

# XV YOUNG SCIENCE SYMPOSIUM

Del 7 al 9 de Julio de 2021



## LIBRO DE COMUNICACIONES





## Bienvenida del Decano

Os damos la bienvenida a esta nueva edición del 15<sup>th</sup> Young Science Symposium, que organiza la Facultad de Ciencias y Tecnologías Químicas de la Universidad de Castilla – La Mancha junto con sus jóvenes investigadores. En esta ocasión, y atendido a la situación ocasionada por el COVID, en formato mixto.

El simposio, nació en el año 2007, como una iniciativa del personal más joven de la Facultad para poner en valor la investigación realizada, en un Centro en el que esta faceta del profesor universitario tiene una muy especial relevancia y nuestros jóvenes investigadores querían reivindicar su papel y contribuir a su excelencia. Ha ido madurando y cogiendo cuerpo con el tiempo y, a día de hoy, es un elemento que trasciende de sus objetivos iniciales y permite mostrar a la Sociedad, desde la óptica de los jóvenes investigadores, la investigación puntera que se realiza en nuestro Centro, sin olvidar la idea base de su concepción original: Promover y divulgar la investigación en los campos científicos y tecnológicos que tiene que ver con la Química, la Ingeniería Química, y la Ciencia y Tecnología de los Alimentos, que son las enseñanzas tradicionales de nuestro Centro. Afortunadamente, y como consecuencia del enorme trabajo desarrollado por los Comités Organizadores, en las últimas ediciones la relevancia ha crecido muy significativamente, y las comunidades investigadoras de otros centros de la Universidad con investigación en la temática se han unido, aumentando la relevancia del evento y permitiendo aumentar su interdisciplinariedad.

El Simposio tiene además una segunda componente importante, en este caso pedagógica. Permite a nuestros titulados introducirse en el mundo de la organización de eventos científicos y en el de la difusión científica, elementos muy importantes de la actividad investigadora. Nuestros jóvenes investigadores pueden trabajar en todas las fases de vertebración de un evento, lo que constituye un aprendizaje muy importante. Conocen desde dentro cómo se organizan los congresos a los que después asisten. Aprenden a discutir resultados en un foro más amigable y entrenan sus actuaciones para la difusión en los eventos internacionales. En este contexto, constituye una actividad formativa para los estudiantes de nuestros programas de doctorado. Y lo que es más... ilusiona a todos nuestros jóvenes investigadores que trabajan de una forma u otra para conseguir que sea un éxito total. En línea con lo que se ha ido haciendo otros años, en esta edición, para incentivar a aquellos jóvenes doctorandos y nuevos doctores que participan como ponentes en estas Jornadas, también se concederán el VI PREMIO CIENCIA JOVEN y cuatro premios en la categoría I PREMIO VIRTUAL-FLASH en categoría TFG, TFM y tesis, con alguna otra sorpresa para los asistentes.

Desde la Facultad, que aporta la infraestructura y los recursos necesarios, hemos de felicitar al grupo de jóvenes que han estado detrás de la organización de esta edición, por su dedicación y entusiasmo. Agradecer a todos los participantes su respuesta y favorable acogida. A los investigadores invitados. A los patrocinadores; incluso bajo las condiciones especiales de

este año. Al Rector, y al Vicerrector de Política Científica de la UCLM, por su apoyo a estos Simposios. Y, así, con estos respaldos, el convencimiento del éxito de esta nueva edición del Simposio Ciencia Joven.

**Manuel Andrés Rodrigo Rodrigo**

*Decano de la Facultad*

## Comité Científico:

**Manuel Andrés Rodrigo Rodrigo**, *Dean of Faculty*

**María Antonia Herrero Chamorro**, *'Vice dean of Faculty & President from STCLM de la RSEQ'*

**Sergio Gomez Alonso**, *'Vice dean of Faculty'*

**Gema Dura Gracia**, *'Inorganic Chemistry'*

**Ana Raquel de la Osa Puebla**, *'Chemical Engineering'*

**Elena Alañón Pardo**, *'Food Sciences and Technology'*

**Antonio M. Rodríguez García**, *'Organic Chemistry, EYCN-JIQ-RSEQ, CM Faculty'*

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**Esther Pinilla Peñalver**, *'Analytical Chemistry'*

**Alba Escalona Verbo**, *'Physical Chemistry'*

**Iván Torres Moya**, *'Organic Chemistry'*

**Raúl López Martín**, *'Physics'*

**Pablo Belmonte López**, *'Chemical Engineering'*

**Margarita María Villar Rayo**, *'Biochemistry'*

Estamos encantados de retomar durante los días 7, 8 y 9 de Julio la iniciativa del **"Young Science Symposium"**, siendo este año su **decimoquinta edición**.

Con este fin, un grupo de **jóvenes doctorandos** pertenecientes a la **Facultad de Ciencias y Tecnologías Químicas de Ciudad Real, Facultad de Ambientales de Toledo, Instituto de Investigación en Recursos Cinegéticos y Facultad de Medicina de Albacete** presentarán una serie de comunicaciones sobre el trabajo que están desarrollando en sus respectivas áreas. También contaremos con algunos investigadores invitados externos que nos darán una visión más general sobre la investigación en España, tanto en instituciones públicas como en la empresa privada.

Con el fin de incentivar y despertar el espíritu investigador entre los alumnos de la facultad, nuestra futura "cantera", la asistencia a las jornadas podrá ser convalidada por un **Crédito de Libre Configuración**. Creemos que esta iniciativa puede ser muy interesante para acercar a los alumnos a la verdadera actividad de los laboratorios de investigación de la facultad.

Por otro lado, a modo de incentivar a aquellos jóvenes doctorandos y nuevos doctores que participan como ponentes en estas jornadas, en esta convocatoria 2021, se concederá el **“VI PRIZE OF YOUNG SCIENCE FACULTY OF SCIENCES AND TECHNOLOGY”**. Asimismo, se otorgará cuatro premios dentro de “I PREMIO VIRTUAL-FLASH en categoría TFG, TFM y tesis” a la mejor flash virtual, ya que este año contamos también con contribuciones en este formato.

Por todo ello, os agradecemos vuestra participación y esperamos que la experiencia os sea de provecho, aunque este año tenga que ser en esta versión online debido a la situación de alerta sanitaria de este año.

No olvidéis visitar nuestra página web donde podréis encontrar las últimas novedades de estas jornadas, instantáneas de las presentaciones, así como el Libro de abstracts en formato electrónico:

<http://www.uclm.es/CR/FQuimicas/>

## ***SYMPOSIUM SCHEDULE***



### Wednesday, 7<sup>th</sup> July 2021

**9:00- Opening ceremony chaired by the Vice-Chancellor for teaching and professional development of the UCLM and the Dean of the Faculty of Chemical Sciences and Technology.**

**10:00- Invited Lecturer: Prof. Jonathan W. Steed (Durham University, UK). "Supramolecular Gels: Tangled Soft Materials".**

#### **10:30- 1<sup>st</sup> session**

- *"Pulsed electric field and supercritical fluid extraction for valorization of almond hull as antioxidant". Manuel Salgado. Organic Chemistry.*
- *"Discrimination and quantification of quercetin nanoemulsions by liquid state SERS analyzer". Cristina Montes. Analytical Chemistry.*
- *"Supercritical CO<sub>2</sub> extraction of natural antioxidants from lavender: process optimization and scaling up". Encarnación Cruz. Chemical Engineering.*
- *"Valorization of agricultural waste and CO<sub>2</sub> into bioderived cyclic carbonates". Maria del Prado Caballero. Inorganic Chemistry.*
- *"Implementation of non-thermal technologies for the control of the wine microbiota". Raquel Muñoz. Food Sciences and Technology.*

**12:15- Break.**

#### **12:45- 2<sup>nd</sup> session**

- *"Bioavailability of long-term low-dose administration of a grape seed extract in healthy male Wistar rats". Eduardo Guisantes. Biochemistry.*
- *"Catalytic fractionation of biomass, a pathway to obtain textiles, biofuels and platform chemicals from renewable sources". Alberto José Huertas. Organic Chemistry.*
- *"Optimization of an extraction methodology of Platinum nanoparticles from road dust". Armando Sánchez. Analytical Chemistry.*
- *"Metal extraction from mine tailings by bioleaching with a acclimatized mixed culture". Hassay Lizeth Medina. Chemical Engineering.*
- *"Synthesis of polycarbonates and terpolymers catalysed by heteroscorpionate indium complexes". Marc Martínez de Sarasa. Inorganic Chemistry.*

#### **16:00- 3<sup>rd</sup> session**

- *"Monitoring air quality in Las Tablas de Daimiel National Park". María Gabriela Viteri. Physical Chemistry.*
- *"Rapid estimation of total polyphenol content and antioxidant activity of natural cork stoppers by NIR spectroscopy". Manuel López. Food Sciences and Technology.*
- *"A new analytical methodology for the assessment of platinum nanoparticles speciation in in vitro toxicological assays". Sergio Fernández. Analytical Chemistry.*

- *“Application of thermoregulating nanopcm slurries for enhancing the thermal comfort of building materials”*. **Daniel López**. *Chemical Engineering*.
- *“Could light treat cancer? New photoactivatable metallocomplexes as an alternative to current chemotherapies”*. **Daniel Martínez**. *Inorganic Chemistry*.

#### 17:15- 4<sup>th</sup> session

- *“Soot characterization using different techniques”*. **María Inmaculada Aranda**. *Physical Chemistry*.
- *“CO<sub>x</sub>-free hydrogen generation from ammonia by electrochemical promotion”*. **Marina Pinzón**. *Chemical Engineering*.
- *“Determination of oxidative stress markers in the blood of *Taeniopygia guttata* using HPLC-MS”*. **Marina Córdoba**. *Analytical Chemistry*.
- *“Safety assessment of LAB strains to be used in food fermentations”*. **Sara Rodríguez**. *Food Sciences and Technology*.
- *“Naturally curved organic crystalline structures for waveguide and photonic circuits”*. **Carlos Tardío**. *Organic Chemistry*.

### Thursday 8th of July 2021

#### 9:00- 5<sup>th</sup> session

- *“Subolesin/Akirin: a multi arthropod vaccine antigen”*. **Sara Artigas**. *Biochemistry (IREC)*.
- *“Magnetic responsive hydrophobic pockets for on-off drug release”*. **Jorge Leganés**. *Organic Chemistry*.
- *“Determination of zinc nanoparticles in yeast samples by spICP- MS”*. **Samah Lahouidak**. *Analytical Chemistry*.
- *“Production of GABA-enriched yoghurt using selected *Lactobacillus* strains”*. **Inés Ramos**. *Food Sciences and Technology*.
- *“Astrochemistry in the laboratory”*. **Sergio Blázquez**. *Physical Chemistry*.

**10:30- Invited Lecturer: Dr. Ana Ferreira-Duarte (Newcastle University, UK)**. *“Research journey from bioinspired biomaterials to tissue engineering constructs”*.

#### 11:45- Break

#### 12:15- Presentation of the Territorial Section of the Royal Spanish Society of Chemistry (STCLM-RSEQ)

#### 12:30- 6<sup>th</sup> session.

- *“Optimum Experimental Design: “Think before you act””*. **Sergio Pozuelo**. *Mathematics and Physics*.
- *“Tuning the Cytotoxicity of bis-phosphino-amines Ruthenium(II) para-cymene complexes for clinical development in Breast Cancer”*. **Elena Domínguez**. *Inorganic Chemistry*.
- *“Electro-scrubbing for the Removal of Volatile Organic Compounds (VOCs) from Gaseous Streams”*. **Andrea Nataly Arias**. *Chemical Engineering*.

- *“New naphthalenimide derivatives with application in organic photonics”*. **Beatriz Donoso**. *Organic Chemistry*.
- *“Kinetic and formation of Secondary Organic Aerosol from ozonolysis of trans- $\beta$ -methylstyrene”*. **Alba Escalona**. *Physical Chemistry*.

**16:00- 7<sup>th</sup> session**

- *“Towards turbulence with a Schwarz domain decomposition Legendre collocation method”*. **Darío Martínez**. *Mathematics*.
- *“Mosquitoes and West Nile Virus”*. **Laia Casades Martí**. *Biochemistry (IREC)*.
- *“Synthesis of metallic nanoparticles by spark ablation. Application in surgical facemasks”*. **Raúl López Martín**. *Physics*.
- *“Nickel electrodes prepared by magnetron sputtering for water and ethanol-water hybrid electrolysis”*. **Ester López**. *Chemical Engineering*.
- *“Photopolymerizable chitosan hydrogels for tissue engineering”*. **Irene San-Millán**. *Organic Chemistry*.

**17:30- Invited Lecturer: Dr. Sergi García Segura (Arizona State University, USA).**  
“Applied electrochemical technologies to decentralized water treatment: Advances within materials, chemistry, and engineering nexus for small scale application”.

**Friday 9th of July 2021**

**9:00- Invited Lecturer: Prof. Miguel Ángel Miranda (Universitat Politècnica de València).** “Oportunidades en la carrera investigadora a través de los programas de la AEI”.

**10:00- Invited Lecturer: Dra. Raquel Mateos (Institute of Food Science, Technology and Nutrition, ICTAN, CSIC).** “Novel nutraceuticals based on combination of oat beta- glucans and green coffee phenolic extract to combat obesity and its comorbidities”.

**11:00- Break**

**11:30- Invited Lecturer: Dr. Francisco Javier Guerra (Universidad de Valladolid).**  
“Building bridges between Academia and Industry. Which are the missing pieces?”.

**12:30- Miguel Martínez, AGROVIN.**

**13:00- Colloquium, Prize winners and Closing Ceremony chaired by the Rector Magnificus of the UCLM, the Dean of the Faculty of Chemical Sciences and Technology, Dr. Ricardo Cuevas (General Director of Universities, Research and Innovation of the Regional Government of Castilla-La Mancha) and Prizes sponsors”.**



# INVITED SPEAKERS



## CI-1

### “Supramolecular Gels: Tangled Soft Materials”

Jonathan W. Steed

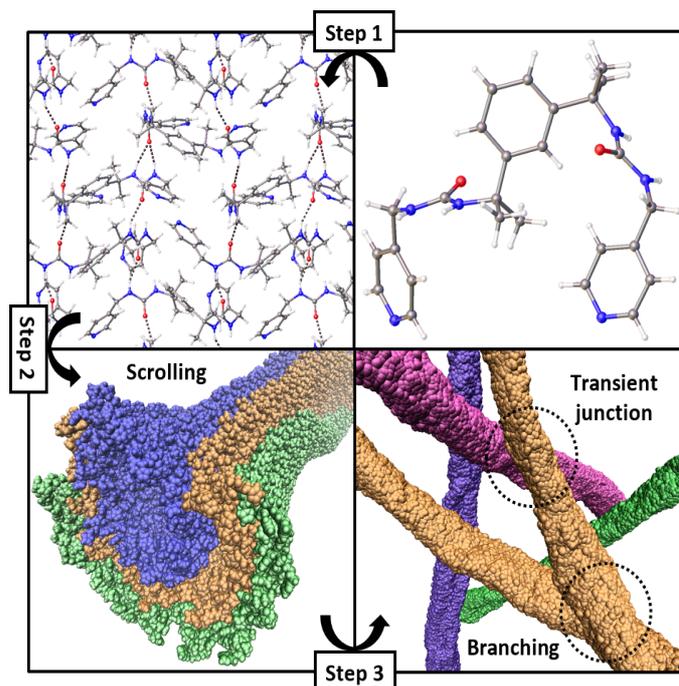
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*Inorganic Chemistry*

Gels are formed by hierarchical self-assembly either because of hydrophobic effects in water or by more directional interactions such as hydrogen bonding in less polar solvents (Fig. 1). Low molecular weight gelators based on small molecules (LMWG) are emerging as pharmaceutical crystallization media. Particular attractions of LMWGs to the scientific community are the reversible nature of the interactions between the gelator molecules, the wide (essentially unlimited) range of solvents that can be gelled and the possibility of tuning the gels' behaviour by introducing responsive or switching functionality.

This presentation focuses on control and crystallization by manipulating the materials properties of small molecule (supramolecular) gels and the nature of the gel fibre surface. We show how concepts firmly rooted in supramolecular host-guest chemistry and supramolecular self-assembly can be married with the materials science of soft matter in order to control and manipulate bulk materials properties.[1] The application of these kinds of switchable gels as novel media for pharmaceutical crystal growth is emerging.



**Figure 1.** Assembly of a supramolecular gel by (1) layering, (2) scrolling and (3) entanglement.

#### References

- [1] Jones, C. D.; Simmons, H. T. D.; Horner, K. E.; Liu, K.; Thompson, R. L.; Steed, J. W., Braiding, branching and chiral amplification of nanofibres in supramolecular gels. *Nature Chem.* **2019**, *11*, 375-381.

## CI-2

### Exploiting natural-based materials for the manufacturing of tissue engineering constructs

Ana Marina Ferreira-Duarte\*

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*Biomaterials & Tissue Engineering*

The extracellular matrix (ECM), the non-cellular portion of a tissue that regulates key bio-functions and cell fate, is damaged, altered, or lost in most human diseases and injuries. The use of biomaterials as tissue constructs is showing promise as a regenerative medicine approach to facilitate new tissue formation by recreating native micro-environments. Particularly, natural polymers are widely used to support or guide cellular function by mimicking the native ECM composition and microenvironment [1-2]. For example, naturally derived materials, such as animal-derived collagen and fibrin, already contain cell adhesion ligands and are susceptible to proteolytic degradation that enables cell infiltration and remodelling [3]. The use and processing of different natural-based materials as functional coatings and scaffolds are studied [2-5], including the exploitation of bio-fabrication technologies like bioprinting for creating bioinspired tissue engineering constructs. In recent works, the importance of bioink composition and cell density in the development of biomimetic and bioinspired tissue engineering constructs was investigated, as these directly impact cellular process and tissue maturation rates [6]. Therefore, the use and processing of different natural-based materials for the creation of biomimetic and tissue engineering constructs will be discussed.

#### References

- [1] Ngadimin, K.D., Stokes, A., Gentile, P. and Ferreira, A.M., *Biomaterials Science* **2021**, 9, pp. 4246-4259
- [2] Dewhurst, R.M., Scalzone, A., Buckley, J., Mattu, C., Rankin, K.S., Gentile, P., Ferreira, A.M. *Frontiers in Bioengineering and Biotechnology* **2020**, 8, art. no. 754
- [3] Montalbano, G., Toumpaniari, S., Popov, A., Duan, P., Chen, J., Dalgarno, K., Scott, W.E., III, Ferreira, A.M. *Materials Science and Engineering C* **2018**, 91, pp. 236-246.
- [4] Upson, S.J., O'Haire, T., Russell, S.J., Dalgarno, K., Ferreira, A.M. *Materials Science and Engineering C* **2017**, 76, pp. 190-195.
- [5] Ferreira, A.M., Gentile, P., Toumpaniari, S., Ciardelli, G., Birch, M.A. *ACS Applied Materials and Interfaces* **2016**, 8 (44), pp. 29923-29932.

[6] Da Conceicao Ribeiro, R., Pal, D., Ferreira, A.M., Gentile, P., Benning, M., Dalgarno, K. *Biofabrication* **2019**, 11 (1), art. no. 015014.

### CI-3

#### **Applied electrochemical technologies to decentralized water treatment: Advances within materials, chemistry, and engineering nexus for small scale application**

*Sergi Garcia-Segura\**

*Nanosystems Engineering Research Center for Nanotechnology-Enabled Water  
Treatment, School of Sustainable Engineering and the Built Environment, Arizona State  
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*Chemical Engineering*

Water scarcity and quality are critical issues on a global scale. Ensuring access to water and sanitation for all is a sustainable development goal identified by the United Nations. Emerging contaminants (e.g., perfluoroalkyl substances, pharmaceuticals, pesticides, etc.) are ineffectively removed by conventional water treatment technologies and may produce waste. Multidisciplinary research efforts are key to succeed in the development of promising transformative water treatment technologies. In this scenario, electrochemically-driven processes emerge as alternative new generation of advanced treatments.

General principles of electrochemical water treatment processes will be introduced as a base to discuss research efforts at different technology readiness levels. Specifically, niche market opportunities of scaled-down devices for point-of-use applications will be presented using three examples. This seminar aims to discuss key questions that drive the research needs of today and tomorrow. How can electrochemical processes and engineering can contribute to advance the next generation of smart and sustainable water treatment? Join us to discover some answers in this seminar.

**CI-4**

**Oportunidades en la carrera investigadora a través de los programas de la  
Agencia Estatal de Investigación**

*Miguel Ángel Miranda*

*Chemical Engineering Department*

Recorreremos en esta charla la actualidad del camino académico en España desde el punto de vista del Presidente del área científica: Ciencias y Tecnologías Químicas (CTQ) de la Agencia Estatal de Investigación de España.

## CI-5

### **Building bridges between Academia and Industry. Which are the missing pieces?**

*Javier Guerra*

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*Organic Chemistry*

The society requires different missions from the Higher education institutions. Beyond teaching duties and research, there is a third mission that is based on the production of knowledge that generates a social and economic development.<sup>1</sup> This interpretation of an entrepreneurial university finds two antagonist views. Universities claim that teaching involves not only knowledge but also values and transversal skills and they should not provide students with specific profiles adjusted to job vacancies. Entrepreneurs sustain that their companies require professionals with capabilities adapted to the job essential functions.

This talk is addressed to empower the doctorate studies as a critical piece to build a bridge between these two sides. Currently, some authors<sup>2</sup> demand for a mind-set revolution among doctoral students and their supervisors to make the students more sympathetic to employment outside academia. Competencies acquired during the PhD training should range from transdisciplinary to cooperative skills and attitudes, integrating knowledge to find solutions to real-life issues and personal skills such as communication, leadership, ability, resilience, change adaptability and creativity.

In the first part of the talk, we will take a glance at the current R&D scenario in Spain followed by a second part where the distinctive features that compose the research performed in the Chemical-Pharmaceutical Industry are studied. Different causes will be formulated to explain the lack of communication between Academia and Industry. The missing dots of a typical doctorate profile working in the private sector will be exemplified by the experience of the speaker in Academia as well as in the Industry.

#### **References**

<sup>1</sup> Tavares, O.; Sin, C.; Soares, D., In *Structural and Institutional Transformations in Doctoral Education: Social, Political and Student Expectations*, Cardoso, S.; Tavares, O.; Sin, C.; Carvalho,

T., Eds. Springer , 2020; pp 347-373. <sup>2</sup> De Grande, H., De Boyser, K., Vandeveldel, K. et al. *J Knowl Econ* 5, 538–561 (**2014**)

## CI-5

### **Novel nutraceuticals based on combination of oat beta- glucans and green coffee phenolic extract to combat obesity and its comorbidities**

*Mateos R\*, Bravo L & Sarriá B*

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*Food Science and Technology*

Obesity and its associated comorbidities are a major public health concern worldwide. Nutraceuticals might be an alternative means to help lose weight without changes in the habitual diet and reduce associated cardiometabolic risk factors. The objective of the present study was to assess the efficiency of nutraceuticals combining oat beta-glucan (BG) extracts with different physicochemical properties and a decaffeinated green coffee bean extract (GCBE) on obesity-related biomarkers in overweight/obese subjects. A randomized, parallel, blind, dose-response pilot study was carried out in four groups of subjects (n=15) who consumed, during 6 weeks, twice a day, a nutraceutical containing low (3 g/d) or high (5 g/d) doses of 35% or 70% BG and a fixed amount of GCBE providing 600 mg/d of phenols. BG-35% presented 10 and 100 times higher molecular weight and viscosity, respectively, compared to BG-70%, which was twice as concentrated than BG-35%. Food intake, anthropometry and different cardiometabolic markers were assessed at the beginning and end of the intervention. According to the general model of variance with repeated measure analysis, levels of total-cholesterol, LDL-cholesterol, VLDL-cholesterol, triglycerides, alanine-aminotransferase, aspartate-aminotransferase, hemoglobin A1c, insulin, systolic blood pressure (SBP), total body fat% (TBF%), visceral fat% and waist and hip circumferences were reduced. Attending to ANOVA and Bonferroni tests, among the treatments, 5g-35%BG produced the greatest reduction in LDL-cholesterol and 5g-70%BG was the most effective in lowering SBP and TBF%. In conclusion, 5g-70%BG was the most effective treatment and additionally, it produced the least bloating according to a subjective questionnaire.

## CI-6

### **The importance of RedOx potential on the wine production processes**

Miguel Martínez

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#### *Potencial RedOX*

The redox potential or electrochemical potential provides data on the oxide-reduction process, indicating whether the species found in it are in an oxidized or reduced state, depending on the  $E^\circ$  of each species (Normal reduction potential). The electrochemical potential will evolve throughout the process and knowing it will give us information on the phenomena that depend on it (oxidation or reduction risks), being able to carry out actions that help us reorient it.

Wine is changeable and to control it you must use equipment that measures the values of its conservation, either in tanks or in barrels. The redox potential is measured in mV, indicating the state of the liquid in terms of oxidation and reduction.

In the case of:

- **Musts:** It will be the moment in which the values are maximum oscillating between 200mV - 300mV. Because we find  $O_2$  dissolved in high proportions, the risk of oxidation is greater.
- **Alcoholic and malolactic fermentation:** The microbiological activity produces a significant drop in the electrochemical potential, reaching minimum values currently.
- **For proper wine conservation,** the values must be between 0 - 150mV, the danger of oxidation beginning at 250mV.

This knowledge prompted AGROVIN to start carrying out research 5 years ago on what would be the measure of the RedOx Potential and that has made it possible to design and market various equipment, including ELECTROWINE that could measure this Potential in the difficult conditions of the winery.



# ORAL SPEAKERS

**(appearance in order according to the SYMPOSIUM PROGRAMME)**



## O-1

### **Non-conventional and sustainable novel approaches for the valorization of lignocellulosic biomass as antioxidant**

M. Salgado,<sup>1</sup> F.J. Martí-Quijal,<sup>2</sup> A.J. Huertas-Alonso,<sup>1</sup> M.P. Sánchez-Verdú,<sup>1</sup> F.J. Barba,<sup>2</sup>  
A. Moreno.<sup>1</sup>

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*Organic and Medical Chemistry*

Innovative alternative technologies are nowadays emerging for the recovery of polyphenols from plants as an alternative tool to traditional methods.<sup>1-3</sup> These techniques produce a low environmental impact since no organic solvent and low temperatures are required. Among these techniques, pulsed electric fields (PEF) and supercritical fluid extraction (SFE) have been shown to be promising for intracellular extraction from plant food materials.

The main goal of this study is the recovery of polyphenols from *almond hull*, an interesting source of antioxidants, by combining both PEF and SFE in a sequential process. For instance, although the combination of PEF + SFE has not been explored before, some previous studies have reported interesting results after the application of other non-conventional techniques, such as ultrasound assisted extraction (UAE). Therefore, the antioxidant activity of almond hull was evaluated after combining both PEF + SFE, thus demonstrating a new alternative route for the valorization of this biomass as source of antioxidants.

#### **References**

1. F. A. Khawli, F. J. Martí-Quijal, N. Pallarés, F. J. Barba and E. Ferrer, *Applied Sciences*, 2021, **11**, 1701.
2. M. Kokkali, F. J. Martí-Quijal, M. Taroncher, M. J. Ruiz, K. Kousoulaki and F. J. Barba, *Molecules*, 2020, **25**.
3. N. Pallarés, F. J. Barba, H. Berrada, J. Tolosa and E. Ferrer, *Applied Sciences*, 2020, **10**, 6989.



## O-2

### **Discrimination and quantification of quercetin nanoemulsions by liquid state SERS analyzer**

C. Montes\*, M.L. Soriano, M.J. Villaseñor, A. Ríos

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*Química Analítica*

In the present work, the encapsulation of a lipophilic flavonoid such as quercetin in nanoemulsions has been optimized and developed by means of the phase inversion temperature (PIT) methodology [1]. The final composition of the synthesis (% w/w) was 5.25% castor oil, 0.25% quercetin, 0.55% ethanol, 5% surfactant mixture (4.5% tween 80 and 0.5% quillaja saponin) and the remaining up to 100% was water. The synthesis showed excellent results related to encapsulation efficiency, 96%. Afterwards, the nanostructural characterization of the quercetin-loaded nanoemulsions was carried out by several techniques such as UV-Vis, Raman spectroscopy, DLS and SEM. Based on raman and SERS profiles it was possible to discriminate between free quercetin and nanoquercetin. While drug or bioactive release systems have been developed, some limitations have should be overcome. One of the most important is the need to develop analytical tools allowing its characterization and quantification without altering its original state [2]. For this reason, a three-dimensional plasmonic sensor in liquid state with gold nanobones has been developed for Q-NEs quantification based on SERS magnification at 1600  $\text{cm}^{-1}$  band. This sensor showed good analytical performance with lineal concentration range of 0.5 – 30  $\mu\text{M}$  and detection limit of 0.4  $\mu\text{M}$ . The developed analytical method was applied to the analysis of nanoquercetin in complex commercial matrices.

