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Facultad de Ciencias y Tecnologías Químicas

Facultad de Ciencias y Tecnologías Químicas
Universidad de Castilla- La Mancha

XVI YOUNG SCIENCE SYMPOSIUM

Del 22 al 24 de Junio de 2022

RSEQ
Sección Territorial de Castilla La Mancha

Yuntero

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LA JARABA

VINICOLADECASTILLA

LIBRO DE COMUNICACIONES

Bienvenida del Decano

Os damos la bienvenida a esta nueva edición del 16th Young Science Symposium, que organizan los jóvenes investigadores de la Facultad de Ciencias y Tecnologías Químicas de la Universidad de Castilla – La Mancha.

El Simposio, que nació en el año 2007, es una iniciativa del personal más joven de la Facultad para poner en valor la investigación realizada y aprender unos de otros, conociendo en que se investiga en nuestros más de treinta grupos de investigación, no solo en temática sino también en la metodología. Precisamente, la investigación tiene una muy especial relevancia en nuestra Facultad, siendo el Centro más competitivo en captación de fondos y en producción científica y nuestros jóvenes investigadores quieren reivindicar su papel y contribuir a su excelencia. Por este motivo, el simposio 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: Favorecer 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 las temáticas se han unido, aumentando la relevancia del evento y permitiendo aumentar su interdisciplinariedad.

El Simposio tradicionalmente no solo ha tenido la visión científica: 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 VII PREMIO CIENCIA JOVEN y cuatros premios en la categoría II PREMIO VIRTUAL-FLASH en categoría TFG, TFM y tesis, con alguna otra sorpresa para los asistentes.

Este año, vamos a aprovechar el Simposio para renombrar uno de nuestros edificios como Edificio Margarita Salas, investigadora de referencia reconocida mundialmente que ha sido un modelo en el que todos nuestros jóvenes investigadores quieren reflejarse

Como en años anteriores, desde la Facultad, Centro que aporta la infraestructura y los recursos necesarios, y anima a la organización, 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. Al Rector por su apoyo a estos Simposios no solo ahora, sino desde que ejercía como Vicerrector de Política Científica. 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’*

Mª Elena Alañón Pardo, *‘Food Sciences and Technology’*

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

Comité Organizador:

Ines Maria Ramos Monje, *‘Food Sciences and Technology’*

Manuel Bartolomé Díaz, *‘Analytical Chemistry’*

María Inmaculada Aranda Díaz-Lucas, *‘Physical Chemistry’*

Josué Muñoz Galindo, *‘Organic Chemistry’*

Pablo Belmonte López, *‘Chemical Engineering’*

María Crespo Gutiérrez, *‘Biochemistry’*

Estamos encantados de retomar durante los días 22, 23 y 24 de Junio la iniciativa del **“Young Science Symposium“**, siendo este año su **decimosexta 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 2022, se concederá el **“VII PRIZE OF YOUNG SCIENCE FACULTY OF SCIENCES AND TECHNOLOGY”**. Asimismo, se otorgará cuatro premios dentro de **“**II PREMIO VIRTUAL-FLASH en categoría TFG, TFM y tesis**”** al 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, 22nd June 2022

9:30- Opening ceremony chaired by the Rector Magnificus of the UCLM, Dr. Ricardo Cuevas (General Director of Universities, Research and Innovation of the Regional Government of Castilla-La Mancha) and the Dean of the Faculty of Chemical Sciences and Technology. (Link to session)

10:00- Invited Lecturer: Prof. Javier García-Martínez (University of Alicante) International Union of Pure and Applied Chemistry (IUPAC) President.

11:00- Invited Lecturer: Dr. Ricardo Cuevas Campos (General Director of Universities, Research and Innovation of the Regional Government of Castilla-La Mancha).

11:30- Coffee Break.

12:00- Rebranding of building "Margarita Salas".

12:30- Invited Lecturer: Dr. María A. Blasco (Director of the Spanish National Cancer Research Centre (CNIO) and Head of the Telomeres and Telomerase Group – CNIO).

16:00- 1st session

- *"A new methodology for the quantification of graphene oxide in water sample". **Elena Briñas.** Organic Chemistry.*
- *"PI3Kα inhibition using nanoparticles conjugated with the anti EGFR antibody Cetuximab for the treatment of Head and Neck Squamous Cell Carcinoma". **Almudena del Campo.** Inorganic Chemistry.*
- *"Persulfates electrogeneration using BDD anodes and 3D-printed reactors". **María del Pilar Castro.** Chemical Engineering.*
- *"Enhanced antitumoral activity when combining PARP inhibitors with encapsulated BET inhibitors for the treatment of BRCA-mutated cancers". **María de Gracia Arenas**. Inorganic Chemistry.*
- *"Improvement of the texture of non-fat yogurt with autochthonous exopolysaccharides-producing lab strains". **Inés María Ramos**. Food Sciences and Technology.*

17:15- 2nd session

- *"Novel and sensitive electrochemical approach based on an assembly nanocomposite with chitosan and ɣ-cyclodextrin-graphene quantum dots modified spces for the full sensing of fluoroquinolones in alimentary samples". **Manuel Bartolomé**. Analytical Chemistry.*
- *"Role of PPARβ/δ in the hippothalamic action of leptin. Implication on the inflammatory response and the control of food intake and energy expediture". **Carmen Soriano**. Biochemistry.*
- *"Strategies for robust designs in toxicologial tests". **Sergio Pozuelo**. Mathematics.*

- *"Atmospheric chemistry of hydrochlorofluoroolefins (HCFO): why is it important?". **Maria Areti**. Physical Chemistry.*
- *"Study of Process variables on the microcellular foaming of different TPUs using supercritical* CO_2*". **Pablo Belmonte**. Chemical Engineering.*

Thursday 23rd of June 2022

9:00- 3rd session

- *"Bilayer hydrogel in drug delivery". **Carlos Martín**. Organic Chemistry.*
- *"Behaviour of oenological microorganism after microwave treatments". **Raquel Muñoz.** Food Sciences and Technology.*
- *"Novel carbon-based catalysts for hydrogen production from ammonia decomposition reaction" **Marina Pinzón.** Chemical Engineering.*
- *"Sulfonate-based hydrogels: new soft scaffolds for biomedical applications". **Josué Muñoz**. Organic Chemistry.*
- *"Calcium complexes as catalysts for activation of small molecules"**. Enrique Francés.** Inorganic Chemistry.*
- *"Fluorescent discrimination between free and nanoencapsulated quercetin by a quenching responsive nanotool based on S,N-graphene quantum dots". **Natalia Villamayor**. Analytical Chemistry.*

10:30- Invited Lecturer: Dr. Jordi Mayneris Perxachs (Girona Biomedical Research Institute (IDIBGI), Spain). *"Feeling Gut? Microbiota, Memory, and Emotions".*

11:30- Break

12:00- 4th session

- *"Effect of glutamate intake during gestation on the cerebellum of pregnant rats and their fetuses: an overview of the state of receptors and oxidative stress". **Adrián Tejero**. Biochemistry.*
- *"Rational design of D-A-D naphthalendiimide and perylenediimide with potential application as N-type semiconductors in organic field-effect transistors". **Abelardo Sánchez.** Organic Chemistry.*
- *"BTX enhancement production through catalytic co-fast pyrolysis of agricultural waste". **Ángel Alcázar**. Chemical Engineering.*
- *"Mango by-products: from waste to functional ingredients". **Rodrigo Oliver.** Food Sciences and Technology.*
- *"Gas-phase reactivity at ultra-low temperatures for the study of interstellar chemistry". **Daniel González.** Physical Chemistry.*
- *"One-component iron complexes for the synthesis of industrial products". **Maria del Prado Caballero**. Inorganic Chemistry.*

16:00- Invited Lecturer: Dr. Daniel Peters (Newcastle Univ., UK). *"A journey through the valley of death: commercialization of academic research from the perspective of a post-doc".*

17:00- 5th session

- *"Production of a heterologous ferulic acid decarboxylase enzyme from Klebsiella Pneumoniae TD 4.7 and application of the enzyme in the production of 4-vinylguaiacol"*. **Maite Bernardo Correia**. *Food Sciences and Technology*.
- *"Comparison of the effect of ozone and chlorine dioxide dosing on hospital urine polluted with pharmaceuticals".* **Ángela Moratalla.** *Chemical Engineering.*
- *"Signal transduction pathways in a tumoral cell line: what about cholesterol metabolism?".* **Clara Fructuoso.** *Biochemistry.*
- *"Potential of sunlight in the treatment of diseases: photodynamic therapy at ultra-low doses to treat cancer".* **Carlos Gonzalo**. *Inorganic Chemistry.*
- *"New materials for soft robots".* **Francisco Javier Patiño**. *Organic Chemistry.*

Friday 24th of June 2022

9:00- 6th session

- *"A novel NiFe/NiFeO catalytic bilayer structure prepared by magnetron sputtering for hydrogen energy saving production via urea assisted water electrolysis"*. **Celia Gómez**. *Chemical Engineering.*
- *"Proteomic evaluation of intestinal function after dietary supplementation with grape seed polyphenols".* **Eduardo Guisantes.** *Food Sciences and Technology.*
- *"Anthropomorphic hydrogel-based phantoms for microwave imaging medical applications".* **Daniel Álvarez**. *Organic Chemistry.*
- *"Kinetic study of the Cl atom reaction of biogenic aldehydes in the atmosphere".* **María Asensio**. *Physical Chemistry.*

10:00- 7th session

- *"Organolithium Chemistry under Sustainable Conditions: Synthesis of Amidines and Guanidines"*. **Blanca Parra. *Inorganic Chemistry.***
- *"Bioleaching of real mine tailings using autochthonous microorganisms: effects of ultrasounds pretreatment".* **Irene Acosta. *Chemical Engineering.***
- *"Chitosan hydrogels: tissue engineering applications and magnetic properties".* **Irene San Millán. *Organic Chemistry.***
- *"Anisotropy Engineering with Highly Corrugated Magnetic Thin Films"***. Rafael Delgado. *Physics.***

11:00- Break

11:30- Presentation of the Territorial Section of the Royal Spanish Society of Chemistry (STCLM-RSEQ). María Antonia Herrero Chamorro

11:45- Raquel Reina. Catedra de Innovación Incarlopsa-UCLM

12:00- Miguel Martínez, AGROVIN.

12:15- ***Invited Lecturer: Ana Belén Cifuentes. Assistant Director for Safety, Environment and Quality at REPSOL.***

13:15- 13:15- Colloquium, Prize winners and Closing Ceremony chaired by the Dean of the Faculty of Chemical Sciences and Technology and Prizes sponsors”.

INVITED SPEAKERS

CI-1

CIRCULAR CHEMISTRY: DESIGNING A NEW ECONOMY AT MOLECULAR SCALE

J. García Martínez

International Union of Pure and Applied Chemistry, email: jgarcia-martinez@iupac.org

Chemistry is usually defined, conceived, and taught as the science of transformation. To adapt to the circular economy, chemistry must evolve towards being the science (and industry) of reuse. We cannot continue to extract, emit, and dispose at the levels we are doing now without compromising our climate, the environment, and our health. If we want to have a viable industry and a healthy planet, the circular economy cannot be just an aspiration but the key objective of chemistry. [1]

Rethinking chemistry for a circular economy involves profound changes, from the way molecules are conceived to how processes are designed to ensure traceability, recyclability, and reuse [2]. Circularity at the molecular level means turning chemistry toward the reuse of atoms, molecules, monomers, polymers, etc—and represents an opportunity to place chemistry at the center of the new circular economy. [3] Several examples of circular economy will be presented, including the design of a new generation of plastics with break-points [4] or dynamic bonds [5] that allow for their disassembly into their monomers and their reconstruction. This process can be done at ca. 100 % yield and multiple times. These and other examples of circular chemistry will be described in detail and an outlook of the area will be provided.

Finally, I will comment on some of the actions that we are promoting from the International Union of Pure and Applied Chemistry (IUPAC) for the promotion of green chemistry and research, education and chemical industry that contribute to the sustainability of our economy. Especially, I will mention the activities that we are carrying out during the International Year of Basic Sciences for Sustainable Development.

References

1. The Circularity Gap Report, CGRi, 2019, https://www.circularity-gap.world/
2. J. García-Martínez, *Angew. Chem. Int. Ed.*, **60** 4956 (2021)
3. P. G. Levi, J. M. Cullen, *Environ. Sci. Technol.* **52** 1725 (2018)
4. M. Häußler et al, *Nature* **590**, 423 (2021)
5. PR Christensen, *Nature Chemistry* **11** 442 (2019)
6. F. Gomollón, J. García-Martínez, *Nature Chemistry*, **14**, 113 (2022)

Javier García Martínez

President of the International Union of Pure and Applied Chemistry. President of the Young Academy of Spain. Professor of Inorganic Chemistry at the University of Alicante and Professor of the Rafael del Pino Foundation. Trustee of the Gadea Foundation for Science.

CI-2

Plan regional de Investigación Científica, Desarrollo Tecnológico e Innovación

Ricardo Cuevas Campos

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JCCM

CI-3

Envejecimiento como origen de las enfermedades

María A. Blasco

Director of the Spanish National Cancer Research Centre (CNIO)
Head of the Telomeres and Telomerase Group – CNIO

16th YOUNG SCIENCE SYMPOSIUM, FACULTY OF CHEMICAL SCIENCES AND TECHNOLOGIES, UCLM

Maria A. Blasco obtained her PhD in 1993 at the *Centro de Biología Molecular "Severo Ochoa"* under the supervision of M. Salas. That same year, Blasco joined the *Cold Spring Harbor Laboratory* in New York (USA) as a Postdoctoral Fellow under the leadership of C. W. Greider. As a postdoc she isolated one of the telomerase essential genes and generated the first telomerase deficient mouse model, which served to demonstrate the importance of telomerase in telomere maintenance, chromosomal instability and disease. In 1997, she returned to Spain to start her own research Group at the *Centro Nacional de Biotecnología* in Madrid. She joined the Spanish National Cancer Research Centre (CNIO) in 2003 as Director of the Molecular Oncology Programme and Leader of the Telomeres and Telomerase Group. In 2005, she was also appointed Vice-Director of Basic Research at CNIO. Since June 2011, she is the CNIO Director.

For more than 20 years, Blasco´s work has focused in demonstrating the importance of telomeres and telomerase in cancer, as well as in age-related diseases. Blasco has published more than 250 papers in international journals and has an h-index of 81. Her achievements have been recognized by the following international and national awards: Josef Steiner Cancer Research Award, Swiss Bridge Award for Research in Cancer, Körber European Science Award, the EMBO Gold Medal, the Rey Jaime I Award in Basic Research, the Fundación Lilly Preclinical Research Award, and the Santiago Ramón y Cajal National Award in Biology. Blasco holds two Doctorate Honoris Causa from the *Universidad Carlos III* of Madrid and from *Universidad de Alicante* and in October 2017 she received the Scientific Merit Award of the *Generalitat Valenciana*.

CI-4

Feeling Gut? Microbiota, Memory, and Emotions

Jordi Mayneris Perxachs

Biosciences Institute, Medical School, Newcastle University, Newcastle upon Tyne, UK;
e-mail: daniel.peters@newcastle.ac.uk

Dr. Jordi Mayneris-Perxachs holds two BSc in Chemistry and Food Science and Nutrition and a PhD in Theoretical and Computational Chemistry. He is an expert in Systems Biology and Omics Sciences, particularly metabolomics, metagenomics and transcriptomics. He acquired most of this expertise during a four-year postdoctoral stay (2011-2015) at the University of Reading and Imperial College London (UK) under a Marie Curie COFUND programme. There, he pioneered the description of gut microbial-derived alterations in Tryptophan metabolism with undernutrition and environmental enteropathy applying a metabolomic approach. In 2015, he was granted a Marie Curie fellowship (Tecniospring programme) to join the Units of Nutrition and Omics Science at the Technology Centre of Catalonia (EURECAT). In 2019, he was granted a Miguel Servet (ISCIII) and joined the Girona Biomedical Research Institute (IDIBGI), where he leads the Integrative Systems Medicine research. He applies cutting edge post-genomic technologies combined with advanced computational techniques (*i.e.,* machine learning) in large human cohorts and pre-clinical models to obtain a holistic view of the holobiont and unravel the molecular mechanisms underlying the pathogenesis of cardiometabolic disease and cognitive performance, with particular emphasis on the complex microbiome-host interplay. He has led the discovery of microbial profiles and functional signatures linked to memory, inhibitory control, depression and fatty liver, publishing the results in high-impact journals such as Cell Metabolism (IF=27.287), Gut (IF=23.059), Cell Host & Microbe (IF=21.023) and Microbiome (IF=14.652).

CI-5

A journey through the valley of death: commercialization of academic research from the perspective of a post-doc

D.T. Peters

Biosciences Institute, Medical School, Newcastle University, Newcastle upon Tyne, UK;
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The “Valley of Death” is a term used to describe the gap between research and its successful commercial application. The challenges involved in this process are immense, and the failure rate of new start-up companies is high. It can be especially daunting for early career researchers, who have often spent many years training to do specialist research, to consider the new skills and mindset needed to develop a successful business. However, there is a great overlap between the skills required by an entrepreneur and those possessed by an early career researcher. Government and industry have also developed programmes and mentorship networks to help researchers transition from academia to business to commercialise their technologies and drive innovation. Finally, as competition for permanent academic positions intensifies, the spin out route can provide an attractive alternative for scientists who are keen to continue their research and make an impact on the wider world.

In this talk, I will describe my experience so far of the journey towards forming a spin-out company and how, as a post-doc, I have begun learning the required skills, including the importance of understanding and identifying the commercial value of a technology, the advantages of market discovery and training programmes, and the benefits of social media for building networks.

References

[1] Overcoming the Valley of Death: A New Model for High Technology Startups. *AA. Gbadegeshin, A. Al Natsheh, K. Ghafel, O. Mohammed, A. Koskela, A. Rimpiläinen, J. Tikkanen, and A. Kuoppala.* ***Sustainable Futures (2022) 4 100077***

CI-6

LIDERAZGO INSPIRADOR: PALANCA CLAVE PARA LA INNOVACIÓN

Ana Belén Cifuentes

Assistant Director for Safety, Environment and Quality at REPSOL

16th YOUNG SCIENCE SYMPOSIUM, FACULTY OF CHEMICAL SCIENCES AND TECHNOLOGIES, UCLM

CI-7

R&D IN INCARLOPSA

R. Reina

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Área de conocimiento

Brief summary of how the R&D department is organized within the Incarlopsa group; as well as an explanation of the main projects that are being worked on.

ORAL SPEAKERS

(Appearance in order according to the SYMPOSIUM PROGRAMME)

O-1

A new methodology for the quantification of graphene oxide in water sample

Elena Briñas Gutiérrez, Viviana Jehová González, María Antonia Herrero, Mohammed Zougagh, Ángel Ríos, Ester Vázquez

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Organic Chemistry

The use of graphene oxide (GO) increases in many products due to its vast number of excellent properties [1]. However, this extensive use in real-world applications has increased their potential release into the environment. In order to evaluate their possible health and ecological risks, there is a need for analytical methods that can quantify these materials at very low concentrations in environmental media such as water. One of the most sensitive analytical techniques is Raman spectroscopy (Fig. 1), specifically its most innovative variant, surface-enhanced Raman scattering (SERS) [2]. SERS is a good alternative for detecting GO with high selectivity and sensitivity. Indeed, given its potential for extremely high enhancement levels, SERS transforms Raman spectroscopy from a structural analytical tool to a structurally sensitive single-molecule probe [3].

Therefore, a new method for detecting and quantifying GO in aqueous samples is showed in this work [4]. The final methodology has been optimized and has shown is simple, useful, and effective in water samples. This method is able to detect GO in the concentration range of 0.1–10.0 ppb (Figure 1). The practical limit of quantification achieved is 0.1 ppb. This method shows high reproducibility and repeatability. Tests have been applied to real samples, showing good selectivity. And finally, in the case of accuracy, the recoveries obtained ranged from 95.66% to 100.47%.

References

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[4] E. Briñas, V. Jehová González, M. A. Herrero, M. Zougagh, A. Ríos, E. Vázquez. *Environmental Science & Technology*. Sent.

O-2

PI3Kα inhibition using nanoparticles conjugated with the anti EGFR antibody Cetuximab for the treatment of Head and Neck Squamous Cell Carcinoma

Almudena del Campo*, Carmen Segrelles, Alberto Juan Ignacio Silva, Iván Bravo, Jorge Peral, Alberto Ocaña, Pilar Clemente-Casares, Carlos Alonso-Moreno, Corina Lorz

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Química inorgánica

Even though surgery approaches, radiation therapy and the use of therapeutic agents, the prognosis of head and neck squamous cell carcinomas (HNSCC) remains poor with tendency to develop recurrence and/or metastasis. In this regard, Inhibition of PI3Kα is a promising therapeutic approach for the treatment of this tumor type[1]. Epidermal growth factor receptor (EGFR) is overexpressed in over 90% of head and neck tumors[2] and, therefore, targeted therapies based on the antibody targeting EGFR is an alternative to be pursued. In this study, by the generation of anti-EGFR conjugated nanoparticles (ACNPs) for the controlled release of Alpelisib, a PI3Kα inhibitor in clinical use, we propose a more efficient therapy for the treatment of HNSCC. Our study shows that the use of ACNPs aim to improve therapeutic efficacy by increasing the tumor concentration of Alpelisib which may reduce drug exposure in disease-free organs. The Alpelisib-loaded nanoparticles generated significantly enhanced efficacy *in vitro* in comparison with the free drug. These results proposed a novel strategy based on nanotechnology to enhance the efficacy of Alpelisib and diminish toxicity in patients with HNSCC.

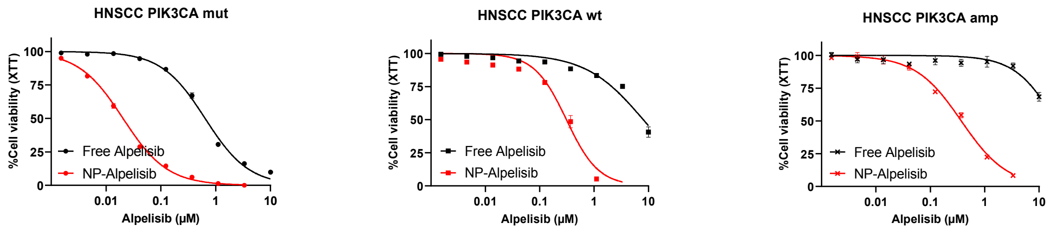

Figure 1. Antiproliferative effects induced by free Alpelisib and Alpelisib encapsulated in nanoparticles in three different cell lines at 72 hours.

References

[1] Elkabets M, Pazarentzos E, Juric D et al. AXL mediates resistance to PI3Kα inhibition by activating the EGFR/PKC/mTOR axis in head and neck and esophageal squamous cell carcinomas. Cancer Cell 27(4), 533–546 (2015).

O-3

Persulfates electrogeneration using BDD anodes and 3D-printed reactors

M. Pilar Castro*, Miguel A. Montiel, Ismael F. Mena, Cristina Sáez, Manuel A. Rodrigo

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Ingeniería Química y Ambiental

Nowadays, one of the most important environmental problems is the pollution of liquid effluents due to the wide variety of refractory species that biological processes cannot treat. In this sense, the generation of oxidant species with high stability and high activity in the degradation of persistent pollutants emerges as an interesting alternative to traditional processes. Among the different technologies, electrooxidation with conductive diamond electrodes is one of the most efficient processes in the generation of oxidants due to the use of these diamond anodes favors the massive generation of strong reactive oxygen species, mostly hydroxyl radicals ($HO^\bullet$), at the surface of the anode [1]. The $HO^\bullet$ produced react with other ions contained in wastewater favoring the production of other powerful oxidants. Among them, persulfates, widely used in many applications, are generated in presence of sulfate ions. Moreover, boron-doped diamond (BDD) anodes present higher chemical and electrochemical stability than other electrode materials, making them a good choice for persulfate generation [2]. Nevertheless, for its large-scale application, there are still many aspects to improve, some of which are addressed in this work. Therefore, this work is focused on the persulfate electrogeneration using BDD anodes with a novel 3D printing designed electrochemical reactor, paying attention to the influence of the key operation parameters (temperature, pH, current density, and electrolyte concentration) to determine the best conditions to produce persulfates efficiently and eco-friendly. This will not only contribute to the optimization of the persulfate generation process but also relevant economic savings in terms of materials and operational time can be achieved. Results show that the conductive diamond electrolysis of 1M of H_2SO_4 generates up to 0.2 M of persulfate with an anodic efficiency of 80%, being current density a key operation parameter with an optimal value of 300 $mAcm^{-2}$.

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O-4

Enhanced antitumoral activity when combining PARP inhibitors with encapsulated BET inhibitors for the treatment of BRCA-mutated cancers

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Química Inorgánica

BRCA1/2 protein deficient or mutated cancers comprise a group of aggressive malignancies. Although PARPis have shown great efficacy in their treatment, the widespread use of these agents in clinic is restricted by various factors, including the development of acquired resistance due to the presence of compensatory pathways [1]. BETis can disrupt the HR pathway completely by repressing the expression of BRCA1 and could aim at generation combination regimes to overcome PARPis resistance and enhance PARPis efficacy [2].

Due to the poor pharmacokinetic profile and short half-life [3], the first in class BETi, JQ1, were loaded into newly developed nanocarrier formulations to improve the effectivity of Olaparib for the treatment of BCA-mutated cancers. First, polylactide polymeric nanoparticles were generated by double emulsion. Also, liposomes were prepared by injection and evaporation solvent method. JQ1-loaded drug delivery systems display optimal hydrodynamic radii between 60 and 140 nm with a very low polydispersity index (PdI), and encapsulation efficiencies of 98 and 45% for lipid- and polymeric-based formulations, respectively. Formulations show high stability and sustained release. We confirmed that all assayed JQ1 formulations display improved anti-proliferative activity compared to the free JQ1 in models of ovarian and breast cancers. In addition, synergistic interaction between JQ1 and JQ1-loaded nanocarriers and Olaparib evidenced the ability of encapsulated JQ1 to enhance antitumoral activity of BETis. In vivo studies validate the encapsulation of JQ1 as an efficient approach to combination therapies for the treatment of BRCA-mutated cancers.

