

Q

CiQUS

Centro Singular de Investigación
en **Química Biolóxica e**
Materiais Moleculares

Annual Scientific Report 2022

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

Table of contents

Foreword	3
1. ORGANIZATION	5
1.1. ORGANIZATIONAL CHART.....	5
1.2. DESCRIPTION AND COMPOSITION (DECEMBER 31, 2022)	5
2. FACTS & FIGURES	9
3. SCIENTIFIC AREAS AND RESEARCH LINES	11
3.1 STRATEGIC SCIENTIFIC PROGRAMME.....	12
3.2 SCIENTIFIC AREAS AND RESEARCH LINES.....	12
4. HUMAN RESOURCES	15
4.1 HUMAN RESOURCES BY CATEGORIES	15
4.2 TALENT RECRUITMENT	15
5. R&D PROJECTS, NETWORKS, AND INTERNATIONAL COLLABORATIONS	19
5.1 R&D PROJECTS.....	19
5.3 RESEARCH NETWORKS.....	23
5.4 INTERNATIONAL COLLABORATIONS.....	25
6. RESEARCH OUTPUT	27
6.1 SCIENTIFIC PRODUCTION.....	27
6.2 AWARDS	31
7. INNOVATION, TECHNOLOGY TRANSFER AND VALORIZATION	33
7.1 VALORIZATION PROJECTS.....	33
7.2 R&D CONTRACTS AND SERVICES IN COLLABORATION WITH COMPANIES.....	33
7.3 INNOVATION & ENTREPRENEURSHIP	33
7.4 PATENTS	34
8. TRAINING	35
9. COMMUNICATION & OUTREACH	41
9.1 COMMUNICATION	41
9.2 OUTREACH	44
9.3 ORGANIZATION OF SCIENTIFIC EVENTS.....	46
10. INFRASTRUCTURES	49
10.1 RESEARCH FACILITIES.....	49
10.2 SINGULAR LABORATORIES	50
10.3 OTHER FACILITIES AND RESOURCES AT THE USC.....	51
ANNEXES	53
ANNEX I: CIQUS MEMBERS (DECEMBER 31, 2022).....	55
ANNEX II: ACTIVE R&D & VALORIZATION PROJECTS DURING 2022.....	65

CiQUS Annual Scientific Report 2022

ANNEX III: ACTIVE R&D CONTRACTS DURING 2022	77
ANNEX IV: LIST OF PUBLICATIONS	79
ANNEX V: THESES DEFENDED.....	93
ANNEX VI: MASTER DISSERTATIONS.....	95
ANNEX VII: BACHELOR FINAL PROJECTS.....	97
ANNEX VIII: INVITED LECTURES GIVEN BY CIQUS RESEARCHERS DURING 2022	101
ANNEX IX: RESEARCH STAYS OF CIQUS MEMBERS DURING 2022.....	105
ANNEX X: PATENTS IN 2022	107
ANNEX XI: 2022 CIQUS LECTURE'S PROGRAMME	109

Foreword

It goes without saying that the past year has been a memorable moment in CiQUS history. The Center celebrated its 10th anniversary with the organization of the 1st Symposium *Chemistry at the Frontier*. Although it was initially scheduled for the year 2021, restrictions derived from the pandemic forced us to move it to 2022. Nevertheless, this scientific meeting that took place from March 30th to April 1st 2022, brought to Santiago de Compostela an extraordinary panel of world-leading scientists as plenary, keynote or invited speakers, and also many good friends who joined our special celebration and made it really unforgettable. Special thanks go to the whole CiQUS community for their commitment, collaboration, and participation on this event. The meeting also entailed the first visit of the recent Nobel laureate David MacMillan to a country other than the US.

By the end of the spring 2022, CiQUS had to face crucial challenges that could significantly influence its progression in the coming years. The programme 2019-2022 for supporting Research Centers of the Galician University Systems reached its end. So, our center underwent the corresponding evaluation process by an external committee appointed by the *Consellería de Cultura, Educación, Formación Profesional e Universidades* of the Xunta de Galicia Government. This committee made an exhaustive evaluation of the progression and results of the eight centers of the Galician research centers network for the period 2019-2022. CiQUS' progress was considered as excellent (score A) and ranked first among all the regional centers. The result of this evaluation determined the basal funding approved for the center to continue its activity during the year 2023. The result of this evaluation confirms the great progress of CiQUS in the last years, which is now well-recognized at national and international levels, with a good number of ongoing projects at the frontier of knowledge, high-quality scientific production, high level of funding and a remarkable incorporation of high-quality junior researchers, as well as with high standards in the organization of the center.

Specifically in 2022, CiQUS researchers have been granted with up to 23 new R&D projects and 6 new Valorization or Proof of Concept projects for a total amount of 7,14 M €. Particularly worth mentioning is the success achieved by the CiQUS' Junior Scientists in the new call for Strategic Projects Oriented to the Ecological Transition and the Digital Transition, launched by the Spanish Research Agency, where they lead the 43% of the total number of proposals granted to the CiQUS. By the end of the year, the European Innovation Council granted two projects to CiQUS' PI J. Montenegro, through the EIC-Pathfinder and an EIC-Transition programmes (the latter being the first project under this framework granted in Galicia). In terms of HHRR competitive public calls, up to 26 CiQUS members were granted under different frameworks.

Regarding our scientific output, it's worth to note that 42% of CiQUS' articles were published in JCR journals with IF higher than 9, including contributions in Nature, Science and Nature Chemistry, that involved international collaborations. In terms of tech transfer, up to 4 new international patents were granted last year.

Finally, once the restrictions applied as consequence of the COVID were suppressed, we are extremely glad to have been able to recover the total normality in the center. This fact led to the CiQUS members to re-establish their normal working schedules, without time limitation or capacity restrictions for the labs and common spaces. Additionally, we were also able to fully restart our outreach and dissemination programmes, recovering the visits of students from primary to high school level, and organizing outreach activities throughout the whole year.

Yours,



José Luis Mascareñas
CiQUS Scientific Director



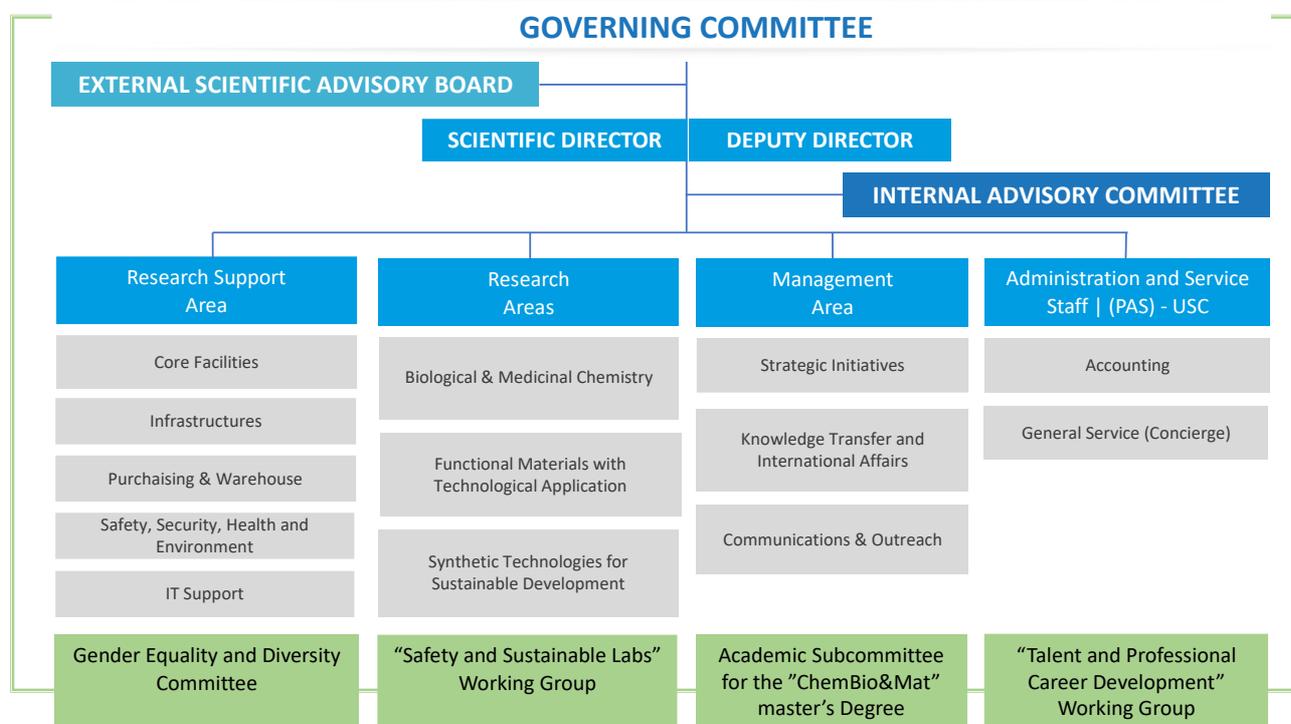
Dolores Pérez
CiQUS Deputy Director

Santiago de Compostela, April 2023

1. ORGANIZATION

1.1. Organizational Chart

The structure of CiQUS is implemented as per the organizational chart shown below.



Organizational Chart at CiQUS

1.2. Description and composition (December 31, 2022)

GOVERNING COMMITTEE

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*

María del Pilar Bermejo Barrera, *Representative of the USC Governing Council*

Cecilia Sierra Rey, *USC Social Council President*

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

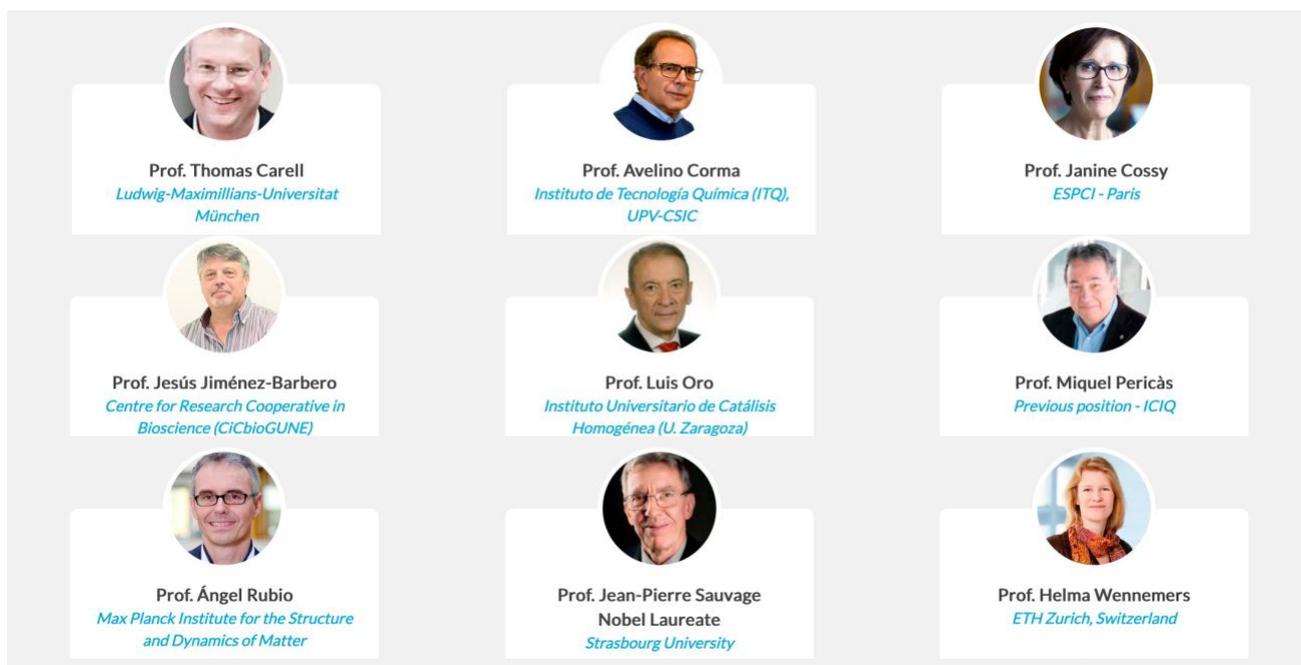
Carlos Closa Montero, *CSIC Vice-President for Organization and Institutional Affairs*

José Luis Mascareñas Cid, *CiQUS Scientific Director*

María Dolores Pérez Meirás, *CiQUS Deputy Director*

Changes affecting the composition of the CiQUS Governing Committee in 2022 were the incorporation of Prof. M. Pilar Bermejo as representative of the USC Governing Council (as on May 25th, 2022) and the designation of Prof. Carlos Closa Montero as representative of CSIC (as on August 17th, 2022).

EXTERNAL SCIENTIFIC ADVISORY BOARD (ESAB)



CiQUS ESAB Members

Prof. Helma Wennemers (ETH Zurich, Switzerland) was appointed as CiQUS ESAB member by the Governing Committee on May 31st, 2022.

DIRECTORS

Scientific Director: José Luis Mascareñas Cid

Deputy Director: María Dolores Pérez Meirás

- **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 an **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 programme aimed at discovering novel methods based on metal catalysis, and a chemical biology programme 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 as Scientific Director of CiQUS in February 2014, being his appointment renewed on September 2019 for an additional period of 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 and Innovation at the USC (2006-2010). In 2010, she was appointed as Commissioner Director of CiQUS, being responsible for the establishment and operation of the center until 2014, when she was appointed as Deputy Director. 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.

The functions and competences of the CiQUS Governing Committee, the CiQUS ESAB and the CiQUS Directors are set out in the [CiQUS Internal Regime Regulations](#), which last version was approved by the USC Governing Council in October 29, 2021.

INTERNAL ADVISORY COMMITTEE

An advisory board representative of the main research areas at the CiQUS, that it is currently constituted by CiQUS PIs *Juan R. Granja, Antonio Fernández-Ramos, Pablo del Pino and María Giménez*. Diego Peña is also part of the internal advisory committee since spring 2022. 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.

RESEARCH AREAS

The CiQUS scientific team is currently organized into 18 research groups, whose research lines are aligned to the three main thematic areas: *i) Biological and Medicinal Chemistry; ii) Functional Materials with Technological Application and iii) Synthetic Technologies for Sustainable Development* ([See CiQUS webpage for more info](#)).

MANAGEMENT AREA

This area integrates 3 different units:

- ✓ **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

This area is 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 5 different units:

✓ Core facilities: provides the scientific instrumentation support needed to carrying out research at CiQUS, ensures the maintenance and optimal use of the equipment, and offers training in the use of the equipment, sample preparation and data processing [Dr. Arcadio Guerra (manager), Laura Acevedo]. Furthermore, a Biological Support Technician (Rebeca Menaya) is responsible for cell culture labs and for assistance on other biological techniques to the CiQUS researchers.

✓ Infrastructures: responsible for the management and maintenance of labs, equipment, furniture, and general spaces at CiQUS [Laura Acevedo (manager)].

✓ Purchasing and Warehouse: centralized purchasing of reagents, solvents, disposable laboratory products and management of the CiQUS' warehouse [Noela Torrente (manager), Andrea López].

✓ Safety, Health and Environment: Updating and implementation of the CiQUS' Safety and Risk Prevention Plan, including training to all new CiQUS members, coordination and training of the emergency teams and management of the laboratories' safety (Noela Torrente).

✓ Information technology: 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 (Adrián Torreiro).

In 2022, our research support team was strengthened by hiring new personnel:

✓ An Advanced Microscopy Lab manager (Dr. Enrica Soprano, part-time dedication to this task): PhD in Materials Science with extensive experience in fluorescence, confocal and hyperspectral microscopy. Responsible for scientific-technical support in the Advanced Microscopy laboratory at CiQUS.

✓ A senior research support technician for the area of Functional Materials (Dr. Víctor Leborán): PhD in Physics with solid background in the construction of thermal and electrical transport measurement devices as well as in the development of scientific instrumentation control software. Responsible for scientific-technical support to the CiQUS Groups working on the development of new materials and thermic and electronic devices.

✓ Two assistant research support technicians (Álvaro Sande and Tamara Vázquez) hired through the INVESTIGO Programme, funded by the Galician regional government. They give general technical support to CiQUS research groups working in the fields of functional materials and chemical biology, respectively.

ADMINISTRATION AND SERVICES STAFF AREA

This area is covered by USC Permanent Staff (PAS category – *Persoal de administración e servizos*) and includes:

✓ Accounting and administrative support (Mercedes Varela, Lucía Rodríguez). Elena Veiga former CiQUS Accounting Manager retired at the end of fall 2022.

✓ Concierge and general services (M. Carmen Rey, Ángel Rama).

As a main novelty of the year 2022, different working teams and/or committees have been launched to analyze and implement new programmes and strategic actions related to transversal issues: i) *Gender Equality and Diversity Committee*; ii) *Safety and Sustainable Lab's Working Group*; iii) *Academic Subcommittee for the ChemBio&Mat master's degree* and iv) *Talent and Professional Career Development Working Group*. These working groups and committees are formed by members of the CiQUS community representing the different categories, areas, and positions at the Center.

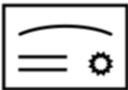
2. FACTS & FIGURES

As an overview, we have listed 8 cumulative key figures to illustrate the performance of CiQUS in 2022:

Ranked **1st** 
CIGUS Centers (*) 2019-2022
Evaluation
() Galician University System Network of Research Centres (CIGUS Network)*


7,84 M€
Income of new Projects & Contracts

23 
New R&D Projects
including **7** TED Projects (*)
() Strategic Projects Oriented to the Ecological and the Digital Transition*

6 
New Proof of Concept Projects
4 New International granted patents

42% 
articles published in JCR-journals with **IF>9**

26 
New Researchers granted with HRRR public competitive programs

14 
PhD Theses defended
50% International Mention

 **3,544** followers
 **2,877** followers
 **2,107** followers
>1,500 New followers in 2022

3. SCIENTIFIC AREAS AND RESEARCH LINES

The CiQUS Strategic Scientific Agenda was developed in alignment with on the Mission, Vision and Strategic Values defined for the Center at the time of its creation, which maintain fully validity now a days:



MISSION

- ✓ To promote the advancement of **science at the frontier of knowledge** in the fields of synthetic chemistry, chemical biology and functional materials
 - ✓ **Training** new scientists, professionals and future leaders
- ✓ To create socio-economic **progress** and **technology transfer**
- ✓ To increase the international **prestige** of the USC and Galicia



VISION

To be an **international reference** center on excellent, interdisciplinary chemical research at the frontier with chemical biology and materials science

STRATEGIC VALUES



- ✓ **Cutting edge science**
- ✓ Multidisciplinarity
- ✓ Intra & inter-collaborative projects
- ✓ Responsible research and innovation
- ✓ Outreach to society



- ✓ **Best researchers and best students**
- ✓ Stimulating scientific environment
- ✓ Competitive recruitment and selection processes
- ✓ Gender balance
- ✓ Excellence in training



- ✓ **Self-demanding model**
- ✓ Professional R&D management
- ✓ Support to researchers
- ✓ Shared resources and facilities

3.1 Strategic Scientific Programme

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, Biology and Materials Science, and on fostering the transfer knowledge and research results to the society. Towards this end we seek an effective Interdisciplinary Integration of Research Topics supported by highly competitive scientists with complementary expertise.



Biological & Medicinal Chemistry

- Bio-Supramolecular Chemistry
- Chemistry & Nanotechnology at the frontier with Cell Biology and Biomedicine
- Pharmacological Agents, cell transport an innovative strategies for the activation of pro-drugs



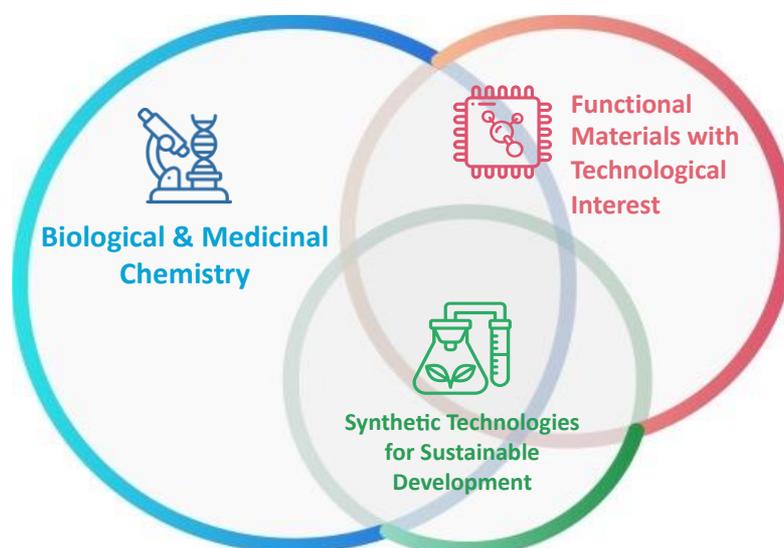
Functional Materials with Technological Application

- Nanostructures with technological applications
- Sensors & thermal and electronic devices



Synthetic Technologies for Sustainable Development

- Catalysis & synthesis for sustainable development
- Chemical technologies for product health



CiQUS Strategic Scientific Areas and Research Lines

3.2 Scientific Areas and Research Lines

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 encouraging 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 or bacterial resistance. Our current organization includes, among others, the following research topics associated to different PIs:

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

I.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) Bioprinting of nanoparticles for medical applications (B. Pelaz). d) Smart biomimetic nano-systems (J. Montenegro, P. del Pino). e) Photocatalytic processes inside cells (M. Tomás). F) Biomimetic cell-derived nanovectors (E. Polo).

I.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 was the incorporation of Dr Beatriz Orosa as *Ramón y Cajal* researcher who joint the CiQUS in spring 2022. She leads a new research line at the Center focused on the development of new **immunity tools by post-translational modifications**.

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.

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

II.2) SENSORS: THERMAL AND ELECTRONIC DEVICES: a) Custom-crafted graphene nanostructures for the design of new nanoscale quantum spintronic devices (D. Peña). b) Fabrication of new electrodes of zinc-air long-life batteries (M. Giménez-López). c) Devices for ultraprecise thermal measurements (F. Rivadulla). d) Stimuli-responsive dynamic polymers (F. Freire/E. Quiñoá). e) Development of portable nanophotonic biosensors based on multifunctional nanoporous graphene for early diagnostics (D. Peña). f) Functional materials for active control of thermal conductivity (F. Rivadulla). g) Engineered conductive proteins for upscaling and using as smart ink-based conductors and ionic electrolytes in energy storage devices (E. Vázquez). h) Development of thin film oxide nanostructures for information, logic and energy management (R. Ramos).

III. SYNTHETIC TECHNOLOGIES FOR SUSTAINABLE DEVELOPMENT

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

III.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). f) Sustainable chemical methods promoted by visible light for greenhouse gases valorization, biodegradable polymers and bioconjugation processes (M. Nappi). g) Simulation of MOFs and related heterogeneous catalytic systems for biomass Upgrading (M. Ortuño).

III.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.

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.

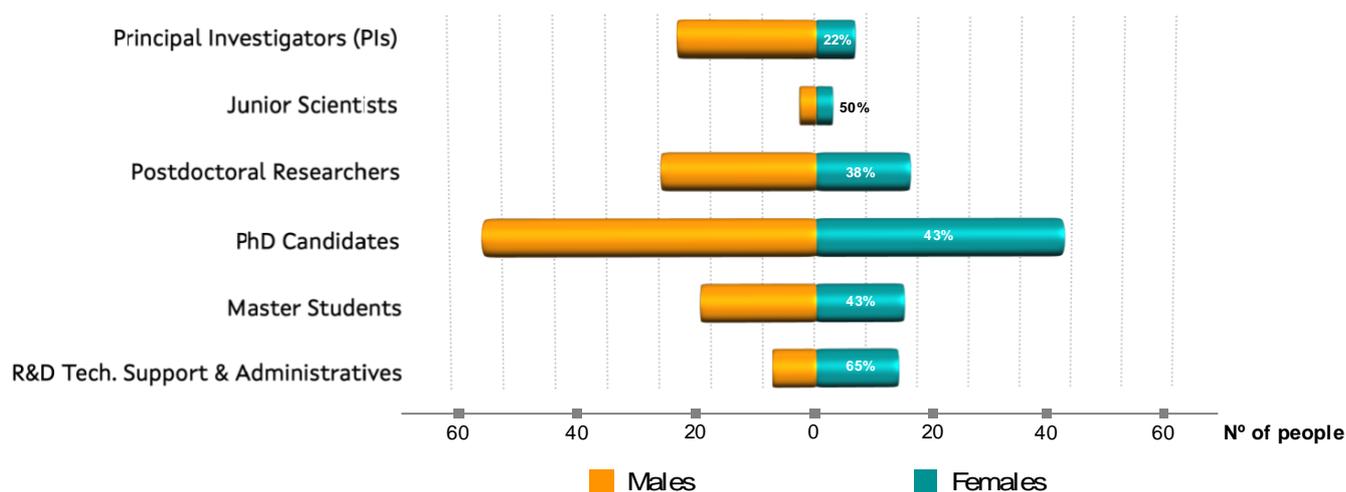
For a more detailed description of the different research lines of the Strategic Scientific Project, see <https://www.usc.es/ciqus/en/research/research-groups>.

4. HUMAN RESOURCES

4.1 Human Resources by Categories

32 Principal Investigators (PIs), 6 Junior Scientists (Junior Group Leader), 45 postdoctoral researchers, 106 PhD candidates, 37 Master students and 23 Technical and administrative assistants (8 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, 2022)

In December 2022, over 250 people (41% female; 7% foreigners from up to 9 different countries) were working at CiQUS: 32 Principal Investigators (3 of them *Ramón y Cajal* associates; 22% female; 6% foreigners), 6 Junior group leaders (4 *Ramón y Cajal* associates, 1 *Xunta de Galicia Distinguished Researcher*, 1 *Manuela Barreiro – USC Distinguished Researcher*, 50% female; 16% foreigners), 45 postdoctoral researchers (4 *Juan de la Cierva*, 2 *MSCA-PF*, 6 *Xunta de Galicia* postdocs, 2 *María de Zambrano* and 5 *Margarita Salas* researchers; 38% female and around 15% of CiQUS postdoctoral researchers coming from abroad), 106 PhD candidates (43% female and 10% foreigners), 37 MSc students (43% female), together with 23 people of technical, management and administration staff (8 of them hired by a research groups). 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 2022) is included in Annex I.



Distribution of human resources by categories

4.2 Talent Recruitment

4.2.1 Human Resources hired under competitive public calls

At the **senior postdoctoral level**, two brilliant young scientists started their position as *Ramón y Cajal Researchers* at the CiQUS in the year 2022 [María Tomás (2020 call) and Beatriz Orosa (2019 call)]. Additionally, 3 other CiQUS researchers, Julián Bergueiro, Andrea Pérez Potti and Ignacio Insua, have been granted with contracts from the same HHRR Programme in the call of 2021 (results published in 2022). Whereas J. Bergueiro and A. Pérez Potti started their *Ramón y Cajal* contracts at the CiQUS in January 2023, I. Insua will move to the USC Department of Pharmacology, Pharmacy and Pharmaceutical Technology to start there his independent research lines.

At the postdoctoral level, Rafael Riego and José M. Vila-Fungueiriño started their contracts as *Juan de la Cierva* researchers at the CiQUS during the year 2022 (2021 call). Furthermore, L. Mateo de Doni has been granted with a Juan de la Cierva Contract in the call of 2022, starting his contract in January 2023.

