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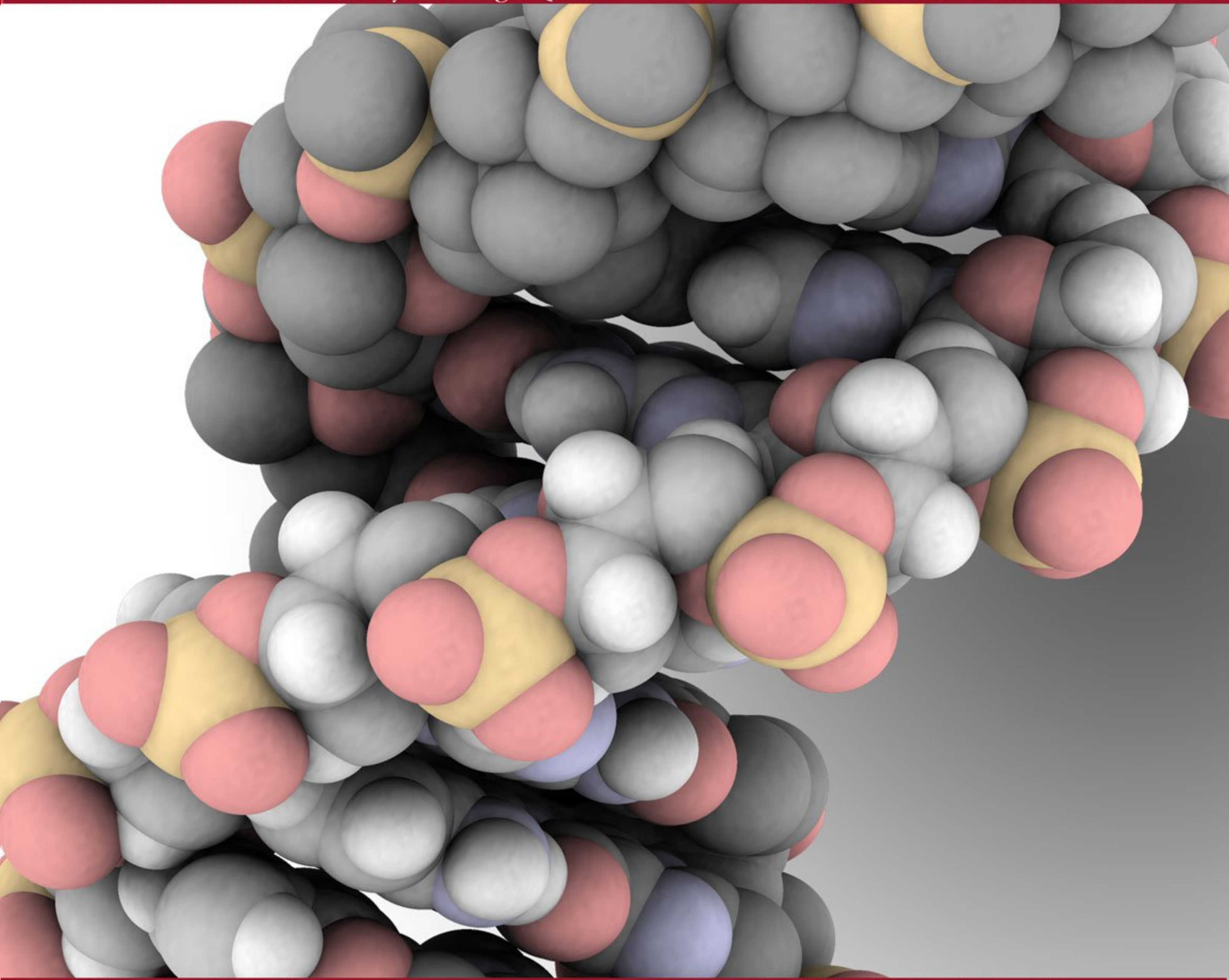

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JORNADAS POSTDOCTORALES UCLM

CONFERENCIA MARÍA A. BLASCO

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PRESENTACIÓN

El número de Junio es un monográfico dedicado al XII Simposio de Ciencia Joven. Este año se ha producido un aumento del número de contribuciones con una sesión de posters por primera vez. Además, este número también recoge información relativa a las Jornadas Postdoctorales de la UCLM y la conferencia de la directora del CNIO, María Blasco.

El comité editorial.

Los químicos noveles de la UCLM comparten sus líneas de investigación en el Simposio de Ciencia Joven

La Facultad de Ciencias y Tecnologías Químicas de la Universidad de Castilla-La Mancha (UCLM) en Ciudad Real acoge desde hoy y hasta el viernes el simposio Ciencia Joven, durante el que los investigadores noveles presentan sus líneas de trabajo a sus colegas del centro universitario. El encuentro, que cumple su duodécima edición, ha sido inaugurado por el rector de la UCLM, Miguel Ángel Collado, quien ha hecho alusión a la importancia que tiene la investigación para seguir creciendo.

Los jóvenes investigadores de la Facultad de Ciencias y Tecnologías Químicas en el Campus de Ciudad Real presentan entre hoy y el viernes a la comunidad académica sus líneas de investigación y los resultados obtenidos durante la celebración del duodécimo Simposio de Ciencia Joven, una iniciativa organizada por ellos mismos que a su vez les supone una oportunidad para acercar a los estudiantes a la tarea investigadora.

El encuentro ha sido inaugurado esta mañana por el rector de la Universidad de Castilla-La Mancha (UCLM), Miguel Ángel Collado, quien ha subrayado el entusiasmo de los jóvenes investigadores por la ciencia y ha felicitado a la Facultad de Químicas por su “compromiso por la investigación en tiempos difíciles”.

El rector ha insistido en que la investigación “es necesaria para todos, para seguir creciendo” y ha reivindicado su apoyo a nivel estatal y regional. En este punto, se ha congratulado, por un lado, de la creación del nuevo Ministerio de Ciencia, Innovación y Universidades, del que espera una regulación y una financiación adecuada para la investigación; y, por otro, de la convocatoria regional de ayudas para proyectos de investigación científica y transferencia, aunque respecto a esta última ha hablado de la necesidad de recuperar su temporalidad.

Por su parte, el decano de la Facultad de Ciencias y Tecnologías Químicas, Ángel Ríos, se ha referido a la celebración del simposio Ciencia Joven como una excelente oportunidad única para los investigadores noveles. “Todo lo hacen ellos, desde la organización del evento, a la recepción y selección de comunicaciones, y, lo que es más importante, la presentación de su propio trabajo, sus líneas y sus resultados”, ha dicho el decano, quien ha indicado que éste es un “pequeño ensayo” que les ayudará a conocer cómo se prepara un congreso científico.

En el simposio, en el que colabora la Real Sociedad Española de Química, se han inscrito un total de 120 investigadores del Campus de Albacete, Ciudad Real y Toledo, así como estudiantes extranjeros de doctorado, y se han admitido 31 comunicaciones orales y 34 contribuciones en formato póster en los distintos ámbitos que abarca la Facultad: Química Inorgánica, Ingeniería Química, Química Orgánica, Química Analítica, Tecnología de los Alimentos, Química Física, Matemáticas y Bioquímica. Entre otras líneas de investigación, durante el simposio se hablará de sensores químicos, control de calidad, catalizadores, medio ambiente, nuevos materiales o control de nanomateriales en alimentos.

Junto a los ponentes, el simposio cuenta con la intervención de cinco ponentes externos invitados de las universidades Rovira i Virgili, Complutense de Madrid y Málaga y del Consejo Superior de Investigaciones Científicas.

Contrato-programa

Por otro lado, y en declaraciones a los medios de comunicación y posteriormente a los participantes en el simposio, el rector ha recordado que la UCLM se encuentra en pleno proceso negociador con el Gobierno regional del contrato-programa. Tras seis meses de negociación, Collado ha asegurado que urge ya firmar el mismo porque “el tiempo juega en contra de la UCLM”, con un importe “razonable” y con un marco temporal amplio, “no de uno o dos años”.

Collado ha indicado que la UCLM ha cumplido con la presentación del Plan Estratégico y corresponde a la Junta poner una cifra al contrato-programa que “nos permita seguir creciendo, no subsistiendo”. “Estamos a mediados de junio, el próximo curso se echa encima y crece la incertidumbre porque se complica el funcionamiento de la Universidad. Necesitamos saber cuanto antes la cuantía del contrato-programa”, ha insistido el rector.

Gabinete Comunicación UCLM. Ciudad Real, 13 de junio de 2018

INNOVACIONES EN EL ESTUDIO DE LA ASTRINGENCIA; IMPACTO DE CIERTAS PRÁCTICAS ENOLÓGICAS SOBRE LA PERCEPCIÓN DE LA ASTRINGENCIA DE LOS VINOS TINTOS. "IN MEMORIAN ISIDRO HERMOSÍN"

Fernando Zamora Marín

La presente conferencia “In memoriam” del Profesor Isidro Hermosín trata de los estudios sobre la astringencia que se han realizado en colaboración entre el grupo de investigación del Profesor Isidro Hermosín en la Universidad de Castilla-La Mancha y nuestro grupo de investigación de la Universidad Rovira i Virgili. En la exposición se abordará la descripción de qué es la astringencia, de cuál es su mecanismo de acción molecular y de coma afectan ciertos aspectos vitivinícolas tales como la madurez de la uva o los procesos de vinificación y crianza del vino tinto sobre dicho atributo sensorial. Finalmente se presentarán los últimos resultados de nuestra colaboración consistentes en la aplicación de la resonancia en superficie de plasmones (Surface Plasmon Resonance - SPR), para el estudio de la interacción molecular entre mucina bovina y diferentes tipos de taninos. La SPR se fundamenta en la capacidad de algunos metales de absorber parte de una radiación laser a un ángulo de incidencia determinado formando una radiación en superficie que se conoce con el nombre de plasmón. El ángulo de incidencia (y el de reflexión) en que se forma el plasmón depende del grosor del metal, incluyendo el otro material adherido a éste. Cuando una molécula se fija a la superficie del metal y otra molécula se pone en contacto con esta superficie, la interacción molecular entre ambas se puede investigar en tiempo real midiendo la variación de este ángulo. Esta técnica permite por tanto determinar el aumento del espesor de una superficie generada por la interacción molecular entre una molécula previamente fija (la mucina) y otra que se inyecta en el sistema (los taninos). El análisis de estas interacciones hace posible la caracterización de las constantes de asociación y disociación cinéticas y termodinámicas entre la mucina y los diferentes taninos, abriendo por tanto una nueva perspectiva para estudio de los factores que afectan a la astringencia.

CONFERENCIA INVITADA

SENORES ÓPTICOS PARA EL ANÁLISIS DE ANTIBIÓTICOS Y DE TOXINAS NATURALES. BÚSQUEDA DE NUEVOS ELEMENTOS DE RECONOCIMIENTO SELECTIVO

Mª Cruz Moreno Bondi

Los biosensores son dispositivos autointegrados que proporcionan información analítica específica, cuantitativa o semicuantitativa, sobre la especie objetivo mediante el uso de un elemento de reconocimiento biológico (un receptor bioquímico) en contacto espacial directo con un elemento transductor. La necesidad de un diagnóstico rápido y la mejora de las características de detección, selectividad, estabilidad operativa, almacenamiento a largo plazo o la facilidad de preparación, han favorecido el desarrollo de receptores sintéticos intrínsecamente estables que imitan a los elementos de biorreconocimiento (es decir, los receptores biomiméticos) manteniendo sus características de afinidad y selectividad [1]. Durante la última década, los polímeros de impronta molecular (MIPs) se han empleado, en sustitución de los anticuerpos y las enzimas, como elementos de reconocimiento selectivo en sensores y otras separaciones analíticas. Los MIPs son altamente robustos, mostrando una excelente estabilidad operacional bajo una amplia variedad de condiciones. Pueden utilizarse en medios orgánicos o acuosos, su coste es inferior y su preparación mucho más sencilla que la de los anticuerpos, evitando el uso de animales de laboratorio o las dificultades asociadas a la producción de anticuerpos para compuestos tóxicos. Además, los MIPs pueden diseñarse para que presenten una buena sensibilidad y especificidad para una amplia gama de analitos mediante una selección adecuada de los componentes de la mezcla de polimerización (molécula de plantilla, monómeros funcionales, entrecruzante, disolvente). Su combinación con la nanotecnología ha demostrado sus ventajas para la detección óptica [2]. En un enfoque diferente, la técnica del desplegado de fagos (“phage display”) ha mostrado un gran potencial en la preparación de péptidos miméticos de epítopos (mimopeptidos) para la detección de toxinas naturales utilizando inmunosensores. Estos mimopéptidos evitan la etapa de conjugación y la toxicidad asociada al empleo de toxinas naturales, como las micotoxinas. Además pueden inmovilizarse a elevadas densidades para la producción de microarrays preservando su estabilidad y especificidad. Por otra parte, su uso evita los riesgos asociados a la manipulación de compuestos peligrosos [3]. Esta presentación presenta algunos ejemplos recientes de nuestro Grupo sobre el desarrollo de microsensores y nanosensores basados en MIP, así como sobre la aplicación de la tecnología “phage display” al desarrollo de microarrays para el análisis de antibióticos y micotoxinas en diferentes matrices [4,5].

Agradecimientos: Estudio financiado por el Ministerio de Economía y Competitividad y el Fondo Europeo de Desarrollo Regional (CTQ2015-69278-C2-1-R MINECO/FEDER) y la UE (SAMOSS; FP7-PEOPLE-2013-ITN; Contrato 607590). R.P. agradece su contrato predoctoral a la UCM.

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TRANSFERENCIA DEL CONOCIMIENTO DESDE EL GIGA AL SECTOR EMPRESARIAL Y VICEVERSA

José Miguel Rodríguez Maroto

En la ponencia se presenta un breve recopilatorio de algunos casos seleccionados de transferencia del conocimiento desde el Grupo de Ingeniería y Gestión Ambiental (GIGA) de Andalucía al sector empresarial. Dichos casos se enmarcan en las líneas de investigación que desarrolla el grupo y se pretende mostrar la diversidad de las actuaciones que un grupo, formado por exclusivamente por profesores y titulados de Ingeniería Química, ha llevado a cabo en su colaboración con las empresas.

Los trabajos de transferencia del conocimiento desarrollados obedecen a tres objetivos básicos: a) Desarrollar soluciones tecnológicas a problemas específicos "Personalización", b) Mejorar la competitividad de las empresas y c) Poner en valor la investigación del grupo.

Se han seleccionado tres parejas de proyectos que recogen casos de transferencia del conocimiento en las líneas de investigación de: Evaluación y tratamiento de suelos contaminados, tratamiento de aguas potables y residuales y aprovechamiento de residuos respectivamente.

En la primera se presenta un estudio de la afección del suelo debida a la actividad desarrollada en relación con el almacenamiento y aprovechamiento de restos de automóviles fuera de uso (sector de desguaces y chatarrerías) en la Comunidad Autónoma de País Vasco (CAPV) y otro sobre el desarrollo de modelos físico-químico-matemáticos y el software correspondiente para la evaluación y el seguimiento de operaciones de tratamiento de suelos contaminados mediante las técnicas de extracción de vapores a vacío y de electrodescontaminación.

En la segunda se presenta un estudio sobre la recuperación de fósforo y nitrógeno en plantas de tratamiento de aguas residuales mediante precipitación controlada de estruvita y otro sobre el uso de energías renovables en la generación electroquímica de Fe(III) para su utilización como coagulante en el tratamiento de aguas potables.

Finalmente, la tercera pareja incluye la aplicación de residuos férricos procedentes de plantas potabilizadoras de agua como adsorbentes de tiomoléculas causantes de malos olores y la formulación de aditivos de alta calidad para la fabricación de hormigón celular in situ.

Por último, se presentan algunas conclusiones alcanzadas a partir de las relaciones mantenidas con las empresas durante un largo periodo de colaboración con las mismas.

ALIMENTÓMICA, INGREDIENTES BIOACTIVOS Y CÁNCER DE COLON: HISTORIA DE UN LARGO VIAJE

Alejandro Cifuentes

One of the main topics in our lab during the last years [1-18], has been the search of new natural compounds with anti-colon cancer activity following a Foodomics evaluation. To carry out this work, transcriptomics, proteomics and/or metabolomics have been employed. This work has included: a) the development of new green extraction processes to obtain bioactive compounds from different natural sources (algae, microalgae, food by-products, plants, etc) [1-4]; b) the determination of the antiproliferative effect of the new extracts against different in vitro and in vivo models of colon cancer [5-8]; c) the development of advanced analytical approaches including metabolomics profiling based on comprehensive LCxLC-MS/MS for the chemical characterization of the bioactive extracts [9,10]; d) the identification of genes, proteins and metabolites differentially expressed in cancer cells using whole-transcriptome microarrays followed by RT-PCR confirmation, nano-LC-MS for proteomics and/or non-targeted whole-metabolome approaches based on LC-MS and CE-MS [11-15] and; e) the development of different algorithms for the comprehensive analysis of these MS-based datasets [16-18]. These strategies represent a good example of the important challenges that still have to be addressed by Foodomics in order to scientifically link Food & Health at molecular level and will allow us to discuss in this work some of the current and future challenges in this area of research.