Overall, these novel formulations may represent an efficient and safer JQ1-delivering alternative to enhance efficacy of Olaparib for BRCA-mutated cancer treatment.

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O-5

Improvement of the texture of non-fat yogurt with autochthonous exopolysaccharides-producing LAB strains

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Food science and technology

Fermented foods have been consumed over the years and during this time they have been modified and improved according to trends and scientific advances. For some time now, consumers have been demanding more healthy and safe foods with as few additives as possible. Among these fermented foods is yogurt, which is consumed by the population almost every day. In the search for healthier foods, non-fat yoghurts were elaborated, which provide the nutrients of a traditional yogurt with less fat. However, the production of this product requires the use of thickeners to obtain the texture characteristics of a full fat yogurt. In the search to improve the texture of non-fat yogurts, exopolysaccharides (EPS) have begun to be used, which are carbohydrate polymers capable of producing thickening or gelling, providing products with pleasant rheological and sensory properties. These compounds are synthesised by microorganisms such as *Leuconostoc* and *Lactobacillus,* which are genera of lactic acid bacteria used in food processing.

In this work, experimental non-fat yogurts were produced with the addition of previously selected autochthonous EPS-producing LAB strains. Two strains of *Leuconostoc* (Ln2 and Ln6) and one of *Lactobacillus* (Lb47) were used to obtain non-fat yoghurts with the texture and organoleptic characteristics of this product, without the addition of thickeners or gelling agents as additives. The experimental yogurts were analysed physico-chemically, microbiologically and sensorially during a storage period of 28 days at 4ºC. EPS production by the inoculated bacteria was found in all of them. Experimental yogurts were obtained with the characteristics of non-fat yogurts and no defects were found in any of them.

O-6

Novel and sensitive electrochemical approach based on an assembly nanocomposite with chitosan and ɣ-cyclodextrin-graphene quantum dots modified SPCEs for the full sensing of fluoroquinolones in alimentary samples

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Química Analítica

Fluoroquinolone (FQs) antibiotics have been used in an abusive way within the alimentary industry in the last decades, leading to the appearance of quinolone resistant microorganisms and reducing so the effectiveness of FQs-based drugs for the treatment of infection diseases at both animal and human levels[1]. In consequence, diverse international organizations have established legislation regarding the maximum amount of quinolones allowed in food[2]. A new electrochemical platform based on screen printed carbon electrodes (SPCE), modified with a nanocomposite material assembled from gamma cyclodextrins functionalized graphene quantum dots and chitosan (δCDs-GQDs-CHI), has been reported and applied for the first time to evaluate the global amount of fluoroquinolones in food samples from animal origin. Electrochemical properties of the sensing nanocomposite were assesed by cyclic voltammetry (CV), showing improved electrocatalytic performance throughout evaluation of relevant electrochemical features as electronic transfer rate (K^0), electroactive area (A) and double capacitance layer (Cdl). 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 a single oxidation mechanism for all FQs, also here elucidated. Developed sensor shows boosted analytical performance in terms of linear range (4 – 250 µM) and lower detection limit (LOD = 1.2 µM). The designed approach allowed the determination of FQs global contain in broths, bouillon cubes and milkshakes at three concentration levels (150, 75 and 37.5 µM) for both equimolar and different ratio FQs mixtures with recoveries values ranging from 90 to 106%.

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O-7

Role of PPARβ/δ in the hypothalamic action of leptin. Implication on the inflammatory response and the control of food intake and energy expenditure.

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Bioquímica

Leptin is an adipokine that acts at the hypothalamic and media level in the maintenance of energy homeostasis and the control of intake. PPARβ/δ is a transcription factor involved in lipid metabolism and the inflammatory response. The relationship between leptin and PPARβ/δ in different peripheral tissues is known, however, at the hypothalamic level it has not been fully clarified. The main objective of this work was to study the role of PPARβ/δ in the action of leptin in the hypothalamus and its relationship with the modulation of the inflammatory response and the production of neuropeptides involved in the control of energy intake and metabolism.

GSK0660, a PPARβ/δ antagonist, was used and administered intraperitoneally (IP) for 7 days to 3-month-old Wistar rats, which were simultaneously administered leptin or saline intracerebroventricularly via osmotic minipumps. On the hypothalamic tissue, the expression levels of PPARβ/δ were analysed together with their targets. Thus, it was observed that the combined administration of leptin and GSK0660 produced a decrease in the levels of these factors, demonstrating that the PPAR antagonist was able to cross the blood-brain barrier. The effect that PPARβ/δ had on the leptin pathway was studied. The transcription factor increased the pathway activation by increasing levels for the adipokine receptors and for SOCS3 and pY727-STAT3. In addition, the involvement of PPARβ/δ in the neuroendocrine activity of leptin was determined. The results obtained showed that GSK0660 caused an increase in the secretion of orexigenic factors (NPY) and a decrease in the anorectic ones (POMC, TRH, CRH), contrary to the effect of leptin. Finally, the involvement of PPARβ/δ in the hypothalamic inflammatory response was determined. Blocking this factor increased the levels of pro-inflammatory factors (CCL5) and microglial and/or macrophages and astrocytes markers (Iba1 and GFAP, respectively). On balance, the values obtained seem to show that PPARβ/δ is involved in the hypothalamic functions of leptin and that it would have an anti-inflammatory effect at this level.

O-8

STRATEGIES FOR ROBUST DESIGNS IN TOXICOLOGICAL TESTS

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Estadística e Investigación Operativa

Toxicological tests are widely used to study toxicity in aquatic environments. Reproduction is a possible endpoint of this type of experiment, whose response variable is given by counts. There is a literature on the most suitable probability distribution to be used for analyzing the data. In the theory of optimal experimental design, the assumption of this probability distribution is essential, and when this assumption is not appropriate, there may be a loss of efficiency in the design obtained. The main objective of this study is to propose robust designs when there is uncertainty about the probability distribution of the response variable. Three different strategies for attaining this goal are introduced and compared, and they are then applied to toxicological tests based on and *Lemna minor*. In addition, a simulation study is performed to test the estimation properties of the robust designs obtained.

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O-9

Atmospheric chemistry of Hydrochlorofluoroolefins(HCFO): Why is it important?

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Química Física

Halogenated unsaturated olefins, i. e., Hydrofluoroolefins (HFO) have been recently proposed as Hydrofluorocarbons (HFC) replacements. Although CFC and HCFC are controlled by the Montreal protocol and its amendments, the high atmospheric reactivity of the double bonds in Hydrochlorofluoroolefins (HCFO) towards atmospheric oxidants like OH radicals or Cl atoms prohibits them from being transferred in the stratosphere leading to short tropospheric lifetimes, very low GWPs[1] and negligible ODPs. Further, the presence of the C-Cl bonds along with the C-F enhances the required physicochemical properties of HCFO,[2] extending the field of their potent applications. As of today, $CF_3CF=(Cl)CH$ and $CF_3CH=(Cl)CH$ are already used as refrigerants and blowing agents.[3, 4] However, HCFO are not included in the Paris Agreement and they are not regulated by the Kigali Amendment of the Montreal Protocol, while at the same time, there are very limited data regarding their atmospheric reactivity and almost none about their oxidation end-products. Prior to their extensive production and use, the full atmospheric lifecycle of HCFO needs to be assessed so as to evaluate their impact on climate change and air quality. In this study the reaction kinetics of OH radicals with $CF_3(Cl)C=CCl_2$, at atmospherically relevant temperatures will be investigated in the department of Physical Chemistry of UCLM, employing the Pulsed Laser Photolysis/Laser Induced Fluorescence (PLP/LIF) technique[5] and a smog simulation chamber[6].

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O-10

STUDY OF PROCESS VARIABLES ON THE MICROCELLULAR FOAMING OF DIFFERENT TPUS USING SUPERCRITICAL CO_2.

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Ingeniería Química

Polyurethanes (PU) are part of the "big six", a group gathering the six most important plastic materials worldwide for their use and economic value. The main problem derivate from the extensive use of these materials is the high number of wastes related to their synthesis and what to do with these materials after their lifetime. For this reason, the present work proposes as an alternative to the traditional recycling of thermoplastic polyurethane the foaming of this material using supercritical CO_2.

The present work is focused on the study of the influence and significance of temperature, pressure, and contact time with the supercritical CO2 in the foaming of thermoplastic polyurethanes (TPU). To carry out the study of these variables, four commercial TPUs were selected.

The following range of conditions were studied, using a design of experiments and an statistical software to analyze the data (Statgraphics):

- Temperature: 100 ºC – 120 ºC
- Pressure: 100 bar – 200 bar
- Contact time: 1 h – 3 h

TPUs were characterized using DSC and TGA analysis to determine the melting point and the thermal degradation temperature of the polymer. Once foaming experiments were done, the density of the foams obtained was measured using a 3D scanner SEM analysis were also performed with the aim of analyzing the foam structure obtained. Using the information provided by the density measurement and SEM, cell density (Nf), average cell size (D), and expansion ratio (**ϕ**) were calculated for the different conditions studied.

O-11

Bilayer hydrogel in drug delivery

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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.[1] 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. In this work, in order to combine the advantages of synthetic and natural hydrogels, a bilayer hydrogel is prepared: a smart synthetic hydrogel layer that will respond to external stimuli attached to a natural hydrogel layer, where the cell culture will be performed (Figure 1). The swelling degree of both gels, their internal structure using the scanning electron microscopy technique and their mechanical properties (Young's modulus and viscoelasticity) have been analyzed. In addition, the release of rhodamine 101 from these gels has been studied in response to a magnetic stimulus.

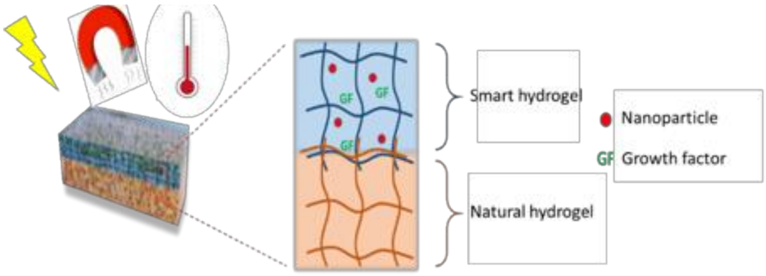

Figure 1: Bilayer hydrogel

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O-12

BEHAVIOUR OF OENOLOGICAL MICROORGANISM AFTER MICROWAVE TREATMENTS

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Tecnología de Alimentos

Microwave has been more frequently used in food industries to enhance or replace conventional techniques. The present study will focus on the application of microwaves (MW) on microorganisms to evaluate its effect with different treatment conditions of power, duration and presence of pulses on Saccharomyces and non-Saccharomyces yeasts and *Lactiplantibacillus plantarum*; studies of viability and vitality were carried out after treatments. MW affected all microorganisms in different ways depending on the applied treatment and on the microorganism. In general, S. cerevisiae and non-Saccharomyces yeast were less resistant than *L. plantarum.* Counts immediately after treatment showed influence reaching even inactivation. Nevertheless, maximum OD after 96h presented values closer to the controls (microorganisms not treated). This effect shows that in some cases the treatment exerts an antimicrobial effect immediately after application, but after some time, microorganisms can restore their biological structures and growth, which is reflected in an increase of lag phase. On a few occasions, treatments were also able to improve the kinetic parameters. Thus, this technique could be useful for inactivation, attenuation, or even activation of associated food microorganisms.

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O-13

NOVEL CARBON-BASED CATALYSTS FOR HYDROGEN PRODUCTION FROM AMMONIA DECOMPOSITION

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Chemical Engineering

Currently the success of the 'hydrogen economy' depends on the current hydrogen (H_2) storage and transport routes, which are characterized by their high costs (high pressures or low temperatures)[1]. A potential solution to this issue comprises the utilization of molecules that contains hydrogen in its structure such as ammonia (NH_3). Because of high hydrogen content, mature technology and relatively low cost (easy liquefaction), and carbon-free molecule, ammonia has gained attention as 'hydrogen carrier' to generate H_2. Unfortunately, H_2 from NH_3 requires an efficient catalyst to achieve high conversion at low reaction temperatures. Recently, attractive results have been obtained with carbon-based materials[2]. In this way, ruthenium (Ru) supported on reduced graphene oxide (rGO) were synthesized, characterized and tested for carbon-free H_2 generation from NH_3. Both amount of pre-reducing agent clearly (*y*C-rGO) and metal loading (*x*Ru/*y*C-rGO) influenced the catalytic properties (Ru particles size, electronic conductivity and basicity) and activity. Therefore, 2.5Ru/10C-rGO catalyst led materials with Ru size of 3.6 nm and the highest total basic sites (1.69 mmol CO_2 g_{cat}^{-1}), which allowed to achieve a 96 % of ammonia conversion at 400 °C. rGO proved to be a suitable support in the development of nanosized Ru catalysts being the optimal one highly active in hydrogen production during more than 60 h of reaction.

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O-14

SULFONATE-BASED HYDROGELS: NEW SOFT SCAFFOLDS FOR BIOMEDICAL APPLICATIONS

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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 trough the combination of natural and synthetic components.[1] In that sense, hydrogels have recently attracted much attention in the field of tissue engineering, having numerous applications, especially as scaffolds for cell cultures.[2] 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.[3]

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.

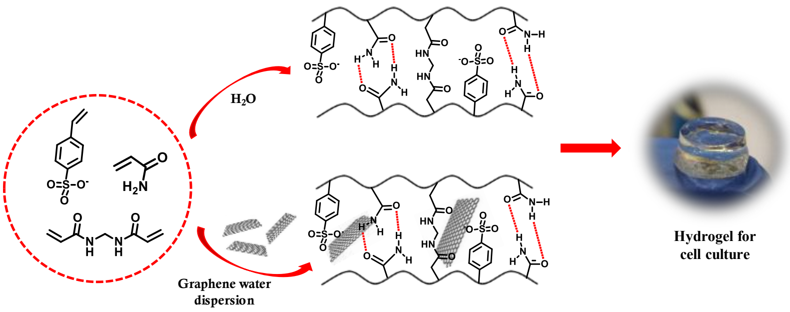

Figure 1. VBS based hydrogels in the presence and absence of graphene.

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O-15

Calcium complexes as catalysts for activation of small molecules

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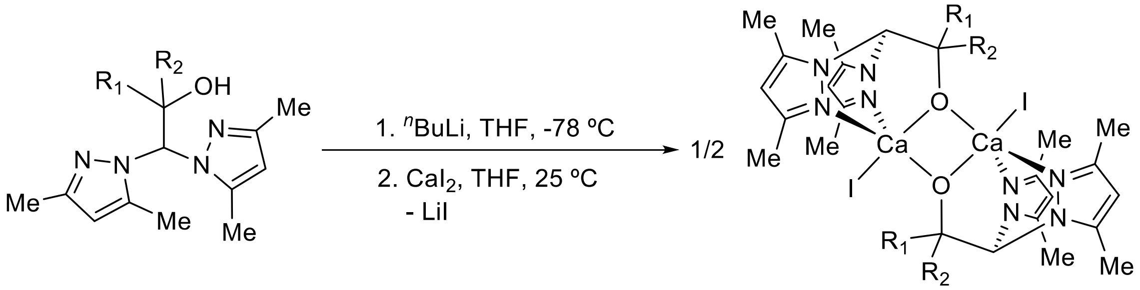
Química Inorgánica

In recent years, great advances have been made in the design of catalysts based on abundant and/or biocompatible metals for their use in the transformation of CO_2 into high value-added products. For instance, metals such as aluminium, iron, or zinc, have shown to be efficient catalysts for the synthesis of new organic molecules and polymeric materials with CO_2 in their structure [1]. In this sense, calcium is a metal that could also be especially useful in this type of catalytic process, considering its abundance, easy availability, and low cost. In addition, it is a biocompatible metal, so its use in processes that involve obtaining materials with subsequent applications in biomedicine is of great interest.

Despite all of this, there are hardly any studies to date on the use of calcium catalysts in CO_2 activation processes, so it is highly relevant to delve into the use of these metal complexes for this type of development [2]. In this context, new calcium complexes supported by heteroscorpionate ligands have been prepared by reaction of CaI_2 with the lithium salt of different bis(3,5-dimethylpyrazol-1-yl)methane-based ligands (Scheme 1). The reactivity of these complexes towards CO_2 and other small molecules has also been evaluated. Furthermore, these calcium compounds have been used as one-component catalysts for the synthesis of cyclic carbonates from epoxides and propargyl alcohols and CO_2 under mild reaction conditions.



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O-16

Fluorescent discrimination between free and nanoencapsulated quercetin by a quenching responsive nanotool based on S,N- graphene quantum dots

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Analytical Chemistry

A new smart nanomaterial based on sulfur and nitrogen co-doped graphene quantum dots (S,N-GQDs) has been synthetized for both detection and discrimination of free and encapsulated quercetin as nanoemulsions-loaded (Q and Q-Nes respectively). The sensing nanoprobe was reached by a hydrothermal single step through a bottom-up approach [1]. The presence of Q-NEs and free Q can quench the S,N-GQDs fluorescent intensity through an inner filter effect (IFE) mechanism exhibiting a dynamic quenching for Q-NEs and static one for free Q (**Figure 1**). A low energy method, such as phase inversion temperature method (PIT) was selected to synthesize Q-NEs [2]. The optimal Q-NEs composition (% w/w) was: 10% Miglyol 812, 0.25 % quercetin, 0.55 % ethanol, 7.4 % tween 80, 0.1 % soy lecithin and to 100 % of aqueous phase (MES buffer pH = 5.9). All synthesized nanomaterials were characterized through DLS, CLSM, SEM, HRTEM, XRD, FTIR, Raman, UV-Vis and fluorescence spectroscopies in order to describe their physic-chemical and nanostructural features.

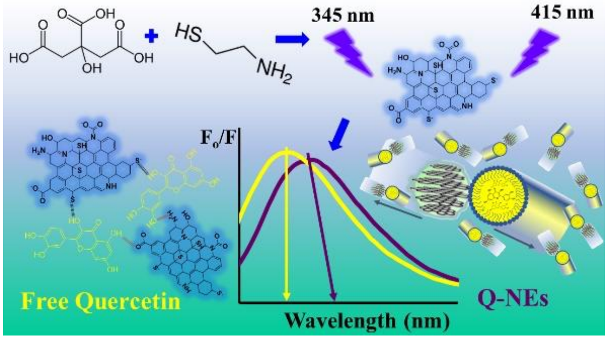

Figure 1. Discrimination between Q and Q-NEs through their quenching behaviour.

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O-17

Effect of glutamate intake during gestation on the cerebellum of pregnant rats and their fetuses: an overview of the state of receptors and oxidative stress.

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Neurochemistry

Glutamate is an amino acid present in proteins that we usually ingest in the diet, but its consumption has increased significantly since it is an important additive, responsible for the umami flavour, that enhances the flavour of foods. This amino acid is needed to synthesize endogenous proteins, but it also plays a fundamental role in the central nervous system (CNS), being the main excitatory neurotransmitter. At physiological concentrations, it participates in learning and memory processes, however, at high concentrations it acts as an excitotoxin producing cell degeneration and death. In fact, high concentrations of this amino acid have been associated with neurodegenerative diseases (ND). Glutamate and adenosine (which modulates glutamate level) receptors have been studied in different ND resulting in a significant alteration of its expression or affinity in different tissues. Not only that, but the study of the oxidative stress correlated with ND such as Alzheimer disease (AD) and Parkinson disease (PD) is key to understand the etiology of these diseases and to reach new strategies of early diagnosis and treatment. Previous studies of this group have shown that there is a change in the receptor expression in the brain of pregnant rats administered glutamate and their fetuses but is unknown what happens in the cerebellum of these animals. Cerebellum is abundant in neurons and it is responsible for motor, cognitive and emotional functions, and this structure can also be useful in the study of AD and PD. Therefore, the aim of this research is not only to analyze the receptors expression in the cerebellum, but also focus on the study of the oxidative stress associated to the consumption of glutamate. The state of the receptors seems to remain unaltered in cerebellum, unlike in brain, however the oxidative damage caused by glutamate consumption is significant as it is seen in enzymatic activities and peroxidation assays carried out on this samples. Further studies will be necessary to elucidate the importance of glutamate intake and its possible excitotoxicity in cerebellum of pregnant rats and their ability to cross the placental barrier.

O-18

RATIONAL DESIGN OF D-A-D NAPHTHALENDIIMIDE AND PERYLENEDIIMIDE WITH POTENTIAL APPLICATION AS n-TYPE SEMICONDUCTORS IN ORGANIC FIELD-EFFECT TRANSISTORS

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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-donor (D-A-D) architectures, making easier intramolecular charge transfer (ICT), necessary for this kind of devices. In this sense, naphthalenediimide (NDI) and perylenediimide (PDI) 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-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, D-A-D napthalenediimide and perylenediimide derivatives (Figure 1) with different alkynyl donor groups were chosen. Firstly, these compounds have been theoretically studied, then they were synthesized, and OFET devices were manufactured under different conditions. The results obtained from this study showed a behavior as n-type semiconductors with high electron mobilities, [1] improving the electrical efficiency with respect to previous D-A naphthalenimide derivatives described by our research group. [2]

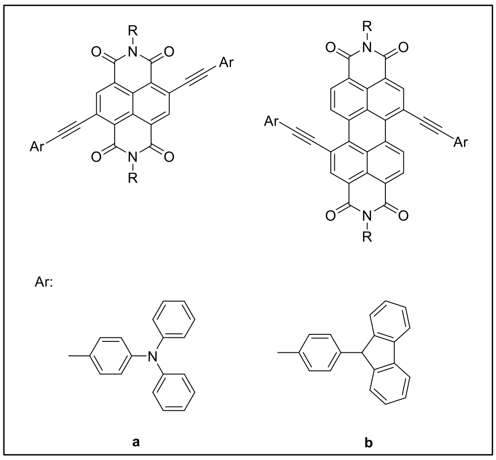

Figure 1. Different series of D-A-D naphthalenediimide and perylenediimide derivatives.

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O-19

BTX ENHANCEMENT PRODUCTION THROUGH CATALYTIC CO-FAST PYROLYSIS OF AGRICULTURAL WASTE

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Tecnología Química

Lignocellulosic biomass is an abundantly renewable feedstock for producing bio-oil with aromatic hydrocarbons via fast pyrolysis [1]. However, the bio-oil yielded has certain disadvantages in comparison to petroleum-derived oil: low calorific value, high viscosity, and thermal instability due to is composed of a mixture of oxygenated compounds. Moreover, the hydrogen-deficient nature of lignocellulosic biomass yields undesirable features in the bio-oil. Therefore, co-pyrolysis with hydrogen-rich material has become a simple way of enhancing both bio-oil quality and yields. To tackle the problems posed by bio-oil, plastic waste is presented herein as a solid feedstock for blending with biomass residue. Among the most used types of plastics, polyvinyl chloride (PVC) has attracted attention due to high consumption in recent years. Worldwide demand for PVC is expected to grow by 3.2% annually until 2023 [2]. To counter harmful emissions in PVC combustion by traditional plastic waste disposal techniques, enhanced recycling techniques that convert solid waste blends into high value-added products are urgently needed. To enhance the bio-oil obtained from co-pyrolysis, firstly, it must undergo catalytic upgrading using efficient catalysts to reduce its oxygen content and heavy hydrocarbons. Catalysts may be incorporated into co-pyrolysis, to remove oxygenated fractions via decarboxylation, dehydration and decarbonylation, to produce enhanced bio-oil. However, in combination with zeolites, some internal minerals in biomass, such as alkali and alkaline earth metals (AAEMs) could interact as catalysts and influence bio-oil yields and their composition [3]. This work addresses enhanced benzene, toluene and xylene (BTX) production by catalytic fast co-pyrolysis from agroindustrial biomass blended with PVC and the use of prepared NaZSM-5 and HZSM-5 zeolites. Moreover, the coupling effect of the AAEMs inherent to the biomass and zeolite on the production of aromatics was evaluated.

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O-20

MANGO BY-PRODUCTS: FROM WASTE TO FUNCTIONAL INGREDIENTS.

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Química analítica y farmacia

Mango (Mangifera indica) is the most harvested tropical fruit in the world and its processing activities generates unavoidable quantities of by-products, which are intrinsically rich in techno- and bioactive compounds. Since mango by-products have demonstrated to be a valuable source of bioactive compounds with antiproliferative activities against several cancer cell lines (1), mango kernel extract were tested in vitro on glioblastoma multiforme T98 and A172 cell lines and also nanoencapsulations of this extract have been developed to analyze its potential as a cosmeceutical ingredient to treat various skin conditions such as ageing or psoriasis.

Results showed that treatment with mango kernel extract (from 10 to 50 µg/ml at 72 h) was the most effective inhibiting cell proliferation in both lines tested, reaching up to 70 % of growth inhibition. Fluorescent microscopy showed dose-dependent deterioration of certain cellular structures, such as the nucleus (Hoescht 33342 dye), as well as the activation of astrogliosis processes (GFAP dye). These results suggests that Mango Kernel Extract might be a promising agent for the treatment of glioblastoma multiforme. In terms of nanovehiculization, all the formulations were executed using soy lecithin as encapsulating lipid and water as dispersant agent. The best performing formulations in terms of particle characteristics, bioactivity potential and skin penetration and diffusion were those containing 20% glycerol and 10% propylenglycol (some these assays are already ongoing at the time of submission of this abstract). Overall, these research lay the groundwork for future researches in which *in vivo* together with clinical studies should be carried out to evaluate the translational performance of this fruit by-product extract.

