ICIQ

Institut Català d'Investigació Química

Annual Scientific Report Summary

'15

BIST

Barcelona Institute of Science and Technology

LETTER FROM THE DIRECTOR

Dear friends,

Thanks for browsing the 2015 ICIQ Scientific Report. I hope you find the information useful.

2015 was the year of creation of the Barcelona Institute of Science and Technology (BIST). The ICIQ together with five other research centres (CRG, IRB Barcelona, ICFO, ICN2 and IFAE) set up BIST to promote joint research strategies, transfer of technology and graduate programmes. BIST is a scientific endeavor that I'm sure will position itself among the leading European research institutions.

I would also like to highlight the institute's success in obtaining ERC funding; Dr. Julio Lloret-Fillol received an ERC Consolidator Grant and Profs. Núria López, Emilio Palomares and José Ramón Galán-Mascarós were each awarded an ERC Proof of Concept. Once again, ICIQ Group Leaders were able to raise funding for promising research projects. Congratulations to all of them!

As for the ICIQ family, one new leader, Dr. Mónica H. Pérez Temprano joined the institute through ICIQ's Starting Career Programme (ICIQ-SCP) for incorporating talented young group leaders and helping them start an

independent research career, while Dr. Julio Lloret- Fillol was appointed ICREA Research Professor and Prof. Piet van Leeuwen retired.

With respect to research achievements, the institute has continued to be very active, and 150 scientific papers were published during the year. The institute reached Hirsch index 101 in December and topped international rankings measuring scientific excellence (excellencemapping.net).

Finally, let's not forget the set up of Ertflow, the ICIQ's new technology development unit that aims to develop proprietary technologies related to catalysis and flow chemistry and to offer products and services to the fine chemical, pharmaceutical and biotechnological industries for the production of new high added value products and processes under flow conditions.

Let's wait and see what next year has in store for us!

Best wishes,

Miquel À. Pericàs

19 RESEARCH GROUPS

1 ERC ADVANCED GRANT

1 ERC CONSOLIDATOR GRANT

5 ERC STARTING GRANTS

3 ERC PROOF OF CONCEPT GRANTS

9 ICREA RESEARCH PROFESSORS

HIGHLIGHTS OF THE YEAR

ERC FUNDING

During 2015, ICIQ received 2,084,000 euros from ERC Grants, which represents around 14 % of the overall funding. In 2015, four ICIQ researchers have been awarded with grants funded by the European Research Council.

- Julio Lloret-Fillol got an ***ERC Consolidator Grant*** to develop the project 'Towards a Greener Reduction Chemistry by Using Cobalt Coordination Complexes as Catalysts and Light-driven Water Reduction as a Source of Reductive Equivalents' (GREENLIGHT_REDCAT).

Worth up to € 2.75 million per grant for up to 5 years, *ERC Consolidator Grants* are designed to support researchers at the stage at which they are consolidating their own independent research team or programme.

- Emilio Palomares received an ***ERC Proof of Concept Grant*** for the project 'Ratiometric FRET Based Nanosensors for Trypsin Related Human Recessive Diseases' (2-NanoSi).
- José Ramón Galán-Mascarós was awarded an ***ERC Proof of Concept Grant*** for the project 'A Solar-Powered Hydrolyzer' (HYDRER).
- Núria López received an ***ERC Proof of Concept Grant*** for the project 'Big Data for Catalysis' (BigData4Cat).

Worth up to €150.000 per grant, *'Proof of Concept'* funding helps ERC grant holders to bridge the gap between their existing frontier research and its commercial applications.

ICIQ JOINS BIST

BIST institutes directors

Six of the top research centres in Catalonia took a step forward in their collaboration by setting up **The Barcelona Institute of Science and Technology** (BIST). The centres involved were: the Centre for Genomic Regulation (CRG); the Institute of Chemical Research of Catalonia (ICIQ); the Catalan Institute for Nanoscience and Nanotechnology (ICN2); the Institute of Photonic Sciences (ICFO); the High Energy Physics Institute (IFAE); and the Institute for Research in Biomedicine (IRB Barcelona).

