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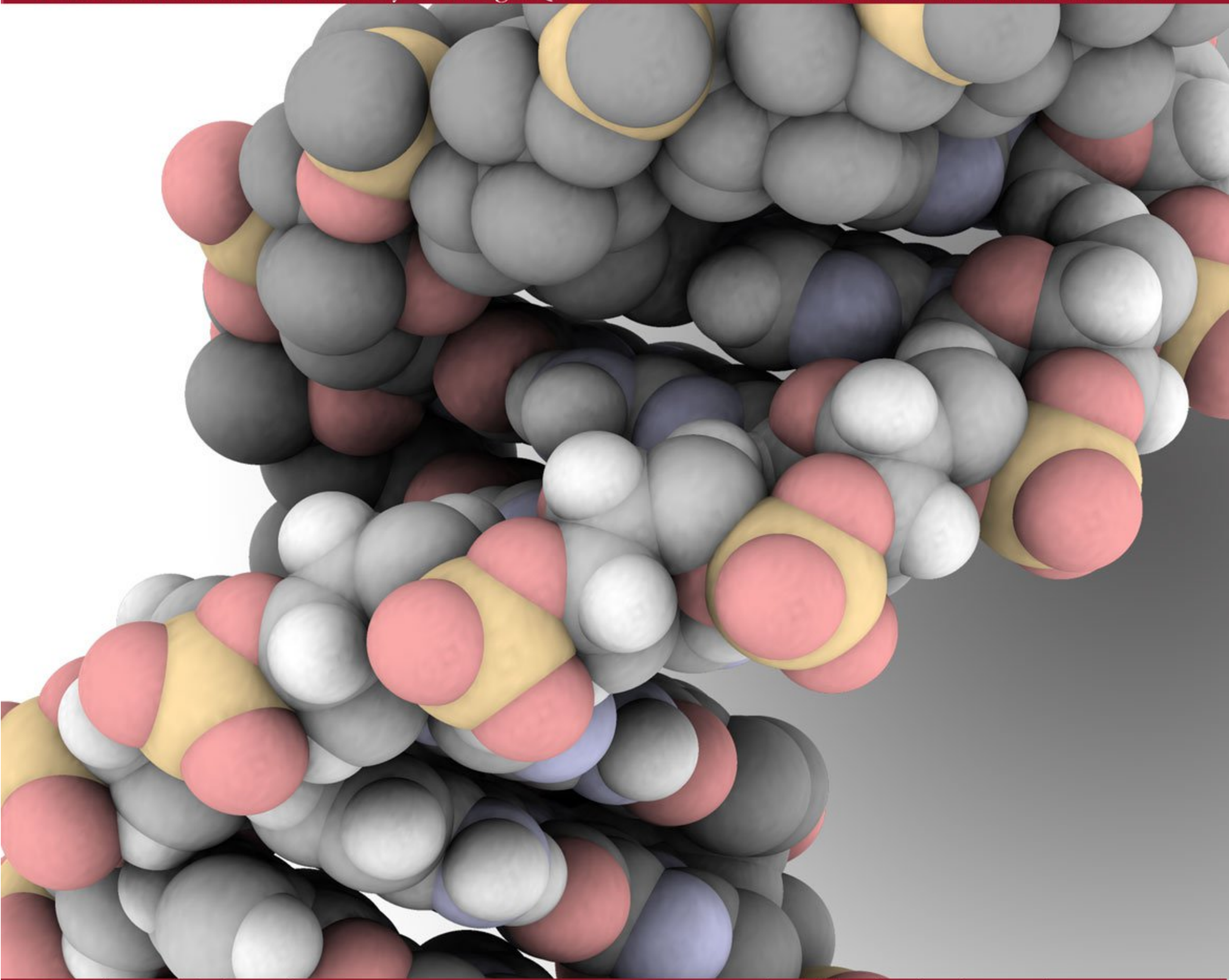

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ÍNDICE

PRESENTACIÓN

El número de Junio es un monográfico dedicado al XIII Simposio de Ciencia Joven, donde se recogen todas las comunicaciones orales y posters que han participado en el evento, además de las conferencias invitadas. Este número también recoge información relativa a los premios otorgados en el simposio.

El comité editorial.

LOS QUÍMICOS NOVELES DE LA UCLM COMPARTEN CON SUS COMPAÑEROS SUS LÍNEAS DE TRABAJO DE INVESTIGACIÓN

El rector de la Universidad de Castilla-La Mancha inaugura el XIII Simposio Ciencia Joven que se celebra en Ciudad Real

La Facultad de Ciencias y Tecnologías Químicas de la Universidad de Castilla-La Mancha (UCLM) en Ciudad Real acoge el Simposio Ciencia Joven desde el 5 al 7 Junio, 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 decimotercera edición, ha sido inaugurado por el rector de la UCLM, Miguel Ángel Collado.