Regarding International HHRR Programmes, up to **4 scientists have been granted with MSCA Postdoctoral Fellowships during the year 2022** (D. Bugallo, N. Tiwari, A. Sánchez and S. Fazal). The result of this call clearly reflects the success of the CiQUS strategic action for supporting MSCA candidates during the application process ([see more info](#)). Through this initiative, highly specialized support is provided to those candidates with outstanding scientific profiles aligned with our scientific strategic agenda in order to complement our research capacities ([See link](#)).

In terms of regional postdoctoral HHRR Programmes, during 2022 up to 5 CiQUS young promising researchers have been granted with postdoctoral contracts within the framework of the Xunta de Galicia HHRR programmes for postdoctoral training. María Maneiro and David Ferro-Costas were granted with Xunta de Galicia Postdoctoral Contracts – Modality B, for two-years research position at CiQUS. Furthermore, Silvia Castro, Jesús Castro and Eva Rivera were granted with Xunta de Galicia Postdoctoral Contracts – Modality A, that will fund their contracts for two years at international research centers abroad [Oxford University (UK), MIT (USA) and Aachen University (Germany), respectively] and, later on, an additionally one-year return contract at the CiQUS.

With regard to pre-doctoral trainees, up to **12 CiQUS PhD candidates** have been granted within the framework of different national and regional HHRR programmes during the year 2022: **4 MECD – FPU Predoctoral Contracts (National Programme)**: Y. Folgar (Supervisor: J. Montenegro), L. Goicoechea (Supervisor: M. Gulías), A. Agulleiro (Supervisor: J. Granja) and A. Garcia (Supervisor: E. Sotelo); **4 AEI – Predoctoral Contracts (National Programme; contracts associated to research projects funded by the AEI)**: M. Piñeiro (Supervisor: M. Fañanas), P. Gulías (Supervisor: J. Montenegro), S. Díaz (Supervisor: F. López) and A. Durán (Supervisor: E. Polo); **3 Xunta de Galicia Predoctoral Contracts (Regional Programme)**: D. Conde (Supervisor: R. García-Fandiño), M.C. Pacín (Supervisor: M. Lazzari) and A.D. Varela (Supervisor: P. del Pino), and **1 Xunta de Galicia Contract for Industrial PhD studies (Regional Programme)**: F. Suárez (Supervisor: R. García-Fandiño). There is currently another AEI - Pre-doctoral contract assigned to a CiQUS group (Supervisor: M. Giménez) which resolution is still pending. Furthermore, Daniel Marcos (Supervisor: J.L. Mascareñas) was granted **with a prestigious mobility Fulbright Spain Fellowship** for a six-months research secondment at UC Berkeley (USA).

It is worth mentioning that during 2022 **up to 81 researchers were funded by competitive public programmes** (more than 54% of CiQUS trainees, considering postdoctoral and predoctoral researchers).

Finally, the new **INVESTIGO call** funded by NextGeneration EU programme and focused to the recruitment of young research support staff and/or technicians in research bodies, public universities, technology centres and other public and private entities involved in research, allowed the incorporation of 2 research support technicians (Álvaro Sande and Tamara Vázquez) in 2022, with 1-year full-time contracts.

4.2.2 Human Resources hired through R&D contracts

During 2022, up to 75 researchers were directly hired by the CiQUS groups through R&D contracts (25 postdoctoral researchers and more than 50 PhD candidates). Additionally, CiQUS funds the R&D contract of 1 Junior Scientist (M. Nappi, *Manuela Barreiro Distinguished Researcher*) and 10 Master Students (CiQUS Part-time Research Initiation contracts. *See section 4.2.3*).

Regarding research support technicians and managers, whereas CiQUS funds the contract of 9 people (CiQUS technical support unit), up to 8 technicians are directly hired by the CiQUS groups.

4.2.3 CiQUS talent attraction programmes

- **Research initiation contracts for CiQUS Master Students:** a strategic initiative aimed at master's students for strengthening some of the center's most active lines of research, as well as providing an unbeatable stimulus and experience to young, prospective researchers during this first training period. The 9th edition of this programme offered 10 part-time research contracts for graduate students. The final awardees were enrolled in the Master of Organic Chemistry (5), the Master in Chemistry at the Interface with Biology and Materials Science (4) and in the Master in Chemical Research and Industrial Chemistry (1). It is worth noting that 8 of the 10 master students granted within the framework of this call during the academic year 2021/2022 are currently performing their PhD studies at the CiQUS. 2 of them having been already granted with HHRR competitive public contracts for performing their PhD studies.

The 10th edition of this programme was launched in November 2022. Up to 8 master students were hired as part-time research initiation staff during 9 months in 2023. The final awardees are currently enrolled in the Master of Organic Chemistry (3), the Master in Biomedical Research (2), the Master in Chemistry at the Interface with Biology and Materials Science (1), the master in Physics (1) and the Master in Chemical Research and Industrial Chemistry (1).

- **CiQUS Summer Fellowships programme:** a strategic initiative aimed at highly motivated undergraduate students (pursuing the last or penultimate academic course of their corresponding University Bachelor's Degree) with excellent academic records, giving them the opportunity to achieve their first research experience in first class labs, using state of the art equipment, and being training under the guidance of the different CiQUS Research groups. Although this initiative was originally launched by the CiQUS in the year 2014, since 2019 the call is jointly published with CiMUS, CiTIUS e IGFAE centers (*USC Research Centers accredited by the Xunta de Galicia as Research Centers of Excellence*) and it is coordinated by the USC central services as a joint programme.

The 8th edition of this programme was launched in spring 2022. Up to 15 undergraduate students (8 of them were females) from 4 different Spanish Universities were granted within this call, and performed their one-month stay at CiQUS in July 2023. All of them presented an average mark on their academic track records above 8.0 points on a scale 0-10. Regarding their bachelor's degrees, 8 of them were enrolled in Chemistry, 1 in Biotechnology, 1 in Pharmacy, 1 in the Physics & Chemistry Double Degree and 4 of them in the Biology and Chemistry Double Degree. Five of these scholarship holders are currently pursuing either their master's or bachelor's dissertations at the CiQUS.

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

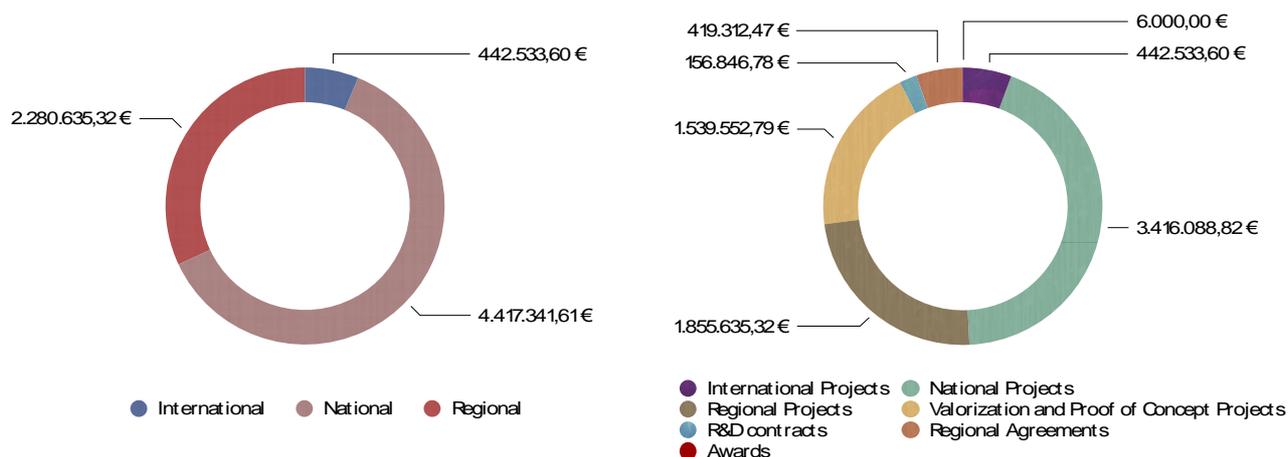
5. R&D PROJECTS, NETWORKS, AND INTERNATIONAL COLLABORATIONS

5.1 R&D Projects

- Total income of R&D projects, grants and contracts raised by CiQUS researchers in 2022, 7,84 M €.
- 15 New R&D Projects funded by the AEI (Spanish Research Agency), including 1 associated predoctoral contract, in 2022 (2,38 M€)
- 6 New Valorization and/or Proof of Concept projects starting in 2022 (1,54 M€)

During 2022, the CiQUS progress continued in consolidating the scientific structure of the center, by obtaining funding through competitive R&D programmes that will sustain the different research lines define as the strategic nucleus of the CiQUS' Scientific agenda for the next 3-5 years.

The year 2022 has been successful both in terms of achieved income (**over 7,84 M€**), as well as regarding the total number of competitive R&D and Valorization/Proof of Concept projects granted to CiQUS Researchers through the different international, national, and regional calls (**7,14 M€** for a total number of **29 projects (6 of them valorization/proof of concept projects)**). A detailed analysis shows that 13 of the 18 CiQUS research groups have been granted with new funds in 2022 (72% of CiQUS' research groups), while up to 20 CiQUS researchers are listed as Principal Investigator (PI) of the different proposals (among them, 16 CiQUS PIs and 4 Junior Scientists).



Left: Distribution of R&D and Valorization/Proof of Concept projects granted in 2022, by source of revenue | Right: CiQUS' 2022 fundraising results, by type of Income

The distribution of the R&D projects and the Valorization/Proof of Concept projects granted to CiQUS research groups in 2022 by source of revenue shows that 62% of them comes from national programmes, 32% from regional programmes and 6% from international programmes. Regarding the type of income 71,5% comes from R&D projects, 19,7% form Valorization/Proof of concept projects, 5,4% correspond to special agreements with the Regional Government, 2% comes from R&D contracts, 1,5% correspond to R&D funds linked to HHRR competitive programmes and over 0,1% comes from awards.

Furthermore, it has been particularly thriving the income granted within the framework of the State Plan for Scientific and Technical Research and Innovation 2021-2023 from the Spanish Research Agency: rising more than 3,13 M € distributed in 15 R&D projects (including 7 Knowledge Generation Projects and 7 Strategic Projects Oriented to the Ecological Transition and the Digital Transition, among them) and 4 Valorization/Proof of Concept Projects.

Regarding International R&D Projects, an EIC-Pathfinder and the first EIC Transition Open of Galicia have been granted to Javier Montenegro at the end of 2022 and beginning of 2023, respectively. Starting in 2023, (the associated income has not been included in the 2022 results), these projects will advance in the preclinical validation of a novel delivery system for therapeutic nucleic acids.

The main R&D projects (including valorization or proof of concept projects) granted to the CiQUS researchers throughout 2022 are listed below:

COMPETITIVE INTERNATIONAL CALLS

1 EIC Pathfinder | 0.5 M€

- **EIC-Pathfinder-101099867 CAR-T REX:** PI: Javier Montenegro. INCOME: **€560,513.** (*) (Starting Spring 2023).

1 EIC Transition Open | 2.5 M€

- **TraffikGene-Tx:** *TraffikGene-Tx: Targeted Peptide Carriers for RNA Delivery.* PI: Javier Montenegro. INCOME: **€2.499,000.** (*) (Starting Spring 2023)

4 MSCA-PF | 0.79 M€

- **DOI: [10.3030/101063432](https://doi.org/10.3030/101063432):** *New Germanium-based materials for Green electronics.* PI: Francisco Rivadulla. INCOME: **€261,380.64.**
- **DOI: [10.3030/101067060](https://doi.org/10.3030/101067060):** *Novel electroactive polymeric materials for dielectric elastomers actuators and soft robots.* PI: Massimo Lazzari. INCOME: **€181,152.96**
- **DOI: [10.3030/101064817](https://doi.org/10.3030/101064817):** *Engineered Exosomes for Stimuli-responsive Image-guided Drug delivery for Cancer Theranostic applications.* PI: Pablo del Pino. INCOME: **€181,152.96** (*) | (Starting September 2023).
- **DOI: [10.3030/101063372](https://doi.org/10.3030/101063372):** *Deep eutectic solvents for membrane transport of nucleic acids.* PI: Javier Montenegro. INCOME: **€165,312.96** (*) | (Starting September 2023).

(*) INCOME not included as 2022 funds.

COMPETITIVE NATIONAL CALLS

7 AEI - Knowledge Generation Projects | 0.97 M€

- **PID2021-122923NB-I00:** *Recovery of scarce and valuable metals from electronic waste using custom-made absorbent materials.* PI: Massimo Lazzari. INCOME: **€121,000.**
- **PID2021-124010OB-I00:** *Multi-target drugs in cancer immunotherapy: Discovery of ligands that act synergistically at two immune checkpoints in the tumor microenvironment.* PI: Eddy Sotelo. INCOME: **€145,200.**
- **PID2021-127341OB-I00:** *Solid state refrigerants, electrocatalysts and metal ion batteries activated by pressure or by confinement in sustainable hybrid materials.* PI: María Giménez-López. INCOME: **€181,500.** Also granted with a Predoctoral Contract.
- **PID2021-127606OA-I00:** *Deciphering cereal immunity mediated by ubiquitination.* PI: Beatriz Orosa. INCOME: **€163,350.**
- **PID2021-127684OB-I00:** *Boronic acids: A round trip between drug transport and NMR characterization.* PI: Eduardo Fernández-Megía. INCOME: **€133,100.**
- **PID2021-127702NB-I00:** *Peptide tools in sensors, catalysis and materials science.* PI: M. Eugenio Vázquez. INCOME: **€114,950.**

- **PID2021-127857NB-I00:** *New strategies for anti-cancer and anti-Covid-19 therapies based on metallopeptide tools.* PI: Miguel Vázquez. INCOME: **€114,950.**

7 AEI - Strategic Projects Oriented to Ecological Transition and Digital Transition | 1.25 M€

- **TED2021-129833A-I00:** *Harnessing the energy of visible light to convert greenhouse gases into valuable chemical products.* PI: Manuel Nappi. INCOME: **€218,500.**
- **TED2021-130930B-I00:** *Thermal memories and thermoregulators based on ionic conductors.* PI: Rafael Ramos Amigo. INCOME: **€152,950.**
- **TED2021-131451B-C21:** *Durable Confined Catalyst with Improved Activity to Solve Cathode Limitations in a Zn-Air Battery - (ENDURANCE).* PI: María Giménez-López. INCOME: **€278,300.**
- **TED2021-131460A-I00:** *Domain-assisted depolymerization in ionic liquids using computational techniques at the atomic level.* PI: Manuel Ortuño. INCOME: **€116,955.**
- **TED2021-131641B-C42:** *Semisynthetic conducting peptides and chemical synthesis.* PI: M. Eugenio Vázquez. INCOME: **€149,500.**
- **TED2021-132388B-C42:** *Design and synthesis of molecular precursors for gas sensors.* PI: Diego Peña. INCOME: **€148,350.**
- **TED2021-132449B-I00:** *Methane valorization promoted by light.* PI: Martín Fañanás-Mastral. INCOME: **€184,000.**

Particularly worth mentioning is the success achieved by the CiQUS Junior Scientists researchers in this call, leading 43% of the total number of proposals achieved. This clearly reflects the center's commitment and support to the consolidation of emerging young researchers.

Finally, two other CiQUS PIs participate as co-PIs in projects also selected for funding under this call. However, funds for these projects are linked to other USC research centers, so they are not account as CiQUS' funds in the present report:

- **TED2021-132522B-I00:** *Nanomaterials Derived from Silicon-Based MOFs for 3D Printing Additive Manufacturing of Next-Generation Anodes for Lithium-Ion Batteries.* PIs: Pablo del Pino (CiQUS), Pablo Taboada (iMATUS). INCOME: **€254,380** (assigned to the USC Faculty of Physics).
- **TED2021-131322B-I00:** *Enzymatic bio-recycling of PET.* PIs: Gemma Maria Eibes (CRETUS), Jose M. Martínez-Costas (CiQUS). INCOME: **€189,750** (assigned to the USC Vicechancellorship for Research and Innovation).

2 AEI - Proof of Concept Projects | 0.29 M€

- **PDC2022-133402-I00:** *Deciphering the human lipidome: Crypt Lipid Codes to predict and diagnose diseases.* PI: Rebeca García-Fandiño. INCOME: **€141,450.**
- **PDC2022-133925-I00:** *ZUPRAenergy - A New Supramolecular Rechargeable Zinc-Bromine Battery for a Sustainable Energy Transition.* PI: María Giménez-López. INCOME: **€149,500.**

It is especially remarkable the success obtaining within this call. The two proposals selected for funding are leading by women. Furthermore, it should be noted that the funding granted to CiQUS female researchers in 2022 have an amount greater than €830,000.

2 AEI – Projects in Public-Private Collaboration | 0.46 M€

- **CPP2021-008390:** *Parallel quantification of multiple immune checkpoint interactions in onco-immunology - PREDICTEAM.* PI: Eddy Sotelo. INCOME: **€181,654.**
- **CPP2021-009090:** *CAPN12-IO: preclinical development and first human clinical trial of a selective calpain-12 inhibitor as a new strategy for cancer immunotherapy.* PI: Eddy Sotelo. INCOME: **€276,948.79.**

This is a new call funded by NextGeneration EU programme and focused to promote synergies and collaboration between research centers and companies. Projects funded within the framework of this programme are led by industrial partners. In these cases, whereas PREDICTEAM is led by **Hawks Biosystems** (in collaboration with the CiQUS, the University of Navarra and Celtarys Research), CAPN12-IO is led by **Landsteiner Genmed** (in collaboration with the CiQUS, the National Center for Biotechnology (CNB) and the 12 de Octubre Hospital).

1 ISCIII-HEALTH 2002 – Seal of Excellence Institute of Health Carlos III | 0.98 M€

- **IHRC22/00009:** *Beyond metalloenzymes: Metal-grafted nanostructures for organometallic catalysis in live settings.* PI: José Luis Mascareñas. INCOME: **€984,251.82.**

1 CaixaResearch Consolidate 2021 (La Caixa Foundation) | 0.30 M€

- **HR21-00232:** *Selectively eliminating cancer stem cells through inhibition of mitochondrial respiration using metal-based small molecules.* PI: José Luis Mascareñas. INCOME: **€300,000**

This project has been selected by La Caixa for funding withing the CaixaResearch Consolidate Programme in the 2021 call (project starting in 2022).

1 AEI International Joint Programming | 0.16 M€

- **PCI2021-122091-2B:** *Engineered Exosomes for Stimuli-responsive Image-guided Drug delivery for Cancer Theranostic applications.* PI: Pablo del Pino. INCOME: **€160,932.**

Finally, national funding also includes the complementary support income associated to the young talent incorporation programmes such as Ramón y Cajal and Juan de la Cierva.

COMPETITIVE REGIONAL PROGRAMMES

Research Centers of the Galician University System | 0.82 M€

- Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CiQUS). PI: José Luis Mascareñas. INCOME: **€823,488.27**

In May 2022, CiQUS passed the evaluation corresponding to the accreditation as Research Center of the Galician University System for the period 2019-2022 (accreditation of Excellence). The evaluation was performed by an external committee of experts who ranked CiQUS as first of the eight centers currently holding this accreditation. Therefore, the activity of the center for the year 2023 will be funded with more than 0.82 M€.

1 IGNICIA Project | 0.49 M€

- **IN855A 2021/06:** *TRAFFIKGENE – Novos vehículos peptídicos para aplicación en terapia xénica.* PI: Javier Montenegro. INCOME: **€490, 200.**

This project has been selected by GAIN (Galician Innovation Agency – Xunta de Galicia Government) for funding withing the IGNICIA Programme in the 2021 call (project starting in 2022). This is a specific

Programme launched by GAIN to support the valorisation phase of R&D methodologies and promoting the development of research innovative technologies.

4 Regional Competitive Grants for Consolidation and structuring of research Groups and Young researchers | 0.83 M€

- **ED431C 2022/21:** Competitive Reference Group: GRC-1608 – *Nanomaterials and Bioactive Molecules*. PI: Emilio Quiñoá. INCOME: **€280,000**.
- **ED431C 2022/27:** Competitive Reference Group: GRC-1603 – *Organometallic Catalysis*. PI: Carlos Saá. INCOME: **€320,000**.
- **ED431F 2022/17:** Modality C (Excellence Projects): *Use of the ubiquitin pathway to induce resistance to pathogens in cereals (iUbc)*. PI: Beatriz Orosa. INCOME: **€115,000**.
- **ED431F 2022/04:** Modality C (Excellence Projects): *Study of interactions between spin-red-electron(ion) in transition metal oxides for the manipulation of thermal conduction and thermoelectric conversion*. PI: Rafael Ramos. INCOME: **€115,000**.

Regional funding also includes the complementary support income associated to the young talent incorporation programme Contratos Predoutorais Xunta de Galicia – Modality B.

Furthermore, CiQUS' income for the year 2022 also includes funds linked to regional agreements (0,42 M€), R&D contracts (0,16 M€), R&D funds associated to HHRR competitive programmes (0,11 M €) and awards (6000 €).

Our figures on December 31st, 2022 show **77 active competitive projects** for a total amount of 24,4 M €. These projects include **5 ERC** (1 SyG, 1 CoG, 2 StG and 1 PoC), **3 FET-Open**, **1 ICT**, **1 MSCA ITN**, **1 H2020 Societal Challenges**, **1 CaixaResearch Consolidate**, up to **27 RETOS or Generación de Conocimiento** national projects, among others. Update information on the complete list of active projects at the center can be found at the following link <https://www.usc.es/ciqus/en/research/projects>.

Additionally, regarding other financial contributions, in 2022 CiQUS received a transfer of €118,429 associated to a USC pilot programme for the partial (20%) return of the overheads to the accredited research centers.

Finally, it is also worth noting the significant financial support associated to the hiring expenses of the 81 CiQUS' trainees holding research contracts under competitive HHRR programmes (Ramón y Cajal, Juan de la Cierva, MSCA-IF, FPU, AEI predoctoral, Galician postdoctoral and predoctoral programmes, etc). This funding is directly managed by the USC central offices, and it has not been included in the INCOME figures disclosed above.

5.3 Research Networks

Regarding **International Research Networks**, CiQUS researchers participate in **two newly COST Actions** approved in Spring 2022 by the European Union:

- **Modelling immunotherapy response and toxicity in cancer (IMMUNO-model)** | CA21135 | Action Chair: Dr. Eva Martínez-Balibrea (Fundació Institut d' Investigació Germans Trias i Pujol, Spain) | CiQUS PIs: **E. Sotelo** and **J.M. Martínez-Costas** | Start date – 02/11/2022; End date – 01/11/2026.



- **Iron-sulphur (FeS) clusters: from chemistry to immunology (FeImmChemNet)** | CA21115 | Action Chair: Dr. Kourosh Ebrahimi (King's College London, UK) | CiQUS PI: **J.M. Martínez-Costas** | Start date – 19/09/2022; End date – 18/09/2026.

Additionally, two other COST Actions remained active in 2022 with participation of CiQUS PIs:

- **European Research Network on Signal Transduction (ERNEST)** | CA18133 | Action Chair: Dr. Jana Selent (GRIB – Research Programme on Biomedical Informatics, Spain) | CiQUS PI: **E. Sotelo** | Start date – 11/03/2019; End date – 10/03/2023.

- **Cancer nanomedicine – from the bench to the bedside (NANO2CLINIC)** | CA17140 | Action Chair: Prof. Sabrina Pricl (University of Trieste – MOSE-DMNR, Italy) | CiQUS PI: **E. Fernández-Megía** | Start date – 13/04/2018; End date – 27/03/2023.

Currently, a new proposal is under evaluation within the Call 2023 (CiQUS PI: M. Fañanas).

In terms of **National Research Networks**, CiQUS researchers participate in **7 newly Research Networks** (Redes de Investigación) which has been provisional approved by the Spanish Research Agency within the Call 2022. Furthermore, 1 of these new research networks is coordinated by a CiQUS PI (M. Lazzari):

- **Science and Technology Network for the conservation of cultural heritage** | RED2022-134287-T | Coordinator: **Massimo Lazzari** (CiQUS PI, Galicia) | Start date 2023; End date 2024.

- **Structures, methodologies and materials based on organometallic complexes** | RED2022-134287-T | Coordinator: Complutense de Madrid University (Madrid) | CiQUS PIs: **C. Saá** and **J.V. Varela** | Start date 2023; End date 2024.

- **Molecular Nanoscience Network (NanoMolNet)** | RED2022-134713-T | Coordinator: ICMOL (C. Valenciana) | CiQUS PIs: **D. Pérez** | Start date 2023; End date 2024.

- **Organic electronic devices: from high-performance materials to advanced applications** | RED2022-134503-T | Coordinator: ICMA (Catalonia) | CiQUS PIs: **D. Peña** | Start date 2023; End date 2024.

- **Asymmetric Catalysis Research Network** | RED2022-134331-T | Coordinator: Euskal Herriko Unibertsitatea (Basque Country) | CiQUS PIs: **M. Fañanás** | Start date 2023; End date 2024.

- **Nanomedicine Network for advancing in the diagnosis and treatment of high social impact diseases (NanoCARE 2.0)** | RED2022-134560-T | Coordinator: University of Granada (Andalucía) | CiQUS PIs: **E. Fernández-Megía** | Start date 2023; End date 2024.

- **(Photo)-electrocatalysis: from the atomic scale to advance devices** | RED2022-134508-T | Coordinator: Euskal Herriko Unibertsitatea (Basque Country) | CiQUS PIs: **M. Giménez** | Start date – 02/11/2022; End date – 01/11/2026.

Furthermore, 3 other National Research Networks with participation of CiQUS researchers were active in 2022. One of them coordinated by a CiQUS PI (E. Vázquez):

- **Peptides in Biomedicine and Nanoscience Network** | RED2018-102417-T | Coordinator: **Eugenio Vázquez** (CiQUS PI, Galicia) | End date – 2022.

- **Molecular Science on Surface: Synthesis and Functionality** | RED2018-102833-T | Coordinator: Asoc. CIC NanoGUNE | CiQUS PIs: **D. Peña** | End date – 2022.

▪ **Organometallic Complexes for the Generation of New Substances, Materials and Transformations** | RED2018-102387-T | Coordinator: Complutense de Madrid University (Madrid) | CiQUS PIs: **C. Saá** | End date – 2022.

Finally, regarding **Regional Research Networks**, CiQUS holds the accreditation of excellence as Research Center of the Galician University System 2019-2022, being 1 of the 8 centers that currently make up the **CIGUS Network** promoted by the Xunta de Galicia. Additionally, CiQUS is 1 of the 5 USC Research Centers included in the Singular Research Centers Network of the University of Santiago de Compostela.

5.4 International Collaborations

CiQUS researchers have demonstrated their commitment with international collaborations, both through the active participation in collaborative projects funded by highly competitive international programmes, and through scientific collaborations resulting in high impact publications. In this context, **46 articles** (51%) of CiQUS scientific production during the year 2022 **resulting from international collaborations**. Among them, it is worth mentioning those results published in top-ranked journals such as **Nature**, **Science** and **Nature Chemistry**. Among the collaborators, there are research groups from up to 17 different countries (USA, UK, The Netherlands, Germany, Switzerland, Sweden, Norway, France, Portugal, Italy, Belgium, Czech Republic, Slovak Republic, Japan, China, Brazil, and Russia).

