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

XIII YOUNG SCIENCE SYMPOSIUM

Del 5 al 7 de Junio de 2019

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LIBRO DE COMUNICACIONES

Bienvenida del Decano

Os damos la bienvenida a esta nueva edición del 13th Young Science Symposium, que organiza la Facultad de Ciencias y Tecnologías Químicas de la Universidad de Castilla – La Mancha junto con sus jóvenes investigadores.

Es el XIII Simposio, que nació con este formato en la edición del año 2013. Previamente, y desde el año 2007, se había desarrollado como jornadas de sesiones cortas a lo largo de los meses de abril a junio. En todos los casos, ha sido siempre un compromiso de la Facultad por la investigación y hacia sus jóvenes investigadores. Promover y divulgar la investigación en los campos científicos y tecnológicos que tiene que ver con la Química, la Ingeniería Química, y la Ciencia y Tecnología de los Alimentos, que son las enseñanzas tradicionales de nuestro Centro.

El objetivo es doble: divulgar y dar a conocer lo que nuestros jóvenes investigadores hacen, e introducirlos en la organización de pequeños eventos científicos, que a escala reducida sirvan de ejemplo de cómo se organizan los congresos a los que después ellos asisten, a nivel nacional e internacional, presentando los resultados de sus trabajos científicos. Constituye también una actividad formativa para los estudiantes de nuestros programas de doctorado, después de los cambios que éstos han experimentado a partir del año 2011. En esta edición se sigue contando con la participación de jóvenes investigadores de otros campus (Toledo y Albacete) de la Universidad de Castilla-La Mancha, cuyos temas de investigación están estrechamente relacionados con los campos científicos y tecnológicos que se desarrollan en este Centro, hecho que fomenta la interdisciplinaridad y el debate entre nuestros jóvenes investigadores. Es buena prueba de la magnífica aceptación del Simposio, que va creciendo de forma muy clara durante los últimos años. A modo de incentivar a aquellos jóvenes doctorandos y nuevos doctores que participan como ponentes en estas Jornadas, en esta convocatoria 2019, se concederá el IV PREMIO CIENCIA JOVEN. Asimismo, se otorgará el II PREMIO CIENCIA JOVEN al mejor póster, ya que este año contamos también con contribuciones en este formato.

Desde la Facultad, que aporta la infraestructura y los recursos necesarios, hemos de felicitar al grupo de jóvenes que han estado detrás de la organización de esta edición, por su dedicación y entusiasmo. Agradecer a todos los participantes su respuesta y favorable acogida. A los investigadores invitados. A los patrocinadores; cada vez en mayor número. Al Rector, y al Vicerrector de Investigación y Política Científica de la UCLM, por su sensibilidad y apoyo a estos Simposios. Y, así, con estos respaldos, el convencimiento del éxito de esta nueva edición del Simposio Ciencia Joven.

Ángel Ríos Castro

Decano de la Facultad

Comité Científico:

Ángel Ríos Castro, *Decano de la Facultad*

Alberto Ramos Alonso *“Inorganic Chemistry”*

Ana Raquel de la Osa Puebla *“Chemical Engineering”*

Elena Alañón Pardo *“Food Sciences and Technology”*

Antonio Manuel Rodríguez García *JIQ-RSEQ - EYCN EuChemS*

María Antonia Herrero Chamorro *STCLM de la RSEQ*

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Virginia Moreno García *“Analytical Chemistry”*

Sergio Blázquez González *“Physical Chemistry”*

Luis Fernando León Fernández *“Chemical Engineering”*

Jorge Leganés Bayón *“Organic Chemistry”*

Javier Toledano Villar *"Simbiosis Producciones" (Photography)*

Estamos encantados de retomar durante los días 5, 6 y 7 de Junio la iniciativa del **“Young Science Symposium“**, siendo este año su **decimotercera edición**.

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

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

Por otro lado, a modo de incentivar a aquellos jóvenes doctorandos y nuevos doctores que participan como ponentes en estas jornadas, en esta convocatoria 2019, se concederá el **"IV PRIZE OF YOUNG SCIENCE FACULTY OF SCIENCES AND TECHNOLOGY"**. Asimismo, se otorgará el **"II PREMIO CIENCIA JOVEN"** al mejor póster, ya que este año contamos también con contribuciones en este formato.

Por todo ello, os agradecemos vuestra participación y esperamos que la experiencia os sea de provecho.

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

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

Programme:

Wednesday, 5th June 2019.

9:00- Welcome reception. Delivery of documentation.

9:30- **Opening ceremony** chaired by the **Rector Magnificus of the UCLM** and the Dean of the **Faculty of Chemical Sciences and Technology**.

10:00- **Invited Lecturer: Prof. Emilio M. Pérez Álvarez (IMDEA Nanoscience).** *"Interfacing molecules and nanomaterials: from carbon nanotube rotaxanes to single-molecule experiments".*

11:00- 1st sesión

- *"Nanomolar Detection of Dopamine in Human Fluids by N-Doped Carbon Nanoparticles".* **Marwa Lauleb.** *Analytical Chemistry.*
- *"Bioelectrochemical systems for the reductive treatment of hazardous pollutants".* **Luis Fernando León.** *Chemical Engineering.*
- *"Reactivity of Zinc Complexes towards Alkynes: Catalytic Intramolecular Hydroalkoxylation of Alkynyl Alcohols".* **Miguel Ángel Gaona**. *Inorganic Chemistry.*
- *"Alternative photosensitizers to enhance the sensitivity of NMR spectroscopy through hyperpolarization methods on microcoils".* **Margarita Ruiz de Castañeda.** *Organic Chemistry.*

12:00- **Invited Lecturer: Prof. Yolanda Pico (University of Valencia).** *"Retos para el control de nanomateriales en alimentos".*

13:00-Poster session.

14:30- Lunch break.

16:00- 2nd session

- *"Another application of yeasts: Biodetoxification of pollutants".* **Beatriz García-Bejar.** *Food Sciences and Technology.*
- *"Functionalization of polymers in supercritical carbon dioxide".* **Sonia López**. *Chemical Engineering.*
- *"Study by AF4-ICP-MS of the PtNPs' behaviour in natural and synthetic freshwaters".* **Armando Sánchez.** *Analytical Chemistry.*
- *"Adenosine receptors, resveratrol and cancer".* **Sonia Muñoz.** *Biochemistry.*

- *"Hydrogels with Iron and Cobalt magnetic Nanoparticles".* **Jesús Herrera**. *Organic Chemistry.*

Thursday 6th of June 2019

9:00- **Invited Lecturer: Prof. Pedro Lozano (Universidad de Murcia).** *"Green Chemistry or 'Dream' Chemistry: procesos biocatalíticos limpios de interés industrial".*

10:00- 3rd session

- *"Electrochemical detection of Rhodamine B by molecularly imprinted polymer modified screen printed carbon electrode and extraction by magnetic multiwalled carbon nanotube poly(styrene-co-divinylbenzene".* **Yassine Benmassaoud** *Analytical Chemistry.*
- *"Yeasts with probiotic potential".* **Pilar Fernández-Pacheco.** *Food Sciences and Technology.*
- *"Smart Materials for sensing and soft robotics applications".* **Ana Martín.** *Organic Chemistry.*
- *"Synthesis of Bio-Derived Cyclic Carbonates from Renewable Resources".* **Felipe de la Cruz.** *Inorganic Chemistry.*

11:00- Coffee break

11:30- **Invited Lecturer: Prof. David Serrano (IMDEA Energy Institute).** *"Investigación en energía: progreso vs circularidad".*

12:30- Act of commemoration of the **International Year of the Periodic Table IYPT2019** chaired by the Dean of the Faculty of Chemical Sciences and Technology:

Pedro Lozano Rodríguez: *"Modelos y ejemplos. La experiencia en la Universidad de Murcia"*

María José Ruiz (UCLM-Toledo): *"Divulgación científica de la Tabla Periódica"*

María Antonia Herrero Chamorro: *"Reseña de la Jornada de la RSEQ"*

14:00- Lunch break

16:00- 4th session

- *Screening and Preliminary Biochemical and Biological Studies of [RuCl(p-cymene)(N,N-bis(diphenylphosphino)-isopropylamine)][BF4] in Breast Cancer models.* **Elena Domínguez**. *Inorganic Chemistry.*
- *"New electroFenton reactors for wastewater treatment".* **José Fernando**. *Chemical Engineering.*

- *"2H-benzo[d][1,2,3]triazole derivatives with application in organic electronics".* **Beatriz Donoso**. *Organic Chemistry*.
- *"Application of the GC-MS/MS technique and laser-based mass spectrometry techniques to the determination of PAH, OPAH and NPAH in the reference and real soot samples".* **Sonia Lara**. *Physical Chemistry.*

17:00- Break

17:30- 5th session

- *"Synthesis of furfural by dehydration of pentoses. Towards full biomass valorisation".* **Manuel Salgado**. *Organic Chemistry.*
- *"Fixation of CO_2 into Cyclic Carbonates for the generation of Polyurethanes free of Isocyanates (NIPUs)".* **Marc Martínez de Sarasa Buchaca**. *Inorganic Chemistry.*
- *"Flexible, multifunctional nanoribbon arrays of palladium nanoparticles for transparent conduction and hydrogen detection".* **Elena Hernández**. *Physics.*
- *"Simple and sensitive method for determining gold nanoparticles and food dyes in samples of different nature using surface-enhanced Raman spectroscopy".* **Esther Pinilla**. *Analytical Chemistry.*
- *"Formation of Secondary Organic Aerosol (SOA)".* **Alba Escalona**. *Physical Chemistry.*
- *"Efficient bilirubin removal by BSA functionalized polymeric particles".* **Mª del Prado Garrido**. *Chemical Engineering.*

Friday 15th of June 2019

9:30- 6th session

- *"Phenolic compounds profile of different berry parts from novel Vitis vinifera L. red grape genotypes and Tempranillo using HPLC-DAD-ESI-MS/MS: a varietal differentiation tool".* **José Pérez**. *Food Sciences and Technology.*
- *"Central leptin protects the heart from lipotoxicity by selectively increasing PPARβ/δ in rats with normal leptin sensitivity".* **Blanca Rubio**. *Biochemistry.*
- *"Evaluation of the atmospheric impact of the use of fuels and biofuels".* **María Inmaculada Aranda.** *Physical Chemistry.*
- *"Valorization of ethanol into value added compounds by electroreforming on a PEM cell".* **Alberto Rodríguez**. *Chemical Engineering.*

- *"Blue Aggregation-Induced Emission by Hydrogelation Process".* **Josue Muñoz**. *Organic Chemistry*.
- *"Resveratrol is a non-selective adenosine receptors agonist: potential role in neurodegeneration".* **Alejandro Sánchez**. *Biochemistry.*

11:00- Coffee break

11:30- 7th session

- *"Synthesis of heterocycle compounds catalyzed by imidazolium salts"*. **Mª del Prado Caballero.** *Inorganic Chemistry.*
- *"Interstellar dark clouds chemistry: Kinetic behaviour of neutral-neutral reactions at very low temperatures".* **Antonio Jesús Ocaña.** *Physical Chemistry.*
- *"Electrochemical properties and sensing capacities of different carbon dots families using screen printed electrodes".* **Cristina Montes**. *Analytical Chemistry.*
- *"Evaluation of chemical volatile profile of mango by-products by HS-SPME-GC-MS as potencial source of flavouring compounds".* **Rodrigo Oliver.** *Food Sciences and Technology.*
- *"Graphene based materials applications".* **Antonio Patón**. *Chemical Engineering.*
- *"Alkynyl 1H-Benzo[d]imidazole derivatives: Applications in Organic Electronics".* **Carlos Tardío**. *Organic Chemistry*.

13:00- Prize winners and closing ceremony chaired by **the Vice-Chancellor of Research and Scientific Policy of UCLM** and **the Dean of the Faculty of Chemical Sciences and Technology.** Words of the Vice-Chancellor about the compromises of the UCLM for promoting research activities.

CONFERENCIAS INVITADAS

CI-1

Interfacing molecules and nanomaterials: from carbon nanotube rotaxanes to single-molecule experiments

Emilio M. Pérez*

IMDEA Nanociencia; Ciudad Universitaria de Cantoblanco, Madrid, Spain.
e-mail: emilio.perez@imdea.org

Organic Chemistry

We will provide a global perspective of the work we have carried out in the last five years in the search for novel strategies to interface molecules (0D), single-walled carbon nanotubes (SWNTs, 1D) and bidimensional materials (2D).

In particular, we will present the synthesis of mechanically interlocked derivatives of SWNTs (MINTs), which are rotaxane-type materials, the first example of, a 0D-1D mixed dimensional heterostructure interfaced through the mechanical bond (see Figure).[1] We will also show that the effect of the mechanical bond on the properties of SWNTs is unique, and clearly different from the noninterlocked, supramolecular compounds.[2] We will also show that encapsulation of organic molecules into SWNTs results in modulation of their electronic properties.[3]

In the flatland area, we will report a method to functionalize graphene covalently with exquisite (>97%) atomic selectivity and yield (92%).[4] We will describe improved methods for the production of 2D materials through liquid-phase exfoliation (LPE),[5] and report simple strategies to construct functioning electronic devices from the resulting nanoflakes.[6] Finally, we will describe a “click” reaction protocol for the covalent modification of TMDCs.[7]

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CI-2

RETOS DEL CONTROL DE NANO MATERIALES EN ALIMENTOS

Yolanda Picó

Grupo de Investigación en Seguridad Alimentaria y Medioambiental (SAMA-UV), Universitat de València, España

Analytical Chemistry

El control de los nanomateriales en los alimentos sigue siendo un reto difícil de abordar pero que debe instaurarse para garantizar la seguridad de los consumidores y fijar algunos aspectos relacionados (por ejemplo, el etiquetado o el control). El mayor reto para la química analítica es que son un nuevo tipo de analitos, cuya caracterización involucran tanto información química (composición, masa y concentración numérica) como física (tamaño, forma y agregación). Además existe una gran variedad de nanomateriales (basados en óxidos inorgánicos, en carbono, moléculas orgánicas) que complica todavía más la determinación de estas sustancias. Por todo ello, en esta charla se analiza la situación actual, evaluando y comparando los métodos analíticos implicados y estudios desarrollados hasta ahora para la identificación y cuantificación de nanomateriales en los alimentos. El papel de cada una de las técnicas empleadas (microscopia electrónica, Raman, fraccionamiento en campo de flujo, plasma de acoplamiento inductivo (partícula única, etc.) se analizará en profundidad. Se valoraran el rango de aplicaciones y las ventajas y limitaciones de cada técnica, así como las perspectivas de futuro haciendo hincapié los principales desafíos específicos que quedan dentro de este tema. Por último, también contemplamos perspectivas futuras que plantea el control de nanomateriales en alimentos.

CI-3

Green Chemistry or 'Dream' Chemistry: Clean biocatalytic processes of industrial interest

Pedro Lozano

Grupo de investigación: Química Sostenible. Departamento de Bioquímica y Biol. Molec. B e Inmunol. Facultad de Química, Campus Regional de Excelencia Internacional "Mare Nostrum". Universidad de Murcia, E-30100 MURCIA, Spain

e-mail: plozanor@um.es

The development of sustainable chemical processes turns around two main axes: the selectivity of catalytic transformations, and the easy and clean separation of pure products. The use of enzymes in ionic liquids (ILs) was reported great advantages (*i.e.* improved activity and enantioselectivity, enhanced stability, etc.),[1] and its combination with supercritical technologies was resulted in synergetic and outstanding platforms for developing (multi)catalytic green chemical processes under flow conditions able to directly provide pure products.**[2]** This has been demonstrated by several examples of flow synthetic processes in IL/$scCO_2$ biphasic systems at 100 bar and 40-100ºC (*e.g.* DKR of *rac*-1-phenylethanol,**[3]** biodiesel,**[4]** monoglycerides,**[5]** etc. Straightforward protocols for carrying out biotransformations, product recovering and biocatalysts/ILs reusing without any loss in the overall greenness character of the process, have been developed in recent years.

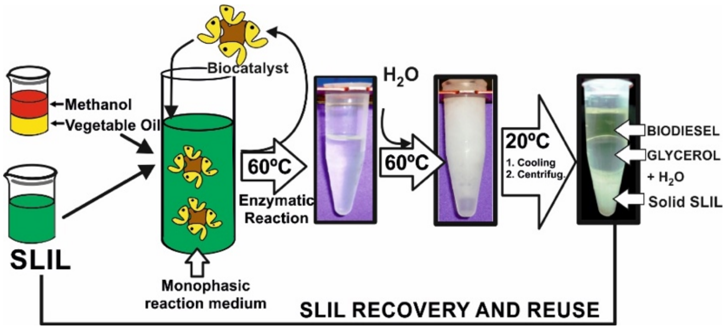

Figure 1. Schema of the protocol for the biocatalytic synthesis of biodiesel in SLIL, and product separation with full recovery and reuse of the SLILs

Sponge-Like Ionic liquids (SLILs) are hydrophobic ILs based on cations with long alkyl side-chains, *e.g*. octadecyltrimethylammoniumbis(trifluoromethylsulfonyl)imide, etc.), which behaves as sponge-like systems by switching from liquid to solid phase with temperature.**[6]** Based on this new property, the SLILs have been applied for developing straightforward and clean approaches for biocatalytic synthesis and extraction of nearly pure compounds of added value (*e.g.* terpene esters,[7] biodiesel,[8] etc.).As can be seen in Figure 1, the SLILs are able for dissolving (soaking) hydrophobic compounds at temperatures compatible with enzyme catalysis (*e.g.* vegetable oil and methanol mixtures are monophasic in $[C_{18}mim][NTf_2]$ at 50°C**[7]**). By cooling reaction mixtures based on these SLILs under room temperature, they are solid phases that can be fractionated by centrifugation, allowing the release (wringing out) of reaction products from the SLIL net, and resulting in two phases: a solid SLIL phase and a liquid phase containing synthetic products (flavour esters, biodiesel, etc.). This approach for product separation can be improved by using centrifugal filters, demonstrating the excellent suitability of this straightforward and green approach for carrying out synthesis and separation of pure products with full recovery and reuse of the reaction system (SLIL and biocatalyst).[6]

Acknowledgements. Work supported by the MINECO CTQ-2015-67927-R, and Fundación SENECA-CARM 20790/PI/18 grants.

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CI-4

Investigación en energía: progreso vs circularidad

David Serrano Granados

Catedrático de Ingeniería Química, Universidad Rey Juan Carlos

Director del Instituto IMDEA Energía

A pesar de los avances que se han producido en los últimos años en el desarrollo e implementación a escala comercial de las energías renovables, todavía en la actualidad más del 80 % de la energía primaria consumida a nivel mundial procede de combustibles fósiles (carbón, petróleo y gas natural). Como consecuencia de las emisiones de gases de efecto invernadero así generadas, la concentración de CO_2 en la atmósfera no deja de crecer año tras año, habiendo superado ya la barrera de las 400 ppm, provocando una aceleración de los efectos del cambio climático.

IMDEA Energía es un instituto de investigación creado por la Comunidad de Madrid con la misión de contribuir a un sistema energético sostenible y de mínimo impacto ambiental, basado en tecnologías energéticas limpias y renovables. Entre las temáticas de investigación que desarrolla y estudia, cabe destacar las siguientes: producción de combustibles sostenibles, energía solar de concentración, sistemas y dispositivos de almacenamiento de energía, redes eléctricas inteligentes, eficiencia energética, valorización de las emisiones de CO_2 y análisis integral de los sistemas energéticos.

El progreso de la investigación en el ámbito de la energía durante las últimas décadas no siempre ha progresado de forma lineal, al estar fuertemente condicionado por factores externos de tipo político y económico. Ello ha llevado a una cierta recurrencia y circularidad en las temáticas de moda que se abordan de forma prioritarias. En este sentido, conceptos, como los de biocombustibles de tercera generación, los vehículos eléctricos, las pilas de combustible, el hidrógeno como vector energético o la valorización de residuos, que en el momento presente son de gran actualidad iniciaron en realidad su desarrollo hace ya bastante tiempo.

PRESENTACIONES

O-1

EVALUATION OF THE ATMOSPHERIC IMPACT OF THE USE OF FUELS AND BIOFUELS

I. Aranda, S. Salgado, P. Martín, B. Cabañas

Dpto. de Química Física, Universidad de Castilla-La Mancha, Avd. Camilo José Cela s/n 13071 Ciudad Real, e-mail: inmaculada.aranda@uclm.es

Physical Chemistry

The combustion of fossil fuels and biofuels generates Volatile Organic Compounds (VOCs), nitrogen oxides (NO_x), CO, CO_2 and particulate matter (PM). These pollutants are causing changes in the climate that affect the environment globally and have an impact in the human health. In addition, fossil fuels are a non-renewable energy source. For those reasons new fuels are being developed from biomass waste (biofuels), which could replace the fossils fuels being used in the same motors, without any modification. In general, the use of biofuels represents lower emissions of compounds such as CO_2 and PM[1], however, in most studies has been observed that biodiesel blends increase NO_x emissions or are similar to diesel fuel[2]. Moreover, some studies have shown that the addition of oxygenated compounds in fuels reduces the formation process of soot[3]. Thus, the use of oxygenated compounds (alcohols, ethers, hydroxyethers…) as additives in fuels is being investigated. In this sense, our research group evaluates the atmospheric impact of the use of these additives in a massive way in new fuels, from the point of view of the chemistry and atmospheric reactivity. Additionally, our group evaluates the atmospheric impact of the gas phase emissions generated in the combustion of these fuels and biofuels, through the kinetic study, evaluation of the Global Warming Potential (GWP), ozone generation capacity and determination of the reaction products. Finally, respect to the PM (soot) emitted, our group carried out studies of physico-chemical characterization and reactivity of these particles with different gases.