Los jóvenes investigadores de la Facultad de Ciencias y Tecnologías Químicas de la universidad de Castilla-La Mancha (UCLM) en el Campus de Ciudad Real, así como otros llegados de Albacete y Toledo, presentan a la comunidad académica sus líneas y resultados de investigación con motivo de la celebración del decimotercer Simposio Ciencia Joven, una iniciativa organizada por ellos mismos que a su vez les supone una oportunidad para acercar a los estudiantes a la tarea investigadora.

El encuentro ha sido inaugurado esta mañana por el rector de la Universidad de Castilla-La Mancha (UCLM), Miguel Ángel Collado, quien ha felicitado a la Facultad de Químicas y a sus organizadores por esta iniciativa, muestra de la “vitalidad” del centro, y por su “entusiasmo, trabajo y compromiso con la investigación pese a las dificultades”.

Para el rector, este encuentro refleja que en la Universidad de Castilla-La Mancha hay gente joven “con talento, capacidad e inteligencia” que aseguran el futuro de la investigación. Frente a ello está el problema de los recursos económicos y materiales, de ahí que el rector haya pedido a los nuevos gobiernos surgidos de las urnas que “asuman con mayor entusiasmo la investigación” y apuesten por “la financiación, la regularidad y consolidación de convocatorias y la divulgación de la ciencia” a fin de que la sociedad valore la tarea investigadora. “La ciencia contribuye a seguir creciendo y a vivir mejor”, ha dicho.

LOS QUÍMICOS NOVELES DE LA UCLM COMPARTEN CON SUS COMPAÑEROS SUS LÍNEAS DE TRABAJO DE INVESTIGACIÓN

Junto al rector de la UCLM, el decano de la Facultad de Ciencias y Tecnologías Químicas, Ángel Ríos, se ha referido a la celebración del simposio de Ciencia Joven como una excelente oportunidad para los investigadores noveles, ya que el mismo les ayudará a conocer cómo se prepara un congreso científico, les servirá de apoyo en su tarea formativa investigadora y les permitirá conocer el trabajo que realizan otros compañeros.

En el simposio, en el que colabora la Real Sociedad Española de Química, se han inscrito un total de 120 investigadores del Campus de Albacete, Ciudad Real y Toledo y se han admitido 35 comunicaciones orales y 28 contribuciones en formato póster en los distintos ámbitos que abarca la Facultad: Química Inorgánica, Ingeniería Química, Química Orgánica, Química Analítica, Tecnología de los Alimentos, Química Física, Matemáticas y Bioquímica. Entre otras líneas de investigación, durante el simposio, según ha explicado en representación de la organización la investigadora Virginia Moreno, se expondrán cuestiones como los nanomateriales en alimentos y medioambiente, fluidos supercríticos sostenibles con el medioambiente, el grafeno o las propiedades del vino, entre otras.

Junto a los ponentes investigadores noveles, el simposio cuenta con la intervención de cinco ponentes externos invitados del Instituto IMDEA Nanoscience, y de las universidades de Valencia y Murcia.

Gabinete Comunicación UCLM. Ciudad Real, 5 de junio de 2019

INTERFACING MOLECULES AND NANOMATERIALS: FROM CARBON NANOTUBE ROTAXANES TO SINGLE-MOLECULE EXPERIMENTS

EMILIO M. PÉREZ

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

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

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

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RETOS DEL CONTROL DE NANO MATERIALES EN ALIMENTOS

YOLANDA PICÓ

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

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GREEN CHEMISTRY OR 'DREAM' CHEMISTRY: CLEAN BIOCATALYTIC PROCESSES OF INDUSTRIAL INTEREST

PEDRO LOZANO

The development of sustainable chemical processes turns around two main axes: the selectivity of catalytic transformations, and the easy and clean separation of pure products. The use of enzymes in ionic liquids (ILs) was reported great advantages (*i.e.* improved activity and enantioselectivity, enhanced stability, etc.),[1] and its combination with supercritical technologies was resulted in synergetic and outstanding platforms for developing (multi)catalytic green chemical processes under flow conditions able to directly provide pure products.[2] This has been demonstrated by several examples of flow synthetic processes in IL/scCO$_2$ biphasic systems at 100 bar and 40-100ºC (*e.g.* DKR of *rac*-1-phenylethanol,[3] biodiesel,[4] monoglycerides,[5] etc. Straightforward protocols for carrying out biotransformations, product recovering and biocatalysts/ILs reusing without any loss in the overall greenness character of the process, have been developed in recent years.

