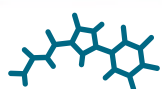




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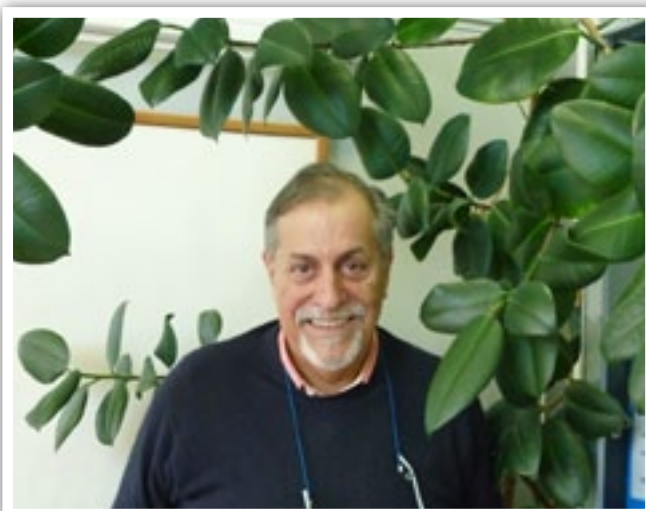
ICIQ<sup>R</sup>

Institut  
Català  
d'Investigació  
Química



www.iciq.es

## Professor Javier de Mendoza retires



Javier de Mendoza

If you have ever come across professor Javier de Mendoza, you know that the interview format is not going to work on him. He loves jumping from one idea to another; from fond memories to solid future projections; from science to art. Giving a concrete answer to a concise question is not in his nature.

“As a student I liked those kind of professors who digressed. I really got impressed by professor Pascual Vila, father of the Catalan organic chemistry, who digressed a lot and made me think. In fact, I’ve been always an autodidact” says de Mendoza.

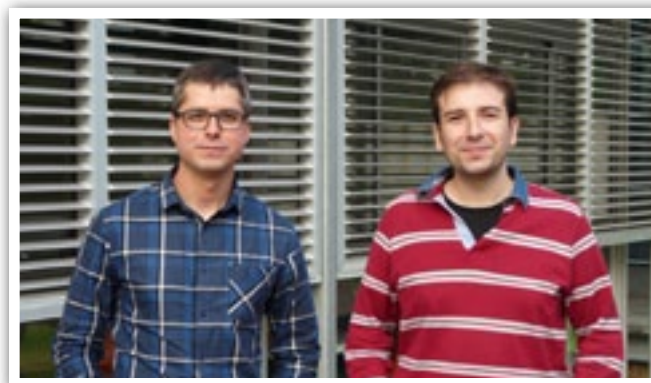
Professor de Mendoza graduated in Pharmacy from University of Barcelona following his father’s advice. “I’m almost deaf from one ear as a consequence of an ear infection when I was a child. Taking that into consideration and being a kid with great interest in science – I was a walking encyclopedia- my father thought that if I owned a pharmacy I would make a living and I could do research on drugs” recalls de Mendoza. **Continues on page 4**

## New group leaders join ICIQ

Dr. Marcos G. Suero and Dr. Julio Lloret-Fillol joined our Institute through [ICIQ's Starting Career Programme \(ICIQ-SCP\)](#), a programme aimed at attracting new talent and help young outstanding researchers to start their independent careers.

Marcos García Suero, postdoctoral Marie Curie fellow from the University of Cambridge, will work on the development of 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.

Julio Lloret-Fillol, Young Research Group Leader at the *Institut de Química Computacional i Catàlisi (UdG)*, will develop a project aimed to merge concepts at the edge of the fields of solar fuels production and catalytic transformation facilitated by coordination complexes to perform new light-driven catalytic transformations of organic substrates.



Dr. Marcos G. Suero and Dr. Julio Lloret-Fillol

They both will carry out part of their research in the [CELLEX-ICIQ HTE Laboratory](#) using High Throughput Experimentation.

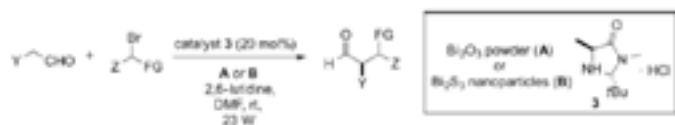
[Suero group](#)

[Lloret-Fillol group](#)

## New bismuth-based photocatalysts

The development of enantioselective catalytic processes that make use of sunlight as the energy source and nontoxic, affordable materials as catalysts represents one of the new and rapidly evolving areas in chemical research. MacMillan and co-workers gave the first step in this direction, when they merged organo- and photoredox catalysis to promote the direct asymmetric  $\alpha$ -alkylation of aldehydes with a ruthenium-based catalyst. The problem is that ruthenium is a scarce and expensive metal and its compounds are highly toxic and suspected carcinogens.

