

**ICIQ**   
Institut  
Català  
d'Investigació  
Química

Annual  
Scientific  
Report  
Summary

'14

# LETTER FROM THE DIRECTOR



Dear friends,

2014 was a major turning point in ICIQ's history. The institute was recognized as Severo Ochoa Centre of Excellence. This award has allowed ICIQ to develop a strategic project based on the discovery of catalysts for generating fuel (hydrogen) through water splitting using solar energy and on the discovery of catalysts for converting molecules which have a strong environmental impact (such as CO<sub>2</sub>) or low reactivity (such as methane) into molecules of interest for the chemical and energy industry. The funds obtained through the Severo Ochoa accreditation have also helped us to consolidate our Starting Career Programme, to launch an international mobility plan for PhD students and to set a training agenda for postdoctoral researchers.

As for the ICIQ family, two new leaders, Drs. Marcos G. Suero and Julio Lloret-Fillol, joined the Institute through ICIQ's Starting Career Programme (ICIQ-SCP) to incorporate young talented group leaders and help them start an independent research career. Profs. Atsushi Urakawa and José-Ramón Galán-Mascarós got tenure and Prof. Javier de Mendoza retired.



With respect to research achievements, the institute has continued to be very active, and about 150 scientific papers were published during the year. The institute reached Hirsch index 97 in December and topped international rankings (Mapping Scientific Excellence and SCImago Institutions Rankings) measuring scientific excellence.

And let's not forget our 10th Anniversary week of celebrations: A Scientific Symposium; ICIQ's 2nd Quinquennial Evaluation (highly positive at the end), the institutional celebration and the inauguration of the CELLEX-ICIQ High Throughput Experimentation laboratory.

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

Best wishes,

**Miquel À. Pericàs**

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21 RESEARCH  
GROUPS

2 ERC ADVANCED  
GRANTS

5 ERC STARTING  
GRANTS

8 ICREA RESEARCH  
PROFESSORS

## HIGHLIGHTS OF THE YEAR



*The Severo Ochoa award*

## ICIQ: SEVERO OCHOA CENTRE OF EXCELLENCE

In March 2014, ICIQ was accredited as a “Severo Ochoa Centre of Excellence” by the Secretary of State for Research, Development and Innovation from Mineco (Ministry of Economy and Competitiveness). The Severo Ochoa accreditation recognizes units and research centres that excel for being situated among the best in the world in their respective fields of research.

The Severo Ochoa accreditation will allow ICIQ to develop a strategic project dealing with the discovery of catalysts for generating fuel (hydrogen) through water splitting using solar energy and the discovery of catalysts for converting molecules which have a strong environmental impact (such as CO<sub>2</sub>) or which have low reactivity (such as methane) into molecules of interest for the chemical and energy industry. It will also allow ICIQ to consolidate its Starting Career Programme and to launch an international mobility plan for PhD students and a training offer for postdoctoral researchers.

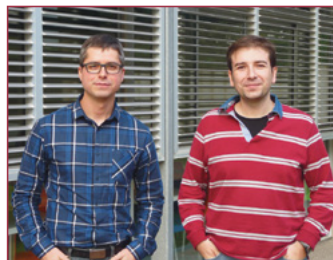
## GROUP LEADER STORIES

### New Group Leaders on Board

Marcos G. Suero and Julio LLoret-Fillol joined ICIQ after being selected through the ICIQ Starting Career Programme.

Dr. Lloret Fillol seeks to merge cutting-edge concepts in the fields of solar fuel production and catalytic transformation facilitated by coordination complexes to perform new light-driven catalytic transformations of organic substrates. This project may open newer and greener avenues toward the application of artificial photosynthetic schemes in catalytic transformations of organic molecules of added value.

Dr. Suero plans to explore new reactivity concepts using catalysis and its applications in solving important synthesis problems. Particularly, he aims to develop new carbon–hydrogen bond functionalization strategies of simple building blocks that could be used for the preparation of complex molecules and biologically privileged structural motifs.



*Marcos G. Suero and  
Julio LLoret-Fillol*



*José Ramón Galán-Mascarós  
and Atsushi Urakawa*

### Atsushi Urakawa and José Ramón Galán-Mascarós Got Tenure

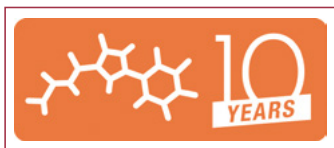
After a demanding evaluation by several members of ICIQ's Scientific Committee, José Ramón Galán-Mascarós and Atsushi Urakawa received tenure at ICIQ.

