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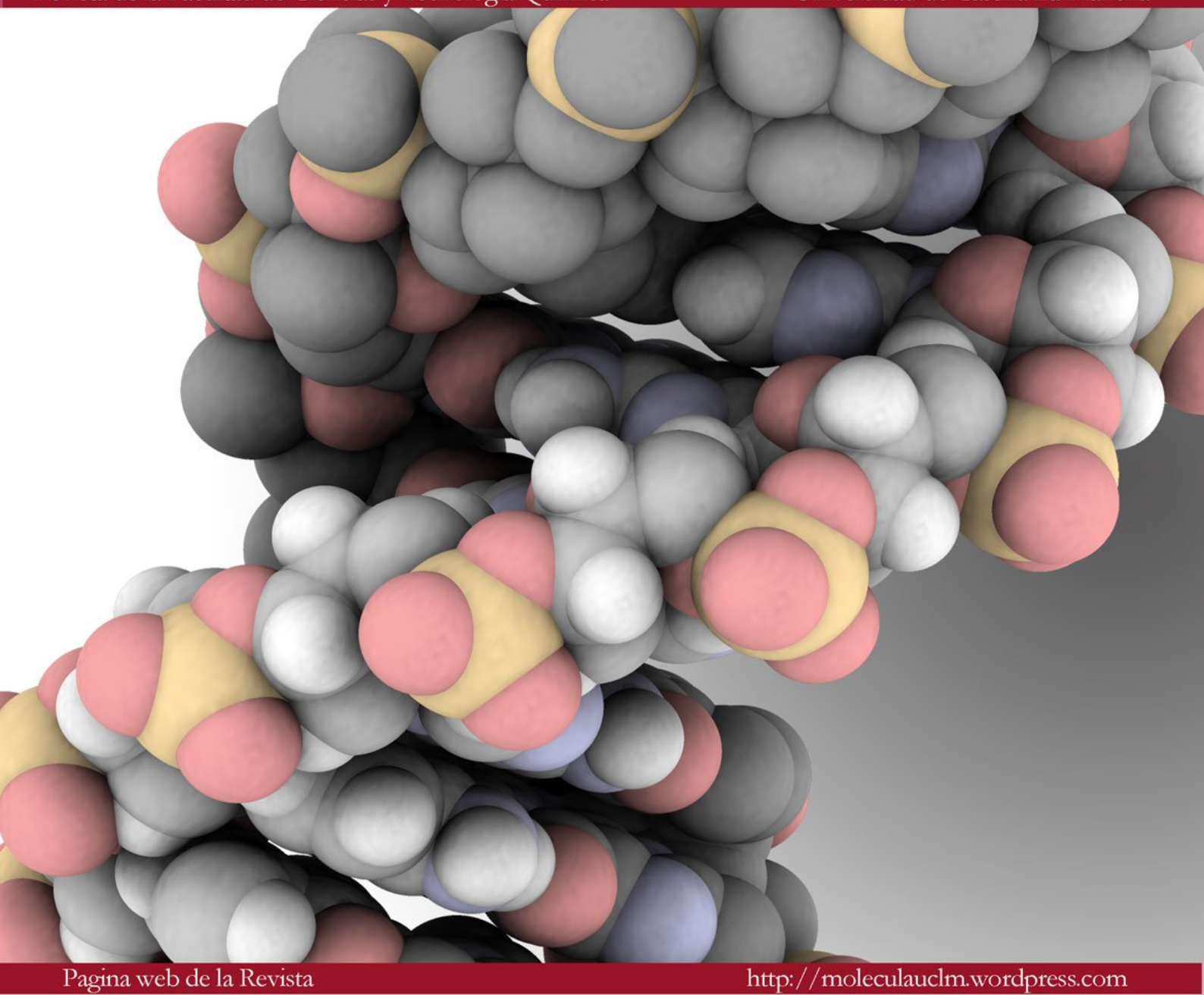

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ÍNDICE

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.

CONFERENCIA INVITADA

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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CONFERENCIA INVITADA

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.