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### O-3

#### **Supercritical CO<sub>2</sub> extraction of natural antioxidants from lavender: process optimization and scaling-up**

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*Chemical engineering*

The continuously growing demand of natural products in sectors such as food and pharmaceuticals has led to the search of natural sources rich in bioactive substances with beneficial properties for the human health. These substances can be added to foods, constituting the so-called nutraceutical products, or they can even be used in the synthesis of drugs, thus replacing the disadvantages of traditional medicines such as side effects or intolerance. One of the main commercial products derived from nature are essential oils, with the lavender essential oil as one of the most widely used. It stands out because it has compounds that have great antioxidant and anti-inflammatory capacity such as the linalool [1]. These properties would make it an effective substance for the treatment of skin diseases. In recent decades, the use of supercritical fluid extraction has proven to be effective for obtaining bioactive compounds from mixtures of several components like essential oils because of its versatility and environmental friendliness, thus overcoming the disadvantages of traditional extraction techniques. Carbon dioxide (CO<sub>2</sub>) is the most widely used supercritical fluid, as it is inert, non-toxic and allows extraction at lower temperatures and pressures [2].

The present work focuses on the supercritical extraction of lavender essential oil for its application in drugs and nutraceuticals. The influence of pressure and temperature on the extraction yield and antioxidant capacity was studied. The composition of the extracts was determined by gas chromatography/mass spectrometry and the DPPH (2,2-diphenyl-1-picrilhidrazil) assay test was carried out in order to evaluate their antioxidant potential. In addition, a model for the simulation of the equilibrium system formed by lavender essential oil and supercritical CO<sub>2</sub> was developed with the aid of Aspen Plus commercial simulator to enable the subsequent scaling up and economic study of the process.

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## O-4

### Valorization of Agricultural Waste and CO<sub>2</sub> into Bioderived Cyclic Carbonates

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*Química Inorgánica*

Society demands the development of new products and chemical processes that make our planet more sustainable. In the last few years, waste production has increased enormously, which has a huge negative impact on the environment. Among the produced agri-residues, vegetable oils have attracted much attention in the last decade for the design of new sustainable catalytic processes. On the other hand, the increase of carbon dioxide emissions in the atmosphere is one the main causes of global warming. For this purpose, highly efficient metal-free bifunctional organocatalysts<sup>1</sup> have been used for the synthesis of waste vegetable oils-derived cyclic carbonates from bio-derived epoxides and CO<sub>2</sub>. In this contribution, epoxidized vegetable oils and carbon dioxide have been used as renewable feedstocks for the synthesis of waste vegetables oils-derived cyclic carbonates in excellent isolated yields using the bifunctional imidazole-based organocatalyst in the optimal reaction conditions without solvent.<sup>2</sup>



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## O-5

### **Implementation of non-thermal technologies for wine microbiota control.**

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*Tecnología de Alimentos*

In the winemaking process, the most important microbial species is undoubtedly *Saccharomyces cerevisiae*, responsible for alcoholic fermentation. On the other hand, lactic bacteria are responsible for carrying out the malolactic fermentation in red wines and some white wines, so they should also be highlighted as beneficial microorganisms. However, there are others that can produce some kind of alteration, among which *Dekkera anomala* is worth mentioning [1]. The aim of this work was to study the effect of different microwave treatments on the vitality and viability of *Saccharomyces cerevisiae*, *Lactobacillus plantarum* and *Dekkera anomala*, chosen as representatives of the microbiota characteristic of the winemaking process [2].

For this purpose, six different treatments were applied on fresh cultures with a population of  $10^6$  cfu/mL, varying the conditions of exposure time, power and pulses. Plate counts were performed to study the effect on viability, while changes in vitality were quantified by obtaining the kinetic parameters of the microorganisms once the treatment was applied. In all cases, YPD and MRS media were used for yeast and bacteria respectively. In parallel, controls were carried out for each of the strains without the application of microwaves. All tests were performed in quadruplicate. The results showed that in some cases the metabolism was attenuated, which was reflected in a longer lag phase, together with a loss of viability. At other times, no significant differences were observed with respect to the controls, and finally, sometimes cell death occurred, mainly in treatments carried out continuously, without the application of pulses.

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## O-6

### **Bioavailability of a long-term low-dose administration of a grape seed extract in healthy male Wistar rats**

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#### *Biochemistry*

Plant-based diets rich on polyphenols have outbreak as a powerful tool to prevent several metabolic disturbances provoked by inadequate diets and sedentary lifestyles. Between them, flavanols are one of the most consumed polyphenols in diets and have been reported to play an important role in health. However, the mechanism of action for these compounds are not fully understood<sup>1</sup>. To establish a clear relationship between intake of flavanols and effects in the prevention of diverse diseases is vital to understand the bioavailability of these compounds in the organism. Thus, we aimed to evaluate serum metabolites after a low-dose dietary administration of a grape seed extract (GSE) (25 mg/kg body weight/ day) in young-male Wistar rats for 28 days.

In first place, we approached the characterization of the GSE by spectrophotometric and chromatographic techniques (HPLC-QToF-MS) showing a high content on polyphenols, mainly flavanols with different degree of polymerization. Then, we proceed to analyse the serum metabolites by UHPLC-HR-MS considering the possible transformations suffered by flavanols through the stages of digestion, intestinal absorption, distribution and metabolization. Our results showed a rapid metabolization and elimination of the flavanols, the prevalence of sulphate and glucuronidated metabolites and the relevance of colonic metabolization, carry out by the microbiota, to increase the bioavailability of these compounds. These data might explain the possible metabolic effects of flavanols.

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O-7

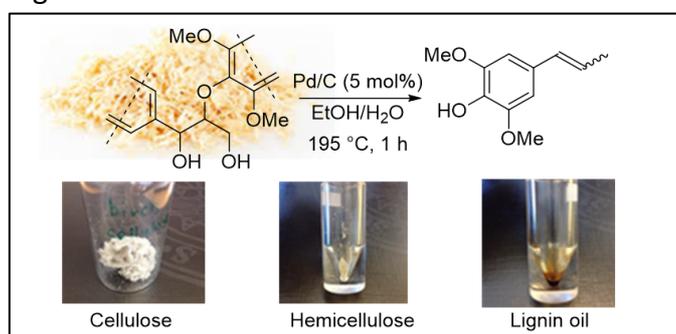
**Catalytic fractionation of biomass, a pathway to obtain textiles, biofuels, and platform chemicals from renewable sources**

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*Química orgánica*

Lignin-first processing is the broadly accepted umbrella term for solvent-based methods in which lignin preservation, together with that of the polysaccharides, is considered upfront, moving away from the current practice of having to deal with an intractable lignin product at the end of a biorefining process. The lignin-first process would be considered as an active stabilisation approach that liberates lignin from the plant cell wall and prevents condensation reactions through either catalysis or protection-group chemistry. Importantly, lignin-first biorefining is not a synonym for lignin valorisation, but rather an integral approach that derives value from both lignin and polysaccharides, towards an atom-efficient and more sustainable utilisation of lignocellulosic biomass. Most commonly, lignin-first processes involve three steps: (i) the lignin is removed from whole biomass using an organic solvent through solvolysis or acid catalysed reactions (similarly to organosolv pretreatment); (ii) the resulting intermediates are stabilised, with the intention of preventing condensation of reactive species generated by lignin depolymerisation, and (iii) further depolymerisation occurs if not fully depolymerised at the stabilisation stage.<sup>1</sup>



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**O-8**

**Extraction and characterization of platinum nanoparticles from road dust**

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*Analytical Chemistry*

In the last decades, metallic nanoparticles (NPs) are being widely applied in a very broad field of applications. Among them, the use platinum nanoparticles (PtNPs) has grown steadily due to their unique properties, especially in automotive catalytic convertors. Mechanical abrasion and chemical reactions occurring at the catalyst surface could lead to their emission all over the environmental compartments. However, information about the fate, bioavailability, or possible transformations that they may undergo once in the environment is very limited [1]. Adequate methods for the detection, characterization, and measurement of PtNPs are needed to understand their behavior and assess possible associated environmental risks. In order to reach reliable information about PtNPs in complex environmental matrixes, a previous sample preparation step is required. This process is the most critical and laborious, especially for solid samples, such as road dust [2]. It should be carefully optimized to preserve all the NP properties (e.g., size, shape, or aggregation state), and concentration. Usually, chemical (an extractant agent) and physical (some type of energy) treatments are required. In the present work, an analytical methodology for the extraction of PtNPs from road dust is presented. Critical parameters, including extractant agent, extraction technique and sample:extractant ratio, have been optimized. Best results were obtained using ultrasonic energy and water as extractant. Single particle inductively coupled plasma mass spectrometry has been used for PtNP characterization and quantification.

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**O-9**

**METAL EXTRACTION FROM MINE TAILINGS BY BIOLEACHING WITH AN  
ACCLIMATIZED MIXED CULTURE**

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*15th Young Science Symposium*

The metal mining sector has been an important pole of economic development in several European countries. However, the accumulation of mine tailings after the closure of the facilities has triggered a negative environmental impact [1], derived from the high accumulation of heavy metals in the soil, the surface and underground water bodies. This situation could be worsened when waste get in contact with different environmental agents, such as wind and water due precipitation [2]. This work has studied the bioleaching of metals contained in mine tailings, using an adapted mixed culture by an acclimation stage to improve metals bioleaching. The mixed culture was taken from a real acid mine drainage. The physicochemical and microbiological parameters were controlled during the bioleaching experiments on the pregnant leach solution (PLS). After the bioleaching process Cu, Cd Pb and Zn were dissolved from the waste demonstrating that it could be possible to recover metals even from the discarded mine tailing [3].

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O-10

**SYNTHESIS OF POLYCARBONATES AND TERPOLYMERS CATALYSED BY  
HETEROSCORPIONATE INDIUM COMPLEXES**

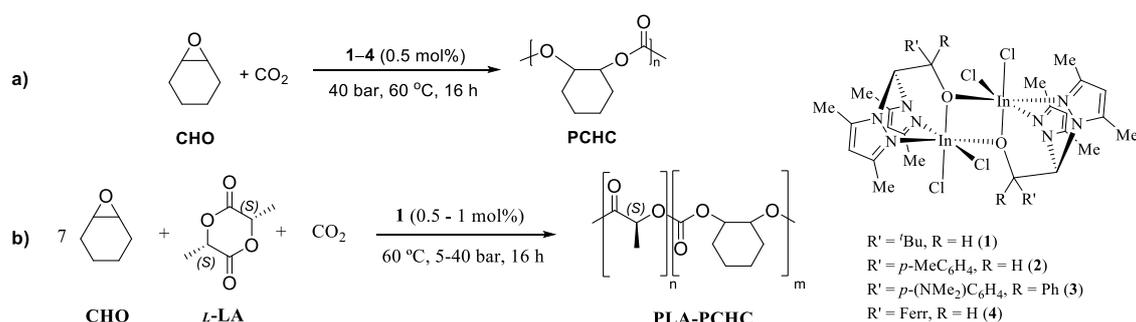
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*Inorganic Chemistry*

During the last years, the scientific and industrial community have focused on the development of new processes to transform CO<sub>2</sub> into high-value added organic chemicals and polymers.<sup>1</sup> In this context, it is worth highlighting the ring opening copolymerisation between epoxides and CO<sub>2</sub> to afford polycarbonates, which have found multiple applications.<sup>2</sup> More recently, terpolymerisation reactions between epoxides, CO<sub>2</sub> and cyclic anhydrides and/or cyclic esters have received much attention due to the possibility to fine-tune the properties of the resulting polymeric materials.<sup>2</sup> In this work, we report the synthesis of a new family of dinuclear chloride indium complexes (**1-4**) which have shown to be very efficient for the ROCOP of epoxides and CO<sub>2</sub> and the terpolymerisation reaction of cyclohexene oxide, CO<sub>2</sub> and *L*-lactide to afford polycarbonate and polyester-polycarbonate materials, respectively, with low to moderate molecular weights and narrow polydispersity values (Scheme 1).



**Scheme 1.** a) Synthesis of PCHC and b) synthesis of PLA-PCHC.

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**O-11**

**Monitoring air quality in Las Tablas de Daimiel National Park**

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*Physical Chemistry*

Air quality is generally measured in urban and industrial sites. Nevertheless, anthropogenic activities can also contribute to the pollution of natural remote areas. The need for assessing such contributions to the air quality of protected areas is the motivation for the present study. This work reports field measurement data of O<sub>3</sub>, NO<sub>x</sub>, SO<sub>2</sub>, CO and PM<sub>2.5</sub> from March 2020 to July 2021 in Las Tablas de Daimiel National Park, within “La Duquesa” weather station that belongs to the park. Pollutants were measured by analysers that were installed inside a thermostatic cabin. Data were registered every ten minutes and hourly, and then downloaded remotely. In addition, meteorological data (temperature, wind direction, wind speed, pressure, and humidity) were provided by “La Duquesa” to have a complete dataset for this study.

The results show a substantial ozone concentration rise during June – September 2020 when the solar radiation intensity is higher than in winter months. Ozone values obtained (annual average= 69.3mg/m<sup>3</sup>) are slightly higher than the concentrations registered in urban monitoring stations (Red de Control y Vigilancia de la Calidad del Aire de la JCCM). This is consistent with other studies that observed higher ozone concentrations in areas far from emission sources. On the other hand, NO<sub>x</sub> concentrations (annual average= 3.1mg/m<sup>3</sup>) are lower than values registered in the surrounding urban areas, also, they are below legal environmental parameters. The same behaviour was also observed for SO<sub>2</sub> and CO, with average values of 0.34 and 135.5 mg/m<sup>3</sup> respectively.

In the case of PM<sub>2.5</sub>, there is no clear pattern during this study. Sahara intrusions have been considered in this study, observing that they present a small contribution to fine particles, which have an average “local” background value of 4.7µg/m<sup>3</sup>. The results show that concentrations of PM<sub>2.5</sub> are below the levels established by the legislation.

## O-12

### **Near-infrared spectroscopy (NIRS) as a potential non-destructive tool in the evaluation of quality parameters of natural cork stoppers**

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*Área de Tecnología de los Alimentos*

The quality control of the cork industry includes different parameters related to the structure of the cork and its chemical composition, such as visual quality, extraction force, compression force, absence of olfactory defects or extractable chemical compounds. In this sense, the production of natural cork stoppers includes different sanitation steps such as hot water or steam washing and the use of hydrogen peroxide to reduce phenolic compounds, mainly tannins, and to eliminate microorganisms that can produce off-flavors [1]. Both, the analysis of off-flavors responsible for the defect known as “cork taint” and the analysis of phenolic compounds are carried out by precise conventional techniques that require time and previous preparation of the sample, so they cannot be included in the production lines. Due to the importance of the presence of olfactory defects in wine attributable to cork, most industries have a gas chromatography-mass spectrometry system, however, they lack analysis systems for phenolic compounds, which, like volatile compounds, can migrate to the wine affecting its color, astringency, and bitterness [2]. On the other hand, cork is a source of phenolic compounds, which poses important antioxidant properties that could also migrate to the wine. Therefore, although a high content of phenolic compounds could modify the chemical and sensory properties of wines, their migration could also increase their antioxidant properties.

The aim of this study was the development of predictive models through the chemometric treatment of the data obtained by NIRS, for the rapid and non-destructive estimation of the total polyphenol content and antioxidant activity of natural cork stoppers, for which 132 samples of different visual qualities and perfectly characterized from its origin were used. The external validations carried out for each model indicated a good fit between the values obtained from the chemical analysis method, and the values estimated by the NIR calibration method. Therefore, NIR spectroscopy could be used as a rapid and non-destructive technique for the simultaneous determination of different chemical parameters in natural cork stoppers, such as total polyphenol content and antioxidant activity, and probably others of interest in the cork industry.

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**O-13**

**A NEW ANALYTICAL METHODOLOGY FOR THE ASSESSMENT OF PLATINUM  
NANOPARTICLES SPECIATION IN *IN VITRO* TOXICOLOGICAL ASSAYS**

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*Analytical Chemistry*

The employment of platinum nanoparticles (PtNPs) has raised in numerous fields, especially in biomedicine due to unique physicochemical properties. Despite their use, there are limited data on their toxicity, and the possible harmful effects on human health [1]. Thus, it is necessary to perform toxicological studies for the assessment of the risks associated to NPs. To get reliable information about NP behavior and transformations in these complex biological media is still a challenging task and the development of new analytical methodologies for this purpose is needed. In that sense, one powerful alternative for metallic NPs is the hyphenation of separation technique, such as high performance liquid chromatography, to specific detector, as inductively coupled plasma-triple quadrupole mass spectrometry (HPLC-ICP-TQ-MS). It provides information about the characterization, and quantification of NPs, and dissolved species in complex matrices in a short period of time at low concentrations. Nevertheless, its applicability for the study of PtNPs in these types of samples should be demonstrated. Therefore, the goal of this work has been to develop and validate a new analytical methodology based on the use of HPLC-ICP-TQ-MS for the PtNP speciation including 5, 30 nm PtNPs, and dissolved Pt species upon dispersion in different cell culture media, such as Dulbecco's Modified Eagle Medium (DMEM), and Roswell Park Memorial Institute, RPMI-1640 suspensions, all supplemented with 10% fetal bovine serum, and antibiotics commonly used in *in vitro* toxicological assays. The presence of the cellular media induced transformations in these nano-sized particles over time (i.e., oxidation, and protein corona formation). Also, complementary techniques as dynamic light scattering, and scanning electron microscopy were used to study the hard, and soft corona formation. These results will be very useful to achieve an appropriate interpretation in future *in vitro*, and *in vivo* toxicological assays.

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**O-14**

**Application of thermoregulating nanoPCM slurries for enhancing the thermal  
comfort of building materials**

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*Chemical Engineering*

It is expected that the world energy consumption rises nearly 50 % by 2050. This quick and high growing energy demand can generate a depletion of resources, supply difficulties and destructive environmental impact. Spain has an average of 2500 hours of sunshine guaranteed per year, which translates into a wide potential for the development of solar thermal energy technologies. However, the intermittency of the solar energy is an important constraint, but the use of thermal energy storage (TES) in buildings can smooth this problem. Latent heat storage (LHS) is the most studied and promising TES technology. The materials used for the LHS are named phase change materials (PCM). These materials are able to absorb, store and release energy during the phase change. However, due to the solid-liquid transition, they must be suitably contained to prevent leakage. Nowadays the efforts of implementing these materials are focused on obtaining nanocapsules (NPCM), in order to increase the thermal energy surface for improving the heat transfer rate. The incorporation of the capsules in construction materials allows utilizing them in passive energy storage systems, reducing the building energy consumption and the CO<sub>2</sub> emissions because the dependence on fossil fuels is diminished.

In this work, a thermoregulating nanoPCM slurry was synthesized, which is constituted by NPCM containing the PCM dispersed in water. This nanoPCM slurry was made in only one single step, avoiding the waste generation. This slurry contains 38.5 wt.% of solid particles being able to be handled as water for producing the desired building materials. In this first approach, gypsum block containing up to 20 wt% of thermoregulating NPCM were produced by mixing this nanoslurry with the hemihydrate obtaining building materials that present a double purpose, the common structural one and as an insulating material having thermal energy saving properties (large TES capacity).

O-15

**Could light treat cancer? New photoactivatable metallocomplexes as an alternative to current chemotherapies.**

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*Química Inorgánica*

Photochemotherapy emerges as a new non-invasive technique to improve the selectivity of current cancer treatments. In this therapy, a photosensitizer is administered, which is ideally harmless in the dark, and activates in the presence of light. This approach has special interest in tumours that can be irradiated by light or cannot be removed by surgery (head, neck, skin...) More precisely, in photodynamic therapy (PDT)  $^1\text{O}_2$  and reactive oxygen species (ROS) are generated, producing cancer cell apoptosis. This allows to design a light-driven chemotherapy in a spatio-temporal way. Iridium complexes with C<sup>N</sup> ligands have been employed as photosensitizers in PDT mechanisms due to their photochemical properties. In this work, a new type of chloro-bridged dimer with  $\pi$ - extended ligands (C<sup>N</sup>= benzo[a]pyrido-[2,3-c]phenazine; bppz) have been synthesized and new complexes  $[\text{Ir}(\text{C}^{\text{N}})_2(\text{N}^{\text{N}})]^+$  are presented as potential candidates for PDT. Furthermore, fluorescence studies demonstrated that these compounds are luminescent, which can be useful to use them as probes in theragnosis devices. Cytotoxicity studies are being carried out.

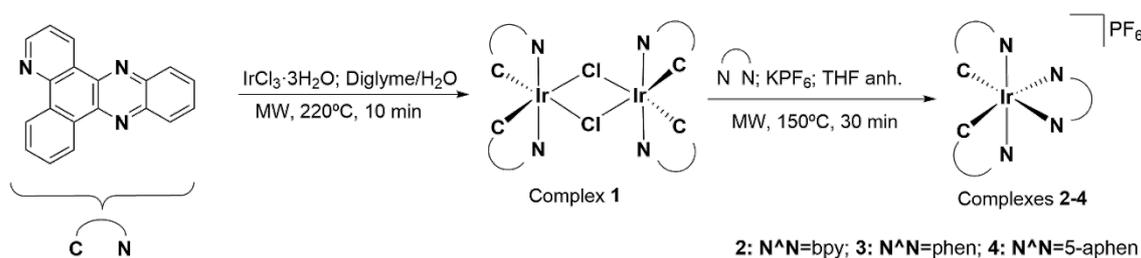


Figura 1. Synthesis scheme of Ir complexes with C<sup>N</sup> (5-aphen: 5-aminephenanthroline).

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## O-16

### Soot characterization using different techniques

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#### *Physical Chemistry*

Soot is the carbonaceous particles formed during the incomplete combustion or pyrolysis of hydrocarbons<sup>1</sup>, such as fossil or biomass fuel. It is well known that this pollutant has negative effects on the human health<sup>2</sup> and cause changes in the Earth's energy balance directly by absorbing the solar radiation and indirectly affecting cloud properties<sup>3</sup>. Depending on the fuel used and the generation conditions, the properties of the generated soot particles may change so it is important to characterize them. In this work, soot samples have been characterized using different techniques:

1. Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) which provides information about the functional groups present in their surface.
2. EC/OC analyser, which allows to determine that mass fraction of elemental carbon (EC) and organic carbon (OC).
3. Scanning Mobility Particle Sizer (SMPS), to determine the particle size distribution.

For investigating the optical properties:

4. Photoacoustic Extinctionmeter (PAX), which measures the absorption and scattering of light at 870 nm.
5. Aethalometer, which measures light attenuation through a filter at seven wavelengths.

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**O-17**

***CO<sub>x</sub>-free hydrogen generation from ammonia by electrochemical promotion***

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*Chemical Engineering*

Hydrogen (H<sub>2</sub>) from renewable source seems to be potential green energy carrier to support a low carbon energy economy, using fuel cells and internal combustion engines by releasing only water such as by products. However, the main drawback related to this compound is its low volumetric energy density which increases storage and transport costs. An alternative to remove these issues is the use of hydrogen carrier compounds. In this respect, ammonia (NH<sub>3</sub>) is a promising hydrogen carrier because of its high volumetric energy density and high hydrogen content, well-known technology for production and distribution and relatively low cost<sup>1</sup>. Moreover, its decomposition only yields hydrogen and nitrogen. Therefore, NH<sub>3</sub> is an exceptional carbon-free hydrogen vector. However, to release H<sub>2</sub> contained in NH<sub>3</sub> it is necessary to develop a robust, efficient, and economic active catalyst at low temperatures, since high purity H<sub>2</sub> is necessary to be used in fuel cells. Promising results of NH<sub>3</sub> decomposition at low temperatures are achieved with ruthenium catalysts<sup>1</sup>, although catalytic activity is influenced by adding promoters. The electrochemical promotion of catalysis (EPOC) is a promising alternative way to explore the in-situ addition of electronic promoters to an heterogeneous catalyst and hence, to enhance catalytic reaction rates <sup>2</sup>.

In this work it has been explored for the first time in the literature, the effect of the electrochemical promotion for low temperature catalytic decomposition of ammonia (250-350 °C). For that purpose, a ruthenium catalyst and an alkaline solid electrolyte (Na-βAl<sub>2</sub>O<sub>3</sub> and K-βAl<sub>2</sub>O<sub>3</sub>) have been used on the catalytic reaction.

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**O-18**

**Determination of oxidative stress markers in the blood of *Taeniopygia guttata* using reversed-phase high-performance liquid chromatography coupled to electrospray ionization-quadrupole-time-of-flight mass spectrometry**

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*Analytical Chemistry*

The objective of the present work is the determination of oxidative stress markers at the systemic level, using birds of the Mandarin diamond species (*Taeniopygia guttata*) as study models, after an experimental induction of oxidative stress. This stress was produced through the contribution of a substance that decomposes into free radicals in the drinking water for 30 days, at the same time that the birds developed their plumage. A reversed-phase high-performance liquid chromatography (RP-HPLC) method coupled to electrospray ionization-quadrupole-time-of-flight mass spectrometry (ESI-QTOF-MS) was developed to identify and quantify the following markers of oxidative damage in plasma and blood cells of birds: 3-nitro-L-tyrosine, 3-chloro-L-tyrosine, 8-hydroxy-2'-deoxyguanosine and o,o'-dityrosine. For this, the different parameters that intervene in RP-HPLC-ESI-QTOF-MS were optimized and calibration curves were made from the pure standards of the indicated compounds. The samples presented a great complexity and a high quantity of interferences, so they were treated, achieving the precipitation of plasma proteins and the opening of blood cells, which allow us to analyze their content.

The analyses show the presence of oxidative stress markers in the samples. The prevalence differs between them, since 8-hydroxy-2'-deoxyguanosine, which is an important indicator of DNA damage, could be identified in relatively high concentrations in all samples, 3-chloro-L-tyrosine and o,o'-dityrosine were only detected in a small number of them. The results therefore indicate the relevance of 8-hydroxy-2'-deoxyguanosine as a global marker of physiological oxidative damage. They also show the production of other markers very poorly determined previously in non-model organisms in blood samples of birds, which opens the door to a greater diversification of potentially useful parameters in oxidative damage studies. These findings will be delivered to the company that requested them in order to carry out different studies on metabolomics and genetics.

**O-19**

**Safety assessment of LAB strains to be used in food fermentations**

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*Food Science and Technology*

Lactic acid bacteria (LAB) are used in the food industry as starters or as probiotic cultures since many years ago, due to their potential beneficial effects on human and animal health. Their presence contributes to enhancing microbiological stability, increasing the conservation time, and to improve the organoleptic characteristics. LABs are considered GRAS (*Generally Recognized as Safe*) but their involvement in the pathogenesis of some infectious processes has been described, contributing to the appearance of bacteremia, endocarditis and localized infections [1]. Therefore, it is essential to assess their safety, before being used in industrial processes. Ninety-eight strains belonging to different LAB species were tested. The safety traits assayed were 1) the antibiotic resistance using the disc diffusion method 2) the presence of antibiotic resistance and amino acid decarboxylase (*tdc*, *odc*, *ldc* and *hdc*) genes by using specific PCRs 3) the production of biogenic amines (BA) by RP-HPLC, and 4) the production of different virulence factors such as the haemolytic, DNase, and coagulase activities by using blood agar, DNase agar and the BD BBL™ Coagulase Plasma, Rabbit Kit, respectively.

Differences between strains belonging to the same species, both in the antibiotic resistance and in the presence of antibiotic resistance genes were observed, confirming that antibiotic resistance is a strain-dependent property. PCR analysis of amino acid decarboxylase genes showed that the *tdc* gene was present in 13.3% of the strains, the *odc* gene was in 10.2%, the *ldc* gene was in 9.2% and the *hdc* gene was in 8.2% of them. Sixty-one percent of the strains were not biogenic amine producers or produced very low amounts of BA. The most produced amine was by far putrescine, followed by tyramine and cadaverine. In the assay for haemolytic activity, none of the strains were  $\beta$ -haemolytic nor showed DNase or coagulase activities.

Based on these results, it can be concluded that the strains, *Levilactobacillus brevis* UCLM-86, *Levilactobacillus brevis* UCLM-47, *Levilactobacillus brevis* UCLM-111, *Lactiplantibacillus plantarum* UCLM-93, and *Lacticaseibacillus paracasei* UCLM-24, were the safest to be used in food fermentations.

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O-20

**Naturally curved organic crystalline structures for waveguide and photonic circuits**

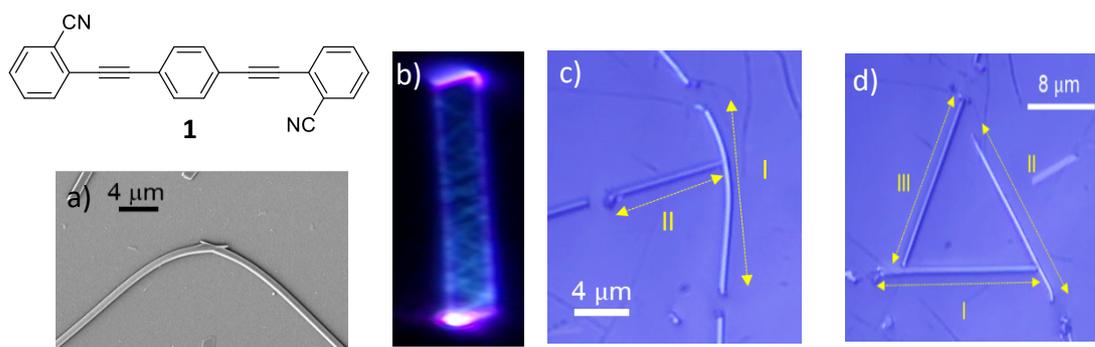
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*Área de Química Orgánica*

Organic crystals are excellent candidates for nanophotonic applications due to the excellent advantages they offer, such as tailor-made synthesis, excellent optical properties, easy processability and lightweight. As a disadvantage, they are usually stiff and fragile. However, the future technologies mandate flexible nanophotonic devices, so we need crystals with higher flexibility.<sup>1</sup>

In this work, we have synthesised an alkynyl derivative of benzene (**1**) that aggregate in naturally bent flexible crystals. In addition, these crystals have optical waveguide behaviour with low values of optical loss. From crystals interconnected and cutting with an AFM cantilever in the desirable locations, we obtained T- and triangular-shaped photonic circuits that allow the flow of light depending upon the excitation point.<sup>2</sup>



**Figure 1:** a) FESEM image of the bent crystal. b) PL image of the crystal. c) T-shaped and d) Triangular-shaped photonic circuits.