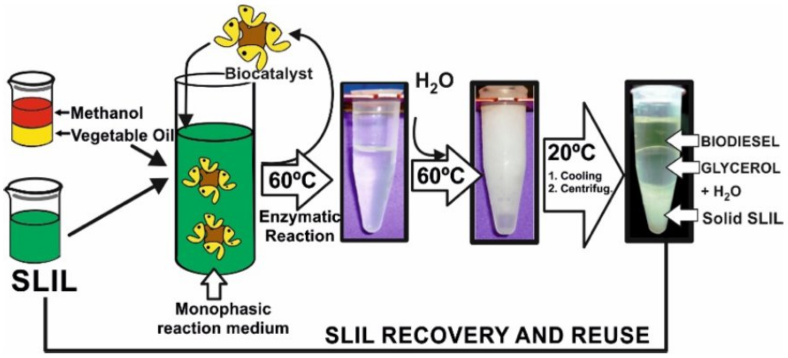

Figure 1. Schema of the protocol for the biocatalytic synthesis of biodiesel in SLIL, and product separation with full recovery and reuse of the SLILs

GREEN CHEMISTRY OR 'DREAM' CHEMISTRY: CLEAN BIOCATALYTIC PROCESSES OF INDUSTRIAL INTEREST

PEDRO LOZANO

Sponge-Like Ionic liquids (SLILs) are hydrophobic ILs based on cations with long alkyl side-chains, *e.g.* octadecyltrimethylammoniumbis(trifluoromethylsulfonyl)imide, etc.), which behaves as sponge-like systems by switching from liquid to solid phase with temperature.[6] Based on this new property, the SLILs have been applied for developing straightforward and clean approaches for biocatalytic synthesis and extraction of nearly pure compounds of added value (*e.g.* terpene esters,[7] biodiesel,[8] etc.). As can be seen in Figure 1, the SLILs are able for dissolving (soaking) hydrophobic compounds at temperatures compatible with enzyme catalysis (*e.g.* vegetable oil and methanol mixtures are monophasic in [C_{18}mim][NTf_2] at 50°C[7]).

By cooling reaction mixtures based on these SLILs under room temperature, they are solid phases that can be fractionated by centrifugation, allowing the release (wringing out) of reaction products from the SLIL net, and resulting in two phases: a solid SLIL phase and a liquid phase containing synthetic products (flavour esters, biodiesel, etc.). This approach for product separation can be improved by using centrifugal filters, demonstrating the excellent suitability of this straightforward and green approach for carrying out synthesis and separation of pure products with full recovery and reuse of the reaction system (SLIL and biocatalyst).[6]

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

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INVESTIGACIÓN EN ENERGÍA: PROGRESO VS CIRCULARIDAD

DAVID SERRANO GRANADOS

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

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

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

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

MARÍA INMACULADA ARANDA

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

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ELECTROCHEMICAL DETECTION OF RHODAMINE B BY MOLECULARLY IMPRINTED POLYMER MODIFIED SCREEN PRINTED CARBON ELECTRODE AND EXTRACTION BY MAGNETIC MULTIWALLED CARBON NANOTUBE POLY(STYRENE-CO-DIVEINYLBENEZNE)

YASSINE BENMASSAOUD

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

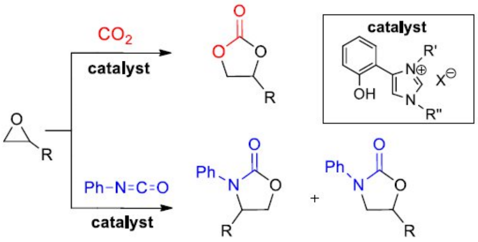
In this study, a molecular imprinted polymer was prepared and used as a screen-printed carbon electrode modifying film for the rapid electrochemical detection of Rhodamine B. A magnetic solid phase extraction was also carried out using magnetic multiwalled carbon nanotubes poly(styrene-co-divinylbenzene)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

SYNTHESIS OF HETEROCYCLE COMPOUNDS CATALYZED BY IMIDAZOLIUM SALTS

MARÍA DEL PRADO CABALLERO

Metal-free organocatalysts based on imidazolium salts showed high efficiency catalyzing the cycloaddition reactions to prepare heterocycle compounds such as cyclic carbonates and oxazolidinones (Scheme 1).[1,2] Imidazolium salts performed as bifuntional catalysts and exhibited improved activity for the fixation of CO_2. Mechanistic studies revealed that the hydroxyl group promoted the activation of the epoxide ring by nucleophilic attack of the iodide.

Oxazolidinones are an important class of heterocycle compounds which are commonly used as precursors to antibacterial medicines. Using the optimal reaction conditions (2 mol% of 5-hidroxyphenylimidazol at 80 °C in toluene for 24 hours) aromatic and aliphatic epoxides were reacted with phenylisocyanate to prepare the corresponding oxazolidinones. The activity[3] of catalysts has an important role in the synthesis since the cyclotrimerization of isocyanates is a competing reaction.



Scheme 1. Synthesis of cyclic carbonates and oxazolidinones.