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O-21

Gas-phase Reactivity at Ultra-low Temperatures for the Study of Interstellar Chemistry

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Química Física

Astrochemistry is a field which has experienced an enormous increase in the last decades due to the development of the radioastronomy which has made it possible that since 1937 more than 270 molecules (as of May 2022) have been detected in the interstellar medium (ISM) or circumstellar shells [1]. The discovery of this unexpected chemistry in the ISM has strengthened the exogenous synthesis hypothesis, in which the prebiotic molecules were synthesized in space and then, delivered to the Earth by meteorites, comets or asteroids [2]. Therefore, it is essential to study the chemistry present in the coldest regions (~10-100 K) of the ISM, known as dark clouds, which provide the raw material for solar systems. Astrochemical networks trying to model the IS chemistry have been improving with the inclusion of the rate coefficients (*k*) for the different processes, such as the bimolecular gas-phase reactions. *k* must be characterized under the appropriate temperature range (10-100 K) in laboratory experiments. For this reason, we have studied the gas-phase reactivity of two species found in the ISM, methylamine (CH_3NH_2) and ammonia (NH_3), towards an abundant IS radical, the hydroxyl radical (OH) between 11.7 and 177.5 K. It is important to know the processes involving these N-bearing species as their chemistry is closely linked to the simplest amino acid, glycine, observed in several comets [4] but undetected in the ISM so far. We have used the CRESU (French acronym for Reactions Kinetics in a Uniform Supersonic Flow) technique, based on supersonic expansions through a Laval nozzle, to experimentally determine *k* [3]. The OH radicals are generated by pulsed laser photolysis (PLP) of H_2O_2 and the OH temporal profile is monitored by laser-induced fluorescence (LIF). The results will be shown at the talk.

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O-22

ONE-COMPONENT IRON COMPLEXES FOR THE SYNTHESIS OF INDUSTRIAL PRODUCTS

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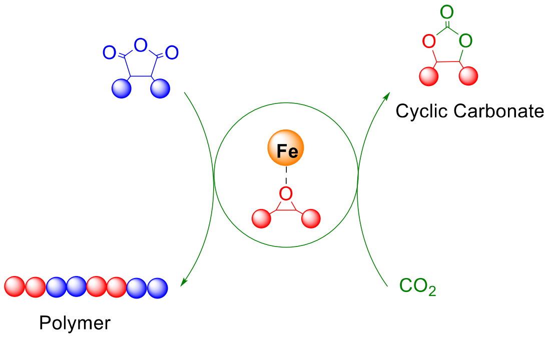
Química Inorgánica

Emissions of carbon dioxide as a consequence of human activity over the last two hundred years have resulted in a huge accumulation of this in the atmosphere which influences in global warming.[1] In this context, the atom-efficient reaction of CO_2 and epoxides for the preparation of cyclic organic carbonates and different polymers is an attractive option in terms of sustainability and atom-economy (Scheme 1). Bifunctional metal systems have been far less studied for the synthesis of cyclic carbonates.[2] Iron-based catalyst systems have recently been gaining attention for these reactions because of their low cost, abundance, and reduced toxicity in comparison to other metal-based catalytic systems. In this work, we design new iron catalytic systems that behave as neutral bifunctional systems that show high catalytic activity for the fixation of CO_2 into cyclic carbonates under mild reaction conditions. In addition, these iron catalysts have shown excellent catalytic activity for the synthesis of fully bio-renewable cyclic carbonates and bio-based polymers.



Scheme 1

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O-23

PRODUCTION OF A HETEROLOGOUS FERULIC ACID DECARBOXYLASE ENZYME FROM KLEBSIELLA PNEUMONIAE TD 4.7 AND APPLICATION OF THE ENZYME IN THE PRODUCTION OF 4-VINYLGUAIACOL

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Ciencia y Tecnología de los Alimentos

4-vinylguaiacol (4-VG), with a spicy clove aroma, is a valuable component in the food and cosmetics industry, particularly in the production of fragrances. However, the industrial demand for 4-VG is not met by extraction from natural sources and synthesis by chemical. As a solution, enzymatic methods can be used to produce these compounds. Bacteria are capable of transforming ferulic acid (FA) into 4-VG, where the bioconversion pathway occurs by the non-oxidative decarboxylation reaction by the action of the enzyme ferulic acid decarboxylase (FAD) (EC 4.1.1.102). The *K. pneumoniae* TD4.7 in the working collection at the Laboratory of Biochemistry and Applied Microbiology of São Paulo State University (UNESP-BRASIL), has an AFD gene. The FAD enzyme gene was amplified and the product was inserted into plasmid pET-28a(+). The pET-28a(+)/fad recombinant vector was transformed into E. coli BL21(DE3), and the induction of 0.2 mM IPTG at 20°C overnight, FAD was highly expressed as a soluble protein. Protein purification was performed and FAD enzyme activity was determined by assays carried out in triplicate, adding 0.05 mL of enzyme extract to 0.45 mL of a solution composed of 0.3 g L^{-1} of FA. The reaction mixture was incubated at 40°C, at pH 5.5, for reaction times of 5, 10 and 15 min. FAD enzyme activity was measured by FA reduction and 4-VG formation. After the heterologous FAD purification process, SDS-PAGE polyacrylamide gel analysis was performed to verify the material, each isoform has a mass of approximately 20 kDa. The enzyme activity test showed that the enzyme maintained its activity after the cloning and heterologous expression processes in *E. coli*, confirming its catalytic efficiency for FA with 4-VG formation.

O-24

COMPARISON OF THE EFFECT OF OZONE AND CHLORINE DIOXIDE DOSING ON HOSPITAL URINE POLLUTED WITH PHARMACEUTICALS

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Chemical Engineering

The inefficiency of conventional biological processes to remove pharmaceutical compounds (PhCs) is leading to their accumulation in aquatic environments. These compounds are characterized by high toxicity, high antibiotic activity and low biodegradability, and their presence is causing serious environmental risks [1]. Hospital effluents have been considered one of the main routes of entry of PhCs into the aquatic environment, as a large part of these compound are consumed by patients and excreted in the urine. [2]. Therefore, it is important to develop efficient technologies to reduce the chemical and biological risk of this type of effluents. In this context, Electrochemical Advanced Oxidation Processes (EAOPs) have demonstrated high performance for degradation of organic compounds in wastewater thanks to the in-situ electrochemical generation of powerful oxidants in liquid and gas phase such as ozone (O_3) and chlorine dioxide (ClO_2). In this context, this work aims to test the feasibility of electrochemically generated O_3 gas and ClO_2 gas for application to hospital urine polluted with several PhCs of similar composition to the effluents of an Intensive Care Unit (ICU) ward.

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O-25

16th YOUNG SCIENCE SYMPOSIUM, FACULTY OF CHEMICAL SCIENCES AND TECHNOLOGIES, UCLM

SIGNAL TRANSDUCTION PATHWAYS IN A TUMORAL CELL LINE: WHAT ABOUT CHOLESTEROL METABOLISM?

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Área de Bioquímica

Transduction pathways are mediated by stimulation or inhibition of receptors, mainly G protein coupled receptors, in the plasma membrane by specific neurotransmitters. Glutamate is the main excitatory neurotransmitter in the Central Nervous System which is involved in physiological action as learning and memory processes. Action of glutamate is evoked by two types of receptors, ionotropic that are ion channel and metabotropic glutamate receptors which has been classified into Group I, II and III. Group I receptors are coupled to stimulation of phospholipase C activity and Groups II and III receptors are coupled to inhibition of adenylyl cyclase activity. At high concentration, glutamate is excitotoxic being responsible for degeneration and neuronal death. To avoid cytotoxic action of glutamate several neuromodulator molecules, such as adenosine, regulate levels of this neurotransmitter. Adenosine is a nucleoside that exert their neuroprotective role through four specific receptor, namely A1, A2A, A2B and A3 receptors. A1 and A3 receptor inhibit adenylyl cyclase activity while A2A and A2B receptors stimulate this enzymatic activity. Both adenosine and glutamate receptor have been involved in neurodegenerative diseases as Alzheimer Disease (AD). Recently, our group have described that cholesterol present in plasma membranes is able to bind and modulate adenosine receptors acting as a non-selective agonist suggesting that cholesterol in brain could be involved in the neurodegeneration characteristic of AD. Therefore, we try to elucidate the role of the metabolism of this lipid and their relationship with adenosine and glutamate receptors in degeneration and cell death using C6 glioma cell as a model. Lipoprotein, enzymes related to the cholesterol metabolism and transduction pathways have been analyzed. Preliminary results show an important relationship between lipid metabolism and signal transduction pathways mediated by adenosine and metabotropic glutamate receptors, mainly by modulation of cAMP levels. Additional studies will be necessary to suggest that the maintaining of cholesterol level not only is important to prevent cardiovascular but neurodegenerative disease.

O-26

Potential of sunlight in the treatment of diseases: photodynamic therapy at ultra-low doses to treat cancer

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Química Inorgánica

Photodynamic therapy (PDT) is a clinically approved non-invasive technique to treat cancer. In this strategy, a photosensitizer (PS) is delivered which is ideally harmless in the dark and activates in the presence of light releasing $^1O_2$ and reactive oxygen species (ROS), which can cause cell death. Octahedral Ir(III) complexes with C^N ligands have been employed as PS in PDT due to their photochemical properties.[1] In this work, new half-sandwich Ir(III) complexes with π-extended C^N ligands and imidazole derivatives (**Fig. 1**) are presented as PDT agents at ultra-low doses.

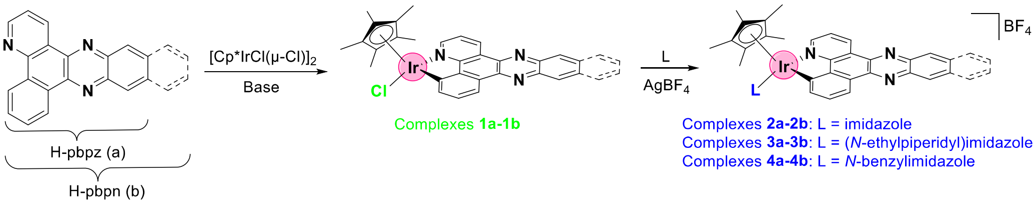

Figure 1. Synthesis of half-sandwich Ir(III) complexes.

Biological studies in A549 cell line show high cytotoxicity in the dark for all complexes (IC_{50} ≤ 8 μM). Under blue light, cytotoxicity hardly improves for pbpz but significantly increases for pbpn complexes ($PI = IC_{50,dark}/IC_{50,light} \leq 1300$) by a great $^1O_2$ generation ($F_{\Delta} \geq 0.81$), achieving $IC_{50,light}$ values up to 190 pM for **4b**. Complexes with pbpn are activated even with red light ($PI \leq 63$), which allows a greater light penetration. These outstanding results confirm the enormous potential of pbpn complexes as $^1O_2$ sensitizers and as a new class of photoactivatable anticancer drugs.

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O-27

New materials for soft robots

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Área de química orgánica

It is beyond doubt that robotics plays an important role in our society, and that this area will be an important part of our future. However, at this moment most of the robots are only used in industry because they are made of hard materials such as metals, which can cause problems when treating with living beings.

In order to expand the application of robotics to animals and humans, it is necessary to prepare soft robots able to adapt to the environment in order to avoid damages to the organisms. Hydrogels are a promising material, as their mechanical properties can be tuned on demand, some of them present self-healing properties and they can be responsive to certain stimulus such us pH, light or electricity. [1]

Here we present a hydrogel, based on [2-(Acryloyloxy)ethyl]trimethylammonium chloride (AETA) monomer. This hydrogel is electrically responsive at 95% water content, producing a finger-like movement and a change in the hydrogel toughness when an electric field is applied. Unlike others electrically responsive hydrogels shown in literature, our gel doesn't need an external aqueous medium to move, which enables us to prepare electrically actuated soft robots outside water (Fig. 1). [2]

However, it remains a challenge the preparation of a suitable electrode, flexible, conductive and stable enough to be used in soft robotics applications. Here we present recent advances in this kind of materials, by metal deposition over hydrogels which leads to flexible and highly conductive composites.

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O-28

A novel NiFe/NiFeO catalytic bilayer structure prepared by magnetron sputtering for hydrogen energy saving production via urea assisted water electrolysis

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Chemical Engineering

In this work different thin films as active catalyst-electrodes have been prepared by magnetron sputtering under oblique angle configuration for green hydrogen production via urea assisted water electrolysis. The films have been characterized by a number of surface analysis techniques and have been tested in half electrochemical cell and in a complete alkaline anion exchange membrane electrolyzer cell (AEM) using urea-water as feeding stream. In this way the oxygen evolution reaction (OER), which requires a high activation energy barrier, is replaced by the oxidation urea (UOR). This enables the hydrogen production at lower overpotentials (i.e., decreasing the energy requirements) and alleviates water contamination problems derived from industrial and urine rich effluents. Among the different prepared catalyst films: pure nickel, Ni/Fe mixture, and NiFe/NiFeO bi-layer, the latter one (**Fig.1a**) showed the best electrocatalytic performance. This electrode was selected as anode in a complete anion exchange membrane water electrolyzer (AEM) for urea oxidation, providing a decrease in 0.13 V in applied potential vs. the conventional water electrolysis to achieve 40 mA·cm^{-2}. These operating conditions permit to produce hydrogen with a electrical energy demand of 47.18 kWh/KgH$_2$, 8% less than for a conventional water electrolysis process. As a proof of concept, the system was coupled with a Photovoltaic Panel (PV) to demonstrate the long time and stable production of a pure hydrogen stream (**Fig. 1b**) via renewable energy.

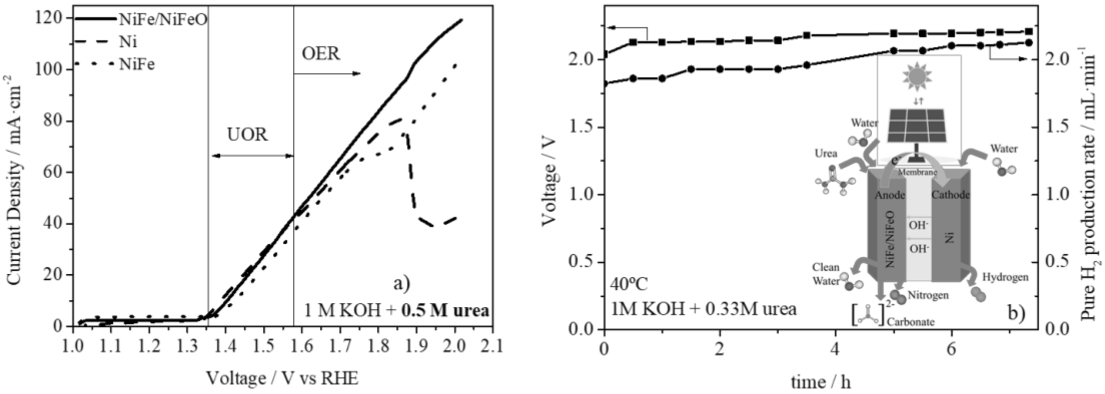

Figure 1. a) Linear sweep voltammetry experiments carried out in a solution of 0.5M urea with 1M potassium hydroxide in half electrochemical cell; b) Proof of concept of hydrogen production via direct PV-AEM coupling

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O-29

Proteomic evaluation of intestinal function after dietary supplementation with grape seed polyphenols

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Food science and technology

Intestinal epithelial barrier has a crucial role in maintenance of the host homeostasis and bioactive compounds such as grape seed polyphenols has been related with lower incidence of many non-infectious diseases [1]. However, the effects of its dietary supplementation in gut homeostasis or its mechanism of action are not fully understood.

Thus, we evaluate the ileal proteome changes of young-healthy Wistar rats that were supplemented with a grape seed extract (GSE) (25 mg of GSE/kg body weight/day) for 28 days through SWATH-MS quantitative proteomics to gain insight into the molecular and cellular processes that were affected by this extract.

After GSE supplementation, 13 proteins were over-represented and 223 proteins under-represented in ileal proteomes. Attending to biological pathways, proteins implicated in intestinal motility and intestinal barrier integrity were over-represented in GSE-treated rats. Moreover, proteins related to energy metabolism, innate immune system and cancer development were under-represented, indicating that GSE supplementation at low doses may improve the intestinal barrier function and prevent aberrant over-activation of immune responses in the ileum.

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O-30

Anthropomorphic hydrogel-based phantoms for microwave imaging medical applications

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Química Orgánica

Hydrogels are being widely used for biomedical applications based on their unique properties, commonly developed to mimic human tissues as image phantoms [1]. These phantoms are designed for medical imaging research, systems' characterization, and images' reconstruction optimization. The proposed work is ongoing for the optimized and valid use of dedicated hydrogel-based phantoms for breast microwave screening, a new medical imaging technique that exploits dielectric properties of tissues.

A literature review was performed to select the desired hydrogel's physical properties (mechanical and dielectric) based on updated data from breast tissues' experimental studies. A full dielectric characterization (to study conductivity and permittivity) of some hydrogel composites based on different monomers were performed via an open-ended coaxial probe [2]. Then, several theoretical models were implemented to reconstruct the dielectric parameters of common breast tissues (skin, adipose, glandular, cancerous) and compare them with measured hydrogels' dielectric properties. Additionally, models for hydrogels 3D printing are on development, based on real human breasts via MRI morphology features' extraction. An optimization of hydrogels' 3D printing is ongoing to assure and keep breast complex morphologies represented by used hydrogels.

Water-content stability, multilayered disposition and dedicated hydrogel-based representation of breast tumors are being studied via different phantom prototypes, which will be studied soon through an operational microwave imaging system.

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O-31

Kinetic study of the Cl atom reaction of biogenic aldehydes in the atmosphere

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Atmospheric Chemistry

Aldehydes are volatile organic compounds (VOCs) recognized as primary and secondary pollutants emitted into the lower atmosphere from several sources. Large quantities of aldehydes are directly emitted into the atmosphere from biogenic and anthropogenic sources and are also formed *in situ* through atmospheric photooxidation reactions of other VOCs[1]. These carbonyl compounds can be removed by tropospheric oxidation initiated by OH radicals (in the day-time), NO_3 radicals (in the night-time), and by Cl atoms (in the marine environment and coastal areas), being important contributors to the formation of peroxyacyl nitrates (PANs), ozone, and other compounds that have a detrimental effect on the environment and human health[2]. Even at low levels, Cl atoms can have a profound impact on tropospheric oxidation, reacting faster with VOCs in comparison to OH. For this reason, in this work we report the gas-phase kinetic study at ground level conditions ($T = 298\pm2K$ and $P = 760\pm5$ Torr of air) of the reactions between Cl and a series of aldehydes (2-methylbutanal, *trans*-2-methyl-2-butenal, 2-methylpentanal and 2-methyl-2-pentenal). For that purpose, an atmospheric simulation chamber coupled to a Fourier Transform Infrared spectrometer was used to determine k_{Cl} by a relative kinetic method[3] in which Cl atoms were generated by photodissociation of Cl_2 by using actinic UV lamps (λ=340-400 nm). Finally, the atmospheric implications of the degradation of these aldehydes will be discussed in terms of its lifetime due to homogeneous reaction with Cl atoms, OH and NO_3 radicals.

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O-32

Organolithium Chemistry under Sustainable Conditions: Synthesis of Amidines and Guanidines

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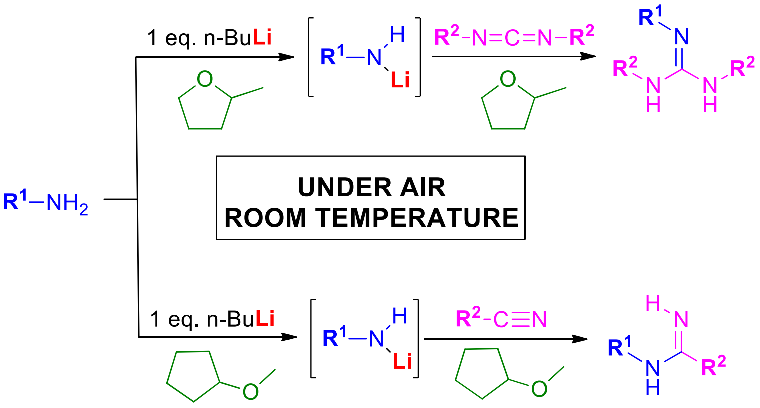
Química Inorgánica

The possibility of using organolithium compounds under-air opens the door to a greener polar organometallic chemistry.[1] In basis to our previous experience in the synthesis of guanidines and amidines,[2] in this work we describe the highly-efficient and selective fast addition of *in-situ* generated lithium amides [LiN(H)R] (obtained *via* acid-base reaction between n-BuLi and the desired amine) into carbodiimides (R-N=C=N-R) or nitriles (R-C≡N), in 2-MeTHF or methylcyclopentylether as ethereal green solvents, at room temperature and in the absence of a protective atmosphere. This alternative synthetic methodology allows the straightforward and successful synthesis of either guanidines or amidines, without the need of isolation or purification steps of any halfway reaction intermediate. The robustness of the method allows the reaction to be carried out on a multigram scale, thus proving that our new and environmentally friendly protocol is amenable for a possible applied synthesis of these highly substituted iminic-type fine chemical products under bench-type reaction conditions.[3]



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O-33

EFECTS OF ULTRASOUNDS AS A PRETREATMENT IN BIOLEACHING OF HIGH POLLUTED MULTI-METAL MINE TAILINGS

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Chemical engineering

The mining industry has produced a vast number of hazardous wastes, which remain abandoned. These wastes combined with the climatic agents lead to the pollution of the soils, water, air, and biota nearby. In Spain, there are 75 abandoned mining sites considered of high risk for human health and the ecosystem. In this research, the used mine tailings were collected from the abandoned Pb/Zn mine of San Quintin Ciudad Real, Spain).

Bioleaching is a process by which an effluent with the metal pollutants of the tailings can be obtained, taking advantage of the microbial remediation. The inconvenience of this process is its slow rate and low yield, most specially compared with other hydrometallurgical process, less ecological but more effective. By the coupling of bioleaching with ultrasounds, we expected to achieve an increase in the overall reaction rate and metal recovery. [1]

The experiments were carried out at laboratory scale. The strategy was the ***biostimulation*** of the autochthonous microorganisms of the mine tailings, therefore conditions were set for the optimal growth. The procedure consisted in two steps, first discontinuous dosages of ultrasounds were applied; next the flasks were incubated at 30 ºC and 150 rpm for 30 days. Two frequencies of ultrasounds were applied (37 kHz and 80 kHz) and different energy dosages (0 – 18 kJ/g).

The use of ultrasounds in this biological process showed a double effect of stimulating but also damaging the microorganisms. The main leached metals were iron (Fe), aluminium (Al) and zinc (Zn). Thus, increasing the energy dosage, the metal extraction incremented until the damaging effect was higher than the stimulating. Once this border was overpassed, the metal extraction decreased for both frequencies.

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O-34

Chitosan hydrogels: tissue engineering applications and magnetic properties

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

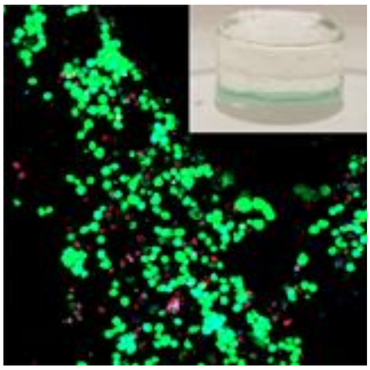

Figure 1. Cell culture in chitosan hydrogels.

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 antimicrobial properties [1]. 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 [2] and magnetic nanoparticles [3] 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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O-35

Permalloy thin films on V-groove patterned substrates for sensoring 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 sensoring 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, $\theta = 55°$) was characterised using SEM [Figure 1]. Permalloy thin films were deposited by DC sputtering with normal incidence on several substrates at a $1.6\ \text{Å}/s$ 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.

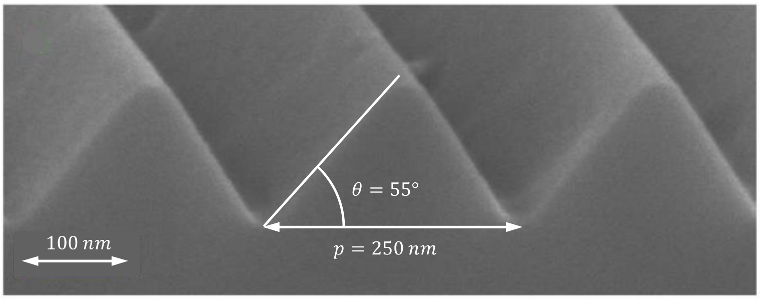

Figure 1. SEM characterization of nanopatterned V-groove silicon substrate.

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PRESENTATIONS FLASH

(Appearance in alphabetic order)

F-1

A new iodometric microwave assisted method for peroxide determination

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16th Young Science Symposium

Peroxides play an important atmospheric role both in the gas and particle phases. Several techniques are available in the literature to measure peroxides in Secondary Organic Aerosols (SOA), although current techniques are very expensive or time consuming. In the present work, a new fast and sensitive iodometric spectrophotometric method has been developed based on the traditional iodometric method (1-2). The proposed method is based on the acceleration by microwave radiation of the reaction of peroxides with potassium iodide in acid medium to liberate iodine, that in the presence of excess of iodide forms triiodide that could be monitored at three different wavelengths (287 nm, 351 nm y 420 nm).

Different analytical parameters including pH, potassium iodide mass, temperature and time of thermostatic bath, microwave power and time, interferences due to oxygen and metals were evaluated. The method has been optimized for H_2O_2 and t-butyl hydroperoxide (one of peroxides that reacts very slowly in the traditional method), in contrast with previous studies that only used H_2O_2 or an organic peroxide that reacts faster with iodide.

The main advantages of the new method in relation to the traditional method are the following: less time-consuming analysis, lower and controlled oxygen interferences, and smaller sensitivity differences between different peroxides.