Furthermore, it is highly remarkable the number of international projects in collaboration active at the CiQUS during the year 2022:

- **ERC-SyG-MoIDAM** (CiQUS PI: D. Peña) | *Single Molecular Devices by Atomic Manipulation* | In collaboration with: IBM Research GMBH (Switzerland) and the Universitaet Regensburg (Germany).
- **ICT-REAP** (CiQUS PI: B. Pelaz) | *Revealing drug tolerant persister cells in cancer using contrasts enhanced optical coherence and photoacoustic tomography* | In collaboration with: 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), Lavisision Biotec GMBH (Germany) and Linoix International BV (The Netherlands).
- **FET-Open e-Prot** (CiQUS PI: E. Vázquez) | *Protein-based conductive materials pave the way for next-generation energy storage devices* | In collaboration with: 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).
- **FET-Open SWIMMOT** (CiQUS PI: B. Pelaz) | *Switchable magneto-plasmonic contrast agents and molecular imaging technologies* | In collaboration with: AIT Austrian Institute of Technology GMBH (Austria), Institut National des Sciences Appliquees de Toulouse (France), Centre National de la Recherche Scientifique CNRS (France), Medizinische Universitaet Wien (Austria) and Universitaet Innsbruck (Austria).
- **FET-Open SPRING** (CiQUS PI: D. Peña) | *Spin Research IN Graphene* | In collaboration with: CiC NanoGUNE (Spain), Technische Universiteit Delft (The Netherlands), IBM Research GMBH (Switzerland), The Chancellor, Masters and Scholars of the University of Oxford (UK) and the DIPIC Foundation (Spain).
- **MSCA-ITN HeatNMof** (CiQUS PI: P. del Pino) | *Heating triggered drug release from nanometric inorganic-metal organic framework composites* | In collaboration with: IMDEA Energy Foundation (Spain), Centre National de la Recherche Scientifique CNRS (France), Univeriteit Antwerpen (Belgium), Immaterial LTD (UK), Institut National des Sciences Appliquees de Toulouse (France), Univeritaet Hamburg (Germany), Fondazione Istituto Italiano di Tecnologia (Italy), Nanoscale Biomagnetics S.L. (Spain) and ISERN Patentes y Marcas M S.L. (Spain).

- **JTC FLAG-ERA LEGOCHIP** (CiQUS PI: D. Peña) | *Multifunctional Nanoporous Graphene Integration in Operational Nanophotonic Biosensor Devices* | In collaboration with: ICN2 (Spain), University of Bologna (Italy) and University of Manchester (UK).

- **JTC EuroNanoMed III PLATMED** (CiQUS Junior Scientist: E. Polo) | *Biomimetic Platelet-Derived Nanomedicines for Treatment of Thromboembolic Stroke* | In collaboration with: IDIS (Spain), University Caen-Normandy, GIP Cyceron (France), McGill University (Canada) and Op2Lysis (France).

- **EIG CONCERT-Japan 5th Joint Call SUPRAPOROUS** (CiQUS PI: J. Montenegro) | *Nanoparticle Supramolecular Frameworks as Advances Nanoporous Materials* | In collaboration with: University of Tokyo (Japan), University of Hamburg (Germany) and UAB Ferentis Company (Lithuania).

Finally, it is also worth noting the active participation of CiQUS researchers as members in evaluation committees for international funding agencies all around the world. Specifically, during 2022 up to 14 CiQUS PIs acted as evaluators for more than 20 international competitive calls, EIC Pathfinder (EU), ERC-SyG (EU), ERC-CoG (EU), ERC-StG (EU), MSCA-PF (EU), Proof of Concept Projects – Okinawa Institute of Science and Technology (Japan), Research Projects – Austrian Academy of Science (Austria), OPUS – National Science Center (Poland), PRELUDIUM BIS - National Science Center (Poland), SONATA - National Science Center (Poland), Hong Kong Research Grants Council (China), ENW Open Competition Domain Science M22-1 -Dutch Research Council–NOW (The Netherlands), Standard Grant Projects – The Czech Science Foundation-GACR (Czech Republic), PAZY Foundation (Israel), ANR 22 – French National Research Agency (France), among others.

6. RESEARCH OUTPUT

6.1 Scientific Production

6.1.1 Scientific publications

CiQUS maintained a good record of scientific contributions in 2022, with 90 articles, 88 of which were published in JCR Journals (98% of all CiQUS publications). From them, **up to 37 articles were published in journals with IF>9**, which represents 42% of CiQUS JCR publications in 2022. It should be especially highlighted the papers published by CiQUS researchers in top impact journals during last year, **1 Nature, 1 Science, 1 Nature Chemistry and 1 Nature Communications**, among many others. Furthermore, up to 7 articles were published in *Angewandte Chemie International Edition* and other 4 in the *Journal American Chemical Society*, which represents the 12% of 2022 CiQUS scientific production.

Journal Name	JCR - IF (*)	nº of published articles
<i>Nature</i>	69,504	1
<i>Science</i>	63,832	1
<i>Advanced Materials</i>	32,086	1
<i>Nature Chemistry</i>	24,274	1
<i>ACS Nano</i>	18,027	2
<i>Nature Communications</i>	17,694	1
<i>Angewandte Chemie-International Edition</i>	16,823	7
<i>Journal of the American Chemical Society</i>	16,383	4
<i>Water Research</i>	13,400	1
<i>Journal for Immunotherapy of Cancer</i>	12,485	1
<i>Nano Letters</i>	12,262	2
<i>Green Chemistry</i>	11,034	2
<i>Science of the Total Environment</i>	10,754	1
<i>Carbohydrate Polymers</i>	10,723	1
<i>Chemical Science</i>	9,969	5
<i>Journal of Colloid and Interface Science</i>	9,965	2
<i>Journal of Nanobiotechnology</i>	9,429	2
<i>ACS Sustainable Chemistry & Engineering</i>	9,224	2

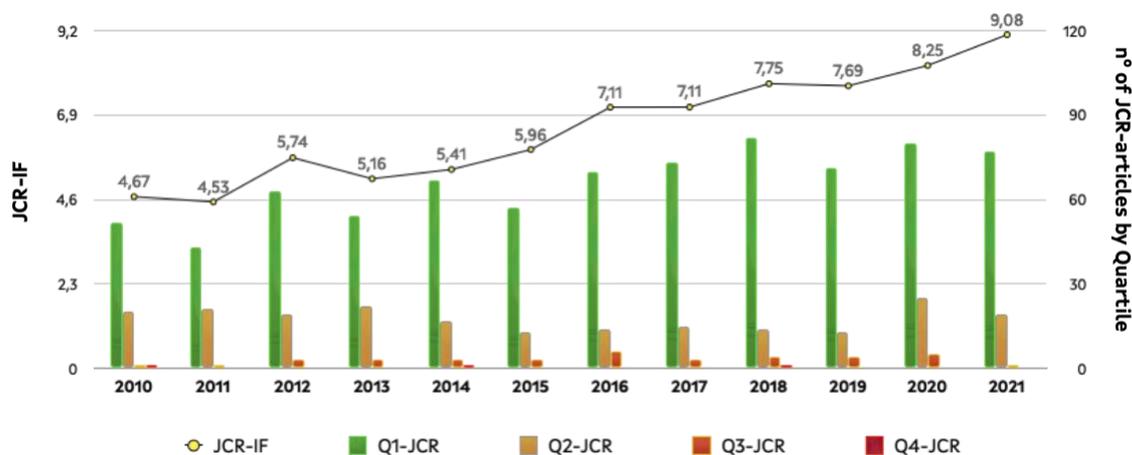
(*) Journal Impact factor values for the year 2022 are based on 2021 Journal Citation Reports (2021 data). 2022 data have not yet been published.

Table 1. Scientific Journals with JCR- IF > 9, in which CiQUS articles were published during 2022 and total number of articles per Journal.

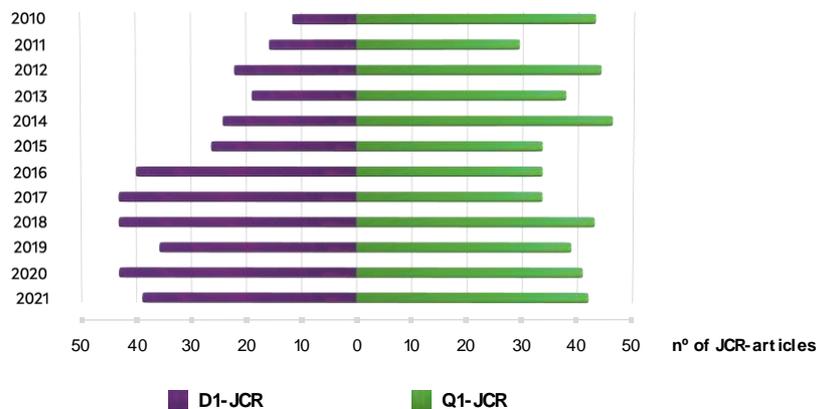
During 2022, 51% of the contributions involved international collaborations, many of them with prestigious research centres and groups. **Annex IV** shows a full listing of the scientific articles in JCR journals published by CiQUS researchers in 2022.

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, 73 articles (83% of the total number of JCR papers) published by CiQUS researchers in 2022 were already Open Access articles. Furthermore, in collaboration with the USC library, CiQUS supports its researchers in archiving their scientific production in the institutional online repository of the University of Santiago de Compostela (Minerva).

Regarding evolution trend of the impact and the quality from CiQUS scientific production, we will focus our analysis on articles published up to the year 2021, since Journal Citation Reports (JCR) and Scimago Rank (SJR) data corresponding to 2022 are not yet published at this moment (April 2023). Thus, the conclusions and values of the indicators for scientific production of 2022 may not be accurate or present deviations from the final values that will be assigned in 2023. During the year 2021, **79% of CiQUS JCR articles were published in journals indexed in the first quartile (Q1)** and, more significantly, **38% 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 9,08**, keeping this impact indicator above 8 for second year in a row and above 7 for seventh year in a row.



Evolution of the number of JCR-publications by quartile and by year and JCR-average impact factor 2010-2021



Evolution trend of the number of publications published in D1 and Q1- not D1 JCR-journals 2010-2021

Looking back to the scientific production in 2022, it is worth to note that the slight decrease in productivity observed, may have been a consequence of the restrictions to experimental work during the COVID-19 pandemic, including shift work until September 2021. Fortunately, we can already find promising signs of recovery from these setbacks, as evidenced by the publication of 36 articles within the first 3.5 months of 2023 (as of April 15th).

6.1.2 CiQUS Scientific Highlights

Among the most outstanding CiQUS scientific results, in 2022 there are remarkable contributions in the three strategic thematic areas of the center. Among the articles published by the center's researchers last year, the following two stand out for their impact:

- **Boron clusters as broadband membrane carriers**, published in the *Nature* journal (<https://doi.org/10.1038/s41586-022-04413-w>). It is the result of an international collaboration between Prof. Javier Montenegro (CiQUS) and Prof. Werner M. Nau from Jacobs University Bremen (Germany). The researchers describe a new strategy for controlling the transport of bioactive molecules across the cell membrane based on boron compounds as superchaotropic carriers.
- **Selectivity in single-molecule reactions by tip-induced redox chemistry**, published in the *Science* journal (<https://doi.org/10.1126/science.abo6471>). It is the result of the long and stable collaboration between Prof. Diego Peña (CiQUS) and Dr. Florian Albrecht and Leo Gross from IBM Research Europe. Research developed on this occasion within the framework of the ERC-Synergy MoDAM project. By applying selective and precise voltages through a scanning probe microscope (STM), researchers are able to induce defined changes in the structure of molecular rings.

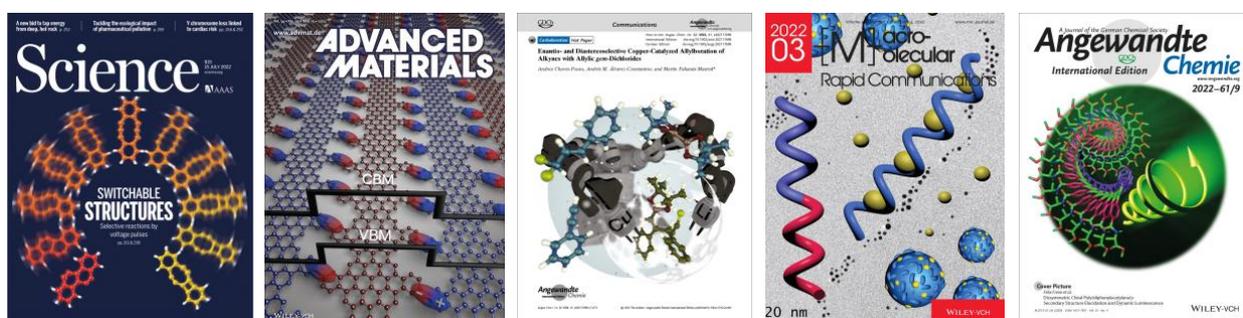
Furthermore, we must also highlight the quality of the publications resulting from the collaboration between groups at the center (83% Q1 JCR, 50% D1 JCR and FI average = 10.6), which highlights the efforts of the leaders of the different research groups that make up the CiQUS to combine capabilities and address new and ambitious challenges from a multidisciplinary approach. A small selection of articles in internal collaboration is summarized below:

- **Chiral Ligands Based on Binaphthyl Scaffolds for Pd-Catalyzed Enantioselective C–H Activation/Cycloaddition Reactions** published in the *Journal of the American Chemical Society* (<https://pubs.acs.org/doi/10.1021/jacs.2c09479>). In this article, Prof. José Luis Mascareñas and Prof. Moisés Gulías (synthetic chemistry and catalysis) and the CiQUS's new distinguished researcher, Dr. Manuel A. Ortuño (theoretical and computational chemistry), describe in their study the development of a new family of ligands (NOBINAC) from computational studies and its application in C-H activation reactions catalyzed by palladium complexes for the enantioselective synthesis of rings of seven membered rings by means of formal (5+2) cycloadditions.
- **Catalytic Lewis Base Additive Enables Selective Copper-Catalyzed Borylative α -C–H Allylation of Alicyclic Amines** published in the *Journal of the American Chemical Society* (<https://doi.org/10.1021/jacs.2c07969>). Prof. Martín Fañanás (synthetic chemistry and catalysis) collaborates in this article with Prof. Jesús Varela (theoretical and computational chemistry) in a complete synthetic and mechanistic study through which the authors carry out the development of a new catalytic process for the borylative α -C-H allylation of O-benzoyl hydroxylamines based on copper complexes.
- **Ag₂ nanoclusters with dual catalytic antiradical activities** published in the *Journal of Colloid and Interface Science* (<https://doi.org/10.1016/j.jcis.2022.07.133>). Prof. María Giménez (inorganic chemistry) and Prof. Massimo Lazzari (physical chemistry) collaborate in this article, where they study the catalytic application of silver nanoclusters to deactivate DPPH (2,2-diphenyl-1-picrylhydrazyl) radicals, with a potential use as scavengers in industrial or biomedical catalytic redox processes.

On the other hand, up to 9 CiQUS articles were selected by different journals as **hot articles / hot topics** in 2022: *The Role of Polymer-AuNP Interaction in the Stimuli-Response Properties of PPA-AuNP Nanocomposites* (*Macromol. Rapid. Commun.*, Hot Topic: Gold); *Dissymmetric Chiral Poly(diphenylacetylene)s: Secondary Structure Elucidation and Dynamic Luminescence* (*Angew. Chem. Int. Ed.*, **Hot Paper**); *Reactive Jetting of High*

Viscosity Nanocomposites for Dielectric Elastomer Actuation (*Adv. Mater. Technol.*, Hot Topic: Robotics); *Enantio- and Diastereoselective Copper-Catalyzed Allylboration of Alkynes with Allylic gem-Dichlorides* (*Angew. Chem. Int. Ed.*, **Hot Paper**); *Palladium-Catalyzed Tandem Cycloisomerization/Cross-Coupling of Carbonyl- and Imine-Tethered Alkylidenecyclopropanes* (*Angew. Chem. Int. Ed.*, **Hot Paper**); *Atomically Sharp Lateral Superlattice Heterojunctions Built-in Nitrogen-doped Nanoporous Graphene* (*Adv. Mater.*, Hot Topic: Carbon, Graphite, and Graphene); *Exporting Homogeneous Transition Metal Catalysts to Biological Habitats* (*Eur. J. Org. Chem.*, Hot Topic: Biocatalysis); *3D Printing: An Emerging Technology for Biocatalyst Immobilization* (*Macromol. Biosci.*, Hot Topic: Biocatalysis); *Magnetic Hyperthermia Enhancement in Iron-based Materials Driven by Carbon Support Interactions* (*Chem. Eur. J.*, Hot Topics: Carbon, Graphite, and Graphene; Magnetic Materials Society).

Finally, 5 CiQUS' articles were selected as **cover image** in the volumes in which they were published: *Science* (<https://doi.org/10.1126/science.abo6471>); *Adv. Mater.* (<https://doi.org/10.1002/adma.202110099>); *Angew. Chem. Int. Ed.* (<https://doi.org/10.1002/anie.202117696>); *Angew. Chem. Int. Ed.* (<https://doi.org/10.1002/anie.202115070>); *Macromol. Rapid Commun.* (<https://doi.org/10.1002/marc.202100616>).



Some examples of CiQUS articles selected as cover

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>). 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.

6.1.3 Other research outputs

• Patent applications

During 2022, CiQUS researchers obtained the approval of four international patents [Ru complexes, EP 3539971B1, US 11471467, PIs: J.L. Mascareñas, E. Vázquez], and two others are European patents [muNS Proteins, EP 2535348B1, PI: J. Martínez-Costas, and Magnetic nanoparticles for treatment of tumors, and EP3790588B1; PI: J. Granja, in collaboration with Italian institutions].

In terms of new applied patents, up to 3 European patents have been presented in the year 2022, two of them within the framework of the ENDOSCAPE European consortium and co-owned by Sapreme Technologies, Charité Universitätsmedizin Berlin and Freie Universität Berlin (EP22193416, EP22193399; PI: E. Fernández-Megía). The third European patent applications comes from the TraffikGene initiative (Peptides

for intracellular delivery, EP22382596; PI: J. Montenegro). Additionally, a new Spanish patent has been applied for (Automated gas monitoring, P202230249; PI: M. Giménez).

• **Software Licences**

Prof. A. Fernández-Ramos and colleagues registered update versions for 1 computer programme developed by his research group during 2022: Torsiflex – a programme for the conformational search in flexible acyclic molecules (<https://github.com/cathedralpkg/TorsiFlex>). This software programme use Python 3 as programming language.

• **PhD Theses**

In 2022, up to 14 PhD Theses were defended under the supervision of CiQUS PIs. All of them obtained a *Sobresaliente cum laude* qualification and 7 of them obtained a *European doctorate/International Mention*. Additionally, 2 of them were international trainees (14%).

Detailed information about CiQUS PhD theses presented in this period can be found in Annex V and on [CiQUS website](#). Up to 71% these PhD candidates were funded from competitive human resources programmes while the rest were hired under R&D contracts linked to their advisor's research grants.

• **Contributions to scientific congresses**

CiQUS Research Staff gave over 47 lectures in 2022. **7 of them as Plenary, 6 as Keynote and 34 as Invited Speakers** at international conferences and meetings from up to 9 different countries (Armenia, Austria, Cuba, Denmark, Portugal, Spain, Switzerland, UK and USA). Furthermore, CiQUS Researchers attended many others national and international scientific meetings from up to 10 different countries (Cuba, Czech Republic, Finland, France, Germany, Italy, Portugal, Spain, The Netherlands, and USA), and presenting there more than 70 oral communications, 21 *flash* communications and more than 135 posters.

• **Research Mobility**

In 2022, up to 20 CiQUS PhD candidates had short stays at prestigious national and international research institutions from 7 different countries: **Germany** (RWTH Aachen University, Freie Universität Berlin); **Spain** (ICN2, ICMOL), **South Korea** (Pusan National University), **Sweden** (Stockholm University, Uppsala University); **The Netherlands** (Eindhoven University of Technology – TU/e), **UK** (University of Cambridge, University of Manchester, University of Oxford, University of Southampton, University of Glasgow and the National Institute of Biological Standards from the UK-Medicines and Healthcare Regulatory Agency) and **USA** (University of California Berkeley, University of Columbia, University of Wisconsin-Madison, Northwester University and Emory University). These short stays were part of their PhD training programme (predoctoral secondments). Furthermore, 2 CiQUS Senior Researchers had short stays at the University of Groningen (The Netherlands) and the University of Zaragoza (Spain) within the framework of scientific collaborative projects.

• **Visiting Researchers**

Despite of the difficulties for mobility and the extended period of lockdown, CiQUS received during the year 2022 up to 26 visiting researchers for short stays at our center (42% female; 1 Senior Researcher and 25 Postdoctoral or PhD candidates), coming from up to 13 different countries (Argentina, Chile, Germany, Greece, India, Italy, Portugal, Romania, Spain, The Netherlands, Ukraine, Tunisia, Venezuela).

6.2 Awards

CiQUS Principal Investigators have received different awards and recognitions during the year 2022, *Prof. José Luis Mascareñas* received the **Vila de Vida** award from the Allariz city council, for his contribution to the promotion of the economic, cultural and social development of the region. Furthermore, José Luis

Mascareñas has been elected as [full member of the Galician Royal Academy of Sciences](#). *Prof. Diego Peña* was invited to attend the [Honour Science & Chemistry](#) event organized by the European Chemical Industry Council (Cefic) and to the recreation of the iconic 1927 Solvay Conference Picture. Prof. Peña also received the [Ernesto Viéitez Cortizo](#) award from the Galician Royal Academy of Science (an award for recognizing original research publications). *Prof. Eddy Sotelo* received the [Fernando Calvet Prats](#) award from the Galician Royal Academy of Science (an award for recognizing excellent ideas for transfer technology) and Dra. Beatriz Pelaz received the [Young Researcher Group Leader](#) award from the Spanish Royal Society of Chemistry. Additionally, Celtarys Research (*a startup led by Prof. Eddy Sotelo*) was recognized as [one of the three best startups in Galicia](#) in the year 2022 within the framework of the Galicia Startup Congress.

Furthermore, *Soraya Learte* (former CiQUS PhD candidate supervised by Prof. J.L. Mascareñas) received an [Honourable mention from the 2022 IUPAC-Solvay International Award for young chemists](#) and *Maria Luisa Juanes* (former CiQUS PhD candidate supervised by Prof. J. Montenegro) received the [Extraordinary Doctorate Prize](#) from the University of Santiago de Compostela. Finally, several other CiQUS researchers have also been awarded for their contributions to different scientific conferences, among others:

- *Rebeca García-Fandiño* (CiQUS PI): Poster prize at the 20th International Cyclodextrin Symposium | Italy.
- *Pilar Suárez de Cepeda* (PhD candidate – González-Bello Group): Poster Prize of the European Federation of Medicinal Chemistry at the XXVII EFMC International Symposium of Medicinal Chemistry | France.
- *Xulían Fernández* (PhD candidate – Mascareñas | López | Gulías Group): Best flash communication at the Chemical tools for Chemical Biology Symposium (XXXVIII Biental RSEQ) | Spain.
- *Martín Piñeiro* (PhD candidate – Fañanás Group): 3rd Best Poster Prize GEQOR at the XXXVIII Biental RSEQ | Spain.
- *Eugenia P. Quirós* (PhD candidate – Giménez Group): Best Poster Prize at the Symposium of Materials for Energy (XXXVIII Biental RSEQ) | Spain.
- *Alejandro Seco* (PhD candidate – Granja | Montenegro | García-Fandiño Group): Best Oral Communication Prize at the XXXVIII Biental RSEQ | Spain.
- *María Valentina Malavé* (Master Student – Guitián | Pérez | Peña Group): Best Scientific Poster Award | XIV Symposium of the master's degree in Organic Chemistry | Spain



7. INNOVATION, TECHNOLOGY TRANSFER AND VALORIZATION

7.1 Valorization Projects

During 2022, CiQUS PI J. L. Mascareñas obtained the support of the prestigious **Caixa Research Consolidate programme** (€300K) to continue progressing in a valorization project based on new therapeutic agents against the stem cells of cancer, previously also funded by the ERC-PoC, and the IGNICIA programmes.

Four AEI-Proof of Concept (PdC) projects of the State Research Agency (AEI) started at the CiQUS during 2022. In the 2022 call, the projects of led by M. C. Giménez (ZUPRAenergy - A New Supramolecular Rechargeable Zinc-Bromine Battery for a Sustainable Energy Transition) and R. García-Fandiño (Deciphering the human lipidome: Crypt Lipid Codes to predict and diagnose diseases) were selected for funding. In the previous call, (2021 call, resolved at the end of that year), other 2 projects led J.L. Mascareñas (Metal-based anticancer agents targeting the mitochondrial respiration of cancer stem cells) and J. Montenegro (GeneVector - A New Chemical Platform for Customized Gene Therapy) were also selected for funding.

Regarding **competitive projects in public-private collaboration**, under the new programme launched in the year 2022 by the Spanish Research Agency (AEI), Prof. E. Sotelo achieved €456K for its participation as a partner in 2 new consortia: CAPN12-IO led by Landsteimer, a project that includes a clinical trial in humans for immunotherapy of the cancer, and PREDICTEAM led by Fastbase Solutions, focused on immune checkpoint interactions in oncoimmunology.

Additionally, it should be noted that in the call for **strategic projects aimed at the ecological and digital transition** (AEI-TED 2022), M. Giménez and the technological center CIDETEC achieved €278K and €234K, respectively, for a collaborative project (BANZAI - Zinc electrode battery -Nanostructured air), which is the continuation of the ERC-PoC ZABCAT project. Under the same AEI-TED 2022 call, it is worth highlighting two other valorization projects selected for funding: i) enzymatic bio-recycling of PET, (led by CRETUS-USC, CiQUS PI: J.M. Martínez-Costas) and ii) new highly sensitive and portable gas sensors, (CiQUS PI D. Peña and coordinated by the ICN2).

7.2 R&D contracts and services in collaboration with companies

During 2022, CiQUS researchers have signed several new R&D contracts for a total budget of € 156K. Among them it should be remarked:

- **MestreLab Research.** As part of a long-term relationship, a new 99,220 € contract has been signed to provide support for the development of chemical software.
- **Landsteiner Genmed S.L.** Following previous agreements since 2018, a new 27,000 € contract has been signed to develop synthetic methodologies and organic molecules libraries.

The full list of active R&D contracts during 2022 is available in Annex III.

7.3 Innovation & entrepreneurship

The spin-off Celtarys (led by CiQUS PI: E. Sotelo) created with the support of the IGNICIA programme, obtained €650K in its first round of financing.

Furthermore, the technology that forms the basis of the TraffikGene initiative (led by CiQUS PI: J. Montenegro) was selected for funding within the 2021 regional call IGNICIA (a programme for transfer technology) at the end

of the year 2021. This initiative has been also granted in 2022 with an **EIC-Pathfinder** (€500K), as part of a consortium of €3 million and more recently with **the first EIC-Transition Open of Galicia** (€ 2,5 millions).

The MD.USE has received a predoctoral contract from the Xunta's Industrial Doctorate 2022 programme. 1 PhD candidate will be funded under this call to develop his doctoral theses on the next topic:

- *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)

Regarding **European Technology Platforms and Networks**, the CiQUS continued during in 2020 with an stable an regular 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' KTT manager attended in person several important sectoral events: Battery Innovation Days (Bruselas), Bionnale (Berlín), ETPN2022 (Braga), ExpoQuímica (Barcelona), Galicia Biodays (A Coruña).