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PRODUCTOS NATURALES: DE LA MAGIA A LA QUÍMICA MODERNA

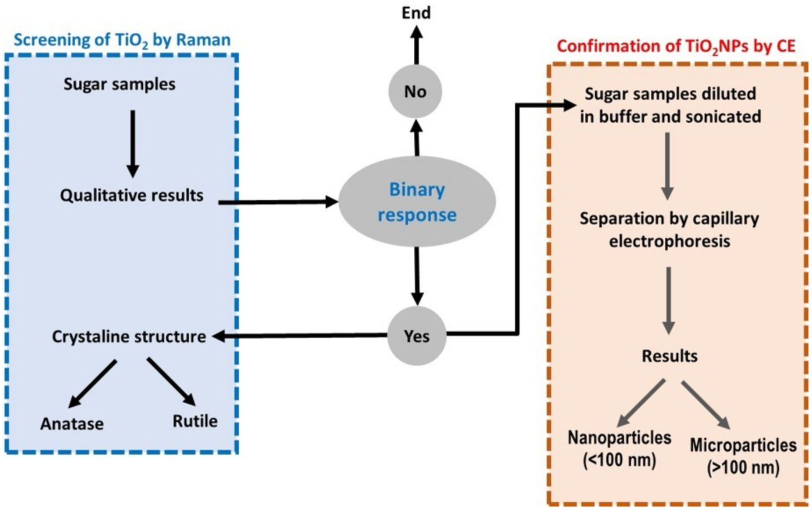
Mª del Carmen de la Torre Egido

Los productos naturales han jugado un papel decisivo en el desarrollo de la especie humana. Usados, en un principio, como remedios para ciertas dolencias, como especias o esencias, o incluso para trascender a lo sobrenatural, los Productos Naturales son una parte fundamental de la Química Orgánica. Con el desarrollo de las técnicas espectroscópicas, especialmente de la resonancia magnética nuclear, el número de nuevos compuestos creció exponencialmente, de tal manera que actualmente se conocen varios cientos de miles de productos naturales. Estos compuestos se caracterizan porque son escasos en la naturaleza, no son comunes a todos los seres vivos y presentan interesantes propiedades biológicas y una enorme variedad estructural. En la actualidad se necesitan, cada vez más, nuevos compuestos que den respuesta a las necesidades de la sociedad en ámbitos como la salud, la energía o el medioambiente. Una de las estrategias para la preparación eficiente de nuevos compuestos es la Síntesis Orientada a la Diversidad. En nuestro grupo de investigación se han desarrollado metodologías sintéticas, basadas en esta estrategia, que permiten la síntesis de nuevos compuestos estructuralmente complejos y con una gran variedad estructural. A lo largo de la presentación se expondrán varios ejemplos en los que, utilizando diferentes productos naturales como materiales de partida, se demuestra la gran versatilidad de esta aproximación sintética.

ANALYTICAL NANOMETROLOGICAL APPROACH FOR SCREENING AND CONFIRMATION OF TITANIUM DIOXIDE NANO/MICRO PARTICLES IN SUGARY SAMPLES BASED ON RAMAN SPECTROSCOPY - CAPILLARY ELECTROPHORESIS

Virginia Moreno García

Analytical nanometrology is a present challenge in today analytical science, particularly from a practical point of view and when it is addressed to routine/control laboratories. In this way, a screening-confirmation approach is described for the characterization and distinction between titanium dioxide nano/micro-particles in sugary food samples. The first step involves the confirmation of the presence of TiO_2 in the sample (used as additive E171 in sugary samples), using a portable Raman spectrometer, in which the crystalline structure of TiO_2 (anatase or rutile) in the positive samples can be also obtained in this step. Then, the second step was only applied to positive samples, and it involves the use of Capillary Electrophoresis (CE), which allows to distinguish between TiO_2-nanoparticles (<100 nm) from TiO_2-microparticles (>100 nm). Additionally, nanoparticles (TiO_2 anatase 5 nm and TiO_2 rutile 60 nm) and microparticles (TiO_2 rutile 0.1-0.2 μm) can be electrophoretically separated. The general procedure is simple, fast and low cost, providing a valuable analytical tool in the field of food safety and control, thus contributing to the development of the analytical nanometrology.



SYNTHESIS OF POLYMER-DRUG CONJUGATES TO CONTROLLED RELEASE OF DRUGS

María José Carrero Menchén

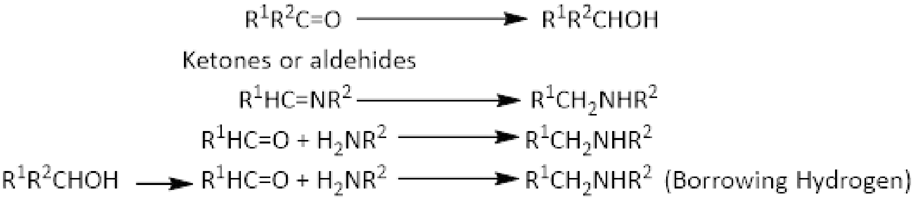
Poly(ethylene oxide)-poly(propylene oxide) (PEO-PPO) block copolymers stand out among amphiphilic molecules due to the possibility of modifying their hydrophilic/hydrophobic character easily, just varying the proportion between the PEO and PPO molecules respectively. This property together with their biocompatibility and biodegradability make them, and their derivatives, suitable for products formulation in industries ranging from agriculture to pharmaceuticals and controlled release of drugs. Thus, these copolymers are able to form thermodynamically stable micelles in aqueous solution above a certain copolymer concentration, CMC (critical micelle concentration) that can improve the poor solubility of the drugs. Moreover, the introduction of glycidyl propargyl ether (GPE), which contains triple bonds, in the copolymer chain allows to obtain functionalized terminal alkynyl-polyethers suitable for future click attachment, with the objective of enlarge the drug lifetime in the body. The ultimate purpose of this work is to obtain a tailor-made polymeric drug carrier able to incorporate the coumarin (anticancer agent) which will provide the two aforementioned benefits.

First, PEO-PPO-GPE triblock copolymers were synthesized through nucleophilic ring-opening polymerization, maintaining the mass ratio between hydrophilic/hydrophobic segments (50/50) in all cases, but changing the ratio for the hydrophobic monomers (PPO and GPE) to increase the GPE mass percentages in the final copolymer from 0 to 15 percent. Subsequently, on the one hand, the coumarin was loaded in polymeric micelles with different percentages of GPE using direct dissolution method. Based on the DLS results, the micelles size was in the suitable range (10-200 nm) to enable its absorbability by the target cells and this size increased when coumarin was added, confirming its incorporation. On the other hand, the click reaction based on the use of Cu (II) as catalyst, between the PEO-PPO-GPE copolymers and azide-coumarin was successfully carried out according to FTIR and NMR analysis.

CATALYTIC TRANSFER HYDROGENATION PROCESSES USING RUTHENIUM AND IRIDIUM ORGANOMETALLIC COMPOUNDS

Margarita Ruiz de Castañeda Álvaro

In the second half of the 20th century the interest toward homogeneous catalysis has increased remarkably with the development of organometallic chemistry. In the past decade, half-sandwich Ru(II) complexes have found applications as active homogeneous catalysts in a large number of organic reactions. Transfer hydrogenation (TH) catalytic processes are an important alternative to catalytic reduction with H_2, involving the formal transfer of H_2 from a donor molecule to a substrate. The use of water makes the process more environmentally friendly. Our group is interested in the development of versatile catalysts active in aqueous media for TH of organic carbonyl and imine compounds using HCOOH/HCOONa as hydrogen source and in the deuterium labelling of the products [1,2]. The use of D_2O has allowed a considerable and selective deuterium labelling of the obtained alcohols or amines. The complexes have been used in processes of direct hydrogenation or in a tandem alternative. Thus, the amination of alcohols is achieved by the use of borrowing hydrogen methodology that has proven to be a highly atom economical method for the production of amines. No external reductant is required for this process, as the alcohol substrate serves as the hydrogen donor.



$$R^1R^2C{=}O \longrightarrow R^1R^2CHOH$$

Ketones or aldehides

$$R^1HC{=}NR^2 \longrightarrow R^1CH_2NHR^2$$

$$R^1HC{=}O + H_2NR^2 \longrightarrow R^1CH_2NHR^2$$

$$R^1R^2CHOH \longrightarrow R^1HC{=}O + H_2NR^2 \longrightarrow R^1CH_2NHR^2 \text{ (Borrowing Hydrogen)}$$

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TUNABLE POLYMERS DERIVED FROM 2H-BENZO[d]1,2,3-TRIAZOLE MONOMERS

Iván Torres Moya

Multifunctionality is greatly desirable in materials science. In this sense, the appropriate choice of substituents allows control not only of the structure of the material but also of its properties. Thus, appropriate control of the starting molecular components enables the formation of supramolecular nanoscopic architectures which combine several properties and have a range of potential applications. [1]

In our research group, we are working with oligomers derived from 2H-benzo[d]1,2,3-triazole because of interesting characteristics due to its acceptor character and specially, its easy modification in the N-H bond of the triazole ring and the easy introduction of donor groups in benzene ring. To check the multifunctionality of these monomeric derivatives, in the last years, we have tested them as optical waveguides[2], organic field-effect transistors (OFETs)[3], liquid crystals or organogels.

In this work, for the first time in our group, we have synthesized six different polymers, keeping constant one fluorene copolymer derivative and changing the monomers derived from 2H-benzo[d]1,2,3-triazole in order to modify the structure and the properties to stablish a relationship between structure and properties, in terms of photophysical properties and in the application as organic semiconductors in organic field-effect transistors (OFETs).

This study is supported by theoretical calculations, which are an essential tool in organic chemistry because they can predict properties and study the topology of frontier molecular orbitals before synthesizing them avoiding unnecessary synthesis and contributing to more economic and sustainable processes.

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YEAST BIODIVERSITY FROM NATURAL SOURCES IN THE CENTRAL REGION OF SPAIN

Beatriz García-Bejar Bermejo

The loss of biodiversity in the world due to human activity is a major concern worldwide because it implies the destabilisation of the ecosystems from which goods and services for human development are obtained. So, the knowledge of the existing microbiological diversity it is important since its plays a significant role in the balance of the ecosystems, food cycles and regeneration of nutrients. However, yeast biodiversity, which is estimated that 99% of the potential it is still unknown, have not been traditionally studied. For these reasons, a study of the yeast diversity presented in samples from different environments of a central region of Spain was carried out, due to these areas have great biological diversity, both animal and plant, as well as specific food.

Samples were collected at different points of Ciudad Real and Madrid region. Yeasts colonies were isolated by traditional microbiology techniques and were cultured and grown during 48 hours at 30ºC on YPD agar plates with antibiotics and antifungals. This process allowed to select and purify the isolated colonies from each sample that were observed using the optical microscope to confirm that were yeasts. The genetic identification was first done at specie level using PCR-RFLP analysis, amplifying the 5.8S rRNA region with ITS1 and ITS4 primers and being confirmed the profiles by sequencing the D1/D2 region. Secondly, strain genetic identification was carried out using the PCR-RAPD technique. All the data were analysed utilising bioinformatics programs like MEGA4 and BioNumerics 7.6.

A total of 392 yeasts were isolated from 24 different environments, identifying 21 species and 215 strains. This study has allowed knowing the yeast diversity from a specific area of Spain that has not been exanimate before. Also, it has been demonstrated the association of some species with determinate environments, while species never before described in this territory have been identified.

GRAPHENE SYNTHESIS: CHEMICAL OXIDATION, EXFOLIATION AND REDUCTION

Antonio Patón Carrero

During the last decade, due to the graphene revolution, the production of graphene precursors have become an important subject of study. Several ways are developed in order to obtain this material, one of the most important route is the chemical reduction. This route implies different chemical and physical procedures with the final aim of obtain an important graphene-based material: reduced graphene oxide. Figure 1 represents the scheme of chemical reduction.

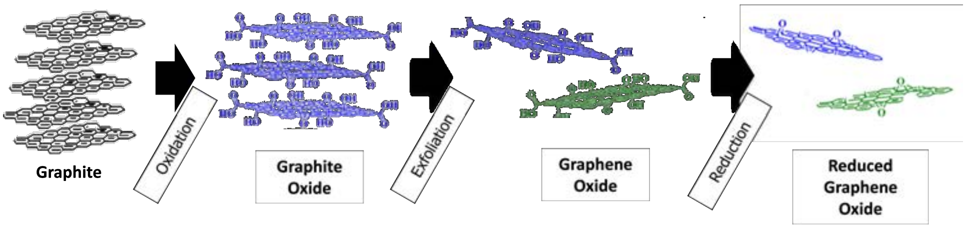


Figure 1. Scheme of chemical reduction

The main problem of this method is the great amount of variables and products that are obtained during the whole chemical reduction. This work summarize the study of three of the main variables in this process in order to improve chemical method and obtain the best possible products. First of all, the morphology and size of starting graphite are studied attending to the characteristics of the final graphite oxide. Other important variable is the oxidizing agent which determine the level of the oxidation and layer distance of graphite oxide. And to conclude this work, different reduction methods are carried out in order to obtain a reduced graphene oxide with the most similar structure than the graphene one.

These results provide new information about different types of graphene-based products and hence make mass production viable.

MODIFIED SCREEN-PRINTED CARBON NANOFIBER ELECTRODE FOR QUANTITATION OF HETEROCYCLIC AMINES IN FOOD

Cristina Montes Correal

An electrochemical sensing method based on a screen printed nanofiber carbon electrode (SPE) modified with silver nanoparticles (AgNPs) and Nafion (Nf) was developed to determine the aromatic heterocyclic amine (HAA) 2-Amino-3,8-dimethylimidazo [4,5-f] quinoxaline (MeIQx) in food samples. Building of sensing electrode platform was firstly performed attending to sensitivity results with regard to analyte by evaluation of different commercial SPEs, different working pHs, different surface coatings (nanomaterials, amounts) and addition of polymeric cationic exchanger electrolyte (Nf).

The surface of this Ag-Nf screen printed carbon nanofiber electrode was nanostructurally characterized by UV-Vis spectrometry, dynamic light scattering (DLS), scanning electron microscopy (SEM) and raman spectroscopy with good agreement between results from the different techniques and the expected results, obtaining an average size of 14.09 nm for AgNPs. The electrochemical characterization of the sensor was performed using the cyclic voltammetry (CV) technique, showing a diffusion controlling electhochemical mechanism. The electrode modified with AgNPs/Nf showed better electrocatalytic properties (in terms of reversibility and faster kinetic of electronic transfer) than the unmodified electrode and the electroactive area increased 0.048 cm^2 with respect to the unmodified electrode. Differential pulse voltammetry (DPV) was selected as the most suitable electrochemical technique for quantification of MeIQx.

Instrumental parameters relative to DPV technique were optimized: ΔE, amplitude, width pulse, width sampling, pulse period and quiet time. Additionally, this DPV analytical signal was sensitized using the first derivative and smoothing. Analytical performance characteristics of the developed method have been satisfactorily evaluated in terms of repeatability and reproducibility, linearity range (0.1 - 100 μM), and detection limits and quantification limits (0.33 10^{-9} g and 1 10^{-9} g, respectively).

COMUNICACIÓN
ORAL

INNOVATIONS IN VINE FERTILIZATION USING WINE DISTILLERY COMPOST

Juan Antonio Delgado Sánchez-Migallón

The high generation of organic wastes together with the increasing interest in developing a sustainable agriculture convert the recycling of these materials as source of organic matter and nutrients in a good option of management. A field experiment was established during 2017 to evaluate the use of a compost made from wastes from the winery and distillery industry in Chelva vine traditionally grown in Castilla-La Mancha region, area where these wastes are generated. A randomized complete-block design was used with four treatments consisting on three doses of compost: 1 (D1), 2 (D2) or 3 (D3) kg compost per linear meter of plantation and a control (D0) without compost application and the aroma profile of wine was studied by chemical and sensory techniques. For making wines, laboratory fermentations were carried out according to traditional winemaking process for white wines. Volatile compounds were isolated using SPE technique and then analyzed by GC-MS. Sensory aroma profile of wines was evaluated using a trained panel of then assessors.

A total of 81 volatile compounds were identified and quantified in studied wines. Significant differences were found between control wines and wines elaborated with grapes fertilized, in general the fertilization treatment increase the concentration of volatile compounds especially when the dose is 2 Kg/m linear related with floral y fruity notes. It can be see that when the dose is of 3 Kg/m linear increase the concentration of C6 compounds related with green notes of the wine. The application of compost derived from winery and distillery wastes resulted in slight increases the concentration of varietal aroma compounds related with the aromatic typicity of wines principally when the dose of compost corresponding to 2 kg of compost per linear meter.