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F-2

EFFECTS OF THE OXIDATION OF SALICYLIC ACID BY PEROXYNITRITE

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Physical chemistry, Kinetic

Non-opioid analgesics and non-steroidal anti-inflammatory drugs, such as salicylic acid derivatives are on the list of essential drugs of the Health Organization [1]. This compound has been the most prescribed against pain and inflammation [2]. Their biological action has been widely studied, however, their reaction at the intracellular level is not so well known. More specifically, there are hardly any studies on their possible mechanism of oxidation of these analgesics. On the other hand, peroxinitrite is an important pro-oxidant in the human body, this molecule is present in organs, tissues, cells… being the first defense at the cellular level against virus and bacterial infections.

Also, it is very important to understand the mechanism of salicylate degradation by peroxynitrite at cellular level. The experimental results have shown a complex order to peroxinitrite and salicylic acid concentrations (Fig. 1).

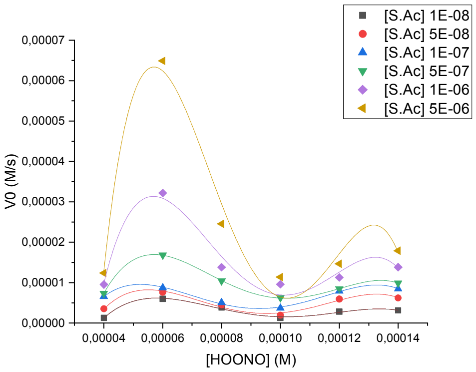

Figure 1- Initial rate versus oxidant concentration, at different substrate concentrations. Experimental conditions: I= 0,15 M; pH= 2;Tª=25ºC.

A thorough knowledge of this mechanism as well as of all intermediates and reaction products can improve their analgesic effect and reduce adverse effects.

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F-3

Optimizing the Supercritical Synthesis of TiO_2 Nanoparticles for CO_2 Photoconversion: Effect of Nature and Concentration of Ti Precursor

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Ingeniería Química

Photoreduction of CO_2 using solar energy and semiconductors such as TiO_2, ZnO, CdS, SiC or WO_3, is an alternative method to reduce emissions of this greenhouse gas. Within these materials, titanium dioxide (TiO_2) is one of the most widely used semiconductors for being efficient and nonthreatening for the environment [1]. One of the possibilities for obtaining these catalysts is to do it under supercritical conditions. Numerous studies have identified an improvement in the properties of catalysts synthesized in supercritical medium [1]. Using this technology, several studies have been carried out regarding the precursor for the synthesis process [2], but very few comparing the resulting physico-chemical characteristics, and fewer, comparing the effects of different ratios of hydrolytic agent (HA)/precursor [3]. For these reasons, this research focused on synthesizing catalysts with 4 different precursors, Diisopropoxytitanium bis (acetylacetonate) (TDB), Titanium (IV) isopropoxide (TIP), Titanium (IV) butoxide (TBO) and Titanium (IV) 2-ethylhexyloxide (TEO), and the HA/precursor ratio were 10, 20, 30 and 40 mol / mol. One of the variables observed is the yield production, where TIP and TBO presented a higher catalyst production (>70%). Also, TIP yield increased with increasing HA/precursor ratio. The physico-chemical characteristics vary differently according to the precursor and the HA/precursor ratio. Regarding the photocatalytic activity of the catalysts, TDB and TEO exhibit a higher production of CO and CH_4, but the influence of AH/precursor ratio was not apparent.

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F-4

Comparative Study between Packed Column and Venturi in the Electro-absorption Process for the Removal of Xylene from Gaseous Streams

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Volatile organic compounds (VOCs) are considered useful raw materials in several industries, especially in the production of paints and solvents. Xylene is used as a solvent and forms part of fossil fuels due to its high octane rating. In organic chemistry, it is used as starting product in the production of phthalic acids. However, it generates polluted gaseous streams that pose a major environmental problem associated with tropospheric chemistry, air quality and human health [1]. Electro-absorption is a novel technology to remove VOCs, such as xylene, from gaseous streams. It combines two stages: absorption in which pollutants pass from the gas to the liquid electrolyte and electro-oxidation where the elimination of them is carried out by oxidation reactions [2]. This study is focused on the evaluation of the electro-absorption process as a novelty treatment for gaseous streams polluted by xylene. To do this, two configurations in absorption steep were used: packed column and venturi, and it was evaluated the influence of current intensity (10, 50 and 100 mA cm^{-2}) in the concentration of the liquid phase and the mass flow of gaseous streams. The inlet gas flow used was 6 L h^{-1}. Results show that in xylene degradations there was obtained higher elimination percentage with the venturi configuration. In the liquid phase, tolualdehyde was identified as the principal intermediate aromatic compound, also there were generated carboxylic acids. However, their concentrations were not significant amounts, it could be established that mineralization is the principal way of xylene in the electro-oxidation process. Meanwhile, there was observed a reduction in the concentration of the pollutant in the outlet streams compared to the inlet ones. This data verifies that electro-absorption is a functional electrochemical application to remove xylene from gaseous streams. When the current density rises, the removal percentage increases but the degradation percentage relative to the energy consumption decreases. This energy efficiency behaviour occurs because mass transport is the limiting stage in the oxidation of diluted organic solutions. This information contributes to the understanding of the kinetics and reaction mechanisms involved in the electro-absorption of xylene.

Acknowledgment
Financial support from the Spanish Ministry of Economy, Industry and Competitiveness, European Union through project PID2019-107271RB-I00 (AEI/FEDER, UE) is gratefully acknowledged.
Andrea N. Arias acknowledge the FPI grant nº PRE2020-094902.

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F-5

Formulation of a nano biofertilizer based on soil yeast and its effects on lettuce crop: Preliminary results.

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Conventional agriculture uses large volumes of agrochemicals, which affects living organisms and ecosystems. Worldwide, agriculture has focused on reducing the use of agrochemicals, improving safety for the population and environment and reducing their costs without affecting crop quality. Nanotechnology, especially nanoparticles, offers an alternative for the sustainable development of agroecosystems. Currently, nano fertilizers, encapsulated agrochemicals and plant growth nano-promoters, have been developed, with potential applications for agriculture. In addition, with this new technology, nature-based alternatives have been developed, where soil microorganisms play an important role in the search for adaptation and mitigation strategies, such abiotic stress. Soil yeasts are microorganisms that offer an alternative as potential plant growth promoters (PGP) through different pathways, alleviating alterations in root architecture, translocation of macro and micronutrients, improving photosynthetic activity, between others, in different crops such as lettuce, one of the most consumed crops worldwide, considered an healthy food, due to their content as antioxidant compounds and fiber.

This research is based on the development of a nano biofertilizer, composed by nanoparticles and soil yeasts. A completely randomized 4x2 design was developed, and two strains *Candida guillermondi* and *Rodothorula mucilaginosa,* and with and without nanoparticle addition. PGP activities as siderophore production, phosphate solubilization and indole acetic acid were evaluated by spectrophotometric methods. Physiological parameters as stomatal conductance, water use efficiency, internal CO_2 concentration in leaves, photosynthetic rate and fluorescence were also evaluated.

The main results of the PGP activities were the presence of siderophores, phosphate solubilization and indole acetic acid production, in both strains. In terms of growth, there are clear visual differences between strains and nanoparticle application. Finally, nano biofertilizers based on yeast has better efficacy in the presence of nanoparticle, with a potential improvement of the physiological and hydric status of crops.

Acknowledgments: FONDECYT 1190585 Project.

F-6

Selective Formation of Highly Emitting Anthracene T-Shaped Excimers allows FLIM imaging in breast cancer cell lines

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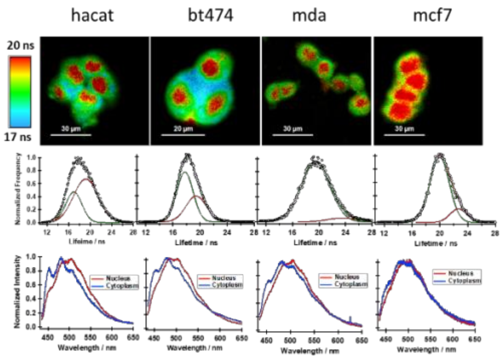
Química Física

We recently reported a new anthracene-guanidine (AG) derivative able to form the rare T-shaped dimer in water solution, and where water molecules play a fundamental role assisting the self-assembly though H-bonds. Such T-shaped dimer formation is easy to be controlled, and stability depends mainly on the response to external stimuli: pH values within 4 – 10, water molar fraction ranging 0.8 – 1, and concentrations < 10 µM reinforce the stability enhancing luminescence properties - extremely high quantum yield (QY≈ 1) and maximum emission at 515 nm and large fluorescence lifetime (≈ 25 ns).

Next, we studied the behaviour of the AG dimers in biological systems, where different physiological factors such as the ionic strength, the presence of biological macromolecules, and the viscosity, among others, may affect their rate of formation or persistence.

Fluorescence Lifetime Imaging Microscopy (FLIM) was used to monitoring populations of GA in human breast cancer (MCF7, BT474 and MDA-MB231). Different populations of monomer, T-shaped and π-π dimers were observed in the cell membrane, cytoplasm and nucleoplasm related to the local viscosity and presence of water (Figure 1). The T-shaped dimer is exclusively formed in the nucleus because of the higher density and viscosity compared to the cytoplasm. In addition, different rate of T-shaped to p-p dimer conversion was observed in the studied cell lines which would allow cell differentiation.

Figure 1. FLIM images of the studied cell lines along with the respective overall histograms of the average emission lifetimes and



the emission spectra collected st selected points in the cell nucleii (red) and cytoplasm (blue).

F-7

REINFORCEMENT PLGA-BASED SCAFFOLDS MANUFACTURING VIA SUPERCRITICAL CO_2 FOAMING.

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Tissue engineering is an important field of regenerative medicine for tissue repair, particularly the repair of bone defects from trauma loss, tumor section, etc. 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, remains a great challenge.

Different polymers are postulated for this application, among them PLGA is one of the most used polymers for fabricating porous scaffolds. PLGA stands out as highly biodegradable and bioabsorbable polymer, in fact, it has been approved by the Food and Drug Administration.

However, one of the problems this polymer exhibits is poor mechanical strength [1]. Many studies have set their goals to reinforce these porous scaffolds by introducing reinforcing agents into the polymer matrix. Various compounds have been used as reinforcing agents as different calcium phosphates, Mg and derivates.

Among the manufacturing techniques for the preparation of polymeric scaffolds, the supercritical CO_2-assisted foaming offers significant advantages because is a solvent-free technique, since CO_2 is a gas non-toxic, chemically stable, non-flammable, and cost-effective. Additionally, CO_2 can achieve its supercritical state at “mild” conditions, $T = 31\ ^{o}C$ and $P = 73$ bar [2].

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F-8

Nitrogen-doped graphene-based aerogels as electrocatalysts

Chemical Engineering

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The increase in CO_2 emissions and the excessive use of fossil fuels (coal, gas and oil) is forcing society to look for sustainable alternatives for obtaining energy. These alternatives are the renewable energies, and an established sustainable energy is the obtained from the energy vector “Hydrogen”. The producing of this molecule is being done by different methods, and a synthesis that obtains green and pure hydrogen is the Hydrogen Evolution Reaction (HER). Traditionally, this reaction has been catalyzed by noble metal catalysts (Pt or Pd) but their high prize and limited availability is an industrial handicap. Nowadays the studies are focused on develop new metal-free electrocatalysts with sustainable materials, such as graphene. The structure of the catalyst is relevant because it involves the active surface area, so the production of materials with high surface area and a well-defined 3D matrix structure is crucial, such as the aerogel disposition. Furthermore, if the graphene-based catalyst is doped with heteroatoms as nitrogen, the physicochemical properties of material change and it generates an n-type semiconductor which electroactivity increased.

In this study graphene-based electrocatalysts were synthesized by using non-nitrogenous (ethylene glycol) and nitrogenous reducing agents (hydrazine monohydrate, 2-chloroethylamine and ethylenediamine). The hydrothermal method was used to obtain the self-assembly of the graphene sheets, and then the freeze-drying generated the 3D carbon matrix. The electrocatalytic performance of the resulting graphene-based aerogels was strongly influenced by porosity, density, crystallinity and the crucial presence of nitrogenous and oxygenated groups. This work concluded that metal-free nitrogen-doped graphene-based aerogel synthesised achieved -12 mA cm^{-2} at -0.15V (vs RHE) with 410 m^2/g of surface area and a density of 0.0061 g/cc.

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F-9

Synthesis of arylethyl pyrazine derivatives. Application as optical waveguides.

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Química Orgánica

Ever since it was shown that light could be confined in a medium[1] and travel through it carrying information,[2] research in this field has continued unabated. The goal is for photonics to overtake electronics in the world of communication because of its many advantages. In this sense, miniaturised photonic devices are being developed, for which the design and synthesis of optical waveguides, which are structures capable of efficiently propagating and confining light, is fundamental.[3]

In this work, four aryletynyl pyrazine derivatives have been synthesised, supramolecular aggregates have been formed using the slow diffusion technique, their morphology has been studied by SEM and those with the best structures have been measured as optical waveguides using a confocal fluorescence microscope. Three of the synthesised compounds have optical waveguide behaviour (Figure 1).

Figure 1. Aryletynyl pyrazine derivatives as optical waveguide.

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F-10

Use of electrogenerated ozone gas in PEM cells for disinfection of urine

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Chemical Engineering

The pollution of the aquatic environment constitutes one of the main problems in our society. In this context, pharmaceutical products have caused significant concern in the environmental field due to their frequent presence in effluent treatment plants (ETEs), with concentrations in the order of $ng \cdot L^{-1}$ to $mg \cdot L^{-1}$ [1]. Moreover, COVID pandemic events have demonstrated the necessity for advanced microbial decontamination as a preventative measure for epidemic control. Similarly, presence of SARS-CoV-2 RNA in urban wastewater has been reported [2]. Among these possible routes of entry to treatment plants, the main one is consumption and excretion in urine and feces. For this reason, it is necessary to develop clean and efficient technologies that reduce the danger from the environmental and health point of view before discharging them into the environment. Electrochemical Advanced Oxidation Processes (EAOP) can be considered a promising alternative. They can generate oxidants (such as ozone) currently used in the remediation of contaminated wastewater. With this background, this work evaluates, on the one hand, ozone electrogeneration by EAOP using boron-doped diamond (BDD) electrodes, and on the other hand, disinfection of hospital urine contaminated with Klebsiella by means of electrogenerated ozone gas. The influence of current density (25, 50 and 75 $mA \cdot cm^{-2}$) on ozone generation and elimination of klebsiella in synthetic urine was studied. The disinfection rate is higher when increasing the current intensity due to the higher production of ozone.

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F-11

A reduced order method for the Rayleigh-Bénard problem

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Matemáticas

Parametrized partial differential equations are standard tools to model many processes in scientific and industrial contexts. For this reason, understanding the solutions of such equations has become of paramount importance in the mathematical community. Two of the better-known techniques developed in this context are the numerical stability and bifurcation studies. However, performing such studies using a high-fidelity numerical scheme –finite difference method, finite element method or spectral techniques– has a huge computational cost, especially if fluid dynamics equations are involved. To overcome this problem, the mathematical community has developed several reduced order techniques, which allow to reduce dramatically the computational cost of stability and bifurcation studies.

Reduced order methods usually work in two steps. First, some solutions of the problem are obtained by a high-fidelity scheme. These solutions are processed to obtain a new basis of energetic solutions. Second, the solutions of the original problem are projected into the new basis. In this way, a new reduced order model is obtained, whose numerical evaluation is really fast, compared to that of the original problem.

In this communication we present a new reduction order technique applied to a classical problem in fluid dynamics: the Rayleigh-Bénard convection problem [1]. This fluid dynamics problem models the convection of a 2D fluid heated from below. Our reduction order technique follows the two steps listed in the above paragraph. The main novelty is the way solutions are obtained in the first step.

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F-12

GENERATION OF CLO_2 FOR REMEDIATION OF SOILS SYNTHETICALLY CONTAMINATED WITH CARBAMATES

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Chemical Engineering

Soil pollution is a challenge that has involved researchers from different fields of science in search of technologies for their recovery. Thus, ex-situ soil washing appears as a simple and efficient solution for the remediation of contaminated soil. However, this treatment generates toxic effluents that cannot be discarded without treatment [1]. Given the need to treat this waste, there is another need to develop technologies capable of efficiently producing oxidizing species capable of completely removing dissolved organics. Among the wide variety of oxidants [2], the electrochemical production of chlorine dioxide from the reduction of chlorate (ClO_3^-) with hydrogen peroxide (H_2O_2), both continuously generated, is proposed in this work as an alternative for the treatment of effluents contaminated with carbamates. Thus, the first part of this work is to study the electrochemical production of ClO_3^- and H_2O_2 at a continuous flow rate, obtaining values of 2.67 mmol h^{-1} and 0.24 mmol h^{-1} with a flow rate of 0.1 L h^{-1}, respectively. This flow rate was chosen as the optimal to maximize the generation of the reagents (ClO_3^- and H_2O_2) responsible for the generation of ClO_2. Another challenge of ClO_2 generation is finding the proper ratio of ClO_3^- to react with H_2O_2. Since this reduction, it can also promote the formation of chlorite and hypochlorous acid, for example [3]. Hence, further studies should be carried out in order to quantify the generation of ClO_2 during the immediate reaction of ClO_3^- and H_2O_2.

Acknowledgments

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F-13

Treatment of Real Acid Mine Drainage for Metal and Energy Recovery by Electrodialysis and Bio-electrochemical Systems

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Chemical Engineering

Pollution is a serious problem that humans are increasingly aware, being one of them abandoned mines, which were used to extract metals in the last centuries. Nevertheless, when ores were exhausted, mines were abandoned irrespective of environmental hazard, polluting soil and water. Regarding water pollution, the effluent is named Acid Mine Drainage (AMD), being characterized by its high metal concentration and low pH. AMD treatment is needed both for ecological consequences and for the elevated valuable material contained, following circular economy recovering the metals. The real AMD (AMDR) that was utilized was from San Quintín mine (Ciudad Real, Spain).

In this research, two technologies were studied to treat AMDR. First, electrodialysis (ED) was used. Voltage and volume ratio between diluate and concentrated were the studied parameters with synthetic AMD (AMDS). Once these optimal conditions were selected, a test with them and AMDR was done. The obtained concentrated effluent was taken to posterior treatment with bio-electrochemical systems (BES).

Afterwards, bio-electrochemical systems treated the real concentrated effluent obtained by electrodialysis. Initially, MFC (Microbial Fuel Cell) configuration was used. The biofilm was on the carbon felt electrode in the anolyte. Biofilm creation lasted a month with growth medium and with activated sludge from a conventional wastewater treatment plan in Ciudad Real. In the catholyte occurred the electrodeposition of copper on the titanium electrode, reduction of Fe(III) to Fe(II) and production of energy.

MFC performance was operated for almost 300 h. Then, it was changed to MEC (Microbial Electrolysis Cell), applying 0.5 V for 48 h, 1.0 V for 96 h and 1.5 V for 96 h. Thanks to this configuration, reducing and recovering the rest of the metals was possible.

F-14

Hydrofluoroethers as eco-friendly candidates for replacing greenhouse gases

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Atmospheric Chemistry

Hydrofluoroethers (HFEs) have been proposed in the last decades as climate-friendly alternatives to potent greenhouse gases, such as hydrofluorocarbons, in several industrial applications (i.e: refrigerants, blowing agents, etc). Assessing the impact on climate change is indispensable to evaluate the suitability of HFEs as environmentally friendly candidates to replace high global-warming (GWP) species. To achieve that objective, it is necessary (*1*) to investigate the temperature and pressure dependence of the absolute rate coefficient, $k_{OH}(T,P)$, for the reaction of HFEs with OH radicals to mimic the tropospheric conditions, which is the main removal process in the atmosphere, and (2) to determine the IR absorption cross sections in the atmospheric window (720-1250 cm^{-1}). With these two parameters the GWP of HFEs can be estimated. In the present work, we present the first kinetic study of the OH-reactions with $CF_3CH_2OCH_3$ (HFE-36 263fb2), $CHF_2CF_2CH_2OCH_3$ (HFE-374pcf) and $CF_3CF_2CH_2OCH_3$ (HFE-365mcf3) as a function of temperature (263-353 K) and pressure (50-500 Torr of helium) using the pulsed laser photolysis/laser induced fluorescence technique[1]. No pressure dependence of the rate coefficient was observed in the studied range and the temperature dependences ($k_{OH}(T)$ in $cm^3 molecule^{-1} s^{-1}$) are well described by the following Arrhenius expressions[1]: $k_{OH}(T) = (3.88 \pm 0.89) \times 10^{-12} \exp[-(508 \pm 69)/T]$ for HFE-263fb2, $k_{OH}(T) = (2.81 \pm 0.33) \times 10^{-12} \exp[-(312 \pm 35)/T]$ for HFE-374pcf and $k_{OH}(T) = (2.60 \pm 0.31) \times 10^{-12} \exp[-(319 \pm 35)/T]$ for HFE-365mcf3. From these results, the atmospheric lifetime (t) for HFE-374pcf, HFE-263fb2, and HFE-365mcf3 due to the OH-reaction are 12, 17, and 13 days, respectively. Considering t and the IR absorption cross sections determined in this work, the radiative for these HFEs were 0.03 W m^{-2} $ppbv^{-1}$. At a time horizon of 100 years, GWP relative to CO_2 for these HFEs results in the range of 0.40-0.76. [1] The drastic reduction in GWP observed with respect to the gases HFEs will replace minimize the effect on the global warming of the planet.

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F-15

MICROFLUIDICS IN SUPRAMOLECULAR CHEMISTRY AND MATERIALS WITH WAVEGUIDE PROPERTIES

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Química Orgánica

Microfluidics is the science of systems that employs small amounts of liquid or gaseous fluids, using channels ranging in size from tens to hundreds of micrometres. The high surface-to-volume ratio of microreactors enables a favored mass and heat transfer as well as an easy diffusion of molecules. The result is a reduction in analysis times, and low reagent consumption and production of undesirable by-products, reducing cost.

In this work, the advantages of this discipline have been used to study the occlusion of naproxen in the supramolecular hydrogel that forms the tripeptide ^{L}Leu-^{D}Phe-^{D}Phe using 3D printed microfluidic devices made of polydimethylsiloxane (PDMS). The waveguide property of this tripeptide is under study.

In addition, focused on preparing a hydrogel with waveguide properties to guide the light inside a microfluidic channel, we started preparing a macroscopic waveguide as first step. These structures are capable of confining and transmitting light through the total internal reflection (TIR) phenomenon and its importance deals because they represent the major component of photonic chips. For the synthesis of the materials, a 1,8-naphthalimide derivative (Fig. 1) has been synthesised, which is characterised by having excellent photostability, being a fluorophore unit, good structural flexibility and a large Stokes shift (a prerequisite to behave like an optical waveguide). A macroscopic organogel that contains the 1,8-naphtalimide derivate in its structure was also prepared. In addition, its waveguide property is under study.

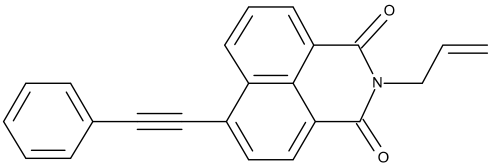

Figure 1. Chemical structure of the synthesised compound.

F-16

Nested supramolecular interactions: guest uptake in cages embedded in tripeptide gels

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Química Orgánica

Supramolecular gels composed of short peptides are very popular thanks to their ease of preparation and their chemical diversity. The appropriate choice of amino acid chirality in D,L-tripeptides has emerged as a useful strategy to fine-tune the supramolecular behavior of these materials.[1] Metal-organic cages are interesting supramolecular structures able to selectively encapsulate guests for a wide variety of uses, including chemical separation between immiscible liquid phases.[2] In this work, we illustrate hybrid gels based on nested supramolecular interactions: guests can be separated from a mixture via encapsulation in their respective host cage embedded in discrete peptide gel phases (Fig. 1). These hybrid materials have been characterized by NMR, Raman, EDX, UV-visible and CD spectroscopies, TEM and rheology. Overall, this investigation represents a general strategy for the immobilization of supramolecular hosts within gels to yield novel materials that could be applied for molecule separation.

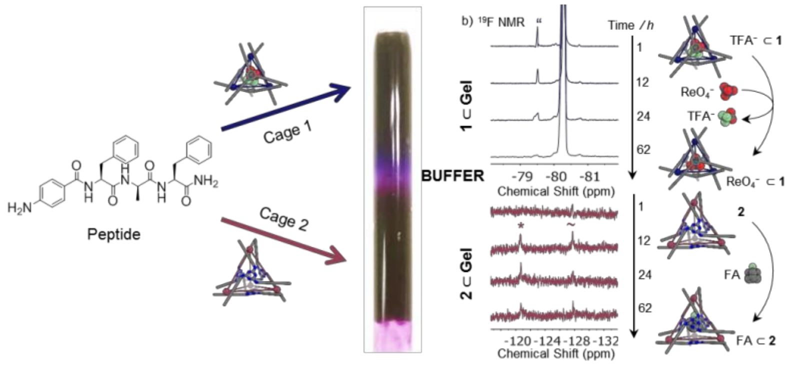

Figure 1. ^{19}F NMR spectra of **1⊂Gel** (blue) and **2⊂Gel** (pink) showing respectively the decrease of the encapsulated TFA$^-$ peak (“) and the increase of the both the encapsulated (*) and free (~) FA over time after addition of a mixture of 1 eq. or FA and ReO_4^-.