Prof. Pericàs and Prof. Palomares groups have achieved the direct asymmetric  $\alpha$ -alkylation of aldehydes with  $\alpha$ -bromocarbonyl compounds using  $\text{Bi}_2\text{O}_3$  and  $\text{Bi}_2\text{S}_3$  as photocatalysts in combination with a second-generation MacMillan imidazolidinone as the chiral catalyst. Bismuth materials are abundant, rather inexpensive and non-toxic. Therefore they represent a promising alternative to ruthenium complexes.



“The idea of collaboration was to combine the expertise of both groups to solve the problem of doing redox catalysis with materials that were cheap and non-toxic alternatives to ruthenium. When two areas of expertise are combined, the result is always more valuable than the two areas separately” –says Prof. Miquel A. Pericàs.

When asked about the collaboration between different groups, Prof. Emilio Palomares says: “The issue is to find a symbiosis between the expertise of different groups. I know very well about my field of research, but I also want to address issues in which I am not an expert. I do not work on catalysis, but if someone asks me to collaborate to do photocatalytic reactions, it seems to me that is an interesting opportunity to bring my experience into a more complex project”.

*Light-Driven Organocatalysis Using Inexpensive, Nontoxic  $\text{Bi}_2\text{O}_3$  as the Photocatalyst*

P. Riente, A. Mata Adams, J. Albero, E. Palomares, M. A. Pericàs  
*Angew. Chem. Int. Ed.*, **2014**, 53, 9613-9616

*Highlighted in Synfacts*

## ICIQ's Fèlix Serratosa medal to professor Luis A. Oro

Professor Luis A. Oro, professor of Inorganic Chemistry in Zaragoza and Director of the *Instituto Universitario de Catálisis Homogénea (IUCH)*, was awarded with the ICIQ's Fèlix Serratosa Medal for his valuable contribution and support as member of ICIQ's Scientific Advisory Board.

Professor Oro served as member of ICIQ's Scientific Advisory Board (SAB) during the period 2002-2013. Members of ICIQ's SAB have the task of giving advice to ICIQ's Board of Trustees on the Institute's scientific policy. They also participate in the selection of group leaders and evaluate the scientific activity of ICIQ and its group leaders.



Prof. Luis A. Oro (left) and ICIQ director, Prof. Miquel A. Pericàs

## Journal Inside Cover



“Enantiopure Narrow Bite-Angle P-OP Ligands: Synthesis and Catalytic Performance in Asymmetric Hydroformylations and Hydrogenations”

**i** [Access to the abstract](#)

*Chem. Eur. J.*, **2014**, 20, 15375-15384

H. Fernández-Pérez, J. Benet-Buchholz, A. Vidal-Ferran

## 2014 International Year of Crystallography

### New methodology to determine the absolute configuration of light-atom molecules

Given the fact that many active pharmaceutical ingredients (APIs) are chiral light-atom compounds and different enantiomers can have different physiological properties, the assignment of the absolute configuration to these materials is crucial. The determination of absolute configuration is usually achieved using “soft” X-ray radiation, most often generated with a copper target. This measurement is facilitated by the presence of atoms heavier than oxygen and for that reason is difficult to determine absolute configurations of molecules made up of atoms no heavier than oxygen (*light-atom molecules*).

Up to now, Cu  $K\alpha$  radiation was supposed to have advantage over Mo  $K\alpha$  radiation because of its larger resonant scattering factors. Nevertheless, the new methodology developed at ICIQ's X-Ray Diffraction Unit allows the unambiguously determination of the absolute structure of crystals constituted exclusively by light atoms using X-ray diffraction data obtained with instruments equipped with molybdenum anodes.



“Given that the instruments equipped with copper anodes are used for the determination of protein structures, laboratories studying small molecules often do not have this equipment. We believe that the main advantage of this methodology is that it makes such studies more accessible because many single-crystal diffractometers used for small-molecule structure determination are equipped with molybdenum anodes” -says Dr. Jordi Benet, ICIQ's X-Ray Diffraction Unit manager.