COMUNICACIÓN ORAL

CAPILLARY ELECTROPHORESIS METHOD FOR THE DISCRIMINATION BETWEEN NATURAL AND ARTIFICIAL VANILLA FLAVOR FOR CONTROLLING FOOD FRAUDS

Samah Lahouidak

A capillary electrophoresis method was developed for the determination of coumarin (COUM), ethyl vanillin (EVA), p-hydroxybenzaldehyde (PHB), p-hydroxybenzoic acid (PHBA), vanillin (VAN), vanillic acid (VANA) and vanillic alcohol (VOH) in vanilla products. The measured concentrations are compared to values obtained by liquid chromatography (LC) method.

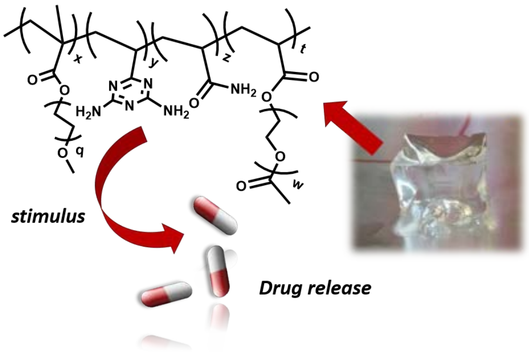
Analytical results, method precision, and accuracy data are presented and limits of detection for the method ranged from 2 to 5 μg/mL. The results obtained are used in monitoring the composition of vanilla flavorings, as well as for confirmation of natural or non-natural origin of vanilla in samples using four selected food samples containing this flavor.

DESIGNING NOVEL TRIAZINE-BASED HYDROGELS FOR DRUG DELIVERY APPLICATIONS

Jorge Leganés Bayón

The introduction of aminotriazines in polymeric hydrogels has been successfully used to strengthen the mechanical properties of gels, bind DNA for reverse gene transfection,[1] or remove metal ions through adsorption. Based on our experience in the preparation of triazine derivatives,[2] we presently carry out the syntheses of 2,4-diaminotriazine-based hydrogels.

Macroscale Drug Delivery Systems (MDDS) are widely employed to load, carry and release compounds of clinical significance in a controlled and directed manner.[3] In this study, we analyze the synthesis, design and drug release behavior of these macroporous diaminotriazine-based hydrogels and evaluate them as a possible candidates for MDD.



Overview scheme of triazine-based MDDS

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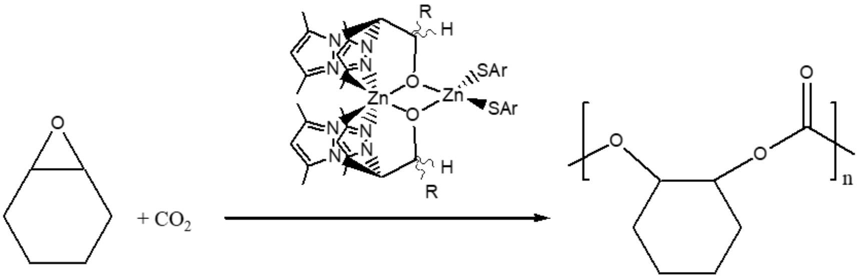
NEW SCORPIONATE ZINC COMPLEXES AS INITIATORS FOR THE SYNTHESIS OF POLYCARBONATES BY ROP COPOLYMERISATION OF CYCLOHEXENE OXIDE AND CARBON DIOXIDE

Sonia Sobrino Ramírez

A series of new alcoxide and tioalcoxide mono- and bimetallic zinc complexes containing heteroscorpionate ligands have been prepared in very high yields. The structures of the complexes were determined by spectroscopic methods, and various single-crystal X-ray structure of these families confirmed a κ^3-NNO, κ^2-NN, κ^2-NN-μO coordination mode of the scorpionate ligand in a mono- and dinuclear molecular arrangement.

These zinc complexes were investigated as catalysts for the synthesis of polycarbonates from epoxides and carbon dioxide in the absence of a cocatalyst.[1] Under the optimal reaction conditions, the complex type $[Zn(\kappa^2NN\text{-}\mu O)_2Zn(SAr)_2]$ acts as an efficient single-component initiator for the ring-opening copolymerisation of cyclohexene oxide and carbon dioxide, at 1% catalyst, 10 bars of CO_2 and 70ºC, yielding polycarbonate materials.



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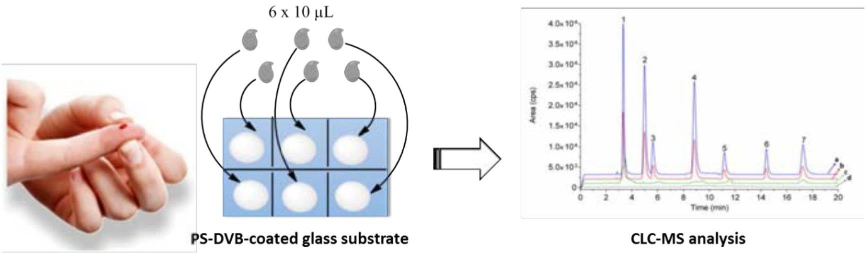
A SIMPLE POLY(STYRENE-CO-DIVINYLBENZENE)-COATED GLASS BLOOD SPOT METHOD FOR MONITORING OF SEVEN ANTIDEPRESSANTS USING CAPILLARY LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY

Khaled Ali Murtada

A simple, rapid, selective and sensitive monitoring method for the simultaneous determination of the widely-prescribed antidepressants agomelatine, bupropion, citalopram, fluoxetine, mirtazapine, paroxetine, trazodone in a unique drop of human blood is here developed and validated. This methodology is based on the use of lab manufactured poly(styrene-co-divinylbenzene)-coated glass (PS-DVB) blood spot for the extraction of the analytes and their subsequent separation and detection by capillary liquid chromatography-mass spectrometry (CLC-MS). Briefly, 10 mm-side squares were punched out from blood spots collected on glass substrate coated by 10 µg of the PS-DVB polymer and eluted with 1.0 mL of 2.0% acetic acid in methanol. The analytes were then separated and detected in less than 20 minutes by capillary CLC-MS using a Jupiter 4µ Proteo 90A column and water: acetonitrile (20:80 v/v) and ammonium acetate (5 mM, pH 3.0) as mobile phase. Limit of detection (LOD) ranged from 0.018 to 0.038 µg mL^{-1}, and precision values for the responses and migration times lower than 5.89% and 1.92% were calculated, respectively. Moreover, accuracy values ranging between 15.0% and -3.8% were obtained. Future validation will focus on the clinical application of the method with blood real samples.



COMUNICACIÓN
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SUSTAINABLE-GREEN ELECTROOXIDATION OF ORGANOCHLORINATED COMPOUNDS

María Millán Espinar

Over the last decades, the environmental concern about pesticides pollution has increased noticeable. Large crop areas present a huge amount of pesticides remaining in soils and groundwater due to filtration processes. Most of these pesticides are organochlorinated compounds which present high toxicity and carcinogenic nature. Furthermore, their low biodegradation and great chemical stability make them resistant to traditional treatments. Advance oxidation processes (AOPs) have been widely studied for the treatment of wastewater effluent polluted by persistent compounds. Among them, the conductive diamond electrochemical oxidation (CDEO) has shown higher efficiencies removing organic compounds due to the great chemical and electrochemical stability of Boron Doped Diamond (BDD) electrodes[1]. Nevertheless, the main handicap of this electrochemical process is the huge electrical energy demand per unit of treated volume. Consequently, the coupling of these electrochemical processes with green energies could overcome this drawback.

The present work shows the degradation of a pesticide, clopyralid, from a soil using an electrolysis technique based on BDD electrodes. A soil polluted with 2g clopyralid per kg soil was washed to remove the pesticide from the soil. Then, the electrolysis of the washing effluent was carried out powering the reactor at galvanostatic mode (constant current) and under a solar profile recorded in Ciudad Real from 26th of January to 9th of February of 2018. The results demonstrate that the use of solar energy attains higher removal efficiencies at sunlight hours, 94 %. On the contrary, these efficiencies dropped sharply overnight as it was expected. Nevertheless, the electrochemical reactor solar powered was able to remove at peak hours a 3 % of pollutant more regarding the reactor supplied at constant current. Additionally, the amount of intermediate species was higher in the last case. Thus, it can be concluded that the solar-electrolysis coupled system can be use for the pesticide removal.

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COMUNICACIÓN
ORAL

WAVEGUIDE BEHAVIOUR IN SELF-ASSEMBLED THIADIAZOLE AND BENZOTHIADIAZOLE-BASED MATERIALS

Raúl Martín Lozano

One dimensional (1D) organic single crystal nano- and micro-wires built of organic semiconducting derivatives have attracted much attention in last decade due to their potential applications in organic opto-electronics.[1] Self-assembly through non-covalent interactions between organic conjugated molecules has shown to be a versatile approach for obtaining these functional organic single crystalline microstructures.[2] In the recent years, our research group has prepared triazole and benzotriazole -based self-assembled aggregates obtaining π-conjugated molecules which have exhibited interesting properties as organic optical waveguides.[3]

Thiadiazole and benzothiadiazole cores have shown to have intense luminescent values with good thermal stability.[4] With the appropriate functionalization, it is possible to obtain dyes with a wide range of colours. We have synthesized four new arylalkynyl derivatives of benzo[c][1,2,5]thiadiazole and 1,3,4-thiadiazole avoiding the use of solvents with the use of microwave irradiation as energy source.[5]

Organized supramolecular structures have been obtained by slow diffusion technique. The ability to propagate light along the supramolecular structures was measured using a fluorescence microscope. Results showed that these aggregates exhibited optical waveguide behavior showing blue, green and red emission. It should be highlighted the ability of these aggregates to emit at various wavelengths.

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ANTHOCYANIN PROFILE OF BRAZILIAN HYBRID GRAPE CULTIVAR BRS NÚBIA ('MICHELE PALIERI' AND 'ARKANSAS 2095')

Yara Paula de Oliveira Nishiyama

BRS Nubia grape is a hybrid cultivar with seeds developed by the Brazilian Agricultural Research Corporation (EMBAPA). This grape was created from the 'Michele Palieri' and 'Arkansas 2095' grapes for the commercialization “in natura”. Its bunches are large and conical with large berries that have firm texture and neutral taste. As there is no knowledge of studies on the detailed anthocyanins composition of this grape skin the study for more knowledge about this cultivar is very import to encourage its production and commercialization. The anthocyanins profile from BRS Núbia grape skin was determined by extracting the compounds of interest and further evaluation of this extract with the aid of high-performance liquid chromatography with diode array detector coupled to mass spectrometry with electrospray ionization chamber and ion trap analyzer (HPLC-DAD-ESI-MS/MS).

Were identify 23 monoglycosylated anthocyanins including glucosylated (glc), acetylated, coumaroylated and caffeoylated compounds derived from the five main anthocyanidins present in grapes: delphinidin, cyanidin, petunidin, peonidin (pn) and malvidin (mv). Non-acylated anthocyanins were the major series found in these grape cultivar (76%) following by coumaroylated derivatives (14%) and caffeoylated derivatives (1%). Mv-3-glc was the principal compound in this cultivar, representing 52% of the anthocyanins, followed by pn-3-glc with 14% of the total. Although it is hybrid grape, it´s possible to observe that the obtained results for anthocyanins profile is similar to that of a vinifera grapes.

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SYNTHESIS OF SECOND GENERATION BIOFUELS FROM AGRO-FOOD WASTES AND ITS ATMOSPHERIC IMPLICATIONS

Almudena Lorente Diezma

Fossil fuel reserves are nowadays decreasing and their use cause high CO_2 emissions. For these reasons lignocellulosic biomass is becoming increasingly recognized as a good feedstock and carbon source with different components and applications.[1]

Plant cell wall is mainly composed by cellulose, hemicellulose and lignin being cellulose the predominant component. These polymers can be transform into biofuels, bio-oils and value-added chemicals with good properties to use in biorefinery. Microwave radiation is a promising technique widely used as heating system into biomass[2] and hydrothermal liquefaction (HTL) is a green thermochemical technique that converts the biomass into a liquid product (bio-oil or bio-crude) at moderate to high temperature and pressure.[3]

Giving the background, the aim of this work is firstly a completely study of microcrystalline cellulose pyrolysis; secondly, the synthesis of hydrolysis and dehydration products (HMF and levulinic acid) of carbohydrates present in agro-food wastes such as melon rind and brewer´s spent grain under microwave radiation and thirdly, the synthesis of bio-oil from brewer´s spent grain by microwave-assisted hydrothermal liquefaction process. Finally, the study of the emissions of these synthetized compounds was carried out to know the emitted compounds and to value the environmental benefits of these products.

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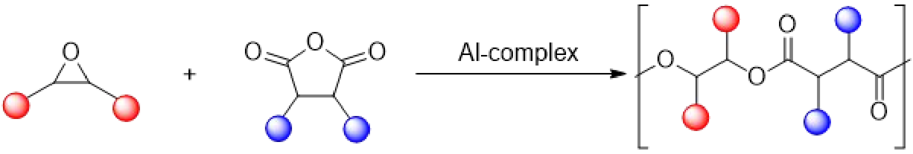
RING-OPENING COPOLYMERIZATION OF CYCLIC ANHYDRIDES AND EPOXIDES CATALYSED BY ALUMINIUM HETEROSCORPIONATE COMPLEXES

Marc Martínez de Sarasa Buchaca

Polyesters are materials produced on a 50 million tonne scale, annually.[1] During the last few decades, a compelling growth of interest in polymers from renewable resources has emerged within the scientific and industrial communities.[2] Aliphatic polyesters, are biodegradable and often, biocompatible, and have multiple applications ranging from bulk packaging to biomedical devices while semiaromatic polyesters, are used within the packaging industry and as liquid crystalline polymers.[3,4] The most promising reaction for the synthesis of this materials is the Ring-Opening Copolymerization (ROCOP) of epoxides and cyclic anhydrides (Scheme 1).

In this work, we report the ROCOP of epoxides and cyclic anhydrides catalysed by organometallic aluminium complexes with a range of co-catalysts. A variety of bio-derived polyesters have been synthesized and fully characterized including a new one which has not been previously reported, limonene succinate.



Scheme 1

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ELECTROCHEMICAL ACTIVATION OF CATALYSTS FOR HYDROGEN PRODUCTION

Estela Ruíz López

Hydrogen is one of the most accepted alternative fuels due to its energetic efficiency and methane steam reforming has been wide used for its production[1]. However, it entails distribution, transport and gas storage difficulties that could be minimized by using a liquid compound. Additionally, the overproduction of bioalcohols due to the legal support has pointed out bioethanol as an interesting replace to the methane for H_2 production. Likewise, the phenomenon of electrochemical activation or promotion of catalysts, known as EPOC, is based on the promotion of catalytic active sites due to the migration of ions to the catalyst film when different potentials are applied. Moreover, it allows to control in a continuous and reversible manner the addition of promoters to the catalyst under reaction conditions.

In this work, the EPOC phenomenon has been studied for the catalytic steam reforming of ethanol. For that purpose, a Pt-$K\beta Al_2O_3$ electrochemical catalyst schemed in Figure 1 a) has been prepared, characterized and tested under reaction conditions. As shown on Figure 1 b), higher reaction rates were obtained by the application of electrical potentials lower than 0 V. At these potentials, the ions K^+ are transferred to the catalyst surface, enhancing the dehydrogenation of ethanol to acetaldehyde, which in a further step reacts with water to yield H_2 and CO_2, thus increasing the H_2 production rate in almost 5 times vs. the un-promoted state. It has been supported by TPO, Raman and SEM-EDX analysis performed after the different polarizations. Furthermore, very interesting, additional experiments have shown the possibility of the catalyst regeneration during the positive polarization steps.

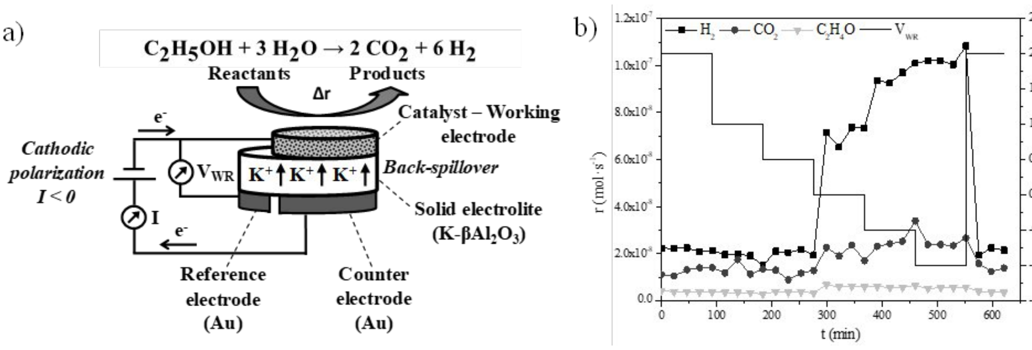

Figure 1.a) Scheme of the electrochemical cell used. b) H_2, CO_2, $C_4H_{10}O$, C_2H_4O production rates vs time under different applied potentials. ESR conditions: H_2O/C_2H_5OH = 9 %/3 %, T = 450 ºC.