BIST is a scientific initiative that seeks to foster interdisciplinary research, to leverage its scientific impact, and to position itself among the leading European institutions. It will display three major lines of work:

- The development of combined research from diverse disciplines and shared infrastructures.
- The development of a joint technology and knowledge transfer strategy.
- The launching of joint international multidisciplinary graduate programs.

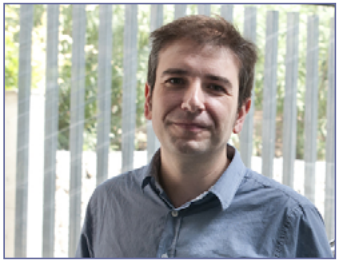
GROUP LEADER STORIES

New group leader on board

Dr. Mónica Pérez-Temprano

Dr. Mónica Pérez-Temprano joined ICIQ in November through the ICIQ's **Starting Career Programme (ICIQ-SCP)**, a programme aimed at attracting new talent and help young researchers to start their independent careers.

At ICIQ, her group will focus on the fundamental understanding of relevant organometallic processes in the context of bimetallic catalysis and C-H activation using first row metals. The long term goal is to provide critical information for the rational design and development of novel catalytic transformations.



Prof. Julio Lloret-Fillol

Julio Lloret-Fillol appointed ICREA Research Professor

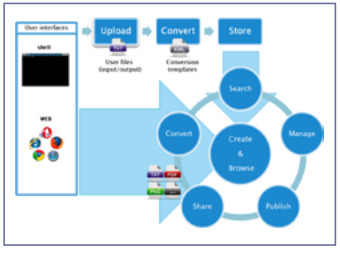
The Catalan Institution for Research and Advanced Studies (ICREA) is a foundation supported by the Catalan Government, which aims to recruit top scientists for the Catalan R&D system. Prof. Lloret-Fillol joined ICIQ in September 2014 and by being appointed as **ICREA Research Professor** he enters the group of ICIQ group leaders that are also part of the ICREA programme: Professors Vidal, Ballester, Palomares, Melchiorre, Martín, Galán-Mascarós, Kleij and Muñiz.

Professor Piet van Leeuwen

Farewell to Professor Piet van Leeuwen

On February 20th, the ICIQ community and friends joined professor Piet van Leeuwen for a symposium in his honour. **Professor van Leeuwen retired from ICIQ** to start a new research adventure as a visiting professor in the UFRGS (Porto Alegre, Brazil). He will be also be holding a Chair in the Chaires d'Attractivité programme of the Université de Toulouse, France.

A TASTE OF OUR 2014 HARVEST



ioChem-BD system overview

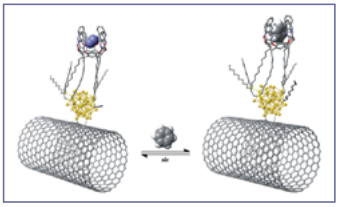
ioChem-BD, a solution for the Big Data problem in computational chemistry

The problem of managing huge amounts of data appears in many scientific research fields. The volume of information that is generated daily, coming from the results of scientific calculations is increasing exponentially and researchers need to have tools to manage it.

In the search for solutions to this problem, researchers at ICIQ and at URV have developed the ioChem-BD platform, **a multi-headed tool aimed at managing large volumes of computational chemistry results** from a diverse

group of already common simulation packages. The platform automates the extraction of relevant data and its conversion into fully tagged information in a distributed database. It provides tools for the researcher to validate, enrich, publish and share information, and tools in the cloud to access it and view it.

A hand-held sensor selective for benzene

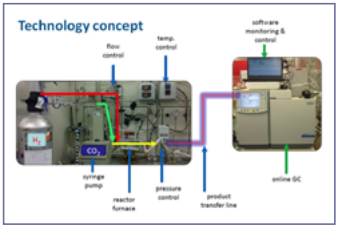


Benzene sensor

The collaboration between the groups of Prof. Pau Ballester at ICIQ and Prof. Eduard Llobet at URV has allowed the **development of a highly selective sensor for benzene in air with a lower limit of detection to the extent permitted by law.**

The researchers have prepared a new sensor based on multi wall carbon nanotubes (MWCNTs) oxygen plasma treated and decorated with gold nanoparticles whose surface was functionalized by quinoxaline-walled deep cavitands. They have found that the presence of benzene induces an increase in the resistance that allows the detection of this aromatic compound.
The sensor is suitable for being integrated in hand-held portable analysers, wearable detectors and semi-passive radio frequency identification tags with sensing capabilities or in the nodes of wireless sensor networks with a wide range of potential applications in environmental monitoring, workplace safety or medical devices, among others.

