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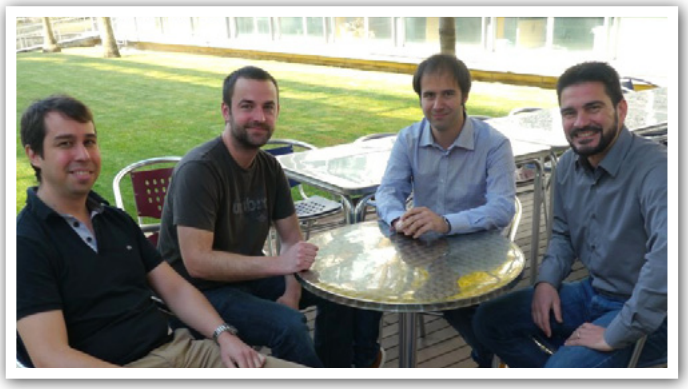
New catalysts mimic human vision



(L-R), Yannick Rey, Charlie Verrier, Luca Buzzetti and Paolo Melchiorre. Mattia Silvi, former group member, is also co-author of the paper.

Prof. Paolo Melchiorre's group published a new photocatalysis paper in *Nature Chemistry*.

Photoreceptors in vertebrates typically consist of two different, colourless parts: an organic pigment and a protein. When both pieces combine, they create a colourful, light-sensitive molecule –an iminium ion– that triggers vision upon light excitation. Inspired by this mechanism, a team of researchers at ICIQ created a new family of sustainable, environmentally friendly catalysts that can be 'switched on' using purple LEDs.

"Despite being a well-known mechanism in biochemistry, the photo-excitation of iminium ions hadn't been used to make chiral molecules yet," says Paolo Melchiorre, ICIQ Group Leader and ICREA Professor, who led the study. "Thanks to this novel approach, triggered by visible light, we can obtain products that were impossible to achieve using traditional thermally-activated transformations," he adds.

"Visible-Light Excitation of Iminium Ions Enables the Enantioselective Catalytic β-Alkylation of Enals."

M. Silvi, C. Verrier, Y.P. Rey, L. Buzzetti, P. Melchiorre.

Nature Chemistry, **2017**, DOI: 10.1038/nchem.2748

A beacon of science outreach

Tarragona's former «Banc d'Espanya» building will become a knowledge-dissemination centre. The announcement was made by Mr. Francesc Roca, Tarragona's councillor for Education, Employment and Economic Development, on April 5th in a press conference.

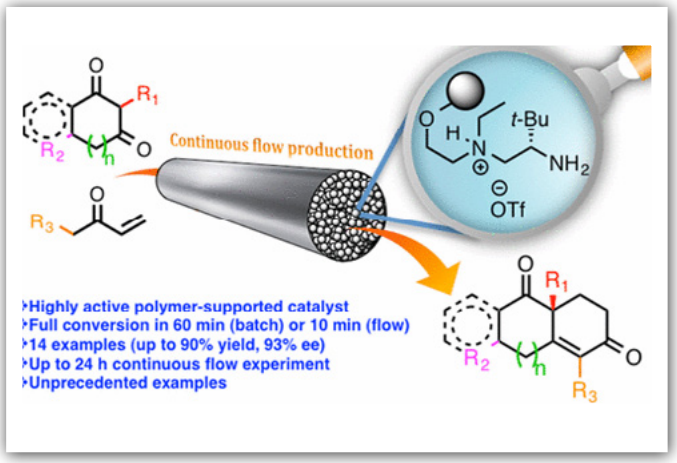
The "Banc d'Espanya" building in Tarragona.

ICIQ will participate in this project by offering its expertise on chemistry outreach. Together with Tarragona's two other main research institutes (IPHES and ICAC) we will collaborate in this ambitious endeavour providing content and materials, as well as acting as advisors during the whole creation process.

Being part of this project and reaching out to Tarragona right from the city center, will facilitate our educational task towards the general public.

The new space will be an interactive centre, not a conventional museum, sharing the excellent research carried out in Tarragona. Prof. Miquel A. Pericàs, ICIQ director, imagines "a space with hands-on laboratories, exhibitions, an auditorium, and of course a café as the main meeting-point." Prof. Pericàs expects the new centre to be "an innovative space, an experience hub that will become an inspirational model."

