ICIQ

Institut Català
d'Investigació Química

Annual Report 2023

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KTT

Communication & Outreach

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Introduction

Prof. Emilio J. Palomares Gil
Director of the Institute of Chemical Research of Catalonia

Dear ICIQ Community,

2023 has been a very fruitful year for our institution, which has continued to thrive thanks to the dedication of our team and the collaboration with the international scientific community.

ICIQ continues to consolidate itself as a reference in the generation of knowledge and innovation, with a total of 171 scientific publications and 81 ongoing research projects. Our initiatives, from the design of new molecules to the creation of pioneering technologies in different areas, continue to set new paradigms and drive the scientific progress significantly.

This year 27 theses have been successfully defended, reflecting one of our fundamental pillars: training the future generations of scientists and contibuting to the development of research career.

This year has also established a new strategy and new directions for the Knowledge and Technology Transfer, and Industrial Projects Department (KTT), which has multiplied the collaborations with the industry offering value-added services and solutions.

We are strongly committed to the society and for this reason, we consider that we have a fundamental responsibility towards scientific education. We have organised outreach activities that have brought together more than 4,000 people, mainly school and high-school students, fostering their interest in science.

In this report, we not only celebrate the successes and contributions of the past, but also outline our strategy to face the challenges of the future. By 2024, we are committed to continue facing scientific challenges to strengthen our influence in the global frontier chemistry research. With an eye to the future, feet on the ground and eyes on the world, we seek to expand our international collaboration, promote diversity and inclusiveness, and make a significant contribution to the scientific advances that will define the coming decades.

Institute of Chemical Research of Catalonia (ICIQ-CERCA) is a public foundation dedicated to chemical research, addressing global challenges such as climate change or energy supply. Recognised with two Severo Ochoa accreditations of excellence since 2014, the centre has 250 researchers distributed in 18 research groups dedicated to sustainable catalysis, renewable energies and molecular medicine, driving excellence through computational and experimental research. ICIQ researchers have obtained a total of 25 projects funded by the European Research Council (ERC) and eight of them are ICREA professors (Catalan Institution for Advanced Research). Located in Tarragona, ICIQ collaborates closely with industry to improve its competitiveness, fostering the development of innovative applications and the training of high-level scientists. As a CERCA centre and member of BIST, ICIQ is committed to sustainable and equitable development, open science and the social impact of research. More information at www.iciq.org

2023 in numbers

171 Total **publications**

2.98
ESI Chemistry Normalised Impact

67%
International Collaborations

2
Highly cited papers

16,5M € **Budget** 2023

- **Catalan Government** 7,878,059.00 €
- **Spanish Government** 3,399,637.42 €
- **European Union** 4,065,047.44 €
- **Others** 1,180,944.93 €

314 **People** staff (FTE)

- **Men** 190
- **Women** 124

250 Research

31 Scientific Core Facilities

64 Management

+6,800 **Training** hours

27
Doctoral Theses Defended

44
Seminars of BASF-ICIQ Seminar Programme

14
Conferences and Symposiums

SHARP
Severo Ochoa PhD Training Programme

1.9M € Revenues from **projects with industry**

18
Active Patents
+3 opportunities

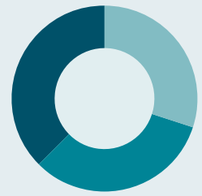
64
Research Projects with industry

3
Technological Development Units

3
Spin-offs

35 **Outreach** activities

4,660
Individuals



- **Adults** 1.741
- **High School Students** 1.518
- **Children** 1.401

Media impact, Social Media and Web

25,383 Followers in Social Media

- 11,269
- 8,230
- 2,871
- 1,463
- 1,550

810
Media Impact

140,946
Website visitors

Research

ICIQ Research

At ICIQ, we conduct research to advance scientific knowledge and promote innovation.

Our research is organized into three main areas that cover a wide variety of research lines. These areas are carefully designed to address global challenges. By aligning our research efforts with these critical areas, we aim to make meaningful contributions that drive positive changes and foster a sustainable future.

Sustainable catalysis

Renewable energies

Molecular medicine

Research Groups

At ICIQ, there are 18 Group Leaders who stand out for meeting the highest standards in conducting their research. These researchers enjoy full autonomy and independence to pursue their activities within the research lines of the Institute, and they receive specialised support from scientific and technical staff to carry out their research.

In addition, the Group Leaders are authors of articles, book chapters, and covers of specialised scientific journals. They have also contributed to the development of patents and innovative technologies.

Prof. Pau Ballester

ICREA Professor

Prof. Pau Ballester group works in the areas of organic chemistry and physical organic chemistry. Their current research focuses on the design, synthesis, study, and characterisation of functional molecular aggregates. The group applies molecular self-assembly processes as a methodology for constructing large and functional interconnected structures. The group also applies the developed receptors as carriers for anions and amino acids across liposomal membranes.

Their second area of interest is the design and application of molecular containers, cages and capsules. These are molecular or supramolecular architectures with an internal cavity large enough to include or encapsulate other molecules. The cavities of the molecular containers are exploited for the stabilization of reactive molecules or in the mediation of chemical reactions among others.

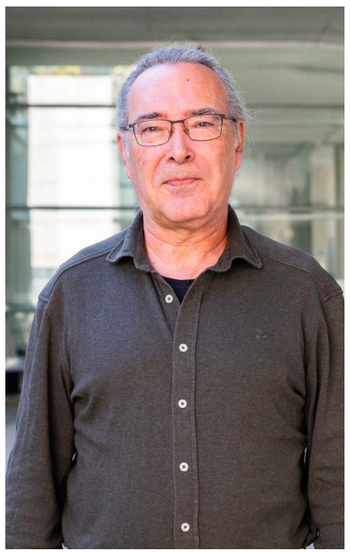
Highlighted publication

Influence of the solvent in the self-assembly and binding properties of [1 + 1] tetra-imine bis-calix[4]pyrrole cages

Mirabella, C. F. M.; Aragay, G.; Ballester, P.

Chem. Sci. **2023**, 4, 186-195

Prof. Carles Bo



Prof. Bo group develops and applies computational methods to address fundamental problems in chemical reactivity and catalysis. The group holds long experience in elucidating mechanisms of transition-metal catalysed homogeneous reactions, in organo-catalytic reactions, CO_2 fixation processes, and in polyoxometalates chemistry. The group uses methods based on density functional theory (DFT), molecular dynamics simulations, and their own developed methods as basic tools to provide new understanding of reaction mechanisms, predict properties of complex systems in solution, and advanced molecular design. The group is actively contributing to open-science through the development of the ioChem-BD platform.

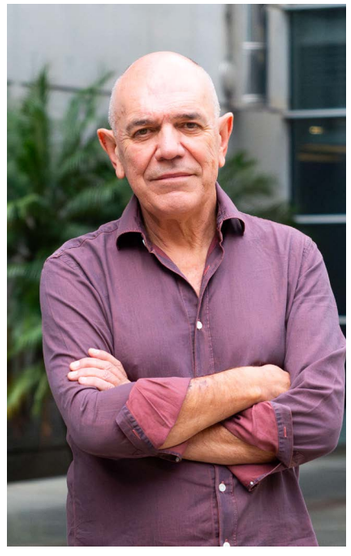
Highlighted publication

Multi-Time-Scale Simulation of Complex Reactive Mixtures: How Do Polyoxometalates Form?

Petrus, E.; Garay-Ruiz, D.; Reiher, M.; Bo, C.

J. Am. Chem. Soc. 2023, **145**, 18920–18930

Prof. Antonio M. Echavarren



ERC Advanced Grant

The group of Prof. Echavarren focuses on the design of catalytic systems and the invention of a new organic synthesis methodology. The most important scientific contributions of the group have been in the field of homogenous gold catalysis, where they have established the mechanistic foundations that have guided the discovery of new transformations and have introduced gold catalysts to the scientific community. They have also demonstrated the usefulness of new synthetic methods in the context of the synthesis of complex molecules, both biologically relevant natural products and molecules of interest in materials science.

Highlighted publication

Enantioselective Catalysis with Pyrrolidinyl Gold(I) Complexes: DFT and NEST Analysis of the Chiral Binding Pocket

Zuccarello, G.; Nannini, L. J.; Arroyo-Bondía, A.; Fincias, N.; Arranz, I.; Pérez-Jimeno, A. H.; Peeters, M.; Martín-Torres, I.; Sadurní, A.; García-Vázquez, V.; Wang, Y.; Kirillova, S. M.; Montesinos-Magraner, M.; Caniparoli, U.; Núñez, G. D.; Maseras, F.; Escofet, I.; Echavarren, A. M.

JACS Au 2023, **3**, 1742–1754

Awards

Premi Rei Jaume I d'Investigació Bàsica 2023

Pedler Award 2023 by the Royal Society of Chemistry (RSC)

Prof. José Ramón Galán-Mascarós

ICREA Professor

The people of Prof. Galán-Mascarós is dedicated to the development of low-cost materials for its implementation in new strategies for the transformation of renewable energies into chemicals and solar fuels. Through the design and selection of materials, they face very different challenges, from intelligent materials for thermal/optical devices to nanostructured electrocatalysts designed to participate in competitive systems on an industrial scale.

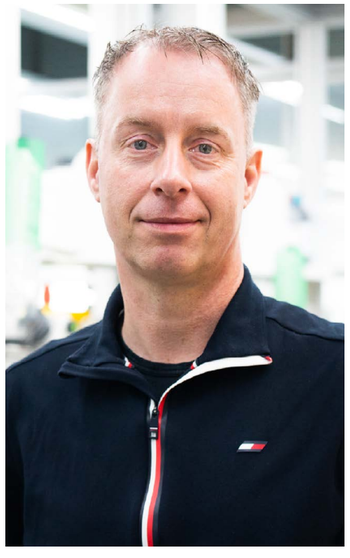
Highlighted publication

Molecular memory near room temperature in an iron polyanionic complex

Moneo-Corcuera, A.; Nieto-Castro, D.; Cirera, J.; Gómez, V.; Sanjosé-Orduna, J.; Casadevall, C.; Molnár, G.; Bousseksou, A.; Parella, T.; Martínez-Agudo, J.M.; Lloret-Fillol, J.; Pérez-Temprano, M.H.; Ruiz, E.; Galán-Mascarós, J.R.

Chem. 2023, **9**, 377-393

Prof. Arjan W. Kleij



ICREA Professor

The group of Prof. Kleij focuses on the conversion of small molecules, such as CO_2, into heterocyclic compounds useful towards the synthesis of fine chemical and pharmaceutical products. The decarboxylative conversion of these heterocycles and related structures is used to discover new stereo- and enantioselective transformations to prepare modular types of pharmacores or advanced precursors. In addition, biomass compounds such as terpenes are used to design novel types of polyesters, polycarbonates and polyethers with mechanical, thermal and optical properties of potential interest to industry.

Highlighted publication

Bicyclic Guanidine Promoted Mechanistically Divergent Depolymerization and Recycling of a Biobased Polycarbonate

Lamparelli, D.H.; Villar-Yanez, A.; Dittrich, L.; Rintjema, J.; Bravo, F.; Bo, C.; Kleij, A.W.

Angew. Chem. Int. Ed. 2023, **62**, e202314659

Awards

European Sustainable Chemistry Award 2023 by European Chemical Society (EUChemS)

Award for Scientific Excellence 2023 by the Catalan Chemistry Society (SCQ)

Prof. Julio Lloret-Fillol

ICREA Professor

Professor Lloret-Fillol's group is focused on developing catalysts for artificial photosynthesis and exploring synthetic methodologies to integrate this emerging field with organic chemistry. In this context, the team has created biomimetic catalysts using abundant metals for the reduction of water and CO_2 into fuels. Furthermore, the group is expanding its research to include the exploration of robust catalysts based on reticular materials or solution combustion for industrial applications and developing tools to automate the discovery of catalysts, streamlining the research process in the field of catalysis.

Highlighted publication

Decoding the CO_2 Reduction Mechanism of a Highly Active Organometallic Manganese Electrocatalyst: Direct Observation of a Hydride Intermediate and Its Implications

Fernández, S.; Franco, F.; Martínez Belmonte, M.; Friães, S.; Royo, B.; Luis, J. M.; Lloret-Fillol, J.

ACS. Catal. 2023 **13** (15), 10375-10385

Awards

GEQO Award for Research Excellence 2023 for the Specialised Group of Organometallic Chemistry (GEQO) of the Spanish Royal Society of Chemistry (RSEQ)

Prof. Antoni Llobet

The group of Prof. Llobet develops research in the field of redox catalysis using transition metal complexes for the oxidation and reduction of organic and inorganic substrates of technological interest. Its general objective is to understand the various factors that affect the efficiency and selectivity of the catalysts, paying special attention to the electronic structure and the spatial arrangement of the transition metals. The group focuses specifically on the catalytic oxidation of water to molecular dioxygen, taking into account the implications of this reaction for new energy conversion schemes based on artificial photosynthesis. The final objective is the generation of clean and renewable fuels with high energy density.

Highlighted publication

Robust Molecular Anodes for Electrocatalytic Water Oxidation Based on Electropolymerized Molecular Cu Complexes

Amthor, S.; Ranu, K.; Bellido, C. G.; Salomón, F. F.; Piccioni, A.; Mazzaro, R.; Boscherini, F.; Pasquini, L.; Gil-Sepulcre, M.; Llobet, A.

Adv. Mater. 2024, **36**, 2308392

Prof. Núria López

The group of Prof. López studies phenomena (thermo, electro, and photo-catalytic) with theoretical models that integrate Density Functional Theory with microkinetic models and other continuous equations. The group is an expert in complex reaction networks that take place in a large plethora of catalytic materials. The group has a particular interest in introducing statistical techniques (machine learning) in its field of research and they are advocates of open data through the ioChem-BD database.

Highlighted publication

Fast evaluation of the adsorption energy of organic molecules on metals via graph neural networks

Pablo-García, S.; Morandi, S.; Vargas-Hernández, R. A.; Jorner, K.; Ivković, Z.; López, N.; Aspuru-Guzik, A.

Nat Comput Sci. 2023, **3**, 433–442

Prof. Rubén Martín

ICREA Professor
ERC Advanced Grant

The research of Prof. Martin focuses on discovering the potential of catalytic functionalisation of raw materials for the synthesis of valuable compounds from simple and abundant precursors. They have contributed extensively to the catalytic functionalisation of C-O and C-H bonds, as well as to the fixation of CO_2 to organic matter. They have described a catalytic technology capable of fixing carbon dioxide in saturated and unsaturated hydrocarbons to prepare fatty acids, key parts in the manufacture of polymers, detergents, cosmetics, and pharmaceuticals.

