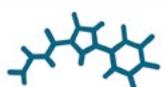




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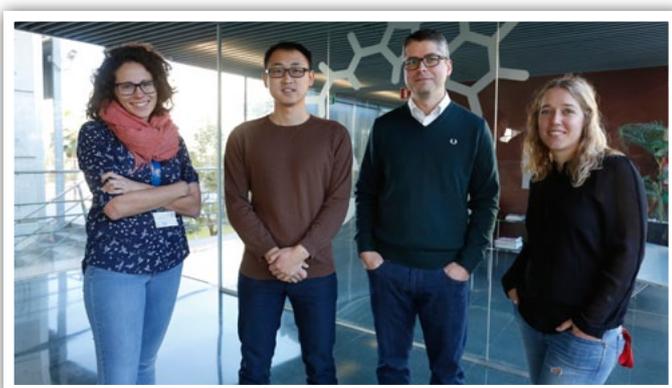


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www.iciq.eu

## Interstellar molecules inspire new transformations



L-R: A.M. del Hoyo, Z. Wang, M.G. Suero and A. Herraiz

Back in the 1930s, astronomers detected one of the first molecules in interstellar space – carbynes. The simplest carbyne, formed by carbon and hydrogen only, is nowadays considered one of the most basic ingredients for life. Despite the impact these molecules could have in synthesis, they have eluded chemists for years. But now, researchers at ICIQ have discovered how to generate carbynes in the lab using visible light and photocatalysts. Led by Dr. Marcos García Suero, they have created a new methodology that allows them to create chiral centres adding, like lego pieces, three different fragments to a carbyne.

Suero and his team used carbynes to add new chiral fragments to already ‘finished’ molecules, without having to alter the whole synthetic process from scratch – which is usually very problematic, expensive and time consuming. Suero’s group demonstrated the potential of their original idea by functionalizing drugs like duloxetine (antidepressant), paclitaxel (anticancer), fingolimod (multiple sclerosis) or ibuprofen.

[Generating carbyne equivalents with photoredox catalysis](#)

Z. Wang, A.G. Herraiz, A.M. del Hoyo, M.G. Suero.

*Nature*, 2018, DOI: 10.1038/nature25185

[Link: See animated video](#)

## Dr. Elisabet Romero, ICIQ’s new group leader

Dr. Elisabet Romero joined our institute through [ICIQ’s Starting Career Programme \(ICIQ-SCP\)](#) aimed at attracting new talent and helping young researchers to start their independent careers. The programme is funded by the Severo Ochoa Excellence grant. Previously, she worked as a researcher in Prof. Rienk van Grondelle’s group at the Vrije Universiteit, Amsterdam.

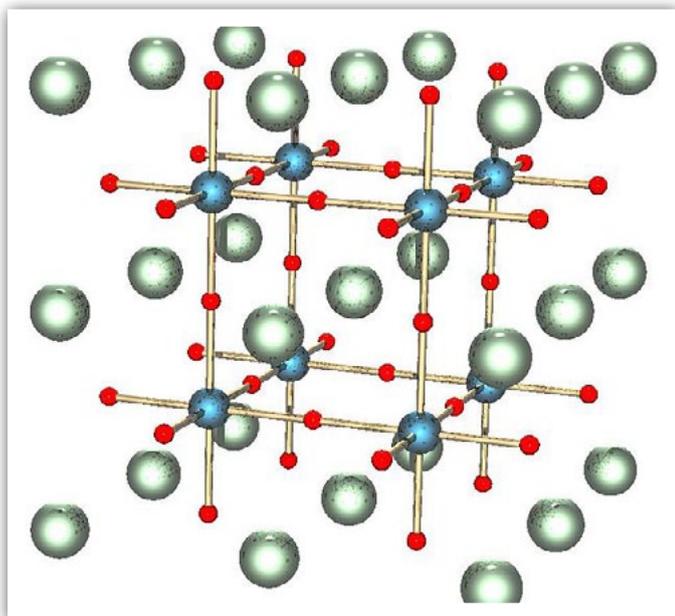


Dr. Elisabet Romero

“I am excited to start this new scientific adventure. ICIQ has everything I could wish for: a wide range of facilities and services for its scientific community, and above all, great professionals and wonderful people,” says Dr. Romero.

