 5 book chapters and supervised 12 PhD theses. 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 conjugated systems and nanographenes. She has been 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. From September 2017 to June 2018, she was also Commissioner of the USC Rector for Campus Vida and for the Coordination of the Singular Research Centres Network.

1.1.2 Management Structure

The CiQUS Management body is organized in several different units which give support to the scientific and non-scientific activity of the centre:

- **Internal Advisory Committee**, which is representative of the main research areas at the CiQUS, is currently constituted by CiQUS PIs *Ricardo Riguera (emeritus), Juan R. Granja, Antonio Fernández-Ramos, Pablo del Pino and María Giménez*. The committee provides advice to the Directors (José Luis Mascareñas and Dolores Pérez) on some key decision-making processes, and is involved in the elaboration, implementation and monitoring of the CiQUS strategic plan.

- **Management Area**: This area integrates 4 different units:

✓ Administration Unit: responsible for the accounting management of R&D activities, secretarial issues and administrative support (*Elena Veiga* and *Lucía Rodríguez*).

✓ Strategic Initiatives: coordination of CiQUS scientific strategic project, talent attraction programmes, training activities, events and writing of scientific and activity's reports. (*Dr. Almudena García*).

✓ Knowledge Transfer & International Affairs: promotion of international R&D initiatives and identification of technology transfer opportunities (*Fernando Casal).*

✓ Communications and Outreach Unit: Maintenance and updating of CiQUS social media, edition of press release and contact with press media. Coordination of outreach and social programme (Mariano Comino).

- **Research Support Area**: responsible for the implementation of the centralized operational model which gives technical support to CiQUS' research activity, aiming at the optimization of the available resources and the improvement of the working conditions at the centre. This area integrates 4 different units:

✓ Core facilities: provides the scientific instrumentation support needed to carry out research at CiQUS, ensures the maintenance and best use of the equipment, and offers 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 labs, equipment, furniture, and general spaces at CiQUS (*Laura Acevedo*).

✓ Purchasing and Warehouse: responsible for the negotiation and purchasing of reagents, 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. Elaboration and maintenance of CiQUS' Self-protection plan, coordination and

training of the emergency teams and management of the laboratories' safety (*Noela Torrente, Pablo Cajaraville*).

✓ A Biological Support Technician (Rebeca Menaya): responsible for cell culture and for assistance on other biological techniques.

✓ An IT Support Technician (Adrián Torreiro): responsible for technical assistance, installation, configuration and maintenance of the computer equipment associated with the scientific instrumentation and the rest of computer and electronic equipment at the Centre.

✓ A Transmission Electron Microscopy (TEM) Manager (Dr. José Manuel Vila): with a contract partially funded by the USC Vicerectorate for Research, Dr. Vila is responsible for the scientific and technical management of the recently acquired high-resolution TEM (JEOL F200).

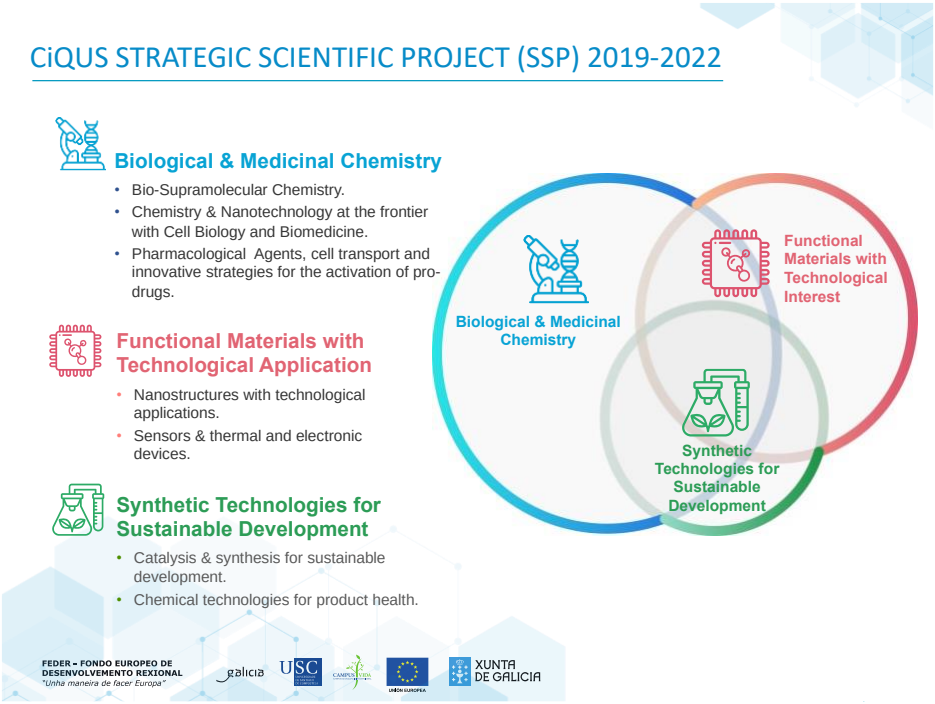
In 2021, our research support team was strengthened by hiring new personnel:

- ✓ An Advanced Microscopy Lab Manager (Dr. Jose R. Couceiro): PhD in Biology, with extensive experience in fluorescence, confocal and hyperspectral microscopy. Responsible for scientific-technical support in the Advanced Microscopy laboratory at CiQUS.
- ✓ Two research technicians (Lluvia Domínguez and Andrea López) for technical assistance to the CiQUS' Research Support Area: maintenance of small laboratory equipment and the scientific instrumentation of the center.

1.2 Scientific Structure

CiQUS research activity is organized to exploit the full potential and quality of its research groups in the most effective way to generate science of high impact at the frontier of knowledge, pursuing innovative solutions and approaches to face societal challenges in the fields of health, environment, or new materials and energies, in line with the priorities established by the European, national and regional R&D strategies. This commitment is supported by our policies to optimize efforts and promote collaborations and synergies between the different research groups and disciplines within the centre with the aim to maximize our scientific and technological competitiveness.

In this context, our Strategic Scientific Project, designed within the "*Centros de Investigación of Galicia (2019-2022)*" framework programme, focuses on the generation of ground-breaking science at the interface between Chemistry, Biological Chemistry and Materials Science, and on the technological transference of some of the results. Towards this end we seek an effective Interdisciplinary Integration of Research Topics supported by highly competitive scientists with complementary expertise.



The CiQUS scientific programme is currently organized around three main thematic areas:

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

The broad scientific background of the CiQUS researchers, from chemists to physics, biologists, pharmacists and biochemists, is a cornerstone to strongly interconnect the scientific areas mentioned above. **The promotion of collaborative research lines between the different areas of knowledge as well as the favouring of the intramural synergies by the participation of all the PIs and groups in each research topic, is crucial to ensure the success of our Strategic Scientific Project**.

Our efforts are focused on the generation of impact, in the development of excellence science to contribute to the socioeconomical progress of the contour and the training of the next generation of research leaders and highly qualified scientists.

A brief description of the CiQUS research areas, sub-areas and the corresponding active research lines is outlined below:

I. BIOLOGICAL AND MEDICINAL CHEMISTRY

Research in this area focuses on the fields of supramolecular, biomolecular and cellular chemistry as well as biomedicine, and addresses pressing medical problems and challenges in cancer, neurodegenerative diseases and bacterial resistance. Our current organization includes, among others, the following research topics associated to different PIs:

A.1) BIO-SUPRAMOLECULAR CHEMISTRY: a) Supramolecular devices based on peptides and biological applications (J. Granja, J. Montenegro). b) Metallopeptides for nucleic acid interactions (E. Vázquez). c)

Dynamics of photoinduced processes (F. Rodríguez Prieto/M.C. Ríos). d) Multiscale simulations of supramolecular systems (R. García Fandiño).

A.2) CHEMISTRY AND NANOTECHNOLOGY AT THE INTERFACE WITH CELL BIOLOGY: a) Metal catalysis in biological habitats (J.L. Mascareñas). b) Molecular fluorescent probes in cell biology (E. Sotelo, J. Montenegro, E. Vázquez). c) Nanobiointeractions (B. Pelaz). d) Smart biomimetic nano-systems (J. Montenegro, P. del Pino). E) Photocatalytic processes inside cells (M. Tomás)

A.3) PHARMACOLOGICAL AGENTS AND NEW STRATEGIES FOR DRUG TRANSPORT AND DELIVERY: a) Cellular transport of proteins, nucleic acids and cytotoxic molecules (J. Montenegro). b) Antibiotics for resistant bacteria (C. González-Bello). c) Combinatorial technologies for drug discovery (E. Sotelo). d) Mitochondria-targeted antitumoral agents (E. Vázquez). f) Dendrimeric nanostructures in drug delivery and diagnosis (E. Fernández-Megía). g) Carbohydrate and peptide-based bioactive compounds (J.C. Estévez/R. Estévez); h) Virus-based biotechnological tools (J.M. Martínez-Costas). i) Anticancer drugs based on helical metallo-peptides (M. Vázquez). j) New materials for nanomedicine application (B. Pelaz).

The main novelty regarding this area is the incorporation of Dr Beatriz Orosa as Ramón y Cajal researcher who will start in 2022 a new research line at CiQUS for developing of new **immunity tools by post-translational modifications**.

It is also worth to noting i) the new research line started by Dr. Beatriz Pelaz based **on bioprinting of nanoparticles for medical applications** and the study of their trafficking behaviour within cells through the ERC-StG "SPACING" project; ii) the promotion of Dr. Ester Polo to Ramón y Cajal researcher leading a **new research line on biomimetic cell-derived nanovectors**; and iii) Prof. Eugenio Vázquez started a new research line focused on the development of **engineered conductive proteins** for upscaling and using **as smart ink-based conductors and ionic electrolytes in energy storage devices** within the framework of the FET-Open "e-Prot" project in collaboration with other research centres and companies from Spain, Portugal, Israel, UK and France.

II. FUNCTIONAL MATERIALS WITH TECHNOLOGICAL APPLICATIONS

Research in this topic aims at the discovery of new organic, inorganic and metallo-organic materials with unique properties, as well as their implementation for the development of devices and technologies with applications in different fields, such as biomedicine, molecular electronics or energy storage and conversion.

B.1) INNOVATIVE MATERIALS AND TECHNOLOGIES: a) Nanoparticles, MOFs and hybrid nanomaterials with applications in drug delivery, theragnostic or as cell reprogramming agents (P. del Pino, B. Pelaz). b) Magnetic and transport properties in transition-metal materials (F. Rivadulla). c) Metal-carbon hybrid nanostructures for catalysis and energy-related applications (M. Giménez-López). d) Bottom-up approaches to graphene materials (D. Peña). e) Functional polycyclic conjugated systems (D. Pérez/E. Guitián). f) Smart helical polymers (F. Freire/E. Quiñoá). g) Nanomaterials with applications in catalysis and sustainability (M. Lazzari). h) Dynamic Chiral Catalysts based on Helical Polymers (F. Freire).

B.2) SENSORS: THERMAL AND ELECTRONIC DEVICES: a) Custom-crafted graphene nanostructures for the design of new nanoscale quantum spintronic devices (D. Peña). b) Devices for ultraprecise thermal measurements (F. Rivadulla). c) Stimuli-responsive dynamic polymers (F. Freire/E. Quiñoá). d) Development of portable nanophotonic bio-sensors based on multifunctional nanoporous graphene for early diagnostics (D. Peña). e) Functional materials for active control of thermal conductivity (F. Rivadulla).

In this context, several new different research lines were initiated at the centre during last year: i) "**MolDAM**" (ERC-SyG): A CiQUS team led by PI. Diego Peña in collaboration with IBM Research GMBH and the Universitaet Regensburg will use scanning tunnelling microscopy to manipulate electron charge within molecules for

studying chemical reactions mechanisms at the single-molecule level. ii) María Giménez launched the ERC proof of concept "**ZABCAT**" for the **fabrication of new electrodes of zinc-air long-life batteries** based on an innovative prototype to overcome cathode degradation through catalyst confinement. iii) Dr. Rafael Ramos was promoted to Ramón y Cajal researcher leading a new line for the development of **thin film oxide nanostructures for information, logic and energy management**.

III. SYNTHETIC TECHNOLOGIES FOR SUSTAINABLE DEVELOPMENT

This area is focused on the discovery of effective catalytic processes and the development of sustainable synthetic methods.

C.1) CATALYSIS AND SYNTHESIS FOR A SUSTAINABLE WORLD: a) Synergistic catalytic processes to transform methane and other abundant feedstocks into high value-added products. b) Metal-based technologies for C-H activation/C-C bond formation (M. Fañanás, M. Gulías). c) Synthetic methods for anticancer agents (J.L. Mascareñas/F. López). d) Catalytic routes for the preparation of doped PAHs and bioactive heterocycles (C. Saá/J. Varela). e) Theoretical methods and mechanistic studies (A. Fernández-Ramos, R. García-Fandiño).

C.2) CHEMICAL TECHNOLOGIES FOR PRODUCT HEALTH (J. Sardina): Application of chemical technologies to the development of safe, sustainable processes in the industry: product health in consumable goods.

The main novelty regarding this area is the reinforcement of the sub-area C.1 in two relevant topics: i) M. Ortuño is launching a new research line based on **simulation of MOFs and related heterogeneous catalytic systems for biomass Upgrading**; and ii) M. Nappi is leading a new research line focused on **sustainable chemical methods promoted by visible light for greenhouse gases valorisation, biodegradable polymers and bioconjugation processes**.

Despite each group focuses on specific thematic and research lines, the scientific organization has been designed to facilitate interactions and synergies between groups of experts on different subjects and thus allow to pursue interdisciplinary projects and relevant scientific challenges from an interdisciplinary perspective.

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.

2. RESOURCES

2.1 Research facilities

The CiQUS building, has 5.900 m^2 built-up area with 22 RESEARCH LABS (90 m^2 each) designed under the criteria of safety, sustainability and flexibility, and equipped with first class laboratory furniture suited to fit the needs of the different research areas: synthetic chemistry, chemical biology and materials science.

Furthermore, over 1000 m^2 are dedicated to shared research support facilities, a highly well-equipped infrastructure to cover the needs of all our research areas and interdisciplinary projects:

- **4 General Support Laboratories** (over 200 m^2 in total) for instrumental equipment, covering a broad range from analytical to preparative experimental techniques: chromatography (HPLC, UHPLC, Recycling GPC, SFC, GC, GC-MS, LC-MS), spectroscopy and spectrometry [UV-Vis, IR, fluorescence, CD, Dynamic Light Scattering [DLS and (MADLS)], NanoDrop spectrophotometers], calorimetry (DSC, TGA), etc.

Representative General Support Laboratories

- **An NMR room** equipped with two 300 MHz and one 500 MHz spectrometers, two of them including a robot module for continuous NMR sample tube handling automation. This equipment is part of the equipment for the Research Infrastructure Area at the USC and also provides service to the rest of the university community. This service works under the supervision of the USC-NMR technical staff.

- **2 Cell Culture Laboratories** equipped with biosafety cabinets (with the certification and validation of Biosafety Level 2, BSL-2), centrifuges, cell culture incubators, among other cell culture stuff.

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

Other facilities and resources include a radioactive facility, two cold rooms, a high-pressure lab (in the roof of the building), glove boxes, solvent purification systems, lyophilizers, Automated Microwave Peptide Synthesizer, a computer cluster and other small equipment.

It is very important to emphasize that the management structure of the centre contributes to 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 general use. Sharing equipment also allows for expert exchange of different instrumental techniques and for the development of scientific collaborations and interdisciplinary projects.

Our central service for purchasing of solvents and other consumables is also very relevant from an economical and safety (reduction of stocks of hazardous and flammable materials) perspective.

A CiQUS' virtual tour is available at our webpage (https://www.usc.es/ciqus/visita-virtual/). Through this section it is possible to visit our laboratories and facilities, additional information and specific features are also included for the different rooms. Implementation of the English version is in progress.

Some screenshots form CiQUS virtual tour

Finally, with regard to audio-visual and IT resources, the center has a lecture room equipped with a digital video production to enable streaming events (e.g., lectures, PhD viva ceremonies…) through Microsoft Teams and Zoom platforms, and even to broadcast open events by our YouTube channel; two seminar rooms fully equipped for hosting online meetings and a computer server for remoting access to the experimental files and the automatic periodic backing up of the experimental data from all CiQUS equipment and the rest of the CiQUS general archive.

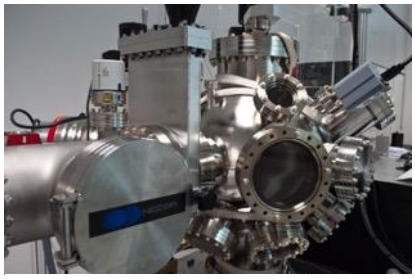
During 2021, the center acquired the programme "*ChemInventory*", a cloud-based software for managing the location and availability of the chemical compounds at the center. This software is available to the different CiQUS research groups for managing and sharing their own inventories with the other groups.

All facilities, resources and laboratories work under the supervision of CiQUS' technical staff.

2.2 Singular Laboratories

• ***Advanced Microscopy Laboratory*** for live-cell imaging equipped with a Hyperspectral Microscope, a Confocal Microscope with Spinning-Disk and TIRF modules "Nikon Dragonfly", an Epifluorescence Microscope and a flow cytometer.

• ***PLD Laboratory***: equipped with a Pulse Laser Deposition (PLD) system and a cryostat system for electrical transport, Seebeck Coefficient and thermal conductivity measurements.



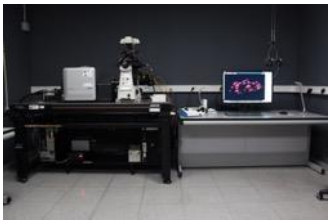
PLD Equipment

• ***Lithography Laboratory:*** equipped with photoresist film (SpinCoater) and metallic and dielectric layers (PECS) deposition systems, mask aligner, a wire-bonding system and a battery testing equipment.

• ***AFM microscopy Laboratory***. Equipped with an AFM NX-10 Park Systems microscope, 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 additional modules of electrical conductivity and thermal conductivity.

• ***Innovative Lab for technology development***. an open space for developing and implementing novel technologies based on CiQUS's knowledge. At this moment, it is dedicated to the development of a system for the measurement of thermal conductivity by frequency-resolved thermoreflectance.





Laboratories for AFM microscopy (left), lithography equipment (centre) and advanced microscopy (right)

2.3 New Equipment

A preparative scale HPLC system, a high range Differential Scanning Calorimeter (DSC) and an Isothermal Titration Calorimeter (ITC; jointly with Prof. P. Taboada) have been acquired within the framework of the *Xunta de Galicia* financial agreement for the acquisition of scientific technical equipment, during the year 2021.

Furthermore, CiQUS' spectroscopic capabilities were strengthened with the acquisition of an enhanced measurement capabilities spectrofluorometer (picosecond lifetimes, NIR spectral coverage, quantum yield measurements) and a high sensibility UV-Vis-NIR spectrophotometer. This instrument was acquired through the national competitive call for acquisition of scientific technical equipment launched in 2019 by the Spanish State Research Agency (Agencia Estatal de Investigación – AEI).

Additionally, a new sizing, charge, and particle concentration measurement system (MADLS) was also acquired to improve the previously available particle measurement equipment.

2.4 New Lab spaces

The recent incorporation of several young researchers leading their own research lines, as well as the increased number of postdoctoral researchers and PhD candidates associated to the starting of many international projects led to a situation of maximum occupation of the CiQUS Labs.

Due to this circumstance, the USC approved that some spaces, available at the CIBUS building, were upgraded for using by CiQUS researchers. The CiBUS is located about 50 meters form the CiQUS, and both buildings are connected by internal corridors. At the CiBUS, CiQUS technical staff is working on the set up of: i) a molecular biology research lab, which will be used by the newly incorporated *Ramón y Cajal* researcher Beatriz Pelaz and other biologists working in different groups at CiQUS; ii) a photochemistry room, equipped with an improved

300 W Xenon lamp and with specific safety elements, iii) new spaces equipped with biological safety cabinets and cell incubation systems for implementing the CiQUS' cell culture capacity, iv) a new laboratory designed and equipped for the assembly and study of new battery prototypes, and v) a new hands-on lab equipped with some scientific instruments for masterclasses, scientific training and outreach activities.

2.5 Other facilities and resources at the USC

In addition to our own facilities, CiQUS researchers have access to the general research support services of the University of Santiago de Compostela (see www.usc.es/gl/investigacion/riaidt/) most of them located at the CACTUS building, 200 m away from CiQUS. These services include a high field NMR (750 MHz), mass spectrometry, electronic and confocal microscopy, X-Ray diffraction, magnetic susceptibility, etc, as well as the associated technologic platforms.

Among them, it is especially crucial for some of our research groups, the new high-resolution Transmission Electron Microscopy (TEM) - specifically, a JEOL JEM- F200CF-HR microscope, acquired in 2019 thanks to the financial support of the Consellería de Cultura, Educación e Universidade. The technical capacities of this instrument are fundamental for the development of research lines at CiQUS related with soft-matter and, in particular, for the area of carbon-based materials (including the ERC-Starting Grant NANOCOMP, PI Dr. María Giménez).

CiQUS researchers working in biological topics have access to the CEBEGA, the Center for Experimental Biomedicine of the USC, when they require experiments which involved animal testing.

For computational studies, CiQUS researcher are regular user of CESGA, the Galician Supercomputing Center (https://www.cesga.es/en/home-2/).

Finally, CiQUS PIs regularly support and/or lead other proposals for the acquisition of equipment for the general R&D services of the University of Santiago (CACTUS). In this context, an application proposal for the acquisition of a SQUID (superconducting quantum interference device) magnetometer, led by Prof. F. Rivadulla (CiQUS PI), was granted by the Spanish State Research Agency through the national competitive call for acquisition of scientific technical equipment launched in 2021 (Ref. EQC2021-007176-P).

3. SCIENTIFIC REPORT 2021

The following chapters describe and summarize CiQUS key research capabilities as well as its scientific activity in 2021. More detailed information is available in the Annexes section and the CiQUS website: www.usc.es/ciqus/en.

3.1 Human Resources

32 Principal Investigators (PIs), 5 Junior Scientists (Junior Group Leader), 41 postdocs, 95 PhD candidates, 39 Master students and 27 Technical and administrative assistants (9 of them are directly hired by CiQUS research groups, under their own R&D research projects, for supporting them with administrative issues and/or technical research tasks) (Dec 31, 2021)

In December 2021, more than 230 people (39% female; 8% foreigners from up to 11 different countries) were working at CiQUS: 32 Principal Investigators (3 of them *Ramón y Cajal* associates; 22% female; 6% foreigners), 5 Junior group leaders (2 Ramón y Cajal associates, 1 Xunta de Galicia *"Distinguished Researcher",* 1 Manuela Barreiro – USC "Distinguished Researcher, 1 JIN researcher; 40% female; 20% foreigners), 41 postdoctoral researchers (3 *Juan de la Cierva* researchers, 1 MSCA-IF and 3 Xunta's postdoctoral researchers; 37% female and around 15% of CiQUS postdoctoral researchers coming from abroad), 95 PhD candidates (42% female and 11% foreigners), 38 MSc students (41% female), together with 12 research support technicians (2 of them hired by a particular group), 15 people for administrative, R&D management and service tasks (7 of them hired by particular groups for administrative support). Furthermore, around 4 USC faculty members collaborate in the scientific activity of different research groups, though they are not officially affiliated at CiQUS. The full list of people (as for December 2021) is included in Annex I.

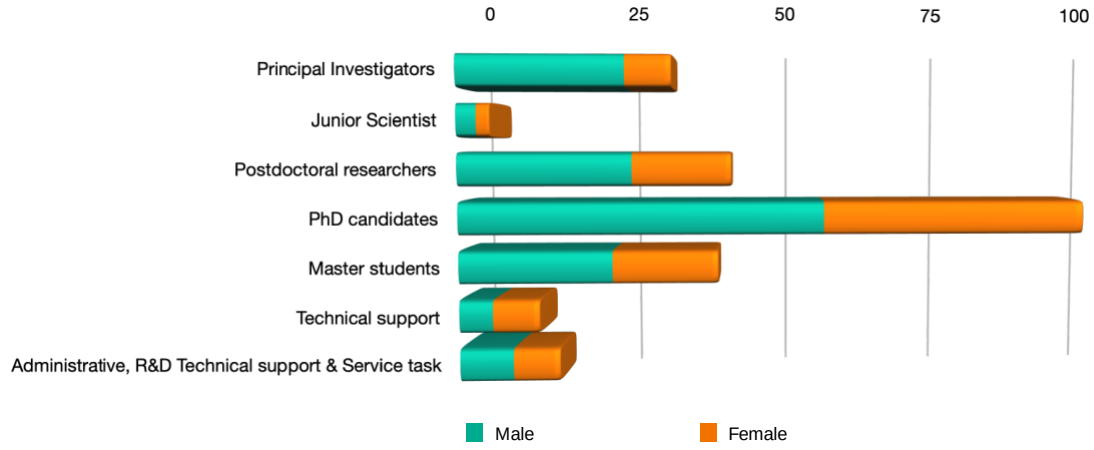


Chart 1. Distribution of human resources by category

3.1.1 Talent Recruitment

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

As a research centre that belongs to the University of Santiago de Compostela, our recruiting strategy to attract new talent as Research Staff is governed by the legal framework of the University access regulation. CiQUS recruitment policies have combined a proven ability to attract talent through competitive HHRR calls (see section 3.1.2) with other specific actions, funded by our own centre's "structural" budget (granted by the Xunta de Galicia).

In this context, CiQUS has implemented a number of initiatives to attract the best researchers at different levels. Some of these actions are detailed below.

- **Junior group leaders and *Ramón y Cajal* researchers:**

Over the years CiQUS has been able to attract and recruit extremely talented young researchers, with long international trajectories, mainly through the ***Ramón y Cajal (RyC) programme***, a tenure track-like program launched by the Spanish Ministry of Science and Innovation within the State Programme for the Promotion of Talent and its Employability in R&D&I framework. Through this highly competitive call based on the attraction, recruitment, support and early promotion of outstanding researchers, up to 6 young promising scientists, whose research profiles were aligned with our scientific agenda, have joined the CiQUS in the last 8 years. Remarkably, 4 of these 6 recruited scientists had no previous relationship with Galicia.

