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

XII YOUNG SCIENCE SYMPOSIUM

Del 13 al 15 de Junio de 2018

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LIBRO DE COMUNICACIONES

Bienvenida del Decano

Os damos la bienvenida a esta nueva edición del 12th 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 XII 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. Ello ha hecho aumentar en media jornada más el Simposio, abriendo por primera vez una sesión de presentaciones en forma de póster. Además, continuaremos con la convocatoria del “III Premio Ciencia Joven” de la Facultad, a fin de que sea un estímulo adicional para nuestros jóvenes investigadores que participan en el evento.

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 Simposia. 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 Organizador:

Ángel Ríos Castro, *Decano de la Facultad*

Alberto Ramos Alonso *"Inorganic Chemistry"*

Ana Raquel de la Osa Puebla *"Chemical Engineering"*

José Pérez Navarro *"Food Sciences and Technology"*

Virginia Moreno García *"Analytical Chemistry"*

Inmaculada Moreno Sanchez-Gil *"Physical Chemistry"*

Antonio Manuel Rodríguez García *"Organic Chemistry" & Jóvenes Investigadores Químicos de la RSEQ & European Young Chemistry Network - EYCN EuCheMS*

Julián Rodríguez López *"Sección Territorial de Castilla - La Mancha de la Real Sociedad Española de Química (RSEQ)"*

Martina Viñuela Delgado, *Photographer*

Estamos encantados de retomar durante los días 13, 14 y 15 de Junio la iniciativa del **"Young Science Symposium"**, siendo este año su **Duodécima 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 2018, se concederá el **"III PRIZE OF YOUNG SCIENCE FACULTY OF SCIENCES AND TECHNOLOGY"**.

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/

PROGRAMA

Programme:

Wednesday, 13th June 2018

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. Fernando Zamora Marín (Universidad Rovira i Virgili). Conference "***In Memorian of Prof. Isidro Hermosín". "Innovaciones en el estudio de la astringencia; impacto de ciertas prácticas enológicas sobre la percepción de la astringencia de los vinos tintos".*

11:00- **Invited Lecturer: Prof. Mª Cruz Moreno Bondi (Universidad Complutense de Madrid**). *"Sensores ópticos para el análisis de antibióticos y de toxinas naturales. Búsqueda de nuevos elementos de reconocimiento selectivo"*.

12:00- Poster session.

14:00- Lunch break.

16:00- 1st session *(Chairman: Alberto Ramos)*

- *"Analytical nanometrological approach for screening and confirmation of TiO2 nano/micro-particles in sugary samples based on Raman spectroscopy-capillary electrophoresis".* **Virginia Moreno García***. Analytical Chemistry.*
- *"Synthesis of Polymer-drug Conjugates to Controlled Release of Drugs".* **María José Carrero Menchén.** *Chemical Engineering***.**
- *"Catalytic Transfer Hydrogenation processes using ruthenium and iridium organometallic compounds".* **Margarita Ruiz de Castañeda Álvaro***. Inorganic Chemistry.*
- *"Tunable polymers derived from 2H-benzo[d]1,2,3-triazole monomers".* **Iván Torres Moya.** *Organic Chemistry.*

17:00- Break

17:30- 2nd session *(Chairman: Alberto Ramos)*

- *"Yeast biodiversity from natural sources in the central region of Spain".* **Beatriz García-Berja Bermejo**. *Food Sciences and Technology.*
- *"Graphene synthesis: Chemical oxidation, exfoliation and reduction".* **Antonio Patón Carrero.** *Chemical Engineering.*
- *"Modified screen-printed carbon nanofiber electrode for quantitation of heterocyclic amines in food".* **Cristina Montes Correal**. *Analytical Chemistry.*

Thursday 14th of June 2018

9:00- 3rd session *(Chairwoman: Inmaculada Moreno)*

- *"Innovations in vine fertilization using wine distillery waste compost".* **Juan Antonio Delgado Sánchez-Migallón.** *Food Sciences and Technology.*
- *"Capillary electrophoresis method for the discrimination between natural and artificial vanilla flavor for controlling food frauds".* **Samah Lahouidak**. *Analytical Chemistry.*
- *"Designing Novel Triazine-based hydrogels for drug delivery applications".* **Jorge Leganes Bayón.** *Organic Chemistry.*
- *"New scorpionate zinc complexes as initiators for the synthesis of polycarbonates by ROP copolymerisation of cyclohexene oxide and carbon dioxide".* **Sonia Sobrino Ramírez**. *Inorganic Chemistry.*

10:00- 4th session *(Chairwoman: Inmaculada Moreno)*

- *"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.** *Analytical Chemistry.*
- *"Sustainable-green electrooxidation of organochlorinated compounds".* **Maria Millán Espinar.** *Chemical Engineering.*
- *"Waveguide Behaviour in Self-assembled Thiadiazole and Benzothiadiazole-based Materials".* **Raúl Martín Lozano.** *Organic Chemistry.*
- *"Anthocyanin profile of brazilian hybrid grape cultivar BRS Núbia ('Michele Palieri' x 'Arkansas 2095')".* **Yara Nishiyama.** *Food Sciences and Technology.*

11:00- Coffee break

11:40- Presentation of the Territorial Section of the Real Sociedad Española de Química (RSEQ), Dr. Julián Rodríguez López and Jóvenes Investigadores Químicos JIQ-RSEQ & EYCN - Dr. Antonio M. Rodríguez.

12:00- **Invited Lecturer: Prof. José Miguel Rodríguez Maroto (Universidad de Málaga**). *"Transferencia del conocimiento desde el GIGA al sector empresarial y viceversa"*

13:00- 5th session *(Chairwoman: Virginia Moreno)*

- *"Synthesis of second generation biofuels from agro-food wastes and its atmospheric implications".* **Almudena Lorente Diezma.** *Organic Chemistry.*
- *"Ring-Opening Copolymerization of Cyclic Anhydrides and Epoxides Catalysed by Aluminium Heteroscorpionate Complexes".* **Marc Martínez de Sarasa Buchaca.** *Inorganic Chemistry.*
- *"Electrochemical activation of catalysts for hydrogen production".* **Estela Ruíz López.** *Chemical Engineering.*
- "*Analysis of gold nanoparticles using inductively coupled plasma mass spectrometry via single particle (SP-ICP-MS) in clinical samples".* **Sergio Fernández Trujillo**. *Analytical Chemistry.*

14:00- Lunch break

16:00- **Invited Lecturer: Prof. Alejandro Cifuentes (CSIC, Madrid**). "Alimentómica, ingredientes bioactivos y cáncer de colon: historia de un largo viaje"***.***

17:00- 6th session *(Chairman: Jose Pérez)*

- "*Screen-printed electrodes used for the determination of drugs of abuse".* **Isabel Lizcano Sanz**. *Analytical Chemistry.*
- *"Effects of seeds and stems grape by-products extracts and colloidal silver as alternative preservatives on white wine quality".* **Lucía Loarce Ortíz**. *Food Science and Technology.*
- *"NMR Sensitivity Enhancement Combining Miniaturized Coils and Hyperpolarization Techniques".* **Rosa María Sánchez Donoso.** *Organic Chemistry.*
- *"Gas Phase Kinetics at temperatures of the interstellar medium".* **Sergio Blázquez González.** *Physical Chemistry.*

Friday 15th of June 2018

9:30- 7th session (*(Chairwoman: Ana Raquel de la Osa)*

- *"Influence of dehydration process on flavonol profile of seedless grape cultivar BRS Vitória (CNPUV 681-29 x BRS Linda)".* **Carolina Olivati**. *Food Sciences and Technology.*
- *"Schwarz domain decomposition method applied to the incompressible Navier-Stokes equations with Boussinesq approximation".* **Ana Fernández Pérez**. *Mathematics.*
- *"Photo-CIDNP: A Tool for In-Situ Monitoring of Structural Changes in Biomolecules".* **José Miguel Mateo González.** *Organic Chemistry.*
- *"Operating membrane electrolytic technology for the direct disinfection of highly fecal-polluted water".* **Julia Isidro Elvira**. *Chemical Engineering.*

10:30- Coffee break

11:00- 8th session *(Chairman: Antonio M. Rodríguez)*

- *"Linking [C60] Fullerene on N-doped Graphene Surface. Synthesis and Characterization".* **Luis Miguel Arellano Castellanos.** *Organic Chemistry.*
- *"Development of hydroxy-containing imidazole organocatalysts for CO2 fixation into cyclic carbonates".* **Mª del Prado Caballero Espinosa.** *Inorganic Chemistry.*
- *O-30"Chemistry of secondary organic aerosol formation from the photolysis and oxidation of α-methylstyrene with hydroxyl radicals".* **María Mercedes Tajuelo Díaz-Pavón.** *Physical Chemistry.*
- *"Use of capillary electrophoresis for characterisation of vinyl- terminated gold nanoprisms and nanooctahedra".* **Carlos Adelantado Sánchez.** *Analytical Chemistry.*

12:00- Invited Lecturer: **Prof. Mª del Carmen de la Torre Egido (CSIC, Madrid).** *"Productos Naturales: de la Magia a la Química Moderna".*

12:50- Act of academic distinction to the Vice-Chancellor of Research and Scientific Policy of UCLM **Prof. José Julián Garde López-Brea**. Intervention of the Vice-Chancellor.

13:30- Prize winners and closing ceremony chaired by the Dean of the Faculty of Chemical Sciences and Technology Prof. Ángel Ríos Castro and Sponsors.

CONFERENCIAS INVITADAS

CI 1

INNOVACIONES EN EL ESTUDIO DE LA ASTRINGENCIA; IMPACTO DE CIERTAS PRÁCTICAS ENOLÓGICAS SOBRE LA PERCEPCIÓN DE LA ASTRINGENCIA DE LOS VINOS TINTOS

Fernando Zamora

Conference “In Memorian of Prof. Isidro Hermosín”
Universitat Rovira i Virgili, Departament de Bioquímica i Biotecnologia, Facultat d'Enologia de Tarragona. Marcelí Domingo, s/n 43007 - Tarragona

Food Science and Technology

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.

CI 2

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

María C. Moreno-Bondi[1]; E. Benito Peña[1]; R. Peltomaa[1]; S. Carrasco[1], F. Navarro[1]; R. Barderas[2]; U. Sauer[3]

[1]Dept. Analytical Chemistry, Faculty of Chemistry, Universidad Complutense de Madrid, Av. Complutense s/n, 28040 Madrid, Spain; mcmbondi@ucm.es [2] Dept. of Biochemistry and Molecular Biology I, Universidad Complutense de Madrid, Av. Complutense s/n, 28040 Madrid, Spain. [3] Center for Health & Bioresources, AIT Austrian Institute of Technology GmbH, Konrad-Lorenz-Straße 24, 3430 Tulln, Austria.

Analytical Chemistry

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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CI 3

TRANSFERENCIA DEL CONOCIMIENTO DESDE EL GIGA AL SECTOR EMPRESARIAL Y VICEVERSA

José Miguel Rodríguez Maroto*

Departamento de ingeniería Química. Universidad de Málaga

Chemical Engineering

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.

CI 4

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

Alejandro Cifuentes

Foodomics Laboratory, CIAL, CSIC, Madrid, Spain. E-mail: a.cifuentes@csic.es

Food Science and Technology

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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CI 5

PRODUCTOS NATURALES: DE LA MAGIA A LA QUÍMICA MODERNA

Mª del Carmen de la Torre Egido*, A. Pérez, J. Gómez, M. Ortiz

Universidad Complutense de Madrid, Consejo Superior de Investigaciones Científicas; Instituto de Química Orgánica General; Departamento de Síntesis, Estructura y Propiedades de Compuestos Orgánicos, Madrid, España

Organic Chemistry

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.

PRESENTACIONES

O-1

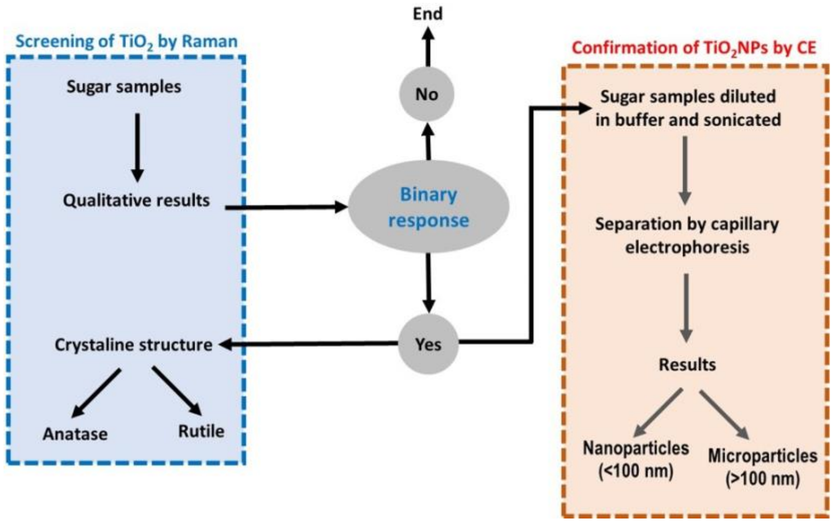
ANALYTICAL NANOMETROLOGICAL APPROACH FOR SCREENING AND CONFIRMATION OF TITANIUM DIOXIDE NANO/MICRO PARTICLES IN SUGARY SAMPLES BASED ON RAMAN SPECTROSCOPY – CAPILLARY ELECTROPHORESIS

V. Moreno*, M. Zougagh, Á. Ríos

Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha, Camilo José Cela Avenue, 13071 - Ciudad Real, Spain; phone number: +34 659798755; e-mail: Virginia.Moreno@uclm.es

Analytical Chemistry

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.



O-2

SYNTHESIS OF POLYMER-DRUG CONJUGATES TO CONTROLLED RELEASE OF DRUGS

M. José Carrero*, M. J. Ramos, J. F. Rodríguez, A. M. Borreguero

Instituto de Tecnología Química y Medioambiental, Universidad de Castilla-La Mancha, Avda. Camilo José Cela, 1A 13004; Tfn: +34 926295300 Ext: 96318; e-mail: mjose.carrero@uclm.es

Chemical Engineering

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.

O-3

CATALYTIC TRANSFER HYDROGENATION PROCESSES USING RUTHENIUM AND IRIDIUM ORGANOMETALLIC COMPOUNDS

M. Ruiz-Castañeda*[1], B. Manzano[1], G. Espino[2], F. Jalón[1]

[1] Dpto. de Química Inorgánica, Orgánica y Bioquímica, Universidad de Castilla-La Mancha, Facultad de Ciencias y Tecnologías Químicas-IRICA. Avda. C. J. Cela, 10, 13071, Ciudad Real; e-mail: Margarita.RAlvaro@uclm.es [2] Dpto. de Química, Universidad de Burgos, Facultad de Ciencias. Plaza Misael Bañuelos s/n, 09001, Burgos.

Inorganic Chemistry

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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O-4

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

I. Torres-Moya*[a], R. Vázquez[b], S. Fernández-Palacios[c], J.R. Carrillo[a], A. Díaz-Ortiz[a], R. Mallavia[b], M. C. Ruiz-Delgado[c], R. Ponce-Ortiz[c], P. Prieto[a]

[a] Department of Organic Chemistry, Faculty of Chemical and Technologies Sciences-IRICA, University of Castilla La Mancha. 13071, Ciudad Real (Spain). [b] Department of Organic Chemistry, Institute of Molecular and Celular Biology, University Miguel Hernández. 03202 Elche (Spain). [c] Department of Physical Chemistry, Faculty of Sciences, University of Málaga. 29071 Málaga (Spain).
e-mail: Ivan.TorresMoya@uclm.es

Organic Chemistry

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 2*H*-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 2*H*-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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O-5

YEAST BIODIVERSITY FROM NATURAL SOURCES IN THE CENTRAL REGION OF SPAIN

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

Dpto. de Química Analítica y Tecnología de los Alimentos, Universidad de Castilla – La Mancha, Avda Camilo José Cela s/n 13071 Ciudad Real, tfno: +34; e-mail: beatriz.gbermejo@uclm.es

Food Science and Technology

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.

O-6

GRAPHENE SYNTHESIS: CHEMICAL OXIDATION, EXFOLIATION AND REDUCTION

A. Paton-Carrero*, J. L. Valverde, M. P. Lavin-Lopez, A. Romero,

Dpto. de Ingeniería Química, Universidad de Castilla La Mancha, Avda. Camilo Jose Cela s/n 13071 Ciudad Real tfno: +34 926 29 53 00 ext. 96322;
e-mail: Antonio.Paton@uclm.es

Chemical Engineering

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.