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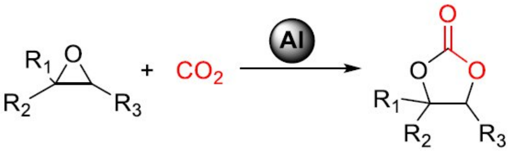
SYNTHESIS OF BIO-DERIVED CYCLIC CARBONATES FROM RENEWABLE RESOURCES

FELIPE DE LA CRUZ

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

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



Highly diastereoselective synthesis;
Excellent yields; Earth-abundant catalyst

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SCREENING AND PRELIMINARY BIOCHEMICAL AND BIOLOGICAL STUDIES OF [RuCl(p-CYMENE)(N,N-BIS(DIPHENYLPHOSPHINO)-ISOPROPYLAMINE)][BF4] IN BREAST CANCER MODELS

ELENA DOMÍNGUEZ

Breast cancer is the second leading cause of cancer death worldwide. Despite progress in drug discovery, identification of the correct population is the limiting factor to develop new compounds in the clinical setting. Therefore, the aim of this study is to evaluate the effects of a new metallodrug, [RuCl(p-cymene)(N,N-bis(diphenylphosphino)-isopropylamine)][BF4] (pnpRu- 14) as a lead pnp-Ru compound by screening and preliminary biochemical and biological studies in different breast cancer subtypes. The results show that complex pnpRu-14 is much more effective in promoting in vitro cytotoxic effect on HER2+ and RH+/HER2- breast cancer than the reference metallodrugs cisplatin, carboplatin or RAPTA-C. It is important to highlight that pnpRu-14 shows an impressive cytotoxicity against BT474 cells. Caspase-dependent apoptosis is the mechanism of action for these compounds. In addition, treatment of SKBR3, BT474, T47D and MCF7 cancer cells with pnpRu-14 caused an accumulation of cells in the G0/G1 phase cells. The Human serum albumin (HSA), DNA and H1 histones binding properties of the lead compound are reported. Pharmacokinetic and biodistribution studies show a quick absorption of pnpRu-14 in serum with no significant accumulation in any of the tested organs. This work provides evidence to support the preclinical and clinical development of pnpRu-14 in breast cancer.

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

BEATRIZ DONOSO

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

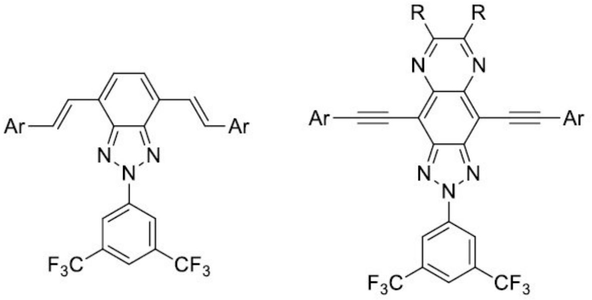

Figure 1. 2*H*-benzo[*d*][1,2,3]triazole derivatives.

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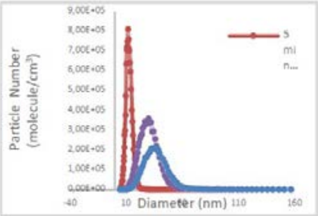
FORMATION OF SECONDARY ORGANIC AEROSOL (SOA)

ALBA ESCALONA

Atmospheric aerosols are considered as one on the main uncertainty sources in the current understanding of the Earth's climate[1]. Previous studies showed that some compound aromatic emitted to the atmosphere give a high SOA (Secondary Organic Aerosol) formation potencial[2,3]. Reaction of the alkenes with ozone proceeds through the formation of a Criegee intermediate (CI). Very recently, it has been found that stabilized CI (sCI) can undergo reactions with SO_2 several orders of magnitude faster than assumed so far[4] producing SO_3, which contributes efficiently to the formation of ground level sulfuric acid[5,6].

We study the ozonolysis reaction of different volatile organic compound following the conditions that lead to the formation and growth of new particles. The effect of water vapor and SO_2 concentrations during the process are also studied and discussed. The reactions have been carried out in a Teflon chamber filled with synthetic air mixtures at atmospheric pressure and room temperature and following the particle formation by SMPS (Scanning Mobility Particle Sizer) and CPC (Condensation Particle Counter).



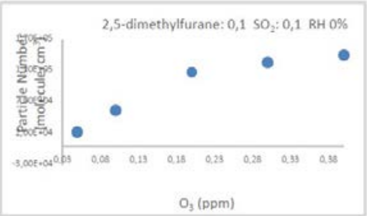


Figure 1. Distribution of particle size at different reaction times. Figure 2. Effect of $[O_3]$ on the production of SOA

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YEASTS WITH PROBIOTIC POTENTIAL