At ICIQ, [her group](#) will focus on the design, construction and investigation of bio-inspired chromophore-protein assemblies with the ability to absorb, transfer and convert solar energy into electrochemical energy. The final goal is to connect these assemblies to catalysts to achieve the efficient conversion of solar energy to fuel. She is joining the ICIQ groups working in the field of artificial photosynthesis, one of the institute’s main research lines.

## Understanding how perovskites work



*The lattice of an imaginary perovskite.*

Perovskite solar cells are becoming increasingly popular. However, the solar cell function behind their high efficiency remain unclear. Perovskite composition is certainly key but, surprisingly, materials with very different cations and halide ratios lead to similar performance results. To better understand this, ICIQ in collaboration with EPFL researchers, propose the use of 'old tricks' to measure novel processes and the relationship between the perovskite structure, the ion motion and the charge transfer processes.

The process, envisioned by Prof. Emilio Palomares' group, is based on photo-induced charge extraction (PICE) measurements. During these experiments, researchers fully charge, then short-circuit solar cells to investigate the details of charge migration processes. Using advanced perovskites and solar cells provided by collaborators from École Polytechnique Fédérale de Laussane (EPFL), they determined that different kinetics in PICE are due to ion migration and recombination processes.

[Photo-Induced Dynamic Processes in Perovskite Solar Cells. The Influence of Perovskite Composition in the Charge Extraction and the Carriers Recombination](#)

N.F. Montcada, M. Méndez, K.T. Cho, M.K. Nazeeruddin, E. Palomares

*Nanoscale* **2018**, DOI: 10.1039/C8NR00180D.

## BASF renews ICIQ's seminar programme

On February 16th [BASF Española](#) renewed sponsorship of the [ICIQ Seminar Programme](#) for training Master and PhD students and postdoctoral researchers. The agreement reflects BASF's commitment to make an annual donation to ICIQ for a period of three consecutive years, from 2018 to 2020. BASF has been funding our seminar programme since 2012.

The ICIQ Seminar Programme is a meeting point for top-class chemists undertaking ground-breaking research. It consists of about 35 scientific seminars per year, scheduled on a weekly basis. Among the most prestigious scientists, including Nobel Prize laureates K.B. Sharpless, R.R. Schrock, R. Grubbs, A. Suzuki and J.P. Sauvage, have presented seminars as part of the programme. Seminars are open to all ICIQ researchers and the scientific public at large.



*Miquel A. Pericàs (left), ICIQ director, and Carles Navarro, CEO at BASF Española signed the agreement.*

## Prof. Antonio M. Echavarren, new RSEQ President



Last January, the [Spanish Royal Society of Chemistry \(RSEQ\)](#) celebrated an election to renew part of its Board. Prof. Antonio M. Echavarren, ICIQ Group Leader and URV Professor, led the winning candidacy. As new RSEQ President, Prof. Echavarren expects an even

more dynamic society that encourages the organisation of more symposia and conferences. The new board will also work towards a better cooperation between young researchers and the different RSEQ divisions.

## ioChem-BD helps authors of Wiley journal to share their data

ioChem-BD is a platform created by researchers at ICIQ and URV. This innovative tool aims to parse, easily organise and publish the results of computational chemistry research projects. Moreover, because ioChem-BD is an open-access initiative, it allows researchers to further analyse data published by their peers, or start new studies based on previously existing work.

Now, the [International Journal of Quantum Chemistry](#), published by Wiley, lists this open-access platform as one of the solutions for publishing computational data about molecules and materials. In their new submission guidelines, the International Journal of Quantum Chemistry highlights the versatility of ioChem-BD for archiving and storing data generated with a variety of simulation packages.



ioChem-BD: the solution to manage computational chemistry Big Data

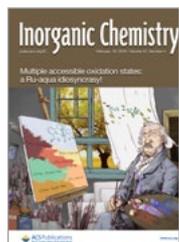
## Journal Covers



[Synthesis and Binding Studies of a Tetra- \$\alpha\$  Aryl-Extended Photoresponsive Calix\[4\] pyrrole Receptor Bearing meso-Alkyl Substituents](#)

L. Escobar, F.A. Arroyave, P. Ballester

*Eur. J. Org. Chem.* **2018**, 1097-1106, DOI: 10.1002/ejoc.201701602.