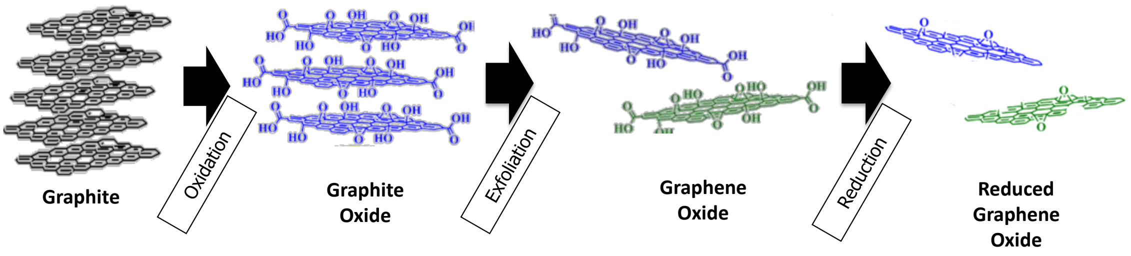


Figure 1. Scheme of chemical reduction

The main problem of this method is the great number of variables and products that are obtained during the whole chemical reduction. This work summarizes 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.

O-7

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

C. Montes*, A. Contento, M.J. Villaseñor, A. Ríos

Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha, Avda. Camilo José Cela 10, 13004 Ciudad Real, Spain, tfno: +34 693631397; e-mail: Cristina.Montes1@alu.uclm.es

Analytical Chemistry

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).

O-8

INNOVATIONS IN VINE FERTILIZATION USING WINE DISTILLERY COMPOST

J. A. Delgado*, E. Sánchez-Palomo, M. A. Ferrer Valverde, M. A. González Viñas

Dpto. de Química Analítica y Tecnología de Alimentos, Universidad de Castilla-La Mancha, Avda Camilo José Cela s/n 13071 Ciudad-Real, tfno: +34 926 295300; e-mail: JuanAntonio.Delgado@alu.uclm.es

Food Science and Technology

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.

O-9

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

S. Lahouidak*, 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 :+34 602105228, e-mail:slahouidak@gmail.com

Analytical chemistry

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 flavourings, as well as for confirmation of natural or non-natural origin of vanilla in samples using four selected food samples containing this flavour.

O-10

DESIGNING NOVEL TRIAZINE-BASED HYDROGELS FOR DRUG DELIVERY APPLICATIONS

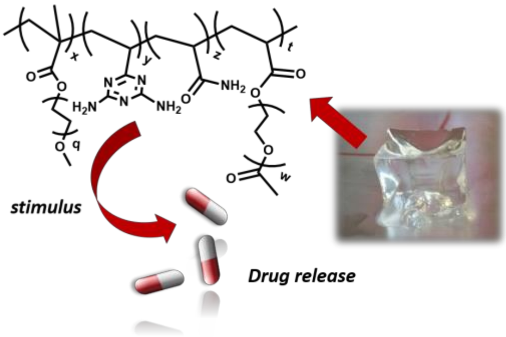
J. Leganés*, J. M. Galindo, A. Sánchez-Migallón, S. Merino, E. Vázquez

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

Organic Chemistry

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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O-11

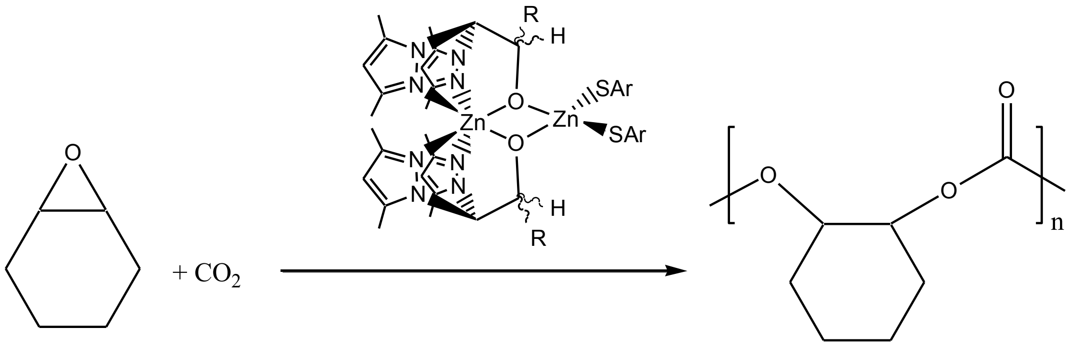
NEW SCORPIONATE ZINC COMPLEXES AS INITIATORS FOR THE SYNTHESIS OF POLYCARBONATES BY ROP COPOLYMERISATION OF CYCLOHEXENE OXIDE AND CARBON DIOXIDE

S. Sobrino,[1] A. Otero,[1*] J. Fernández-Baeza,[1*] L. F. Sánchez Barba,[2*] A. Garcés,[2] A. Lara Sánchez,[1] J. A. Castro Osma,[1] A. M. Rodríguez[1]

[1]Dpto. Química Inorgánica, Orgánica y Bioquímica. Facultad de Ciencias y Tecnologías Químicas. Universidad de Castilla-La Mancha. Avda. Camilo José Cela, S/N. 13071 Ciudad Real. 636699976, Sonia.Sobrino@uclm.es [2]Dpto. Biología y Geología, Física y Química Inorgánica. Campus de Móstoles. Universidad Rey Juan Carlos. Calle Tulipán. s/n. 28933-Móstoles-Madrid.

Inorganic Chemistry

A series of new alcoxide and tioalcoxide mono- and bimetallic zinc complexes containing heteroscorpionate ligands have been prepared in very high yields. The structures of the complexes were determined by spectroscopic methods, and various single-crystal X-ray structure of these families confirmed a κ^3-NNO, κ^2-NN, κ^2-NN-μO coordination mode of the scorpionate ligand in a mono- and dinuclear molecular arrangement. These zinc complexes were investigated as catalysts for the synthesis of polycarbonates from epoxides and carbon dioxide in the absence of a cocatalyst.[1] Under the optimal reaction conditions, the complex type $[Zn(\kappa^2NN\text{-}\mu O)_2Zn(SAr)_2]$ acts as an efficient single-component initiator for the ring-opening copolymerisation of cyclohexene oxide and carbon dioxide, at 1% catalyst, 10 bars of CO_2 and 70ºC, yielding polycarbonate materials.



O-12

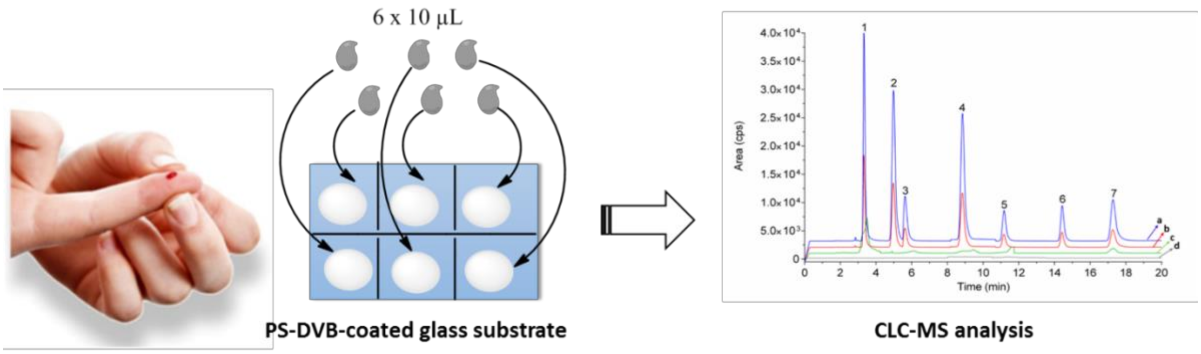
A SIMPLE POLY(STYRENE-CO-DIVINYLBENZENE)-COATED GLASS BLOOD SPOT METHOD FOR MONITORING OF SEVEN ANTIDEPRESSANTS USING CAPILLARY LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY

K. Murtada*, F. de Andrés, M. Zougagh, Á. Ríos

Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha, Ciudad Real 13071, tfno: +34 632097107; e-mail: Khaled.Ali@alu.uclm.es

Analytical Chemistry

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.



O-13

SUSTAINABLE-GREEN ELECTROOXIDATION OF ORGANOCHLORINATED COMPOUNDS

M. Millán*, M.A. Rodrigo, C.M. Fernández-Marchante, P. Cañizares, J. Lobato

Department of Chemical Engineering, University of Castilla-La Mancha, Avda Camilo José Cela, 12 13071 Ciudad Real, Tel: 926 295 300 Ext: 96352
email: maria.millan@uclm.es

Chemical Engineering

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 used for the pesticide removal.

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O-14

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

R. Martín*, P. Prieto, J. R. Carrillo, Á. Díaz

Department of Inorganic, Organic and Biochemistry, University of Castilla La Mancha,
Avda de Camilo José Cela, 10 13071 Ciudad-Real, tel. +34 926 295370; email:
Raul.Martin@uclm.es

Organic Chemistry

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 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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O-15

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

Y. P. O. Nishiyama*, C. Olivati, J. Pérez-Navarro, R. T. Souza, S. G. Alonso, I. Hermosín-Gutierrez, R. Da-Silva, E. S. Lago-Vanzela

Universidade Estadual Paulista, Instituto de Biociências, Letras e Ciências Exatas, Departamento de Engenharia e Tecnologia de Alimentos, São José do Rio Preto, SP, 15054-000, Brasil, tfno: +34 695 796 317; e-mail: yaranishy@gmail.com

Food Science and Technology

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.

O-16

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

A. Lorente*, M. P Sánchez-Verdú, B. Cabañas, A. Moreno

Department of Inorganic, Organic, Biochemistry and Physics chemistry. University of Castilla–La Mancha, Avda Camilo José Cela, 10. phone: 926 295300; e-mail: Almudena.lorente@uclm.es

Organic Chemistry

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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O-17

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

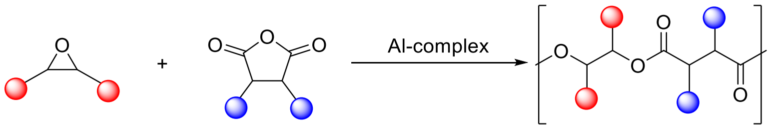
M. Martínez de Sarasa Buchaca[1], J. A. Castro-Osma[2]*, A. Lara-Sanchez,[1]*, A. Otero[1]

[1]Dpto. Química Inorgánica y Bioquímica. Facultad de Ciencias y Tecnologías Químicas. Universidad de Castilla-La Mancha. Avda. Camilo José Cela, S/N. 13071 Ciudad Real.
[2]Dpto. Química Inorgánica, Orgánica y Bioquímica. Facultad de Farmacia. Universidad de Castilla-La Mancha. Avda. Cronista Francisco Ballesteros, 1. 02071 Albacete.
Marc.MartinezSarasa@uclm.es

Inorganic Chemistry

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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O-18

ELECTROCHEMICAL ACTIVATION OF CATALYSTS FOR HYDROGEN PRODUCTION

E. Ruiz-López*, F. Dorado, A. De Lucas-Consuegra

Dpto. de Ingeniería Química, Universidad de Castilla la Mancha, Avda Camilo José Cela
12 13071 Ciudad Real, tfno: +34 926 295300; e-mail: Estela.Ruiz@uclm.es

Chemical Engineering

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.

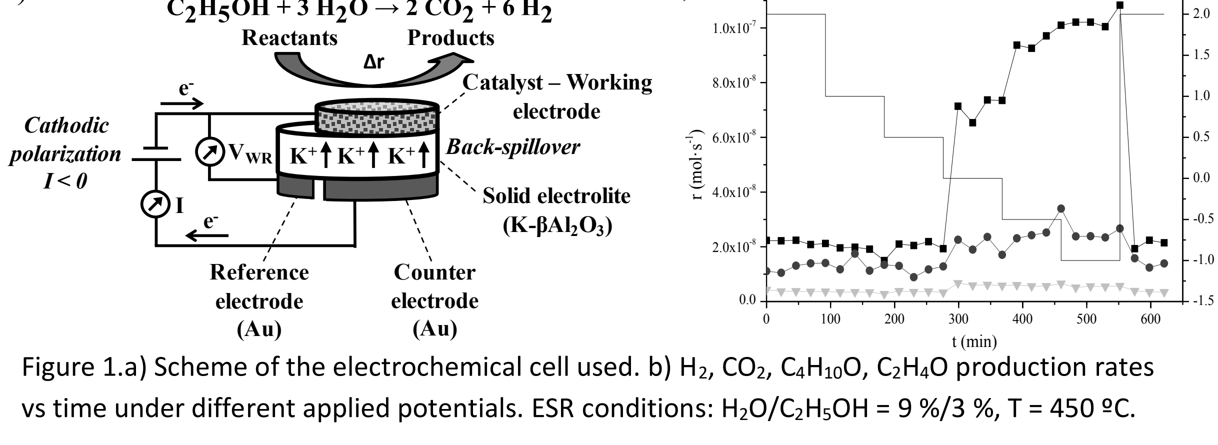

Figure 1.a) Scheme of the electrochemical cell used. b) H_2, CO_2, $C_4H_{10}O$, C_2H_4O production rates vs time under different applied potentials. ESR conditions: H_2O/C_2H_5OH = 9 %/3 %, T = 450 ºC.

O-19

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

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

[1]Department of Analytical Chemistry and Food Technology, Faculty of Environmental Sciences and Biochemistry, University of Castilla-La Mancha, Avda. Carlos III s/n, 45071 Toledo, Spain [2]Department of Analytical Chemistry and Food Technology, Faculty of Chemical Sciences and Technologies, University of Castilla-La Mancha, Avda. Camilo José Cela s/n, 13071 Ciudad Real, Spain; e-mail: Sergio.Fernandez@uclm.es

Analytical Chemistry

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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O-20

SCREEN-PRINTED ELECTRODES USED FOR THE DETERMINATION OF DRUGS

I. Lizcano*, J. Rodríguez, G. Castañeda

Dpto. de Química Analítica y Tecnología de los Alimentos, Universidad de Castilla La Mancha, Avda Camilo José Cela 10, 13071 Ciudad Real, tfno: +34 926295300; e-mail: Isabel.Lizcano@uclm.es

Analytical Chemistry

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.

O-21

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

L. Loarce *[1], L. Marchante [1], M. E. Alañón [1], P. M. Izquierdo [2], E. García [2], M. C. Díaz-Maroto [1], M. S. Pérez-Coello [1]

[1] Area of Food Technology. Faculty of Sciences and Chemical Technologies. University of Castilla la Mancha. Avenida Camilo José Cela 10. 13071. Ciudad Real. Spain.

[2] Regional Institute of Agrifood and Forestry Research and Development of Castilla-La Mancha (IRIAF-IVICAM). Crta. Toledo-Albacete s / n. 13700 Tomelloso (Ciudad Real). Spain. E-mail: lucia.loarce@uclm.es

Food Science and Technology

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.

O-22

NUCLEAR MAGNETIC RESONANCE SENSITIVITY ENHANCEMENT COMBINING MINIATURIZED COILS AND HYPERPOLARIZATION TECHNIQUES

R. M. Sánchez*[a,b], M. Mompeán[a], A. de la Hoz[a], V. Saggiomo[b],
A. Velders[a,b], M.V. Gómez[a]

[a] Instituto Regional de Investigación Científica Aplicada (UCLM), Avda. Camilo José Cela s/n, 13071 Ciudad Real, +34 926295300 Ext.6740; e-mail: rosamaria.sanchez@uclm.es
[b] Laboratory of BioNanoTechnology, Wageningen University, The Netherlands

Organic Chemistry

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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O-23

GAS PHASE KINETICS AT TEMPERATURES OF THE INTERSTELLAR MEDIUM

S. Blázquez*[1], A. J. Ocaña[1], B. Ballesteros[1,2], M. Antiñolo[2], J. Albaladejo[1,2], E. 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 C. Real, Spain.
[2] Instituto de Investigación en Combustión y Contaminación Atmosférica (ICCA).
Universidad de Castilla-La Mancha, Camino de Moledores s/n, 13071 C. Real, Spain.
e-mail: Sergio.Blazquez@uclm.es

Physical Chemistry

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:

$$k(T = 21 - 107\text{ K}) = (2.1 \pm 0.5) \times 10^{-11}\,(T/300\text{ K})^{-(0.71 \pm 0.10)}\ \text{cm}^3\ \text{molecule}^{-1}\ \text{s}^{-1}$$

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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O-24

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

C. Olivati*[1], Y.P.O. Nishiyama[1], J. Pérez-Navarro[2], S. Gomez-Alonso[2], I. Hermosín-Gutierrez [2], R. Da-Silva [1], E.S. Lago-Vanzela[1]

[1]Department of Food Engineering and Technology at the São Paulo State University - UNESP, Sao Jose do Rio Preto - SP, Brazil, [2] Instituto Regional de Investigación Científica Aplicada, Universidad de Castilla-La Mancha, Campus Universitario s/n, 13071 Ciudad Real, Spain; e-mail: carolinaolivati@gmail.com

Food Science and Technology

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.