PILAR FERNÁNDEZ-PACHECO

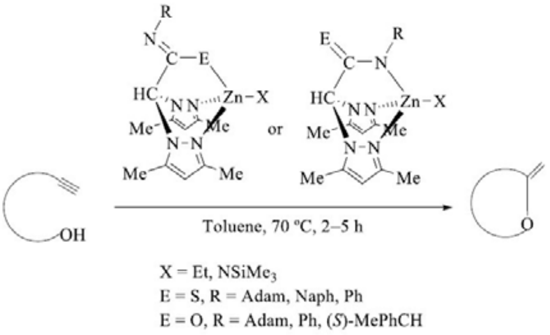
The intestinal microbiota is the most populated community of the human body in which trillions of microorganisms live in symbiosis, contributing to the normal functioning of the organism through its interactions with the host. However, a dysbiosis can cause multiple alterations. One of the most widely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

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

REACTIVITY OF ZINC COMPLEXES TOWARDS ALKYNES: CATALYTIC INTRANOLECULAR HYDROALKOXYLATION OF ALKYNYL ALCOHOLS

MIGUEL ÁNGEL GAONA

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



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ANOTHER APPLICATION OF YEASTS: BIODETOXIFICATION OF POLLUTANTS

BEATRIZ GARCÍA-BÉJAR

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

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

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

EFFECIENT BILIRUBIN REMOVAL BY BSA FUNCTIONALIZED POLIMERIC PARTICLES

MARÍA DEL PRADO GARRIDO

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

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

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

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

ACKNOWLEDGEMENTS

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FLEXIBLE, MULTIFUNCTIONAL NANORIBBON ARRAYS OF PALLADIUM NANOPARTICLES FOR TRANSPARENT CONDUCTION AND HYDROGEN DETECTION

ELENA HERNÁNDEZ

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

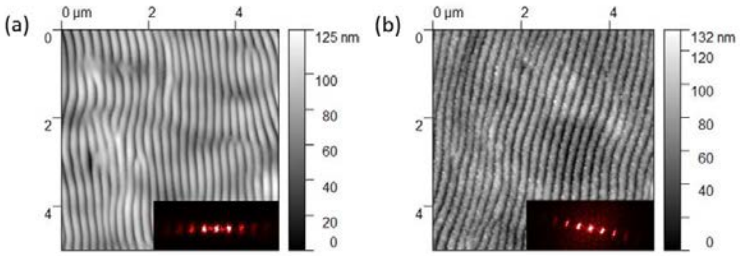

Figure 1: AFM height images (5 x 5 μm^2 size) of (a) PET substrate with LIPSS and (b) Pd nanoparticles on PET substrate with LIPSS. The inset images correspond to the Fast Fourier Transform of each height image.

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HYDROGELS WITH IRON AND COBALT MAGNETIC NANOPARTICLES

JESÚS HERRERA

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

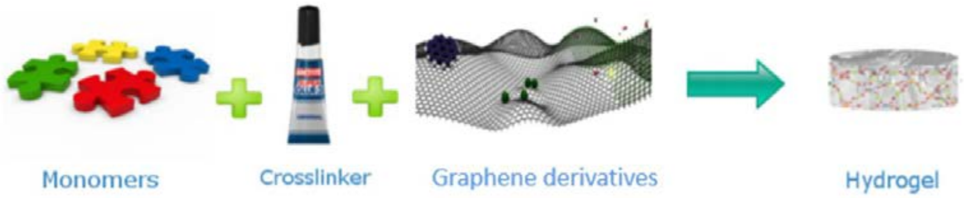

Figure 1. General scope of hydrogels synthesis.

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APPLICATION OF THE GC-MS/MS AND LASER-BASED MASS SPECTROMETRY TECHNIQUES FOR THE DETERMINATION OF POLYCYCLIC AROMATIC HYDROCARBONS (PAH) AND THEIR DERIVATIVES (OPAH AND NPAH) IN REFERENCE AND REAL SOOT SAMPLES

SONIA LARA

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

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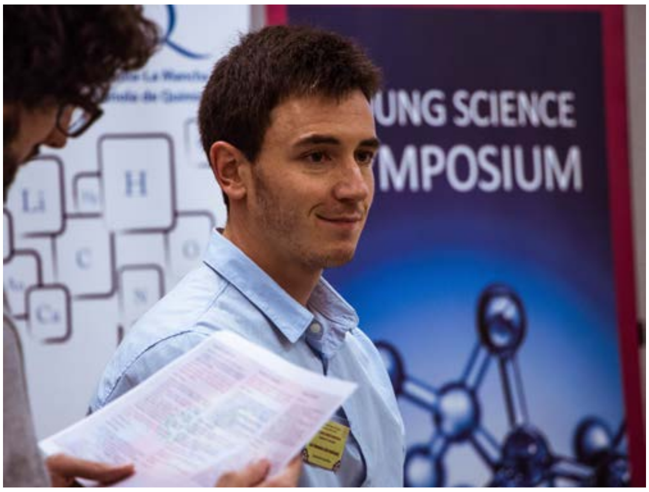
CAPILLARY ELECTOPHORESIS METHOD FOR THE DISCRIMINATION BETWEEN BIOELECTROCHEMICAL SYSTEMS FOR THE REDUCTIVE TREATMENT OF HAZARDOUS POLLUTANTS