CONFERENCIA INVITADA

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

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

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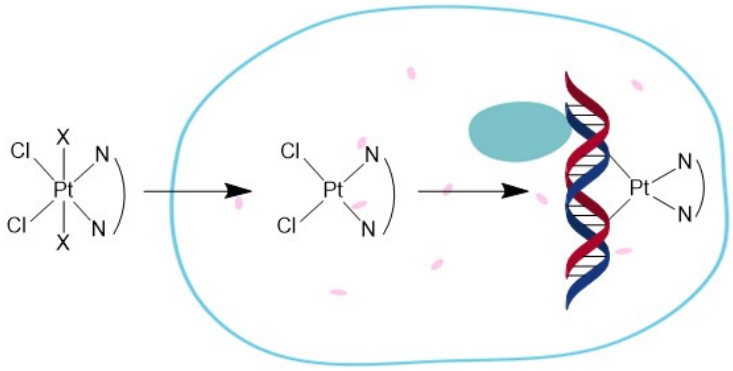
SYNTHESIS OF Pt(II) AND Pt(IV) COMPOUNDS AS POTENTIAL ANTICANCER DRUGS

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

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

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

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

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

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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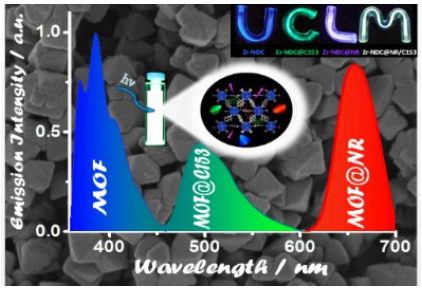


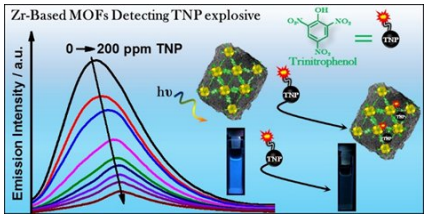
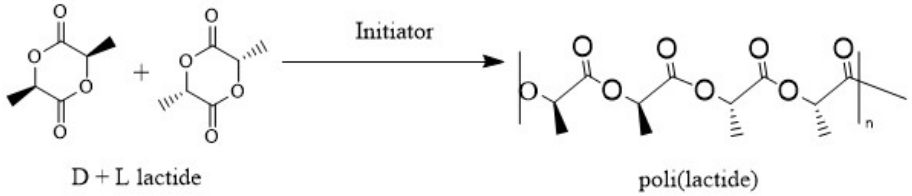


Figure 1. A) White light emission of Zr-NDC MOF containing C153 and NR dyes. B) Emission quenching of Zr-NDC/Tz MOF in presence of TNP explosive molecules.

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

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

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.

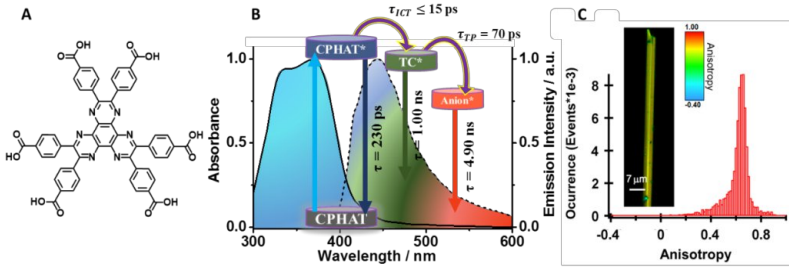

Figure 1. A) Scheme of CPHAT. B) Absorption and emission spectra of CPHAT in DMF solutions. C) Dependence of the emission anisotropy on the orientation of single crystal of CPHAT-1a.

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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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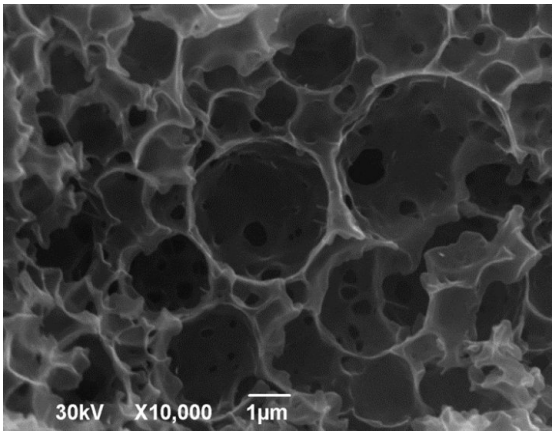