Patent issued for Urakawa's work on CO_2 conversion to methanol



A patent for the high-pressure process for the hydrogenation of CO_2 to methanol developed by Dr. Urakawa Research Group at ICIQ has been issued by the United States Patent and Trademark Office.

The work describes a continuous flow process for close-to-quantitative one-pass hydrogenation of CO_2 to methanol where conventional and commercial methanol synthesis catalysts are used. The process developed allows **a highly productive conversion of CO_2 to methanol achieving close to full one pass conversion.**

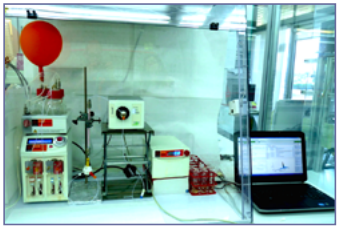
The CSOL team

FROM THE LAB TO THE MARKET

The ICIQ aims to bridge this gap through the valorisation of research results. For this reason the **CSOL (Catalyst Selection and Optimization Laboratory)** platform was created. In 2015, **Obra Social "la Caixa"** financed, for the second consecutive year, valorisation projects of the research conducted at ICIQ. The projects were selected according to their relevance, technological interest and social impact. In 2015 the following projects were developed:

- 'Hydrogen production by water electrolysis using renewable energies' (under the scientific supervision of Prof. J. R. Galán-Mascarós)
- 'Methanol formation by hydrogenation of carbon dioxide at high pressures' (under the scientific supervision of Dr. A. Urakawa)
- 'In-silico studies for the formation of pharmaceutical co-crystals' (under the scientific supervision of Crysforma and Prof. C. Bo)

The objective is that the projects move along the Technology Readiness Level metrics and are better positioned, so that they can contribute to the creation of a spin-off company, be licensed more easily or achieve new sources of funding.



Set-up for flow chemistry

ICIQ'S NEW TECHNOLOGY DEVELOPMENT UNIT

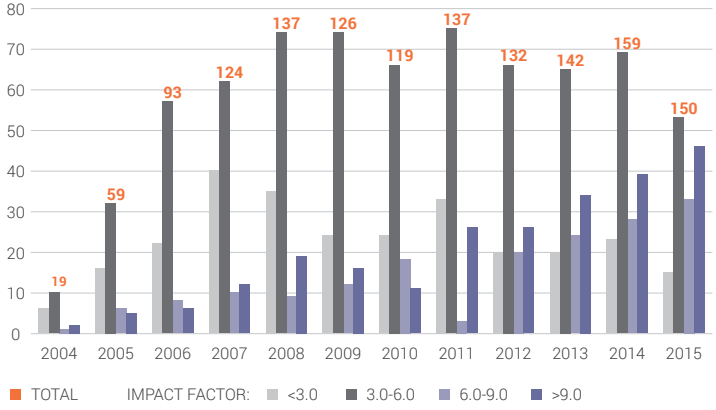
ERTFLOW aims at developing proprietary technologies related to catalysis and flow chemistry and **offering products and services to the fine chemical, pharmaceutical and biotechnological industries** for the production of new high added value products and processes under flow conditions.

Batch processing, the most usual production scheme in the pharmaceutical and fine chemical industries, presents important disadvantages such as low intensification, waste generation problems in scale-up and risks associated to large volumes. Flow techniques solve most of those problems and present a series of advantages -increased heat transfer, faster mixing or flexible production among others- that make them a very convenient alternative for the production of organic compounds.

SCIENTIFIC PRODUCTION

In 2015, the web application Mapping Scientific Excellence ranked ICIQ in second position on "Best Paper Rate" (proportion of highly cited papers published by an institution) and third on "Best Journal Rate" (ratio of papers published in the most influential journals) in the field of Chemistry worldwide.