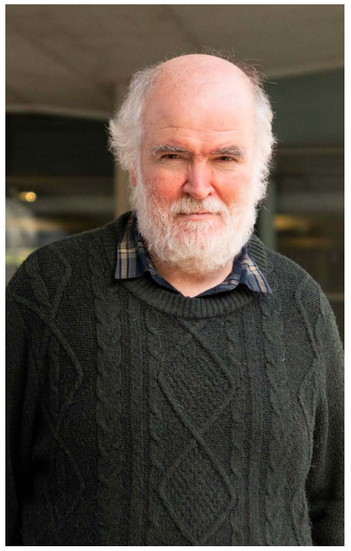
Highlighted publication

Native amides as Enabling Vehicles for Forging sp3–sp3 Architectures via Interrupted Deaminative Ni-catalyzed Chain-Walking

Rodrigalvarez, J.; Wang, H.; Martin, R.

J. Am. Chem. Soc. 2023, **145**, 3869–3874

Prof. Feliu Maseras



The group of Prof. Maseras applies computational chemistry to the study of the structure and reactivity of transition metal complexes, with special emphasis on homogeneous catalysis. Some of the reactions in which they have achieved the most relevant results are in cross-coupling and the activation of C-H bonds. The group works on oxidative coupling reactions, reductive coupling, organocatalysis, photocatalysis and mechanochemistry. They are also interested in the application of statistical models to the treatment of massive amounts of computational results.

Highlighted publication

Charge-controlled Pd catalysis enables the meta-C–H activation and olefination of arenes

Mondal, A.; Díaz-Ruiz, M.; Deufel, F.; Maseras, F.; van Gemmeren, M.

Chem, 2023, **9**, 1004–1016

Prof. Emilio J. Palomares Gil

ICREA Professor
ERC Advanced Grant

The group of Prof. Palomares works on the design, synthesis and characterisation of molecules and materials with optical and electrical properties for energy applications. Through these materials, the group manufactures (opto) electronic devices, including solar cells, light emitting diodes and photo/ electrocatalysts. The understanding of the device behaviour is completed by the characterisation of the charge transfer reactions using advanced photo-induced transient and steady-state spectroscopy under operating conditions. On the other hand, the characterisation of the charge kinetics in photo or electron induced catalytic reduction of CO_2 has allowed to gain deeper insight into the efficiency of hybrid electrodes. Finally, the group has reported their results as well in the application of sunlight as an energy source and as an initiator of catalytic reactions in the conversion of CO_2 and H2 generation.

Highlighted publication

Self-assembled molecules for hole-selective electrodes in highly stable and efficient inverted perovskite solar cells with ultralow energy loss

Li, W.; Cariello, M.; Méndez, M.; Cooke, G.; Palomares, E.

ACS Appl. Energy Mater. 2023, **6**, 1239-1247

Prof. Mónica H. Pérez-Temprano

The group of Prof. Pérez-Temprano is focused on the development of new synthetic catalytic methods with cobalt through detailed knowledge of the catalytic process. To develop their research projects, they apply different approaches, from synthetic organic chemistry to mechanical studies, including the capture of highly reactive reaction intermediates.

Highlighted publication

Protocol Synthesis and characterisation of highly diluted polyanionic iron(II) spin crossover systems

Moneo-Corcuera, A.; Nieto-Castro, D.; Cirera, J.; Gómez, V.; San-josé-Orduna, J.; Casadevall, C.; Molnár, G.; Bousseksou, A.; Parella, T.; Martínez-Agudo, J. M.; Lloret-Fillol, J.; Pérez-Temprano, M. H.; Ruiz, E.; Galán-Mascarós, J. R.

STAR Protoc. 2023, **4**, 102394

Dr. Elisabet Romero

ERC Consolidator Grant

Dr. Romero aims at developing a new generation of bio-inspired macromolecular systems able to convert solar energy to fuel. The group objective is to design and construct chromophore-protein assemblies based on abundant and biodegradable materials with the capacity to absorb, transfer and convert sunlight into electrochemical energy with high efficiency. The resulting energy and electron transfer dynamics in these assemblies will be investigated by ultrafast laser spectroscopy. Ultimately, the optimised systems will be incorporated into devices to provide a renewable, safe and inexpensive energy solution towards a sustainable future.

Highlighted publication

Engineering Excitonically-Coupled Dimers in an Artificial Protein for Light Harvesting via Computational Modelling

Curti, M.; Maffeis, V.; Teixeira Alves Duarte, L. G.; Shareef, S.; Hallado, L. X.; Curutchet, C.; Romero, E.

Protein Sci. 2023, **32**, e4579

Prof. Marcos García Suero

ICREA Professor
ERC Consolidator Grant

The main objective of Prof. Suero is to catalytically generate reactive carbon species not yet explored and study their behaviour on organic compounds. His goal is to discover new rules of reactivity of carbon, not only for the design and discovery of new chemical reactions, but also for its use to build molecular complexity. The group has been a pioneer in the catalytic generation of diazomethyl radicals as direct equivalents of monovalent carbine species. This discovery allows the design of innovative disconnection strategies for the construction of chiral centres in drugs, agrochemicals and materials. In addition, the group is interested in the use of high throughput techniques for the synthesis of libraries of bioactive molecules that cannot be obtained by conventional routes, precision medicine with PET imaging and in the development of new chemical reactions with application in chemical biology.

Highlighted publication

Late-Stage Aryl C-H Bond Cyclopropenylation with Cyclopropenium Cations

Tu, H.-F.; Jeandin, A.; Bon, C.; Brocklehurst, C.; Lima, F.; Suero, M. G.

Angew. Chem., Int. Ed. 2023, **62**, e.202308379.

Dra. Katherine Villa

The research of Dr. Villa group is focused on a rational design of nanostructured photocatalytic systems based on multicomponent heterojunctions that can efficiently convert polluting compounds into high-value chemicals and fuels. On the other hand, they are also devoted to the development of light-driven micro/nanomotors for environmental applications. Both approaches are in line with the sustainable development goals from the EU, including clean energy generation and water decontamination.

Highlighted publication

Bubble-propelled micromotors for ammonia generation

Ferrer Campos, R.; Bachimanchi, H.; Volpe, G.; Villa, K.

Nanoscale, 2023, **15**, 15785-1579.

Awards

Young Researcher Award - Modality "Group Leader" 2023 by the Spanish Royal Society of Chemistry (RSEQ)

New member of the Spanish Young Academy 2023

The Melchiorre's group

The research of Prof. Paolo Melchiorre group aims to identify novel reactivity concepts that could redefine the synthetic potential of venerable organic processes. Expanding upon our recent results, we are investigating further applications of photo-organocatalysis, where key transient intermediates of organocatalytic processes in the ground state actively participate in the photo-excitation of substrates, without the need for an external metal-based photosensitiser.

Highlighted publication

Stereoselective conjugate cyanation of enals by combining photoredox and organocatalysis

Berger, M.; Ma, D.; Baumgartner, Y.; Hin-Fung Wong, T.; Melchiorre, P.

Nat. Catal. 2023, **6**, 332–338

Dr. José A. Berrocal

The group of Dr. Berrocal combines the chemistry of small molecules and macromolecules to build functional materials. We are particularly interested in controlling the (mechanical) properties of the prepared materials by rational design. In our approach, chemistry is the thread that connects (macro)molecular structure, morphology, and function. Our efforts are aimed at developing strategies potentially applicable to sustainable development.

✳ Highlighted publication

Closed-loop recycling of vinylogous urethane vitrimers

Ma, Y.; Jiang, X.; Yin, J.; Shi, Z.; Berrocal, J. A.; Weder, C.

Angew. Chem. Int. Ed. Engl. **2023**, e202306188

Prof. Beatriz Prieto-Simón

Prof. Prieto-Simón group aims to deliver diagnostic solutions by pushing the boundaries of the performance of biosensors, as powerful diagnostic tools, by harnessing advances in materials science and nanotechnology driven by principles found in nature.

✳ Highlighted publication

Towards the rapid detection of haze forming proteins

Cetó, X.; McRae, J. M.; Mierczynska-Vasilev, A.; Voelcker, N. H.; Prieto-Simón, B.

Talanta, 2023, **268**, 125305.

ICREA Professor

NEW RESEARCH GROUPS

Associated researchers

Dr. Casadevall's group aims to develop functionalised polymeric microreactors and catalysts based on abundant materials on the planet for the production of solar fuels and chemical products, driving new conceptual developments in the field of artificial photosynthesis.

✳ Highlighted publication

Imidazole-derived carbenes and salts boost nickel-catalyzed ester carbonylation activity

Casadevall, C.

Chem Cat. 2023, **3** (12), 10086

◯ Awards

Young Researcher Award - Modality "Postdoctoral Researcher" 2023 by the Spanish Royal Society of Chemistry (RSEQ)

Emerging Scientific Talent Award 2023 by the Catalan Society of Chemistry (SCQ)

Dr. Kherzi group focuses its research lines on sustainable energy and nano/microbots. On the one hand, she investigates the development of multifunctional materials for sustainable energy technologies, focusing on improving the efficiency and activity of electrocatalysts for selective energy production. On the other hand, it studies the design of programable microbots for environmental and biomedical applications.

✳ Highlighted publication

A survey of Earth-abundant metal oxides as oxygen evolution electrocatalysts in acidic media (pH < 1)

Yu, J.; Giancola, S.; Khezri, B.; Nieto-Castro, D.; Redondo, J.; Schiller, F.; Barja, S.; Spadaro, M. C.; Arbiol, J.; Garcés-Pineda, F.A.; Galán-Mascarós, J. R.

EES Catal., 2023, **1**, 765

Highlighted research

ioChem-BD, the ICIQ Open Data platform, moves towards market

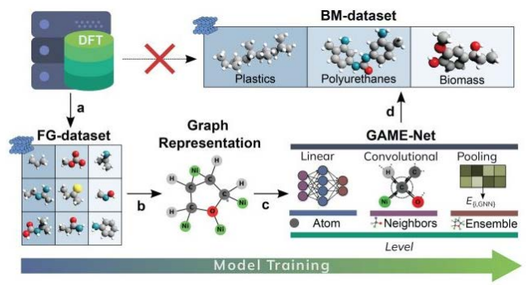
The open software platform ioChem-BD, which analyses, stores, and labels computational chemistry data, has reached a new milestone with 500 open datasets linked to journal research articles identified by DOIS and more than 300K indexed structures of molecules and materials.

Prof. Emilio J. Palomares Gil receives an ERC Advanced Grant up to €2.5 million to study the quantum coherence phenomena

The European Research Council (ERC) Advanced Grants will help outstanding research leaders across Europe to explore their most innovative and ambitious ideas. With this latest award, the Institute of Chemical Research of Catalonia (ICIQ-CERCA) has accumulated a sum of 25 grants from the ERC.

How can AI reduce the carbon footprint in the environment?

Researchers from Prof. Núria López's group, together with researchers from the University of Toronto (Canada), have made create a new model called GAME-Net, which uses an advanced artificial intelligence tool: graph neural networks.

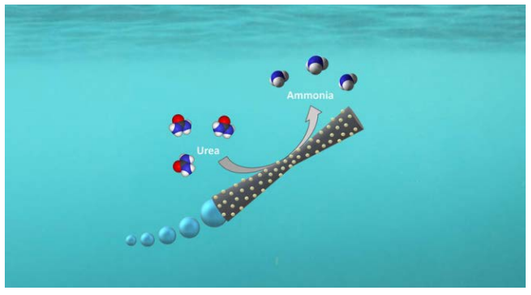


ICIQ and IDIBGI join forces in a pioneering collaboration to discover new therapeutic targets against cancer

This collaboration explores new therapeutic targets and developing new drugs for cancer treatment. This cooperation has become one of ICIQ strategic projects with the goal of advancing research in this field.

New water treatment method can generate green energy

Researchers from Dr. Katherine Villa Group have designed micromotors that move around on their own to purify wastewater. The process creates ammonia, which can serve as a green energy source. A machine learning method developed at the University of Gothenburg will be used to tune the motors to achieve the best possible results.



ICIQ researchers describe a more sustainable process to recycle biobased polycarbonates

Prof. Arjan W. Kleij, Prof. Bo and Dr. Fernando Bravo describe a circular process to recycle polycarbonates, a specific polymer often used in plastic applications, using less chemicals and user-friendly conditions. The study was carried out on a biobased polycarbonate generated from limonene obtained from citrus peel oil.

Publications

Scientific publications are an essential part of the research activities carried out at ICIQ and serve as a key indicator of excellence and progress in research.

Furthermore, they provide a platform for international collaborations allowing the tackling of complex scientific challenges, and the establishment of links with industry. In a centre of international reference, scientific publications are a key tool to maintain and consolidate our reputation and impact within the global scientific community.[1]

171
Publications[2]

2
Highly Cited Papers

67%6
International Collaborations

%
With industry

11%
Women Lead Papers

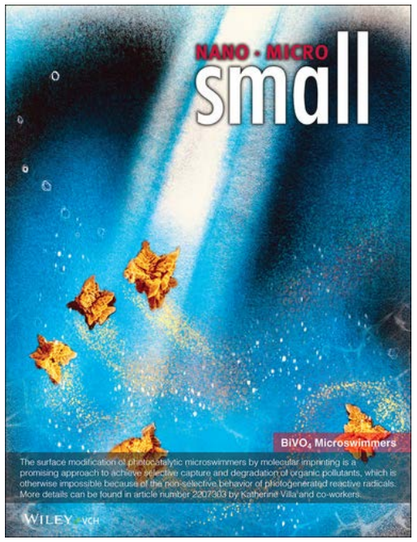
2,98
ESI Chemistry Normalised Impact

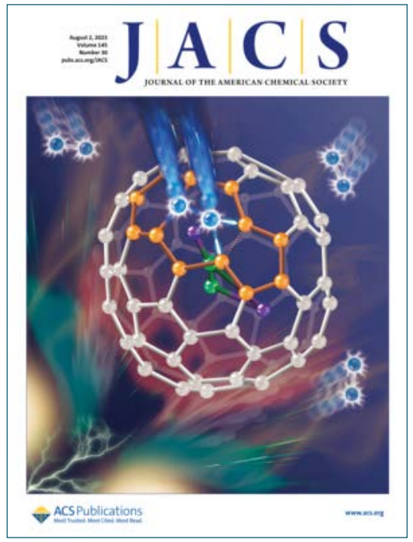
TOP 5 Journals where ICIQ has published most frequently in 2023

Journal	No. of publications
Angewandte Chemie - International Edition	16
ACS Catalysis	10
Journal of the American Chemical Society	10
Chemical Science	7
Chemical Communications	5

417 Citations of published articles 2023

The normalized impact of ICIQ in the ESI field “Chemistry” is 2.98. This figure is a comparison of the world average of citations per publication, ESI field and year of publication. Two articles have received a large number of citations, in addition to four that have been reviewed in journal covers.