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F-17

Novel boron-doped diamond electrodes development for environmental applications

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Materials Science/ Environmental techonologies

Electrochemical Advanced Oxidation Process (EAOPs) includes cheap and environmentally friendly methods with high efficiency in organic degradation with the production of highly oxidative species. In these techniques, although the hydroxyl radical is the main oxidizing formed agent, it can interact with other ions forming other oxidizing agents, which can be more stable than the hydroxyl radical. As they are multidisciplinary techniques, they depend on the knowledge such as material surface, electrochemistry, solid-state physics, and optics. Thus, EOPs are completely related to materials science. A material with a wide application in EAOPs is the boron-doped diamond (BDD). Its excellent mechanical properties, chemical stability, corrosion resistance, high oxidation potential, and low background current, make BDD a singular material for these applications. Besides, the methods of BDD growth allow the deposition above several substrates, ranging its grain size from micro to ultrananocrystalline morphologies. These different diamond composite properties can influence the pollutant degradation process as well as the oxidizing species generation, combining different morphologies and material characteristics to improve the final result. In this sense, we aimed at improving the BDD growth on porous materials by the deposition of novel boron-doped ultrananocrystalline on titanium dioxide nanotubes (TDN). From the perspective to grow diamond film from the chemical vapor deposition (CVD) technique, the porous substrate of the TDN is extremely advantageous, allowing to obtain a homogeneous film and distributed along the substrate to keep the substrate porosity motivated by the conversion of TiO2 to TiC, which occurs in the diamond reactor. As result, we developed three different boron doped diamond electrodes that can be applied in EAOPs: 1) an ultrananocrystaline diamond electrode with porosity associated with TDN expose morphology and that presented photoresponse; 2) an ultrananocrystaline diamond electrode developed without seeding with the obtention of a homogeneous layer of diamond film that respects the porosity of the film and that have two different planes of diamond growth, also improving the electrode area; and 3) micro and ultrananocrystalines tridimensional diamond electrode grown on Ti grid with a titanium dioxide nanotube layer. All the electrodes were morphological, physical, and electrochemically characterized, proving their quality and potentiality for EAOP applications.

F-18

Synthesis of 2D nanomaterials with metallic nanoparticles

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Química Orgánica

Different synthesis methods emerged over the years, first for graphene and then for other 2D nanomaterials. With the addition of nanoparticles, these materials can be tuned surface and properties [1] to enhance catalytic, magnetic, electrical, and optoelectronic properties [2]. These hybrid nanomaterials can be synthesized by solution mixing [3], sol-gel processes [4], microwave irradiation [5], etc. However, these methodologies have disadvantages, such as using hazardous and non-environmentally friendly reactants, time-consuming, and yields [6]. Here in a simple, one-step, and environmentally friendly methodology, we report a new ball milling procedure for synthesizing hybrid 2D nanomaterials (graphene to dichalcogenides) with metallic nanoparticles.

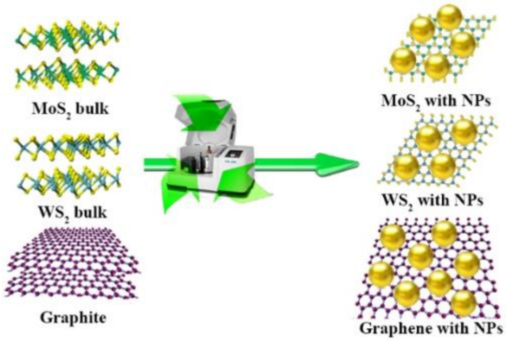

Figure 1. *Synthesis of hybrid 2D nanomaterials.*

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F-19

Production of oxidants in an electro-absorber designed by 3D printing for the degradation of benzene from gaseous streams polluted

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Electrochemistry

The main objective of this work is the design of an integrated absorption column and electrochemical reactor in a single unit (electro-absorber) generated by 3D printing. Different materials for the fabrication of the electro-absorber were evaluated until getting a useful and contaminant-resistant prototype. A transparent resin was used allowed observe internal hydrodynamic features during the experiment. In this case, the electrodes used were Boron-Doped Diamond (BDD) and titanium for anode and cathode, respectively, sulfuric acid as electrolyte and absorbent, and benzene as a pollutant. A flow-rate gas inlet of 6.0 L h^{-1} and different current densities were tested (50, 100, and 150 mA cm^{-2}) and complete characterization of the liquid and gaseous phases were carried out by CG-MS. Benzene removal occurs by the production of a cocktail of oxidants during electrolysis in the electrochemical cell and by physical absorption itself. An evaluation of these oxidants of the liquid and gaseous phases were carried out by the standard iodometric titration method (Method I^-/I_2) [1,2].

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F-20

SYNTHESIS AND FORMULATION OF BIO-BASED FREE-ISOCYANATE POLYURETHANES

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Chemical Engineering

Over the years, the development of new materials that meet human needs in different applications fields, with the paradigm of the great climate and environmental concerns, has irremediably led the progress of technologies and production processes towards alternatives that are increasingly sustainable and respectful with our ecological-social environment.

Faced with the toxicological implications and environmental repercussions associated with certain materials such as traditional polyurethanes, polymers synthesized from isocyanates, sustainable alternatives arise to replace them in each and every one of their applications.

This project focuses on the study of the synthesis and formulation of isocyanate-free polyurethanes, also known as *NIPUs,* from a polyaddition reaction between raw materials of renewable origin such as carbonated soybean oil (CSBO) and diamines derived from dimerized fatty acids.

To do this, the optimization of the synthesis conditions and curing process of the materials is first studied, analyzing the influence of the molar ratio between reagents, temperature and curing time, setting the optimal conditions at 90ºC, 6 hours and a molar ratio equal to 1.1.

Furthermore, it is proposed a modification of the chemical structure of the precursors through an original procedure that consist of the partial blocking of the active polymerization sites, thus allowing to obtain materials with a wide range of tailor-made properties. This study also allows to synthesize NIPUs with a 100% renewable origin, using as precursors CSBO and a reagent as simple and sustainable as water.

Finally, a foaming process assisted by supercritical CO_2 ($scCO_2$) is studied, which allows the reprocessing of the elastomers obtained previously and the obtaining of flexible NIPU foams, leaving the door open to further investigation on the optimal foaming conditions.

F-21

Functionalized carbon nanohorns with SERS activity

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Nanochemistry

In the last decades, organic chemists have developed numerous functionalization routes to fine tune the properties of carbon nanomaterials including carbon nanotubes, graphene, or carbon nanohorns. Carbon nanohorns are spherical aggregates of horn-shaped carbon nanotubes. Their size distribution, low toxicity and electrical properties make them very interesting for their application in sensing and bioimaging. This contribution will show the functionalization of carbon nanohorns with a series of thiophene derivatives and their potential use in Surface Enhanced Raman Spectroscopy (SERS).[1,2] In particular, it will focus on the fast and efficient eco-friendly covalent functionalization of carbon nanohorns *via* the 1,3-dipolar cycloaddition and their unique spectroscopic features. The work combines experimental and *in silico* studies to understand the Raman enhancement.

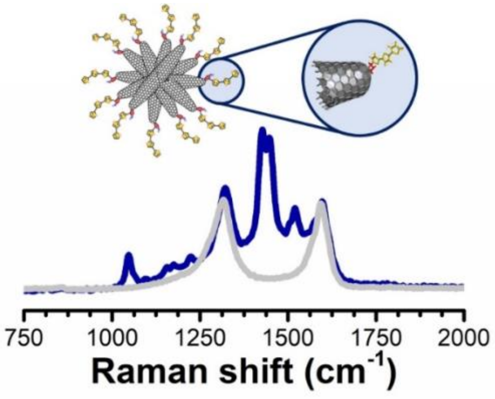

Figure 1. Schematic representation of covalently functionalized carbon nanohorns with thiophene derivatives and the comparison of the Raman spectra of the pristine and the functionalized materials.

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F-22

Strategies for the synthesis and analytical control of Coenzyme Q_{10} nanoformulations

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Química Analítica

Nanoformulations have generated great interest in research due to their applications as carriers and bioactive release systems[1]. This is the case of nanomicelles, which are used as colloidal nanocarriers based on surfactants that improve the bioavailability and solubility of lipophilic bioactives[2]. For this reason, it emerges the need to apply analytical chemistry to improve the quality control of these nanoproducts as well as their identification, characterization, and quantification, through the development of new analytical methods and tools. For this purpose, Coenzyme Q_{10} nanomicelles were synthesized with two different surfactants (Kolliphor® HS15 y Tween 80®) by heating at 50ºC in a water bath with constant stirring for 15 minutes. Then, a stabilizer consisting of 2% Glucose and 0.1538M NaCl was added, and the pH was adjusted to 4. These syntheses were characterized to compare the data with both surfactants, to optimize the CoQ_{10}/surfactant ratio, to measure the encapsulation efficiency (%EE) of the bioactive, as well as the stability of the micelles and reproducibility of the synthesis. The characterization was carried out by absorption (UV-Visible) and emission (Fluorescence) spectroscopic techniques, dynamic light scattering (DLS), and scanning electron microscopy (SEM). Once optimized, the 1:10 ratio was chosen as the average size (18.76±1.39 nm and 176.70±2.65 nm obtained with Kolliphor® HS15 and Tween 80®, respectively) and polydispersity (0.21±0.05 and 0.09±0.04 obtained with Kolliphor® HS15 and Tween 80®, respectively). As for the encapsulation efficiency, it turned out to be 96.28% and 95.15% for the micelles formed with Kolliphor® HS15 and Tween 80®, respectively. Finally, according to their UV-vis and fluorescence spectra, as well as their sizes and polydispersity, measured for 1 month, the nanomicelles were relatively stable and reproducible.

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F-23

STIMULI-RESPONSIVE MULTI-LAYERED HYDROGELS FOR TISSUE ENGINEERING

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Química Orgánica

Hydrogels are three-dimensional networks of natural or synthetic polymers, capable of absorbing large amounts of water or biological fluids.[1] These systems are highly versatile due to their unique properties, which can be modified depending on the nature of the monomer units, the crosslinking agent or dopants molecules. One of the most promising applications of these systems is their use in tissue engineering for tissue and organ regeneration, bioactive molecules controlled release, living cells encapsulation or wound dressings among others.[2]

In particular, the aim of this research is the synthesis of a multi-layered hydrogel system consisting of two concentric layers: a magnetic synthetic hydrogel derived from 2-vinyl-4,6-diamino-1,3,5-triazine (DAT) surrounding a core with a biodegradable natural polymer of hyaluronic acid functionalized with methacrylic anhydride (HAMA) (Figure 1). This combination can be suitable, as the external magnetic field stimulus can induce the release of active molecules towards the inner natural hydrogel layer to stimulate cell proliferation and differentiation.

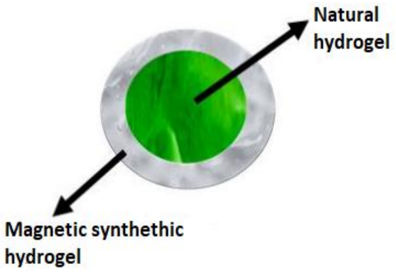

Figure 1. Bilayer hydrogel.

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F-24

Método de descomposición de dominios Schwarz para mejorar soluciones de colocación Legendre

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Matemáticas aplicadas. Mecánica de fluidos.

Fluids are all around us, from gases to liquids. Therefore, it is important to understand them mathematically. The only way to study them nowadays is by numeric methods like Legendre collocation. Each numeric method has its own advantages and disadvantages. The Legendre collocation method is ill-conditioned, which means the computational complexity of the problem grows exponentially. The Schwarz decomposition method (SDM) is then used to overcome this issue. With SDM, the whole domain is split into several smaller subdomains where we can apply Legendre collocation independently. Thanks to SDM, we have been able to reach solutions never obtained before with a collocation method. The particular problem we are studying is the Rayleigh-Bénard problem, a fluid in a rectangular domain is heated from below keeping the upper tape at constant temperature. With the mathematical formulas there are two parametres that will define the fluid behaviour, the aspect ratio (Γ) and the Rayleigh number (Ra). Our main goal is to reach turbulence dynamics, which is a part of the field not very well known. Turbulence occurs with high Ra ($\sim 10^7$). With SDM and Legendre collocation Ra can be increased drastically. We are still studying these methods to their full potential, but the results already accomplised are very good and may be usefull to show the huge impact SDM has alongside the Legendre collocation method.

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F-25

INFLUENCE OF ELECTRIC FIELDS (AC AND DC) TO ENHANCE PHYTOEXTRACTION OF METALS USING *LOLIUM PERENNE* FROM MULTI-METAL POLLUTED MINE-TAILINGS

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Chemical Engineering

The presence of heavy metals in water and soils remains an important challenge being a risk for the environment and humans. The mining sector activities have led to the accumulation of mine tailings and other wastes abandoned and exposed to the environmental agents which contribute to the spread of pollution. Electro-phytoremediation emerges as interesting new technology for the treatment of polluted soil and rehabilitation of abandoned mining areas. This technology was tested in this research using real mine tailings. The experimental design was composed of 5 experimental series using ryegrass (*Lolium perenne*) as plant species and different types of the electric field that started to be applied 44 days after sowing and kept for 14 days with a voltage gradient of 1 V.cm^{-1}. The treatments were: alternate current with plants (EKPhAC) and without plants (EKAC), direct current with plants (EKPhDC) and without plants (EKDC), and plants without electric current (Ph). The physicochemical parameters were controlled in liquid samples from electrode wells, soil pore water, soil, and plant biomass. The reversal polarity mode in DC current treatment was efficient to avoid those extreme pH changes that could affect plant growth and rhizosphere development[1]. *Lolium perenne* grew up in highly polluted mine tailings. However, it showed phytotoxicity symptoms like chlorosis and early wilting in the growth period[2]. The metals accumulated to a higher extent in ryegrass tissues were Zn, Pb, and Cu. The application of electric current did not affect the biomass production of ryegrass. The application of alternate electric current (EKPhAC) improved mainly the metal bioavailability and uptake by *Lolium perenne*.

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F-26

Synthesis and characterization of self-healing materials.

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Química Orgánica

Soft materials such as polymers, elastomers or hydrogels can be easily damaged, for that reason their lifetime, in most of the cases, is too short. This problem has led to the study of self-healing materials.

In the last years, many materials with different self-healing mechanisms have been studied. The most important mechanisms are: i) encapsulation of self-healing agents, ii) metal-ligand coordination bonds, iii) reversible covalent bonds such as Diels-Alder reactions, iv) non covalent bonds such as hydrogen bonds or ionic interactions or hydrophobic interactions.[1]

Some of the previous mechanisms are not autonomous, that means that the material must receive an external stimulus like light, heat, or an electromagnetic field in order to self-heal. For that reason, these materials do not have many applications.

The objective of this work is to find hydrogels with self-healing and with good mechanical proprieties. The starting point is the SHAP hydrogel (*Self-Healing AETA-based Polymer),*[2] this hydrogel was synthesized by the MSCO Nanochemistry group; it was synthesized by photopolymerization of (2-(Acryloyloxy)ethyl)trimethylammonium chloride (AETA) using *N,N'*-Methylenebisacrylamide (MBA) as the chemical crosslinker and sodium 2,4,6-trimethylbenzoylphosphonate (NaTPO) as photoinitiator using water as solvent. The self-healing capacity of this hydrogel is given by the hydrogen bonds that form the water molecules inside the structure. To improve the self-healing capacity of the SHAP hydrogel, monomers with diverse charges were added to the SHAP chemical structure producing an additional electrostatic interaction between the different monomers. Different hydrogels were synthesized using various types of negatives and positives monomers and different molar concentrations.

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F-27

Guanidines as catalysts for the reduction of CO_2 using hidroboranes

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Química inorgánica

In last years, the scientific community has shown a huge interest for the use of CO_2 as C1 feedstock with the objective of reduce its concentration in the atmosphere. One of its most interesting transformations is the reduction into methanol, which can be used as fuel or as a building block to synthesize valuable chemicals.[1] To carry out this reduction, several reducing agents have been studied with homogeneous catalysts, where hydroboranes stand out for favoring mild reaction conditions and enabling the use of organocatalysts.[2]

In this work, we use four different trisubstituted guanidines [R^1–N=C(NHR^2)(NHR^3)] (R = alryl or alkyl groups) as catalysts for the reduction of CO_2 to methanol using two commercial hydroboranes ($BH_3{\cdot}SMe_2$, 9-borabicyclo-[3:3:1]-borane (HBBN)) as reductant agents. Several experiments have been carried out to optimize the catalytic conditions, as well as catalysts' recycling experiments to prove their activity. Furthermore, stoichiometric experiments helped us to identify the intermediates of the catalytic reactions.

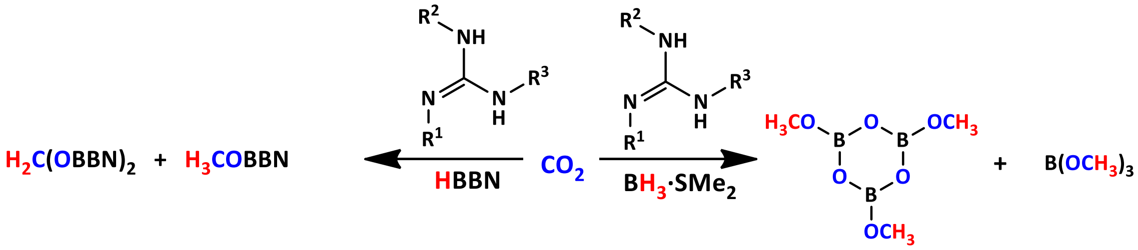

Figure 1: Catalytic reduction of CO_2 with HBBN and $BH_3{\cdot}SMe_2$

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F-28

Reactions of N-phosphinoguanidines with calcium amides

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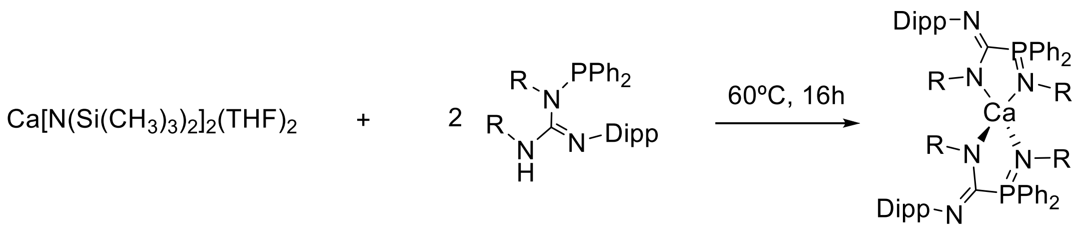
Química Inorgánica.

We have studied the reactivity of N-phosphinoguanidines with metal derivatives of the main groups, having previously used aluminium, zinc or magnesium alkyls. In the present work, a calcium amide has been used, $Ca[N(Si(CH_3)_3)_2]_2(THF)_2$ **(1)**, which has allowed us to broaden our knowledge of the reaction mechanism with these ligands, detecting previously undocumented intermediates and isolating more phosphinoimine-amidinate complexes. As with the other metals, by using two equivalents of N-phosphinoguanidines, $(HNR)(Ph_2PNR)C(NAr)$ (Ar = $2,6\text{-}^{i}Pr_2C_6H_3$ [Dipp]) (R = *i*-Pr, **2a**; Cy, **2b**), per equivalent of the calcium amidide and heating under mild conditions (16h at 60ºC), the phosphinoimine-amidinate complexes, $Ca\{k^2,N,N'\text{-}(N\text{-}R)(N\text{-}R))C(=NDipp)PPh_2\}_2$ **(3a, b)**, are obtained after ligand rearrangement. To understand the mechanism of this reaction, involving the rearrangement of the ligand, we also decided to follow the progress of the reaction at 50ºC through $^{31}P\{^1H\}$ NMR spectroscopy, identifying different intermediates and how they underwent Schlenk-type equilibria. [1, 2]



1

R = iPr, 2a; Cy, 2b

R = iPr, 3a; Cy, 3b

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F-29

Studying the aromatic profile of dealcoholized rosé wines of the Cencibel variety

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Área de Química Analítica y Tecnología de Alimentos

Recently, an increased ethanol concentration in wines has been observed, mainly because of climate change. On the other hand, consumers are increasingly demanding wines with reduced or null alcohol content due to the negative effects that it has in health. In this context, the winemaking industry has developed different techniques to reduce alcohol content in wine, among which post-fermentation techniques stand out because they are the ones that least modify the sensory profile of the wines. In this way, we have analyzed three rosé Cencibel wines with different alcohol content (control wine with a normal ethanol content, partially fermented wine and a dealcoholized "wine") in order to determine the main impact compounds and aromatic series of the aroma of the three studied wines, as well as to determine if the partial or total dealcoholization process produces changes in these profiles.

Volatile components were analysed by GC-MS with a previous isolation by solid phase extraction (SPE) [1]. Once the compounds were identified and quantified, the active aroma value (OAV = c/t) was calculated for each of them. In addition, aromatic descriptors were assigned to each of the compounds, allowing us to group those with similar descriptors into aromatic series. The intensity of each series was calculated as the sum of the VAOs of all compounds assigned to each of the aromatic series. Out of the 26 compounds with a OAV > 0.1, only some of them were found in concentrations above their corresponding olfactory perception threshold, so these were the compounds that were considered potential contributors to wine bouquet (acetaldehyde, ethyl octanoate, isoamyl acetate, ethyl butyrate, β-damascenone, etc.).The main aromatic series that determined the bouquet of the wines, regardless of the winemaking process, were the same (fruity, fatty and sweet), showing only differences in their intensity. The dealcoholized "wine" was the one that presented the lowest intensities of the sweet and fruity series, probably due to the lower concentration of esters.

We can conclude that dealcoholization process does not modify the aromatic composition of the wine, but it does affect the intensity of the profile.

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F-30

Study of the capacity of fungal and bacterial laccases for the degradation of ochratoxin A in different reaction media

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Introduction. Ochratoxin A is a food toxin that can be found in different crops such as cereals, cocoa beans, coffee, grapes, etc. This toxin has nephrotoxic, immunosopressive, genotoxic, teratogenic, etc. effects, classified by the IARC as a possible human carcinogen. One of the methods of removing this toxin is the application of laccases of diverse nature on contaminated food. The presence of some compounds, which are called mediators, can intervene and improve the reaction of degradation of this toxin.

Objectives. The main objective of this study was to evaluate and compare the effect of the laccases *Trametes versicolor* and *Lactobacillus casei* on the reduction of ochratoxin A in the presence of different mediators and in different reaction media.

Methodology. Oxidation reactions were carried out in volumes of 100µL in microtubes of 1.5 mL. Duplicates of both the control samples and the degradation tests were performed. Some mediators used were phenolic compounds, such as catechin or ferulic acid. The reaction media used were sodium acetate buffer 50 mM at pH=4 and synthetic wine (12% ethanol and 5 g/L tartaric acid). The samples were prepared and subjected to a stirring reaction for 24 hours at 28ºC. The reactions were stopped after this time by azide sodium 100 mM. The determination of ochratoxin A degradation was carried out using an HPLC coupled to a Q-TOF mass spectrometer.

Results. The results showed that in the absence of a mediator there is no degradation of ochratoxin A, while in the presence of mediators such as catechin, epicatechin and ferulic acid significant degradation values are observed. On the other hand, the degradation values of this toxin were higher when the reaction medium was carried out in sodium acetate buffer.

Conclusions. It can be concluded that these enzymes allow the reduction of the concentration of ochratoxin A under the conditions studied, always in the presence of a mediator. The influence of the reaction medium on the action of the different lacasas was also confirmed.

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F-31

Remove of antibiotic resistant bacteria on air with electrochemically oxidants generated

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XVI Young Science Symposium

The research of biologic aerosols (bioaerosols) has increased strongly due to the world pandemic of SARS-CoV-2. The bioaerosols are suspended particle on the air whose size is in 0,1 to 100 µm and they expel them to the nose and/or the mouth of illness person when sneeze, talk or cough. These droplets in suspension can be constituted for diverse compounds of biological origin like bacteria, fungi or virus [1]. In this context, is very important to resalt the high frequency of hospital outbreaks for nosocomial infections that can be lethal and transmitted for airborne pathogens [2]. The nosocomial infections more frequent are the urine infections for bacteria like Escherichia coli or Klebsiella spp. And the respiratory infections for microorganisms like Staphylococcus aureus, Legionella spp. or Aspergillus spp., or viruses like respiratory syncytial virus. Have been used radiation technologies like the UV light, active filtration with HEPA filters or the fumigation with gas oxidants like ozone or hydrogen peroxide for control the extension of airborne pathogens [3]. In this study, the electrochemically technologies have been evaluated as alternative to conventional treatments. In a first step, the simulation of bioaerosols that contain E. coli will make in controlled conditions to laboratory scale using commercial hydraulic nebulizers commons and others more specific like the Collison nebulizer. To continue, the bioaerosols will recollect in a sterile liquid phase and they will treat direct or indirectly with electrochemically oxidants generated (ozone, hydrogen peroxide and chlorine dioxide). The production of this gas oxidants will develop with electrochemical cells capable of working to high pressure (until 10 bares) and with electrodes of flow through of them. In both cases, the ultraviolet light can be coupled to for knowing the synergic effect between treatment technologies.

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F-32

Addition of biomass combustion ashes in ceramic materials: influence on composition, properties and environmental aspects

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Área de conocimiento: Química Física

In this work, it is analysed the influence of the addition of biomass ash, specifically olive pomace ash, on the properties of ceramic material. This possibility has been raised due to the high potassium content of these ashes and their possible behaviour as a fluxing material. They could be used as a substitute for alkaline feldspars, as these ashes have a potassium content 30% higher than that of feldspars (12-15%)[1,2].

To this end, physical, chemical and mineralogical analyses have been carried out in order to characterize the ashes to be used, the raw material clays and the ash-clay mixtures made in the laboratory (ash content 5% or less)[3].

Fluorescence and X-ray diffraction studies, thermal methods such as thermogravimetry or optical heating microscopy have been carried out on the different raw materials and new mixtures. These studies carried out at laboratory level, together with the performance of tests at industrial level, will make possible to determine whether the ashes show fluxing behaviour[4].

The results are related with i) the possibility to reduce the high firing temperatures of the ceramic production process, ii) the possible reduction of carbon dioxide emissions into the atmosphere, iii) the possible contamination or not by other compounds and iv) the assessment of the mechanical properties of the new mixtures produced.