ANALYSIS OF GOLD NANOPARTICLES USING INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY VIA SINGLE PARTICLE (SP-ICP-MS) IN CLINICAL SAMPLES

Sergio Fernández Trujillo

Nanotechnology is currently a field of an utmost importance to the scientific community. Metallic nanoparticles, especially, gold nanoparticles (AuNPs) have emerged as biological targets in several applications such as therapy, biosensors and drug delivery in pharmaceuticals and biomedical research due to their unique physicochemical and optical properties. Despite their benefits, there are serious concerns about their potential harmful effects on human health. For these reasons, it is necessary to develop new analytical methodologies for the assessment of the risks associated to NPs in clinical studies.

Single particle-inductively coupled plasma-mass spectrometry (SP-ICP-MS) is an emerging analytical tool to face new challenges for the detection and characterization of NPs in biological fluids. SP-ICP-MS offers substantial advantages for detecting NPs, which involves the determination of size distribution, chemical composition and/or concentration [1].

The objective of this study has been to develop a new analytical method based on the use of SP-ICP-MS for the identification and characterization of AuNPs. The applicability of the method to clinical samples was evaluated in cell culture medium. This methodology allows the characterization of AuNPs of different sizes in complex media which enables the correct interpretation of biological and toxicological tests.

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SCREEN-PRINTED ELECTRODES USED FOR THE DETERMINATION OF DRUGS

Isabel Lizcano Sanz

Screen-printed electrodes (SPEs) are disposable sensors based on the screen-printing technology. They are constructed by printing several types of inks on different ceramic or plastic substrates. The main advantages of these electrodes are related to their operation simplicity, reliability, potential portability, small instrumental setups comprising the reference, working, and auxiliary electrodes, and modest cost. Furthermore, the same electrode surface can be safely used for successive analyses.

The most commonly used pastes are carbon, silver, and gold inks. Carbon paste is preferred over the gold paste as it is inexpensive, chemically inert, adaptable, and easily modifiable.

Drug determination is an important field of analytical chemistry. Consequently, developing accurate, reliable, rapid, and economic methods for quantitative determination of drug in biological fluids is important.

A sensitive square wave voltammetry (SWV) method at screen-printed carbon electrodes has been developed to determine imatinib in human urine using prepared multi-walled carbon nanotubes modified with carboxyl groups (MWCNT-COOH) as working electrode. Quantitative analysis was carried out through its oxidation process at + 0.7 V, pH 7 and accumulation time of 120 s. The SWV method was linear in the range 50 nM - 912 nM.

The method was successfully applied for the determination of imatinib in real clinical urine samples from patients with chronic myeloid leukemia.

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EFFECTS OF SEEDS AND STEMS GRAPE BY-PRODUCTS EXTRACTS AND COLLOIDAL SILVER AS ALTERNATIVE PRESERVATIVES ON WHITE WINE

Lucía Loarce Ortíz

Sulfur dioxide is one of the most used preservatives in wine industry for its powerful antioxidant and antimicrobial activity. Particularly, the use of sulfur dioxide is essential for the production of white wines to avoid oxidation reactions, which entail browning and chemical composition changes in detriment of its sensorial quality. But in turn, it is well known the existence of allergies due to this compound and the production of defects in wine organoleptic characteristics. Therefore, alternatives to the use of sulfur in winemaking are being found and one of them is the use of grape by-products as preservatives due to their already proven antioxidant and antimicrobial activity. In this sense, the objective of this work was the evaluation of extracts from grape seeds and stems of Vitis vinifera L. cv. Tempranillo solely or in combination with colloidal silver as substitutes of sulfurous in winemaking. To carry out the essay, the effects of the extracts on physical-chemical and sensory characteristics of white wines were evaluated.

Wines were elaborated with the addition of 0.5 g/L of seeds and stems extracts, and 1 g/L of colloidal silver. In parallel, wines with SO_2 were also elaborated and used as “control”. The use of extracts and sulfurous had a similar effect against the microbial growth, observing some inhibition effects in wines with colloidal silver. Wines with seeds extracts showed higher antioxidant activity and content of catechins and flavonols. Regarding to the volatile fraction, the addition of extracts produced an increase in acids, esters and some benzenic compounds, while the absence of sulfur caused a decrease in acetaldehyde. To sum up, the use of these natural extracts as a substitute for sulfur dioxide seems to be potentially applicable in wine industry.

COMUNICACIÓN ORAL

NUCLEAR MAGNETIC RESONANCE SENSITIVITY ENHANCEMENT COMBINING MINIATURIZED COILS AND HYPERPOLARIZATION TECHNIQUES

Rosa María Sánchez Donoso

Nuclear Magnetic Resonance (NMR) is a powerful tool which gives information about molecular structures or reaction mechanisms among other applications, but it suffers from an intrinsic low sensitivity. The use of miniaturized coils[1] (microcoils) are a good approach to tackle mass-sensitivity issues. Alternatively, hyperpolarization schemes have been devised to overcome concentration-sensitivity limitations. Here, we present the combination of solenoidal microcoils with photo-chemically induced dynamic nuclear polarization[2] (photo-CIDNP), resulting in an surprising boost of sensitivity, pushing the limit of detection down to sub-picomole amounts of material at moderate (9.4 T) B_0 fields.

Moreover, this novel set up overcomes the main photo-CIDNP drawbacks. For instance, we work under continuous flow conditions, which avoid accumulation of photodegraded flavin in the detection region. In addition, we show that our system enables rapid and efficient, in-situ mixing of sample components, which opens new avenues for more sophisticated applications.

To sum up, the present work not only rekindles the realm of the photo-CIDNP technique, but also illustrates the potential of microcoils as an alternative to cryoprobe technologies and the use of higher magnetic fields[3].

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GAS PHASE KINETICS AT TEMPERATURES OF THE INTERSTELLAR MEDIUM

Sergio Blázquez González

Although the interstellar medium (ISM) is a harsh environment full of energetic particles and photons, it has been recognized for a long time that molecules, even complex, could survive inside particular areas known as interstellar clouds. The development of radioastronomy revealed an unsuspected richness of species, currently, around 200 most of them organic molecules, like ethanol (CH_3CH_2OH) detected in 1975 by Zuckerman et al. in Sagittarius B2. The interpretation of the observed abundances of these species in ISM requires a large amount of kinetic and photochemical data (Jiménez et al, 2015). The kinetics of the reaction between ethanol (CH_3CH_2OH) and hydroxyl (OH) radical between 21 and 107 K is the objective of this work. To achieve ISM temperatures (10 – 100K) the pulsed and continuous CRESU (French acronym for Cinétique de Réaction en Ecoulement Supersonique Uniforme) technique has been used. This technique involves the isentropic expansion of a gas passing through a Laval nozzle, separating a high pressure volume from a low pressure chamber. This expansion provides a supersonic jet with an isentropic core, where very low and constant temperature and pressure are maintained along a certain distance from the nozzle exit to the detection zone (typically 20-30 cm). The gas phase reaction under study takes place in this uniform supersonic jet.

The obtained T-expression in this temperature range is:
$k(T = 21 – 107\ K) = (2.1 \pm 0.5) \times 10^{-11}\ (T/300\ K)^{-(0.71 \pm 0.10)}\ cm^3\ molecule^{-1}\ s^{-1}$

In this work, we present for the first time the pressure and temperature dependence of the rate coefficients for the CH_3CH_2OH + OH reaction at temperatures below 54 K. No evident pressure dependence of k(T) was observed in the gas density range investigated between 21 and 107 K (Ocaña et al, 2018).

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INFLUENCE OF DEHYDRATION PROCESS ON FLAVONOL PROFILE OF SEEDLESS GRAPE CULTIVAR BRS VITÓRIA (CNPUV 681-29 X BRS Linda)

Carolina Olivati

Among the dehydrated fruits consumed all over the world, raisins are one of the most important due to their high consumer acceptance. Moreover, grapes are considered an important source of compounds that claim functional properties as the phenolic compounds. On the other hand, the drying process to obtain the raisins can degraded these compounds. In Brazil, the Brazilian Agricultural Research Corporation (EMBRAPA) had developed among the past years various seedless grapes cultivars that can be used for the elaboration of raisins, such as BRS Vitória grape. Aiming knowing more about the potential health benefits of raisins, the study of the drying process effects on the phenolic compounds is appropriate. Thus, this research aimed evaluate the qualitative changes on flavonol profile in raisins produced from BRS Vitória (CNPUV 681-29 x BRS Linda) cultivar after dehydration in a drying oven with forced air convection (60ºC), with and without application of olive oil as pre-treatment, in order to accelerate the dehydration process and improve the raisin quality.

The grape and its raisins showed a flavonol profile covering the glucoside of the six principal flavonols aglycones (Myricetin, Quercetin, Laricitrin, Kaempferol, Isorhamnetin and Syringetin). After the drying process, regardless, a processing time reduction of 38% for the pre-treated raisins, no difference was found in flavonol profile between the two raisins produced. However, in comparison with the fresh grape, the Myricetin glucuronide and galactoside were degraded in the raisins and quercetin free aglycone had appeared. These changes on the flavonol profile had occurred during the dehydration process probably due to thermal degradation and oxidation by endogenous polyphenoloxidases, since the temperature used in the process was not very high. The quantification of the flavonols present in the fresh grape and its raisins is being carried out to clarify how the drying process affected the flavonol profile.

SCHWARZ DOMAIN DECOMPOSITION METHOD APPLIED TO THE INCOMPRESSIBLE NAVIER-STOKES EQUATIONS WITH BOUSSINESQ APPROXIMATION

Ana Fernández Pérez

The aim of this work is to present a theoretical and numerical study of the Schwarz domain decomposition method, based on Legendre collocation spectral methods, in order to solve a two-dimensional Rayleigh-Bénard convection problem. This convection problem is modelled by the incompressible Navier-Stokes equations together with the heat equation, using the Boussinesq approximation. The problem is defined in a rectangular domain, which is divided into two subdomains. The solution is calculated using suitable transmission conditions at the interface between the subdomains considered. It is also important to highlight that depending on the nature of the decomposition, it can be distinguish overlapping and nonoverlapping methods. We focus in the one who includes overlap. According to the numerical resolution, we employ a second order time discretization scheme. In each temporal step, a Schwarz domain decomposition method is used to solve the problem in both subdomains. It could be pointed out that one of the interests of considering this domain decomposition technique resides in the shape of the domain that it is going to be considered. Using Legendre polynomial approximation is straightforwardly related with the domain, since this technique requires a rectangular domain. Therefore domain decomposition will be very helpful when our domain it is not a rectangle, but it can be decomposed into rectangular subdomains.
The theoretical convergence study of the decomposition method is done with a Fourier technique (Blayo, Cherel, & Rousseau, 2016), and the numerical approach is similar to the stationary problem solved in (Herrero, Pla, & Ruiz-Fernández, 2018), although with the pertinent adjustments to the temporal approach that is going to be taken into account in this work.

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COMUNICACIÓN ORAL

PHOTO-CIDNP: A TOOL FOR IN-SITU MONITORING OF STRUCTURAL CHANGES IN PROTEINS

José Miguel Mateo González

Photo-chemically induced dynamic nuclear polarization (photo-CIDNP) Nuclear Magnetic Resonance (NMR) spectroscopy is a hyperpolarization technique that allows the investigation of solvent-accessible amino acids in proteins.[1] Some amino acids, especially those that present aromatic side chains, are responsible for most of the interactions that take place between proteins and other molecules. In the presence of a photosensitizer and under light irradiation, the NMR signal intensities of these residues are enhanced, reflecting which amino side chains are either exposed or buried to the solvent, and thus facilitating the structure elucidation of the protein for a specific experimental conditions.

Therefore, we use photo-CIDNP NMR spectroscopy to study the structural transition of the LytA239-252 peptide, a fragment of the LytA autolysin that switches between β-hairpin and α-helix conformations upon micelle-modulated interactions,[2] a structural change that is considered a key step in biological processes and degenerative diseases.[3,4]

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OPERATING MEMBRANE ELECTROLYTIC TECHNOLOGY FOR THE DIRECT DISINFECTION OF HIGHLY FECAL-POLLUTED WATER

Julia Isidro Elvira

Disinfection is probably the core stage of a typical treatment scheme for surface water supplies. It is important to note that disinfection using electrochemical technologies emerges as an environmentally friendly, economically and operationally competitive technology to be applicable against a wide range of microbiological contamination[1]. Thus, powerful oxidants such as chloride, sulfate, phosphate or carbonate compounds generated by direct electrolysis can attack microorganisms without adding additional chemicals. Likewise, the cathodic production of hydrogen peroxide and the formation of other oxidants such as ozone helps to improve the disinfection. Among the different electrode materials, the bored doped diamond (BDD) has shown remarkable properties in water disinfection but, unfortunately, it can lead to the formation of undesirable chloro-species, which have a possible carcinogenic effect on human health.

Taking this into account, the present work studies the efficiency of the CabECO® electrochemical cell, for the direct disinfection of surface water. Electrolysis tests were carried out galvanostatically at current densities ranging from 0.0 to 833.3 A m^{-2} in discontinuous mode and from 416.7 to 1666.7 A m^{-2} in continuous mode. During the test it was monitored the concentration of total coliforms, pseudomonas aeruginosa, total aerobic microorganisms, total organic carbon, trihalomethanes (THM) and ionic species (including chloro-especies, sulfate, nitrate, ammonium…).

Results show that CabECO is a very efficient technology for disinfection regardless of the operation mode used, although efficiency depends strongly on the applied current density. The higher the current density, the higher is the rate of disinfection. Different conditions are required to disinfect and to remove TOC, being more exigent the removal of organics. A positive point is that organochlorinated species were not detected (detection limit of 6 ppb). Besides ozone produced in the cell, chlorinated species are formed and they generate persistent disinfection. The formation of chlorate and perchlorate can be minimized by working at low current density and continuous mode.

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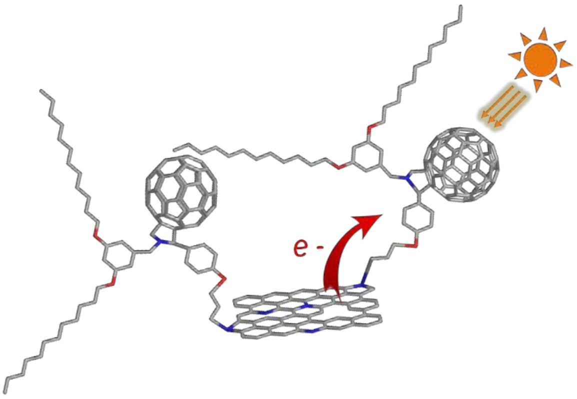
LINKING FULLERENE C_{60} ON N-DOPED GRAPHENE SURFACE. SYNTHESIS AND CHARACTERIZATION

Luis Miguel Arellano Castellanos

Graphene, one of the most relevant materials along the last decade, has attracted massive attention due to their unique properties, like mechanical resistance and good stability under chemical and thermal treatments [1]. Unfortunately, the absence of an electronic band-gap and its extreme chemical inertness significantly compromise their use as an active element in electronic devices; the introduction of dopants onto graphene layer via substitutional doping is one of the most feasible methods to tailor its electronic properties, which makes able graphene as a new interesting material for a great number of technological applications [2].
Recently, in our research group, we reported an efficient method to functionalize N-doped graphene by N-alkylation, demonstrating the influence of the electronic properties of the anchored group for the modulation of the band gap of the material [2]. With this aim, in this communication, we present herein our results on the synthesis and the study of the electronic properties of new nanohybrid involving N-doped graphene and fullerene C_{60} unit using N-alkylation reaction.



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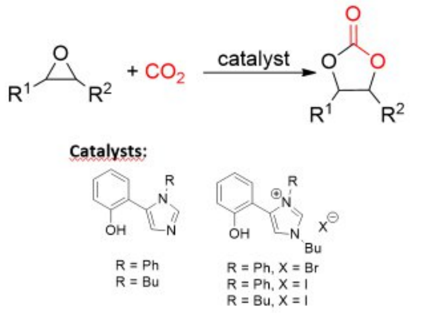
DEVELOPMENT OF HYDROXY-CONTAINING IMIDAZOLE ORGANOCATALYSTS FOR CO_2 FIXATION INTO CYCLIC CARBONATES

María del Prado Caballero Espinosa

Highly efficient neutral and ionic imidazole-based organocatalysts have been developed for the synthesis of cyclic carbonates from epoxides and carbon dioxide (Scheme 1).[1] The ionic derivates performed as bifuncional catalysts and exhibited improved activity for the fixation of CO_2 compared to the neutral compounds. Mechanistic studies revealed that the hydroxyl group promoted the activation of the epoxide ring by nucleophilic attack of the iodide.[2]



Scheme 1. Synthesis of cyclic carbonates.