Our commitment with career development defines a solid policy to support these junior scientists on the development of independent and new research lines. Those with excellent performance are promoted after positive evaluation by the CiQUS ESAB. Thus, 3 RyC researchers recruited in 2015-2016 (M. Fañanás, J. Montenegro, P. del Pino), were promoted to PIs in 2016. Later on, **three brilliant RyC female researchers** were recruited in the period 2018-2019, M. Giménez, who joined CiQUS after 10 years in U. Nottingham, was promoted to PI in 2018, and R. García Fandiño and B. Pelaz both promoted to PIs in September 2020. It is highly remarkable that 4 of these researchers (Fañanás, Montenengro, Giménez, Pelaz) are currently ERC Grantees, while del Pino and García-Fandiño lead international and national projects.

As a result of the 2020 Ramón y Cajal call, 3 new RyC researchers joined the CiQUS throughout the year 2021, Ester Polo, Rafael Ramos and Beatriz Orosa. As a result of the 2021 RyC call, María Tomás joined the CiQUS as RyC in January 2022. It is worth mentioning CiQUS' commitment to attract and retain young talent and achieve a gender balance as shown by the fact that 6 of the 10 researchers recruited through the Ramon y Cajal Programme over the last 8 years are female.

The new 4 RyC grantees were promoted to Junior Scientists within CiQUS organization, together with Manuel Ortuño and Manuel Nappi, researchers hired as part of the CiQUS own career development scheme. This category has been defined for young researcher who launch and lead new research lines at the CiQUS.

- **Postdoctoral researchers and PhD Candidates:**

During 2021, up to 78 researchers were directly hired by the CiQUS groups through R&D contracts. 31 Research Associates (postdoctoral level) and 47 PhD candidates.

Furthermore, a number of postdoctoral researchers and PhD candidates were hired in 2021 through different HHRR competitive calls funded by public agencies:

- *2 Postdoctoral researchers: 1 MSCA (call 2021), 2 "Juan de la Cierva - Incorporación contracts (JdC)*" (call 2019) and 6 Margarita Salas. 1 María Zambrano, 1 Margarita Salas and 2 JdC will join the CiQUS in 2022 as a result of different calls launched in 2021 (see section 3.1.2).

- *22 PhD candidates:* 11 "Xunta de Predoutoral" fellowships, 5 FPU and 6 Predoctoral Contracts funded by the Spanish State Research Agency (AEI, former FPI). (See section 3.1.2 for further details)

- **Master students:**

- *Research initiation contracts for CiQUS Master Students*: 10 part-time contracts were offered during the year 2021 for the development of a Master Research Project under the supervision of 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 relationship with the University of Santiago.

- **Undergraduate students:**

  - *7th 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. For the second time, the application process was coordinated by the University of Santiago de Compostela Service for R&D Human Resources Calls and the call was jointly launched with the CiMUS, the CiTIUS and the IGFAE centers.

The CiQUS Summer Fellowships were granted to 15 students (6 of them female) from 5 different universities, all with an average mark on their academic track record above 8.0 points on a scale 0-10. Significantly, 47% of CiQUS summer 2021 fellows are currently continuing their training activity linked to CiQUS. 7 of them were enrolled in the bachelor's in chemistry, 4 in biotechnology, 2 in the double bachelor's degree in physics and Chemistry and the other 2 in the double bachelor's degree in biology and Chemistry.

Remarkably, 5 of these scholarship holders are currently pursuing their master's degree at the center (33%) and another 2 are developing their bachelor thesis dissertations at the CiQUS (13%).

3.1.2 Human Resources Competitive Public Funding

Several grants have been awarded to young **postdoctoral** researchers in 2021 to carry out their research activity at CiQUS:

- **Ramón y Cajal Programme***:* Dr María Tomás ***PhD in Chemistry from the University of Oviedo*** in 2011 and over 3 years of Postdoctoral research at Ludwig München Universität under the supervision of Prof. Thomas Carell. Her research will be focus on the use of light as energy source for the development of novel bioorthogonal catalytic transformations.
- Dr Manuel Nappi was hired as a **Manuela Barreiro Distinguished researcher position** at the University of Santiago de Compostela.
- The result of the 2020 "**Juan de la Cierva – Incorporación**" call will lead to the recruitment of Dr. Rafael Rodríguez Riego (expected to join CiQUS in Spring 2022; supervisor: E. Quiñoá & F. Freire) and Dr. José Manuel Vilas Fungueiriño (expected to join CiQUS in Summer 2022; supervisor: F. Rivadulla)] as postdoctoral research associates at CiQUS, respectively. Additionally, Dr. Jéssica Rodríguez (supervisor: J.L. Mascareñas) and Dr. Jaime Mateos started their Juan de la Cierva – Incorporación contracts during the year 2021 (Call 2019).
- Dr. Adrián Sánchez (supervisor: J. Montenegro) will join the CiQUS in 2022 as a result of the **new call "María Zambrano"** for postdoctoral researchers launched by the Ministry of Universities.
- Up to 7 young researchers were granted within the **new "Margarita Salas" postdoctoral programme**. 6 of them (David Bugallo; David Cagiao; Zulema Fernández, Jacobo Gómez, Eva González, Iago Pozo) will expend the next two year in a research institution abroad, and later on they will come back for a third year at the CiQUS. Carlos Lázaro will expend the first 2 years at the CiQUS (supervisor: J.L. Mascareñas) and he will leave to another institution during the third year.

With regard to **predoctoral** trainees and master students, thirteen new competitive research contracts have been awarded to CiQUS PhD students in 2021:

- *MECD – FPU Predoctoral fellowships*: Lucía Vizcaíno (supervisor: M. Giménez), Antía Fernández (supervisor: B. Pelaz), Iván Huertas (supervisor: M. Gulías), Axel Sarmiento (supervisor: M. Vázquez and E. Vázquez) and Andrés Arribas (supervisor: J.L. Mascareñas).

- *AEI Predoctoral Contracts (former FPI)*: Noa Varela (supervisor: F. Rivadulla), Adrián Martínez (supervisor: D. Peña), Xulián Fernández (supervisor: J.L. Mascareñas), Manuel Fernández (supervisors: E. Quiñoá and F. Freire), Jesús Janeiro (supervisor: D. Pérez), and Ezequiel Troncoso (supervisor: J. Granja).

- *Xunta de Galicia – Predoctoral contracts*: Andrés Álvarez (supervisor: M. Fañanás); Antonio Andújar, Lucía Campos, Aitor García, Darío Pastoriza (supervisor: E. Sotelo); Bruno Delgado (supervisor: E. Fernández-Megía); Sara Illodo (supervisor: F. Rodríguez); Alejandro Jiménez (supervisors: J.C. Estévez and R. Estévez); José María Martínez (supervisor: J. Montenegro); Laura Martínez (supervisors: E. Vázquez and M. Vázquez) and Alejandro Rey (supervisor: J.L. Mascareñas). Additionally, Antía Fernández (supervisor: B. Pelaz); Axel Sarmiento (supervisors: M. Vázquez and E. Vázquez); Noa Varela (supervisor: F. Rivadulla) and Lucía Vizcaíno (supervisor: M. Giménez) were awarded with this grant but declined after receiving the corresponding FPU grants or AEI Predoctoral Contracts, respectively.

Competitive Predoctoral Fellowships and Contracts awarded in 2021		
Program	**Funding Agency**	**No. grants awarded**
Xunta de Galicia – Predoctoral contracts	Xunta de Galicia	15(*)
MECD – FPU	AEI	5
AEI Predoctoral Contracts (former FPI)	AEI	6
Total		**26** (*)

(*) 4 of them were declined.

Competitive Postdoctoral Contracts awarded in 2021		
Program	**Funding Agency**	**No. contracts awarded**
Ramón y Cajal	AEI	1
Juan de la Cierva – Incorporación	AEI	2
"Manuela Barreiro" Distinguished Researcher	USC	1
Margarita Salas	Ministry of Universities	7
María Zambrano	Ministry of Universities	1
Total		**12**

Ongoing Competitive Contracts 2021		
Program	**Funding Agency**	**No. of active contracts**
Ramón y Cajal	AEI	6
Distinguished Researcher	Xunta de Galicia	1
"*Manuela Barreira*" Distinguised Researcher	USC	1
Juan de la Cierva Incorporación	AEI	5
MSCA Postdoctoral Fellowships	European Research Executive Agency (REA)	2
Xunta de Galicia – Mod. A	Xunta de Galicia	5
Margarita Salas	Ministry of Universities	6
MECD - FPU	AEI	17
AEI Predoctoral Contracts (former FPI)	AEI	17
Xunta de Galicia - Predoctoral Contracts	Xunta de Galicia	25
MSCA-ITN	European Research Executive Agency (REA)	4
Total		**89**

In addition to these new competitive fellowships, an important number of research contracts have been drawn in 2021 under different funded research projects and contracts.

It is worth mentioning that, in 2021, **up to 89 researchers were funded by competitive public programs** (more than 51% of CiQUS researchers considering postdoctoral researchers and PhD Candidates).

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

3.2 Research Funding

- Funding associated to new R&D projects starting in 2021 reached 9,9 M € (54,9% international projects, 13,1% national projects, 22,8% regional projects, 7,0% R&D contracts & valorisation projects, 2,2 % correspond to special agreements with the Regional Government and over 0,1% of patent licensing).
- 1 ERC-SyG, 1 ERC-StG, 2 ERC-PoC, 1 FET Open, 1 ICT, among others.
- 10 AEI (*Retos*, *Generación de Conocimiento* and *Prueba de Concepto* – including 4 associated predoctoral contracts), among others.

CiQUS has proved to have an excellent fundraising capacity despite the difficult financial circumstances, increasing not only the regional and national funds but also international funding. Quite remarkable is also the increase observed in the funds for R&D services and valorisation projects from public sources. This trend clearly shows CiQUS' commitment to strengthen its knowledge transfer capacity. Our figures as of December 31st, 2021, show 66 active projects and 21 contracts for a total amount of 16,7 M €.

Regarding new funds raised **in 2021, CiQUS started 26 new projects and 9 new R&D contracts or Proof of Concept projects for a total amount of 9,6 M €**. If the income granted from regional agreements and patent licensing is also included, the total funds raised by the CiQUS researchers during the year 2021 amounts to 9,8 M €, where up to 54,9% came from international projects, 13,1% from national projects, 22,8% from regional projects, 7,0% from R&D contracts and valorisation projects, 2,2% correspond to special agreements with the Regional Government and over 0,1% derived from patent licensing). This represents an increase of 26% in the funds raised by CiQUS researchers respect of 2020 and more than 72% regarding the funds raised in 2019. We must highlight the remarkable increase observed for the international funding sources as well as the number of international projects granted during the year 2021.

A retrospective analysis over the past five years clearly shows the remarkable rising and stable fundraising capacity in terms of international budget, specially from the European Research Council (ERC). Since 2014, CiQUS PIs have been granted with 10 ERCs (1 SyG, 1 AdG, 1 CoG, 3 StG and 4 PoC). Furthermore, CiQUS PIs have also participated in several international collaborative projects over the past years (1 ICT, 3 FET-Open, HFSP, H2020-Societal Challenges…).

The following table and chart show the increasing fundraising capacity of the CiQUS during the last 5 years. More detailed information regarding 2021 is shown in Annex II and Annex III**.**

Table 5. R&D fundraising evolution at the CiQUS since 2016

	2016	2017	2018	2019	2020	2021
1. International Projects	1.670.215,20 €	757.574,89 €	1.795.300,60 €	1.269.235,87 €	3.031.951,36 €	5.411.879,73 €
2. National Projects	833.017,00 €	1.666.424,00 €	712.488,00 €	827.602,00 €	2.254.575,00 €	1.291.500,00 €
3. Regional Projects	709.766,74 €	2.165.000,00 €	850.000,00 €	1.950.000,00 €	1.887.260,40 €	2.246.862,36 €
4. R&D Contracts and Valorization Projects	1.084.723,75 €	1.278.285,80 €	885.310,00 €	1.203.540,20 €	544.886,47 €	685.900,00 €
5. Regional Agreements (*)	278.750,00 €	140.000,00 €	203.877,83 €	439.900,00 €	77.500,00 €	219.000,00 €
6. Patents & Licensing				28.000,00 €		7.381,00 €
7. Donations & Crowdfunding					30.000,00 €	
Total	**4.576.472,69 €**	**6.007.284,69 €**	**4.446.976,43 €**	**5.718.278,07 €**	**7.826.173,23 €**	**9.862.523,09 €**

(*) Regional agreement refers to specific non-competitive Regional funding link to ERC-grantees Programme and Centro de Investigación do SUG accreditation.

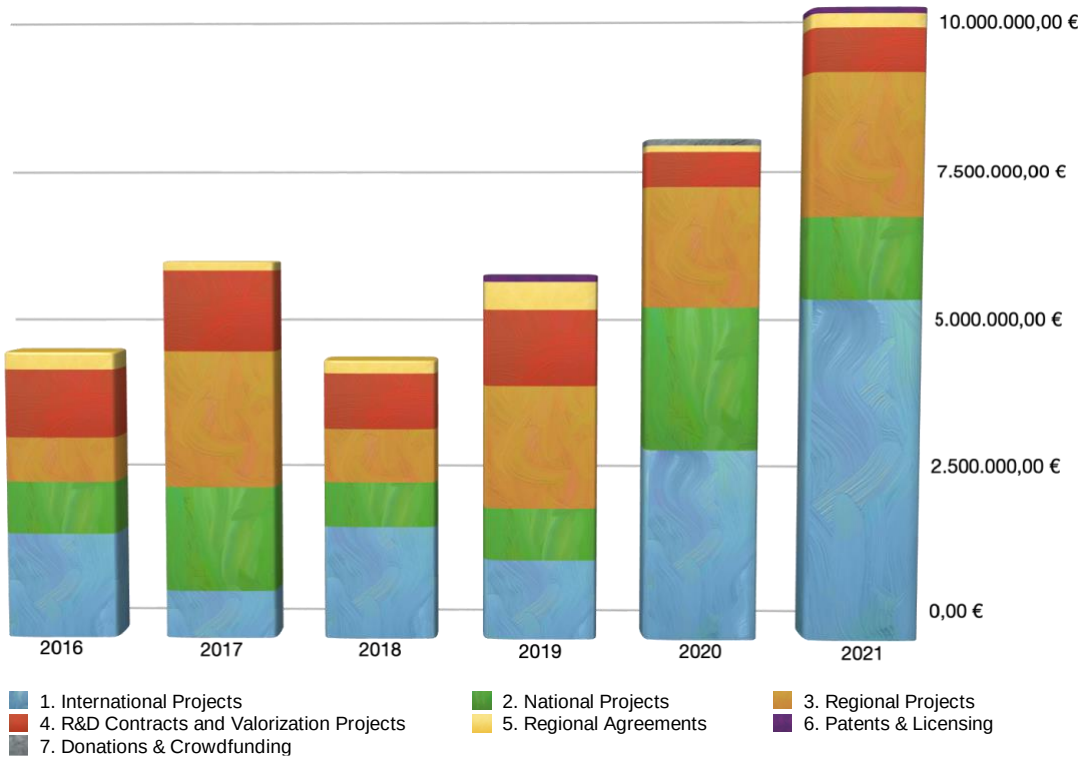


Chart 3. Evolution of the fundraising capacity, 2016-2021 (*)

(**) HR Programs are not included in this chart

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

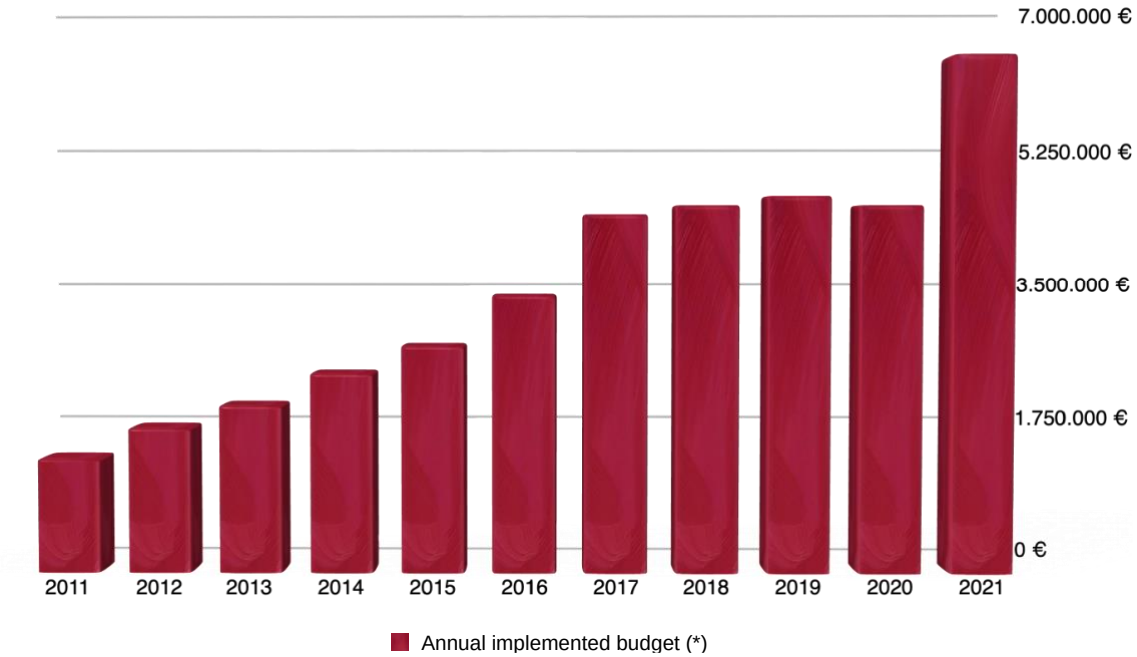


Chart 4. Evolution of the annual implemented budget, 2011-2021 (*)

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

Our annual implemented budget has continuously increased from 1,4 M € in 2011 (CiQUS creation date) up to 4,6 M € in 2019. Remarkably, despite of the lockdown period due to the COVID-19 pandemic crisis, 2020 results remained practically constant compared to the previous year (4,5 M €), which is quite exceptional and shown that CiQUS research groups were able to keep its research activity in spite of all the difficulties over that year. Finally, it is worth noting the remarkable increase observe of the CiQUS implemented budget for the year 2021, that rises up to more than 6,3 M €, which represent an increase over the previous year of more than 40%. This increase is mainly due to the international projects that were launched during the whole year 2021.

Regarding the projects starting in 2021, these are the key facts:

- **International Projects: 5,4 M €**. The year 2021 has been especially successful in terms of new international projects. Among others, Prof. D. Peña started the **ERC-SyG project "MolDAM"** (Single Molecular Devices by Atomic Manipulation), that involves the participation of researchers from IBM Research GMBH (Switzerland), the Universitaet Regensburg (Germany) and CiQUS-USC; Dr. B. Pelaz started the **ERC-StG project "SPACING"** (Spatially-Controlled ligand arrNGement by origami-based naoprinters) and the ICT project "REAP" (Revealing drug tolerant persister cells in cancer using contrats enhanced optical coherence and photoacoustic tomography), that involves the participation of researchers from the Medizinische Universitaet Wien, the AIT Austrian Institute of Technology GMBH, the Picophotonics Oy (Finland), the Tampereen Korkeakoulusaatio SR (Finland), the Politecnico di Torino (Italy), Innolas Laser GMBH (Germany), Lavision Biotec GMBH (Germany), Linoix International BV (The Netherlands) and CiQUS-USC; and Prof. E. Vázquez started the **FET-Open "e-Prot"** (Protein-based conductive materials pave the way for next-generation energy storage devices), that involves the participation of researchers from CiC biomaGUNE (Spain), Universidade de Aveiro (Portugal), Ben-Gurion University of the Negev (Israel), University of Alicante (Spain), CiC EnergiGUNE (Spain), Smart Fabric Inks Limited (UK) and Specific Polymers (France)

- **National Projects: 1,3 M €**. CiQUS researchers successful competed in the National Research Program (8 projects: 5 of them associated with the RETOS (societal challenges) call and 3 of them associated to the GENERACIÓN DE CONOCIMIENTO call, both of which work in a 3-year cycle). Remarkably, 3 of them were awarded to CiQUS Junior Scientists (E. Polo, M. Nappi and M. Ortuño). Additionally, 4 of these projects have also been granted with a Predoctoral Contract.

The national funding also included the young talent incorporation program Ramón y Cajal (awarded to E. Polo, R. Ramos), and the Juan de la Cierva Incorporación (awarded to J. Rodríguez and J. Mateos).

CiQUS PIs got also funds through other national highly competitive calls. A project of Prof. M. Vázquez was granted within the framework of the "IDEAS Semilla 2021" programme of the Spanish Association Against Cancer (AECC). In this project, a new family of anticancer drugs will be developed based on selective cleavage of DNA three-way junctions by Cu(II) peptide helicates acting as nucleases.

- **Regional Funding: 2,2 M €**. 43% (0,96 M €) accounts for the support of the Xunta de Galicia to the CiQUS as accredited *Research Centre* of the Galician University System (SUG), co-funded by the European Regional Development Fund – (ERDF), project ED431G 2019/03. Additionally, CiQUS Researchers were granted with up to 5 projects from competitive calls launched by the Regional Government for a total amount of 1,29 M €.

- **R&D and Valorisation contracts: 0,69 M €.** In 2021, Prof. J.L. Mascareñas started the **ERC-PoC "antiCSC" project** (Targeting the cancer stem cell (CSC) metabolism with designed, reactive metal complexes) and, Dr. M. Giménez started the **ERC-PoC "ZABCAT" project** (A New Zn-Air Battery Prototype to Overcome Cathode Degradation Through Catalyst Confinement) in collaboration with the CIDETEC Foundation in January 2021. These 2 ERC-PoC projects are the second ERC-grants awarded to J.L. Mascareñas and to M. Giménez, respectively. They are also the third and fourth ERC-PoC grants that will be developed at CiQUS. Remarkably, the only 4 ERC-PoC granted in the Galician Region so far belongs to CiQUS PIs.

Furthermore, CiQUS researcher successful competed in the new call “Proof of Concept - R&D&I Projects” launched by the Spanish Research Agency (AEI). The projects “Metal-based anticancer targeting mitochondrial respiration of cancer stem cells” (led by J.L. Mascareñas) and “A new chemical platform for customized gene therapy (GeneVector) (led by J. Montenegro) were funded within this new call. Additionally, CiQUS researchers signed 5 R&D contracts during 2021 (0.22 M €) with different companies.

Finally, it is also worth noting the income associated to the contracts of some of CiQUS researchers (e.g., RyC researchers, JdC postdoctoral researchers; MSCA postdoctoral researchers and predoctoral researchers from regional and national calls) awarded through Human Resources Competitive public calls.

3.3 Research Output

3.3.1 Scientific publications

CiQUS maintained a good record of scientific contributions in 2021, with **99 articles,** 95 of which were published in JCR Journals (96% of all CiQUS publications). **83% of CiQUS JCR articles were published in journals indexed in the first quartile (Q1)** and, more significantly, **45% in the first decile (D1)** of their respective thematic areas of the Web of Science database (WoS) (see Annex IV). In 2021, the **average impact factor of CiQUS JCR articles was 8,44,** keeping this impact indicator above 8 for second year in a row and above 7 for seventh year in a row.

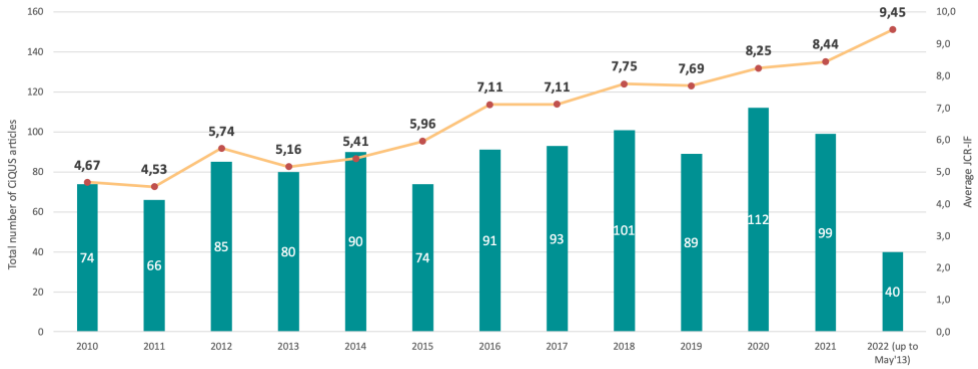


Chart 5. Evolution of the number of publications and JCR-average impact factor (*) 2010-2022

Chart 6. Distribution of the number of publications by JCR-quartiles (*) 2010-2022

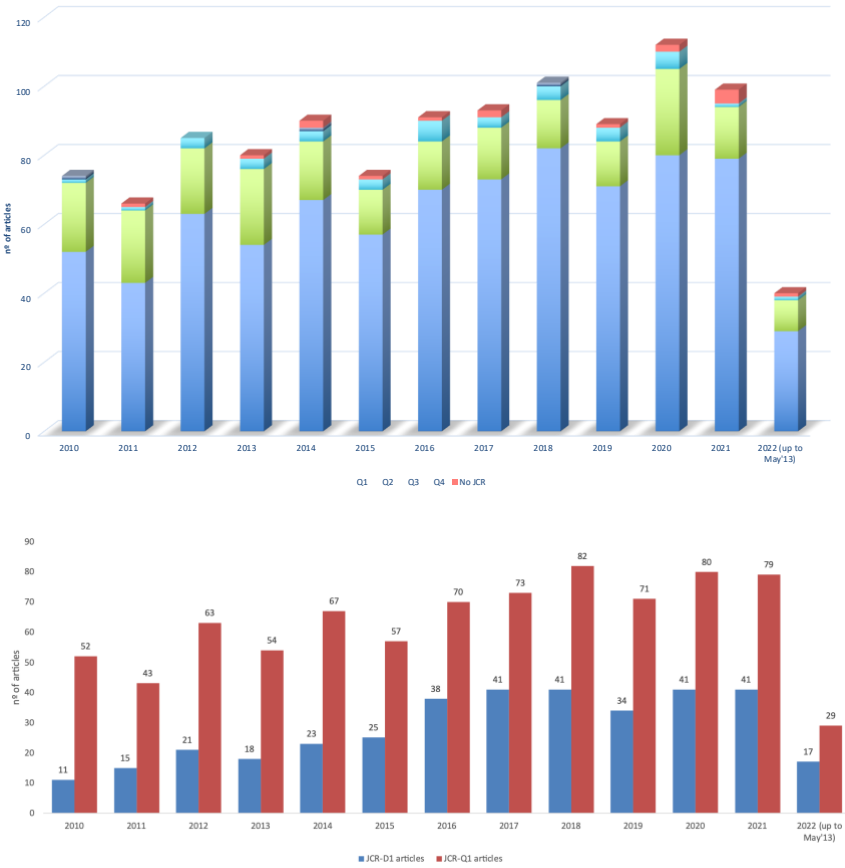


Chart 7. Evolution of the number of publications published in D1 and Q1 journals (*) 2010-2022 (**)

(*) Journal Impact factor values and quartiles for the years 2021 and 2022 are based on *2020 Journal Citation Reports (2020 data)*. 2021 data have not yet been published. (**) For Q1 articles we also consider those articles published in D1 journals.