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F-33

Enhanced separation of seven biologically active compounds by capillary electrophoresis with carbon-based nanoparticles as additive

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Química Analítica

Biologically active compounds can be defined as nutrients and non-nutrients present in food matrices. These compounds are characterized by influencing cellular and physiological activities, showing a beneficial effect for health related to disease prevention and even forming part of therapeutic treatments [1]. In view of the growing worldwide usage associated with their health benefits, their efficacy and safety, sensitive and selective analytical methods are required for the determination of such food components and those related compounds that nullify the beneficial effects [2]. Herein, a highly reliable separation and determination of various health-promoter compounds was achieved by capillary electrophoresis (CE) based on β-cyclodextrin-functionalized graphene quantum dots (βcd-GQDs) as the background electrolyte additive. βcd-GQDs was successfully prepared and characterized for the first time, showing to enhance the separation efficiency of all the analytes studied, as the result of decreasing their apparent mobility and increasing their migration time. Up to eight consecutives' runs were acquired with high precision for the separation of resveratrol, pyridoxine, riboflavin, catechin, ascorbic acid, quercetin, curcumin and even of several of their structural analogues. Baseline separation was achieved within just 13 min as a result of the effective mobility of the analytes along the capillary owing to the differential interaction with the additive. By the proposed analytical method, detection limits lower than 0.3 $\mu g\ mL^{-1}$ and precision values were in the range of 2.1 – 4.0% for all analytes. The usefulness of the GQDs-assisted selectivity-enhanced CE method was verified by the analysis of food and dietary supplements. The applicability to such complex matrices and the easy and low-cost GQDs preparation opens the door for routine analyses of food and natural products.

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F-34

Valorization of Polluted Vegetal Waste for Manufacturing Sustainable Cathode Materials for the Production of Hydrogen Peroxide

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Dpto. de Ingeniería Química

Electrochemical production of H_2O_2 is an area of research that has grown in importance in recent years due to the wide availability of this reagent and the high environmental impact of its production using traditional anthraquinone processes. The main direction of research is the cathodic production of H_2O_2 from oxygen reduction using carbonaceous materials, usually coated with a mixture of polytetrafluoroethylene (PTFE) and carbon black (CB) [1]. On the other hand, restoration of contaminated environments through electro-, bio-, and phytoremediation techniques is a viable alternative to restore large-scale contaminated sites. Nevertheless, the grown biomass accumulates the target pollutants and becomes a new contaminant.

In this context, this work proposes the utilization of heavy metal-contaminated plant biomass during phytoremediation of mining waste as a feedstock for the synthesis of carbonaceous materials that can be used as a substitute for CB for hydrogen peroxide production. This transformation is achieved by applying a hydrothermal carbonization (HTC) step to produce hydrochar that can be further transformed through thermal or chemical activation processes [2]. This approach, based on the concept of a circular economy, can simultaneously achieve two important milestones: recycling a wide range of polluting wastes and reducing the environmental impact of CB production influences.

Based on this, the HTC process and subsequent thermal activation were performed on *Spergularia* contaminated with Zn, Pb, and Cu to obtain materials with high specific surface area (around 400 m^2/g) and high electrical conductivity. To correlate the properties of the material with the proposed application, structural and physicochemical characterizations, including thermogravimetric analysis, N_2 adsorption isotherms, surface conductivity, Raman spectroscopy, and elemental analysis, were performed. Finally, hydrogen peroxide production was evaluated with the most electrocatalytically active material in a continuous flow reactor with an electrode surface area of 64 cm^2, comparing the hydrogen peroxide production efficiency of the synthetic material and commercial CB with succesful results.

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F-35

A NOVEL BIOINSPIRED HYDROGEL SYSTEM IMPROVES THE QUALITY OF SHEEP OOCYTES AFTER IN VITRO MATURATION

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Química Orgánica

The global assisted reproductive technology (ART) market is expected to reach $50.32 Billion in 2027 due to the increasing incidence of infertility and growing awareness. Despite being one of the most promising ARTs, oocyte *in vitro* maturation has become a major limiting factor for the *in vitro* production of viable embryos in different mammalian species.

To improve the standard *in vitro* models within oocyte maturation, we have developed a new 3D culture system based on binding two hydrogels that closely mimic the mechanical characteristics of the mammalian ovary. Thus, DNA fragmentation studies, confocal microscopy, and quantitative real-time PCR demonstrated that the double hydrogel system significantly improved the quality of matured sheep oocytes.

According to these results, the proposed system is potentially a novel tool for reproductive technologies and livestock production applications.

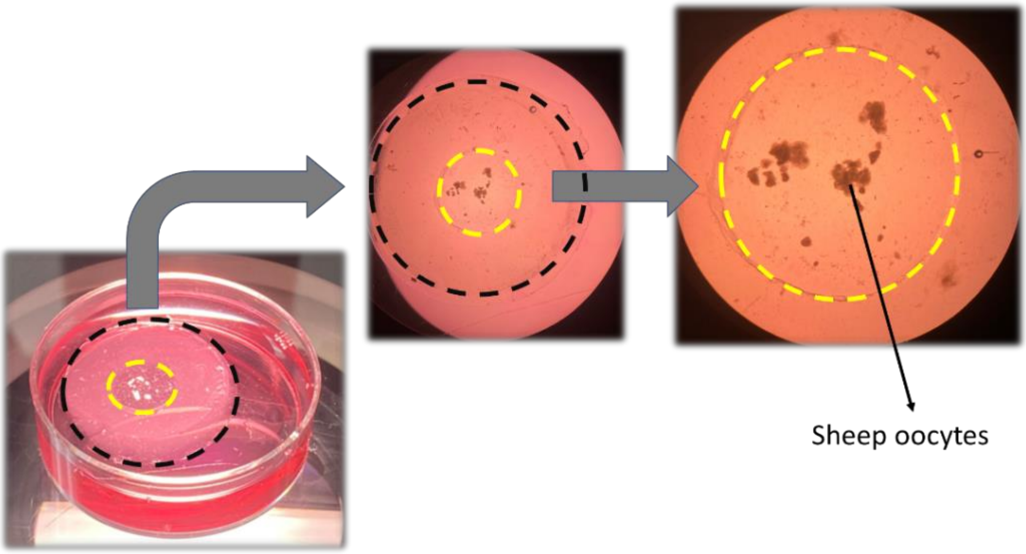

Figure 1. Novel hydrogel system during oocyte in vitro maturation.

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Electro-reforming of bioethanol streams produced by sugar fermentation on an optimized Pt-Ni anodic catalyst supported on graphene nanoplatelets

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Ingeniería Química

The continuous increment in gaseous pollutants has created the need to find new and cleaner ways to fulfill the global energy demand. In this sense, green hydrogen has gained importance as an energy carrier alternative to fossil fuels, since it can be obtained by alcohol electro-reforming in an electrolyzer. Ethanol is the main product obtained by the fermentation of carbohydrates from biomass [1]. In ethanol electro-oxidation reaction (EOR), ethanol is oxidized in the anode, obtaining acetaldehyde, ethyl acetate and acetic acid; whereas the protons from EOR are reduced in the cathode into hydrogen.

Taking this into account, the electro-reforming of real bioethanol streams was performed in a Proton Exchange Membrane (PEM) electrolyzer containing a Membrane Electrode Assembly (MEA), in order to study the progress in ethanol production over fermentation time. The anodic catalyst employed was a 40 wt.% Pt-Ni (Pt/Ni 2/1) supported on graphene nanoplatelets, with an anode loading of 1.5 $mg_{Pt\text{-}Ni}\cdot cm^{-2}$, as studied in a previous work of our group as a technical and economically appropriate alternative to commercial anodes. Then, three bioethanol streams were produced by fermentation at room temperature without stirring, with initial sugar concentrations of 150, 200 and 250 $g\cdot L^{-1}$ and an initial dry yeast concentration of 5 $g\cdot L^{-1}$. A general tendency in the increase in ethanol concentration given on each fermentation day was found as initial sugar concentration decreases. Conversely, larger ethanol yields and longer fermentation times were achieved as sugar concentration rises, achieving the 200 $g\cdot L^{-1}$ bioethanol stream the best compromise between bioethanol production and fermentation time. Additionally, this stream accomplished the highest current density (~285 $mA\cdot cm^{-2}$ at 1.2 V, on the 21st of fermentation), hence proving the promising use of this anodic catalyst in the electro-reforming of real bioethanol streams.

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F-37

DESIGN AND DEVELOPMENT OF A HARD/SOFT DOUBLE HYDROGEL SYSTEM TO IMPROVE REPRODUCTIVE BIOTECHNOLOGIES

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Química Orgánica

Conventionally, cell culture is developed in 2D environments, which can affect the cell morphology, the communication between cells and with the extracellular matrix and cause several changes. In order to reduce cell culture and physiological environment, 3D scaffolds have been developed, partially maintaining the mechanical and biochemical cues of the original tissue. In particular, *in vitro* fertilization is usually also performed in 2D environments and half of the embryos fail to develop. In this project, we aim to create a 3D biocompatible scaffold for 3D cell culture by using hydrogels.

Hydrogels are three-dimensional polymeric materials chemically or physically cross-linked which can absorb water without dissolving in it. They are also very porous materials, which allows the exchange of nutrients and cellular wastes.[1, 2]

Our scaffold consists of a natural part in the middle that will contain the oocyte, and another natural or synthetic part surrounding it, trying to mimic the natural environment of oocytes. The central part is made of alginate, which is highly biocompatible. The external part can be made of three different kinds of hydrogels: one of them is based on 2-Vinyl-4,6-diamino-1,3,5-triazine (VDT); the second one is based on sodium 4-vinylbenzenesulfonate (VBS) and the third one is based on a natural polymer, i.e., chitosan. These hydrogels can link to alginate through physical interactions.

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F-38

Ruthenium (II) polypyridine complexes as potent PACT agents for selective therapy

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Química Inorgánica

The problematic of cancer as the second leading cause of death globally and the increase of antimicrobial resistance (AMR), due to ineffective treatments, have led to a wide variety of lines of research on novel pharmacological drugs to solve these issues. More effective and selective compounds are required to deal with the drawbacks of traditional chemotherapy: multidrug resistance and severe side effects. Photochemotherapy (PCT) has emerged as a promising therapy, a prodrug (usually named as photosensitizer) is used to treat the pacient, this compound becomes active in presence of light while it remains innocuous in dark conditions. Photoactivated chemotherapy (PACT), which stems from PCT, uses a prodrug which suffers a photocleavage process (also known as photodissociation) when irradiated at a certaing wavelenght. These mechanism leads to one or more active species originated from the previous innocuous compound, which eventually triggers cellular death through an oxygen-independent mechanism. In this work, a series of ruthenium (II) compounds of formula $[Ru(tpy\text{-}R)(Me_2bpy)(L)]A_2$, potentially active as PACT agents, have been synthesized. The terpyridine ligand has been extensively studied as it gives unique electronic properties to the metal center, enhancing the photodissociation process. The 6,6´-dimethyl-2,2´-bipyridine (Me_2bpy) ligand generates a great steric hindrance produced by the methyl groups, improving photodissociation. The L ligand is a cytotoxic compound which is innocuous when caged in the metallic complex. Clotrimazole, an antifungical commercial drug, has showed interesting cytotoxic properties in several cancer cell lines. For this reason, it has been used as the cytotoxic compound (L).[1]

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F-39

Air quality assessment in the ecological area of Las Tablas de Daimiel National Park, in Spain

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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 areas. Although these areas may be far away from urban or industrial sites, remote transport of persistent pollutants to national parks or protected areas has been reported in previous studies [1,2]. This work shows that national parks and other protected natural areas require in situ tools to monitor and detect local and remote air pollution sources which are a threat to natural resources. The main objective of this work is to perform a field campaign inside a national park involving the measurement of the air criteria pollutants, O_3, NO_2, NO, SO2, CO $PM_{2.5}$ and VOCs from anthropogenic sources and meteorological parameters to assess the air quality inside the park Las Tablas de Daimiel and to identify local or distant sources of pollutants which could endanger its preservation.

The study was carried out from March 2020 to July 2021, involving the continuous measurement of meteorological data, gaseous pollutants, and $PM_{2.5}$ inside the park with one hour time resolution. Twelve campaigns, one week duration, were also performed to sample air in sorbent tubes to analyse VOCs. The results are discussed considering meteorology, especially wind and speed direction together with the assessment of back-trajectories of remote air masses. The results show that, excepting for the high levels of ozone, air quality in the park is slightly affected by local and remote air pollution sources.

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F-40

What exists inside a beehive?

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Ciencia y tecnología de los alimentos

At present, beekeeping occupies a very representative place in the agri-food sector, with the products obtained emerging with increasing force, both in the national market and in the international market under the idiosyncrasy of "clean technology", propitiating an increase in demand by new consumers, concerned about a healthy life and a respect for the environment [1]. Inside a hive the main products found are: honey, pollen, royal jelly and propolis. Since ancient times, all of them have been used for their medicinal and nutritional properties, being recognized for their benefits in pollination and indirect pest control by competing with insects for plant food (nectar and pollen) [2].

Materials and methods

In order to know the microorganisms that are found both in the beekeeping environment (surface of the hive, atmosphere, bees and flowers) and in the products generated (honey, pollen and honeycomb), a sampling has been carried out in 4 apiaries and in a total of 23 honeys of different varieties. A count of bacteria, yeasts and molds has been carried out, taking 5 g of previously homogenized honey together with 45 ml of YPD broth (Yeast Peptone Dextrose) in a sterile flask. For ambient samples, the amount of sample is weighed and the same volume of YPD broth is added to make a 1:1 dilution in a stomacher bag. They were incubated with shaking (200 rpm) at 30ºC for yeasts and molds and 37ºC for bacteria for 24 hours. They were seeded on YPD agar and incubated at the same temperatures for 2/10 days. To carry out the identification of yeasts, the RAPD-PCR technique is performed together with the RFLP-PCR technique, thus identifying at the species level and the strain level. The databases used for the results of the two PCR techniques are Blast ® and Yeast-ID, respectively.

Results and discussion

The results obtained in the present work indicate that both in the environment and in the products of the beehives there is a growth of organisms, whose average counts obtained are 2.72 log cfu/g for bacteria and 0.84 log cfu/g for yeasts. Generally formed by bacteria of the genus *Bacillus*, and yeasts of the genus *Saccharomyces*, the most frequent being *S. bisporus*, *S.rouxii* and *S. bailii* and other *non-Saccharomyces* yeasts such as *Zygosaccharomyces* spp. and *Candida* spp. [3]. In addition, the presence of molds has been observed, which is associated with the intestinal content of bees, as well as with the environment, recognizing among them genders such as *Aspergillus*, *Chaetomium*, *Penicillium* and *Mucor* [2]. Finally, it should be noted that honey has been recognized as a source of *Clostridium botulinum* spores and is sometimes associated with ingested infant botulism [4].

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Ultraviolet (UV) photolysis study of Furan-based compounds in the gas phase under exposure on solar radiation.

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Química Física

Biomass burning (BB) due to wildfires, agricultural burning, and domestic fuel use are substantial both biogenic and anthropogenic sources of a series of volatile organic compounds that impact the air-quality and human health. Recent field studies[1, 2] have measured a series of furanoids, at significant levels, despite their high tropospheric reactivity. Furans are heterocyclic, semi- or low-volatile oxygenated compounds that can be aromatic or not. Besides, their inherent toxicity furans atmospheric degradation could lead to ozone formation, a strong greenhouse gas and/or to secondary organic aerosols (SOAs) formation and thus a substantial source of the atmospheric particulate matter.[3] The presence of the heteroatom on the five-member ring, along with the several optically active groups that have been proved to contain, e. g. carbonyl-, alkyl or alkoxy- groups, could make them potent UV absorbers in the actinic wavelength range. In this work, the UV photolysis of furan derivatives and the formation of oxidation products are being studied by exposing the furans on solar radiation using a solar simulator, as an irradiation source, and a proton transfer time-of-flight mass spectrometer to monitor the loss of furan compound and formation of gaseous products. The size-distribution of formed SOAs is monitored by a fast mobility particle sizer.[4] The UV absorption cross sections are also determined in the UV actinic solar region ($\lambda > 290$ nm) in order to evaluate the UV absorption capability of these compounds and their potential atmospheric degradation by photolysis.

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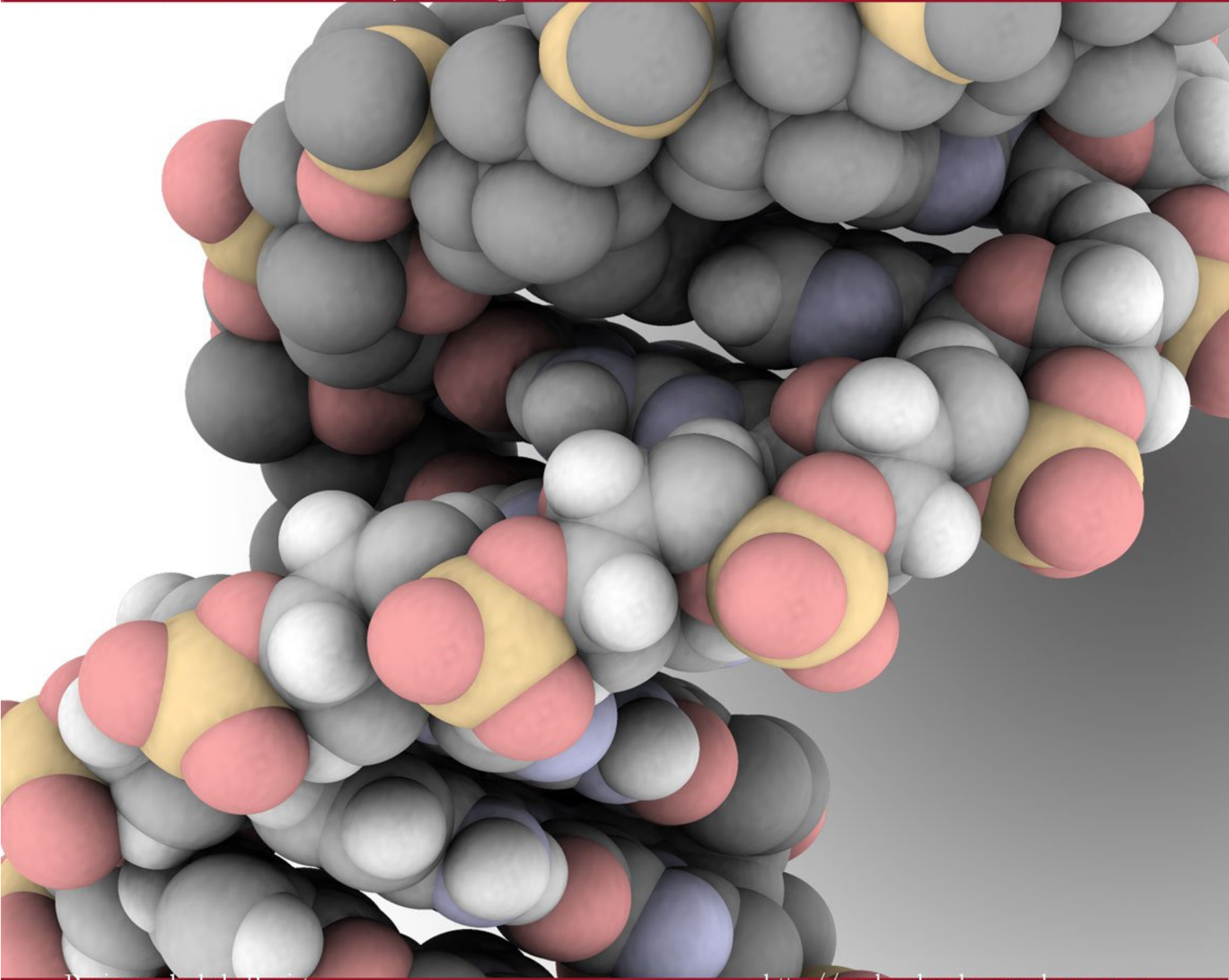
CÓMO FUE LA EDICIÓN DEL AÑO PASADO...

REVISTA MOLÉCULA

Revista de la Facultad de Ciencias y Tecnología Química
Universidad de Castilla La Mancha



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ÍNDICE

PRESENTACIÓN

El mes de Julio esta dedicado al XV Young Science Symposium donde se recoge el transcurso de este interesante evento. Se muestran las conferencias de prestigiosos invitados, comunicaciones orales y comunicaciones flash, todo ello con el fin de conocer el increíble trabajo que se realiza.

Aparte de lo mencionado, se recogen los premios otorgados y experiencias vividas en el symposium.

¡Deseamos que lo disfrutéis!

El comité editorial.

PRESENTACIÓN XV YOUNG SCIENCE SYMPOSIUM

Los noveles investigadores de la UCLM comparten sus líneas de trabajo en el Simposio Ciencia Joven

Marian Herrero (i), Ana Briones (c) y Manuel Andrés Rodrigo.

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Organizado por la Facultad de Ciencias y Tecnologías Químicas, se celebra en formato híbrido desde el 7 de Julio 2021 y hasta el 9 de Julio 2021.

La Facultad de Ciencias y Tecnologías Químicas de la Universidad de Castilla-La Mancha (UCLM) en Ciudad Real celebra entre el 7 y el 9 de Julio el XV Simposio Ciencia Joven, durante el que los investigadores noveles presentan sus líneas de trabajo a sus colegas de la institución académica a fin de conocer qué están desarrollando. El encuentro, que cumple su decimoquinta edición, se celebra en forma híbrido y congrega a unos 170 investigadores.

Los jóvenes investigadores de la Facultad de Ciencias y Tecnologías Químicas en el Campus de Ciudad Real, así como de otros llegados de distintos centros de la Universidad de Castilla-La Mancha (UCLM), presentaron entre el miércoles 7 de Julio y el viernes 9 de Julio a la comunidad académica sus líneas y resultados de investigación con motivo de la celebración del XV Simposio Ciencia Joven, una iniciativa que en esta edición se celebró en formato híbrido (presencial y en línea) y que a su vez les supone una oportunidad para acercar a los estudiantes a la tarea investigadora.

El encuentro reunió a alrededor de 170 investigadores y en él tuvieron cabida 35 comunicaciones orales de noveles investigadores, además de seis charlas de ponentes externos invitados de la Durham University (UK), Newcastle Universtity (UK), Arizona State University (USA), Universitat Politécnica de Valencia, Institute of Food Science, Technology and Nutrition y Universidad de Valladolid. Asimismo, y por primera vez en estos años, los pósteres han sido sustituidos por flash virtuales de vídeos de unos tres minutos de duración que pueden verse en las redes sociales de la Facultad de Ciencias y Tecnologías Químicas.

PRESENTACIÓN XV YOUNG SCIENCE SYMPOSIUM

Las líneas de investigación a presentar son "muy variadas", tal y como ha explicado la vicedecana de Estudiantes de la Facultad de Ciencias y Tecnologías Químicas y una de las organizadoras del evento, Marian Herrero, y pasan por las propias relacionadas con la Química, la Ingeniería Química y la Tecnología de Alimentos que pueden cursarse en el propio centro, a otras que tienen que ver con la sostenibilidad, la atmósfera o los hidrogeles. Ello da cuenta del carácter multidisciplinar que tiene este evento que en palabras de Herrero supondrá "una oportunidad para que los jóvenes investigadores interaccionen y conozcan qué hacen sus compañeros de Universidad, qué se investiga aquí".

Precisamente, la vicerrectora de Profesorado, Ana Briones, encargada de inaugurar el simposio, ha insistido en la importancia que tiene conocer el trabajo de investigación que realizan otros y relacionarse con investigadores distintos a los de su centro y campus, porque "el conocimiento pertenece a la Humanidad". Asimismo, ha señalado que eventos científicos y divulgativos como éste son "un buen escaparate" para que los jóvenes se entusiasmen por la Ciencia.

En su intervención, Briones ha indicado que la Ciencia "es conocimiento, saber" y que "es la investigación la que permite incrementar el conocimiento". En este punto, ha recordado la apuesta continua de la UCLM por hacer una investigación de excelencia y ha apuntado a la Facultad de Ciencias y Tecnologías Químicas como "ejemplo de esfuerzo y formación en jóvenes doctores, que se extiende al resto de centros" de la institución académica.

Junto a la vicerrectora, el decano de la Facultad de Ciencias y Tecnologías Químicas, Manuel Rodrigo, ha hecho también alusión a la importancia de este simposio para "motivar e ilusionar a los jóvenes para que hagan carrera investigadora", porque la ciencia "es atractiva, conlleva un esfuerzo y sacrificio, pero a la vez es gratificante". "Hay que intentar concienciar a la sociedad de la importancia que tiene la Ciencia y de cómo nuestros investigadores, en especial los más jóvenes, pueden ayudar a mejorar nuestra calidad de vida", ha manifestado.

El XV Simposio de Ciencia Joven incluye los premios a la Mejor Comunicación Oral, al Mejor Flash Virtual en las categorías de TFG, TFM y doctorado, y el Premio Social Media al vídeo con mayor impacto y viralización, patrocinados por Agrovin, Dilabo, la sección territorial de Castilla-La Mancha de la Real Sociedad Española de Química y Mervilab.

Gabinete Comunicación UCLM. Ciudad Real, 7 de julio de 2021

PRESENTACIÓN XV YOUNG SCIENCE SYMPOSIUM

Marian Herrero: “La participación y el nivel de los investigadores hacen del Congreso de Ciencia Joven un acontecimiento relevante para nuestra Facultad»

Simposio de Ciencia Joven

La vicedecana de Estudiantes de la Facultad de Ciencias y Tecnologías Químicas, Marian Herrero, defiende la relevancia adquirida por el XV Simposio de Ciencia Joven que se celebra en el campus de Ciudad Real, por el incremento de la participación y la presencia de relevantes investigadores. Herrero, como organizadora de este evento, destaca el hecho de contar con la participación de grupos de toda la UCLM, la participación con presentaciones flash/virtual y la ampliación del número de premios. Hasta el viernes 9 de Julio, los investigadores nóveles presentaron sus líneas de trabajo para dar a conocer los proyectos en los trabajan.