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COMUNICACIÓN
ORAL

CHEMISTRY OF SECONDARY ORGANIC AEROSOL FORMATION FROM THE PHOTOLYSIS AND OXIDATION OF ALPHAMETHYLSTYRENE WITH HYDROXYL RADICAL

María Mercedes Tajuelo Díaz-Pavón

Ambient aerosol can adversely affect human health, atmospheric visibility and the climate. Aerosols are generally classified as primary and secondary according to their formation processes. The secondary organic aerosol (SOA) is a key component in secondary aerosols and accounts for as much as 50% of the total aerosol mass. For most atmospheric volatile organic compounds (VOCs), reaction with the hydroxyl radical (OH) is the principal step initiating the mechanism to SOA formation. Initial reaction products may, themselves, react further with OH, leading eventually to the suite of semivolatile and nonvolatile products that constitute SOA.

The formation and composition of SOA generated by irradiating α-methylstyrene (AMS) in the presence and/or absence of OH, water vapour, oxides of nitrogen (NO_x) and seed particle has been investigates for the first time. The AMS is a VOC with abundant anthropogenic sources released into atmosphere from activities such as petroleum refining, food industry and motorized vehicles.

Experiments were performed in a smog chamber at 298 K and atmospheric pressure. The temporal evolution of the aerosol was monitored using a Fast Mobility Particle Sizer (FMPS) spectrometer was used to measure of SOA, the AMS concentration was monitored by using gas chromatography-mass spectrometry (GC-MS), the NO_x evolution was followed by a chemiluminescence analyzer and the seed aerosols were generated by aspirating aqueous solution through an atomizer (TSI 3076). Finally, the particle composition was analyzed offline using a filter/denuder sampling system (UGR-2000-30FG) which simultaneously collecting gas and particle-phase products.

The aim of this study was to determine the extent to which the SOA yield was affected by presence and/or absence of OH radical, water vapour, NO_x and seed aerosols as previously mentioned. In addition, the particulate products of the α-methylstyrene SOA were obtained, and the possible reaction mechanisms leading to these products will be also discussed.

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USE OF CAPILLARY ELECTROPHORESIS FOR CHARACTERISATION OF VINYL-TERMINATED GOLD NANOPRISMS AND NANOOCTAHEDRA

Carlos Adelantado Sánchez

It is described a simple, rapid and efficient methodology to characterise and separate gold nanoprisms and nanooctahedra by capillary electrophoresis. This technique is suitable to distinguish between morphologies and it can be used as a powerful separation tool after a customised synthesis of both structures [1]. This synthesis was carried out by amending two parameters, temperature and pH, and a sharp decrease was found in nanotriangles when temperature was increased from 70 up to 95ºC. However, when the synthesis was performed at a given temperature, an increase in pH did not promote an important change in isolation of any structure until pH=9.5, critical in the final morphology of the nanoparticle. Gold nanoprisms and nanooctahedra were successfully separated by capillary electrophoresis according to differences in charge-to-mass ratio of the morphologies. Final particle morphology was confirmed by transmission electron microscopy analysis. Under optimal working conditions, a mixture containing both shapes of gold nanoparticles was initially injected and two major peaks were obtained for each structure. Capillary electrophoresis allowed to study pH and temperature influence on both morphologies. It was inferred that the ratio between triangles and octahedra decreased to a great extent when increasing both temperature and pH. To the best of our knowledge, all reports involving gold nanoparticles and capillary electrophoresis are focused on the separation of gold nanoparticles and their conjugates by their sizes [2]. This study describes characterisation and separation of gold nanoparticles by shapes for the first time.

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COMUNICACIÓN
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IONIC LIQUIDS FOR EXTRACTION AND PRECONCENTRATION OF CORTISOL AND CORTISONE FROM SALIVA

Feras Abujaber

Cortisone and cortisol are the major steroid hormones secreted from the adrenal glands. Recently, they have been considered as a biomarker of psychological stress and levels may be related to mental or physical disease. The determination of cortisone and cortisol in saliva is easy and the sample collection is non-invasive compared to other biological fluids.

In recent years, liquid chromatography (LC) coupled to tandem mass spectrometry has emerged as the technique of choice for the determination of steroid hormones because it offers high selectivity. Despite its benefits, this technique is sophisticated, expensive and does not avoid sample preparation. LC with ultraviolet-visible (UV/vis) detection is a feasible approach after sample preparation to reach typical salivary cortisone and cortisol levels. Among sample preparation techniques, dispersive liquid–liquid microextraction (DLLME) provides several advantages over conventional extraction techniques, such as rapidity, ease of operation, high recovery and enrichment factor [1]. Moreover, the use of ionic liquids (IL) instead of organic solvents gives to a more environmentally friendly approach.

In this work, IL-DLLME method for the extraction of cortisone and cortisol from human saliva samples was developed for the first time. The extracts were analyzed by LC-UV/vis. Limits of detection were 0.11 (cortisone) to 0.16 (cortisol) µg L^{-1}. Adequate enrichment factors and quantitative recoveries in spiked saliva samples in a short time were obtained.

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COMUNICACIÓN
PÓSTER

PROTECTIVE EFFECTS OF BEER COMPOUNDS IN C6 GLIOMA AND SH-SY5Y NEUROBLASTOMA CELLS

Patricia Alonso Andrés

Alzheimer and Parkinson are the main neurodegenerative diseases in the elderly. Together with these pathologies, cancer and cardiovascular diseases constitute the major challenge in our society. Although causes of Alzheimer and Parkinson diseases are unknown, excitotoxicity and oxidative stress seem to be involved. However, a good nutrition and the intake of several nutrients have showed beneficial effects and they can reduce the probability of developing these pathologies or slow down its progression. Moderate consume of alcoholic drinks, like wine or beer, have benefit effects in cancer or cardiovascular diseases. However, there are few studies about beer consume and neurological diseases. Benefits of beer can be due to the wide kind of compounds present in this beverage as antioxidants, polyphenols or flavonoids. Previous results of our group have shown altered levels of receptors implicated in memory and neuromodulation, as metabotropic glutamate (mGluRs) or adenosine receptors (AdoRs). In Alzheimer disease, mGluRs are decreased with the illness progression while AdoRs are increased since early stages which are asymptomatic. For this reason, these receptors and other related metabolites have been studied in two cellular models, C6 glioma and SH-SY5Y neuroblastoma cells which have been subjected to different insults related to AD (oxidative stress, excitotoxicity..) and the effect of beer (extract of beer, hop and polyphenols) was studied. Viability results show cell death due to these insults and a recovery of life cells after beer exposure. On the other hand, gene expression of receptors which are altered in AD was modified in cells after treatment with beer. These results demonstrate a protective effect of beer in these cell cultures and the ability of beer to modulate the expression of these GPCRs, suggesting that a moderate consume of beer could be protective versus oxidative stress and other factors associated to neurodegeneration.

GEMCITABINE-IMPREGNATED PLGA SCAFFOLDS PROCESSED WITH SUPERCRITICAL CO_2

Irene Álvarez Lara

The use of controlled delivery systems reduces the undesirable and toxic effects produced by conventional drug administration. They are made up of biodegradable polymers capable of incorporating drugs into their structure.

Production of polymeric foams or scaffolds is carried out at temperatures above the melting point of the polymer to increase the mobility of its chains, but this can lead to degradation of the polymer itself and the drug. On the other hand, when foaming is carried out from polymer solutions, the coil expands and behaves like a molten polymer[1]. In this context, the use of supercritical fluids, specifically $scCO_2$, allows the total elimination of solvent residues on polymeric scaffolds[2]. This is the best alternative to avoid thermal degradation of the compounds and reduce energy consumption.

Therefore, the objective of this research is the synthesis and impregnation of polymeric foams with a drug using $scCO_2$. The polymer used was poly (lactic - co - glycolic acid) (PLGA). The solvent used is Ethyl Lactate, a "green" solvent approved by the FDA for use in the food and pharmaceutical industry. Gemcitabine, a chemotherapeutic agent used in the treatment of various types of cancer such as lung and pancreatic cancer, has been selected as the drug[3].

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TROPOSPHERIC REACTIVITY OF 3-ETHOXY-1-PROPANOL

María Inmaculada Aranda Díaz-Lucas

Glycol ethers are used in paints, coatings, inks, cleaners and polished and in blends with diesel fuel polished (Gómez-Cuenca et al, 2011). They are also emitted to the atmosphere during the combustion of diesel/biodiesel blends (Fisher and VanPeppen, 2001). In this work, rate coefficients for the reactions of OH and NO_3 radicals, and Cl atoms, with 3-ethoxy-1-propanol have been determined using a relative rate technique with FTIR (Fourier Transform Infrared Spectroscopy) as detection system. Relative rate coefficients obtained were (units cm^3 $molec^{-1}$ s^{-1}): $(3.4\pm0.2)x10^{-10}$, $(3.4\pm0.1)x10^{-11}$ and $(1.6\pm0.1)x10^{-14}$ for Cl, OH and NO_3 reactions respectively. Experiments were developed using at least three reference compounds. As an example, Figure 1 shows the relative kinetic data plotted for Cl reactions with 3-ethoxy-1-propanol with two reference compounds. Qualitative product analysis for Cl reaction in the presence of NOx was determined using FTIR and GC-MS (Gas Chromatography/Mass Spectrometry) obtaining carbonyl compounds such as ethyl formate and formaldehyde as the main products. These results suggest a mechanism involving initial Cl attack at the methylene groups followed by the subsequent reactions of the resulting radicals. Tropospheric lifetimes calculated for Cl, OH and NO_3 suggest that the dominant loss process for 3-ethoxy-1-propanol is the daytime reaction with the OH radical.

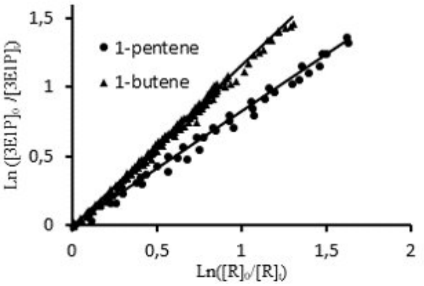

Figure 1. Relative rate plots for the reaction of 3-ethoxy-1-propanol (3E1P) with Cl atoms using two reference compounds

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COMUNICACIÓN PÓSTER

IONIC LIQUID AND MAGNETIC NANOPARTICLES FOR EXTRACTION OF CARBAMATE PESTICIDES FROM WATER SAMPLES PRIOR THEIR DETERMINATION BY CAPILLARY ELECTROPHORESIS

Jihane Ben Attig

A rapid and simple method for the extraction of six N-methylcarbamate pesticides (carbaryl, carbofuran, isoprocarb, promecarb, BDMC and methomyl) in water samples was developed. The procedure is based on temperature controlled ionic liquid dispersive liquid phase microextraction and magnetic nanoparticles combined with capillary electrophoresis. In this method, no centrifugation separation step was involved. Some parameters that affected the extraction efficiency such as type and volume of extractant solvent, temperature, sample volume and extraction time were investigated in order to found the optimal extraction conditions.

RAPID SAMPLE SCREENING METHOD FOR AUTHENTICITY CONTROLLING VANILLA FLAVOURS USING LIQUID CHROMATOGRAPHY WITH ELECTROCHEMICAL DETECTION AT ALUMINIUM DOPED ZIRCONIA NANOPARTICLES-MODIFIED ELECTRODE

Yassine Benmassaoud

Considered a major flavoring product, natural vanilla faces many frauds. Thus, several analytical methods have been optimized in order to determine its chemical constitution. Moreover, the use of screen-printed electrodes as electrochemical sensors capable of detecting several compounds in numerous sectors have significantly increased over last years due to their high selectivity, reproducibility, low-cost production, simple modification surface and the increasing miniaturization challenge. In the present work, a screen-printed carbon electrode (SPCE) was modified using a composite film of AlO_2 nanoparticles doped with Zr (Zr/AlO_2NPs) in the aim of providing a high sensitive and selective electrochemical sensor for the amperometric quantification and detection of adulterations in vanilla flavors. Zr/AlO_2NPs were synthetized and characterized by X-ray diffraction. SPCE was then modified using an optimal volume of Zr/AlO_2NPs and compared with non-modified SPCE by cyclic voltammetry on dopamine. Further, the home-made sensor was employed for the development and validation of a new analytical method using high pressure liquid chromatography with amperometric detection of six phenolic compounds of vanilla flavors namely; vanillin, p-hydroxybenzoic acid, p-hydroxybenzaldehyde, vanillyl alcohol, vanillic acid and ethyl vanillin. The proposed method allowed the quantification of vanilla compounds at 0.5- 10 mg/L linear range. The limit of detection, limit of quantification and relative standard deviations were inferior to 0.14 mg/L, 0.48 mg/L and 4.76%, respectively. The natural origin of real samples was finally investigated by discriminating the vanilla phenolic compounds where several cases were obtained and discussed.

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GRAPE SEED OIL EPOXIDATION IN SUPERCRITICAL CO_2

Juan Catalá Camargo

Castilla La-Mancha has one of the largest wine industries in the world. Approximately 100,000 tonnes of grape seed oil per year are obtained as a by-product from solvent extraction or pressing.

This oil can be functionalized easily, due to its high content of unsaturated fatty acids, transforming its double bonds into different functional groups, thus becoming a potential raw material for a multitude of bioproducts. In particular, epoxy-vegetable oils are one of the main intermediates in the production of lubricants, plasticizers and non-isocyanate polyurethanes (NIPU).

The most widely used epoxidation method is based on the use of peroxides formed in situ from traditional solvents, such as acetic or formic acids. However, the possibility of carrying it out without the use of these solvents is recently explored, thanks to the formation of peroxycarbonic acid, from the reaction between supercritical CO_2 and H_2O_2.

In this work, the supercritical epoxidation of grape seed oil is carried out mainly at 150 bar, 40ºC and 15h. The influence of the quantity and type of additives (such as phase transfer catalysts, PTC) and pressure on the conversion and selectivity of the obtained product is studied.

The results obtained show yields similar to those observed in the literature for supercritical epoxidation of soybean oil and represent an important advance in the development of a safer, and more sustainable method of vegetable oil epoxidation.

A DIRECT SCREENING OF AgNPs FROM DECORATION OF PASTRY

Ana Isabel Corps Ricardo

Metallic silver as a food additive (E174) is authorized by the European Commission to be used in the external coating of pearls meant for decoration of pastry [1]. These silver coated pearls can release silver as ions and eventually, as nanoparticles (AgNPs) and the subsequent exposure to the consumer may cause health risks [2]. At present, the use of AgNPs in food is not regulated, but it is important to develop methods that cover future needs for qualitative and/or quantitative information about AgNPs in food. Current analytical methods provide a lot of information (i.e. number, mass concentration, size range) with high sensitivity and selectivity. However, the information needs are often much less demanding. Screening methods, which are based on a binary response, are rapid, simple, cost-effective and they are a valuable option for this purpose. Nevertheless, to our knowledge, no screening methods for AgNPs have been reported so far.

The aim of this work is to develop an instrumental screening method of AgNPs in different type of silver coated pearls meant for decoration of pastry based on the enhanced chemiluminiscence of the luminol/ $AgNO_3$ in the presence of AgNPs in alkaline media. Limits of detection were around 1 µg L^{-1} of AgNPs and the unreliability zone was between 0.07 and 2.58 µg L^{-1}. Several samples were used for the final demonstration of the reliability and usefulness of the method.

References:

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EFFECT OF HYPERTHERMIA-INDUCED SEIZURES ON MOTOR COORDINATION AND GAIT IN BOTH ADOLESCENT AND ADULT RATS

María Crespo Gutiérrez

Febrile seizures (FS) is one of the most common convulsive disorders in infants and young children that only occurs in children between 3 months and 6 years-old, when the cerebellum is still developing.

In the present work, we have analyzed the consequences of febrile seizures on motor coordination and gait from adolescent and adult rats using balance beam and footprint test. In balance beam test motor coordination and balance were analyzed by measuring the ability of the rat to traverse a graded series of narrow beams to reach an enclosed safety platform in balance beam test. On the other hand, footprint test was used to compare the gait in different rats. The hind- and forefeet of the rats were inked with orange and pink nontoxic paints, respectively, and the rats were allowed to walk along a 50-cm-long, 10-cm-wide runway (with 10-cm-high walls). The footprint patterns were analysed in terms of the following parameters: a) stride length that represent the average distance of forward movement between each stride; b) Hindpaw and forepaw base that correspond to the average distance between left and right hind footprints and left and right front footprints and c) forepaw/hindpaw overlap, the distance between forepaw and hindpaw print, was used to measure uniformity of step alternation.