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O-2

Electrochemical detection of Rhodamine B by molecularly imprinted polymer modified screen printed carbon electrode and extraction by magnetic multiwalled carbon nanotube poly(styrene-co-divinylbenzene)

Y. Benmassaoud, K. Murtada, R. Salghi, M. Zougagh, Á. Ríos

Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha, Ciudad Real 13071, Spain; E-mail : angel.rios@uclm.es

Analytical Chemistry

Due to its potential health risks on human bodies, the use of Rhodamine B, as well as several other dyes, is banned from food industry. thus, several analytical methods were developed for its determination. furthermore, molecularly imprinted polymers are synthetic receptors for a targeted molecule allowing a better discrimination in a complex matrix.

In this study, a molecular imprinted polymer was prepared and used as a screen-printed carbon electrode modifying film for the rapid electrochemical detection of Rhodamine B. A magnetic solid phase extraction was also carried out using magnetic multiwalled carbon nanotubes poly(styrene-co-divinylbenzene) composite (MMWCNTs-PS-DVB) as sorbent. The MIPs synthesis was optimized by varying the activated TiO_2 and MWCNTs amounts. SPCE electrode was then modified using an optimum volume of TiO_2-MWCNTs-MIP and compared to a non-modified SPCE, a TiO_2-SPCE and a MWCNTs-SPCE by cyclic voltammetry. The magnetic solid phase extraction and detection conditions were optimized as well. the developed method provided a quantification linear range from 5-100 µg L^{-1}. The limit of detection, limit of quantification and relative standard deviation were respectively 1.44 µg L^{-1}, 4.81 µg L^{-1} and 6.59 %. Finally, the present method was applied in real food samples analysis.

O-3

Synthesis of heterocycle compounds catalyzed by imidazolium salts

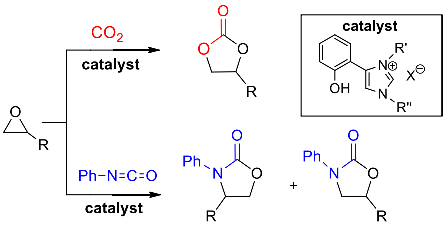
María P. Caballero, Fernando Carrascosa, José A. Castro-Osma, Antonio Otero, Agustín Lara-Sánchez and Juan Tejeda.

Dpto. de Química Inorgánica, Orgánica y Bioquímica, Universidad de Castilla-La Mancha-Centro de Innovación en Química Avanzada (ORFEO-CINQA), Facultad de Ciencias y Tecnologías Químicas, Avd. Camilo José Cela, nº 10, 13071, Ciudad Real.
E-mail : prado.caballero@uclm.es

Inorganic Chemistry

Metal-free organocatalysts based on imidazolium salts showed high efficiency catalyzing the cycloaddition reactions to prepare heterocycle compounds such as cyclic carbonates and oxazolidinones (Scheme 1).1,2 Imidazolium salts performed as bifuntional catalysts and exhibited improved activity for the fixation of CO2. Mechanistic studies revealed that the hydroxyl group promoted the activation of the epoxide ring by nucleophilic attack of the iodide.

Oxazolidinones are an important class of heterocycle compounds which are commonly used as precursors to antibacterial medicines. Using the optimal reaction conditions (2 mol% of 5-hidroxyphenylimidazol at 80 °C in toluene for 24 hours) aromatic and aliphatic epoxides were reacted with phenylisocyanate to prepare the corresponding oxazolidinones. The activity3 of catalysts has an important role in the synthesis since the cyclotrimerization of isocyanates is a competing reaction.



Scheme 1. *Synthesis of cyclic carbonates and oxazolidinones.*

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O-4

SYNTHESIS OF BIO-DERIVED CYCLIC CARBONATES FROM RENEWABLE RESOURCES

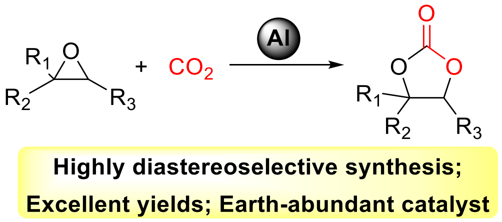
F. De la Cruz-Martínez, J. Martínez, J. Fernández-Baeza, A. Otero, J.A. Castro-Osma, A. Lara-Sánchez

Dpto. de Química Inorgánica, Orgánica y Bioquímica, Universidad de Castilla-La Mancha, Avd. Camilo José Cela s/n 13071 Ciudad Real; e-mail: felipe.cruz@uclm.es

Inorganic Chemistry

The development of bio-based high-value added chemical products to replace petrol-based molecules is one of the main objectives for the scientific community and industry. In this context, a range of new platform molecules derived from waste biomass have been developed and used as monomers for the production of polymeric materials, as solvents and as chemical intermediates.[1] One of the most abundant form of carbon on Earth is carbon dioxide (CO_2) and it is a potential sustainable feedstock for the chemicals industry.[2] The most important transformation of carbon dioxide is its catalytic coupling with epoxides to prepare cyclic carbonates.[3] This reaction has been widely studied over the last decade with the development of a wide range of highly efficient metal- and organic catalysts for this reaction.[3]

In this contribution we report the aluminum catalyzed coupling reaction of carbon dioxide with bio-derived epoxides under mild reaction conditions to afford highly-substituted natural-derived cyclic carbonates with excellent diastereoselectivity, obtaining in some cases one diastereoisomer as the major product.



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O-5

Screening and preliminary biochemical and biological studies of [RuCl(p-cymene)(N,N-bis(diphenylphosphino)-isopropylamine)][BF_4] in Breast Cancer models

E. Domínguez-Jurado, J. A. Castro-Osma, F. de Andrés, I. Bravo, A. Lara-Sánchez, C. Alonso-Moreno, A. Ocaña.

Dpto. de Inorgánica, Orgánica y Bioquímica, Facultad de Farmacia de Albacete, UCLM, 02006, Albacete, España. tfno: +34 687257587; e-mail: elenadj97@gmail.com

Inorganic Chemistry

Breast cancer is the second leading cause of cancer death worldwide. Despite progress in drug discovery, identification of the correct population is the limiting factor to develop new compounds in the clinical setting. Therefore, the aim of this study is to evaluate the effects of a new metallodrug, [RuCl(p-cymene)(N,N-bis(diphenylphosphino)-isopropylamine)][BF_4] (pnpRu-14) as a lead pnp-Ru compound by screening and preliminary biochemical and biological studies in different breast cancer subtypes. The results show that complex pnpRu-14 is much more effective in promoting in vitro cytotoxic effect on HER2+ and RH+/HER2- breast cancer than the reference metallodrugs cisplatin, carboplatin or RAPTA-C. It is important to highlight that pnpRu-14 shows an impressive cytotoxicity against BT474 cells. Caspase-dependent apoptosis is the mechanism of action for these compounds. In addition, treatment of SKBR3, BT474, T47D and MCF7 cancer cells with pnpRu-14 caused an accumulation of cells in the G0/G1 phase cells. The Human serum albumin (HSA), DNA and H1 histones binding properties of the lead compound are reported. Pharmacokinetic and biodistribution studies show a quick absorption of pnpRu-14 in serum with no significant accumulation in any of the tested organs. This work provides evidence to support the preclinical and clinical development of pnpRu-14 in breast cancer.

O-6

2*H*-Benzo[*d*][1,2,3]triazole derivatives with application in organic electronics

B. Donoso, I. Torres, A. Díaz-Ortiz, P. Prieto, J.R. Carrillo

Department of Organic Chemistry, Faculty of Chemical Sciences and Technologies, University of Castilla La Mancha, Av. Camilo José Cela 10, 13071 Ciudad Real, Spain. tfno: 926 295 370; e-mail: Beatriz.Donoso@uclm.es

Organic Chemistry

In the last decades, organic electronics has attracted great attention due to the development of organic semiconductor materials. These materials have practical applications in the latest generation devices organic field effect transistors (OFETs)[1], organic light emitting diodes (OLEDs), organic photovoltaic devices (OPVs), as well as optical waveguides[2] which are essential elements for their implementation in photonic circuits. In our research group, we have studied the preparation and self-assembly properties of different 2*H*-benzo[*d*][1,2,3]triazole derivatives with the aim to determine their behavior as organic waveguides and semiconductors in OFETs (**Figure 1**). As a green approach, we have used computational calculations to avoid unnecessary synthesis. We have calculated the energy and topology of frontier molecular orbitals, and the photophysical properties of a set of derivatives. The selected compounds have been synthesized using cross-coupling reactions. Currently, we are studying the behavior of these compounds as semiconductors in OFETs and optical waveguides.

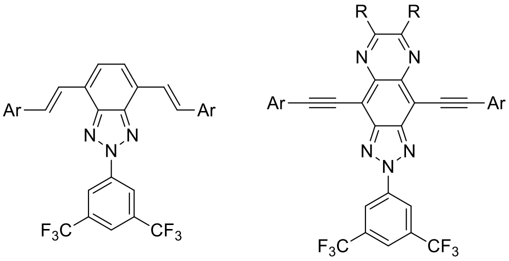

Figure 1. 2*H*-benzo[*d*][1,2,3]triazole derivatives.

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O-7

FORMATION OF SECONDARY ORGANIC AEROSOL (SOA)

Alba Escalona[1], Yolanda Díaz de Mera[1], Alfonso Aranda[1], Diana Rodríguez[2], Ana Mª Rodríguez[2]

[1]Dpto. de Química Física, Universidad de Castilla-La Mancha, Facultad de Ciencias y Tecnologías Químicas, Avd. Camilo José Cela s/n, 13071, Ciudad Real, España.
[2]Universidad de Castilla-La Mancha, Facultad de Ciencias Ambientales y Bioquímica, Avenida Carlos III s/n, 45071 Toledo, España e-mail: alba.escalona@uclm.es
Physical Chemistry

Atmospheric aerosols are considered as one on the main uncertainty sources in the current understanding of the Earth's climate[1]. Previous studies showed that some compound aromatic emitted to the atmosphere give a high SOA (Secondary Organic Aerosol) formation potencial[2,3]. Reaction of the alkenes with ozone proceeds through the formation of a Criegee intermediate (CI). Very recently, it has been found that stabilized CI (sCI) can undergo reactions with SO_2 several orders of magnitude faster than assumed so far[4] producing SO_3, which contributes efficiently to the formation of ground level sulfuric acid[5,6]. We study the ozonolysis reaction of different volatile organic compound following the conditions that lead to the formation and growth of new particles. The effect of water vapor and SO_2 concentrations during the process are also studied and discussed. The reactions have been carried out in a Teflon chamber filled with synthetic air mixtures at atmospheric pressure and room temperature and following the particle formation by SMPS (Scanning Mobility Particle Sizer) and CPC (Condensation Particle Counter).

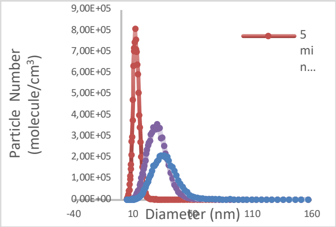

Figure 1. Distribution of particle size at different reaction times.

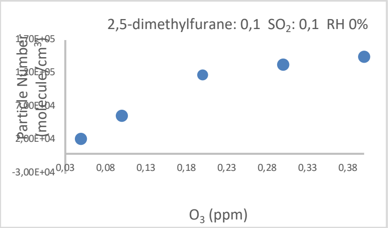

Figure 2. Effect of [O3] on the production of SOA

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O-8

YEASTS WITH PROBIOTIC POTENTIAL

P. Fernández-Pacheco, B. García-Béjar M. Arévalo-Villena, A. Briones

Dpto. de Química Analítica y Tecnología de los Alimentos. Universidad de Castilla-La Mancha, Avd. Camilo José Cela s/n 39005 Ciudad Real.
E-mail: Pilar.FRodriguez@uclm.es

Food Science and Technology

The intestinal microbiota is the most populated community of the human body in which trillions of microorganisms live in symbiosis, contributing to the normal functioning of the organism through its interactions with the host. However, a dysbiosis can cause multiple alterations. One of the most widely used current approaches in the modulation of intestinal microbiota balance is based on the administration of probiotics. Currently, a wide range of probiotic products are marketed, almost all of them are bacteria, but there is also a probiotic yeast (*Saccharomyces boulardii)*. For this reason and due to the increased of researching in this field, the aim of this work was to study the behavior of potential probiotic yeasts already selected by previous works under *in vitro* and *in vivo* conditions. The study was carried out with 5 strains belonging to *Saccharomyces cerevisiae* (2), *Hanseniaspora osmophila* (2) and *kluyveromyces thermotolerans* (1), isolated from food ecosystems and selected due to their good probiotic characteristics *in vitro*. All of them underwent gastrointestinal conditions in studies *in vitro* through the use of Simgi® equipment. It allows the dynamic emulation of the different physiological variables (peristaltic movements, pH, gastrointestinal fluids, etc.) getting effects very similar to those occurred in humans. The results showed that two strains (*S. cerevisiae* and *H. osmophila*) were the most resistant to the process showing a minimal loss of viability. Both were used for experiments *in vivo* with mice and contributed to the recolonisation of gut microbiota process after the use of antibiotics. On the other hand, they showed a transitory adhesion capacity to the mucosa since their concentration decreased drastically after their administration was stopped, besides, they did not show ability to invade tissues by hyphae formation, as show the pathogenic yeasts.

These strains could be used to produce probiotic products (foods and drugs).

O-9

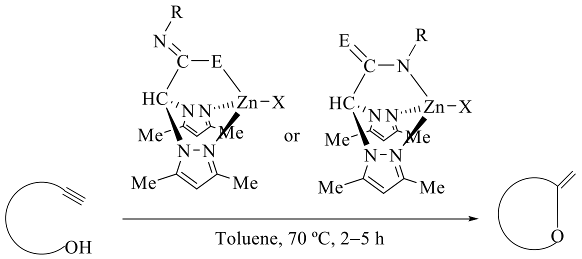
Reactivity of Zinc Complexes Towards Alkynes: Catalytic Intramolecular Hydroalkoxylation of Alkynyl Alcohols

M. A. Gaona, A. Lara-Sánchez, J. A. Castro-Osma, A. Otero, J. Fernández-Baeza, A. M. Rodríguez

Dpto. de Química Inorgánica, Orgánica y Bioquímica. Facultad de Ciencias y Tecnologías Químicas. Universidad de Castilla-La Mancha. Avd. Camilo José Cela, S/N. 13071. Ciudad Real.
e-mail: miguel.gaona@uclm.es

Inorganic Chemistry

Alkyne is a very interesting functional group, as it can be used as a building block to many useful compounds through the generation of new C-C, C-H or C-X bonds.[1] There transformations are usually catalyzed by transition metals, establishing efficient and selective procedures under a variety of conditions. One of these reactions is the intramolecular hydroalkoxylation of alkynyl alcohols for the synthesis of oxygen-containing heterocycles, with several applications in the ppharmaceutical and the fine chemicals industries.[2] However, these catalysts usually involve expensive and/or toxic metals, making them less attractive. In this scenario, zinc-based have grown in interest, due to its abundance and low toxicity.[3] Herein, we describe the synthesis of a series of heteroscorpionate alkyl and amido zinc complexes, their reactivity towards a variety of alkyne compounds and their catalytic activity towards the intramolecular hydroalkoxylation of alkynyl alcohols.



X = Et, $NSiMe_3$
E = S, R = Adam, Naph, Ph
E = O, R = Adam, Ph, (*S*)-MePhCH

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O-10

ANOTHER APPLICATION OF YEASTS: BIODETOXIFICATION OF POLLUTANTS

B. García-Béjar, A. Briones, E. Guisantes-Batan, J. Rodríguez-Flores, P. Fernández-Pacheco, M. Arévalo-Villena

Dep. of Analytical Chemistry and Food Technology, University of Castilla – La Mancha, Camilo José Cela Avenue no number 13071, Ciudad Real, Tel: +34 926285300 Ext: 3423;
E-mail: beatriz.gbermejo@uclm.es

Food Science and Technology

Over the past years, biodetoxification has become a new elimination alternative of compounds such as microbial toxins, chemical pollutant and waste industrial products. Detoxification techniques used in the present are catalogued by the elimination mechanisms carried out: chemical, physical or microbial. Microbial detoxification methods could be a useful and a specific action tool that provide a new way for reducing the presence of pollutants from industrial waste, as heavy metals, or dangerous biotoxins such as mycotoxins. This capability has been traditionally studied in bacteria and microalgae, being the fungi clade barely investigated.

In this study, 213 yeast strains from 20 different species, isolated from Castilla – La Mancha region, were incubated in separated minimal contaminated media supplied with 2 important pollutants for the industry, Aflatoxin B_1 and Zinc. Incubation process was carried out during 5 days at 30ºC. At the end of the process, aliquots were selected and analysed by HPLC and voltammetric techniques respectively. Additionally, strains with the best activity were subjected to complementary assays: biocontrol capability against mycotoxigenic moulds and heavy metal tolerance.

The results show that detoxification capability is toxin and strain dependant. Also, it has been noticed that is not directly related with cell growth, which could indicate that there are mechanisms of bioaccumulation or bioadpsorption involved. In general, yeasts were able to remove more percentage of Zinc than Aflatoxin B_1, higher than 50% of this heavy metal. Regarding the biocontrol activity, almost 50% of the strains presented an inhibition of the mycotoxigenic moulds' mycelium. On the other hand, most of the strains grew at 100 ppm concentration of Zinc. Promising strains will be further studied in order to know more about the mechanisms involved in biodetoxification process.

O-11

EFFICIENT BILIRUBIN REMOVAL BY BSA FUNCTIONALIZED POLYMERIC PARTICLES

M.P. Garrido[1], J.F. Rodríguez[1], A.M. Borreguero[1], M.J. Ramos[1], M. Carmona[1], F.J. Redondo[2], D. Padilla[2]

[1]Dpto. de Ingeniería Química, Universidad de Castilla-La Mancha, Avd. Camilo José Cela 12 13071, tfno: +34 926 29 53 00 ext. 96318; [2] Unidad de Investigación Traslacional, HGUCR, SESCAM, Ciudad Real. e-mail: mariaprado.garrido@uclm.es

Chemical Engineering

Hyperbilirubinemia is an illness caused by a hepatic failure, inducing a dramatic increase of bilirubin concentration in blood. In addition, the majority of patients with hyperbilirubinemia are also affected by kidney failure. Existing systems for the treatment of these patients are complex, expensive and not selective towards bilirubin. Hence, the development of a new material for efficient bilirubin removal is justified.

The main objective of this research was the syntesis of P(St-co-MMA) particles on whose surface PEGMA was incorporated at the identity point of a suspension polymerization reaction, making the particles more compatible with blood. After that, in order to improve the selectivity towards bilirubin, the biofunctionalization of the particles took place by the immobilization of Bovine Serum Albumin (BSA) in its surface.

First of all, polymeric particles with a proper particle diameter to avoid the coagulation of blood during its passing through the particles bed were synthesized. After that, the immobilization of BSA in the particles took place. Finally, some *in vitro* and *in vivo* tests were carried out, obtaining bilirubin removals of 83% and 72%, respectively, in a short period of time.

Considering these results, it can be stated that the new synthesized particulate material is suitable for an efficient and fast bilirubin removal completely compatible with a conventional hemodialysis system.

ACKNOWLEDGEMENTS

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O-12

Flexible, multifunctional nanoribbon arrays of palladium nanoparticles for transparent conduction and hydrogen detection

Elena H. Sánchez, Peter S. Normile, Jose A. De Toro, Rubén Caballero, J. Canales-Vázquez, Esther Rebollar, Marta Castillejo, Jose M. Colino

Instituto Regional de Investigación Científica Aplicada and Depto. de Física Aplicada, Universidad de Castilla-La Mancha, 13017, Ciudad Real; e-mail: elena.hsanchez@uclm.es

Physics

A multifunctional material system consisting of planar arrays of nanoribbons was made with Pd nanoparticles (NPs) obliquely deposited on polyethylene terephthalate (PET) substrates. The PET substrates were first irradiated with a linearly polarized 266 nm laser to obtain a laser-induced periodic surface structure (LIPSS)[1]. As-prepared specimens were comprised of large area, high coherence nanoripple pattern with a mean spacing 200 nm and average amplitude 46 nm. Separately, in a gas phase aggregation vacuum equipment, the Pd NPs (diameter 5 nm) were deposited on the LIPSS at an incidence angle 60-65° directed as to become partially shadowed by the ripple ridges. This resulted in the formation of an array of NP ribbons (thickness ~ 20 nm) on the ripple ridges, the mean ribbon width depending on the deposition incidence angle. After the NPs deposition the surface pattern preserved the spacing and the analysis of AFM and SEM images confirmed the shadow effect and the Pd NPs deposition. These planar arrays were studied as candidate for both flexible, transparent conductors and hydrogen sensors.