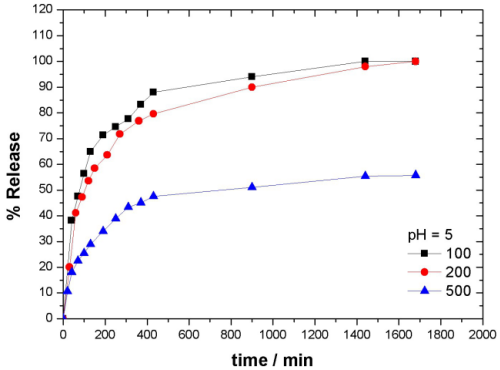


Figure 1. (a) SEM micrograph of PCL-FIII, 10000X. (b) DOX-released profile for PCL-FIII at pH=5

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

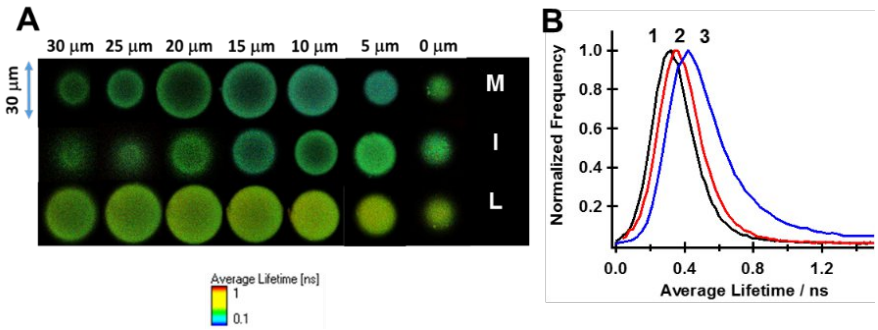
C.S. Gondim*, G.M. Durán, A.M. Contento, A. Ríos

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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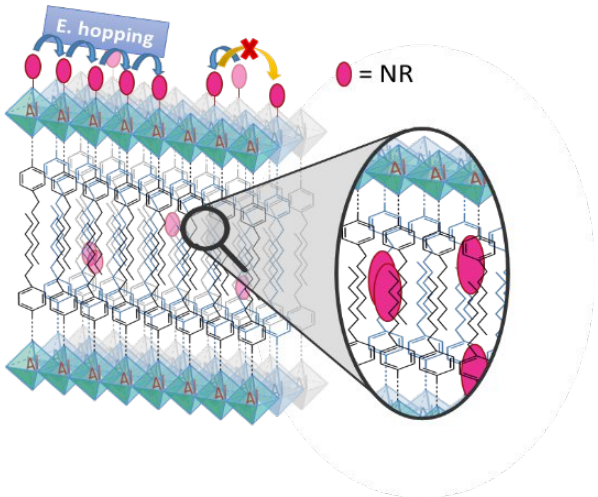

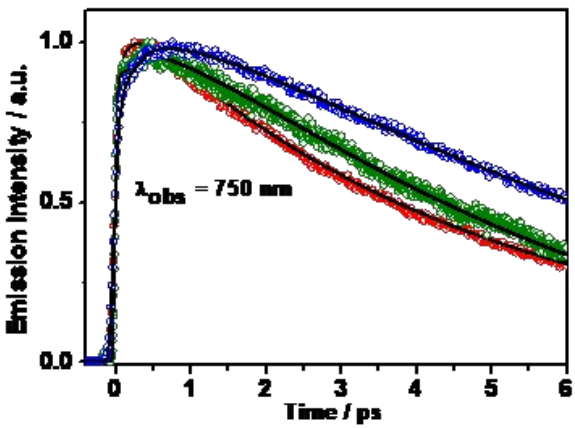

(A) Schematic representation of NR distribution and its dynamics when interacting with Al-ITQ-HB. (B) Emission decays of NR@Al-ITQ-HB observed at 750 nm and excited at different wavelengths: 470 nm (blue circles), 550 nm (green circles and 635 nm (red circles).

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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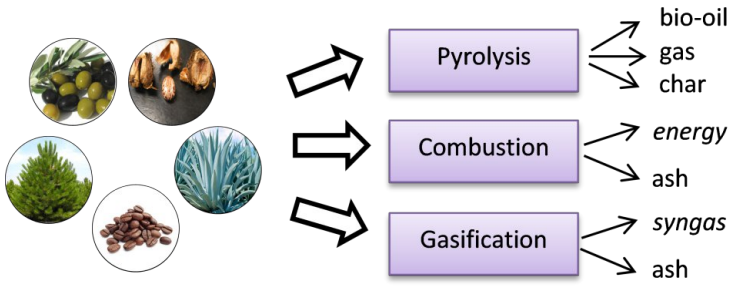