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**O-21**

**SUBOLESIN/AKIRIN: A MULTI ARTHROPOD VACCINE ANTIGEN**

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Ticks are obligate hematophagous arthropod vectors of pathogenic viruses, bacteria, protozoa and helminths responsible for highly prevalent tick-borne diseases (TBDs) with animal and human growing incidence worldwide. Ticks are the second most common arthropod vectors, after mosquitos, for human health and the most important in domestic animals. Vaccines constitute the most environmental-friendly and efficient approach against ticks and TBDs in comparison with other traditional methods. Although vaccine efficacy against these and other arthropods had been previously described, the necessity of improving vaccine formulations combining protective antigens, as interacting proteins involved in the interactome or key physical or functional proteins interactions, is more evident every day. Subolesin/Akirin are proteins that have been conserved throughout the metazoan and play an important role in the cell interactome and regulome in response to pathogen infection and other biological processes. The conserved functional evolution of Subolesin/Akirin correlates with the protective capacity shown by these proteins in vaccine formulations for the control of different arthropod and pathogen species [1]. The identification and characterization of these proteins regulome and interactome is crucial to advance in the complete physiological context improving new vaccine formulations by combining Subolesin/Akirin with their interacting proteins for the control of multiple ectoparasite infestations and pathogens infection. Furthermore, we proposed a novel combined scientific and artistic approach for the advanced characterization of Akirin2 interactome. Thus, focusing on proteins involved in cell interactome and regulome through protein-protein interactions for the regulation of multiple biological processes involved in vector-host-pathogen interactions led to Quantum Vaccinomics, the combination of protective epitopes or immunological quantum to develop vaccines “to control them all” [2].

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O-22

**MAGNETICALLY RESPONSIVE HYDROPHOBIC POCKETS FOR ON-OFF DRUG  
RELEASE**

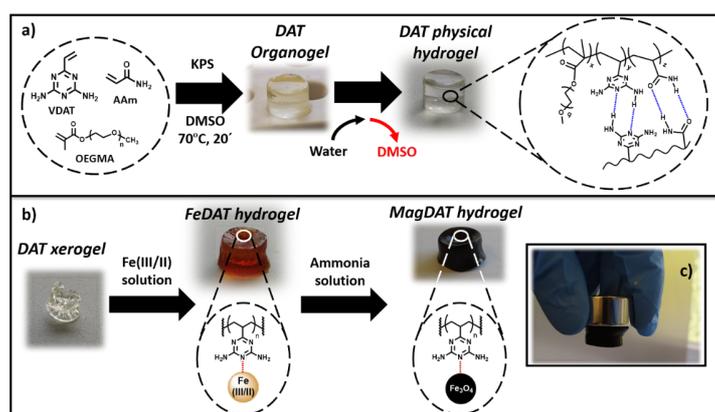
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The vast majority of drugs available on the market are hydrophobic compounds. As a result, their poor water solubility can critically compromise the overall absorption of these drugs by patients. Although numerous different strategies have been developed to improve their bioavailability, the controlled delivery of these drugs is still a challenge. In this sense, stimuli-responsive hydrogels could be a solution to improve administration and stable release. However, the strategies required to render hydrogels hydrophobic mostly rely on weak hydrophobic interactions, which can lead to disassembly of the system and undesired burst discharge. Accordingly, the on-demand release of poorly water-soluble drugs is still a major milestone in this field. To circumvent these setbacks, we present for the first time a hydrophobic, magnetically responsive hydrogel based on the diaminotriazine (DAT) skeleton. The versatility of DATs in terms of H-bond formation and metal complexation simultaneously endows the hydrogel with hydrophobicity and magnetic responsiveness, thus allowing both the efficient loading and on-off release of a model hydrophobic drug as well as of a hydrophobic growth factor. Theoretical calculations further suggested stable formation of DAT aggregates that operate as efficient hydrophobic cavities or “pockets” for these compounds.



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**O-23**

**Determination of ZnO NPs in Yeast and wheat flour sample by single particle  
ICP-MS**

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*Analytical chemistry*

Single-particle inductively coupled plasma mass spectrometry (spICP-MS) is a potential approach for detecting metal-containing nanoparticles (NPs) and quantifying their size and content. Whereas previous research has mostly focused on NPs suspended in aqueous matrices, nothing is known regarding the applicability of sp-ICPMS for NP identification in complex matrices such as yeast and wheat flour samples. In the current research, Alkaline and Enzymatic treatments were used to solubilize yeast and wheat flour samples that had been spiked intravenously with Zinc nanoparticles (ZnONPs). The finding revealed that regardless of the sample preparation techniques employed, comparable size distribution of ZnONPs produced. Furthermore, the quantitative findings for ZnONPs mass concentration obtained with spICP-MS after enzymatic digestion pre-treatment agreed with the findings for total zinc concentration obtained from acid-digested samples using conventional ICP-MS. However, the recovery of ZnONPs from alkaline degraded samples was substantially lower.

**O-24**

**Production of GABA-enriched sheep's milk yoghurt using selected  
*Lactobacillus* strains**

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Gamma-aminobutyric acid (GABA) is an inhibitory neurotransmitter of the mammalian central nervous system, found in plants, animals and microorganisms. GABA has numerous health-promoting functions, including lowering blood pressure, modulation of mood, memory and mood disorders, as well as beneficial effects in the treatment of epilepsy, diabetes and cancer. The production of this amino acid by lactic acid bacteria (LAB) has been demonstrated. Within these, the genera most commonly used in food production are *Lactobacillus*, *Leuconostoc* y *Lactococcus*. In particular, the genus *Lactobacillus* has been the subject of numerous studies on GABA production since, in addition to being a group of bacteria considered GRAS (*Generally Recognized as Safe*), there is a wide variety of strains of the different species capable of producing this compound. Therefore, the production of foods fermented by these bacteria, which can also be a source of GABA for the consumer, has recently been sought.

The aim of this work was, on the one hand, to evaluate the capacity to produce GABA by different strains belonging to the genus *Lactobacillus*, in order to select the most productive ones to be used in the production of yoghurt. And, on the other hand, to produce yoghurts from semi-skimmed sheep's milk with these bacteria in order to obtain health-promoting products with significant amounts of GABA. The experimental yoghurts elaborated presented high concentrations of GABA significantly higher ( $P < 0.05$ ) than the controls, and showed good sensory characteristics and were positively valued by the sensory panel.

## O-25

### Astrochemistry in the Laboratory

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### *Physical Chemistry*

In 1953, Stanley L. Miller<sup>1</sup> conducted an experiment where, from simple molecules, obtained prebiotic molecules as amino acids. This experiment that simulated the first moments of the primitive Earth may be a possible explanation for the origin of life. These simple molecules, in addition to many others, have been found in molecular clouds in the interstellar medium (ISM). The study of chemistry in such extremely cold environments ( $T = 10 - 100$  K) is fundamental to understand how more complex molecules can be generated, just as it happened in the Miller's experiment. In our laboratory, gas-phase kinetics of the reactions of OH radical (ubiquitous in the ISM) with simple molecules present in ISM are carried out with the pulsed CRESU system.<sup>2-6</sup> To reach the typical temperatures of the ISM the gas mixture is expanded through a Laval nozzle from a high to a low pressure chamber. Currently, our CRESU system achieves temperatures between 11.7 and 177.5 K, avoiding gas condensation on the reactor walls. This technique, together with the *Pulsed Laser Photolysis* coupled to *Laser Induced Fluorescence* technique, allows us to determine the rate coefficient of these reactions in gas-phase at ultra-low temperature, contributing to the improvement of astrophysical models to have a greater and better knowledge of the evolution of the cosmos.

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**O-26**

**Optimum Experimental Design: “Think before you act”**

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*Matemáticas*

There is currently a growing interest in the study of experimental design, since it is a fundamental part of the scientific method. Data analysis will be informative only if the data themselves are informative [1]. Experimental sciences and engineering are fields of knowledge especially interested in obtaining models that adequately explain the phenomena under study. Obtaining accurate estimators of the model parameters is, among others, a desirable property to obtain the best quality of statistical inference. For this reason, the data collection strategy becomes a crucial point for the good development of the study where economic factors and practical constraints come into play. The main objective of the Optimal Design of Experiments (DOE) is to determine where to take the observations and how often to optimize some aspect of the model in an efficient way. This paper presents a general introduction to this theory, highlighting some of the models approached by the Optimum Experimental Design group [2] from this perspective. Some of them are used for the calibration of instruments used in radiotherapy, to explain the effect of a drug on tumor cell death, to detect the phenomenon of hormesis or for survival analysis.

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**O-27**

**Tuning the Cytotoxicity of bis-phosphino-amines Ruthenium(II) para-  
cymene complexes for clinical development in Breast Cancer**

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XV SIMPOSIO DE CIENCIA JOVEN

Even knowing the severe toxic side effects and the intrinsic or acquired resistance manifested in various types of cancers, platinum compounds as therapeutic agents are held in high regard. In this context, organometallic ruthenium(II) compounds are proposed as a viable alternative to the platinum therapy because they are less toxic and present an ideal template for both high-throughput and rational drug design. To support the preclinical development of bis-phosphino-amine ruthenium compounds in the treatment of breast cancer, we carry out chemical modifications in the structure of these derivatives to aim at the design of less toxic and more efficient therapeutic agents. We report new bis-phosphino-amine ligands and the synthesis of their ruthenium counterparts. The novel ligands and compounds were fully characterized, studied their water stability, and evaluated their cytotoxicity *in vitro* against a panel of tumour cells which compile the three breast cancer subtypes. The mechanism of action of the lead therapeutic of the series was studied. *In vivo* toxicity assessment was accomplished for further clinical evaluation. The results obtained might pave the way for the clinical development of these compounds in breast cancer therapy.

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## O-28

### ELECTRO-SCRUBBING FOR THE REMOVAL OF VOLATILE ORGANIC COMPOUNDS (VOCS) FROM GASEOUS STREAMS

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#### *Electrochemical technologies for environmental applications*

At the present time, one of the most relevant environmental issues is removal of volatile organic compounds (VOCs), and electro-scrubbing has been found to be very promising technology to face this challenge (1). The main objective of this study is to evaluate the benzene removal from gaseous streams through a process which combine absorption and electro-oxidation (electro-scrubber). The experimental setup consists of a packed absorption column and a flow electrochemical cell (BDD as anode and stainless steel as cathode). Influencing factors such as gas flow rate and current density had been studied. The evolution of the concentrations of benzene and reaction intermediates, in liquid and gaseous streams, were measured by gas chromatography with mass spectroscopy (GC-MS) and high-performance liquid chromatography (HPLC). Results showed that, at 3 and 6 l/h of inlet gas flow rate, the absorption rate of benzene is greater than its degradation rate. Additionally, the optimized flow was determined to be 1,5 l/h. In all cases, electro-scrubbing demonstrated to be functional to absorb and eliminate benzene through anodic oxidation mechanisms. On the other hand, it was found that using a current density from 30 to 100 mA/cm<sup>2</sup> the elimination efficiency of benzene was over 90% and phenol, quinones and carboxylic acids were identified as intermediates. These findings allowed to suggest a mechanistic model for the benzene degradation which consists at first in its transformation into phenol to start phenolic oxidation pathways where carboxylic acids are produce from quinones before their mineralization. This study gives valuable information about the performance of electro-scrubbing, and results conclude that this gas treatment device can be a powerful technique for benzene removal.

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**O-29**

**New naphthalenimide derivatives with application in organic photonics**

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*Organic Chemistry*

We live in an increasingly technological world, where technologies based on light and photonics have been fundamental in the vertiginous development of many disciplines such as communications, medicine and robotics.[1]

This evolution would not have been possible without the parallel development of new materials with improved performance, among which organic compounds have played a very prominent role. Organic materials have attracted increasing attention due to their low cost, easy fabrication, and tunable properties.

In this sense, we have synthesized three new compounds based on the branched nucleus of 1,8-naphthalimide with different alkynyl donor groups and we have studied their ability to transmit and amplify incident light, that is, their ability to behave as optical waveguides [2] and lasers [3]. Two of these compounds have shown behavior as lasers and one of them as a red and green optical waveguide.

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**O-30**

**Kinetic and formation of SOA from ozonolysis of trans- $\beta$ -methylstyrene**

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*Physical Chemistry*

Atmospheric aerosols are considered as one of the main uncertainty sources in the current understanding of the Earth's climate<sup>1</sup>. The formation of aerosols can be observed from the reaction of different VOCs (Volatile Organic Compounds) with atmospheric pollutants. In the present work, we have studied the kinetic rate constant and formation of SOA (Secondary Organic Aerosol) from the ozonolysis of alkene; this reaction proceeds through the formation of a Criegee intermediate (CI). Recently, it has been found that stabilized CI (sCI) can undergo reactions with SO<sub>2</sub> several orders of magnitude faster than assumed so far<sup>2</sup> producing SO<sub>3</sub>, which contributes efficiently to the formation of ground level sulfuric acid<sup>3</sup>. Styrene and derivatives as  $\alpha$ -methylstyrene or trans- $\beta$ -methylstyrene are toxic to humans and considered to be one of the most important secondary organic aerosol (SOA) precursor<sup>4</sup>. These aromatic compounds can be emitted into the atmosphere from different sources such as solvents, combustion, building materials, adhesives and industrial processes<sup>5</sup>. In this context, the formation and growth of new SOA are evaluated in this work from ozonolysis of trans- $\beta$ -methylstyrene.

The reactions have been carried out in a Teflon chamber filled with synthetic air mixtures at atmospheric pressure and room temperature. The kinetic rate constant has been studied with absolute and relative methods by GCMS (Gas Chromatography Mass Spectrometry) and the particle formation has been followed by a SMPS (Scanning Mobility Particle Sizer) and a CPC (Condensation Particle Counter). The main parameters for their characterization are nucleation, influence of different amounts of reagents including effect of water vapor and effect of different SO<sub>2</sub> concentration.

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**O-31**

**Towards turbulence with an alternating Schwarz Legendre collocation  
method for a convection problem**

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*Matemática Aplicada*

An alternating Schwarz domain decomposition Legendre collocation method for a Rayleigh-Bénard problem is presented in this work [1,2]. The problem is modeled with the incompressible Navier-Stokes equations coupled with a heat equation in a rectangular domain. The Boussinesq approximation is considered. The nonlinearity is solved with a Newton method. Each iteration of the Newton method is dealt with an alternating Schwarz domain decomposition method in the horizontal variable, where each domain is solved with Legendre collocation. Thanks to this domain decomposition the aspect ratio and the Rayleigh number can be increased without limitation by adding domains. The computational cost is affordable because the method is parallelizable. Other advantage is high order.

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**O-32**

**Mosquitoes and West Nile**

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*Sanidad y Biotecnología*

West Nile Virus (WNV) is a neuropathic virus for humans, horses and birds transmitted by mosquitoes. Wild birds are natural reservoirs for WNV and, in liaison with competent mosquitoes, responsible for their maintenance and transmission. In Spain, the link between species involved is not yet understood, especially in areas without declared outbreaks. Aiming to deepen in the ecology of flaviviruses at the wildlife-livestock-human interface, we carried out several samplings in horse farms in 1) Ciudad Real and 2) Toledo between 2018 and 2019. We differentiated three sites per farm: i) the farm; ii) a site 500-1,000m away from the farm; and iii) a site at a 3-5 km distance from the farm without livestock. Mosquitoes were captured with specific traps fortnightly. Additionally, blood samples, oral and cloacal swabs, and growing feathers from wild birds (n=580) were sampled. Specific antibodies anti-WNV were detected with a commercial blocking ELISA Kit and WNV RNA was amplified through PCR. Furthermore, sera of 2418 wild ungulates (*Cervus elaphus* and *Sus scrofa*) from Doñana National Park (A1), Western Sierra Morena (A2), Central Sierra Morena (A3), Guadiana river Valey (A4) and Toledo Mounts (A5) between 2005-2019 were tested with the same ELISA Kit. Regarding wild birds, anti-WNV specific IgGs were detected in 28/451 (6.2%), the highest proportion of positives occurring in the farms (8.1%) in comparison to sites ii and iii (4.6% and 5.8%, respectively). Besides, four of 503 (0.8%) were positive to Flavivirus in PCR test. The proportion of exposed ungulates was higher in A1 (33.5%) and A2 (35.3%) than in A3 (18.7%), A4 (20.3%) and A5 (18.7%), shaping the contrasting reported incidence of WNV outbreaks in southern (n=189) and south-central (n=2) Spain. Mosquitoes are currently under analysis. The presence of *Culex pipiens*, the main transmitter of the virus, has been confirmed in sites 1 and 2. These findings corroborate the active circulation of flaviviruses in continental Spain and, especially, close to horse farms. In addition, wild ungulates prove to be efficient predictors for Flavivirus spatiotemporal dynamics.

**O-33**

**Synthesis of metallic nanoparticles by spark ablation. Application in surgical facemasks**

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*Physics*

Spark ablation is a simple, quick, and easy scalable technique for gas-phase synthesis of nanoparticles. By applying a high voltage between two electrodes an aerosol of the desired nanoparticles can be produced, in contrast with the usual liquid solution obtain by 'wet chemistry' methods. The size of these nanoparticles as well as the agglomeration between them can be tuned by varying the operational parameters<sup>1</sup>. Said nanoparticles can be collected into a porous substrate by passing the aerosol through it. In this case, Ag nanoparticles have been deposited in commercial surgical facemasks to study the promising antiviral performance against SARS-CoV2. In this communication the versatility of a spark ablation source when producing multielement nanoparticles is also pointed out as it enables both simultaneous and sequential production<sup>2</sup>.

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O-34

**Nickel electrodes prepared by magnetron sputtering for water and ethanol- water hybrid electrolysis**

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*Chemical Engineering*

Hydrogen is considered as a feasible alternative energy vector and can be obtained by different process. Water electrolysis is recognized as a sustainable and environmentally friendly alternative to produce hydrogen. On the other hand, ethanol electrolysis has been proposed as a promising method to produce hydrogen with lower power demands, since part of the energy required for electrolysis is provided by the organic molecule. We have proposed the use of Magnetron Sputtering (MS) technique to prepare nickel-based electrodes. The developed electrodes have been tested for water electrolysis and for ethanol-water hybrid electrolysis (simultaneous water and ethanol electrolysis). In this study, the influence of different fabrication and operation parameters of nickel electrodes has been tested in a three-electrode glass cell and in an Anion Exchange Membrane Water Electrolysis (AEMWE) cell (see Fig. 1 a)). The current density obtained for the same voltage is higher for hybrid water electrolysis than that for the pure water splitting (see Fig. 1 b)). Finally, a great stability and efficiency in relation to the amount of catalyst has been obtained demonstrating the high potentiality of the MS method.

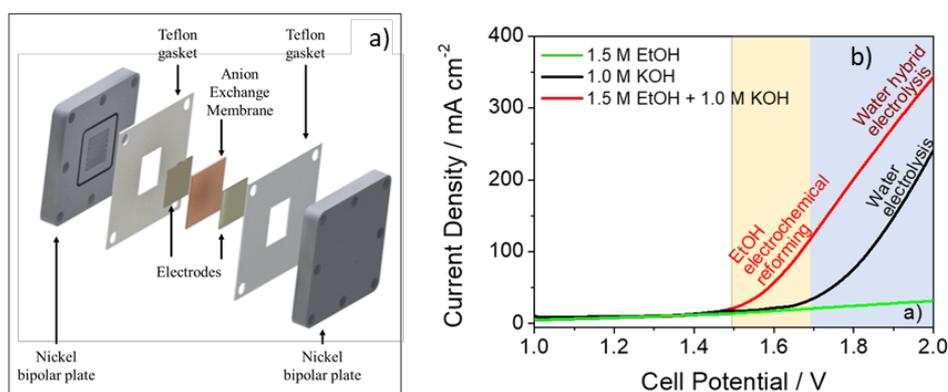


Figure 1. a) Exploded view of a complete electrolysis cell and b) current-potential curves for water and ethanol-water hybrid electrolysis.

O-35

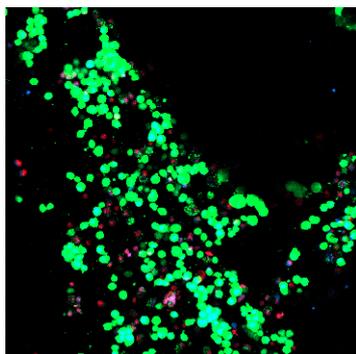
PHOTOPOLYMERIZABLE CHITOSAN HYDROGELS FOR TISSUE ENGINEERING

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*Organic Chemistry*

The field of tissue engineering has the potential to transform how we treat pathologies and diseases that cause tissue damage, by repairing, regenerating, or improving the function of the damaged tissue. A key concept in tissue engineering is the use of biomaterials to support the growth of new cells and promote repair. Of the many types of materials that have been used in tissue engineering, hydrogels have emerged as one of the most prominent and versatile. Hydrogels can be designed to support cell proliferation, migration, and differentiation, to permit oxygen and nutrient transport, and to provide cells with a 3D, highly hydrated environment that



**Figure 1.** Cell culture in chitosan hydrogels.

mimics native soft tissues. Careful design of the underlying polymer scaffold is therefore vital, dictating both the physical and biological properties of a hydrogel [1].

In this work, we highlight chitosan-based hydrogels as suitable scaffolds for tissue engineering applications (Figure 1). Chitosan is a partially deacetylated form of chitin and it occupies a distinct position amongst other biomaterials due to its abundance, versatility, biocompatibility and anti-fungal properties [2]. To increase the mechanical strength and structural integrity of this biomaterial, we have introduced acrylamide as a copolymer. Besides, the addition of nanomaterials such as graphene [3] and magnetic nanoparticles [4] will allow us to tune the biological response of cell cultures in our scaffold by increasing cell adhesion and controlling cell fate using external stimulation.

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# PRESENTATIONS FLASH

(appearance in alphabetic order)



F-1

**VALORIZATION OF BIOMASS WASTE THROUGH FAST PYROLYSIS FOR VALUE-  
ADDED BIOPRODUCTS**

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*Ingeniería Química*

A great deal of research into renewable energy has been undertaken in recent years due to the rising global energy demand and the need to reduce environmental damage caused by excessive use of fossil fuels. Lignocellulosic biomass is an attractive feedstock for producing renewable energy, which can mitigate dependence on fossil fuels because of its potential to generate zero CO<sub>2</sub> emissions, as well as its abundant availability and low price. The International Energy Agency (IEA) suggests that bioenergy has enough resources to provide 10% of the global primary energy supply by 2035 [1]. Biomass has been considered a remarkable renewable energy source because it is the only one that can be stored directly and transported. Using bioenergy waste may also help greatly to achieve a future energy system with net-zero or negative emissions [2]. However, biomass may vary in composition depending on where they are grown and the type of industrial processing. Pyrolysis is one of the most promising and effective methods, among different thermochemical routes for turning lignocellulosic biomass into high added-value products. Depending on heating rate, reaction temperature, and residence time, pyrolysis can be classified as slow, intermediate, or fast. The latter is a promising method for converting lignocellulosic biomass into high-energy forms for use as an energy carrier, mainly bio-oil [3]. It is striking those interactions between inherent traces of mineral matter in all biomass wastes could catalyze different reactions that occur during pyrolysis. That is, they may enhance reaction yields such as cracking, decarbonylation, or decarboxylation [4]. Depending on the final target of the products, pre-treating biomass feedstock or using potential catalysts could therefore enhance bio-oil properties. It would give a new insight for the understanding biomass pyrolysis for high quality liquid fuel and chemicals, which is important for the development of biomass pyrolysis technology and the utilization of biomass resources.

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F-2

**Tropospheric degradation of 2-methylbutanal initiated by OH radicals, Cl atoms and sunlight**

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*Química Física*

The biogenic oxygenated volatile compound 2-methylbutanal (2MB) is emitted into the low atmosphere from several natural sources such as microbiological processes, wildland fires, or emissions from vegetation [1]. During the day, the oxidation of 2MB can be initiated by sunlight, hydroxyl (OH) radicals or chlorine (Cl) atoms in marine atmospheres. Up to date, gas-phase kinetics of OH with 2MB has only been studied at room temperature [2]. The photolysis rate coefficients ( $J$ ) of 2MB initiated by sunlight have also been reported [3]. However, there is no available data for the reaction of Cl atoms with 2MB. In this work, the photolysis rate coefficient ( $J$ ) of 2MB has been measured using a solar simulator in a Pyrex cell coupled to a Fourier Transform Infrared (FTIR) spectrometer to monitor the loss of 2MB. Moreover, the gas-phase kinetics of the reaction of 2MB with Cl ( $k_{Cl}$ ) and OH ( $k_{OH}$ ) have been investigated to evaluate the contribution of these homogeneous degradation routes to the total loss of 2MB in the atmosphere. All the kinetic experiments were carried out under free-NO<sub>x</sub> conditions (simulating a clean atmosphere). Regarding the relative kinetic study on the Cl-reaction, an atmospheric simulation chamber coupled to a FTIR spectrometer was used at 298 K and T60 Torr [4] of air, whereas for the absolute kinetics of the OH-reaction,  $k_{OH}$  was determined as a function of temperature and pressure ( $T = 263$ - $353$  K and  $P = 50$ - $600$  Torr of helium) by using a pulsed laser photolysis-laser induced fluorescence system. Finally, in addition to FTIR, gas chromatography coupled to mass spectrometry and proton transfer time-of-flight mass spectrometry were used to detect the gas-phase reaction products when 2MB was exposed to Cl.

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F-3

**Voltammetric sensing of fluoroquinolones in commercial food daily products  
at chitosan/ $\gamma$ -cyclodextrin-graphene quantum dots modified carbon screen  
printed electrodes**

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*Analytical Chemistry*

A new electrochemical sensor based on screen printed carbon electrodes (SPCE) modified with gamma cyclodextrin functionalized graphene quantum dots (GQDs- $\delta$ CDs) and chitosan (CHI) for the determination of fluoroquinolones (FQs) global amount has been reported for the first time. Developed sensor exhibited an extraordinary electrochemical behaviour towards oxidation of fluoroquinolones due to excellent conductivity of GQDs incorporated in chitosan film. Additionally,  $\delta$ CDs became an excellent recognition element allowing the size based selective discrimination of FQs over other drugs [1]. For the design of the electrochemical sensing system, GQDs functionalized with different kinds of CDs ( $\alpha$ -CDs,  $\beta$ -CDs and  $\delta$ -CDs) were synthesized and later evaluated over the performance of the sensor, finally selecting  $\delta$ CDs-GQDs as the most suitable ones.  $\delta$ CDs-GQDs were characterized by TEM, DLS, FTIR and XRD. The electrochemical properties of the sensing system were assessed by cyclic voltammetry (CV) using potassium ferricyanide as redox probe, showing an increase on kinetic constant ( $k^0$ ) and electroactive area ( $k^0$ ) in presence of  $\delta$ CDs-GQDs, improving thus its performance. Electrochemical mechanism of the redox process was also studied on four representative quinolones attending to their distinctive chemical structures, obtaining in all cases the same number of  $e^-$  (2) and  $H^+$  (2) involved in their oxidation process, which suggested us a single oxidation mechanism for all FQs. Selection of physic-chemical and instrumental conditions were carried out using enrofloxacin as representative model analyte of the global FQs behaviour. Finally, the individual response of the four representative FQs, and that of their binary and quaternary mixtures has been evaluated too to perform global determinations. Analytical performance features and applications in commercial samples are now in progress.

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**F-4**

**Foaming of thermoplastic polyurethanes using supercritical CO<sub>2</sub>.**

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*Chemical Engineering*

Polyurethanes are usually foamed with traditional blowing agents such as azodicarbonamide and hydrofluorocarbon [1]. However, these blowing agents can leave some chemical residue in the polymer, and release toxic gas [2]. For this reason, alternative methods are being studied, like supercritical fluid foaming. Carbon dioxide (CO<sub>2</sub>) is the most widely used supercritical fluid, due to the mild conditions needed to reach its supercritical state compared to other substances and it is environmentally friendly properties, as it is inert and non-toxic, and offers the versatility needed to treat different raw materials.

Thermoplastic polyurethane (TPU) combines the excellent properties of the soft and hard segments in the macromolecular chain, which provides the material with many superior properties, including high elasticity and resilience [3]. In addition, TPU foams show a promising future in many industrial fields such as athletic footwear and automotive accessory. The present work focuses on the influence of temperature, pressure, and contact time in the foaming of TPU using supercritical CO<sub>2</sub>.