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)

7.4 Patents

- *4 New international patents have been granted in 2022:*

- Ru complexes | EP 3539971B1, US 11471467 | PIs: J.L. Mascareñas, E. Vázquez.

- Proteínas muNS | EP 2535348B1 | PI: J. Martínez-Costas

- Magnetic nanoparticles for treatment of tumors | EP3790588B1 | PI: J. Granja, in collaboration with Italian institutions

- *3 International extensions were applied for the next patents in 2022:*

- 2 of them within the framework of the ENDOSCAPE European consortium and co-owned by Sapreme Technologies, Charité Universitätsmedizin Berlin and Freie Universität Berlin | EP22193416, EP22193399 | PI: E. Fernández-Megía

- Peptides for intracellular delivery | EP22382596 | PI: J. Montenegro

- *1 National patent has been applied in 2022:*

- Automated gas monitoring | P202230249 | PI: M. Giménez

- *Patent Licensing:* the startup Celtarys Research has licensed the Fluorotools patent (PI: E. Sotelo).

⋮

8. TRAINING

8.1 Bachelor

Up to 51 bachelor final projects defended by 45 undergraduate students in 2022 were developed at CiQUS under the supervision of CiQUS PIs. A complete list of the final projects presented yearly can be found in Annex VII.

Most of the undergraduate students (28) were enrolled in the bachelor's degree in Chemistry. The rest of students were enrolled in the bachelor's degree in Pharmacy (2), in Biotechnology (4), in the Double Degree in Physics & Chemistry (3) and in the Double Degree in Chemistry & Biology (8).

Regarding the distribution by thematic areas, 64% of the projects were focused in Biological & Medicinal Chemistry, 20% in Functional Materials with Technological Application and 16% in Synthetic Methodologies for Sustainable Development.

Furthermore, it is noteworthy that the 48% of the undergraduate students continue nowadays their research training at CiQUS as Master students or PhD candidates.

In terms of training actions aimed to undergraduate students, CiQUS annually launched its **Summer Fellowships Programme** (See section 4.2.3 CiQUS Talent Attraction Programmes). Within this framework, 15 undergraduate students spent 1 month research stays at the CiQUS during July 2022.

Full Name	Bachelor's degree	University
<i>Balboa López, Manuel</i>	Chemistry	U. of Santiago de Compostela
<i>Bao Camacho, Inés</i>	Biology & Chemistry	U. of Coruña
<i>Barbosa de Bessa, Jorge Francisco</i>	Chemistry	U. of Santiago de Compostela
<i>Calviño Sanlés, Esther</i>	Biology & Chemistry	U. of Coruña
<i>Corral Sertal, Javier</i>	Physics & Chemistry	U. of Santiago de Compostela
<i>Lomba Riego, Lucía</i>	Biology & Chemistry	U. of Coruña
<i>Martín Gómez, Beatriz</i>	Chemistry	U. of Valladolid
<i>Martín Polo, Ainhoa</i>	Chemistry	U. of València
<i>Mato Domínguez, Sergio</i>	Chemistry	U. of Valladolid
<i>Montoto Pintos, David</i>	Dobre grao en Química e Bioloxía	U. of Santiago de Compostela
<i>Pérez Sánchez, Carla</i>	Chemistry	U. of Valladolid
<i>Rodríguez Pampín, Iván</i>	Pharmacy	U. of Santiago de Compostela
<i>Ruíz Caamaño, Nilia</i>	Biotechnology	U. of Santiago de Compostela
<i>Sanabria Montalbán, Javier</i>	Chemistry	U. of València
<i>Sanmiguel Vázquez, Lourdes Patricia</i>	Chemistry	U. of Santiago de Compostela

Table 2. Undergraduate students granted with a CiQUS Summer Fellowships in 2022

On this occasion, up to 12 CiQUS research groups participated in the summer programme, supervising the research projects of the fellows and hosting them in their laboratories. Their stays at the CiQUS began with a reception and welcome event for the fellows on Monday, July 4, 2022, which included a short presentation by CiQUS about the center and its capabilities, a guided tour of the CiQUS facilities, and a welcome coffee and socialization. Afterwards, the fellows attended the prevention and safety course, which is mandatory for all the center's staff and, once they passed the corresponding test, they immediately joined the different recipient research groups.



2022 CiQUS Summer Fellowships holders

Summer Fellowship holders had the opportunity to participate in the different activities scheduled at CiQUS during their whole stay at the center: invited lectures, internal seminars, thesis defenses, etc. On Friday, July 29, a closing seminar took place in the CiQUS auditorium, during this event summer fellows presented to the community of the center (directors, principal researchers, postdoctoral researchers, and PhD candidates) a summary of the research project in which they had collaborated during their stay at CiQUS. It is worth noting the high level of the presentations given by the fellows and the good atmosphere of the scientific discussion during the day.

8.2 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 Master in Theoretical Chemistry and Computer Modelling (Erasmus Mundus) and the Master in Drug Research and Development is also relevant. CiQUS annually offers between 30 and 35 vacancies for the Master Project. Approximately, 65% of the students for the master's degree in Chemistry from USC are trained at the CiQUS.

During 2022, 30 master dissertations were defended by CiQUS master students (38% of them were female). Most of the students (13) were enrolled in the Master's degree in Organic Chemistry at the USC, 10 student were enrolled in the Master in Chemistry at the Frontier with Biology and Materials Science, 6 in the master's in Chemical Research and Industrial Chemistry (2nd promotion of this master programme) and 1 student in the Master in Theoretical Chemistry and Computer Modelling, all of them are Master Programmes at the USC. A complete list of 2022 CiQUS master dissertations can be found in Annex VI.

Currently, over the 65% of the 2022 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: 50% were focused on the field of Biological & Medicinal, 33% on the Functional Materials with Technological Application area and 17% on the field of Synthetic Methodologies for Sustainable Development.

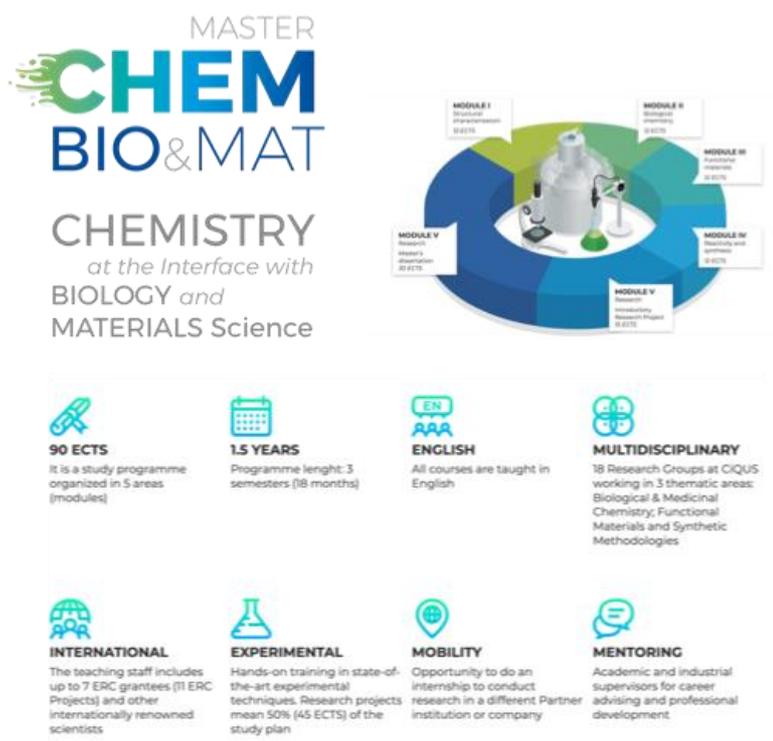
Additionally, up to 9 master students enrolled in the Master in Chemistry at the Interface with Biology and Materials Science (1,5 years duration) presented their master dissertations last February 2023.

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 fourth promotion of the Master's Degree in Chemistry at the Interface with Biology and Materials Science (ChemBio&Mat) started the academic course 2022/2024 with 11 students, who were graduated alumni of the Universities of Santiago, Coruña, Vigo, Málaga, the Basque Country, Valladolid and two African universities, coming from degrees in chemistry, biochemistry and chemical engineering. 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>), where 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 | ECTS distribution by thematic modules of the study programme

Other special feature of this Master Programme is the possibility to host experts as invited professor for highly specialized courses. In this context, during 2022 Prof. Margarita Bastos (CiQUP and Universidade de Porto, Portugal) lectured a Master Course on *Biocalorimetry: theoretical considerations and practical applications*, in spring 2022. Furthermore, special lectures and scientific events were organized within the framework of the master programme:

- In February 2022, Prof. Jesús Jiménez-Barbero, delivered the lecture *Breaking the limits in understanding glycan recognition by NMR*, closing the graduation of the second promotion of the master's degree.

- In July 2022, a special scientific programme was organized for closing the academic year 2021/2022, which included:

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

- A **Closing Lecture**: Prof. David Amabilino delivered the lecture *Dynamic supramolecular gels* which was attended by master's students and other CiQUS researchers.

Finally, as part of the Tutored Training Activities subject, the master students attended several complementary courses focused on transversal skills: *i)* Introduction to Intellectual Property Rights for Chemists, *ii)* Introducing to Scientific Publishing & How to Read a Paper, *iii)* Becoming a Scientific Writer: Putting Why? Before How?, *iv)* Graphic Design for scientific communication, and *v)* the thematic Lecture Series: Industrial Days, among others.

8.3 Doctoral programmes

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

Most of the students (85%) are enrolled in the interuniversity PhD programme *Chemical Science and Technology*. Other doctoral programmes are *Drug Research and Development*, *Materials Science* or *Biology*. Regarding the gender distribution, currently 42% of doctoral students are women and over 10% come from abroad. Remarkably, 48% of CiQUS PhD candidates are currently granted with competitive public HHRR contracts.

In 2022, 14 theses were defended by CiQUS students, all of them obtained *cum laude* top marks. A complete list of theses presented yearly can be found in Annex V. Importantly, the 54% of the PhD theses defended during this period received the International Mention.

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 programme 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 Programme, with top level international speakers from many different scientific disciplines. (See Annex XI for the complete list of speakers in 2022)

The success of the training activity is evident in the awards and recognitions received by our PhD students (see section 6.2 Awards) and their success in accessing the best international centres.

8.4 Postdoctoral programmes

Up to 51 postdoctoral researchers (35% women and 14% international from 6 different countries Switzerland, India, Brazil, Italy, Mexico and Hungary) developed their advanced training at CiQUS in 2022. 33% of CiQUS postdoctoral researchers were beneficiaries of a competitive HR programme. During 2022, 2 Xunta postdoctoral

contracts of modality B (already incorporated as researchers at CiQUS) were obtained, as well as 2 Ramón y Cajal contracts and 4 MSCA contracts, which will start their contracts throughout 2023. Finally, up to 3 researchers from the CiQUS have been selected in modality A of postdoctoral grants from the Xunta de Galicia, and will receive funding to work for 2 years in foreign institutions, returning to CiQUS during the third year of the grant.

8.5 Other training activities and courses

- **Cross-disciplinary training courses:** in 2022, CiQUS continue with its own career development programme, 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:

- *Beyond the Bench: Career Development for Scientists* (aimed to PhD candidates and postdocs): a course focused at improving the strategies in HHRR recruitment processes, either inside or outside of the academic environment. Participants learnt and acquired tools to promote their success in professional job interview or to improve of their professional profile and competitiveness in personnel selection processes.

- *Managing myself and working with my team: A skills upgrade for Group Leaders (2 Editions)* (aimed to PIs and Junior Scientists): The content of this course offered researchers an important battery of advice and recommendations for managing human teams, time management and assertive communication tools for conflict management. The course had an important practical component where participants were able to receive individual personal advice on their own experiences.

- *Graphic Design for Scientists* (aimed to researchers and technical staff): through the development of this course, CiQUS members learned about recommendations for the preparation of graphic materials (presentations, posters, graphical abstracts, etc.), as well as instructions on the use of graphic design tools and software.

- **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 2022, specific seminars on the advanced management of spectrofluorometer, spectrophotometer, ITC, SFC-Mas, and microwave reactor were organized.

- **CiQUS Lecture Programme:** During the year 2022 the programme of lectures given by top national and international scientists included up to 23 research talks at the CiQUS. Invited speakers included Sébastien Perrier (University of Warwick | UK), Olga Garcia Mancheño (University of Münster | Germany), Michael Haley (University of Oregon | USA), Paolo Samorì (Université de Strasbourg | France), Joost Reek (Van't Hoff Institute of Molecular Sciences | Netherlands), among many others. (See full list: <https://www.usc.es/ciqus/en/ciqus-lectures>).

- **CiQUS Seminar Programme:** We also continue with the internal fortnightly programme of seminars with the participation of PhD candidates, and postdoctoral researchers. (See complete list: <https://www.usc.es/ciqus/en/internal-seminar-programme>).

- **1st Symposium Chemistry at the Frontier:** this scientific event was organized on the occasion of the CiQUS 10th anniversary. It was also envisioned as a training activity for young researchers (postdoctoral researchers, PhD candidates and master students) who attended the corresponding organized lectures (3 plenary, 6 keynote and 6 invited).

Finally, in 2022 CiQUS researchers (PIs and Junior Scientists) were invited to participate as lecturers in up to 27 different scientific training seminars or doctoral programmes at several department at national and international institutions.

8.6 Other strategic training initiatives

In the year 2022, CiQUS launched the second edition of its **mobility grant's programme**. A strategic initiative focused on supporting the mobility of the center's research staff, with the idea of promoting short research stays associated to the development of the center's scientific agenda and the establishment of new international collaborations. In the context of this call, CiQUS financially supported the trips and stays abroad of 3 PIs to attend scientific meetings and networking events in the USA (Metal in Medicine – Gordon Research Conference), Italy (20th International Cyclodextrin Symposium) and Spain (1st School – group of Carbohydrates, RSEQ). Additionally, several CiQUS researchers were granted within the framework of this programme for carrying out analysis associated to collaborative work [1 PI, 1 Research support technician and 1 PhD Candidate at the [ALBA Synchrotron](#) [a national Strategic infrastructure (Spain)], 1 Postdoctoral researcher at the QEM2022 (France), 1 postdoctoral researcher at the Stratingh Institute for Chemistry-University of Groningen (Netherlands) and 1 PhD candidate at the ICMOL (Spain)], and 3 PhD candidates were granted for research secondments at international reference institutions [RWTH Aachen (Germany), TU/e (Netherlands) and NIBSC (UK)].

9. COMMUNICATION & OUTREACH

9.1 Communication

CiQUS Governing Committee approved in spring 2022 our Communication Plan. This document contextualizes and defines the center's communication and dissemination strategy and establishes its priority objectives and the set of actions to achieve them. The plan has been approved as a dynamic document, likely for updating during its period of validity. Furthermore, a specific and detailed review will be performed once the CiQUS Strategic Plan will be approved in 2023 (currently under final preparation).

9.1.1 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 shows update information about research areas, scientific production, research groups, facilities, job offers, training programmes 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.

In 2022, CiQUS website was implemented with an INTRANET section with authorized access for CiQUS members. From this section, it is possible to access to all the documentation and operating regulations of the center, as well as reservation forms, equipment catalogues or shared folders for the different commissions and work groups that operate in the center (in this case, the access is only authorized for the members of the corresponding committees or working groups).

Tracking traffic and web visitors are monitored through Google analytics. During 2022, CiQUS website has received more than 179,097 visits. Approximately, 90,78% correspond to new visitors. The majority age range of visitors is between 25 and 34 years old (22%) and 50,7% of the visitors were female. CiQUS website has received visits from up to 150 different countries, mainly Spain (73%), USA (3%), India (3%), Mexico (2%), UK (2%), Germany (2%), Portugal (2%), Argentina, Chile, The Netherlands, Italy, and France (1%).

On the other hand, CiQUS website is complemented with the corresponding social networks: Facebook (2011), LinkedIn (2012), YouTube (2013), and Twitter (2014). CiQUS accounts on these platforms kept in 2022 a rising trend both in followers as well as number of generated interactions:

- **Twitter.** 2,877 followers (514 new followers since 2021). 252 new posts and more 451,600 total impressions reached.
- **LinkedIn:** 3,544 followers (856 new followers since 2021). 117 new posts. 5,059 people visited the profile, reaching more than 195,000 impressions, 9,475 clicks and 3,404 feedback. Different entries were shared up to 175 times.
- **Facebook.** 2,107 followers and 1,919 Likes (179 new followers since 2021).
- **YouTube:** 410 subscriptions (72 Subscriptions since 2021). 4 new entries. 8,871 views (viewing time: 250 h).

Regarding presence in the media, over 38 items were published in 2022 in the news section of the Centre's website (<https://www.usc.es/ciqus/en/news>). The news covered the activities's programme 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 País, El Mundo, La Vanguardia, La Voz de Galicia, El Correo Gallego,...), news agencies (Eurekalert, Europapress, EFE, Agencia SINC, etc), dissemination portals

(Gciencia, Diario Médico, Madri+d, Xataka, etc), specialized technology portals (Biotech,...) and other international platforms (Chemistry World, PHYS.org, Le Parisien, etc.). A brief summary is shown below:

Press

<https://elpais.com/ciencia/2022-03-23/descubierta-una-nueva-manera-de-penetrar-en-las-celulas-humanas.html>

<https://www.elmundo.es/ciencia-y-salud/ciencia/2022/07/14/62d0504221efa0a07e8b45c1.html>

<https://www.lavanguardia.com/ciencia/20220131/8022613/obtener-terapias-celulas-madre-cancer.html>

https://www.lavozdeg Galicia.es/noticia/santiago/santiago/2022/03/30/ciqus-celebra-diez-anos-trasapando-fronteras-investigacion/0003_202203G30P27991.htm

<https://www.elcorreogallego.es/galicia/ciqus-una-decada-de-avances-y-prestigios-en-el-ambito-cientifico-KC10659726>

News agencies

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

<https://www.infosalus.com/salud-investigacion/noticia-disenan-nanopartcula-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/universidade-gl/soraya-learte-tese-ciqus/>

<https://www.diariomedico.com/medicina/oncologia/metal-rutenio-recubierto-contrametastasis-y-recidivas.html>

<https://www.xataka.com/investigacion/ultimo-avance-quimica-modificar-moleculas-atomo-a-atomo-responsables-estos-investigadores-gallegos>

<https://www.gciencia.com/perspectivas/investigadora-beatriz-pelaz-foi-premiada-pola-real-sociedade-espanola-quimica/>

<http://www.madrimasd.org/notiweb/noticias/logran-por-primera-vez-modificar-los-enlaces-entre-atomos-una-molecula>

<https://biotech-spain.com/es/articulos/nueva-estrategia-inmuno-terap-utica-en-la-lucha-contrael-c-ncer-dise-ada-por-investigadores-del-ciqus-de-la-usc/>

Others international platforms

<https://www.chemistryworld.com/news/combining-expertise-to-develop-remote-controlled-nanomaterials/4015986.article>

<https://phys.org/news/2022-03-cell-superchaotropic-properties-boron-clusters.html>

<https://www.infobae.com/america/agencias/2022/03/23/descubierto-un-nuevo-sistema-para-transportar-farmacos-a-las-celulas/>

<https://www.leparisien.fr/sciences/voici-les-toutes-premieres-images-de-molecules-extraterrestres-01-02-2022-A6XNYGMBQJHYPM2ZM562YSOM2E.php>

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

EL PAÍS

Ciencia / Materia

La humanidad logra por primera vez modificar los enlaces entre átomos de una única molécula

El avance permitirá construir máquinas moleculares inimaginables hoy en día, capaces de realizar tareas como la distribución inteligente de fármacos

PHYS ORG

Solving stability problems of relevant graphene derivatives

REACTIVE RIBBON

PROTECTED RIBBON

La tesis de Soraya Learte, investigadora de la USC, galardonada como una de las mejores del mundo en química en 2021

20 minutos ECONOMÍA

Feijóo participa en la inauguración de Simposio Chemistry at the Frontier

CHEMISTRY WORLD

NEWS NOBEL PRIZES RESEARCH OPINION FEATURES CULTURE CAREERS PODCASTS WEBINARS

Combining expertise to develop remote-controlled nanomaterials

BY VICTORIA ATKINSON | 12 AUGUST 2022

Beatriz Pelaz is a chemist at the University of Santiago de Compostela in Spain

EL PAÍS

Descubierta una nueva manera de penetrar en las células humanas

El ingenioso mecanismo tiene el potencial de revolucionar la medicina, al permitir introducir fármacos o moléculas tóxicas capaces de matar el cáncer

O CIQUS cumple 10 años á vangarda da investigación internacional en química

EL MUNDO

Unas pinzas para mover átomos 'hechas en Galicia' acercan el sueño de crear las máquinas más diminutas del mundo

Un grupo internacional de científicos, con participación española, publica una nueva técnica para manipular moléculas «como si fueran piezas de Legos». Ayudará a crear fármacos, nuevos materiales y mecanismos a escala diminuta

CIQUS

LAVANGUARDIA

¿Se puede obtener terapias contra las células madre del cáncer?

Some examples of CIQUS' news in Press media

9.2 Outreach

9.2.1 Outreach aimed at the general public

- 2022 Ciencia Singular – Open Door's Day:** In November, the sixth 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 Government. Over 221 people (46% kids) visited the center on November 19th, attended the lectures and talks with CiQUS Researchers and participated in the chemical games and workshops included in the programme.



Ciencia Singular 2022

Up to 80 volunteers were collaborating for the celebration of this event. Among them, 10 Principal Investigators (PIs), 1 Junior Scientists, 15 Postdoctoral Researchers, 33 PhD candidates, 9 Master's students, 13 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.

- 1st Andaina en Marcha,** a solidarity event organized by the Spanish Association against Cancer (AECC) which included a scientific fair for raising funds for investment in cancer research. CiQUS researchers participated with information stands on the CiQUS advances on cancer research and related.

<https://www.contraelcancer.es/es/actualidad/noticias/inscripciones-abiertas-andaina-solidaria-santiago-compostela-marcha-contra-o-cancro>

- G-Night European Researchers' Night:** on September 30th, CiQUS participated for the second time in a row together in this worldwide outreach event (<https://gnight.gal/>). On this occasion, CiQUS researchers and technical staff prepared and organized a workshop on molecular cuisine aimed to children.

- Pint of Science:** CiQUS researchers participated both as organizers and speakers of this international dissemination initiative organized annually during Spring. Additionally, the CiQUS center participate as sponsor of the event held in Santiago de Compostela.

- ConCiencia Programme – Prof. David MacMillan:** Introduction by Prof. José Luis Mascareñas. CiQUS researchers keep a regular collaboration with the ConCiencia Programme throughout the years. This is an outreach event of the USC (<https://www.usc.gal/en/conciencia-program>) originally launched in the year 2006. This initiative is aimed to *i*) disseminate scientific advanced by Nobel Laureates/ Fields Medal / Abel Prize among the general non-specialized audience (free access for the attendants), *ii*) to promote the image of Santiago de Compostela as scientific reference space and *iii*) to expand the networking of USC researchers and scientific

world leaders. CiQUS researchers participate in the official invitation process as well as making the introductory presentation of the speaker and the corresponding talk.

9.2.2 Outreach aimed to promote scientific vocations among young students

- **International Day of Women and Girls in Science:** an activity aimed at STEM high school students, organized on February 11, within the framework of the *International Day of Women and Girls in Science*. CiQUS programme was based on initiatives for bringing experiences of female researchers of different profiles and professional stages to the participants, with the aim of promoting scientific vocations among young students with especial focus on female students. A total of 43 students and 4 teachers from two Galician high school centers attended to the event. Additionally, in the same context, the center also participated in the organization of the musical *CHRISTIANE. Scientific bio-musical*. A joint initiative of CiQUS, CiMUS, CiTIUS and IGFAE aimed at primary, secondary and high school schools, with a reach of about 150 students and 7 teachers, from six educational centers in Galicia.

<https://www.cidadedacultura.gal/gl/evento/christiane-un-bio-musical-cientifico-dia-da-muller-e-nena-na-ciencia-2022>

- **CiQUS annual programme for school visits:** in the year 2022 CiQUS recovered the full operativity of the programme of visits to the center aimed at primary, secondary and high school students. The activity included a guided tour of the facilities, a presentation of the center's scientific agenda and the main research lines and talks and interviews with the researchers at the laboratories. The center received the visit of 12 centers from all over the Galician community. More than 360 students and teachers attended the programme.

- **Research in Chemistry: Creative Science for a better world – Online Edition (Pilot test):** this initiative was launched for the first time through the Zoom Platform. A science high school class from the IES Rosalía de Castro in Santiago de Compostela had the opportunity to witness live the basic tasks of a chemical experimentation laboratory and learn about the main lines of research of one of the center's groups. In this initiative participated CiQUS Pls **Dolores Pérez** and **Diego Peña**, together with their team members Jesús Castro, Berta Álvarez and Javier Besteiro.

Finally, it is also worth mentioning the presence and collaboration of CiQUS researchers in different dissemination initiatives organized by other USC units or by other public institutions (City Councils, Provincial Councils, Schools, etc.). Thus, CiQUS researchers participated during 2022 in more than 50 outreach events. Among them:

- **A Ponte Programme:** **Concepción González-Bello** [*Chemistry Facing the Challenge of Superbacteria* – IES A Carballeira-Marcos Valcárcel (Ourense), IES Lamas de Castelo (Carnota) and IES Porto do Son (A Coruña)]; *How to design drugs using computers?* – CPR Plurilingüe Compañía de María (Santiago de Compostela), IES Ricardo Carvalho Calero (Ferrol), IES A Carballeira-Marcos Valcárcel (Ourense), IES Ortigueira (Ortigueira), IES Johan Carballeira (Bueu), colegio Pablo IV (A Rúa), IES nosa Sra. Dos Ollos Grandes (Lugo)]; **Diego Peña** [*Serendipity in Chemical Research* – IES Chamoso Lamas (Ourense)], **Félix Freire** [*Molecular cuisine: chemical reactions at the kitchen* – several high school centers in Ourense, Coristanco, Santiago de Compostela, Silleda, Pontearreas, melide, Muros and Cambados], and **Ricardo Riguera** [several high school centers in A Guarda, Ourense, Becerreá, A Estrada, As Pontes, Cee and Vigo].

- **Mulleres STEM do século XXI – Building a future in feminine: emergent sectors and pending challenges** [**Dolores Pérez**, Santiago de Compostela]

- **II Nanocar Race:** a joint team formed by researchers from CiQUS (led by [Diego Peña](#)), CFM (Center for Physics of Materials, UPV/EHU – CSIC) and DIPC (Donostia International Physics Center) participated in this event organized by the CNRS, in which molecular machines compete on a nano-sized racetrack.

- **Outreach and dissemination scientific lectures:** [STEM Bach Programme \[Accelerated course in Organic Chemistry\]](#) by [Diego Peña](#)- IES de Valga (Pontevedra); [Science in feminine](#) [[Natalia Barreiro – Mondoñedo](#)]; [Ciencia e tal - Twitch Chanel](#) [[The Galician vaccine against Covid](#) by [J.M. Martínez-Costas](#)]; [A pandemia Silenciosa](#) by [Concepción González-Bello](#) (Santiago de Compostela).

- **Bay Area Scientists Inspiring Students – BASIS** [[Daniel Marcos](#), California]

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.