Furthermore, the CiQUS has achieved a sharp increase in the number of publications in top-ranked journals. In 2021, CiQUS published a total number of **32 papers with IF>9**, which represents 34% of CiQUS JCR publications in 2021. It should be especially highlighted the number of articles published by CiQUS researchers in the prestigious journal Angewandte Chemie International Edition during the year 2021. Up to 12 articles (which represents the 12% of 2021 CiQUS scientific production) were published in Angewandte Chemie International Ed. along 2021.

Table 6. Scientific Journals with JCR- IF > 9, in which CiQUS articles were published during 2021 and total number of articles per Journal

Full Journal Name	JCR | IF (*)	nº of published articles
Trends in Chemistry	24,081	1
Advanced Science	16,806	1
ACS Nano	15,881	5
Journal of the American Chemical Society	15,419	3
Angewandte Chemie-International Edition	15,336	12
Nature Communications	14,919	3
ACS Catalysis	13,084	1
Nano Letters	11,189	1
Chemistry of Materials	9,811	1
Carbohydrate Polymers	9,381	1
ACS Applied Materials & Interfaces	9,229	3
Total nº of CiQUS articles		32

(*) Journal Impact factor values for the year 2021 are based on *2020 Journal Citation Reports (2020 data)*. 2021 data have not yet been published.

Table 7 shows the list of scientific journals in which CiQUS articles were published in 2021. These journals are listed according to the total number of CiQUS articles published in each journal during 2021 and by alphabetical order.

Table 7. Scientific Journals in which CiQUS articles were published during 2021 and total number of articles per Journal.

Journal Name	JCR | IF(*)	nº of published articles
2D Materials	7,103	1
ACS Appl. Mater. Interfaces	9,229	3
ACS Appl. Nano Mater.	5,097	1
ACS Appl. Poly. Mater.	No JCR	1
ACS Catal.	13,084	1
ACS Macro Lett	6,903	1
ACS Nano	15,881	5
ACS Omega	3,512	1
Adv. Sci.	16,806	1
Adv. Therap.	No JCR	1
Angew. Chem. Int. Ed.	15,336	12
Antibiotics	4,639	1
Appl. Phys. Lett.	3,791	2
Bioconjugate Chem.	4,774	1

Bioorg. Chem.	5,275	1
Carbohydr. Polym.	9,381	1
Chem. Commun.	6,222	2
Chem. Eur. J.	5,236	2
Chem. Mater.	9,811	1
ChemSusChem	8,928	1
Colloid Surf. B-Biointerfaces	5,268	1
Eur. J. Org. Chem.	3,021	1
Front. Chem.	5,221	1
Front. Immunol.	7,561	1
Front. Microbiol.	5,64	1
Front. Pharmacol.	5,81	1
Fuel	6,609	1
Giant	No JCR	1
Int. J. Pharm.	5,875	1
J. Am. Chem. Soc.	15,419	3
J. Antimicrob. Chemother.	5,79	1
J. Cheminformatics	5,514	1
J. Eur. Ceram. Soc.	5,302	1
J. Med. Chem.	7,446	3
J. Mol. Liq.	6,165	3
J. Org. Chem.	4,354	3
J. Organomet. Chem.	2,369	1
J. Phys. Chem. C	4,126	1
J. Phys. Chem. Lett	6,475	1
J. Phys. Photonics	0,94	1
Jove-J Vis Exp	1,355	1
Langmuir	3,882	1
Mol. Pharmaceut.	4,939	1
Molecules	4,411	1
Nano Lett.	11,189	1
Nanomaterials	5,075	1
Nanoscale	7,79	3
Nanoscale Adv	4,553	1
Nat. Commun.	14,919	3
New. J. Chem.	3,591	1
Org. Lett.	6,005	3
Pharmaceutics	6,321	1
Pharmacol. Res.	7,658	1
Phys. Chem. Chem. Phys.	3,676	1
Phys. Rev. Applied	4,985	1
PLoS Comput. Biol.	4,475	1

Polym. Chem.	5,582	2
Polymers	4,329	2
RSC Chem Biol	No JCR	1
Sci. Rep.	4,379	3
Trends Chem.	24,081	1
Total nº of CiQUS articles		99

(*) Journal Impact factor values for the year 2021 are based on *2020 Journal Citation Reports (2020 data)*. 2021 Data have not yet been published.

It is very important to note that many of the publications in top journals are the result of research carried out exclusively in the centre, which demonstrates that the CiQUS' groups can themselves be highly competitive, and do not depend on others. Also, there is a progressive increase in publications arising from internal collaborations.

However, we are firm believers of scientific collaboration to pursue cutting-edge challenges. Therefore, 49% of the contributions during the period of reference involve international collaborations, many of them with prestigious research centres and groups. It is also true that, in most of them, the main corresponding author is also from CiQUS. **Annex IV** shows a full listing of the scientific articles in JCR journals published by CiQUS researchers in 2021.

Although, the total number of articles published in 2021 was slightly below 100, it is important to point out that the restrictions and limitations applied on experimental work derived from the COVID-19 pandemic (i.e., the effect of the two months of confinement in 2020, and the shift work policy maintained at our center in 2021) to comply with the measures of personal distancing, limited the number of working hours in the CiQUS facilities, clearly affected the CiQUS productivity. However, the slight reduction in the number of publications is more than offset by the very remarkable increase in the quality of published articles.

Finally, in line with the commitments of the National and European R&D funding agencies regarding Open Access policy, CiQUS encourages its research groups for publishing under Open Access models. According to Web of Science database, over 77 articles (81% of the total number of JCR papers) published by CiQUS researchers in 2021 were already Open Access articles. Furthermore, in collaboration with the USC library, supports its researchers in archiving their scientific production in the institutional online repository of the University of Santiago de Compostela (Minerva).

3.3.2 CiQUS Scientific Highlights

Among the most outstanding CiQUS scientific results, in 2021 there are remarkable contributions in the three major thematic areas of the center. We should also highlight the quality of the publications resulting from the collaboration between groups of the center (100% Q1 JCR, 80% D1 JCR and average JCR-FI = 12.6), which shows the effort of the leaders of the different research groups that make up CiQUS to combine capabilities and address new and ambitious challenges from a multidisciplinary approach. A short selection of articles derived from internal collaboration is shown below:

- *Dynamic Stereoselection of Peptide Helicates and Their Selective Labeling of DNA Replication Focus in Cells* (*Angew. Chem. Int. Ed.*). In this article, the Vázquez/Vázquez and Martínez-Costas groups, both associated with the area of Biological and Medicinal Chemistry of the center, combine the experience of Profs. E.Váquez and M.Vázquez in the synthesis of metal peptides with the biochemical expertise of Prof. J. Martínez-Costas for the designing of new Fe(II) peptide helicates and their study for the labelling of the DNA replication process inside the cell.

- A New Type of Supramolecular Fluid Based on H_2O – Alkylammonium / Phosphonium Solutions (*Angew. Chem. Int. Ed.*). The CiQUS groups led by Prof. F. Rivadulla (Physical Chemistry group) and M.

Giménez (Inorganic Chemistry group), respectively, both associated with the area of Functional Materials with Technological Application, have shown that it is possible to induce a particular structure of water using certain types of organic molecules, which confers interesting physicochemical properties to the liquid. The authors suggest that from the results published in this article, an original approach may emerge for the design of a new class of supramolecular liquids, based on aqueous solutions of small molecules containing a hydrophobic part, with potential advanced technological applications such as solvents and electrochemical media, sequestering agents of small non-polar molecules, among others.

• *3,4-Dihydropyrimidin-2 (1H) -ones as Antagonists of the Human A (2B) Adenosine Receptor: Optimization, Structure-Activity Relationship Studies, and Enantiospecific Recognition* (*J. Med. Chem.*). In this publication, the authors present the design and characterization of a "library" of 3,4-dihydropyrimidin-2 (1H) -onas as antagonists of the human adenosine A (2B) receptor A2BAR, as agents for (immune) therapy studies. cancer. The compounds presented in this article are the result of the collaboration between the group of Prof. E. Sotelo, associated with the area of Biological and Medicinal Chemistry, with extensive experience in the development of pharmacological molecules and the group of Prof. J. Sardina, associated with the area of Synthetic Technologies for Sustainable Development, with extensive experience in the design of synthetic pathways and the use of advanced NMR characterization techniques.

• *Plasmonic-Assisted Thermocyclizations in Living Cells Using Metal –Organic Framework Based Nanoreactors* (*ACS Nano*). In this paper, the authors describe the design of a microporous plasmonic nanoreactor to carry out cyclothermic cyclization reactions inside living cells. Photothermal transformation allows the generation of cyclic fluorescent products inside the cell, which can be observed by fluorescence microscopy. The strategy presented by the authors may have potential application in the specific and localized activation of prodrugs. The results achieved in this project arise from the collaboration and synergy of the groups Mascareñas / López (associated with the areas of Biological and Medicinal Chemistry and Synthetic Technologies, with extensive experience in the development of new catalytic reactions in biological media) and del Pino / Pelaz (associated with the areas of Functional Materials, with extensive experience in the design of molecular nanostructures and nanoparticle-based materials).

On the other hand, up to 7 CiQUS articles were recognized by different journals as "**Hot articles / hot topics**" in 2021: "Transition Metal - promoted Reactions in Aqueous Media and Biological Settings" (*Chem. Eur. J.*, Hot Topic: Biocatalysis); "A New Type of Supramolecular Fluid Based on H_2O – Alkylammonium / Phosphonium Solutions" (*Angew. Chem. Int. Ed.*, Hot Paper); "Photochemical Electrocyclization of Poly (phenylacetylene)s: Unwinding Helices to Elucidate their 3D Structure in Solution" (*Angew. Chem. Int. Ed.*, Hot Paper); "Bioorthogonal Azide - Thioalkyne Cycloadditions Catalyzed by Photoactivatable Ru (II) Complexes" (*Angew. Chem. Int. Ed*., Hot Topic: Click Chemistry); "Palladium Nanoparticles Hardwired in Carbon Nanoreactors Enable Continually Increasing Electrocatalytic Activity During the Hydrogen Evolution Reaction" (*ChemSusChem*, Hot Topic: Carbon, Graphite and Graphene & Hot Topic: Sustainable Chemistry Society Volumes: Spain), Highly Enantioselective Iridium (I) - Catalyzed Hydrocarbonation of Alkenes: A Versatile Approach to Heterocyclic Systems Bearing Quaternary Stereocenters" (*Angew. Chem. Int. Ed*., Hot Topic: C-H Activation); "Exporting Metal-Carbene Chemistry to Live Mammalian Cells: Copper-Catalyzed Intracellular Synthesis of Quinoxalines Enabled by N − H Carbene Insertions" (*Angew. Chem. Int. Ed*., Hot Paper: Bioorthogonal Catalysis).

Finally, 5 articles were selected as **cover image** in the volumes in which they were published: 2 *Angew. Chem. Int. Ed*. (https://doi.org/10.1002/anie.202015800, https://doi.org/10.1002/anie.202014780), *RSC Chem. Biol.* (https://doi.org/10.1039/D0CB00103A), *ChemSusChem* (https://doi.org/10.1002/cssc.202101236), *Chem. Eur. J*. (https://doi.org/10.1002/chem.202004127).

Some examples of CiQUS articles selected as cover

Finally, a complete list of articles, with links to their respective journal websites, can be found in CiQUS web page (https://www.usc.es/ciqus/en/research/publications). Additional information about the selected articles, considered as significant scientific contributions of that period, can be found in the News section of the website (https://www.usc.es/ciqus/en/news). Additionally, these findings and other relevant announcements were disseminated by our Communication and Outreach unit through the CiQUS' website (news section), social networks (Twitter, Facebook, Youtube, and LinkedIn) and, in some cases, through the press media.

3.3.3 Other research outputs

• ***Patent applications***

During 2021, CiQUS researchers obtained the approval of three international patents [*Proteins muNS*, US 11174485B2, PI J.M. Martínez-Costas; *Ru Complexes*, MX 385760, PIs J.L. Mascareñas, E. Vázquez and *Use of a boron cluster compound as transmembrane carrier*, WO/2021/259668, PI J. Montenegro], and 4 national patents [Fragmentos peptídicos de CX43 para su uso como agentes senolítico, ES2804039A1, PIs J.L. Mascareñas, M.E. Vázquez; Heterogeneous metal ceramic catalysts with three-dimensional structure obtained by 3D printing, ES2824324B2, PI E. Sotelo; Compound for batteries, ES2796448B2, PI M. Giménez; Supramolecular fluid, ES2797556B2, PIs M. Giménez and F. Rivadulla]. The corresponding international extension was applied for the next 3 patents: *Battery Compound*; *Supramolecular Fluid*; and *Fluorotools* (PI. E. Sotelo).

• ***Software Licences***

Prof. A. Fernández-Ramos and colleagues registered update versions for 2 computer programmes developed by his research group during 2021: "Torsiflex" – a programme for the conformational search in flexible acyclic molecules (https://github.com/cathedralpkg/TorsiFlex); and "Pilgrim" – a thermal rate constant calculator and kinetics Monte Carlo Simulator (https://github.com/cathedralpkg/Pilgrim). These software programmes use Python 3 as programming language.

• ***PhD Theses***

In 2021, up to 19 PhD Theses were defended under the supervision of CiQUS PIs. All of them obtained a *Sobresaliente cum laude* qualification and 9 of them obtained a *European doctorate/International Mention*; 9 of the new doctors were female (47%) and 2 of them were international trainees (11%).

Detailed information about CiQUS PhD theses presented in this period can be found in Annex V and on CiQUS website. Up to 63% these PhD candidates were funded from competitive human resources programs while the rest were hired under R&D contracts linked to their advisor's research grants.

• ***Contributions to scientific congresses***

The COVID-19 crisis still had a huge impact on scientific events during 2021. Many of them were finally cancellated or converted to virtual events. Nevertheless, CiQUS Research Staff gave 14 lectures in 2021 as Invited Speakers at international conferences and meetings from 3 different countries (Germany, France and Spain) and over 50 oral communications. Furthermore, it is worth noting the total number of CiQUS scientific contributions at congresses (more than 70).

• ***Research Mobility***

In 2021, up to 14 CiQUS PhD candidates had short stays at prestigious national and international research institutions from 9 different countries: Portugal (International Iberian Nanotechnology Laboratory – INL); France (CNRS), Switzerland (University of Zurich); USA (Scripps Research Institute), Germany (Max Planck Institut für Kohlenforschung, Mullheim an der Rür); Sweden (Stockholm University, Uppsala University); The Netherlands (Stratingh Instute for Chemistry), UK (University of Cambridge, University of St Andrews), Spain (CIC NanoGUNE, CIC BioGUNE, ICN2). These short stays were part of their PhD training program (predoctoral secondments).

• ***Visiting Researchers***

Despite of the difficulties for mobility and the extended period of lockdown, CiQUS received during the year 2021 up to 17 visiting researchers for short stays at our center (47% female; 2 Associate Professors, 7 Postdoctoral researcher, 6 PhD candidates and 2 Master Students for internship), coming from up to 10 different countries (Spain, Portugal, France, Italy, The Netherlands, Lithuania, Ukraine, Tunisia, Venezuela and Argentina).

3.3.4 Awards

CiQUS Principal Investigators has received different awards and recognitions during the year 2021, *Prof. José Martínez-Costas* was awarded the **Zendal prize** under the *Human Health* category for his project on the "SARS-CoV-2 vaccine"; Prof. Concepción González-Bello received the **Ignacio Ribas Medal** from the GEQOR-RSEQ; Dra. Beatriz Pelaz has been named a new **member of the Spanish Youth Academy (AJE)** and Prof. Eddy Sotelo was awarded by BIOGA for **the best business idea in biotechnology**.

Regarding CiQUS young researchers, Dr Natalia Barreiro, postdoctoral researcher (supervisor: J. Martínez-Costas), received the "Young Talent Award of the Xunta de Galicia" in the Science category, in recognition for her excellent career in the field of molecular virology.

Furthermore, two of the three 2021 RSEQ-Lilly awards for the for PhD students were awarded to CiQUS researchers Soraya Learte (supervisor: J.L. Mascareñas) and Eva Rivera-Chao (supervisor: M. Fañanás). These prizes recognize research excellence in the fields of Organic, Pharmaceutical and Analytical Chemistry.

Finally, several postdoctoral researchers and PhD candidates have also been awarded for their contributions to different scientific conferences, among others:

- *Marc Font* (Postdoctoral researcher – Mascareñas | López | Gulías Group): 1st Winner Poster Award in the ACS Pubs Symposium: The power of Chemical Transformations (virtual) |Honk Kong

- *Andrés Arribas* (PhD candidate – Mascareñas | López | Gulías Group): 3rd Winner Poster Award (3º premio) I GEQOR Young Researcher Simposium (virtual) | Spain

- *Ignacio Insua* (MSCA Posdoctoral researcher – Granja | Montenegro | García-Fandiño): Best Oral Communication | XVII Simposio de Investigadores Jóvenes RSEQ | Spain

Awarded CiQUS Researchers in 2021

3.4 Training

3.4.1 Bachelor

Up to 42 bachelor final projects defended in 2021 were developed at CiQUS under the supervision of CiQUS PIs (51% of them were female). A complete list of the final projects presented yearly can be found in Annex VII.

Most of the undergraduate students (21) were enrolled in the bachelor's degree in Chemistry. The rest of students were enrolled in the bachelor's degree in Pharmacy (1), Double Degree in Physics & Chemistry (3) and Double Degree in Chemistry & Biology (9).

Regarding the distribution by thematic areas, 60% of the projects were focused in Biological & Medicinal Chemistry, 24% in Functional Materials with Technological Application and 16% in Synthetic Methodologies for Sustainable Development.

Furthermore, it is noteworthy that the 50% of the undergraduate students continue nowadays their research training at CiQUS as Master students or PhD candidates.

3.4.2 Master

Most of CiQUS PIs participate in the *Master's Degree in Chemistry at the Interface with Biology and Materials Science*, the *Master in Organic Chemistry* (with the UCM and the UAM), and the *Master in Chemical Research and Industrial Chemistry* (in collaboration with the University of Vigo and the University of A Coruña). The participation of some of them in the (Erasmus Mundus) and the Master in Drug Research and Development is also relevant. CiQUS annually offers between 25 and 30 vacancies for the Master Project. Approximately 60-65% of the students for the master's degree in Chemistry from USC are trained at the CiQUS.

During 2021, 36 master dissertations were defended by CiQUS master students (44% of them were female). A complete list of 2021 CiQUS master dissertations can be found in Annex VI.

Most of the students (21) were enrolled in the Master's degree in Organic Chemistry at the USC, 6 students were enrolled in the master's in Chemical Research and Industrial Chemistry and 9 student was enrolled in the Master in Chemistry at the Frontier with Biology and Materials Science (1st promotion of this master programme), both of them are also Master Programmes at the USC. Currently, the 42% of the 2021 master student's promotion continues their research training at CiQUS as PhD candidates.

These research training projects were aligned with the CiQUS' main thematic areas: 44% were focused on the field of Biological & Medicinal, 28% on the Functional Materials with Technological Application area and 28% on the field of Synthetic Methodologies for Sustainable Development.

Additionally, up to 10 master students enrolled in the Master in Chemistry at the Interface with Biology and Materials Science (1,5 years duration) presented their master dissertations last February 2022.

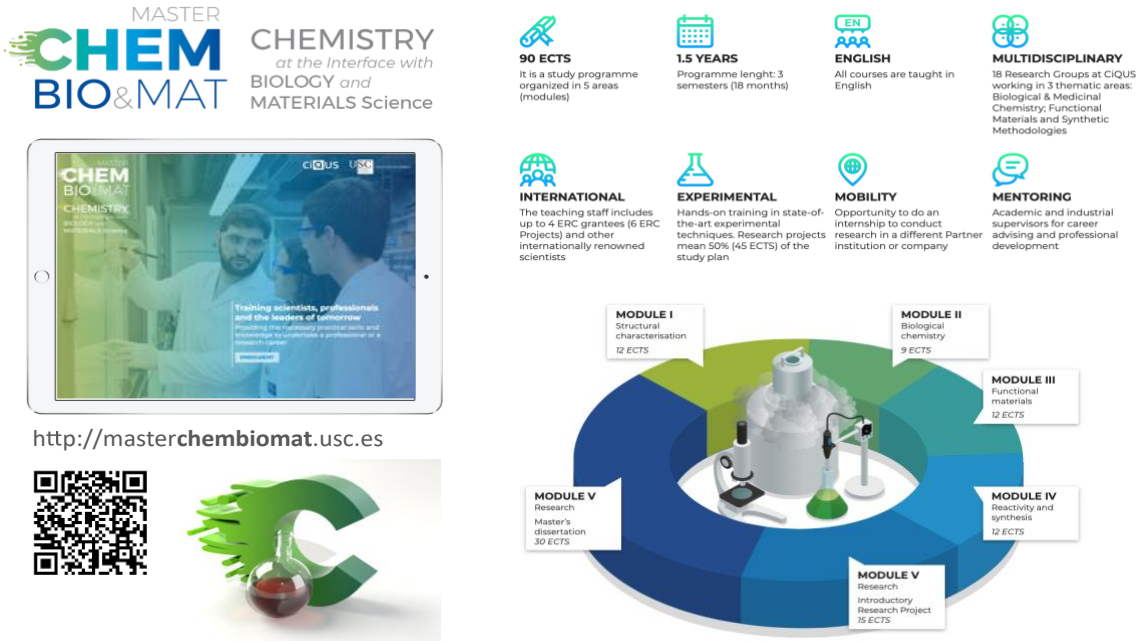
Outstandingly, the Master's degree in Organic Chemistry was ranked as the third-best Master's degree in Spain within the category of "Experimental and Technological Sciences", and the best Master in Chemistry according to the ranking annually published by "El Mundo" newspaper (https://www.elmundo.es/especiales/mejores-masters/ciencias-experimentales-y-tecnologicas.html#quimica-organica).

It is also very important to note that the third promotion of the Master's Degree in Chemistry at the Interface with Biology and Materials Science (ChemBio&Mat) started the academic course 2021/2022 with 11 students, 3 of them already coming from outside of the Galician Region (2 of the from other Spanish provinces and 1 from Mexico). This Master Programme launched in 2019 by the CiQUS, the Faculty of Chemistry and the USC is the

first example of an academic offer aligned with the scientific research agenda of a Research Centre accredited by the Galician University System (SUG).

This Master is coordinated by CiQUS PI Prof. Juan Granja. It is a 1.5-year programme (90 ECTS) aimed at providing first-class multidisciplinary training at the frontier of chemistry, biomedicine and materials sciences, from a molecular approach and giving the students the necessary practical skills and knowledge to undertake a professional or a research career.

CiQUS has created a specific website for this Master Programme (http://masterchembiomat.usc.es), were visitors have access to complete and detailed information about the academic programme, the Lecturers and many other interesting details. Posters and graphic material were designed for advertising the new Master's Programme. Furthermore, a specific Twitter account (https://twitter.com/ChemBioMatMSc) and an Instagram account (https://www.instagram.com/chembiomatmsc/) were open to promote the Master Programme among the undergraduate students and the rest of the scientific community.



Master's Degree official logo, website and ECTS distribution by thematic modules of the study program

Other special feature of this Master Programme is the possibility to host external scientific leaders as invited Professor for highly specialized course. In this context, during 2021 Prof. Margarita Bastos (CiQUP and Universidade de Porto, Portugal) taught the online Master Course "*Biocalorimetry: theoretical considerations and practical applications*" in March 2021. Furthermore, special lectures and scientific events were organized within the framework of this master programme:

- In February 2021, Prof. Nazario Martín, through the zoom platform, gave the lecture "*Carbon Nanostructures for Emergent Viruses: Ebola and beyond*", closing the graduation of the first promotion of the master's degree.

- In July 2021, a special scientific programme was organized for closing the academic year 2020/2021, which included:

- A **round table** "*Science and Research in the post-COVID era*", which was attended by *María Jesús Tallón* (Deputy Director General of Scientific Promotion and University Technology – Xunta de Galicia Government), *Luis Liz-*

Marzán (Scientific Director of the CIC biomaGUNE), *Pilar Bermejo* (Dean of the Faculty of Chemistry - USC) and *José Luis Mascareñas* (Scientific Director of CiQUS).

- A **Scientific Panel Session**: the master's degree students presented the results achieved in the subject "*Research Initiation Project*" in a poster session. Students had the opportunity to discuss their results with Prof. Luis Liz-Marzán (guest speaker at the closing lecturer).

- A **Closing Lecture**: Prof. Liz-Marzán gave the lecture "*Colloidal BioNanoPlasmonics*" which was attended by master's students and other CiQUS researchers and could also be followed via the zoom platform.

Finally, as part of the "Tutored Training Activities", the master students attended a 2-day online course on "Effective Reading & Scientific Writing" organized by CiQUS in May 2021 and several workshop for career development and transversal skills (ej: "Career guidance [online]" and "Introduction to Intellectual Property Rights for Chemists").

It is important to note that in spite of the uncertainty about the evolution of the COVID-19 pandemic, the *Master in Chemistry at the Interface with Biology and Materials Science* was carried out during the academic year 20-21 without any problem. Teaching involved a blend of in-person and online lecturing, adapting to the circumstances at each moment. Training process and quality were not compromised at any time or circumstance.

3.4.3 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.

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 over 10% of doctoral students come from abroad. 55% of CiQUS PhD candidates are currently granted with competitive public HHRR contracts.

19 theses were defended by CiQUS students in 2021 all of which obtained *cum laude* top marks. 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 centre, but also thanks to the stimulating and competitive environment of CiQUS, the biweekly interdisciplinary seminars program or the training in transferable skills. Additionally, our MSc and PhD students, together with the rest of CiQUS members, have the opportunity to attend the CiQUS Lectures Program, with top level international speakers from many different scientific disciplines. (See Annex XI for the complete list of speakers in 2021)

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 centres.

3.4.4 Postdoctoral programs

In 2021, 55 researchers developed their postdoctoral training at CiQUS, 38% were female and 15% of them came from other countries (Italy, The Netherlands, Switzerland, Hungary, Turkey, India and Mexico).