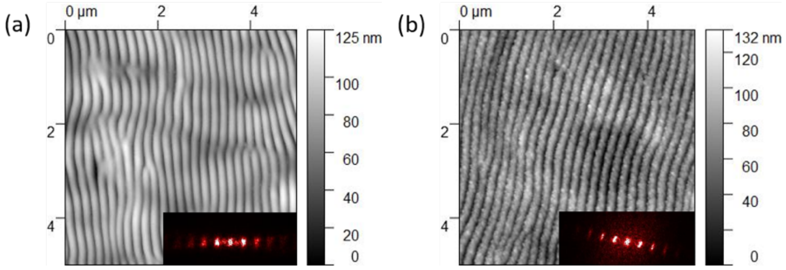

Figure 1: AFM height images (5 x 5 μm^2 size) of (a) PET substrate with LIPSS and (b) Pd nanoparticles on PET substrate with LIPSS. The inset images correspond to the Fast Fourier Transform of each height image.

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O-13

Hydrogels with Iron and Cobalt magnetic Nanoparticles

J. Herrera,[1] V. J. González,[2] P. Prieto,[1] E. Vázquez[2]

[1]Departament of Organic Chemistry, Faculty of Chemical Sciences and Technologies, Castilla-La Mancha University, Camilo José Cela Avenue, S/N, 13071, Ciudad Real, Spain
[2] Instituto Regional de Investigación Científica Aplicada (IRICA), UCLM, 13071 Ciudad Real, Spain. Email: Jesus.Herrera@uclm.es

Organic Chemistry

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 hydrogel (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 communication, 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. Furthermore, graphene is expected to contribute to the mechanical, electrical and thermal properties, and at the same time, cellular adhesion can be increased.

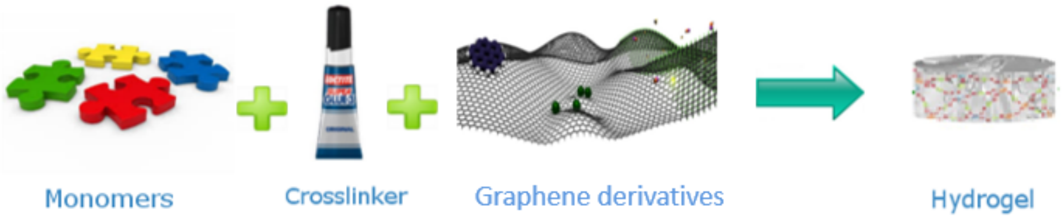

Figure 1. General scope of hydrogels synthesis.

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O-14

Application of the GC-MS/MS and laser-based mass spectrometry techniques for the determination of polycyclic aromatic hydrocarbons (PAH) and their derivatives (OPAH and NPAH) in reference and real soot samples

S. Lara[a], F. Villanueva[a], P.Martin,[a] C. Focsa[b]

[a]Instituto de Investigación en Combustión y Contaminación Atmosférica. Universidad de Castilla La Mancha, Camino de Moledores s/n 13071 Ciudad Real. [b]Laboratorio de física de Láseres, Átomos y Moléculas (PhLAM), Universidad de Lille, CNRS, UMR 8523, Lille, Francia. e-mail: Sonia.LaraGomez@uclm.es

Physical Chemistry

The incomplete combustion processes contribute to a great extent generating atmospheric pollutants in gas phase and particles in suspension. The main source of particulate matter is traffic (May et al, 2014). Their emissions are constituted by soot that is mainly composed of black carbon and SOF (soluble organic fraction) where organic compounds such as Polycyclic Aromatic Compounds (PACs) are adsorbed. They are considered as toxic persistent substances (WHO, 2010). Soot has been classified as the second largest contributor to global warming after CO_2 (IPCC, 2013). Therefore, to know the chemical composition of soot is important in order to evaluate its impact on human health and climate change. In this study, an analytical methodology (microwave assistant extraction, MAE and GC-MS/MS) has been developed and validated for the analysis of PACs (PAH, OPAH, NPAH) from soot particles generated from fuels and biofuels combustion. For that, three soot samples have been investigated Printex-U, a standard reference material (SRM NIST1650b) and a real diesel soot sample. The results showed that the SRM and real sample present differences regarding the adsorption of the heaviest and NPAH since the recoveries of internal standards were 50-136% and 1-41%, respectively. In addition, total PACs retained in the diesel soot was markedly poorer (9 ng/mg- 27 ng/mg) than the extracted from SRM (699 ng/mg). Laser-based mass spectrometry techniques (L2MS and HR-LMS) were also applied to the soot samples in order to obtain more information about the composition of SOF. The results obtained confirmed that diesel soot had a low content of SOF since the PACs were strongly retained, particularly the heavy ones. These differences in the composition of soot samples can be attributed to the conditions in which the diesel soot was produced.

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O-15

CAPILLARY ELECTROPHORESIS METHOD FOR THE DISCRIMINATION BETWEEN BIOELECTROCHEMICAL SYSTEMS FOR THE REDUCTIVE TREATMENT OF HAZARDOUS POLLUTANTS

Luis Fernando León, Francisco Jesús Fernández, José Villaseñor, Pablo Cañizares, Manuel Andrés Rodrigo

Dept. of Chemical Engineering. Faculty of Chemical Sciences and Technologies. Ciudad Real. Spain. E-mail : LFernando.Leon@uclm.es

Chemical Engineering - Bioelectrochemistry

Conventional Bioelectrochemical Systems (BESs) consist in biological anodes and abiotic cathodes, in which bacteria attached to the electrode is able to catalyze the anodic reaction. Commonly, BESs working as Microbial Fuel Cells (MFCs) have been used to produce electrical energy from organic compounds in wastewater, using oxygen as oxidant at the cathode. Applications in BESs have been shooting up in recent decades, as well as improving the materials used in their design.

In this study, several hazardous compounds from different wastewaters have been treated through a reductive process at the cathode of our BESs, seizing the catalytic activity of the biofilm at the anode to reduce the energy input for the electrolysis.

O-16

FUNCTIONALIZATION OF POLYMERS IN SUPERCRITICAL CARBON DIOXIDE

S. López, M.T. García, J.F. Rodríguez, I. Gracia, M.J. Ramos.

Dpto. de Ingeniería Química, Universidad de Castilla-La Mancha, Avd. Camilo José Cela 12, 13071 Ciudad Real; e-mail: Sonia.Lopez@uclm.es

Chemical Engineering

The growing demand for "intelligent" polymers has led to the continuous search for simple and efficient methods for their generation. Polymer-drug conjugates are finding increasing use as novel anticancer agents. Polymeric systems conjugated with a drug result in the controlled release of drugs as this occurs when a carrier material, specifically a polymer, is combined with an active principle so that it is released from the system in a pre-designed way. The release of drugs achieves more effective therapies as it eliminates the administration of both overdoses or doses below the minimum effective dose. In this context, click chemistry emerges as a simple and extremely powerful methodology due to its ability to easily and effectively interconnect different substructures. This has resulted in a wide range of applications in biomedical sciences, organic synthesis and materials science. Click chemistry has the advantage of being a highly reliable methodology, clean, with excellent performance and compatible with a large number of functional groups. One of the most well-known reactions is copper(I)-catalyzed alkyne azide cycloaddition (CuAAC). Terminal alkyne group reacts with an azido group to form a thermally and hydrolytically stable triazole ring, where N, N-dimethylformamide (DMF) or tetrahydrofuran (THF) are the most common solvents used to achieve the conjugation of chemical product. This work aims to find an option that avoids the use of toxic solvents such as THF or DMF, and to use a solvent that can protect medicines from degradation and is additionally environmentally sustainable, using supercritical technology. In recently, considerable attentions have been focused on using supercritical carbon dioxide ($scCO_2$) as a reaction medium for organic reactions due to their attractive physical and toxicological properties. This research focuses on the conjugation of a polymer, polyethylene glycol (PEG), with an active ingredient, coumarin, by means of click chemistry, carrying it out for the first time using supercritical technology without the use of a ligand being necessary for the reaction to be carried out satisfactorily. In order to carry out the reactions corresponding to click chemistry based on Cu catalysis, it is necessary that the polymers previously incorporate azide or alkyne groups on which to carry out the functionalization

O-17

Nanomolar Detection of Dopamine in Human Fluids by N-Doped Carbon Nanoparticles

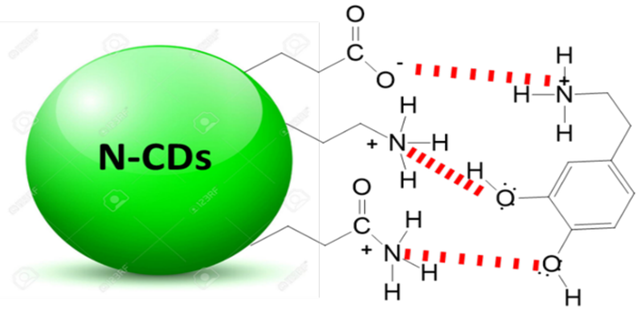
M. Louleb∗, M. Algarra, C. S. Alves, E. Rodriguez-Castellón, L. Latrous, A. Rios, M. Zougagh

Department of Analytical Chemistry and Food Technology. University of Castilla-La Mancha, Avd. Camilo José Cela s/n 13001, Ciudad Real, tfno: +34632466448, e-mail: marwa.louleb@alu.uclm.es

Analytical chemistry

Nitrogen doped carbon nanoparticles, obtained by an easiest hydrothermal and eco-friendly process, was applied as fluorescence sensor for dopamine in urine and serum human fluids at nanomolar concentration range. The HR-TEM images demonstrated well dispersed nanoparticles with 19 nm as mean size, and the ATR and XPS analysis demonstrated the surface composition based in carboxylate and amide/amine functionals groups. The obtained nanoparticles were excitation wavelength dependent, with an optimal emission at 438 nm, which is the basis of the quantification of dopamine when quenches the signal. A linear trend between 0-652 nM was the range of application with a detection limit at 4 nM, acceptable accuracy (>80%) and precision (RSD<10%), showing a highest selectivity with related analytes and acceptable accuracy.

Keywords: N-doped carbon dots, dopamine, quenching, human fluids.



Scheme 1. Schematic representation of the interaction between N-CDs and DA.

O-18

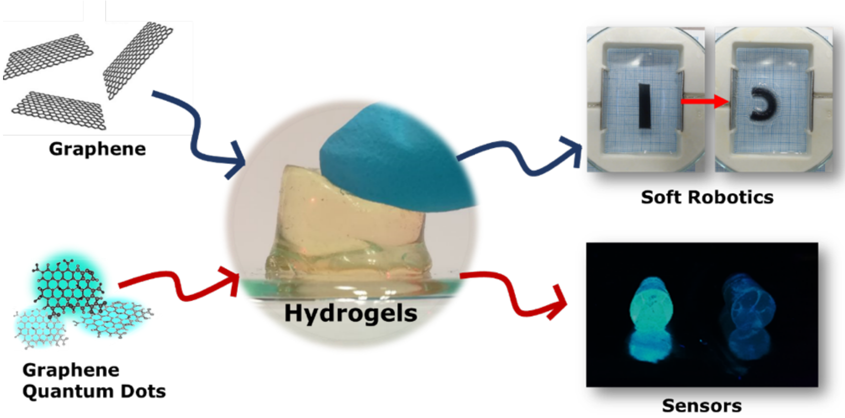
SMART MATERIALS FOR SENSING AND SOFT ROBOTICS APPLICATIONS

A. Martín-Pacheco*, M.A. Herrero, S. Merino, E. Díez-Barra, E. Vázquez

Facultad de Ciencias y Tecnologías Químicas- Instituto Regional de Investigación Científica Aplicada, UCLM, Ciudad Real. E-mail: Ana.MPacheco@uclm.es

Organic Chemistry

Hydrogels, three-dimensional polymeric networks, have been extensively studied as suitable materials for a wide range of applications, from agriculture to biological uses. In recent times, composite hydrogels have been developed as the combination between hydrogels and fillers, improving the properties of the final material. Specially, graphene derivative-based hydrogels have recently opened a new field in science and technology because of their unique properties [1]. In this work, graphene (G) and graphene quantum dots (GQDs) were used to prepare composite hydrogels in order to understand their role in the hydrogel structure, regarding their sizes and chemical surfaces, in comparison with GO [2]. These nanomaterial-based composite hydrogels have been thoroughly characterised and applied in several applications, that range from sensing to soft robotics. For instance, a GQD-based hydrogel can be used as sensor for polyaromatic compounds in water [3], because of their fluorescent properties. In its case, G-based hydrogels can be used as a soft actuator or as fingertips, modulating the precision of gripping in robotics hands [4].



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O-19

FIXATION OF CO_2 INTO CYCLIC CARBONATES FOR THE GENERATION OF POLYURETHANES FREE OF ISOCYANATES (NIPU)s

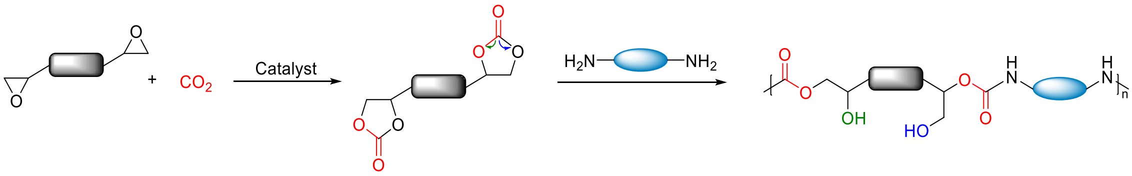
M. Martínez de Sarasa Buchaca, J. Fernández-Baeza, A. Otero, J. A. Castro-Osma, A. Lara-Sánchez

Dpto. Química Inorgánica y Bioquímica. Facultad de Ciencias y Tecnologías Químicas.
Universidad de Castilla-La Mancha. Avd. Camilo José Cela, S/N. 13071 Ciudad Real.
e-mail: Marc.MartinezSarasa@uclm.es

Inorganic Chemistry

In the past few years, a compelling growth of interest has emerged within the plastic industry for the production of polyurethane materials using greener intermediates and processes to substitute the classical route first reported by Otto Bayer during the late 1940s.[1-4] One of these processes is the polyaddition between di-cyclic carbonates and diamines.[5] These polymers combine numerous properties (light weight, excellent strength, energy absorbing performance, comfort features etc.) required in different fields such as medical, automotive and industrial.[6]

In this work, we report the synthesis of a wide range of new polyurethanes free of isocyanates from CO_2, bis-epoxides and diamines derivates with different thermal properties for their specific use within industry (Scheme 1).



Scheme 1

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O-20

ELECTROCHEMICAL PROPERTIES AND SENSING CAPACITIES OF DIFFERENT CARBON DOTS FAMILIES USING SCREEN PRINTED ELECTRODES

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

Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha,
Avd. Camilo José Cela s/n 13004 Ciudad Real, tfno: +34 926 29 53 70;
e-mail: Cristina.Montes@uclm.es

Analytical chemistry

The novelty of this work lays in the comparison of the electrochemical properties of three new carbon-based nanodots species with different structures thus involving diverse crystallinity and quantum confinement degree: carbon nanodots (CNDs), carbon quantum dots (CQDs) and graphene carbon dots (GQDs), here employed as potential sensing tools on screen printed electrodes. The three carbon-based nanodots species were synthesized by different routes, top-down and bottom-up [1, 2] and characterized by TEM, FTIR, Raman, UV-Vis and fluorescence. Measured sizes by TEM were similar between them being the smaller diameter found for CQDs (around 3 nm) while the highest one was found for GQDs (9 nm). All structures were passivated with different functional groups of oxygenated species. Since the aim of this work is to elucidate the potential effect of the carbogenic core structure (crystalline or amorphous) on their electrocatalytic properties, cyclic voltammetry assays were carried out using different specific redox probes such as: potassium hexacyanoferrate(III), hexaammine-ruthenium(III) chloride and dopamine hydrochloride, everyone with specific surface active degree. Better electrocatalytic properties were obtained for the CND, CQD and GQD modified electrodes compared to the bare one. However, CND and GQD electrodes showed better electrochemical features than CQD electrode in terms of reversibility and electronic transfer rate. The electroanalytical capabilities of these carbogenic nanodots as sensing tools were also considered for the detection of bioactives analytes like different vitamins such as ascorbic acid (Vit C), tocopherol isomers (Vit E) and several kind of aminoacids (lysine, arginine, histidine, cysteine, methionine, tyrosine, etc) present in biological samples like food products and biological fluids.

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O-21

BLUE AGGREGATION-INDUCED EMISSION BY HYDROGELATION PROCESS

J. M. Galindo, J. Leganés, M. A. Herrero, E. Díez-Barra, S. Merino, A. Sánchez-Migallón, E. Vázquez

Instituto Regional de Investigación Científica Aplicada (IRICA). Facultad de Ciencias y Tecnologías Químicas. Universidad de Castilla-La Mancha, 13071, Ciudad Real, Spain,
e-mail: Josue.MGalindo@uclm.es

Organic Chemistry

A novel stable physical hydrogel was prepared by radical polymerization of a monomer system including acrylate monomers and a vinyltriazine derivative. For the first time, a phenyltriazine compound is used as monomer in the construction of a hydrogel. The strong interactions between the triazine molecules[1] are the origin of the blue fluorescence that the gel exhibits when being excited under UV-light (Figure 1). Restricted Intramolecular Rotation (RIR) caused by polymer formation and Restricted Intramolecular Motion (RIM) engendered by H-bonds operate as Aggregation-Induced Emission (AIE)-mechanisms.[2] Fluorescence response with respect to the pH change has been studied. The idea of combining soft materials and AIE properties expands the applications of these materials, being able to be used as sensor for ions or molecules capable of interacting with the different functional groups of the polymer network. As well as, the possibility of incorporating other substances into the hydrogel may also allow the development of light-emitting soft materials.

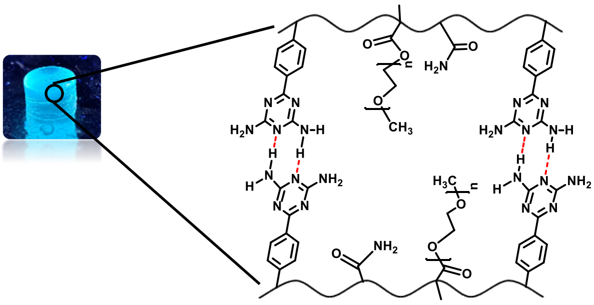

Figure 1: Digital image and chemical hydrogel structure.

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O-22

ADENOSINE RECEPTORS, RESVERATROL AND CANCER

S. Muñoz-López, A. Sánchez-Melgar, J. L. Albasanz, M. Martín

Department of Inorganic, Organic Chemistry and Biochemistry. Faculty of Chemistry Sciences and Technologies. University of Castilla-La Mancha, Avenida Camilo José Cela 10, 13071, Ciudad Real; e-mail: sonia.mlopez@ulcm.es

Biochemistry

Extracellular adenosine is one of the major constituents of the tumor microenvironment and plays a crucial role in apoptosis, angiogenesis and metastasis in cancer. The effects of this purine are triggered through four G-protein coupled receptors: A_1, A_{2A}, A_{2B} and A_3. A_1 and A_3 receptors inhibit adenylyl cyclase activity through $G_{i/o}$ protein whereas A_{2A} and A_{2B} receptors activate this enzymatic system through G_s protein. Current efforts are focused on resveratrol (RSV), a diet polyphenolic phytoalexin found in many plant species such as grapes, peanuts and berries and also in red wine. This molecule has shown promising effects in inhibiting proliferation and cancer progression in several tumoral models. However, its molecular mechanisms are poorly understood. Recently, our group has found that RSV acts as a non-selective adenosine receptor agonist. This study provides strong evidence that adenosine receptors are a primary target for RSV. Adenosine receptor have been involved in cancer. Therefore, the aim of the present work was to study the antitumoral effect of RSV and the possible mechanism involving adenosine receptors. To this end, two tumoral cell lines were used, rat C6 glioma and human HeLa epithelioma cervix cells which is one of the most aggressive cancer in woman. Cell viability assays shown that RSV inhibited proliferation in a time and concentration dependent manner in both tumoral cell lines. RSV was also able to modulate these receptors and their corresponding transduction pathway. All together these results suggest that antitumoral effect of RSV could be through adenosine receptors activation.

O-23

INTERSTELLAR DARK CLOUDS CHEMISTRY: KINETIC BEHAVIOUR OF NEUTRAL-NEUTRAL REACTIONS AT VERY LOW TEMPERATURES

A. J. Ocaña[1,], S. Blázquez[1], D. González[1], B. Ballesteros[1,2], M. Antiñolo[1,2], J. Albaladejo[1,2] and E. Jiménez[1,2]

[1]Departamento de Química Física. Facultad de Ciencias y Tecnologías Químicas. Universidad de Castilla-La Mancha, Avd. Camilo José Cela, 1B. 13071 Ciudad Real, Spain. [2]Instituto de Combustión y Contaminación Atmosférica (ICCA). Universidad de Castilla-La Mancha, Avd. Moledores s/n. 13071 Ciudad Real, Spain. tfno: +34 926 29 53 00. Ext. 96337;

e-mail: antoniojesus.ocana@uclm.es

Physical Chemistry

In the field of astrochemistry, complex organic molecules (COMs), are defined as molecules which are formed by C, H, O and/or N atoms and have 6 or more of atoms[1] Understanding how the COMs which are present in interstellar dark clouds are formed and destroyed is crucial in order to model the abundances of them. Usually, the rate coefficient (*k*) values used in modelling are extrapolations from temperature dependences reported at $T > 200$ K but it is known that these reactions are much faster than estimated by Arrhenius equations obtained at $T > 200$ K[2].