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F-5

**PLGA foaming via supercritical CO<sub>2</sub> for tissue engineering applications**

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*Chemical Engineering*

Tissue engineering is an important field of regenerative medicine for tissue repair, particularly the repair of bone defects from trauma loss, tumor section, infection debridement and congenital skeletal abnormalities. Traditionally, bone implants have been made with metals or their alloys, but they are not absorbed by the body and require subsequent surgeries. In addition, they prevent bone regeneration due to the space they occupy. Therefore, the manufacture of porous scaffolds from biocompatible and biodegradable polymers, as poly(lactic-co-glycolic acid) (PLGA), remains a great challenge. The scaffold structure should meet several design criteria: (1) the surface should allow cell adhesion and promote cell growth; (2) the porosity should be high enough to provide sufficient space for cell adhesion and extracellular matrix regeneration; (3) the scaffolds should be biocompatible and biodegradable; (4) the scaffolds should be mechanically strong.

Among the manufacturing techniques for the preparation of polymeric scaffolds, the supercritical CO<sub>2</sub>-assisted foaming offers significant advantages because is a solvent-free technique, since CO<sub>2</sub> is a gas non-toxic, chemically stable, non-flammable, and cost-effective. Additionally, CO<sub>2</sub> can achieve its supercritical state at “mild” conditions, T = 31 °C and P = 73 bar<sup>1</sup>. In this process, in a first step, the polymer is saturated with supercritical fluid at constant temperature and pressure conditions. Subsequently, the system is led to a supersaturated state by rapidly reducing pressure resulting in the nucleation and growth of gas bubbles inside the polymer matrix. The sc-foaming method allows the tuning of their porous morphology (porosity, mean pore size, and pore size distribution) to fit certain target specifications. Processing temperature and pressure, CO<sub>2</sub> contact time and depressurization rate are the main foaming parameters able to adjust the pore size and homogeneity<sup>2</sup>.

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F-6

**CHLOR-ALKALI CELLS: A CLASSIC FOR A NEW WAY OF STORING ENERGY**

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*Electrochemistry*

Global concern has increased about the excessive dependence on fossil fuels and the pollution associated with their use is currently one of the main concerns worldwide. One of the greatest concerns is global warming driven by uncontrolled greenhouse gas emissions. Among them, carbon dioxide (CO<sub>2</sub>) is the most important, because of its huge production<sup>1</sup>. Furthermore, although there is no perfect energy source, renewable energies can be a good alternative to conventional power sources. However, the electricity production is not easily adapted to demand. In this sense, in recent years, many electrochemical technologies are being developed to solve this supply problem. One of these novel technologies is that which uses hydrogen to produce energy. The aim of this work is to integrate a chlor-alkali PEM reversible fuel cell powered with renewable energy with a novel system of spray-drying absorber<sup>2</sup> to remove carbon dioxide from gases. In the first stage, the electrochemical PEM cell produces hydrogen and chlorine, and subsequently these reagents are used to regenerate electricity leading to a sustainable process. In the second stage, one of the by-products obtained during the chlor-alkali electrolysis (NaOH) is used as absorbent, whose hydroxyl ions combine with CO<sub>2</sub> and fix efficiently it as bicarbonates or carbonates. Details of the technology as well as results of a case study are shown in this work.

**Acknowledgments**

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F-7

**Effects on different agroenvironmental practices on the female reproductive parameters of Iberian hare (*Lepus granatensis*)**

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*Bioquímica (IREC)*

During the 20th century agriculture underwent important changes based on the search for maximum productivity, which has led, on the one hand, to an important homogenization of the landscape due to the concentration of land, and on the other hand, to the use of a large amount of pesticides and fertilizers in the environment [1]. This change in agricultural management has been linked to the loss of plant and wildlife biodiversity. In the specific case of pesticides, there are significant gaps in the knowledge of their secondary or sub-lethal effects on wildlife [2]. Under this context, the aim of this study was to evaluate the impact of different agricultural management models, based on the use or not of pesticides, on the reproductive success of the Iberian hare (*Lepus granatensis*), as a sentinel species of the potential effects that the use of pesticides can have on the wildlife of the Iberian agrarian ecosystems. To carry out this study, the ovaries of female Iberian hares from hunting areas free of pesticides (control 1 and 2, n=18) and from others where pesticides are used (treated 1 and treated 2, n=32) were weighed, measured and processed for a subsequent follicle and corpora lutea count. Hares from pesticide-treated areas showed significant lower ovarian size and weight than hares from pesticides-free areas. Significant differences were also detected in the number of secondary and atresic follicles, being, this last, particularly high in individuals from treated areas. As a conclusion, we can say that intensive agricultural management, based on the use of pesticides, has a negative impact on the reproductive function of the Iberian hare, for which may be one of the factors responsible for its population decline.

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F-8

**EXPLORING THE POTENTIAL OF LACTIC ACID BACTERIA STRAINS AS HEALTH  
PROMOTERS**

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*Área de microbiología*

The current relevance of the consumption of foods with a positive impact on health and the changes in eating habits, cause the search for new products. Probiotics are a clear example of this type of products, and the search for new strains of bacteria to which this denomination is attributed is recurrent <sup>[1]</sup>. Because of this, the present Master's Thesis aims to search for lactic acid bacteria strains (LAB) that exhibit health-promoting properties such as phenol tolerance, antioxidant activity, cholesterol-lowering capacity and antifungal activity. In this study, a collection of LAB strains was analyzed. Specifically, the bacteria belonged to different isolated species from various fermented foods in previous works, *Levilactobacillus* (3), *Lactobacillus* (4), *Lacticaseibacillus* (9) and *Lactiplantibacillus* (22) <sup>[2]</sup> and were preserved frozen at -80°C. It was proved that 36 of the strains studied showed tolerance to a concentration of 0.4% phenol, however, only two strains tolerated 0.6% phenol. The strains of the genus *Lactiplantibacillus*, belonging to the species *Lpb. plantarum*, showed a high antioxidant activity with respect to the rest of the strains studied. On the other hand, the strain that eliminated the greatest amount of cholesterol from the medium was *Lb. acidophilus* UCLM-Lb70. Unlike the rest of the assays, where the results were variable, no strain showed antifungal capacity. The results obtained in this master's thesis have shown a great variability in the behavior of the strains evaluated. This fact demonstrates that each strain of lactic acid bacteria has its own mechanisms of action against exposure to reactive oxygen species (ROS), toxics and to reduce or eliminate some compounds from the medium such as cholesterol, meaning the properties tested are strain-dependent .

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F-9

**Combined processes as an alternative for water and air treatment**

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*Chemical Engineering*

The exposure to polluted air containing volatile organic compounds (VOC) is related with a several illnesses, i.e., headache, respiratory illness, fatigue, nerve damage and others. In addition, the long exposure poses the risk of cancer. The adsorption treatment is regarded as one of the most promising technologies due the cost-effectiveness, flexible operation, and low energy consumption [1]. On the other hand, electrochemical treatment of contaminated solutions can lead to complete mineralization of the organic compounds. It means that it is able to oxidize the molecules to CO<sub>2</sub> and H<sub>2</sub>O, which are much less harmful to the environment and to humans [2]. This work proposes the combination of adsorption technology with electrochemical treatment to treat air and water streams contaminated with VOCs. First, 50 L of a solution with 100 mg L<sup>-1</sup> of benzene was submitted to the adsorption in granular activated carbon (15.9 g). This step showed that 70% of benzene can be removed from water. This polluted adsorbed was easily desorbed with 1 L of methanol and this solution was electrochemically treated using a boron-doped diamond electrode and a current density of 50 mA cm<sup>-2</sup>. Our results suggest that the difference between treat 50 L of solution with low concentration of benzene and 1 L of methanol solution with a great amount of benzene was negligible. This becomes a great advantage for the treatment of benzene in gas phase.

**Acknowledgements**

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F-10

**Permalloy thin films on V-groove patterned substrates for sensing and  
biological applications**

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*Física Aplicada y Nanotecnología*

The magnetic properties of advanced materials, such as soft magnetic nano-undulated films[1], offer innovative possibilities for sensing and biological applications. For example, the morphologic and anisotropic characteristics of magnetic-coated V-groove substrates could be used for measuring perpendicular magnetic fields or guided control of cell movement [2]. For this purpose, Permalloy (Py) thin films were grown in V-groove (VG) patterned silicon substrates. Silicon substrates were processed through a multistep procedure involving photolithography, laser interference and reactive ion-etching techniques. The resulting pattern ( $p = 250$  nm,  $\theta = 55^\circ$ ) was characterised using SEM [Figure 1]. Permalloy thin films were deposited by DC sputtering with normal incidence on several substrates at a  $1.6 \text{ \AA/s}$  deposition rate.

The deposited Py-VG thin films were characterised using scanning probe microscopies and a vectorial Kerr magnetometer for the study of the resulting morphology and magnetic anisotropy.

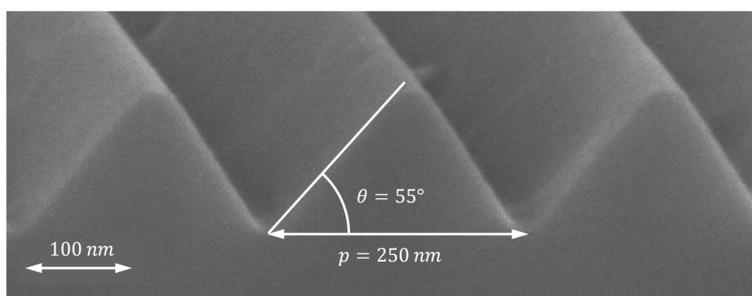


Figure 1. SEM characterization of nanopatterned V-groove silicon substrate.

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F-11

**Real Acid Mine Drainage Treatment by Bioelectrochemical Systems**

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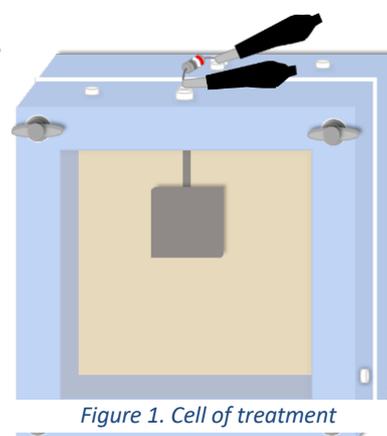
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*Chemical Engineering*

The electrodeposition has been studied since a century ago. [1] Due to the interest of scientific community, from then on, the electrodeposition has been improved, developing new electrodes, configurations, types of wastewater inputs, among others.

The objective of this work is to treat a real acid mine drainage (AMD) from San Quintín mine using a Bioelectrochemical system, both Microbial Fuel Cell (MFC) and Microbial Electrolysis Cell (MEC). The configuration of the cell is shown in the Figure 1, where the titanium electrode can be seen, in which the metals from the AMD are electrodeposited.

The microorganisms are in the anode, which in MFC configuration, can reduce metal and generate energy simultaneously, and the real AMD is in the cathode. The AMD is composed, mostly, of Zn, Al, Cu, Fe, Cd and Mn.



In order to obtain the metals' reduction, the MFC configuration was used for a period of 5 days, generating electrical current, reducing the  $\text{Fe}^{3+}$  to  $\text{Fe}^{2+}$  and recovering all the copper on the cathode surface. Then, the configuration is changed to MEC to get a total electrodeposition of metals.

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**F-12**

**Study by spectroscopic techniques of the process of protein corona formation  
onto platinum nanoparticles in biological media**

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*Analytical Chemistry*

For the past decades, the use of nanotechnology has been on the rise, and more specifically, metallic nanoparticles (NPs) are an interesting option to use thanks to their unique structural, electrical, optical, and magnetic properties. Recently, platinum nanoparticles (PtNPs) are attracting high interest in the biomedical field, in applications such as gene delivery or antitumoral therapies, among others [1]. When these PtNPs are in contact with a biological media, they do not act as inert entities, in fact, different macromolecules present in this media can be adsorbed onto the nanomaterial surface. Out of all the interactions, protein adsorption is the most relevant one, resulting in a dynamic structure called protein corona. This structure is described to have two parts, known as hard corona (macromolecules interact strongly with the NPs) and soft corona (weaker interactions are established between proteins that form multilayers around the NP). The study of the protein corona is of great importance to understand the behavior, fate, pharmacological profile, and toxicological risk of PtNPs in biological systems, but the available information is still very scarce [2].

In this work, we aimed to study by spectroscopic techniques, such as dynamic light scattering (DLS), UV-vis absorption, and fluorescence emission, the process of formation of hard and soft protein corona using 30 nm PtNPs with albumin protein, from bovine serum, as a model using different analytical methodologies.

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F-13

**Hydrofluoroethers as new alternative compounds of Chlorofluorocarbons:  
How do we study them?**

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*Physical Chemistry*

The worldwide concern about the strong environmental impact of Chlorofluorocarbons (CFCs) led to the application of the Montreal Protocol in 1987, which banned the use of CFCs in various industrial applications such as carried fluids, cleaning of electronic equipment, foam blowing agents and heat transfer agents in refrigeration. Hydrofluoroethers (HFEs) are considered a new alternative to this type of compounds as they do not contain chlorine atoms that cause ozone layer degradation.<sup>[1]</sup>

To assess the suitability of HFEs as potential candidates for replacing this greenhouse species is essential to evaluate their expected impact on climate change prior to their widespread. For that purpose, the rate coefficient ( $k_{OH}$ ) for the reaction of a certain HFE with OH radicals, the main diurnal atmospheric oxidant, and its infrared (IR) absorption cross sections is determined. With this experimental data we obtain the Global Warming Potential (GWP), which is expected to be considerably lower than majority of CFCs.<sup>[2]</sup> To determine  $k_{OH}(T,P)$  the pulsed laser photolysis/laser-induced fluorescence technique was used.<sup>[3]</sup> In addition, Fourier transform IR spectroscopy was used to determine the IR absorption cross sections between 500 and 4000  $\text{cm}^{-1}$ . The atmospheric lifetime of HFEs will be calculated along the troposphere and their suitability as potential CFC replacements will be discussed in terms of the calculated GWP.

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**F-14**

**BIOACTIVE PARTICLES FOR THE SELECTIVE ELIMINATION OF BILIRUBIN IN  
HEMODIALYSIS PATIENTS IN A CRITICAL STATE**

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*Chemical Engineering*

Bilirubin is an indicator of liver function levels derived primarily from the metabolites of hemoglobin that are released by red blood cells. A distinction can be made between indirect or non-conjugated bilirubin, which is transported to the liver as a complex with albumin, and direct or conjugated bilirubin which is excreted as bile. The two types of bilirubin together are known as total bilirubin. The normal level of total bilirubin in the blood is between 0.3-1.2 mg/dL, however, successive disturbances in its metabolism and/or in its excretion can cause an excessive accumulation of non-conjugated bilirubin in the blood, causing liver disease or even death. <sup>[1]</sup>

In recent decades, plasma perfusion has proven to be a very effective strategy to reduce bilirubin levels and has been used as a reference for liver diseases. Several bilirubin adsorbents have now been developed because the adsorption system is a critical component of plasma perfusion. Nevertheless, these adsorbents have limited hemocompatibility making it necessary to research and develop new materials that provide a solution to this problem.

One of the main problems facing this research is the biocompatibility and selectivity of materials against bilirubin. For this reason, new materials are being investigated to solve this difficulty, by tackling two possible routes for extracorporeal adsorption of bilirubin based on the cationic surfactant system of tricoctylmethylammonium chloride (TOMAC).

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F-15

**Potential probiotic and food protection role of wild yeasts isolated from  
pistachio fruits (*Pistacia vera*)**

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Ciencia y Tecnología de los Alimentos

Biotechnological capability of yeasts isolated from pistachio fruits has not been studied in deep, despite of their potential industrial application. The interest on probiotic capacity of yeast has been increased in the last years, as well as their use as biocontrol agents. So, the main objective of this study was to determinate both capabilities of wild yeasts isolated from pistachio fruits harvested in Castilla – La Mancha.

A total of 15 strains were identified by molecular techniques (PCR-RAPD) which were catalogued in 7 different species by ITS region sequencing. These strains were subjected to an invitro intestinal conditions test in order to select those with the best probiotic potential (65%). The evaluation of their kinetic parameters showed that some of the wild strains had better behavior than *Saccharomyces boulardii*, used as positive control since is the only commercial probiotic yeast. Complementary assays were done in order to know their auto-aggregation capacity, cell surface hydrophobicity, behavior in a sequential simulated digestion, biofilm formation capability and carbon sources assimilation. Finally, their biocontrol activity was evaluated against mycotoxigenic moulds and pathogenic yeasts, together with their antioxidant ability.

Results showed that *Diutina rugosa* **14**, followed by *Diutina rugosa* **8**, were the best ones as potential probiotic and in carbon sources utilisation. In contrast, *Hanseniaspora guilliermondii* **6** and *Aureobasidium proteae* **5** could be used to improve food or feed products preservation thanks to their notable biocontrol and antioxidant capability.

**F-16**

**A simple preliminary design of self-support power supply based on Hydrogen  
and Photovoltaic technology**

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*Ingeniería Química*

The use of renewable energy and hydrogen technology is a sustainable way to help reducing the impact of fossil fuels and can be the solution for the intermittent feature of renewable energies. Hence, the aim of the present work is to design a self-sufficient system for a one-family house by coupling a solar photovoltaic array and an anion exchange membrane water electrolyzer (AEMWE). The first step is the selection of the photovoltaic panel for supplying the electrical demand of the house during the daylight time by using a commercial software PV-SYST 7.0. Then, the hydrogen production system (via AEMWE) is calculated by coupling the electrolyzer and photovoltaic panel current-potential curves. A fuel cell is selected to use the hydrogen produced when the solar energy is not available (i.e., at nights or cloudy days) to self-sufficient the electrical power of the house. Finally, the hydrogen storage tank is also estimated in order to store hydrogen for a design basis of four consecutive cloudy days according to the hydrogen consumption of the fuel cell. The whole system is calculated and designed by a simple procedure for a specific location in Ciudad Real (Spain) for January, known as the coldest (the lowest radiation level) month of the year. The general and simple procedure described in this work could be used elsewhere for other similar applications and demonstrated that the hydrogen production at low scale is a suitable technology to use renewable energy for self-energy supporting in a residential application without any connection to the grid.

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F-17

## Synthesis of 2D Nanomaterials

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*Nanoscience and nanotechnology*

Graphene has peculiar mechanical and electronic properties, [1] important from microelectronics to biosensing, nano-medicine, and biology. From their discovery, it has been possible to find near of 150 exotic 2D layered nanomaterials [2] such as Transition metal dichalcogenides (TMDs), hexagonal boron nitride (h-BN), borophene (2D boron), MXenes (2D carbides/nitrides), and others. [3] Single layers of Transition metal dichalcogenides (TMDs) have attracted notable interest due to their unique properties and natural abundance, all these conferring promising applications. [4] Here, we summarize of the different nanomaterials synthesized in the laboratory, including some interesting applications. Also, we report an environmentally friendly, cheap, and simple approach for the synthesis of aqueous soluble nanomaterials through ball milling synthesis.[5-7]

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F-18

**Study of the Gas-phase Reactivity of the OH+CH<sub>3</sub>NH<sub>2</sub> Reaction at Interstellar  
Temperatures**

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*Química Física*

The hostile conditions present in the interstellar medium (ISM), *i.e.* the space between two star systems, have not been an obstacle to detect more than 200 different species of molecules [1]. In the coldest regions (~10 K) of the ISM, *i.e.* the dense molecular clouds, just a few complex organic molecules (COMs) have been observed. Some of them contain C-O or C-N bonds, which are considered potential precursors of prebiotic molecules, such as sugars or amino acids [2]. For example, methylamine (CH<sub>3</sub>NH<sub>2</sub>) was first detected in 1974 in Sgr B2 and Ori A [3]. Understanding the gas-phase chemistry of CH<sub>3</sub>NH<sub>2</sub> at ultra-low temperatures is of great importance to elucidate the formation of other species, such as CH<sub>3</sub>NH or CH<sub>2</sub>NH<sub>2</sub> radicals, which can further contribute to the formation of larger COMs. One of the reactions to consider is the reaction of CH<sub>3</sub>NH<sub>2</sub> with hydroxyl (OH) radicals, first detected in 1963 [4] and ubiquitous in the ISM. In this work, the experimental kinetics of the gas-phase reaction between CH<sub>3</sub>NH<sub>2</sub> and OH have been studied between 21.7 K and 177.5 K for the first time, using the most powerful pulsed CRESU (French acronym for Reaction Kinetics in a Uniform Supersonic Flow) worldwide [5]. The CRESU technique is based on supersonic expansions through a specifically designed Laval nozzle. The OH radicals are generated in the cooled jet by pulsed laser photolysis (PLP) of H<sub>2</sub>O<sub>2</sub> and the OH temporal profile is monitored by laser induced fluorescence (LIF). An increase of the rate coefficient as the temperature decreases was observed in the investigated temperature range.

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F-19

**“Half-sandwich” Ir complexes as potential candidates for light-mediated therapy**

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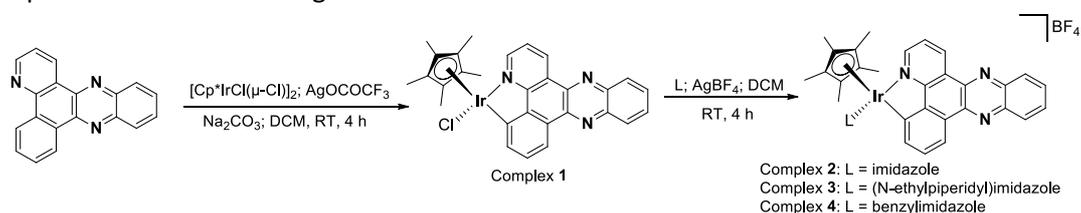
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Cancer has become the second leading cause of mortality in the world. However, its mortality has decreased due to the advance of new detection and treatment techniques. Photochemotherapy emerges as a new non-invasive technique to improve the selectivity of current cancer treatments. In this therapy, a photosensitizer is delivered which is ideally harmless in the dark and activates in the presence of light. Action can take place through different mechanisms: photodynamic therapy (PDT) in which  $^1\text{O}_2$  and reactive oxygen species (ROS) are generated<sup>1</sup>, and photoactivated therapy (PACT) in which irradiation leads to photodissociation of the molecule to give rise to one or two active species<sup>2</sup>. This allows to design a light-controlled chemotherapy in a spatio-temporal way. Iridium complexes with C<sup>N</sup> ligands have been employed as photosensitizers in PDT mechanisms due to their photochemical properties<sup>1</sup>. In this work we present Ir(III) complexes with  $\pi$ -extended C<sup>N</sup> ligands and imidazole derivatives (**Figure 1**) which are expected to generate ROS after light irradiation. The introduction of  $\pi$ -extended C<sup>N</sup> ligands enables their intercalation into DNA<sup>1</sup>, while cytotoxic imidazole derivatives ligands could improve their activity via PACT.

Optimization of the synthesis method was necessary because the conventional methods described in the literature were not successful. The X-ray diffraction structure of complex **2** was determined. Biological studies are in progress. Preliminary results show high cytotoxicity of complexes **1-3** in human lung carcinoma cell line.



**Figure 1.** Synthesis of Ir complexes with C<sup>N</sup> ligands.

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F-20

**Design of Electrochemical Reactors for the Removal of Pollutants from  
Gaseous Streams**

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*Electrochemistry*

Currently, waste gaseous streams have become an important issue of environmental concern, therefore society is demanding more sustainable technologies to clean up these streams. A novel technology for remove odorous substances, organic and inorganic pollutants and VOCs from gaseous streams, is known as electro-scrubbing or electro-absorption process. Which combines two separated treatment stages: absorption process and reactive electrochemical system. These treatment technologies need more research to increase the technology readiness level (TRL), as it is currently at a low TRL [1] [2]. Therefore, this work tries to unify the two stages in a single unit to improve gas-liquid mass transfer efficiency and optimization of parameters with use of aqueous metal solutions to promote the electrochemical oxidation. 3D printers offer the possibility of making come true the complex mechanical concepts and upscaling, because of the complexity associated to the heterogeneity of the gas-liquid and electrolyte-electrode interfaces. In these sense, different prototypes have been made with 3D filament printers in our laboratory, using mechanically and environmentally stable thermoplastics, polylactic acid (PLA) or polyethylene terephthalate glycol- modified (PET-G). Using 3D printers can enable more sustainable modes of production and consumption.

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**F-21**

**Magnetic acrylamide hydrogels: SPIONs in situ.**

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*Organic Chemistry*

Hydrogels have been extensively studied by the scientific community due to its excellent properties, what make them useful for such a big number of applications. Hydrogels are three-dimensional networks, physically or chemically crosslinked, that can absorb water though not soluble in it. The properties of these soft systems can be tuned by changing its composition or by introducing nanoparticles.<sup>1</sup> On the other hand, superparamagnetic iron oxide nanoparticles (SPIONs) for medical applications have been reported in such a big number of reports in the last few years.<sup>2</sup> On this regard, SPIONs have been introduced into the acrylamide hydrogels by *co-precipitation in situ* method in different concentrations. These hydrogels have been characterized and studied in order to know their properties, which are shown in this work.

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## F-22

### Design of flexible electrodes based on organogels for biomechanical purposes

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#### Organic Chemistry

Robotics has been an important part of our lives for a long time. The robotic systems traditionally used are rigid and heavy, so they can be dangerous for humans. This problem has been solved with the development of soft robotics.[1] Among the different materials that can be used in acted soft structures, hydrogels with response to stimuli are of special interest. The MSOC Nanochemistry research group has extensive experience in the design and synthesis of different types of hydrogels.[2, 3] In addition, they have studied an actuator based on a [2-(acryloyloxy)-ethyl] trimethylammonium chloride hydrogel that is able of bending in the presence of electrodes, without the need to immerse it in an external aqueous medium.[4]

For a material to act as a flexible electrode, it must have high electrical conductivity. For this reason, it was decided to deposit different metals by sputtering on a 2-hydroxyethyl acrylate (2-HEA) organogel.[5] In this way, a metallic conductivity is achieved, making this organogel an excellent electrode (Figure 1).



**Figure 1.** Electrode based on a 2-HEA organogel with silver deposited by sputtering.

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**F-23**

**Design of a bioreactor for bioleaching of metals from solid mine tailings**

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*Chemical Engineering*

There are many sites that the mining industry, once its work is finished, has left abandoned over the years and in these, a large amount of solid mining waste<sup>1</sup>. This type of waste can contain large amounts of metallic sulfides and heavy metals, which are harmful to the environment<sup>2</sup>, so in recent years it has been necessary to develop different plans and directives for their decontamination. The bioleaching process is a feasible and possibly very efficient method for the recovery of these metallic sulfides and heavy metals. This method allows the conversion of an insoluble metal into a soluble form<sup>3</sup>.

The objective of the work is to carry out the design of a bioreactor for the bioleaching of metals from solid mining wastes. The following steps were followed: review in the literature the state of the technique and study the conditions under which it is carried out; select the operating conditions; design the bioreactor based on experimental data obtained in the literature, design the necessary auxiliary services; finally, estimate the cost of the proposed technology. The main advantage of this technology is its moderate cost and low environmental impact, while its main disadvantage is its slowness, as is often the case with environmental bioprocesses. To improve treatment capacity, it is proposed to increase the number of reactors to be worked with, instead of increasing the size of a single reactor. Using reactors that are not excessively large would facilitate their transport and use at different mining sites.

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**F-24**

**Formaldehyde, acrolein and other carbonyls in dwellings of university students. Levels and source characterization**

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Fifteen carbonyl compounds were investigated in the living rooms and bedrooms of 25 university student flats in the urban area of Ciudad Real (Central Southern Spain) in wintertime. Carbonyls were sampled using Radiello® passive samplers refilled in the laboratory according to the method described in ISO 16000-3 Standard (1). The most abundant carbonyls at living rooms and bedrooms were formaldehyde, acetone, acetaldehyde, hexaldehyde and butyraldehyde. The median concentration levels in the living rooms and bedrooms were: 28.6 and 34.2 µg m<sup>-3</sup> for formaldehyde, 18.3 and 23.1 µg m<sup>-3</sup> for acetone, 14.3 and 15.8 µg m<sup>-3</sup> for acetaldehyde, 11.4 and 14.1 µg m<sup>-3</sup> for hexaldehyde and 10.8 and 12.4 µg m<sup>-3</sup> for butyraldehyde. The median concentration of formaldehyde, benzaldehyde, valeraldehyde and hexaldehyde was significantly higher in the bedrooms than in the living rooms. Indoor concentrations were significantly higher than outdoor concentrations for all carbonyl measured, indicating that sources in the indoor environment are prevailing in all flats. Principal component analysis, multiple linear regressions and Spearman correlation coefficients were used to investigate the origin, the indoor pollutants determinant, to establish common sources between carbonyls or the possible influence of different factors such as floor characteristics, type of heating or smoking. Formaldehyde, acetaldehyde, acrolein, acetone, propionaldehyde and benzaldehyde concentrations were compared with relevant international guidelines, being their concentrations below recommended values except acrolein, where all measured flats exceed the reference levels; it would be important to focus on the characterization of emissions sources of acrolein in indoor air in order to minimise the exposition and health risk.