Continous flow: an alternative towards sustainable drugs



Researchers in Prof. Miquel A. Pericàs lab published the first **asymmetric Robinson annulation in continuous flow**, which allows the synthesis of utmost important building blocks in organic synthesis, such as the Wieland–Miescher ketone or the Hajos–Parrish ketone. For instance, the Wieland–Miescher ketone has been used as the precursor for more than 50 natural products like steroids, antibiotics, and the world-famous anti-cancer drug paclitaxel (Taxol®).

This paper represents the first example of a Robinson annulation reaction carried out in continuous flow. Pericàs and his collaborators developed a supported chiral catalyst that shows very high activity and enantioselectivity. The reactions can be carried out at mild temperatures (under 60ºC) and most of them in very short periods of time (1-2 hours).

The catalysts developed can be used non-stop during 24h to prepare some of the products in a multigram scale, with turn over numbers of as much as 117. The catalyst are sustainable because they can be cleaned and recycled without affecting their efficiency.

A Highly Active Polymer-Supported Catalyst for Asymmetric Robinson Annulations in Continuous Flow

S. Cañellas, C. Ayats, A.H. Henseler, M.A. Pericàs.

ACS Catal., **2017**, DOI: 10.1021/acscatal.6b03286

ERC and ITN projects awarded

ERC PoC to Prof. Ruben Martin got funding for his project LABEL-DIOX (Latestage catalytic carboxylation techniques with labelled carbon dioxide: new opportunities for radiolabeling). The Proof of Concept (PoC) grants for projects between 12 and 18 months long and up to 150.000€. They are designed to explore the innovation potential of results obtained by ERC grantees. Prof. Martin is currently developing another PoC project, OLE-DIOX, and will start this new one at the end of the year.

The ITN project entitled ELCOREL (Electrochemical Conversion of Renewable Electricity into Fuels and Chemicals) is coordinated by Dr. Petr Krtil from the J. Heryrovský Institute of Physical Chemistry (Czech Republic) and its main aim is to train young researchers in the conversion of water and carbon dioxide into fuels and chemicals. **Prof. Núria López**, ICIQ group leader, will participate in the project hosting 2 PhD students to perform detailed density functional calculations to gain insight into reaction pathways of CO_2 reduction.

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Celebrating ERC's 10th anniversary

ICIQ's "ERC Day" took place on Thursday, March 16th, at ICIQ Auditorium. The event featured invited talks by Prof. Andreu Mas-Colell (BIST President and former ERC Secretary General), Dr. Esther Rodríguez Blanco (ERC National Contact Point), and Prof. Antonio Echavarren (ICIQ Group Leader and ERC Advanced grantee). In addition to that, Prof. Miquel A. Pericàs (ICIQ Director) moderated a panel between Prof. José Ramón Galán-Mascarós, Prof. Rubén Martín, Prof. Paolo Melchiorre and Prof. Julio Lloret-Fillol, all of them both ICIQ Group Leaders and ERC Grantees. They discussed their experience applying for ERC Grants and how ERC funds helped them consolidate their research groups.

Since ERC started, ICIQ has been awarded 15 projects, meaning **more than €17 million in competitive funding**. This money helped ICIQ create a total of 125 jobs between PhD students, Postdocs and Technicians. Thanks to ERC funding, groups were able to buy state of the art equipment to develop their research, a total of 71 devices. And last but not least, ICIQ published 215 peer-reviewed paper and was granted two patents thanks to ERC funding.

BIST updates

BIST Founding conference

On March 31st at CCCB Barcelona took place the BIST Founding Conference, the first international scientific meeting organized by BIST. The conference brought together some of the world's leading experts in the four areas that BIST has identified as strategic for the development of multidisciplinary projects: chemical biology, graphene, big data and microscopy. The opening keynote address was delivered by Prof. Jean-Pierre Sauvage, Nobel Prize in Chemistry 2016.

Prof. Jean-Pierre Sauvage, Nobel Prize in Chemistry 2016.