### Javier de Mendoza Retired

Professor de Mendoza joined ICIQ in 2004. On December 2014 ICIQ organized a Mini-symposium honouring him on the occasion of his retirement.



*Javier de Mendoza*



## CELEBRATION OF ICIQ'S 10TH ANNIVERSARY

After its official inauguration in July 2003, research activities started at the Institute of Chemical Research of Catalonia (ICIQ) in the spring of 2004. In 2004 the whole ICIQ community celebrated 10 years of hard and promising work, and also plenty of achievements and personal accomplishments.

The week of celebrations (July 15th-19th) started with the 2nd Quinquennial Evaluation of the Institute (highly positive!) and continued with a Scientific Symposium, that included lectures delivered by a selection of the most recognised chemists nowadays. The celebrations concluded with an institutional event with representatives of industry and different administrations and with the inauguration of the CELLEX-ICIQ High Throughput Experimentation laboratory. ICIQ also recognised the dedicated work of the ICIQ people. Particularly of those who also celebrated 10 years working at the institute.

## ICIQ'S NEW HTE LABORATORY

On July 18th, 2014, Andreu Mas-Colell, conseller d'Economia i Coneixement, inaugurated the CELLEX-ICIQ High Throughput Experimentation (HTE) laboratory, funded by Fundació Cellex. This is the only HTE laboratory of this type in Europe. Two other similar laboratories are in the University of Princeton and University of Pennsylvania.

The HTE laboratory provides ICIQ researchers with the instrumentation and know-how to speed up run processes in the development of new drugs and catalysts. The facility offers the possibility to run and analyze a large number of reactions in a very short time, which accelerates the optimization and discovery of new processes. Moreover, the possibility of running many reactions in a short time also allows to follow unexplored ways and to study difficult processes with, a priori, little chance of success.



*Inauguration of ICIQ's new HTE laboratory*

## CRAZY ABOUT CHEMISTRY

ICIQ trained 21 high-school students who were (and totally are) crazy about chemistry. They were selected to participate in the first edition of this course sponsored by Catalunya-La Pedrera Foundation. This is a year-long chemistry course to make sure students don't recover from their craziness. "It's a unique opportunity to learn chemistry in a different way than we are used to," says Irene. "We've seen a new world we barely knew and we've lived experiences you don't learn in books", adds Marina.

Throughout the course ICIQ researchers and technicians shared their knowledge and their respective career's experiences with students. The ICIQ staff shed light and supported them through theoretical and practical classes conducted by Dr. Laia Pellejà, ICIQ's science outreach officer. "It's chemistry from first hand. You get to know the real chemistry," says Raimon. "You don't only meet researchers but also fantastic classmates. It has helped me to decide my career," added Júlia. "And let's not forget the fun experiments we perform in the laboratory... like toothpaste for elephants!" pointed out Josep.

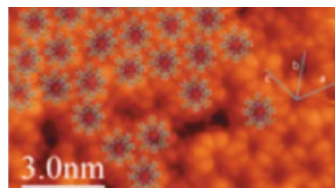
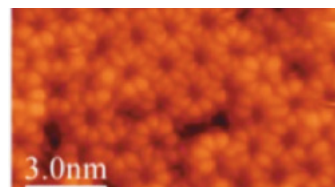


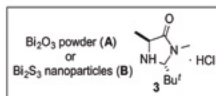
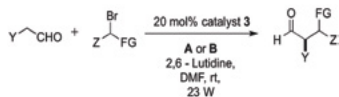
## A TASTE OF OUR 2014 HARVEST

### Strong collaborations between ICIQ groups

#### Easily processable Single-Molecule Magnets

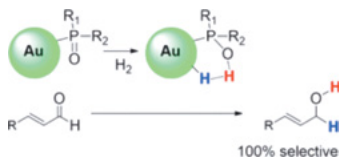
In the search for molecule-based materials for novel applications in the fields of materials sciences, P. Ballester and J. R. Galán-Mascarós teams have designed, synthesised and characterised a new family of complexes that exhibit single-molecule magnet (SMM) behaviour. Currently there is growing interest in such compounds as they could be used in the future for high-density information storage, which would allow us to increase the storage capacity of computer hard disks.