The success in attracting postdoctoral researchers through national and international calls is shown by the recruitment in 2021 of 1 Ramón y Cajal researcher, 1 MSCA-IF-ST fellow, 2 Juan de la Cierva Incorporación fellows, 1 María de Zambrano and 7 Margarita Salas fellows. Moreover, 2 Ramón y Cajal researchers, 2 Juan del

Cierva Incorporación fellows and 1 María de Zambrano will join the CiQUS in 2022. All these grants were awarded under the corresponding 2020 or 2021 calls, respectively.

3.4.5 Funding for training programmes (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 (CiQUS Research Initiation Contracts). In 2021, CiQUS launched the 9th edition of this Programme offering 10 part-time contracts for graduate students. 10 students performing their Master Thesis Dissertation at CiQUS were awarded with research contracts under this call, 5 of them enrolled in the Master in Organic Chemistry, 4 in the Master's in Chemistry at the Interface with Biology and Materials Science, and 1 in the Master in Chemical Research and Industrial Chemistry.

Regarding the doctoral stage, 63 PhD students were developing their theses supported by competitive national grants and contracts during 2021 [17 AEI Predoctoral Contracts (former FPI), 17 FPU, 25 Predocs by the Xunta de Galicia, 4 by the MSCA-ITN, among others]. Most of the remaining doctoral students have contracts linked to research projects.

As far as postdoctoral researchers are concerned, in addition to those hired through national and regional competitive programs (see 3.1.2) and international exchange programs, they all have contracts linked to research projects. It is worth mentioning the recent success in applying for new programme Margarita Salas. Up to 7 CiQUS researchers were granted under this call.

3.4.6 Other training activities and courses

- **Cross-disciplinary training courses**: in 2021, CiQUS launched its own career development program, which included the organization of different courses and workshops to provide CiQUS researchers and technical staff with cross-curricular tools that complement and improve the competitiveness and professional profile. Among others:

- ***Empowering Women in Science: a workshop for women and men*** (focused to predocs, postdocs, IPs and Technical Staff): The content of this course addressed various topics of special interest in the field of emotional intelligence. Among them, learning to manage relationships with other members of the group, correcting inherited gender roles or knowing how to see how we are sometimes limited by our own course. In addition to acquiring resources and practical tools to know how to deal with the emotional challenges faced by researchers and technical staff.

- **The Road to Competitive Funding: tools, perspectives, and processes** (focused to postdoctoral researchers, Junior Scientists and IPs): The content of this course offered researchers an important set of tips and recommendations for preparing applications for international calls of the Europe Horizon, ...) and of the national plan. The course had an important practical component in which participants were able to receive individual personal advice on their own proposals.

- **Career Guidance** (focused to master's students and pre-doctoral researchers): Through the development of this course, students learned recommendations for the preparation of their CVs and how they should face the challenge of job interviews to maximize their chances of success.

- **Prevention and risk course**: all the centre's staff must attend a general security course, taught by the centre's security manager (Noela Torrente), before joining the CiQUS facilities, in order to know the basic rules of work in the laboratory and the safety and evacuation plan of the center.

- **Technical training courses**: the CiQUS technical support team regularly organizes workshops and seminars on the operation and management of the centre's instrumental equipment. These seminars are mandatory for

all new users. Among others, in 2021, specific seminars on the management of the hyperspectral microscope, the Zetasizer Advance Ultra Red (MADLS), HPLC Prep., DSC, etc. were organized.

- **CiQUS Lecture Program**: During the year 2021 we will continue with the program of lectures given by top national and international scientists. The corresponding global mobility limitations have forced CiQUS to maintain its conference program in virtual sessions, open to the entire scientific community through the online conference mode, using the Zoom platform. It should be noted that a high percentage of participants, usually more than 50% of attendees belonged to other centers or institutions, both national and international, which clearly shows the openness undertaken by CiQUS in relation to the visibility of its scientific training activities (see complete list: https://www.usc.es/ciqus/gl/gl/conferencias-ciqus).

- **CiQUS Seminar Program**: We also continue with the internal fortnightly program of seminars in the format of virtual sessions through Microsoft Teams, with the participation of predoctoral, postdoctoral, and principal investigators. (See complete list: https://www.usc.es/ciqus/gl/gl/gl/programa-seminarios-internos).

3.4.7 New strategic initiatives

In the year 2021, two additional strategic actions were launched:

- **CiQUS 2021 Workshop**: An internal workshop was held last October at the center. During two days, we developed an intense scientific program, with 25 presentations by CiQUS IPs and junior scientists, as well as spaces for debate and discussion, open to all researchers at the center (see https://www.usc.es/ciqus/gl/eventos/ciqus-workshop-2021). The organization of this scientific meeting had 3 main objectives: ***1)*** share updated information on research and active projects in CiQUS, the most outstanding scientific results and the capabilities of our researchers, in order to promote new synergies and collaborations, ***2)*** reactivate the team spirit and foster cooperation and collaboration among the community of the center, and ***3)*** be the official opening of a program of activities related to the celebration of the 10th anniversary of CiQUS. The event was a success both from a scientific point of view and from a point of view of training.

- **Mobility grants "pilot" programme**: in order to promote internationalization of CiQUS researchers and favor the mobility and strength collaborations with international institutions and research centers, the CiQUS funded the trips and stays abroad of 3 PIs (in Switzerland, Portugal and Turkey), 1 associate researcher (in France) and 7 PhD Candidates (Germany (Max Plank Institute für Kohlenforshung), Switzerland University of Zurich), United Kingdom (University of St Andrews) and Spain (Universitat de València, CIC bioGUNE and CIC nanoGUNE)].

3.5 Internationalization

- 2021: 49% of the papers include some international collaboration (33% D1, 83% Q1) (WoS database)
- 1 ERC-SyG (MOLDAM), 1 ERC-StG (SPACING), 2 ERC-PoC (antiCSC and ZABCAT), 1 FET-Open (e-Prot), 1 ICT (REAP).

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

49 Papers (49%) resulting from international collaborations, **83% of them in the first quartile (Q1)** and **33% in the first decile (D1)**. Among the collaborators, there are a number of research groups from prestigious research centres, including the Universidade de Porto (Portugal), the Tohoku University and the University of Tokyo (Japan), the Philipps Universitat Marburg (Germany) or IBM Research (Switzerland).

It is highly remarkable the number of international projects started at the CiQUS during the year 2021: ***4 new ERC grants were awarded to CiQUS PIs during the period January 2020 – January 2021***: **an ERC-SyG** (MolDAM, PI. Prof. D. Peña); **an ERC-StG** (SPACING, PI. Dr. B. Pelaz), **two ERC-PoC projects** (antiCSC, PI. Prof. J.L. Mascareñas; ZABCAT, PI. M. Giménez). A FET-Open project (e-Prot, PI. Prof. E. Vázquez), an **ICT project** (REAP, PI. Dr. B. Pelaz), and **an ERA-Net Cofund "EuroNanoMed3" project** (*Biomimetic platelet-derived nanomedicines for treatment of thromboembolic stroker* – AES, PI. Dr. E. Polo). [See section 3.2 for further details regarding budget and collaborations].

In 2021, despite the mobility restrictions derived of the COVID-19 pandemic, CiQUS received up to 17 visiting researchers (47% female and 83% foreigners) from 10 different countries (Spain, Portugal, France, Italy, The Netherlands, Lithuania, Ukraine, Tunisia, Venezuela and Argentina). They were 2 Associate Professors, 7 Postdoctoral researcher, 6 PhD candidates and 2 Master Students for internship.

As part of their PhD training program, up to 14 CiQUS PhD candidates carried out secondments at prestigious international research institutions from 9 different countries: Portugal (International Iberian Nanotechnology Laboratory – INL); France (CNRS), Switzerland (University of Zurich); USA (Scripps Research Institute), Germany (Max Planck Institut für Kohlenforschung, Mullheim an der Rür); Sweden (Stockholm University, Uppsala University); The Netherlands (Stratingh Instute for Chemistry), UK (University of Cambridge, University of St Andrews), Spain (CIC NanoGUNE, CIC BioGUNE, ICN2).

European Technology Platforms (ETP). Since 2012, CiQUS is a member of SusChem Spain, which is part of the **ETP for Sustainable Chemistry (SusChem)**. Since 2015, CiQUS also belongs to the **ETP Nanomedicine** (ETPN) and **MATERPLAT**, the Advanced Materials and Nanomaterials Spanish Technological Platform. Throughout the year, the head of CiQUS knowledge transfer and international affairs unit regularly attends a number of national and international networking events organized by all of these technology platforms.

CiQUS Lectures Programme. In 2021, our Lecture programme was still affected by the mobility restrictions derived from COVID-19 pandemic. While during the first half of the year, we kept active the lecture programme through online sessions using the Zoom platforms, CiQUS lecture were hosted *in-person* at the center during the second half of the year 2021. Among others, the Programme included names as Prof. Nazario Martín (IMDEA-Nanoscience), Prof. Igor Larrosa (University of Manchester) or Prof. Michinori Suginome (Kyoto University). Online lectures were open to the whole scientific community, thus we received a high percentage of attendants from many different national and international research institutions.

Finally, in 2021, 13% of CiQUS members (PIs, junior scientists, postdoctoral researchers and PhD candidates) came from 14 foreign countries (USA, New Zeeland, Switzerland, The Netherlands, Italy, Hungary, Portugal, Rumania, India, Turkey, Vietnam, Mexico, Cuba, and Chile).

3.6 Technology Transfer and Valorisation

3.6.1 Valorization projects

In terms of valorisation projects, the 3rd and 4th ERC-Proof of Concepts granted to CiQUS researchers started in 2021:

- **ERC-PoC-antiCSC** | *Novel metal compounds as anti-cancer agents - antiCSC* will assess the feasibility of using metal-based compounds as new antitumor agents. In this project, Prof. Mascareñas in collaboration with cell biologists at the Autonomous University of Madrid (UAM), will test and validate the potential behaviour of these compounds for selectively acting on the metabolism of cancer stem cells and thus eliminate their carcinogenic characteristics.

- **ERC-PoC-ZABCAT** | *A new Zn-air battery prototype to overcome cathode degradation through catalyst confinement*. This project led by Dr. M. Giménez-López will developed in collaboration with CIDETEC (an important Basque Technological Centre with broad experience in the production of batteries) new electrodes which will be manufactured and later tested in pre-industrial battery prototypes. An innovative approach based on a technology developed at Giménez-López Group at the CiQUS.

Furthermore, during the year 2021 CiQUS researchers also applied to the new call of Proof-of-Concept Projects launched by the Spanish Research Agency (AEI). Up to two CiQUS initiatives have been granted within this framework:

- **PDC2021-121192-I00** | *A new chemical platform for customized gene therapy (GeneVector)*. PI J. Montenegro.

- **PDC2021-121508-I00** | *Metal-based anticancer agents targeting the mitochondrial respiration of cancer stem cells*. PI J.L. Mascareñas

3.6.2 R&D contracts and services in collaboration with companies and entities

During 2021, CiQUS researchers have signed 5 new R&D contracts for a total budget of € 169K. Among them it should be remarked:

- **Landsteiner Genmed S.L**. Following previous agreements since 2018, a new 65,000 € contract has been signed to develop synthetic methodologies and organic molecules libraries.

- **MestreLab Research**. As part of a long-term relationship, a new 66,550 € contract has been signed to provide support for the development of chemical software.

Additionally, several other small contracts were also signed during 2021 with Sigillum Knowledge Solutions, and Celtarys, among others. Although the total budget raised from these small contracts is not so remarkable, they are very important in terms of employability. They do not only support innovative SMEs or spin-offs but also open new qualified job positions. In this context, an important number of CiQUS alumni have been hired by these companies throughout the last years.

The full list of active R&D contracts during 2021 is available in Annex III.

- **Entrepreneurship**

Following the successful participation in BioIncubaTech, the high-tech incubator for biotechnology transfer, led by the USC with the support of GAIN, the project **FluoroTools** (E. Sotelo) gave rise in 2021 to the ***spin-off Celtarys*** (https://www.celtarys.com/), which obtained € 650K in its first round of funding, and the **TraffikGene** (J. Montenegro) initiative was also proposed for funding in the IGNICIA program at the end of the year 2021.

Additionally, CiQUS Spin-Offs MD.USE and Celtarys have been granted within the new Industrial Doctorate programme launched by GAIN and the Xunta de Galicia. 2 PhD candidates will be funded under this call to develop their doctoral theses on the next topics, respectively:

- *A computational platform for the design of drugs and pharmaceutical formulation based on cyclodextrins. Application to anti-aging drugs* | MD.USE (Supervisor: R. García-Fandiño)

- *New conjugation strategies for the development of PROTACs Drugs and fluorescent tools for their characterization* | Celtarys (Supervisor: E. Sotelo)

On the other hand, the CiQUS spin-off MD.USE Innovative Solutions, SL continues to expand CiQUS's scientific collaborations, producing 3 joint publications with companies in 2021 (Ligand Pharmaceuticals and Underdog Pharmaceuticals, both in the US).

Finally, the start-up companies **Sigillum Knowledge Solutions** (http://sigillumks.com), promoted by the PI. Prof. Javier Sardina and founded at the end of 2018, and **Celtarys** (https://www.celtarys.com/), promoted by the Prof. E. Sotelo and founded at the beginning of 2021, have played a key role providing employment opportunities to CiQUS former PhD students and postdoctoral researchers. The companies respectively focus on the growing need of fashion companies to comply with the dynamic international regulations, as well as evaluating the health, safety, quality and sustainability of their products (SKS); and the development of innovative chemical tools that improve the efficiency of the High Throughput Screening (HTS) process in early drug discovery (Celtarys).

3.6.3 Patents

- *3 New international patents granted in 2021*:

- Proteins muNS, US 11174485B2, PI J.M. Martínez-Costas.
- Ru Complexes, MX 385760, PIs J.L. Mascareñas, E. Vázquez
- *Use of a boron cluster compound as transmembrane carrier*, WO/2021/259668, PI J. Montenegro]

- *4 New Spanish patents granted in 2021*:

- Fragmentos peptídicos de CX43 para su uso como agentes senolítico, ES2804039A1, Pis J.L. Mascareñas, M.E. Vázquez.
- Heterogeneous metal ceramic catalysts with three-dimensional structure obtained by 3D printing, ES2824324B2, PI E. Sotelo.
- Compound for batteries, ES2796448B2, PI M. Giménez
- Supramolecular fluid, ES2797556B2, PIs M. Giménez and F. Rivadulla

- *International extensions were applied for the next 3 patents:*

- Battery Compound, PI M. Giménez
- Supramolecular Fluid, PIs M. Giménez and F. Rivadulla
- Fluorotools, PI. E. Sotelo

- *Patent Licensing*: **the multinational MERCK** (*a global pharmaceutical, chemical and life science company with a history that began in 1668 and a future shaped by approximately 50,000 employees in 66 countries*) **has licensed the "Mitoblue" patent (PIs: J.L. Mascareñas, E. Vázquez, J.M. Martínez-Costas) incorporating this product into its commercial catalog**. Fluorotools (PI: E. Sotelo) was also licensed to the spin-off Celtarys. Finally, a "first choice" contract was signed with Abcam PLC (UK) for the possible licensing of the "muNS" patent family (PI: J.M. Martínez-Costas).

Furthermore, CiQUS researchers has signed 3 MTA and 6 Confidential agreements over different technologies during the year 2021.

3.6.4 European Technology Platforms and Networks

In 2021, CiQUS continued its stable participation in the meetings and networking actions of ETP SusChem (European Technology Platform for Sustainable Chemistry), ETP Nanomedicine (European Technology Platform for Nanomedicine), and MATERPLAT (Spanish Technology Platform for Advanced Materials and Nanomaterials).

In addition, CiQUS attended in person several important sectoral events: ExpoQuimia (Barcelona), FarmaForum (Pamplona) and BioSpain (Madrid). In these last two he was part of the Galician delegation accompanying Bioga, the Galician Biotechnology Cluster.

In terms of networking actions, CiQUS has been present at more than 20 events (mostly online due to the pandemic), both linked to the launch of new programs on Horizon Europe and on the subject of batteries, advanced materials and nanomedicine. including ExpoQuimia, BioSpain and Farmaforum.

Finally, it should be noted that at the regional level, CiQUS PIs M. Giménez, M. Fañanás, J. Martínez-Costas and P. del Pino attended the working tables for the new Smart Specialization Strategy (RIS3) of Galicia 2021-2027.

Finally, it is worth mentioning that CiQUS website provides detailed and accessible information about all the activity of the centre, 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).

3.7 Outreach

3.7.1 CiQUS website and presence in the media

CiQUS website (www.usc.es/ciqus/es) is a fully trilingual web page, with an adaptive design (web responsive) for facilitating the access and correct display from any electronic device (computer desktops, mobiles, or tablets). It shown update information about research areas, scientific production, research groups, facilities, job offers, training programs and comprehensive information about the centre's activities and research outputs. Additionally, you can find specific sections on transparency, structure and organization and other information regarding CiQUS policies and commitments. It is currently complemented with social networks: Facebook (2011), LinkedIn (2012), YouTube (2013), and Twitter (2014).

Tracking traffic and web visitors are monitored through Google analytics. During 2021, CiQUS website has received more than 179,097 visits. Approximately, 68% correspond to new visitors. The majority age range of visitors is between 25 and 34 years old (22%) and 55% were female. CiQUS website has received visits from up to 146 different countries, mainly Spain (71%); USA (3%); UK, India, Mexico, Argentina (2%); Portugal, Germany, France, The Netherlands, Italy, and Chile (1%). Regarding electronic devices, 57% of the visitors used desktops, 42% mobiles and 1% tablets.

- **Facebook**. 1,928 followers and 1812 "Likes" (110 new followers since November 2021). 121 posts published and 42,796 total impressions reached.

- **Twitter**. 2,363 followers (418 new followers since November 2021). 160 new posts and 487,500 total impressions reached.

- **LinkedIN**: 2,688 followers (797 new followers since November 2020). 102 new posts. 1,830 people visited the profile, reaching 112,318 impressions, 4,392 "clicks" and 1,718 feedback. Different entries were shared up to 149 times.

- **YouTube**: 338 subscriptions (184 Subscriptions since November 2020, which represents a 119% increase in the number of subscribers). 21 new entries. 25,867 views (viewing time: 877.7 h).

During 2021, over 40 items were published in the news section of the Centre's website (https://www.usc.es/ciqus/es/noticias). The news covered the activities's program developed at the CiQUS during the whole year (e.g., scientific highlights, lectures and seminars, Theses defense, awards, training outreach activities, etc.). Furthermore, more than 12 were also published as press releases and disseminated to media. This generated numerous impacts in newspapers (El Correo Gallego, El Español,...), news agencies (Eurekalert, InfoSalud, GaliciaPress,...), dissemination portals (Mappingignorance, GCiencia,...), specialized technology portals (Biotech,...) and others. A brief summary is shown below:

Press
https://www.elcorreogallego.es/galicia/crean-una-nanoparticula-que-contribuye-a-prevenir-la-perdida-de-la-memoria-FC7316337
https://www.elespanol.com/quincemil/articulos/actualidad/investigadores-de-la-usc-disenan-una-nanoparticula-que-previene-el-alzheimer-en-ratones
https://www.lavozdegalicia.es/noticia/ciencia/2021/05/26/cientificos-universidade-desarrollan-potenciador-antibioticos/0003_202105S26C3996.htm
https://www.elcorreogallego.es/santiago/pese-a-las-dificultades-en-galicia-es-posible-hacer-investigacion-excelente-FD6500160
https://www.youtube.com/watch?v=Pa6SMPnOGcs

News agencies

https://www.eurekalert.org/news-releases/934156

https://www.infosalus.com/salud-investigacion/noticia-disenan-nanoparticula-previene-ratones-fase-inicial-alzheimer-20210419162709.html

https://www.galiciapress.es/texto-diario/mostrar/2253506/consejo-europeo-investigacion-apoyara-proyecto-usc-explorar-potencial-baterias-sostenibles

Scientific outreach platforms

https://www.gciencia.com/ciencia/ciqus-tecnoloxia-funcions-celulares-controlar/

https://www.gciencia.com/ciencia/traballo-ciqus-anticorpos-celula-membrana/

https://mappingignorance.org/2021/09/23/topological-graphene-nanoribbons/

Technological specialist portals:

http://biotech-spain.com/es/articles/un-potenciador-de-antibi-ticos-para-hacer-frente-a-las-superbacterias-/

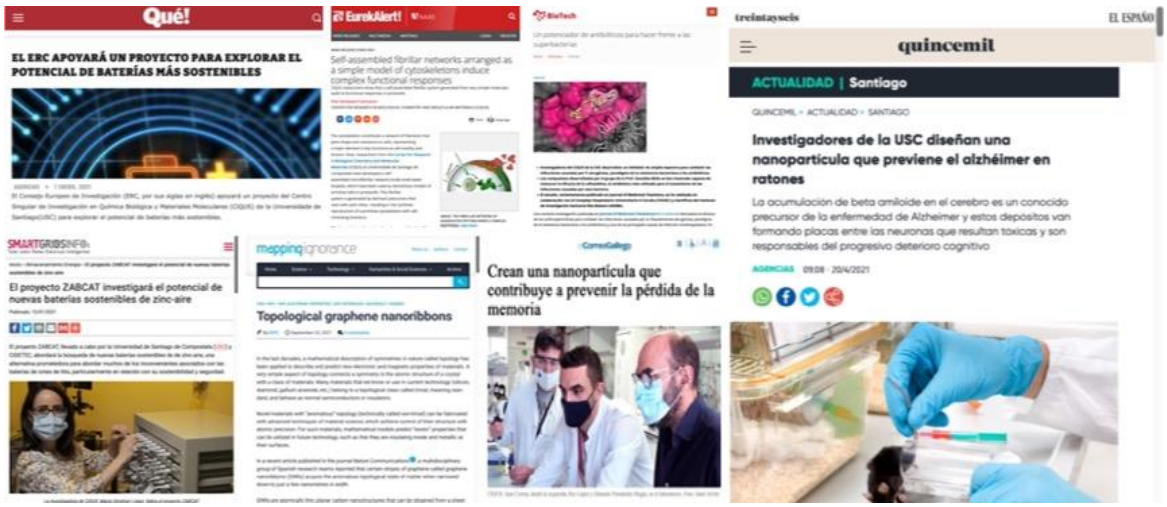
https://www.smartgridsinfo.es/2021/01/12/proyecto-zabcat-investigara-potencial-nuevas-baterias-sostenibles-zinc-aire

Others

https://www.newtral.es/de-que-estan-hechas-las-vacunas-covid/20210615/

https://www.que.es/2021/01/07/erc-proyecto-baterias-sostenibles/

Every press released and news were always support by coverage on the Centre's social networks (Twitter, LinKedIn and Facebook).



Some examples of CiQUS' news in Press media

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

- **2021 "Ciencia Singular" – Open Door's Day**: In November, the fifth edition of the "Singular Science" Open Day was organized by CiQUS jointly with CiMUS, CiTIUS and IGFAE (https://cienciasingular.usc.es/). An event sponsored through a specific agreement with the *Consellería de Cultura, Educación e Universidade* of the Xunta de Galicia Governement. Over 218 people (46% kids) visited the center on November 20th, attended the lectures and talks with CiQUS Researchers and participated in the chemical games and workshops included in the programme.

"Ciencia Singular" 2021

Up to 70 volunteers were collaborating for the celebration of this event. Among them, 10 Principal Investigators (PIs), 5 Junior Scientists, 7 Postdoctoral Researchers, 20 PhD candidates, 13 Master's students, 15 members of the CiQUS research support team and the concierge staff. The volunteers carried out experiments, demonstrations and workshops, gave talks and guided the groups (adults and children) for the visit, as well as other tasks for the organization and general coordination of the activity.

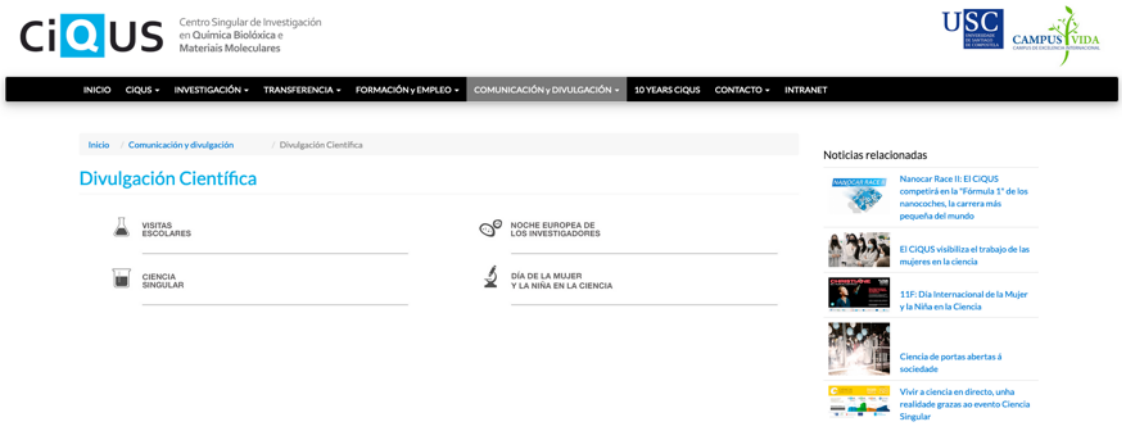
- **From girls to researchers: the path of Science**: a virtual round table (zoom platform), organized on the occasion of "February 11, International Day of Women and Girls in Science", with the aim of bringing the experiences of researchers of different profile and professional stage to the students of primary, secondary and baccalaureate of Galicia, with the aim of promoting scientific vocations. The event was jointly organized by CiQUS, CiMUS, CiTIUS and IGFAE and was attended by 12 schools in Galicia, with a reach of about 490 students.

- **G-Night "European Researchers' Night"**: on September 24th, CiQUS participated together with other entities in an outreach event funded by the Horizon 2020 Research and Innovation Program, Marie Sloklodwska-Curie Actions of the European Union under the agreement of grant 101035979-G-NIGHT (https://gnight.gal/). CiQUS researchers and technical staff actively participated in the organization and development of scientific experiment workshops for children. Multimedia material was also published in the programme website. CiQUS PIs Diego Peña (on the ERC-SyG-MolDAM project) and Martín Fañanás (on the ERC-CoG-BECAME project) took part, among others.