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F-25

**Potential use of coumarin conjugates via click chemistry as a novel anticancer  
and antioxidant agent**

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Ingeniería Química*

Chemotherapy is the main treatment option for early stages of cancer and is also used in combination with surgery and radiation therapy for late stages of cancer. However, chemotherapy is associated with unavoidable side effects, leading to toxicity in patients and the development of drug resistance. The emergence of advanced drug delivery systems has shown great potential for greater therapeutic efficacy.

Systems based on polymer-drug conjugates have many advantages as a powerful platform for cancer drug delivery, such as improved availability, high drug loading efficiency, resistance to recrystallisation, and spatially and temporally controllable release. In order to carry out the union between polymer and drug, click chemistry was employed. Click chemistry has the advantage of being a highly reliable methodology, clean, with excellent performance and compatible with a large number of functional groups. One of the most well-known reactions is copper(I)-catalyzed alkyne azide cycloaddition (CuAAC). Terminal alkyne group reacts with an azido group to form a thermally and hydrolytically stable triazole ring, where N, N-dimethylformamide (DMF) or tetrahydrofuran (THF) are the most common solvents used to achieve the conjugation of chemical product. This work aims to find an option that avoids the use of toxic solvents such as THF or DMF, and to use a solvent that can protect medicines from degradation and is additionally environmentally sustainable, using supercritical technology. In this research PEG supported coumarin were synthesized via click chemistry and their aggregation properties were studied.

On the other hand, due to the hydrophilic character of self-assemblies composed of PEG, the study was carried out to incorporate two cytotoxic (Paclitaxel, PTX and Curcumin, CUR) drugs via non-covalent interactions to aim to form micelles.

Several reports clearly reveal the ability of micelles to overcome cytotoxic drug resistance and their broad applicability in cancer therapy. In conclusion, micelles of the mPEG-coumarin conjugate are promising delivery systems to enhance the anticancer activity of PTX and CUR, thereby reducing their side effects, and may act as potential carriers for other chemotherapeutic agents.

F-26

## Multilayer hydrogels for tissue engineering

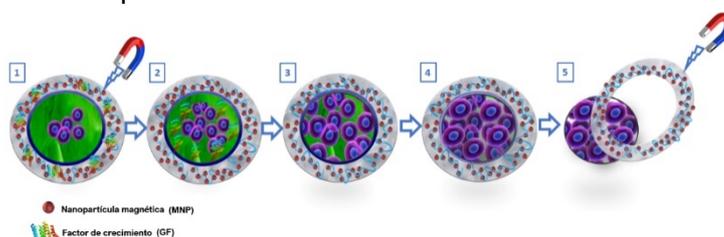
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*Área de Química Orgánica*

Tissue engineering is an interdisciplinary field in continuous development, combining progress in technology and life sciences. This area has great potential in regenerative medicine, and its greatest achievement could be to generate artificial organs from cells, supports and biological factors. Among the different materials that can be used in tissue engineering, hydrogels represent a class of macromolecules of particular interest because they possess unique physicochemical characteristics, which make them the synthetic biomaterials that most closely resemble living tissues.<sup>1</sup> Hydrogels prepared from natural polymers do not have good mechanical properties, although they have the advantage of being biocompatible and biodegradable. On the other hand, synthetic hydrogels can be synthesized with greater control of their mechanical properties: their highly porous structure can be easily tailored by controlling the crosslink density and the type of functional groups in the gel matrix. However, they are not as biocompatible as natural hydrogels, and their biodegradation is difficult and/or they can produce toxic degradation compounds. Therefore, our proposal aims to produce a multilayer hydrogel system consisting of two concentric layers: a hydrogel layer, magnetically sensitive, will surround a core of a natural biodegradable polymeric network. The synthetic magnetic response layer will serve to load and release bioactive molecules on demand. This layer will be removed once it has achieved its purpose, leaving the tissue in a biodegradable system that could be implanted.



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**F-27**

**Incubation with cAMP Modulators Before In Vitro Maturation Increases DNA Integrity and Developmental Potential of Sheep Oocytes**

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*Producción Animal*

To date, the underlying mechanisms by which cAMP modulators act during in vitro maturation to improve oocyte developmental competence are poorly understood. Here, we sought to fill this knowledge gap by evaluating the use of phosphodiesterase inhibitor 3-isobutyl-1-methylxanthine (IBMX) and adenylyl cyclase activator forskolin during a culture period of 2 h before in vitro maturation (pre-IVM) on the nuclear and cytoplasmic maturation features in essential organelles, cumulus cells activity, and in vitro developmental potential of sheep oocytes. Results showed that pre-IVM treatment significantly improved ( $p < 0.05$ ) the DNA integrity of mature oocytes and increased blastocyst rates compared to the control. Considering that oocytes are highly vulnerable to the accumulation of DNA damage because of exposure to in vitro culture conditions, our results suggest that the modulation of intra-oocyte cAMP levels with forskolin and IBMX before IVM might give oocytes a more effective DNA repair mechanism to overcome damage obstacles and ultimately improve developmental competence. This previously unappreciated action of cAMP modulators could help develop improved methods for assisted reproduction technologies in animal and clinical research.

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F-28

**Biomass and Lipid Production by the Native Green Microalgae *Chlorella sorokiniana***

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*Chemical engineering- Biotechnology*

Biodiesel produced from microalgal lipids is a promising alternative energy source. Production of biomass and lipids by microalgae depend on several factors such as nutrients supply, light intensity, and CO<sub>2</sub>. Freshwater microalgae *Chlorella* sp. is widely used in biotechnology because of their high lipid content and wide spectrum of applications, that includes microalgae Microbial Fuel Cells (MFC). Genome-Scale Metabolic models (GEM) allows for a quantitative view of the transport and metabolism of compounds within a particular microorganism and association Gene-Protein-Reaction. *Chlorella sorokiniana* was isolated from a freshwater lake using Chu13 medium on agar plates. The microalgae were identified using molecular analysis of the Ribosomal Internal Transcribed Spacer (ITS). Response surface methodology (RSM) with a 3<sup>2</sup> factorial design (light intensity of 1000, 3000, and 5000 lux and CO<sub>2</sub> concentrations of 0.03, 10, and 20%) was used to model the biomass concentration, lipid content, and specific growth rates, in glass tubular 200mL photobioreactors (PBR). A genome-scale metabolic model for *Chlorella sorokiniana* was constructed based on the KEGG database and Rapid Annotation of Photosynthetic Systems (RAPS) methodology, subsequently Flux Balance Analysis (FBA) study on the lipid and biomass production of the microalgae was carried out. Microalgae can efficiently modify their metabolism in response to changes in environmental conditions. Under optimal growth conditions, large amounts of biomass were produced but with relatively low lipid contents. In contrast, under stress conditions, microalgae altered their biosynthetic pathways towards lipid production and accumulation. Optimal conditions to maximize lipid content and biomass concentration were obtained using the desirability function as 20% CO<sub>2</sub> and 2300 lux, with a theoretical biomass concentration of 2g / L and 31% of lipids. Validation tests of these conditions achieved a biomass concentration of 1.66 ± 0.09 g/L and lipid content of 32.8 ± 5.9%. A Metabolic mode with 1246 annotated genes of *C. sorokiniana* was developed FBA reveals that light intensity above 1000luxes limits biomass production, and the model adjusted reasonably to experimental data.

F-29

**Improving the biodegradability of hospital urines by electrochemical advanced oxidation processes**

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*Chemical Engineering*

The presence of antibiotics in aquatic environments, related to its high consumption and the inefficiency of conventional biological processes to remove this type of compounds, is one of the main subjects of environmental concerns nowadays [1]. In this context, hospital urine effluents represent one of the main sources of pollution contamination in the environment and its proper management is seen as critical to solving this serious environmental problem. In the last years, Electrochemical Advanced Oxidation processes (EAOPs) are an interesting alternative to conventional technologies. This technology is mainly based on the production of powerful oxidants to contribute to the degradation of pollutants.

Within this background, this work proposes the design of an electrochemical reactor to improve the biodegradability, reduce toxicity and remove the antibiotic activity of these effluents. For the development of the reactor, the type of electrode, type of cell and flow and operation conditions were considered.

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### Acknowledgements

This work has been supported by the Spanish Ministry of Science and Innovation, Junta de Comunidades de Castilla-La Mancha (JCCM) and European Union (European Regional Development Fund) through the projects PID2019-110904RB-I00 and SBPLY/17/180501/000396.

F-30

## GRAPHENE-BASED SULFONATE HYDROGELS: SOFT SCAFFOLDS FOR CELL CULTURE

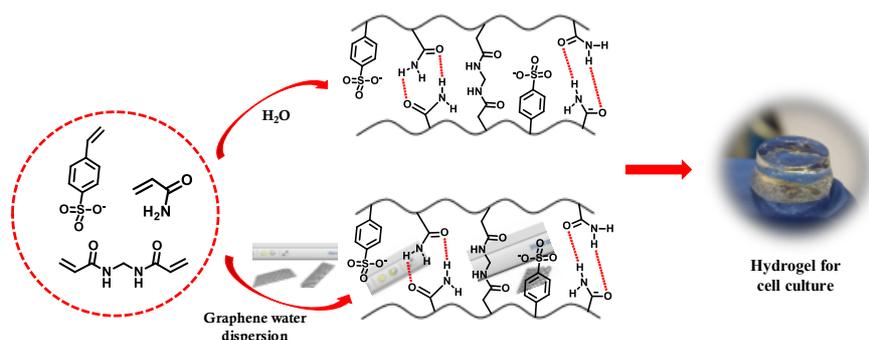
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*Química Orgánica*

The concept of tissue engineering has been widely studied. It involves from the field of biomaterials to scaffolds for cell culture. The final goal is to design materials which will be able to mimic human organs or tissues that can replace or repair damaged or diseased tissues with scaffolds made through the combination of natural and synthetic components.<sup>1</sup> In that sense, hydrogels have recently attracted much attention in the field of tissue engineering, having numerous applications, especially as scaffolds for cell cultures.<sup>2</sup> We have shown that the introduction of graphene in the hydrogel structure improves their biocompatibility supporting the growth of cultured brain cells and allowing neuronal adhesion.<sup>3</sup>

In this work, novel graphene hybrid hydrogels based on sodium 4-vinylbenzenesulfonate (VBS) have been prepared in order to study their capacity to support living neurons.



**Figure 1.** VBS based hydrogels in the presence and absence of graphene.

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**F-31**

**Resveratrol as a possible modulator of adenosinergic system in HeLa and SH-SY5Y cells**

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*Biochemistry and Molecular Biology*

Resveratrol (3,4',5-trihydroxystilbene - RSV) is a polyphenolic phytoalexin found in grapes, berries, peanuts and also red wine. This natural compound exerts a beneficial role in the prevention and progression of many diseases, such as cancer. However, its molecular mechanisms are still unclear. Adenosinergic system, including adenosine receptors (A<sub>1</sub>, A<sub>2A</sub>, A<sub>2B</sub> and A<sub>3</sub>) and ectonucleotidases (5'-Nucleotidase), has emerged as a promising target in cancer due to its involvement in various stages of tumorigenesis, such as proliferation, angiogenesis and metastasis. We have previously described that RSV acts as an agonist of adenosine receptors [1]. Therefore, the aim of the present work was to study the antitumoral effect of RSV and the possible mechanism involving adenosinergic system in two different human cell lines: HeLa epithelioma cervix cells and SH-SY5Y neuroblastoma cells. To this end, cell viability by XTT method, adenosine receptors quantification by Western-blotting, gene expression by real time PCR and 5'-Nucleotidase activities were assayed. Results herein showed a significant decrease on HeLa and SH-SY5Y cell viability in a concentration-dependent manner after treatment with RSV. Accordingly, there was a reduction in the number of treated cells. In addition, this polyphenol caused an increase in A<sub>1</sub> and A<sub>2A</sub> gene expression in HeLa cells, whereas there were no changes in SH-SY5Y cells. Regarding the quantification of adenosine receptors, A<sub>2B</sub> protein levels were significantly decreased after RSV exposure in HeLa cells, whereas protein levels in SH-SY5Y cells remained unaltered. Furthermore, it was observed that RSV significantly reduced 5'-Nucleotidase activity in plasma membrane in both cell lines. Moreover, this polyphenol increased 5'-Nucleotidase activity in the cytosolic fraction in SH-SY5Y cells. These findings suggest that antitumoral effects of RSV might be explained by the activation and modulation of the adenosinergic system.

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**F-32**

**Mango by-products extracts as a promising therapy for glioblastoma T98 and A172 cells: communicating science through the viral TikTok platform.**

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*Tecnología de Alimentos*

Mango (*Mangifera indica*) is the world most harvested tropical fruit whose processing activities generates unavoidable amounts of by-products which are rich in valuable compounds (1). Mango by-products have demonstrated to be a valuable source of bioactive compounds with antiproliferative activities against several cancer cell lines (2). Mango peel, kernel and pulp extracts have been tested on in vitro glioblastoma cancer cells to elucidate whether any of them have the potential to become a new drug for glioblastoma cancer therapies. The mango kernel extract performed the best results, so complementary flow cytometry and immunofluorescence assays were also conducted for a better understanding of the action mechanisms of the mango kernel extract.

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**F-33**

**Impact of reducing alcohol techniques in the aromatic chemical profile of rosé  
Tempranillo wines**

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*Tecnología de Alimentos*

In the last decades, the oenological industry has developed different techniques to reduce alcohol concentration in wines due to the increasing consumers' demand of wines with low or non-existing alcohol content mainly due to the negative effects that alcohol has in human health. Based on this, the principal aim of this study was to investigate the effect of partial and total dealcoholisation in the chemical aromatic profile of rosé wines from Cencibel grape variety. Wines were elaborated following the traditional red-wine winemaking process, and they were divided in three sets: one control, and two destined to the elaboration of low alcohol and dealcoholized wine. For dealcoholized wine, it was used a spinning cone column technique (SCC). Traditional analysis were done following the OIV method proposed in 2014 <sup>[1]</sup>. Volatile components were analysed by GC-MS with a previous isolation by solid phase extraction (SPE) <sup>[2]</sup> Volatile compounds were grouped in aromatic series and the total intensity of each aromatic series was calculated by the summatory of the OAVs of the compounds assigned to each series. The results of this study show how the total concentration of volatile compounds is affected by the partial or total alcohol reduction. Esters and alcohols have been the most affected fermentation components, and C<sub>6</sub> compounds have been the most affected varietal components, followed by benzenic compounds. The principal aromatic series that describe wine aroma have been fruity, fatty, and sweet. The application of the dealcoholisation technique modifies quantitatively but not qualitatively the intensity of aromatic series. These wines mean an alternative to the traditional wine-making process that can satisfy consumers' demand and can compete in national and international markets with dealcoholized and low alcohol products.

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**F-34**

**Degradation study of Ochratoxin A by laccases obtained from *Botrytis cinerea***

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*Tecnología de Alimentos*

Laccases are multicopper proteins involved in oxygen transport and electron transfer in redox processes, oxidizing a wide variety of substrates. This means that its use in the food industry allows the oxidation of organic polluting compounds, such as ochratoxin A. Some substrates on which the laccases act are not capable of directing the redox reaction by themselves, so the addition of certain low molecular weight molecules called mediators would be required.

The objective of this work was to study the degradation capacity of ochratoxin A, a contaminant present in a wide variety of food and drinks such as wine, by the laccase extracted from *Botrytis cinerea* [1,2]. For this, different conditions of ethanol, SO<sub>2</sub> and mediators (e.g. catechin, ferulic acid or caftaric acid) were tested [3], and the quantification of this mycotoxin was carried out in a HPLC-QTOF-MS system.

The results obtained indicate that redox mediators exert an essential action in the oxidation process of Ochratoxin A, resulting in different percentages of residual mycotoxin according to the mediator used. In addition, the different oenological conditions evaluated had a significant effect on the activity of the laccase and, therefore, on the degradation of this undesirable substance.

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F-35

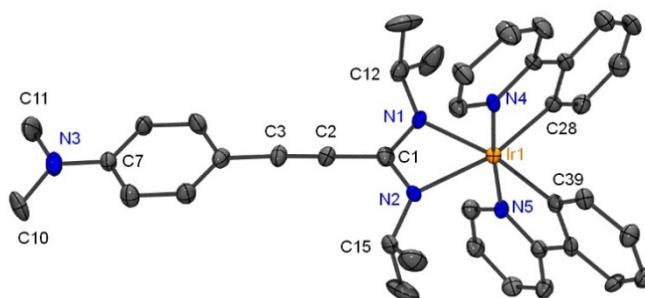
**Boron a Iridium-derived luminescent compounds with amidine ligands**

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*Química Inorgánica*

The Chemistry of luminescent molecular compounds has become one of the growing-interest fields in chemical synthesis, since they can be used in the preparation of luminescent devices or biological probes [1, 2]. Propiolamidines are organic compounds whose chemical formula is  $R^1N=C(C\equiv CR^2)(NHR^3)$  and include a conjugated triple bond C-C with the amidine system. This group of compounds can be obtained in a very efficient way, just by addition of terminal alkynes to carbodiimides, using  $ZnEt_2$  as pre-catalyst [3], which allows to obtain potential ligands with different electronic and steric properties. In this communication, the synthesis of new luminescent boron and iridium-derived compounds with formula  $[BPh_2\{\kappa^2-N,N-ArC\equiv CC(N^iPr)_2\}]$  and  $[Ir\{\kappa^2-C,N-(C_6H_4-py)\}_2\{\kappa^2-N,N-ArC\equiv CC(N^iPr)_2\}]$  is described by using this type of ligands.



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F-36

### Hydrogels in soft robotics

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#### Química Orgánica

Nowadays, is beyond doubt that robotics plays an important role in our society, and they will be an important part of our future. However, at this moment most of them are only used in industry because they are made of hard materials such as metals, which can cause problems when treating with living beings.<sup>1</sup> In order to expand the application of robotics to animals and humans, is necessary to prepare a soft robot able to adapt himself in order to avoid damages to the organism. Hydrogels are a promising material, as their mechanical properties can be turned on demand and they can be responsive to certain stimulus such us pH, light or electricity.<sup>2</sup>

Here we present an electrically responsive hydrogel actuator, able to emulate the finger movement (Fig. 1).<sup>3</sup> Also, we propose the use of malachite green carbinol base as a photoswitch,<sup>4</sup> in order to produce an hydrogel responsive to light. This could be useful to simplify the components of the robot.

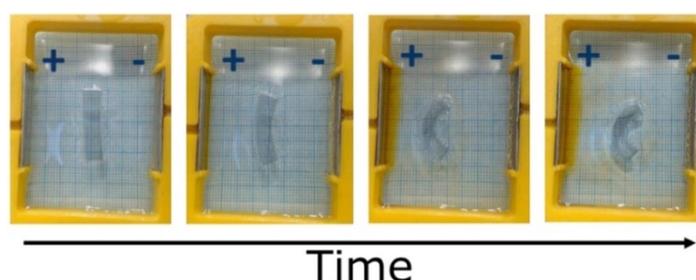


Figura 2: Hydrogel movement

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**F-37**

**Treatment of bioaerosol with electrochemically generated oxidants**

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*Ingeniería Química*

Person-to-person transmission of airborne pathogens, such as tuberculosis, smallpox, or SARS, can have serious economic and social impacts. For this reason, the study and treatment of bioaerosols is important [1]. To do this, radiation, physical capture or chemical disinfection technologies have been used as control measures [2]. In this work, electrochemical technologies are evaluated as alternative to conventional treatment.

In a first stage, it is carried out the development of electrochemical cells capable to operate at high pressures (up to 10 bars) to produce powerful oxidants such as ozone, hydrogen peroxide or chlorine dioxide. Then, in a second stage, the electrogenerated oxidants are used to decrease the riskiness of bioaerosol polluted with *E. Coli* in both gaseous phase and in liquid phase. In the first scenario, the treatment system must be optimized to maximize the contact among small droplets containing pathogens and gaseous oxidants (ozone and chloride dioxide) electrogenerated in an electrochemical cell. In the second case, bioaerosols are collected in liquid-phase and then the polluted solution is electrolyzed in an electrochemical cell equipped with an electrode of metal mixed oxide as anode and a mesh titanium covered with CB-PTFE as cathode to maximize the electrogeneration of hydrogen peroxide from oxygen reduction. In both cases, UV light may be also coupled to check the synergistic effect among technologies.

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**Acknowledgements**

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**F-38**

**Resveratrol adsorption at graphene quantum dots surface: a promoting strategy to increase its photochemical stability in food products**

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*Analytical Chemistry*

Resveratrol is a natural polyphenolic compound, specifically a stilbenoid, which displays beneficial properties such as cardioprotective, neuroprotective, antioxidant and anti-inflammatory activities [1]. Food sources of resveratrol include the skin of grapes, blueberries, raspberries, and blackberries. However, such health benefits are mainly associated with the *trans*-isomer. Despite the positive effects attributed to *trans*-resveratrol, there are several factors that limit its effectiveness, including chemical instability [2]. *Trans*-resveratrol is rapidly transformed into *cis*-resveratrol, less biologically active isomer, when exposed to light. For this reason and to overcome this limitation, it would be advisable to protect *trans*-isoform from light to prevent or delay the quick isomerization as far as possible. This work includes a new role provided by a carbon nanomaterial synthesized from uric acid as the only precursor. The application consists of the adsorption of resveratrol on graphene quantum dots in such a way that it confers photostability to the polyphenol, producing a partial inhibition in the conversion of *trans*- into *cis*-resveratrol when irradiated with UV light. This effect was monitored by an electrophoretic method using corrected peak areas as analytical signal. Toxicity studies revealed a non-toxic effect on model microorganisms by the nanomaterial, even at high concentrations. In addition, its adsorption on the carbonaceous material causes an increase in the antioxidant capacity of the bioactive, which adds to its healthy properties. This effect was tested in several beverages and food supplements rich in resveratrol, producing a slowdown of isomerization of up to 10 times in some of them. Finally, the content of *trans*-resveratrol present in the selected food samples was quantified, obtaining concordant results by two calibration methods as well as very similar to those declared on the product labels.

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F-39

## PUSH-PULL QUINAZOLINES CHROMOPHORES: SYNTHESIS, PHOTOPHYSICAL PROPERTIES, AND USE FOR WHITE LIGHT EMISSION.

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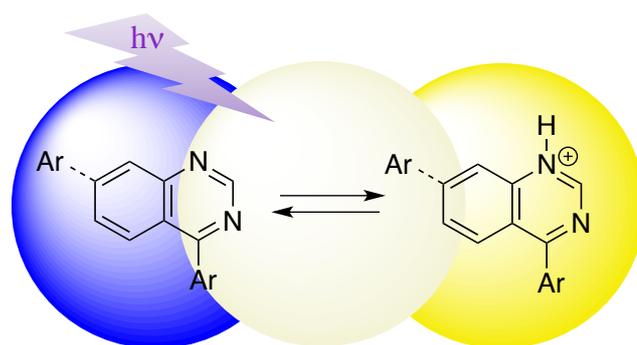
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Organic Chemistry

There is great interest in the design of conjugated push-pull molecules that incorporate nitrogen heterocycles because of their intense luminescence properties.<sup>1</sup> In this context, p-deficient nitrogen heterocycles act as moderate-to-strong electron-withdrawing groups. Engaging the electron lone pair of the nitrogen atoms provides a way to increase the electron-withdrawing character of the heterocycle, which induces substantial changes in the photophysical properties of the chromophore. Thus, these molecules have demonstrated to be highly sensitive to changes in polarity, pH, and the presence of metal cations. Although sensitivity to acids has been used primarily for sensing applications, a more recent application concerns white light emission.<sup>2</sup>

In this flash communication, we will describe a new series of push-pull 4-substituted and 4,7-disubstituted quinazolines that show multicolor photoluminescence, including white light, both in solution and in thin film by the controlled protonation of the initially blue emitting materials. This methodology has potential applications in the fabrication of white OLEDs based on only one material.<sup>3</sup>



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<sup>2</sup> Achelle, S.; Rodríguez-López, J.; Bureš, F.; Robin-le Guen, F. *Chem. Rec.* **2020**, *20*, 440-451.

<sup>3</sup> Plaza-Pedroche, R.; Georgiou, D.; Fakis, M.; Fihey, A.; Katan, C.; Robin-le Guen, F.; Achelle, S.; Rodríguez-López, J. *Dyes Pigm.* **2021**, *185*, 108948.

**F-40**

**Development of baits for oral administration of vaccines and other drugs in  
wild boar**

D. Relimpio

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The Eurasian wild boar (*Sus scrofa*) is a natural reservoir of shared pathogens. Innovative disease control tools will alleviate the consequences of diseases such as swine fever. Oral vaccination has the potential to control infections in wild reservoirs and to prevent outbreaks in other species. For an oral vaccination strategy to be effective, bait characteristics and bait deployment strategies need to be suitable for containing the vaccine, stable under a range of environmental conditions, species-specific, and able to achieve optimal uptake rates [1]. Our starting point is the IREC bait developed by Ballesteros et al. [2], with paraffine and sugar as key components. The matrix of the new baits consists of 41% piglet feed (Piensos Inalsa S.A., Ciudad Real, Spain), 17% corn flour, 15% saccharose and 25% honey. To further improve these baits, different protective layers are being tested to protect baits from environmental humidity but also, to improve their mechanical properties.

Once the final composition of these baits has been fixed, fieldwork is ongoing to observe the preferences of wild boar regarding the influence of different shapes, scents, and colorants in baits, thus finding an effective and specific final formula for this species. These baits are further tested for bacterial viability and physical stability, where their resistance to humidity, temperature and impact is studied. The following step will consist of testing immunogenicity of different forms of antigen presentation (in vials or mixed in the bait matrix). Finally, selected prototypes will be assessed for uptake rates in field experiments.

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**F-41**

**Study and Characterization of Chemical Pigments for Artistic Painting**

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*Química Orgánica*

The objective of this research work is to deepen the knowledge of the materials used in the creation of artistic painting. From a greater knowledge, as always, all the improvement, conservation and restoration actions are born for the future enjoyment of the public. Let us point to pre-e-historical research milestones of painting since that wild pig was painted in a remote valley on an Indonesian island 45,500 years ago. The artist who painted geometric anthropomorphic figures on quartzite rock some 4000 years ago in Peña Escrita or La Batanera, fantasizes about believing that he knew that the material used would reach us. The clay had always been there, unalterable. At the end of the 14th century, Cennino Cennini wrote his treatise, "The Book of Art", perhaps one of the first technical painting manuals. Shortly after, Leonardo, the Renaissance-Man, in the 15th century, invented, created, and of course, investigated artistic techniques and materials. In the 17th century, Newton investigated and deepened the theory of color. At the end of the 18th century, a physicist named J.A.C. Charles applied examination methods to paintings in the Louvre Museum. In November 1895, Röntgen discovered RXs that are immediately applicable to works of art. Since then, there has been a huge amount of research studies, although their generalization through instrumental techniques occurs in the last decades of the 20th century. And of course, in the XXI century<sup>1-3</sup>. Today and here, we want to continue this line, studying pigments and materials, in our case, the paintings of an artist from La Mancha, close to the generation of 27, Gregorio Prieto.

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**F-42**

**Unravelling the interface: farm connectivity provided by spotless starling  
(*Sturnus unicolor*) movements**

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Highly Pathogenic Avian Influenza Viruses (HPAIV) are relevant pathogens for wild and domestic birds. Strict biosecurity is vital for outbreak prevention in domestic poultry and gamebird production. While aquatic birds are considered the reservoir of avian influenza viruses, circumstantial evidence and results from experimental infections suggest that passerine peridomestic birds that frequently enter barns and production facilities could act as bridge species for the introduction of HPAIV. Potential for such transmission has been experimentally demonstrated for the tree sparrow (*Passer montanus*) and Eurasian starling (*Sturnus vulgaris*). The spotless starling, a close relative of the European starling, is a frequent farm bird in Europe which forms large flocks especially in winter.

We captured 27 starlings on a red-legged partridges farm (*Alectoris rufa*), took samples for pathogen detection, and equipped 21 with Pinpoint GPS Argos transmitters. We were able to track the movements of 17 spotless starlings, during 3-5 days in July and November. Though our sample size of tagged birds is small, these individuals belong to a large flock of starlings (i.e. roughly 500 individuals) and thus represent the movements of a much larger number of birds which potentially move together.

None of the starlings tested positive for HPAIV by RtPCR on cloacal and oral swabs or had Salmonella, also none had antibodies against AIV. One individual was positive against West Nile (WNV), or cross-reacting Flaviviruses and one carried a multiresistant strain of *Escherichia coli*. Satellite transmitter data revealed mostly local movements of the starlings, connecting different types of farms with crops, several small waterbodies or streams and a village. Specifically, movements included visits to most different livestock farms in the region, such as pig, poultry, sheep farms as well as a horse stable. This suggests that the starlings could act as vectors for enteropathogens or AIV.