## Enantioselective organo-photocatalysis with bismuth-based materials as photocatalysts

The development of chemical transformations that make use of sunlight as the energy source are currently subject of intense research, specially in the area of asymmetric catalysis. By working collaboratively, Miquel Pericàs and Emilio Palomares groups have used bismuth-based materials as photocatalysts in combination with a second-generation MacMillan imidazolidinone as the chiral catalyst to perform the  $\alpha$ -alkylation of aldehydes with  $\alpha$ -bromo-carbonyl compounds with good yields and very high enantioselectivities. At first, the reaction was performed with simulated sunlight, but it also proved to proceed with high efficiency when the reaction vial was exposed to the morning sunlight on a clear day in Tarragona.



## Research on gold nanoparticles stands out

Piet van Leeuwen, Atsushi Urakawa et al. have synthesised air-stable and homogeneous gold nanoparticles (AuNPs) stabilized by a secondary phosphine oxide (SPO). This is the first case that describes the use of SPOs as stabilizing ligands for AuNPs, but it is also the first that aims to investigate the role of these ligands in catalysis. This work represents a clear demonstration of the ligand-metal cooperative effect, where the nature of the SPO ligand plays a crucial role and is directly related to the catalytic activity.



## TARGET-DRIVEN CHEMISTRY TO FULFIL INDUSTRIAL NEEDS

We put our expertise and research results at the service of the chemical and pharmaceutical industries to improve their competitiveness and performance.

During 2014, ICIQ's technology development unit CSOL has been involved in several collaborative projects with industry in the field of homogeneous catalysis as well as performing valorization projects to develop the inventions made by ICIQ's research groups into technologies that are ready to be transferred to industry. It's worth mentioning that Fundació Obra Social "la Caixa" extended its funding for the development of projects for one further year. Crysforma continued expanding its capabilities in the field of pharmaceutical solid state development and it started its own internal research lines to develop new co-crystals of high demand APIs with improved solubility and bioavailability properties.



KNOWLEDGE  
AND  
TECHNOLOGY  
TRANSFER

Research projects

12

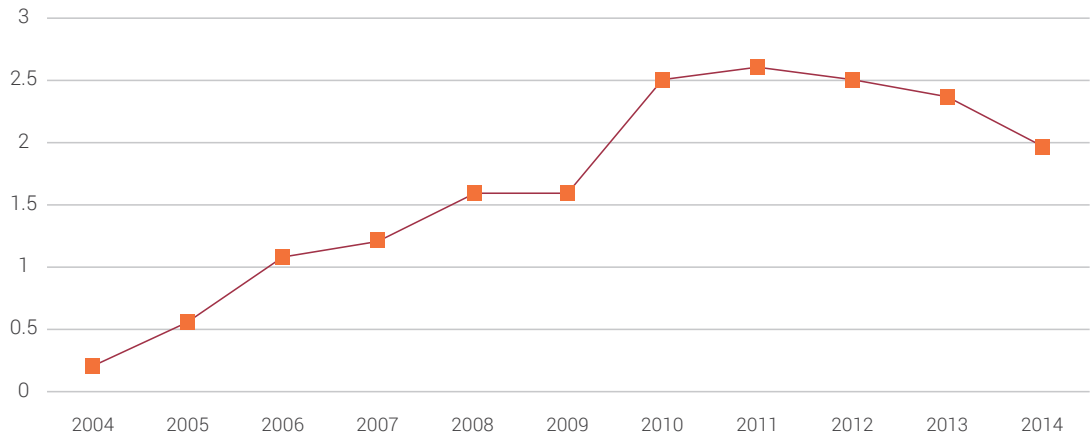
Patents

12

And last but not least, one more year we have continued our tight collaboration with Henkel and Esteve under the strategy of the ICIQ-Industry joint units.



## EVOLUTION OF REVENUES FROM INDUSTRIAL COLLABORATIONS IN M€



## 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.



EXCELENCIA  
SEVERO  
OCHOA

Severo Ochoa-ICIQ International  
Graduate Students Programme



UNIVERSITAT  
ROVIRA I VIRGILI

ICIQ-URV Master on Synthesis,  
Catalysis and Molecular Design



Obra Social "la Caixa"