Ignite projects awarded

Four ICIQ groups have been awarded an Ignite grant to carry out multidisciplinary projects with researchers from other BIST centres. The projects awarded were:

- Transport of small molecules and ions across lipid bilayers using synthetic carriers (CALIX4TRANS), Pau Ballester (ICIQ) and Manuel Palacín (IRB Barcelona)
- Pushing the tumour's detection limits in positron emission tomography (PET): developing novel materials with high-Z value (ZPro), Federico Sánchez (IFAE) and Emilio Palomares (ICIQ)
- Continuous flow oxidation processes via plasmon-assisted photocatalysis (OxiFlowPas), Romain Quidant (ICFO) and Miquel A. Pericàs (ICIQ)
- In-situ atomic resolution transmission electron microscopy of heterogeneous water oxidation catalysts (inWOC), José Ramón Galán-Mascarós (ICIQ) and Jordi Arbiol (ICN2)

BIST PhD visits

BIST PhD fellows visited ICIQ facilities on April 19th. They got acquainted with ICIQ research and life first hand through ICIQ staff and PhD students.

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Face to Face with Ben Davis

Ben Davis is a Professor of Chemistry at the University of Oxford. He's a leading expert in biological and carbohydrate chemistry and has received the most prestigious awards in the field. He sits on the Editorial Boards of several journals like ChemBioChem or ACS Central Science and has founded a couple of biotech companies. Ben Davis is also member of the Royal Society since 2015.

When did you decide to become a scientist?

When I was a child, I was interested in lots of things that seemed different, I was curious. Until I was 17 years old I was going to study law. With law I could make a difference, fight for what's right, which is really important for me. I then realised it's possible to make a big difference through chemistry, so I changed my mind just before we had to fill out our [application] forms.

What are the more promising areas in Science?

This may have become a cliché, but I think now is the best time to be a chemist. Every discipline has become incredibly aware of the importance of molecules. I sit on the Editorial Board of 'ACS Central Science', and it's a wonderful idea. Carolyn [Bertozzi, Editor-in-Chief] has this clear vision of how chemistry is at the very heart of science and how it makes a difference in almost everything. Chemists know this, but often other people don't appreciate to what extent this is true.

Can we learn chemistry lessons from looking at biology?

Absolutely. We can learn a lot about how biology controls questions of selectivity and reactivity, specially in the context of catalysis. We can be guilty as chemists of trying to make nature do what we want, and actually for me is much more fun to look at what nature shows you, and use experiments to probe that. You're an explorer in nature.

What would you say to young researchers...?

I think you've got to love what you do. [...] When we explore a new project, it feels very much like trying to make a piece of art. Genuinely, when I read the reports from my group, when I attend group meetings, I just feel incredibly excited, it feels very similar to when I go around an art gallery and I see a beautiful piece of art. It's an emotional connection.

People consider a PhD to be a qualification. But a PhD is a doctorate in philosophy, you should learn about yourself, and find a passion. I encourage people to find that. If you love something, there's a great chance you will do something important.

What are your thoughts about open access and peer review?

Open access is vital, so there is no market in science and data, they have to be owned by all. We need to find a mechanism for open access that works. Journals like 'ACS Central Science' have taken a step [forward].

And peer review has never been more important. The idea that it's a hurdle is completely false. People that complain about that are often bitter, and haven't thought deeply about the process. A non-peer-reviewed system would be madness. In the origins of the Royal Society everything was peer review meetings, and that [collective] guidance made science better. That will be our legacy.

Proust Questionnaire

A chemical element: *Don't have one.*

Favourite scientist: *Emil Fischer.*

Your favourite invention: *Buildings. I can think of several buildings that just inspire me. Good architecture.*

If you hadn't been scientist... *I'd love to spend more time exploring the aesthetics of art. I love how art is intended to make a lot of people think differently, similar to the way that science can work.*

A book: *Jane Eyre.*

A movie: *Koyaanisqatsi.*

Science is... *Art.*

MSCA Grants

Three postdoctoral researchers have been awarded with an individual fellowship (MSCA-IF) to carry out their 2-year projects at ICIQ:

- Dr. Adela I. Carrillo from the Pericàs Research Group will start her project Pho- CuS-Flow (Photocatalysis induced by copper complexes supported on Silica materials-Study in Flow processes).

- Dr. Kaisa J. Helttunen will join the Ballester Research Group to carry out the project MAREXT (Macrocyclic receptors for selective anion extraction).