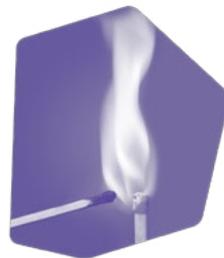
[Synthesis, Structure, and Redox Properties of a trans-Diaqua Ru Complex That Reaches Seven-Coordination at High Oxidation States](#)

R. Matheu, J. Benet-Buchholz, X. Sala, A. Llobet

*Inorg. Chem.* **2018**, 57, 1757-1765, DOI: 10.1021/acs.inorgchem.7b02375.

## BIST updates

### SOLHYCAT gets ignited



The 2017 [BIST Ignite Program](#) awarded five projects for their multidisciplinary and high level of scientific excellence. The winners will have eight months to develop their projects, at which point they will be eligible to apply for the second phase of the 2017 Ignite Program. One of the awarded projects is SOLHYCAT (“Carbon Materials as Charge Transfer Platforms to Convert Sunlight into Fuel with a Nanocrystal-Molecular Catalyst hybrid”), led by Antoni Llobet of ICIQ and Víctor F. Puntes of ICN2.

### Leadership in Action course



BIST postdoctoral researchers gathered in Collbató, at the foot of the mountain of Montserrat, for an intensive three day course (April 11<sup>th</sup>-13<sup>th</sup>) focused on the development of leadership skills for successful self-management and progress in a professional career.

### BIST Colloquium series



On April 9<sup>th</sup>, BIST’s Master students came to ICIQ to attend Prof. Serena DeBeer’s (Max Planck Institute for Chemical Energy Conversion) talk on “X-ray spectroscopic studies of biological methane oxidation.” They also had time to discuss research with her. Moreover, they participated in a workshop about planning a participatory dialogue activity by Dr. Carolina Llorente (Universitat Pompeu Fabra).

## Face to Face with David Leigh



David A. Leigh is a Royal Society Research Professor and, since 2014, the Sir Samuel Hall Chair of Chemistry at the University of Manchester, UK. Previously, he worked as a postdoc in Ottawa, and as the chair of synthetic chemistry in Warwick and then organic chemistry in Edinburgh. Leigh's research focuses on new approaches to functional molecule synthesis and the influence of non-covalent interactions on structure and function from biology to materials science. Over the last 20 years, Leigh has pioneered the development of molecular machines and motors, notably molecular knots.

### ■ What is being a scientist for you?

It's a great job, a fantastic way to live your life. Because science is about finding out what's true. Even though we live in the age of 'fake news', thanks to science we know more truth than ever about the way the world really is and how it works. Moreover, I am lucky to work every day with young people to see how far we can be creative and, using science, create things that didn't exist before. Hopefully, we're changing the world for the better.

### ■ Why did you decide to become a chemist?

I never thought about it as a kid, or even while in University. Back then, I used to believe I was going to become a high school teacher. Most lecturers in the UK were really old, so becoming one didn't seem like an option at all. But then I did a postdoc in Canada and made a lot of friends who were physical and theoretical chemists. They helped me develop a much broader image of chemistry, and I learnt to apply my skills in organic chemistry to solve the problems of my colleagues in those different fields. When I went back to the UK, I saw an opportunity in

collaborating with other disciplines. To be honest, I wasn't the smartest organic chemist, didn't know a lot about mechanisms or the names of the reactions, but I had something that made me different. I could see a bit further, I was open to new ideas, and thus I was able to tackle problems that were interesting for my colleagues. And all this was quite new, back in the nineties!

### ■ What are the most promising areas in Science?

For organic chemists, I see a lot of interest in C-H activation, photochemistry, and electrochemistry. It is wonderful how young chemists in the US like Baran and Macmillan are re-inventing subjects that, although they were known, they were clearly not mature enough. It is nice to see there is still a big chance to be creative, and I am really excited to see this 'renaissance' of organic synthesis.