ICIQ's privileged position in this list confirms the Institute's strong evolution towards scientific excellence since the beginning of its research activities in 2004. Since then, ICIQ has published more than 1300 scientific articles. About 90 % of them have been published in the most influential chemical research journals in the world, those ranked in the first quartile (25%).



Articles in 2015

150

Total articles (2004-2015)

1396

h-Index

102

Citations in 2015

9530

Total citations (2004-2015)

53,409

Average citations (2004-2015)

35,92

KNOWLEDGE AND TECHNOLOGY TRANSFER

Research projects

13

Patents

18

Technology Development Units

3

Joint Units ICIQ-Industry

2

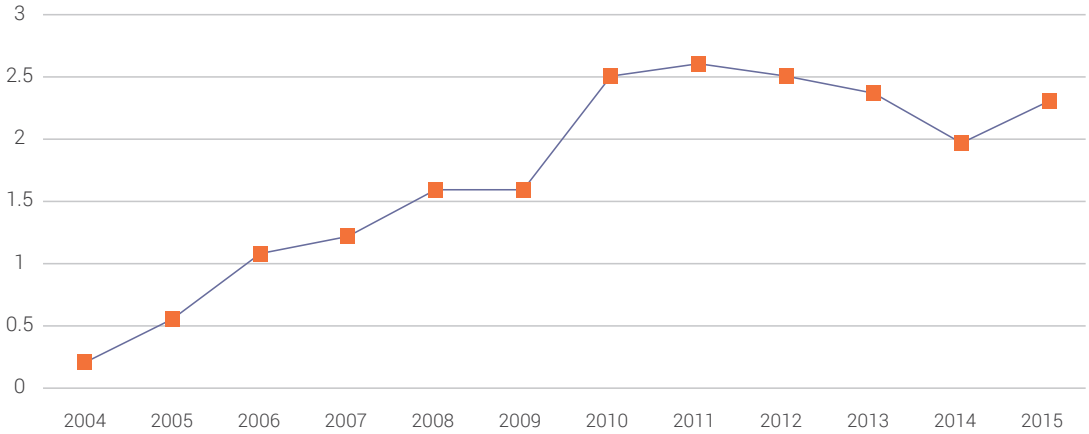
TARGET-DRIVEN CHEMISTRY TO FULFIL INDUSTRIAL NEEDS

Transfer of knowledge and technology to the industrial sector is an integral part of the institute's activities. During 2015, the technology development unit **CSOL** has been involved in one collaborative project with industry in the field of homogeneous catalysis as well as performing five valorization projects to develop the inventions made by ICIQ's research groups into technologies that are ready to be transferred to the industry.

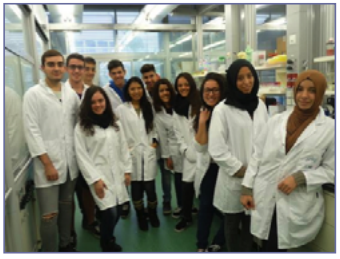
As for **Crysforma**, it continues expanding its capabilities in the field of pharmaceutical solid state development. During 2015, **Crysforma** continued with its own internal research lines to develop new co-crystals of high demand APIs with improved solubility and bioavailability properties, and started a collaboration with the group of Carles Bo in the area of prediction of co-crystal formation.

Moreover, a new technology development unit was created: **ERTFLOW**, which works in the area of catalysis and flow chemistry, to develop and implement technical solutions in process intensification for sustainable Chemistry. And we have continued out tight collaboration with **Henkel** and **Esteve** under the strategy of the ICIQ - Industry joint units.

EVOLUTION OF REVENUES FROM INDUSTRIAL COLLABORATIONS IN M€



PUBLIC ENGAGEMENT



ICIQ Teaching and Learning Laboratory

ENGAGING YOUTH TO PURSUE A CAREER IN CHEMISTRY

ICIQ seeks to raise public awareness of chemical research as a key factor in the progress of our society. Our purpose is to sensitize citizens to the benefits of chemistry research in terms of health, energy and environmental sustainability. We are also committed to engaging and encouraging youngsters to pursue a career in chemistry research. To this end in 2015 we have displayed a science outreach programme addressed to audiences of all ages as a way to position the joy of chemistry within reach of many more people and to explain the research we're carrying out at ICIQ.