The aim of this work is to provide new kinetic data for the gas phase reactions of OH radicals with COMs at dark clouds temperatures (10-100K), using the continuous and pulsed[3] CRESU (French acronym that stands for Reaction Kinetics in Uniform Supersonic Flow) technique. This technique is based on the isentropic gas expansion through a Laval nozzle from a high-pressure region to a low-pressure region to cool down the gas to get uniform jets in temperature and total gas density over several tens of cm. The impact of the measured rate coefficients will be discussed at the conference.

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O-24

EVALUATION OF CHEMICAL VOLATILE PROFILE OF MANGO BY-PRODUCTS BY HS-SPME-GC-MS AS POTENCIAL SOURCE OF FLAVOURING COMPOUNDS

R. Oliver-Simancas[1], M.C. Díaz-Maroto[1,2], M.S. Pérez-Coello[1], Alañón, M.E.[2]

[1] Department of Food Technology, University of Castilla-La Mancha, Avd. Camilo José Cela 10, 13071, Ciudad Real, Spain; tfno: ext. 96340; e-mail: Rodrigo.Oliver@uclm.es

[2]Area of Food Technology, Regional Institute for Applied Scientific Research (IRICA), University of Castilla-La Mancha. Avd. Camilo José Cela, 10, 13071 Ciudad Real, Spain.

Food Science and Technology

Mango (*Mangifera indica L.)* is an appreciated tropical fruit for its unique characteristics of aroma and flavor. During its processing stages, large quantities of bio-wastes are produced which represent from 25 to 60 % of the fruit approximately. Several studies have reported the value-added of mango wastes especially as a natural source of functional and nutraceutical ingredients derived from the vast variety of bioactive compounds existing in those discarded fractions (Jahurul et al., 2015). However, other different potential applications of mango by-products in the food industry have already not been addressed until now.

Therefore, due to the appreciated sensory characteristics of mango, it is thought that revalorization of mango wastes as a source of natural flavourings may be considered an alternative for exploiting those by-products. For that scope, the chemical composition of outstanding mango by-products (skin, seed) in comparison with mango pulp were analysed by HS-SPME-GC-MS with the aim to characterize their volatile composition and evaluate the flavouring potential of mango by-products.

Results showed that mango peel exhibited large quantities of volatile compounds (monoterpens, sesquiterpens, alcohols, aldehydes,…) in higher concentrations than in mango pulp. Furthermore, the odor activity values (OAVs) indicated that mango peel was also the part of mango with the highest values in herbaceous green and floral features. Therefore, mango peel by-product is proposed as a natural source of volatile compounds for prospective applications in the food industry.

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O-25

GRAPHENE BASED MATERIALS APPLICATIONS

A. Patón-Carrero, J.L. Valverde, V. Gonzaga, S. Ordoñez-Lozoya, A. Romero

Dpto. de Ingeniería Química, Universidad de Castilla La Mancha, Avd. Camilo Jose Cela s/n 13071 Ciudad Real tfno: +34 926 29 53 00 ext. 96322;

e-mail: Antonio.Paton@uclm.es

Ingenería Química

Since Geim and Novoselov won the Nobel Prize in physics for the isolation of one perfect atomic layer of graphene in 2010, the interest of researchers towards graphene field has awakened. In the search for the best way to synthesize graphene, a large number of new carbon nanomaterials have been discovered. One of the most important materials discover around graphene is graphene oxide (GO), which can be defined as few functionalized layers of graphene with molecules of carbon, oxygen and hydrogen attached to the structure [1]. This material and its derivatives are widely used in a wide range of applications, from electronic devices and medical treatments to adsorber media.

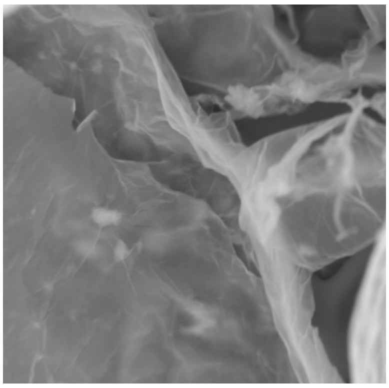

Figure 1: SEM Image of graphene oxide

The development of this applications is one of the new research area for this new material. Two of the most important applications for graphene oxide are the adsorption of chemical molecules and the electrochemical applications. On one side, the adsorption capacity of this new materials provides a reusable resource for harmful molecules as dyes, heavy metals or organic compounds. On the other side, the electrochemical applications based on the doping of heteroatoms as catalyst for oxygen reduction reaction (ORR) provide new green free-metal catalyst for this purpose.

O-26

New electroFenton reactors for wastewater treatment

J.F. Pérez, A. Moratalla, C. Sáez, J. Llanos, C. López, P. Cañizares, M.A. Rodrigo

Dpto. de Ingeniería Química, Universidad de Castilla-La Mancha, Avd. de Camilo José Cela, Edificio Enrique Costa, Ciudad Real, tfno: +34 926 295 300 ext 96319;
e-mail: josefernando.perez@uclm.es

Chemical Engineering

ElectroFenton has been extensively studied on laboratory scale for the abatement of hardly-biodegradable organic pollutants in wastewater. However, most of the works are carried out on a laboratory scale. The objective of the present work is the design and construction of electroFenton reactors with potential to be scale up and applied on an industrial scale. Figure 1 shows schematically the final prototype which integrates synergistically different technological solutions:

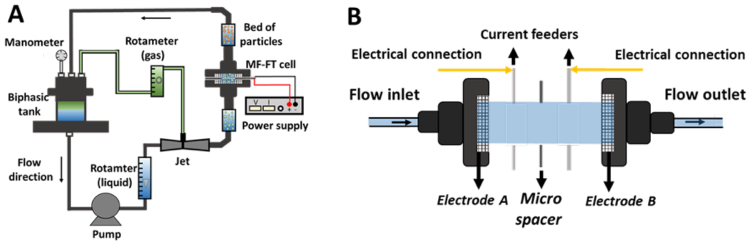

Figure 1. A) Schematic setup of the system; B) A micro-fluidic flow-through cell

In particular, the reactor incorporates an efficient pressurized-jet aerator to supply large oxygen flow rates at moderate pressure, a microfluidic flow-through reactor to simultaneously minimize ohmic resistance and maximize mass-transfer, equipped with state-of-the-art electrodes and a fluidized bed of particles to promote Fenton reaction.

Results show an outstanding performance of the microfluidic flow-through cell in comparison to a commercial flow-by, a synergistic combination of anodic oxidation and electroFenton in this reactor [1] or the lowest specific energy consumption ever reported under similar conditions for the production of hydrogen peroxide. The communication summarizes the development and current application of this reactor.

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O-27

PHENOLIC COMPOUNDS PROFILE OF DIFFERENT BERRY PARTS FROM NOVEL *VITIS VINIFERA* L. RED GRAPE GENOTYPES AND TEMPRANILLO USING HPLC-DAD-ESI-MS/MS: A VARIETAL DIFFERENTIATION TOOL

J. Pérez-Navarro[a], P.M. Izquierdo-Cañas[b], A. Mena-Morales[b], J. Martínez-Gascueña[b], J.L. Chacón-Vozmediano[b], E. García-Romero[b], I. Hermosín-Gutiérrez[a], S. Gómez-Alonso[a]

[a]Instituto Regional de Investigación Científica Aplicada, Universidad de Castilla-La Mancha, Av. Camilo José Cela s/n, 13071 Ciudad Real. [b]Instituto Regional de Investigación y Desarrollo Agroalimentario y Forestal de Castilla-La Mancha (IRIAF), Ctra. Albacete s/n, 13700 Tomelloso, Ciudad Real. e-mail: jose.pnavarro@uclm.es

Food Science and Technology

Phenolic compounds are bioactive secondary metabolites found in plants and fruits with potential beneficial effects on human health. In addition, these compounds are regarded as antioxidants and antimicrobials in food. Grape phenolic composition is a determinant factor for red wine quality, since it is related to important sensory attributes such as color, bitterness and astringency, and also to aging aptitude. Moribel and Tinto Fragoso are two novel red grape genotypes (*Vitis vinifera* L.) recently identified in Castilla-La Mancha, which are not previously registered in any national or international data base. They have been studied genetically but until now, no deep studies are still available about their phenolic composition. The aim of this work was to perform a comprehensive study of the phenolic profile of Moribel and Tinto Fragoso red grape genotypes (*V. vinifera* L.) for the first time and compare them to that of Tempranillo using HPLC-DAD-ESI-MS/MS over two consecutive vintages (2016 and 2017).

More than 50 phenolic compounds were identified in different berry parts from these grapes, of which, as far as we know, some anthocyanin and flavonol dihexosides were reported for the first time in *V. vinifera* grapes. According to phenolic composition, these novel red grape cultivars have interesting oenological properties. Tinto Fragoso may be a potential source of anthocyanins, which are responsible for the bluish-red and purple color of young red wines, and Moribel genotype was characterized by having a phenolic profile similar to Tempranillo cultivar, which may be due to a genetic relationship. Application of Principal Component Analysis (PCA) to experimental data showed a good separation of the novel grape genotypes and Tempranillo according to the phenolic profile of skins and seeds, mainly based on the proportion of trisubstituted anthocyanin derivatives, flavonols and flavan-3-ols, being a useful tool to differentiate these grape genotypes.

O-28

SIMPLE AND SENSITIVE METHOD FOR DETERMINING GOLD NANOPARTICLES AND FOOD DYES IN DIFFERENT SAMPLES USING SURFACE-ENHANCED RAMAN SPECTROSCOPY

E. Pinilla, M.J. Villaseñor, A.M. Contento and A. Ríos

Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha, Avenue Camilo José Cela s/n 13071 Ciudad Real, Tfno: +34 926 295 370;
e-mail: Esther.Pinilla@uclm.es

Analytical Chemistry

Metallic nanoparticles, especially, gold nanoparticles (AuNPs) are used in several applications such as photoelectrochemical materials, optical sensors, diagnostic tests with biomedical imaging or catalysts showing unique physicochemical and optical properties due to the oscillation of localized surface plasmons (LSP). Despite their benefits, there are serious concerns for their possible environmental and biological impact. For these reasons, it is necessary to develop analytical methodologies controlling these particles.

SERS (Surface-Enhanced Raman Spectroscopy) has emerged thanks to the incorporation of noble metal nanoparticles to common Raman spectroscopy, providing so an enhanced signal due to the resonant excitation of LSP on metal nanoparticles surface that generates a magnification of electromagnetic field.[1]

In this report, on the one hand SERS signal has been indirectly used to determine AuNPs, incorporating on the substrate different organic molecules that belong to the family of synthetic food dyes with good ability to be adsorbed on metallic gold surfaces and that could be suitable candidates as AuNPs-sensor. Erythrosine B showed to be the best candidate producing a good SERS activity in presence of this nanomaterial. The proposed analytical method has been thoroughly validated for determining AuNPs in environmental, cosmetic and biological samples considering the principles of analytical nanometrology.[2] The obtained results were satisfactory with a lineal range between 1-12 ng L^{-1}, detection limit of 1 ng L^{-1} and precision (%RSD) of 4.2 for 8 replicates of 6.8 ng L^{-1} AuNPs solution. In the opposite way, this method was also used for determining erythrosine in food samples. This last method was also validated with a lineal range between 5-150 µg L^{-1} and a detection limit of 4.7 µg L^{-1} as figures of merit.

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O-29

Valorization of ethanol into value added compounds by electroreforming on a PEM cell

A. Rodríguez, A.R. de La Osa, A. de Lucas-Consuegra, J.L. Valverde

Department of Chemical Engineering. University of Castilla-La Mancha Avd. Camilo José Cela, 1213071, Ciudad Real, España. Tlf: 926 295300 Alberto Rodríguez Gómez:
E-mail: Alberto.RGomez@uclm.es

Chemical engineering

In recent years bioethanol has become one of the most promising alternatives to traditional fossils fuels. However, the overproduction on a global scale (biodiesel crisis) and also on a national scale (surplus in wine production and industrial waste of alcohol production) have required the search of different strategies for the valorization of this compound. In this research work, the electrochemical reforming process is proposed as an alternative, which presents some advantages (less deactivation and selectivity limitations) compared to conventional catalytic processes. Using a polymer membrane electrochemical reactor (PEM cell), in the anodic compartment the oxidation reaction of ethanol takes place, producing protons and organic compounds of industrial interest. Reduction reaction takes place in the cathodic compartment, generating high purity hydrogen. It is well known that no special attention is given to the organic compounds in the available literature [1]. For that reason, the aim of this research work is to maximize the production of valuable liquids obtained in the anodic compartment, derived from the ethanol oxidation, in order to improve the valorization of this compound. Some of these products are acetaldehyde, acetic acid and ethyl acetate. Acetaldehyde is an important intermediate in organic synthesis, used as a raw material for the production of acetic acid, acetic anhydride, ethyl acetate, pyridine, medicines or plastics. Industrially, it is obtained from the direct catalytic oxidation of ethylene through Wacker process, which is very intensive in terms of energy, so the electrocatalytic alternative is presented as a more efficient option. Under this scenario, ethanol electro-reforming process was carried out at 80 ºC, 1 atm and 1.15 ml/min of flow rate for cathodic and anodic chamber. In order to verify the viability of the system, different experiments were carried out: linear voltametries, chronopotenciometries at various levels of intensity, stabilities essays to estimate the total consume and impedance spectroscopy essays. Commercial Pt/C was used for the cathode and PtRu/C (synthetized through the modified polyol method) for the anode.

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O-30

LEPTIN. “FROM 1969 TO THE PRESENT DAY”

B.M. Rubio, L. Mazuecos, N. Gallardo, A. Andrés

Dpto. de Química Inorgánica, Orgánica y Bioquímica, Universidad de Castilla La Mancha (UCLM), Avd. Camilo José Cela 10 13005 Ciudad Real, tfno: +34 655064734;
e-mail: altajagra@gmail.es

Biochemistry

The development of cardiovascular diseases (CVD) is the main cause of death and disability of the elderly world population, being some of the major risk factors obesity or Diabetes Mellitus (DM). In search of preventive strategies, and after its discovery as a regulator of body fat reserves (Halaas JL et al., 1995), leptin began to be studied as a point of control of energy metabolism. This hormone is produced mainly by the white adipose tissue, but the receptors for the hormone are distributed in a great variety of tissues, being very important its discovery in the hypothalamic nuclei related to the appetite control, metabolism and thermoregulation.

Our group tries to respond to the effects caused by the use of central leptin in peripheral tissues; however, and unlike other studies, our measures are based on the activation of the sympathetic nervous system as an intermediary of the effects of leptin. In this case we have shown that central leptin causes alterations in the heart metabolism, such as favoring the metabolic fuel change, reducing lipotoxicity or generating a specific pattern of cardiac atrophy (Mora et al., 2018). Similarly, white adipose tissue is able to guide a browning model by increasing the metabolic rate, favoring oxidative metabolism and thermogenesis.

Our current studies focus on the use of nuclear PPAR receptors as intermediates of the action of central leptin, based on the use of the specific PPARβ / δ antagonist.

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O-31

ALTERNATIVE PHOTOSENSITIZERS TO ENHANCE THE SENSITIVITY OF NMR SPECTROSCOPY THROUGH HYPERPOLARIZATION METHODS ON MICROCOILS

M. Ruiz-Castañeda, B. Donoso, M. Mompeán, A. Velders, J. R. Carrillo, A. Díaz, A. de la Hoz, V. Gómez

Dpto. de Química de Inorgánica, Orgánica y Bioquímica, Universidad de Castilla-La Mancha,
Avd. Camilo J. Cela, 10, 13071 Ciudad Real;

E-mail: Margarita.RAlvaro@uclm.es

Organic Chemistry

Nuclear Magnetic Resonance (NMR) Spectroscopy is one of the most powerful and versatile analytical techniques available today used in chemistry, physics, biology and medicine. NMR is widely employed to probe the local structure and dynamic properties of atoms. However, NMR suffers from an intrinsically low sensitivity, precluding the application of NMR spectroscopy to mass- and volume-limited samples.

Here, we present the use of hyperpolarization methodology to enhance the NMR sensitivity. These experiments are initiated with the excitation of a photosensitizer by an external laser source.

Furthermore, we have combined the use of microcoils with the hyperpolarization methodology to provide a breakthrough in both mass and concentration sensitivity for the study of low solubility samples. In previous works, our group have been able of detecting subpicomole quantities of sample and a sample concentration in the µM range for a fluorinated compound.[1]

The most common photosensitizers are flavins. However, flavins are prone to photoreduction during the hyperpolarization experiments as the process is not perfectly cyclic and they form aggregates. Thus, we are focusing on the development of alternative photosensitizers as triazines derivatives and organometallic compounds of ruthenium.

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O-32

SYNTHESIS OF FURFURAL BY DEHYDRATION OF PENTOSES. TOWARDS FULL BIOMASS VALORISATION

M. Salgado, A.J. Huertas-Alonso, A. Lorente, M.P. Sánchez-Verdú, A. Moreno

Dpto. de Química Inorgánica, Orgánica y Bioquímica, Universidad de Castilla-la Mancha, Avd. Camilo José Cela nº10, 13071 Ciudad Real.
E-mail: Manuel.Salgado@uclm.es

Organic Chemistry

Furfural (FF), or furan-2-carbaldehyde, is a green key compound which has been recognized as a top-value bio-based chemical by United States Department of Energy[1]. Therefore, it is useful to be employed in a wide range of applications, from the chemical industry to the agrochemical sector[2], as well as in the production of bio-fuels and solvents. FF production is generally carried out by the initial dehydration of pentoses, such as xylose. This process usually involves acidic conditions, for instance, with inorganic mineral acids, heterogeneous catalysts or sulfonic acids. Moreover, the mechanism for FF production has been also suggested by many researches[3].

Particularly, FF can be obtained from C_5-sugars found in hemicelluloses, one of the three major components in lignocellulosic biomass, including cellulose and lignin [2]. Nowadays, due to the diminishing of fossil fuel reserves, together with the detrimental augmentation of greenhouse effects, the worldwide scientific community has focused on novel routes employing sustainable C-sources for the synthesis of the top platform chemicals [4]. Regarding to the top, the main goal of this work is the optimization of some variables (temperature, time, solvent, catalyst…) in order to achieve the best yield of FF from xylose, as well as the influence of these variables over the valorization of some lignocellulosic wastes, always keeping the Green Chemistry Principles.

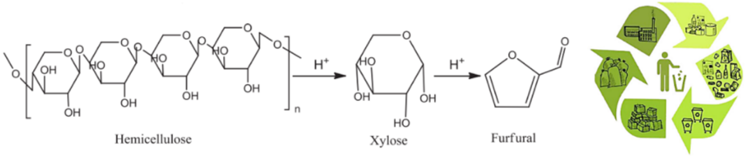

Figure 1. General chemical path from biomass to furfural

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O-33

STUDY BY AF4-ICP-MS OF THE PtNPs' BEHAVIOUR IN NATURAL AND SYNTHETIC FRESHWATERS

A. Sánchez-Cachero[1], N. Rodríguez Fariñas[1], A. Ríos[2], R. C. Rodríguez Martín-Doimeadios[1]

[1] Environmental Sciences Institute (ICAM), 45071, Toledo, Spain.
[2] Faculty of Chemical Sciences and Technologies, Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha, 13071, Ciudad Real, Spain.

E-mail: armando.sanchez@alu.uclm.es

Analytical Chemistry

Platinum nanoparticles (PtNPs) present exceptional catalytic reactivity which makes them useful for automotive catalysts. However, mechanical abrasion and chemical reactions at the catalyst surface may cause PtNPs' emission through exhaust gasses of vehicles, leading to dispersion and accumulation of PtNPs all over environmental compartments [1]. The study of these NPs in relevant environmental samples is necessary to know the potential associated risks. This is indeed a challenging task for analytical chemistry, and the development of novel and powerful analytical techniques is necessary [2]. New analytical strategies based on the coupling of hydrodynamic separation techniques with elemental specific detectors have been recently proposed. One of the most promising combination is asymmetric flow field flow fractionation hyphenated to inductively coupled plasma mass spectrometry (AF4-ICP-MS). This system can give simultaneous information about particle size range, concentration and composition, but there are nearly not applications for PtNPs, especially in environmental samples. In this work a methodology based on AF4-ICP-MS has been developed for the study of PtNPs in water samples. Once the optimization of the separation and acquisition conditions in AF4-ICP-MS is done, PtNPs (5, 30 and 50 nm) were separated in one single fractogram run. It was also possible to detect transformations of these PtNPs in natural and synthetic freshwaters samples under the influence of relevant environmental factors such organic matter, pH, ionic strength or incubation time.