During 2021, the restrictions on mobility and capacity arising from the COVID-19 pandemic forced us to suspend our program of face-to-face outreach activities (school visits and workshops for 2º high school students). Looking for an alternative, the Center is working on the development of a new dissemination section, which will allow us to maintain and strengthen our commitment to the dissemination and promotion of scientific culture through a virtual format, 3D experiences and multimedia galleries.

This new section, which is still under construction, will cover the different activities that make up the centre's outreach program. Visitors will be able to access content related to the purpose of the activities, multimedia material from old editions or participation registration forms. In the year 2022 we will recover the program of face-to-face school visits (currently all available dates of the program are reserved) and we will launch a virtual visit format and online conversations with CiQUS researchers focused on encouraging interest in focused university studies the sciences.

It is also worth mentioning the presence and collaboration of CiQUS researchers in different dissemination initiatives organized by other public institutions (City Councils, Provincial Councils, Schools, etc.). Recent examples include:



https://www.usc.es/ciqus/gl/gl/comunicacion-e-divulgación/divulgacion-cientifica

- **"A Ponte" Programme**: Diego Peña (several educational centers in Vigo, Santiago de Compostela, Padrón and Quiroga (Lugo): "Accelerated course in organic chemistry"; "Graphene ... a miraculous material?"; "Serendipity in Chemical Research"], Concepción González-Bello [IES Campo de San Alberto (Noia), IES Pontepedriña (Santiago de Compostela): "Chemistry Facing the Challenge of Superbacteria"], Félix Freire [CIFP Coroso (Ribeira) , IES A Guía (Vigo), IES Eduardo Pondal (Santiago de Compostela), IES Ramón Cabanillas (Cambados): "Molecular Gastronomy: Chemical Reactions in the Kitchen"], among others.

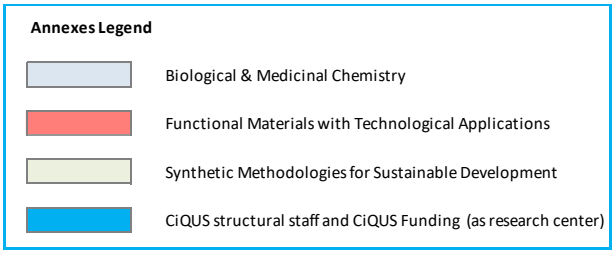
- **Outreach and dissemination scientific lectures**: (IES de Cacheiras-Santiago, CPI de Vedra) - Natalia Barreiro: "What is the use of science that is useless?"

On the other hand, CiQUS strongly supports other scientific dissemination initiatives that have arisen in our environment, such as those organized by the Galician Youth Society of Chemistry (SXGQ), which> 80% is currently made up of predoctoral researchers from CiQUS.

- **Other collaborations** with educational centers: the school "Plurilingüe Divina Pastora Franciscanas" of Ourense, recognized the outreach commitment of CiQUS and its researchers for the promotion of scientific vocations among schoolchildren over the last years, by giving the name of our director (the Prof. José Luis Mascareñas Cid) to its science laboratory.

(https://twitter.com/franciscanasOU/status/1459077446058360862?s=20).

ANNEXES


Annexes Legend
Biological & Medicinal Chemistry
Functional Materials with Technological Applications
Synthetic Methodologies for Sustainable Development
CiQUS structural staff and CiQUS Funding (as research center)

ANNEX I: CiQUS Members (December 31, 2021)

CiQUS Principal Investigators (December 31, 2021)		
Area	**Name**	**Academic Category**
	Del Pino, Pablo	Associate Professor (PIS)
	Estévez Cabanas, Ramón J.	Full Professor
	Estévez Cabanas, Juan Carlos	Associate Professor (Profesor Titular)
	Fañanás Mastral, Martín	Associate Professor (Profesor Titular)
	Fernández Megía, Eduardo	Full Professor
	Fernández Ramos, Antonio	Associate Professor (Profesor Titular)
	Freire Iribarne, Félix Manuel	Associate Professor (PCD)
	García Fandiño, Rebeca	Ramón y Cajal Researcher
	Giménez López, María del Carmen	Ramón y Cajal Researcher
	González Bello, Concepción	Associate Professor (Profesor Titular)
	Granja Guillán, Juan Ramón	Full Professor
	Guitián Rivera, Enrique	Full Professor
	Gulías López, Moisés	Associate Professor (PCD)
	Lazzari, Massimo	Associate Professor (Profesor Titular)
	López García, Fernando	CSIC Tenure Scientist
	Martínez Costas, José Manuel	Associate Professor (Profesor Titular)
	Mascareñas Cid, José Luis	Full Professor
	Montenegro García, Javier	Associate Professor (Profesor Titular)
	Pelaz, Beatriz	Ramón y Cajal Researcher
	Peña Gil, Diego	Full Professor
	Pérez Meirás, María Dolores	Full Professor
	Quiñoá· Cabana, Emilio	Full Professor
	Riguera Vega, Ricardo Jesús	Emeritus Professor
	Ríos Rodríguez, María del Carmen	Associate Professor (Profesor Titular)
	Rivadulla Fernández, Francisco	Associate Professor (Profesor Titular)
	Rodríguez Prieto, María Flor	Full Professor
	Saá Rodríguez, Carlos	Full Professor
	Sardina López, Francisco Javier	Full Professor
	Sotelo Pérez, Eddy	Associate Professor (Profesor Titular)
	Varela Carrete, Jesús	Associate Professor (Profesor Titular)
	Vázquez López, Miguel	Associate Professor (Profesor Titular)
	Vázquez Sentís, Eugenio	Associate Professor (Profesor Titular)

Junior Scientists (December 31, 2021)		
Area	**Name**	**Position**
	Nappi, Manuel	*Manuela Barreiro* Distinguished Researcher
	Ortuño Maqueda, Manuel Ángel	Xunta Distinguished Researcher
	Polo, Ester	Ramón y Cajal Researcher
	Ramos, Rafael	Ramón y Cajal Researcher
	Tomás Gamasa, María	JIN Research Associate

Postdoctoral Researchers (December 31, 2021)		
Area	**Name**	**Position**
	Acuña Barros, José Ángel	R&D Research Contract
	Ageitos Martínez, José Manuel	R&D Research Contract
	Barreiro Piñeiro, Natalia	R&D Research Contract
	Bergueiro Álvarez, Julián	"Juan de la Cierva - Incorporación" Researcher
	Bernárdez Alfaya, Rodrigo	R&D Research Contract
	Bouzada Reborado, David	R&D Research Contract
	Bugallo Ferrón, David	FPI
	Castiñeira Reis, Marta	"Xunta Mod. A" Researcher - (period at foreign institution)
	Correa Chinea, Juan Francisco	R&D Research Contract
	Daudey, Geert	R&D Research Contract
	Ferro Costas, David	R&D Research Contract
	Font Molins, Marc	R&D Research Contract
	Fuertes García, Alberto	R&D Research Contract
	Gutiérrez Hernández, Sara	R&D Research Contract
	Herreros Lucas, Carlos	R&D Research Contract
	Insua López, Ignacio	MSCA Postdoctoral Researcher
	Juanes Carrasco, María Luisa	R&D Research Contract
	Learte Aymamí, Soraya	FPI
	Leborán Álvarez, Víctor	R&D Research Contract
	Lence Quintana, Emilio José	R&D Research Contract
	Lostalé Seijo, Irene	R&D Research Contract
	Maneiro Rey, María	"Xunta Mod. A" Researcher
	Mateo de Doni, Luis Manuel	R&D Research Contract
	Mateos Gil, Jaime	“Juan de la Cierva – Incorporación” Researcher
	Molina Cebeiro, Alba	R&D Research Contract
	Navarro Poupard, María Fernanda	R&D Research Contract
	Parcero Bouzas, Samuel	R&D Research Contract
	Pérez Potti, André	R&D Research Contract
	Rama Martínez, Gustavo	R&D Research Contract
	Rellán Piñeiro, Marcos	Margarita Salas Researcher
	Rodríguez Pérez, Manuel	R&D Research Contract
	Rodríguez Riego, Rafael	"Xunta Mod. A" Researcher - (period at foreign institution)
	Rodríguez Villar, Jessica	“Juan de la Cierva – Incorporación” Researcher
	Sánchez Sordo, Irene	R&D Research Contract
	Seoane Fernández, Andrés	“Juan de Cierva – Incoporación” Researcher

	Tóth, Balázs	R&D Research Contract
	Vilas Varela, Manuel	R&D Research Contract
	Villarino Palmaz, Lara	"Xunta's Mod. B" Researcher
	Zampini, Giulia	R&D Research Contract

PhD CANDIDATES (December 31, 2021)		
Area	**Name**	**Funded by**
	Alcalde Ordoñez, Ana	FPI
	Álvarez Constantino, Andrés Manuel	Predoctoral Xunta
	Álvarez Lorenzo, Aitor	FPU
	Álvarez Pérez, Berta	AEI Predoctoral Contract (former FPI)
	Andújar Arias, Antonio	Predoctoral Xunta
	Arribas Domingo, Andrés	R&D Research Contract
	Barbeiro Arán, Sergio	Student
	Bayón Fernández, Alfonso	Predoctoral Xunta
	Bello García, Jesús	R&D Research Contract
	Campos Prieto, Lucía	Predoctoral Xunta
	Canabal Falcón, Rafael	R&D Research Contract
	Castro Esteban, Jesús Alfonso	AEI Predoctoral Contract (former FPI)
	Cedrún Morales, Manuela	FPU
	Cendón Mariño, Borja	AEI Predoctoral Contract (former FPI)
	Chaves Pouso, Andrea	R&D Research Contract
	Colchón Pierna, Esther	R&D Research Contract
	Da Concepción Vicente, Eduardo	Predoctoral Xunta
	D'Avino, Cinzia	R&D Research Contract
	Delgado González, Bruno	Predoctoral Xunta
	Díaz Arias, Sandra Natalia	Predoctoral Xunta
	Domínguez Ramos, Lidia	R&D Research Contract
	Fariña Torres, Víctor	R&D Research Contract
	Fernández Casanova, Andrés	Student
	Fernández Castro, Saleta	Predoctoral Xunta
	Fernández González, Xulian	AEI Predoctoral Contract (former FPI)
	Fernández Iglesias, Antía	FPU
	Fernández Míguez, Manuel	AEI Predoctoral Contract (former FPI)
	Fernández Vega, Javier	Predoctoral Xunta
	Fojo Carballo, Hugo	Predoctoral Xunta
	Gallego Gómez, Iván	FPU
	García Rey, Aitor	Predoctoral Xunta
	Gioe, Claudia	R&D Research Contract
	Gómez Ojea, Rebeca	R&D Research Contract
	González González, José Manuel	Predoctoral Xunta
	González Pico, Lucía	Student
	Grela Casal, Uxía	Student

	Guillén Soler, Melanie	R&D Research Contract
	Gutiérrez González, Alejandro	FPU
	Huertas Morales, Iván	FPU
	Illodo Brea, Sara	Predoctoral Xunta
	Janeiro Rodríguez, Jesús	AEI Predoctoral Contract (former FPI)
	Jiménez López, Cecilia	R&D Research Contract
	Jiménez Vázquez, Alejandro	Predoctoral Xunta
	Lago Silva, María	Predoctoral Xunta
	Lamas Pérez, Alejandro	AEI Predoctoral Contract (former FPI)
	Lema Saavedra, Anxo	Student
	Le thi Thanh, Hiep	R&D Research Contract
	López Blanco, Roi	R&D Research Contract
	López Bueno, Carlos	Predoctoral Xunta
	López Carracedo, Pablo	R&D Research Contract
	López Corbalán, María Victoria	Predoctoral Xunta
	Mackay Anderson, Amelia	Student
	Mallo Abreu, Ana	R&D Research Contract
	Marcos Atanes, Daniel	FPU
	Martínez Balart, Pol	R&D Research Contract
	Martínez Castrillón, Adrián	AEI Predoctoral Contract (former FPI)
	Martínez Castro, Laura	Predoctoral Xunta
	Martínez Parra, José María	Predoctoral Xunta
	Migliavacca, Martina	R&D Research Contract
	Miguel Ávila, Joan	FPU
	Miranda Pastoriza, Darío	Predoctoral Xunta
	Monteiro Santás, Adrián	R&D Research Contract
	Narayanan Kolusu, Sai Rohini	R&D Research Contract
	Osorio Celis, Marcelo	Predoctoral Xunta
	Otero Riesgo, Sergio	R&D Research Contract
	Panaite, Ana María	MSCA-ITN
	Pérez Maseda, Marta	FPU
	Piñeiro Suárez, Martín	Student
	Prieto Díaz, Rubén	Predoctoral Xunta
	Quirós Díez, Eugenia Pilar	Predoctoral Xunta
	Rey López, Alejandro	Predoctoral Xunta
	Rey Tarrío, Francisco	Predoctoral Xunta
	Reza Ramos, David	Predoctoral Xunta
	Rioboo Vidal, Alicia	FPU
	Rivadulla Cendal, Elena	R&D Research Contract
	Rivera Chao, Eva	Predoctoral Xunta

	Rodiño Balboa, Ricardo	FPU
	Rodríguez Costa, Ángela	AEI Predoctoral Contract (former FPI)
	Rodríguez García, Carlos	R&D Research Contract
	Sabater Algarra, Yolanda	R&D Research Contract
	Salluce, Giulia	AEI Predoctoral Contract (former FPI)
	Sarmiento Fuentes, Axel	FPU
	Seco González, Alejandro	R&D Research Contract
	Soprano, Enrica	R&D Research Contract
	Suárez de Cepeda Fuentes, Pilar	R&D Research Contract
	Suárez García, Juan	R&D Research Contract
	Suárez Lustres, Alejandro	R&D Research Contract
	Tarrío Cordeiro, Juan José	FPU
	Troncoso Mondragón, Ezequiel	AEI Predoctoral Contract (former FPI)
	Varela Domínguez, Noa	AEI Predoctoral Contract (former FPI)
	Vázquez Galiñanes, Nuria	AEI Predoctoral Contract (former FPI)
	Velasco Rubio, Álvaro	Predoctoral Xunta
	Vidal Pereira, Xandro	FPU
	Vilela Góñez, Karen	R&D Research Contract
	Vilela Picos, Marcos	R&D Research Contract
	Vizcaíno Anaya, Lucía	FPU

MASTER STUDENTS (December 31, 2021)		
Area	**Name**	**Funded by**
	Aguilleiro Beraza, Amaia	CiQUS' Research Initiation Contract
	Cabezón Vizoso, Alfonso	CiQUS' Research Initiation Contract
	Casabella Amieiro, Braulio	CiQUS' Research Initiation Contract
	Cora Calvo, Diego	CiQUS' Research Initiation Contract
	Díaz Alonso, Sergio	CiQUS' Research Initiation Contract
	Folgar Cameán, Yeray	CiQUS' Research Initiation Contract
	Fulias Guzmán, Patricia	R&D Research Contract
	Funes Hernando, Samuel	CiQUS' Research Initiation Contract
	López Ferreiro, Miriam	CiQUS' Research Initiation Contract
	Losada Castro, Pablo	CiQUS' Research Initiation Contract
	Luaces Calví, Antón	CiQUS' Research Initiation Contract
	Malavé Fernández, Valentina	CiQUS' Research Initiation Contract
	Pérez Pérez, Manuel	R&D Research Contract
	Rodríguez Romero, Manuel	R&D Research Contract
	Salgado Barca, Jesús Fernando	R&D Research Contract
	Torrón Celada, Alba María	CiQUS' Research Initiation Contract
	Troncoso Afonso, Lara	CiQUS' Research Initiation Contract

TECHNICAL STAFF (December 31, 2021)		
Area	**Name**	**Position**
	Acevedo Arteaga, Laura Alicia	Infrastructure's manager
	Barros Frieiro, Manuela	Administrative support (CiQUS' Research Group)
	Cajaraville Ares, Pablo	Purchasing & Warehouse / HSE Support Technician
	Casal Garea, Fernando	Head of International Affairs and Knowledge Transfer
	Comino León, Mariano	Communication and Outreach manager
	Domínguez Villalobos, Lluvia	Core Facilities support technician
	Fernández Aguiño, Carmen	Lab Technician (CiQUS' Research Group)
	García Fernández, Almudena	Head of Strategic Initiatives
	Giner Rajala, Óscar Vicent	Lab Technician (CiQUS' Research Group)
	Guerra Fandiño, Arcadio J.	Core Facilities manager
	Jiménez Balsa, Adrián	Administrative support (CiQUS' Research Group)
	Lago Rama, Patricia	Administrative support (CiQUS' Research Group)
	López Ulloa, Andrea	Purchasing & Warehouse support technician
	Menaya Vargas, Rebeca	Biological Techniques' manager
	Pereira Rodríguez, María Begoña	Administrative support (CiQUS' Research Group)
	Porto Vence, César	Lab Technician (CiQUS' Research Group)
	Reif López, Rubén	Administrative support (CiQUS' Research Group)
	Rey Ramos, María Carmen	Concierge
	Rey Uzal, María José	Lab Technician (CiQUS' Research Group)
	Rodríguez Couceiro, José M.	Advanced Microscopy Lab Manager
	Rodríguez Martínez, Lucía	Administrative support
	Torreiro Cea, Adrián	IT Support manager
	Torrente Filgueira, Noela	Purchasing & Warehouse / HSE manager
	Veiga Álvarez, Elena	Administrative support - Account manager (shared with CiTIUS)
	Vidal Ocampo, Ildefonso Martín	Concierge
	Vila Fungueiriño, José Manuel	TEM Manager

ANNEX II: Active R&D & Valorziation Projects during 2021

Active International R&D Projects in 2021							
Area	**PI**	**Title**	**Program**	**Funding Agency**	**Start**	**End**	**Budget**
	Peña, Diego	Single Molecular Devices by Atomic Manipulation (MolDAM)	ERC-SyG	ERC	01-10-21	30-09-27	2.820.106 €
	Vázquez, Eugenio	Protein-based conductive materials pave the way for next-generation energy storage devices (e-Prot)	FET-Open	REA	01-09-21	31-08-25	337.106 €
	Pelaz, Beatriz	SPAtially-Controlled lIgand arraNGement by origami-based nanoprinters (SPACING)	ERC-StG	ERC	01-01-21	31-03-26	1.498.866 €
	Pelaz, Beatriz	Revealing drug tolerant persister cells in cancer using contrast enhanced optical coherence and photoacoustic tomography (REAP)	H2020 | ICT-36-2020 - Disruptive photonics technologies	REA	01-01-21	31-12-24	453.903 €
	Polo, Ester	Biomimetic Platelet-Derived Nanomedicines for Treatment of Thromboembolic Stroke	ISCIII-Programación Conjunta Internacional	AEI-ISCIII	01-01-21	31-12-23	140.965 €
	Montenegro, Javier	Dynamic bonds and polyion complex (PIC) nanoparticles for targeted intracellular peptide delivery	MSCA-IF-EF	MSCA Actions	01-01-21	31-12-22	160.932 €
	Pelaz, Beatriz	Switchable magneto-plasmonic contrast agents and molecular imaging technologies (SWIMMOT)	FET-Open	REA	27/10/20	30/9/24	546.035 €
	Fañanás, Martín	Bimetallic Catalysis for Diverse Methane Functionalization (BECAME)	ERC-CoG	ERC	1/9/20	31/8/25	1.999.679 €
	Rivadulla, Francisco	Spin-Phonon interaction for Energy Conversion (SPEC)	MSCA-IF-ST	MSCA Actions	15/9/20	14/9/22	172.932 €
	Peña, Diego	Síntesis en disolución para la integración del grafeno nanoporoso multifuncional en biosensores nanofotónicos	FLAG ERA 3	PCI-AEI	1/3/20	28/2/23	62.400 €
	Del Pino, Pablo	Heating triggered drug release from nanometric inorganic-metal organic framework composites (HeatNMof)	MSCA-ITN	MSCA Actions	0/7/2020	29/2/24	250.905 €
	Fernández-Megía, Eduardo	ENDOSCAPE, a clinicalyy applicable non-viral gene deliveri technology	H2020	REA	1/1/19	31/12/22	444.238 €
	del Pino, Pablo	21QBIONEURO Impulso de una red de I+i en química biológica para diagnóstico y tratamiento de enfermedades	POCTEC	EU	1/1/18	31/12/21	224.058 €
	Peña, Diego	Spin Research IN Grahene (SPRING)	FET-Open	REA	1/10/19	30/9/23	500.940 €

	J. Montenegro	Redes Supramoleculares de Nanopartículas como Materiales Nanoporosos Avanzados	EIG Concert-Japan	PCI-AEI	1/4/19	31/02/22	100.000 €
	Giménez López, María	Complex Dinamic of Clusters in High-Aspect Hollow Nanostructures (NANOCOMP)	ERC-StG	ERC	1/2/18	31/1/22	1.571.692 €
	Rivadulla, Francisco	Spin conversion, logic storage in oxide-based electronics (SPICOLOST)	MSCA-Rise	MSCA Actions	1/3/17	28/2/21	102.021 €
	Montenegro, Javier	Dynamic Penetrating Adaptamers (DYNAP)	ERC-StG	ERC	1/2/16	31/7/22	1.432.824 €

Active National R&D Projects in 2021							
Area	PI	Title	Program	Funding Agency	Start	End	Budget
	Ramos, Rafael	Thin film oxide nanostructures for information, logic and energy management	Dotación "Ramón y Cajal"	AEI	01-09-21	31-08-25	40.000 €
	Montenegro, Javier	Conceptually New Chemical Tools for the Next Generation of Nucleic Acid Delivery Vehicles	RETOS	AEI	01-09-21	31-08-24	242.000 €
	Fañanás, Martín	Catalytic hydrocarbon valorization into multifunctional building blocks	RETOS	AEI	01-09-21	31-08-24	193.600 €
	Saá, Carlos / Varela, Jesús A.	Organometallic/Photo Catalysis: Sustainable Routes to Non-natural Peptides and PAHs (PhotocatPePPAH)	GENERACIÓN	AEI	01-09-21	31-08-24	181.500 €
	López, Fernando	Enantioselective synthetic methods based on transition metal catalysis and applications thereof	GENERACIÓN	AEI	01-09-21	31-08-24	145.200 €
	del Pino, Pablo	Plasmonic Nanocomposites for Photothermophoretic Manipulation of Molecules inside Living Cells	RETOS	AEI	01-09-21	31-08-24	121.000 €
	Polo, Ester	Biomimetic dendritic-cell-derived nanovectors for targeting the immune system (NanoDCell)	RETOS	AEI	01-09-21	31-08-24	96.800 €
	Nappi, Manuel	Sustainable chemical methods promoted by visible light: greenhouse gases valorisation, biodegradable polymers synthesis and novel bioconjugation methodologies	GENERACIÓN	AEI	01-09-21	31-08-24	84.700 €
	Ortuño, Manuel	Metal–organic frameworks for biomass Upgrading via SImulations of CAtalytic systems (MUSICA)	RETOS	AEI	01-09-21	31-08-24	84.700 €
	Orosa, Beatriz	Improving plant immunity using post-translational modifications	Dotación "Ramón y Cajal"	AEI	01-09-21	31-08-25	40.000 €
	Vázquez, Miguel	A new family of anticancer drugs: selective cleavage of DNA three-way junctions by Cu(II) peptide helicates acting as nucleases	Programa - "IDEAS Semilla 2021"	AECC	15-11-21	14-11-23	10.000 €

	Mateos, Jaime	-	Dotación "Juan de la Cierva - Incorporación"	AEI	2021	2023	6.000 €
	Rodríguez, Jessica	-	Dotación "Juan de la Cierva - Incorporación"	AEI	2021	2023	6.000 €
	Polo, Ester	Synthetic biomimetic cell-derived nanostructures	Dotación "Ramón y Cajal"	AEI	01-01-21	31-12-25	40.000 €
	Fernández-Ramos, Antonio	Simulación de Biocombustibles y Aditivos de Gasolina	RETOS-Mod. B	AEI	1/6/20	31/5/24	60.500 €
	González-Bello, Concepción	Combatiendo las bacterias resistentes a los antibióticos y controlando su evolución in vivo mediante estrategias innovadoras y nuevos tests de diagnóstico clínico	RETOS-Mod. B	AEI	1/6/20	31/5/23	169.400 €
	Martínez-Costas, Jose	Nuevos enfoques de la encapsulación de proteínas en micro/nanoesferas basadas en viroplasmas para aplicaciones industriales, terapéuticas e immunoterapia (VIROSPHERE)	RETOS-Mod. B	AEI	1/6/20	31/5/23	121.000 €
	Rivadulla, Francisco	Materiales funcionales para el control activo de la conductividad térmica	RETOS-Mod. B	AEI	1/6/20	31/5/23	151.250 €
	Seoane, Andrés	Desarrollo de reacciones catalizadas por metales en el entorno celular	Juan de la Cierva - Incorporación	AEI	1/7/20	30/6/23	6.000 €
	Font Molins, Marc	Desarrollo y optimización de nuevos métodos de sintesis orgánica basados en la actividad	Juan de la Cierva - Incorporación	AEI	27/3/19	26/3/21	6.000 €
	García Melo, Fátima	Preparación de hidrocarburos policíclicos aromáticvos, incluyendo acenos de gran tañama	Juan de la Cierva - Incorporación	AEI	1/3/19	28/2/21	6.000 €
	Pelaz García, Beatriz	Sintesis y caracterización de nanomateriales para el desarrollo de nanomedicinas	Ramón y Cajal	AEI	4/2/19	3/2/23	40.000 €