9.3 Organization of Scientific Events

▪ **1st Symposium Chemistry at the Frontier** (<https://www.usc.es/ciqus/es/10-years-ciqus>): a strategic initiative both from the scientific point of view and from the international visibility and projection of CiQUS and the USC. It was designed with the vision of consolidating itself as a quadrennial scientific meeting, being a reference conference for the international research community. The symposium took place between **March 30 and April 1, 2022**, in the *Edificio Fontán* of the *Cidade da Cultura* in Santiago de Compostela. The first edition of this event was organized to coincide with the celebration of the tenth anniversary of the beginning of scientific activity at CiQUS.

The organizing committee was formed by the CiQUS Directors and a selection of CiQUS Principal Investigators (PIs), representatives of all the scientific strategic areas of the center:

- **Prof. José Luis Mascareñas**, CiQUS Scientific Director | President of the Organizing Committee
- **Prof. Dolores Pérez**, CiQUS Deputy Director
- **Dr. Fernando López**, CiQUS PI associated to the area of Synthetic Methodologies for Sustainable Development | Treasurer of the Organizing Committee
 - **Dr. María Giménez-López**, CiQUS PI associated to the area of Functional Materials for Technological Application
 - **Prof. M. Eugenio Vázquez**, CiQUS PI associated to the area of Biological & Medicinal Chemistry

Furthermore, the organizing committee had the collaboration of a group of volunteers, made up of 5 PhD candidates or postdoctoral researchers; [Jesús Bello](#), [Jesús Castro](#), [Soraya Learte](#), [Samuel Parceró](#) and [Nuria Vázquez](#); and the technical support staff of CiQUS. The services of the USC Event Management Office were hired for the technical secretarial tasks.

The symposium programme included two types of activities:

1) Scientific events, which included **3 plenary lectures** [[Prof David W. MacMillan](#) (Nobel Laureate in Chemistry 2021, Princeton University, USA), [Prof Helma Wennemers](#) (ETH Zurich, Switzerland) and [Prof Harry Anderson](#) (University of Oxford, UK)], **6 keynote lectures** and **6 other invited lectures**.

Regarding the selection of the speakers, the organizing committee considered **i)** the balanced representation of the Center's 3 strategic research lines (Biological and Medical Chemistry; New Materials of Technological Interest and Synthetic Methodologies for sustainable development), **ii)** the gender balance between the participants (7 women and 8 men), and **iii)** the international character of the speakers (53.3% of the speakers carry out their research activity in foreign institutions). Thus, the meeting brought together a brilliant panel of

scientists, from up to 5 different countries, among which was the latest Nobel Prize in Chemistry and a large number of ERC Grantees. The book of abstracts (accessible from the symposium website) includes detailed information regarding speakers and brief summaries of the lecture's content:

https://www.usc.es/ciqus/sites/default/files/eventos/ciqus_10years_bookofabstracts.pdf

2) Social events: aimed at strengthening networking through various activities of a social nature (welcome cocktail, gala dinner, and traditional Galician music concert).

Up to 252 participants attended the symposium. Among the institutions or research centers from which the participants come from outside the USC were, among others, the CINBIO (UVigo), the CICA (UDC) of Galicia, the University of Oviedo, the Instituto de Investigaciones Químicas (IIQ, CSIC-U. Seville), the ICIQ (Tarragona), the Rijksuniversiteit Groningen (Netherlands), the Philipps-Universität Marburg (Germany), etc. Moreover, researchers from different multinationals in the chemical sector (i.e., Lilly, Janssen | Johnson&Johnson) also attended to the symposium.

The inauguration ceremony was attended by the President of the Xunta de Galicia (Mr. Alberto Núñez Feijoo), the Galician Minister of Culture, Education, Training and Universities (Mr. Román Rodríguez), the Vice-Chancellor of Scientific Policy of the USC (Mr. Vicente Pérez Muñuzuri) and the President of the Royal Spanish Chemical Society (RSEQ, D. Antonio Echavarren).



1st Symposium Chemistry at the Frontier – 2022

Additionally, during the year 2022 CiQUS researchers participated as members of the organizing committees of different scientific meetings, among others:

-XXXVIII Reunión Bienal RSEQ | Granada, June 2022 | J.L. Mascareñas

-XX National Meeting of the Spanish Society of Medicinal Chemistry (SEQT) | Santiago de Compostela, June 2022 | Eddy Sotelo

-XIII International School on Organometallic Chemistry *Marcial Moreno Mañas* | Santiago de Compostela, June 2022 | C. Saá (Chair), J.L. Mascareñas, J. Granja, J.A. Varela, F. López, M. Gulías, M. Fañanás-Mastral

-New Trends in Polymer Science: Health of the Planet, Health of the People | Italy, May 2022 | M. Lazzari (Scientific Committee)

-XVIII National School on Molecular Materials | Santiago de Compostela, March 2022 | M. Giménez, D. Peña, F. Rivadulla and F. Freire

-XIII Conference of Young Researchers in Atomic and Molecular Physics (J^2IFAM) | Santiago de Compostela, March 2022 | David Ferro, Jéssica Rodríguez, Sara Illodo.

10. INFRAESTRUCTURES

10.1 Research facilities

The CiQUS building, has 5.900 m² built-up area with 22 RESEARCH LABS (90 m² 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 m² are dedicated to shared research support facilities, a highly well-equipped infrastructure to cover the needs of all our research areas and interdisciplinary projects:

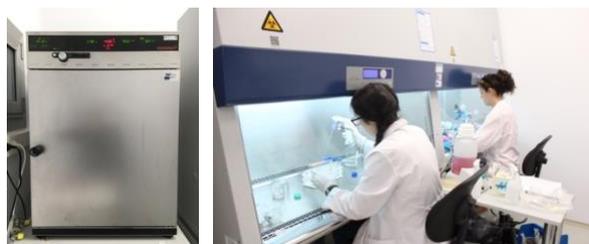
- **4 General Support Laboratories** (over 200 m² in total) for instrumental equipment, covering a broad range from analytical to preparative experimental techniques: chromatography (HPLC, UHPLC, Recycling GPC, SFC, GC, GC-MS, LC-MS), spectroscopy and spectrometry [UV-Vis, IR, fluorescence, CD, Dynamic 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.

- **3 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.



PLD 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. In this context, since 2022 a detailed catalogue with full info of CiQUS' equipment is available in the webpage of the center (https://www.usc.es/ciqus/sites/default/files/instalaciones/listado_equipamento_ciqus.pdf).

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 from 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.

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

10.2 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.

- **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.
- **2 Innovative Labs for technology development.** open spaces for developing and implementing novel technologies based on CiQUS's knowledge. At this moment, they are dedicated to the development of a system for the measurement of thermal conductivity by frequency-resolved thermoreflectance and to the development of new battery prototypes.



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

A full description of CiQUS equipment (and core facilities is available at the CiQUS webpage:

[-https://www.usc.es/ciqus/en/ciqus/facilities](https://www.usc.es/ciqus/en/ciqus/facilities)

[-https://www.usc.es/ciqus/sites/default/files/instalaciones/listado_equipamento_ciqus.pdf](https://www.usc.es/ciqus/sites/default/files/instalaciones/listado_equipamento_ciqus.pdf)

10.3 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 internal and external proposals for the acquisition of equipment for the general R&D services of the University of Santiago (CACTUS).

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, 2022)

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

Junior Scientists (December 31, 2022)

Area	Name	Position
	<i>Nappi, Manuel</i>	<i>Manuela Barreiro</i> USC -Distinguished Researcher
	<i>Orosa Puente, Beatriz</i>	Ramón y Cajal Researcher
	<i>Ortuño Maqueda, Manuel Ángel</i>	Xunta Distinguished Researcher
	<i>Polo, Ester</i>	Ramón y Cajal Researcher
	<i>Ramos, Rafael</i>	Ramón y Cajal Researcher
	<i>Tomás Gamasa, María</i>	Ramón y Cajal Researcher

Postdoctoral Researchers (December 31, 2022)

Area	Name	Position
	<i>Ageitos Martínez, José Manuel</i>	R&D Research Contract
	<i>Barreiro Piñeiro, Natalia</i>	R&D Research Contract
	<i>Bergueiro Álvarez, Julián</i>	R&D Research Contract
	<i>Bouzada Reboredo, David</i>	R&D Research Contract
	<i>Bugallo Ferrón, David</i>	MSCA-PF_Period Abroad Researcher
	<i>Castiñeira Reis, Marta</i>	Posdoutural Xunta Mod. A - Period at CiQUS Researcher
	<i>Castro Esteban, Jesús Alfonso</i>	Posdoutural Xunta_Mod. A_Period Abroad Researcher
	<i>Castro Fernández, Silvia</i>	Posdoutural Xunta_Mod. A_Period Abroad Researcher
	<i>Correa Chinaea, Juan Francisco</i>	R&D Research Contract
	<i>Fazal, Sajid</i>	R&D Research Contract
	<i>Fernández Villar, Zulema</i>	Posdoutural Xunta_Mod. A_Period Abroad Researcher
	<i>Ferro Costas, David</i>	Posdoutural Xunta Mod. B Researcher
	<i>Fuertes García, Alberto</i>	R&D Research Contract
	<i>Gómez González, Jacobo</i>	Margarita Salas_Period Abroad Researcher
	<i>Herreros Lucas, Carlos</i>	R&D Research Contract
	<i>Insua López, Ignacio</i>	MSCA-PF Researcher
	<i>Juanes Carrasco, María Luisa</i>	R&D Research Contract
	<i>Lázaro Milla, Carlos</i>	Margarita Salas Researcher
	<i>Mallo Abreu, Ana</i>	R&D Research Contract
	<i>Maneiro Rey, María</i>	Posdoutural Xunta Mod. B Researcher
	<i>Mateo de Doni, Luis Manuel</i>	R&D Research Contract
	<i>Mateos Gil, Jaime</i>	Juan de la Cierva - Incorporación Researcher
	<i>Molina Ceberio, Alba</i>	R&D Research Contract
	<i>Mora Fuentes, Juan Pedro</i>	R&D Research Contract
	<i>Navarro Poupard, María Fernanda</i>	R&D Research Contract
	<i>Padín González, Esperanza</i>	Margarita Salas Researcher
	<i>Parcero Bouzas, Samuel</i>	R&D Research Contract
	<i>Pérez Potti, André</i>	R&D Research Contract
	<i>Piñero Vargas, Juan José</i>	Margarita Salas Researcher
	<i>Pozo Míguez, Iago</i>	Margarita Salas_Period Abroad Researcher
	<i>Rama Martínez, Gustavo</i>	R&D Research Contract
	<i>Rivera Chao, Eva</i>	Posdoutural Xunta_Mod. A_Period Abroad Researcher
	<i>Rodríguez Pérez, Manuel</i>	R&D Research Contract
	<i>Rodríguez Riego, Rafael</i>	Juan de la Cierva - Incorporación Researcher
	<i>Rodríguez Villar, Jessica</i>	Juan de la Cierva - Incorporación Researcher
	<i>Sánchez Fernández, Adrián</i>	María Zambrano Researcher

	<i>Sánchez Sordo, Irene</i>	R&D Research Contract
	<i>Santos Claro, Marcel</i>	María Zambrano Researcher
	<i>Seoane Fernández, Andrés</i>	Juan de la Cierva - Incorporación Researcher
	<i>Soprano, Enrica</i>	R&D Research Contract
	<i>Velasco Rubio, Álvaro</i>	R&D Research Contract
	<i>Vilas Varela, Manuel</i>	R&D Research Contract
	<i>Vilela Góñez, Karen</i>	R&D Research Contract
	<i>Villarino Palmaz, Lara</i>	R&D Research Contract
	<i>Zampini, Giulia</i>	R&D Research Contract

PHD CANDIDATES (December 31, 2022)

Area	Name	Funded by
	<i>Alcalde Ordóñez, Ana</i>	AEI Predoctoral Contract (former FPI)
	<i>Álvarez Constantino, Andrés Manuel</i>	Predoutoral Xunta Contract
	<i>Álvarez Lorenzo, Aitor</i>	FPU
	<i>Andújar Arias, Antonio</i>	Predoutoral Xunta Contract
	<i>Arribas Domingo, Andrés</i>	FPU
	<i>Barbeira Arán, Sergio</i>	R&D Research Contract
	<i>Bayón Fernández, Alfonso</i>	R&D Research Contract
	<i>Bello García, Jesús</i>	R&D Research Contract
	<i>Besteiro Sáez, Javier</i>	R&D Research Contract
	<i>Blanco González, Alexandre</i>	R&D Research Contract
	<i>Cabezón Vizoso, Alfonso</i>	R&D Research Contract
	<i>Campos Prieto, Lucía</i>	Predoutoral Xunta Contract
	<i>Canabal Falcón, Rafael</i>	R&D Research Contract
	<i>Casabella Amieiro, Braulio</i>	R&D Research Contract
	<i>Ceballos Guzmán, Juan Manuel</i>	MSCA-ITN
	<i>Cedrún Morales, Manuela</i>	FPU
	<i>Chaves Pouso, Andrea</i>	R&D Research Contract
	<i>Colchón Pierna, Esther</i>	R&D Research Contract
	<i>Conde Piñeiro, Adrián</i>	R&D Research Contract
	<i>Conde Torres, Daniel</i>	Segundo Gil Dávila Foundation Fellowship Holder
	<i>Cool, Leonard G.</i>	R&D Research Contract
	<i>D'Avino, Cinzia</i>	R&D Research Contract
	<i>Da Concepción Vicente, Eduardo</i>	R&D Research Contract
	<i>Delgado González, Bruno</i>	Predoutoral Xunta Contract
	<i>Díaz Alonso, Sergio</i>	AEI Predoctoral Contract (former FPI)
	<i>Díaz Arias, Sandra Natalia</i>	R&D Research Contract
	<i>Domínguez Ramos, Lidia</i>	R&D Research Contract
	<i>Durán Bravo, Álvaro</i>	AEI Predoctoral Contract (former FPI)
	<i>Falcón Fariña, Sara</i>	R&D Research Contract
	<i>Fariña Torres, Víctor</i>	R&D Research Contract
	<i>Fernández Castro, Saleta</i>	Predoutoral Xunta Contract
	<i>Fernández González, Xulián</i>	AEI Predoctoral Contract (former FPI)
	<i>Fernández Iglesias, Antía</i>	FPU
	<i>Fernández Míguez, Manuel</i>	AEI Predoctoral Contract (former FPI)
	<i>Fojo Carballo, Hugo</i>	R&D Research Contract
	<i>Folgar Cameán, Yeray</i>	FPU

	<i>Fulias Guzmán, Patricia</i>	AEI Predoctoral Contract (former FPI)
	<i>García Abuín, Lucas</i>	R&D Research Contract
	<i>García Morales, Elvira</i>	R&D Research Contract
	<i>García Rey, Aitor</i>	Predoutoral Xunta Contract
	<i>Gioe, Claudia</i>	R&D Research Contract
	<i>Goicoechea Crespo, Laura</i>	FPU
	<i>Gómez Ojea, Rebeca</i>	R&D Research Contract
	<i>Gómez Roibás, Patricia</i>	R&D Research Contract
	<i>González González, Carmen</i>	R&D Research Contract
	<i>González González, José Manuel</i>	R&D Research Contract
	<i>González Pico, Lucía</i>	R&D Research Contract
	<i>Grela Casal, Uxía</i>	R&D Research Contract
	<i>Guillén Soler, Melanie</i>	R&D Research Contract
	<i>Gutiérrez González, Alejandro</i>	FPU
	<i>Huertas Morales, Iván</i>	FPU
	<i>Illodo Brea, Sara</i>	Predoutoral Xunta Contract
	<i>Janeiro Rodríguez, Jesús</i>	AEI Predoctoral Contract (former FPI)
	<i>Jiménez Vázquez, Alejandro</i>	Predoutoral Xunta Contract
	<i>Lago Silva, María</i>	Predoutoral Xunta Contract
	<i>Le Thi Thanh, Hiep</i>	R&D Research Contract
	<i>Lema Saavedra, Anxo</i>	R&D Research Contract
	<i>López Blanco, Roi</i>	R&D Research Contract
	<i>López Carracedo, Pablo</i>	R&D Research Contract
	<i>López Corbalán, María Victoria</i>	R&D Research Contract
	<i>Lorenzo Fojón, Carla</i>	R&D Research Contract
	<i>Losada Castro, Pablo</i>	R&D Research Contract
	<i>Luaces Calví, Antón</i>	R&D Research Contract
	<i>Mackay Anderson, Amelia</i>	R&D Research Contract
	<i>Malavé Fernández, María Valentina</i>	R&D Research Contract
	<i>Marcos Atanes, Daniel</i>	FPU
	<i>Matínez Balart, Pol</i>	R&D Research Contract
	<i>Martínez Castrillón, Adrián</i>	AEI Predoctoral Contract (former FPI)
	<i>Martínez Castro, Laura</i>	Predoutoral Xunta Contract
	<i>Martínez Parra, José María</i>	Predoutoral Xunta Contract
	<i>Méndez Gómez, Lucía</i>	R&D Research Contract
	<i>Migliavacca, Martina</i>	R&D Research Contract
	<i>Miranda Pastoriza, Darío</i>	Predoutoral Xunta Contract
	<i>Narayanan Kolusu, Sai Rohini</i>	R&D Research Contract
	<i>Ortigueira Noya, Sandra</i>	Other Fellowship Holder

	<i>Osorio Celis, Marcelo</i>	R&D Research Contract
	<i>Otero Riesgo, Sergio</i>	R&D Research Contract
	<i>Pacín Salvador, María del Carmen</i>	R&D Research Contract
	<i>Pérez Maseda, Marta</i>	FPU
	<i>Prieto Díaz, Rubén</i>	Predoutoral Xunta Contract
	<i>Rey López, Alejandro</i>	Predoutoral Xunta Contract
	<i>Reza Ramos, David</i>	Predoutoral Xunta Contract
	<i>Rioboo Vidal, Alicia</i>	FPU
	<i>Rivadulla Cendal, Elena</i>	R&D Research Contract
	<i>Rodiño Balboa, Ricardo</i>	FPU
	<i>Rodríguez Costa, Ángela</i>	R&D Research Contract
	<i>Rodríguez García, Carlos</i>	R&D Research Contract
	<i>Sabater Algarra, Yolanda</i>	R&D Research Contract
	<i>Salgado Barca, Jesús Fernando</i>	Predoutoral Xunta Contract
	<i>Salluce, Giulia</i>	AEI Predoctoral Contract (former FPI)
	<i>Sánchez Gascón, Paula</i>	R&D Research Contract
	<i>Sánchez-Brunete Gayoso, Diego</i>	R&D Research Contract
	<i>Sarmiento Fuentes, Axel</i>	FPU
	<i>Seco González, Alejandro</i>	R&D Research Contract
	<i>Serantes Otero, Sergio</i>	R&D Research Contract
	<i>Suárez de Cepeda Fuentes, Pilar</i>	R&D Research Contract
	<i>Suárez García, Juan</i>	R&D Research Contract
	<i>Suárez Lestón, Fabián</i>	R&D Research Contract
	<i>Suárez Lustres, Alejandro</i>	R&D Research Contract
	<i>Torrón Celada, Alba María</i>	R&D Research Contract
	<i>Troncoso Mondragón, Ezequiel</i>	AEI Predoctoral Contract (former FPI)
	<i>Varela Domínguez, Noa</i>	AEI Predoctoral Contract (former FPI)
	<i>Vázquez Galiñanes, Nuria</i>	AEI Predoctoral Contract (former FPI)
	<i>Vilela Picos, Marcos</i>	FPU
	<i>Villar Castro, Daniel</i>	R&D Research Contract
	<i>Vizcaíno Anaya, Lucía</i>	FPU

TECHNICAL STAFF (December 31, 2022)		
Area	Name	Position
	<i>Acevedo Arteaga, Laura Alicia</i>	Infrastructure's manager
	<i>Barros Frieiro, Manuela</i>	Administrative support (CiQUS' Research Group)
	<i>Casal Garea, Fernando</i>	Head of International Affairs and Knowledge Transfer
	<i>Comino León, Mariano</i>	Communication and Outreach manager
	<i>Fernández Aguiño, Carmen</i>	Lab Technician (CiQUS' Research Group)
	<i>García Arrese, Ana María</i>	Lab Technician (CiQUS' Research Group)
	<i>García Fernández, Almudena</i>	Head of Strategic Initiatives
	<i>Guerra Fandiño, Arcadio J.</i>	Core Facilities manager
	<i>Jiménez Balsa, Adrián</i>	Administrative support (CiQUS' Research Group)
	<i>Lago Rama, Patricia</i>	Administrative support (CiQUS' Research Group)
	<i>López Ulloa, Andrea</i>	Purchasing & Warehouse support technician
	<i>Menaya Vargas, Rebeca</i>	Biological Techniques' manager
	<i>Rama Rivera, Ángel</i>	Concierge
	<i>Pereira Rodríguez, María Begoña</i>	Administrative support (CiQUS' Research Group)
	<i>Reif López, Rubén</i>	Administrative support (CiQUS' Research Group)
	<i>Rey Ramos, María Carmen</i>	Concierge
	<i>Rodríguez Maqueda, Elena María</i>	Lab Technician (CiQUS' Research Group)
	<i>Rodríguez Martínez, Lucía</i>	Administrative support
	<i>Sande Barreira, Álvaro</i>	Research Specialist Technician (INVESTIGO PROGRAMME)
	<i>Torreiro Cea, Adrián</i>	IT Support manager
	<i>Torrente Filgueira, Noela</i>	Purchasing & Warehouse / HSE manager
	<i>Varela Señarís, Mercedes</i>	Administrative support - Account manager (shared with CiTIUS)
	<i>Vazquez Zas, Tamara</i>	Research Specialist Technician (INVESTIGO PROGRAMME)

ANNEX II: Active R&D & Valorization Projects during 2022

Active International R&D Projects in 2022							
Area	PI	Title	Programme	Funding Agency	Start	End	Budget
	Lazzari, Massimo	Novel electroactive polymeric materials for dielectric elastomers actuators and soft robots (EPOMA DESO)	MSCA-PF	MSCA Actions	01-09-22	31-08-24	181.153 €
	Rivadulla, Francisco	New Germanium-based materials for Green electronics (NeGeMat)	MSCA-PF	MSCA Actions	01-07-22	30-06-25	261.381 €
	Peña, Diego	Single Molecular Devices by Atomic Manipulation (MoIDAM)	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 Ilgand 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 €
	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 €
	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 clinically applicable non-viral gene delivery technology	H2020	REA	1/1/19	31/12/22	444.238 €
	Peña, Diego	Spin Research IN Graphene (SPRING)	FET-Open	REA	1/10/19	30/9/23	500.940 €
	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 €
	Montenegro, Javier	Dynamic Penetrating Adaptamers (DYNAP)	ERC-StG	ERC	1/2/16	31/7/22	1.432.824 €

Active National R&D Projects in 2022

Area	PI	Title	Programme	Funding Agency	Start	End	Budget
	<i>Mascareñas, José Luis</i>	Beyond metalloenzymes: Metal-grafted nanostructures for organometallic catalysis in live settings	Sello de Excelencia ISCIII-HEALTH 2022	ISCIII	2022	2024	984.252 €
	<i>del Pino, Pablo</i>	Engineered Exosomes for Stimuli-responsive Image-guided Drug delivery for Cancer Theranostic applications	Programación Conjunta Internacional - MSCA-PF-EF	AEI	2022	2024	160.932€
	<i>Tomás, María</i>	Desarrollo de nuevas herramientas y sondas para el estudio de procesos biológicos. traslado de fotocátalisis al contexto de la química bioortogonal.	Dotación Ramón y Cajal	AEI	2022	2026	42.000 €
	<i>Lazzari, Massimo</i>	Recuperación de metales escasos y valiosos de residuos electrónicos mediante materiales adsorbentes preparados a medida	Generación de Conocimiento	AEI	2022	2025	121.000€
	<i>Sotelo, Eddy</i>	Fármacos multi-diana en la inmunoterapia del cáncer: Descubrimiento de ligandos que actúan sinérgicamente en dos puntos de control inmunitarios en el microambiente tumoral	Generación de Conocimiento	AEI	2022	2025	145.200 €
	<i>Giménez-López, M. Carmen</i>	Refrigerantes de estado sólido, electrocatalizadores y baterías de iones metálicos activados por presión o mediante confinamiento en materiales híbridos sostenibles	Generación de Conocimiento	AEI	2022	2025	181.500 €
	<i>Orosa, Beatriz</i>	Descifrando la inmunidad de los cereales mediada por la ubiquitinación	Generación de Conocimiento	AEI	2022	2025	163.350€
	<i>Fernández-Megía, Eduardo</i>	Acidos borónicos: Un viaje de ida y vuelta entre transporte de fármacos y caracterización por RMN	Generación de Conocimiento	AEI	2022	2025	133.100€
	<i>Vázquez, Eugenio</i>	Herramientas peptídicas en sensores, catálisis y ciencia de materiales	Generación de Conocimiento	AEI	2022	2025	114.950€
	<i>Vázquez, Miguel</i>	Nuevas estrategias para terapias anticáncer y contra el Covid-19 basadas en herramientas	Generación de Conocimiento	AEI	2022	2025	114.950€
	<i>Nappi, Manuel</i>	Aprovechar la energía de la luz visible para convertir los gases de efecto invernadero en valiosos productos químicos	Transición Ecológica y Transición Digital	AEI	2022	2024	218.500€

Ramos, Rafael	Memorias térmicas y termoreguladores basados en conductores iónicos	Transición Ecológica y Transición Digital	AEI	2022	2024	152.950 €
Giménez-López, M. Carmen	Catalizador Confinado Duradero con Actividad Mejorada para Resolver las Limitaciones del Cátodo en una Batería de Zn-Aire - (ENDURANCE)	Transición Ecológica y Transición Digital	AEI	2022	2024	278.300 €
Ortuño, Manuel	Depolimerización asistida por dominios en líquidos iónicos usando técnicas computacionales a nivel atómico	Transición Ecológica y Transición Digital	AEI	2022	2024	116.955 €
Vázquez, Eugenio	Péptidos conductores semisintéticos y de síntesis química	Transición Ecológica y Transición Digital	AEI	2022	2024	149.500€
Peña, Diego	Diseño y síntesis de precursores moleculares para sensores de gases	Transición Ecológica y Transición Digital	AEI	2022	2024	148.350 €
Fañanás, Martín	Valorización de metano promovida por luz	Transición Ecológica y Transición Digital	AEI	2022	2024	184.000 €
Rodríguez, Rafael	-	Dotación Juan de la Cierva Incorporación	AEI	2022	2025	6.300 €
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 €
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 €
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 €