Figure 1. Thermochemical processes of biomass

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

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

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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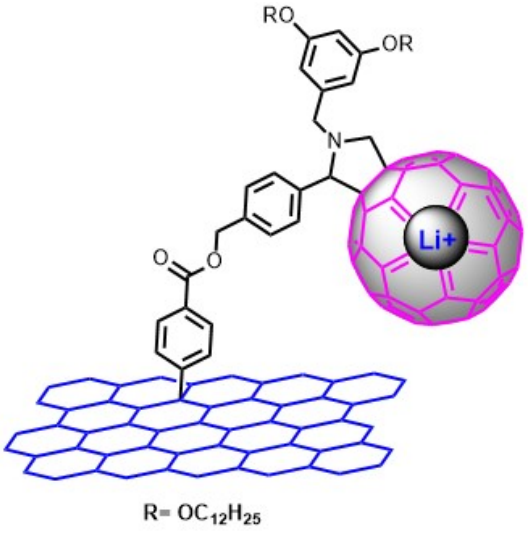

MODIFIED MAGNETIC NANOPARTICLES IN THE TARGET ANALYSIS OF SOME EMERGING POLLUTANTS

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

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

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%.

Acknowledgment: Spanish Ministry of Economy and Competitiveness CTQ2016-78793-P) and Junta de Comunidades de Castilla-La Mancha (PEIC-2014-001-P).

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

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

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.

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

Xth International School on Organometallic Chemistry "Marcial Moreno Mañas"

This event is an annual activity organized by the ORFEO-CINQA team. The meeting aims to get together young students, early career researchers and well recognized, world-leading scientists from academy and industry, to facilitate and generate exchange of scientific information and knowledge.

The first School took place in Ciudad Real, in 2008. This edition of the school will be held, once again, at the Ciudad Real Campus of the University of Castilla-La Mancha. The campus is located in a human-size and welcoming city, well-connected to the rest of the country by highway and high-speed train.

The school will feature:

- 8 plenary lectures,
- 15 oral contributions,
- 40 flash presentations,
- around 70 poster presentations,

The oral contributions and flash presentations will be selected from the attendants.

We look forward to see you at the School next July 2017 in Ciudad Real!

Despedida a Ana Isabel García Fernández

Temprano levantó la muerte el vuelo,

Ningún docente imagina que, algún día, entre sus tareas se encontrará la de escribir unas palabras póstumas para despedir a uno de sus estudiantes; pero hoy, los profesores de Ciencia y Tecnología de Alimentos tenemos esa difícil tarea, la de rendir, desde Molécula, un homenaje póstumo a una de nuestras estudiantes: **Ana Isabel García Fernández**.

La muerte es siempre inoportuna y dolorosa por esperada que sea, pero es todavía más sobrecogedora e inexplicable cuando se trata de alguien en plena juventud.

Ana, empezó sus estudios en nuestra Facultad hace unos años y la recordamos con sus grandes ojos, su amplia sonrisa, su cola de caballo y sus gafillas, sentada en los primeros bancos en el aula, siempre atenta y trabajadora. No sin esfuerzo llegó entusiasmada a cuarto curso del Grado de Ciencia y Tecnología de Alimentos y animosa por ver el fin de sus estudios, por poder recompensar el esfuerzo de su familia, y esperanzada con la posibilidad de un contrato cercano y por otros anhelos e ilusiones propios de su juventud, los inexplicables hados le susurraron: ahora no Ana, ahora hay que empezar otro viaje.

Y ahí empezó su lucha, sabemos que titánica, hasta tal punto que fiel a su estilo realizó los exámenes de sus últimas asignaturas, confiada en que ganaría el pulso a su terrible enfermedad. No obstante, a pesar de su empeño, su coraje, su ánimo y sobretodo de su esperanza, el caprichoso destino no le ha permitido cumplir sus sueños.

Te despedimos con unos versos de Miguel Hernández,

Ana, *un manotazo duro, un golpe helado,*
un hachazo invisible y homicida,
un empujón brutal te ha derribado.

Pero confiamos y esperamos que:

Volverás a tu huerto y a tu higuera,
y por los altos andamios de las flores
pajareará tu alma colmenera

En el próximo número de Molécula...

En el número de julio incluiremos las noticias y trabajos más relevantes presentados en la décima edición de la Escuela de Química Organometálica y las impresiones de dos de los finalistas de la primera edición del concurso "Tesis en 3 minutos" organizada por la Escuela Internacional de Doctorado. También contaremos con nuestras habituales secciones de investigación y cafetería.