Results obtained have shown that in adolescent rats the time required to cross the 18 mm-round section and 12 mm-round section beam were significantly higher in hyperthermic group than in control animals. Similar results were obtained in adult rats when 35 mm-square section was used. Concerning footprint test, forepaw/hindpaw overlap resulted significantly higher in adolescent rat whereas stride lenght, forepaw and hindpaw base were altered in adult rats exposed to HIS.

We conclude that hyperthermia-induced seizures evoked fine motor coordination impairment and gait disturbances in both adolescent and adult rats.

TRANSFORMING THE NON-EXPENSIVE LIGNIN INTO A HIGH-ADDED VALUE BIOPOLYOL

Juan Carlos de Haro

The non-expensive natural lignin, which is the second most abundant natural polymer, is an amorphous, highly branched, and irregular three-dimensional phenolic polymer (Figure 1). The annual production of lignin is around 72 million tons produced mainly as a by-product of the paper industry. This material is used as fuel for power generation and only a 2% of the lignin is usually used as raw material to obtain higher-added value products. However, due to its structure, lignin could be a good source of biopolyols to produce polyurethane foams (PUF).

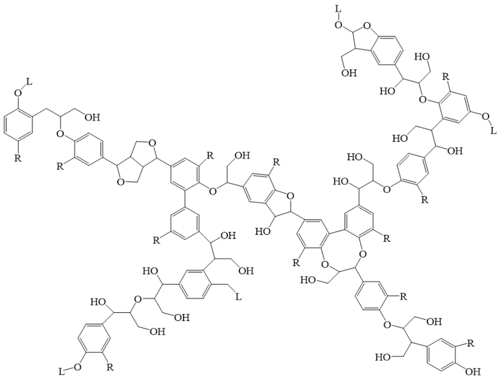

Figure 1. Chemical structure of lignin

Different methods have been proposed in literature for obtaining the biopolyols such as acid/basic depolymerization, sub- and supercritical hydrolysis, oxidation in presence of H_2O_2 and liquefaction. From these techniques, lignin liquefaction in presence of PEG400 and glycerol have received a great attention due to its low operating temperature and pressure. Hence, the main object of this work is the obtention of a lignin-based biopolyol that could be suitable for the synthesis of rigid PU foams (RPUF). The influence of reaction temperature (90-150 ºC), the reaction time (up to 8h) and the mass ratio lignin/glycerol/PEG400 was studied. As a result, a biopolyol having a hydroxyl number and a molecular weight of 630 mg KOH/g and 4400 g/mol, respectively, was obtained. The polyol yield was >99% and using this polyol was possible to produce RPUF substituting up to a 50% of traditional petroleum-based polyols by lignin-based ones without modifying the internal structure of the RPUF.

KINETICS OFTHE ATMOSPHERICALLY RELEVANT GAS-PHASE REACTIONS OF ALLYL CYANIDE

Rafael del Olmo Martínez

Allyl cyanide was found in 1863 in mustard oil and since then, it has also been detected in cruciferous vegetables such as cabbage, broccoli, cauliflower and sprouts, being its production higher when the leaves of these vegetables are damaged. (L. G. West et al., JAFC, 25, pp. 1234-1238 (1997); H. Tanii et al., FCT, 42, pp. 453-458 (2004)) Moreover, allyl cyanide is one of the nitriles widely used in the manufacture of plastics, solvents, and synthetic intermediates. In fact, thermal degradation of acrylonitrile-based plastics leads to the emissions of a large variety of nitriles, including allyl cyanide. (M. M. Shapi et al., JCB, 562, pp. 681-696 (1991)) Therefore, allyl cyanide may be released into the atmosphere from both biogenic and anthropogenic sources and it is important to now its reactivity towards the different tropospheric oxidants.

The aim of this work is to determine the rate coefficients and reaction products of the gas-phase reactions of ally cyanide with tropospheric oxidants, such as chlorine (Cl) atoms, hydroxyl (OH) radicals, and ozone (O_3). An atmospheric simulation chamber has been used for the study of the proposed reaction at 298 ± 2 K and 760 ± 5 Torr under free-NOx conditions. A relative kinetic method has been employed in which Fourier transform infrared spectroscopy (FTIR) has been used as quantification technique of allyl cyanide and the reference compound (cyclohexane or ethanol). (A. A. Ceacero-Vega et al., JPCA, 116, pp. 4097-4107 (2012)) FTIR and gas chromatography-mass spectrometry coupled to solid phase micro-extraction (GC-MS/SPME) have been used to detect and quantify, when possible, the reaction products.

ALKENYL DERIVATIVES OF 2H-BENZO[D][1,2,3]TRIAZOLE WITH APPLICATION IN ORGANIC ELECTRONICS

Beatriz Donoso Jurado

The self-assembly of organic π-conjugated systems has recently gained considerable attention in the broader area of supramolecular chemistry as a technique for obtaining functional structures that exhibit enhanced optical and/or electronic properties in comparison to the isolated molecules. We have studied the preparation and self-assembly properties of alkenyl 2H-benzo[d][1,2,3]triazole derivatives with the aim to determine their photophysical behaviour and to compare with the alkynyl analogs recently prepared in our research group.

The synthesis of alkenyl derivatives of 2H-benzo[d][1,2,3]triazole required the previous preparation of 2-(3,5-bis(trifluoromethyl)phenyl)-4,7-dibromo-2H-benzo[d][1,2,3]triazole and arylethylenes. To avoid unnecessary synthesis, the compounds synthesized were selected using computational calculation.

Organized supramolecular structures of alkenyl derivatives of 2H-benzo[d][1,2,3]triazole have been obtained by using a slow diffusion technique. The formation of these aggregates has been visualised by using SEM on glass substrates.

The photophysical features of these compound have been also investigated. The optical waveguiding behaviour of the aggregates formed upon self-assembly of benzotriazole derivatives has been determined by using confocal optical microscopy coupled to a camera.

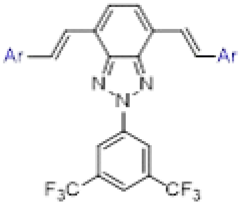

Figure 1. Alkenyl derivatives of 2H-benzo[d][1,2,3]trizole.

PROBIOTIC CAPABILITY IN YEAST: SET-UP OF A SCREENING METHOD

Pilar Fernández-Pacheco Rodríguez

Due to the interest of the food industry in the selection of new probiotic strains, the objective of the present study was to establish an adequate method for evaluating the probiotic potential of Saccharomyces and non-Saccharomyces strains isolated from food ecosystems. A new laboratory protocol was designed by studying of the kinetics parameters. Each decision was made based on multifactorial statistical assay results. The yeast strains used were belong to the culture collection of Yeast Biotechnology Laboratory (UCLM) and to the “Colección Española de Cultivos Tipo” (CECT). In addition to Saccharomyces boulardii, commercial probiotic, used as positive control. Set-up of the method was carried out bearing in mind the following objectives: selection of positive and negative controls and establishment of the best conditions for simulating intestinal gut digestion to obtain a rapid, reproducible and reliable screening method. The most important parameters calculated using the model described by Warringer and Blomberg (2003) were lag phase (λ), generation time (G), maximum optical density (ODmax) and specific growth rate constant (μmax). S. cerevisiae strain 3 was chosen as positive control and T. delbrueckii strain 1567 as negative control, both of them selected because of their performances and growth kinetic. The simulation conditions of the stomach and intestine were: a first step with static conditions for 3 h. at pH 2 and 37ºC in the presence of pepsin; and a second step which was a growth assay in the presence of bile salts and pancreatin for 22 h. at pH 8 and 37ºC to simulate the intestine. The best yeast evaluated was number 39, one S. cerevisiae isolated from wine. The preliminary screening indicates that S.cerevisiae strains are more resistant to the conditions than non-Saccharomyces ones, which seems to indicate that the probiotic character of Saccharomcyes yeasts is more accentuated. The results obtained in the present study showed that the protocol set-up is adequate and it can be useful for evaluating the probiotic characteristics and studying the growth kinetic along the sequential process throughout the intestinal gut while being.

INFLUENCE OF ECOLOGICAL FERTILIZATION ON SENSORY CHARACTERISTICS OF LA MANCHA TRUJILLO MELONS

Manuel Ángel Ferrer Valverde

Generally, humans prefer sweet and aroma-rich fruits, but an optimal sensory quality is the result of a balance of sweetness and sourness, sweetness and bitterness as well as sweetness and aroma, respectively. Sensory quality is a difficult concept to define, as it comprehends not only the intrinsic attributes of the product, but also the interaction between the product and the consumer. This interaction is made up of several factors relative to food characteristics, consumer features and background. Moreover, it is also necessary to establish a relationship between the sensory perceptions and the acceptability for the consumer. The aim of this study was research the influence of compost made from wastes from the winery and distillery industry and phosphorus on sensory profile of fresh-cut La Mancha melons and investigate the consumer preferences of these melons. A randomized complete-block design was used with four treatments consisting on one doses of compost, phosphorus and compost+phosphorus:, 2 kg compost per linear meter of plantation (D2), 120 kg/ha of P_2O_5 (phosphoric acid) (P) or D2+P and a control (C) without compost application and the sensory profile of melons and consumers acceptance were evaluated. Descriptive Sensory Analysis of melons was carried out by an expert panel of melon tasters. The sensory evaluation of the melon samples was made with a group of trained panelists. The application of compost made from wastes from the winery and distillery industry and phosphorus as fertilization treatment influence the sensory characteristics of La Mancha Trujillo melons principally when the phosphorus is use. Acceptance tests demonstrated that there has been no significant difference ($p \geq 0.05$) in relation to the grade of acceptance between the melons corresponding to the control and fertilized samples.

SWEET GREEN GRAPHENE: EXFOLIATION OF GRAPHITE AND PREPARATION OF GLUCOSE-GRAPHENE COCRYSTALS THROUGH MECHANOCHEMICAL TREATMENTS

Viviana J. González Velázquez

Graphene has peculiar mechanical and electronic properties, [1] important from microelectronics to biosensing, nano-medicine, and biology area. The use of cocrystals is important to get biologically active compounds into viable products solving most of the problems involved in this area.[2, 3] Cocrystals are supramolecular structures of, at least, two neutral organic molecules interacting via intermolecular interactions. This can be synthetized mechanochemically,[4] which has also gained importance for the exfoliation and functionalization of nanomaterials like graphene. [5]

Here, we present the comparison between different carbohydrates studied by density functional theory (DFT) calculations and experimental method to provide useful insights on the decision making of which carbohydrate to use to exfoliate graphene. Also, we report environmentally friendly, cheap and simple approach for the synthesis of aqueous soluble graphene, in the form of cocrystal with glucose.

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FUNCTIONALIZATION OF PLA WITH COUMARIN VIA CLICK CHEMISTRY IN scCO2

Eulalio Gracia Cortés

Polylactic acid (PLA) is a biodegradable and biocompatible polymer which belongs to aliphatic polyesters. These properties, make it an important candidate in medical applications. Furthermore, PLA is also characterized by other properties like mechanical properties, thermal properties, barrier properties and processability.

Among different polymers functionalization where toxic organic solvents are used, click chemistry has emerged as one of the most promising reactions because it is classified as a very specific, efficient and versatile reaction which allow to obtain high products yields. It consists on the reaction of an azido group to an alkyne group (AAC) catalyzed by copper (CuAAC) in organic media, where DFM or THF are the most common solvents. The compound chosen for PLA functionalization is coumarin. This substance is well-known by its pharmacological properties such as anti-inflammatory, anticoagulant or antiviral activity.

The main advantage of using supercritical technology for PLA functionalization is the elimination of organic solvents in the reaction being substituted by a solvent at supercritical conditions, which in this case is supercritical carbon dioxide ($scCO_2$). This solvent appears as a solution to carry out environmental friendly processes due to its lack of reactivity, high diffusivity and good transport properties.

In this work, PLA functionalization via click chemistry with coumarin in supercritical conditions CO_2 has been achieved [1]. Click reaction was performed at atmospheric pressure and $scCO_2$ for comparison being observed that is possible to obtain similar yields, higher than 95% in both cases.

1. Gracia, E., et al., Functionalization and optimization of PLA with coumarin via click chemistry in supercritical CO2. Journal of CO2 Utilization, 2017. 20: p. 20-26.

HYDROGELS WITH MAGNETIC PROPERTIES

Jesús Herrera Herreros

Hydrogels are physically or chemically crosslinked hydrophilic 3D polymer networks, which absorb and retain large amounts of water, though not soluble in it, with maintenance of shape[1]. Our research group has a large experience synthesizing hydrogels (Figure 1). It is well known that hydrogels can store drugs inside and, depending on the structure and composition, they can deliver the drug in response of a certain stimulus[2]. In this poster, we show the synthesis of hydrogels functionalized with Co and Fe Nanoparticles and also with Few Layer Graphene (FLG) and Graphene Oxide (GO). These hydrogels will be applied to the design of scaffolds for 3D cell cultures. The presence of nanoparticles makes them sensitive to a magnetic stimulus, in order to deliver, for example, grown factors. Furthemore, graphene is expected to contribute to the mechanical, electrical and thermal properties, and at the same time, cellular adhesion can be increased.

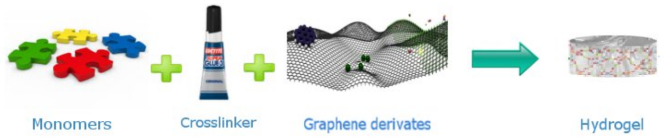

Figure 1. General scope of hydrogels synthesis.

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RICH SUGAR BIOMASS AS RAW MATERIAL FOR CATALYTIC CONVERSION OF GLUCOSE INTO BIOFUEL

Alberto José Huertas Alonso

The continuous depletion of fossil fuel reserves has urged the current society to search for new energy feedstocks, not only for the necessity of new fuels, but also for the synthesis of chemicals. In addition, increasing concern about global warming has pointed out that these new energy feedstocks must be obtained according to environmentally friendly processes, which result in a reduction of atmospheric CO_2 emissions. Nowadays, biomass has emerged as the most affordable source of a wide range of chemical compounds,[1] being lignocellulosic biomass the main element. Lignocellulosic biomass is rich in carbohydrates, and therefore is a valuable starting point for their catalytic conversion into platform chemicals,[2] mainly 5-hidroxymethyfurfural (5-HMF) and levulinic acid (LA). Both 5-HMF and LA could be transformed into biofuels such as 2,5-dimethylfuran (2,5-DMF)[3] and γ-valerolactone,[4] respectively, via hydrogenation.

In this work we present the catalytic dehydration of glucose under microwave heating and their extraction from high sugar biomass, concretely Opuntia Ficus-Indica, aimed to develop an easy method to obtain 5-HMF and LA selectively from this starting material.

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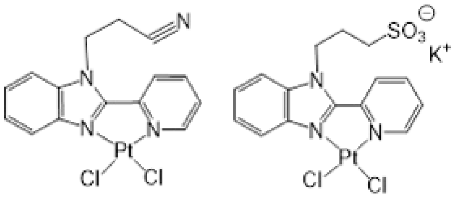
SYNTHESIS AND CYTOTOXICITY OF Pt(II) PYRIDYL BENZIMIDAZOLE COMPOUNDS BEARING FUNCTIONALIZED TAILS. IMPORTANCE OF THEIR INTERACTION WITH SEROALBUMIN

Jorge Leal Cruz

Cisplatin, along with other Pt(II) coordination compounds, has been widely used in cancer treatment due to their great cytotoxic properties. However, their poor selectivity towards tumoral cells leads to undesirable side effects. It is necessary to design new organometallic compounds that overcome these problems while having good cytotoxic properties. In this work, we report two Pt(II) organometallic compounds with ligands derivated from pyridyl benzimidazole, bearing functionalized tails included to affect their properties, especially the lipophilicity and hydrophilicity balance that could influence their cellular uptake.



We have studied their cytotoxic properties and the ability to bind to dGMP, DNA and albumin models. It has been found that the nature of the lateral chain has a great influence on the properties of these complexes. We have verified that compounds that have a strong interaction with albumin have lower cellular uptake, being less cytotoxic. Other studies with compounds synthesized in our group with functionalized bypyridine ligands are in agreement with these results.

Financial support acknowledgment: MINECO of Spain (CTQ2014-58812-C2-1-R), MRC thanks to FEDER founds and Plan Propio de I+D+i-UCLM (2014/10340) for a predoctoral contract.

FUNCTIONALIZATION OF PEG WITH COUMARIN VIA CLICK CHEMISTRY IN SUPERCRITICAL CO_2

Sonia López Quijorna

The field of natural products with an anticarcinogenic profile is currently being exploited with the aim of developing drugs to reduce side effects, as the clinical application of chemotherapy drugs is limited due to these effects. Natural coumarins or synthetic analogues, are of great interest due to their pharmacological properties. In particular, their physiological, bacteriostatic and anti-tumor activity makes these compounds attractive and screening as novel therapeutic agents.