[1] See the full list of publications on ICIQ website.
[2] Source: Web of Science Core Colleciton 2023. Last access: 20/02/2024

Competitive funding

Projects, Fellowships and Individual Research Grants

Competitive funding is essential to face global challenges and establish collaborations with other international institutions. 2023 was quite exceptional in terms of the number and relevance of the projects and grants awarded to ICIQ and research personnel, achieving a total competitive funding of **11,214,874.20.3€**. This positive evolution over the last few years reflects the continued commitment to research and innovation.

In the European arena, highlight a new ERC advacned project, **EXCITED** from Prof. Palomares group, together with the participation of Prof. Llobet, Prof. Lloret and Prof. Palomares groups in three new projects within the Cluster 5 of Horizon Europe: **SUNGATE**, **PHOTOSINT** and **PEARL**, respectively.

Additionally, for the first time, the Institute participates in a new MSCA Staff Exchange project: **ENRICH**, with the participation of Prof. Ballester group.

Moreover, ICIQ coordinates a new collaborative project: **SUPERVAL**, led by Prof. Galán-Mascarós, with the participation also of Prof. López group. The project has been selected within the EIC-Pathfinder Challenges 2022 call and forms part of the EIC portfolio on carbon dioxide and nitrogen management.

On the national scene, we are glad to participate in a new public-private Collaborative project funded by the State Research Agency (Spanish Ministry of Science, Innovation and Universities). ICIQ Innovation and Valorisation laboratory within the KTT and Industrial projects department, together with the HTE (High Throughput Experimentation) laboratory, participate in a consortia led by the pharmaceutical company Hemostatics Pharmaceuticals.

Finally, we would also like to highlight a new *Innovadors* project, ioChemBD-EXPAND, from Prof. Bo group. Funded by AGAUR (Catalan Agency for Management of University and Research Grants), the project aims to explore commercialisation paths for the automated data management tool created by ICIQ computational groups, ioChem-BD, which facilitates the efficient creation, curation and sharing of computational data in various fields of knowledge, following FAIR principles.

The **D-CARBONIZE** project, funded under the HORIZON-TMA-MSCA-DN programme, has started in March 2023. ICIQ is one of the collaborators of the programme, recruiting 2 of the 12 PhD students that will train the project. Each doctoral student will be hosted at two institutions in different countries, and will receive additional training at the facilities of the associated industrial partners.

Regarding fellowships and grants for research personnel, in 2023 we obtained 17 grants for the hiring of pre-doctoral researchers, of which 2 Joan Oró Research Staff Training (FI), 1 University Faculty Training (FPU) and 14 Research Staff Training (FPI). Regarding postdoctoral grants, during the year 2023, 9 Marie Skłodowska-Curie Actions - Postdoctoral Fellowships (HE-MSCA-PF), 1 grant Beatriu de Pinós (H2020-MSCA-COFUND, AGAUR), 4 grants Juan de la Cierva (MICIU) and 1 grant Ramon y Cajal (MICIU) were obtained. In addition, during 2023 the number of grants in force was 92, including 8 grants Investigo (AGAUR).

Competitive funding achieved during 2023

11,214,874.20€

[3] You can see the full list of research projects and grants to research staff achieved during 2023 in Annex 1.

ENRICH aims to develop new, more economical, fast and efficient tools for the enrichment of post-translationally modified proteins. Scientific studies have highlighted the pivotal role of histone post-translational modifications (PTMs) in cellular processes, including transcription and DNA repair. To better understand these processes and their implications in human diseases such as cancer, schizophrenia and diabetes, the ability to detect PTMs is crucial.

The **SUPERVAL** project proposes to design and implement an autonomous solar-powered installation to capture pollutants from flue gases, with the aim of converting them into valuable raw materials for the chemical industry, using water as a source of electrons and protons.

D-CARBONIZE aims to train the next generation of scientists who represent the future leaders in the field of sustainable polymers and depolymerisation strategies, biocarbon valorisation and innovative catalytic strategies.

Scientific Core Facilities

Scientific Core Facilities are organised into 10 specialised units, each dedicated to a specific technique or group of related techniques. These units are articulated between the Characterisation Technologies Department and the Reaction Technologies Department (CTD and RTD, respectively). The Characterisation Technologies Department achieved significant milestones in 2023. The spectroscopy unit developed customized accessories, improved cryogenic temperature research capabilities, and upgraded the circular array equipment with a new APD detector. The introduction of the highly sensitive GC-PDHID detector by the Energy Laboratory improved the accuracy of gas analysis. Another highlight was the establishment of Europe first three-dimensional electrodiffraction service, marking a breakthrough in crystallography. In addition, advances in photophysics and mass spectrometry, including new systems for photovoltaic stabilization and IPCE analysis, underscore the department dedication to cutting-edge research and technological development.

On the other hand, the Department of Reaction Technologies provided support to ICIQ researchers in terms of High Throughput Experimentation (HTE), reactions in conditions that require special equipment (high pressure, reactive gases, microons...) and design and fabrication of customised pieces to assemble any experiment needed by the researchers. Regarding the new instrumentation in the department, it is worth mentioning the complete implementation of the automatic solids dispenser in the HTE Unit, which helps to speed up the preparation of multi-position reaction plates, minimises errors, increases the precision in the quantities dispensed and frees the unit personnel from this task. As for the laboratories, the complete renovation of the mechanical workshop took place in 2023. The new workshop, with more space than the previous one, allows a new organisation of the facilities: there is a bench dedicated to 3D printing, a special bench to prepare new assemblies, a bench dedicated to repairs, office space for two people, space to discuss issues with the researchers and more accessibility to air and materials. This new disposition translates directly into a more efficient work flow, which ultimately results in better service to the researchers.

CRTU, Diffraction, NMR, Mass, E-Lab, ChromTae, Photophysics, SMCU

106,640
experiments

HTE

4,789
reactions

Glass Blowing Workshop

752
new pieces

1,083
repaired pieces

Mechanical Workshop

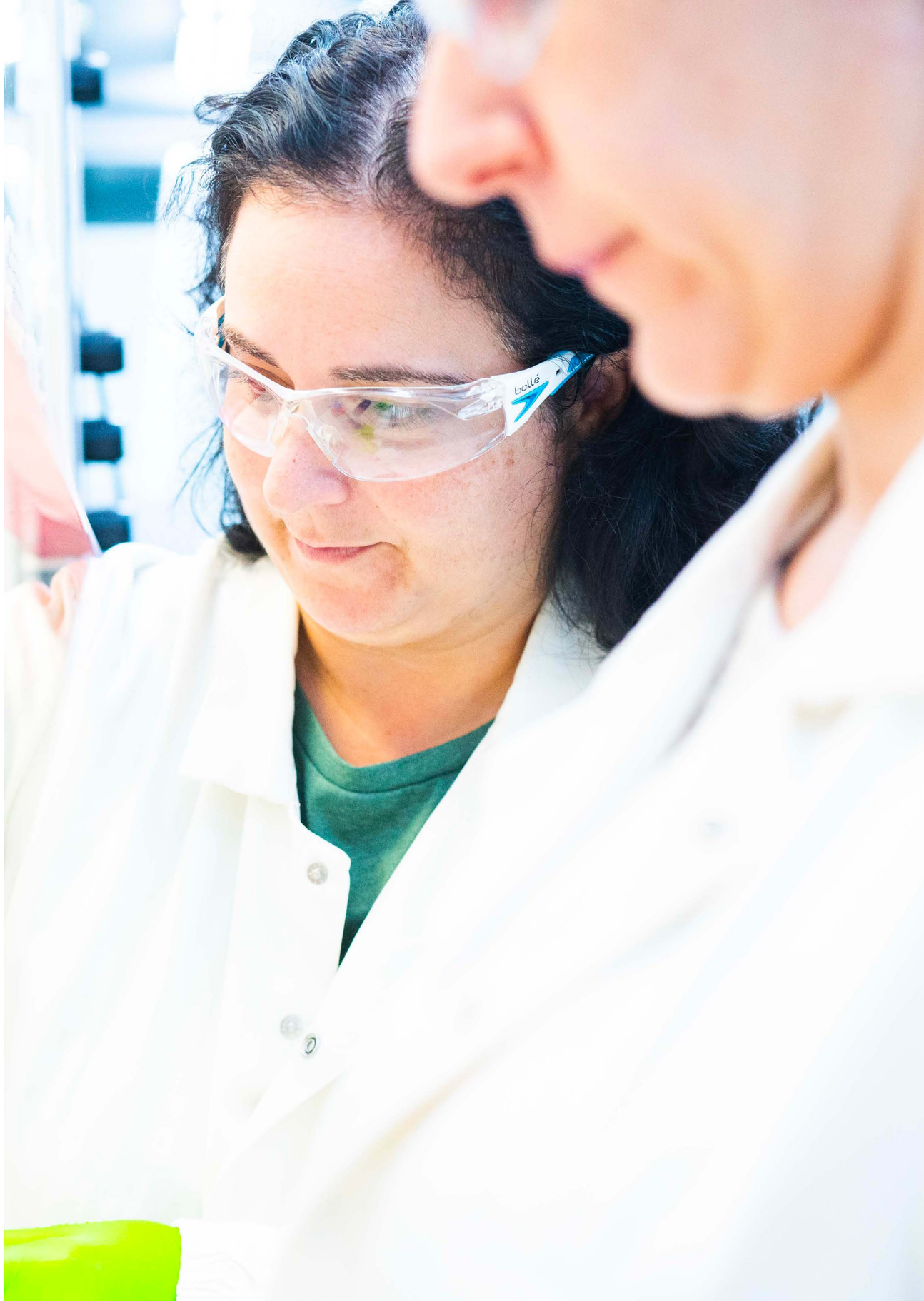
190
projects

1,215
manufactured pieces

254
repaired equipment

Equipment acquisitions:

- Electron diffractometer for structural determination of nanocrystalline matter
- High resolution mass spectrometer with ionic mobility
- Renovation and extension of the mechanical workshop
- Scientific stations for computational calculation and processing of laboratory data



Institutional

The institutional scope of ICIQ is the fundamental basis of its mission, values and purpose. It is within this framework that the strategic guidelines are defined and the policies that promote excellence in chemical research are developed.

Governance

This section details the structure and governing bodies that guide ICIQ policies and strategic decisions, guaranteeing the achievement of its objectives and the promotion of its commitment to scientific excellence and innovation. Through transparency, participation and accountability, the governing bodies of ICIQ ensure efficient and responsible management of all aspects of the institution, contributing to its success and prestige at national and international level.

The **Board of Trustees** is the highest body in the administration, representation and governance of ICIQ Foundation.

President / Vice-president

Dr. Joaquim Nadal i Farreras	Minister for Research and Universities of the Government of Catalonia
Dr. Josep Pallarès	Rector of the Universitat Rovira i Virgili

Members

Dr. Lluís Rovira i Pato	Director of CERCA Research Centres of Catalonia
Montserrat Vallverdú	Coordinator Renewable Fuels and Circular Economy of I.C., Repsol S.A.
Dr. Álvaro Gordillo	Business Development & Technical Sales Leader EMEA & Americas, BASF Española, S.L.

Secretary

Dr. Joan Gómez Pallarès	General Director of Research of the Government of Catalonia

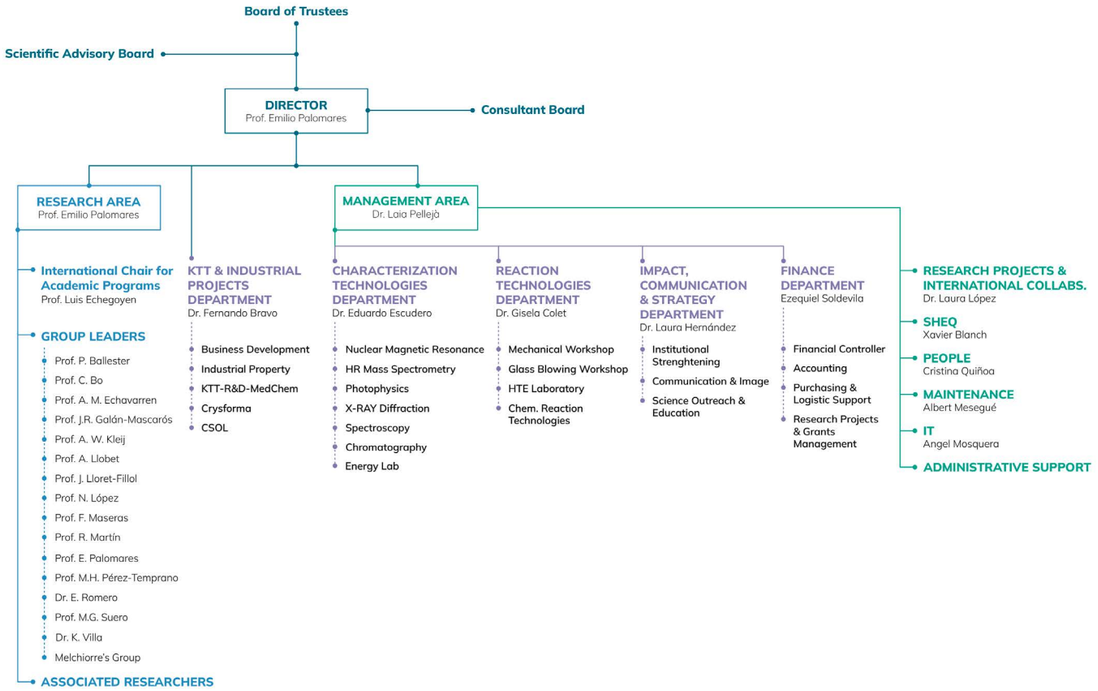
The **Scientific Advisory Board** (SAB) is the body in charge of advising the Board of Trustees on the scientific policy of the Foundation, as well as of periodically recruiting and evaluating the principal investigators. It ensures that the scientific management of ICIQ meets international standards of excellence. The SAB is composed of scientists of international prestige in the field of chemistry.