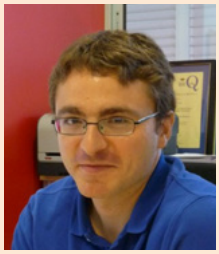
- Dr. Xiao-Li Pei joined the Echavarren Research Group last September. She will soon start working on her project PGOLDCAT (Polynuclear Gold Cluster Catalysis).

ETSF Young Researchers Meeting

The ETSF Young Researchers' Meeting (YRM) will be held at ICIQ from June 5th to 9th, 2017. The YRM is an annual workshop for postdocs, PhD students and Master students, who work on state-of-the-art theoretical and computational methods for the study of the electronic and optical properties of materials. It addresses problems and recent advances in method development, algorithms and implementations as well as applications to real materials. Young researchers are given a chance to showcase their work, exchange ideas with others at their own level, learn novel techniques, start new collaborations, and improve their presentation skills.

News in brief

Thesis: Drs. Marta Rodríguez, Cayetana Zárate, Ruth Dorel, Víctor Fernández, Martín Romero, José Ramón Romero, Carmen A. Mak, Sergio Roso, Patricia LLanes and Pilar Calleja, predoctoral students at ICIQ have defended their PhD thesis. They were all awarded the highest honours for their work.



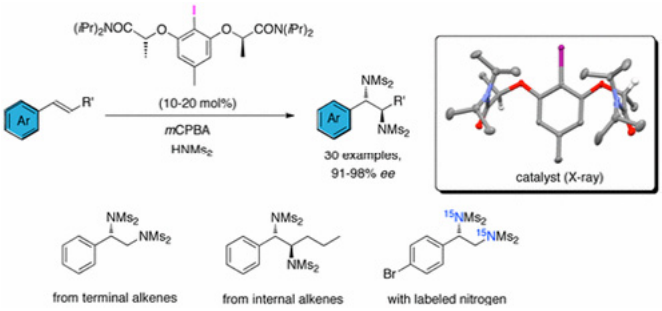
Prof. Rubén Martín, ICIQ group leader and ICREA professor, received the prestigious OMCOS award recognising a scientist under the age of 40 who has made significant contributions to the field of organometallic chemistry and organic synthesis. He is the first Spanish Chemist ever to win this award.

Prof. Kilian Muñiz was honoured with this year's Synthesis Best Paper Award for his feature "Enantioselective Vicinal Diacetoxylation of Alkenes under Chiral Iodine(III) Catalysis" (*Synthesis*, **2016**, *48* (6), 816-827). Prof. Paul Knochel, Editor-in-Chief of Synthesis, commented how "the development of new catalytic asymmetric synthesis of chiral molecules is especially important for pharmaceutical and fine chemistry in general."

ChemSusChem Special issue: Profs. Arjan W. Kleij and Atsushi Urakawa (ICIQ group leaders), together with Prof. Michael North (University of York, UK) have co-edited the latest issue of *ChemSusChem* (**2017**, 10, 6) on 'Catalysis for CO_2 conversion'. The aim of this Special Issue is to highlight recent work that illustrates the importance of catalysis as a key enabling technology for CO_2 conversion.

A-Leaf website: check out its new website! A-Leaf: a photo-electro-catalytic cell from earth-abundant materials for sustainable solar production of CO_2-based chemicals and fuels.

Catalytic and enantio-selective diamination of styrenes



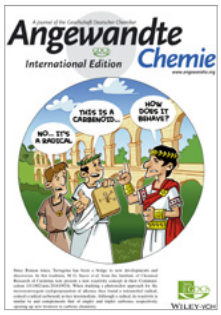
Diamination reactions are often hard to catalyse because nitrogen atoms strongly coordinate to transition metals. However, vicinal diamines are valuable for the pharmaceutical industry, as they are important building blocks for the synthesis of various alkaloids and drugs. Now, the group of Prof. Kilian Muñiz discovered the first catalytic example for an asymmetric diamination of styrenes. Thanks to iodine(I/III) redox catalysis, our researchers achieved enantioselectivities of over 91% in 30 different examples.