[\*The use of Mo  \$K\alpha\$  radiation in the assignment of the absolute configuration of light-atom molecules; the importance of high-resolution data\*](#)

E. C. Escudero-Adán, J. Benet-Buchholz, P. Ballester  
*Acta Cryst. B*, 2014, 70, 660-668

### Explaining crystallography to high-school students

The week of November 17<sup>th</sup> ICIQ welcomed high-school students to shed light on crystallography. They learnt what is crystallography, the applications of this technique and they had the chance to see crystals grow. The students also visited ICIQ's X-ray laboratory and van Leeuwen's group laboratory to learn why researchers need to crystallized compounds.



Jordi Benet and Laia Pellejà

## Professor Javier de Mendoza retires



The turning point of his career was when he met professor Jean-Marie Lehn. After working in the field of heterocyclic chemistry ( "I learned a lot from professor José Elguero in Montpellier" ) he was enlightened by Lehn's supramolecular chemistry. "That changed my life! I had a deep admiration for my father, a very Cartesian man. But I discovered my mother's creative print in my genoma through supramolecular chemistry" he says.

So when he took over the department of organic chemistry at the *Universidad Autónoma de Madrid* (UAM) he decided to gear it towards supramolecular chemistry, a new window of research that remained closed until then in Spain.

"I ended having a big research group of 40 people or so. Although the pyramidal system of the Spanish university is not the best model to encourage great research work, I think we did a good job. I've always told my students not to be afraid of making mistakes, that they must be brave in expressing their ideas. If you don't practice errors you will never have good ideas" says de Mendoza.

Joining ICIQ in 2004 was for him a great responsibility. It was a total change of paradigma. A research model based on meritocracy and primed for collaboration. An institute offering state-of-the art facilities and equipment.

*"To work at ICIQ you must be a self-demanding person. You must take risks because you're not expected to carry out routine research. My years at ICIQ have been the best years. We might have not published a lot but I did very creative and risky research that others have followed."*

To publish and where you publish. An issue with different nuances for the scientific community. When it refers to a way to evaluate the scientific performance of a given scientist, professor de Mendoza makes it clear. "I don't agree with the way science is evaluated. This bibliometric obsession is ridiculous. The thing is that now we're obsessed with media even when we do science" he says with regret.

Professor de Mendoza is a few weeks from retirement. He has looked back and forward seated in his office. His paintings are off the wall, the round table once for meetings is covered with chemical products from his lab. His books are waiting to be stuffed in boxes. Only the enormous ficus plant touching the ceiling is allowed to remain there.

*"What I've learnt being a scientist (and it applies for any kind of work) is that the result of your work has also to do with a rich and comforting personal life. And fortunately, I realized on time that combining my work with other interests and, most importantly, with quality time with my family makes a difference."*

## Professor Javier de Mendoza retires

### Proust questionnaire

**A chemical element:**

Nitrogen.

**Favourite scientist:**

Those who have fought against the incomprehension of his time such as Darwin and Galileo.

**Your favourite invention:**

Years ago I would have said the Tipp-Ex (correction paper for typos made on typewriters) but now I think that it is Internet.

**If you had not been scientist...**

I would have liked to be a pianist.

**Favourite destination:**

When I was young I liked the mountain but now I prefer the sea. Both give time for solitude.

**A book:**

Those of my childhood. Any book by Alejandro Dumas, Zola or Salgari.

**A movie:**

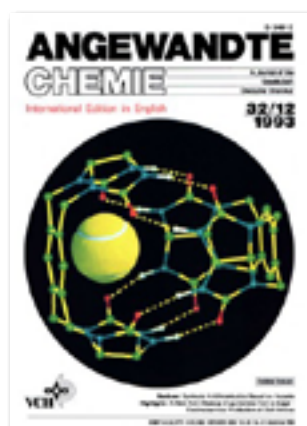
The Godfather, I can watch it many times. Any Italian Neorealism film.

**A dream:**

I don't know, we live in a better time than our parents.

**Science is...**

One of the most human activities that exists.