F-43

**RATIONAL DESIGN OF NAPHTHALENIMIDE AND PERYLENIMIDE DERIVATES WITH APPLICATION IN ORGANIC FIELD-EFFECT TRANSISTORS (OFETS)**

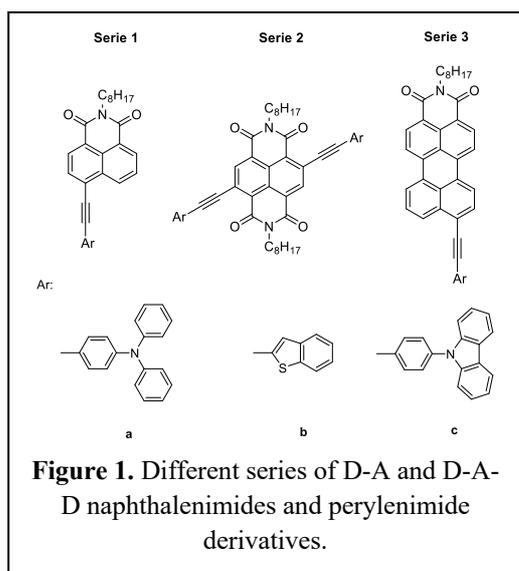
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*Organic Chemistry*

In the last decades, organic molecules have attracted the interest of the research due to their enormous potential in electronic devices like organic field-effect transistors (OFETs). In this way, an interesting strategy is to build donor-acceptor (D-A) architectures, making easier intramolecular charge transfer (ICT), necessary for this kind of devices. In this sense, naphthalenimide and perylenimide derivatives are very interesting due to their planar

structure, their acceptor character, their self-assembling capacity and the possibility of combining with different donor groups, to obtain D-A or D-A-D systems. Furthermore, Computational Chemistry is a powerful tool in Organic Chemistry because it can predict properties of compounds before synthesizing them avoiding unnecessary synthesis and contributing to more economic and sustainable processes.



Taking into account all these premises, in this work, three different series of D-A or D-A-D naphthalenimide and perylenimide derivatives (Figure 1) with different alkynyl donor groups

have been studied theoretically in order to predict the best derivatives for their application in OFETs. The most promising candidates have been synthesized and tested as organic semiconductors in OFETs, corroborating the previous results by theoretical calculations.

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**F-44**

**Perovskites as catalytic precursors in ammonia decomposition**

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*Chemical Engineering*

The main energy sources that the current society uses are based on fossil fuels and the energy demand is growing incessantly. All this, together with the inevitable depletion of these energy sources, means that current society is facing a huge challenge. In this scenario, the concept of Sustainable Development has emerged, which pursues, in the energy sector, the decarbonization of the energy supply <sup>1</sup>. The use of hydrogen as an energy vector is a fascinating solution to that problem because it can store and deliver energy in a usable form. However, the H<sub>2</sub> economy need to establish a safe, reliable, and economically viable transportation and storage system. In this framework, a possible solution would be the use of green ammonia as a H<sub>2</sub> carrier, which could be transformed into H<sub>2</sub> in-situ through suitable conversion processes. Green NH<sub>3</sub> is a carbon free H<sub>2</sub> vector, with large infrastructures, safe, easy to transport and store. However, ammonia decomposition reaction occurs at high temperatures, and the application of NH<sub>3</sub> as a H<sub>2</sub> vector requires acceptable conversion temperatures <sup>2</sup>.

Therefore, the present work aims to develop new catalysts with a high catalytic activity that allow ammonia to be decomposed into hydrogen at low temperatures and at a reasonable cost. In this work, LaNiO<sub>3</sub> and LaCoO<sub>3</sub> perovskites synthesized by the self-combustion method were used as catalytic precursors in the ammonia decomposition reaction. As-prepared nickel and cobalt perovskites-derived catalysts resulted in excellent H<sub>2</sub> production associated with an ammonia conversion close to 100 % at 450°C and provided good performance stability after one day of reaction.

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**F-45**

**Synthesis and analytical characterization of quercetin nanoemulsions**

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*Analytical Chemistry*

Nanotechnology is a new subject of interest in the field of food industry. Particularly, nanoemulsions are suitable for commercial applications with the aim to increase the bioavailability of hydrophobic bioactives such as quercetin, whose poor water solubility has limited its applications as nutraceutical in food industry. For this reason, current research reports the development, optimization, and evaluation of Quercetin (Q) loaded nanoemulsions (NEs). The work here developed addresses the synthesis of Q-NEs using the Phase Inversion Temperature method (PIT)[1]. After optimizing all components, the suitable final composition (expressed as mass/mass percentage) for Q-NEs was 10% Miglyol 812 oil, 0.25% quercetin, 0.55% ethanol, 7.5% surfactant mixture (7.4% Tween 80 and 0.1% soy lecithin) and 81.7% aqueous phase (pH = 5.9, MES 10mM). The formulation with optical transparency consistent with a reduced droplet diameter nanoemulsion was characterized in terms of dispersed phase droplet diameter, morphology, polydispersity index, composition, and encapsulation efficiency of Q-NEs, all these obtained by DLS, UV-Vis and Raman spectroscopies, Scanning Electron Microscopy (SEM) and Confocal Laser Scanning Microscopy (CLSM) techniques. By DLS, it was obtained a Q-NEs nanoparticle diameter of  $10.41 \pm 1.08$  nm ( $n=3$ ) with a polydispersity index of  $0.25 \pm 0.01$  ( $n=3$ ). The UV-Vis spectroscopy allowed us to discriminate between free quercetin and Q-NEs based on their displayed absorption bands for free quercetin (256 and 376 nm) and those ones for quercetin loaded nanoemulsion (229 and 376 nm) respectively. Encapsulation efficiency for the synthesized Q-NEs was also determined by UV-Vis spectroscopy with very good results, 99.6%. On the other hand, Raman spectra of Q-NEs showed a typical band at  $1628\text{ cm}^{-1}$  whereas when it was unencapsulated, only a wider band appears at  $1616\text{ cm}^{-1}$ . Finally, both SEM and CLSM techniques reported pseudospherical shapes droplets.

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**F-46**

**Transfer of *Escherichia coli*, *Staphylococcus aureus* and *Campylobacter* spp. by cross contamination in a kitchen**

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*Ciencia y Tecnología de los Alimentos*

One of the major risks in the food industry is cross-contamination, which consists of the transfer of microorganisms from food to other foodstuff or utensils that are in contact with them or vice versa.

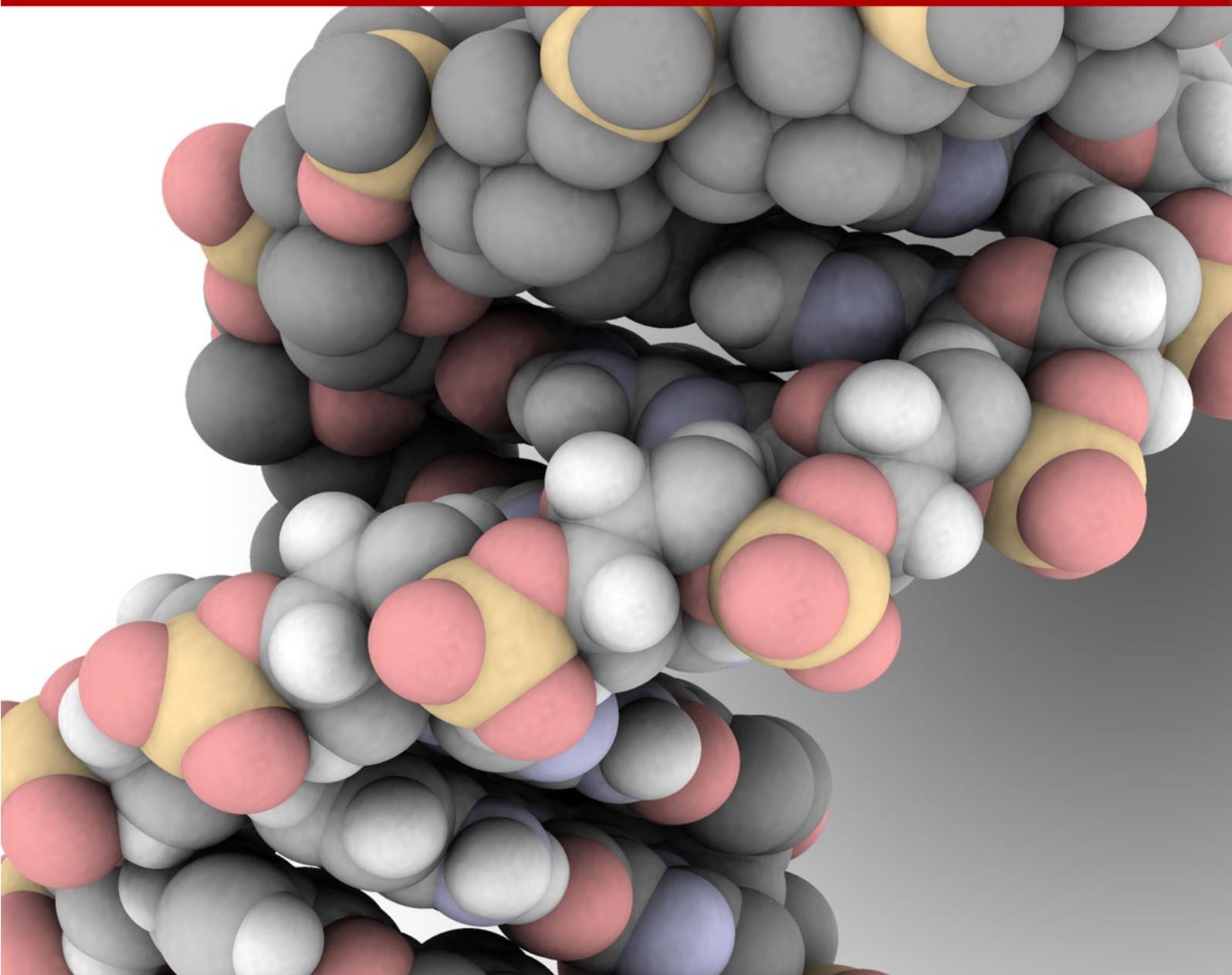
In this flash presentation is shown the procedure carried out to analyse the possible cross-contamination that could happen during turkey meat preparation in the kitchen. For this purpose, the utensils used to slice the meat (board and knife) are sampled to determine the presence of quality indicator microorganisms such as (*Escherichia coli*) and emerging pathogens such as (*Staphylococcus aureus* and *Campylobacter* spp.).

The results obtained concluded that these microorganisms are transferred from meat to the utensils which confirmed the possibility of consumption of these bacteria due to cross contamination. In the table there is a higher prevalence than in the knife.



This can cause serious diseases for the consumer, campylobacteriosis. To reduce this risk is important to establish and follow some hygienic measures not only in the food industry but also at home.

# CÓMO FUE LA EDICIÓN DEL AÑO PASADO...



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## PRESENTACIÓN

Después de una larga pausa debido al confinamiento y el verano volvemos con el número de septiembre. Hemos recogido las actividades de todo este periodo, incluyendo las Tesis doctorales, algunas de ellas defendidas on-line; diversos reconocimientos personales y colectivos, artículos y reseñas de libros que pueden interesaros y un resumen de Ciencia Joven 2020 que se celebró on-line.

Esperamos poder seguir publicando mensualmente la revista aunque suponemos que con menos actividades que habitualmente.

El comité editorial.

## Efectos de la leptina central y la restricción calórica en la reprogramación metabólica del tejido adiposo

**Doctoranda:** Lorena Mazuecos

**Directores:** Dr. Antonio Andrés y Dra. Nilda Gallardo

**Área de Bioquímica**

El tejido adiposo es un órgano dinámico que actúa como sensor nutricional de la energía almacenada. La flexibilidad de los adipocitos para indicar exceso o demanda de energía tiene su origen en un coordinado control transcripcional, indicativo de adaptaciones metabólicas y fisiológicas de un organismo. La hormona leptina, secretada por el tejido adiposo, es de las señales más importantes capaz de actuar a nivel central e indicar un estado de exceso de energía. Por ello, las alteraciones metabólicas son generalmente acompañadas de daños en su señalización debido a un fenómeno conocido como resistencia a leptina. Sin embargo, los mecanismos moleculares que conducen al desarrollo de estos estados patológicos no se encuentran definidos de forma precisa.

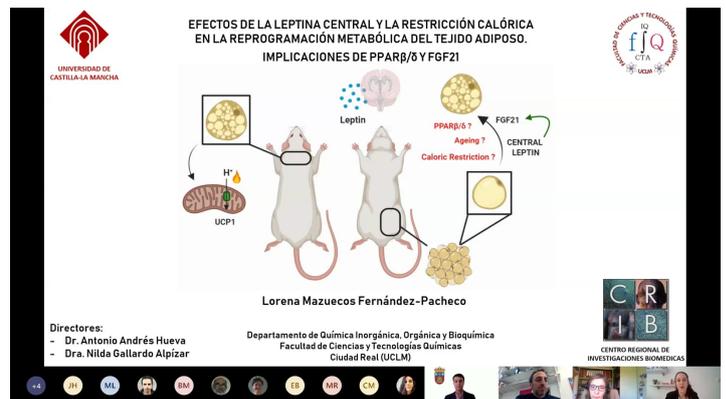
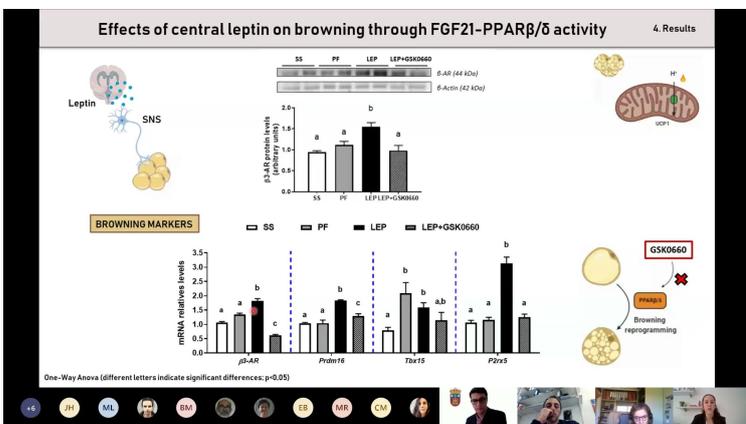
En este trabajo, hemos estudiado posibles efectos derivados de la leptina central en la reprogramación metabólica del tejido adiposo visceral, dependientes de la actividad del receptor PPAR $\beta/\delta$ , factor de transcripción perteneciente a la familia de receptores nucleares activados por proliferadores de peroxisomas (PPAR) implicado en la homeostasis lipídica y glucídica. El estudio fue llevado a cabo en ratas Wistar de 3 meses. El tratamiento central de leptina (0,2  $\mu\text{g}/\text{día}$ , 7 días) fue administrado mediante cirugía intracerebroventricular (ICV) y mini-bombas osmóticas implantadas en el espacio interescapular. La inhibición del receptor PPAR $\beta/\delta$  "in vivo" fue realizada a través de la administración farmacológica intraperitoneal del antagonista selectivo GSK0660.

Por otra parte, hemos estudiado los efectos en esta reprogramación metabólica en tejido adiposo e hígado de otros factores como son la restricción calórica moderada y el envejecimiento en animales de 7 y 24 meses de edad. Además, hemos analizado la situación de ayuno y la respuesta postprandial a una sobrecarga aguda de lípidos (1 ml/kg) para evaluar la eficacia y capacidad de activación transcripcional de un protocolo de restricción en estos dos órganos con altas demandas metabólicas.

Los resultados obtenidos muestran como la actividad metabólica del receptor PPAR $\beta/\delta$  es requerida en los efectos anorexigénicos a nivel central de leptina, y en sus acciones lipolíticas ejercidas sobre el tejido adiposo a través del sistema nervioso. Además, la inhibición de la actividad de este receptor promueve la acumulación lipídica, el incremento de la adiposidad e inhibe parcialmente el proceso de browning en el tejido adiposo blanco, afectando al estado oxidativo y funcional de los adipocitos. Un tratamiento de leptina a nivel central durante 7 días disminuye los valores circulantes del factor de crecimiento 21 (FGF21), al mismo tiempo que incrementa notablemente su expresión endógena en los adipocitos blancos, concurriendo con el incremento en marcadores termogénicos, también relacionados con el proceso de la lipólisis. Curiosamente, el tratamiento con el antagonista GSK0660 inhibe la expresión endógena de FGF21 en el tejido adiposo blanco, sugiriendo una interacción regulatoria entre el factor de transcripción PPAR $\beta/\delta$  y la hormona FGF21 no descrita con anterioridad.

Por otra parte, mostramos cómo los valores circulantes de FGF21 aumentan con el envejecimiento, y son potenciados bajo una restricción calórica moderada en animales de edad joven-media (7mFR). Nuestros resultados indican que una restricción calórica a esta edad, es capaz de modificar la actividad transcripcional del hígado y al tejido adiposo, así como los niveles circulantes de FGF21, en respuesta a cambios nutricionales; la cual es parcialmente inhibida en animales de 24 meses. La dislipidemia postprandial aumenta progresivamente con el envejecimiento, correlacionando con un aumento de la actividad transcripcional del factor lipogénico ChREBP, puesta de manifiesto por el aumento en la expresión de genes diana, sugiriendo una activación de este factor sensible a glucosa también con la entrada de lípidos o metabolitos derivados. Curiosamente, una restricción calórica moderada reduce la adiposidad y evita la hipertrigliceridemia postprandial en ratas Wistar de 7 y 24 meses, estrechando la asociación entre los niveles de triglicéridos y la adiposidad tras la ingesta. En consecuencia, el grado de adiposidad podría correlacionar con el transporte de triglicéridos y el metabolismo de las lipoproteínas plasmáticas.

Los resultados obtenidos en este estudio ayudan a descifrar las bases moleculares de patologías metabólicas asociadas a la obesidad, contribuyendo a definir los estados de resistencia a leptina, a insulina y el emergente concepto de resistencia a FGF21. Con los datos observados, sugerimos que la leptina central promueve la señalización autocrina/paracrina de FGF21 en el tejido adiposo, y que la actividad del factor de transcripción PPAR $\beta/\delta$  es esencial en la funcionalidad y fisiología de los adipocitos. Además, nuestros datos apuntan a un importante papel de la restricción calórica en el estado energético postprandial y la resistencia a insulina con el envejecimiento, en la que el tejido adiposo blanco podría incrementar su capacidad termogénica en respuesta a una sobrecarga aguda de grasa, potenciada en animales de 24 meses sometidos a una reducción en la ingesta.



## Benzothiadiazole and thiophene derivatives in Organic Photonics and Photocatalysis. Computational study of carbon nanomaterials



**Doctorando: Raúl Martín Lozano**

**Directores: Dra. Pilar Prieto Núñez-Polo y Dr. José Ramón Carrillo Muñoz**

**Área de Química Orgánica**

El pasado 10 de Septiembre tuvo lugar en el campus de Ciudad Real la defensa de la Tesis Doctoral de Raúl Martín Lozano, estudiante del programa de Doctorado en Química, titulada "Benzothiadiazole and thiophene derivatives in Organic Photonics and Photocatalysis. Computational study of carbon nanomaterials". La tesis, supervisada por la Dra. Pilar Prieto Núñez-Polo y el Dr. José Ramón Carrillo Muñoz, obtuvo mención internacional y calificación de sobresaliente Cum Laude por parte del tribunal compuesto por la Dra. Mari Carmen Ruiz (Universidad de Málaga), el Dr. David Curiel (Universidad de Murcia), y la Dra. Ana Belén Muñoz (Universidad Federico II de Nápoles).

Este trabajo de investigación se ha dividido en dos partes claramente diferenciadas.

En la primera parte, se ha llevado a cabo la síntesis de derivados de 1,3,4-tiadiazol, benzo[c][1,2,5]tiadiazol y 2,2'-bitiofeno, estudiando sus propiedades como nuevos materiales orgánicos en campos como el de las guías de onda óptica, los láseres o los fotocatalizadores, es decir, procesos donde la interacción luz-materia juega un papel muy importante. Además, la síntesis de estos derivados ha podido enmarcarse como medioambientalmente benigna ya que en ella se han empleado catalizadores reutilizables de paladio, se ha minimizado el empleo de disolventes y se ha utilizado la irradiación microondas como fuente de energía.

Cabe destacar el papel fundamental de la Química Computacional para poder justificar muchos de los resultados experimentales observados, pudiendo establecer interesantes relaciones estructura-propiedad necesarias para el diseño de futuros materiales. Además, el carácter predictivo de esta disciplina ha permitido diseñar a priori algunos de los productos finales, seleccionando aquellos que mejores propiedades presentaban y evitando síntesis innecesarias.



En la segunda parte, se han llevado a cabo distintos estudios computacionales basados en nanoestructuras de carbono, incluyendo grafeno, quantum dots y nanocuernos. Estos estudios se centran en la adsorción no covalente de moléculas orgánicas sobre estas nanoestructuras y en su relación estructura-propiedad, ayudando a entender aún más sus propiedades y justificando algunos resultados experimentales.

Cabe destacar que durante el transcurso de esta Tesis se ha realizado una breve estancia nacional a la Universidad de Zaragoza bajo la dirección del Dr. Jesús Orduna (Julio 2015) y una estancia internacional a la Universidad Federico II de Nápoles, bajo la dirección del Dr. Michele Pavone (Abril-Junio 2016).

Como fruto de esta Tesis Doctoral se han publicado, hasta la fecha, 7 artículos en distintas revistas de interés científico. Además, el trabajo realizado ha sido presentado distintos congresos de índole nacional e internacional, consiguiendo en uno de ellos el accésit a la mejor contribución y trayectoria científica.

## Biotechnological and Proteomic Characterisation of Yeast from Natural Environments

**Doctoranda:** Beatriz García-Béjar Bermejo

**Directoras:** Dras. María Arévalo Villena y Ana Briones Pérez

**Área de Tecnología de alimentos**

El pasado 26 de marzo se defendió la tesis titulada “Biotechnological and Proteomic Characterisation of Yeast from Natural Environments” de manera online debido al confinamiento producido por la actual pandemia. Esta ha sido dirigida y supervisada por la Dr. María Arévalo Villena y la Dr. Ana Briones Pérez.

La presente tesis doctoral se centró en el estudio de la biodiversidad de levaduras de la provincia de Ciudad Real y su aplicación en nuevos aspectos biotecnológicos aplicados a la descontaminación del medio ambiente o la industria de los alimentos.

Por todo ello, se seleccionaron 20 puntos de muestreo diferentes agrupados en 4 grupos: Flores, animales, productos alimentarios y muestras ambientales. Se obtuvieron un total de 702 aislados los cuales se clasificaron por especies y cepas gracias a técnicas moleculares. La PCR-RFLP y la posterior secuenciación de la región D1/D2 permitieron identificar 35 especies diferentes y, gracias a la PCR-RAPD, se determinaron un total de 329 cepas. La especie mayoritaria aislada fue *Diutina rugosa* y la que estaba presente en mayor número de muestras fue *Rhodotorula mucilaginosa*. El estudio de los parámetros de biodiversidad realizados indicó que los ambientes con más riqueza de especies eran el agua procedente de una poza seguido del ambiente de una quesería. Así mismo la mayor variabilidad genética se observó en las especies que menor número de aislados tuvieron.

Una vez realizada esta clasificación, aquellas cepas procedentes de muestras ambientales, florales y animales se estudiaron para su aplicación como agentes de detoxificación de metales pesados y micotoxinas, mientras que las aisladas de alimentos se utilizaron para buscar nuevos usos en la industria de los alimentos.

Para la prueba de detoxificación, se ajustaron tanto los parámetros de incubación como los de análisis. Para ello, se seleccionaron representantes de toxinas inorgánicas (Zinc) y orgánicas (*Aflatoxina B1*) a las que se expusieron las cepas. Los resultados indicaron que la capacidad de eliminación de la toxina es cepa dependiente y que las cepas no usaban para crecer estos compuestos, es decir, las rutas metabólicas no son el mecanismo de acción utilizado. Además, un 18% y un 16% de las cepas fueron capaces de eliminar >50% del Zn y la AFB1, respectivamente. Cabe destacar a *D. rugosa* y *Rh. mucilaginosa*, las cuales fueron las especies con mejor habilidad para detoxificar el Zn y la AFB1, respectivamente. Estas cepas con la mejor capacidad de biodetoxificación fueron sometidas a dos pruebas complementarias: Biocontrol de mohos micotoxigénicos y tolerancia en medio sólido de Zn.

Con el objetivo de ahondar en el mecanismo que las levaduras usan para eliminar este tipo de contaminantes. Se decidió caracterizar el proteoma de 8 cepas (1 *Saccharomyces cerevisiae* y 7 *no-Saccharomyces*) que habían detoxificado >50% de alguna de las 2 toxinas y habían superado las pruebas complementarias. Primero, las cepas se expusieron a altas concentraciones de ambos contaminantes durante 24 horas. Pasado este tiempo, las proteínas se extrajeron y se determinaron con el espectrómetro de masas Q-Exactive. Los resultados en bruto se analizaron por técnicas bioinformáticas usando los programas MaxQuant, Perseus y Blast2Go.

En el caso del Zn, el análisis indicó que la presencia de este ion metálico provocaba una alteración en el proteoma de las cepas estudiadas, llegando a cambiar hasta el 44% del proteoma de alguna cepa (*Candida tropicalis AK11*). El aumento de proteínas con sitios de unión de iones metálicos y la disminución de transportadores de iones de la membrana y la vacuola revelaron que uno de los posibles métodos de eliminación del Zn es la bioacumulación en el interior de la célula y su asociación a determinados orgánulos. Dicha hipótesis se pudo confirmar mediante un ensayo con el SEM-EDS y un análisis de la presencia de este ion en el citoplasma y la pared celular de dichas cepas.

En cuanto a la AFB1, hubo ausencia de cambio en el proteoma al exponer las células a esta toxina, lo cual indicaba que la eliminación de las micotoxinas puede llevarse a cabo por adsorción a la pared celular. Por ello, se caracterizaron y cuantificaron los componentes de la pared celular, tanto proteínas como polisacáridos. Este rol de la pared se pudo confirmar mediante la utilización del antimicótico caspofungin, que es capaz de dañarla, pudiendo observarse que el efecto tóxico de la AFB1 no perjudica al crecimiento de la cepa con la pared intacta como si lo hace con aquella tratada con *caspofungin*.

Por último, se buscaron nuevos usos para aquellas cepas procedentes de alimentos. Se ha podido conocer que algunas cepas presentan capacidad antioxidante, así como actividad de biocontrol frente a mohos y levaduras alterantes, por lo que podrían ser usados como potenciales protectores de alimentos. Además, se ha estudiado su capacidad probiótica y prebiótica, viendo resultados favorables en el primer screening en el 47% de las cepas y destacando las cepas de las especies *Pichia kudriavzevii* (K41, K49, K51) y *Wickerhamomyces anomalus* (SD25). Por último, se ha comprobado que algunas cepas son idóneas para la producción de volátiles como las de las especies *Debaryomyces hansenii*, *Candida zeylanoides* y *S. cerevisiae*.



## Utilización de CO<sub>2</sub> como fuente de carbono para la síntesis de productos de interés industrial



**Doctoranda:** Felipe de la Cruz Martínez

**Directores:** Dres. Agustín Lara Sánchez y José Antonio Castro Osma

**Área de Química Inorgánica**

El pasado 24 de Septiembre tuvo lugar en el Aula Magna de la Biblioteca General del Campus de Ciudad Real la defensa de la Tesis Doctoral de Felipe de la Cruz Martínez titulada “Utilización de CO<sub>2</sub> como fuente de carbono para la síntesis de productos de interés industrial”. La tesis, supervisada por el Prof. Agustín Lara Sánchez y el Dr. José Antonio Castro Osma, obtuvo la máxima calificación por parte del tribunal constituido por el Prof. Juan Carlos Flores Serrano (Universidad de Alcalá), el Dr. Joaquín García Álvarez (Universidad de Oviedo) y la Dra. Giulia Fiorani (Università Ca’ Foscari Venezia).

Actualmente, existe un interés creciente en la transformación de los residuos generados por la sociedad en productos de elevado valor añadido. Tal es el caso del dióxido de carbono, considerado como una fuente renovable de carbono y cuyo uso se encuentra limitado debido a su baja reactividad. Por ello, resulta de gran importancia el desarrollo de procesos catalíticos sostenibles que involucren el uso de este gas en la obtención de productos de interés industrial.

La primera parte de la Tesis se ha centrado en el diseño de nuevas entidades organometálicas de metales abundantes como hierro y aluminio, y de otros metales como zinc y elementos de las tierras raras. En este sentido, se han sintetizado, caracterizado y estudiado una amplia variedad de complejos para estos metales con ligandos heteroescorpionato derivados del bis(pirazol-1-il)metano coordinados al centro metálico. En la segunda parte de este trabajo, se ha evaluado la actividad catalítica de algunos de estos complejos en procesos de utilización de CO<sub>2</sub> para la síntesis de productos de interés industrial, tales como carbonatos cíclicos, carbamatos, policarbonatos y terpolímeros.

Cabe destacar que durante la Tesis Doctoral se ha realizado una estancia internacional en el “Green Chemistry Centre of Excellence” de la Universidad de York, bajo la dirección del Prof. Michael North. El trabajo durante este periodo se ha centrado en el estudio de la actividad catalítica de la base orgánica triazabicyclodeceno para la preparación de carbamatos por reacción de carbonatos cíclicos procedentes de la biomasa y aminas alifáticas.