Sustainability is key to this new method. Mainly because it does not require the use of expensive, toxic metals, but also because it uses catalytic amounts of the chiral iodine and clean, non-chlorinated solvents. The new conditions uncovered by Muñiz et al. reduce the amount of side products of the reaction, maximizing the yield of diamines over undesired epoxides and aminoalcohols.

This research was recently highlighted in Chemistry Views.

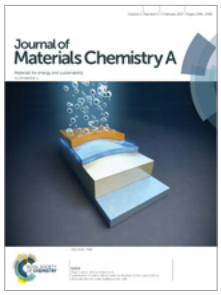
Catalytic Asymmetric Diamination of Styrenes
K. Muñiz, L. Barreiro, R. Martín-Romero, C. Martínez.
J. Am. Chem. Soc. **2017**, DOI: 10.1021/jacs.7b01443.

Journal Covers



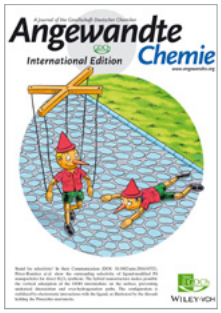
A Stereoconvergent Cyclopropanation Reaction of Styrenes

A.M. del Hoyo, A.G. Herraiz, M.G. Suero
Angew. Chem., Int. Ed., **2016**, *56*, 1610-1613. DOI: 10.1002/anie.201610924



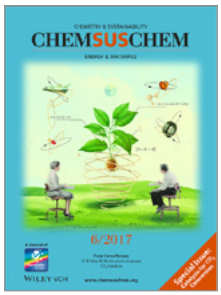
Substitution of native silicon oxide by titanium in Ni-coated silicon photoanodes for water splitting solar cells

Yuanyuan Shi, Tingting Han, Carolina Gimbert, Xiaoxue Song, Mario Lanza and Antoni Llobet
J. Mater. Chem. A **2017**, *5*, 1996-2003. DOI: 10.1039/C6TA08774D.



Hybrid Palladium Nanoparticles for Direct Hydrogen Peroxide Synthesis: The Key Role of the Ligand

G.M. Lari, B. Puértolas, M. Shahrokhi, N. López, J. Pérez-Ramírez
Angew. Chem., Int. Ed. **2016**, *56*, 1775-1779. DOI: 10.1002/anie.201700066



CO_2 Catalysis (ChemSusChem 6/2017) (page 1034)

Prof. Arjan W. Kleij, Prof. Michael North and Prof. Atsushi Urakawa
ChemSusChem **2017**, *10*, 1036-1038. DOI: 10.1002/cssc.201700379.

"Aportando Valor al CO_2"

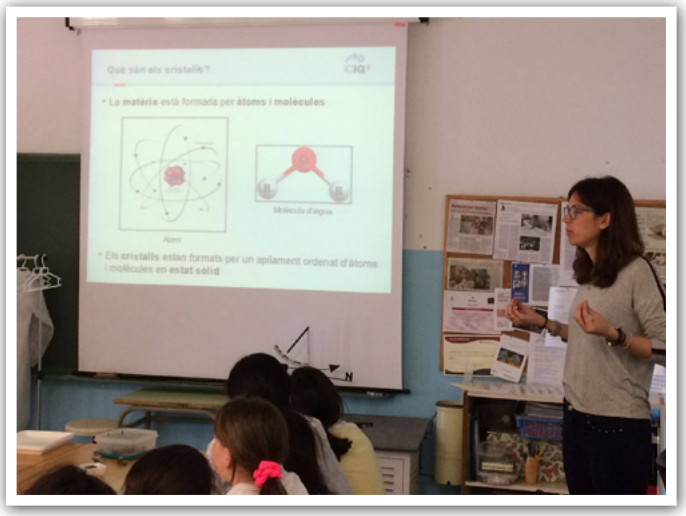
From May 9th to 10th 2017, ICIQ will host the second edition of the congress "Aportando Valor al CO_2" which is organized by "Plataforma Tecnológica Española del CO_2" (PTECO2), "Plataforma Tecnológica Española de Química Sostenible" (SusChem-España) and ICIQ.

The congress is aimed at offering a global view of the different approaches in the technologies of use and transformation of CO_2: from its foundations to its applications in the market. Discussions will be centered in five areas: political and strategic motivation; CO_2 to materials (use of CO_2 and biomass); CO_2 to fine chemicals and polymers; CO_2 to energy vectors and CO_2 direct uses.