	Martínez-Costas, Jose	Desarrollo de una vacuna contra SARS-COV-2 mediante micro/nanoesferas de muNS-Mi	Vaccines Development	ISCIII	13/4/20	16/5/21	150.000 €
	Montenegro, Javier	An Efficient Peptide Vector for mRNA Vaccination Against COVID19	Vaccines Development	ISCIII	30/4/20	30/8/21	126.425 €
	Martínez-Costas, Jose	Desarrollo de una vacuna contra SARS-COV-2 mediante micro/nanoesferas de muNS-Mi (DEVASARMIC)	FONDO SUPERA COVID-19	CRUE-B.Santander	2020	2021	200.000 €
	Freire, Félix	Chiral Dynamic Catalysts based on Helical Polymers	Becas Leonardo	BBVA Foundation	30/10/20	29/4/22	40.000 €
	Pelaz, Beatriz	Nanoimpresoras basadas en origamis para controlar la disposición espacial de ligandos en nanopartículas: estudio de su influencia en procesos intracelulares (ORIGARITMO)	RETOS-Mod. B	AEI	1/6/20	31/5/23	84.700 €
	Granja, Juan	Materiales Supramoleculares Dinámicos Funcionales Basados en Ciclopéptidos. Una Aproximación a Terapias Supramoleculares	RETOS-Mod. B	AEI	1/6/20	31/5/23	1963.600 €
	Gulías, Moisés	Nuevos Métodos de Síntesis Química Mediante la Funcionalización de Enlaces C-H con Catalizadores Metálicos	Generación de Conocimiento	AEI	1/6/20	31/5/23	84.700 €
	Pérez, Dolores	Lego Molecular Basado en Arinos: Aplicación a la Síntesis de Hidrocarburos Policíclicos Conjugados y Materiales π-Funcionales	Generación de Conocimiento	AEI	1/6/20	31/5/23	127.050 €
	Freire, Félix; Quiñoá, Emilio	Materiales quirales con propiedades-estimulo respuesta: Diseño, síntesis y aplicaciones	Generación de Conocimiento	AEI	1/6/20	31/5/23	205.700 €
	Mascareñas, José Luis	Herramientas basadas en metales para su uso en química biológica y biomedicina. Desarrollo de nuevas estrategias anticancer	RETOS-Mod. B	AEI	1/6/20	31/5/23	363.000 €
	Peña, Diego	Síntesis en disolución para sistemas moleculares funcionales (FunMolSys)	RETOS-Mod. B	AEI	1/6/20	31/5/23	151.250 €

	Tomás, María	Fotocatalisis Bioortogonal Mediada Por Luz Visible	RETOS-JIN	AEI	1/8/19	31/12/21	181.500 €
	García Fandiño, Rebeca	Diseño De Agentes Antitumorales A Partir De Simulaciones De Dinamica Molecular, Analisis Big Data E Inteligencia Artificial Validados Por Experimentos Biofisicos	RETOS-Mod. A	AEI	1/1/19	31/12/22	121.000 €
	Vázquez Sentís, Eugenio; Vázquez López, Miguel	Plataformas Peptidicas Para Aplicaciones En Quimica (Bio)Supramolecular Y De Materiales, Catalisis Y Sensores (Swissknife)	RETOS-Mod. B	AEI	1/1/19	31/12/21	157.300 €
	Giménez López, María	Almacenamiento Y Conversion De Energia Sostenible Mediante Confinamiento En Nanocontenedores Huecos De Carbono Y En Nanocajas Con Interacciones De Tipo Receptor-Huesped	RETOS-Mod. A	AEI	1/1/19	31/12/21	96.800 €
	Fernández Megía, Eduardo	Ensamblaje Jerarquico De Complejos Poliionicos Dendriticos Como Protocelulas Y Bioreactores	RETOS-Mod. B	AEI	1/1/19	30/12/21	106.722 €
	Lazzari, Massimo	Nuevos Materiales Porosos Para La Separacion Selectiva De Contaminantes Industriales En Efluentes Gaseosos Y Liquidos	Generación de Conocimiento	AEI	1/1/19	31/12/21	82.280 €
	E. Vázquez	Red de Péptidos en Biomedicina y Nanociencia	Redes de Investigación	AEI	1/12/19	31/12/21	20.000 €
	García Río, Luis	Control de la adinidad, dinámica y estructura de sistemas supramoleculares	RETOS-Mod. B	AEI	1/1/18	31/12/21	102.850 €
	Saá Rodríguez, Carlos	Nuevas rutas cataliticas a PAHs	RETOS-Mod. B	AEI	1/1/18	30/6/21	170.610 €
	Montenegro García, Javier	Péptidos hídridos para el transporte selectivo y entrega de proteínas terapéuticas	RETOS-Mod. B	AEI	1/1/18	30/6/21	145.200 €
	Pino, Pablo del	Nanocápsulas biomiméticas para la administración dirigida de nanomedicinas	RETOS-Mod. A	AEI	1/1/18	30/6/21	71.269 €

	Fañanás Mastral, Martín	Generación no convencional de reactivos organometálicos catalíticos para el uso de hidrocarburos	RETOS-Mod. A	AEI	1/1/18	30/6/21	71.269 €
	Giménez López, María	Synthesis and characterisation of a new class of functional hydrid metal-carbon nanostructures	Ramón y Cajal	AEI	1/5/18	30/4/22	40.000 €
	García Fandiño, Rebeca	Trabajos de simulación computacional de sistemas de interés biológico a nivel de membrana	Ramón y Cajal	AEI	10/6/18	9/6/22	40.000 €

Active Regional R&D Projects and Signed Agreements in 2021							
Area	**PI**	**Title**	**Program**	**Funding Agency**	**Start**	**End**	**Budget**
	C. González-Bello	GRC GI 2155 Inhibidores Enzimáticos e Ferramentas Químicas	CONSOLIDACIÓN - GRC	Xunta de Galicia	1/1/21	30/11/24	280.000 €
	J.R. Granja	GRC GI-2132 Química supramolecular e nanotubos peptídicos (QSNP)	CONSOLIDACIÓN - GRC	Xunta de Galicia	1/1/21	30/11/24	400.000 €
	J.L. Mascareñas	GRC GI-1611 Química Biolóxica e Supramolecular (BCS)	CONSOLIDACIÓN - GRC	Xunta de Galicia	1/1/21	30/11/24	400.000 €
	M. Giménez-López	GPC GI 2170 Materia Condensada & Materiais Funcionais (MAT2)	CONSOLIDACIÓN - GPC	Xunta de Galicia	1/1/21	30/11/23	90.000 €
	E. Polo	CONSOLIDACION 2021 - Mod. D "Excelencia"	EMERXENTES	Xunta de Galicia	1/1/21	30/11/24	115.000 €
	Ortuño, Manuel	Axuda Complementaria para o desenvolvemento da liña de investigación asociada as axudas para atracción e retención de talento investigador na categoría de persoal investigador distinguido nas universidades do SUG	Distinguised Researchers	Xunta de Galicia	1/12/20	30/11/24	160.000 €
	Guitián, Enrique	GI-1595_Catálisis Organometálica y Materiales Moleculares Orgánicos	Grupo de Referencia Competitiva	Xunta de Galicia	1/1/20	30/11/23	280.000 €
	Sotelo, Eddy	GI-1597 Descubrimiento y síntesis de fármacos - DESINFARMA-COMBIOMED	Grupo de Potencial Crecimiento	Xunta de Galicia	1/1/20	30/11/22	90.000 €
	Pelaz, Beatriz	Desarrollo de tecnologías basadas en ADN para ingeniería de nanomedicinas inspiradasen las cápsides víricas: ADNanoVir	Consolidación – Mod.D “Excelencia”	Xunta de Galicia	1/1/20	30/11/23	90.000 €
	García-Fandiño, Rebeca	Estudio de la intersección entre la infección y el cáncer a través de enfoque sinérgico in-silico	Consolidación – Mod.D “Excelencia”	Xunta de Galicia	1/1/20	30/11/23	115.000 €
	Fernández-Megía, Eduardo	Affidendrons anti-SARS-CoV-2 S: herramientas multivalentes para diagnóstico temprano y terapia antiviral	COVID-19 GAIN Rescate ISCIII	GAIN, Xunta de Galicia	1/1/20	31/12/22	233.100 €

	González-Bello, Concepción	Novos axentes antivirais baseados en aminoquinolinas para o tratamento da pandemia actual por SARS-COV-2	COVID-19 GAIN Rescate ISCIII	GAIN, Xunta de Galicia	1/1/20	31/12/22	140.300 €
	Mascareñas, José Luis	Acretiación Centro de Investigación do SUG (2019-2022)	CIGUS (Centros de Investigación del Sistema Universitario Gallego)	Xunta	1/12/19	30/11/22	2.880.000
	Sardina López, Fco Javier	Consolidación e estructuración 2018 GRC GI-1935 Reactividade e Catálise (RyC)	Grupo de Referencia Competitiva	Xunta de Galicia	1/1/19	30/11/21	400.000 €
	Saá Rodríguez, Carlos E	Consolidación e estructuración 2018 GRC GI-1603 Catálise Organometálica (Cat Organomet)	Grupo de Referencia Competitiva	Xunta de Galicia	1/1/19	30/11/21	200.000 €
	Quiñoá Cabana, Emilio	Consolidación e estructuración 2018 GRC GI-1608 Nanomateriais e Moléculas Bioactivas	Grupo de Referencia Competitiva	Xunta de Galicia	1/1/19	30/11/21	280.000 €
	Rodríguez Prieto, M. Flor	CONSOLIDACIÓN 2019 GPC GI-1586 Química Biofísica, Fotofísica e Espectroscopía - Química Biofísica	Grupo de Potencial Crecimiento	Xunta de Galicia	1/1/19	20/11/21	90.000 €
	Giménez López, María	Convenio de colaboración Consellería Cultura, Educación e Ordenación Universitaria e a USC	Consellería de Educación, Universidade e Formación Profesional	Convenio	1/1/18	31/12/21	199.878 €
	del Pino, Pablo	Consolidación e estructuración 2017 Modalidade D (Excelencia)	Mod. D (Excelencia) - RyC	Xunta de Galicia	1/1/17	30/11/21	115.000 €

Active Valorization Projects in 2021							
Area	**PI**	**Title**	**Program**	**Funding Agency**	**Start**	**End**	**Budget**
	J. Montenegro	A new chemical platform for customized gene therapy (GeneVector)	PROYECTOS DE I+D+i "PRUEBAS DE CONCEPTO"	AEI	1/12/21	30/11/23	143.750 €
	J.L. Mascareñas	Metal-based anticancer agents targeting the mitochondrial respiration of cancer stem cells	PROYECTOS DE I+D+i "PRUEBAS DE CONCEPTO"	AEI	1/12/21	30/11/23	108.100 €
	M. Giménez-López	A New Zn-Air Battery Prototype to Overcome Cathode Degradation Through Catalyst Confinement (ZABCAT)	ERC-PoC	ERC	01/10/2021	31/03/2023	85.500 €
	J.L. Mascareñas	Targeting the cancer stem cell (CSC) metabolism with designed, reactive metal complexes (antiCSC)	ERC-PoC	ERC	01-01-21	30-06-22	130.000 €

ANNEX III: Active R&D Contracts during 2021

Active R&D Contracts in 2021						
Area	**PI**	**Title**	**Partnert/Client**	**Start**	**End**	**Budget**
	Martínez-Costas, José Manuel	Etiquetado e inclusión de antígenos recombinantes seleccionados del virus del síndrome reproductivo y respiratorio porcino (PRRSV) en microesferas de reovirus aviar para su posterior validación en modelo murino y modelo porcino como candidato vacunal frente a esta enfermedad	UNIVERSIDAD DE CORDOBA	28/12/21	27/9/23	20.000 €
	Sardina Lopez, Francisco Javier	Creación e implantación dunha matriz de riscos para o control da conformidade de artigos de moda (téxtil, coiro, calzado e complementos) axustada aos requisitos de Saúde de produto do Grupo TENDAM	SIGILLUM KNOWLEDGE SOLUTIONS, S.L.	22-01-21	31-01-21	15.000 €
	Sotelo Pérez, Eddy	Puesta a punto y desarrollo de metodologías sintéticas y obtención de quimiotecas de moléculas orgánicas	LANDSTEINER GENMED, S.L	03-03-21	04-03-22	65.000 €
	Sotelo Pérez, Eddy	ADENDA: Realización de los servicios de puesta a punto y desarrollo de metodologías sintéticas y la obtención de quimiotecas de moléculas orgánicas	Oncostellae	01-01-21	31-12-22	62.000 €
	Sotelo Pérez, Eddy	Servicios de consultoría técnica, síntesis de colecciones de ligandos y análisis estructural relacionados con los ligandos fluorescentes desarrollados por CELTARYS	Celtarys Research S.L.	25/10/21	24/1/23	22.890 €
	Sardina Lopez, Francisco Javier	Deseño e desenvolvemento de algoritmos para a análise e interpretación asistidas por intelixencia artificial de datos e información química para o seu uso en entornos de aplicacións Web e prestación de servizos analíticos cualitativos, cuantitativos e de asignación estrutural	Mestrelab Research	01-02-21	31-12-23	66.550 €
	Sardina Lopez, Francisco Javier	Avaliación científica, técnica, normativa e comercial de novas tecnoloxías e metodoloxías de ensaio e análise no campo do control da saúde de produtos de consumo	APPLIED MASS SPECTROMETRY LABORATORY, SLU (AMSLAB)	1/2/20	31/1/22	18.150 €
	Sotelo Pérez, Eddy	Puesta a punto y desarrollo de metodologías sintéticas y obtención de quimiotecas de moléculas orgánicas.	LANDSTEINER GENMED, SL	5/3/20	4/3/22	105.000 €
	Sotelo Pérez, Eddy	Puesta a punto y desarrollo de metodologías sintéticas y la obtención de quimiotecas de moléculas orgánicas	ONCOSTELLAE, SL	1/1/21	31/12/22	30.000 €

	Sardina Lopez, Francisco Javier	Deseño e desenvolvemento de algoritmos para a automatización de tarefas de recollida, interpretación e análise de datos para o seu uso nun entorno de libreta de laboratorio electrónica que inclúa a prestación de servizos analíticos cualitativos e cuantitativos dentro do contexto do Proxecto Futurelab	MESTRELAB RESEARCH, SL	1/1/20	31/12/23	66.550 €
	Sardina Lopez, Francisco Javier	Asesoramiento para la elaboración de un plan de acción en sostenibilidad	SIGILLUM KNOWLEDGE SOLUTIONS, SL	24/2/20	28/2/21	1.170 €
	Sardina Lopez, Francisco Javier	Nuevas técnicas analíticas de control para la transición industrial hacia unha economía circular (CdTI-Misiones)	TORUS SOFTWARE SOLUTIONS SL	1/8/20	31/12/23	60.000 €
	Sardina Lopez, Francisco Javier	Nuevas técnicas analíticas de control para la transición industrial hacia unha economía circular (CdTI-Misiones)	SIGILLUM KNOWLEDGE SOLUTIONS, SL	1/8/20	31/12/23	60.000 €
	Sardina Lopez, Francisco Javier	Nuevas técnicas analíticas de control para la transición industrial hacia unha economía circular (CdTI-Misiones)	APPLIED MASS SPECTROMETRY LABORATORY, SLU (AMSLAB)	1/8/20	31/12/23	120.000 €
	Sardina Lopez, Francisco Javier	Apoyo en la notificación a Poison Centers de mezclas clasificadas como peligrosas de acuerdo a lo establecido en el Reglamento (CE) 1272/2008 (CLP)	SIGILLUM KNOWLEDGE SOLUTIONS, SL	15/9/20	15/10/21	17.520 €
	Sardina Lopez, Francisco Javier	Soporte en el análisis del marco regulatorio aplicable a sustancias de uso en investigación (RUO)	SIGILLUM KNOWLEDGE SOLUTIONS, SL	3/11/20	5/11/21	1.152 €
	Estevez Cabanas, Ramon Jose	Asesoría técnica para a realización e elucidación das análises de Resonancia Magnética	GALCHIMIA S.A.	1/1/21	31/12/22	9.999 €
	Garcia Fandiño, Rebeca	Caracterizacion estructural e enerxetica das interaccions entre o remdesivir, farmaco empregado no COVID•-19, e o excipiente Captisol	MD. USE INNOVATIONS SL	1/12/20	30/1/22	15.000 €
	Sardina Lopez, Francisco Javier	Apoyo en la notificación a Poison Centers de mezclas clasificadas como peligrosas de acuerdo con lo establecido según el Reglamento (CE) 1272/2008 [CLP]	SIGILLUM KNOWLEDGE SOLUTIONS, SL	28/12/20	29/12/21	1.944 €
	Estevez Cabanas, Juan Carlos	Síntesis de glicósidos	FUNDACION KERTOR	1/1/20	30/6/21	36.700 €
	Sardina López, Francisco Javier	Deseño e desenvolvemento de algoritmos para a automatización de tarefas de recollida, interpretación e análise de datos para o seu uso nun entorno de libreta de laboratorio electrónica e dun sistema de xestión de prestación de servizos deslocalizados de análise por RMN	Mestrelab Research, S.L.	01-01-19	31-12-21	60.000 €

	Sardina López, Francisco Javier	Deseño e desenvolvemento de algoritmos para a automatización de tarefas de recollida, interpretación e análise de datos para o seu uso nun entorno de libreta de laboratorio electrónica e un sistema de xestión de ensaios de saúde de produto e calidade	Mestrelab Research, S.L.	01-01-18	31-12-21	45.000 €

ANNEX IV: List of Publications

2021 List of CiQUS Publications						
Area	**Authors**	**Title**	**Journal**	**Vol.**	**Pages**	**DOI**
	J. Arca-Suárez, C. Lasarte-Monterrubio, B.-K. Rodiño-Janeiro, G. Cabot, J. C. Vázquez-Ucha, P. M. Rodríguez-Iglesias, F. Galán-Sánchez, A. Beceiro, C. González-Bello, A. Oliver, G. Bou	Molecular mechanisms driving in vivo development of OXA-10-mediated resistance to ceftolozane/tazobactam and ceftazidime/avibactam during treatment of extensively drug-resistant Pseudomonas aeruginosa infection	*J. Antimicrob. Chemother.*	**76**	91-100	10.1093/jac/dkaa396
	J. Gómez-González, Y. Pérez, G. Sciortino, L. Roldán-Marín, J. Martínez-Costas, J.D. Maréchal, I. Alfonso, M. Vázquez López, M.E. Vázquez	Dynamic Stereoselection of Peptide Helicates and Their Selective Labeling of DNA Replication Foci in Cells	*Angew. Chem. Int. Ed.*	**60**	8859-8866	10.1002/anie.202013039
	J. Azuaje, A. Rama, A. Mallo-Abreu, M.G. Boado, M. Majellaro, C.R. Tubío, R. Prieto, X. García-Mera, F. Guitián, E. Sotelo, A. Gil	Catalytic performance of a metal-free graphene oxide-Al2O3 composite assembled by 3D printing	*J. Eur. Ceram. Soc.*	**2**	1399-1406	10.1016/j.jeurceramsoc.2020.10.010
	E. González-Freire, F. Novelli, A. Pérez-Estévez, R. Seoane, M. Amorín, Juan R. Granja	Double orthogonal click reactions for the development of antimicrobial peptide nanotubes	*Chem. Eur. J.*	**27**	3029-3038	10.1002/chem.202004127
	P. Destito, C. Vidal, F. López, J.L. Mascareñas	Transition Metal-promoted Reactions in Aqueous Media and Biological Settings	*Chem. Eur. J.*	**27**	4789-4816	10.1002/chem.202003927
	M. Pazo, G. Salluce, I. Lostalé Seijo, M. Juanes, F. González, R. García-Fandiño, J. Montenegro	Short Oligoalanine Peptides for Supramolecular Nanopore Assembly and Protein Cytosolic Delivery	*RSC Chem Biol*	**2**	503-512	10.1039/D0CB00103A
	T. Pose-Boirazian, G. Eibes, N. Barreiro-Piñeiro, C. Díaz-Jullien, J.M. Lema, J. Martínez-Costas	Chemical and thermal stabilization of CotA laccase via a novel one-step expression and immobilization in muNS-Mi nanospheres	*Sci. Rep.*	**11**	2802	10.1038/s41598-021-82468-x
	X. Alvarez, A. Alves, M.P. Ribeiro, M. Lazzari, P. Coutinho, A. Otero	Biochemical characterization of Nostoc sp. exopolysaccharides and evaluation of potential use in wound healing	*Carbohydr. Polym.*	**254**	1173030	10.1016/j.carbpol.2020.117303
	R. Steeno, A. Minoia, M.C. Giménez-López, M.O. Blunt, N.R. Champness, R. Lazzaroni, K.S. Mali, S. De Feyter	Molecular dopant determines the structure of a physisorbed self-assembled molecular network	*Chem. Commun.*	**57**	1454-1457	10.1039/d0cc07338e

	R. García-Fandiño, A. Piñeiro	Delving Into the Origin of Destructive Inflammation in COVID-19: A Betrayal of Natural Host Defense Peptides?	*Front. Immunol.*	**11**	610024	10.3389/fimmu.2020.610024
	A. Fierro, L. García-Río, S. Arancibio-Opazo, J.J. Alcázar, J.G. Santos, M.E. Aliaga	Cucurbit[7]uril as a Supramolecular Catalyst in Base-Catalyzed Reactions. Experimental and Theoretical Studies on Carbonate and Thiocarbonate Hydrolysis Reactions	*J. Org. Chem.*	**86**	2023-2027	10.1021/acs.joc.0c02728
	H. Meer, F. Schreiber, C. Schmitt, R. Ramos, E. Saitoh, O. Gomonay, J. Sinova, Baldrati, M. Kläui	Direct Imaging of Current-Induced Antiferromagnetic Switching Revealing a Pure Thermomagnetoelastic Switching Mechanism in NiO	*Nano Lett.*	**21**	114-119	10.1021/acs.nanolett.0c03367
	C. López-Bueno, C. Herreros-Lucas, M. Suárez-Rodríguez, M.R. Bittermann, A. Amigo, S. Woutersen, M. Giménez-López, F. Rivadulla	A New Type of Supramolecular Fluid Based on H2O–Alkylammonium/Phosphonium Solutions	*Angew. Chem. Int. Ed.*	**60**	7540-7546	10.1002/anie.202015800
	A. Domínguez-Celorrio, M. Vilas-Varela, D. Peña, V. Langlais, D. Serrate	Symmetry-Driven Formation of Chiral Boroxine-Based Organometallic Oligomers on Ag(001)	*J. Phys. Chem. C*	**125**	2015-2021	10.1021/acs.jpcc.0c08039
	E. Da Concepción, I. Fernández, J.L. Mascareñas, F. López	Highly Enantioselective Cobalt-Catalyzed (3+2) Cycloadditions of Alkynylidenecyclopropanes	*Angew. Chem. Int. Ed.*	**60**	8182-8188	10.1002/anie.202015202
	J.M. González, B. Cendón, J.L. Mascareñas, M. Gulías	Kinetic Resolution of Allyltriflamides through a Pd-Catalyzed C–H Functionalization with Allenes: Asymmetric Assembly of Tetrahydropyridines	*J. Am. Chem. Soc.*	**143**	3747-3752	10.1021/jacs.1c01929
	E. Lence, C. González-Bello	Bicyclic Boronate β-Lactamase Inhibitors: The Present Hope against Deadly Bacterial Pathogens	*Adv. Therap.*	**4**	2000246	10.1002/adtp.202000246
	Z. Fernández, B. Fernández, E. Quiñoá, F. Freire	The Competitive Aggregation Pathway of an Asymmetric Chiral Oligo(p-phenyleneethynylene) Towards the Formation of Individual P and M Supramolecular Helical Polymers	*Angew. Chem. Int. Ed.*	**60**	9919-9924	10.1002/anie.202100162
	M.E. Navas Guimaraes, R. López-Blanco, J. Correa, M. Fernández-Villamarin, M.B. Bistué, P. Martino-Adami, L. Morelli, V. Kumar, M.F. Wempe, A.C. Cuello, E. Fernández-Megía, M.A. Bruno	Liver X Receptor Activation with an Intranasal Polymer Therapeutic Prevents Cognitive Decline without Altering Lipid Levels	*ACS Nano*	**15**	4678-4687	10.1021/acsnano.0c09159
	L. Cruz, J. Correa, N. Mateus, V. de Freitas, M.H. Tawara, E. Fernández-Megía	Dendrimers as Color-Stabilizers of Pyranoanthocyanins: The Dye Concentration Governs the Host–Guest Interaction Mechanisms	*ACS Appl. Poly. Mater.*	**3**	1457-1464	10.1021/acsapm.0c01321
	F. Rey-Tarrío, R. Rodríguez, E. Quiñoá, R. Riguera, F. Freire	Photochemical Electrocyclization of Poly(phenylacetylene)s: Unwinding Helices to Elucidate their 3D Structure in Solution	*Angew. Chem. Int. Ed.*	**60**	8095-8103	10.1002/anie.202014780
	A. Hammid, J.K. Fallon, T. Lassila, G. Salluce, P.C. Smith, A. Tolonen, A. Sauer, A. Urtti, P. Honkakoski	Carboxylesterase Activities and Protein Expression in Rabbit and Pig Ocular Tissues	*Mol. Pharmaceut.*	**18**	1305-1316	10.1021/acs.molpharmaceut.0c01154

	P. Jiménez-Cavero, I. Lucas, D. Bugallo, C. López-Bueno, R. Ramos, P.A. Algarabel, M.R. Ibarra, F. Rivadulla, L. Morellón	Quantification of the interfacial and bulk contributions to the longitudinal spin Seebeck effect	*Appl. Phys. Lett.*	**118**	92404	10.1063/5.0038192
	C. Lasarte-Monterrubio, J.C. Vázquez-Ucha, M. Maneiro, J. Arca-Suárez, I. Alonso, P. Guijarro-Sánchez, J.D. Buynak, G. Bou, C. González-Bello, A. Beceiro	Activity of imipenem, meropenem, cefepime, and sulbactam in combination with the β-lactamase inhibitor In-1-255 against acinetobacter spp	*Antibiotics*	**10**	210	10.3390/antibiotics10020210
	M. Lazzari, D. Reggio	What Fate for Plastics in Artworks? An Overview of Their Identification and Degradative Behaviour	*Polymers*	**13**	883	10.3390/polym13060883
	A. Perez-Potti, H. Lopez, B. Pelaz, A. Abdelmonem, M.G. Soliman, I. Schoen, P.M. Kelly, D.A. Dawson, W.J. Parak, Z. Krpetic, M.P. Monopoli	In depth characterisation of the biomolecular coronas of polymer coated inorganic nanoparticles with differential centrifugal sedimentation	*Sci. Rep.*	**11**	6433	10.1038/s41598-021-84029-8
	E. Vieira Silveria, R. Monteciones, L. Scorsin, L.García-Río, M. Medeiros, V. Nascimento, F. Nome, R.F. Affeldt, G.A. Micke	Supramolecular kinetic effects by pillararenes: the synergism between spatiotemporal and preorganization concepts in decarboxylation reactions	*New. J. Chem.*	**45**	6486-6494	10.1039/D1NJ00551K
	M. Majellaro, W. Jespers, A. Crespo, M.J. Núñez, S. Novio, J. Azuaje, R. Prieto-Díaz, C. Gioé, B. Alispahic, J. Brea, M.I. Loza, M. Freire-Garabal, C. Garcia-Santiago, C. Rodríguez-García, X. García-Mera, O. Caamaño, C. Fernandez-Masaguer, J.F. Sardina, A. Stefanachi, A. El Maatougui, A. Mallo-Abreu, J. Åqvist, H. Gutiérrez-de-Terán, E. Sotelo	3,4-Dihydropyrimidin-2(1H)-ones as Antagonists of the Human A(2B)Adenosine Receptor: Optimization, Structure-Activity Relationship Studies, and Enantiospecific Recognition	*J. Med. Chem.*	**64**	458-480	10.1021/acs.jmedchem.0c01431
	A. Stefanucci, J. Amato, D. Brancaccio, B. Pagano, A. Randazzo, F. Santoro, L. Mayol, S. Learte-Aymamí, J. Rodríguez, J.L. Mascareñas, E. Novellino, A. Carotenuto, A. Mollica	A novel β-hairpin peptide derived from the ARC repressor selectively interacts with the major groove of B-DNA	*Bioorg. Chem.*	**112**	104836	10.1016/j.bioorg.2021.104836
	J. Lawrence, M.S.G. Mohammed, D. Rey, F. Aguilar-Galindo, A. Berdonces-Layunta, D. Peña, D.G. de Oteyza	Reassessing Alkyne Coupling Reactions While Studying the Electronic Properties of Diverse Pyrene Linkages at Surfaces	*ACS Nano*	**15**	4937-4946	10.1021/acsnano.0c09756