One of the most commonly used polymer groups in drug conjugation is polyethylene glycol due to its excellent properties: non-toxic, non-immunogenic, non-antigenic, highly flexible and high hydrophobicity. Nowadays, polymer-pharmaceutical conjugate is used as a potent therapeutic agent because it provides greater biological activity and specificity. Among the most common procedures to carry out the synthesis of the polymer drug conjugate is the click chemistry.

Click chemistry has been used in the synthesis of polymers with pharmaceutical, biomedical applications and modification nanoparticles. In addition to that, click chemistry has the advantage of being a highly reliable methodology, clean, with excellent performance and compatible with a large number of functional groups, when compared with other conventional polymer-pharmaceutical conjugation methods. Combined with the use of supercritical technology, we will protect drugs from degradation and avoid the use of toxic solvents. The aim of this work was to synthesize a polymer-pharmaceutical conjugate (PEG-coumarin) using supercritical click chemistry ($scCO_2$)[1]. Different reaction conditions were evaluated in order to find the optimal conditions to obtain the best reaction performance.

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NOVEL METAL NANOPARTICLE-ENHANCED FLUORESCENCE FOR DETERMINATION OF DOPAMINE IN URINE SAMPLES

Marwa Louleb

A simple, rapid and highly sensitive fluorimetric method for the determination of dopamine in urine samples is developed. In addition, a new type of gold nanoparticles (AuNPs) was synthesized with simple and easy synthetic processes and environmentally friendly compound. The as-synthesized AuNPs were further characterized by UV-Vis absorption spectroscopy. The effects of different concentrations of AuNPs on the fluorescence behaviours of dopamine in aqueous solutions were investigated. An enhancement or quenching of the fluorescence can also be observed, depending on the exact conditions.

FROM NANO TO MACROSCALE: GRAPHENE QUANTUM DOT-AEROGELS FOR SENSING POLYAROMATIC COMPOUNDS

Ana Martín Pacheco

Graphene Quantum Dots (GQDs) have received a great deal of attention due to their photoluminiscent properties, high water solubility and biocompatibility. Furthermore, these nanoparticles present planar surfaces that are able to bind other molecules by π-π interactions. These excellent properties make that GQDs can be used as materials for solar cells, in analytical science or in biomedical applications. However, the tendency for aggregation of GQDs in dry states is a limiting factor that can affect the photoluminiscent behavior. To prevent this agglomeration, nanoparticles can be incorporated into appropiate matrices. In particular the incorporation of nanoparticles within three-dimensional polymer matrices such as hydrogels to form nanocomposites is a useful strategy not only to preserve the photoluminiscent properties, but also to enhance the mechanical properties or the response to certain stimuli.

In this work, a hydrogel based on GQDs is prepared. This nanocomposite is completely characterized and their sensing properties are also studied at different pH media and in the presence of several molecules. Our GQDs-based nanocomposite has also been proven to be a sensor for polyaromatic compounds in water.[1]

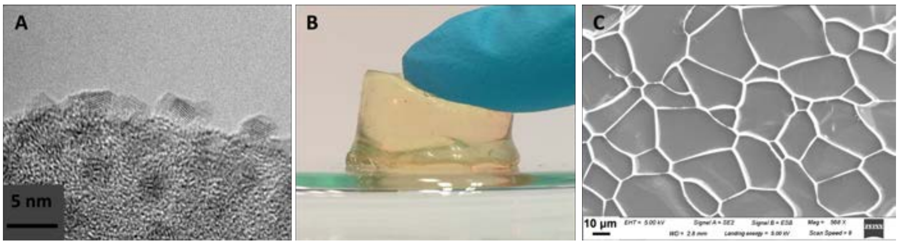

Figure: a) Transmission Electron Microscopy (TEM) of GQDs; b) Digital photo and c) Cryo-Scanning Electron Microscopy (Cryo-SEM) of the nanocomposite.

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FOOD RESTRICTION-ASSOCIATED INCREASES IN ChREBP BETA ISOFORM OF AGED- WISTAR RATS HAVE MARKEDLY IMPLICATION IN GLUCOSE HOMEOSTASIS

Lorena Mazuecos Fernández-Pacheco

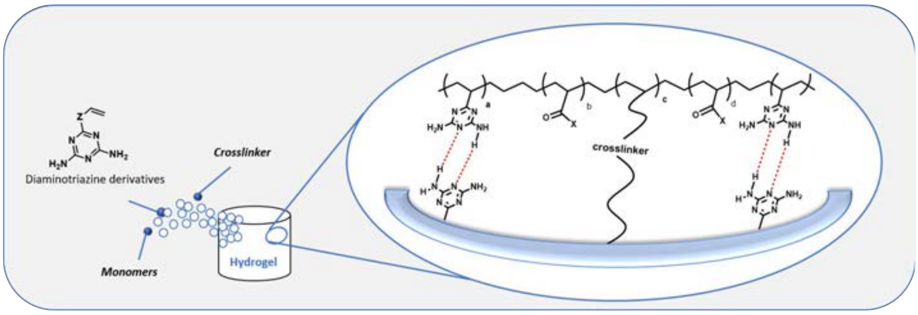
Ageing in rodents and humans is associated with obesity and insulin resistance. Food restriction, which delays the aging process in mammals ameliorated insulin resistance and inflammation. Recently, it have been shown that a shorter ChREBP isoform (ChREBP-β) links glucose transport to lipogenesis and insulin sensitivity in white adipose tissue, but not in the liver. The aim of this study was to dilucidate the mechanism by which food restriction avoid hyperglycaemia in 24-month-old Wistar rats when challenged with a high fat meal. The experiments were performed in male 3- , 8- and 24-month-old Wistar rats fed ad libitum or food restricted, from our in-house colony (Centre of Molecular Biology, Madrid, Spain). Animals were fasted 16h before the oral fat tolerance test. Then the bolus of olive oil (0.1 ml / 100 g body weight) was orally administered. Blood aliquots from the tail vein at the following times 0, 30, 60, 90, 120, 180 and 240 minutes be taken for measuring glucose and insulin levels. 4 h after fat load animals were sacrificed and liver and visceral adipose tissue were rapidly excised. We found that high fat meal produces hyperglycaemia in 24-month-old rats fed ad libitum but not in their food restricted littermate. In addition food restriction lead to a different pattern of expression of ChREBP isoforms in liver and adipose tissue. Interestingly, ChREBP beta expression markedly increased in liver from 24mFR rats, in parallel with the expression of key lipogenic genes (Scd-1, ACC, Elovl6), also regulated by this transcription factor. Surprisingly, ChREBP beta expression is also altered in adipose tissue from 24m rats as well as the genes related to glyceroneogenesis, and glucose uptake Pck1 and Glut4 respectively. This suggest that ChREBP might be involved in the control of glyceroneogenesis, lipogenesis and glucose uptake under a high fat meal.

NOVEL HYDROGELS BASED ON TRIAZINE AS Fe(III) SENSORS

Josué Muñoz Galindo

The 1,3,5-triazine moiety has received a great deal of attention in supramolecular chemistry due to the large number of interactions it presents, i.e., coordination links, hydrogen bonding, π-π interactions, etc. [1] Considering these properties, and based on the group's experience in the preparation of triazine derivatives,[2] we have carried out the syntheses of new hydrogels based on diaminotriazine.

Both chemical and physical hydrogels have been prepared showing luminescent properties upon UV light exposure. It was observed that the fluorescence intensity of these gels were quenched in the presence of Fe (III) cation, proving them as potential sensors. The pore size of these materials was performed by Scanning Electron Microscopy (SEM).



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IMPROVING THE EFFICIENCY OF ELECTROLYTIC REMEDIATION PROCESSES THROUGH THE CONCENTRATION OF GASEOUS EFFLUENTS

Martín Muñoz Morales

Recently, many research works have been focused on the development of new electrochemical processes with the aim to increase the removal efficiency of organochlorinated pesticides contained in soil and water effluents. One of the main drawbacks were the limitations of mass transfer due to the low concentration of these compounds in the sewage plants and the treatment of dangerous vapours that appear during their treatment that sometimes could be more dangerous than parental compounds.

In this work, it is proposed a novel and environmentally- friendly system to concentrate and remove gaseous effluents that combine the adsorption properties of granular active carbon (GAC) with an electroxidation process using boron doped diamond as anode [1, 2]. It was observed different behaviors in methanol and water solvents to desorb perchloroethylene as a model of non-polar and semi-volatile compounds. To do this, firstly it has been evaluated the adsorption isotherms in both solvents with different quantities of GAC particles to determine the level of pre-concentration of pollutants. Afterwards, it was desorbed using methanol as organic solvent and the solution obtained was treated in an electrolytic cell using a conductive diamond electrochemical oxidation (CDEO) process. This solution contains sodium chloride and sodium hydroxide as electrolyte to increase the conductivity in methanol media. Results obtained showed that it is possible to remove perchloroethylene from methanol solution, and re-use the GAC particles and methanol solution after removing the chlorinated compound. Additionally, it was monitored the intermediates compounds also removed in the process using GC-MS.

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3D-PRINTING: MODELING HYDROGELS

Alicia Naranjo Chacón

In the last few years, the interest of the novel techniques of 3D-printing has increased. These approaches allow an efficient process for the manufacture of on demand complex products through computer-designed 3D models. Thereby, it is becoming more common to implement those techniques in different sectors and areas of knowledge as industry, building trade, architecture, civil engineering, jewellery and footwear, and specially in scientific research.

The 3D-printing methodology can be used to prepare materials with application in energy store, flexible electronics or sensors,[1] as well as materials production for tissue engineering.[2] Hence, the study and the preparation of inks for 3D-printing has become one of the most interesting topics nowadays.

Following this trend, in this project we have used the 3D printing technology to prepare hydrogels without the need for molds and with the require features depending on the final application. Hydrogel precursor-based inks have been also designed and their rheological properties have been analysed.

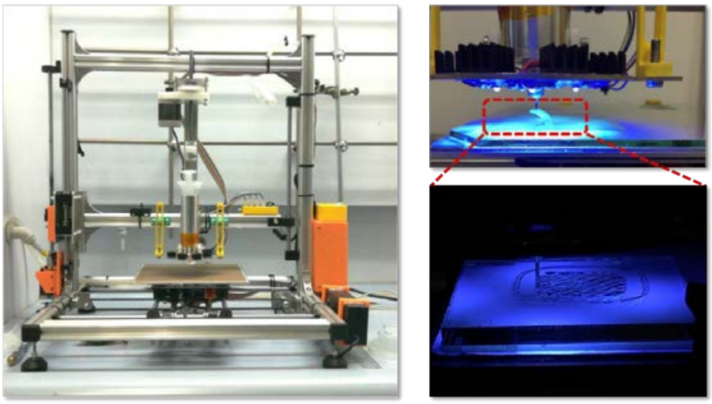

Figure. 3D printer and printing process.

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A PRESSURIZED JET-AERATED MICROFLUIDIC FLOW-THROUGH REACTOR FOR WASTEWATER TREATMENT BY EO-BDD AND HETEROGENEOUS EF

José Fernando Pérez

Electrochemical advanced oxidation technologies (EAOPs) have demonstrated a high efficiency in the removal of organic compounds in a number of effluents. However, most of the works are carried out on a laboratory scale. Thus, the objective of the present work is to design an electrochemical reactor integrating EAOPs with potential to be scaled-up for the remediation of wastewater under real conditions at a reasonable cost.

In particular, the reactor integrates the anodic oxidation with a boron-doped diamond (AO-BDD) with the electroFenton (EF) technology in such a way that both electrodes contribute to the decontamination of the effluent thanks to the generation of hydroxyl radicals ($^\bullet$OH), a powerful oxidant (Fig. 1A):

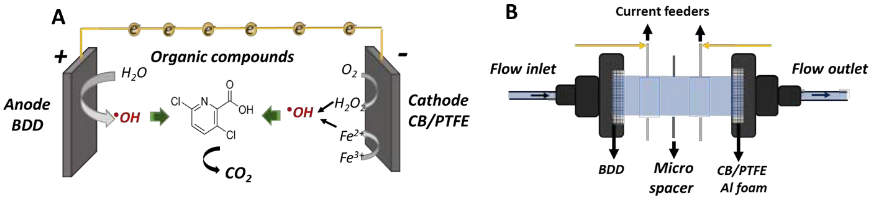

Figure 1. A) Generation of $^\bullet$OH vía AO-BDD y EF; B) MF-FT cell configuration

The electrochemical cell presents a novel configuration microfluidic flow-through to simultaneously minimize ohmic drop in the electrolyte and maximize mass-transfer [1] (Fig 1.B). In addition, the aeration system is a combination of a pressurized circuit and a jet aerator, allowing a fast and efficiency generation of H_2O_2 for the EF process. A fluidized-bed of iron particles act as the catalyst for the Fenton reaction, minimizing the addition of chemicals, preventing the secondary pollution and reducing the water and CO_2 foot-print of the treatment.

Acknowledgments: Financial support from the Spanish Ministry of Economy, Industry and Competitiveness and European Union through project CTM2016-76197-R (AEI/FEDER, UE) is gratefully acknowledged

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INTEGRAL VALORIZATION OF OLIVE OIL BYPRODUCTS THROUGH CO-GASIFICATION PROCESS

María Puig Gamero

The development of alternative renewable energies has taken importance due to the growing concern of climate change owing to greenhouse gas emission. In addition, population growth and their socio-economic development require large amounts of energy, converting the biomass in one of the most viable option for a sustainable future. In this sense, the waste of olive industry is a suitable candidate due to olive oil industry is one of the most important economic activity in Spain, which produces large amount of seasonal waste.

On the other hand, steam gasification is considered to be one of the most effective and efficient techniques for generating hydrogen from biomass and electric power. In addition, the product gas from biomass gasification can be also used in methanol or Fischer-Tropsch synthesis that yields liquid fuels. Currently, renewable chemicals industries have taken tremendous interests from both an economical and ecological perspective since they can reduce the use of fossil resource. However, the industrialization of biomass gasification is limited due to its lower calorific value and energy density, its higher tar yield, its heterogeneity as raw material and its unstable supply. In this sense, the co-gasification of coal, petcoke and biomass is one of the alternatives to solve problems associated with gasifying each of them separately. Biomass and coal gasification could achieve synergistic effects, combining some of the characteristics of each feedstock to improve the characteristics of the gasification process such as tar formation or char reactivity.

Although the main aim of this research is to produce a high quality syngas, by-product such as biochar is obtained. Therefore, the integral use of all by-products can improve the efficiency and economy of the gasification plants. Among the different possibilities of using biochar, its use as an adsorbent is one of the most promising options that can be carried out due to the analogies the mechanism of the formation of active carbon obtained through physical activation and biochar. In this sense, other important objective of this study is the use of bio-char as an adsorbent of greenhouse gases such as CO_2 and CH_4.

ELECTROCATAYTIC PROCESSES FOR THE TRANSFORMATION OF BIOETHANOL INTO HIGH ADDED VALUE PRODUCTS

Alberto Rodríguez Gómez

In recent years bioethanol has become one of the most promising alternatives to traditional fossil fuels. However, the overproduction on a global scale (biodiesel crisis) and on a national scale (surplus in wine production and industrial waste of alcohol production) cause that different alternatives are being considered for the valorisation of this compound.

In this research work, the use of electrocatalytic processes is proposed sine it presents some advantages (less deactivation and selectivity limitations) compared to conventional catalytic processes. The bioethanol reforming process is carried out in a polymer membrane electrochemical reactor (PEM cell), at atmospheric pressure and temperature below 100ºC. Under this configuration, in the anodic compartment the oxidation reaction of ethanol takes place, producing protons and organic compounds of industrial interest, while in the cathodic compartment reduction reaction takes place, generating high purity hydrogen.

Recent researches has shown the viability of light alcohols for the generation of hydrogen, through the technology described above, so it is important to note that the current research will be focused on maximizing the liquid product obtained in the anodic compartment, derived from the ethanol oxidation on supported metal catalysts. Some of this compounds are acetaldehyde, acetic acid and ethyl acetate. Acetaldehyde is an important intermediate in the organic synthesis that is used as a raw material for the production of acetic acid, acetic anhydride, ethyl acetate, pyridine, medicines, plastics… Industrially, it is obtained from the direct catalytic oxidation of ethylene through the Wacker process, which is very intensive in terms of energy. Therefore, the electrocatalytic route is presented as a more efficient and less expensive alternative. Also, changes in the operation variables (flow rates, temperature, amperage, MEA configuration) allow to vary the selectivity of the organic compound obtained in the reaction.