LUIS FERNANDO LEÓN



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

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

FUNCTIONALIZATION OF POLYMERS IN SUPERCRITICAL CARBON DIOXIDE

SONIA LÓPEZ

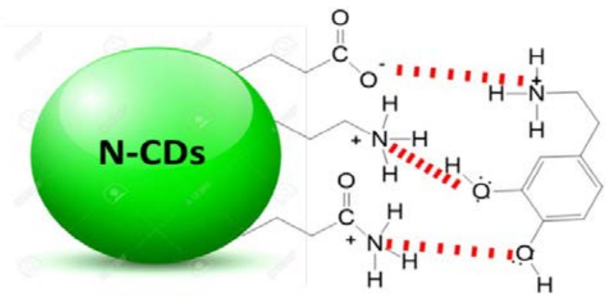
The growing demand for "intelligent" polymers has led to the continuous search for simple and efficient methods for their generation. Polymer-drug conjugates are finding increasing use as novel anticancer agents. Polymeric systems conjugated with a drug result in the controlled release of drugs as this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

NANOMOLAR DETECTION OF DOPAMINE IN HUMAN FLUIDS BY N-DOPED CARBON NANOPARTICLES

MARWA LAULEB

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

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

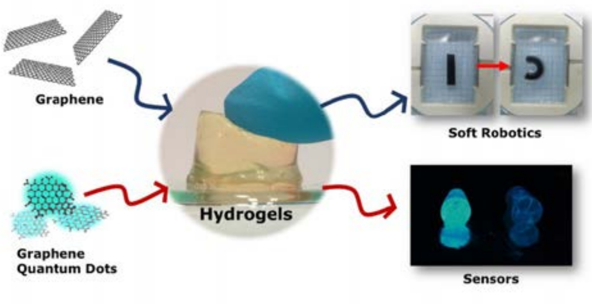


Scheme 1. Schematic representation of the interaction between N-CDs and DA.

SMART MATERIALS FOR SENSING AND SOFT ROBOTICS APPLICATIONS

ANA MARTÍN

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



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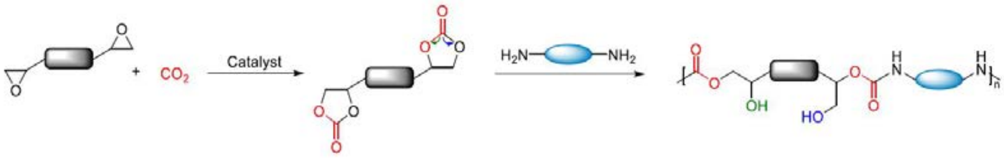
FIXATION OF CO_2 INTO CYCLIC CARBONATES FOR THE GENERATION OF POLYURETHANES FREE OF ISOCYANATES (NIPU)s

MARC MARTÍNEZ DE SARASA

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

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



Scheme 1

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

CRISTINA MONTES

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

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BLUE AGGREGATION-INDUCED EMISSION BY HYDROGELATION PROCESS

JOSUE MUÑOZ

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

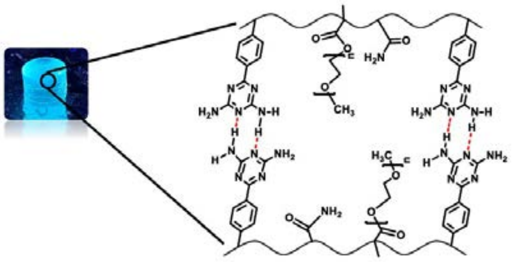

Figure 1. Digital image and chemical hydrogel structure

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ADENOSINE RECEPTORS, RESVERATROL AND CANCER

SONIA MUÑOZ

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

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

ANTONIO JESÚS OCAÑA

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

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

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

RODRIGO OLIVER

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

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

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

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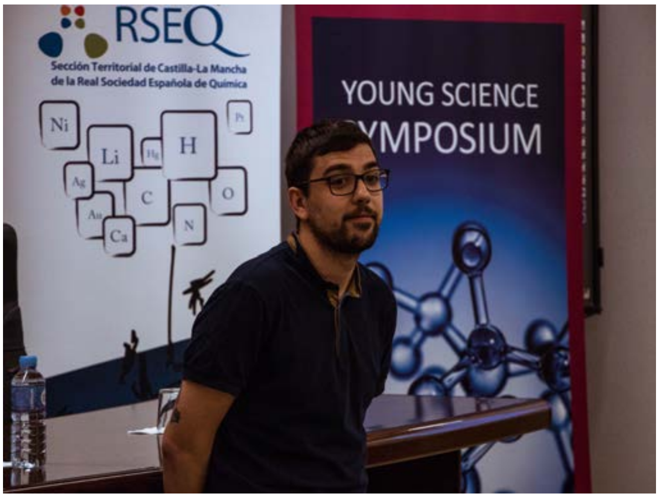
GRAPHENE BASED MATERIALS APPLICATIONS