### ■ Why do you use magic in your lectures?

It's funny to see the reaction of scientists when they see something that just doesn't add up. But I do it mostly to entertain, this way if people are not interested in my research, at least they will have a good time! I also think that magic has a lot in common with chemistry. You know what you put in your flask, then you see your products... but most of the times you don't know what happens in between, even if you draw a ton of tiny arrows and intermediates to 'explain' the mechanism. And it teaches us something beautiful: sometimes the obvious explanation for what happened may not correspond to reality.

## Proust Questionnaire

**Favourite scientist:** *I would have to choose between James Clerk Maxwell or Richard Feynman. Maxwell amazes me, he drew the laws electromagnetism without even knowing that atoms really existed, and the things he came up with are still considered true today! This doesn't happen with other scientists of the same time, like Lord Kelvin.*

**Your favourite invention:** *Two of the most impactful are the motorcar and mass communication, like TV or the Internet.*

**If you hadn't been scientist...** *I would have been a professional poker player.*

**A book:** *Lord of the Rings.*

**A movie:** *I always cry with 'Schindler's List'.*

**Science is...** *the truth about the way things are.*

## Eight MSCA go to ICIQ!

Eight postdoctoral researchers have been awarded with a MSCA (Marie Skłodowska Curie Actions) – IF (Individual Fellowship)-2017 to carry out their research projects at ICIQ. Dr. Sahoo Basudev (Martin group), Dr. Giacomo Crisenza (Melchiorre group), Dr. Catherine Holden (Melchiorre group), Dr. Liyin Jiang (Suero group), Dr. Xiaoming Jie (Echavarren group) and Dr. Sudipta Raha (Melchiorre group), will be starting their two-year projects in the following months at ICIQ. The MSCA-IF fellowships aim to help experienced researchers boost their career by working abroad.



Two of these MSCA fellowships are global fellowships, carried out in collaboration with a third country outside of Europe, where the fellows spend their first 1 or 2 years before joining ICIQ for one more year. Dr. Sergio Gonell, currently at the University of North Carolina Chapel Hill (Miller group), will join Lloret-Fillol group next year. While, Dr. Christopher Sandford, currently at the University of Utah (Sigman group), will join Martin group in 2020.

## Impulsion, ICIQ's new COFUND



The European Commission COFUND Programmes aim to co-fund new or existing regional, national and international programmes to provide international, intersectorial and interdisciplinary (the triple “i”) research training. This COFUND project is dubbed I<sub>2</sub>:ICIQ Impulse, wants to “impulse” the research career of 12 postdoctoral researchers in the next 4 years through two competitive calls. The first call will be launched at the end of this year. I<sub>2</sub>:ICIQ Impulse is ICIQ's second COFUND programme after IPMP (International PostDoctoral Mobility Programme) which has just been finished in April 2018.

## News in brief

**Thesis:** Drs. Lidia Clot, Sergio Sopeña, Marcos Rellán, Rohit Gaikwad, Shoulei Wang and Eduardo C. Escudero, predoctoral students at ICIQ defended their PhD thesis. Congrats!



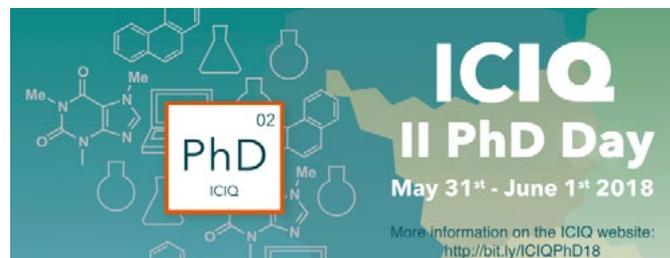
**Congrats! Dr. Ruth Dorel** (Prof. Echavarren's group, now a Ramón Areces post-doc fellow at Prof. Feringa's lab) and **Dr. Ignacio Funes** (Prof. Maseras' group, now working as a postdoctoral researcher), were awarded the 'Josep Castells' award for best PhD theses by the [Catalan section of the Spanish Royal Society of Chemistry \(RSEQ\)](#).