A Synthetic Cavity Assembles Through Self-Complementary Hydrogen Bonds

R. Wyler, J. de Mendoza, J. Rebek Jr.  
*Angew. Chem. Int. Ed.*, **1993**, 32, 1699-1701



Inclusion of cavitands and calix[4]arenes into a metallobridged para-(1H-imidazo[4,5-f][3,8]phenanthrolin-2-yl)-expanded calix[4]arene

E. Botana, E. Da Silva, J. Benet-Buchholz, P. Ballester, J. de Mendoza

*Angew. Chem., Int. Ed.*, **2007**, 46, 198-201



Autoencapsulation Through Intermolecular Forces: A Synthetic Self-Assembling Spherical Complex

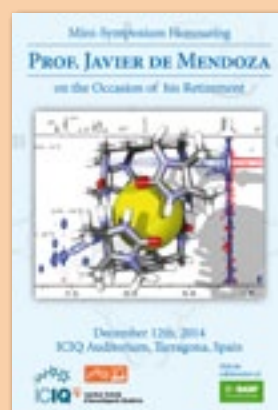
R. S. Meissner, J. Rebek Jr., J. De Mendoza

*Science*, **1995**, 270, 1485-1488

## A tribute to professor Javier de Mendoza

ICIQ organized a Mini-symposium honouring professor Javier de Mendoza on the occasion of his 70<sup>th</sup> birthday and retirement.

The invited speakers were professors Jean-Pierre Sauvage (University of Strassbourg), Roeland Nolte (Nijmegen University), Tomás Torres (Universidad Autónoma de Madrid), Jean-Marie Lehn (University of Strassbourg) and Javier de Mendoza (ICIQ).



The symposium took place on December 12<sup>th</sup>, from 9am to 13.45 pm, at ICIQ Auditorium.

## Exceptionally mild conditions for ATRA reactions

In their search of metal-free photochemical processes, Melchiorre's group has found that an organic molecule as simple as *p*-anisaldehyde, working as a photosensitizer, can efficiently catalyse the intermolecular atom-transfer radical addition of a variety of haloalkanes onto olefins. The chemistry only requires irradiation from a household 23 W compact fluorescent light bulb to proceed, and ambient temperature is sufficient for achieving functionalized olefins with synthetically useful results.



“This is an historical reaction that usually requires oxidants, radical initiators and thermal activation with average temperatures of 100 °C. What we have found is that we can promote this reaction in a very mild way. We are using a really simple molecule (*p*-anisaldehyde) in catalytic amount and a simple fluorescent light bulb that is easily available. And what probably is the most important point, the reaction is conducted at room temperature”—says professor Paolo Melchiorre.

These findings are expected to open new avenues for reactions design in the field of radical processes and represent and advance in sustainable, environmentally friendly radical reactions.

### [Photo-Organocatalysis of Atom-Transfer Radical Additions to Alkenes](#)

E. Arceo, E. Montroni, P. Melchiorre  
*Angew. Chem. Int. Ed.*, **2014**, 53, 12064-12068

## News in brief

**PhD theses defended:** Drs. Xinyuan Fan, Fernando Castro, Manuel Nappi, Asraa Ziadi and Antoni Bautista, pre-doctoral students at ICIQ have defended their PhD thesis. They were all awarded the highest honours for their work.

**Piet van Leeuwen, Doctor Honoris Causa:** Professor van Leeuwen was invested *Doctor Honoris Causa* by the Universidade Federal do Rio Grande do Sul (UFRGS). Professor van Leeuwen said that he felt very honoured with the distinction and emphasized his professional and personal relationship with professors of UFRGS.



**Lilly on campus recruitment:** Representatives from [Eli Lilly and Company](#) came to ICIQ to interview doctoral and post-doctoral students so they can be taken into account as potential candidates for an R+D open position in the company. This programme is aligned with ICIQ's commitment to give industries the opportunity of meeting/recruiting bright researchers and at the same time, help our young researchers to start a professional career.

**Antonio M. Echavarren honoured for prestigious career:** He is a recipient of the prestigious 2015 Arthur C. Cope Scholar Awards given by the American Chemical Society. The award recognizes excellence in organic chemistry over the trajectory of the recipient's career.



**ICIQ, 1st position in Excellence with Leadership worldwide:** The 2014 [SCImago Institutions Rankings \(SIR\)](#) places ICIQ as the leading government research centre worldwide according to the ratio of Excellence with Leadership.

Excellence and Leadership indicates the amount of documents in the Excellence rate in which the institution is the main contributor. Excellence rate represents the amount (in %) of an institution's scientific output that is included into the set of the 10 % of the most cited papers in their respective scientific fields.

## Reaching out

### Crazy about Chemistry, so far

We're approaching the closing event of the programme Crazy about Chemistry and still no sign of recovery. Our first 21 students participating in this year-long course funded by Fundació Catalunya-La Pedrera have had the unique opportunity of learning chemistry in a total different way.

They have learned Chemistry from ICIQ researchers and technicians and they have put it into practice in one of ICIQ's research laboratories.