O-25

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

A. Fernández*, H. Herrero, F. Pla

Dpto. de Matemáticas, Universidad de Castilla-La Mancha, Avda. Camilo José Cela 10,
13071 Ciudad Real, tfno: +34 926295412; e-mail: Ana.Fernandez20@alu.uclm.es

Applied Mathematics

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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O-26

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

J. M. Mateo*, M. Mompeán, P. Nitschke, M. Á. Jiménez, R. M. Gschwind, M. V. Gómez

Faculty of Chemical Sciences and Technologies, University of Castilla-La Mancha, Avda
Camilo José Cela 10, 13071 Ciudad Real, tfno: +34 926 295300 Ext.: 96345;
e-mail: josemiguel.mateo@uclm.es

Organic Chemistry

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 specific experimental conditions.

Therefore, we use photo-CIDNP NMR spectroscopy to study the structural transition of the $\text{LytA}_{239-252}$ peptide, a fragment of the LytA autolysin that switches between ⍰-hairpin and ⍰-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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O-27

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

J. Isidro*, C. Sáez, J. Llanos, P. Cañizares, M.A Rodrigo

Department of Chemical Engineering, University of Castilla La Mancha,
Avda. Camilo José Cela, 12 13079 Ciudad Real, tfno: +34 926 295 300 ext: 96352;
e-mail: julia.isidro@uclm.es

Chemical Engineering

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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O-28

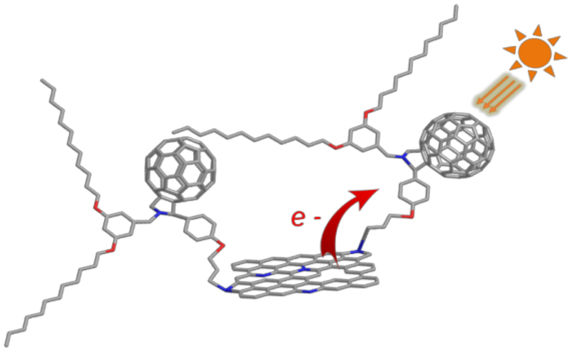
LINKING FULLERENE C_{60} ON *N*-DOPED GRAPHENE SURFACE. SYNTHESIS AND CHARACTERIZATION

L. Miguel Arellano*, M. Barrejón, M. J. Gómez-Escalonilla, F. Langa

Instituto de Nanociencia, Nanotecnología y Materiales Moleculares (INAMOL),
Universidad de Castilla-La Mancha, 45071, Toledo, Spain; e-mail:
LuisMiguel.Arellano@uclm.es

Organic Chemistry

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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O-29

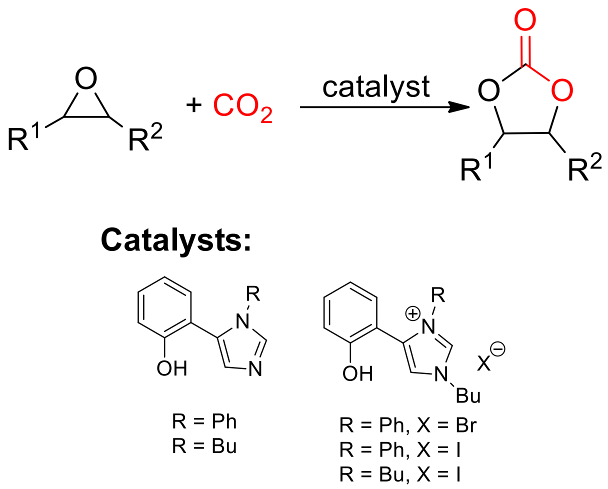
DEVELOPMENT OF HYDROXY-CONTAINING IMIDAZOLE ORGANOCATALYSTS FOR CO_2 FIXATION INTO CYCLIC CARBONATES

P. Caballero*, J. A. Castro-Osma, J. Martínez, F. de la Cruz-Martínez, J. Fernández-Baeza, A. Otero, A. Lara-Sánchez, J. 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, Avda Camilo José Cela s/n 13071, Ciudad Real,
e-mail: prado.caballero@uclm.es

Inorganic Chemistry

Highly efficient neutral and ionic imidazole-based organocatalysts have been developed for the synthesis of cyclic carbonates from epoxides and carbon dioxide (Scheme 1).[3] 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.[4]



Scheme 1. Synthesis of cyclic carbonates.

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O-30

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

M. Tajuelo, D. Rodríguez, A. Rodríguez

Dpto. de Química Física, Universidad de Castilla-La Mancha, Avda Carlos III s/n 45071 Toledo, tfno: 925268800, Ext: 5790; e-mail: mercedes.tajuelo@uclm.es

Physical Chemistry

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 vapor, oxides of nitrogen (NOx) and seed particle has been investigated 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 NOx 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 vapor, NOx 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.

O-31

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

C. Adelantado*, M. Algarra, M. Zougagh, Á. Ríos

Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha, Camilo José Cela Avenue, 13071 - Ciudad Real, Spain; phone number: +34 692881998; e-mail: carlos.adelantado@uclm.es

Analytical Chemistry

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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POSTERS

P-1

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

F. Abujaber [1*], A.I. Corps[1], F.J. Guzmán [1], A. Ríos [2] R.C. Rodríguez [1]

Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha.

[1] Environmental Sciences Institute (ICAM), E-45071, Toledo, Spain.
[2] Faculty of Chemical Sciences and Technologies, E-13071, Ciudad Real, Spain, e-mail: feras.abujaber@alu.uclm.es

Analytical Chemistry

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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P-2

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

P. Alonso-Andrés[1], J. L. Albasanz[1], M. Martín[1]

Área de Bioquímica. Dpto de Química Inorgánica, Orgánica y Bioquímica. Facultad de Ciencias y Tecnologías Químicas. UCLM.

Biochemistry

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.

P-3

GEMCITABINE-IMPREGNATED PLGA SCAFFOLDS PROCESSED WITH SUPERCRITICAL CO_2.

I. Álvarez*, C. Gutiérrez, J. F. Rodríguez, A. de Lucas and M. T. García.

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

Chemical Engineering

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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P-4

TROPOSPHERIC REACTIVITY OF 3-ETHOXY-1-PROPANOL

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

Dpto. Química Física, Universidad de Castilla La Mancha, Facultad de Ciencias y Tecnologías Químicas, Avda Camilo José Cela s/n 13071,
Minmaculada.aranda@alu.uclm.es

Physical Chemistry

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}): $(3.4\pm0.2)\times10^{-10}$, $(3.4\pm0.1)\times10^{-11}$ and $(1.6\pm0.1)\times10^{-14}$ 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 NO_x 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.

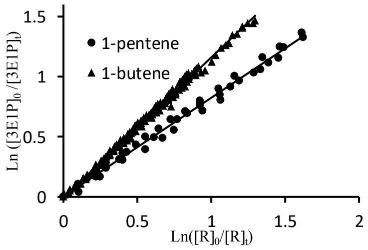

Figure 1. Relative rate plots for the reaction of 3-ethoxy-1-propanol (3E1P) with Cl atoms using two reference compounds

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P-5

IONIC LIQUID AND MAGNETIC NANOPARTICLES 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 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 find the optimal extraction conditions.

P-6

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

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

Department of Analytical Chemistry and Food Technology, Faculty of Chemical Science and Technologies, University of Castilla-La Mancha, tfno: +34 631985414; e-mail: Yassine.Benmassaud@uclm.es

Analytical Chemistry

Considered a major flavouring 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.

P-7

GRAPE SEED OIL EPOXIDATION IN SUPERCRITICAL CO_2

J. Catalá*, M.J. Ramos, J. F. Rodríguez, M. T. García.

Dpto. de Ingeniería Química, Universidad de Castilla La Mancha,
Avda Camilo José Cela 12, 13071 Ciudad Real.
tfno: +34 926 295 300 Ext: 96350; e-mail: juan.catala@uclm.es

Chemical Engineering

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.

P-8

A DIRECT SCREENING OF AgNPs FROM DECORATION OF PASTRY

A. I. Corps [1*], F.J. Guzmán [1], R.C. Rodríguez [1], A. Ríos [2]

Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha.[1] Environmental Sciences Institute (ICAM), E-45071, Toledo, Spain. [2] Faculty of Chemical Sciences and Technologies, E-13071, Ciudad Real, Spain, e-mail: Anaisabel.corps@uclm.es

Analytical Chemistry

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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P-9

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

M. Crespo [1], D. A. León-Navarro [1], M. Martín [1]

[1]Facultad de Ciencias y Tecnologías Químicas / Facultad de Medicina de Ciudad Real.
Universidad de Castilla-La Mancha. Spain.

Biochemistry

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.

P-10

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

J. C. de Haro*, A. López, A. Pérez, M. Carmona, J. F. Rodríguez

Instituto de Tecnología Química y Medioambiental, Universidad de Castilla-La Mancha, Avda. Camilo José Cela, 1A 13004; Tfn: +34 926295300 Ext: 96318; e-mail: JCarlos.Haro@uclm.es

Chemical Engineering

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).

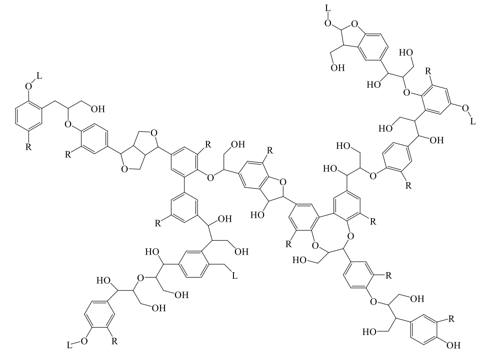

Figure 1. Chemical structure of lignin

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.

P-11

KINETICS OFTHE ATMOSPHERICALLY RELEVANT GAS-PHASE REACTIONS OF ALLYL CYANIDE

M. Antiñolo[1,2], R. del Olmo[1,2], E. Jiménez[1,2], J. Albaladejo[1,2]

[1] Instituto de Investigación en Combustión y Contaminación Atmosférica. Universidad de Castilla-La Mancha, Camino de Moledores, s/n. 13071 Ciudad Real, Spain.
[2] Departamento de Química Física. Facultad de Ciencias y Tecnologías Químicas. Universidad de Castilla-La Mancha, Avda. Camilo José Cela, 1B. 13071 Ciudad Real, Spain.

Physical Chemistry

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-NO_x 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.

P-12

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

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

Dpto. de Química Orgánica, Universidad de Ciencias y Tecnologías Químicas,
Universidad de Castilla La Mancha, Avda Camilo José Cela 10, 13071, Ciudad Real. Tfno:
+34 926295300; e-mail: Beatriz.Donoso@uclm.es

Organic chemistry

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 2*H*-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 2*H*-benzo[*d*][1,2,3]triazole required the previous preparation of 2-(3,5-bis(trifluoromethyl)phenyl)-4,7-dibromo-2*H*-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 2*H*-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 compounds 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.

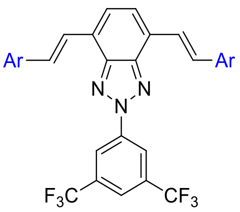

Figure 1. Alkenyl derivatives of 2*H*-benzo[*d*][1,2,3]trizole.

P-13

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

P. Fernández-Pacheco*, M. Arévalo-Villena, A. Briones Pérez

Food Science and Technology Department, Universidad Castilla-La Mancha, Ciudad Real, Avda Camilo José Cela s/n 13071 Ciudad Real. +34 926 29 53 00 ext.96332
Pilar.Fernandezpacheco@alu.uclm.es

Food Science and Technology

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.

P-14

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

M.A. Ferrer Valverde*, E. Sánchez-Palomo, J.A. Delgado, M.A. González Viñas

Dpto. de Química Analítica y Tecnología de Alimentos, Universidad de Castilla-La Mancha, Avda Camilo José Cela, 10, 13071 Ciudad-Real, tfno: +34 295300; e-mail: ManuelAngel.Ferrer@alu.uclm.es

Food Science and Technology

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.

P-15

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

V. J. González[a]*, A. M. Rodríguez[a], V. León[a], E. Vázquez[a,b]

[a] Instituto Regional de Investigación Científica Aplicada (IRICA), UCLM, 13071 Ciudad Real, Spain. [b] Fac. CC y Tecnol. 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-16

FUNCTIONALIZATION OF PLA WITH COUMARIN VIA CLICK CHEMISTRY IN $scCO_2$

E. Gracia*, I. Gracia, M.T. García, A.M. Borreguero, A. De Lucas, J.F. Rodríguez

Dpto. de Ingeniería Química, Universidad de Castilla-La Mancha, Avda Camilo José Cela, 12; 13005 Ciudad Real; e-mail: Eulalio.gracia@uclm.es

Chemical Engineering

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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P-17

HYDROGELS WITH MAGNETIC PROPERTIES

J. Herrera, V. J. González, P. Prieto, E. Vázquez.

Dpto. de Química Orgánica, Facultad de Ciencias y Tecnologías Químicas-IRICA,
Universidad de Castilla-La Mancha, Avda. Camilo José Cela, s/n, C.P. 13071, Ciudad
Real, Tfno:926-295300; e-mail: 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 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.

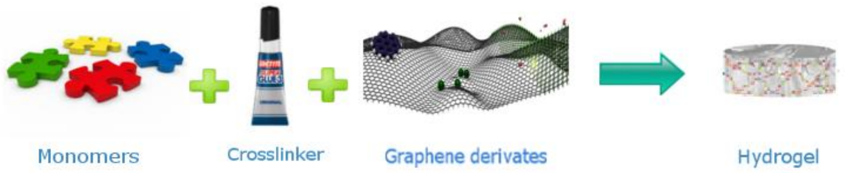

Figure 1. General scope of hydrogels synthesis.

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P-18

RICH SUGAR 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-19

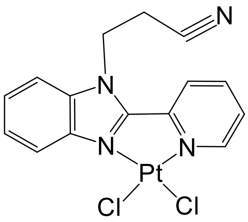
SYNTHESIS AND CYTOTOXICITY OF Pt(II) PYRIDYL BENZIMIDAZOLE COMPOUNDS BEARING FUNCTIONALIZED TAILS. IMPORTANCE OF THEIR INTERACTION WITH SEROALBUMIN

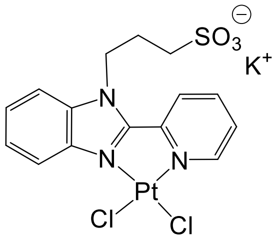
J. Leal,[†] C. Pérez-Arnaiz,[‡] N. Busto,[‡*] M. del Carmen Carrión,[†] A. R. Rubio,[‡] G. Barone[§], Javier Santolaya,[‡] J. M. Leal,[‡] M. Vaquero,[‡] F. A. Jalón,[†] B. R. Manzano,[†*] B. García[‡*]

[†]Universidad de Castilla-La Mancha, Facultad de Ciencias y Tecnologías Químicas-IRICA, Avda. Camilo J. Cela 10, 13071 Ciudad Real, Spain. [‡]UBU, Departamento de Química, Plaza Misael Bañuelos s/n, 09001, Burgos, Spain. [§]Dipartimento di Scienze e Tecnologie Biologiche, Chimiche e Farmaceutiche, Università degli Studi di Palermo, Viale delle Scienze Ed. 17, 90128, Palermo, Italy

Inorganic Chemistry

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 *d*GMP, 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.

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P-20

FUNCTIONALIZATION OF PEG WITH COUMARIN VIA CLICK CHEMISTRY IN SUPERCRITICAL CO_2.