**CompCAT Registration to CompCat:** Computational Catalysis for Sustainable Chemistry conference is open!



## ICIQ's 2nd PhD Day

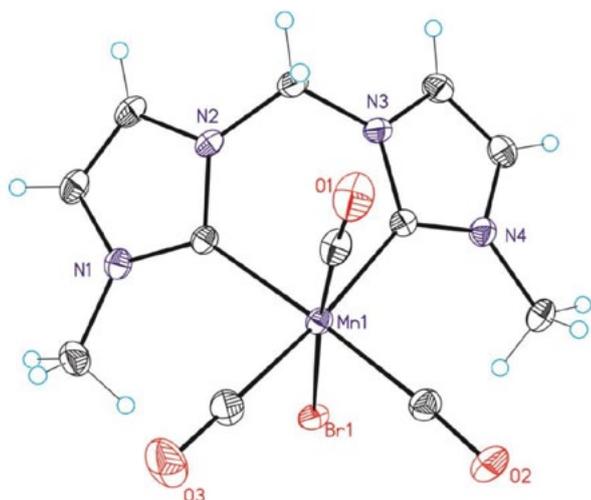
The ICIQ PhD Day is an event designed for and by ICIQ PhD students featuring interesting invited conferences, flash presentations and poster and networking sessions.



This year's programme includes talks by former ICIQ researchers such as Drs. Gerald Metselaar (BASF), Marçal Capdevila-Cortada (Editor in Nature Catalysis) and Eugenia Martínez (Eurecat) who will share their career experience and explain their current work. It will also feature talks about ICIQ's staff members. Dr. Ignacio Funes will shed light on science outreach and Dr. Lorena Tomás will show the nuts and bolts of project management.

## Magnese carbenes- key for effective CO<sub>2</sub> reduction

Imagine transforming carbon dioxide into a sustainable feedstock for the production of value added chemicals. This could be possible thanks to efficient catalysts that could reduce CO<sub>2</sub> using renewable energy. Some homogeneous catalysts based on earth abundant metals like manganese and bipyridine ligands show promising results for a selective conversion of CO<sub>2</sub> to CO. On the other hand, reported manganese-based catalysts containing non-diimine ligands are rare and usually inefficient, including systems with mixed pyridyl/*N*-heterocyclic carbene moieties.



*New highly active Mn(I) complex for the selective electrocatalytic reduction of carbon dioxide to CO with excellent TOF values.*

Now, ICIQ researchers, in collaboration with chemists at Nova University in Lisbon, Portugal, have developed a novel manganese(I) complex featuring a bidentate *N*-heterocyclic carbene that outperforms all the electrocatalysts synthesized to date. The octahedral complex was fully characterized using NMR, IR, and X-ray crystallography, and showed spectroscopic features in concordance with previously reported manganese carbenes.

### [A Highly Active \*N\*-heterocyclic Carbene Mn\(I\) complex for Selective Electrocatalytic CO<sub>2</sub> Reduction to CO](#)

F. Franco, M.F. Pinto, B. Royo, J. Lloret-Fillol.  
*Angew. Chem. Int. Ed.* **2018**, DOI: 10.1002/anie.201800705.

## “Young Researcher” award

Dr. Marcos G. Suero, ICIQ Group Leader, was recognized with the RSEQ ‘Young Researchers’ award. The award acknowledges great individual research that has been performed and enhanced by a Young Researcher (<40 years old). The RSEQ also awarded its 2018 Gold Medal to Prof. Jesús Jiménez Barbero, one of the members of our Scientific Committee. Congratulations!



*Dr. Marcos G. Suero.*

## Journal Covers



### [A Domino Process towards Functionally Dense Quaternary Carbons through Pd-Catalyzed Decarboxylative Csp<sup>3</sup>-Csp<sup>3</sup> Bond Formation](#)

W. Guo, R. Kuniyil, J.E. Gómez, F. Maseras, A.W. Kleij

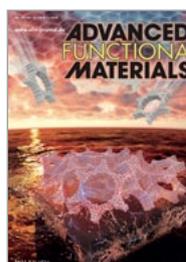
*J. Am. Chem. Soc.* **2018**, *140*, 3981-3987, DOI: 10.1021/jacs.7b12608.



### [XBphos-Rh: A Halogen-Bond Assembled Supramolecular Catalyst](#)

L. Carreras, M. Serrano-Torné, P.W.N.M. van Leeuwen, A. Vidal-Ferran

*Chem. Sci.* **2018**, DOI: 10.1039/C8SC00233A.