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O-34

RESVERATROL IS A NON-SELECTIVE ADENOSINE RECEPTOR AGONIST: POTENTIAL ROLE IN NEURODEGENERATION

A. Sánchez-melgar, J.L. Albasanz, M. Martín

Dpto. de Química Inorgánica, Orgánica y Bioquímica, Universidad de Castilla La-Mancha, Avd. Camilo José Cela 10 13071 Ciudad Real, tfno: +34 926295 ext: 96343; e-e-mail: alejandro.sanchez@uclm.es

Biochemistry

Aged population is increasing fast in the last decades. Hence, neurodegeneration is one of the greatest global challenges for health research in the next future due to the major risk factor is the age. Currently, it is described that around 50 million of people live with any kind of dementia. By 2050, the incidence of neurodegeneration-associated diseases is estimated to be triplicated, which supposes an over cost for health services. Resveratrol (RSV) is a natural polyphenolic compound produced by plants under stressful conditions that has shown multiple beneficial properties for human health, including neurodegeneration. Unfortunately, the precise molecular mechanisms by which this phytochemical exhibits its biological functions remain still unclear. Therefore, the aim of this work was to investigate whether RSV was able to induce modulation on adenosine-mediated signaling. Our results strongly indicated, by biochemical and informatics approaches, that RSV acts as a non-selective adenosine receptor agonist, which affects to adenosine-mediated signaling in rat glioma C6 cell line. On the other side, long-term RSV supplementation in diet reversed the age-related effect on adenosinergic system in total brain from SAMP8 mice, an animal model of Alzheimer's disease. Accordingly, plasma membrane-expressed A_1 receptor was found to be increased whereas no changes on plasma membrane-expressed A_{2A} receptors were detected in RSV-treated mice as compared to their age-matched controls. Moreover, an increase of A_1 receptor-mediated signaling was observed, but a desensitization of A_{2A} receptor-mediated signaling was induced by RSV. On the other side, adenosine production/degradation carried out by the enzymes 5'-Nucleotidase and Adenosine Deaminase, respectively, were both found to be significantly reduced in RSV-treated mice, suggesting an alteration on adenosine level. In conclusion, RSV acts as a non-selective agonist, exerting a tissue-dependent biological effect. Taking all of this into account, adenosine receptors should be considered as a primary target for resveratrol and, although further experimentation is required, new therapeutic strategies involving resveratrol and adenosine-mediated signaling should be aimed in the future for neurodegeneration-associated diseases.

O-35

ALKYNYL 1*H*-BENZO[*d*]IMIDAZOLE DERIVATIVES: APPLICATIONS IN ORGANIC ELECTRONICS

C. Tardío, R. Martín, A. de la Hoz, J. R. Carrillo, P. Prieto

Department of Organic Chemistry, University of Castilla-La Mancha, Avenue Camilo José Cela 10 13071 Ciudad Real, Tfno: +34 926 29 53 70;
e-mail: carlos.tardio@uclm.es

Organic Chemistry

In the last years, self-assembly of π-conjugated organic molecules has undergone a big growth due to the improvement of the optoelectronic properties offered by these structures with respect to isolated molecules. The shape, morphology and photophysical properties play a fundamental role in the applicability of the structures.[1] Multifunctionality is a desirable objective in these new structures. In this context, we have synthesised a series D-A-D of alkynyl compounds using 2*H*-benzo[*d*]triazole and benzo[*c*][1,2,5]thiadiazole as the acceptor cores. Self-assembly of these derivatives has generated structures with a high applicability in organic electronics as waveguides[3] and OFETs.[2] With the aim to define the structure-property relationship, in this report we have changed the acceptor moiety to 1*H*-benzo[*d*]imidazole (Figure 1). The structures resulting from self-assemble were studied by SEM and PL microscopy. The main objective is to study the applicability of these compounds as organic semiconductors in OFETs, or in the field of nanophononics as optical waveguides.

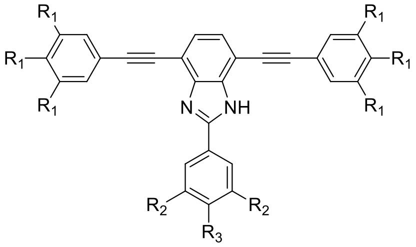

Figure 1. Structure of alkynyl 1*H*-benzo[*d*]imidazole derivatives.

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POSTERS

P-1

ELECTROCHEMICALLY-ASSISTED DEWATERING FOR THE REMOVAL OF OXYFLUORFEN FROM A COAGULATION/FLOCCULATION SLUDGE

G. Acosta-Santoyo[1,2], A. Raschitor[1], E. Bustos[2], P. Cañízares[1], M.A. Rodrigo[1], J. Llanos[1]*

[1]Dpto. de Ingeniería Química, Universidad de Castilla-La Mancha, Edificio Enrique Costa Novella, Campus Universitario s/n 13071 Ciudad Real; [2]Centro de Investigación y Desarrollo Tecnológico en Electroquímica, Parque Tecnológico Querétaro s/n 76090 Querétaro, México
e-mail: Javier.Llanos@uclm.es

Chemical Engineering / Water Electroremediation

Electrochemical dewatering is an emerging and energy-efficient alternative technology that provides improved liquid/solid separation for the treatment of wastewater sludge. This work focuses on the evaluation of the electrochemical dewatering of sludge obtained from electrocoagulation of water polluted with oxyfluorfen. To do this, sludge samples from electrocoagulation assays were treated using this approach in order to reduce the contaminated volume of reclaimed water and, at the same time, facilitating the degradation of oxyfluorfen in the remaining sludge via electrolysis using boron-doped diamond electrodes at different electric field treatments.

P-2

POTENTIAL APPLICATIONS OF OENOLOGICAL BY-PRODUCTS AS ANTIOXIDANTS IN PROCESSED MEAT PRODUCTS

M. Alarcón, A. Soriano, M. E. Alañón, M. S. Pérez-Coello

Area of Food Science and Technology, University of Castilla-La Mancha, Avda. Camilo José Cela 10, 13071, Ciudad Real, Spain. tfno: ext.96340
e-mail: Marina.Alarcon@alu.uclm.es

Food Science and Technology

One of the major causes of quality deterioration of meat products are the oxidative phenomena. Lipid oxidation is the main reaction produced which entails losses in nutritional and organoleptic quality reducing meat self-life. This fact causes the essential use of antioxidants in meat products. In order to decrease the use of synthetic antioxidants, in recent years, research about antioxidants of natural origin has increased and, in particular, the by-products revalorization generated during the processing of food, show a wide interest in the food industry. Therefore, the aim of this work was to study the antioxidant capacity of several oenological by-products in different meat products.

Different types of meat products were carried out: pork and venison burger patties, pork cooked model system and "salchichon". In all products two control samples were assayed: C (without antioxidants) and AC (with 400 ppm sodium ascorbate). Likewise, oenological by-products were employed as natural antioxidants in different concentrations (1-5 %): oak wood, stems, vine-shoots and lees. Development of lipid oxidation during self-life of the different products was evaluated. Lipid oxidation was determined by the thiobarbituric acid reactive substances content (TBARs), and hexanal was evaluated as the volatile compound indicator of lipid oxidation by GC-MS throughout the manufacturing process and store.

A significant reduction of lipid oxidation (TBARs) was found in the different meat products using oenological by-products. This effect was appreciated immediately after the natural antioxidant addition in samples. Furthermore, the inhibition of oxidation was reflected on the hexanal content which showed lower values compared to control samples. In all cases, natural antioxidants were more effective than sodium ascorbate.

Therefore, oenological by-products could be employed as natural antioxidants against lipid oxidation in meat products.

P-3

IONIC LIQUID AND MULTIWALLED CARBON NANOTUBES FOR EXTRACTION OF CARBAMATE PESTICIDES FROM WATER SAMPLES PRIOR THEIR DETERMINATION BY CAPILLARY ELECTROPHORESIS

J. Ben Attig, L. Latrous, M. Zougagh, A. Ríos

Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha,
Avda Camilo José Cela s/n 13001 , Ciudad Real ,tfno :+34632301546,

e-mail: jihenebenatig@gmail.com

Analytical chemistry

A rapid and simple method for the extraction of five N-methylcarbamate pesticides (carbaryl, carbofuran, promecarb, BDMC and methomyl) in water samples was developed. The procedure is based on temperature controlled ionic liquid dispersive liquid phase microextraction and multiwalled carbon nanotubes combined with capillary electrophoresis. Some parameters that affected the extraction efficiency such as type and volume of extractant solvent, temperature and sorbent mass were investigated in order to find the optimal extraction conditions.

P-4

BILIRUBIN METABOLISM IN HUMAN BODY AND ITS POSSIBLE CONTROL WITH SILICA MATERIALS

A. Bórnez, M.J. Ramos, M. Salvador

Dpto. de Ingeniería Química, Universidad de Castilla-La Mancha, Avda. Camilo José Cela 12 13071, tfno: +34 926 29 53 00;
e-mail: abornezg@gmail.es

Chemical Engineering

The increase in serum bilirubin levels can be caused by several issues: haemolysis, impaired hepatic metabolism, liver failure in dialysis patients with critical illness, etc. Bilirubin builds up in tissues like skin and muscle (jaundice). It can even get into the brain and cause neurological damage (kernicterus). In our project, we suggest the use of nanosilica materiales as possible treatment for serum bilirubin removal in critical patients. Silica by itself has a low capacity of bilirubin removal, so it is convenient to attach a functional agent with amine groups that interact with bilirubin carboxylic groups.

Difficulties in the synthesis of amino-organo functionalized NanoSiO2 particles have stopped us from getting results in bilirubin adsorption in PBS or serum. Therefore, we need to optimize the synthesis method to get a significant amount of silica material in order to perform the adsorption assays.

P-5

Assessment of Reversible Hydrogen-Chlorine PEM fuel cell

M. Carvela*; S. Díaz; J. Lobato; C.M. Fernández-Marchante; M. A. Rodrigo.

Department of Chemical Engineering, Faculty of Chemical Sciences and Technologies,
University of Castilla-La Mancha, 13005, Ciudad Real, Spain
e-mail: Mireya.carvela@uclm.es

Electrochemistry

Reversible Hydrogen-Chlorine cells are a promising type of devices for the regulation of the energy produced by solar PV panels and wind turbines. In the electrolytic mode, this type of cell transforms hydrochloric acid into hydrogen and chlorine, which can be stored helping to regulate the exceeding energy. In fuel cell mode, the reversible reactions occur, and hydrochloric acid is regenerated. Thus, the compounds which have been produced during the electrolysis of hydrochloric acid are fed to the same cell operating as a fuel cell to produce energy. Integration of the both modes of operation into the same cell is an important handicap which has been faced in this work, using different Mixed Metal Oxides anodes in order to determine the most efficient formulation, which are characterized by XRD and by EDX-SEM (physical characterization), and by cyclic voltammetry and by electrochemical impedance spectroscopy (electrochemical characterization), different proton exchange membranes and operation conditions. This work reports some of the most interesting results obtained in this promising technology.

P-6

OBTENTION OF HIGH VALUABLE COMPOUNDS FROM LOW-COST MATERIALS OF THE AGROINDUSTRIAL SECTOR OF CASTILLA-LA MANCHA THROUGH $scCO_2$

E. Cruz*, J. M. García, I. Gracia, M. T. García

Department of Chemical Engineering. University of Castilla-La Mancha. Faculty of Chemical Sciences. Avda. Camilo José Cela 12, 13071 Ciudad Real, Spain.
e-mail: Encarnacion.Cruz@uclm.es

Chemical Engineering

Nowadays, the increase in the demand of nutraceutical and pharmaceutical products of natural origin has led to the search of sources of bioactive products. In this sense, the agro-food sector of Castilla La Mancha offers the possibility of obtaining these products from low-value materials or residues, allowing both to satisfy the current need of natural products and promote a key economic sector of the region. Special interest has been paid to compounds with antioxidant and anti-inflammatory potential for the treatment of skin-related diseases such as atopic dermatitis, which affects approximately 20% of the world's population. Various studies have shown that extracts from the wine, essential oil from different plants and garlic industries have compounds with these properties. Bioactive compounds are usually extracted with organic solvents. However, these methods have certain limitations such as high energy costs, high temperatures and low selectivity. For this reason, alternative methods are being studied, like supercritical fluid extraction (SFE). This technology is environmentally friendly and offers the versatility needed to treat different raw materials. Carbon dioxide (CO_2) is the most widely used supercritical fluid, it is inert, non-toxic and allows extraction at lower temperatures and pressures. In addition, this option is interesting because allows not only to isolate the compounds, but also to subject them to chemical transformation in order to enhance their therapeutic properties. The present project will focus on the SFE and chemical transformation of the following products: essential lavender oil, for its topical use to promote wound healing ; garlic oil, because garlic-derived compounds such as thiosulfinates and sulfonates have antioxidant, anti-inflammatory and bactericidal characteristics; and different wine waste flows, due to the fact that the wine industry produces a large quantity of residual by-products containing polyphenols which are very interesting from a dermatological point of view.

P-7

GLYCOLYSIS PROCESS FOR POLYURETHANE WASTE RECYCLING

J. del Amo*, J.F. Rodríguez, A.M. Borreguero, M.J. Ramos

Dpto. de Ingeniería Química, Universidad de Castilla-La Mancha, Avda. Camilo José Cela 12 13071, tfno: +34 926 29 53 00 ext. 96318; e-mail: Jesus.delAmo@uclm.es

Chemical Engineering

Polyurethanes (PUs) are generally thermoset polymers resulting from the addition between a polyol and an isocyanate. The characteristic functional group obtained by the nucleophilic addition of the oxygen of the polyalcohol to the carbon of the cyano group is the urethane. Based on their applications, PUs can be classified into foams (flexible or rigid) and CASEs (Coatings, Adhesives, Sealants, Elastomers).

PUs are the sixth group of polymers most used in the world and generate a large volume of waste, whose correct management is an environmental challenge, due to its low biodegradability. Traditionally, PUs waste has been deposited in landfills but due to the constant increase and the lower availability in landfills, make it necessary to find new and more environmentally friendly alternatives.

Physical recycling processes are successfully used in thermoplastic polymers, but they are useless for most PUs due to their thermostable nature, therefore, chemical recycling processes are of special interest, making possible to obtain chemical products from the PUs foams waste, such as polyether polyol, for the synthesis of new PUs foams.

Glycolysis is the most widely used chemical recycling process for PUs and it is applied to elastomers, coatings, rigid foams, flexible foams and PU RIM (injection molding foams with reinforced reaction). It consists of a transesterification reaction, in which the ester group bonded to the carbonyl carbon of the urethane is exchanged for the hydroxyl group of the glycol. This reaction results in the formation of a polyol and an unstable carbamate at the reaction temperatures, which promotes the formation of secondary amines and carbon dioxide. In addition, with an excess of glycol in the reaction a biphasic product is obtained, where the upper phase is formed mainly by the recovered polyol and the bottom phase by the excess of glycolysis agent and by-products of the reaction; improving the quality of the recovered polyol. Besides, our research has demonstrated that the polyurethane foams synthesized from the recovered polyol meet the conditions and specifications for which are designed.

P-8

EFFECT OF PROCESS PARAMETERS IN A SO_2 DEPOLARIZED ELECTROLYSIS CELL

S.Diaz-Abad*, M.Millán, M.A.Rodrigo and J.Lobato

Dpto. de Ingeniería Química, Universidad de Castilla-La Mancha, Avda Camilo José Cela, Ciudad Real, 13071, Spain 13071; e-mail: sergio.diazabad@uclm.es

Chemical Engineering

Hydrogen is a promising energy carrier for the future. Production of Hydrogen from renewable sources is one of the main challenges of researches. The ideal raw material for its production is water, however an effective technique for the separation of H2 and O2 is needed. One promising technique is the Westinghouse cycle, also called Hybrid Sulfur (HyS) process, which combines a electrochemical step in which the SO2 is introduced in the anode together with water which reduces the standard equilibrium potential from 1.23V vs RHE (water electrolysis) to 0.16V vs RHE (SO2 depolarized electrolysis) to form sulfuric acid, electrons and ions (equation 1). In the cathode, the ions are combined to form hydrogen (equation 2). The other step of the Westinghouse cycle is a thermochemical step in which the produced sulfuric acid is decomposed in O2, water and SO2 which is recirculated to the electrolyzer.

$$SO2(aq) + 2\ H2O \rightarrow H2SO4(aq) + 2H+ + 2\ e- \qquad (1)$$

$$2H+ + 2\ e- \rightarrow H2(g) \qquad (2)$$

The typical PEM used in the electrolysis cell is a Nafion membrane. However, Nafion based membranes show several limitations, including the inability to operate at elevated temperatures and the decreased performance observed when exposed to high acid concentrations [5]. This work is focused on the study of the SO2 depolarized electrolysis at high temperature (100-200 °C) using a phosphoric acid doped PBI membrane as PEM. The tests are performed in a 25 cm2 SO2 depolarized electrolysis cell using a commercial PBI membrane (DAPAZOL, supplied by DPS, Denmark) doped in 85 wt% H3PO4. 0.9 mg Pt/cm2 were deposited on both electrodes (anode and cathode) using 40 % Pt/Vulcan carbon XC72 as catalyst. Different operation conditions are evaluated such as temperature, SO2 flow and the SO2/H2O molar ratio. Polarization curves and impedance spectroscopy analysis are carried out to evaluate the performance of the cell and the ohmic and charge transfer resistances. A preliminary stability test will be performed to assess the stability of the different components of the cell (membrane and electrodes).

P-9

TRANSESTERIFICATION OF WASTE OIL USING A BIFUNCTIONAL CATALYST

V. Enguilo Gonzaga[1], R. Romero1, R. Natividad[1], R. Gómez1, S.L. Martínez[2], A. Romero[3]

[1]Centro Conjunto de Investigación en Química Sustentable UAEM-UNAM, Carretera Toluca Atlacomulco Km 14.5, Unidad San Cayetano, Toluca, Estado de México 50200, México. [2]Facultad de Química, Universidad Autónoma del Estado de México, Paseo Colon esq. Paseo Tollocan. Residencial Colón, Toluca, Estado de México C.P. 50 000, México. [3]Departamento de Ingeniería Química.Universidad de Castilla la Mancha, Avenida Camilo José Cela 12, Ciudad Real, Spain

Chemical Engineering

Biodiesel is one of the most important sources of sustainable energy, is a form of biofuel used as a substitute for fossil diesel, chemically consists of a mixture of methyl esters of fatty acids (FAMEs). Biodiesel is obtained, mainly from transesterification of triglycerides (TG). Biodiesel has several chemical advantages over fossil diesel, it is biodegradable, renewable and reduce the emission of polluting particles. Despite the advantages, the industrial production of biodiesel is limited due to high production costs with the current technology, specifically when used basic homogeneous catalysts [1]. Several researches have proposed the use of waste oils as raw material and the synthesis of new catalysts is of vital importance for that. Bifunctional heterogeneous catalysts contain both acid and basic sites, therefore can simultaneously carry out esterification of free fatty acids and transesterification of triglycerides [2]. These catalysts are promising in the production of biodiesel from used cooking oil and they could to reduce production costs.

In this work, the catalytic activity of iron oxide (III) doped with calcium oxide (Fe2O3/CaO) as a bifunctional heterogeneous catalyst for the biodiesel production using waste oil as raw material was investigated. The optimal conditions for the synthesis of catalysts (temperature of activation, percentage of impregnated iron (III), and iron (III) precursor specie) were determined. Additionally, the conditions of reaction process (molar ratio alcohol-oil, temperature of reaction, catalyst loading and reaction time) were optimized. The Fe_2O_3/CaO was characterized by SEM-EDS, XPS and TGA. The final Biodiesel samples were analyzed by gas chromatography follow the European Regulation (UNE-EN14103) and ICP analysis was made to determinate the leaching of calcium and iron. In summary, a bifunctional catalyst was successfully synthesized to transform the waste oil into high quality biodiesel without soap formation.

P-10

STUDY OF DIFFERENT PRESERVATIVES FOR THE PLATINUM NANOPARTICLES STABILIZATION IN COMPLEX CLINICAL MATRICES

S. Fernández-Trujillo[1], M. Jiménez-Moreno[1], Á. Ríos[2], R.C. Rodríguez Martín-Doimeadios[1]

Department of Analytical Chemistry and Food Technology, UCLM
[1]Faculty of Environmental Sciences and Biochemistry (Toledo, Spain)
[2]Faculty of Chemical Sciences and Technologies (Ciudad Real, Spain)
e-mail: Sergio.Fernandez@uclm.es

Analytical Chemistry

Engineered nanoparticles (NPs) are applied in a wide array of fields, such as biomedicine, cosmetics, pharmaceuticals, environment and clinical research. In particular, platinum nanoparticles (PtNPs) are highly remarkable due to their intrinsic physicochemical and antibacterial properties making them an effective candidate towards biomedical applications [1]. In order to have an adequate control of these applications it is necessary to study of PtNPs in complex clinical samples. These studies are challenging for current analytical methodologies and there are still important open questions that starts even from the stability of metallic NPs in the presence of biological fluids.

Thus, the goal of this work is to evaluate the effect of several preservatives (tetramethylammonium hydroxide (TMAH) and Triton X-100) for PtNPs of different sizes (50 and 70 nm) over time in human urine and blood serum. The characterization of PtNPs in terms of both particle size and concentration was carried out by inductively coupled plasma mass spectrometry in single particle mode (SP-ICP-MS). This study suggested that TMAH is the most adequate preservative and different concentrations (from 1 to 10%) have also been tested. The conclusions of this work will allow to perform a correct analytical characterization of PtNPs and interpretation of preclinical trials in the future.