Como fruto de esta Tesis Doctoral, se han publicado hasta la fecha 9 artículos científicos y se han presentado 9 comunicaciones a congreso nacional e internacional. Además, se ha logrado el premio Ciencia Joven de la edición 2020.

## La fundación Domingo Martínez concede al Departamento de Ingeniería Química de la Universidad de Castilla La Mancha un proyecto de investigación para la producción de Hidrógeno mediante electrólisis de agua

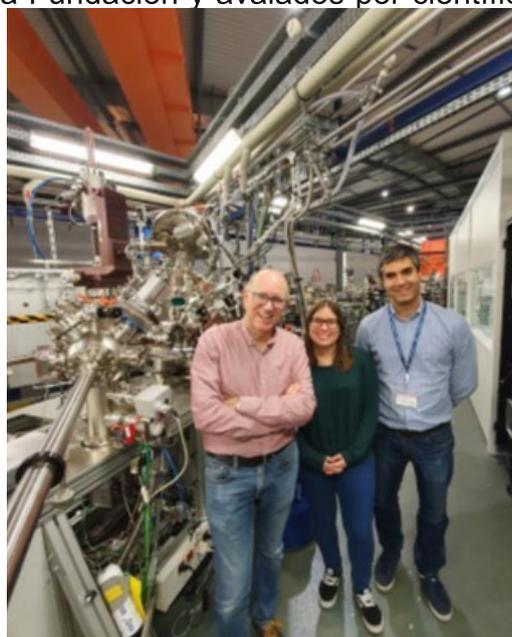
La Fundación Domingo Martínez, ha resuelto recientemente la convocatoria de proyectos de investigación del año 2020, financiando con una cuantía de 50.000 euros/año, el proyecto de investigación titulado: “Desarrollo de electrolizadores más eficientes y competitivos basados en electrodos preparados mediante la técnica de pulverización catódica”. El profesor del Departamento de Ingeniería Química de la Universidad de Castilla La Mancha, Antonio de Lucas Consuegra, coordina el equipo de investigación de este proyecto, formado por investigadores del Departamento de Ingeniería Química de la Universidad de Castilla La Mancha y del Instituto de Ciencia de Materiales de Sevilla del Consejo Superior de Investigaciones Científicas (CSIC).

El objetivo final del proyecto es contribuir a una mayor gestión de las energías renovables, empleando el Hidrógeno como vector energético y la electrólisis de agua como método de producción. De este modo se pretende desarrollar un nuevo tipo de electrolizador, más eficiente, económico y competitivo, para la producción renovable y sostenible de hidrógeno. Para ello, se emplearán membranas comerciales de intercambio aniónico (conductoras de iones  $\text{OH}^-$ ), que permitirán trabajar con ánodos y cátodos basados en metales no nobles de bajo coste económico como son: níquel, óxidos de níquel, óxidos de cobalto, óxidos de cobre, entre otros. Adicionalmente se emplearán técnicas de pulverización catódica (“magnetron sputtering”), para la preparación de estos electrodos en forma de láminas ultradelgadas, lo que permitirá reducir considerablemente el contenido metálico de los mismos.

La Fundación Domingo Martínez (FDM) es una entidad privada benéfico-docente, que fue constituida en 1971. Entre los principales fines de la fundación, esta la promoción y fomento de la investigación científica y técnica en los campos que se relacionan con las aplicaciones de los gases industriales y medicinales, y con las otras áreas correspondientes a las actividades que fueron objeto de la empresa ‘Autógena Martínez, Industrias de la Soldadura S.A., (AMSA). Actualmente la Fundación Domingo Martínez Convoca anualmente ayudas a la investigación proponiendo los temas a investigar, los cuales son fijados por el Comité Técnico de la Fundación y avalados por científicos de reconocido prestigio.



Parte del equipo investigador del proyecto de la UCLM



Parte del equipo investigador del Proyecto (UCLM-CSIC) en las instalaciones del Sincrotrón Alba

## PREMIOS DE LA SECCIÓN TERRITORIAL DE LA RSEQ

La sección territorial castellano-manchega de la Real Sociedad Española de Química ha distinguido hoy al profesor de la Universidad de Castilla-La Mancha (UCLM) Ernesto Martínez Ataz con su Premio a la Trayectoria Científica Química, en reconocimiento a su dilatada carrera investigadora. Durante la entrega del premio, que ha tenido lugar en el Campus de Ciudad Real, se ha distinguido también a varios jóvenes investigadores.

El catedrático de Química Física de la Universidad de Castilla-La Mancha (UCLM) Ernesto Martínez Ataz ha recibido hoy el Premio a la Trayectoria Científica que concede la sección territorial castellano-manchega de la Real Sociedad Española de Química. La entrega ha tenido lugar en el Campus de Ciudad Real durante el transcurso de la II Jornada de Divulgación en Químicas, cuya inauguración ha presidido el rector de la Universidad regional, Miguel Ángel Collado; junto con la presidenta de sección territorial de la RSEQ, la profesora de la UCLM María Antonia Herrero.

El profesor Martínez Ataz se ha mostrado “agradecido” y “halagado” por este premio que llega de manos de “mis compañeros, de quienes me conocen” y que viene a ser un reconocimiento “a los que tuvimos el placer de formar”. Durante el acto, Martínez Ataz ha subrayado la importancia de la investigación en Químicas y de la ciencia en general, como “un modo de ser y enfrentarse al mundo, especialmente en estos momentos, muy necesaria”.

Ernesto Martínez Ataz acumula una dilatada carrera investigadora en la espectroscopia láser, fluorescencia inducida por láser, estudio de la dinámica de estados excitados de moléculas pequeñas y dinámica de reacciones rápidas en fase gaseosa y estudios de química atmosférica. El que también fuera rector de la UCLM entre 2003 y 2011, llegó a la institución académica en 1988, tras realizar su tesis doctoral en el Instituto de Química Física Rocasolano del Consejo Superior de Investigaciones Científicas (CSIC), doctorarse en Ciencias Químicas por la Universidad Complutense de Madrid (1977), y realizar una estancia postdoctoral de dos años en las universidades de Londres (Queen Mary College) y Cambridge (Physical Chemistry Laboratory).

A lo largo de la jornada, la organización que agrupa a los químicos castellano-manchegos también ha premiado a otros dos investigadores de la UCLM, Carlos Romero Nieto, como Joven Investigador Químico; y Antonio Manuel Rodríguez García, como mejor divulgador en química. A estos reconocimientos se suman el Premio al Mejor Trabajo Fin de Máster que ha recaído en Rodrigo Plaza Pedroche; y el Premio a la Mejor Tesis Doctoral para Iván Torres Moya, mientras que el accésit ha sido para Almudena Lorente Diezma.

En la inauguración de las jornadas, el rector de la UCLM ha felicitado a la sección territorial castellano-manchega de la Real Sociedad Española de Química por su “impulso a la investigación” y porque con el acto de hoy “se reconoce a los mejores”, en el caso del profesor Martínez Ataz “su trayectoria académica que tanto valoramos”. Collado ha asegurado que hoy “es un día de alegría para la ciencia y la divulgación”.

**Gabinete Comunicación UCLM. Ciudad Real, 18 de septiembre de 2020**

# PREMIOS



## La OMS publica el trabajo de la investigadora de la UCLM Florentina Villanueva sobre contaminantes en colegios y escuelas infantiles

La Organización Mundial de la Salud (OMS) ha publicado un trabajo de la investigadora de la Universidad de Castilla-La Mancha (UCLM) Florentina Villanueva sobre contaminantes en colegios y guarderías que sistematiza métodos de muestreo y control de distintos compuestos que se han demostrado nocivos para la salud.

En un contexto especialmente sensibilizado como consecuencia de la pandemia por el SARS-CoV-2, la Organización Mundial de la Salud (OMS) acaba de publicar un detallado estudio realizado por la investigadora de la Universidad de Castilla-La Mancha (UCLM) Florentina Villanueva pensado para hacer un seguimiento de los contaminantes presentes en centros escolares y guarderías, evaluar sus efectos adversos y, como consecuencia, prevenirlos.

El informe detalla los procedimientos de muestreo de un total de diecisiete productos químicos y otros cuarenta contaminantes presentes en el aire interior de los colegios y escuelas infantiles. Entre ellos, compuestos orgánicos volátiles que se originan principalmente de fuentes interiores como pinturas, productos de construcción, muebles, colas o barnices; y otros contaminantes propios del aire exterior, como el dióxido de nitrógeno y el ozono, que penetran en los ambientes interiores.

Según la investigadora del Instituto de Investigación en Combustión y Contaminación Atmosférica, la determinación de las concentraciones de contaminantes del aire interior resulta fundamental para evaluar los riesgos para la salud de los niños expuestos, identificar la contribución de fuentes interiores y exteriores (en este caso, las mediciones exteriores también son necesarias), observar las tendencias temporales y espaciales de la calidad del aire interior, evaluar el cumplimiento de las pautas y estándares de calidad del aire interior, y desarrollar y justificar medidas de reducción de riesgos.

Según la investigadora, con esta publicación, la OMS pone en manos de los gobiernos “una herramienta para evaluar la presencia de contaminantes con efectos negativos sobre la salud en espacios tan sensibles como los colegios y las guarderías y realizar las acciones necesarias para reducir su presencia”. Entre los procedimientos más eficaces de prevención, Villanueva apunta una adecuada ventilación de los espacios interiores, una medida que se está generalizando como consecuencia de la pandemia y que, por tanto, tendría beneficios añadidos a los de evitar la propagación del coronavirus.

“La calidad del aire es muy importante –explica Villanueva. Ahora ha aumentado la concienciación social como consecuencia de la COVID, pero la contaminación interior provoca también graves daños en la salud a largo plazo, por lo que resulta imprescindible su seguimiento y control”.

El trabajo de Florentina Villanueva forma parte de un proyecto de la OMS para desarrollar una herramienta que permita evaluar los riesgos del efecto combinado de la exposición a múltiples sustancias químicas.



Gabinete Comunicación UCLM

## ARTÍCULO DEL MES CENTRO DE INVESTIGACIONES CIENTÍFICAS ISLA DE LA CARTUJA

**Un artículo científico de D. Ester López Fernández seleccionado como mejor “Artículo del Mes” de abril de 2020, por el Centro de Investigaciones Científicas Isla de la Cartuja.**

El trabajo científico titulado “Robust label-free  $\text{Cu}_x\text{Co}_y\text{O}_z$  electrochemical sensors for hexose detection” ha sido desarrollado en el laboratorio de Catálisis y Materiales del Departamento de Ingeniería Química de la UCLM en colaboración con el Instituto de Ciencia de Materiales de Sevilla (CSIC-US). Este trabajo científico fue publicado el pasado mes de Febrero en la revista Sensors and Actuators B: Chemical y ha sido elegido como “Artículo del Mes” de abril del 2020 en el Centro de Investigaciones Científicas Isla de la Cartuja (cicCartuja), centro mixto del CSIC, Universidad de Sevilla (US) y Junta de Andalucía.

En este trabajo de investigación, en el que han participado los investigadores del Departamento de Ingeniería Química de la UCLM, Antonio de Lucas Consuegra y Ester López Fernández, se propone el uso de electrodos fabricados mediante la técnica de magnetron sputtering (tecnología de plasma) como sensores electroquímicos de hexosas. Se ha demostrado su fiabilidad en el seguimiento de un proceso de fermentación de vino sintético en sus diferentes etapas, así como en otros productos agroalimentarios. Este trabajo se enmarca dentro de la tesis doctoral de Dña. Ester López Fernández, becaria del programa nacional de Formación Universitario del Departamento de Ingeniería Química de la UCLM (FPU 2017). Esta investigadora en formación realiza sus estudios de doctorado en colaboración con el grupo de investigación de Nanotecnología en Superficies, ubicado en Sevilla, que se encuentra especializado en el uso de plasma en la Tecnología de Lámina Delgada.

Las investigaciones de este trabajo cobran una importancia determinante hoy día ya que la monitorización de la cinética de fermentación es un requisito clave para garantizar la calidad del vino y otras bebidas y ayudar a los productores a tomar medidas correctivas para evitar la fermentación lenta o estancada. El presente trabajo está motivado por la necesidad de desarrollar sensores robustos para la detección selectiva de azúcares en alimentos líquidos y, en particular, su uso para la monitorización del proceso de fermentación del vino.



## MINAS DE ALMADÉN. EuChemS Historical Landmarks Award 2019



Las minas de Almadén han sido galardonadas con el EuChemS Historical Landmarks Award 2019 – European Level, en reconocimiento al papel que han jugado en la historia de la química y en el sentido de pertenencia de las personas e ideas en Europa.

El Parque Minero de Almadén, ubicado en la provincia de Ciudad Real (Castilla la Mancha), representa uno de los mayores yacimientos de mercurio a nivel mundial. Constituyen las minas más antiguas del mundo y muestran el avance tecnológico de los métodos relacionados con la producción de mercurio. Sus pozos, edificios e instalaciones son Patrimonio de la Humanidad desde el año 2012 y están inscritos bajo el nombre de Patrimonio del Mercurio. Almadén e Idrija.

El Historical Landmarks Programme de la EuChemS busca reforzar el sentido de pertenencia de los químicos europeos y recordarles que en la historia de la química, las ideas se han compartido y dado forma a través de reuniones y comunicaciones. Así mismo, pretende transmitir al público en general la visión de que la química es parte del patrimonio histórico y cultural de cada ciudadano europeo.

## SELLO INTERNACIONAL DE CALIDAD

**Los grados de Química e Ingeniería Química y el Máster en Ingeniería Química de la UCLM, reconocidos con el sello internacional de calidad.**

Los grados en Química e Ingeniería Química y el Máster en Ingeniería Química de la Universidad de Castilla-La Mancha (UCLM) han sido reconocidos con el sello internacional de calidad Chemistry Eurobachelor, EUR-ACE Bachelor y EUR-ACE Master, por este orden. La certificación concedida por ANECA tras un riguroso procedimiento de evaluación acredita el cumplimiento de calidad académica e investigadora según estándares europeos y eleva a seis las titulaciones de la Universidad regional que cuentan con este certificado.

Tres nuevos títulos, dos de grado y uno de máster, de la Universidad de Castilla-La Mancha (UCLM) han sido reconocidos con los sellos internacionales de calidad que en España concede la Agencia Nacional de Evaluación de la Calidad y Acreditación (ANECA). Se trata de los grados en Química e Ingeniería Química que han obtenido los sellos Chemistry Eurobachelor y EUR-ACE Bachelor, respectivamente; y del Máster en Ingeniería Química, reconocido con el EUR-ACE Master, que se imparten en la Facultad de Ciencias y Tecnologías Químicas del Campus de Ciudad Real.

Los sellos EUR-ACE de Ingeniería y Chemistry Quality Eurabel son certificados concedidos por una agencia autorizada por la European Network for the Accreditation of Engineering Education (ENAE) y la European Chemistry Thematic Network Association (ECTN), respectivamente, a una universidad respecto a un título evaluado según una serie de estándares definidos de acuerdo con los principios de calidad, relevancia, transparencia, reconocimiento y movilidad contemplados en el Espacio Europeo de Educación Superior. Dichos sellos reconocen y acreditan la calidad de la docencia e investigación, la internalización y la adecuada orientación profesional a los estudiantes que cursan los grados y el máster.

El rector de la Universidad de Castilla-La Mancha (UCLM), Miguel Ángel Collado, ha felicitado a la Facultad de Ciencias y Tecnologías Químicas y al Departamento de Ingeniería Química por los reconocimientos obtenidos y ha asegurado que los sellos “son una muestra más de la excelencia de vuestro trabajo, del que estamos muy orgullosos”.

Hasta la fecha eran tres las titulaciones de la UCLM que contaban con un sello de calidad internacional: el Grado en Ingeniería Civil y Territorial y el Máster Universitario en Ingeniería de Caminos, Canales y Puertos, con el EUR-ACE; y el Grado en Ingeniería Informática, con el EURO-INF. Éste último lo concede una agencia, -en España la ANECA-, autorizada por la European Quality Assurance Network for Informatics Education (EQANIE).

**Gabinete Comunicación UCLM. Ciudad Real, 16 de junio de 2020**

## RANKING UNIVERSIDAD DE TAIWAN



### **Ingeniería Química en la UCLM logra el puesto 207 del mundo en el “ranking” de la Universidad Nacional de Taiwan**

La disciplina de Ingeniería Química en la Universidad de Castilla-La Mancha (UCLM) aparece en la posición 207 del mundo en la última edición del “ranking” NTU, elaborado por la Universidad Nacional de Taiwan con criterios que valoran la producción científica y el impacto y la excelencia de la investigación.

La clasificación elaborada por la National Taiwan University (NTU), que selecciona las trescientas mejores universidades del mundo en catorce disciplinas científicas, sitúa en 2019 a Ingeniería Química de la Universidad de Castilla-La Mancha (UCLM) en la posición 207 a nivel mundial, siendo la Ingeniería mejor calificada de toda la Universidad de Castilla La Mancha.

El ranking NTU, que emplea bases bibliométricas, está basado en tres criterios que consideran la producción científica, impacto de la investigación y excelencia en la investigación. Para ello se emplean una serie de indicadores objetivos que permiten comparar la calidad investigadora de las diferentes disciplinas científicas de la universidad en términos como productividad científica e impacto y excelencia de la investigación, tanto a largo como a corto plazo.

De este modo, la disciplina de Ingeniería Química obtiene una puntuación combinada de 50,5 puntos en el caso de la Universidad de Castilla-La Mancha, que la sitúa en el sexto lugar entre las universidades españolas.

La mayoría de los profesores del Departamento de Ingeniería Química participan en la docencia en los tres niveles universitarios: Grado en Ingeniería Química, Máster en Ingeniería Química y Doctorado en Ingeniería Química y Ambiental, que se imparten en Ciudad Real.

**Gabinete Comunicación UCLM. Ciudad Real, 11 de mayo de 2020**

## Desarrollan una célula solar que podría alcanzar un 50% de eficiencia



Científicos del Laboratorio Nacional de Energía Renovable de Estados Unidos (NREL) han desarrollado una célula solar que podría llegar a alcanzar una eficiencia de hasta el 50%. En la actualidad, este récord de eficiencia lo ostenta la célula solar de seis uniones que alcanza el 47,1% y cuya eficiencia fue medida bajo iluminación concentrada.

John Geisz, científico principal en el Grupo de Fotovoltaica de Alta Eficiencia en NREL y autor principal del artículo, asegura que el dispositivo demuestra el extraordinario potencial de las células solares multifuncionales. El proyecto ha sido financiado por Oficina de Tecnologías de Energía Solar del Departamento de Energía de los Estados Unidos.

### Construcción de la célula solar

La célula solar está basada en los materiales III-V, que reciben este nombre debido a su ubicación en la tabla periódica. Estos elementos poseen una amplia gama de propiedades de absorción de luz. Por ello, cada capa de la célula está desarrollada con el objetivo de capturar la luz de una parte en concreto del espectro solar.

La célula solar está formada por cerca de 140 capas totales de varios materiales III-V que apoyan el rendimiento entre las uniones. Estos materiales, que son más finos que un cabello humano, tienen una propiedades que brindan una alta y costosa eficiencia, por lo que suelen ser utilizados en la construcción de sistemas de alimentación para satélites.

Sin embargo, Ryan France, coautor del estudio y científico en NREL, afirma que la célula solar de seis uniones es altamente válida para su uso en paneles fotovoltaicos en la Tierra. De hecho, se muestra muy optimista en el hecho de alcanzar ese 50% de eficiencia, descartando alguna vez llegar al 100% por los meros límites que la termodinámica impone.

### Obstáculos para el desarrollo de esta tecnología

Los principales obstáculos para el desarrollo de la tecnología de alta eficiencia son las barreras que hacen resistencia y que, por tanto, impiden el flujo de corriente dentro de la misma.

Javier López de Benito

## Ciencia y Técnica de Castilla-La Mancha



**Azafea del astrónomo Azarquiel/ J.Jurado**

Una azafea del gran astrónomo andalusí Azarquiel -nacido en Toledo- es la foto que ilustra la portada de «Ciencia y Tecnología en Castilla-La Mancha. Diccionario biográfico»

**«Ciencia y Técnica de Castilla-La Mancha» pone luz y reconocimiento sobre los investigadores y científicos de la región desde el siglo XI**

Astrónomos, inventores, naturalistas, médicos, farmacéuticos, agrónomos y veterinarios de esta Comunidad Autónoma o vinculados a ella, desde el siglo XI hasta la actualidad, forman parte de “Ciencia y Técnica en Castilla-La Mancha”, una obra colectiva que reúne 320 entradas, básicamente biografías y referencias a empresas e instituciones relacionadas con la tecnología y la investigación científica. Este trabajo, coordinado por Alfonso González Calero y Enrique Díez Barra y editado por Almud, será presentado el próximo 14 de octubre en Ciudad Real.

¿Por qué abordar un «Diccionario de Ciencia y Técnica en Castilla-La Mancha»? se preguntan los coordinadores de este libro, Enrique Díez y Alfonso González Calero, en la introducción de una obra colectiva que cuenta con más de 70 colaboradores y reúne 320 entradas, entre biografías de científicos e investigadores nacidos en esta región o vinculados a ella, además de referencias a empresas e instituciones relacionadas con la tecnología y la investigación científica.

Es más. Los coordinadores de este diccionario biográfico llegaron a preguntarse si ¿acaso era esta región -interior, deprimida, no especialmente desarrollada ni culta- proclive a estas aventuras del intelecto?. Y en la respuesta salieron a luz los nombres de médicos y profesores, investigadores, científicos e inventores que trabajaron desde el siglo XI hasta la segunda mitad del siglo XX, gracias a las aportaciones realizadas desde las cinco provincias castellano-manchegas.

### **Astrónomos, inventores, naturalistas...**

Así, el libro recoge los nombres de astrónomos como Azarquiel o Jiménez Coronado; inventores como Blasco de Garay, Mónico Sánchez, Imedio o Juanelo Turriano; naturalistas como Hernández, Gómez Menor, Gómez Ortega o Sánchez Labrador; médicos como Chirino, Creus, Hernando, Muñoz Urra; farmacéuticos como Palacios y Bayá, agrónomos como Alonso de Herrera o Álvarez Ugena; veterinarios como García Izcara, o Morcillo; matemáticos como Balanzat, Sixto Ríos o Martínez Sancho; químicos como Del Campo Cerdán o Mascareña o ingenieros como Díaz Marta, Ortiz Echagüe, y tantos otros.

Estos nombres y otros muchos ofrecen una cierta aproximación a una realidad poco conocida hasta ahora como es la creatividad científica y técnica desarrollada durante nueve siglos en Castilla-La Mancha o en otros territorios lo que no es óbice para darlos a conocer y reconocer su labor.

## **Iniciativas tecnológicas**

El libro se detiene, también, en algunas iniciativas tecnológicas como la minería (Almadén y Hellín), las Reales Fábricas impulsadas en el siglo XVIII (Riópar-Alcaraz, Toledo, Alcázar), los molinos de papel (Cuenca), la automovilística La Hispano Suiza (Guadalajara) o la industria petroquímica de Puertollano en la segunda mitad del siglo XX.

Los coordinadores del trabajo definen la tradición científica y tecnológica en Castilla-La Mancha durante este largo período como de «a salto de mata», sin un plan concreto y como consecuencia de iniciativas y entregas personales muy costosas y, en ocasiones, como reflejo del momento en el que España quiere sumarse a la corriente europea del desarrollo del conocimiento científico, en los siglos XVII-XVIII.

## **Centros de investigación de la UCLM**

Sin embargo, el desarrollo del Estado de las Autonomías y la integración de España en Europa posibilitaron que el gobierno de Castilla-La Mancha diseñara su avance científico, aunque la «Edad de Plata» -como la llaman- de su producción científica empezó con la consolidación de la Universidad de Castilla-La Mancha (UCLM). «Y para este diccionario, hemos tenido la suerte de contar con las descripciones que han realizado los responsables de sus principales centros de investigación», explican los coordinadores.

Para ellos, no solo estos centros de la UCLM han contribuido a la europeización de Castilla-La Mancha en cuanto a ciencia y tecnología, sino que iniciativas privadas y públicas para aplicar la energía solar, los nuevos vectores energéticos o el aprovechamiento de residuos, están contribuyendo a las energías limpias y la economía circular en Castilla-La Mancha.

«Confiamos en que este Diccionario ayude al reconocimiento social y al impulso financiero sostenido que la ciencia y la técnica necesitan», señalan Enrique Díez y Alfonso González quienes fraguaron este proyecto durante el confinamiento por la pandemia de coronavirus. Editado por Almud ediciones de Castilla-La Mancha, el libro está dedicado a Isidro Sánchez y será presentado el próximo 8 de octubre en Toledo y el día 14 en Ciudad Real.

## **La azafea de Azarquiel**

Una azafea del gran astrónomo andalusí Azarquiel -nacido en Toledo- es la foto que ilustra la portada de este Diccionario biográfico de casi 600 páginas y de consulta obligada para conocer este pasado tan brillante de muchas individualidades científicas de Castilla-La Mancha.

La azafea es un instrumento de observación astronómica que mejoraba los cálculos realizados con el astrolabio construido por Azarquiel (Toledo, c. 1029 – Sevilla, 1087). Su uso permitía realizar observaciones y el cómputo desde cualquier latitud terrestre, frente a ceñirse a una latitud específica como exigía el astrolabio.

## El hombre que creó el método para exterminar humanos a escala industrial



El primer ataque con gas de la historia arrasó a las tropas francesas atrincheradas cerca del pequeño pueblo de Ypres, en Bélgica. Al despertar en la madrugada del jueves 22 de abril de 1915, los soldados vieron una enorme nube verdosa que reptaba hacia ellos por la Tierra de Nadie. Dos veces más alta que un hombre y tan densa como la niebla invernal, se estiraba de un lado a otro del horizonte, a lo largo de seis kilómetros. A su paso las hojas de los árboles se marchitaban, las aves caían muertas desde el cielo y el pasto se teñía de un color metálico enfermizo. Un aroma similar a piña y lavandina cosquilleó las gargantas de los soldados cuando el gas reaccionó con la mucosa de sus pulmones, formando ácido clorhídrico. A medida que la nube se empozaba en las trincheras, cientos de hombres se desplomaron convulsionando, ahogándose en sus propias flemas, con mocos amarillos burbujeando en su boca, su piel azulada por la falta de oxígeno. «Los meteorólogos tenían razón. Era un día hermoso, el sol brillaba. Donde había pasto, resplandecía verde. Debiéramos haber estado yendo a un picnic, no haciendo lo que íbamos a hacer», escribió Willi Siebert, uno de los soldados que abrió parte de los seis mil cilindros de gas cloro que los alemanes derramaron esa mañana en Ypres. «De pronto escuchamos a los franceses gritando. En menos de un minuto comencé a oír la mayor descarga de municiones de rifle y ametralladoras que escuché en mi vida. Cada cañón de artillería, cada rifle, cada ametralladora que tenían los franceses tiene que haber sido disparado. Jamás oí un estruendo similar. La lluvia de balas que pasaba silbando sobre nuestras cabezas era increíble, pero no estaba deteniendo el gas. El viento seguía empujándolo hacia las líneas francesas. Escuchamos a las vacas berrear y los caballos relinchar. Los franceses siguieron disparando. Era imposible que vieran a qué estaban disparando. En unos quince minutos el fuego comenzó a detenerse. Después de media hora, solo disparos ocasionales. Entonces todo volvió a estar tranquilo. En un rato el aire se había despejado y caminamos más allá de las botellas de gas vacías. Lo que vimos fue la muerte total. Nada estaba vivo. Todos los animales habían salido de sus agujeros para morir. Conejos, topos, ratas y ratones muertos en todas partes. El olor del gas aún flotaba en el aire. Colgaba de los pocos arbustos que habían quedado. Cuando llegamos a las líneas francesas, las trincheras estaban vacías, pero a media milla los cuerpos de los soldados franceses estaban esparcidos por todas partes. Fue increíble. Luego vimos que había algunos ingleses. Uno podía ver cómo los hombres se habían arañado la cara y el cuello, tratando de volver a respirar. Algunos se habían disparado a sí mismos. Los caballos, aún en los establos, las vacas, los pollos, todo, todos estaban muertos. Todo, incluso los insectos estaban muertos.»