	A. Berdonces-Layunta, J. Lawrence, S. Edalatmanesh, J. Castro-Esteban, T. Wang, M.S.G. Mohammed, L. Colazzo, D. Peña, P. Jelínek, D.G. de Oteyza	Chemical Stability of (3,1)-Chiral Graphene Nanoribbons	*ACS Nano*	**15**	5610-5617	10.1021/acsnano.1c00695
	M. Calvelo, C.I. Lynch, J.R. Granja, M.S.P. Sansom, R. García-Fandiño	Effect of Water Models on Transmembrane Self-Assembled Cyclic Peptide Nanotubes	*ACS Nano*	**15**	7053-7064	10.1021/acsnano.1c00155
	R. Zuzak, I. Pozo, M. Engelund, M. Vilas-Varela, J.M. Alonso, E. Guitián, D. Pérez, D. Peña, s. Golewski	Microscopic Visualization of Porous NanographenesSynthesized through a Combination of Solution and On-Surface Chemistry	*Jove-J Vis Exp*	**169**	e62122	10.3791/62122
	J.J. Alcázar, N. Geue, V. Valladares, A. Cañete, E.G. Pérez, L. García-Río, J.G. Santos, M.E. Aliaga	Supramolecular Control of Reactivity toward Hydrolysis of 7-Diethylaminocoumarin Schiff Bases by Cucurbit[7]uril Encapsulation	*ACS Omega*	**6**	10333-10342	10.1021/acsomega.1c00683
	M.S.G. Mohammed, J. Lawrence, F. García, P. Brandimarte, A. Berdonces-Layunta, D. Pérez, D. Sánchez-Portal, D. Peña, D.G. de Oteyza	From starphenes to non-benzenoid linear conjugated polymers by substrate templating	*Nanoscale Adv*	**3**	2351-2358	10.1039/D1NA00126D
	J.C. Vázquez-Ucha, D. Rodríguez, C. Lasarte-Monterrubio, E. Lence, J. Arca-Suárez, M. Maneiro, E. Gato, A. Perez, M. Martínez-Guitián, C. Juan, A. Oliver, G. Bou, C. González-Bello, A. Beceiro	6-Halopyridylmethylidene Penicillin-Based Sulfones Efficiently Inactivate the Natural Resistance of Pseudomonas aeruginosa to β-Lactam Antibiotics	*J. Med. Chem.*	**64**	6310-6328	10.1021/acs.jmedchem.1c00369
	T. Wang, J. Lawrence, N. Sumi, R. Robles, J. Castro-Esteban, D. Rey, M.S.G. Mohammed, A. Berdonces-Layunta, N. Lorente, D. Pérez, D. Peña, M. Corso, D.G. de Oteyza	Challenges in the synthesis of corannulene-based non-planar nanographenes on Au(111) surfaces	*Phys. Chem. Chem. Phys.*	**23**	10845-10851	10.1039/D1CP01212F
	M. L. Picchio, J. Bergueiro, S. Wedepohl, R.J. Minari, C.I. Alvarez Igarzabal, L.M. Gugliotta, J.C. Cuggino, M. Calderón	Exploiting cyanine dye J-aggregates/monomer equilibrium in hydrophobic protein pockets for efficient multi-step phototherapy: an innovative concept for smart nanotheranostics	*Nanoscale*	**13**	8909-8921	10.1039/D0NR09058A

	M.Liu, A.J. Deloria, R. Haindl, Q. Li, G. Szakacs, A. Csiszar, S. Schrittwieser, P. Muellner, R. Hainberger, B. Pelaz, E. Polo, P. del Pino, A. Penttinen, M. Guina, T. Niemi, K. Meiburger, F. Molinari, C. Menhard, J. Heidelin, V. Andresen, D. Geuzebroek, W. Drexler	REAP: Revealing drug tolerant persister cells in cancer using contrast enhanced optical coherence and photoacoustic tomography	*J. Phys. Photonics*	**3**	21001	10.1088/2515-7647/abf02f
	A. Gutiérrez-González, P. Destito, J.R. Couceiro, C. Pérez-González, F. López, J.L. Mascareñas	Bioorthogonal Azide-Thioalkyne Cycloadditions Catalyzed by Photoactivatable Ru(II) Complexes	*Angew. Chem. Int. Ed.*	**60**	16059-16066	10.1002/anie.202103645
	M. Núñez-Martínez, S. Arias, E. Quiñoá, R. Riguera, F. Freire	Dynamic Chiral PPA–AgNP Nanocomposites: Aligned Silver Nanoparticles Decorating Helical Polymers	*Chem. Mater.*	**33**	4805-4812	10.1021/acs.chemmater.1c00805
	J.M. Rodrigues, B. Cendón, M. Gulías, J.L. Mascareñas, M. Queiroz	Rhodium(III)-catalyzed formal cycloaddition between thienopyridine/thienopyrazine carboxylic acids and alkynes, triggered by C-H activation	*Eur. J. Org. Chem.*		3234-3240	10.1002/ejoc.202100439
	N. Dib, C.M.O. Lépori, N.M. Correa, J.J. Silber, R.D. Falcone, L. García-Río	Biocompatible Solvents and Ionic Liquid-Based Surfactants as Sustainable Components to Formulate Environmentally Friendly Organized Systems	*Polymers*	**13**	1378	10.3390/polym13091378
	E. Rivera-Chao, M. Fañanás-Mastral	Stereoselective Synthesis of Highly Substituted 1,3-Dienes via 'à la carte' Multifunctionalization of Borylated Dendralenes	*Angew. Chem. Int. Ed.*	**60**	16922-16927	10.1002/anie.202104741
	W. Frost, T. Seki, T. Kubota, R. Ramos, E. Saitoh, K. Takanashi, A. Hirobata	Evaluation of edge domains in giant magnetoresistive junctions	*Appl. Phys. Lett.*	**118**	172405	10.1063/5.0049315
	A. Gómez, J.M. Vila-Fungueiriño, C. Jolly, R. García-Bermejo, J. Oró-Solé, E. Ferain, N. Mestres, C. Magén, J. Gazquez, J. Rodríguez-Carvajal, A. Carretero-Genevrier	Crystal engineering and ferroelectricity at the nanoscale in epitaxial 1D manganese oxide on silicon	*Nanoscale*	**13**	9615-9625	10.1039/D1NR00565K
	D. Gomez-Diaz, M. Parajo, O. Richoux, M.D. La Rubia, A. Rumbo	Kinetics, absorption and regeneration of biphasic solvent with ethylpiperidine for carbon dioxide absorption	*Fuel*	**300**	121020	10.1016/j.fuel.2021.121020
	M. Aygün, M. Guillen-Soler, J.M. Vila-Fungueiriño, A. Kurtoglu, T. Chamberlain, A.N. Khlobystov, M.C. Giménez-López	Palladium Nanoparticles Hardwired in Carbon Nanoreactors Enable Continually Increasing Electrocatalytic Activity During the Hydrogen Evolution Reaction	*ChemSusChem*	**19**	4973-4984	10.1002/cssc.202101236
	A. Arribas, M. Calvelo, D.F. Fernández, C.A.B. Rodrigues, J.L. Mascareñas, F. López	Highly Enantioselective Iridium(I)-Catalyzed Hydrocarbonation of Alkenes: A Versatile Approach to Heterocyclic Systems Bearing Quaternary Stereocenters	*Angew. Chem. Int. Ed.*	**60**	19297-19305	10.1002/anie.202105776

	A. Mallo-Abreu, I. Reyes-Resina, J. Azuaje, R. Franco, A. García-Rey, M. Majellaro, D. Miranda-Pastoriza, X. García-Mera, W. Jespers, H. Gutiérrez-de-Terán, G. Navarro, E. Sotelo	Potent and Subtype-Selective Dopamine D2 Receptor Biased Partial Agonists Discovered via an Ugi-Based Approach	*J. Med. Chem.*	**64**	8710-8726	10.1021/acs.jmedchem.1c00704
	A. Pardo, B. Pelaz, P. del Pino, A. Al-Modlej, A. Cambón, B. Velasco, R. Domínguez-González, A. Moreda-Piñeiro, P. Bermejo-Barrera, S. Barbosa, P. Taboada	Monodisperse superparamagnetic nanoparticles separation adsorbents for high-yield removal of arsenic and/or mercury metals in aqueous media	*J. Mol. Liq.*	**335**	116485	10.1016/j.molliq.2021.116485
	M. Mirjolet, F. Rivadulla, P. Marsik, V. Borisov, R. Valentí, J. Fontcuberta	Electron–Phonon Coupling and Electron–Phonon Scattering in $SrVO_3$	*Adv. Sci.*	**8**	2004207	10.1002/advs.202004207
	F. Noveli, M. Vilela, A. Pazó, M. Amorín, J.R. Granja	Molecular Plumbing to Bend Self-assembling Peptide Nanotubes	*Angew. Chem. Int. Ed.*	**60**	18838-18844	10.1002/anie.202107034
	X. Vidal, J.L. Mascareñas, M. Gulías	Assembly of Tetrahydroquinolines and 2-Benzazepines by Pd-Catalyzed Cycloadditions Involving the Activation of C(sp3)–H Bonds	*Org. Lett.*	**23**	5323-5328	10.1021/acs.orglett.1c01594
	B. Fernández, Z. Fernández, E. Quiñoá, F. Freire	From oligo(Phenyleneethynylene) monomers to supramolecular helices: The role of intermolecular interactions in aggregation	*Molecules*	**26**	3530	10.3390/molecules26123530
	S. Leiras, E. Suárez-Picado, E. Quiñoá, R. Riguera, F. Freire	Tuning the helical sense and elongation of polymers through the combined action of the two components of tetraalkylammonium-anion salts	*Giant*	**7**	100068	0.1016/j.giant.2021.100068
	J.A. Rubiolo, E. Lence, C. González-Bello, M. Roel, J. Gil-Longo, M. Campos-Toimil, E. Ternon, O.P. Thomas, A. González-Cantalapiedra, H. López-Alonso, M.R. Vieytes, L.M. Botana	Crambescin C1 Acts as A Possible Substrate of iNOS and eNOS Increasing Nitric Oxide Production and Inducing In Vivo Hypotensive Effect	*Front. Pharmacol.*	**12**	694639	10.3389/fphar.2021.694639
	C. Ruiz Martínez, J.M. Pérez, F.M. Arrabal-Campos, M. Batuecas, M.A. Ortuño, I. Fernández	Cyclic polylactide synthesis initiated by a lithium anthraquinoid: understanding the selectivity through DFT and diffusion NMR	*Polym. Chem.*	**12**	4083-4092	10.1039/D1PY00547B
	J. Bello-García, D. Padín, J.A. Varela, C. Saá	Nonplanar Tub-Shaped Benzocyclooctatetraenes via Halogen-Radical Ring Opening of Dihydrobiphenylenes	*Org. Lett.*	**23**	5539-5544	10.1021/acs.orglett.1c01881
	C. Correa-Paz, A. da Silva-Candal, E. Polo, J. Parcq, D. Vivien, D. Maysinger, B. Pelaz, F. Campos	New Approaches in Nanomedicine for Ischemic Stroke	*Pharmaceutics*	**13**	757	10.3390/pharmaceutics13050757

	L. Altenschmidt, S. Sánchez-Paradinas, F. Lübkemann, D. Zámbó, A.M. Abdelmonem, H. Bradtmüller, A. Masood, I. Morales, P. de la Presa, A. Knebel, M.A. García García-Tuñón, B. Pelaz, K.D.J. Hindricks, P. Behrens, W.J. Parak, N.C. Bigall	Aerogelation of Polymer-Coated Photoluminescent, Plasmonic, and Magnetic Nanoparticles for Biosensing Applications	*ACS Appl. Nano Mater.*	**4**	6678-6688	10.1021/acsanm.1c00636
	X. Wang, W. Jespers, R. Prieto-Díaz, M. Majellaro, A.P. Ijzerman, G.J.P. van Westen, E. Sotelo, L.H. Heitman, H. Gutiérrez-de-Terán	Identification of V6.51L as a selectivity hotspot in stereoselective A2B adenosine receptor antagonist recognition	*Sci. Rep.*	**11**	14171	10.1038/s41598-021-93419-x
	A. Velasco-Rubio, R. Bernárdez, J.A. Varela, C. Saá	Enantioenriched α-Vinyl 1,4-Benzodiazepines and 1,4-Benzoxazepines via Enantioselective Rhodium-Catalyzed Hydrofunctionalizations of Alkynes and Allenes	*J. Org. Chem.*	**86**	10889-10902	10.1021/acs.joc.1c01268
	T. Kikkawa, D. Reitz, H. Ito, T. Makiuchi, T. Sugimoto, K. Tsunekawa, S. Daimon, K. Oyanagi, R. Ramos, S. Takahashi, Y. Shiomi, Y. Tserkovnyak	Observation of nuclear-spin Seebeck effect	*Nat. Commun.*	**12**	4356	10.1038/s41467-021-24623-6
	M.A. Ortuño, A. Lledós	How acid can become a dihydrogen complex in water? A DFT study	*J. Organomet. Chem.*	**949**	121957	10.1016/j.jorganchem.2021.121957
	P. Zamora-Perez, B. Pelaz, D. Tsoutsi, M.G. Soliman, W.J. Parak, P. Rivera-Gil	Hyperspectral-enhanced dark field analysis of individual and collective photo-responsive gold-copper sulfide nanoparticles	*Nanoscale*	**13**	13256-13272	10.1039/D0NR08256B
	J.M. Liñeira del Río, E.R. López, F. García, J. Fernández	Tribological synergies among chemical-modified graphene oxide nanomaterials and a phosphonium ionic liquid as additives of a biolubricant	*J. Mol. Liq.*	**336**	116885	10.1016/j.molliq.2021.116885
	E. Lence, C. González-Bello	Molecular Basis of Bicyclic Boronate β-Lactamase Inhibitors of Ultrabroad Efficacy – Insights From Molecular Dynamics Simulation Studies	*Front. Microbiol.*	**12**	721826	10.3389/fmicb.2021.721826
	S. Gutiérrez, M. Tomás-Gamasa, J.L. Mascareñas	Exporting Metal-Carbene Chemistry to Live Mammalian Cells: Copper-Catalyzed Intracellular Synthesis of Quinoxalines Enabled by N−H Carbene Insertions	*Angew. Chem. Int. Ed.*	**60**	22017-22025	10.1002/anie.202108899
	A. Bacle, P. Buslaev, R. Garcia-Fandino, F. Favela-Rosales, T. Mendes Ferreira, P.F.J. Fuchs, I. Gushchin, M. Javanainen, A.M. Kiirikki, J.J. Madsen, J. Melcr, P. Milán Rodríguez, M.S. Miettinen, O.H. Samuli Ollila, C.G. Papadopoulos, A. Peón, T.J. Piggot, A. Piñeiro, S.I. Virtanen	Inverse Conformational Selection in Lipid–Protein Binding	*J. Am. Chem. Soc.*	**143**	13701-13709	10.1021/jacs.1c05549

	V.G. Vegas, A. Latorre, M.L. Marcos, C.J. Gómez-García, O. Castillo, F. Zamora, J. Gómez, J. Martínez-Costas, M. Vázquez López, A. Somoza, P. Amo-Ochoa	Rational Design of Copper(II)–Uracil Nanoprocessed Coordination Polymers to Improve Their Cytotoxic Activity in Biological Media	*ACS Appl. Mater. Interfaces*	**13**	36948-36957	10.1021/acsami.1c11612
	J. Gómez-González, D. Bouzada, L.A. Pérez-Márquez, G. Sciortino, J.-D. Maréchal, M. Vázquez López, M.E. Vázquez	Stereoselective Self-Assembly of DNA Binding Helicates Directed by the Viral β-Annulus Trimeric Peptide Motif	*Bioconjugate Chem.*	**32**	1564-1569	10.1021/acs.bioconjchem.1c00312
	A. Blanco-González, M. Calvelo, P.F. Garrido, M. Amorín, J.R. Granja, A. Piñeiro, R. García-Fandiño	Transmembrane Self-Assembled Cyclic Peptide Nanotubes Based on α-Residues and Cyclic δ-Amino Acids: A Computational Study	*Front. Chem.*	**9**	704160	10.3389/fchem.2021.704160
	G.C. Dubed Bandomo, S. Sekhar Mondal, F. Franco, A. Bucci, V. Martin-Diaconescu, M.A. Ortuño, P.H. van Langevelde, A. Shafir, N. López, J. Lloret-Fillol	Mechanically Constrained Catalytic $Mn(CO)_3Br$ Single Sites in a Two-Dimensional Covalent Organic Framework for CO_2 Electroreduction in H_2O	*ACS Catal.*	**11**	7210-7222	10.1021/acscatal.1c00314
	A.M. Anderson, T. Kirtadze, M. Malanga, D. Dinh, C. Barnes, A. Campo, D.M. Clemens, R. Garcia-Fandiño, A. Piñeiro, M.S. O'Connor	Cyclodextrin dimers: A versatile approach to optimizing encapsulation and their application to therapeutic extraction of toxic oxysterols	*Int. J. Pharm.*	**606**	120522	10.1016/j.ijpharm.2021.120522
	B. Claro, A. Peón, E. González-Freire, E. Goormaghtigh, M. Amorín, J.R. Granja, R. García-Fandiño, M. Bastos	Macromolecular assembly and membrane activity of antimicrobial D,L-α-Cyclic peptides	*Colloid Surf. B-Biointerfaces*	**208**	112086	10.1016/j.colsurfb.2021.112086
	I. Pozo, A. Cobas, D. Peña, E. Guitián, D. Pérez	Toward 2-Thiophyne: Ketocarbene versus Hetaryne Intermediates from 2-(Trimethylsilyl)thiophen-3-yl Triflate	*Org. Lett.*	**23**	7376-7380	10.1021/acs.orglett.1c02552
	L. Martínez-García, G. Prado, K.V. Góñez, M.R. Paleo, F.J. Sardina	Stereoselective Synthesis of Hydrindane and Hydroazulene Derivatives by Transannular Cyclization of Nine- and Ten-Membered Carbocycles	*J. Org. Chem.*	**89**	13684-13692	10.1021/acs.joc.1c01751
	D. Bugallo, E. Langenberg, E. Ferreiro-Vila, E.H. Smith, C. Stefany, X. Batlle, G. Catalan, N. Domingo, D.G. Schlom, F. Rivadulla	Deconvolution of Phonon Scattering by Ferroelectric Domain Walls and Point Defects in a PbTiO3 Thin Film Deposited in a Composition-Spread Geometry	*ACS Appl. Mater. Interfaces*	**38**	45679-45685	10.1021/acsami.1c08758
	J. Li, S. Sanz, N. Merino-Díez, M. Vilas-Varela, A. Garcia-Lekue, M. Corso, D.G. de Oteyza, T. Frederiksen, D. Peña, J.I. Pascual	Topological phase transition in chiral graphene nanoribbons: from edge bands to end states	*Nat. Commun.*	**12**	5538	10.1038/s41467-021-25688-z

	A. Piñeiro, J. Pipkin, V. Antle, R. Garcia-Fandiño	Aggregation versus inclusion complexes to solubilize drugs with Cyclodextrins. A case study using sulphobutylether-β-cyclodextrins and remdesivir	*J. Mol. Liq.*	**343**	117588	10.1016/j.molliq.2021.117588
	P.F. Garrido, P. Rodríguez-Dafonte, L. García-Río, Á. Piñeiro	Simple ApproximaTion for Aggregation Number Determination by Isothermal Titration Calorimetry: STAND-ITC	*Langmuir*	**37**	11781-11792	10.1021/acs.langmuir.1c01727
	A. Velasco-Rubio, J.A. Varela, C. Saá	Pd-Catalyzed allylic C–H activation to seven-membered N,O-heterocycles	*Chem. Commun.*	**57**	10915-10918	0.1039/D1CC04056A
	J. Hieulle, S. Casto, N. Friedrich, A. Vegliante, F. Romero Lara, S. Sanz, D. Rey, M. Corso, T. Frederiksen, J.I. Pascual, D. Peña	On-Surface Synthesis and Collective Spin Excitations of a Triangulene-Based Nanostar	*Angew. Chem. Int. Ed.*	**60**	25224-25229	10.1002/anie.202108301
	C. Carrillo-Carrión, R. Martínez, E. Polo, M. Tomás-Gamasa, P. Destito, M. Ceballos, B. Pelaz, F. López, J.L. Mascareñas, P. del Pino	Plasmonic-Assisted Thermocyclizations in Living Cells Using Metal–Organic Framework Based Nanoreactors	*ACS Nano*	**15**	16924-16933	10.1021/acsnano.1c07983
	C.F.F. Sousa, E. Fernández-Megía, J. Borges, J.F. Mano	Supramolecular dendrimer-containing layer-by-layer nanoassemblies for bioapplications: current status and future prospects	*Polym. Chem.*	**12**	5902-5930	10.1039/D1PY00988E
	D.M.A. Mackenzie, M. Galbiati, X.D. de Cerio, I.Y. Sahalianov, T.M. Radchenko, J. Sun, D. Peña, L. Gammelgaard, B.S. Jessen, J.D. Thomsen, P. Bøggild, A. Garcia-Lekue, L. Camilli, J.M. Caridad	Unraveling the electronic properties of graphene with substitutional oxygen	*2D Materials*	**8**	45035	10.1088/2053-1583/ac28ab
	X. Vidal, M. Font, B. Cendón, J.L. Mascareñas, M. Gulías	(4 + 2) Cycloadditions via Pd C(sp3)–H activation	*Trends Chem.*	**3**	1102-1103	10.1016/j.trechm.2021.08.009
	J. Castro-Esteban, F. Albrecht, S. Fatayer, D. Pérez, L. Gross, D. Peña	An on-surface Diels-Alder reaction	*Angew. Chem. Int. Ed.*	**6**	26346-26350	10.1002/anie.202110311
	R. Booth, I. Insua, S. Ahmed, A. Rioboo, J. Montenegro	Supramolecular fibrillation of peptide amphiphiles induces environmental responses in aqueous droplets	*Nat. Commun.*	**12**	6421	10.1038/s41467-021-26681-2
	R. Novoa-Carballal, M. Martin-Pastor, E. Fernández-Megía	Unveiling an NMR-Invisible Fraction of Polymers in Solution by Saturation Transfer Difference	*ACS Macro Lett*	**10**	1474-1479	10.1021/acsmacrolett.1c00628
	I. Raïch, R. Rivas-Santistesban, A. Lillo, J. Lillo, I. Reyes-Resina, X. Nadal, C. Ferreiro-Vera, V.S. de Medina, M. Majellaro, E. Sotelo, G. Navarro, R. Franco	Similarities and differences upon binding of naturally occurring Δ9-tetrahydrocannabinol-derivatives to cannabinoid CB1 and CB2 receptors	*Pharmacol. Res.*	**174**	105970	10.1016/j.phrs.2021.105970
	Z. Fernández, B. Fernández, E. Quiñoá, F. Freire	Merging Supramolecular and Covalent Helical Polymers: Four Helices Within a Single Scaffold	*J. Am. Chem. Soc.*	**143**	20962-20969	10.1021/jacs.1c10327

	D. Bugallo, E. Langenberg, E. Carbó-Argibay, N. Varela Dominguez, A. O. Fumega, V. Pardo, I. Lucas, L. Morellón, F. Rivadulla	Tuning Coherent-Phonon Heat Transport in $LaCoO_3/SrTiO_3$ Superlattices	*J. Phys. Chem. Lett*	**12**	11878–11885	10.1021/acs.jpclett.1c03418
	A.R. Araújo, J. Correa, V. Domínguez-Arca, R.L. Reis, E. Fernández-Megía, R.A Pires	Functional Gallic Acid-Based Dendrimers as Synthetic Nanotools to Remodel Amyloid-β-42 into Noncytotoxic Forms	*ACS Appl. Mater. Interfaces*	**13**	59673-59682	10.1021/acsami.1c17823
	W. Jespers, L.H. Heitman, A.P. Ijzerman, E. Sotelo, G.J.P. van Westen, J. Åqvist, H. Gutiérrez-de-Terán	Deciphering conformational selectivity in the A2A adenosine G protein-coupled receptor by free energy simulations	*PLoS Comput. Biol.*	**17**	e:1009152	10.1371/journal.pcbi.1009152
	M. Corso, R.E. Menchón, I. Piquero-Zulaica, M. Vilas-Varela, J.E. Ortega, D. Peña, A. Garcia-Lekue, D.G. de Oteyza	Band Structure and Energy Level Alignment of Chiral Graphene Nanoribbons on Silver Surfaces	*Nanomaterials*	**11**	3003	10.3390/nano11123303
	F. Schreiber, H. Meer, C. Schmitt, R. Ramos, E. Saitoh, L. Baldrati, M. Kläui	Magnetic Sensitivity Distribution of Hall Devices in Antiferromagnetic Switching Experiments	*Phys. Rev. Applied*	**16**	64023	10.1103/PhysRevApplied.16.064023
	D. Ferro-Costas, I. Mosquera-Lois, A. Fernández-Ramos	TorsiFlex: an automatic generator of torsional conformers. Application to the twenty proteinogenic amino acids	*J. Cheminformatics*	**13**	100	10.1186/s13321-021-00578-0