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

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

Chemical Engineering

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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P-21

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

M. Louleb*, 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: +34 632 466448, e-mail: marwa.lauleb@gmail.com

Analytical chemistry

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.

P-22

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

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

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

Organic Chemistry

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]

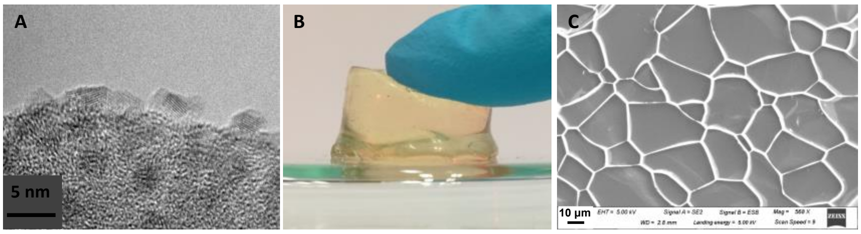

Figure: a) Transmission Electron Microscopy (TEM) of GQDs; b) Digital photo and c) Cryo-Scanning Electron Microscopy (Cryo-SEM) of the nanocomposite.

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P-23

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

L. Mazuecos, B. M. Rubio, A. Fernández, C. Pintado, C. Arribas, A. Andrés, N. Gallardo

Área de Bioquímica. Dpto de Química Inorgánica, Orgánica y Bioquímica. Facultad de Ciencias y Tecnologías Químicas. UCLM.

Biochemistry

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.

P-24

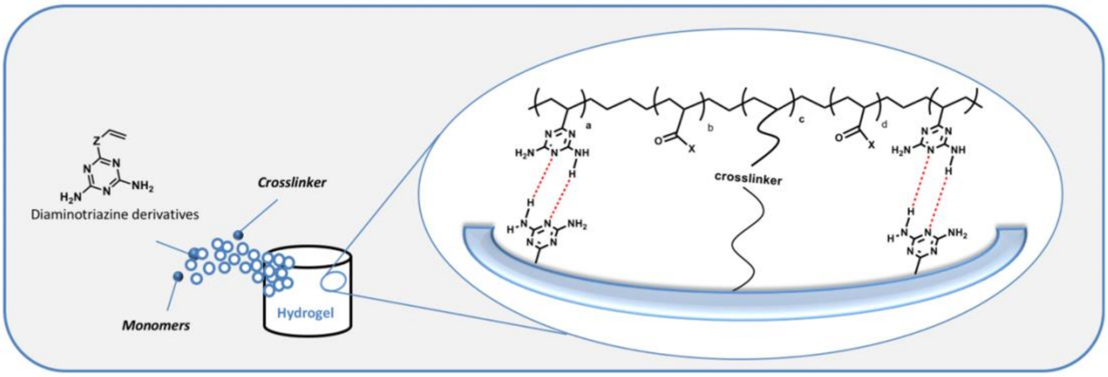
NOVEL HYDROGELS BASED ON TRIAZINE AS Fe(III) SENSORS

J. Muñoz Galindo*, J. Leganés, S. Merino, A. Sánchez-Migallón, E. Vázquez

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

Organic Chemistry

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

M. Muñoz-Morales, C. Sáez, P. Cañizares, M.A. Rodrigo*

Dpto. de Ingeniería Química, Universidad de Castilla-La Mancha, Avda. Camilo José Cela s/n 13071 Ciudad Real; e-mail: martin.munoz@uclm.es

Chemical Engineering

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

A. Naranjo*, A. Martín-Pacheco, A. M. Rodríguez, E. Díez-Barra, M. A. Herrero, E. Vázquez

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

Organic Chemistry

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.

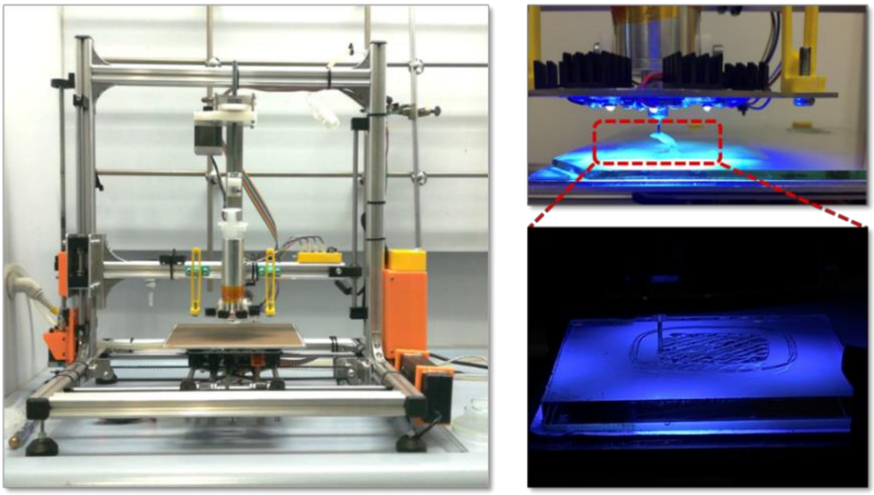

Figure. 3D printer and printing process.

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P-27

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

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

Dpto. de Ingeniería Química, UCLM, Avda de Camilo José Cela. Edificio Enrique Costa
13071 Ciudad Real, tfno: 926 29 53 00; e-mail: joseferfernando.perez@uclm.es

Chemical Engineering

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

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

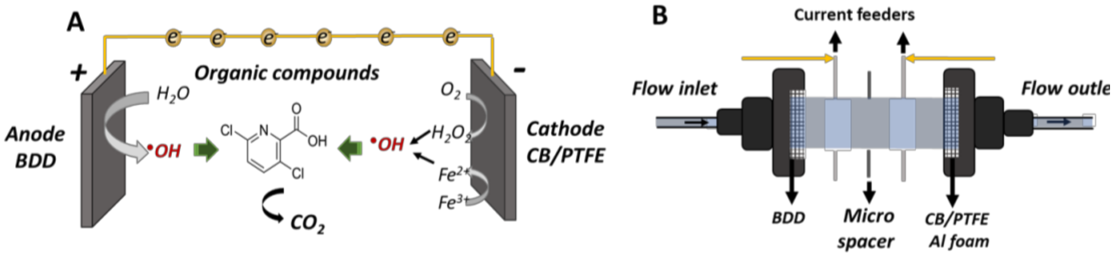

Figure 1. A) Generation of $^{\bullet}OH$ vía AO-BDD y EF; B) MF-FT cell configuration

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

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

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INTEGRAL VALORIZATION OF OLIVE OIL BYPRODUCTS THROUGH CO-GASIFICATION PROCESS

M. Puig-Gamero*, M.L. Sánchez-Silva, J.L. Valverde, P. Sánchez

Dpto. de Ingeniería Química, Universidad de Castilla-La Mancha, Avda Camilo Jose Cela s/n 13071 Ciudad Real, tfno: +34 926 29 53 00 ext: 6419; e-mail: maria.puig@clm.es

Chemical Engineering

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 .

P-29

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

A. Rodríguez,* A.R. de La Osa, J.L. Valverde

[1] *Deparment of Chemical Engineering. University of Castilla-La Mancha*
Avd. Camilo José Cela, 12 13071, Ciudad REAL, España
e-mail: Alberto.RGomez@uclm.es

Chemical Engineering

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 research 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 these 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.

P-30

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

B. M. Rubio, L. Mazuecos, C. Pintado, A. Fernández, C. Mora, V. López, C. Arribas, N. Gallardo, A. Andrés

Área de Bioquímica. Dpto de Química Inorgánica, Orgánica y Bioquímica. Facultad de Ciencias y Tecnologías Químicas. UCLM.

Biochemistry

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.

P-31

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

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

Department of Inorganic, Organic and Biochemistry. University of Castilla-la Mancha. Faculty of Chemical Sciences and Technologies. Ciudad Real (Spain)

Organic Chemistry

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

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

Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha [1] Environmental Sciences Institute (ICAM), 45004, Toledo, Spain.[2] Faculty of Chemical Sciences and Technologies, 13005, Ciudad Real, Spain, e-mail: armando.sanchez@alu.uclm.es

Analytical Chemistry

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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P-33

RESVERATROL MODULATES GPCRS GENE EXPRESSION IN SAMP8 MICE

A. Sanchez-Melgar[1], J. L. Albasanz[1], M. Pallàs[2], M. Martín[1]

[1] Department of Inorganic, organic and biochemistry. Faculty of Chemistry Sciences and Technologies. School of Medicine of Ciudad Real. CRIB. University of Castile-La Mancha. [2] Pharmacology Section and Institute of Neuroscience, University of Barcelona, Barcelona, Spain.

Biochemistry

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 $A_{2A}R$ were decreased, a significant increase on A_3R mRNA levels was detected without changes on the $A_{2B}R$ gene expression. In the glutamatergic system, group I metabotropic glutamate receptors were analyzed, showing a significant increase only on $mGluR_5$ gene expression. In the case of dopaminergic system, no changes were detected on D_2R mRNA levels. Therefore, we conclude that RSV differentially modulates these three neurotransmission systems, which may suggest that protective role of this polyphenol could be related to GPCR-mediated signaling modulation.

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CATHODIC CATALYST FOR THE ELECTROCHEMICAL HYDROGENATION OF CINNAMALDEHYDE

M.J. Torres*, A.R. De La Osa, A. De Lucas- Consuegra, J.L. Valverde, P. Sánchez

Facultad de Ciencias y Tecnologías Químicas, Departamento de Ingeniería Química, Universidad de Castilla-La Mancha, Avda. Camilo José Cela 12, 13071 Ciudad Real; e-mail: MariaJose.Torres@uclm.es

Chemical Engineering

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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CÓMO FUE LA EDICIÓN DEL AÑO PASADO…

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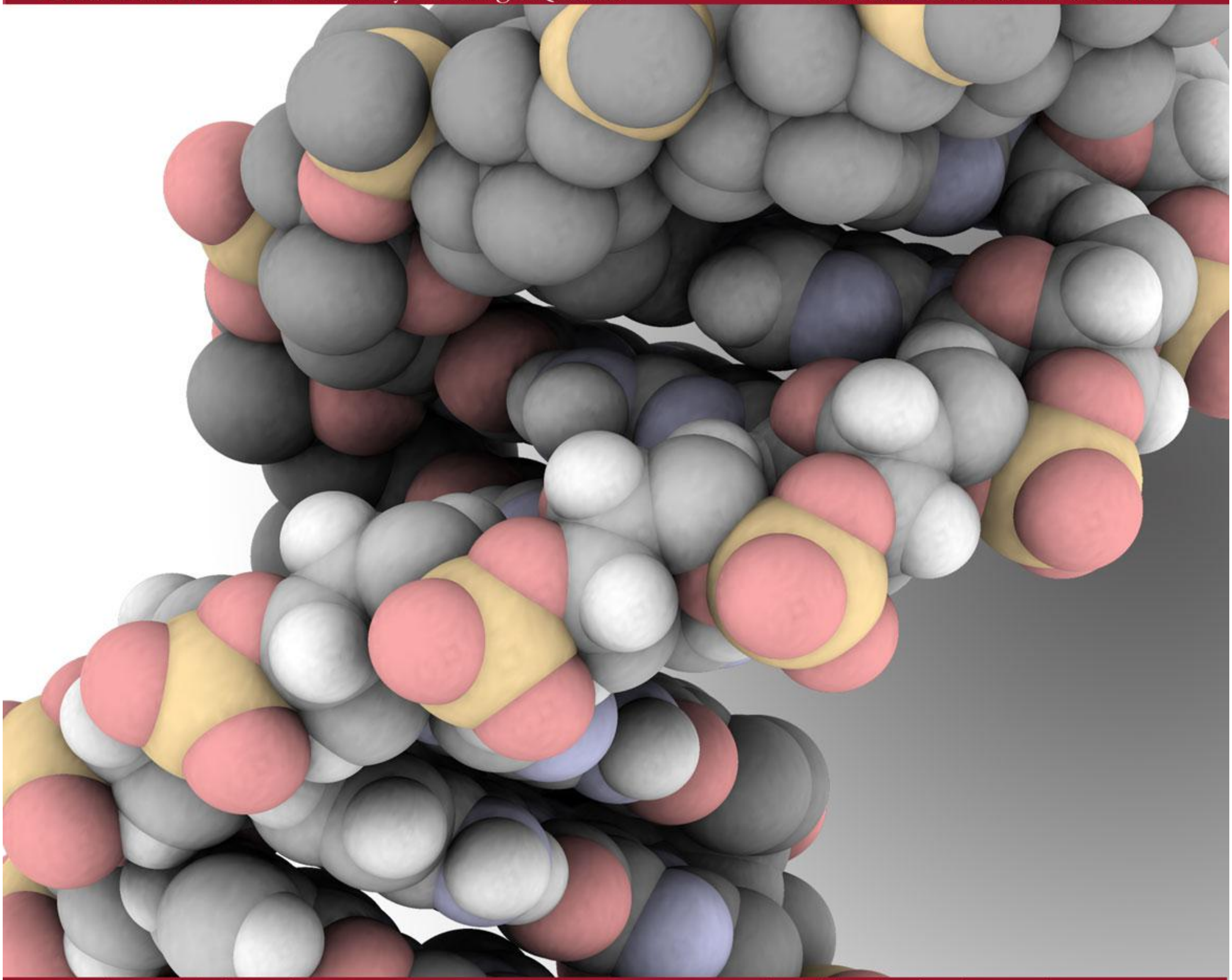

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E-mail de contacto: Antonio.Hoz@uclm.es

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ÍNDICE

PRESENTACIÓN

El número de Junio es un número monográfico dedicado a las jornadas de Ciencia Joven. Este año se ha producido un aumento del número de contribuciones y hay una serie de conferencias de gran interés.

Además, en este número también se recoge la información relativa a la décima edición de la Escuela de Química Organometálica "Marcial Moreno Mañas" y la despedida del profesorado del Grado en de Ciencia de Tecnología de los Alimentos, Ana Isabel García Fernández, a la cual nos unimos todos los miembros del Comité Editorial.

El comité editorial..

Los investigadores noveles de la Facultad de Ciencias Químicas exponen sus líneas de trabajo

La Facultad de Ciencias y Tecnologías Químicas de la Universidad de Castilla-La Mancha (UCLM) en Ciudad Real acoge desde ayer y hasta mañana viernes el simposio Ciencia Joven, durante el que los investigadores noveles presentan sus líneas de trabajo a sus colegas del Campus, así como a otros llegados de fuera. El encuentro, que cumple su undécima edición, ha sido inaugurado por el rector de la UCLM, Miguel Ángel Collado, quien ha expuesto las dificultades de financiación pública que atraviesa la investigación en la región.

Los jóvenes investigadores de la Facultad de Ciencias y Tecnologías Químicas en el Campus de Ciudad Real trabajan desde ayer en el undécimo Simposio de Ciencia Joven, una iniciativa impulsada y organizada por ellos mismos que les sirve de plataforma de presentación de sus líneas de investigación y de discusión de los resultados obtenidos, al tiempo que es una oportunidad para acercar a los estudiantes la tarea investigadora.

El encuentro ha sido inaugurado formalmente hoy por el rector de la Universidad de Castilla-La Mancha (UCLM), Miguel Ángel Collado, quien ha puesto el acento en el carácter intergeneracional de esta iniciativa ya consolidada y que año tras año es un éxito dado que en ella colaboran conjuntamente investigadores seniors y noveles, que son quienes asegurarán el desarrollo de la ciencia. Precisamente, a estos últimos el rector les ha animado a seguir trabajando porque “sois el futuro de la Universidad, de la región y del conocimiento”, ha dicho.

En su intervención, el rector ha asegurado que este simposio no viene sino a reafirmar la convicción universitaria de la importancia que tiene la investigación y ha expuesto las dificultades de financiación para proyectos de investigación en la región. En este sentido, ha indicado que la paralización de la aprobación de los presupuestos de Castilla-La Mancha ha impedido que a día de hoy se haga efectiva la convocatoria de ayudas regionales para investigación por importe de 12 millones de euros en cuatro años comprometida por el Gobierno autonómico.

Para intentar paliar la falta de financiación pública, Collado ha recordado que a finales de 2014 la institución se dotó de un Plan Propio de Investigación del que recientemente se concedieron 30 contratos predoctorales para la formación de personal investigador. En la actualidad son 90 los jóvenes investigadores que disfrutan de un contrato de este tipo.