ANTONIO PATÓN



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

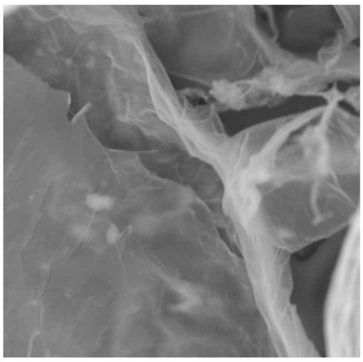


Figure 1: SEM Image of graphene oxide

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

NEW ELECTROFENTON REACTORS FOR WASTEWATER TREATMENT

JOSÉ FERNANDO PÉREZ

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

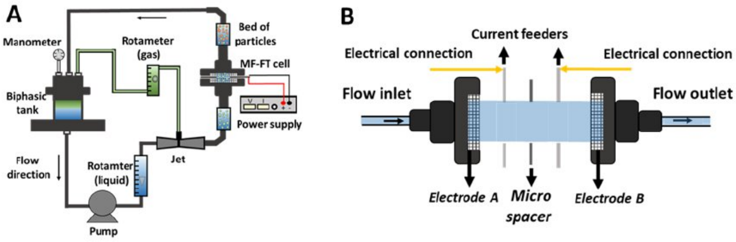


Figure 1. A) Schematic setup of the system; B) A micro-fluidic flow-through cell

In particular, the reactor incorporates an efficient pressurized-jet aerator to supply large oxygen flow rates at moderate pressure, a microfluidic flow-through reactor to simultaneously minimize ohmic resistance and maximize mass-transfer, equipped with state-of-the-art electrodes and a fluidized bed of particles to promote Fenton reaction. Results show an outstanding performance of the microfluidic flow-through cell in comparison to a commercial flow-by, a synergistic combination of anodic oxidation and electroFenton in this reactor[1] or the lowest specific energy consumption ever reported under similar conditions for the production of hydrogen peroxide. The communication summarizes the development and current application of this reactor.

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

JOSÉ PÉREZ

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

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

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

ESTHER PINILLA

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

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

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

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VALORIZATION OF ETHANOL INTO VALUE ADDED COMPOUNDS BY ELECTROREFORMING ON A PEM CELL

ALBERTO RODRÍGUEZ

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

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LEPTIN. "FROM 1969 TO THE PRESENT DAY"

BLANCA RUBIO

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

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

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

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

MARGARITA RUIZ DE CASTAÑEDA

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

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

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

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

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

MANUEL SALGADO

Furfural (FF), or furan-2-carbaldehyde, is a green key compound which has been recognized as a top-value bio-based chemical by United States Department of Energy [1]. Therefore, it is useful to be employed in a wide range of applications, from the chemical industry to the agrochemical sector [2], as well as in the production of bio-fuels and solvents. FF production is generally carried out by the initial dehydration of pentoses, such as xylose. This process usually involves acidic conditions, for instance, with inorganic mineral acids, heterogeneous catalysts or sulfonic acids. Moreover, the mechanism for FF production has been also suggested by many researches [3]. Particularly, FF can be obtained from C_5-sugars found in hemicelluloses, one of the three major components in lignocellulosic biomass, including cellulose and lignin [2]. Nowadays, due to the diminishing of fossil fuel reserves, together with the detrimental augmentation of greenhouse effects, the worldwide scientific community has focused on novel routes employing sustainable C-sources for the synthesis of the top platform chemicals [4]. Regarding to the top, the main goal of this work is the optimization of some variables (temperature, time, solvent, catalyst…) in order to achieve the best yield of FF from xylose, as well as the influence of these variables over the valorization of some lignocellulosic wastes, always keeping the Green Chemistry Principles.

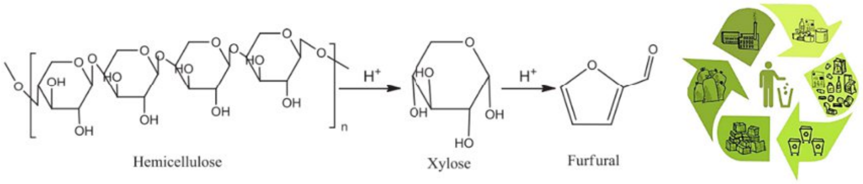

Figure 1. General chemical path from biomass to furfural

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

ARMANDO SÁNCHEZ

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

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

ALEJANDRO SÁNCHEZ

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

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

CARLOS TARDÍO

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

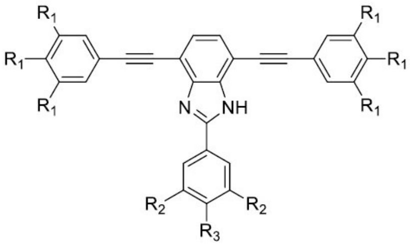

Figure 1. Structure of alkynyl 1*H*-benzo[*d*]imidazole derivatives

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

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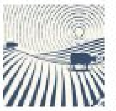
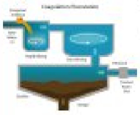
Introduction

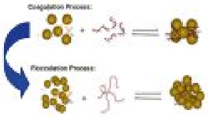


Use of **herbicides** in developed countries is an essential part of **agricultural production**, it is aimed to improve indirectly crop yield by killing or inhibiting the growth of weeds that compete with the desirable main plants for nutrition.