### [Increasing the Efficiency of Organic Dye-Sensitized Solar Cells over 10.3% Using Locally Ordered Inverse Opal Nanostructures in the Photoelectrode](#)

L. Xu, C. Aumaitre, Y. Kervella, G. Lapertot, C. Rodríguez-Seco, E. Palomares, R. Demadrille, P. Reiss

*Adv. Funct. Mater.* **2018**, *28* (15), 1706291, DOI: 10.1002/adfm.201706291.

## Science Fairs

We went to [YOMO](#) (The Youth Mobile festiva, February 27<sup>th</sup>-March 2<sup>nd</sup>, Barcelona) and [Recerca en directe](#) (April 11<sup>th</sup>-14<sup>th</sup>, CosmoCaixa, Barcelona). In both science fairs we presented our brand new game on artificial photosynthesis, one of the main research fields at ICIQ. The game reproduces a



ICIQ's racing cars at YOMO

chemical reactor that converts CO<sub>2</sub> and water into a fuel using a catalyst. The fuel obtained is used to power two cars that release CO<sub>2</sub> which we'll use to refill our reactor. So the cycle is closed! Science fairs are an excellent place to showcase our research to students of all ages from many places.

## Chemical expression

A poster for "Missatges" (Messages) at Banc d'Espanya. The title "MISSATGES" is in large white letters. Below it, it says "Expressió prehistòrica, romana i química". The date is "23 d'abril 2018" from 10:00 to 13:00. Logos for ICIQ, ICAC, and IPHES are visible. The background features chemical symbols and a stylized figure.

On April 23<sup>rd</sup> (Sant Jordi) we invited several schools from Tarragona to participate in a series of chemical experiments related to writing. Within the framework of the science outreach programme "Ciència al Banc d'Espanya" we presented, together with ICAC and IPHES, three different workshops to commemorate the day where books are given as a gift. Primary school and ESO students made messages disappear and reappear. They also had the opportunity to write as Romans did and paint as cavemen/women did.

## Casal d'Estiu



[Registration](#) to our Summer Camp in chemistry is now open. We are offering two courses: **Fem química**, introduction to chemistry from experiments that help to understand our daily life from the perspective of chemistry, and **M'agrada la recerca**, where students learn different laboratory techniques and see the potential of chemistry to improve the world.