Precisamente, el decano de la Facultad de Ciencias y Tecnologías Químicas, Ángel Ríos, se ha mostrado agradecido durante la inauguración del simposio Ciencia Joven por esa iniciativa de la UCLM, porque “en época de sequía financiera para la investigación, ésta es una apuesta valiente y decisiva de la que nos beneficiamos como centro investigador”. En relación al simposio, se ha referido a él como una gran oportunidad para el aprendizaje de los investigadores noveles.

En el simposio, en el que colabora la Real Sociedad Española de Química y en el que este año participan no sólo investigadores del Campus de Ciudad Real, sino también de Albacete y Toledo, se han inscrito un total de 140 investigadores y se han admitido treinta y dos comunicaciones en los distintos ámbitos que abarca la Facultad: Química Inorgánica, Ingeniería Química, Química Orgánica, Química Analítica, Tecnología de los Alimentos, Matemáticas y Bioquímica.

El simposio se completa con la intervención de los prestigiosos investigadores externos como el director del departamento de Ingeniería Química y Tecnología de los Alimentos de la Universidad de Cádiz, Enrique Martínez de la Ossa Fernández; la directora del Grupo de Reactividad Fotoquímica del Instituto de Ciencia Molecular de la Universidad de Valencia, Julia Pérez Prieto; la investigadora del Grupo de Bioactividad y Alergenicidad de Proteínas y Péptidos del Instituto de Investigación en Ciencias de la Alimentación, Lourdes Amigo Garrido; y el investigador del Departamento de Química Analítica de la Universidad de Córdoba Feliciano Priego Capote.

Gabinete Comunicación UCLM. Ciudad Real, 8 de junio de 2017

CONFERENCIA INVITADA

LOS FLUIDOS SUPERCRÍTICOS EN LA INGENIERÍA QUÍMICA

Enrique Martínez de la Ossa

De todas las sustancias que se pueden utilizar como fluidos supercríticos (FSC), las más usadas en procesos de Ingeniería Química son el dióxido de carbono y el agua. El CO_2-SC presenta unas extraordinarias propiedades de transporte y un elevado poder disolvente y se puede usar como medio de reacción en procesos químicos (p.e. transesterificación de triglicéridos para fabricar biodiesel) y como disolvente/ antisolvente en operaciones unitarias de separación, como extracción y precipitación. El H_2O-SC se usa como medio de reacción en dos procesos: la oxidación supercrítica (OASC), para la depuración completa de residuos orgánicos, tóxicos o peligrosos (que por ser muy exotérmica, es además generadora de energía), y la gasificación supercrítica (GASC), para la producción de gases combustibles con un alto contenido en Hidrógeno a partir de residuos lignocelulósicos.

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NIR-RESPONSIVE SMART NANOHYBRIDS BASED ON LANTHANIDE-DOPED NANOPARTICLES

Julia Pérez-Prieto

Nanoparticles consisting of a matrix doped with rare earth ions can present upconversion luminescence after near-infrared (NIR) excitation. These upconversion nanoparticles (UCNPs) are interesting for biomedicine (biosensing, bioimaging), medicine (photodynamic therapy) photocatalysis, and security [1-3]. UCNPs are particularly promising in biomedicine since they can be excited by NIR light directly with much less absorption and scattering in tissues, resulting in deeper tissue penetration than visible light. These nanoparticles can be assembled with functional systems (dyes, polymers, drugs, etc.) following different strategies, thus providing functional nanohybrids benefiting from synergistic effects between the components. In this presentation, various strategies for modifying the surface of UCNPs and proof-of-concepts of their applicability will be presented [4]. For instance, $NaYF_4$: Yb^{3+}, Er^{3+} UCNPs have been functionalized with photosensitizers, fluorophores, and functional polymers by either their direct interaction with the nanoparticle surface or by using a rigid macromolecule as the anchoring unit. Some of the resulting nanosystems have been assayed in photodynamic therapy as well as in strong acidic conditions showing the resistance of the assembly under these conditions and/or their potential application for building release systems.

Acknowlegements: We thank the Spanish Ministry of Economy and Competitiveness (CTQ2014-60174-P) and COST-CM1403 Action.

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PEPTIDOS LÁCTEOS CON FUNCIONALIDAD BIOLÓGICA: DEL LABORATORIO AL CONSUMIDOR

Lourdes Amigo

Durante la digestión de los alimentos, se genera una gran variedad de péptidos a partir de proteínas alimentarias mediante hidrólisis enzimática. Algunos de estos péptidos son estructuralmente similares a los péptidos endógenos que juegan un papel crucial en el organismo como hormonas, neurotransmisores o antibióticos. Por lo tanto, los péptidos alimentarios pueden interactuar con los mismos receptores que los péptidos endógenos y ejercer un efecto agonista o antagonista en el organismo. Las funcionalidades biológicas beneficiosas de los péptidos derivados de la leche incluyen actividad antimicrobiana, antihipertensiva, inmunomoduladora, opioide, etc., aunque el nivel de evidencia para algunas de estas actividades es todavía escaso. Debido a su versatilidad fisiológica y fisicoquímica, los péptidos derivados de alimentos se consideran componentes altamente importantes para alimentos o aplicaciones farmacéuticas que promueven la salud. Sin embargo, el desarrollo de estos nuevos ingredientes debe basarse en criterios científicos capaces de demostrar inequívocamente sus propiedades biológicas.

Esta conferencia revisará nuestros últimos resultados sobre el desarrollo de ingredientes funcionales basados en péptidos bioactivos derivados de la leche, que ejercen principalmente una actividad antihipertensiva o con efecto sobre el tracto intestinal. Se prestará especial atención a la identificación de nuevas secuencias activas, la supervivencia de los péptidos a la digestión gastrointestinal, la absorción y la búsqueda de la forma activa en el organismo. Finalmente, se considerará la incorporación a los ingredientes desarrollados en un producto final, la estabilidad de los péptidos a los procesos tecnológicos aplicados en la industria alimentaria y la estabilidad durante la vida propia del producto. Para ilustrar estos aspectos, se mostrarán varios ejemplos de ingredientes. Por ejemplo, la identificación de nuevos péptidos antihipertensivos en un hidrolizado de caseína se presentará junto con la evaluación de la actividad en modelos animales y estudios clínicos.

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NIR-RESPONSIVE SMART NANOHYBRIDS BASED ON LANTHANIDE-DOPED NANOPARTICLES

Feliciano Priego Capote

El objetivo primordial de la metabolómica consiste en analizar el conjunto de compuestos de bajo peso molecular presentes en un fluido biológico, célula, tejido u organismo, en unas condiciones fisiológicas específicas o en respuesta a diferentes perturbaciones o estímulos. La metabolómica ha sido la última de las disciplina ómicas que integran la Biología de Sistemas (junto a la genómica, la transcriptómica y la proteómica) en ser desarrollada y, en este sentido, se ha aprovechado del camino recorrido por el resto de disciplinas mucho más establecidas.

Una de las áreas donde la metabolómica está empezando a jugar un papel primordial es la clínica ya que la metabolómica parece ser una herramienta adecuada para el desarrollo de herramientas de diagnóstico, pronóstico o cribado de pacientes. En este ámbito, el análisis de biomarcadores juega un papel clave siempre que se desarrolle con rigor experimental, analítico y estadístico. El protocolo genérico utilizado para el análisis de biomarcadores consta de tres etapas básicas que son: (a) diseño del estudio, con el fin de obtener datos finales representativos; (b) adquisición de datos mediante la aplicación del(los) método(s) de análisis; y (c) análisis estadístico. Este esquema ha sido utilizado para el análisis y configuración de paneles de marcadores para la discriminación de individuos afectados por dos tipos de cáncer muy extendidos en la población española, el cáncer de prostata y el de pulmón. Para ello se seleccionaron dos muestras clínicas diferentes por sus características. En el caso del cáncer de próstata se utilizó la orina, ejemplo de muestra clínica convencional ampliamente utilizada. Para el cáncer de pulmón se utilizó el condensado de aire exhalado, muestra novedosa y poco caracterizada. En ambos casos se obtuvieron modelos de discriminación de pacientes caracterizados por altos niveles de sensibilidad y especificidad y, por tanto, con potencial para ser evaluados en una segunda fase con cohortes de mayor tamaño.

USE OF OAK EXTRACT AS A NATURAL ANTIOXIDANT IN BURGER PATTIES

M. Alarcón*, L. Marchante, A. Soriano, M. S. Pérez-Coello

The use of antioxidants in meat products is essential to delay or prevent oxidative phenomena that reduce their useful life. In this sense, there is a growing demand for the use of natural products in order to reduce the addition of chemical additives on food. Therefore, the aim of this work was to study the antioxidant capacity of lyophilized oak wood extracts added on hamburgers.

Five types of pork burger patties were prepared from a basic formulation. Control (C) was prepared with no added extract. The remaining 4 types were prepared by adding 400 ppm of sodium ascorbate (CA), and 0.5, 5 and 10 g/kg of lyophilized oak extract (R1, R2 and R3), respectively. The oak extracts were obtained by Accelerated Solvent Extraction (ASE) using water under subcritical conditions, previously optimized. The samples were packaged in modified atmospheres (80% O_2 and 20% CO_2) and stored at 4-5 ° C with a 12 h/day light exposition. The lipid oxidation was determined by the thiobarbituric acid reactive substances content (TBARS), the volatile composition was evaluated by GC-MS; and color (L*, a*, b*), pH and moisture analysis were performed; sampling at 0, 4, 8 and 12 days.

An intense inhibition of lipid oxidation was found in burger patties with added extract. This antioxidant activity was effective immediately after the extract addition to the samples (0 days). Furthermore, the antioxidant activity of the extracts was reflected in the volatile composition of the burger patties, observing a smaller amount of typical compounds of lipid oxidation such as hexanal and other aldehydes. The L* values decreased as the extract concentration increased, and the a* and b* values were similar among all samples. A significant decrease in pH values was observed between 8 and 12 days in all samples. There were not significant differences for moisture between samples.

Therefore, the incorporation of a concentration equal or greater than 0.5 g/kg of lyophilized extract of oak wood protects from lipid oxidation more effectively than sodium ascorbate in pork burger patties.

SYNTHESIS OF POLYMERIC SCAFFOLDS FOR DRUG DELIVERY SYSTEMS USING SUPERCRITICAL CO_2

I. Álvarez*, C. Gutiérrez, J. F. Rodríguez, A. de Lucas and M. T. García

JAVIERTORRES (2017)

Polymers can be used as biomaterials in order to synthesize scaffolds for tissue engineering and medical devices in the field of regenerative medicine. They are selected for many different biomedical applications depending on their molecular weight, structure, solubility, biodegradability or hydrophilicity/hydrophobicity. In addition to this, they are capable to integrate other substances which promote tissue growth or even drugs for the synthesis of controlled release systems, either microparticles or scaffolds/foams. Controlled drug delivery occurs when a polymer and a drug are combined in a way that the active agent is released from the material in a predesigned manner: constant over a period that varies from hours to months, cyclic or it could be provoked by a change in pH, temperature or drug concentration.

Techniques to produce drug delivery systems such as emulsion, spray-drying or solvent evaporation have disadvantages in relation with total solvent removal. This problem is solved by the employment of supercritical fluids (SCFs). Among the most important reasons to use SCFs are: SCFs leads to the complete solvents elimination, the formation of smaller particles and the control of pore size, distribution and morphology of the foams. Moreover, by using SCFs it is possible to carry out drug impregnation in a clean and efficient way. The most commonly used SCF in this field is CO_2.

The aim of this research is to synthesize medical devices for drug delivery by using Poly (lactic-co-glycolic acid) (PLGA).This polymer is interesting because it has good biodegradability and biocompatibility and it is toxicological safe. The investigation has been focus on the generation of this devices in two different ways: micro and nanoparticles and microcellular foams.

OPTIMIZED RADIOTHERAPY PROTOCOLS DELAY THE MALIGNANT TRANSFORMATION OF LOW-GRADE GLIOMAS IN-SILICO

A. Henares-Molina,*, S.Benzekry, P.C. Lara, M. García-Rojo,
V.M. Pérez-García and A. Martínez-González

JAVIERTORRES (2017)

Grade II gliomas are slowly growing primary brain tumors that affect mostly young patients and become fatal only several years after diagnosis. Cytotoxic therapies such as radiotherapy and/or chemotherapy are used initially only for patients having a bad prognosis. These therapies are planned following the “maximum dose in minimum time” principle (Maximum Tolerated Dose, or MTD paradigm), the same schedule used for high-grade brain tumors in spite of their very different behavior. These tumors transform after a variable time into high-grade tumors, what decreases significantly the patient’s life expectancy. The incurable profile of this disease motivated us in using mathematical models in order to maximize the time to the malignant transformation through the optimization of radiotherapy schemes.

A series of previous studies [1,2] has developed a PDEs model describing the basic features of grade II glioma progression and response to radiotherapy. We found the model predicted that there was a much more effective fractionation scheme, protracted metronomic fractionations [3], i.e. therapeutical schedules enlarging the time interval between low-dose radiotherapy fractions, may lead to a better tumor control without an increase in toxicity. Other non-standard fractionations such as protracted or hypoprotracted schemes may also be beneficial. The potential survival improvement depends on the tumor proliferation rate and can be even of the order of years. A conservative metronomic scheme, still being a suboptimal treatment, delays the time to malignant progression of at least one year when compared to the standard scheme.

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SYNTHESIS OF Pt(II) AND Pt(IV) COMPOUNDS AS POTENTIAL ANTICANCER DRUGS

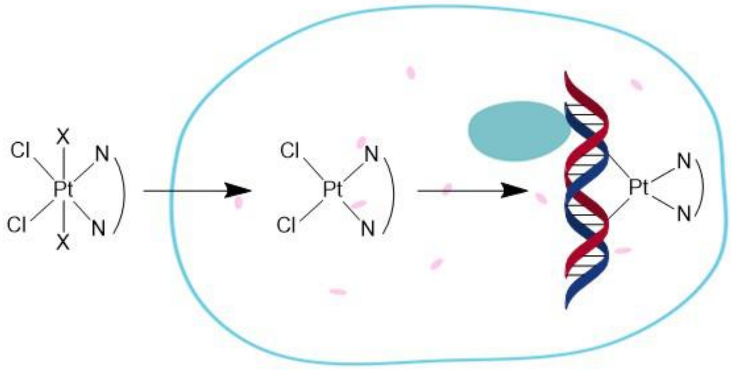
J.Leal*, M. C. Carrión, F. Jalón, B. Manzano

JAVIER TORRES (2017)

Pt(II) Organometallic compounds have been widely used in cancer treatment. Cisplatin is one of the most successful and widely used drug against many types of cancer. However, its poor selectivity towards tumour cells lead to undesirable side effects. Pt (IV) compounds have properties that help to overcome these problems.

Pt(IV) compounds are more stable, leading to higher lifetime and lower side effects. . These compounds act as a pro-drug, being reduced inside the cell to their Pt (II) analogs, which are the ones that have cytotoxic activity. These Pt(II) drugs usually bind covalently to the DNA double helix, starting cell death by apoptosis.

In our group we synthesize Pt(II) and Pt (IV) coordination compounds with different chelating ligands. Chelating ligands have been used in order to force the cis configuration in the complexes, which is known to have best cytotoxic properties. The use of different ligands is useful to tune up the properties of the compounds, achieving more soluble and stable drugs.



VOLATILE AND SENSORY CHARACTERIZATION OF TINTO DE LA PAMPANA BLANCA RED WINES

M. Trujillo, E. Sánchez-Palomo*, M.A. González Viñas


JAVIERTORRES (2017)

Background and Aims: This study characterizes the oenological potential of Tinto de la Pámpana Blanca red wines from La Mancha region.

Methods and Results: The oenological potential of these wines was characterized by their conventional parameters, phenolic composition, chromatic characteristics volatile composition and sensory analysis. With regard to the concentration of polyphenol compounds all the studied wines had normal values to be considered young red closely connected with their colour characteristics. Based on the volatile compounds profile these wines presented a complex chemical profile with a wealth of aromas in its aromatic composition. All wines showed highest aroma contribution of the fruity and fatty series followed by sweet. Sensory profile of Tinto de la Pámpana Blanca wines was caracterized by red friut, liquorice, leather, coffee and Green aromas with floral notes

Conclusions: This study showed that this grape variety provides a viable alternative to traditional grape varieties cultivated in La Mancha region, increasing the offer to the consumer, which favors the differentiation of La Mancha wines on the national and international market.