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P-11

POLYMERIC NANOPARTICLES FOR CONTROLLED DASATINIB DELIVERY IN BREAST CANCER THERAPY

E. García,[1,] E. Niza,[1] S. Castañeda,[1] C. Alonso,[1] J.A. Castro-Osma,[1] C. Nieto,[2] A. Ocaña[2]

[1]Departamento de Química Inorgánica, Orgánica y Bioquímica, Facultad de Farmacia, Av. Dr. Jose María Sánchez Ibáñez s/n, 02006, Albacete [2]Oncología traslacional, CRIB/Unidad de investigación Complejo Universitario de Albacete (CHUA).

e-mail: Erika.Garcia1@alu.uclm.es

Inorganic Chemistry

Dasatinib (DAS) is an inhibitor of the BCR-ABL kinase and of the SRC family kinases together with other specific oncogenic kinases including c-KIT, the ephrin receptor kinases (EPH) and the PDGFβ receptor. This mechanism of action makes it a great candidate for the treatment of breast cancer, but presents serious problems of solubility and primary metabolization by oral route.[1] In order to avoid these problems and perform targeted therapy, in this work, we carried out the encapsulation of Dasatinib in polymeric nanoparticles made from a new biodegradable polymer never tested in drug delivery, poly(cyclohexene phthalate) (CHO + PA) and also a biodegradable polymer approved by the FDA as a PLA. The PLA nanoparticles were used to form an Antibody Drug Conjugate by binding with Trastuzumab (Herceptin).[2] Cytotoxicity and flow cytometry studies of the nanoparticles were performed against the non-encapsulated drug in triple negative breast cancer cell lines (MDA-MB-231, HS578T, BT549) and BT474 cells and BT747 HER2 resistant. The results showed a greater cytotoxic effect of the nanoparticles compared to the free drug.

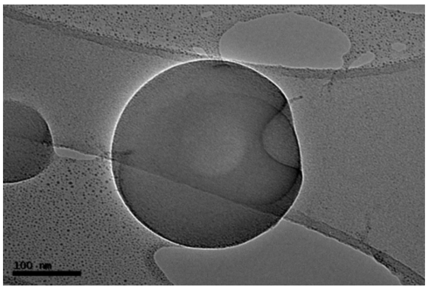

Fig. 1. TEM micrograph of CHO+PA Nanoparticle

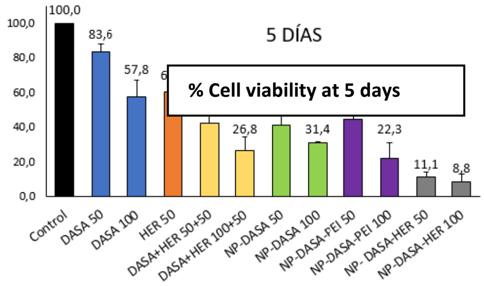

Fig. 2. MTT Assays in BT474 cells

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P-12

MECHANOCHEMISTRY IN THE SYNTHESIS OF NANOMATERIALS

W. E. García-Lorefice*, J. L. Valverde, V. Lopez

Dpto. de Ingeniería Química, Universidad de Castilla La Mancha, Avda Camilo Jose Cela s/n
13071 Ciudad Real, tfno: +34 926 295300 ext. 96322;
e-mail: Wendy.garcia@uclm.es

Chemical Engineering

During the past decades, engineers and materials scientists have developed a great number of methods for synthesizing nanomaterials, engineered particles with improved physical, chemical and biological properties. Fig. 1 shows a typical classification of nanomaterials synthesis methods.

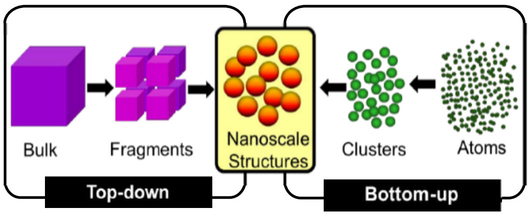

Figure 2. Top-down and Bottom-up techniques.

On the one hand, top-down techniques use an external force to break-up larger initial solid structures into nanoparticles. On the other hand, bottom-up techniques produce nanoparticles by the precipitation or atomic transformation starting from molecular solutions. Nowadays, the mechano-chemical treatment is the least expensive, most simple and powerful way to produce nanoparticles on a commercial scale. One of the nanomaterials with special interest in different applications is Zirconia (ZrO2). Zirconia is an important advanced ceramic with unique properties as the outstanding chemical stability, high strength, wear resistance, flexibility, high toughness, good refractory properties and ionic conductivity.

The properties of the nanomaterial obtained in a milling process and its subsequent calcination are function of several parameters: type of ball mill and mill material, balls material, ball to powder ratio, milling time, milling operating conditions (temperature, pressure and frequency) and heat treatment. According to recent studies, milling time and the subsequent heat treatment are the most important parameters. In this sense, this work analyses different procedure of synthesis where several parameters were varied to find out the optimal way to prepare nanomaterials by mechanical treatment. These results are providing new ideas that allow to define new routes of nanomaterials, which has not been considered enough so far.

P-13

GAS-PHASE REACTIVITY OF ACETONE TOWARDS OH RADICALS AT INTERSTELLAR TEMPERATURES (11.7-64.4 K). ASTROPHYSICAL IMPLICATIONS

Daniel González[1], Sergio Blázquez[1], Antonio J. Ocaña[1], Alberto García[1], Bernabé Ballesteros[1,2], André Canosa[3], María Antiñolo[2], José Albaladejo[1,2], Elena Jiménez[1,2]

[1]Departamento de Química Física, Facultad de Ciencias y Tecnologías Químicas, Universidad de Castilla-La Mancha, Avda. Camilo José Cela 1B, 13071 Ciudad Real.
[2]Instituto de Investigación en Combustión y Contaminación Atmosférica, Edificio Polivalente, Camino de Moledores s/n, 13071 Ciudad Real.
[3]Département de Physique Moléculaire, Institut de Physique de Rennes, UMR CNRS-UR1 6251, Université de Rennes 1, Campus de Beaulieu, 263 Avenue du Général Leclerc, 35042 Rennes Cedex, France.
e-mail : Daniel.GPerezMadrid@uclm.es

Physical Chemistry

Acetone ($CH_3C(O)CH_3$) and hydroxyl (OH) radicals have been found in many sources of the Interstellar Medium, such as Sagittarius B2. The gas-phase kinetics of the $CH_3C(O)CH_3$ + OH reaction have been studied at atmospheric temperatures (down to 202 K)[1] and at interstellar temperatures (79-148 K)[2]. At temperatures of the atmosphere was observed a curvature in the Arrhenius plot, indicating a negative temperature dependence of the *k*. It was confirmed by Shannon et al.[2], reporting the rate coefficient at 146 K and 79 K, with an increase of 2 order of magnitude between both temperatures. They also observed a strong pressure dependence of *k* at around 80 K, while at 140 K was less pronounced. Hence, the importance of study the title reaction at temperatures of the cold dense molecular clouds (T~10–100 K). The CRESU (French acronym for *Reaction Kinetics in an Uniform Supersonic Flow*) system developed in Ciudad Real allows us to achieve ultra-low temperatures, by cooling down the gases below the freezing point without their condensation.

In this work, we have carried out this reaction in the temperature range (11.7-64.4 K), in order to verify if the *k* still continues increasing below 79 K. The CRESU technique was coupled to PLP-LIF (Photolysis Laser Pulsed/Laser Induced Fluorescence) to perform the kinetic study. This technique has been described extensively[3], especially in OH reactions at interstellar temperature. Temperature and pressure dependence of *k* have been investigated and the astrophysical implications will be discussed.

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P-14

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

V. J. González[1], A. M. Rodríguez[1], V. León[1], E. Vázquez[1,2]
[1] Instituto Regional de Investigación Científica Aplicada (IRICA), UCLM, 13071 Ciudad Real, Spain. [2] Facultad de Ciencias y Tecnologías Químicas, UCLM, Avda. Camilo José Cela S/N, 13071, Ciudad Real, Spain.
e-mail: vivianaj.gonzalez@uclm.es

Organic Chemistry

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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P-15

Unusual ligand rearrangement of a *N*-phosphinoguanidinato ligand

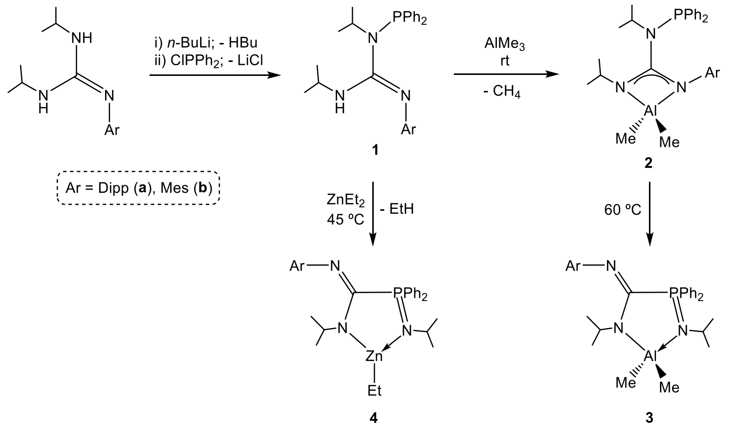
E. Huergo, R. Fernández-Galán, A. Ramos, A. Antiñolo, F. Carrillo-Hermosilla, A. Rodríguez-Diéguez, D. García-Vivó

Dpto. de Química Inorgánica, Orgánica y Bioquímica, Universidad de Castilla-La Mancha, 13071 Ciudad Real

e-mail: estefania.huergo@uclm.es

Inorganic Chemistry

In the last years our group has focused on the development of catalytic methods to prepare guanidines and the coordination chemistry of guanidinato ligands with transition metals and main group elements.[1] As an extension of this work and encouraged by the lack of examples of anionic *N*-phosphinoguanidinato compounds, we aimed to prepare novel *N*-phosphinoguanidines from available trisubstituted guanidines to study their coordination chemistry through protonolysis reactions with different metal alkyls. Here we report the synthesis of *N*-phosphinoguanidines (**1**) and their reactivity towards metal alkyls, such as $AlMe_3$ and $ZnEt_2$, which unexpectedly leads to the formation of stable phosphinimine-amidinato compounds, after an unprecedented rearrangement under mild conditions of the initially formed *N*-phosphinoguanidinato intermediate. A mechanism has been proposed for this transformation in the reaction with $AlMe_3$, supported by DFT calculations, involving cabodiimide de-insertion followed by a [3+2] cycloaddition.[2]



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P-16

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

A.J. Huertas-Alonso, M. Salgado, A. Lorente, M.P. Sánchez-Verdú,
B. Cabañas,[a] A. Moreno.

Dept. of Inorganic, Organic and Biochemistry & Dept. Physical Chemistry,
[a]University of Castilla-La Mancha. Faculty of Chemical Sciences and Technologies.
Av. Camilo José Cela, Nº 10. 13071. Ciudad Real;
e-mail: Alberto.HAlonso@uclm.es

Organic Chemistry

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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P-17

GRAPHENE QUANTUM DOTS FOR ENHANCEMENT OF FLUORIMETRIC DETECTION COUPLED TO CAPILLARY ELECTROPHORESIS FOR DETECTION OF OFLOXACIN

S. Lahouidak, M. Laura Soriano, R.Salghi, M. Zougagh, A. Ríos

Department of Analytical Chemistry and Food Technology University of Castilla-La Mancha,
Avda Camilo José Cela s/n 13001 , Ciudad Real ,tfno :+34602105228,
e-mail: slahouidak@gmail.com

Analytical chemistry

A new CE method with fluorescence detection is reported on the determination of ofloxacin in milk samples using graphene quantum dots (GQDs) for sensitivity enhancement. Injection of GQDs prior the standards/sample is crucial to increase the antibiotic fluorescence response. Clean-up and preconcentration steps allowed for a good linear correlation in a concentration range between 50 and 1000 ng mL^{-1} for the ofloxacin, detection and quantification limits being 10.7 ng mL^{-1} and 35.5 ng mL^{-1}, respectively. Optimal CE conditions for the seven-fluoroquinolone separation method were assessed in terms of buffer type, pH and voltage. The selective interaction of GQDs with ofloxacin as model analyte was subsequently studied finding a significant sensitivity improvement; therefore, the analytes would be detected at low concentrations by means of a commercial CE device equipped with a multiwavelength photoluminescence detector. Due to the different maximum emission wavelengths of the target compounds and the limitations shown by the single-wavelength photoluminescence detector coupled to the CE system, we demonstrated the usefulness of the GQD-assisted sensitivity-enhanced CE method to determine ofloxacin in milk samples. This work opens an interesting possibility of using GQDs in separation techniques combined with photoluminescence detectors for lowering sensitivity levels typically provided by the mere device.

P-18

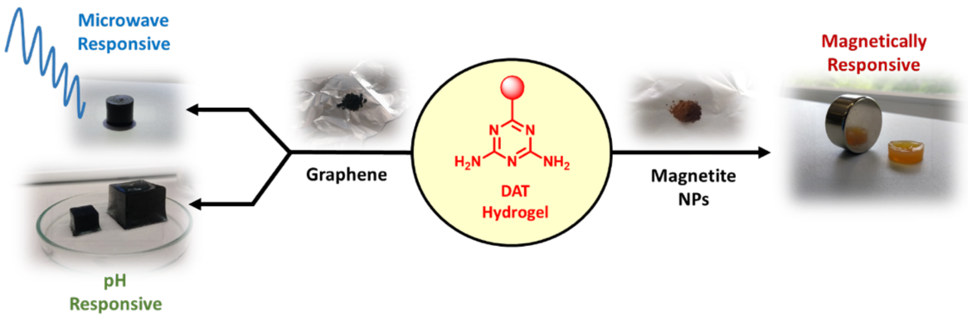
STIMMULI RESPONSIVE HYDROGELS FOR DRUG DELIVERY APPLICATIONS

J-Leganés[a], S. Merino[a], A. Sánchez-Migallón[a], E. Vázquez [a,b]

[a]Instituto Regional de Investigación Científica Aplicada (IRICA), Edificio Marie Curie, Universidad de Castilla-La Mancha; 13071, Ciudad Real, España. [b]Facultad de Ciencias y Tecnologías Químicas, Universidad de Castilla-La Mancha, 13071, Ciudad Real, España
e-mail: jorge.leganes@uclm.es

Organic Chemistry

Hydrogels are three-dimensional crosslinked polymer networks able to swell and incorporate high contents of water. Their biocompatibility and their ability to offer spatial and temporal control over the release of therapeutic agents have placed these soft materials in the spotlight of drug delivery disciplines.[1] However, hydrogels have been traditionally limited to the delivery of water-soluble drugs, since their nature is intrinsically hydrophilic.[2] Diaminotriazines (DAT) are resourceful molecules that stand out for their ability to build supramolecular hydrophobic constructions. In addition, these structures respond to environmental changes, which has expanded the scope of DAT-based materials to the field of controlled delivery.[3,4] In this work, we highlight triazine-based hydrogels as suitable responsive soft materials for drug delivery applications. We have proven DAT-based hydrogels successfully release drugs in response to physiochemical stimuli such as magnetic fields, microwave radiation, or environmental pH. The versatility of DAT-based interactions has encouraged us to further fabricate hybrid graphene-diaminotriazine hydrogels, which have proven to enhance the mechanical and stimuli responsive properties of these materials.



Diaminotriazine (DAT)-based stimuli responsive hydrogels

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P-19

GC-MS ANALYSIS OF THE CORKY OFF-FLAVOUR COMPOUNDS FROM PLANKS USED FOR PRODUCING WINE STOPPERS

L. Loarce, M.S. Pérez-Coello, M.E. Alañón, M.C. Díaz-Maroto

Área de Tecnología de los Alimentos, Universidad de Castilla-La Mancha, Campus Universitario s/n, 13004 Ciudad Real, tfno: +34 926 295300;
e-mail: Lucia.Loarce@uclm.es

Food Science and Technology

Normally, the cork is the closure chosen for wine bottles, and will represent one of the multiple factors that influence its quality. Due to the development of instrumental analytical techniques, such as gas chromatography and mass spectrometry, several scientists attributed to the cork certain off-flavours that sometimes appear in wine, with aromas of moisture and mould. This aroma defect was called "cork taint". The objective of this work was to identify the corky off-flavour compounds in planks that will be used for producing wine stoppers.

The harvested cork planks were supplied by the company Gruart La Mancha, S.A. (Valdepeñas, Ciudad Real), following a previously established sampling plan. They were reduced to powder and volatile extracts were obtained by accelerated solvent extraction (ASE) with dichloromethane as solvent. The extracts were analysed by GC-MS in SIM mode.

Several compounds responsible for the sensory defect called “cork taint”, as alkylmethoxypyrazines, chloroanisoles, chlorophenols, methylisoborneol and geosmin were detected in the newly harvested cork planks. However, their concentration decreased during their storage outside the cork industry before processing, which highlights the importance of this stage to reduce the risk of contamination.

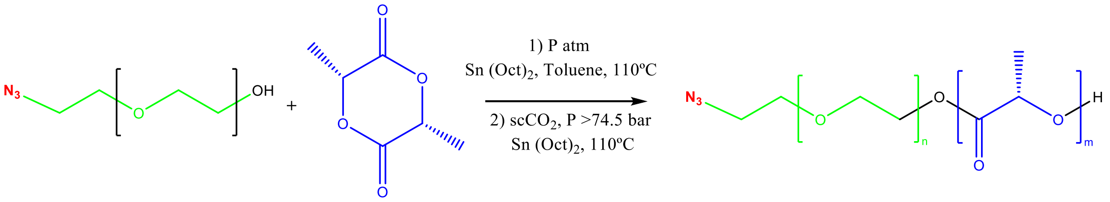
P-20

SYNTHESIS AND FUNCTIONALIZATION OF COPOLYMERS OF L-LACTIDE AND POLY (ETHYLENE GLYCOL) α -HYDROXY-ω-AZIDO TERMINATED

S. López*, M.T. García, J.F. Rodríguez, I. Gracia, M.J. Ramos.

Dpto. de Ingeniería Química, Universidad de Castilla-La Mancha, Avda Camilo José Cela 12, 13071 Ciudad Real; e-mail: Sonia.Lopez@uclm.es

In the last decade, amphiphilic block copolymers consisting of poly ethylene glycol (PEG) and poly lactide (PLA) have gained considerable attention in pharmaceutics and biomedical applications and furthermore have great potential for development drug delivery systems. The design of these copolymers is important for their versatility for potential treatment of a wide range of diseases including cancer. PLA has been successfully implemented in many pharmaceutics applications, but its broader utilization as a biomaterial is limited due to its hydrophobicity and difficulties with encapsulation of significant loadings of polar drugs. A common method to overcome these limitations and improve the hydrophilicity of the hydrophobic polymers is copolymerization with a hydrophilic block such as PEG. PLA-PEG can be copolymerized by polycondensation, anionic polymerization or ring opening polymerization (ROP). In this work, the synthesis and characterization of PLA-b-PEG-N_3 was carried out. It was used the ring-opening polymerization where L-lactide acted as monomer in the presence of poly (ethylene glycol) α-hydroxy-ω-azido terminated used as macroinitiator and stannous octoate as the catalyst. The reaction is shown in scheme 1.



Scheme 1. Synthesis of PLA-b-PEG-N_3 block copolymer.

Copolymerization was carried out in different conditions: at atmospheric pressure and with supercritical CO_2 ($scCO_2$). The $scCO_2$ represents a viable solvent choice for step growth polymerizations. When the environmental advantages of CO_2 are combined with its ability to be used as a solvent medium for a wide variety of chemical reactions, it becomes clear that CO_2 may be the solvent of the future for the polymer industry. The idea was to synthesize a "clickable" PLA-b-PEG-N_3 copolymer that subsequently reacts via copper (I)-catalyzed alkyne azide cycloaddition (CuAAC) with therapeutic ligand with the corresponding alkyne terminal, necessary to form the triazole ring. One of the most promising procedures to carry out the synthesis of the conjugated polymer-drug is click chemistry. Click chemistry has the advantage of being a highly reliable methodology, clean, with excellent performance and compatible with a large number of functional groups, comparing it with other conventional methods of polymer-pharmaceutical conjugation. Combined with the use of supercritical technology, we will be able to protect drugs from degradation and avoid the use of toxic solvents.

P-21

17-β Estradiol degradation in aqueous medium using boron doped diamond electrodes

S. Maldonado*, G. Roa, C. Barrera, J.Ramirez, M. A. Rodrigo, C. Sáez

Dpto. de Ingeniería Química, Universidad de Castilla-La Mancha , Avda Camilo Jose Cela s/n 13071 Ciudad Real, España; Facultad de Química, Universidad Autónoma del Estado de México, Avda Paseo Colón s/n 50120, Toluca , México tfno: +34 942 202020;*

e-mail: sandramaldom@gmail.com, smaldonadod096@alumno.uaemex.mx

Electrochemistry

Nowadays, the appearance of natural and synthetic pollutants in water is a very important problem as many living organisms are being affected.

Emerging contaminants such as 17β- estradiol interferes with the functioning of the endocrine system. It is now observed that these pollutants are complex molecules, and aren't able to be removed in water treatment plants, so new advanced oxidation process are a necessary alternative.