CENTRAL LEPTIN PROTECTS THE HEART FROM LIPOTOXICITY BY SELECTIVELY INCREASING PPARβ/δ IN RATS WITH NORMAL LEPTIN SENSITIVITY

Blanca María Rubio Muñoz

Recent evidences have shown that central and/or peripheral leptin infusion is required to reverse cardiac steatosis in obese leptin-deficient (ob/ob) mice. However, the mechanism by which leptin regulates lipid accumulation in cardiac tissue remains unknown. Here we analyzed the effects of intracerebroventricular leptin infusion for 7 days (0.2µg/day) on cardiac lipid metabolism in 3-month-old Wistar rats with normal leptin sensitivity. Thus, we analyze the fatty oxidation rates and the expression of key enzymes and proteins involved in cardiac lipid metabolism. In addition, we examined the effects of the pharmacological inhibition of PPARβ/δ with the specific antagonist GSK0660 in leptin infused rats. Central leptin infusion markedly decreased TAG levels in cardiac tissue accompanied by the selective up-regulation of gene and protein expression of PPARβ/δ, without influence on PPARα protein levels, while no significant changes were observed in vehicle-infused pair-fed (PF) rats or in leptin infused rats treated with the specific antagonist GSK0660. In addition, although cardiac total fatty acid oxidation rates between groups were not significantly different, central leptin increased myocardial intracellular lipolysis and peroxisomal (CPT1-independent) vs mitochondrial (CPT1-dependent) fatty acid oxidation rates, in parallel to the increased expression of ATGL, HSL and Acox1. Our findings suggest that central leptin increases medium and/or short chain fatty acid availability rates for complete mitochondrial oxidation and demonstrate that the selective up-regulation of PPARβ/δ and the stimulation of peroxisomal fatty acid oxidation contribute to the antisteatotic effects of central leptin in cardiac tissue independently of its effects on body weight. These results support a model where PPARβ/δ overexpression by central leptin protects the heart from lipotoxicity.

SUGAR DEHYDRATION UNDER MICROWAVE-ASSISTED RADIATION: A NEW GREEN METHOD FOR THE SYNTHESIS OF PLATFORM CHEMICALS

Manuel Salgado Ramos

Furfural (FF) is an organic compound which can be produced from the dehydration of pentoses, such as xylose, and it is mainly obtained under acid catalysis. Brønsted and Lewis acid, e.g. H_2SO_4 and $AlCl_3$, respectively, are normally appropriated for this reaction.[1,2] Besides, this molecule is also employed for the synthesis of many interesting compounds, such as furfuryl alcohol, and it is useful for biofuel production. Levulinic acid (LA) and 5-hydroxymethylfurfural (5-HMF) can be also mentioned as platform chemicals in order to obtain biofuel. These precursors can be also produced under acid catalysis and both are generated from hexoses, such as glucose. They are recognized as high value materials for the preparation of many desired compounds (e.g. 2,5-dymethylfuran and γ-valerolactone, which have been already used as biofuels).[3] Diminishing fossil fuel resources and climate change have caused the greater use of lignocellulosic biomass for the production of FF, 5-HMF and LA.[4] Agroindustrial food wastes are one of the most valuable resource of this biomass, which is mainly compound by cellulose, hemicellulose and lignin, therefore it supposes an essential renewable resource in order to reduce CO_2 emissions. The main goal of this work is the synthesis of platform chemicals previously mentioned (FF, 5-HMF and LA) from agroindustrial food wastes, as almond shell and dry grape marc. Furthermore, microwave radiation as a tool for sugar hydrolysis and dehydration is an environmental friendly technique that provide us shorter reaction time, better yield and elimination of by-products.[5]

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OPTIMIZATION OF AN ANALYTICAL METHOD FOR PLATINUM NANOPARTICLES DETERMINATION BY AF4-ICP-MS

Armando Sánchez Cachero

Engineered nanomaterials are extensively used in different fields of nanotechnology. Among them metallic nanoparticles (NPs) and, more specifically platinum nanoparticles (PtNPs), exhibit excellent catalytic reactivity which depends on the size and shape of NPs and makes them useful for catalytic converters in vehicles. However, chemical reactions at the catalyst surface are responsible for emission of PtNPs through exhaust gasses of vehicles [1]. PtNPs emissions could lead to dispersion and accumulation of these NPs in different environmental compartments. Due to the current lack of knowledge on their fate and potential environmental risk more research is necessary in this field.

New analytical techniques for determination and characterization of PtNPs in environmental samples are required. The combination of separation and detection techniques represents an advance on sensitivity, selectivity and representativity of NPs analysis. One of the most promising combination is asymmetric flow field flow fractionation coupled to inductively coupled plasma mass spectrometry (AF4-ICP-MS). AF4 has some advantages over other separation techniques, like wide application range, minimal sample preparation and low sample interaction with the analytical system. The use of ICP-MS as a detector is also advantageous over other techniques because of its high sensitivity, selectivity and multielement capability. The AF4-ICP-MS hyphenated system provides simultaneous information concerning particle size range, composition and concentration.

The aim of this work has been the development of a sensitive and selective analytical method for the determination of PtNPs by AF4-ICP-MS. Separation conditions such as the carrier flow and composition, cross flow or the injection time were optimized to achieve adequate resolution and quantitative recoveries. The developed method will be used for the analysis of water samples.

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RESVERATROL MODULATES GPCRS GENE EXPRESSION IN SAMP8 MICE

Alejandro Sánchez Melgar

Resveratrol (RSV) is a polyphenol produced by plants under stressful conditions in the environment. This compound seems to exhibit some protective roles in several diseases ranging from cancer, metabolic and immune disorders, cardiovascular and neurodegenerative diseases, among others. However, the molecular mechanism by which is acting remain still unclear. Focusing on the Central Nervous System, it has been reported that this polyphenol is able to modulate the neurotransmitters release, suggesting a role through their respective receptors which most of them belong to the G-protein coupled receptor (GPCR) family. Adenosine, dopamine and group I metabotropic glutamate receptors have been found to be altered in neurodegenerative diseases such as Alzheimer's and Parkinson's disease. The aim of this study was to determine whether RSV intake was able to modulate the gene expression of these three GPCR receptor types by using SAMP8 mice which have been considered as Alzheimer disease model. Our results clearly show some significant differences on the gene expression modulation after RSV supplementation in 5 months old mice when compared to untreated mice. In the adenosinergic system, while A_1R and A_2AR were decreased, a significant increase on A_3R mRNA levels was detected without changes on the A_2BR gene expression. In the glutamatergic system, group I metabotropic glutamate receptors were analyzed, showing a significant increase only on $mGluR_5$ gene expression. In the case of dopaminergic system, no changes were detected on D_2R mRNA levels. Therefore, we conclude that RSV differentially modulates these three neurotransmission systems, which may suggest that protective role of this polyphenol could be related to GPCR-mediated signaling modulation.

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CATHODIC CATALYST FOR THE ELECTROCHEMICAL HYDROGENATION OF CINNAMALDEHYDE

María José Torres

The selective hydrogenation of α, β-unsaturated aldehydes to their respective unsaturated alcohols is a critical step in flavours, fragrances and pharmaceutical industries. The hydrogenation of cinnamaldehyde (CMA) mainly produces hydrocinnamaldehyde (HCMA) that has been found to be an important intermediate in the preparation of pharmaceuticals used in the treatment of HIV, and cinnamyl alcohol (CMO), which is widely used in the production of perfumes[2]. Since the C=C hydrogenation is thermodynamically preferred compared to CMO, more attention has been focused on promoting the selectivity towards the unsaturated alcohol. This process could be carried out by heterogeneous catalysis under high pressure conditions due to the low H_2 solubility in the reactants. Other critical issues of this process are the corrosive nature of solvents, the large amount of catalysts used and the need of an external source of hydrogen gas. By contrast, electrocatalytic hydrogenation offers a sustainable alternative for the production of fine chemicals at mild reaction conditions (low temperature and room pressure). Proton Exchange Membrane (PEM) cells are actually a promising alternative to provide highly pure hydrogen (in–situ generation) to carry out the selective hydrogenation of cinnamaldehyde in the cathode chamber[3]. Therefore, the present work was focused on the study of the influence of the cathodic catalysts and conditions on the selectivity electrochemical hydrogenation of cinnamaldehyde in a PEM reactor.

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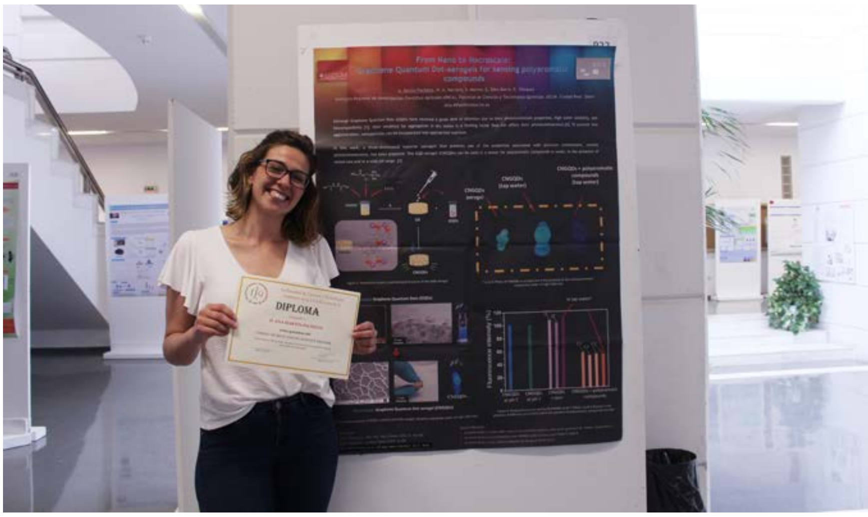
III PREMIO CIENCIA JOVEN

I PREMIO CIENCIA JOVEN POSTER

Como en ediciones anteriores, el comité organizador del XII Simposio de Ciencia Joven hizo entrega del III Premio Ciencia Joven en el acto de clausura del evento. En esta edición, el premio ha sido otorgado a Iván Torres Moya con el trabajo titulado "Tunable polymers derived from 2H-benzo[d]1,2,3-triazole monomers". También se hizo una mención especial como finalista a Raúl Martín Lozano, con el trabajo "Waveguide behaviour in self-assembled thiadiazole and benzothiadiazole-based materials". Por primera vez se hizo entrega del I Premio Ciencia Joven al mejor póster a Ana Martín Pacheco, con el póster titulado "From nano to macroscale: ghaphene quantum dot-aerogels for sensing polyaromatic compounds".

¡Enhorabuena a los premiados!



Investigadores de la UCLM se reúnen en las I Jornadas postdoctorales

El Vicerrectorado de Investigación y Política Científica, junto al colectivo de investigadores SECTI-UCLM, contratados bajo la modalidad de acceso al Sistema Español de Ciencia, Tecnología e Innovación, han organizado las I Jornadas Postdoctorales, que se celebran durante el día de hoy en el Campus de Albacete con un total de 56 participantes, 28 de ellos investigadores y otras 28 investigadoras. Este encuentro pretende propiciar un espacio para compartir su trabajo con el resto de participantes y difundir las áreas de investigación actualmente desarrolladas en la UCLM.

El salón de actos de la Escuela Técnica Superior de Ingenieros Agrónomos y de Montes (ETSIAM) de Albacete acoge la primera edición de las jornadas postdoctorales de la Universidad de Castilla-La Mancha, que han sido presentadas por el vicerrector de Investigación y Política Científica, Julián Garde, junto al director de la ETSIAM, Rodolfo Bernabéu, y Eva María Galán, miembro de la comisión organizadora de la jornada.

Estas jornadas, en palabras de Eva María Galán, suponen una plataforma para reivindicar la investigación “como motor de desarrollo de nuestra esta región y del país y para mostrar las líneas de investigación que se llevan a cabo en la UCLM”, dijo, a la vez que añadía que esta actividad podría ser “la semilla de muchos proyectos multidisciplinares entre nosotros”.

Por su parte, el vicerrector felicitaba a la organización por el trabajo y esfuerzo realizado en estas primeras jornadas, que demuestran, según indicó que “tenemos una masa crítica de doctores vinculados a la Universidad regional en diferentes fases de la carrera investigadora y que hacen investigación por esta universidad y región”. Esta primera edición contará con dos sesiones divulgativas, otra sesión centrada en la exposición de póster y, para finalizar, se llevará a cabo la mesa redonda: “Evaluación de la investigación en España: En busca de la investigación de excelencia", que servirá para clausurar la actividad.

Gabinete de Comunicación UCLM. Albacete, 6 de junio de 2018

La directora del CNIO, María Blasco, explica en la UCLM cómo la longitud de los telómeros determina la longevidad

La directora del Centro Nacional de Investigaciones Oncológicas (CNIO) y jefa del grupo de Telómeros y Telomerasa, María Antonia Blasco, ha visitado este jueves el Campus de Toledo de la Universidad de Castilla-La Mancha (UCLM) para ofrecer la conferencia 'El papel de los telómeros en el cáncer y en el envejecimiento'. Entre otros aspectos, ha señalado la relación entre el acortamiento telomérico y la longevidad y marcado la singularidad del cáncer frente a otras patologías relacionadas con el envejecimiento.

La científica alicantina ha participado en la iniciativa del Vicerrectorado de Investigación y Política Científica '12 meses 12 investigadoras' incidiendo en su trabajo de más de 20 años centrado en demostrar la relevancia de los telómeros y de la telomerasa en el cáncer, así como en enfermedades relacionadas con el envejecimiento.

En este sentido, señaló la importancia de conocer las causas moleculares del envejecimiento para diseñar estrategias contra las patologías asociadas. Entre otras, señaló la que constituye su área de especialidad, que es la erosión de las estructuras que protegen los extremos de los cromosomas humanos, los telómeros, "esenciales para la vida". Su acortamiento, dijo, "es una causa primaria que desencadena otras", y se acortan "a consecuencia de cómo está diseñada la vida" a través de los procesos de división celular.

En su intervención se refirió también a la telomerasa, una enzima que compensa el acortamiento telomérico cuyos descubridores, Elizabeth H. Blackburn, Carol W. Greider y Jack W. Szostak recibieron en 2009 el Premio Nobel de Medicina. En este punto, señaló la singularidad del cáncer frente a otras enfermedades asociadas al envejecimiento. "La diferencia fundamental es que en el cáncer las células dañadas son inmortales gracias a la telomerasa", dijo.

Blasco afirmó que la longitud de los telómeros determina la longevidad y apuntó que si un individuo nace con estas estructuras más cortas debido a una mutación, aumenta la probabilidad de desarrollar de forma prematura enfermedades relacionadas con la degeneración de los tejidos. Insistió en que los telómeros no son iguales en todos los individuos, de forma que las personas con los telómeros más cortos tienen mayor riesgo de desarrollar patologías relacionadas con el envejecimiento como el infarto de miocardio. Por otra parte, explicó las investigaciones llevadas a cabo con ratones sin telomerasa, que se mostraron resistentes al cáncer, lo que ha conducido al desarrollo de inhibidores de esta enzima para el tratamiento de esta patología.

María A. Blasco obtuvo su doctorado en 1993 en el Centro de Biología Molecular ‘Severo Ochoa’ bajo la supervisión de Margarita Salas. Ese mismo año se trasladó a Cold Spring Harbor Laboratory en Nueva York (EE.UU.) para incorporarse al laboratorio dirigido por Carol W. Greider en calidad de becaria posdoctoral. En 1977 regresó a España para establecer su propio grupo de investigación en el Centro Nacional de Biotecnología (CSIC, Madrid). En 2003 se trasladó al Centro Nacional de Investigaciones Oncológicas (CNIO, Madrid) como directora del programa de Oncología Molecular y jefa del grupo de Telómeros y Telomerasa. En 2005 fue nombrada vicedirectora de Investigación Básica del CNIO y en junio de 2011 directora.

Blasco ha publicado más de 250 artículos científicos en revistas internacionales y nacionales con un h-index de 81. Sus logros han sido reconocidos a través de premios como ‘Josef Steiner Cancer Research Award’, ‘Swiss Bridge Award for Research in Cancer’, ‘Körber European Science Award’,’ the EMBO Gold Medal’, el Premio “Rey Jaime I” en Investigación Básica, el premio de la ‘Fundación Lilly en investigación Preclínica’ y el Nacional en Biología ‘Santiago Ramón y Cajal’, entre otros. Además, tiene dos doctorados honoris causa de la Universidad Carlos III de Madrid y de la Universidad de Alicante, respectivamente. En octubre de 2017 recibió la Distinción al Mérito Científico de la Generalitat Valenciana.

Gabinete de Comunicación UCLM. Toledo, 7 de junio de 2018

En el próximo número de Molécula...

El próximo número de MOLÉCULA incluirá todo sobre GIENOL 2018: XIV Congreso Nacional de Investigación Enológica, información del concurso "Tesis en 3 minutos" y otras muchas secciones.