Prof. Thomas Carell	Ludwig - Maximilians - Universität München (Munich, Germany)
Prof. Bo Albinsson	Chalmers University of Technology (Gothenburg, Sweden)
Prof. Christopher A. Hunter	University of Cambridge (Cambridge, United Kingdom)
Prof. James R. Durrant	Imperial College of London (London, United Kingdom)
Prof. Jeremy Harvey	KU Leuven (Leuven, Belgium)
Prof. Erick M. Carreira	ETH Zentrum (Zürich, Switzerland)
Prof. Siglinda Perathoner	Università degli Studi di Messina (Messina, Italy)
Prof. Beatriz Roldán	Max-Planck - Gesellschaft (Munich, Germany)
Prof. Hernán Míguez	Institute of Materials Science of Sevilla CSIC (Sevilla, Spain)
Prof. John F. Hartwig	University of California (Berkeley, USA)
Prof. Cristina Nevado	University of Zurich (Zürich, Switzerland)

According to the **organisational chart**, ICIQ is structured in two main areas: Research and Management.

Research Area: This area is lead by the Director of ICIQ, Prof. Emilo J. Palomares Gil, and it includes 18 independent research groups each headed by a Group Leader. Recently, this area has incorporated associated researchers to the centre. Also, the department of Knowledge and Technology Transfer, and Industrial Projects (KTT).

Management Area: Dr. Laia Pellejà, Administrative and Communication Director, leads this area which includes different departments among which are Finance; Impact, Communication and Strategy; and, Characterisation Technologies and Reaction Technologies. Also linked to this area are the units of Research Projects and International Collaborations, Safety and Labour Risks, Human Resources, Maintenance, Information Technology and Communications, and Administrative Support. In addition, Prof. Luis Echegoyen has joined the management area as International Chair for Academic Programmes.



Accreditations of excellence

The awards of excellence reinforce ICIQ commitment to the highest standards in scientific research, innovation and academic training, while serving as a guide to continue leading scientific excellence and making a significant contribution to international chemical research.

EXCELENCIA SEVERO OCHOA
2020 - 2024

On July 2020, ICIQ received the accreditation as a Severo Ochoa Centre of Excellence for the second time, a recognition awarded by the State Research Agency (AEI) of the Ministry of Science, Innovation and Universities (MICIU). This prestigious accreditation, obtained for the first time in 2014, demonstrates the scientific excellence of ICIQ and positions it as one of the main references in chemical research in Spain. The designation as a Severo Ochoa Centre of Excellence is not only a testimony of the institute commitment to scientific excellence, but also constitutes a significant source of funding, providing resources for the development of innovative research projects, the acquisition of unique equipment, the strengthening of the management area and the promotion of the research career.

HR EXCELLENCE IN RESEARCH

ICIQ remains committed to excellence in human resources for research during 2023, highlighting its distinction with the Human Resources Strategy for Researchers (HRS4R).

After a rigorous internal analysis to align itself with the principles of the *European Charter for Researchers and the Code of Conduct for the Recruitment of Researchers*, ICIQ obtained this prestigious recognition from the European Commission in 2017.

The 2020-2023 Action Plan was supervised by a working group that implemented 16 key actions to reflect the adoption of policy practices to reduce the gaps between ICIQ existing practices and the principles established by the European Commission.

Finance

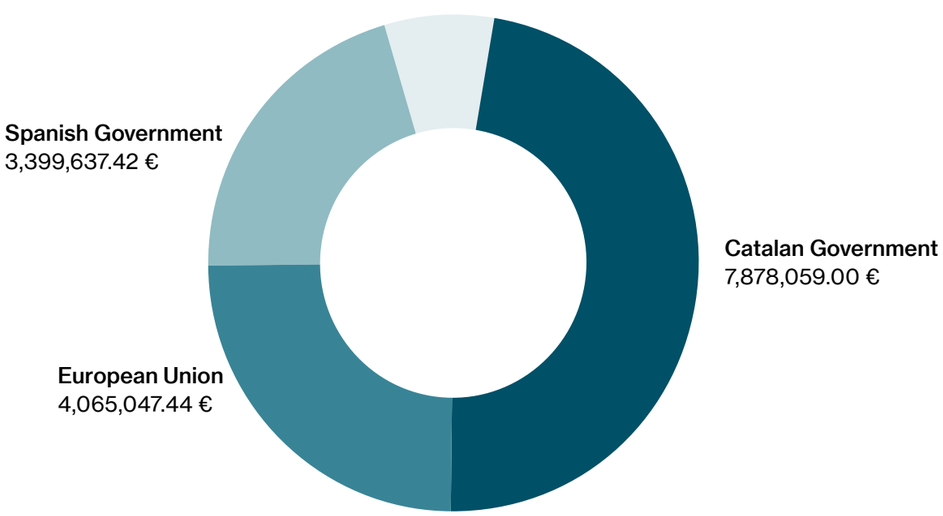
During the year 2023, ICIQ managed a total budget of 16,523,688.79€ from different funding sources that will facilitate the deployment of its research and ongoing operational activities.

These numbers reflect ICIQ continued commitment to excellent scientific research, as well as the diversity and stability of its funding sources. Through this diversified financial support, ICIQ has been able to maintain and promote its research, training and innovation programmes.

Budget 2023

16,523,688.79€

Disaggregation by **source of financing**



Policies

Policies provide an important overview of the organisation values, practices and directions, while establishing clear and specific guidance for the different areas.

Research integrity:

Highlights ICIQ commitment to ethical research practices, prevention of scientific fraud and quality assurance in scientific production.

Environmental policy:

Shows ICIQ efforts to minimize the environmental impact of its activities through initiatives such as waste reduction.

Equality Plan:

Promotes actions and initiatives to encourage the participation of women and other groups in science.

Personnel selection policy:

Underscore the principles and criteria that guide the personnel selection process, placing emphasis on equal opportunities and diversity.

Working groups

The working groups at ICIQ are a fundamental pillar in fostering the progress, cohesion and well being of our scientific community. Each group plays a key role in specific areas, contributing to building a dynamic environment to achieve collective success.

- **Academic Committee:** It is responsible for evaluating academic programmes, ensuring the quality and rigor of training and research at the centre.
- **Equality Comission:** It works actively to promote policies and initiatives aimed at achieving equal treatment and opportunities for men and women, with the aim of creating a fair and inclusive working environment. During the year 2023, the Equality Commission will monitor the actions of the Equality Plan 2019-2023. At the end of the year, a new group of the Equality Commission was set up, made up of 10 members of the Workers Committee and company representatives. This group will support the development of the Equality Plan (2024-2027), which will be officially registered on 28th December at the Directorate for Civil Service. Through this initiative, the Commission continues to reinforce ICIQ commitment to the promotion of gender equality and the elimination of inequalities in the workplace.
- **Safety and Health Committee:** This is a partisan and collegiate body aimed at regular and periodic consultation of the institute actions in terms of risk prevention. It aims to ensure that the installations and practices carried out at ICIQ comply with the highest safety and health standards for all personnel. The constitution of the Committee was carried out in compliance with article 388 of Law 31/1995 of 8 November, on the Prevention of Occupational Risks, and is made up of 6 members, three representatives of the Workers Committee and three members representing the centre. The Health and Safety Committee was updated at the beginning of 2023, when the new prevention delegates were also appointed.
- **Workers Committee:** is the representative and collegiate body of all the workers at the Institute, addressing labour issues and participating in the decision-making that affect the personnel. On 16th November 2023 a new committee was set up composed by 13 members from the different areas of the centre, including scientific and management staff.
- **Green ICIQ:** With a sustainable approach, this voluntary group works to implement ecological and environmentally conscious practices in the daily activities of ICIQ. During 2023, they have focused on three fundamental pillars:

1. Assessment of the environmental impact of the ICIQ activities by calculating the centre carbon footprint for the year 2022.
2. Participation in working groups:

   a. SuRe Catalonia: Sustainable Research Catalonia, a working group of 18 Research Centres in Catalonia that collaborate to make their research more sustainable.

   b. Sustainability Working Group of the BIST: a working group of all the centres of the Barcelona Institute of Science and Technology, which has prepared a common Sustainability Handbook for all the centres.
3. Evaluation of current sustainable measures:

   a. Use of electric vehicle charging equipment.

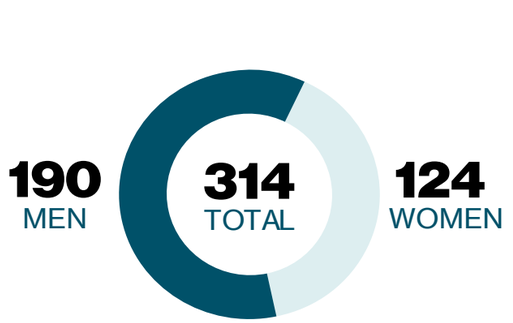
   b. Waste recycling.

People

In 2023, ICIQ have had a staff of 314 FTE professionals who will make possible the success and contributions to science and society.

The community is diverse and brings together more than 40 different nationalities. Thus, 42% of the staff is international, contributing to a diverse perspectives and experiences. With a strong commitment to gender equality, ICIQ has 124 women, representing 39.5% of the staff.

42% of professionals coming from **40** different nationalities



250 Research
164 | 86

64 Management
25 | 39

13 Senior Group Leaders
11 | 2

2 Starting Career Programme Group Leaders
1 | 1

1 Junior Group Leaders
1

78 Postdoctoral researchers
61 | 17

4 Group Scientific Coordinator
4

13 Project Researchers
7 | 6

92 PhD Students
56 | 36

12 Master Students
8 | 4

5 Lab Technicians
3 | 2

31 Research Support Area Technicians
18 | 13

Talent attraction

At the end of 2023, a total of **161 positions** have been opened in different areas, departments and educational levels, from summer fellowships to opportunities for postdoctoral researchers and professionals in areas such as research support, knowledge transfer and management. Some of these people have been incorporated thanks to competitive grants such as the MSCA, Juan de la Cierva or Beatriu de Pinós.

14	18	52	46	10	6	15
Summer Fellows	Master Students	PhD	Postdocs	Scientific Core Facilities	KTT	Management

Training

At ICIQ we offer training programmes for master students, doctoral and postdoctoral researchers to provide them with the necessary tools to achieve outstanding research results. In addition to comprehensive training in chemical research, we offer training to improve and develop interpersonal skills.

Defended theses

At the end of 2023, 27 doctoral theses were defended.[4]

Scientific career development

ICIQ reaffirms its commitment to personal and professional growth by providing training and career development opportunities. Through various initiatives, both students and researchers have access to specialised programmes in scientific project management, communication skills, leadership and other areas relevant to professional development. During 2023, ICIQ has offered a total of 6,802 hours of training.

SHARP Training Programme for PhD students

SHARP Programme (Severo-ocHoA PhD Training Programme) is an initiative that seeks to complement scientific areas that are not included in the traditional curricula of doctoral programmes. A total of 76 students took part in this training, which focused on various key aspects:

› **Introduction to research and technical skills:**

The first week dealt with fundamental aspects of developing a successful doctorate, including scientific and technical modules, team building, programming and open science.

› **Communication skills:**

These sessions will focus on the refinement of crucial skills for effective communication, including technical written and oral communication, audience segmentation, dissemination and the ethical aspects.

› **Innovation:**

Emphasis was placed on knowledge and technology transfer (KTT) activities, with a focus on technology transfer to industry.

› **Careers:**

This session focused on professional development, offering a curriculum adaptation course to prepare students for their professional future, whether in academia or industry.

Severo Ochoa

› **ICIQ Summer Fellowship Programme**

The Summer Fellowship Programme is an initiative of ICIQ to offer a unique experience to undergraduate students, providing them with the opportunity to immerse themselves in an academic environment of excellence. With a significant demand, with more than 150 applications, only 14 students from around the world were selected to participate in this learning opportunity. This group had the opportunity to experience first-hand scientific research in an international and collaborative environment.

› **Severo Ochoa International Mobility Programme:**

The Severo Ochoa International Mobility Programme is an international call aimed exclusively at ICIQ students. The main objective of this programme is to support doctoral students in the second, third or fourth year of their doctoral studies, who are offered a research stay at an international institution abroad.

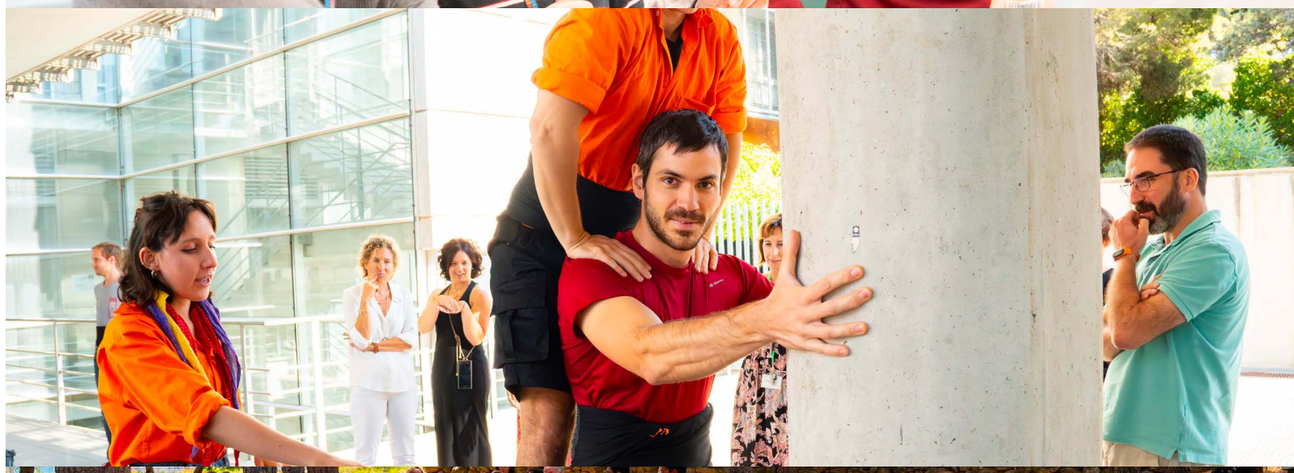
Candidates are free to propose a research project they wish to carry out at a host institution of their choice. This opportunity allows them to strengthen their research skills, establish international collaborations and contribute to their professional development in a global scientific environment. In 2023, three students will benefit from these grants to carry out research stays in Berkeley (United States of America), Manchester (United Kingdom) and Princeton (United States of America).

[4] See the full list of theses defended in 2023 in Annex 2.

ICIQ Community

ICIQ community represents a fundamental pillar in the daily life of the institute. Its main objective is to foster integration and cohesion among all the members of the centre.

Throughout the year, different activities have been organised, including the celebration of Catalan traditions such as castells, Sant Jordi, castanyada, Santa Tecla and the Christmas festivities. Sports activities such as volleyball tournaments have also been promoted. These moments are not only occasions for enjoyment, but also help to strengthen personal and professional bonds within the centre and to promote a culture of collaboration and learning beyond research.