A great example is electrocinetic process using boron doped diamond electrodes given that have useful properties such as high anodic stability, conductivity and low adsorption. It's also observed that 17β- estradiol can be broken down in carboxilic acids, a process which is less complex in high percentages.

P-22

POTENTIAL OF DIFFERENT OENOLOGICAL PRODUCTS TO INHIBIT 1-HYDROXYETHYL RADICAL IN WINE

L. Marchante [a], K. Márquez [b], D. Contreras [b], P. M. Izquierdo-Cañas [a],
E. García-Romero [a], M. C. Díaz-Maroto [c]

[a] Instituto Regional de Investigación y Desarrollo Agroalimentario y Forestal de Castilla-La Mancha (IRIAF-IVICAM). Crta. Toledo-Albacete s/n. 13700 Tomelloso (Ciudad Real), España. [b] Centro de Biotecnología y Facultad de Ciencias Químicas, Universidad de Concepción, Concepción, Chile. [c] Área de Tecnología de los Alimentos, Facultad de Ciencias y Tecnologías Químicas, Universidad de Castilla-La Mancha, Avda. Camilo José Cela 10, 13071. Ciudad Real, España.
e-mail: lmarchantec@jccm.es

Area of Food Science and Technology

The elaboration of wines without SO_2 is a complex challenge, since the free radicals produced in wine oxidation reactions can cause a great deterioration in its composition and organoleptic characteristics. Among the free radicals formed during the oxidation of wine, it has been shown that the 1-hydroxyethyl radical is the most abundant and could be the main agent responsible for the oxidation of other organic substances in wine. The objective of this work was to study the potential of different oenological products to inhibit 1-hydroxyethyl radical in wines without SO_2.

The oenological products studied were ascorbic acid, glutathione, chitosan, inactive dry yeast and grape seed extract. The capacity of the different products to prevent the oxidation of the wine was evaluated in two concentrations (0.5 g/L and 2 g/L) and in two wines elaborated without SO_2: Sauvignon Blanc and Cabernet Sauvignon. The Fenton reaction was carried out in the wine after the addition of the different products, and the 1-hydroxyethyl radical was monitored for 30 min by Electron Paramagnetic Resonance (EPR) using α-(4-pyridyl-1-oxide)-N-tert-Butylnitrone (POBN) as spin trap.

The results showed that the addition of grape seed extract and chitosan offered higher percentages of radical inhibition in red wine. While the effect of the inactive dry yeast to inhibit the radical was only observed in white wine. The ascorbic acid, in the concentration of 0.5 g/L, showed a pro-oxidant effect at the beginning of the reaction in white wine. Therefore, the efficacy of the oenological products studied to inhibit the 1-hydroxyethyl radical in wines without SO_2 is influenced by both the concentration used and the type of wine.

P-23

DEGRADATION OF ANTIBIOTICS BY ELECTRO-FENTON PROCESS

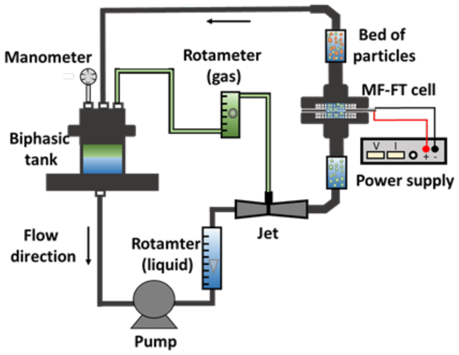
A. Moratalla, J. F. Pérez, C. Sáez, P. Cañizares, M. A. Rodrigo

Departamento de Ingeniería Química, Universidad de Castilla-La Mancha, Edificio Enrique Costa Novella, Av. Camilo José Cela nº 12, Ciudad Real (España).
e-mail: angela.moratalla@uclm.es

Chemical Engineering

The electrochemical advanced oxidation technologies (EAOPs) have been extensively studied on laboratory scale for the efficient abatement of recalcitrant organic pollutants in wastewater. The objective of the present work is the combination of two EAOPs, namely anodic oxidation and electroFenton, on a bench-scale reactor with potential to be scaled up for hospital effluents. An important amount of these effluents contains large amounts of pharmaceuticals as antibiotics.

In particular, the main features of the system are *i)* a pressurized-jet aeration system, a powerful and synergistic combination of a jet aerator and a pressurized circuit *ii)* a microfluidic flow-through electrochemical cell, which combines a low ohmic resistance, a high mass transfer and *iii)* state-of-the-art 3D electrodes, to maximize the mass transfer rate and *iv)* a fluidized bed of iron particles, to promote the Fenton reaction avoiding the issues related to the use of an heterogeneous catalyst .



P-24

SELF-HEALING MATERIALS: MODULATING THE PROPERTIES OF HYDROGELS

A. Naranjo, C. Martín, S. Merino, M.A. Herrero, E. Vázquez

Instituto Regional de Investigación Científica Aplicada, Facultad de Ciencias y Tecnologías Químicas, UCLM, Ciudad Real;
e-mail: Alicia.Naranjo@alu.uclm.es

Organic Chemistry

In the last few years, many scientific researchers have developed novel and smart materials for different applications. In the field of composite materials, hydrogels have got the attention of many sectors from soft robotics[1] to biomedical applications as drug delivery.[2]

Hydrogels, as 3D polymeric networks which are able to absorb aqueous solutions inside, are shown as one of the most novel materials due to their interesting properties. Recently, a new property has been studied, named as self-healing ability.[3] This self-healing materials can inherently repair several times internal or external damages, recovering their properties after the harm (Figure 1).

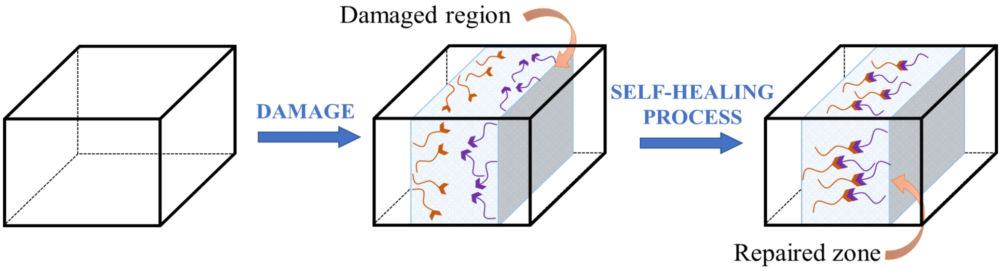


Figure 3. Scheme of the self-healing process.

Following this trend, in this project different hydrogels have been prepared and their main properties have been fully characterized. Graphene based-hydrogels have also been synthesized to compare their self-healing ability with the pristine ones.

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P-25

CATALYTIC AMMONIA DECOMPOSITION OVER RU/SIC

M. Pinzón-García*, A. Romero, P. Sanchez

Dpto. de Ingeniería Química, Facultad de Ciencias y Tecnologías Químicas, Universidad de Castilla-La Mancha, Avda Camilo José Cela s/n 13071 Ciudad Real, tfno: +34 926 295 300; e-mail: Marina.PGarcia@uclm.es

Chemical Engineering

Hydrogen is used as an energy vector and is known as "eternal fuel" as it is the simplest and the most common element of the Universe. Moreover, it can be used as an environmentally clean energy carrier to power fuel cells and internal combustion engines. However, this compound presents serious challenges related to storage and distribution. In this scenario, NH_3 has been investigated for storing hydrogen safely and in an economically feasible way. This compound presents multitude of advantages associated to the low cost of production, a high availability and NH_3 includes at 17% in weight of H_2 atoms. To be able to use H_2, stored in NH_3, it is necessary to decompose the ammonia (Eq.1) into hydrogen (H_2) and nitrogen (N_2) by employing heterogeneous catalyst.

In this work, the reaction of ammonia decomposition over ruthenium using SiC as support with different metal loading (1-7.5% w/w) and at different reaction conditions was studied. Figure 1 shows the TPR-H_2 of the catalysts. As it can be observed in this figure, Ru was easily reduced ($Ru^{3+} \rightarrow Ru^0$) if it was previously calcinated in nitrogen atmosphere. Air calcinated catalyst showed a first peak associated to the reduction of Ru^{3+} to Ru^0 and a second one related to the reduction of RuO_2. Figure 2 presents the ammonia conversion as a function of reaction temperature. The best performance was achieved by the 2.5 Ru/SiC catalyst calcinated in N_2 atmosphere. In this case, 95% of conversion was reached at 450ºC.

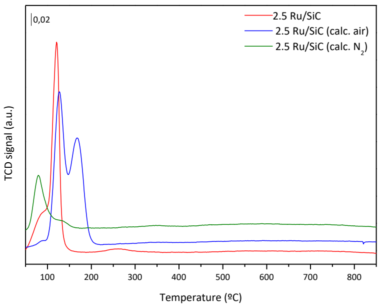


Figure 1. TPR-H_2.

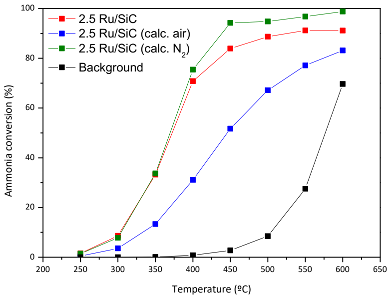


Figure 2. Ammonia conversion presented as a function of reaction temperature.

P-26

2-Hydroxyphenyl-4,6-styrylpyrimidines. Synthesis and Optical Properties

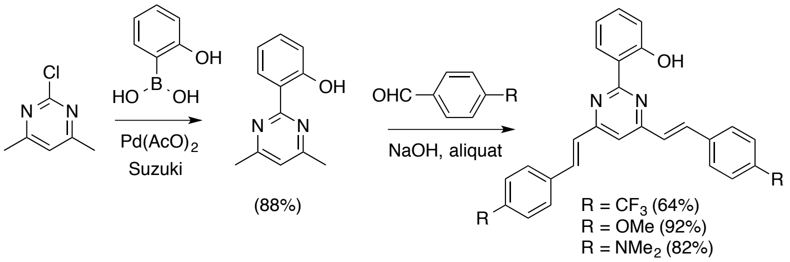
R. Plaza-Pedroche, V. Muñoz-Canales, J. Rodríguez-López

Dpto. de Química Inorgánica, Orgánica y Bioquímica, Universidad de Castilla-La Mancha, Avda. Camilo José Cela 10, 13071, Ciudad Real, Spain;
e-mail: rodripedroche@gmail.com

Organic Chemistry

During the last decade, there has been great interest in the synthesis of chromophores based on pyrimidines by part of the scientific community.[1] The pyrimidine ring is a highly π-deficient aromatic heterocycle that can be used as electron-withdrawing unit in donor-acceptor structures to obtain intramolecular charge transfer. In general, charge transfer along the structure of a molecule has a significant impact on its luminescent properties and is also necessary for non-linear optic processes. In addition, the incorporation of pyrimidine rings in the skeleton of a π-conjugated structure leads the energy difference between HOMO and LUMO of the molecule to be reduced appreciably.[2]

In this work, a series of 2-hydroxyphenyl-4,6-styrylpyrimidines have been efficiently prepared by a combination of Suzuki and aldol condensation reactions (Scheme 1). Their optical absorption and emission properties were studied in different solvents and media. The abilities of these molecules to function as colorimetric and luminescence pH sensors were demonstrated with dramatic color changes and luminescence switching upon the introduction of acid.



Scheme 1. Preparation of 2-hydroxyphenyl-4,6-styrylpyrimidines.

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P-27

MEMBRANE-LESS ELECTROLYZER: A NEW CONCEPT FOR H2 PRODCUTION VIA ALCOHOL ELECTROCHEMICAL REFORMING

E. Ruiz-López[1]*, E. Amores[2], F.Dorado[1], A. De Lucas-Consuegra[1]

[1]Dpto. de Ingeniería Química, Universidad de Castilla-La Mancha, Avda Camilo José Cela 12
13071 Ciudad Real, tfno: +34 926 295300;
[2]Centro Nacional del Hidrógeno, Puertollano, Ciudad Real
e-mail: Estela.Ruiz@uclm.es

Chemical Engineering

The increasing demand of worldwide energy joint to the environmental problems encourages the development of clean and renewable energy such as hydrogen. Water electrolysis is the most established technology to produce pure and free carbonaceous H_2 in a single step, although it requires high cell voltages which mean high energy consumption. In the latest years, alcohol electrochemical reforming has become an attractive alternative due to the high energy contained in these fuels. These conventional studies typically include a membrane electrode assembly (MEA) configuration which separates the anodic compartment from the cathodic one [2]. The membrane is the critical component of the electrochemical reformer limiting the cell life-time and attaining its high cost. In order to contribute for the practical application of this technology, in this work a new concept of alcohol electrochemical reforming was developed, using a membrane-less electrolyzer configuration, i.e., where the anode and the cathode are in a single chamber configuration. For that purpose, Pd supported on carbon Vulcan and Pt on carbon black (20% Pd/C, 20% Pt/C; Alfa Aesar) were used as the anodic and cathodic catalysts respectively. Both catalysts were mixed with an isopropanol solution and sprayed on Carbon Paper (Fuel Cell Earth). A wide variety of experimental tests were carried out in an electrolysis cell (Figure 1 a)) in order to study the viability of the new system (Figure 1 b) is shown as an example).

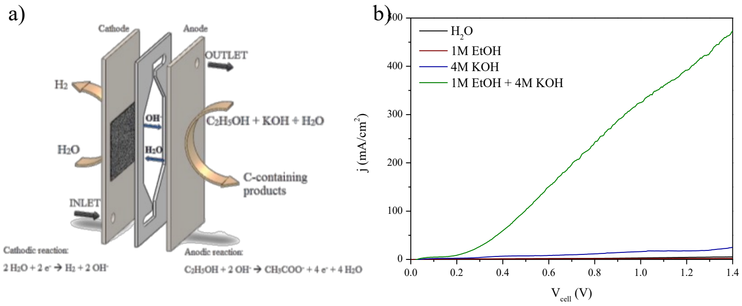

Figure 1. a) Membrane-less system scheme, b) Polarization curves. Scan rate = 5 mV·s^{-1}. T = 85 ºC

P-28

ORGANOGELS FROM 2*H*-BENZO[*d*]1,2,3-TRIAZOLE DERIVATIVES IN THE CRYSTALLIZATION OF DRUGS

I.Torres-Moya[1], B. Saikia[2], P. Prieto[1], J. R. Carrillo[1], J. W. Steed[2].

[1] Department of Organic Chemistry, Faculty of Chemical Sciences and Technologies, University of Castilla La Mancha, 13071 Ciudad Real, Spain. [2] Department of Chemistry, Durham University, South Road, Durham, DH1 3LE, United Kingdom. E-mail: ivan.torresmoya@uclm.es

Organic Chemistry

2*H*-benzo[*d*]1,2,3-triazole is an interesting moiety for Materials Science due to the good acceptor of electrons character, its easy alkylation or arylation in the N-H bond and its easy modification in the benzene ring with electrodonor or electroacceptor groups. In our research group, 2*H*-benzo[*d*]1,2,3-triazole derivatives have been previously tested as optical waveguides,[1] OFETs[2] and polymers in bioimaging.[3] In this work, they have shown organogel formation with a range of different chemical functionalities, highlighting the case of a bis-amide derivative which showed high thermal stability and high mechanical resistance, corroborated by rheology experiments. The obtained gels were totally characterized by SEM, IR, critical gelation concentration (CGC) o Gel to sol transition temperature (T_{sol}). Due to the great properties for these gels, organogels of the bis-amide derivative were used in the crystallization of the pharmaceutical drugs theophylline, sulfathiazole, sulfamerazine and niflumic acid. In the case of sulfathiazole, the gel induces a change in the polymorphic form observed in comparison to solution crystallization under the same conditions.[4] These gels offer significant scope for expanding the rage of current polymorph discovery methods particularly in the pharmaceutical industry.

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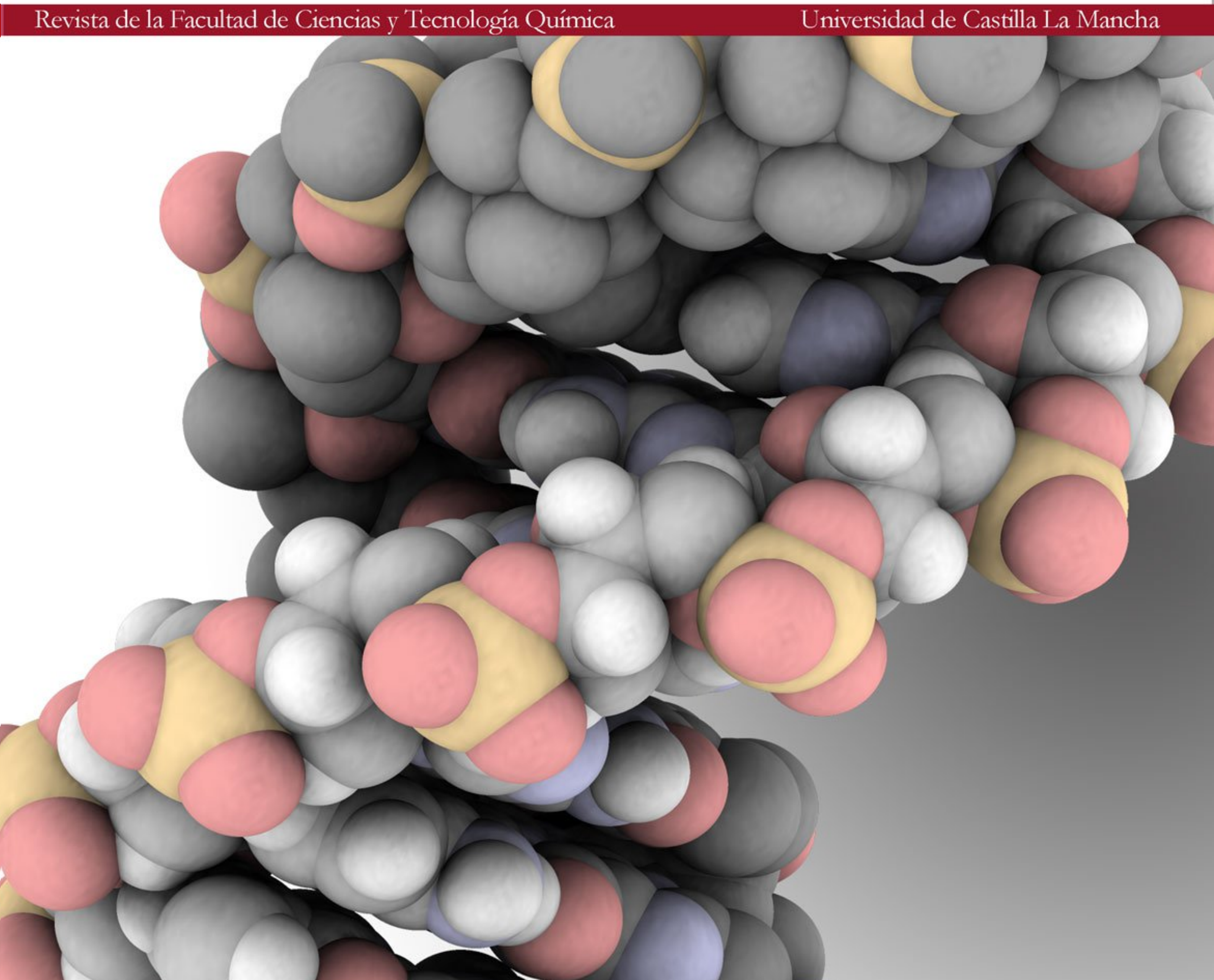

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JORNADAS POSTDOCTORALES UCLM

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E-mail de contacto: Antonio.Hoz@uclm.es

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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.

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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CONFERENCIA INVITADA

PRODUCTOS NATURALES: DE LA MAGIA A LA QUÍMICA MODERNA

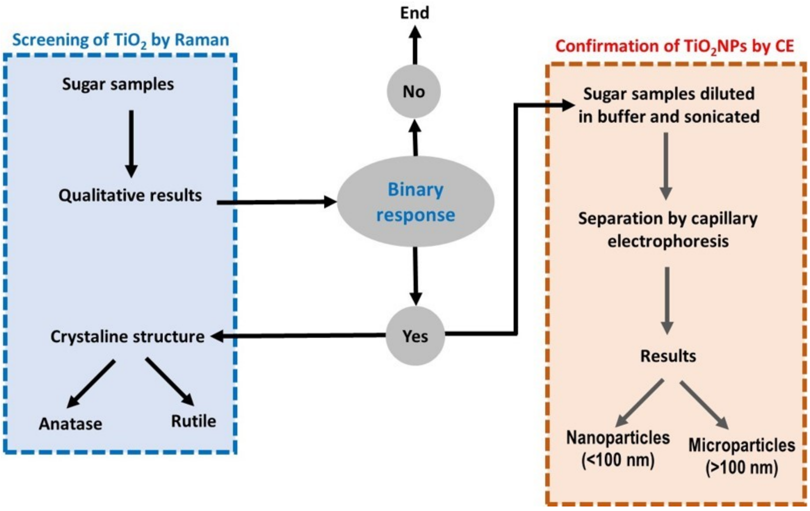
Mª del Carmen de la Torre Egido

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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COMUNICACIÓN ORAL

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.