	<i>Polo, Ester</i>	Biomimetic dendritic-cell-derived nanovectors for targeting the immune system (NanoDCell)	RETOS	AEI	01-09-21	31-08-24	96.800 €
	<i>Nappi, Manuel</i>	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 €
	<i>Ortuño, Manuel</i>	Metal-organic frameworks for biomass Upgrading via Simulations of CAlytic systems (MUSICA)	RETOS	AEI	01-09-21	31-08-24	84.700 €
	<i>Orosa, Beatriz</i>	Improving plant immunity using post-translational modifications	Dotación Ramón y Cajal	AEI	01-09-21	31-08-25	40.000 €
	<i>Vázquez, Miguel</i>	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 €
	<i>Mateos, Jaime</i>	-	Dotación Juan de la Cierva - Incorporación	AEI	2021	2023	6.000 €
	<i>Rodríguez, Jessica</i>	-	Dotación Juan de la Cierva - Incorporación	AEI	2021	2023	6.000 €
	<i>Polo, Ester</i>	Synthetic biomimetic cell-derived nanostructures	Dotación Ramón y Cajal	AEI	01-01-21	31-12-25	40.000 €
	<i>Fernández-Ramos, Antonio</i>	Simulación de Biocombustibles y Aditivos de Gasolina	RETOS-Mod. B	AEI	1/6/20	31/5/24	60.500 €
	<i>Peña, Diego</i>	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 €
	<i>González-Bello, Concepción</i>	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 €
	<i>Martínez-Costas, Jose</i>	Nuevos enfoques de la encapsulación de proteínas en micro/nanoesferas basadas en viroplasma para aplicaciones industriales, terapéuticas e inmunoterapia (VIROSPHERE)	RETOS-Mod. B	AEI	1/6/20	31/5/23	121.000 €

<i>Rivadulla, Francisco</i>	Materiales funcionales para el control activo de la conductividad térmica	RETOS-Mod. B	AEI	1/6/20	31/5/23	151.250 €
<i>Seoane, Andrés</i>	Desarrollo de reacciones catalizadas por metales en el entorno celular	Juan de la Cierva - Incorporación	AEI	1/7/20	30/6/23	6.000 €
<i>Pelaz García, Beatriz</i>	Síntesis y caracterización de nanomateriales para el desarrollo de nanomedicinas	Ramón y Cajal	AEI	4/2/19	3/2/23	40.000 €
<i>Freire, Félix</i>	Chiral Dynamic Catalysts based on Helical Polymers	Becas Leonardo	BBVA Foundation	30/10/20	29/4/22	40.000 €
<i>Pelaz, Beatriz</i>	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 €
<i>Granja, Juan</i>	Materiales Supramoleculares Dinámicos Funcionales Basados en Ciclopéptidos. Una Aproximación a Terapias Supramoleculares	RETOS-Mod. B	AEI	1/6/20	31/5/23	1963.600 €
<i>Gulías, Moisés</i>	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 €
<i>Pérez, Dolores</i>	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 €
<i>Freire, Félix; Quiñóá, Emilio</i>	Materiales quirales con propiedades-estimulo respuesta: Diseño, síntesis y aplicaciones	Generación de Conocimiento	AEI	1/6/20	31/5/23	205.700 €
<i>Mascareñas, José Luis</i>	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 €
<i>Peña, Diego</i>	Síntesis en disolución para sistemas moleculares funcionales (FunMolSys)	RETOS-Mod. B	AEI	1/6/20	31/5/23	151.250 €
<i>García Fandiño, Rebeca</i>	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 €

	<i>J. Montenegro</i>	Redes Supramoleculares de Nanopartículas como Materiales Nanoporosos Avanzados	EIG Concert-Japan	PCI-AEI	1/4/19	31/02/22	100.000 €
	<i>Giménez López, María</i>	Synthesis and characterisation of a new class of functional hybrid metal-carbon nanostructures	Ramón y Cajal	AEI	1/5/18	30/4/22	40.000 €
	<i>García Fandiño, Rebeca</i>	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 2022							
Area	PI	Title	Programme	Funding Agency	Start	End	Budget
	<i>C. Saá</i>	GRC GI-1603 - Catálisis organometálica	CONSOLIDACIÓN - GRC	Xunta de Galicia	2022	2025	320.000 €
	<i>E. Quiñoa</i>	GRC GI-1608 - Nanomateriais e Moléculas Bioactivas	CONSOLIDACIÓN - GRC	Xunta de Galicia	2022	2025	278.772 €
	<i>R. Ramos</i>	Estudio de interacciones entre spin-red-electrón(ion) en óxidos de metales de transición para la manipulación de la conducción térmica y conversión termoelectrónica	PROXECTOS DE EXCELENCIA	Xunta de Galicia	2022	2026	115.000 €
	<i>B. Orosa</i>	-	PROXECTOS DE EXCELENCIA	Xunta de Galicia	2022	2026	115.000 €
	<i>D. Peña</i>	Convenio de colaboración entre a Consellería de Cultura, Educación e Universidade e a Universidade de Santiago de Compostela (USC) para Completar as axudas ao Persoal Investigador Principal dos Programas Grant do Consello Europeo de Investigación (ERC)	Agreement	Xunta de Galicia	2022	2022	80.000,00 €
	<i>M. Fañanás</i>	Convenio de colaboración entre a Consellería de Cultura, Educación e Universidade e a Universidade de Santiago de Compostela (USC) para Completar as axudas ao Persoal Investigador Principal dos Programas Grant do Consello Europeo de Investigación (ERC)	Agreement	Xunta de Galicia	2022	2022	65.000,00 €
	<i>B. Pelaz</i>	Convenio de colaboración entre a Consellería de Cultura, Educación e Universidade e a Universidade de Santiago de Compostela (USC) para Completar as axudas ao Persoal Investigador Principal dos Programas Grant do Consello Europeo de Investigación (ERC)	Agreement	Xunta de Galicia	2022	2022	50.000,00 €
	<i>M. Carmen Giménez-López</i>	Convenio de colaboración entre a Consellería de Cultura, Educación e Universidade e a Universidade de Santiago de Compostela (USC) para Completar as axudas ao Persoal Investigador Principal dos Programas Grant do Consello Europeo de Investigación (ERC)	Agreement	Xunta de Galicia	2022	2022	50.000,00 €

	<i>D. Pérez</i>	Accións Transversais I+D+i. Accións dinamización: Xornadas de portas abertas e bolsas de verán. Convenio Accións I+D. Acción 4.2.2 (Xunta 2022)	Agreement	Xunta de Galicia	2022	2022	24.000,00 €
	<i>C. González-Bello</i>	GRC GI 2155 Inhibidores Enzimáticos e Ferramentas Químicas	CONSOLIDACIÓN - GRC	Xunta de Galicia	1/1/21	30/11/24	280.000 €
	<i>J.R. Granja</i>	GRC GI-2132 Química supramolecular e nanotubos peptídicos (QSNP)	CONSOLIDACIÓN - GRC	Xunta de Galicia	1/1/21	30/11/24	400.000 €
	<i>J.L. Mascareñas</i>	GRC GI-1611 Química Biolóxica e Supramolecular (BCS)	CONSOLIDACIÓN - GRC	Xunta de Galicia	1/1/21	30/11/24	400.000 €
	<i>M. Giménez-López</i>	GPC GI 2170 Materia Condensada & Materiais Funcionais (MAT2)	CONSOLIDACIÓN - GPC	Xunta de Galicia	1/1/21	30/11/23	90.000 €
	<i>E. Polo</i>	CONSOLIDACION 2021 - Mod. D Excelencia	EMERXENTES	Xunta de Galicia	1/1/21	30/11/24	115.000 €
	<i>Ortuño, Manuel</i>	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	Distinguished Researchers	Xunta de Galicia	1/12/20	30/11/24	160.000 €
	<i>Gutián, Enrique</i>	GI-1595_Catálisis Organometálica y Materiales Moleculares Orgánicos	Grupo de Referencia Competitiva	Xunta de Galicia	1/1/20	30/11/23	280.000 €
	<i>Sotelo, Eddy</i>	GI-1597 Descubrimiento y síntesis de fármacos - DESINFARMA-COMBIOMED	Grupo de Potencial Crecimiento	Xunta de Galicia	1/1/20	30/11/22	90.000 €
	<i>Pelaz, Beatriz</i>	Desarrollo de tecnologías basadas en ADN para ingeniería de nanomedicinas inspiradas en las cápsides víricas: ADNanoVir	Consolidación – Mod.D Excelencia	Xunta de Galicia	1/1/20	30/11/23	90.000 €
	<i>García-Fandiño, Rebeca</i>	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 €
	<i>Fernández-Megía, Eduardo</i>	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 €
	<i>González-Bello, Concepción</i>	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 €

	<i>Mascareñas, José Luis</i>	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
--	----------------------------------	--	--	-------	---------	----------	-----------

Active Valorization Projects in 2022

Area	PI	Title	Programme	Funding Agency	Start	End	Budget
	J.L. Mascareñas	Selectively eliminating cancer stem cells through inhibition of mitochondrial respiration using metal-based small molecules	La Caixa Research Consolidate 2021	La Caixa Foundation	2022	2025	300.000 €
	J. Montenegro	TraffikGene	IGNICIA	GAIN	2022	2025	490.000 €
	M. Carmen Giménez-López	A New Supramolecular Rechargeable Zinc-Bromine Battery for a Sustainable Energy Transition (ZUPRAenergy)	PROYECTOS DE I+D+i PRUEBAS DE CONCEPTO	AEI	2022	2024	149.500 €
	R. García-Fandiño	Descifrando el lipidoma humano: CRYPT LIPID CODES para predecir y diagnosticar enfermedades	PROYECTOS DE I+D+i PRUEBAS DE CONCEPTO	AEI	2022	2024	141.450 €
	E. Sotelo	Cuantificación en paralelo de múltiples interacciones de puntos de control inmunitario en onco-inmunología. PREDICTEAM	Proyectos de colaboración público-privada 2021	AEI	2022	2025	181.654 €
	E. Sotelo	CAPN12-IO: preclinical development and first human clinical trial of a selective calpain-12 inhibitor as a new strategy for cancer immunotherapy	Proyectos de colaboración público-privada 2021	AEI	2022	2025	276.948 €
	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 2022

Active R&D Contracts in 2022						
Area	PI	Title	Partnert/Client	Start	End	Budget
	<i>E. Sotelo</i>	Puesta a punto y desarrollo de metodologías sintéticas y obtención de quimiotecas de moléculas orgánicas.	LANDSTEINER GENMED, SL	5/3/18	3/8/23	27.083 €
	<i>F.J. Sardina</i>	Diseño e desenvolvemento de algoritmos e bases de datos espectroscópicas 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 estrutura	MESTRELAB RESEARCH, SL	1/1/22	31/12/25	99.220 €
	<i>E. Sotelo</i>	Apoio técnico no deseño de novas ferramentas químicas e soporte no proceso de desenvolvemento de intermedios químicos. InnovaPeme	CELTARYS RESEARCH SL	19/5/22	30/9/23	10.482 €
	<i>E. Sotelo</i>	Servicios de consultoría técnica, síntesis de colecciones de ligandos y análisis estructural relacionados con los ligandos fluorescentes desarrollados por CELTARYS	CELTARYS RESEARCH SL	2/6/22	1/7/23	19.561 €
	<i>D. Peña</i>	<i>Síntesis de compostos policíclicos aromáticos</i>	<i>ABCR GMBH</i>	1/1/21	31/12/25	500 €
	<i>Martínez-Costas, José Manuel</i>	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 €
	<i>Sotelo Pérez, Eddy</i>	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 €
	<i>Sotelo Pérez, Eddy</i>	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 €
	<i>Sotelo Pérez, Eddy</i>	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 €

	<i>Sardina Lopez, Francisco Javier</i>	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 €
	<i>Sardina Lopez, Francisco Javier</i>	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 €
	<i>Sotelo Pérez, Eddy</i>	Puesta a punto y desarrollo de metodoloxías sintéticas y obtención de quimiotecas de moléculas orgánicas.	LANDSTEINER GENMED, SL	5/3/20	4/3/22	105.000 €
	<i>Sotelo Pérez, Eddy</i>	Puesta a punto y desarrollo de metodoloxías sintéticas y la obtención de quimiotecas de moléculas orgánicas	ONCOSTELLAE, SL	1/1/21	31/12/22	30.000 €
	<i>Sardina Lopez, Francisco Javier</i>	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 €
	<i>Sardina Lopez, Francisco Javier</i>	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 €
	<i>Sardina Lopez, Francisco Javier</i>	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 €
	<i>Sardina Lopez, Francisco Javier</i>	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 €
	<i>Estevez Cabanas, Ramon Jose</i>	Asesoría técnica para a realización e elucidación das análises de Resonancia Magnética	GALCHIMIA S.A.	1/1/21	31/12/22	9.999 €
	<i>Garcia Fandiño, Rebeca</i>	Caracterización estrutural e enerxética das interaccións entre o remdesivir, farmaco empregado no COVID•-19, e o excipiente Captisol	MD. USE INNOVATIONS SL	1/12/20	30/1/22	15.000 €

ANNEX IV: List of Publications

2022 List of CiQUS Publications						
Area	Authors	Title	Journal	Vol.	Pages	DOI
	J.M. Priegue, I. Louzao, I. Gallego, J. Montenegro, J.R. Granja	1D alignment of proteins and other nanoparticles by using reversible covalent bonds on cyclic peptide nanotubes	<i>Org. Chem. Front.</i>	9	1226-1233	10.1039/D1QO01349A
	T. Pose-Boirazian, J. Martínez-Costas, G. Eibes	3D Printing: An Emerging Technology for Biocatalyst Immobilization	<i>Macromol. Biosci.</i>	22	2200110	10.1002/mabi.202200110
	I. Gallego, J. Ramos-Soriano, A. Méndez-Ardoy, J. Cabrera-González, I. Lostalé-Seijo, B.M. Illescas, J.J. Reina, N. Martín, J. Montenegro	A 3D Peptide/[60]Fullerene Hybrid for Multivalent Recognition	<i>Angew. Chem. Int. Ed.</i>	61	e202210043	10.1002/anie.202210043
	X. Xu, T. Pose-Boirazian, G. Eibes, L.E. McCoubrey, J. Martínez-Costas, S. Gaisford, A. Goyanes, A.W. Basit	A customizable 3D printed device for enzymatic removal of drugs in water	<i>Water Res.</i>	208	117861	10.1016/j.watres.2021.117861
	J. Bergueiro, A.E. Glitscher, M. Calderón	A hybrid thermoresponsive plasmonic nanogel designed for NIR-mediated chemotherapy	<i>Biomater. Adv.</i>	137	212842	10.1016/j.bioadv.2022.212842
	A.H.M. Tay, R. Prieto-Díaz, S. Neo, L. Tong, X. Chen, V. Carannante, B. Önfelt, J. Hartman, F. Haglund, M. Majellaro, J. Azuaje, X. Garcia-Mera, J.M. Brea, M.I. Loza, W. Jaspers, H. Gutiérrez-de-Teran, E. Sotelo, A. Lundqvist	A _{2B} adenosine receptor antagonists rescue lymphocyte activity in adenosine-producing patient-derived cancer models	<i>J. Immunoter. Cancer</i>	10	e004592	10.1136/jitc-2022-004592
	S.P. Amaral, J. Correa, E. Fernández-Megía	Accelerated synthesis of dendrimers by thermal azide-alkyne cycloaddition with internal alkynes	<i>Green Chem</i>	24	4897-4901	10.1039/D2GC00473A

N. Friedrich, R.E. Menchón, I. Pozo, J. Hieulle, A. Vegliante, J. Li, D. Sánchez-Portal, D. Peña, A. Garcia-Lekue, J.I. Pascual	Addressing Electron Spins Embedded in Metallic Graphene Nanoribbons	<i>ACS Nano</i>	16	14819-14826	10.1021/acsnano.2c05673
I.R. Arias, D. Buceta, G. Barone, M.C. Giménez-López, H. Lozano, M. Lazzari, M.A. López-Quintela	Ag ₅ nanoclusters with dual catalytic antiradical activities	<i>J. Colloid Interface Sci.</i>	628	437-447	10.1016/j.jcis.2022.07.133
D. Ferro-Costas, M.N.D.S. Cordeiro, A. Fernández-Ramos	An integrated protocol to study hydrogen abstraction reactions by atomic hydrogen in flexible molecules: application to butanol isomers	<i>Phys. Chem. Chem. Phys.</i>	24	3043-3058	10.1039/D1CP03928H
M. Tenorio, C. Moreno, P. Febrer, J. Castro-Esteban, P. Ordejón, D. Peña, M. Pruneda, A. Mugarza	Atomically Sharp Lateral Superlattice Heterojunctions Built-in Nitrogen-doped Nanoporous Graphene	<i>Adv. Mater.</i>	34	2110099	10.1002/adma.202110099
M.R. Bittermann, C. López-Bueno, M. Hilbers, F. Rivadulla, F. Caporaletti, G. Wegdam, D. Bonn, S. Woutersen	Austen in Amsterdam: Isotope effect in a liquid-liquid transition in supercooled aqueous solution	<i>J. Non-Cryst. Solids: X</i>	13	100077	10.1016/j.nocx.2021.100077
A. Sundar, D. Bugallo Ferrón, Y.-J. Hu, L. Qi	Automated hierarchical screening of refractory multicomponent alloys with high intrinsic ductility and surface passivation potency	<i>MRS Commun.</i>	12	1086-1095	10.1557/s43579-022-00241-1
T. Wang, A. Berdonces-Layunta, N. Friedrich, M. Vilas-Varela, J.P. Calupitan, J.I. Pascual, D. Peña, D. Casanova, M. Corso, D.G. de Oteyza	Aza-Triangulene: On-Surface Synthesis and Electronic and Magnetic Properties	<i>J. Am. Chem. Soc.</i>	144	4522-4529	10.1021/jacs.1c12618
N. Vázquez-Galiñanes, I. Velo-Helena, M. Fañanás-Mastral	Bifunctional Skipped Dienes through Cu/Pd-Catalyzed Allylboration of Alkynes with B ₂ pin ₂ and Vinyl Epoxides	<i>Org. Lett.</i>	24	8244-8248	10.1021/acs.orglett.2c03390
E. Soprano, E. Polo, B. Pelaz, P. del Pino	Biomimetic cell-derived nanocarriers in cancer research	<i>J. Nanobiotechnol</i>	20	538	10.1186/s12951-022-01748-4

A. Barba-Bon, G. Salluce, I. Lostalé-Seijo, K.I. Assaf, A. Henning, J. Montenegro, W.M. Nau	Boron clusters as broadband membrane carriers	<i>Nature</i>	603	637-642	10.1038/s41586-022-04413-w
I. Insua, J. Bergueiro, A. Méndez-Ardoy, I. Lostalé-Seijo, J. Montenegro	Bottom-Up Supramolecular Assembly in the Second Dimension	<i>Chem. Sci.</i>	13	3057-3068	10.1039/D1SC05667K
B. Pérez-Saavedra, A. Velasco-Rubio, E. Rivera-Chao, J.A. Varela, C. Saá, M. Fañanás-Mastral	Catalytic Lewis Base Additive Enables Selective Copper-Catalyzed Borylative α -C-H Allylation of Alicyclic Amines	<i>J. Am. Chem. Soc.</i>	35	16206-16216	10.1021/jacs.2c07969
J.M. González, X. Vidal, M.A. Ortuño, J.L. Mascareñas, M. Gulías	Chiral Ligands Based on Binaphthyl Scaffolds for Pd-Catalyzed Enantioselective C-H Activation/Cycloaddition Reactions	<i>J. Am. Chem. Soc.</i>	144	21437-21442	10.1021/jacs.2c09479
M. Núñez-Martínez, E. Quiñoá, F. Freire	Chiroptical and Colorimetric Switches Based on Helical Polymer-Metal Nanocomposites Prepared via Redox Metal Translocation of Helical Polymer Metal Complexes	<i>Nanoscale</i>	14	13066-13072	10.1039/D2NR03807B
J. Lawrence, A. Berdonces-Layunta, S. Edalatmanesh, J. Castro-Esteban, T. Wang, A. Jiménez-Martin, B. de la Torre, R. Castrillo-Bodero, P. Angulo-Portugal, M.S.G. Mohammed, A. Matěj, M. Vilas-Varela, F. Schiller, M. Corso, P. Jelinek, D. Peña, D.G. de Oteyza	Circumventing the stability problems of graphene nanoribbon zigzag edges	<i>Nat. Chem.</i>	14	1451-1458	10.1038/s41557-022-01042-8
D. Valdeperez, N. Wutke, L.-M. Ackermann, W.J. Parak, M. Klapper, B. Pelaz	Colloidal stability of polymer coated zwitterionic Au nanoparticles in biological media	<i>Inorg. Chim. Acta</i>	534	120820	10.1016/j.ica.2022.120820

T. Kikkawa, K. Oyanagi, T. Hioki, M. Ishida, Z. Qiu, R. Ramos, Y. Hashimoto, E. Saitoh	Composition-tunable magnon-polaron anomalies in spin Seebeck effects in epitaxial $\text{Bi}_x\text{Y}_{3-x}\text{Fe}_5\text{O}_{12}$ films	<i>Phys. Rev. Mater.</i>	6	104402	10.1103/PhysRevMaterials.6.104402
M.A. Ortuño, M. Rellán-Piñeiro, R. Luque	Computational Mechanism of Methyl Levulinate Conversion to γ -Valerolactone on UiO-66 Metal Organic Frameworks	<i>ACS Sustain. Chem. Eng.</i>	10	3567-3573	10.1021/acssuschemeng.1c08021
S. Learte-Aymamí, P. Martín-Malpartida, L. Roldán-Martín, G. Sciortino, J.R. Couceiro, J.-D. Maréchal, M.J. Macias, J.L. Mascareñas, M.E. Vázquez	Controlling oncogenic KRAS signaling pathways with a Palladium-responsive peptide	<i>Commun. Chem.</i>	5	75	10.1038/s42004-022-00691-7
L. Cruz, S. Parcerobouzas, E. Fernández-Megía, N. Mateus, V. Freitas	Corrigendum to pH-regulated interaction modes between cyanidin-3-glucoside and phenylboronic acid-modified alginate [Carbohydr. Polym. 280 (2022) 119029]	<i>Carbohydr. Polym.</i>	287	119423	10.1016/j.carbpol.2022.119423
J. Rodríguez, C. Pérez-González, M. Martínez-Calvo, J. Mosquera, J.L. Mascareñas	Deactivation of a dimeric DNA-binding peptide through a palladium-mediated self-immolative cleavage	<i>RSC Adv.</i>	12	3500-3504	10.1039/D1RA09180H
S. Daimon, K. Tsunekawa, S. Kawakami, T. Kikkawa, R. Ramos, K. Oyanagi, T. Ohtsuki, E. Saitoh	Deciphering quantum fingerprints in electric conductance	<i>Nat. Commun.</i>	13	3160	10.1038/s41467-022-30767-w
A. Sánchez-Fernández, S. Prevost, M. Wahlgren	Deep eutectic solvents for the preservation of concentrated proteins: the case of lysozyme in 1:2 choline chloride : glycerol	<i>Green Chem</i>	24	4437-4442	10.1039/D1GC04378A
P. Martínez-Balart, B.L. Tóth, Á. Velasco-Rubio, M. Fañanás-Mastral	Direct C–H Allylation of Unactivated Alkanes by Cooperative W/Cu Photocatalysis	<i>Org. Lett.</i>	24	6874-6879	10.1021/acs.orglett.2c02887

M. Panicera, E. Lence. A. Rodríguez, B. Gracia, J.A. Aínsa, C. Marco-Marín, V. Rubio, C. Roque Duarte Correira, C. González-Bello	Discovery of 3 <i>H</i> -pyrrolo[2,3- c]quinolines with activity against Mycobacterium tuberculosis by allosteric inhibition of the glutamate-5-kinase enzyme	<i>Eur. J. Med. Chem.</i>	232	114206	10.1016/j.ejmech.2022.1 14206
J.J. Tarrío, R. Rodríguez, B. Fernández, E. Quiñoá, F. Freire	Dissymmetric Chiral Poly(diphenylacetylene)s: Secondary Structure Elucidation and Dynamic Luminescence	<i>Angew. Chem. Int. Ed.</i>	13	e202115070	10.1002/anie.202115070
H. Fernández-Caro, A. Méndez-Ardoy, J. Montenegro	Dynamic nanosurface reconfiguration by host-guest supramolecular interactions	<i>Nanoscale</i>	14	3599-3608	10.1039/D1NR05315A
L.N.J. de Windt, Z. Fernández, M. Fernández-Míguez, F. Freire, A.R.A. Palmans	Elucidating the Supramolecular Copolymerization of N- and C- Centered Benzene-1,3,5- Tricarboxamides: The Role of Parallel and Antiparallel Packing of Amide Groups in the Copolymer Microstructure	<i>Chem. Eur. J.</i>	28	e2021036	10.1002/chem.20210369 1
A. Chaves-Pouso, A.M. Álvarez- Constantino, M. Fañanás-Mastral	Enantio- and Diastereoselective Copper-Catalyzed Allylboration of Alkynes with Allylic <i>gem</i> -Dichlorides	<i>Angew. Chem. Int. Ed.</i>	61	e202117696	10.1002/anie.202117696
I. Bolognino, A. Carrieri, R. Purgatorio, M. Catto, R. Caliandro, B. Carrozzini, B.D. Belviso, M. Majellaro, E. Sotelo, S. Cellamare, C.D. Altomare	Enantiomeric Separation and Molecular Modelling of Bioactive 4- Aryl-3,4-dihydropyrimidin-2(1 <i>H</i>)-one Ester Derivatives on Teicoplanin- Based Chiral Stationary Phase	<i>Separations</i>	9	7	10.3390/separations9010 007

D. Miranda-Pastoriza, R. Bernárdez, J. Azuaje, R. Prieto-Díaz, M. Majellaro, A.V. Tamhankar, L. Koenekoop, A. González, C. Gioé-Gallo, A. Mallo-Abreu, J. Brea, M.I. Loza, A. García-Rey, X. García-Mera, H. Gutiérrez-de-Terán, E. Sotelo	Exploring Non-orthosteric Interactions with a Series of Potent and Selective A3 Antagonists	<i>ACS Med. Chem. Lett.</i>	13	243-249	10.1021/acsmchemlett.1c00598
A. Seoane, J.L. Mascareñas	Exporting Homogeneous Transition Metal Catalysts to Biological Habitats	<i>Eur. J. Org. Chem.</i>	-	e202200118	10.1002/ejoc.202200118
J. Correa, A. Garcia-Barandela, L. Socias-Pinto, E. Fernández-Megia	Filtering the NMR Spectra of Mixtures by Coordination to Paramagnetic Cu ²⁺	<i>Anal. Chem.</i>	94	10907-10911	10.1021/acs.analchem.2c01983
S. Boso, J.-L. Santiago, P. Gago, E. Sotelo, I. Álvarez-Acero, M.C. Martínez	Flavanol Content and Nutritional Quality of Wastes from the Making of White and Rosé Wines from Mountain Vineyards	<i>Am. J. Enol. Vitic</i>	73	255-265	10.5344/ajev.2022.22002
R. Rodríguez, E. Rivadulla, M. Fernández-Míguez, B. Fernández, K. Maeda, E. Quiñoá, F. Freire	Full Control of the Chiral Overpass Effect in Helical Polymers: P/M Screw Sense Induction by Remote Chiral Centers After Bypassing the First Chiral Residue	<i>Angew. Chem. Int. Ed.</i>	61	e202209953	10.1002/anie.202209953
A. Miranda, R. López-Blanco, J. Lopes-Nunes, A.M. Melo, M.P. Cabral Campello, A. Paulo, M.C. Oliveira, J.-L. Mergny, P.A. Oliveira, E. Fernández-Megía, C. Cruz	Gallic Acid–Triethylene Glycol Aptadendrimers Synthesis, Biophysical Characterization and Cellular Evaluation	<i>Pharmaceutics</i>	14	2456	10.3390/pharmaceutics14112456
I. Gallego Gómez, J. Montenegro	Glycan Shields for Penetrating Peptides	<i>Chem. Commun.</i>	58	1394-1397	10.1039/D1CC06252B