Marian Herrero, vicedecana de Estudiantes de la Facultad de Químicas del campus de Ciudad Real

La **vicedecana de Estudiantes** de la Facultad de Ciencias y Tecnologías Químicas, Marian Herrero, pone el valor la decimoquinta edición del Simposio de Ciencia Joven que ha sido inaugurada el miércoles 7 de Julio en el campus de Ciudad Real por el incremento de la participación, así como la presencia en el mismo de investigadores de relevancia lo que “lo hacen más multidisciplicar y adquiere otro carisma”, señala en esta entrevista con este digital.

Líneas de investigación

La también presidenta de la Sección Territorial de Castilla-La Mancha de la Real Sociedad Española de la Química y una de las organizadoras de este encuentro participaba la mañana del 7 de Julio en la inauguración del congreso, junto al decano de la Facultad de Químicas, Manuel Rodrigo, y la vicerrectora de Profesorado, Ana Briones, donde ha señalado que las líneas de investigación que presentadas son variadas y pasan por las relacionadas con la Química, la Ingeniería Química y la Tecnología de Alimentos que se pueden cursar en el propio centro, a otras que tienen que ver con la sostenibilidad, la atmósfera o los hidrogeles.

La Facultad de Ciencias y Tecnologías Químicas de la Universidad de Castilla-La Mancha (UCLM) en Ciudad Real celebra la edición número 15 del Simposio Ciencia Joven, durante el que los investigadores noveles presentaron sus líneas de trabajo a sus colegas para que se conozca qué están desarrollando.

7 Julio 2021. Lanza Digital

PRESENTACIÓN XV YOUNG SCIENCE SYMPOSIUM

PREGUNTA ¿Qué evolución ha tenido el Congreso de Ciencia Joven a lo largo de estas XV ediciones?

RESPUESTA.- Ha sido un congreso que ha evolucionado mucho, se comenzó como unas charlas que empezamos organizando los estudiantes de doctorado para conocer la investigación que se llevaba a cabo en la Facultad de Ciencias y Tecnologías Químicas e intentar fomentar la colaboración entre los diferentes grupos (uno de los impulsores es Javier Guerra que será un conferenciante del viernes).

Primero se celebraba los viernes de mayo y junio con una charla por jornada. Posteriormente se empezó a concentrar mas las charlas, luego se pasó a celebrarse durante tres días seguidos y a invitar a investigadores relevantes de otros centros, incluso se empezaron a convocar premios para los doctorandos que daban estas charlas. Y actualmente hemos propuesto mas premios, hemos pasado a extender la participación a los diferentes centros de la UCLM en la rama de ciencias, con una modalidad mixta on line/presencial.

PREGUNTA- Este congreso comenzó para tener interacción entre los jóvenes y ha llegado a tener un importante nivel de relevancia. ¿Cuáles son las claves para llegar a ese nivel?

RESPUESTA- Pues porque hemos incrementando la participación y por tanto se ha convertido en un congreso relevante para nuestro centro y por consiguiente para los demás centros que han comenzado a participar, de igual forma la presencia de otros investigadores relevantes, lo hacen más multidisciplinar y adquiere mayor carisma.

De igual forma hemos contado con la presencia de diferentes autoridades, este año hemos contado en la inauguración con la presencia de la vicerrectora de profesorado, Ana Briones, y en la clausura estará el rector de la UCLM, Julián Garde y del director general de universidades, Ricardo Cuevas.

PREGUNTA- Esta edición, ¿qué novedades aporta?

RESPUESTA- Una de las novedades principales es haber podido contar con la participación de grupos de toda la UCLM y otras de las más destacadas es la incorporación de la participación con presentaciones flash/virtual y la ampliación del numero de premios a esta categoría con diferencia de si el participante es de TFM, TFG o doctorando y también una entrega de premios por likes en redes sociales, igualmente también vamos a realizar una porra con obsequios para los que acierten los ganadores.

Imagen de los asistentes a la inauguración del Simposio de Ciencia Joven en el campus de Ciudad Real/ J.Jurado

PRESENTACIÓN XV YOUNG SCIENCE SYMPOSIUM

PREGUNTA- El congreso está dirigido a estudiantes de la UCLM o ¿también participan de otras universidades?

RESPUESTA- Pueden participar de todos sitios, pero con comunicación solo de la Universidad de Castilla-La Mancha.

PREGUNTA- ¿Cuántos son los participantes?

RESPUESTA- Tenemos casi 100 ponencias entre las dos categorías hay alrededor de 170 inscritos.

PREGUNTA- ¿Qué temas se abordarán durante estas tres jornadas?

RESPUESTA- Los temas son temas muy diversos, tenemos comunicaciones desde los tres grados de la facultad y por tanto tenemos participantes desde matemáticas, física, diferentes áreas de la química, tecnología de alimentos, ingeniería química, agrónomos, farmacia, centros como el IREC, de muy diversa temática y eso lo va hacer un congreso realmente enriquecedor.

PREGUNTA- Intervienen ponentes tanto de la UCLM como de otras universidades

RESPUESTA- Intervienen ponentes de toda la UCLM en las orales y flash y luego tenemos 6 charlas invitadas que 3 de ellas son on line porque son de ponentes que están en el extranjero y también 3 presenciales que serán el próximo viernes y la presencia de los sponsors como Agrovin que ademas dará una pequeña charla o la Sección Territorial de Castilla-La Mancha de la Real Sociedad Española de la Química que también dará una pequeña charla.

En este encuentro tendrán cabida seis charlas de ponentes externos invitados de la Durham University (UK), Newcastle Universtity (UK), Arizona State University (USA), Universitat Politécnica de Valencia, Institute of Food Science, Technology and Nutrition y Universidad de Valladolid. También, y por primera vez en estos años, los pósteres han sido sustituidos por flash virtuales de vídeos de unos tres minutos de duración que pueden verse en las redes sociales de la Facultad de Ciencias y Tecnologías Químicas.

“Supramolecular Gels: Tangled Soft Materials”

Jonathan W. Steed

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.

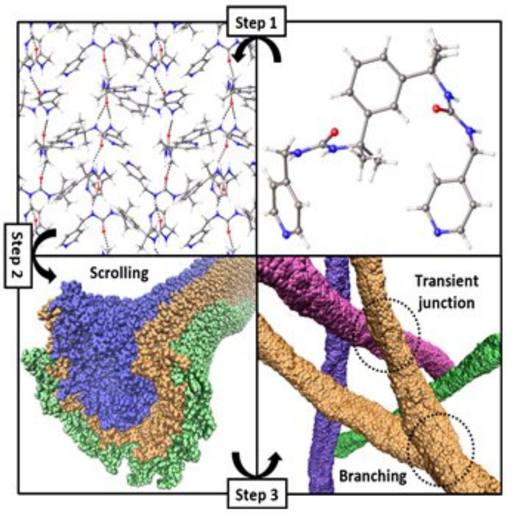

Figure 1. Assembly of a supramolecular gel by (1) layering, (2) scrolling and (3) entanglement.

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

Ana Marina Ferreira-Duarte

Universidad de Castilla-La Mancha
15th YOUNG SCIENCE SYMPOSIUM, FACULTY OF CHEMICAL SCIENCES AND TECHNOLOGIES, UCLM
Newcastle University

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

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From Newcastle. For the world.

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.

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

Sergi Garcia-Segura

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.

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

Miguel Ángel Miranda

Recorremos 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.

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

Javier Guerra

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.[1] 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[2] 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.

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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

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 great estreduction 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.

Potencial RedOX

Miguel Martínez

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 ° 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 have to 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 at this time.

- 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.

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

Manuel Salgado Ramos

Innovative alternative technologies are nowadays emerging for the recovery of polyphenols from plants as an alternative tool to traditional methods.[1-3] 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 us 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.

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Discrimination and quantification of quercetin nanoemulsions by liquid state SERS analyzer

Cristina Montes Correal

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, then a no structural 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 cm^{-1} band. This sensor showed good analytical performance with lineal concentration range of 0.5 - 30 µM and detection limit of 0.4 µM. The developed analytical method was applied to the analysis of nanoquercetin in complex commercial matrices.

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Supercritical CO_2 extraction of natural antioxidants from lavender: process optimization and scaling-up

Encarnación Cruz Sánchez-Alarcos

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_2) 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_2 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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Valorization of Agricultural Waste and CO_2 into Bioderived Cyclic Carbonates

María del Prado Caballero Espinosa

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[1] have been used for the synthesis of waste vegetable oils-derived cyclic carbonates from bio-derived epoxides and CO_2. 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.[2]

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COMUNICACIONES ORALES

Implementation of non-thermal technologies for wine microbiota control

Raquel Muñoz García

In the wine making 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 wine sand 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 wine making process [2].

For this purpose, six different treatments were applied on fresh cultures with a population of 106 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 alonger 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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Bioavailability of a long-term low-dose administration of a grape seed extract in healthy male Wistar rats

Eduardo Guisantes Batan

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 [1]. 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 seedextract (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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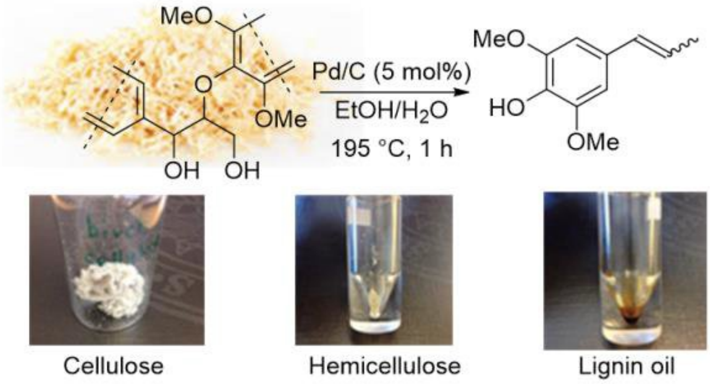
Catalytic fractionation of biomass, a pathway to obtain textiles, biofuels, and platform chemicals from renewable sources

Alberto José Huertas Alonso

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.[1]



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Extraction and characterization of platinum nanoparticles from road dust

Armando Sánchez Cachero

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 growns teadily 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 on cein 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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Metal extraction from mine tailings by bioleaching with an acclimatized mixed culture

Hassay Lizeth Medina Díaz

The metal mining sector has been an important pole of economic development inseveral European countries. However, the accumulation of mine tailings after the closure of the facilities has tiggered 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 discardedmine tailing [3].

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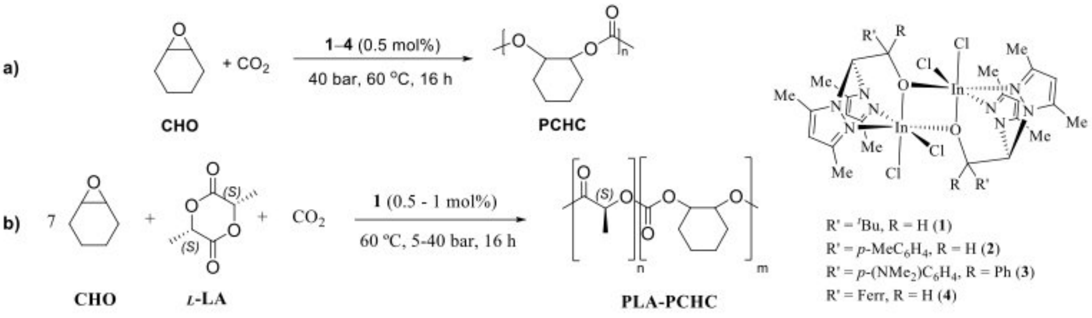
Synthesis of polycarbonates and terpolymers catalysed by heteroscorpionate indium complexes

Marc Martínez de Sarasa Buchaca

During the last years, the scientific and industrial community have focused on the development of new processes to transform CO_2 into high-value added organic chemicals and polymers.[1] In this context, it is worth highlighting the ring opening copolymerisation between epoxides and CO_2 to afford polycarbonates, which have found multiple applications.[2] More recently, terpolimerisation reactions between epoxides, CO_2 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.[2] 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_2 and the terpolymerisation reaction of cyclohexene oxide, CO_2 and L-lactide to afford polycarbonate and polyester-polycarbonate materials, respectively, with low tomoderate molecular weights and narrow polydispersity values (Scheme 1).



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

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Monitoring air quality in Las Tablas de Daimiel National Park

Gabriela Viteri Tovar

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_3, NO_X, SO_2, CO and $PM_{2.5}$ 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 data set 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= 69.3 mg/m^3) 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_x concentrations (annual average = 3.1 mg/m^3) 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_2 and CO, with average values of 0.34 and 135.5 mg/m^3 respectively.

In the case of $PM_{2.5}$, 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 4.7 $\mu g/m^3$. The results show that concentrations of $PM_{2.5}$ are below the levels established by the legislation.

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

Manuel López Viñas

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 in order 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 posess 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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A new analytical methodology for the assessment of platinum nanoparticles speciation in in vitro toxicological assays

Sergio Fernández Trujillo

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

Daniel López Pedrajas

It is expected that the world energy consumption rises nearly 50 % by 2050. This quick and high growing energy demand can generated 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_2 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).

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

Daniel Martínez Domínguez

Photochemotherapy emerges as a new non-invasive technique to improve the selectivity of current cancer treatments. In this therapy, a photosenitizer is administrated, 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)$^1O_2$ 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^N 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 π-extended ligands (C^N= benzo[a]pyrido-[2,3-c]phenazine; bppz) have been synthetized and new complexes $[Ir(C^\wedge N)_2(N^\wedge N)]^+$ 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.

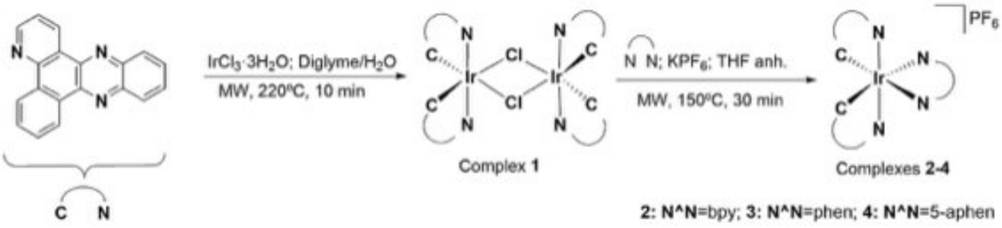

Figura 1. Synthesis scheme of Ir complexes with C^N (5-aphen: 5-aminephenanthroline).

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Soot characterization using different techniques

Inmaculada Aranda Díaz-Lucas

Soot is the carbonaceous particles formed during the incomplete combustion or pyrolysis of hydrocarbons[1], such as fossil or biomass fuel. It is well known that this pollutant has negative effects on the human health[2] and cause changes in the Earth's energy balance directly by absorbing the solar radiation and indirectly affecting cloud properties[3]. 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. Photoacustic Extinctiometer (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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CO_x-free hydrogen generation from ammonia by electrochemical promotion

Marina Pinzón García

Hydrogen (H_2) 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_3) 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[1]. Moreover, its decomposition only yields hydrogen and nitrogen. Therefore, NH_3 is an exceptional carbon-free hydrogen vector. However, to release H_2 contained in NH_3 it is necessary to develop a robust, efficient, and economic active catalyst at low temperatures, since high purity H_2 is necessary to be used in fuel cells. Promising results of NH_3 decomposition at low temperatures are achieved with ruthenium catalysts[1], 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[2].

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-ßAl_2O_3 and K-ßAl_2O_3) have been used on the catalytic reaction.

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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

Marina Córdoba Aceituno

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 interferents, 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.

Safety assessment of LAB strains to be used in food fermentations

Sara Rodríguez Sánchez

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 β-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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Naturally curved organic crystalline structures for waveguide and photonic circuits

Carlos Tardío Rubio

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 stiffand fragile. However, the future technologies mandate flexible nanophotonic devices, so we need crystals with higher flexibility.[1]

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.[2]

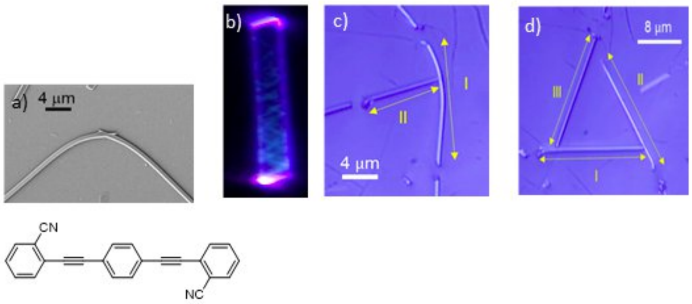

Figure 1: a) FESEM image of the bent crystal. b) PL image of the crystal. c) T-shaped and d)Triangular-shaped photonic circuits.

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Subolesin/Akirin: A multi arthropod vaccine antigen

Sara Artigas Jerónimo

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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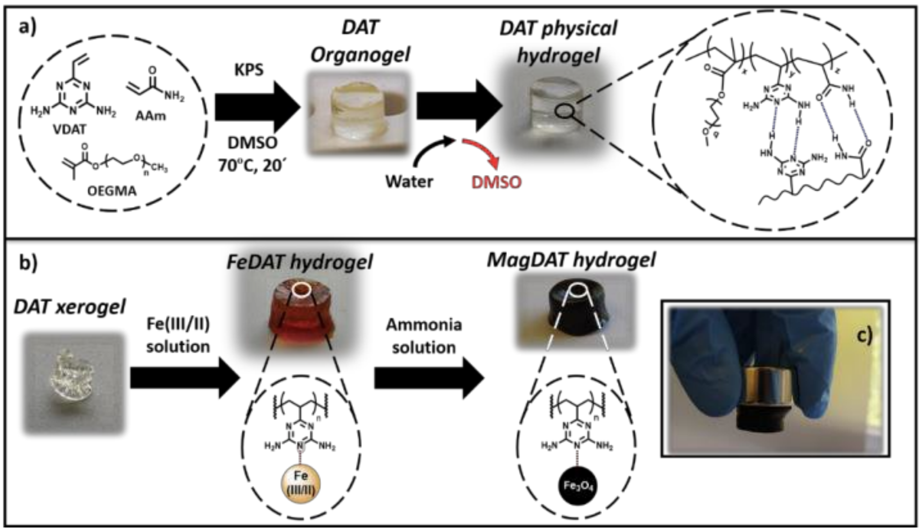
Magnetically responsive hydrophobic pockets for on-off drug release

Jorge Leganés Bayón

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

Samah Lahouidak

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.

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

Inés María Ramos Monge

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.

Astrochemistry in the Laboratory

Sergio Blázquez González

In 1953, Stanley L. Miller[1] 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.[2-6] 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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Optimum Experimental Design: “Think before you act”

Sergio Pozuelo Campos

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

Elena Domínguez Jurado

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-phoshino-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-phoshino-amine ligands and the synthesis of their ruthenium counterparts. The novel ligands and compounds were fully characterized, studied their water stability, and evaluated their citotoxcity *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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Electro-scrubbing for the removal of Volatile Organic Compounds (VOCs) from gaseous streams

Andrea Nataly Arias Sánchez

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^2 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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Acknowledgements

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New naphthalenimide derivatives with application in organic photonics

Beatriz Donoso Jurado

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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Kinetic and formation of SOA from ozonolysis of trans-ß-methylstyrene

Alba Escalona Verbo

Atmospheric aerosols are considered as one on the main uncertainty sources in the current understanding of the Earth's climate[1]. 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_2 several orders of magnitude faster than assumed so far[2] producing SO_3, which contributes efficiently to the formation of ground level sulfuric acid[3]. Styrene and derivates as a-methylstyrene or trans-ß-methylstyrene are toxic to humans and considered to be one of the most important secondary organic aerosol (SOA) precursor[4]. These aromatics compounds can be emitted into the atmosphere from different sources such as solvents, combustion, building materials, adhesives and industrial processes[5]. In this context, the formation and growth of new SOA are evaluated in this work from ozonolysis of trans-ß-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 method 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_2 concentration.

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

Dario Martínez

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 abordable because the method is parallelizable. Other advantage is high order.

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Mosquitoes and West Nile

Laia Casades Martí

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.

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

Raúl López Martín

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[1]. 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[2].

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

Ester López Fernández

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.

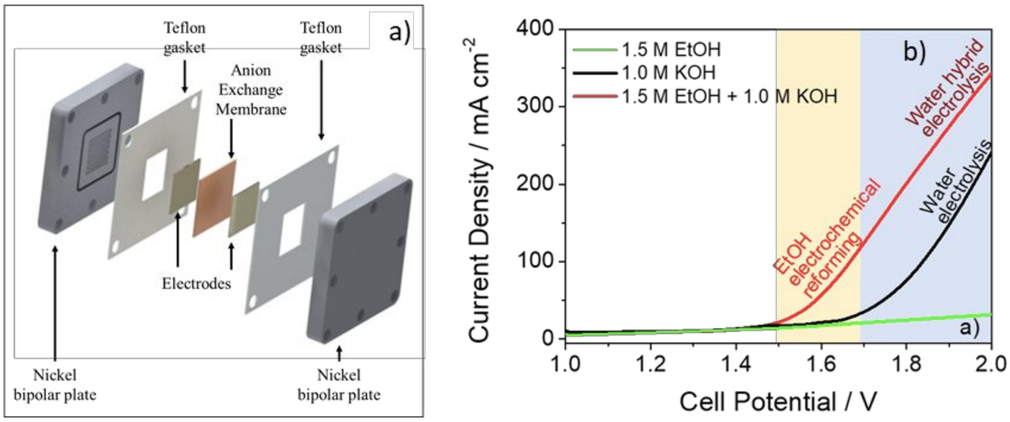

Figure 1. a) Exploded view of a complete electrolysis cell and b) current-potential curves for water andethanol-water hybrid electrolysis.

Photopolymerizable chitosan hydrogels for tissue engineering

Irene San Millán Rodríguez

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 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.

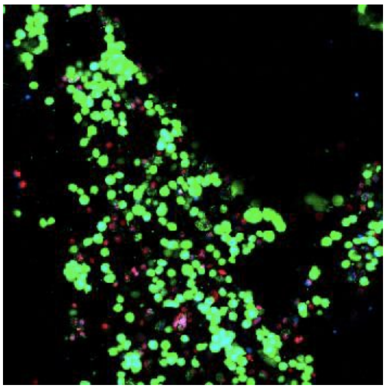

Figure 1. Cell culture in chitosan hydrogels.

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Categoría TFG

José Manuel Chinchilla Cañaveras

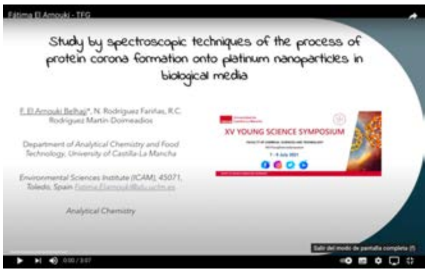
"Agricultural Management Effects on Reproductive Parameters of Iberian Hare (Lepus granatensis)"

AGRICULTURAL MANAGEMENT AFFECTS FEMALE REPRODUCTIVE PARAMETERS OF IBERIAN HARE (*LEPUS GRANATENSIS*)

José Manuel Chinchilla, María Ángeles Risalde, Vanesa Alzaga, Pablo R. Camarero, Francisca Talavera, Jose Alberto Viñuelas, Pelayo Acevedo, Rafael Mateo & Mónica Martinez-Haro

Fátima El Amouki Belhaji

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



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

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Environmental Sciences Institute (ICAM), 45071, Toledo, Spain

Analytical Chemistry

Víctor Lara Avia

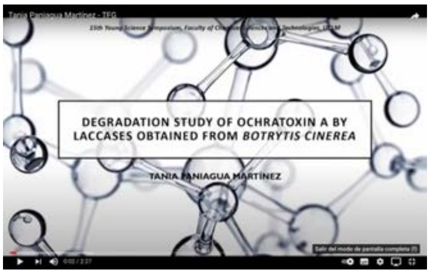
"Design of a biorreactor for bioleaching of metals from solid mine tailings"

María Osorio Alises

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

Tania Paniagua Martínez

"Study of the degradation of Ochratoxin A by lacases obtained from Botrytis cinérea"



DEGRADATION STUDY OF OCHRATOXIN A BY LACCASES OBTAINED FROM *BOTRYTIS CINEREA*

TANIA PANIAGUA MARTÍNEZ

COMUNICACIONES FLASH

Haz click en el vídeo para ver la comunicación flash

Categoría TFG

Natalia Villamayor Moreno

“Synthesis and analytical characterization of quercetin nanoemulsions”

Síntesis y caracterización analítica de nanoemulsiones de quercetina

Autor: Natalia Villamayor Moreno
Tutores: Mª Jesús Villaseñor Llerena
Ángel Ríos Castro

Noelia Viveros Lizondo

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

MICROBIOLOGÍA DE LA CARNE DE PAVO

NOELIA VIVEROS LIZONDO
FACULTADA DE CIENCIAS Y TECNOLOGÍAS QUÍMICAS

COMUNICACIONES FLASH

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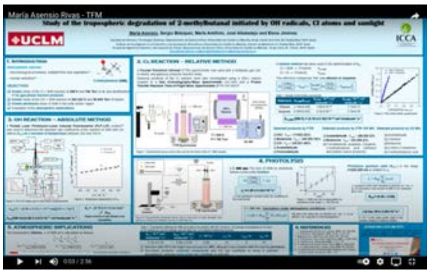
Categoría TFM

María Asensio Rivas

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



Cristina de los Reyes Ramos

"Exploring the potential of lactic acid bacteria strains as health promoters"

Sara Espinosa Gómez

"Hydrofluoethers as new alternative compounds of Chlorofluorocarbons: How do we study them?"