COMUNICACIÓN ORAL

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.

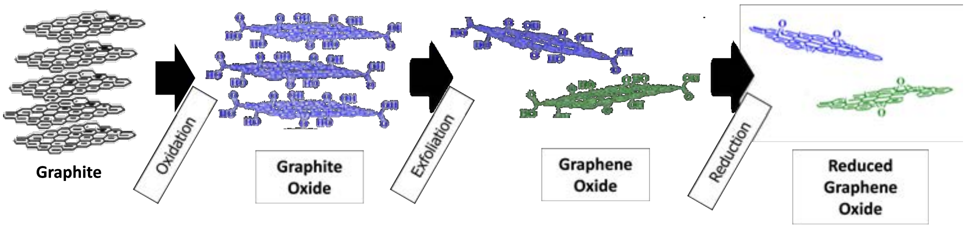


Figure 1. Scheme of chemical reduction

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).

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.

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.

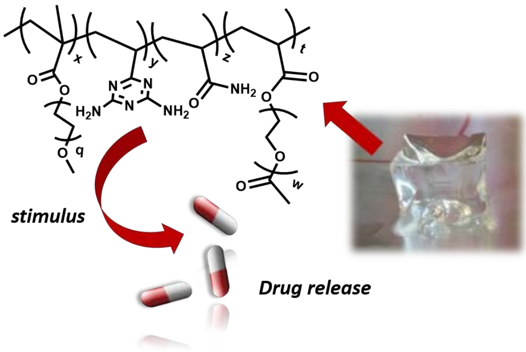
Analytical results, method precision, and accuracy data are presented and limits of detection for the method ranged from 2 to 5 µg/mL. The results obtained are used in monitoring the composition of vanilla flavorings, as well as for confirmation of natural or non-natural origin of vanilla in samples 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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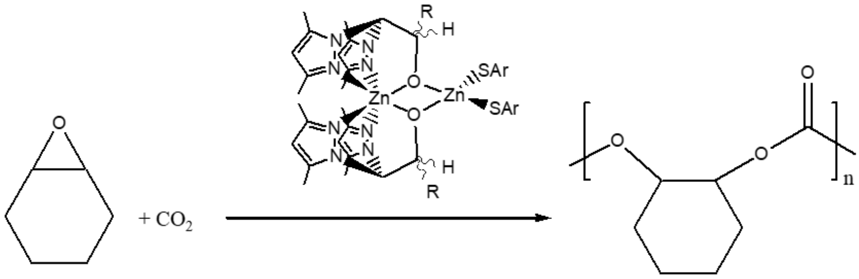
NEW SCORPIONATE ZINC COMPLEXES AS INITIATORS FOR THE SYNTHESIS OF POLYCARBONATES BY ROP COPOLYMERISATION OF CYCLOHEXENE OXIDE AND CARBON DIOXIDE

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.

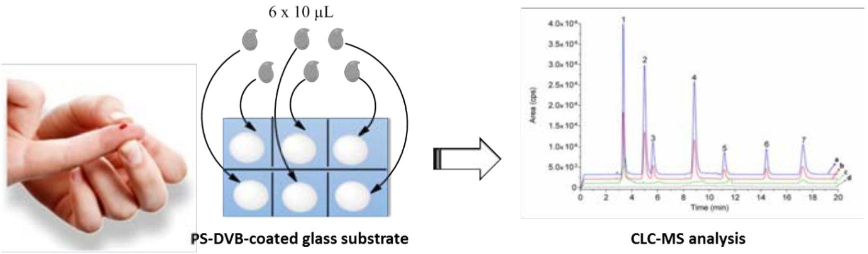
These zinc complexes were investigated as catalysts for the synthesis of polycarbonates from epoxides and carbon dioxide in the absence of a cocatalyst.[1] Under the optimal reaction conditions, the complex type [Zn(κ^{2}NN-μO)$_2$Zn(SAr)$_2$] acts as an efficient single-component initiator for the ring-opening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



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
ORAL

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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COMUNICACIÓN ORAL

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.

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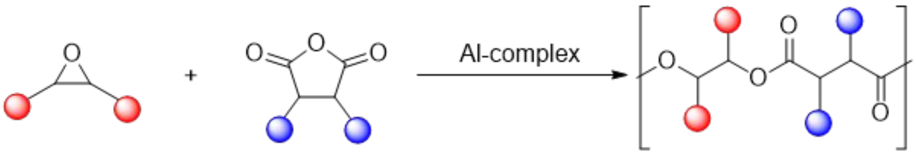
RING-OPENING COPOLYMERIZATION OF CYCLIC ANHYDRIDES AND EPOXIDES CATALYSED BY ALUMINIUM HETEROSCORPIONATE COMPLEXES

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.

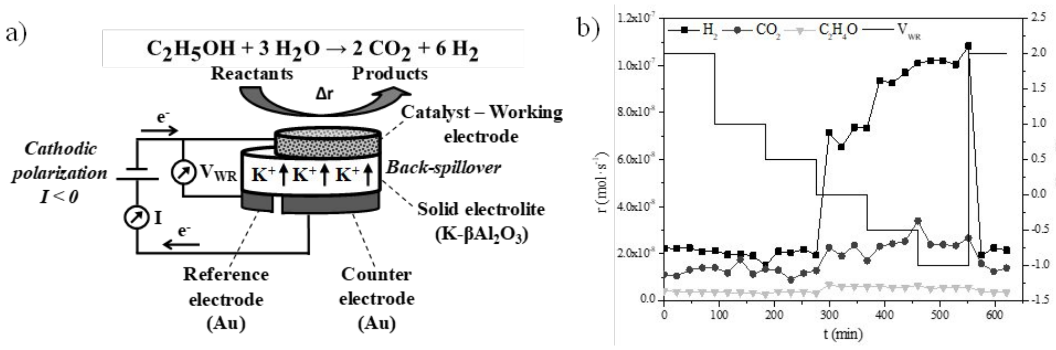

Figure 1.a) Scheme of the electrochemical cell used. b) H_2, CO_2, $C_4H_{10}O$, C_2H_4O production rates vs time under different applied potentials. ESR conditions: H_2O/C_2H_5OH = 9 %/3 %, T = 450 ºC.

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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COMUNICACIÓN
ORAL

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.

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.

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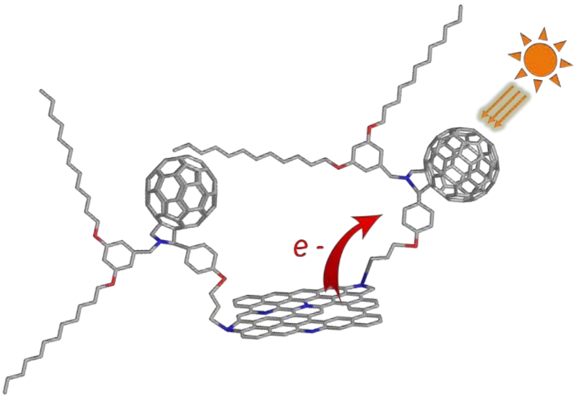
LINKING FULLERENE C_{60} ON N-DOPED GRAPHENE SURFACE. SYNTHESIS AND CHARACTERIZATION

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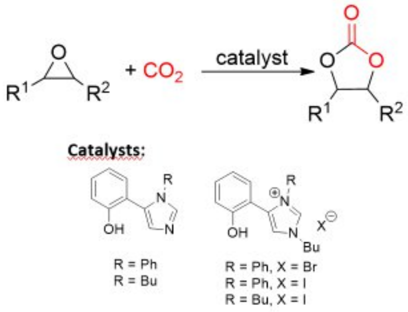
DEVELOPMENT OF HYDROXY-CONTAINING IMIDAZOLE ORGANOCATALYSTS FOR CO_2 FIXATION INTO CYCLIC CARBONATES

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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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.

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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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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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.

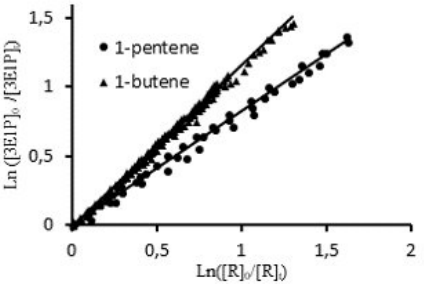

Figure 1. Relative rate plots for the reaction of 3-ethoxy-1-propanol (3E1P) with Cl atoms using two reference compounds

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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.

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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.

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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).

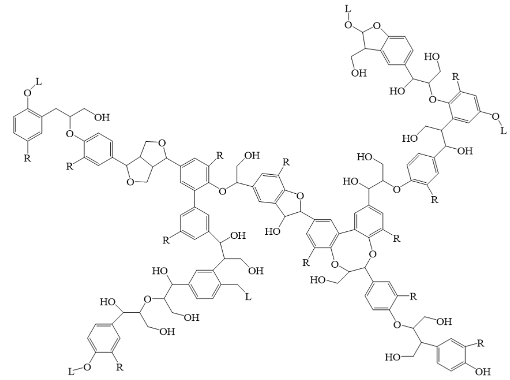

Figure 1. Chemical structure of lignin

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.

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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.

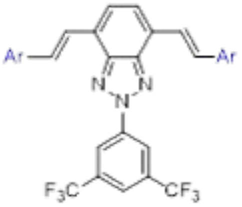

Figure 1. Alkenyl derivatives of 2H-benzo[d][1,2,3]trizole.

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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.

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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.

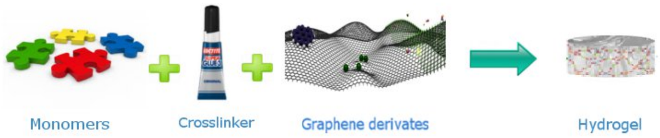

Figure 1. General scope of hydrogels synthesis.

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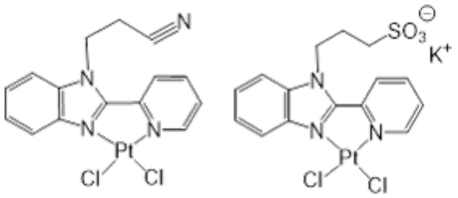
SYNTHESIS AND CYTOTOXICITY OF Pt(II) PYRIDYL BENZIMIDAZOLE COMPOUNDS BEARING FUNCTIONALIZED TAILS. IMPORTANCE OF THEIR INTERACTION WITH SEROALBUMIN

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.

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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]

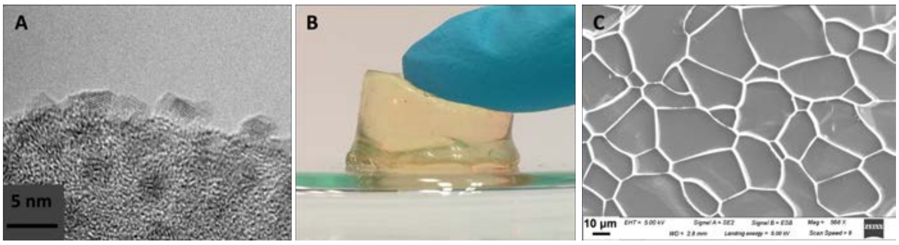

Figure: a) Transmission Electron Microscopy (TEM) of GQDs; b) Digital photo and c) Cryo-Scanning Electron Microscopy (Cryo-SEM) of the nanocomposite.

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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

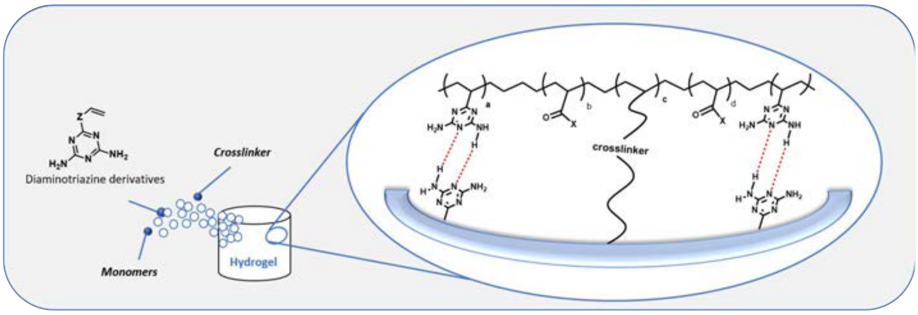
Ageing in rodents and humans is associated with obesity and insulin resistance. Food restriction, which delays the aging process in mammals ameliorated insulin resistance and inflammation. Recently, it have been shown that a shorter ChREBP isoform (ChREBP-β) links glucose transport to lipogenesis and 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.

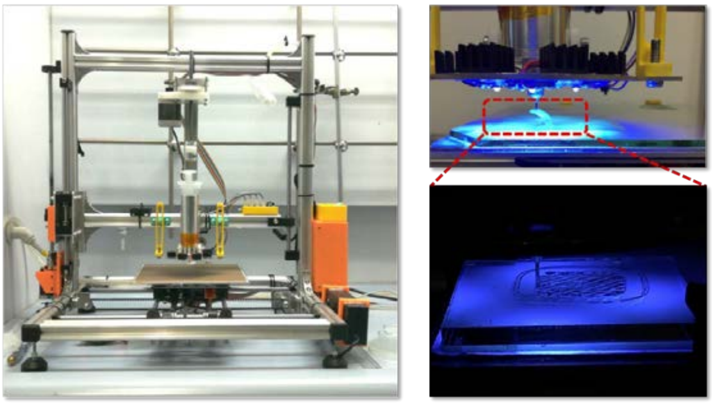

Figure. 3D printer and printing process.

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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):

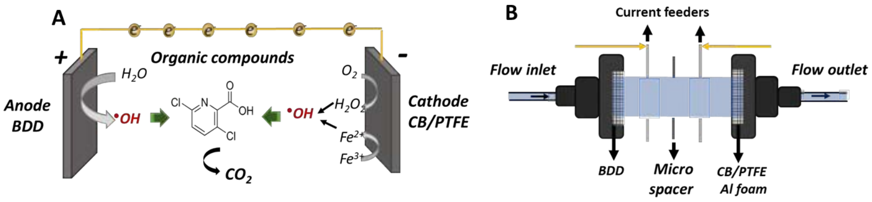

Figure 1. A) Generation of $^{\bullet}OH$ vía AO-BDD y EF; B) MF-FT cell configuration

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.

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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.

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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.

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".

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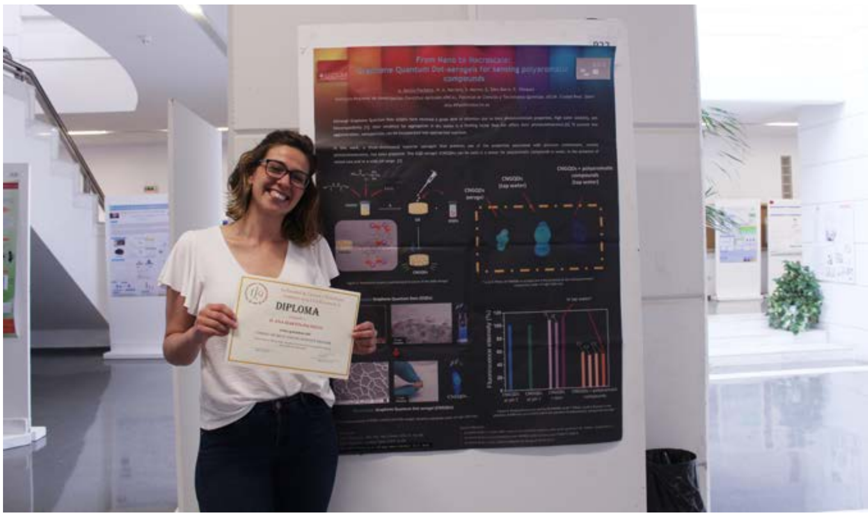

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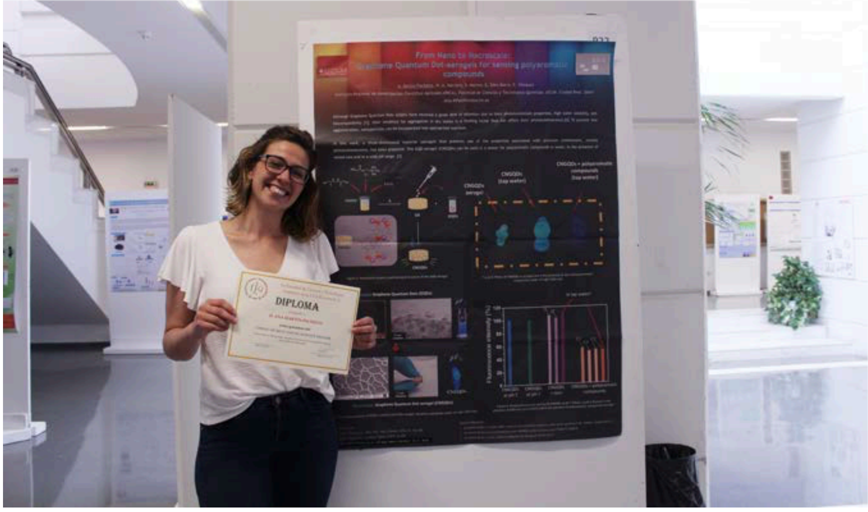

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Jornadas de Ciencia Joven:

FECHA	ACTUACIÓN
Abril de 2007	CIENCIA JOVEN. Un foro de debate de jóvenes investigadores
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De abril a junio de 2011	V JORNADAS DE CIENCIA JOVEN. Un foro de debate de jóvenes investigadores
De mayo a junio de 2012	VI JORNADAS DE CIENCIA JOVEN. Encuentro de jóvenes investigadores
23-24 de mayo de 2013	VII SIMPOSIO CIENCIA JOVEN
22-23 de mayo de 2014	VIII SIMPOSIO CIENCIA JOVEN
21-22 de mayo de 2015	IX SIMPOSIO CIENCIA JOVEN
Del 8 al 10 de junio de 2016	X SIMPOSIO CIENCIA JOVEN
Del 3 al 5 de Junio de 2017	XI SIMPOSION CIENCIA JOVEN
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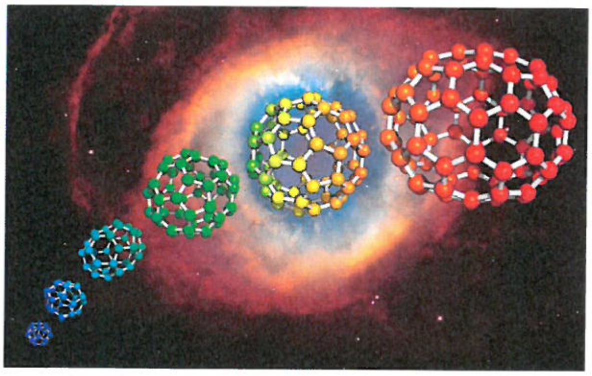

JORNADAS DE CIENCIA JOVEN

Comité Organizador:

Nombre	Apellidos	email
María Elena	Alañón Pardo	mariaelena.alanon@uclm.es
Sergio	Blázquez González	Sergio.Blazquez@uclm.es
Ana Raquel	de la Osa Puebla	AnaRaquel.Osa@uclm.es
María Antonia	Herrero Chamarro	MariaAntonia.Herrero@uclm.es
Luis Fernando	León Fernández	LFernando.Leon@uclm.es
Virginia	López Gómez	Virginia.Moreno@uclm.es
José	Pérez Navarro	Jose.PNavarro@uclm.es
Alberto	Ramos Alonso	Alberto.Ramos@uclm.es
Ángel	Ríos Castro	Angel.Rios@uclm.es
Antonio M.	Rodríguez García	AntonioM.Rodriguez@uclm.es

Participantes

Nº contribución	Apellidos	Nombre
CI-1	Pérez Álvarez	Emilio M.
CI-2	Pico	Yolanda
CI-3	Lozano	Pedro
CI-4	Serrano	David
O-1	Aranda Díaz-Lucas	Mª Inmaculada
O-2	Benmassaoud	Yassine
O-3	Caballero Espinosa	Mª del Prado
O-4	de la Cruz Martínez	Felipe
O-5	Domínguez Jurado	Elena
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O-7	Escalona Verbo	Alba
O-8	Fernández-Pacheco Rodríguez	Pilar
O-9	Gaona Fernández	Miguel Ángel
O-10	García-Béjar Bermejo	Beatriz
O-11	Garrido	Mª Prado
O-12	Hernández Sánchez	Elena
O-13	Herrera Herreros	Jesús
O-14	Lara Gómez	Sonia
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O-18	Martín Pacheco	Ana
O-19	Martínez de Sarasa Buchaca	Marc

O-20	Montes Correal	Cristina
O-21	Muñoz Galindo	Josué
O-22	Muñoz López	Sonia
O-23	Ocaña Fernández	Antonio Jesús
O-24	Oliver Simancas	Rodrigo
O-25	Patón	Antonio
O-26	Pérez	José Fernando
O-27	Pérez Navarro	José
O-28	Pinilla Peñalver	Esther
O-29	Rodríguez	Alberto
O-30	Rubio	Blanca
O-31	Ruíz-Castañeda	Margarita
O-32	Salgado Ramos	Manuel
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P-1	Acosta-Santoyo	Gustavo
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P-3	Atig Jihène	Ben
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P-9	Enguilo Gonzaga	Vania
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P-19	Loarce Ortíz	Lucía
P-20	López	Sonia
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