Annex V: Theses Defended

2021 – Theses Defended					
Area	**Author**	**Title**	**Supervisor(s)**	**European/International Doctorate**	**Date**
	Tomás Pose Boirazian	*Novel protein immobilization approaches for the development of vaccine candidates and enzymatic reactors*	J.M. Martínez-Costas	No	22/12/2021
	David Bouzada Reboredo	*Artificial peptides for DNA recognition and controlled gold clusters formation*	M. Vázquez, E. Vázquez	No	17/12/2021
	Álvaro Velasco Rubio	*New Catalytic Routes to Benzofused Seven-Membered Azaheterocycles*	C. Saá, J. Varela	Yes	03/12/2021
	Marta Pazo Pascual	*Structural control of membrane-targeted peptides for delivery of functional properties*	J. Montenegro	Yes	26/11/2021
	Carlos López Bueno	*Study and control of thermal transpor in complex fluids*	F. Rivadulla	Yes	12/11/2021
	Daniela Reggio	*Testing, optimization and validation of Surface Enhanced Raman (SERS) sensors for the detection of small molecules in cultural heritage materials*	M. Lazzari	No	26/10/2021
	Manuel Núñez Martínez	*Nanomateriales Quirales con Propiedades Quirópticas Modulables*	E. Quiñoá, F. Freire	No	14/10/2021
	Ana Mallo Abreu	*New Ligands and Pharmacological Tools for the Study of G Protein Protein-Coupled Receptors using Multicomponent Reactions*	E. Sotelo	Yes	16/07/2021
	Adolfo Otero Fumega	*Interplay between Electronic, Magnetic and Structural degrees of freedom in Crystalline Transition Metal Compounds*	V. Pardo, F. Rivadulla	Yes	07/07/2021
	David Bugallo Ferrón	*Thermal conductivity of superlattices and ferroelectric thin films. Effect of boundary sizes and vacancies*	F. Rivadulla, E. Langerberg	No	02/06/2021
	David Cagiao Marcote	*Novas Estratexias Sintéticas Baseadas en Catálise de Ouro*	J.L. Mascareñas, F. López	No	28/05/2021
	Alba Pereira Vilar	*Synthesis and characterization of pillar[n]arenes for their use as molecular receptors*	L. García-Río, N. Basílio	Yes	21/05/2021
	Dulce M. Rey Vieites	*Diseño y síntesis de nuevos compuestos aromáticos derivados del pireno, del antraceno y del trifenileno*	D. Pérez, D. Peña	No	21/05/2021
	Soraya Learte Aymami	*Metallopeptides and Metalloproteins in Chemical Biology: From DNA binding to Intracellular Catalysis*	J.L. Mascareñas	Yes	30/04/2021

	Martín Calvelo Souto	*Computational methods for the design and applications of self-assembled cyclic peptide nanotubes*	J.R. Granja, R. García-Fandiño	Yes	09/04/2021
	Samuel Parcero Bouzas	*Aplicaciones de la Química Click y Ácidos Borbónicos en la Síntesis y Funcionalización de Copolímeros de Bloque Dendríticos para la Encapsulación-Liberación Controlada de Fármacos*	R. Riguera, E. Fernández-Megía	No	08/04/2021
	Beatriz Fariña Fraga	*Preparación de muestras de referencia y síntesis de surrogados deuterados de sustancias legalmente reguladas. Desarrollo de nuevos métodos de análisis aplicables en entornos industriales*	F.J. Sardina, C. González	No	26/03/2021
	María Fernanda Navarro Poupard	*Porous Nanosystems for biological applications*	P. Taboada, P. del Pino	No	08/02/2021
	Zulema Fernández Villar	*Covalent and Supramolecular Helycal Polymers: The Dawn of Matryoshka Materials*	E. Quiñoá, F. Freire	Yes	28/01/2021

Annex VI: Master Dissertations

2021 – Master final projects				
Area	**Author**	**Title**	**Supervisor(s)**	**MSc Programme**
	Andrés Manuel Álvarez Constantino	Anelación oxidante [4+2] catalizada por Rh (III) cara HAPs azulénicos dopados con N	J.A Varela, C. Saá Rodríguez	Chemistry at the interface with Biology and Materials Science
	Adrián Martínez Castrillón	Deseño e síntesis de novos precursores moleculares de grafeno poroso	D. Peña	Chemistry at the interface with Biology and Materials Science
	Axel Sarmiento Fuentes	Un enfoque basado na química de coordinación cara o entrelazamento mecánico de nanotubos de carbono	M.E. Vázquez, M. Vázquez	Chemistry at the interface with Biology and Materials Science
	Manuel Fernández Míguez	Loita polo poder en polímeros helicoidais completamente quirais	F. Freire, E. Quiñoá	Chemistry at the interface with Biology and Materials Science
	Tania Prieto González	NanoZIFs cargados con colorantes para aplicación biolóxicas	P. Del Pino	Chemistry at the interface with Biology and Materials Science
	Antía Fernández Iglesias	Desenvolvemento de materiais biomiméticos	B. Pelaz, E. Polo	Chemistry at the interface with Biology and Materials Science
	Xulián Fernández González	Combinando catálise metálica con MOFs	J.L. Mascareñas, M. Tomás	Chemistry at the interface with Biology and Materials Science
	Charlene María Harriswangler Harriswangler	Controlando o espesor de nanoláminas supramoleculares de péptidos cíclicos	J. Montenegro	Chemistry at the interface with Biology and Materials Science
	Lucía Viñes García	Estratexias de autoblocaxe dirixidas ao encima LpxB para desbloquear a resistencia bacteriana en axentes patóxenos prioritarios	C. González-Bello	Chemistry at the interface with Biology and Materials Science
	Rebeca Calviño Fachal	Cara a síntese de cables moleculares basados en oligoacenos que conteñen aneis de ciclobutadieno	D. Pérez	Organic Chemistry
	Jorge Millán Lema	Péptidos anfilíticos baseados en ácidos 2-aminometilciclopentanocarboxílicos	J.C. Estévez, R.J. Estévez	Organic Chemistry

	Iván Huertas Morales	Cicloadición entre alquenil aminas e dienos catalizada por Pd(II) mediante activación C(sp2)-H	M. Gulías, J.L. Mascareñas	Organic Chemistry
	Sergio Barbeira Arán	Síntese rexio e enantioselectiva de derivados quirais de biciclo (1.1.1) pentano mediante alquilación alílica asimétrica catalizada por cobre	M. Fañanás	Organic Chemistry
	Paula Martín González	Síntese diverxente de iminociclohexitoles e ácidos pipecólicos polihidroxilados	J.C. Estévez, R.J. Estévez	Organic Chemistry
	Adrián Martínez Abelairas	Síntese de novos precursores de grafenos nanoporosos	D. Peña	Organic Chemistry
	Lucía Martínez Reiriz	Química verde: procesos acelerados de síntese de dendrímeros	E. Fernández-Megía	Organic Chemistry
	Martín Piñeiro Suárez	Ensamblaxe asimétrico de moléculas multifuncionais mediante catálise de cobre enantioselectiva	M. Fañanás	Organic Chemistry
	Daniel Villar Castro	Síntese de novas ciclopentadienonas e óxidos de tiofeno	E. Guitián, D. Pérez	Organic Chemistry
	Alejandro Suárez Lustres	Benzazepinas azólicas mediante activaciones C-H catalizadas por metais	C. Saá, J.A. Varela	Organic Chemistry
	Alejandro de Manueles Bogajo	Capsulas supramoleculares baseadas en péptidos cíclicos con tapas	J.R. Granja, M. Amorín	Organic Chemistry
	Patricia Fulías Guzmán	Deseño e síntese de sondas sensoras do pH intracelular	J. Montenegro	Organic Chemistry
	Noemí Fiz Alvar	Oligo(p-fenilenetinileno) derivatizado con aleno como indutor quiral en polímeros helicoidais	E. Quiñoá, F. Freire	Organic Chemistry
	Pablo Cid Prieto	Control remote do sentido de xiro en polímeros helicoidais dinámicos	F. Freire, E. Quiñoá	Organic Chemistry
	Sandra Baúlde Arán	Desenvolvemento de dominios WW catalíticos de Pd(II)	J.L. Mascareñas, M.E. Vázquez	Organic Chemistry
	Jesús Fernando Salgado Barca	Ruthenium promoted deprotection reactions in the Golgi Apparatus	J.L. Mascareñas, M. Tomás	Organic Chemistry
	Borja Alvariño Ferreiro	Nanotubos peptídicos tipon Venturi basados en delta aminoácidos	J.R. Granja, M. Amorín	Organic Chemistry
	Estela Sánchez Santos	Desenvolvemento de ligandos irreversibles a EPSP sintasa para o tratamento da tuberculose	C. González-Bello	Organic Chemistry
	José Valdivia Pinaque	Catálise organometálica: novas rutas sostibles a amidas e macrolactamas	C. Saá, J.A. Varela	Organic Chemistry
	Alejandro Seco González	Mutacións in-silico de nanotubos peptídicos transmembranais: impacto nas propiedades internas da canle	R. García-Fandiño	Organic Chemistry
	Cayetana Gullón Conde	Alpha hélices superenrolladas a través de aminoácidos cromofóricos no canónicos	J. Montenegro, J. Bergueiro	Organic Chemistry
	Luis Antonio Pesquera Lorenzo	Polímeros intelixentes (Smart Polymers) e a súa resposta aos estímulos da luz	E. Quiñoá, F. Freire	Chemical Research and Industrial Chemistry

	Paula Pastor Calvo	Síntese de helicados trinucleares de Co (III) con propiedades de unión ao ADN de tres vías	M. Vázquez, J. Gómez	Chemical Research and Industrial Chemistry
	Ana García Barandela	Cobre como axente PSR (relaxación de xiro paramagnético) na supresión selectiva de sinais en RMN	E. Fernández-Megía	Chemical Research and Industrial Chemistry
	David García Martínez	Complexos quirais de rutenio en catálisis: ciclacións enantioselectivas	C. Saá, J.A. Varela	Chemical Research and Industrial Chemistry
	Antía del Río Otero	Cicloadicións 2+2 de alquinos e iminas a betalactamas catalizadas por rutenio	C. Saá, J.A. Varela	Chemical Research and Industrial Chemistry
	Pilar Suárez de Cepeda Fuentes	Desenvolvemento dun antibiótico adxuvante para restaurar a eficacia da fosfomicina	C. González-Bello	Chemical Research and Industrial Chemistry

Annex VII: Bachelor final projects

2021 – Bachelor final projects				
Area	Author	Title	Supervisor(s)	Bacherlor Degree
	Lucas García Abuín	Polímeros helicoidais supramoleculares con amplificación da quiralidade	F. Freire, E. Quiñoá	Chemistry
	Samara Abad González	Optimización da síntese de dendrímeros GATG: supresión de agregador	E. Fernández-Megía	Chemistry
	Patricia Gómez Roibás	Estudo da reactividade de 4,4-dicloro-2-butenoatos de alquilo en catálise de cobre	M. Fañanás	Chemistry
	Diego Cora Calvo	Os efectos isotópicos na química física	M.F. Rodríguez Prieto	Chemistry
	Silvia Santos Aldao	HAPs dopados: acoplamentos cruzados con substratos N-borilados catalizados por metais	J.A. Varela, C. Saá	Chemistry
	Sara Falcón Fariña	Xiros peptídicos inducidor pro B-aminoácidos cicloalcánicos	J.C. Estévez, R.J. Estévez	Chemistry
	Álvaro Arufe López	Sostenibilidade e catálise: novas rutas sintéticas a macrolactamas catalizadas por rutenio	C. Saá, J.A. Varela	Chemistry
	María Valentina Malavé Fernández	Diseño e síntese de precursores de cicloarenos	D. Peña, D. Pérez	Chemistry
	Miriam Nogueira Lorenzo	Síntese de péptidos cíclicos para ensamblaxe supremolecular de nanomateriais	J. Montengro , I. Insúa	Chemistry
	Braulio Casabella Amieiro	Desenvolvemento de sulfonopenicilinas para restaurar a acción dos antibióticos fronte ás superbacterias	C. González-Bello	Chemistry
	Alba María Torrón Celada	Síntese e estudo do ciclopéptido [L-Lys-D-Ser-L-His-D-Ala-BetaAla-L-Lys(Acetil-alcoxiamina)-D-Ala-L-His-D-Ser] para avaliar seu proceso de autoensamblaxe mediante a incorporación de fluoróforos nas cadeas laterais dos seus alfa-aminoácidos	M. Amorín, J. R. Granja	Chemistry
	Alberto Gómez Yáñez	Síntesis e aplicacións catalíticas de tiociclodextrinas	L. García-Río, M. Parajó	Chemistry
	Miguel Ferrer Arufe	Aplicación da síntese cianoacética a preparación de ácidos 2-aminometilciclopentanocarboxílicos polihidroxilados	J.C. Estévez, R.J. Estévez	Chemistry
	Carmen Villar Vázquez	Estudo da conductividade térmica en nanoestructuras mediante microscopía de forzas atómicas (AFM)	F. Rivadulla	Chemistry
	Clara Pose Insúa	Recoñocemento molecular de estructuras de ADN de tres vías	M. Vázquez, J. Gómez	Chemistry
	Li'Ann Rarís Blanco	Ciclacións enantioselectivas catalizadas por complexos quirales de rutenio	C. Saá, J. Varela	Chemistry
	Antón Luaces Calví	Síntese e reactividade do 2,3-dideshidrofenantreno	E. Guitián, D. Pérez	Chemistry
	Lara Troncoso Afonso	Fotocatálise bioortogonal promovida pola luz visible	J.L. Mascareñas, M. Tomás	Chemistry

	José Alejandro Gandarela González	Reaccións de cicloadición [3+2] de alquilidenciclopropanos catalizadas por complexos organometálicos de cobalto	J.L. Mascareñas, F. López	Chemistry
	Antonio Morgade de Arcos	Caracterización e fabricación de micro e nanoplásticos modelo	M. Lazzari	Chemistry
	Pablo Losada Castro	Síntese sostenible de aza-heterociclos bioactivos mediante activación catalítica de enlaces C-H	M. Gulías, J.L. Mascareñas	Chemistry
	Manuel Rodríguez Romero	Novos metaloencimas artificiais unidos a microesferas proteicas como reactores bioortogonais (Parte B)	J.M. Martínez Costas, N. Barreiro	Double degree - Chemistry & Biology
		Novos metaloencimas artificiais unidos a microesferas proteicas como reactores bioortogonais (Parte A)	J.L. Mascareñas, M. Tomás	
	Sandra Carreiras Suárez	Estudo do envellecemento de máscaras cirúrxicas desbotables	M. Lazzari, M. Torneiro	Double degree - Chemistry & Biology
	Alba Barreiro Lusquiños	Síntese e evaluación biolóxica de derivados de fosfonio policíclicos (Parte B)	A.Vidal, E. Vázquez	Double degree - Chemistry & Biology
		Síntese e evaluación biolóxica de derivados de fosfonio policíclicos (Parte A)		
	Anxo Rey Blanco	Péptidos híbridos para transfección de células do sistema inmune (Parte A)	J. Montenegro	Double degree - Chemistry & Biology
		Péptidos híbridos para transfección de células do sistema inmune (Parte B)	J. Montenegro, I. Lostalé	
	Marco Pardo Freire	Formación de biopelículas por bacterias multirresistentes e o seu control mediante bacteriófagos	J.A. López Romalde, C. González-Bello	Double degree - Chemistry & Biology
		Inhibición da formación de biopelículas en patóxenos multirresistentes mediante a desactivación da comunicación bacteriana	C. González-Bello	
	Verónica Feteira Montero	Nanocarriers para o transporte de moléculas con relevancia biolóxica: ARN	B. Pelaz, E. Polo	Double degree - Chemistry & Biology
	Iría Esperón Abril	Desenvolvemento de protocélulas de tipo complexo poliiónico: estudo da comunicación intercelular	E. Fernández-Megía	Double degree - Chemistry & Biology
		Desenvolvemento de protocélulas de tipo complexo poliiónico: estudo de tamaño e estabilidade		
	Adrián Conde Piñeiro	Análise xenómica de Acinetobacter spp. con resistencia a B-lactámicos	J.A. López Romalde, C. González-Bello	Double degree - Chemistry & Biology
		Desenvolvemento dun Kit de diagnóstico clínico para a identificación de bacterias multirresistentes	C. González-Bello	
	Sergio Serantes Otero	Péptidos cíclicos antimicrobianos (Parte A)	J.R. Granja	Double degree - Chemistry & Biology
	Daniel Conde Torres	Nanotubos peptídicos en membranas lipídicas: un estudo computacional a través de simulacións de dinámica molecular	R. García Fandiño, M. Calvelo	Double degree - Physics & Chemistry
	Sara Díaz Rodríguez	Estabilización e propiedades catalíticas de nanoestructuras de paladio	P. del Pino, B. Pelaz	Double degree - Physics & Chemistry
		Síntese e caracterización de composites híbridos nanopartícula-nanoMOFs		

	Lucía Camila Tasende Rodríguez	Autoensamblaxe de nanocristais de perovskitas de haluros de cesio e chumbo. Síntese e caracterización	P. del Pino, B. Pelaz	Double degree - Physics & Chemistry
		Perovskitas de haluros de cesio e chumbo. Síntese, caracterización e estabilización en medios acuosos		
	Lucía González Pico	Descubrimento de ligandos selectivos do receptor A2B de Adenosina por alquilación de derivados pirimidínicos	E. Sotelo	Pharmacy

ANNEX VIII: Invited Lectures given by CiQUS Researchers during 2021

Invited Lectures					
Area	**Author(s)**	**Title**	**Type**	**Conference**	**Place**
	C. González Bello	*Antibiotic adjuvants - A booming strategy to unlock bacterial resistance*	Invited Lecture	GP$_2$A Meeting on "Drug discovery in the era of antimicrobial resistance"	France, online
	C. González Bello	*Facing the Superbug Challenge with Innovative Approaches*	Plenary Lecture	Universitat Jaume I	Spain
	Félix Freire	*Axial to Axial Helix Induction in PPAs Using Allenes as a Chiral Source*	Keynote Lecture	Symposium on Foldamers	France
	Majellaro, M., Azuaje, J., Brea, P., Loza, M.I, Sotelo, E.	*Innovative chemistry to illuminate biology: Novel fluorescent ligands to study GPCRS binding and signaling*	Invited Lecture	Fourth ERNEST meeting: Insights from structures of signalling complexes and computational modelling of GPCR signalling	Online
	Rafael Ramos	*Enhancement of the spin thermoelectric conversion in insulating-magnet/metal heterostructures*	Invited Lecture	one-day international online workshop: Oxides for Spin-Orbitronics and Spin-Caloritronics 2021	France
	Javier Montenegro	*Supramolecular Lessons for New Biomaterials in Gene Delivery and Cytoskeleton Mimic*	Invited Lecture	Spring Meeting 2021	Online
	Javier Montenegro	*Supramolecular Organic Chemistry for Chemical and Synthetic Biology*	Invited Lecture	PhD course_Industrial Chemmistry	Online
	Javier Montenegro	*Desingning functional biomolecular assemblies: Beyond Biology*	Invited Lecture	EMBO Courses and workshops	Germany
	Soraya Learte Aymamí	*Metallopeptides and metalloproteins in Chemical Biology: From DNA binding to intracelular catalysis*	Invited Lecture (Research Lilly Doctorate Award 2021)	RSEQ Symposium	Online
	Eva Rivera-Chao	*New synthetic routes towards alkenylboronates via catalytic alkyne allylborations reactions*	Invited Lecture (Research Lilly Doctorate Award 2021)	RSEQ Symposium	Online
	Martín Fañanás-Mastral	*Turning simple hydrocarbons into multifunctional building blocks*	Invited Lecture	*Young Investigator Workshop 2021 – EuCheMS Organic Division*	Spain

	Beatriz Pelaz	*Efficient Nanocarriers*	Plenary Lecture	4th Spanish Conference on Biomedical Applications of Nanomaterials	Online
	Beatriz Pelaz	*Remotely controlled colloidal nanosystems*	Invited Lecture	11th Early Stage Researchers Workshop in Nanoscience	Online
	Ester Polo	*Functionalized Plasmonic Nanoparticles for Bio-Applications*	Invited Lecture	Plasmonic NPs: synthesis, characterization and applications"	Online

ANNEX IX: Research stays of CiQUS members during 2021

Area	Researcher	Position	Hosting Institution	Country	Funding	Start	End
	Adrián Martínez Castrillón	PhD Candidate	CIC Nanogune	España	CiQUS	15/9/21	30/9/21
	Rubén Prieto Díaz	PhD Candidate	Universidad de Upsala	Suecia	Xunta de Galicia	1/5/21	31/7/21
	Sara Illodo Brea	PhD Candidate	University of St Andrews	Reino Unido	CiQUS	4/10/21	30/10/21
	Giulia Salluce	PhD Candidate	University of Cambridge, Department of Chemistry	United Kingdom	AEI	6/9/21	6/12/21
	Alicia Rioboo Vidal	PhD Candidate	Stratingh Institute for Chemistry, Groningen	Netherlands	MECD	6/9/21	5/12/21
	Xandro Vidal Pereira	PhD Candidate	Stockholm University	Noruega	MECD	1/3/21	31/5/21
	Alejandro Gutiérrez González	PhD Candidate	Max Planck Institut für Kohlenforschung, Mullheim an der Rür	Alemania	MECD	25/2/21	1/6/21
	Eduardo DaConcepción Vicente	PhD Candidate	Max Planck Institut für Kohlenforschung, Mullheim an der Rür	Alemania	Xunta de Galicia	1/5/21	31/7/21
	Jose Manuel González González	PhD Candidate	Scripps Research Institute, La Joya CA	Estados Unidos de América	Xunta de Galicia	31/5/21	2/9/21
	Andrés Arribas Domingo	PhD Candidate	Universidad de Zurich	Suiza	Xunta de Galicia	1/7/21	30/9/21
	Xulián Fernández González	PhD Candidate	ICN2 (Institut Català de Nanociència i Nanotecnologia), Barcelona	España	CiQUS	15/9/21	15/11/21
	Daniel Marcos Atanes	PhD Candidate	CIC BioGUNE, Bilbao	España	CiQUS	1/10/21	31/10/21
	Manuel Ceballos	PhD Candidate	CNRS	France	MSCA-ITN	2/6/21	30/7/21
	Aitor Álvarez Lorenzo	PhD Candidate	International Iberian Nanotechnology Laboratory – INL	Portugal	MECD	13/9/21	12/12/21

ANNEX X: Patents in 2021

Area	Title	Country / Region	Publication Number	Date	Inventors	Owner
	Protein muns that can form inclusions in the endoplasmic reticulum, methods for the use thereof and uses of same	**EU**	US 11174485B2		**José Manuel Martínez** Costas, Natalia Barreiro, **Francisco Javier Benavente**	USC
	Ruthenium complexes for treating cancer which comprises cancer stem cells	**MX**	MX 385760		Jessica Rodríguez Villar, **José Luis Mascareñas Cid**, José Rodríguez Couceiro, Jesús Mosquera Mosquera, **Marco Eugenio Vázquez Sentís**, Bruno Sainz Anding	USC (80%) UAM (20%)
	Fragmentos peptídicos de CX43 para su uso como agentes senolíticos	**ES**	ES2804039A1	**02/02/21**	María D. Mayán Santos, Marta Varela Eirín, Alejandro Castro Iglesias, **M. Eugenio Vázquez Sentis, José Luis Mascareñas Cid**, Soraya Learte Aymami, José Ramón Caeiro Rey, Elena Pazos Chantero	F. Novoa Santos (65%) USC (25%) UDC (7,5%) Servizo Galego de Saúde (2,5%)
	Catalizadores heteroxéneos metal cerámicos con estructura tridimensional obtida por 3D printing	**ES**	ES2824324B2	**27/09/21**	Francisco Gitián, Alvaro Gil, M. Carmen Rial Tubio, **Eddy Sotelo**, Alberto Coelho	USC
	Composto para pilas	**ES**	ES2796448B2	**08/04/21**	**María Giménez López**, Eugenia P. Quirós Diez, Melanie Guillen Soler	USC
	Fluído supramolecular	**ES**	ES2797556B2	**20/04/21**	**María del Carmen Giménez López, José Francisco Rivadulla Fernandez**, Carlos Herreros Lucas, Carlos Lopez Bueno	USC
	Use of a boron cluster compound as transmembrane carrier	**ES WO**	EP20182648 WO/2021/259668	**30/12/21**	Werner Nay**, Javier Montenegro**	Jacobs Univ. Bremen GGMBH, USC
	FluoroTools	**ES**	EP20382684		**Eddy Sotelo**	USC

ANNEX XI: 2021 CiQUS Lecture's Programme

Area	Lecturer	Topic	Institution	Country	Date
	Dr. Luís Mafra	Unveiling CO_2 chemisorption mechanisms in porous adsorbents via surface-enhanced NMR: Quo vadis?	University of Aveiro | CICECO	Portugal	22/01/21
	Prof. Nazario Martín	Carbon Nanostructures for Emergent Viruses: Ebola and beyond	IMDEA-Nanoscience	Spain	05/02/21
	Prof. Hermenegildo García	Getting closer to a large-scale process. Photocatalysts for light-assisted CO_2 hydrogenation	Institute of Chemical Technology (ITQ) | University of Valencia	Spain	12/03/21
	Prof. Michinori Suginome	Asymmetric Amplification Using Dynamic Helical Macromolecule PQX as a Catalyst Platform	Department of Synthetic Chemistry and Biological Chemistry | Kyoto University	Japan	04/06/21
	Prof. Luis M. Liz-Marzán	Colloidal BioNanoPLasmonics	CIC biomaGUNE | BRTA | Ciber-BBN Ikerbasque	Spain	06/07/21
	Prof. Miguel López	New targets for obesity treatment: hypothalamic AMPK	CiMUS | USC	Spain	10/11/21
	Laura M. Salonen, PhD	Covalent organic frameworks – From design to applications	International Iberian Nanotechnology Laboratory (INL)	Portugal	30/11/21
	Prof. Igor Larrosa	Transition metal catalyzed C-H activation: reactivity and selectivity control and late-stage functionalization	University of Manchester	UK	02/12/21
	Alberto García-Fernández, PhD	Synchrotron-based photoelectron spectroscopy of hybrid perovskites. From surface to device characterization	KTH – Royal Institute of Technology	Sweden	21/12/21
	Patricia Barral, PhD	Lipids: friend or foe in tissue homeostasis	The Francis Crick Institute and the Peter Gorer Deparment of Immunology | King's College London	UK	22/12/21