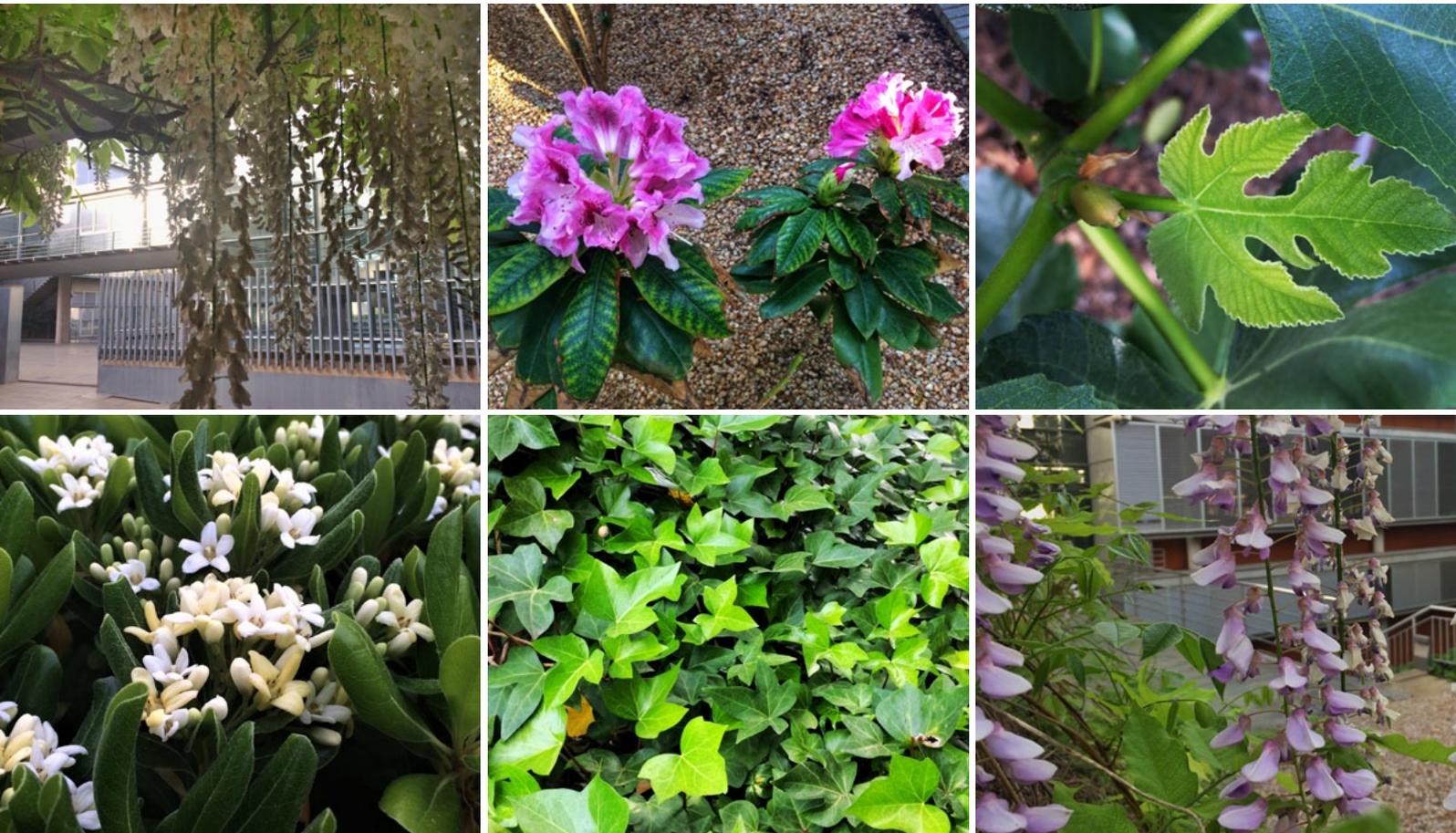
### ■ Courses

**Fem Química:** 5th and 6th grade of primary school, from June 25<sup>th</sup> to June 29<sup>th</sup> 2018. (9am-1.30pm).

**M'agrada la Recerca:** 1st and 2nd grade of ESO, from July 30<sup>th</sup> to August 3<sup>rd</sup> 2018 (9am-1.30pm).

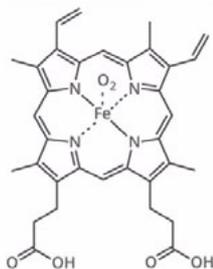
A poster for "La Ciència de la Xocolata" (The Science of Chocolate). The title is in large white letters on a dark background. Below it, it says "TALLERS CIENTÍFICS AL VOLTANT DEL CACAU I DEL DOLÇ MÉS POPULAR". Logos for ICIQ, URV, and the library are visible. The background features a chocolate bar.

## ICIQ Spring



# FELIÇ DIA DE SANT JORDI

## EL COLOR I L'OLOR DE LA SANG



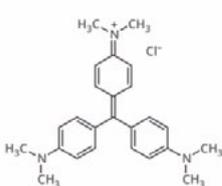
HEMO B (FORMA OXIGENADA)

El color vermell de la sang es deu a les unitats hemo que contenen ferro i que formen l'hemoglobina. El compost que dona l'olor metàl·lica característica a la sang és el *trans*-4,5-epoxi-(E)-2-decenal.

TRANS-4,5-EPOXI-(E)-2-DECENAL

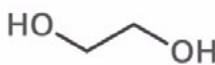


## EL COLOR I L'OLOR DE LA TINTA

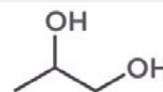


VIOLETA DE METIL

Les tintes negres es basen en negre de carboni o en una barreja de compostos de colors. El color de la tinta blava prové dels colorants amb trifenilmetà com el violeta de metil. L'olor ve donada pels diferents dissolvents que s'utilitzen en la tinta com ara l'etilenglicol i el propilenglicol.



ETILENGLICOL



PROPILENGLICOL

## PINT OF SCIENCE TARRAGONA



PINTOFSCIENCE.ES

Click and see the full programme and schedule!