M. Ceballos, M. Cedrún-Morales, M. Rodríguez-Pérez, S. Funes-Hernando, J.M. Vila-Fungueiriño, G. Zampini, M.F. Navarro Poupard, E. Polo, P. del Pino, B. Pelaz	High-yield halide-assisted synthesis of metal-organic framework UiO-based nanocarriers	<i>Nanoscale</i>	14	6789-6801	10.1039/D1NR08305H
A. Sanchez-Fernandez, M. Basic, J. Xiang, S. Prevost, A.J. Jackson, C. Dicko	Hydration in Deep Eutectic Solvents Induces Non-monotonic Changes in the Conformation and Stability of Proteins	<i>J. Am. Chem. Soc.</i>	144	23657-23667	10.1021/jacs.2c11190
J. Barbazán, M. Majellaro, A.L. Martínez, J.M. Brea, E. Sotelo, M. Abal	Identification of A _{2B} AR as a potential target in colorectal cancer using novel fluorescent GPCR ligands	<i>Biomed. Pharmacother.</i>	153	113408	10.1016/j.biopha.2022.113408
T.Y. Baum, S. Fernández, D. Peña, H.S.J. van der Zant	Magnetic Fingerprints in an All-Organic Radical Molecular Break Junction	<i>Nano Lett.</i>	22	8086-8092	10.1021/acs.nanolett.2c02326
L. Vizcaíno-Anaya, C. Herrero-Lucas, J.M. Vila-Fungueiriño, M.C. Giménez-López	Magnetic Hyperthermia Enhancement in Iron-based Materials Driven by Carbon Support Interactions	<i>Chem. Eur. J.</i>	28	e004592	10.1002/chem.202201861
T. Wang, S. Sanz, J. Castro-Esteban, J. Lawrence, A. Berdonces-Layunta, M.S.G. Mohammed, M. Vilas-Varela, M. Corso, D. Peña, T. Frederiksen, D.G. de Oteyza	Magnetic Interactions Between Radical Pairs in Chiral Graphene Nanoribbons	<i>Nano Lett.</i>	22	164-171	10.1021/acs.nanolett.1c03578
W. Zhang, M. Guillén-Soler, S. Moreno-Da Silva, A. López-Moreno, L.R. González, M.C. Giménez-López, E.M. Pérez	Mechanical interlocking of SWNTs with N-rich macrocycles for efficient ORR electrocatalysis	<i>Chem. Sci.</i>	13	9706-9712	10.1039/D2SC02346F
S.R.N. Kolu, M. Nappi	Metal-free Deoxygenative Coupling of Alcohol-Derived Benzoates and Pyridines for Small Molecules and DNA-Encoded Libraries Synthesis	<i>Chem. Sci.</i>	14	8069-8077	10.1039/D2SC01621D

J.A. Vallejo, N. Trigo-Tasende, S. Rumbo-Feal, K. Conde-Pérez, A. López-Oriona, I. Barbeito, M. Vaamonde, J. Tarrío-Saavedra, R. Reif, S. Ladra, B.K. Rodiño-Janeiro, M. Nasser-Ali	Modeling the number of people infected with SARS-COV-2 from wastewater viral load in Northwest Spain	<i>Sci. Total Environ.</i>	811	152334	10.1016/j.scitotenv.2021.152334
D. Conde, P.F. Garrido, M. Calvelo, A. Piñeiro, R. García-Fandiño	Molecular Dynamics Simulations of Transmembrane Cyclic Peptide Nanotubes Using Classical Force Fields, Hydrogen Mass Repartitioning, and Hydrogen Isotope Exchange Methods: A Critical Comparison	<i>Int. J. Mol. Sci.</i>	23	3158	10.3390/ijms23063158
L. Jiménez-Cabello, S. Utrilla-Trigo, N. Barreiro-Piñeiro, T. Pose-Boirazian, J. Martínez-Costas, A. Marín-López, J. Ortego	Nanoparticle- and Microparticle-Based Vaccines against Orbiviruses of Veterinary Importance	<i>Vaccines</i>	10	1124	10.3390/vaccines10071124
S. Mishra, S. Fatayer, S. Fernández, K. Kaiser, D. Peña, L. Gross	Nonbenzenoid High-Spin Polycyclic Hydrocarbons Generated by Atom Manipulation	<i>ACS Nano</i>	16	3264-3271	10.1021/acsnano.1c11157
F. Suárez-Lestón, P.F. Garrido, A. Piñeiro, R. García-Fandiño	Not so rigid capsids based on cyclodextrin complexes: Keys to design	<i>J. Colloid Interface Sci.</i>	623	938-946	10.1016/j.jcis.2022.05.098
A. Domínguez-Celorrio, C. García-Fernández, S. Quiroga, P. Koval, V. Langlais, D. Peña, D. Sánchez-Portal, D. Serrate, J. Lobo-Checa	On-surface synthesis of Mn-phthalocyanines with optically active ligands	<i>Nanoscale</i>	14	8069-8077	10.1039/D2NR00721E

C. Val, C. Rodríguez-García, R. Prieto-Díaz, A. Crespo, J. Azuaje, C. Carbajales, M. Majellaro, A. Díaz- Hoguín, J.M. Brea, M.I. Loza, C. Gioé- Gallo, M. Contino, A. Stefanachi, X. García-Mera, J.C. Estévez, H. Gutiérrez-de- Terán, E. Sotelo	Optimization of 2-Amino-4,6- diarylpyrimidine-5-carbonitriles as Potent and Selective A1 Antagonists	<i>J. Med. Chem.</i>	65	2091-2106	10.1021/acs.jmedchem.1 c01636
S. Gutiérrez, M. Tomás-Gamasa, J.L. Mascareñas	Organometallic catalysis in aqueous and biological environments: harnessing the power of metal carbenes	<i>Chem. Sci.</i>	13	6478-6495	10.1039/D2SC00721E
F. Verdugo, R. Rodiño, M. Calvelo, J.L. Mascareñas, F. López	Palladium-Catalyzed Tandem Cycloisomerization/Cross-Coupling of Carbonyl- and Imine-Tethered Alkylidenecyclopropanes	<i>Angew. Chem. Int. Ed.</i>	61	e202202295	0.1002/anie.202202295
B. Claro, E. González-Freire, J.R. Granja, R. García-Fandiño, J. Gallova, D. Uhríková, A. Fedorov, A. Coutinho, M. Bastos	Partition of antimicrobial D-L- α - cyclic peptides into bacterial model membranes	<i>Biochim. Biophys. Acta- Biomembr.</i>	1864	183729	10.1016/j.bbamem.2021. 183729
R.J. Vandebriel, S. Remy, J.P. Vermeulen, E.G.E. Hurkmans, K. Kevenaer, N.G. Bastús, B. Pelaz, M.G. Soliman, V.F. Puntes, W.J. Parak, J.L.A. Pennings, I. Nelissen	Pathways Related to NLRP3 Inflammasome Activation Induced by Gold Nanorods	<i>Int. J. Mol. Sci.</i>	23	5763	10.3390/ijms23105763
F. Rey-Tarrío, S. Guisán-Ceinos, J.M. Cuerva, D. Miguel, M. Ribagorda, E. Quiñoá, F. Freire	Photostability and Dynamic Helical Behavior in Chiral Poly(phenylacetylene)s with a Preferred Screw-Sense	<i>Angew. Chem. Int. Ed.</i>	61	e202207623	10.1002/anie.202207623

U. Thupakula, X. Bouju, J. Castro-Esteban, E. Dujardin, D. Peña, C. Joachim	Planar bridging an atomically precise surface trench with a single molecular wire on an Au(111) surface	<i>Chem. Phys. Lett.</i>	806	140029	10.1016/j.cplett.2022.140029
F. Fernández, A.G. Fernández, R. Balo, V.M. Sánchez-Pedregal, M. Royo, R.G. Soengas, R.J. Estévez, J.C. Estévez	Polyhydroxylated Cyclopentane β -Amino Acids Derived from d-Mannose and d-Galactose: Synthesis and Protocol for Incorporation into Peptides	<i>ACS Omega</i>	7	2002-2014	10.1021/acsomega.1c05468
P.N. Trigo-Tasende, M. Vaamonde, K. Conde-Pérez, Á. López-Oriona, E.F. Álvarez, B. Freire, M. Nasser-Ali, I. Barbeito, S. Rumbo-Feal, R. Reif, B.K. Rodiño, J. Parama, L. Tomás, P. Gallego, G. Bou, J. Tarrío-Saavedra, I.I. Corras, D. Posada, I. López de Ulibarri, J.A. Vallejo, S. Ladra, R. Cao, M. Poza	Proyecto COVIDBENS. Seguimiento de la pandemia de COVID-19 en aguas residuales del área metropolitana de A Coruña	<i>Rev. Salud Ambient.</i>	22	50-56	N/A
G.A. Pizzio, C. Mayordomo, J. Lozano-Juste, V. Garcia-Carpintero, M. Vazquez-Vilar, S.G. Nebauer, K.P. Kaminski, N.V. Ivanov, J.C. Estevez, M. Rivera-Moreno, A. Albert, D. Orzaez, P.L. Rodriguez	PYL1-and PYL8-like ABA Receptors of <i>Nicotiana benthamiana</i> Play a Key Role in ABA Response in Seed and Vegetative Tissue	<i>Cells</i>	11	795	10.3390/cells11050795
D. González, A. Lema-Saavedra, S. Espinosa, E. Martínez-Núñez, A. Fernández-Ramos, A. Canosa, B. Ballesteros, E. Jiménez	Reaction of OH radicals with CH ₃ NH ₂ in the gas phase: Experimental (11.7-177.5 K) and computed rate coefficients (10-1000 K)	<i>Phys. Chem. Chem. Phys.</i>	24	23593-23601	10.1039/D2CP03414J

A. Malas, E. Saleh, M.C. Giménez-López, G.A. Rance, T. Helps, M. Taghavi, J.M. Rossiter, C.J. Tuck, I.A. Aschcroft, R.D. Goodridge	Reactive Jetting of High Viscosity Nanocomposites for Dielectric Elastomer Actuation	<i>Adv. Mater. Technol.</i>	7	21001111	10.1002/admt.202101111
F. Pedroso de Lima, E. Lence, P. Suárez de Cepeda, C. Correia, M.A. Carvalho, C. González-Bello, M.F. Proença	Regioselective Synthesis of 2-Aryl-5-cyano-1-(2-hydroxyaryl)-1H-imidazole-4-carboxamides Self-Assisted by a 2-Hydroxyaryl Group	<i>ACS Omega</i>	7	23289-23301	10.1021/acsomega.2c01399
A. Piñeiro, J. Pipkin, V. Antle, R. García-Fandiño	Remdesivir interactions with sulphobutylether- β -cyclodextrins: A case study using selected substitution patterns	<i>J. Mol. Liq.</i>	346	117157	10.1016/j.molliq.2021.117157
H. Montes-Campos, T. Méndez-Morales, L.M. Varela, M.A. Ortuño	Role of Anions in 5-Hydroxymethylfurfural Solvation in Ionic Liquids from Molecular Dynamics Simulations	<i>Adv. Theory Simul.</i>	5	2200522	10.1002/adts.202200522
A. Ruedas-López, I. Alonso-García, C. Lasarte-Monterrubio, P. Guijarro-Sánchez, E. Gato, J.C. Vázquez-Ucha, J.A. Vallejo, P.A. Fraile-Ribot, B. Fernández-Pérez, D. Velasco, J.M. Gutiérrez-Urbón, M. Oviaño, A. Beceiro, C. González-Bello, A. Oliver, J. Arca-Suárez, G. Bou	Selection of AmpC β -Lactamase Variants and Metallo- β -Lactamases Leading to Ceftolozane/Tazobactam and Ceftazidime/Avibactam Resistance during Treatment of MDR/XDR <i>Pseudomonas aeruginosa</i> Infections	<i>Antimicrob. Agents. Ch.</i>	66	e02067-21	10.1128/AAC.02067-21

J. Gómez-González, L. Martínez-Castro, J. Tolosa-Barrilero, A. Alcalde-Ordóñez, S. Learte-Aymamí, J.L. Mascareñas, J.C. García-Martínez, J. Martínez-Costas, J.-D. Maréchal, M. Vázquez López, M.E. Vázquez	Selective recognition of A/T-rich DNA 3-way junctions with a three-fold symmetric tripeptide	<i>Chem. Commun.</i>	58	7769-7772	10.1039/D2CC02874C
F. Albrecht, S. Fatayer, I. Pozo, I. Tavernelli, J. Reep, D. Peña, L. Gross	Selectivity in single-molecule reactions by tip-induced redox chemistry	<i>Science</i>	377	298-301	10.1126/science.abo6471
C. Correa-Paz, M.F. Navarro Poupard, E. Polo, M. Rodríguez-Pérez, M. Migliavacca, R. Iglesias-Rey, A. Ouro, E. Maqueda, P. Hervella, T. Sobrino, J. Castillo, P. del Pino, B. Pelaz, F. Campos	Sonosensitive capsules for brain thrombolysis increase ischemic damage in a stroke model	<i>J. Nanobiotech hnol</i>	20	46	10.1186/s12951-022-01252-9
S. Illodo, C. Pérez-González, R. Barcia, F. Rodríguez-Prieto, W. Al-Soufi, M. Novo	Spectroscopic Characterization of Mitochondrial G-Quadruplexes	<i>Int. J. Mol. Sci.</i>	23	925	10.3390/ijms23020925
R. Balo, A.G. Fernández, A. Chopdat, S. El Ayadi, A. Kato, R.J. Estévez, G.W.J. Fleet, J.C. Estévez	Stable d-xylose ditriflate in divergent syntheses of dihydroxy prolines, pyrrolidines, tetrahydrofuran-2-carboxylic acids, and cyclic β -amino acids	<i>Org. Biomol. Chem.</i>	20	9447-9459	10.1039/D2OB01255C
H. Meer, O. Gomonay, C. Schmitt, R. Ramos, L. Schnitzspan, F. Kronast, M.-A. Mawass, S. Valencia, E. Saitoh, J. Sinova, L. Baldrati, M. Kläui	Strain-induced shape anisotropy in antiferromagnetic structures	<i>Phys. Rev. B</i>	106	94430	10.1103/PhysRevB.106.094430

F. Suarez-Leston, M. Calvelo, G.F. Tolufashe, A. Muñoz, U. Veleiro, C. Porto, M. Bastos, A. Piñeiro, R. Garcia-Fandiño	SuPepMem: A database of innate immune system peptides and their cell membrane interactions	<i>Comput. Struct. Biotec.</i>	20	874-881	10.1016/j.csbj.2022.01.025
S. Gutiérrez-Tarriño, S. Rojas-Buzo, M.A. Ortuño, P. Oña-Burgos	Sustainable Synthesis of Silicon Precursors Coupled with Hydrogen Delivery Based on Circular Economy via Molecular Cobalt-Based Catalysts	<i>ACS Sustain. Chem. Eng.</i>	10	16624-16633	10.1021/acssuschemeng.2c04444
L. Tamarit, M. El Ouardi, E. Lence, I. Andreu, C. González-Bello, I. Vayá, M.A. Miranda	Switching from ultrafast electron transfer to proton transfer in excited drug–protein complexes upon biotransformation	<i>Chem. Sci.</i>	13	9644-9654	10.1039/D2SC03257K
E.A. Glitscher, J. Bergueiro, M. Calderón	Synthesis and anisotropic growth of glycerol-based thermoresponsive NIR plasmonic nanogels	<i>Eur. Polym. J.</i>	175	111342	10.1016/j.eurpolymj.2022.111342
M. Núñez-Martínez, S. Arias, J. Bergueiro, E. Quiñoá, R. Riguera, F. Freire	The Role of Polymer-AuNP Interaction in the Stimuli-Response Properties of PPA-AuNP Nanocomposites	<i>Macromol. Rapid. Commun.</i>	43	2100616	10.1002/marc.202100616
A. Anadón, E. Martín, S. Homkar, B. Meunier, M. Vergés, H. Damas, J. Alegre, C. Lefevre, F. Roulland, C. Dubs, M. Lindner, L. Pasquier, O. Copie, K. Dumesil, R. Ramos, D. Preziosi, S. Petit-Watelot, N. Vieart, J.-C. Rojas Sánchez	Thermal Spin-Current Generation in the Multifunctional Ferrimagnet Ga _{0.6} Fe _{1.4} O ₃	<i>Phys. Rev. Applied</i>	18	54087	10.1103/PhysRevApplied.18.054087
A. Sánchez-Fernández, J. Larsson, A.E. Leung, P. Holmqvist, O. Czakkel, T. Nylander, S. Ulvenlund, M. Wahlgren	Topological Dynamics of Micelles Formed by Geometrically Varied Surfactants	<i>Langmuir</i>	38	10075-10080	10.1021/acs.langmuir.2c00230

	M. Font, M. Gulías, J.L. Mascareñas	Transition-Metal-Catalyzed Annulations Involving the Activation of C(sp ³)-H Bonds	<i>Angew. Chem. Int. Ed.</i>	61	e202112848	10.1002/anie.202112848
	A. Blanco- González, A. Piñeiro, R. García- Fandiño	Unravelling hierarchical levels of structure in lipid membranes	<i>Comput. Struct. Biotech.</i>	20	2798-2806	10.1016/j.csbj.2022.05.04 2
	K. Kaiser, F. Schulz, J.F. Maillard, F. Hermann, I. Pozo, D. Peña, H.J. Cleaves II, A.S. Burton, G. Danger, C. Afonso, S. Sandford, L. Gross	Visualization and identification of single meteoritic organic molecules by atomic force microscopy	<i>Meteorit. Planet. Sci.</i>	57	644-656	10.1111/maps.13784

Annex V: Theses Defended

2022 – Theses Defended					
Area	Author	Title	Supervisor(s)	European/International Doctorate	Date
	Francisco Rey Tarrío	Photoreactivity and Novel Designs in Smart Chiral Materials	E. Quiñoá, F. Freire	No	December 12nd
	Juan José Tarrío Cordeiro	Poly(Diphenylacetylene)s: Design, Synthesis and Applications	E. Quiñoá, F. Freire	No	October 20th
	Joan Miguel Ávila	Transition Metal-Catalyzed Annulations in Biological Media	J.L. Mascareñas, M. Tomás	Yes	July 14th
	Borja Cendón Mariño	Assembly of azaheterocycles via transition metal-catalyzed annulations involving the activation of C-H bonds	J.L. Mascareñas, M. Gulías	Yes	June 10th
	Karen Vilela Góñez	FeCl ₃ como catalizador en reacciones de formación de enlaces C-C y C-O a partir de alquenos	F.J. Sardina, M. Rita Paleo	No	May 16th
	Iván Gallego Gómez	Diseño de nuevos materiales orgánicos híbridos para el reconocimiento proteico y el control de procesos celulares de transporte	J. Montenegro, J.R. Granja	No	May 13th
	Xandro Vidal Pereira	Azaheterocycles through Pd(II)-catalyzed formal cycloadditions involving C–H activation	J.L. Mascareñas, M. Gulías	Yes	April 22nd
	Alejandro Lamas Pérez	Novel supramolecular designs of cyclic peptides that contain γ - or δ -amino acids	J.R. Granja, M. Amorín	Yes	April 20th
	Alberto G. Fernández Fernández	Contribución o estudio de péptidos de beta 2,2 y beta 2,3 aminoácidos cicloalcanicos y azacicloalcanicos: síntesis, estudio estructural e propiedades	J.C. Estévez, R.J. Estévez	No	April 7th

	Enrica Soprano	Smart biomimetic nanosystems for stimuli-responsive drug delivery carriers	B. Pelaz, E. Polo	No	April 6th
	Berta Álvarez Pérez	Síntese e Estudo de Novos Hidrocarburos Policíclicos Aromáticos (HPAs) Funcionais con Aneis de Catro Membros	D. Pérez, D. Peña	No	April 5th
	Fábio Daniel Pedroso de Lima da Conceição	Novel Chromene and Imidazole Derivatives: Synthesis, Biological Evaluation and Computational Studies	M.F. Proença, C. González-Bello	Yes	March, 13rd
	Jesús Alfonso Castro Esteban	Design and synthesis of helicenes and graphene nanostructures	D. Pérez, D. Peña	Yes	February 18th
	Eva Rivera Chao	New synthetic routes towards 1,4-dieneylboronates via catalytic alkyne allyboration reactions	M. Fañanás	Yes	January 27th

Annex VI: Master Dissertations

Area	Author	Title	Supervisor(s)	Master Programme
	A.C.V.	Herramientas computacionales de vanguardia aplicadas a péptidos cíclicos en infección: hacia el desarrollo de nuevas terapias antimicrobianas.	R.García Fandiño, J.R. Granja Guillán	Chemistry at the interface with Biology and Materials Science
	J.B.S.	Química de arinos hacia el estarfeno mas largo	D. Peña Gil	Chemistry at the interface with Biology and Materials Science
	Y.F.C.	Péptidos penetrantes celulares basados en ciclobutanos con localización mitocondrial	J. Montenegro	Chemistry at the interface with Biology and Materials Science
	S.F.H.	Síntesis con control de tamaño de nanopartículas de UiO	P. Del Pino	Chemistry at the interface with Biology and Materials Science
	C.G.G.	Desarrollo de Nuevas Sondas Peptídicas Inteligentes para el Estudio de Interacciones Proteína-Proteína	M.E. Vázquez Sentís	Chemistry at the interface with Biology and Materials Science
	C.L.F.	Amplificación Quiral de Polímeros Supramoleculares Helicoidales	E. Quiñoá, F.M. Freire Iribarne	Chemistry at the interface with Biology and Materials Science
	P.S.G.	Optimización del reensamblaje de fragmentos de GFP mediante la metodología IC-Tagging	J.M. Martínez Costas	Chemistry at the interface with Biology and Materials Science
	E.G.M.	Click chemistry as a tool for nanoparticle-cell tracking	P. Del Pino	Chemistry at the interface with Biology and Materials Science
	D.S.G.	Diseño, síntesis y caracterización de un péptido b-hairpin para el estudio de la formación de híbridos POM-peptido	M. Vázquez López	Chemistry at the interface with Biology and Materials Science
	J.V.B.	Síntesis de un linker rígido para la optimización de fluorescencia en el marcaje de oligonucleótidos de DNA	M. Fañanás Mastral	Chemistry at the interface with Biology and Materials Science
	R.G.P.	Nuevas rutas sintéticas sostenibles a HAPs azulénicos heteroaromáticos	C.E. Saá Rodríguez, J.A. Varela Carrete	Organic Chemistry
	P.G.R.	Síntesis de productos altamente funcionalizados a partir de derivados de 4,4-dicloro-2-buteonatos de alquilo	M. Fañanás	Organic Chemistry
	P.L.C.	Diseño y síntesis de nuevos ligandos quirales para el desarrollo de reacciones de funcionalización C-H asimétricas	M. Gulías, J. L. Mascareñas	Organic Chemistry
	A.M.T.C.	Nuevos diseños de nanotubos peptídicos supramoleculares para estudios de self-sorting	J.R. Granja Guillán, M. Amorín	Organic Chemistry
	S.F.F.	Amidas Polihidroxi/Alquil anfífilicas. Síntesis y estudios IRI	J. C. Estévez Cabanas, R. J. Estévez Cabanas	Organic Chemistry
	M.V.M.F.	Hacia la síntesis de nuevos cicloarenos mediante reacciones de cicloadición de arinos	D. Peña, S. Castro	Organic Chemistry

A.A.L.	Poliacetilenos quirales disustituidos asimétricamente con luminógenos de emisión inducida por agregación	E. Quiñoá, F.M. Freire Iribarne	Organic Chemistry
S.D.A.	Nuevas reacciones de alquilidenociclopropanos promovidas por oro(III): Desde nuevos complejos de oro(III) a sus aplicaciones catalíticas	J. L. Mascareñas, F.J. López García	Organic Chemistry
A.C.P.	Impacto de las Modificaciones de la Secuencia Aminoacídica en la Eficacia Catalítica de las beta-Lactamasas de Clase D	C. González Bello	Organic Chemistry
L.G.A.	Estudio por ¹ H y ¹¹ B RMN de las interacciones entre ácidos borónicos tipo Wulff y 1,2-dioles: aplicaciones a sistemas de transporte de fármacos	E. Fernández Megía	Organic Chemistry
J.A.G.G.	Polímeros Helicoidales como Catalizadores Quirales Dinámicos en Síntesis Asimétrica	F.M. Freire Iribarne, E. Quiñoá	Organic Chemistry
A.L.C.	Hacia el antikekuleno: aproximación a la síntesis y reactividad de precursores de arino derivados de [N]fenilenos	M. D. Pérez Meirás, D. Peña Gil	Organic Chemistry
I.R.R.	Materiales porosos de tetrafenilmetano para procesos de adsorción de fullerenos	M. Torneiro, M. Lazzari	Organic Chemistry
B.E.S.	Reactividad de complejos de tipo iridio(III)-(k ² -NSi) con derivados de 2,2'-bipiridina	M. Vázquez López	Chemical Research and Industrial Chemistry
C.P.I.	Identificación de metalopéptidos catalíticos de lámina beta mediante cribado combinatorio SPOT	M. E. Vázquez Sentís, S.C. Learte	Chemical Research and Industrial Chemistry
R.O.L.	Desarrollo de modelos matemáticos de predicción de parámetros nutricionales en matrices alimentarias mediante tecnología hiperespectral VIS-NIR	J. C. Estévez Cabanas	Chemical Research and Industrial Chemistry
C.N.B.	Polímeros helicoidales supramoleculares.	F.M. Freire Iribarne, E. Quiñoá	Chemical Research and Industrial Chemistry
B.C.A.	Desarrollo de inhibidores Basados en sulfonopenicilinas para reducir el impacto las b Lactamasas en las superbacterias	C. González Bello	Chemical Research and Industrial Chemistry
D.G.S.	Caracterización, identificación y cuantificación de Nuevas Sustancias Psicoactivas (NPS) mediante espectroscopía RMN de bajo campo	E. Sotelo Pérez	Chemical Research and Industrial Chemistry
F.S.L.	Autoensamblaje jerárquico en sistemas basados en ciclodextrinas. Estudio mediante técnicas de Dinámica Molecular.	S.A. Vázquez Rodríguez, R. García Fandiño, A. Piñeiro	Theoretical Chemistry and Computer Modelling