Knowledge and Technology Transfer, and Industrial Projects Department (KTT)

KTT

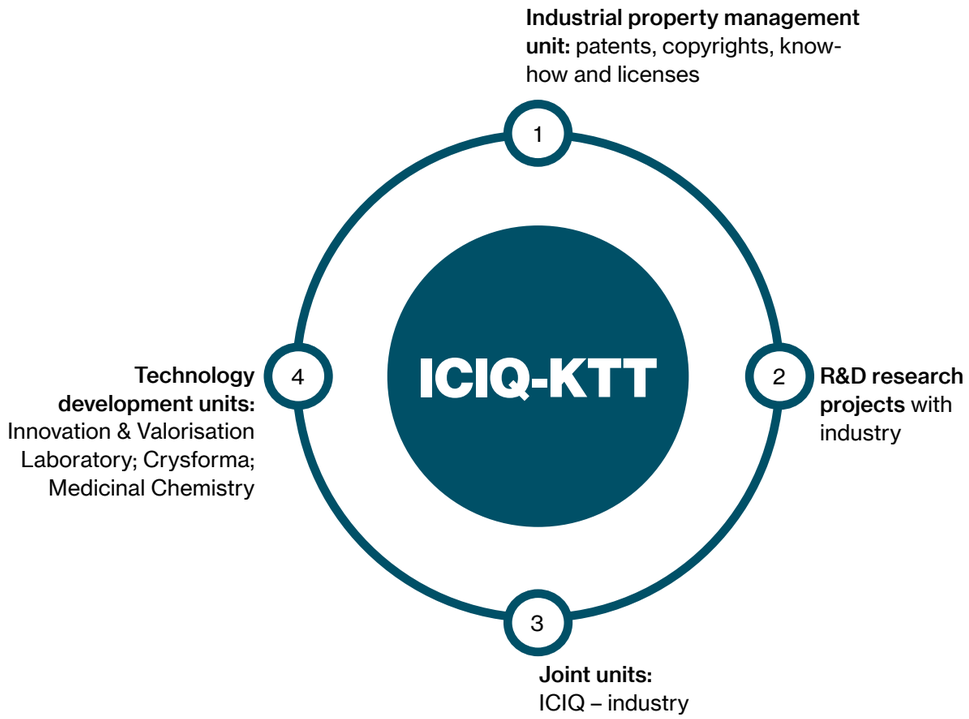
This 2023, ICIQ – Knowledge and Technology Transfer and Industrial Projects ICIQ – KTT) Department put its efforts on collaborative projects with industries and other research institutions related to sustainable catalysis, renewable energies and molecular medicine. The area also has prioritised ICIQ **technologies transfer to market and society** with industry contracts patents and licences, and spin-off companies, contributing to solve global problems related to **climate change and public health**.

The knowledge transfer is one of the main pillars of ICIQ activity, and accomplishes these three objectives:

1. To transfer knowledge and technologies from ICIQ to industry, seeking collaborations and promoting the creation of spin-offs to develop new products and industrial procedures.
2. To generate incomes to carry on industrial collaborations and licensing new patents.
3. To raise awareness and train ICIQ research personnel in innovation management, fostering vocations for technological entrepreneurship.

The area includes three development units related to innovation, industrial collaborations and with other research institutions, and public health projects: Crysforma, focused on the chemical solid state; Medicinal Chemistry, focused on the development of small molecules; and the Innovation & Valorisation Laboratory. This year, this third unit has changed its name (formerly CSOL) to reflect its purpose for being: to work on the valorisation of ICIQ projects and to develop projects with industrial partners.

To unify the tasks of all these three units under the brand ICIQ – KTT, a new logo design has been created that includes ICIQ logo with the specific name of each unit, as well as a generic KTT logo.



ICIQ – KTT Expertise

Valorisation of cutting-edge technology

Evaluation of the technologies from ICIQ research results

IP protection

Incubation and valorisation

Licenses and spin-offs

Transfer to society

Jolt, ICIQ's spin-off, secures €6 million in funding to boost its green hydrogen technology

R&D research projects with industry partners

CO_2 capture, use and storage (CCU)

Artificial photosynthesis

Hydrogen and sustainable fuels

Materials and polymers

Solar cells

ICIQ – KTT collaborates with Hemostatics and CUN to optimise a revolutionary therapy against disabling and lethal hemorrhages

Health research for pharma companies and research institutions

Drug discovery and development

Custom synthesis

Molecular modelling and computational chemistry

Polymorphism, salts, and co-crystals screening

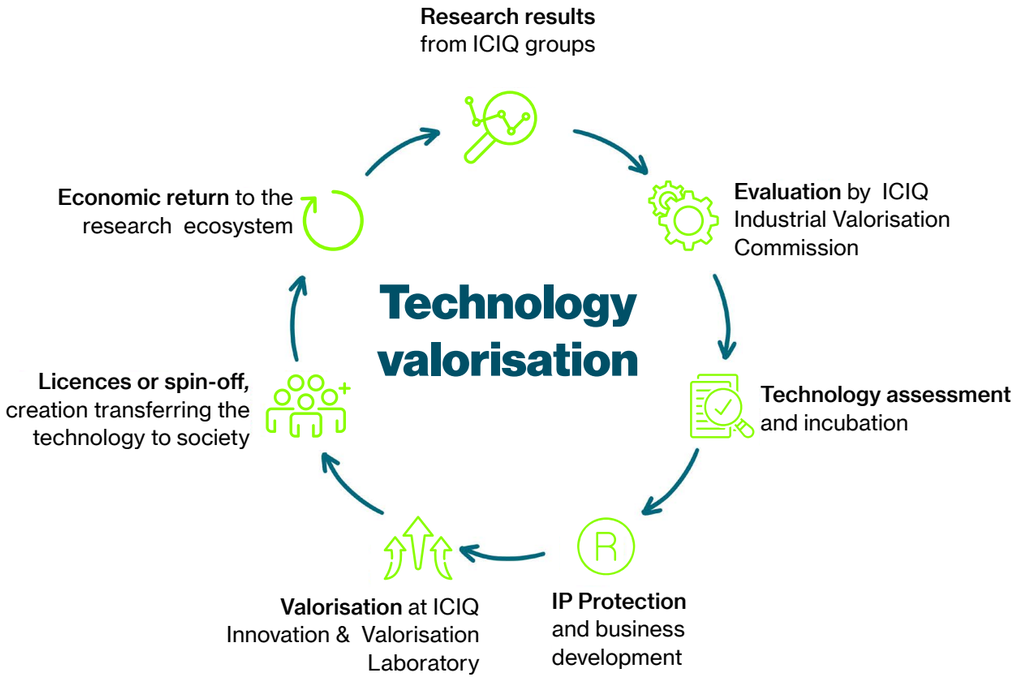
Crystallisation

ICIQ and IDIBGI join forces in a pioneering collaboration to discover new therapeutic targets against cancer

Industrial & Intellectual Property

ICIQ – KTT identifies, with the research groups, the technologies with significant commercial or social value. A solid intellectual and industrial property management strategy is developed through a process of patenting and other forms of protection to ensure that research results are legally protected and successfully commercialised.

In addition to intellectual property protection, industrial property is also managed with licensing agreements and other forms of technology transfer with companies to ensure that research results reach the market and have a social impact.



ICIQ has 18 active patent families, and three licensing opportunities:

PCT/EP2022/085791 PCT Priority: 15/12/2021

BIO-BASED EPOXY RESIN COMPOSITION FOR ADHESIVE AND COATINGS APPLICATIONS

Inventors: Arjan Kleij; Jeroen Rintjema; Fernando Bravo Lara; Carles Alemán Llansó; Elaine Armelin Diggroc

Technology: Post-modification of copolymer derived from limonene and CO_2 through cross-linking strategies.

Application: Obtaining epoxy resins of natural origin for the manufacture of thermostable materials.

Relevant technology transfer activities: Market study through the Gínjol fund patents 2022. AGAUR Innovators project request for the optimisation of obtaining raw materials. Scaling study and validation tests with a leading global polymers company.

EP22382472.3 European Application Priority: 17/05/2022

CYCLOPROPENIUM COMPOUNDS, PROCESS FOR THEIR PREPARATION AND USE

Inventors: Marcos García Suero; Hangfei Tu; Aliénor Jeandin

Technology: New reagent used for the cyclopropanation reaction.

Application: Drug synthesis, late-stage functionalization.

Relevant technology transfer activities: Thermal stability studies to determine the feasibility and industrial process safety. Contact with companies in the pharmaceutical, chemical and venture capital sectors.

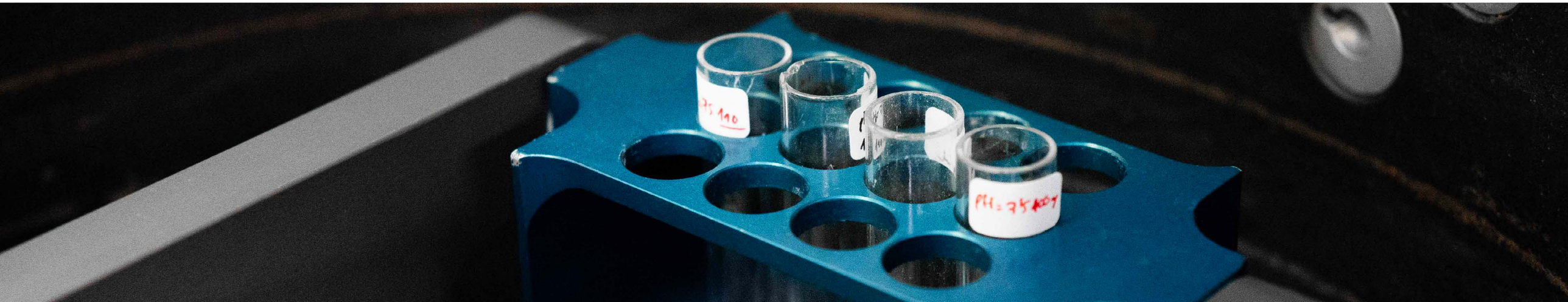
EP 23382578.5 European Application Priority: 15/12/2023

METHOD OF SYNTHESIS OF TRANSITION METAL NITRIDES AND THEIR USE WHEN THEY HAVE TWO, THREE OR FOUR METALS AS CATALYSTS FOR THE OXYGEN EVOLUTION REACTION

Inventors: José Ramón Galán-Mascarós

Technology: One-step synthesis of multimetallic transition metal nitrides (TMNs) using readily available and inexpensive metal salt precursors.

Application: Catalyst that reduces hydrogen production costs by increasing its lifespan and reducing energy consumption.



Research projects with industry

Contract research projects with industry are an opportunity to apply ICIQ research to solving specific problems and advanced processes of companies and other interested parties. During 2023, more than 60 external R&D&I collaborations have been developed, which are detailed below according to the Technology Development Units of ICIQ – KTT:

Technology Development Units ICIQ-KTT	Projects and services	Total income 2023
ICIQ- Crysforma Development of the pharmaceutical solid state	55	1,942,371.13 €
ICIQ - Innovation & Valorisation Lab Transfer of ICIQ research to society	6	
ICIQ - Molecular Medicine Drug discovery and development	3 (one with industry, two with research institutes)	

Technology Development Units

The Technology Development Units are an essential part of ICIQ – KTT. They design and develop new products with added value and a multidisciplinary vision.

ICIQ Knowledge and Technology Transfer
Crysforma

A unit specialised in the development of technologies and services related to the pharmaceutical solid state. This unit collaborates with national and international fine chemical and pharmaceutical companies. During 2023, Crysforma has collaborated with 32 companies.

ICIQ Knowledge and Technology Transfer
Innovation & Valorisation Laboratory

Unit dedicated to the valorisation and innovation projects of ICIQ technologies to optimise, scale and transfer them to industry and society. The unit also develops R&D&I projects with industry, either as punctual projects or long-term collaboration in which research groups from the centre can also participate. During 2023, the unit name was changed from CSOL to adapt it to its purpose.

ICIQ Knowledge and Technology Transfer
Medicinal Chemistry

Unit that works on drug discovery and drug development processes, specialising in molecules with therapeutic potential, using a combination of synthetic chemistry, biology and computational modelling. Its goal is to discover new drugs to treat diseases such as cancer and infectious diseases, collaborating closely with the pharmaceutical industry and other research centres to innovate in therapeutic solutions.

Spin-offs

ICIQ provides support in the protection, commercialisation and application of the technologies developed by the institute researchers. It offers them support and advice during the initial stages of their creation, as well as technical support and access to the centre facilities and resources. In addition, ICIQ maintains a close relationship with its spin-offs for a period to guarantee the business success of the project. The centre currently has 3 spin-offs:

JOLT

Created in 2022, the most recent spin-off of ICIQ has the objective of developing catalytic solutions for water electrolysers.

During 2023, it secured 7 million euros from investors to start large-scale production and enter the market. The spin-off will open a new headquarters in Hospitalet de Llobregat in 2024.

Orchestra Sci.
Well-Tempered Tech

Created in 2017, the spin-off offers a disruptive innovation arising from a patented additive that allows CO_2 to be separated and purified under a wide range of working conditions.

TREELLUM TECHNOLOGIES

Established in 2020, it produces scientific instruments for photochemistry, designing parallel photoreactors that contribute to improving chemical research.

Networks and technology platforms

Participation in networks and technology platforms is part of the strategy of ICIQ - KTT to guarantee visibility, dissemination and knowledge exchange with other institutions.

ICIQ establishes institutional relationships and attends activities and events to promote collaborations within the technological field of chemistry. Among other networks and platforms, the following stand out:

biocat

The life sciences cluster in Catalonia, which promotes and supports structures for knowledge and innovation transfer.

bist
SCIENTIFIC COMMUNITY

It is a collaboration initiative among several research centres aimed at promoting scientific and technological research of excellence in Catalonia.

ChemMed Tarragona
MEDITERRANEAN CHEMICAL CLUSTER

Industrial, logistics, academic and scientific chemical cluster in the Tarragona area. It includes over 100 companies in its industrial and logistics area of influence, and research centres such as ICIQ or Rovira i Virgili University.

ACCIÓ Generalitat de Catalunya
tecnio catalonia
Vigència: 30/12/2024

This is the seal awarded by the Generalitat de Catalunya, through ACCIÓ, to identify and give visibility to technology developers of the Catalan R&D&I system. They possess technological capabilities and the ability to transfer them to strengthen the business fabric and enhance the Catalan innovation ecosystem internationally.

SUSCHEM ES
Química Sostenible • by Feique

As part of SusChem España, ICIQ is also a member of the European Technology Platform for Sustainable Chemistry.