TREATING SOIL-WASHING POLLUTED WITH LINDANE BY ELECTROLYSIS WITH DIAMOND ELECTRODES

M. Muñoz Morales*, C. Sáez, P. Cañizares, M. A. Rodrigo


JAVIERTORRES (2017)

In last years, the removal from soils of hazardous species is an environmental priority in order to avoid the further magnification of the problem with the later pollution of water reservoirs. In this work, it is studied the treating of soils polluted with lindane using surfactant-aided soil-washing (SASW). Lindane has been banned in Europe due to the problems that generate in the environment and on human health. Regarding to this, the removal of lindane from solvents has been faced with different AOPs technologies [1-3] but in this work, it is evaluated the complete treatment of polluted soils.

Fluids generated in SASW process consist of complex mixtures of surfactant SDS, lindane and micelles whose composition (and size of micelles) depends on the surfactant/soil ratio applied. Results show that lindane in the washing fluid can be efficiently mineralized during the electrolysis with diamond electrodes and also was observed the generation of an intermediate during this mineralization. Micelles particle size decreases continuously during the treatment down to the mean size of soil particles and SDS oxidation lead to the formation of sulfates that, in turn, are further oxidized to persulfate, showing a key role on the performance of the treatment technology. In addition, two different stirring conditions were evaluated after detecting an important effect in the results of lindane extraction. The removal of lindane is faster than SDS, and hence, the re-use of the surfactant in the SASW process can be proposed.

Acknowledgements

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FORMATION OF SECONDARY ORGANIC AEROSOL FROM THE REACTION OF STYRENE WITH OH

M. Tajuelo, D. Rodríguez, A. Rodríguez

Air pollution is one of the most serious environmental problems at local and global scales. A wide spectrum of inorganic and organic chemical compounds are emitted from automotive use, from combustion to evaporative processes. They include the obvious water vapor and carbon dioxide (CO_2), as well as carbon monoxide (CO), oxides of nitrogen (NO_x), oxides and oxyacids of sulfur, reduced sulfur compounds, a wide variety of volatile organic compounds (VOCs) and particulate matter. [1] Styrene is one of the most aromatic compounds emitted by motor vehicles. [2] Because of its unsaturated characteristics, styrene is highly reactive in the atmosphere, and can be attacked readily by reactive oxygen species, such as hydroxyl radical (OH), O_3, and nitrate radical (NO_3). [3] This results in secondary pollution like secundary organic aerosol (SOA). [4] SOA not only impoverishes air quality but also has an impact on climate via scattering and, absorption of light as well as aerosol-cloud interactions. [5]

In this work, SOA formation from the photooxidation of styrene has been investigated. The overall aim of this study was to perform a series of experiments under a range of different reaction conditions (varying styrene, radical OH, NOx concentrations and relative humidity) in order to measure the SOA formation yield.

Experiments were performed in a 500 L Teflon environmental chamber. A Fast Mobility Particle Sizer (FMPS) spectrometer was used to measure of SOA, the styrene concentration was monitored by using gas chromatography-mass spectrometry (GC-MS), and the NOx evolution was followed by a chemiluminescence analyzer.

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SUBSTANTIALLY INHIBITION OF FGF21 SECRETION BY CENTRAL LEPTIN INFUSION IN WISTAR RATS

B. M. Rubio Muñoz

Leptin and fibroblast growth factor 21 (FGF21) were introduced as adipokines with potent antidiabetic properties. Leptin, a hormone derived from white adipose tissue, is one of the major signals that relay the status of fat stores to the hypothalamus and plays a significant role in energy homeostasis. FGF21 is a member of the fibroblast growth factor family of proteins, mainly secreted by liver and adipose tissue. FGF21 was originally found to stimulate insulin-independent glucose uptake in adipocytes. Circulating levels of both hormones leptin and FGF21 have been shown to correlate positively with body mass index (BMI), hence, obese and overweight individuals have usually high levels of leptin and FGF21 and develop insulin resistance. Indeed it has been proposed that obesity is a state of leptin and FGF21 resistance. Nevertheless, the real physiological significance of circulating FGF21 remains to be elucidated. Studies from our laboratory indicated that hypothalamic leptin administration reduced the ability of adipose tissues to capture glucose, hence, central leptin decreased lipogenesis and adiposity. Based on these observations, we hypothesized that central leptin decreases the secretion of FGF21 by adipose tissues. In this manner, central leptin reduces glucose uptake in adipocytes. In addition we suggest that the increase in FGF21 levels that accompanies obesity may be due to impaired hypothalamic regulation of adiposity and FGF21 secretion by central leptin.

DESIGN AND SYNTHESIS OF ORGANIC FIELD-EFFECT TRANSITORS (OFETS)

I.Torres*, P.Prieto, J.R. Carrillo, Á. Díaz-Ortiz, I.Arrechea, R. Ponce

JAVIERTORRES (2017)

In the last years, organic electronic has attracted great attention due to the development of semiconductor materials. These materials have practical applications in the latest generation device, like OLEDs, OFETs, Liquid Crystal, etc. Organic field-effect transistors (OFETs) are devices formed with an organic semiconducting layer, a gate insulator layer, and three terminals (source, drain and gate electrodes). [1] OFETs are essential building blocks for the next generation of cheap and flexible organic circuits. Additionally, they also provide an important insight into the charge transport of -conjugated systems.

To design an OFET with good properties, organic chemistry plays an important role, studying the most accurate characteristics of desired organic compounds. Furthermore, an important fact in this research is the theoretically study of their properties to avoid unnecessary synthesis. For this goal, computational chemistry is a crucial tool to evaluate their properties without synthesizing them. In this sense, computational calculations can be used to the determination of the energy and topology of frontier molecular orbitals, calculations of oxidation-reduction potentials, Raman spectra, reorganization energies and theoretical UV-vis spectra. [2]

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ANTIOXIDANT CAPACITY OF JABUTICABA FRUITS

M. C. Paludo*, C. A. Ballus, H. T. Godoy, I. Hermosín

JAVIERTORRES (2017)

Brazil is recognized by your unique biodiversity, which includes a diversity of native fruits, like Jabuticaba. This fruit is rich in several components, like phenolic compounds and mainly the class of anthocyanins, which have high antioxidant capacity and are associated with the prevention of diseases such as cancer, heart disease, premature aging and others. Methodologies have been developed in order to evaluate the capacity of vegetable extracts in oppose free radicals that are normally produced by human metabolism as H_2O_2, $O_2^{\bullet -}$, HOCL, ONOO- e ROO-. Thereby, in this work, the deactivation capacity of radicals ROS (oxygen reactive species) and RNS (Reactive nitrogen species) present in peels and seeds extracts of five Jabuticaba varieties were evaluated. The evaluated varieties were Myrciaria jaboticaba (Vell.) O. Berg (Sabará), Myrciaria cauliflora (DC.) O. Berg (Paulista), Myrciaria coronata Mattos (Coroada), Myrciaria cauliflora (DC.) O. Berg (Hibrida) and Plinia ssp. (Pintada). ROS and RNS were evaluated using the method as hypochlorous acid-scavenging, peroxynitrite-scavenging, superoxide radical-scavenging, hydrogen peroxide-scavenging and oxygen Radical Absorbance Capacity. The mainly results were: deactivation of HOCL in extract of peel Sabará (IC50 9,24 μg.mL-1), $O_2^{\bullet -}$ in extract of seed Paulista (IC50 16,15 μg.mL-1), ONOO- without NaHCO3 in extract of peel Coroada (IC50 3,84 μg.mL-1), and with $NaHCO_3$ in extract of peel Coroada (IC50 5,88 μg.mL-1), ROO- in extract of peel Sabará (918,16 μmol TE g-1) and for of H_2O_2 in extract of seed SF (49,11% Inhibition in the concentration of 125 μg extract.mL-1). The results show up that Jabuticaba fruit can be considered as an excellent source of exogenous antioxidants and also can be useful as data base for development of new products by food, cosmetic and pharmaceutical industries. Moreover, the results indicated that these fruits could be included in the population diet, in order to assist in the prevention of several chronic diseases.

LUMINESCENT ZR-BASED MOFS FOR SENSING AND OPTOELECTRONIC APPLICATIONS

M. Gutiérrez, B. Koen, R. Navarro, F. Sánchez, A. Douhal

Metal-Organic Frameworks (MOFs), a class of highly porous and crystalline compounds, have aroused as smart materials with a wide range of uses and applications. Among all, their excellent luminescence properties combined with their porous structure and synthetic flexibility, make them ideal candidates for solid-light emitting and chemical sensing applications.[1] The photophysical characterization of MOFs is paramount not only to improve the synthesis of more efficient MOF materials, but also for their implementation in the related fields.[2-6] Herein, armed with spectroscopic and ultrafast time-resolved techniques, we decipher the spectral and photodynamical behavior of a series of Zr-MOFs and dyes@MOF composite materials as well as we demonstrate their applications as light emitting diode (LED)[5] and luminescent sensor.[6] We show that the Zr-NDC MOF emission is due to NDC monomers and excimers.[3] By encapsulating different dyes (C153, DCM and NR) into Zr-NDC MOF, we observed an energy transfer process from the MOF to the dyes, and we used this concept to fabricate white light emitting materials (Figure 1A). [2] These composites were incorporated into polymeric films which allow us to fabricate the first OLED based on Zr-MOFs. [4,5] On the other hand, we have also explored the photoproperties of Zr-NDC/Tz and Zr-NDC/CN MOFs, demonstrating that both MOFs detect efficiently and selectively a highly explosive molecule (trinitrophenol, Figure 1B).[6] These results evidence the importance of spectroscopic investigations for further applications of MOFs.

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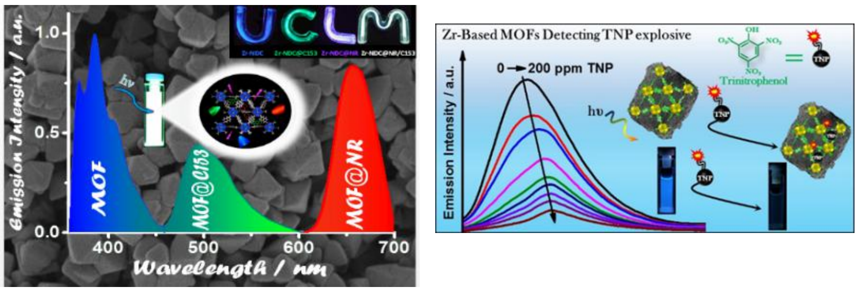


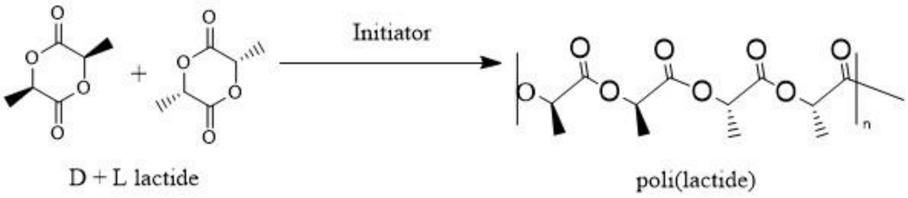
Figure 1. A) White light emission of Zr-NDC MOF containing C153 and NR dyes. B) Emission quenching of Zr-NDC/Tz MOF in presence of TNP explosive molecules.

NEW CHIRAL N,N,O-SCORPIONATE ZINC ALKYLS AS EFFECTIVE INITIATORS FOR THE LIVING ROP OF LACTIDES

S. Sobrino, A. Otero, J. Fernández-Baeza, L. F. Sánchez-Barba, A. Garcés, A. Lara-Sánchez and A. M. Rodríguez


JAVIERTORRES (2017)

During the last years, our research group has contributed widely in the preparation of efficient catalysts bearing heteroscorpionte ligands derived from bis(pyrazol-1-yl)methane moieties for the preparation of biodegradable polymers by a well-controlled ring-opening polymerization (ROP) of cyclic esters, such as lactide (LA), an inexpensive annually renewable natural feedstock.[1] The biocompatible nature of the polylactides (PLAs) have attracted our attention, and consistently, we have employed biocompatible metals such zinc for the design of these catalysts. In the present work, we described the synthetic accessibility of zinc metal complexes bearing a racemic NNO-scorpionate ligands, as well as their catalytic behavior as single-component initiators for the efficient and stereoselective ROP of rac-lactide in the production of heterotactic-enriched polylactides.[2]



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MAGNETIC/NON-MAGNETIC ARGAN PRESS CAKE NANOCELLULOSE FOR THE SELECTIVE EXTRACTION OF SUDAN DYES IN FOOD SAMPLES PRIOR TO THE DETERMINATION BY CAPILLARY LIQUID CHROMATOGRAPHY

Y. Benmassaou *, M. J. Villaseñor, R. Salgh, S. Jodeh, M. Algarra, M. Zougagh, A. Ríos


JAVIERTORRES (2017)

Sudan dyes are a class of azo dyes widely used in the chemical industry as coloring materials. Due to their intense red color and low price, these compounds have illegally been used as food dyes to intensify the color. Although the use of Sudan compounds, as food dyes, has been banned by the European Community [2].

In this contribution, two methods for the determination of Sudan dyes in food samples, by solid phase extraction - capillary liquid chromatography, are developed. Both methods use nanocellulose (NC) extracted from bleached argan press cake (APC), as a nano-adsorbent recycled from an agricultural waste material. One of the methods involves the dispersion of NC in food sample extracts, along with the waste and eluents being separated by centrifugation. In the other method, NC was modified by magnetic iron nanoparticles before using it in the extraction of Sudan dyes. The two proposed methods allows the determination of Sudan dye amounts at the 0.25–2.00 µg L−1 concentration range, with limit of detections lower than 0.1 µg L−1. Both methods were applied to the determination of Sudan dyes in barbeque and ketchup sauce samples, obtaining recoveries between 93.4% and 109.6%.

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CATALYST SYNTHESIS FOR THE ELECTROCHEMICAL HYDROGENATION OF CINNAMALDEHYDE

M.J. Torres, A.R. De La Osa, J.A. Díaz, A. De Lucas- Consuegra, J.L. Valverde, P. Sánchez

The selective hydrogenation of α, β-unsaturated aldehydes such as cinnamaldehyde (CMA) to their respective unsaturated alcohols is a problem that has received considerable attention due to its utility in the flavours, fragrances and pharmaceutical industries. This process could be carried out by heterogeneous catalysis, which is a typical example of ecologically friendly technologies against homogeneous catalytic process[1]. The hydrogenation of CMA mainly produces its saturated aldehyde, hydrocinnamaldehyde (HCMA) that has been found to be an important intermediate in the preparation of pharmaceuticals used in the treatment of HIV, and its unsaturated alcohol, cinnamyl alcohol (CMO), which is widely used in the production of perfumes[2] . Since the formation of HCMA is thermodynamically preferred and can be achieved easily compared to CMO, more attention has been focused on promoting the selectivity towards the unsaturated alcohol.

On the other hand, Proton Exchange Membrane (PEM) cells are actually a promising reactorsfor water electrolysis, providing a sustainable solution for highly pure hydrogen production at the anodic chamber, and protons that pass through the membrane offers the possibility of carry out the selective hydrogenation of unsaturated organic compounds inside the PEM cell cathode[3].

Therefore, this study was focused on the influence of the cathodic Platinum catalysts on the electrochemical hydrogenation of cinnamaldehyde in order to maximize the selectivity to valuable product, especially cinnamyl alcohol.

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LASER SPECTROSCOPY AND MICROSCOPE OF A NEW HOF BASED ON HEXAAZATRIPHENYLENE

E. Gomez*, B. Cohen, I. Hisaki, A. Douhal

Hydrogen-bonded Organic Frameworks (HOFs) are currently attaching interest in the fields of materials chemistry and crystal engineering due to its high crystallinity and theirs applications in optoelectronic devices. [1] In this work, a new HOF based on a heterocyclic π-conjugated system, the hexaazatriphenylene (HAT), is studied. To resolve the photobehaviour of the crystalline framework (CPHAT-1a) it is necessary first to understand the photodynamics of its fundamental unit, CPHAT, Figure 1A. The photobehaviour of this molecule was studied by using steady-state and time-resolved spectroscopy in DMF solutions. A Stokes shift (4650 cm-1) was observed suggesting that an intramolecular charge transfer (ICT) in the excited state is happened, Figure 1B. Four decay components of 70 ps, 0.23, 1.00 and 4.90 ns were found in the time-resolved emission decays. The shortest component one is assigned to an intermolecular proton transfer reaction (PT), after the ultrafast ICT (<15 ps), to generate an anion species that relax to the ground state in 4.90 ns. The intermediate components are assigned to the initially emission lifetimes of the excited CPHAT (0.23 ns) and to the charge transfer species (TC, 1.00 ns). Fluorescence microscopy study at single crystal level in solid state was also performed, revealing an ordered crystalline structure with preferential orientation of the molecular dipole moments, Figure 1C.