El hombre que había planificado el ataque con gas en Ypres era el creador de esa nueva forma de hacer la guerra, el químico Fritz Haber. De raíces judías, Haber era un verdadero genio, y tal vez la única persona en ese campo de batalla capaz de comprender las complejas reacciones moleculares que volvieron negra la piel de los mil quinientos soldados muertos en Ypres. El éxito de su misión le valió un ascenso al rango de capitán, una promoción a la jefatura de la sección de Química del Ministerio de Guerra y una cena con el mismísimo káiser Guillermo II. Pero al volver a Berlín Haber fue confrontado por su esposa. Clara Immerwahr –la primera mujer en recibir un doctorado en química de una universidad alemana– no solo había visto el efecto del gas sobre animales en el laboratorio, sino que había estado muy cerca de perder a su marido, cuando el viento cambió de súbito en una de las pruebas de campo. El gas sopló directo hacia la colina desde la cual Haber, montado sobre su caballo, dirigía a sus tropas. Fritz se salvó de milagro, pero uno de sus ayudantes no pudo escapar de la nube tóxica; Clara lo vio morir en el suelo, retorciéndose como si hubiera sido invadido por un ejército de hormigas hambrientas. Cuando Haber regresó victorioso de la masacre de Ypres, Clara lo acusó de haber pervertido la ciencia al crear un método para exterminar humanos a escala industrial, pero Fritz la ignoró por completo: para él, la guerra era la guerra y la muerte era la muerte, fuera cual fuera el medio de infligirla. Aprovechó su permiso de dos días para invitar a todos sus amigos a una fiesta que duró hasta la madrugada, al final de la cual su mujer bajó al jardín, se quitó los zapatos y se disparó en el pecho con el revólver de servicio de su marido. Murió desangrada en los brazos de su hijo de trece años, quien corrió escaleras abajo al escuchar el balazo. Aún en estado de shock, Fritz Haber fue obligado a viajar al día siguiente para supervisar un ataque de gas en el frente oriental. Durante el resto de la guerra continuó refinando métodos para desplegar el veneno con mayor eficacia, acosado por el espectro de su mujer. «Realmente me hace bien, cada tantos días, estar en el frente, donde las balas vuelan. Allí lo único que importa es el instante, y el único deber es hacer lo que uno pueda dentro de los límites de la trinchera. Y luego, de vuelta en el centro de comando, encadenado al teléfono, donde escucho en mi corazón las palabras que la pobre mujer me dijo una vez, y en una visión nacida del agotamiento, veo su cabeza emerger entre los telegramas. Y sufro.»

Luego del armisticio de 1918, Fritz Haber fue declarado criminal de guerra por los aliados, a pesar de que ellos habían utilizado el gas con el mismo fervor que las potencias del Eje. Tuvo que escapar de Alemania y refugiarse en Suiza, donde recibió la noticia de que había obtenido el Premio Nobel de Química por un descubrimiento que había hecho poco antes de la guerra, y que en las décadas siguientes alteraría el destino de la especie humana.

En 1907, Haber fue el primero en extraer nitrógeno –el principal nutriente que las plantas necesitan para crecer– directamente del aire. Con ello, solucionó, del día a la mañana, la escasez de fertilizantes que a principios del siglo XX amenazaba con desencadenar una hambruna global como no se había visto nunca antes; de no haber sido por Haber, cientos de millones de personas que hasta entonces dependían de sustancias naturales como el guano y el salitre para abonar sus cultivos podrían haber muerto por falta de alimentos.

En siglos anteriores, la demanda insaciable de Europa había llevado a bandas inglesas a viajar hasta Egipto para saquear las catacumbas de los antiguos faraones no en busca de oro, joyas, o antigüedades, sino del nitrógeno contenido en los huesos de los miles de esclavos con que los reyes del Nilo se habían inhumado para que continuaran sirviéndolos más allá de la muerte. Los ladrones de tumbas ingleses ya habían agotado las reservas de Europa continental; desenterraron más de tres millones de esqueletos, incluyendo las osamentas de cientos de miles de soldados y caballos muertos en las batallas de Austerlitz, Leipzig y Waterloo, para enviarlos en barco al puerto de Hull, en el norte de Inglaterra, donde eran molidos en los trituradores de huesos de Yorkshire para fertilizar los campos verdes de Albión. Al otro lado del Atlántico, los cráneos de más de treinta millones de bisontes masacrados en las praderas norteamericanas eran recogidos uno a uno por campesinos e indios pobres, para venderlos al Sindicato de Huesos de Dakota del Norte, que los amontonaba hasta formar una pila del tamaño de una iglesia antes de transportarlos a la fábrica que los molía para producir fertilizante y «negro-hueso», el pigmento más oscuro que se podía encontrar en esa época. Lo que Haber había logrado en el laboratorio, Carl Bosch, el ingeniero principal del gigante químico alemán BASF, lo convirtió en un proceso industrial capaz de producir cientos de toneladas de nitrógeno en una fábrica del tamaño de una pequeña ciudad, operada por más de cincuenta mil trabajadores. El proceso Haber-Bosch fue el descubrimiento químico más importante del siglo XX: al duplicar la cantidad de nitrógeno disponible, permitió la explosión demográfica que hizo crecer la población humana de 1,6 a 7 mil millones de personas en menos de cien años. Hoy, cerca del cincuenta por ciento de los átomos de nitrógeno de nuestros cuerpos han sido creados de forma artificial, y más de la mitad de la población mundial depende de alimentos fertilizados gracias al invento de Haber. El mundo moderno no podría existir sin el hombre que «extrajo pan del aire», según palabras de la prensa de su época, aunque el uso inmediato de su milagroso hallazgo no fue alimentar a las masas hambrientas, sino proveer a Alemania de la materia prima que necesitaba para seguir fabricando pólvora y explosivos durante la Primera Guerra Mundial, luego de que la flota inglesa cortara su acceso al salitre chileno. Con el nitrógeno de Haber, el conflicto europeo se prolongó dos años más, aumentando las bajas de ambos lados en varios millones de personas.

Uno de los que sufrió debido a la extensión de la guerra fue un joven cadete de veinticinco años; aspirante a artista, había rehuido el servicio militar obligatorio de todas las formas posibles, hasta que la policía llegó a buscarlo al número 34 de la calle Schleissheimer, en Múnich, en enero de 1914. Bajo amenaza de prisión, se presentó al examen médico en Salzburgo, pero lo declararon «no apto, demasiado débil e incapaz de portar armas». En agosto de ese año –cuando miles de hombres se inscribían voluntariamente en las fuerzas armadas, sin poder contener sus ganas de participar en la guerra venidera–, el joven pintor tuvo un súbito cambio de actitud: le escribió una petición personal al rey Luis III de Baviera para poder servir como austriaco en el ejército bávaro. El permiso llegó al día siguiente.

Adi, como lo llamaban cariñosamente sus compañeros del Regimiento List, fue enviado directamente a la batalla que en Alemania llegó a ser conocida como Kindermord bei Ypern, la matanza de los inocentes, ya que cuarenta mil jóvenes recién enlistados murieron en solo veinte días. De los doscientos cincuenta hombres que formaban su compañía, solo cuarenta lograron sobrevivir; Adi fue uno de ellos.

Recibió la Cruz de Hierro, fue promovido a cabo y nombrado mensajero de la Sede de su Regimiento, por lo que pasó los siguientes años a una cómoda distancia del frente, leyendo libros de política y jugando con un fox terrier que adoptó y llamó Fuchsl, zorrito. Ocupaba sus tiempos muertos pintando acuarelas azuladas y haciendo bocetos a carboncillo de su mascota y de la vida en las barracas. El 15 octubre de 1918, mientras languidecía esperando nuevas órdenes, fue momentáneamente cegado por un ataque con gas mostaza lanzado por los ingleses, y pasó las últimas semanas de la guerra convaleciendo en un hospital del pequeño pueblo de Pasewalk, en Pomerania, sintiendo que sus ojos se habían convertido en dos carbones al rojo vivo. Cuando supo las noticias de la derrota de Alemania y la abdicación firmada por el káiser Guillermo II sufrió un segundo ataque de ceguera, muy distinto al que le había causado el gas: «Todo se volvió negro ante mis ojos. Volví al pabellón a tientas y tambaleando, me lancé en mi litera, y hundí mi cabeza ardiendo en mi almohada», recordó años después, en una celda de la prisión de Landsberg, acusado de traición por dirigir un fallido golpe de Estado. Allí pasó nueve meses consumido por el odio, aún humillado por las condiciones impuestas a su país de adopción por las potencias vencedoras, y por la cobardía de los generales, que se habían rendido en vez de pelear hasta el último hombre. Desde la cárcel planeó su venganza: escribió un libro sobre su lucha personal y detalló un plan para alzar a Alemania sobre todas las naciones del mundo, algo que estaba dispuesto a hacer con sus propias manos si llegase a ser necesario. En el periodo de entreguerras, mientras Adi escalaba hasta la cima del Partido Nacionalsocialista Obrero, gritando las arengas del discurso racista y antisemita que lo acabaría coronando como el Führer de toda Alemania, Fritz Haber hacía sus propios esfuerzos por recomponer la gloria perdida de su patria.

Envalentonado por el éxito que había tenido con el nitrógeno, Haber se propuso reconstruir la República de Weimar y pagar las reparaciones de guerra que estrangulaban su economía mediante un proceso tan prodigioso como el que le había valido el Nobel: cosechar oro de las olas del mar. Viajando con una identidad falsa para no levantar sospechas, recolectó cinco mil muestras de agua de diversos mares del mundo, trozos de hielo del Polo Norte y témpanos de la Antártida. Estaba convencido de que podía minar el oro disuelto en los océanos, pero luego de años de arduo trabajo tuvo que aceptar que su cálculo original había sobrestimado el contenido de este metal precioso en varias órdenes de magnitud. Volvió a su país con las manos vacías.

En Alemania se refugió en su trabajo como director del Instituto Kaiser Wilhelm de Química-Física y Electroquímica mientras el antisemitismo iba creciendo a su alrededor. Momentáneamente protegido en el oasis académico, Haber y su equipo produjeron múltiples nuevas sustancias; una de ellas usaba el cianuro para formar un pesticida en gas cuya acción era tan violenta que lo bautizaron Zyklon, la palabra alemana que designa los vientos de un huracán. La efectividad radical del compuesto asombró a los entomólogos que lo utilizaron por primera vez, para despiojar un barco que cubría la ruta entre Hamburgo y Nueva York, quienes le escribieron directamente a Haber para elogiar «la extremada elegancia del proceso de erradicación». Haber fundó el Comisionado Nacional para el Control de Pestes; desde allí organizó la matanza de chinches y pulgas en los submarinos de la armada y ratas y cucarachas en las barracas del ejército.

Luchó contra una verdadera legión de polillas que atacaba la harina que el gobierno acumulaba en silos repartidos a lo largo de todo el territorio nacional, y que Haber describió a sus superiores como «una plaga bíblica que amenazaba el bienestar del espacio vital germano», sin saber que ellos habían comenzado a implementar la persecución de todos los que compartían las raíces judías de Haber.

Fritz se había convertido al cristianismo a los veinticinco años. Estaba tan identificado con su país y sus costumbres que sus hijos solo se enteraron de su ascendencia cuando él les dijo que debían escapar de Alemania. Haber huyó después de ellos y pidió asilo en Inglaterra, pero fue violentamente repudiado por sus colegas británicos, quienes conocían el rol que había jugado en la guerra química. Tuvo que abandonar la isla poco después de llegar. Desde allí se escabulló de un país a otro, intentando alcanzar Palestina, con el pecho apretado por el dolor, ya que sus vasos sanguíneos no eran capaces de llevar suficiente sangre a su corazón. Murió en Basel, en 1934, abrazado al cilindro con el que dilatava sus arterias coronarias, sin saber que pocos años más tarde el pesticida que él había ayudado a crear sería utilizado por los nazis en sus cámaras de gas para asesinar a su media hermana, a su cuñado, a sus sobrinos, y a tantos otros judíos que murieron en cuclillas, con los músculos agarrotados y la piel cubierta de manchas rojas y verdes, sangrando por los oídos, echando espuma por la boca, con los más jóvenes aplastando a los niños y a los ancianos en su intento por escalar la pila de cuerpos desnudos y poder respirar unos minutos más, unos segundos más, ya que el Zyklon B se empozaba cerca del suelo luego de ser vertido por ranuras en el techo. Una vez que la niebla de cianuro era disipada por ventiladores, los cadáveres eran arrastrados a enormes hornos e incinerados. Sus cenizas fueron enterradas en fosas comunes, vertidas en ríos y estanques o esparcidas como abono en los campos de los alrededores.

Entre las pocas cosas que Fritz Haber tenía consigo al morir hallaron una carta escrita a su mujer. En ella, Haber le confiesa que siente una culpa insoportable; pero no por el rol que jugó en la muerte de tantos seres humanos, directa o indirectamente, sino porque su método para extraer nitrógeno del aire había alterado de tal forma el equilibrio natural del planeta que él temía que el futuro de este mundo no pertenecería al ser humano sino a las plantas, ya que bastaría que la población mundial disminuyera a un nivel premoderno durante tan solo un par de décadas para que ellas fueran libres de crecer sin freno, aprovechando el exceso de nutrientes que la humanidad les había legado para esparcirse sobre la faz de la tierra hasta cubrirla por completo, ahogando todas las formas de vida bajo un verdor terrible.

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'Un verdor terrible'

Autor: Benjamín Labatut

Editorial: Anagrama

## CIENCIA JOVEN 2020

### Los químicos noveles de la UCLM comparten con sus compañeros sus líneas de investigación

La Facultad de Ciencias y Tecnologías Químicas de la Universidad de Castilla-La Mancha (UCLM) en Ciudad Real ha acogido el Simposio Ciencia Joven, durante el que los investigadores noveles presentan sus líneas de trabajo. El encuentro que, se ha desarrollado en modalidad on-line, ha sido inaugurado por el rector de la UCLM, Miguel Ángel Collado.

Los jóvenes investigadores de la Facultad de Ciencias y Tecnologías Químicas de la universidad de Castilla-La Mancha (UCLM) en el Campus de Ciudad Real, así como otros de Albacete y Toledo, han presentado a la comunidad académica sus líneas y resultados de investigación con motivo de la celebración decimocuarto Simposio Ciencia Joven, una iniciativa que supone una oportunidad para acercar a los estudiantes a la tarea investigadora. Los trabajos, en esta edición, están relacionados con el tratamiento de suelos, electroquímica, catálisis, materiales, analítica, alimentos y bioquímica, entre otras temáticas.

El encuentro, que esta edición se ha celebrado de manera no presencial, ha sido inaugurado por el rector de la Universidad de Castilla-La Mancha (UCLM), Miguel Ángel Collado, quien ha felicitado a la Facultad de Químicas y a sus organizadores por esta iniciativa, muestra de la “vitalidad” del centro, y por su “entusiasmo, trabajo y compromiso con la investigación pese a las dificultades”.

Para el rector, este encuentro se celebra en un momento óptimo, ya que coincide con la aprobación de los fondos regionales de investigación y con el debate en las Cortes de la Ley de la Ciencia que, según Collado, debe estar dotada de una financiación “suficiente, estable y planificada”.

Junto al rector de la UCLM, el decano de la Facultad de Ciencias y Tecnologías Químicas, Ángel Ríos, se ha referido a la celebración del simposio de Ciencia Joven como una excelente oportunidad para los investigadores noveles, ya que el mismo les ayuda a conocer cómo se prepara un congreso científico, les servirá de apoyo en su tarea formativa investigadora y les permitirá conocer el trabajo que realizan otros compañeros.

En el simposio, en el que colabora la Real Sociedad Española de Química, se han inscrito un total de 170 investigadores del Campus de Albacete, Ciudad Real y Toledo y se han admitido 35 comunicaciones orales y 32 contribuciones en formato póster en los distintos ámbitos que abarca la Facultad: Química Inorgánica, Ingeniería Química, Química Orgánica, Química Analítica, Tecnología de los Alimentos, Química Física, Matemáticas y Bioquímica.

Junto a los ponentes investigadores noveles, el simposio cuenta con la intervención de cinco ponentes externos invitados. Se trata de Rafael Van Grieken, de la Universidad Rey Juan Carlos; Teresa Garde, del Instituto de Ciencias de la Vid y el Vino; Juan Ignacio Cirac, del Instituto Max Planck; David Medina, Northeastern University; y Jesús Martínez de la Fuente, del Instituto de Ciencia de Materiales de Aragón.

**Gabinete Comunicación UCLM. Ciudad Real, 8 de julio de 2020**



## 14ª EDICIÓN SIMPOSIO CIENCIA JOVEN (XIV YOUNG SCIENCE SYMPOSIUM)

08 – 10 Julio 2020

El pasado mes de Julio, tuvo lugar la celebración de la decimocuarta edición del Simposio Ciencia Joven (XIV Young Science Symposium) organizado por la Facultad de Ciencias y Tecnologías Químicas de Ciudad Real. Por primera vez, se realizó en modalidad on-line con un formato similar al de ediciones anteriores, adaptados a la no presencialidad.

El objetivo de este Simposio es divulgar y dar a conocer lo que hacen los jóvenes investigadores, e introducirlos en la organización de pequeños eventos científicos, que a escala reducida sirvan de ejemplo de cómo se organizan los congresos a los que después ellos asisten, a nivel nacional e internacional, presentando los resultados de sus trabajos científicos. En esta edición, se contó con la participación de jóvenes investigadores de otros campus (Toledo y Albacete) de la Universidad de Castilla-La Mancha, cuyos temas de investigación están estrechamente relacionados con los campos científicos y tecnológicos que se desarrollan en este Centro, hecho que fomenta la interdisciplinariedad y el debate entre jóvenes investigadores.

Esta edición virtual estuvo compuesta por 35 comunicaciones orales y 32 comunicaciones posters, 19 en formato flash, superando los 170 inscritos. Junto a los jóvenes investigadores, se contó con la intervención de los cinco ponentes invitados: Rafael Van Grieken, de la Universidad Rey Juan Carlos; Teresa Garde, del Instituto de Ciencias de la Vid y el Vino; Juan Ignacio Cirac, del Instituto Max Planck (Alemania); David Medina de la Universidad del Nordeste (EEUU) y Jesús Martínez de la Fuente, del Instituto de Ciencia de Materiales de Aragón.

Además, a modo de incentivar a aquellos jóvenes doctorandos y nuevos doctores que participan como ponentes en estas jornadas, en esta convocatoria 2020, se concedió el “V Prize of Young Science Faculty of Chemical Sciences and Technology” a Felipe de la Cruz con la ponencia titulada “Bimetallic Zinc catalysts for ring-opening copolymerization processes”. Asimismo, se otorgó el “III Poster Prize of Young Science Faculty of Chemical Sciences and Technology” a Viviana J. González, con la mejor presentación flash del póster titulado “Mechanochemical preparation of piezoelectric nanomaterials: BN, MoS<sub>2</sub> and WS<sub>2</sub> 2D materials and their glycine-cocrystals”.

## Friday 10<sup>th</sup> of July 2020

9:00- Invited Lecturer: Dr. Jesús Martínez de la Fuente (Aragón Materials Science Institute). "Hybrid Nanoparticles for Therapy and Diagnosis: New Biotechnological Challenges for Hyperthermia".

10:00- 6<sup>th</sup> session

- "Effect of oenological by-products as natural antioxidants and flavourings in meat products". Marina Alarcón. Food Sciences and Technology.
- "A screening method for the assessment of the release of silver nanoparticles from food containers". Ana Isabel Corps. Analytical Chemistry.
- "Effect of COVID-19- lockdown on the air quality of different cities". Maria Gabriela Viteri. Physical Chemistry.
- "Electrochemical technologies for the elimination of antibiotics in hospital urine". Ángela Moratalla. Chemical Engineering.
- "Graphene-based sulfonate hydrogels: Soft scaffolds for cell culture". Josué Muñoz. Organic Chemistry.
- "Antitumoral effects of resveratrol through adenosinergic system on cervical cancer cell line". Sonia Muñoz. Biochemistry.

12:00- 7<sup>th</sup> session

- "Bimetallic Zinc Catalysts for Ring-Opening Copolymerization Processes". Felipe de la Cruz. Inorganic Chemistry.
- "Accurate quantification of polycyclic aromatic compounds adsorbed on soot samples". Sonia Lara. Physical Chemistry.
- "Determination of biological markers oxidative stress by capillary liquid chromatography mass spectrometry". Yassine Benmassaoud. Analytical Chemistry.
- "Applying statistics criteria in rational selection of probiotic Lactobacillus strains to be used as biocontrol agents". Sara Rodríguez. Food Sciences and Technology.
- "CO<sub>2</sub> reduction by simulated sunlight and TiO<sub>2</sub>-based catalysts". Verónica Rodríguez. Chemical Engineering.
- "Tumor lockdown: how to beat cancer through confinement measures". Miriam Nuncia. Biochemistry.

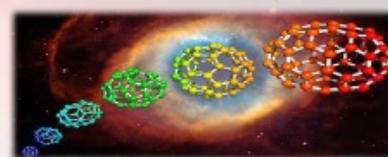
13:30- Colloquium, Prize winners and Closing Ceremony chaired by the Vice-Chancellor of Research and Scientific Policy of UCLM, the Dean of the Faculty of Chemical Sciences and Technology and Ricardo Jurado (AGROVIN, sponsor of the V Prize of Young Science) who presents "Aplicación de ultrasonidos en la elaboración de vinos de calidad".

## SPONSORS:



Further information and abstracts book will be available in: <https://www.uclm.es/ciudad-real/quimicas/Actividad/Simposio-Ciencia-Joven>

Send registrations to: <https://bit.ly/3FXGgR> until 30<sup>th</sup> June



## XIV YOUNG SCIENCE SYMPOSIUM 2020



Virtual edition- Faculty of Chemical Sciences and Technology  
8-10<sup>th</sup> of July 2020

FREE ELECTIVE CREDIT: University of Castilla-La Mancha grants 1 Free Elective Credit  
CERTIFICATE OF ATTENDANCE FOR ALL PARTICIPANTS

V PRIZE OF YOUNG SCIENCE FACULTY OF SCIENCES AND TECHNOLOGY  
and  
III POSTER PRIZE OF YOUNG SCIENCE FACULTY OF SCIENCES AND TECHNOLOGY

*Scientific committee:*  
Ángel Ríos Castro, Dean of Faculty  
María Antonia Herrero Chamorro, 'STCLM de la RSEQ'  
Alberto Ramos Alonso, 'Inorganic Chemistry'  
Ana Raquel de la Osa Puebla, 'Chemical Engineering'  
Elena Alañón Pardo, 'Food Sciences and Technology'  
Antonio Manuel Rodríguez García, 'IIC-RSEQ - EYCN EuChemS'  
*Organization committee:*  
José Pérez Navarro, 'Food Sciences and Technology'  
Cristina Montes Correal, 'Analytical Chemistry'  
Sergio Blázquez González, 'Physical Chemistry'  
Alberto José Huertas Alonso, 'Organic Chemistry'  
María del Prado Caballero, 'Inorganic Chemistry'  
Luis Fernando León Fernández, 'Chemical Engineering'

## Wednesday 8<sup>th</sup> of July 2020

9:00- Opening ceremony chaired by the Rector Magnificus of the UCLM and the Dean of the Faculty of Chemical Sciences and Technology.

9:30- Invited Lecturer: Prof. Rafael Van Grieken (Rey Juan Carlos University). "La carrera académica: luces y sombras de un complejo camino".

10:30- 1<sup>st</sup> session

- "Plasmonic nanosensing based on AuNPs for UV-Vis/Colorimetric assessment of global aminoacids amount in food supplements". Manuel Bartolomé. Analytical Chemistry.
- "Nanostructured electrodes prepared by magnetron sputtering for water electrolysis". Ester Lopez. Chemical Engineering.
- "Ring-Opening Polymerization of Cyclohexane Oxide Catalyzed by Scorpionate Aluminium Complexes". Miguel Angel Goana. Inorganic Chemistry.
- "Benzoxazoles as two-photon absorbing chromophores". Beatriz Donoso. Organic Chemistry.

11:30- Break.

12:00- Invited Lecturer: Dr. Teresa Garde-Cerdan (Institute of GrapeVine and Wine Science). "Foliar application of biostimulants in the vineyard: A tool to improve grape and wine quality and attenuate the effects of climate change".

13:00-14:30- Poster session I.

16:00- 2<sup>nd</sup> session

- "Grape seed extract supplementation modulates hepatic lipid metabolism in healthy rats and could be effective for preventing the progression of overweight-related metabolic disorders". Eduardo Guisantes. Food Sciences and Technology.
- "Kinetics on Supercritical Epoxidation of Vegetable Oils". Juan Catalá. Chemical Engineering.
- "Speciation of a polyphenolic pigment in free solution and encapsulated into a nanocarrier system. Quantification of this bioactive in micellar medium in nutraceuticals". Esther Pinilla. Analytical Chemistry.
- "Effects of central leptin on metabolic reprogramming of adipose tissue. Role of PPAR $\beta$  and FGF21". Lorena Mazneco. Biochemistry.
- "Substituted Alkylbenzenes and Biphenylene-Based Crystalline Structures: X-Ray Study and Optical Waveguide Behaviour". Carlos Tardío. Organic Chemistry.

## Thursday 9<sup>th</sup> of July 2020

9:00- Invited Lecturer: Prof. Juan Ignacio Cirac (Director and Scientific Member Max Planck Institut of Quantum Optics). "Ordenadores cuánticos: Como, cuando y para que".

10:00- 3<sup>rd</sup> session

- "Analytical control of gold and platinum nanoparticles in clinical and toxicological matrices". Sergio Fernández. Analytical Chemistry.
- "Flavan-3-ol composition of chocolate parmed raisins". Carolina Olivati. Food Sciences and Technology.
- "Microwave-responsive Graphene-based hydrogels for drug delivery applications". Jorge Leganés. Organic Chemistry.
- "Characterization and reactivity with NO<sub>2</sub> of diesel soots generated under different combustion conditions". María Inmaculada Aranda. Physical Chemistry.
- "Development of organocatalysts for the synthesis of oxazolones for potential antibiotics". María del Prado Caballero. Inorganic Chemistry.

11:15- Break.

11:45- Presentation of the Territorial Section of the Royal Spanish Society of Chemistry (STCLM-RSEQ)

12:00- 4<sup>th</sup> session

- "Glycolysis process for polyurethane composites recycling". Jesús del Amo. Chemical Engineering.
- "Push-pull azaheterocyclic chromophores: Synthesis, photophysical properties and use for white light emission". Rodrigo Plaza. Organic Chemistry.
- "Why and how do we study the interstellar chemistry?". Sergio Blázquez. Physical Chemistry.
- "Influence of ultrasounds on wine microbiota". Raquel Muñoz. Food Sciences and Technology.

13:00-14:30- Poster session II.

## Thursday 9<sup>th</sup> of July 2020

16:00- Invited Lecturer: David Medina Cruz (Ph.D. Northeastern University at Boston, USA, The Green Chemistry Lab). "Green Nanobiotechnology and Biofactories: from a laboratory curiosity to a market product helping society".

17:00- 5<sup>th</sup> session

- "Resistance to oxidation of SO<sub>2</sub> free red wines elaborated with natural antioxidants". Lourdes Marchante. Food Sciences and Technology.
- "Acrylamide magnetic hydrogels: different methods for the introduction of magnetic nanoparticles". Jesús Herrera. Organic Chemistry.
- "Emerging contaminants treatment in a real waters matrix by AOP processes". Jihane Ben. Analytical Chemistry.
- "Comparative study about formation of Secondary Organic Aerosol from ozonolysis of organic compounds". Alba Escalona. Physical Chemistry.
- "Development of a combined electro-scrubbing process for the treatment of volatile organic compounds". Florymar Escalona. Chemical Engineering.

**En el próximo número de Molécula...**

El próximo número de MOLÉCULA incluirá las actividades realizadas y resúmenes de tesis defendidas en este mes.

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<https://moleculauclm.wordpress.com/>

**V PREMIO CIENCIA JOVEN  
2020**



Como en ediciones anteriores, el comité organizador del XIII Simposio de Ciencia Joven hizo entrega del *V Premio Ciencia Joven* en el acto de clausura del evento. En esta edición, el premio ha sido otorgado a **Felipe de la Cruz** el trabajo titulado "*Bimetallic Zinc catalysts for ring-opening copolymerization processes*". También se hizo entrega del *III Premio Ciencia Joven al mejor póster* a **Viviana J. González Velázquez**, con el póster titulado "*Mechanochemical preparation of piezoelectric nanomaterials: BN, MoS<sub>2</sub> and WS<sub>2</sub> 2D materials and their glycine-cocrystals*".

¡Enhorabuena a los premiados!





## Jornadas de Ciencia Joven:

FECHA	ACTUACIÓN
Abril de 2007	CIENCIA JOVEN. Un foro de debate de jóvenes investigadores
De mayo a junio de 2008	II JORNADAS DE CIENCIA JOVEN. Un foro de debate de jóvenes investigadores
De abril a junio de 2009	III JORNADAS DE CIENCIA JOVEN. Un foro de debate de jóvenes investigadores
De abril a junio de 2010	IV JORNADAS DE CIENCIA JOVEN. Un foro de debate de jóvenes investigadores
De abril a junio de 2011	V JORNADAS DE CIENCIA JOVEN. Un foro de debate de jóvenes investigadores
De mayo a junio de 2012	VI JORNADAS DE CIENCIA JOVEN. Encuentro de jóvenes investigadores
23-24 de mayo de 2013	VII SIMPOSIO CIENCIA JOVEN
22-23 de mayo de 2014	VIII SIMPOSIO CIENCIA JOVEN
21-22 de mayo de 2015	IX SIMPOSIO CIENCIA JOVEN
Del 8 al 10 de junio de 2016	X SIMPOSIO CIENCIA JOVEN
Del 3 al 5 de Junio de 2017	XI SIMPOSIO CIENCIA JOVEN
Del 13 al 15 de Junio de 2018	XII SIMPOSIO CIENCIA JOVEN
Del 5 al 7 de Junio de 2019	XIII SIMPOSIO CIENCIA JOVEN
Del 8 al 10 de Julio de 2020	XIV SIMPOSIO CIENCIA JOVEN