SOMM
EXCELLENCE
ALLIANCE

SOMMa is the alliance of Severo Ochoa Centres and María de Maeztu Units aimed at promoting Spanish excellence in research and enhancing its social impact at both national and international level.

CERCA
Centres de Recerca de Catalunya

Network of reference research centres in Catalonia that promotes quality research and collaboration between members. ICIQ is part of this network and is committed to scientific excellence and the development of research in Catalonia.

Communication & Outreach

Media

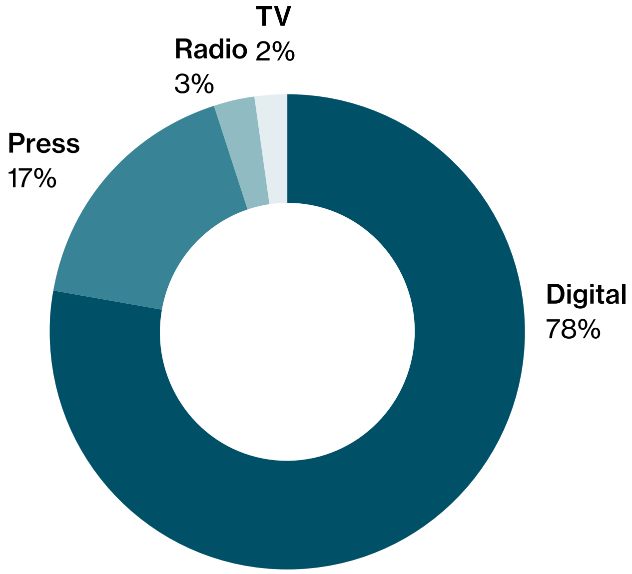
During the year 2023, ICIQ Communication and Image Unit has determinedly pursued the objective of disseminating the mission of the Institute and achievements, as well as the contributions of its research groups to society. Through close collaboration with journalists from the mainstream media, we have managed to generate a considerable number of journalistic impacts, going beyond the 800 impacts in traditional media and other platforms, such as blogs.

In terms of audience, our initiatives have reached a total of 265,920,466 people. In terms of number of publications, ICIQ has occupied a prominent place in 71 international media, far from the presence in national media, where 739 impacts have been registered. In this sense, we recognize an opportunity to expand ICIQ position at the international level, especially in the field of science communication.

In line with our diversity of contents, institutional news have occupied the first position with more than 600 impacts, followed by other topics such as research, knowledge transfer and outreach.

It is relevant to underline that these data reflect a significant upward trend, above the 2022 results, on media impact was established at 399 media appearances.

Media presence by typology



Webpage

ICIQ website is presented as a comprehensive platform that encapsulates all of the ICIQ contents, with accessibility ranging from the main scientific publications to the highlights and events section.

According to the data collected by Google Analytics 4 more than 71,000 users explored more than 522,000 pages (from 4th May until the end of the year due to changes in the Google Analytics service). It is remarkable that the pages dedicated to research groups and scientific publications have been the most visited. The comparison with the 2022 data is not feasible, as the data for 2023 is presented with a slight slippage at the beginning of the collection of these data. Even so, this analysis provides a clear view of the attractiveness and intensive use of the scientific content on the website.

71,000
users

522,719
pages visited

This high level of interaction makes the website an essential and well-used tool for the community, which not only seeks information on the latest research but also a deeper understanding of scientific advances and the results of the research carried out at ICIQ. Thus, the website continues to be a key source of knowledge about ICIQ research to a wide and diverse audience.

Social Media

Through our Social Media profiles, we continue to share ICIQ discoveries, initiatives and inspiring stories, connecting with diverse audiences and promoting the dissemination of scientific knowledge.

2023 has been an extraordinarily positive year for ICIQ presence with an increase in followers on all channels.

Particularly, LinkedIn has experienced exponential growth, with a 28% increase in followers compared to the previous year. On the other hand, Instagram, despite being the platform with the fewest followers, has indexed more engagement, demonstrating that the quality of the content is as important as the number of followers.

#ICIQWomen

In the digital sphere, an annual campaign was carried out to raise the visibility of ICIQ Women with the aim of encouraging scientific vocations in young people and girls. Twelve nominated researchers took part in the campaign on Twitter, achieving more than 29,000 impressions.

11,269
Followers in X (Former Twitter)

8,230
Followers in LinkedIn

2,871
Followers in Instagram

1,463
Followers in Facebook

1,550
subscribers in YouTube

Events

Events are an essential part of ICIQ, as they provide opportunities for dialogue, collaboration and exchange of scientific knowledge, but they are also a platform for positioning and attracting new audiences. Through a wide range of activities and events, ICIQ fosters interaction between researchers, students, professionals and the community in general. From seminars and conferences to cultural celebrations, events at ICIQ reflect the institutional commitment to the dissemination of knowledge, interdisciplinary collaboration and community integration.

BASF-ICIQ Seminar Programme

The BASF-ICIQ Seminar Programme is a joint initiative between BASF and ICIQ, with the aim of highlighting significant advances in chemical research and development. Initiated in 2004, this programme consists of a series of specialised seminars that address diverse topics related to the ICIQ research areas. Each session, led by renowned international experts, provides a platform for the exchange of knowledge and exploration of the latest trends in the world of chemistry. This collaboration strengthens the links between academic research and industry, contributing to the continuous advancement of chemical science and its practical application. [5]

Conferences and Symposiums:

07/03/23

Frontiers in Renewable Fuels and Chemicals

Dr. Carla Casadevall, Prof. Julio Lloret-Fillol

The “Frontiers in Renewable Fuels and Chemicals” event will highlight innovations in green technologies for the production of sustainable fuels and chemicals. World experts addressed the challenges and opportunities in this emerging field, exploring solutions for a more sustainable future.

11/05/23

OpenData Day

Prof. Carles Bo

At the First ICIQ’s Open Data Day, participants will explore the importance of open access to scientific data. Strategies were discussed to improve transparency and collaboration in the chemical research, fostering a culture of data sharing for scientific progress.

05-09/06/23

4th International Conference on Proton-Coupled Electron Transfer

Prof. Antoni Llobet, Dr. Carlos García Bellido, Dr. Anne Mary Beiller

The 4th PCET Conference brought together international experts to discuss the latest trends in the fundamentals of PCET (Proton-CoupledElectron Transfer). The event highlighted innovative research in this field, exploring applications in energy conversion, catalysis and other relevant areas of chemistry.

[5] See the full list of all the seminars and their speakers in Annex 3.

09/06/23

UCB Lecture Award

Prof. Marcos García Suero

The first UCB Lecture Award, organised by ICIQ and UCB Biopharma, recognised Professor Matthew Gaunt from the University of Cambridge. This event highlighted advances in organic chemistry and the synthesis of natural products, and provided a platform for collaboration and exchange of expertise between experts in the field.

21/06/23

2nd Edition of BASF-ICIQ Awards in Innovation and Entrepreneurship

ICIQ

The second edition of the BASF-ICIQ Awards recognised talent and innovation in chemistry in three categories: best doctoral thesis, best patent and entrepreneurship project. This event will be an opportunity to celebrate exceptional contributions to science and encourage collaboration between industry and academic research.

3/07/23

Industrial decarbonisation: a priority for Catalonia

ICIQ-URV

The conference on industrial decarbonisation organised by ICIQ brought together business leaders, research centres, public authorities and representatives of society to address the challenges and opportunities related to the decarbonisation of the industrial sector. This event will highlight the importance of multi-sectoral collaboration to move towards a more sustainable future and reduce carbon emissions.

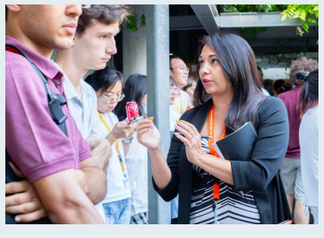
18/07/23

Open LICROX Symposium

Prof. Antoni Llobet, ICIQ Projectes

LICROX, a European project coordinated by ICIQ, ended with a symposium to share the progress made throughout the project, highlighting the results and contributions of the project in the field of chemistry, underlining the importance of collaboration and interdisciplinary research in solving scientific challenges.

13-15/09/23



ICIQ School

Prof. Rubén Martín, Prof. Marcos García Suero

ICIQ inaugurated the 12th edition of the ICIQ School with a prestigious international chemistry symposium. This event marked the beginning of a first-class educational programme, offering a platform for dialogue and exchange of ideas between researchers from all over the world.

18-22/09/23

Solar2Chem Conference

Prof. Núria López, Solar2Chem Consortium

The Solar2Chem 2023 conference inaugurated a pioneering revolution in solar conversion to chemicals. The event brought together experts from around the world to explore the latest innovations in this crucial area for a sustainable future.

22/09/23

ICIQ Alumni Day

ICIQ

ICIQ held the third edition of Alumni Day, reinforcing connections and sharing success stories among former members of the community. The event served as a platform to inspire and encourage collaboration between current and former ICIQ members, highlighting their achievements and contributions to science and society.

04-05/10/23

Hydrogen Horizons

ICIQ

ICIQ brought together European leaders in the field of hydrogen to discuss its energy potential. The event served as a platform to explore the opportunities and challenges related to the use of hydrogen as a sustainable energy source, highlighting the key role of research and collaboration in this emerging field.

23-26/10/23

3D-ED Workshop

Characterisation Technologies Department (ICIQ-CTD)

Researchers from several European centres took part in a training session at ICIQ to learn about the advances of 3D electron diffraction (3D-ED). This innovative technology offers new perspectives in the determination of complex molecular structures, consolidating ICIQ position as a leading research centre in this field.

30-31/10/23

Phd Day

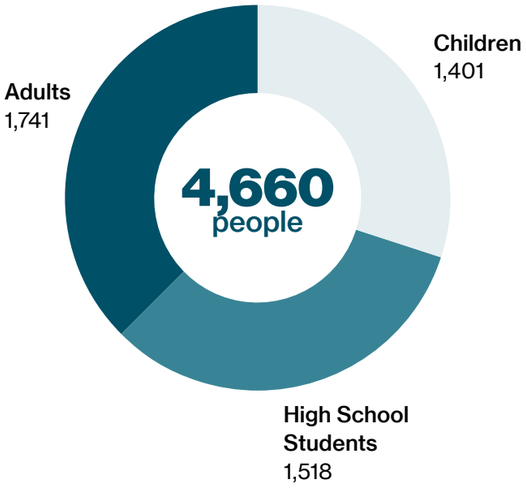
ICIQ-URV

The 7th edition of the ICIQ-URV PhD Day was a success, offering a platform for PhD students to present their research work in front of experts and peers. This event promoted interdisciplinary collaboration and showcased innovation and emerging talent in chemical research.

Outreach and Scientific Education

At ICIQ we recognise the importance of connecting the community and fostering a broader understanding of chemical research. Through different activities in different formats we work to disseminate research to different audiences and encourage dialogue on the challenges and opportunities offered by science.

35 Outreach Activities



Schools and institutes

The best way to bring science closer to young people is through experimentation. That is the reason why we participate in different innovative programmes in collaboration with entities such as Catalunya-La Pedrera Foundation and La Canonja City Council.

- **Bojos per la química:** In 2023, the 10th edition of this programme was held, which allows bright students to enjoy an experimental learning experience during 13 Saturdays a year. The programme encourages critical thinking and involves different people from the school, offering them an overview of research in chemistry.
- **Young people and science:** Programme to welcome three students for two weeks in July to three research groups at the centre.

- **La Canonja green, educational and scientific project:** The collaboration with La Canonja City Council represents a valuable opportunity to further the promotion of young researchers in their pre-doctoral stage. In addition, from January to June, an educational programme focused on green chemistry was held at La Canonja school, which included presentations and practical experiments, thus strengthening the link between the educational community and the world of science. A glass blowing workshop was also held this year for the La Canonja Science Week.
- **Summer camps:** The aim of the summer camps is to introduce boys and girls to the world of chemistry, offering them a real experience in the outreach laboratory. The aim of this stay is for them to have a first contact with the world of chemistry, to carry out experiments in the scientific laboratory and to learn how to make oral presentations of the results obtained.
- **Workshops:** ICIQ offers themed science workshops in which schools and institutes approach curricular concepts of chemistry as aspects of everyday life. In 2023, 22 high school workshops and 10 primary school workshops were held, bringing together more than 1,000 students.
- **Inspira STEAM:** This is a pioneering project aimed at 5th and 6th grade students that offers sessions in different schools based on awareness-raising and guidance actions, given by professionals from the world of research, science and technology. In 2023 the programme will reach around 1,200 children.
- **Experimenta Challenge:** Training programme promoted by the URV and financed by the FECYT, which aims to provide training in different areas. From ICIQ we are in charge of the final award “Campus Experimenta” of the training programme, where the 3 winning teams enjoy a workshop in which they are scientific police. In the first edition, ICIQ participated with a workshop on emulsions.

General Public

- **Day of Women and Girls in Science - 11th February:** Every year ICIQ joins celebrations of this day with the aim of promoting gender equality and inspire women and girls in the field of STEAM. Among other things, there were informative workshops, collective breakfasts and other dissemination activities to create an inclusive and egalitarian environment in science.
- **European Research Night:** ICIQ participated in the 6th edition of this international event, in which more than 3,000 persons gathered to enjoy scientific events. Concretely, ICIQ has organised four workshops: 1) Electrons; 2) The colours of chemistry; 3) Glass blowing workshop; and 4) The use of light to produce hydrogen fuel, in collaboration with the H2CAT network. ICIQ has also participated in the "microexerrades" held in Reus with the slogan: "Nanorobots to decontaminate water".
- **Science Week:** The 28th Science Week held in November 2023 included workshops and guided visits, as well as a lecture on "Chemistry of money" in collaboration with the Bank of Spain.

Blau de Prússia: a scientific divulgation podcast

During 2023, the second season of podcast 'Blau de Prússia' was launched with great success, offering 15 new episodes and accumulating more than 50,000 reproductions. The season counted with the participation of 32 researchers from ICIQ, who shared their knowledge on different topics with a wide and diverse audience. Moreover, in recognition of the quality of the project, 'Blau de Prussia' was selected as a finalist in the second edition of the Sonor Awards, standing out among over 200 applications. Finally, in June, the podcast was selected among the three finalists of the Local Communication Awards 2023 in the category of "Best multimedia and transmedia content", reinforcing its prestige and impact in the world of media and science communication.