Alicia Jimenez de la Torre

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

Carlos Gonzalo

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

COMUNICACIONES FLASH

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Categoría TFM

Blanca Parra

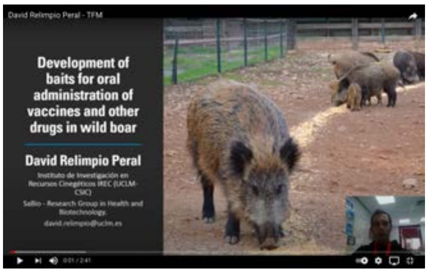
"Derivados luminiscentes de Boro e Iridio con ligandos amidina"


Blanca Parra - TFM

DERIVADOS LUMINISCENTES DE BORO E IRIDIO CON LIGANDOS AMIDINA

David Relimpio Peral

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


David Relimpio Peral - TFM

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

David Relimpio Peral

Instituto de Investigación en Recursos Cinegéticos IREC (UCLM-CSIC)

SaBio - Research Group in Health and Biotechnology.

david.relimpio@uclm.es


Abelardo Sánchez Oliva - TFM

DISEÑO RACIONAL DE DERIVADOS DE NAFTALENIMIDA, NAFTALENDIIMIDA Y PERILENIMIDA CON APLICACIÓN COMO TRANSISTORES DE EFECTO DE CAMPO ORGÁNICOS

UNIVERSIDAD DE CASTILLA LA MANCHA

Facultad de Ciencias y Tecnologías Químicas

Química Orgánica

Autor: Abelardo Sánchez Oliva

Abelardo Sánchez Oliva

"Rational Design of Naphthalenimide and perylenimide derivatives with application in organic field-effect transistors (OFETs)"


Álvaro Sánchez Sánchez - TFM

Perovskitas como precursores catalíticos para la descomposición de amoniaco

Álvaro Sánchez Sánchez

Directoras:
Paula Sánchez Paredes
Ana Raquel de la Osa Puebla

Álvaro Sánchez Sánchez

"Perovskites as catalytic precursors in ammonia decomposition"

COMUNICACIONES FLASH

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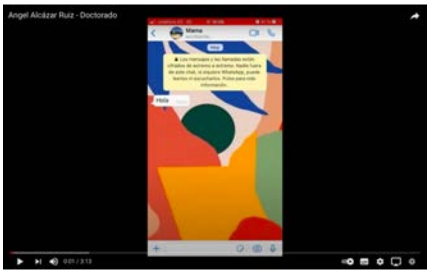
Categoría Doctorado

Ángel Alcázar Ruiz

"Value-added bioproducts production through waste biomass fast pyrolysis"

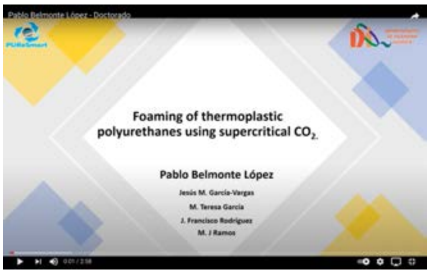


Manuel Bartolomé Díaz

“Voltammetric sensing of fluoroquinolones in commercial food daily products at chitosan - gamma cyclodextrin - graphene quantum dots modified carbon screen printed electrodes”

Voltammetric sensing of FQs in commercial food daily products at CHI-γCDs-GQDs modified SPCEs

Manuel Bartolomé Diaz



Foaming of thermoplastic polyurethanes using supercritical CO_2.

Pablo Belmonte López

Jesús M. García-Vargas
M. Teresa García
J. Francisco Rodríguez
M. J Ramos

Pablo Belmonte López

"Foaming of thermoplastic polyurethanes using supercritical CO_2"

PLGA foaming via supercritical CO_2 for tissue engineering application.

F. Carrascosa*, I. Gracia, J.F. Rodriguez,
J.M. Garcia, M.T. Garcia

Fernando.Carrascosa@uclm.es

Fernando Carrascosa Simón

"PLGA foaming via supercritical CO_2 for tissue engineering application"

Rodrigo de Mello

"Combination of adsorption and electrochemical oxidation processes to remove VOCs"

COMBINED PROCESSES AS AN ALTERNATIVE FOR WATER AND AIR TREATMENT

Rodrigo de Mello
Cristina Sáez
Artur de Jesus Motheo
Manuel Andres Rodrigo Rodrigo

COMUNICACIONES FLASH

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Categoría Doctorado

Rafael Delgado García

"Permalloy thin films on V-groove patterned substrates for sensoring and biological applications"

Rafael Delgado García - Doctorado

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

XV YOUNG SCIENCE SYMPOSIUM

Yelitza Delgado Gonzalez

"Real Acid Mine Drainage Treatment by Bioelectrochemical System"

Yelitza Delgado Gonzalez - Doctorado

Real Acid Mine Drainage Treatment by Bioelectrochemical Systems

Y. Delgado, J. Llanos and F. J. Fernandez

15th YOUNG SCIENCE SYMPOSIUM

Introduction

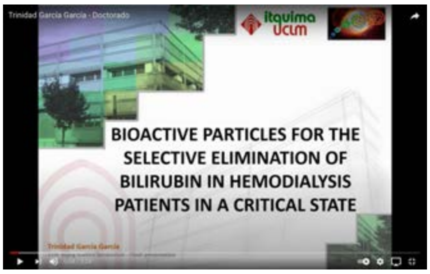
Active technology

Passive technology

Materials and Methods

Results

MFC operation



Trinidad García García - Doctorado

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

Trinidad García García

"Bioactive particles for the selective elimination of bilirubin in hemodialysis patients in a critical state"

Celia Gómez Sacedón - Doctorado

A SIMPLE PRELIMINARY DESIGN OF SELF-SUPPORT POWER SUPPLY BASED ON HYDROGEN AND PHOTOVOLTAIC TECHNOLOGY.

C. G. Sacedón*, E. López-Fernández, A.R. de la Osa, F. Dorado, E. Amores, A. de Lucas-Consuegra

Departamento de Ingeniería Química, Facultad de Ciencias y Tecnologías Químicas,
Universidad de Castilla-La Mancha, E-13071, España

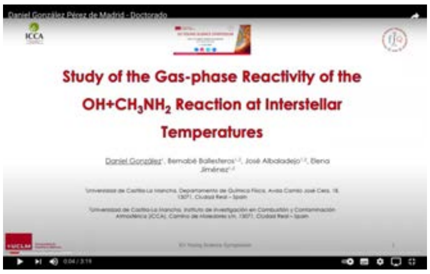
Introduction

Celia Gómez Sacedón

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

Daniel González Pérez de Madrid

"Study of the Gas-phase Reactivity of the $OH+CH_3NH_2$ reaction at Interstellar Temperatures"



Daniel González Pérez de Madrid - Doctorado

Study of the Gas-phase Reactivity of the $OH+CH_3NH_2$ Reaction at Interstellar Temperatures

Daniel González, Bernabé Ballesteros, José Albaladejo, Elena Jiménez

COMUNICACIONES FLASH

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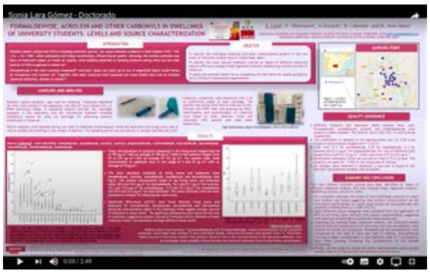
Categoría Doctorado

Rafael Granados Fernández

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

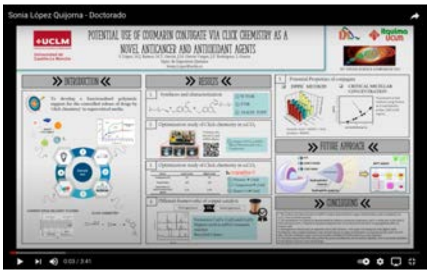
Jesús Herrera Herreros

"Magnetic acrylamide hydrogels: SPIONs in situ"



Sonia Lara Gómez

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



Sonia López Quijorna

"Potential use of coumarin conjugates via click chemistry as a novel anticancer and antioxidant agents"

Carolina Montoya Vallejo

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

COMUNICACIONES FLASH

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Categoría Doctorado

Víctor Pertegal Perez

"Treatment of bioaerosols with electrochemically generated oxidants"


Victor Pertegal Pérez - Doctorado

Treatment of bioaerosol with electrochemically generated oxidants

15th YOUNG SCIENCE SYMPOSIUM, FACULTY OF CHEMICAL SCIENCES AND TECHNOLOGIES, UCLM

Esther Pinilla Peñalver

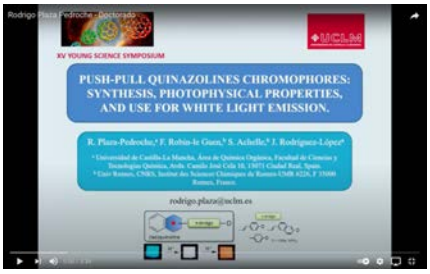
"Resveratrol adsorption at graphene quantum dots surface: a promoting strategy to increase its photochemical stability in food products"


Esther Pinilla Peñalver - Doctorado

RESVERATROL ADSORPTION AT GRAPHENE QUANTUM DOTS SURFACE: A PROMOTING STRATEGY TO INCREASE ITS PHOTOCHEMICAL STABILITY IN FOOD PRODUCTS

XVI Young Science Symposium
Ciudad Real, July 2021

ESTHER PINILLA PEÑALVER


Rodrigo Plaza Pedroche - Doctorado

XV YOUNG SCIENCE SYMPOSIUM

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

R. Plaza-Pedroche, F. Robin-le Guen, S. Achelle, J. Rodríguez-López

rodrigo.plaza@uclm.es

Rodrigo Plaza Pedroche

"Push Pull quinazolines chromophores: synthesis, photophysical properties and use for white light emission"


Carlos Rivera Cabanillas - Doctorado

Carlos Rivera Cabanillas

"Study and Characterization of Chemical Pigments for Artistic Painting"

Alberto Sánchez Cano

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


Alberto Sánchez Cano - Doctorado

Desentrañando la interfaz:

Conectividad entre granjas proporcionada por movimientos de estornino negro

(Sturnus unicolor)

COMUNICACIONES FLASH

Haz click en el vídeo para
ver la comunicación flash

Categoría Doctorado

Ángela Moratalla Tolosa

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


Ángela Moratalla Tolosa - Doctorado

XV Young Science Symposium 2021

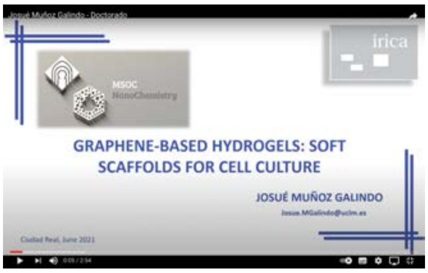
Faculty of Chemical Sciences and Technology
7-9th of July 2021

Improving the biodegradability of hospital urines
by electrochemical advanced oxidation processes

Ángela Moratalla¹*, Engracia Lacasa², Sonia Ruiz³, Pablo Cañizares¹, Manuel A. Rodrigo¹, Cristina Sáez¹

Josue Muñoz Galindo

"Graphene-based sulfonate hydrogels: Soft scaffolds for cell culture"


Josué Muñoz Galindo - Doctorado

GRAPHENE-BASED HYDROGELS: SOFT
SCAFFOLDS FOR CELL CULTURE

JOSUÉ MUÑOZ GALINDO
Josue.MGalindo@uclm.es

Ciudad Real, June 2021


Sonia Muñoz - Doctorado

¿Pueden las moléculas naturales
prevenir el cáncer?

XV Young Science Symposium
7 – 9 July 2021

Doctoranda: Sonia Muñoz López
Directores: Mairena Martín, José Luis Albasanz y Alejandro Sánchez
Área: Bioquímica y Biología Molecular

Sonia Muñoz López

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

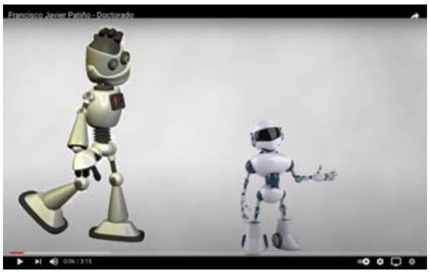

Rodrigo Oliver Simancas - Doctorado

Rodrigo Oliver Simancas

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

Francisco Javier Patiño

"Hydrogels in soft robotics"


Francisco Javier Patiño - Doctorado

COMUNICACIONES FLASH

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ver la comunicación flash

Categoría Doctoras

Beatriz García-Bejar Bermejo

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

Viviana González Velázquez

"Synthesis of 2D Nanomaterials"

PREMIOS DEL XV YOUNG SCIENCE SYMPOSIUM

Como en ediciones anteriores, el comité organizador del XV Simposio de Ciencia Joven hizo entrega del VI Premio Ciencia Joven en el acto de clausura del evento. En esta edición, el premio ha sido otorgado a **Marc Martínez de Sarasa Buchaca** con el trabajo titulado "Synthesis of polycarbonates and terpolymers catalysed by heteroscorpionate Indium complexes" del área de Química Inorgánica.

¡Enhorabuena!

PREMIOS DEL XV YOUNG SCIENCE SYMPOSIUM

Por primera vez, en esta edición existe una nueva categoria denominda Flash Presentation. Esta se divide en categoría de redes, categoría doctorados, categoría TFM y categoría TFG.

El **I Premio Redes Sociales** se otorgó a:

Sonia Muñoz López

En la categoria de Redes Sociales se hizo una mención especial como finalista a:

Blanca Parra

PREMIOS DEL XV YOUNG SCIENCE SYMPOSIUM

El I Premio virtual Flash Communication en la categoría de **Estudiante de Doctorado (PhD)** se le otorgó a:

Rodrigo Oliver Simancas

El I Premio virtual Flash Communication en la categoría **Trabajo de Fin de Máster (TFM)** se le otorgó a:

Alicia Jiménez de la Torre

El I Premio virtual Flash Communication en la categoría de **Trabajo de Fin de Grado (TFG)** se le otorgó a:

Victor Lara Avia

¡Enhorabuena a los premiados!

PREMIOS DEL XV YOUNG SCIENCE SYMPOSIUM

Comité Científico y organizador

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’

PREMIOS DEL XV YOUNG SCIENCE SYMPOSIUM

Comité Científico y organizador

Comité Organizador:

Eduardo Guisantes Batán, ‘Food Sciences and Technology’

Esther Pinilla Peñalver, ‘Analytical Chemistry’

Alba Escalona Verbo, ‘Physical Chemistry’

Iván Torres Moya, ‘Organic Chemistry’

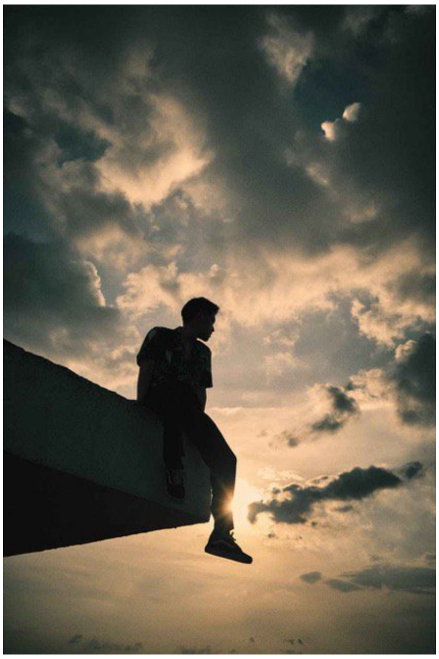
Raúl López Martín, ‘Physics’

Pablo Belmonte López, ‘Chemical Engineering’

Margarita María Villar Rayo, ‘Biochemistry’

EXPERIENCIA EN EL SYMPOSIUM

Nuestro mejor futuro



La semana pasada tuve ocasión de participar como jurado de unos vídeos de divulgación científica dentro del Simposio Ciencia Joven, que organiza la Facultad de Ciencias y Tecnologías Químicas de Ciudad Real. En concreto, los videos pretendían mostrar durante tres minutos la labor que se realiza en Trabajos Fin de Grado, Trabajos Fin de Máster y en Doctorado. No se consideraba en este caso el contenido científico de los resultados, eso ya tiene otra valoración con premio incluido. Lo que se reconoce es la calidad a la hora de la divulgación, la originalidad (no exenta de rigor ni de resultados), la capacidad de enganchar, de llamar la atención como paso previo a esa misteriosa cosa que es la difusión de los resultados. Pero destinado a la sociedad real, no a cuatro casposos que leen revistas elitistas cuyo contenido poco o nada trasciende al pagano de a pie. **Esas revistas que sirven para establecer el ranking también docente y que se supone que jamás están dominadas por lobbies equivalentes en ciencia a los de los negocios o la política**. En absoluto, juas, juas.

Pues participar como jurado me ha permitido reconciliarme con el género humano. He tenido ocasión de conocer gran parte de las líneas de investigación que desarrollamos en la facultad. Son fascinantes, estudios aplicados, no teóricos. Soluciones viables a problemas medioambientales, para eliminar residuos o aprovechar subproductos. Para darles uso combatiendo enfermedades como el cáncer o desarrollando nuevos materiales que permitirán desarrollar mejores fármacos o que los robots similares a los humanos sean una realidad. **El futuro que soñamos y la labor lógica a la que destinar los dineros que todos hemos exigido en los tiempos de covid, ¿verdad?** Pero eso no es nada. Lo auténticamente importante es la pasión con la que la gente hace y habla de su trabajo. Estos eslabones de la cadena de conocimiento y del desarrollo de la ciencia, los más nuevos, son los mejores. **Los más altruistas, los más desinteresados, los más solidarios y los más comprometidos con lo que se hace para mejorar el mundo. Me descubro.**

Photo by Public Domain Pictures on Pexels.com

Nuestro mejor futuro

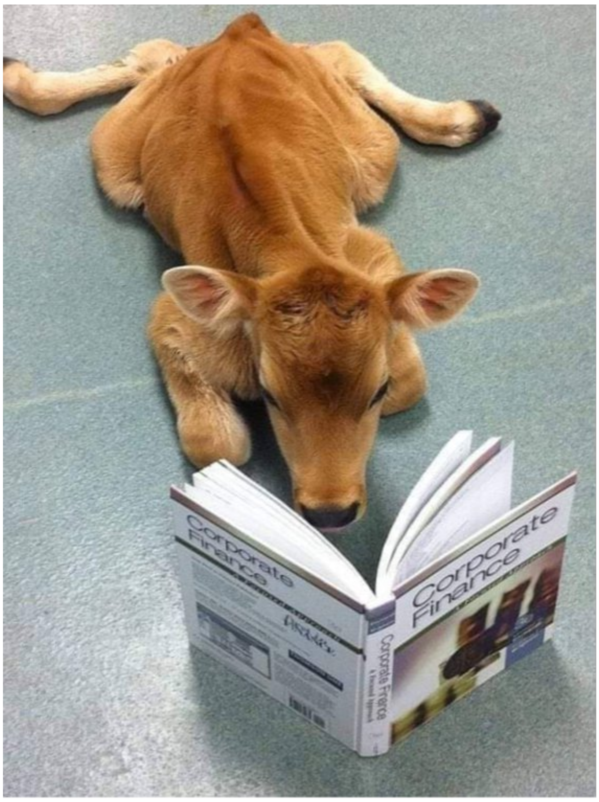
Con un par, amigos. Pero, además, está la labor de difusión a la que aludía. La mayor parte de esos 44 vídeos son impresionantes, y no hablo como profesor. Hablo como espectador, como masa social. Muchos de ellos no es que sean buenos, es que son de lo mejor que he visto en cualquier medio de comunicación.

Te cuentan una historia que conmueve, te enganchan y te dan una solución. Son brillantes. Al mejor nivel de las mejores cosas que ves por la tele. Algo por lo que por supuesto pagarías por ver en una plataforma, la prueba del algodón. Prueba superada con creces. Y con la gran reflexión dolorosa, la comparación con nosotros los viejos, o también llamados investigadores seniors. Las presentaciones no es ya que sean buenas, en que son mejores que cualquiera de las nuestras. Cualquiera de cualquier científico que haya visto en un congreso internacional de prestigio. Eso es bueno, muy bueno. Significa lo que significa. **Que hay una generación que viene detrás de nosotros que más que empujar fuerte está arrasando. Que sois mejores que nosotros, que es lo que tiene que ser.**

Este es a mi juicio el mayor tesoro que puede tener un país, por eso estoy absolutamente orgulloso de vosotros. Y por eso nuestra es la responsabilidad de apoyaros hasta el final, que es donde viene el problema. Que me fijo en vosotros y miro el otro extremo de la cadena y me pongo a llorar. **No es posible que este enorme talento se desperdicie por falta de medios**. Por poner un ejemplo, seguimos valorando las vacunas frente al COVID cuando tenemos en España al mejor experto, desarrollador de las dos vacunas previas en el 2002 y 2012 para los SARS I y II (la famosa Gripe Aviar va en el cajón), con un mísero presupuesto de cuatro millones de euros, que hace que la mejor vacuna no haya estado a punto a tiempo. Y no es culpa de él, que trabaja después de jubilado por amor al arte; bastante tiene con buscar fondos para su equipo. Es que compite con monstruos que dedican miles de millones. Pero es que somos mejores que ellos, y eso es lo que duele. **Que no tengamos algo más de recursos. Posiciones estables, tranquilidad, algo de tranquilidad. Conciliación de la vida laboral y familiar. O por lo menos respeto y algo de consideración por la sociedad,** que os aseguro que esto es un sacerdocio, algo vocacional de gente muy especial. De gente que no se rinde. Que cuando se marcha de España, os lo aseguro, es porque ya no puede más con su hambre. Y se marchan reclamados a los mejores sitios, pero con la cara mirando a este país y los ojos llenos de lágrimas.

Nuestro mejor futuro

Todos tenemos una responsabilidad. Vosotros la de no cambiar nunca, la de nunca rendiros. Nosotros la de exigir que vuestro futuro sea justo, con medios justos. Tanto en lo económico como en lo administrativo y social. A nuestra generación nos toca en el ámbito científico exigir y pasar miserias para que vosotros os podáis ubicar en el lugar que os corresponde. Del mismo modo que nuestros abuelos nos colocaron del tercer al primer mundo hace poco. Y os aseguro que es difícil, pero quiero pensar que tenemos que reclamar a punta de navaja si hace falta lo que consideramos imprescindible para vuestro futuro. A quien corresponda y de la forma que sea, porque ya no podemos desperdiciar una generación más. Debemos reclamar la importancia de lo que es la ciencia para salvar el futuro. **Y si eso implica menos fútbol o menos dinero para estupideces, a lo mejor tenemos de enfrentarnos al mismísimo demonio**. Habrá que hacerlo, nuestros abuelos así lo hicieron y vosotros os lo merecéis.



En el próximo número de Molécula...

El próximo número de MOLÉCULA incluirá las actividades que tengan lugar durante el mes de Septiembre, así como publicaciones de grupos de investigación de la facultad, noticias interesantes y curiosidades. Mientras tanto, os deseamos un feliz verano ¡cuidaos mucho!

¡FELICES VACACIONES!

#DivulgaUCLM

https://moleculauclm.wordpress.com/

VI PREMIO CIENCIA JOVEN
2021

Como en ediciones anteriores, el comité organizador del XIII Simposio de Ciencia Joven hizo entrega del *VI Premio Ciencia Joven* en el acto de clausura del evento. En esta edición, el premio ha sido otorgado a **Marc Martínez de Sarasa Buchaca** el trabajo titulado " *Synthesis of polycarbonates and terpolymers catalysed by heteroscorpionate Indium complexes"*. Por primera vez, en esta edición existe una nueva categoria denominda Flash Presentation. Esta se divide en categoría de redes, categoría doctorados, categoría TFM y categoría TFG.

¡Enhorabuena a los premiados!

El I Premio Redes Sociales se otorgó a:

Sonia Muñoz López

En la categoria de Redes Sociales se hizo una mención especial como finalista a: Blanca Parra

El I Premio virtual Flash Communication en la categoría de Estudiante de Doctorado (PhD) se le otorgó a:

Rodrigo Oliver Simancas

El I Premio virtual Flash Communication en la categoría Trabajo de Fin de Máster (TFM) se le otorgó a:

Alicia Jiménez de la Torre

El I Premio virtual Flash Communication en la categoría de Trabajo de Fin de Grado (TFG) se le otorgó a:

Victor Lara Avia

¡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
Del 7 al 9 de Julio de 2021	XV SIMPOSIO CIENCIA JOVEN

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CI-5	Daniel	Peters
CI-6	Ana Belén	Cifuentes
CI-7	Raquel	Reina
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O-4	María De Gracia	Arenas Moreira
O-5	Inés María	Ramos Monge
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O-12	Raquel	Muñoz García
O-13	Marina	Pinzón García
O-14	Carlos	Martín Andreu
O-15	Enrique	Frances Poveda
O-16	Adrián	Tejero Pérez
O-17	Abelardo	Sánchez Oliva
O-18	Ángel	Alcázar Ruiz
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O-20	Daniel	González Pérez De Madrid
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O-22	Blanca	Parra Cadenas
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F-3	Oscar Ramiro	Andrade
F-4	Andrea Nataly	Arias Sánchez
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F-6	Cristina	Blasco-Navarro
F-7	Fernando	Carrascosa Simón
F-8	Javier	Cencerrero Fernandez Del Moral
F-9	Irene	Chacón Jiménez
F-10	Sergio Enmanuel	Correia Alonso
F-11	Jesús	Cortes

F-12	Leticia Mirella	Da Silva
F-13	Yelitza	Delgado
F-14	Sara	Espinosa Gómez
F-15	Sara	Gallardo López
F-16	Ana María	García Fernández
F-17	Lais	Gimenes Vernasqui
F-18	Viviana Jehová	González Velázquez
F-19	Rafael	Granados Fernández
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F-24	Darío	Martínez
F-25	Hassay	Medina-Diaz
F-26	Alicia	Morcillo Mora
F-27	Alberto	Moreno Fernandez
F-28	Jesús	Naranjo
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F-30	Tania	Paniagua Martinez
F-31	Victor	Pertegal Pérez
F-32	María Teresa	Pinés Pozo
F-33	Esther	Pinilla Peñalver
F-34	Álvaro	Ramírez Vidal
F-35	Irene	Sánchez Sánchez Ajofrín
F-36	Jesús	Serrano Jimenez
F-37	Francisco Manuel	Soria López
F-38	Antonio José	Troyano
F-39	María Gabriela	Viteri Tovar
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