We carried out our traditional **Química en Família** workshop for the little ones; wekkly chemistry workshops addressed to high-school in the **ICIQ Teaching and Learning Laboratory**; ICIQ's **"From the Lab to the Classroom Programme"** to inspire and train teachers in new topics and methodologies to teach chemistry; participation in **science fairs** and **visits to primary schools** to perform chemistry experiments.

We also organized the second edition of **Crazy about Chemistry**. A year-long course in chemistry addressed to high-school students with a special interest and talent on chemistry and research, and who want to expand their scientific knowledge through hands-on experiments in an excellent research centre. This training activity is funded by the Crazy about Science programme of the Catalunya-La Pedrera Foundation.

ADVANCED TRAINING

PREPARING THE NEXT GENERATION OF TOP RESEARCHERS

ICIQ has a strong commitment to offer training programmes for undergraduates, graduate students and doctoral researchers. We prepare a new generation of researchers with the skills and knowledge needed to tackle the most important challenges in chemical research. We are also eager to prepare graduate and post-graduate students to undertake research careers in chemistry. Our **Career Development Programme** offers complementary training such as weekly scientific seminars, technical workshops, international research stages, language courses, ICIQ Summer School, and other soft skills courses and activities.

Programmes

ICIQ Summer Fellowship

ICIQ-URV Master in Synthesis, Catalysis and Molecular Design

SO-ICIQ International Graduate Students Programme

ICIQ-International PostDoctoral Mobility Programme

CELLEX- ICIQ Postdoctoral Programme on High Throughput Experimentation

Seminars
34

ICIQ Seminar Programme funded by BASF The Chemical Company

Theses defended
16

PhD students
94

Postdoctoral researchers
71

FUNDING

Projects

50

European Comission

67.8%

MINECO

30%

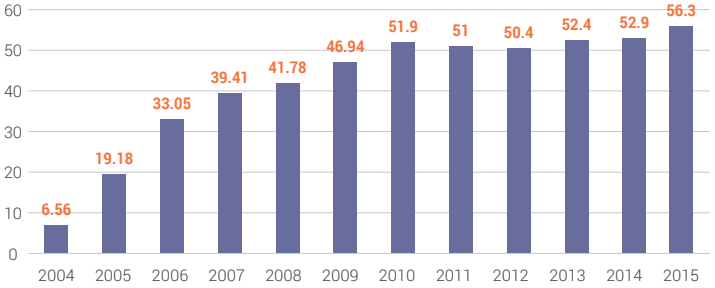
AGAUR

1.2%

Other

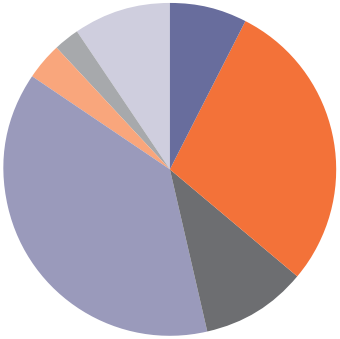
1%

PERCENTAGE OF COMPETITIVE FUNDING AND INDUSTRY INCOME OVER THE TOTAL ICIQ FUNDS



STAFF

SCIENTIFIC AREA



Employees
303

Women
42%

Personnel from abroad
34.5%

Scientific personnel
81.5%

ICIQ

Institut Català d'Investigació Química

Institute of Chemical Research of Catalonia

Av. Països Catalans 16,
43007 Tarragona (Spain)
Tel. +34 977 920 200
iciq@iciq.es
www.iciq.es

Trustees:

Generalitat de Catalunya
Departament d'Economia i Coneixement

covestro

BASF
The Chemical Company

ESTEVE

REPSOL

With the support of:

Ministerio de Economía y Competitividad

Excelencia Severo Ochoa

Unió Europea
Fons Europeu de Desenvolupament Regional
Una manera de fer Europa