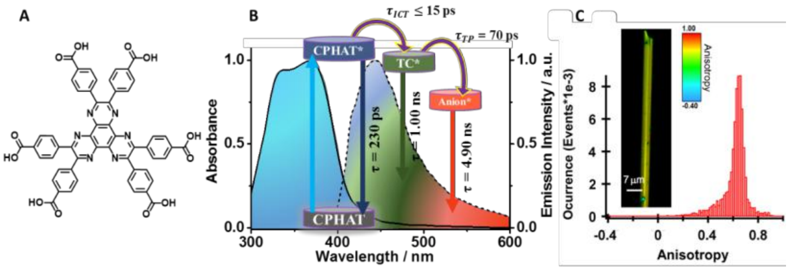

Figure 1. A) Scheme of CPHAT. B) Absorption and emission spectra of CPHAT in DMF solutions. C) Dependence of the emission anisotropy on the orientation of single crystal of CPHAT-1a.

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FABRICATION OF NANO-ALUMINUM/TITANIUM DIOXIDE MODIFIED SCREEN PRINTED CARBON ELECTRODE FOR ELECTROCHEMICAL DETECTION OF VANILLIN IN FOOD SAMPLES

K. Murtadaa*, S. Jodeh, M. Zougaghb, A. Ríos

A new chemically modified electrode based on aluminium nanoparticles (Al-NPs) has been constructed. Titanium was incorporated into the Al-NPs to prepare titanium oxide doped nano-aluminium. Titanium oxide/ nano-aluminium screen printed carbon electrode (TiO_2/Al-NPs-SPCE) was employed as simple, efficient and rapid sensor for electrochemical detection of vanillin in various types of food samples. TiO_2/Al-NPs were characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM) analyses showing that the average particle sizes varied for the Al-NPs (7.63 nm) and TiO_2/Al-NPs (7.47 nm) with spherical crystal. The liner sweep voltammetry (LSV) and cyclic voltammetry (CV) were used to optimize the analytical procedure and a detection limit of 0.985 µM for vanillin was found. A relative standard deviation of 2.09 % was calculated for a 250 µM concentration of vanillin. The electrochemical behavior of other compounds (vanillic acid, vanillic alcohol, p-hydroxybenzaldehyde and p-hydroxybenzoic, etc.), generally present in natural samples, were also studied, to check the interferences with respect to vanillin voltammetric signal. To validate the methodology and efficacy of proposed sensor, detection of vanillin was also examined in food samples. The obtained results were compared with those provided by a reference method based on liquid chromatography.

CURRENT PERSPECTIVES OF THE USE FROM CASTOR (RICINUS COMMUNIS) IN MEXICO

N. Gómez Falcón

The castor (Ricinus commnunis), is an evergreen shrub of the euphorbiaceous family, of fast growth, growth of wild form and in Mexico it is considered weed, due to its rapid propagation in any type of soil. It grows in most climates, is obtained at low cost, has a great tolerance to the environment and its annual production exceeds one million tons. Its main use was medicinal, currently is used how ornamental plant and for the production of industrial oils in several countries of the world. Economically, castor is a crop that contributes nearly 1.0% of the world's total production of oilseeds. However, ingestion of the seeds causes severe intoxication and can be fatal (0.18 g / kg mass), because they contain a toxin called ricin. In this situation, different types of detoxification have been proposed, such as chemical, biological, enzymatic or thermal treatments.

In Mexico the interest for the use from castor as industrial crop, it's due to high content of oil (40-50% from seed weight). In this sense, the oil is used in the manufacture of lubricants, plastics, soaps, hydraulic liquids, paints, varnishes and recently it is promoted for the production of biodiesel. These attributes increase their possibilities as an alternative crop in the oil supply for different types of industries. However, as by-product of the extraction of oil, a product known as castor cake is generated, that once detoxified is used mainly as fertilizer and as a source of protein for the production of feed for livestock. Some studies verify the possibility of its use for human consumption. Another use that is arousing interest in the country is the use of biomass for biofuel purposes. The perspectives of use of this species in Mexico and worldwide have diversified to a large extent, since it has begun to be used as a phytoremediation agent and as biological control agent. However, research continues to grow in the improvement of methods of simultaneous extraction and detoxification, as well as in improvement of methods of elimination of the toxin.

FROM REACTOR TO TUMOR

E. Niza*, J.A. Castro-Osma, C. Alonso-Moreno, I. Bravo,a A. Otero, A. Lara-Sánchez

Drug delivery system (DDS) is the method or process of administering a pharmaceutical compound to achieve a therapeutic effect in humans or animals. DDS allows to decrease the number of doses and to maintain effective for long periods of time without reaching toxic levels, which achieves an improvement in the patient's comfort.

A series of alkyl organoaluminium initiators based on heteroscorpionate ligands have been prepared to increase the catalytic activity in Ring-Opening Polymerization (ROP) of ε-caprolactone without sacrificing control over the Mw/Mn.1 The easy-to-make polycaprolactones of controlled molecular weight and molecular weight distribution were chosen to manufacture biodegradable devices for drug delivery. Amongst the different formulations evaluated, porous polycaprolactone microspheres showed interesting advantages for application as doxorubicin delivery systems. Finally, a copolymer of ε-caprolactone and L-lactide has been designed, which displayed a pH-independent mechanism of doxorubicin release.

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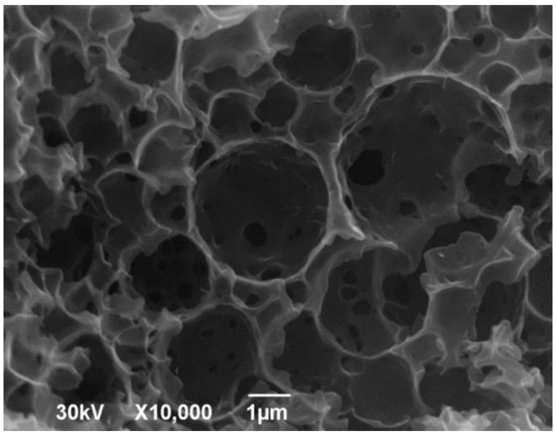


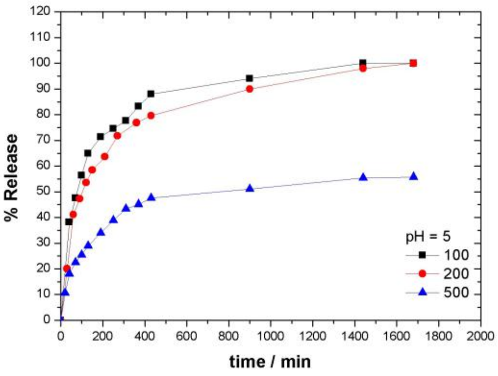


Figure 1. (a) SEM micrograph of PCL-FIII, 10000X. (b) DOX-released profile for PCL-FIII at pH=5

DEVELOPMENT OF A SCREENING METHOD FOR DETECTION OF SULPHONAMIDE RESIDUES USING AN ELECTROCHEMICAL SENSOR

C.S. Gondim*, G.M. Durán, A.M. Contento, A. Ríos

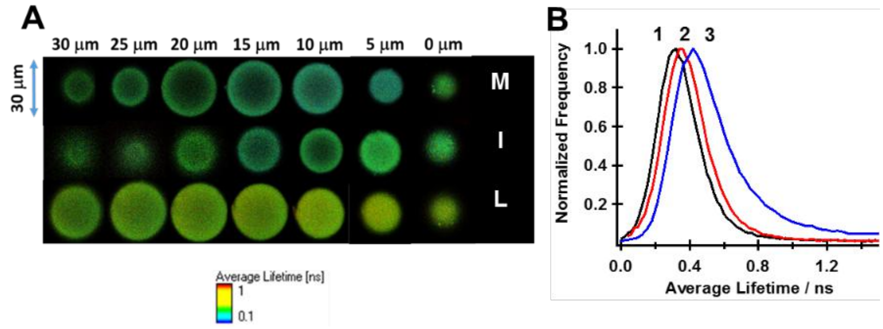
JAVIER TORRES (2017)

The objective of this work was to propose a screening method based on electrochemical measurements that could be applied in detection of sulphonamide residues in milk samples, using a graphene quantum dots modified glassy carbon electrode (G-QDs@Nafion/GCE) for improving sensibility. After optimization, the qualitative method was validated. The performance parameters estimated were false positive, false negative, selectivity and sensitivity rates; accordance, concordance, unreliability region, detection limit and selectivity in presence of potential interferents. Six sulfonamides were evaluated: sulfadimethoxine, sulfadiazine, sulfamethazine, sulfamethoxypyridazine, sulfapyridine and sulfathiazole. Sulphonamide standard solutions at concentrations between 25 and 150 µg L^{-1} were analyzed. The electrochemical technique employed was differential pulse voltammetry. The G-QDs@Nafion/GCE demonstrated satisfactory values for repeatability, reproducibility and stability; with a significant increase on the sensitivity comparing with the glassy carbon electrode. A satisfactory performance related to the false-positive results and precision (accordance and concordance values) was observed. The selectivity was demonstrated for potassium chloride, magnesium sulfate, calcium chloride, sucrose, citric acid and lactose. However, the antimicrobial oxytetracycline was considered a interferent. Sulphonamides were detected at the maximum residue limit (MRL) recommended by the Codex Alimentarius for sulfamethazine (25 µg L^{-1}) and at the MRL established by the European Union for the sum of sulphonamides in milk (100 µg L^{-1}). These results demonstrated the potential applicability of the developed method in detection of sulphonamides residues in milk samples.

FLUORESCENCE-LIFETIME IMAGING MICROSCOPY OF CLOFAZIMINE WITHIN MESOPOROUS SILICA PARTICLES

L. Angiolini, S. Valetti, A. Feiler, B, Koen, A, Douhal

Clofazimine (CLZ) is an antibiotic recommended as primary agent by the World Health Organization for the treatment of leprosy and it is also active against mycobacteria and various Gram-positive bacteria. The low solubility (10 mg/L) in water decreases CLZ bioavailability and triggers its crystallization in the body tissues, which is the cause of various side effects. Mesoporous silica particles (MSP) are stable and biocompatible drug delivery systems able to successfully improve the loading, stability and bioavailability of CLZ. In this work, we characterized the distribution of CLZ within MSP pores with hydrophilic and hydrophobic (low concentration of Si-OH groups) surfaces and studied their effect on CLZ spectroscopic properties. A combination of Fluorescence lifetime imaging (FLIM) microscopy, Time correlated single photon counting and UV-Vis spectroscopy techniques showed a CLZ concentration quenching effect on its emission intensity and emission average lifetime. CLZ presented a stronger quenching effect when encapsulated in the hydrophobic MSP, due to its high affinity for the hydrophobic pores that could retain higher amount of CLZ. This was observed in shorter emission lifetime (0.5 ns), compared to the CLZ within hydrophilic particles (1.2 ns). These findings provide useful information to design MSP delivery systems in order to control the release of CLZ, while increasing the bioavailability without affecting its stability.



UNRAVELING THE INTERNAL AND SURFACE PHOTOBEHAVIOUR OF NILE RED INTERACTING WITH A NOVEL METAL ORGANIC FRAMEWORK

E. Caballero-Mancebo*, B. Cohen, J. M. Moreno, U. Díaz, A. Corma, A. Douhal

In this communication, we unravel the photodynamics of Nile Red (NR) interacting with ITQ-HB, a new layer-structured Metal Organic Framework (MOF) with potential catalytic and photonic applications. This MOF is formed by an oxide metal (Al) cluster and heptane benzoic acid (HB) as linker (Scheme A). Steady-state and time-resolved observations show that the NR behaviour interacting with this MOF is dictated by its location in the material, showing remarkable differences in the photophysical processes when the dye is inside or on the surface of the MOF. A broad absorption band reveals the presence of several species in the ground state, while a narrow emission band indicates processes occurring in the excited state. Furthermore, the time-resolved emission experiments provide more details on the photodynamics of the dye (Scheme B). Our data suggest the occurrence of energy hopping processes leading to shorter emission lifetimes when the NR concentration increases. Our results shed new light on the photodynamics of a new composite and open the door to further researches of encapsulation of relevant molecules within this material, a better understanding of photocatalysts and photonic processes with MOFs.

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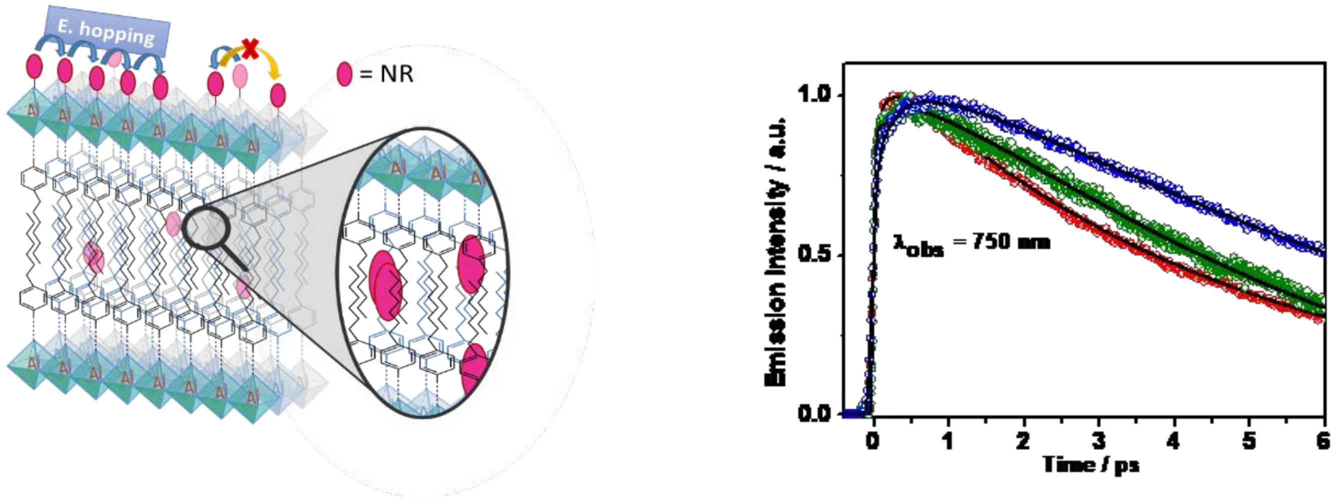
Acknowledgments: This work was supported by the MINECO through Projects MAT2014-57646-P and MAT2014-52085-C2-1-P and JCCM PEII-2014-003-P. E.C.M. thanks the MINECO for the FPI fellowship.



(A) Schematic representation of NR distribution and its dynamics when interacting with Al-ITQ-HB. (B) Emission decays of NR@Al-ITQ-HB observed at 750 nm and excited at different wavelengths: 470 nm (blue circles), 550 nm (green circles and 635 nm (red circles).

NEUROPROTECTIVE PROPERTIES OF BEER COMPOUNDS IN CELLS

P. Alonso-Andres, JL. Albasanz, M. Martín

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.

LIFE CYCLE ASSESSMENT OF BIOMASS THERMOCHEMICAL CONVERSION PROCESSES

M.M. Parascanu*, G. Soreanu, J.L. Valverde Palomino, M.L Sánchez Silva

In recent years, there has been an increasing interest in valorisation of biomass to produce useful fuels and chemicals. Biorenewable feedstocks can be used as solid fuel or converted into gaseous or liquid forms in order to produce energy, chemicals, heat or gaseous or liquid fuels. Biomass conversion can be carried out through a wide range of processes. The most important thermochemical conversion processes of biomass to useful end products are: pyrolysis, combustion and gasification [1].

The set of all inputs of raw material and energy and the outputs of waste and emissions constitutes the environmental impact of the product. Life cycle assessment (LCA) is a very useful tool to evaluate different impact categories quantitatively and qualitatively involved in life cycle of the end products [2]. The SimaPro software is a professional tool to evaluate the environmental impacts of products, processes and services throughout their life cycle.