Sweet science

La "Ciència de la Xocolata" is an educational project aimed at engaging primary school students to pursue a scientific career. The project has been designed in collaboration with the Universitat Rovira i Virgili (URV) and is being carried out at Pau Delclòs School in Tarragona.

The project is intended to focus in particular on raising girls' interest. Seminars are delivered by female researchers who are currently carrying out leading research in the URV and ICIQ. Both the research they carry out and their life experience are important for becoming points of reference for the children. The five theoretical-experimental seminars programmed show the research and knowledge behind chocolate, bringing to light the value of research from different perspectives. Specifically, URV and ICIQ researchers approach the DNA of cocoa, the origin and crystals of chocolate, as well as chocolate as a food and as art.



Dr. Marta Martínez from ICIQ's X-Ray Diffraction Unit delivered a talk about crystals on April 25th.

Summer Camp

ICIQ is offering the following two courses for this year's summer camp:

- ***"Fem Química":*** let's do chemistry is an introductory course to the world of chemistry. Participants have the chance to carry out experiments in our learning laboratory, doing group work and learning how to present their work and results obtained in public.

Age: children finishing 5th and 6th year of primary education

Dates and timetable: 24th – 28th July, 9 AM – 1:30 PM

- ***"M'agrada la Recerca":*** I like research is addressed to children wishing to investigate the world of the laboratory by means of the research carried out at ICIQ. They find out about laboratory techniques and see all the possibilities that chemistry can offer.

Age: children finishing 1st and 2nd year of secondary education.
Dates and timetable: 26th- 30th June, 9 AM – 1:30 PM

BIYSC

Once again ICIQ will be participating in BIYSC, an international scientific challenge aimed at connecting the most passionate science students with the best researchers. We'll be offering the workshop entitled "Artificial Photosynthesis" where students will learn how to copy the natural photosynthesis process in the lab to discover different ways to use and store solar energy. "Artificial Photosynthesis" counts with the collaboration of the Galán-Mascarós Research group at ICIQ.

BIYSC was created by the Fundació Catalunya-La Pedrera to inspire bright young scientists to apply their minds to multidisciplinary research so they can pursue their research passions.

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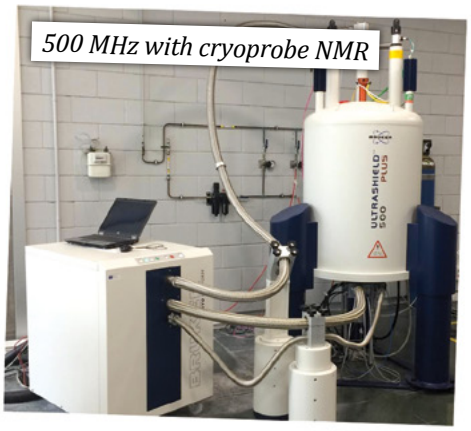
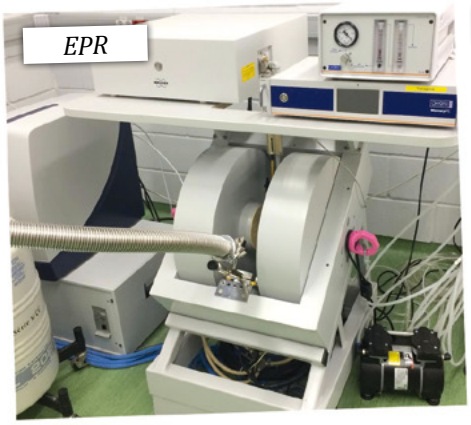
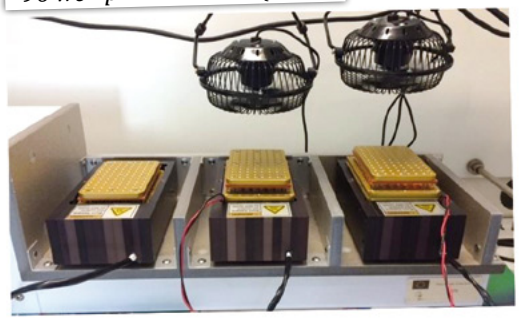
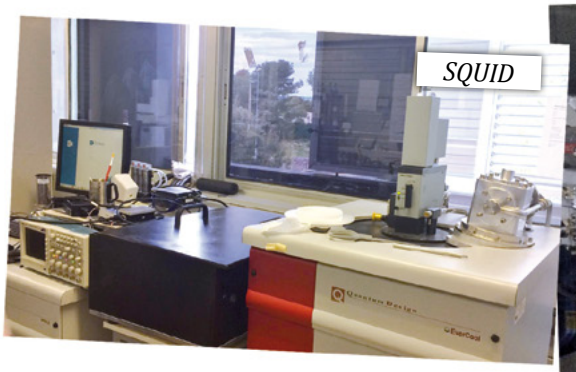
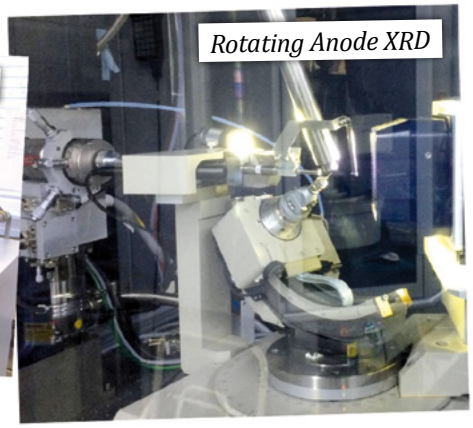
Selected ICIQ equipment