>28,000
listeners

Annex 1
Projects and Grants

Table 1. European competitive research projects obtained during the year 2023

Project title	Project type	Organisation	Amount (€)	PI
Molecular receptors enrich methylated and acetylated peptides for ultra-sensitive proteomics to explore the hidden modified proteome in disease (101131120-ENRICH)	MSCA-SE	European Commission	69,000	P. Ballester
Sustainable Photo-ElectRochemical VALorization of flue gases (S101115456-SUPERVAL)	EIC-Pathfinder-Challenges	European Commission	650,750	JR.Galán-Mascarós
PHOTOelectrocatalytic systems for Solar fuels energy INTegration into the industry with local resources (101118129-PHOTOSINT)	HORIZON EUROPE-CL5	European Commission	467,812.6	J. Lloret- Fillol
Engineering Excited States, Orbital Coupling and Quantum Coherence Phenomena in Photoelectrochemical Energy Conversion Devices (101097684-EXCITED)	ERC-AdG	European Commission	2,500,000	E. Palomares
Flexible Perovskite Solar Cells with Carbon Electrodes (101122283-PEARL)	HORIZON EUROPE-CL5	European Commission	420,312.5	E. Palomares

Table 2. Competitive research projects of the Spanish Government obtained during the year 2023

Project title	Project type	Organisation	Amount (€)	PI
New inter- and intramolecular reactions catalyzed by gold (PID2022-136623NB-I00 -	Proyectos I+D Generación de conocimiento	MICIU	450,000	A. Echavarren
A new catalytic platform for the enantioselective functionalizations of CC bonds (PID2022-140286NB-I00 - FUN-C)	Proyectos I+D Generación de conocimiento	MICIU	243,750	M. García-Suero
Molecular Redox Catalysts for Green Energy Applications (PID2022-140143OB-I00 - EnergyCat)	Proyectos I+D Generación de conocimiento	MICIU	312,500	T. Llobet
Engineering Selective and Durable Catalysts for Artificial Photosynthesis towards Sustainable Chemistry Production (PID2022-140142OB-I00 - ESDuCAPS)	Proyectos I+D Generación de conocimiento	MICIU	281,250	J. Lloret-Fillol
Electrovoltaic materials for CO_2 reduction (PID2022-139866NB-I00 - ElectroVolt)	Proyectos I+D Generación de conocimiento	MICIU	332,500	E. Palomares
Photoactive microswimmers for selective catching, detection and removal of emerging pollutants (PID2022-136886OA-I00 - PhotoClean)	Proyecto I+D Generación de conocimiento	MICIU	137,500	K. Villa
Ensayo clínico fase I de un nuevo agente antifibrinolítico, el compuesto CM-352, con una ruta de síntesis eficiente, dirigido al control de hemorragias discapacitantes y letales (CPP2022-009643)	Colaboración-Público Privada	MICIU	355,575	F. Bravo (CSOL)
Semiconductors with perovskite crystalline structure with null o residual content of lead for light emitting memories (LEMOSKITES) (CNS2022-135483)	Consolidación Investigadora	MICIU	191,967	E. Martínez (Prof. Palomares group)

Table 3. Competitive research projects of the Generalitat de Catalunya obtained during the year 2023

Project title	Project type	Organisation	Amount (€)	PI
Expanding the commercialization of ioChemBD Premium to new geographical markets and customer segments (2022 INNOV 00019 - ioChemBD-EXPAND)	Innovadors	AGAUR	84,000	C. Bo

Table 4. Competitive research projects from other financing agents obtained during 2023

Project title	Project type	Organisation	Amount (€)	PI
Proyectando los límites de la electrocatálisis de CO_2 a combustibles mediante el desarrollo automatizado de catalizadores (ElectroFuel)	Fundación Ramón Areces	Ramón Areces	128,000	J. Lloret-Fillol
Photo-rechargeable Nanorobots for Fungal Biofilm Eradication (NanosFun)	Fundación BBVA	Fundación BBVA	40,000	K. Villa

Tables 5-8 show all the projects funded by public agencies in force during 2023, as well as the amount obtained and the principal investigator (PI).

Table 5. Competitive research projects of the NCCR Catalysis in force in 2023

Project title	Amount (€)	Time period	PI
Statistical learning for converging strategies in thermal and electrochemical conversion of small molecules	120,000	01/04/2021-31/07/2024	N. López
Smart characterisation of heterogeneous catalysts: EXAFS for Single Atom Catalyst	102,406	01/08/2022-31/07/2024	N. López

Table 6. Competitive research projects of the Generalitat de Catalunya in force by 2023

Project title	Amount (€)	Time period	PI
Química Supramolecular Interdisciplinar (2021 SGR 00851)	40,000	2022-24	P. Ballester
Organometallic Chemistry in Organic Synthesis (2021 SGR 01256)	60,000	2022-24	A. Echavarren
GdCA (2021 SGR 01154)	60,000	2022-24	J.R. Galán-Mascarós M. H. Perez-Temprano
Research Group Kleij (2021 SGR 00853)	60,000	2022-24	A. Kleij
Theoretical Heterogeneous Catalysis Group (T-HeCat) (2021 SGR 01155)	60,000	2022-24	N. López
Grup de Catàlisis Redox (Red-Cat) (2021 SGR 01583)	48,555	2022-24	T. Llobet
Prof. Lloret research laboratory (2021 SGR 01260)	40,000	2022-24	J. Lloret-Fillol
Grup d'activació catalítica d'enllaços inerts - CATINERT (2021 SGR 01258)	60,000	2022-24	R. Martín
Grup de recerca en materials i dispositius optoelectrònics (2021 SGR 01261)	40,000	2022-24	E. Palomares E. Romero
Desenvolupament de plataformes de detecció electroquímica per a la determinació selectiva in situ de disruptors endocrins (2021 PROD 00026 - SelSens)	48,555	2022-24	T. Llobet
Intelligent flow photoreactor to industrialize photochemical reactions (2021 PROD 00043 - PHOTOSCALE)	99,961	2022-24	J. Lloret-Fillol
Artificial Intelligence for Safe Medicines (2021 PROD 00042 - AI4SAFEMEDS)	100,000	2022-24	F. Maseras

Table 7. Competitive research projects of Spanish Government in force in 2023

Project title	Project type	Amount (€)	PI
Molecular Containers with Polar Cavities and Versatile Functions (PID2020-114020GB-100 - COMPOFUN)	Proyectos I+D Generación conocimiento	217,800	P. Ballester
Solar catalysis for a renewable energy Future (PLEC2021-007906 – SOLFuture)	Proyectos Líneas Estratégicas	169,075	E. Palomares P. Ballester
Difractómetro de Electrones para la Determinación Estructural de Materia Nanocristalina (EQC2021-006956-P)	Equipamiento científico-técnico	1,495,000	J. Benet (X-Ray unit)
Computational Chemistry 4.0 for a Sustainable Development (PID2020-112806RB-100)	Proyectos I+D	121,000	C. Bo
Linked chemical databases to boost materials discovery (TED2021-132850B-I00 - Data4Mat)	Proyectos Transición Ecológica y Digital	172,500	C. Bo
Movilidad iónica y Espectrometría de Masas con fuentes de ionización ESI/MALDI: un escenario para afrontar nuevos retos (EQC2021-007052-P)	Equipamiento científico-técnico	861,803	N. Cabello (HRMS unit)
Catalytic methods based on gold or other electrophilic metals (PID2019-104815GB-100 - CATMETGOLD)	Proyectos I+D	339,300	A. Echavarren
FUNDACIO INSTITUT CATALA D'INVESTIGACIO QUIMICA (CEX2019-000925-S)	Severo Ochoa	4,000,000	A. Echavarren
New carbyne transfer catalysis in organic chemistry (PID2019-104101GB-100 - CARBYNOID)	Proyectos I+D	145,200	M. García-Suero
Late-stage diazomethylations to impact urgent & unmet medical needs (PDC2021-121180-I00 - Late-need)	Prueba de concepto	109,250	M. García-Suero
New boundary conditions for advanced electrocatalysis: from magnetic field effects to solventless configurations (PID2021-124796OB-I00 - NEWBOUND)	Proyectos I+D	314,600	J. R. Galán-Mascarós
Low-pressure CO_2 CAPture technology for the fermentation industry (PDC2022-133214-I00 - COCAP)	Prueba de Concepto	149,500	J. R. Galán-Mascarós

Advancing the Catalytic Construction of Quaternary Stereocenters (PID2020-112684GB-100)	Proyectos I+D Generación conocimiento	217,800	A. Kleij
Design and Scale Up of Biobased Functionalized Polycarbonates for Adhesive and Coating Applications (PDC2021-120952-I00 - MacroLemon)	Prueba de Concepto	120,750	A. Kleij
Simulations of dynamic materials for photo-electro-catalytic processes (PID2021-122516OB-I00 - SMELT)	Proyectos I+D	181,500	N. López
Development of Molecular Catalysts Relevant for Solar Fuels Generation (PID2019-111617RB-100 - CatFuel)	Proyectos I+D	254,100	A. Llobet
Development of new catalysts for oxidation and reduction chemistry in the context of Artificial Photosynthesis (PID2019-110050RB-100 - AP2Chem)	Proyectos I+D	1694,00	J. Lloret-Fillol
Fabrication of Highly Efficient Electrodes and Test for the Production of Hydrogen under Industrial Relevant Conditions in Anionic Membrane Exchange Electrolyzers (PDC2021-121185-I00 - Electra H2)	Pruebas de Concepto	143,750	J. Lloret-Fillol
Towards Automatized Development of Electrocatalysts for CO_2-to-Fuels (TED2021-132790B-I00 - Auto4Fuel)	Proyectos Transición Ecológica y Digital	302,450	J. Lloret-Fillol
Fabrication of Highly Efficient Electrodes for the Production of CO under Industrial Relevant Conditions in Electrolyzers (PDC2022-133451-I00 - Electra-4-Fuel)	Prueba de Concepto	115,000	J. Lloret-Fillol
De novo sp3 carbon-carbon and carbon-heteroatom bond-forming reactions via catalytic functionalization of native functional groups (PID2021-123801NB-I00 - CAT-NAT)	Proyectos I+D	387,200	R. Martín
Computational sustainable chemistry (PID2020-112825RB-100)	Proyectos I+D	145,200	F. Maseras
New Synthetic Methods Enabled by the Photochemistry of Organic Molecules and Their Use in Drug Discovery and Bioconjugation (PID2019-106278GB-100 - PHOTO-N-TOOLS)	Proyectos I+D	254,100	P. Melchiorre

Solar catalysis for a renewable energy Future (PLEC2021-007906 - SOLFuture)	Proyectos líneas estratégicas	198,500	E. Palomares
Photocatalytic CO_2 Reductions by Green Hydrogen (PLEC2021-007831 - PHOTORED)	Proyectos Transición Ecológica y Digital	198,500	E. Palomares
Solar Energy Driven CO_2 Reduction(TED2021-130206B-C21 - SOLARCO)	Proyectos Transición Ecológica y Digital	234,485	E. Palomares
Mechanism-driven Design of 3d Transition Metal Catalyzed CH Functionalization Reactions (MD3dCAT - PID2020-1 12733GB-100)	Proyectos I+D Generación conocimiento	157,300	M. H. Pérez-Temprano
The role of coherence in photosynthetic light-harvesting: does energy transfer proceed via a quantum-coherent mechanism? (NatureQuantumET) (PID2021-129065OA-I00)	Proyectos I+D	169,400	E. Romero
Design and construction of bio-inspired chromophore-protein assemblies for efficient and sustainable solar-energy conversion to charge separation (SolarBioCharges) TED2021-132747A-I00	Proyectos Transición Ecológica y Digital	189,750	E. Romero
De la gestión de proyectos a la gestión de la investigación (NEXT-ICIQ) GPE2022-000953	Preparación y Gestión de Proyectos Europeos 2022	248,540	L. López (RPIC)

Table 8. Competitive research projects of the European Union in force in 2023

Project title	Project type	Amount (€)	PI
Bioinspired Catalytic Metallofoldamers (835080-Foldmetcat)	ERC-AdG	2,500,000	A. Echavarren
DistributEd Chemicals And fuels production from CO_2 in photoelectrocatalytic Devices (862030-DECADE)	NMBP	538,937.5	J. R. Galán-Mascarós E. Palomares
Novel photo-assisted systems for direct Solar-driven redUctioN of CO_2 to energy rich CHEMicals (884444-SUN2CHEM)	LC-SC3	323,750	J. R. Galán-Mascarós
New carbon reactivity rules for molecular editing (865554-CARBYNE)	ERC-CoG	2,000,000	M. García-Suero

Training the next generation of scientists in solar chemicals for a sustainable Europe by hybrid molecule/semiconductor devices (861151-SOLAR2CHEM)	MSCA-ITN	498,324	N. López
Heterogenous Photo(electro)-catalysis in Flow using Concentrated Light: modular integrated designs for the production of useful chemicals (862453-FlowPhotoChem)	NMBP	492,500	N. López
Cooperation towards a sustainable chemical industry (859910-CO_2PERATE)	MSCA-ITN	501,809.76	R. Martín
Escaping from Flatland by "de novo" Catalytic Decarboxylation Techniques (883756-NOVOFLAT)	ERC-AdG	2,500,000	R. Martín
Light assisted solar fuel production by artificial CO_2 Reduction and water Oxidation (951843-LICROX)	FETPROACT	631,937	A. Llobet
COmbined suN-Driven Oxidation and CO_2 Reduction for renewable energy storage (101006839-CONDOR)	LC-RES	448,118.75	A. Llobet
Inhalable Aerosol Light Source for Controlling Drug-Resistant Bacterial Lung Infections (863102-Light4Lungs)	FETOPEN	372,500	E. Palomares
Innovative photocatalysts integrated in flow photoreactor systems for direct CO_2 and H_2O conversion into solar fuels (101022202-NEFERTITI)	LCE-RES	363,750	E. Palomares
Engineering Bio-Inspired Systems for the Conversion of Solar Energy to Hydrogen (805524 - BioInspired_SolarH2)	ERC-StG	1,500,000	E. Romero
SUNER-C: SUNERGY Community and eco-system for accelerating the development of solar fuels an chemicals (101058481 - SUNER-C)	RESILIENCE	245,075	RPIC

Reversible Heterocyclic Mechanophores for Dynamic Bulk Materials (101041759 - ReHuse)	ERC-StG	1,498,401	J. Berrocal
Biocarbon based Polymers for Sustainable Material Development (101073223 - D-Carbonize)	MSCA-DN	503,942	A. Kleij
Optimised Halide Perovskite nanocrystalline based Electrolyser for clean, robust, efficient and decentralized pRoduction of H_2 (101071010 - OHPERA)	EIC-Pathfinder-Challenges	450,313	N. López
Breaking the barrier - An integrated multidisciplinary approach to kill Gram-negative bacteria through existing antibiotics by making their outer membrane permeable (101072632 - BREAKthrough)	MSCA-DN	251,971	R. Martín
Engineering of Photo-rechargeable Nanoswimmers using Multicomponent Heterojunctions (101076680 - PhotoSwim)	ERC-StG	1,500,000	K. Villa