Annex VII: Bachelor final projects

Area	Author	Title	Supervisor(s)	Bachelor Degree
	V.A.M.	Efecto de la distribución de defectos en la conductividad térmica de películas delgadas de SrTiO ₃ .	J.F. Rivadulla, R. Ramos	Chemistry
	S.M.R.	Estabilización de estructuras de G-cuadrupejos en el ARN genómico del SARS-CoV-2 con metalopéptidos artificiales.	M. Vázquez López	Chemistry
	M.B.L.	Nuevos catalizadores organometálicos para transformar nitrógeno molecular(N ₂) en amoníaco (NH ₃).	J.L. Mascareñas, F. López	Chemistry
	P.V.A.	Simulación computacional aplicada al ensamblaje supramolecular de nanomateriales.	R.García, J. Montenegro	Chemistry
	A.V.D.	Elaboración de plan de síntesis de la decorticasina	V.M. Sánchez, R. Estévez	Chemistry
	H.L.G.	Polímeros Helicoidales supra metalomoleculares	E.Quiñoá, F. Freire	Chemistry
	A.P.M	Interacción de complejos metálicos con ADN G-cuadrupejos	M. Vázquez López, G. Rama	Chemistry
	D.R.P.	Ensamblaje estereoselectivo de 1,4-dienos trifuncionales.	M. Fañanás	Chemistry
	D.D.L.C.R.	Polimerización supramolecular de OPEs quirales para la obtención de un agregado helicoidal	F. Freire, E. Quiñoá	Chemistry
	A.P.L.	Contribución a la química de sales de iminio de azúcares: síntesis estereoselectiva de iminociclohexitoles	R.J. Estévez Cabanas	Chemistry
	D.C.V.	Medidas experimentales de efecto Seebeck de spin en películas delgadas de Y ₃ Fe ₅ O ₁₂ .	J.F. Rivadulla, R. Ramos	Chemistry
	D.P.A.	Nuevos métodos fotoquímicos sostenibles	C.E. Saá Rodríguez, M.Nappi	Chemistry
	J.V.V.	Síntesis y estudio de tiofenos sustituidos	E. Guitián, D. Pérez	Chemistry
	A.R.S.	Síntesis y caracterización de péptidos conductores alfa-helicoidales	M.E. Vázquez Sentís, D. Bouzada	Chemistry
	D.V.C.	Estudio cinético de la reacción de descarboxilación de la N-X-alanina (X=Cl, Br)	J. Crugeiras, M.C. Ríos	Chemistry
	S.M.E.	Caracterización del diagrama de fases sólido-líquido de disolventes eutécticos utilizados en la industria farmacéutica	M.C. Ríos Rodríguez, A. M. Ríos Rodríguez	Chemistry
	R.T.L.	Química computacional como herramienta en la investigación contra el cáncer y las enfermedades infecciosas.	R. García Fandiño, J.R. Granja Guillán	Chemistry
	A.C.V	Generación y reactividad de cetocarbenos derivados del benzotiofeno: acceso a nuevos sistemas heterocíclicos de interés en ciencia de materiales	M.D. Pérez Meirás, A. Cobas	Chemistry
	D.P.P.	Nanopartículas híbridas de metales y polímeros helicoidales.	F.M Freire, E. Quiñoá,	Chemistry
	L.I.P.	Química Computacional como herramienta en la investigación de péptidos antimicrobianos que actúan a nivel de membrana celular	R. García Fandiño, M. Calvelo	Chemistry
	N.R.B.	Diseño y síntesis de tripticenos mediante reacciones de cicloadición de arinos.	D. Peña Gil, M. Vilas	Chemistry
	P.B.G.	Estudio del mecanismo de evasión inmune del SARS-CoV-2. Simulación computacional de la formación de complejos aberrantes con el marcador vírico ORF8.	C. González Bello	Chemistry
	R.V.O.	Síntesis de aminas y aminoácidos derivadas del ácido (-)-sikímico.	J.C. Estévez Cabanas, R.J. Estévez Cabanas	Chemistry

S.S.M.	Síntesis de precursores péptidos para el diseño de cápsulas supramoleculares.	M. Amorín, J.R. Granja	Chemistry
A.H.P.	Estudio fotofísico do 6-amino-2-ciano-1,3-benzotiazol como sonda fluorescente solvatocrómica	F. Rodríguez Prieto	Chemistry
F.B.C.	Síntesis sostenible de aza-heterociclos bioactivos mediante activación catalítica de enlaces C(SP ³)-H.	M. Gulías, J.L. Mascareñas	Chemistry
L.L.L.	HAPs dopados con átomos de B y N: síntesis y propiedades de isómeros B,N-Naftalénicos	C. Saá Rodríguez, J.A. Varela	Chemistry
J.P.D.	Resolución de la ecuación de Schorödinger para la partícula en un cilindro	A. Fernández Ramos	Chemistry
Y.M.C.	Vesículas dendríticas de tipo complejo poliiónico: desarrollo de biorreactores enzimáticos	E. Fernández Megía	Chemistry & Biology
D.R.P.	Péptidos híbridos para la transfección de ácidos nucleicos (Parte B)	J. Montenegro,	Chemistry & Biology
A.V.G.	Expresión de enzimas celulares para la creación de redes metabólicas artificiales mediante su combinación con catalizadores metálicos. Parte B.	J.M. Martínez Costas	Chemistry & Biology
M.B.B.	Desarrollo de Nuevos Antibióticos Antipseudomónicos Mediante la Inhibición Irreversible del Enzima EPSP Sintasa.	C. González Bello	Chemistry & Biology
M.C.D.D.	Alquilamidas derivadas de ácidos 2-aminociclohexanocarboxílicos. Síntesis y estudio de sus propiedades gelificantes.	J.C. Estévez Cabanas, R.J. Estévez Cabanas	Chemistry & Biology
Y.M.C.	Química Verde: Síntesis acelerada de dendrímeros a gran escala.	E. Fernández Megía	Chemistry & Biology
A.M.B.	Micelas poliméricas para el transporte de fármacos antitumorales	E. Fernández Megía	Chemistry & Biology
D.R.P.	Péptidos híbridos para la transfección de ácidos nucleicos (parte A)	J. Montenegro,	Chemistry & Biology
M.E.J.R.	Orientación selectiva de muNS-NS a células cancerosas mediante la interacción con receptores específicos de integrina	J.M. Martínez Costas, N. Barreiro	Chemistry & Biology
M.E.J.R.	Nanopartículas híbridas de metales y polímeros helicoidales. Síntesis del cloruro cíclico-(RGDFK) para la conjugación de HaloTag.	M. Fañanás	Chemistry & Biology
M.B.B.	Análisis comparativo de genomas de cinco cepas de Pseudomonas spp con potencial patogénico para peces.	J.A. López Romalde, C. González-Bello	Chemistry & Biology
E.P.L.	Materiales porosos basados en tetrafenilmetano para la captura de contaminantes orgánicos	M. Torneiro, M. Lazzari	Chemistry & Biology
A.V.G.	Construcción de redes metabólicas artificiales mediante la combinación de catálisis enzimática y metálica. Parte A.	J.L. Mascareñas, M. Tomás	Chemistry & Biology
I.P.G.	Determinación de la estabilidad de membranas lipídicas de diferente composición a través de simulaciones de dinámica molecular	A. Piñeiro, R. García-Fandiño	Physics & Chemistry
I.P.G.	Química computacional como herramienta en la investigación contra el cáncer y la infección	R. García Fandiño,	Physics & Chemistry
C.F.G.	HAPs dopados en células solares: Rutas catalíticas hacia sistemas ulazínicos	C.E. Saá, J.A. Varela Carrete	Physics & Chemistry
J.C.S.	Medidas de conductividad térmica en materiales bidimensionales	F. Rivadulla, R. Ramos	Physics & Chemistry

A.L.T.	Aplicación de la metodología IC-Tagging en la expresión de enzimas de interés industrial.	J.M. Martínez Costas, N. Barreiro	Biotechnology
P.M.C.	Dendrímeros funcionalizados con ácidos borónicos: Síntesis y evaluación como agentes de transporte de material genético	E. Fernández Megía	Biotechnology
A.M.B.	Optimización de la expresión de proteínas en <i>Pichia pastoris</i> (<i>Komagataella phaffii</i>)	C. Díaz Jullien, J. Martínez-Costas	Biotechnology
D.A.L.	Explorando nuevas aplicaciones biotecnológicas del sistema IC-Tagging	J.M. Martínez Costas, N. Barreiro	Biotechnology
C.G.Z.	Protacs: Una aproximación innovadora para el desarrollo de nuevos fármacos	E. Sotelo Pérez	Pharmacy
L.M.G.	Hidrogeles peptídicos sensibles al pH	J.Montenegro	Pharmacy

ANNEX VIII: Invited Lectures given by CiQUS Researchers during 2022

Area	Author(s)	Title	Type	Conference	Place
	J.L. Mascareñas	<i>Exporting transition metal catalysis to celular habitats</i>	Plenary Lecture	55th Bürgenstock Conference 2022, SCS Conference on Stereochemistry	Switzerland
	J. L. Mascareñas	<i>Biocompatible Transformations Involving Organometallic Catalysis</i>	Plenary Lecture	Gordon Research Conference: Metals in medicine	USA
	C. González-Bello	<i>Facing the Superbug Challenge with Innovative Approaches</i>	Plenary Lecture	XXVIII Reunión Bienal del Grupo Especializado de Química Orgánica	Spain
	C. González-Bello	<i>La Batalla Contra las Superbacterias – Retos y Nuevas Estrategias Terapéuticas</i>	Plenary Lecture	Real Academia Nacional de Farmacia	Spain
	D. Pérez	<i>Aryne Chemistry in the Graphene Era</i>	Plenary Lecture	Thieme WebCheminar, presented by Synthesis	Online
	D. Pérez	<i>An aryne-based 'molecular Lego': application to the synthesis of non-conventional aromatics and π-functional materials</i>	Plenary Lecture	XXVI Encontro Galego-Portugués de Química, Santiago de Compostela	Spain
	B. Pelaz	<i>Smart Materials for Biological Applications</i>	Plenary Lecture	XVIII JIQ, RSEQ	Spain
	J.L. Mascareñas	<i>Biocompatible Transformations Involving Organometallic Catalysis</i>	Keynote Lecture	Girona Seminar 2022	Spain
	J.L. Mascareñas	<i>Translating transition metal catalysis to biological environments</i>	Keynote Lecture	INAM annual symposium	Spain
	C. González-Bello	<i>Innovative Strategies to Unlock Bacterial Resistance to Antibiotics</i>	Keynote Lecture	XX National Meeting of the Spanish Society of Medicinal Chemistry (SEQT), From Early Discovery to Translational Medicinal Chemistry	Spain
	C. González-Bello	<i>Antibiotic Adjuvants – A Booming Strategy to Unlock Bacterial Resistance</i>	Keynote Lecture	<i>Drug Development: From Design to Customer (DDDC 2022)</i>	Armenia
	B. Pelaz	<i>Efficient Colloidal Nanosystems for Bioapplications. Nanomaterials applied to life sciences</i>	Keynote Lecture	<i>NALS Conference</i>	Spain
	M.C. Gimenez Lopez	<i>A New Porous Supramolecular Liquid for Energy-Storage Applications</i>	Keynote Lecture	<i>5th Annual UK Porous Materials Conference (UKPorMat 2022). Royal Society</i>	UK
	M. Gulías	<i>Transition metal catalyzed C-H functionalization for the synthesis of heterocycles</i>	Invited lecture	<i>ACS Spring 2022</i>	USA
	J.L. Mascareñas	<i>Organometallic catalysis in cellular habitats</i>	Invited Lecture	<i>The power of chemical synthesis and characterization. Symposium in Honor of Prof. Víctor S. Martín</i>	Spain
	J.L. Mascareñas	<i>Merging metal catalysis with Chemical Biology</i>	Invited Lecture	<i>iMed.Ulissboa-CiQUS Seminar</i>	Portugal
	J.L. Mascareñas	<i>Exporting transition metal catalysis to celular habitats</i>	Invited Lecture	<i>Center for Medicinal Chemistry (Grand-Opening Symposium), University of Copenhagen</i>	Denmark

	M. Tomás-Gamasa, J.L. Mascareñas	<i>Conducting chemistry in living cells</i>	Invited lecture	V Annual Meeting CINBIO	Spain
	F. López	<i>Desarrollo y aplicaciones de nuevos métodos basados en catalizadores metálicos</i>	Invited Lecture	<i>Conferencia Invitada en III Ciclo de Conferencias Punto de Encuentro</i>	Spain
	C. González-Bello	<i>Exploring New Bacterial Niches for Facing the Silent Pandemic</i>	Invited Lecture	<i>XIV Spanish Drug Discovery Network Meeting (SDDN)</i>	Spain
	D. Peña	<i>Surface science to address long-standing challenges in organic chemistry</i>	Invited Lecture	<i>1st Symposium CiQUS Chemistry at the Frontier</i>	Spain
	D. Peña	<i>Bottom-up approach to Carbon Nanomaterials: from Solution chemistry to On-surface synthesis</i>	Invited Lecture	<i>ChemOnTubes 2022-8th International Meeting on Chemistry of Carbon Nanomaterials, San Sebastian</i>	Spain
	D. Peña	<i>Combining Organic Synthesis with Surface Science: from Nanographenes to Single-Molecule Reactions</i>	Invited Lecture	<i>European School on Molecular Nanoscience</i>	Spain
	D. Peña	<i>Building nanographenes by combining organic synthesis and surface science</i>	Invited Lecture	<i>EuChemS Chemistry Congress</i>	Portugal
	D. Peña	<i>Combinando la Química Orgánica con la Ciencia de Superficies: del bencino al grafeno y más allá</i>	Invited Lecture	<i>XXIV Semana Científica Antonio González, La Laguna</i>	Spain
	D. Peña	<i>Combining Organic Chemistry with Surface Science: from Benzene to Graphene and Single-Molecule Reactions</i>	Invited Lecture	<i>III Jornadas del Doctorado en Química Avanzada</i>	Spain
	D. Ferro-Costas, A. Fernández Ramos	<i>New computational tools for chemical kinetics: the Cathedral package</i>	Invited Lecture	<i>Electronic Structure: Principles and Applications</i>	Spain
	E. Polo	<i>Bioactive Colloidal Nanosystems. Invited speaker. Advanced materials and devices for nanomedicine</i>	Invited Lecture	<i>AM4MED Conference</i>	Online
	B. Pelaz	<i>Advanced Bioactive Materials</i>	Invited Lecture	<i>1st Symposium Chemistry at the Frontier</i>	Spain
	B. Pelaz	<i>Active Nanomaterials for Bioapplications</i>	Invited Lecture	<i>XIII Young Investigator Workshop (TIW 2021/2022)-EuChemS Division of Organic Chemistry</i>	Portugal
	E. Fernández-Megía	<i>Polymeric Nanostructures for Biomedical Applications</i>	Invited Lecture	<i>VIII ENCUESTRO SOBRE DENDRÍMEROS</i>	Spain
	M. Fañanás Mastral	<i>Catalytic Approaches for Stereoselective Hydrocarbon Difunctionalization</i>	Invited Lecture	<i>I Simposio Chemistry at The Frontier</i>	Spain
	M.C. Giménez López	<i>Confined Electrocatalyst for Sustainable Energy Conversion</i>	Invited Lecture	<i>Materials for Sustainable Development Conference (MAT-SUS), Symposium #SusEnergy - Sustainable materials for energy storage and conversion (nanoGe Fall Meeting 2022).</i>	Spain
	M.C. Giménez López	<i>Advanced Energy Materials for Sustainable Future</i>	Invited Lecture	<i>8th EuChemS Chemistry Congress (ECC8)</i>	Portugal

	M.A. Ortuño,	<i>Mechanistic understanding of biomass conversion using metal-organic framework catalysts</i>	Invited Lecture	ACS Spring 2022 – Bonding Through Chemistry (online)	USA
	C. Saá	<i>New Oportunities in Catalytic Ruthenium Carbene/Alkyne Metathesis (CAM)</i>	Invited Lecture	Spanish-Italian Symposium on Organic Chemistry	Spain
	M. Eugenio Vázquez	<i>Application of SPOT Combinatorial Libraries for the Identification of Catalytic Metallopeptides</i>	Invited Lecture	XII Reunión Científica de Bioinorgánica, Madrid,	Spain
	M. Lazzari, S. Balboa	<i>Is the presence of microplastics in the water cycle a real environmental concern?</i>	Invited Lecture	12th Micropol & Ecohazard Conference	Spain
	D. Ferro-Costas, A. Fernández Ramos	<i>New computational tools for chemical kinetics: the Cathedral package</i>	Invited Lecture	Electronic Structure: Principles and Applications	Spain
	J.R. Granja	<i>Supramolecular Chemistry with Cyclic Peptides</i>	Invited Lecture	XXXVIII Reunión Bienal de la Sociedad Española de Química	Spain
	J.R. Granja	<i>Cyclic Peptide Nanotubes: a versatile supramolecular platform</i>	Invited Lecture	36th European Peptide Symposium and 12th International Peptide Symposium	Spain
	J. Montenegro	<i>Fibrillar Synthetic Systems Towards Simple Cytoskeleton Mimics</i>	Invited Lecture	Workshop LifeHUB.CSIC	Spain
	J. Montenegro	<i>New synthetic materials for delivering biomolecules to cells with therapeutic applications</i>	Invited Lecture	New synthetic materials for delivering biomolecules to cells with therapeutic applications	Cuba
	J. Montenegro	<i>The exo-helical symmetry of the α-Helix</i>	Invited Lecture	Alpabach Workshop on Coiled Coils 2022	Austria
	J. Bergueiro	<i>UNREVEALING THE α-HELIX EXO-TOPOLOGIES</i>	Invited Lecture	XXXVIII Reunión Bienal de la Sociedad Española de Química	Spain
	I. Insua	<i>Synthetic peptide designs for biomimicry: from cellular membranes to cytoskeletons</i>	Invited Lecture	IUBMB Advanced School and Workshop	Cuba
	I. Insua	<i>Hierarchical peptide self-assembly from 1D to 2D: Geometrical control of peptide interactions towards supramolecular nanosheets</i>	Invited Lecture	GRC	USA

ANNEX IX: Research stays of CiQUS members during 2022

Area	Researcher	Position	Hosting Institution	Country	Funding	Start	End
	Adrián Martínez Castrillón	PhD Candidate	Instituto Catalán de Nanociencia y Nanotecnología (ICN2)	Spain	AEI	17/7/22	30/7/22
	Alejandro Rey López	PhD Candidate	University of Manchester	UK	Xunta de Galicia	1/7/22	30/9/22
	Alfonso Bayon Fernandez	PhD Candidate	Emory University	USA	Xunta de Galicia	1/4/22	30/6/22
	Andrés Manuel Álvarez Constantino	PhD Candidate	University of Wisconsin-Madison	USA	Xunta de Galicia	1/8/22	31/10/22
	Bruno Delgado González	PhD Candidate	Eindhoven University of Technology (TU/e)	The Netherlands	Xunta de Galicia	18/7/22	18/10/22
	Carla Lorenzo Fojón	PhD Candidate	Eindhoven University of Technology (TU/e)	The Netherlands	CiQUS	9/9/22	29/10/22
	Daniel Marcos Atanes	PhD Candidate	University of California Berkeley	USA	FPU, Fulbright España	15/8/22	14/2/23
	Jose María Martínez Parra	PhD Candidate	Universidad Libre de Berín (FU)	Germany	Xunta de Galicia	1/4/22	30/6/22
	Juan Carlos Estévez	CiQUS PI	Universidad de Zaragoza	Spain	CiQUS	7/6/22	10/6/22
	Lara Villarino Palmaz	Postdoctoral Researcher	University of Groningen	The Netherlands	CiQUS	4/7/22	18/7/22
	Lucía Méndez Gómez	PhD Candidate	University of Glasgow (UoG)	UK	-	3/11/22	18/11/22
	Manuel Ceballos	PhD Candidate	University of Cambridge, Department of Chemical Engineering and Biotechnology, Adsorption & Advanced Materials Group	UK	H2020, ITN	5/4/22	24/6/22
	Manuela Cedrún	PhD Candidate	University of Cambridge, Department of Chemical Engineering and Biotechnology, Adsorption & Advanced Materials Group	UK	FPU	2/5/22	30/7/22

CiQUS Annual Scientific Report 2022

	Marcos Vilela Picos	PhD Candidate	Northwestern University	USA	FPU	20/8/22	20/11/22
	María Lago Silva	PhD Candidate	University of Southampton	UK	Xunta de Galicia	11/4/22	10/7/22
	Maria Victoria López Corbalán	PhD Candidate	Srockholm University	Sweden	Xunta de Galicia	1/8/22	31/10/22
	Paula Sánchez Gascón	PhD Candidate	National Institute of Biological Standards (Medinices and Healthcare Regulatory Agency of the UK	UK	CiQUS & AECC	19/9/22	2/12/22
	Pol Martínez Balart	PhD Candidate	RWTH Aachen University	Germany	CiQUS	20/8/22	9/10/22
	Ricardo Rodiño Balboa	PhD Candidate	University of Columbia	USA	FPU	1/8/22	31/10/22
	Saleta Fernández Castro	PhD Candidate	Universidad de Oxford	UK	Xunta de Galicia	13/6/22	13/9/22
	Sara Illodo Brea	PhD Candidate	Pusan National University, Busan	South Korea	Xunta de Galicia & Pusan National University	1/3/22	31/8/22
	Victor Fariña Torres	PhD Candidate	ICMol, University of Valencia	Spain	CiQUS	11/7/22	22/7/22

ANNEX X: Patents in 2022

Area	Title	Country / Region	Publication Number	Date	Inventors	Owner(s)
	Ruthenium complexes for treating cancer which comprises cancer stem cells	EU	EP 3539971B1	20/07/22	J. Rodríguez, J.L. Mascareñas , J. Rodríguez-Couceiro, J. Mosquera, M.E. Vázquez , B. Sainz	USC UAM
		US	US 11471467	18/10/22		
	Applications of the protein muns and the derivates thereof	EU	EP 2535348B1	04/05/2022	A. Brandariz, R. Menaya, F.J. Benavente , J.M. Martínez-Costas	USC
	Magnetic nanoparticles for use in the treatment of tumors	EU	EP3790588B1	13/04/2022	M. Barthel, M. Cssani, M. Fignini, J. Granja , T. Pellegrino, A. Quarta	USC, CNR, Universita degli Studi di Genova, Fondazione IRCCS Istituto Nazionale dei Tumori, Fondazione Istituto Italiano di Tecnologia
	Topic: delivery of nucleic acids into a cell (within the framework of ENDOSCAPE project)	EU	EP 22193416.9	Applied 2022	R. Postel; H. Fuchs; G. Nagel; A. Weng; M. K. Tröger; J. F. Correa Chinae; E. P. Fernández Megía ; R. López Blanco	USC, Sapreme Technologies, Charité, Universitätsmedizin Berlin, Freie Universität Berlin
	Topic: delivery of nucleic acids into a cell (within the framework of ENDOSCAPE project)	EU	EP 22193399.7	Applied 2022	R. Postel; H. Fuchs; G. Nagel; A. Weng; M. K. Tröger; J. F. Correa Chinae; E. P. Fernández Megía ; R. López Blanco	USC, Sapreme Technologies, Charité, Universitätsmedizin Berlin, Freie Universität Berlin
	Topic: intracelullar delivery	EU	EP22382596	Applied 2022	J. Montenegro	USC
	Topic: gas monitorization	ES	P202230249	Applied 2022	M.C. Giménez López , V. Leborán, C. Herrerros, M. Guillen	USC

ANNEX XI: 2022 CiQUS Lecture's Programme

Area	Lecturer	Topic	Institution	Country	Date
	Prof. Johannes F. Teichert	Homoaromatic Hydrocarbons as structurally new photoswitches	Technische Universität Chemnitz · Fakultät für Naturwissenschaften, Institut für Chemie	Germany	01/12/22
	Dr. Emilio Cocinero	Unravelling the structures of biomolecules by high-resolution spectroscopies	Biofisika Institute (CSIC – UPV/EHU) Microwave Region Spectroscopy Group	Spain	15/11/22
	Prof. Michael Haley	The Interplay Between Antiaromaticity and Diradical Character in Diarenoindacenes and Diindenoarenes	Richard M. & Patricia H. Noyes Professor Department of Chemistry & Biochemistry University of Oregon	USA	17/10/22
	Prof. Edvinas Orentas	Exploitation of The Hydrogen Bond: Dynamic Tubular Supramolecular Systems	Department of Organic Chemistry Vilnius University	Lithuania	26/09/22
	Prof. Joost Reek	Supramolecular approaches for gene delivery and catalysis in living cells	Van 't Hoff Institute for Molecular Sciences University of Amsterdam	The Netherlands	23/09/22
	Dr. Josep Cornella	Bismuth redox catalysis	Max-Planck-Institut für Kohlenforschung	Germany	23/09/22
	Prof. Young Min Song	Colorimetric sensing platform for Bioparticles	School of Electrical Engineering and Computer Science at the GIST Wangju	Korea	18/07/22
	Prof. Olga García Mancheño	An Enlightening Journey: from Photocatalyst's Design to Late-Stage Functionalization	Department of organic chemistry at the University of Münster (WWU)	Germany	14/07/22
	Prof. David Amabilino	Dynamic supramolecular gels	Intitut de Ciència de Materials de Barcelona CSIC	Spain	12/07/22
	Prof. Vicent P. Conticello	Self-assembly of Peptide-based Nanomaterials: Structural Insights into the Self-Assembly of Helical Peptide Filaments and Tubes	Department of Chemistry Emory University of Atlanta	USA	06/07/22
	Jun. Prof. Dr. Alicia Casitas	An organometallic perspective to first-row transition metal catalysis: searching for unconventional reactivity patterns	Philipps-Universität Marburg	Germany	10/06/22
	Prof. Hai-Lung Dai	Molecular Processes and Dynamics at Colloidal Surfaces and Biological Membranes	Department of Chemistry Temple University, Philadelphia	USA	19/07/22
	Prof. Eric Borguet	Single Molecule Switching and Sensing	Department of Chemistry Temple University, Philadelphia	USA	19/07/22
	Prof. Daniel Kalafatović	Design of short peptides and peptide assemblies aided by machine learning and genetic algorithms	Department of Biotechnology, University of Rijeka	Croatia	12/05/22
	Dr. Mónica Giménez Marqués	Biohybrid MOFs: boosting the delivery of active bioentities	ICMOL University of Valencia	Spain	11/05/22

Prof. Paolo Samorì	Boosting electrical properties of 2D materials with molecules	Distinguished Professor at the Université de Strasbourg Director of the Institut de Science et d'Ingénierie Supramoléculaires (ISIS) Director of the Nanochemistry Laboratory	France	06/05/22
Prof. M.A. Fernández Ibáñez	S,O-Ligand-promoted Pd-catalyzed C-H Functionalization Reactions	Van 't Hoff Institute for Molecular Sciences University of Amsterdam	The Netherlands	22/04/22
Prof. Sébastien Perrier	Cyclic peptide / polymer conjugates for therapeutic and materials applications	University of Warwick	UK	21/04/22
Dr. Loretta L. del Mercato	Multifunctional Stimuli-Responsive Systems for Sensing and Therapy	Institute of Nanotechnology of CNR	Italy	06/04/22
Prof. Esther Lete	Transition-metal catalyzed C-C bond forming reactions. From cross-coupling to C-H activation	Department of Organic and Inorganic Chemistry Euskal Herriko Unibertsitatea	Spain	04/04/22
Dr. Begoña Abad Mayor	Thermal transport and mechanical properties of complex materials by non-contact laser-based techniques	Nanophononics Lab University of Basel	Switzerland	21/02/22
Prof. Manuel Souto	Electroactive Molecular Materials for Electronics: From Donor-Acceptor Dyads to Redox-Active Porous Frameworks	CICECO Aveiro Institute of Materials	Portugal	17/02/22
Prof. Jesús Jiménez Barbero	Breaking the limits in understanding glycan recognition by NMR	Ikerbasque Research Professor - Scientific Director CIC bioGUNE	Spain	08/02/22
Dr. André Pérez Potti	From nanoparticle-shaped antibody repertoires to COVID-19 T cell responses	Karolinska Institutet	Sweden	26/01/22