*"It's chemistry from first hand. You get to know the real chemistry,"* says Raimon, from IES Jaume Callís, Sant Joan de Vilatorta. *"You don't only meet researchers but also fantastic classmates. It has helped me to decide my career,"* adds Júlia, from INS Manuel de Pedrolo, Tàrrrega.

### Teachers and Science: Effervescent Learning

On October 8<sup>th</sup> and 10<sup>th</sup> Dr. Laia Pellejà, conducted a workshop for high-school teachers on how to make the synthesis of the aspirin. The purpose of this 6-hour long workshop is to train teachers on this subject so they can transfer this knowledge to their students. ICIQ also offered its outreach lab to the participants to perform the synthesis with their students.

*Teachers and Science* is a Catalunya-La Pedrera Foundation programme that offers secondary teachers of high schools in Catalunya the opportunity to participate in specialised workshops delivered by researchers at different research centers in Catalunya.



*Pellejà and the high-school teachers before starting the synthesis of the aspirin*

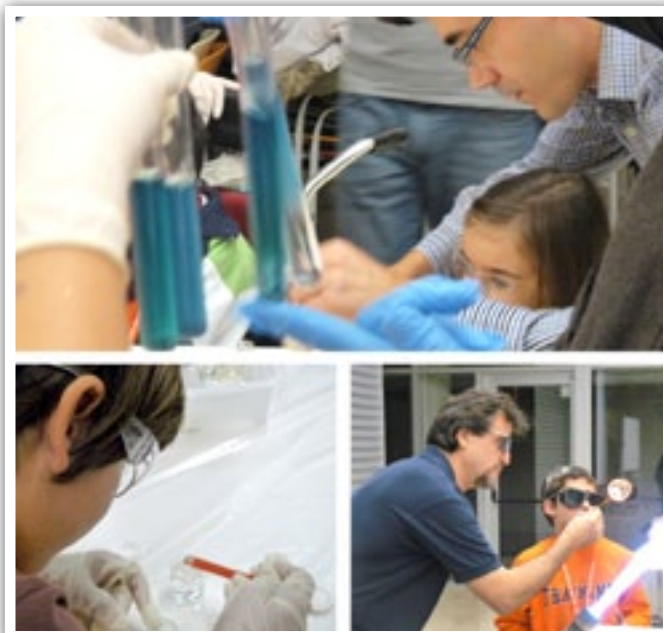


*Our Crazy about Chemistry students*

Dr. Laia Pellejà, ICIQ's science outreach officer, has conducted the course guiding the students through inspiring theoretical and classes. For this journey she has counted with the support of Lluís Lanzetta, who first visited ICIQ as high-school student for a short stay in Prof. Palomares' group. He is currently a master student at Imperial College London.

*"We've seen a new world we barely knew and we've lived experiences you don't learn in books",* adds Marina from IES Josep Tapiró, Reus.

### Química en Família



Full house! We welcomed to our chemistry workshop more than 100 kids over two days with their families and friends. We all enjoyed an evening of chemistry, experiments and glass blowing.

Children made soap, they grew a chemical garden, they wrote a secret message and they created a fantastic rainbow. Pictures speak for themselves.

 [Química en família](#)

## Through the microscope

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 Phone +34 977920200 - Fax +34 977920235



## Sports

### The rain didn't stop them!

ICIQ runners took part of Tarragona's Mitja Marató (November 30<sup>th</sup>).

Sergio Sopeña, Víctor Laserna (PhD students from Kleij's group), Mara Cruz (HR unit), Lluís Solà (ICIQ Manager), Fred Ratel (IP unit), Carles Rodríguez (Pericàs' group coordinator), Javi Izquierdo (postdoctoral researcher from Pericàs' group), Beatriz Martín (administrative support to research groups), Emilio Palomares (group leader), Marcos Rellán (PhD student from López's group) and Kerman Gómez (NMR unit). They all did their best and they went far beyond the finish line.



### The Mappazonos got ICIQ's first beach volley tournament



Fantastic beach day and even more fantastic players. Those who were there on Saturday September 27<sup>th</sup> really enjoyed it. Good games and a gorgeous beach day. Volley, swimming, beer and good conversation under the parasols.

12 teams competed and at the end, as usual, three teams got the first three places: The K-Team & Co. (K stands for Kleij) got the third place; in second place was MarcAntonis and Cleopatra (one Marc two Tonis and a girl with good foot skills) and the winners were... The Mappazonos!!! from Melchiorre's group, led by the "bravissimo" Manuel.

Great organization (Carles, Bala and Aurélien). Now, we are all looking forward to next september.