Table 9. Predoctoral Grants obtained at ICIQ during 2023

Name of Programme	Organisation	No. of Grants	Total Amount (€)
Formació de Personal Investigador Joan Oró (FI)	AGAUR	2	143,536.8
Formación de Profesorado Universitario (FPU)	MICIU	1	103,796.96
Formación de Personal Investigador (FPI)	MICIU (AEI)	14	1,564,612.00

Table 10. Postdoctoral grants awarded to ICIQ during 2023

Project title	Project type	Organisation	Amount (€)	PI
S/P-Coordinated Transition Metal Single Sites-doped Carbon Matrices as Electrocatalysts for Nitrogen Reduction (101106683 - GREEN)	MSCA-PF	European Commission	165,312.96	J. R. Galán-Mascarós
New late-stage functionalization reagents for the construction of chiral centers to impact drug discovery (101110735 - NAKED-C)	MSCA-PF	European Commission	165,312.96	M. García-Suero
The development of bio-supported homogeneous organocatalysts with improved recycling potential through sequential de- and re-polymerization and their use in CO_2 valorization catalysis (101110356 - RECIRCULATE)	MSCA-PF	European Commission	181,152.96	A. Kleij
Photocatalyzed enantiodivergent synthesis of homoallylic and carboxylic acids featuring heterodiaryl quaternary carbon stereocenters (101105057 - PEACE)	MSCA-PF	European Commission	165,312.96	A. Kleij
Molecular Catalyst Immobilized into Porous Photocathode for production of Solar fuel (101104639 - MolPPS)	MSCA-PF	European Commission	165,312.96	T. Llobet
Photoelectrochemical Oxidation of Methane using Single Atom Catalysts (101105451 - POMASAC)	MSCA-PF	European Commission	181,152.96	J. Lloret-Fillol
Fuel forming electrocatalysis: Devising multifunctional covalent organic frameworks with vinylenic linkage for electrocatalytic CO_2 reduction and water oxidation (101105393 - COFPOR-4-fuels)	MSCA-PF	European Commission	181,152.96	J. Lloret-Fillol
Development of new sp3 C–H carboxylation strategies via interrupted Ni-catalyzed chain-walking catalysis (101105032 - CARBO-CHAIN)	MSCA-PF	European Commission	165,312.96	R. Martín
Design of Bioinspired Chromophore-Protein Complexes for Color Converting Layers of Organic Light Emitting Diodes (101107810 - deBioLED)	MSCA-PF	European Commission	165,312.96	E. Romero
Expanding mechanochemistry through computationally-driven mechanistic understanding (2022 BP 00055)	BdP	AGAUR	152,348	F. Maseras
Organ-on-a-chip from tailor engineered bionanomaterials (RYC2022-035783-I)	RyC	MICIU (AEI)	244,350	A. Bachhuka
Aromative decarbenation reaction (JDC2022-049049-I)	JdlC	MICIU(AEI)	67,400	A. Echavarren
Development of carbyne transfer catalysis to impact health care and material science. (JDC2022-048825-I)	JdlC	MICIU (AEI)	67,400	M. García-Suero
Synthesis and applications of biobased polymers (JDC2022-048812-I)	JdlC	MICIU (AEI)	67,400	A. Kleij
First-row transition metal-catalyzed C-H functionalization reactions (JDC2022-048535-I)	JdlC	MICIU (AEI)	67,400	M. H. Pérez-Temprano

Table 11. Grants for hiring of personnel in force in 2023

Name of Programme	Organisation	No. of Grants
Marie Curie Individual Fellowships- Marie Sklodowska-Curie Actions	European Commission	19
Beatriu de Pinós	AGAUR	6
Formació de Personal Investigador Joan Oró (FI)	AGAUR	11
Formación de Profesorado Universitario (FPU)	MICIU (AEI)	7
Formación de Personal Investigador (FPI)	MICIU (AEI)	27
INPhINIT Incoming	Obra Social "La Caixa"	1
Ramon y Cajal	MICIU (AEI)	1
Juan de la Cierva	MICIU (AEI)	7
Investigo	AGAUR	8
Feodor Linen	Humbolt Foundation	1
Personal Técnico de Apoyo	MICIU (AEI)	1
Doctorat Industrial	AGAUR	1
Tecniospring Industry	Acció	1

Annex 2
Doctoral theses

Author	Title	Supervisor 1	Supervisor 2
Adriana Faraone	New Reactions in Metal-based amd Emzymatic Catalysis	Prof. Paolo Melchiorre	-
Fei Cong	Forging sp3 Architectures via sp3 C-C Bond Cleavage and 1,2-Alkylboration Strategies	Prof. Ruben Martín	-
Luis Gutiérrez Victoriano	Metal-Organic Frameworks and Covalent Organic Frameworks as Single-Site Catalysts for Organic Transformations	Prof. Julio Lloret-Fillol	-
Diego Garay Ruiz	Unweaving Complex Reactivity: Graph-Based Tools to Handle Chemical Reaction Networks	Prof. Carles Bo	-
David Pascual Gascón	Photoredox catalysis mediated by transition metal complexes. Towards challeging organic reductions.	Prof. Julio Lloret-Fillol	-
Jiahao Yu	Water Splitting Electrocatalysts in Acidic Media: In the Search for Non-noble Metal Alternatives	Prof. José Ramón Galán Mascarós	-
Alba Helena Pérez Jimeno	Studies on Gold(I) Complexes: from Chiral Catalysts to Elusive Intermediates	Prof. Antonio M. Echavarren	-
Ana Arroyo Bondía	Design of New Gold(I) Catalysts: Dissecting Electronic and Steric Effects	Prof. Antonio M. Echavarren	-
Aleria García Roca	Mechanistic Investigations on Transition Metal-Catalyzed Asymmetric Allylic and Propargylic Substitution Reactions	Prof. Arjan W. Kleij	-
Andrés Romero Navarro	Covalent & Supramolecular Phosphorus Ligands for Linear-Selective Hydroformylations	Prof. Anton Vidal Ferran	-
Emilien Le Saux	Photochemistry and Organocatalysis for Radical-Based Carbon-Carbon Bond-Forming Processes	Prof. Paolo Melchiorre	-
Eleni Georgiou	Photocatalytic strategies for the functionalization of pyridines	Prof. Paolo Melchiorre	-
Sara López Resano	Uncovering the Mechanistic Scenarios of Nucleophilic Couplings in Cp*Co Systems	Prof. Feliu Maseras	Prof. Mónica H. Pérez Temprano
Laura Talavera Codina	Functionalisation of sp3 C-O bonds and olefins enabled by nickel catalysis	Prof. Ruben Martín	-
Pavle Nikacevic	Atomistic Insights into Photocatalytic Mechanisms: Modeling Selected Processes with Density Functional Theory	Prof. Núria López	-

Xuetong Li	Silver-Catalyzed Cascade Conversions of CO_2 into Heterocycles	Prof. Arjan W. Kleij	-
Jordi Morales Vidal	Modelling of Catalytic Systems Towards Green Fuels	Prof. Núria López	Dr. Manuel A. Ortuño
Wei Zhou	New Photochemical Methods for Catalytic Radical Processes	Prof. Paolo Melchiorre	-
Xinyang Lyu	Nickel/Copper-Catalyzed C-C and C-N Bond Forming Reactions to Forge sp3 Carbon Linkages	Prof. Ruben Martín	-
Carlota Odena	Unravelling Mechanistic Underpinnings of Organometallic Nickel Chemistry and Applications into Medicinal Chemistry	Prof. Ruben Martín	-
Jiayu Zhang	Discovery of new reaction modes in organic synthesis triggered by HFIP	Prof. Mónica H. Pérez Temprano	-
Jixiang Ni	Ring-Opening of Cyclic Carbonates: From Fine Chemicals to CO_2-based Polymers	Prof. Arjan W. Kleij	-
Andrea Rivoli	Aryl-Extended Calix[4]Pyrrole Receptors with Metal Centers: Organometallic Receptors and Metallo-Macrocycles Based on Coordination Bonds	Prof. Pablo Ballester	-
Aliénor Jeandin	Synthesis of cyclopropenium cations by carbyne transfer catalysis and applications in novel cyclopropene syntheses	Dr. Marcos García Suero	-
Wenyun Yue	New Platforms for Incorporation of Fluorine-Containing Motifs	Prof. Ruben Martín	-
Eduardo García Padilla	Computational Guided Exploration into Gold(I)-Catalysed transformations	Prof. Antonio M. Echavarren	Prof. Feliu Maseras
Lucía Morán González	Decoding Chemical Processes: The Power of Data-Driven Descriptors	Prof. Feliu Maseras	-

Annex 3
BASF-ICIQ
Seminar Programme

Data	Speaker	Seminar title
17/1/23	**Prof. Dr. Javier Pérez-Ramírez**	Catalysis Engineering for Sustainable Development
27/1/23	**Prof. Eduardo Peris**	N-Heterocyclic carbenes as toolkits for the preparation of supramolecular assemblies and switchable catalysts
9/2/23	**Prof. Ian Tonks**	Ti-Catalyzed Nitrene Transfer Reactions: A Platform for Fundamental Reaction Discovery and Exploration
21/2/23	**Prof. Marta Sales Pardo**	A Bayesian Approach to Learning Mathematical Models from Data
23/2/23	**Prof. Naoto Chatani**	Chelation-Assisted C-F and C-H Functionalization Reactions
24/2/23	**Prof. Claudia Höbartner**	Fluorescent Functional Nucleic Acids by Chemical Synthesis and in Vitro Selection
3/3/23	**Prof. Silvia Osuna**	Can We Rationally Design Efficient Enzymes?
7/3/23	**Prof. Marc Robert**	CO_2 Cascade Electroreduction with 6 Electrons and 6 Protons. Why Can Co Phthalocyanine Catalyze the Reduction of CO to Methanol, While Using CO_2 as Substrate it Mainly Affords CO?
7/3/23	**Prof. Marcella Bonchio**	Molecular Photosynthesis: Such Stuff as Dreams are Made On
7/3/23	**Prof. Vincent Artero**	Proton Relays in Molecular Electrocatalysis: How do They Allow for Reversible Behaviour?
7/3/23	**Prof. Erwin Reisner**	Solar Panels for Light-to-Chemical Conversion
21/3/23	**Prof. Andy McNally**	Selective Functionalization of Pyridines, Diazines and Pharmaceuticals via Unconventional Intermediates
14/4/23	**Dr. Teresa Ortner**	Publishing in Nature Portfolio Journals
20/4/23	**Prof. Guillem Aromí**	Heterometallic Lanthanide Complexes as Molecular Quantum Processors
28/4/23	**Prof. Thibault Cantat**	Formic Acid and CO as Key 'Power Molecules' in the Catalytic Conversion of CO_2 to Chemicals
4/5/23	**Prof. Amanda C. Garcia**	Electrolyte Effect in Electrocatalytic Reactions
4/5/23	**Prof. Marc T. M. Koper**	Mechanisms of Electrocatalytic Hydrogen Evolution
5/4/23	**Prof. Frank Neese**	Insight into the Nature of High Valent Iron Centers as Reaction Intermediates in Biological and Homogeneous Catalysis from a Combination of Spectroscopy and Quantum Chemistry
12/5/23	**Prof. Gonçalo Bernardes**	Translational Chemical Biology
1/6/23	**Prof. Ben Feringa**	The Art of Building Small
2/6/23	**Prof. Alex Miller**	Electrifying Nitrogen Splitting for Ammonia Synthesis
5/6/23	**Prof. Sascha Ott**	Cation-Coupled Electron Hopping and Catalysis of Electrochemical Reactions in Metal-Organic Frameworks
6/6/23	**Prof. Dr. Sven Schneider**	Electro- and Photochemical Strategies for N2 Splitting
16/6/23	**Prof. Jana Roithova**	Mass Spectrometry in Catalysis Research
23/6/23	**Prof. Sylvestre Bonnet**	Soapy Molecules for Supramolecular Photocatalysis: A Multidisciplinary Approach Towards Solar Fuels
28/6/23	**Prof. Dr. Benjamin List**	Universal Organocatalysts for our World
6/7/23	**Prof. Osvaldo Gutiérrez**	The Advent and Recent Developments of Fe-Catalyzed Multicomponent Cross-Coupling Reactions
17/6/23	**Prof. Vladimir Gevorgyan**	Development of Novel C–H Functionalization Methodologies
21/7/23	**Prof. Christopher Uyeda**	Catalysis at Metal-Metal Bonds
12/9/23	**Dr. L. C. Campeau**	Changing the World One Reaction at a Time
19/9/23	**Prof. Lutz Ackermann**	Metallaelectro-Catalyzed Bond Activations
21/9/23	**Prof. Igor Larrosa**	Mechanistic Understanding-Led Transition Metal Catalyzed C-H Functionalization
16/10/23	**Prof. Martín Fañanás-Mastral**	Catalytic Stereoselective Hydrocarbon Difunctionalization
17/10/23	**Prof. Eva Hevia**	Tailoring Alkali-Metal Nickelates for Synthetic and Catalytic Applications
20/10/23	**Prof. Dr. Serena DeBeer**	Making and Breaking Bonds: Advanced X-ray Spectroscopic Studies of Energy Converting Enzymes
27/10/23	**Prof. Olalla Vázquez**	A ChemBio Toolbox to Enlighten Biological Processes
3/11/23	**Prof. Daniel Maspoch**	Clip-off Chemistry: Synthesis by Bond Cleavage
8/11/23	**Prof. Miquel Salmeron**	The Structure of Solid-Liquid Interfaces
10/11/23	**Prof. Julia Pérez-Prieto**	Preparation of Lead and Lead-Free Metal Halides and their Performance in Photocatalysis
17/11/23	**Prof. Ana C. Albéniz**	Palladium Catalyzed C-H Functionalization of Arenes via Metal-Ligand Cooperation
24/11/23	**Prof. M. Concepción Gimeno**	Illuminating Metal Complexes: From Synthesis to Practical Applications
28/11/23	**Prof. Bartholomäus Pieber**	The Wavelength Matters – Controlling the Selectivity of Photocatalytic Reactions Using Different Colors of Light
1/12/23	**Dr. Anna Company**	Modelling the Chemistry of Enzymes: Synthesis and Reactivity of High-Valent Oxoiron Species
4/12/23	**Dr. Sergio Pablo-García**	Orchestration Software and Cheap Open Devices to Accelerate the Adoption of Self-Driving Laboratories

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