Summer stays: ICIQ Summer  
Fellowship Programme



ICIQ-Unicat Summer School



PhD Students Exchange  
Programme with the University of  
Michigan

## TRAINING

Seminars

34

ICIQ Seminar Programme funded by

 **BASF**  
The Chemical Company

Theses defended

21

## PUBLIC ENGAGEMENT

### ENGAGING YOUTH TO PURSUE A CAREER IN CHEMISTRY



*High-school students during a  
research stay at ICIQ*

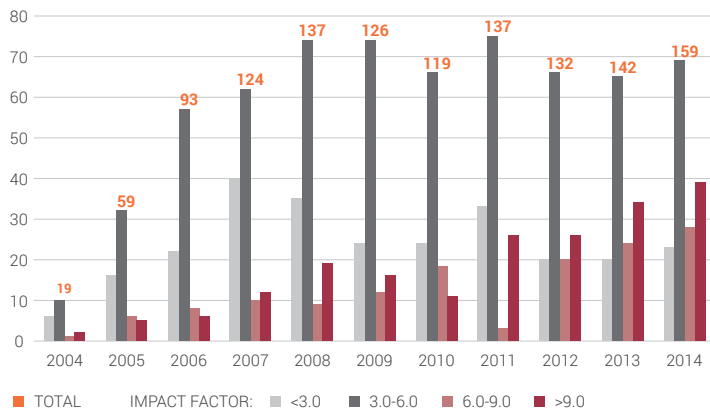


*The "Crazy about Chemistry"  
students*

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 2014 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 Familia workshop for the little ones; a crystallography and synthesis of the aspirin workshop; guided visits to ICIQ facilities; visits to primary schools to perform chemistry experiments; and training courses for secondary school teachers.

In 2014 we organised the first 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.

## PAPERS



## FACTS AND FIGURES

Articles in 2014

159

Total articles (2004-2014)

1247

Citations in 2014

8861

Total citations (2004-2014)

46224

Average citations (2004-2014)

33,57

h-Index in Dec. 2014

97

## SCIENTIFIC PROJECTS

Total funding

€4,252,202

European Union

66%

MINECO

30,4%

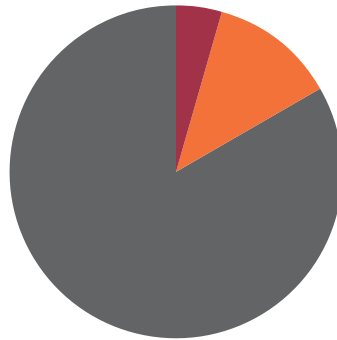
AGAUR

2,24%

Other

1,36%

European Union (VII FP)



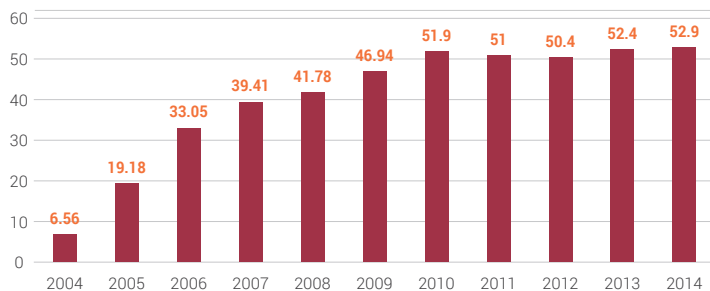
■ EU: VII Framework Programme

■ EU: VII FP-Marie Curie Actions

■ EU: VII FP-ERC

## FUNDING

Percentage of competitive funding and industry income over the total ICIQ funds



Competitive funding from public calls

31,60%

Research projects with industry

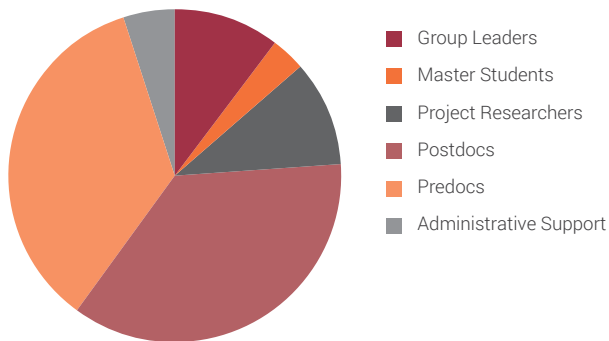
14,72%

Donations from industry and private foundations

8,24%

## STAFF

Research area



ICIQ people

276

Women

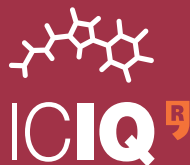
42%

Scientific personnel

74%

Personnel from abroad

31%



**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](mailto:iciq@iciq.es)

[www.iciq.es](http://www.iciq.es)

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