Taking into account all these aspects, this work aims to identify the environmental impacts generated by the production of various products (char, gas, energy, etc.) through the thermochemical processes using as raw material different types of biomass such as olive pomace, castor husk, castor stems, agave bagasse, pinus sawdust, coffee pulp etc.

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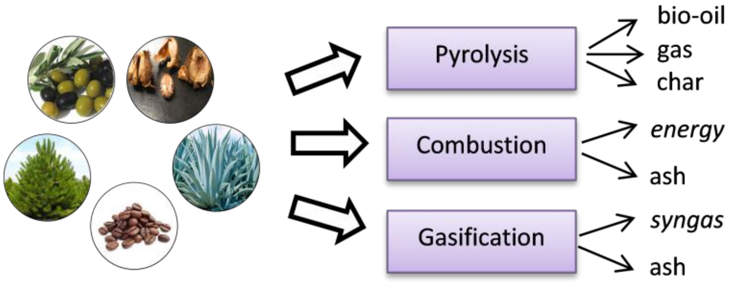

Figure 1. Thermochemical processes of biomass

KINETICS OF THE DEPLETION OF CH3CH2OH BY REACTION WITH OH RADICALS AT TEMPERATURES OF INTERSTELLAR DENSE MOLECULAR CLOUDS (22-107 K)

A. J. Ocaña, M. Antiñolo, S. Blázquez, A. Canosa, E. Jiménez, B. Ballesteros and J. Albaladejo

JAVIERTORRES (2017)

Up to now, more than 180 chemical species (molecules, ions and radicals) have been detected in the interstellar medium (ISM). In order to interpret the observed abundances, gas-phase astrochemical models include the rate coefficients (k) for the potential formation and depletion processes of each species. However, for most gas-phase reactions, k is not known at the temperatures of the dense molecular clouds in the ISM (10-100 K). Usually k values used in modelling the abundances are estimates or extrapolations from temperature dependences reported at T > 200 K. Particularly, the last method is not valid for many radical-molecule reactions due to the observed enhancement of k at low temperatures [1].

Ethanol (CH_3CH_2OH) was first detected in $SgrB_2$ by Zuckermann et al in 1975 [2] and the purpose of this work is to determine k for the gas phase reactions of OH radicals with CH_3CH_2OH at very low temperatures (22-107K), using the CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme or Reaction Kinetics in a Uniform Supersonic Flow) technique. This technique has been described in detail by Jiménez et al [3]. It 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 in terms of their impact on astrochemical models.

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PHYSICOCHEMICAL CHARACTERIZATION AND YIELD ASPECTS IN NEW TABLE GRAPE CULTIVARS IN SUBTROPICAL AREAS

R.C. Colomboa*, J. Pérezb, I. Hermosínb, S.R. Robertoa

JAVIERTORRES (2017)

The traditional table grape cultivars, when cultivated in subtropical areas can be to present some adaptation problems that affect the plants growth and the bunches quality. In Brazil, the EMBRAPA Grape and Wine carry out a grape breeding program since 90s and new grape cultivars were released in the last years to against some of these problems. However, there are a demand in studies to evaluated these new cultivars in subtropical areas where it is possible to obtain two crops a year (regular and out season crops). Among the cultivars recently released by EMBRAPA Grape and Wine, highlights ‘BRS Vitoria’, a seedless table grape (Vitis spp.), recommended for cultivation in tropical and subtropical areas, with excellent horticultural performance, high bud fecundity and tolerance to downy mildew, the most important disease which affects grapevines in humid subtropical areas; presents high yield, and it is an excellent option for overseas market. Due to high yield and the production of two crops a year, bunches quality can be affected and occurs, i.e. a decrease in soluble solid contents when the source/drain relation was lower. In this context, the aim of this study was evaluated the bunches physicochemical characteristics in ‘BRS Vitoria’ table grapes under the production system of two crops a year. The trial was conducted in commercial field of ‘BRS Vitoria’ seedless table grape at Marialva, state of Paraná (South Brazil), vines were trained using an overhead trellises system and spaced at a distance of 2.5 x 5.0 m apart. The treatments consisted in kept bunches density around to four, five and six bunches per m^2. At the harvest was assessed soluble solids contents (SS), titratable acidity (TA), SS/TA ratio, bunches mass, production per plant (kg) and yield (ton ha-1) The results showed that there was no significant difference between treatments for the physicochemical variables evaluated, so it is not necessary to reduce the number of bunches per m2. In out season crop was recorded a yield around to 15 ton ha^{-1} and 25 ton ha^{-1} in the regular crop.

JOINING TOGETHER GRAPHENE AND FULLERENE

L. Miguel Arellano*, F. Langa

Since the discover of graphene in 2004, this material has attracted massive attention due to their unique properties, like mechanical resistance and good stability under chemical and thermal treatments, and emerging as a new interesting field for a great number of technological applications.[1] On the other hand, fullerene C60 is other carbon nanostructure, which have been studied along the last two decades, maintaining great attention owing its remarkable reactivity and optical properties.

Recently, hybrids combining different carbon nanostructures such as carbon nanotubes (CNTs),[2] graphene oxide (GO)[3] and carbon nanohorns with C60 via either covalent or noncovalent functionalization have been developed, driven by the possibility of combine the outstanding properties in a single material.

In this communication, we present our results on the synthesis and study of the properties of new nanohybrids involving graphene and fullerene C60 or endohedral-metallofullerene Li@C_{60}.

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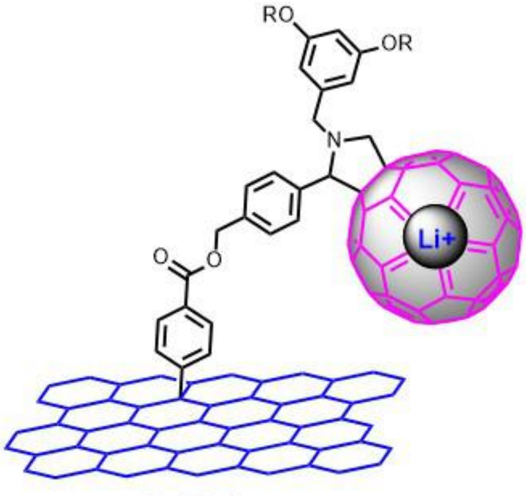

R= $OC_{12}H_{25}$

MODIFIED MAGNETIC NANOPARTICLES IN THE TARGET ANALYSIS OF SOME EMERGING POLLUTANTS

F. Abujer*, F. J. Guzmán, R. C. Rodríguez, Á. Ríos

JAVIERTORRES (2017)

The increasing use of pharmaceutical products has turned into an environmental problem. Analgesic and nonsteroidal anti-inflammatory drugs (NSAIDs) are the most widely prescribed drugs, so their discharge from pharmaceutical factories, hospitals and private household effluents produces a big burden on the environment, especially in water resources. Their concentration in natural waters is typically from ng^{L-}1 to gL^{-1}, so sample preparation techniques that provide adequate sensitivity and selectivity are needed prior to instrumental analysis.

The use of magnetic materials in solid phase extraction has received considerable attention in recent years, taking into account many advantages arising from the inherent characteristics of magnetic particles. Magnetic solid phase extraction (MSPE) methodology overcomes problems such as column packing and phase separation, which can be easily performed by applying an external magnetic field.

In this work, magnetic cellulose nanoparticles (MCNPs) coated with 1-butyl-3-methylimidazolium hexafluoro phosphate ionic liquid (IL) are proposed for the first time as sorbents for MSPE method for the determination of paracetamol, ibuprofen, naproxen and diclofenac in natural waters. This approach can be considered as environmentally friendly because the MCNPs-IL material is made up of cellulose, a renewable material, the IL is not toxic and only a little volume of organic solvent as dispersive agent is required. HPLC with ultra violet (UV) and fluorescence (FD) detector was used after the sample preparation.

The optimized MCNPs-IL-HPLC method showed limits of detection in the range 0.11–0.25 μg L^{-1} with excellent linearity ($R \geq 0.9985$), relative standard deviation below 5%, enrichment factors from 29 to 34 and recoveries close to 100 %.

AGGLOMERATION OF NANOPARTICLES FOR IMPROVED PROCESS SAFETY USING SPRAY-DRYING

J. Martin-Campo*, M. Carmona, J.F. Rodriguez, A.M. Borreguero

JAVIERTORRES (2017)

Nanosized particles are of great scientific interest due to their small size and high surface area, what provide them with unique physical and chemical properties. However, the exposure to these materials supposes potential safety and health hazards. The scaling-up of the production process of nanoparticles requires the use of suitable technologies for its safe handling and transportation.

The main way of entrance of nanomaterials into the organism is by inhalation. The deposition of the particles in the respiratory system highly depends of the particle size. Thus, the goal of this work is the increase of the particle size of the product through agglomeration by using the spray drying technology, obtaining non-respirable micron-sized granules [1].

The nanoparticles are synthesized by means of the sol-gel process, using an alkoxide as precursor [2]. As a result, a liquid suspension of nanoparticles is obtained, that is then dried by means of a spray-dryer. The suspension is sprayed in small drops into a drying chamber where a hot nitrogen stream dries the solvent, which is further recovered. The particles, in the form of agglomerated dry dust are recovered by means of a high efficiency cyclone [3].

The process of agglomeration of nanoparticles is developed in two different scales. First, the optimisation of the operation conditions at laboratory scale was carried out. After that, the process has been scaled-up to pilot plant scale.

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BENEFITS OF CARBON NANOTUBE BASED MAGNETIC SOLID PHASE EXTRACTION IN THE SELECTIVITY OF SAMPLE PREPARATION FOR POLLUTANTS

A.I. Corps*, M. Jiménez, F. J. Guzmán, R. C. Rodríguez, Á. Ríos

A key step in analytical process is sample preparation. A number of techniques have been used for this purpose in relation to analytes that are typically found at trace levels in complex samples. Novel methodologies based on the use of new nanomaterials have been developed and an interesting option is the combination of magnetic nanoparticles coated with carbon nanotubes (CNTs) for magnetic solid-phase extraction (MSPE). MSPE provides a fast and easy separation of analytes using an external magnet and avoids the time-consuming traditional on-column SPE procedures and CNTs provides selectivity. The potential of this combination has been explored for the analysis of different pollutants in several water samples.

Firstly, a rapid and reliable method based on MSPE and ultra-high performance liquid chromatography (UHPLC) analysis was developed and validated for the quantitative determination of seven polycyclic aromatic hydrocarbons (PAHs) in water samples. Magnetic nanoparticles (MNPs) coated with multi walled carbon nanotubes (MWCNTs) were tested as adsorbent materials. Parameters that affect the extraction efficiency were carefully investigated. The instrumental LODs and LOQs achieved were in the range of 0.025–0.73 and 0.04–2.4 ng mL-1 respectively. The recoveries of PAHs were from 76.4 up to 106.5 %. To evaluate the performance, the method was applied to synthetic and real water samples.

Secondly, mercury speciation analysis was carried out in water samples. Not only is this analysis challenging because mercury is present at ultra-trace levels, but also because the most toxic and important mercury species (monomethylmercury, MMHg) is around 5% of the total concentration. In this work, the speciation analyses were carried out by gas chromatography coupled to atomic fluorescence detection (GC-pyro-AFS) after derivatization by ethylation. We studied the performance of MNPs coated with different types of CNTs. After a careful optimization, the developed method allowed the selective determination of MMHg and the clean-up of other mercury species. The LOD and LOQ achieved for MMHg were 5.4 and 17.9 pg L-1, respectively. The methodology was validated analyzing several spiked real water samples with recoveries close to 100%.

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BIOPROSPECTING OF AGROINDUSTRIAL RESIDUES FROM SOLID STATE FERMENTATION WITH SUBSEQUENT PRODUCTION AND ENZYMATIC PURIFICATION

Rosa, Z., Isabel, A.*, Gomes E., Silva, R.

JAVIERTORRES (2017)

Due to the expansion of the industrial applications of lignocellulosic enzymes, the interest in the production of these enzymes by microorganisms through processes that promote high yields at low cost is increasing. Lignocellulosic raw materials are the most abundant renewable sources found in nature, so they are mostly comprised of agroindustrial, urban waste and wood from angiosperms and gymnosperms. The three main polymeric fractions that make up the lignocellulosic biomass are lignin, hemicellulose and cellulose, which are linked together by covalent and non-covalent bonds, forming a complex network resistant to microbial attacks. The biodegradation of cellulose is made by a complex of oxidative and hydrolytic enzymes that act synergistically in the transformation of the molecule into monomers and glucose dimers. This complex is formed by endoglucanases, exoglucanases and β-glycosidase, classified according to their place of action on the cellulosic substrate: a) Endoglucanases, which cleave internal bonds of the cellulosic fiber; b) Exoglucanases, which act in the external region of the cellulose; and c) β-glycosidases, which hydrolyze glucose-soluble oligosaccharides. Among the microbial biodiversity existing on the planet, filamentous fungi present a wide capacity of adaptation in the most varied solid substrates. Due to this characteristic, the industrial production of enzymes can be performed from solid-state fermentation processes using agroindustrial residues and by-products as a substrate for the growth of these fungi, which stand out as producers of enzymes of degradation of lignocellulose. The adaptation of a given microorganism to thermophilicity involves the adjustment of the cytoplasmic membrane, proteins and DNA to temperatures above the mesophilic range. This thermophilic molding has aroused great interest in biotechnology, considering that thermoresistance mechanisms of the biomolecules of these microorganisms may be interesting models for bioengineering and bioprocesses. Thus, knowing and purifying the thermostable enzymes of these microorganisms would bring advances and boost new research. Thus, separation and purification techniques such as electrophoresis and high performance liquid chromatography using LCMS / MS mass spectrometer coupled detectors were employed in order to obtain these proteins from a pure was for their subsequent application in several sectors.

HYPERTERMIA-INDUCED SEIZURES AFFECTS THE BEHAVIOR IN RATS

Crespo M., León-Navarro D.A. and Martín M.


JAVIERTORRES (2017)

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.

BIFUNCTIONAL ALUMINIUM(HETEROSCORPIONATE) CATALYSTS FOR THE FORMATION OF CYCLIC CARBONATES FROM EPOXIDES AND CARBON DIOXIDE

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

The use of carbon dioxide (CO_2) as a universal renewable resource is a challenge for chemists. It requires efficient strategies for the conversion of CO_2 into economically competitive products to help to stabilize and reduce atmospheric carbon dioxide levels to mitigate the greenhouse effect and to develop an alternative and sustainable raw material.[1] One of the most promising reactions in this field is the synthesis of cyclic carbonates from epoxides and CO_2 (Scheme 1). Even though this reaction is highly exothermic due to the release of the epoxide strain energy, it requires a suitable catalyst to lower the high activation barrier. Among these catalysts, bifunctional systems or one-component catalysts, have been less developed probably owing to their more synthetically demanding preparation.[2]

Inspired by the high catalytic activity displayed by the aluminium complexes,[3] this work reports the design of new iodide heteroscorpionate precursors that makes the synthesis of mono- and bimetallic bifunctional aluminium complexes and their application as catalysts for the conversion of epoxides into their corresponding cyclic carbonates.

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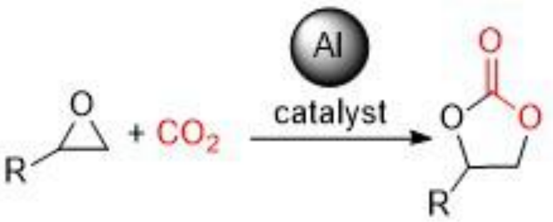

Scheme 1

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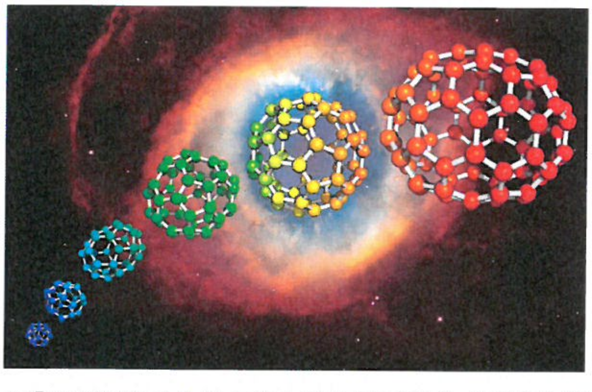

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Inmaculada	Moreno Sánchez Gil	Inmaculada.Moreno@uclm.es

Participantes

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