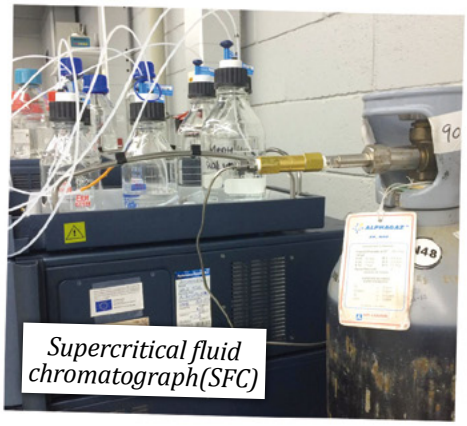

500 MHz with cryoprobe NMR


EPR


96 well plate reactors (HTE)

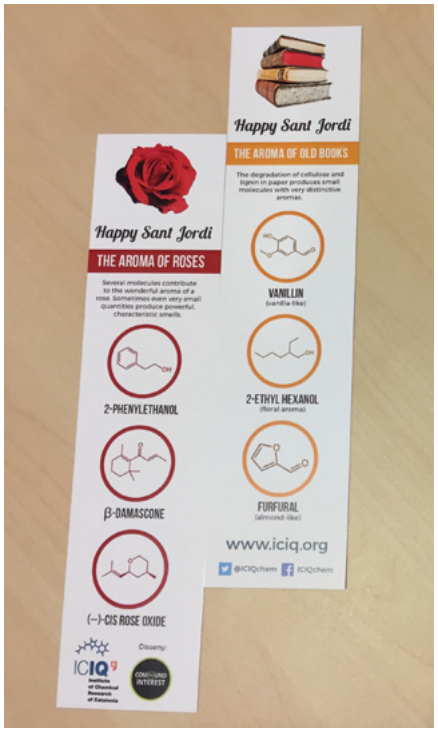

SQUID


Rotating Anode XRD


Supercritical fluid chromatograph(SFC)

Celebrating Sant Jordi

Chemistry bookmarks



Empowering ICIQ PhD students

ICIQ
PhD Day
15-16 June 2017

Some ICIQ PhD students are organizing an event for the ICIQ community featuring interesting invited conferences, flash presentations and poster and networking sessions. It will take place at ICIQ on the 15th–16th June 2017. It represents a good opprtunity to overview the chemistry carried out in different sectors. The invited speakers are Dr. Mónica Pérez-Temprano (ICIQ Group Leader), Dr. Anna Homs (Ferrer); Dr. David Wilcke (Bayer Crop Science), César Palmero (MDPI); Víctor Molina Navas (Gadis) and Dr. Ana M. Castaño (Eli Lilly & Co.).