Oxyfluorfen is one of the most commonly used herbicides. It is a hazardous organochlorinated diphenyl-ether compound that has been used to control certain annual broadleaf and grassy weeds.

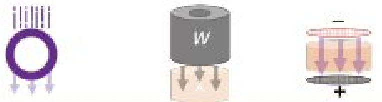


The use of these chemical compounds is associated with **undesirable impacts** in the environment, and many **technologies have been developed and** tested to remove this kind of compounds from synthetic and real water effluents.



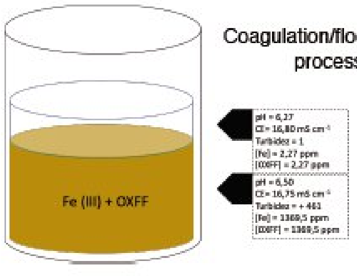
Nowadays, one of the priorities in the field is to **reduce the waste amounts** of sludges from the different treatments including electrochemical processes.

This work explores the **effect of electrochemical dewatering**, to **reduce and oxydize pollutants such as oxyfluorfen from sludges** procedent from a coagulation/flocculation process.

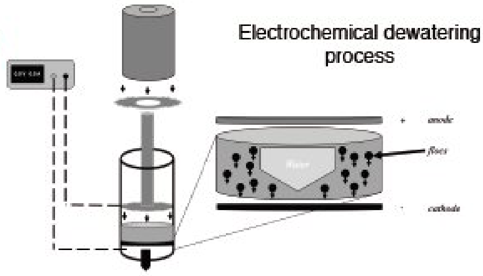


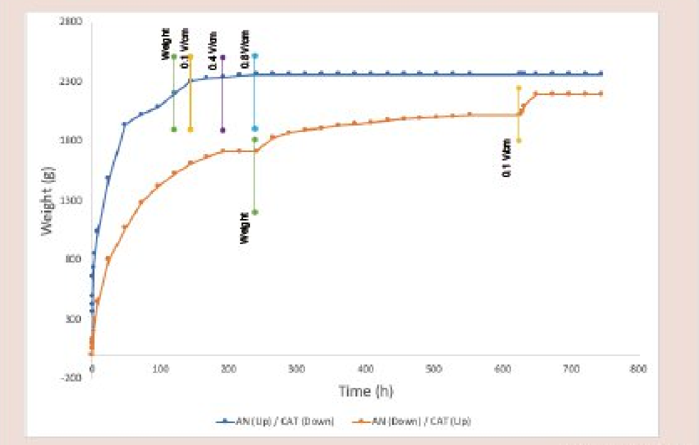
Materials and methods

① Coagulation/flocculation process



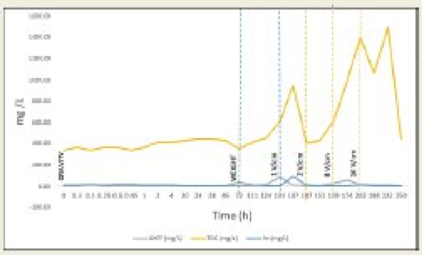
② Electrochemical dewatering process





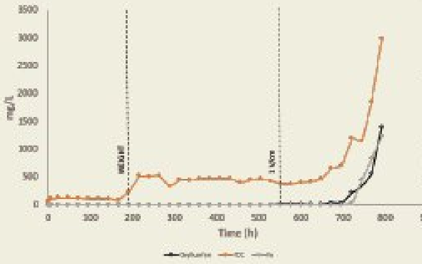
WATER REMOVAL

a



Anode (Up) and Cathode (Down) experiments show that there more energy needed to complete the dewatering of the sludge, but there is almost no oxyfluorfen liberation. TOC is liberated to the liquid sample when electric field is increased.

b



Anode (Down) and Cathode (Up) experiments show almost all water is extracted from the sample when applying 0.1 V/cm, but there is oxyfluorfen liberation that is correlated with TOC and Fe, and a decrease in pH values due to electrokinetic events.

OXYFLUORFEN REMOVAL

Conclusions

1. The application of electric fields enhances the dehydration of polluted sludges and has influence on the movement of the pollutant species in the water flux.
2. The anode – cathode orientation has a relevant influence both in the species mobility and in pH, and also it has an influence in the dryness of the final cake.
3. It has been proven that the electrochemical dehydration of iron-coagulation sludges can reduce the amount of polluted wastes to a great extent.

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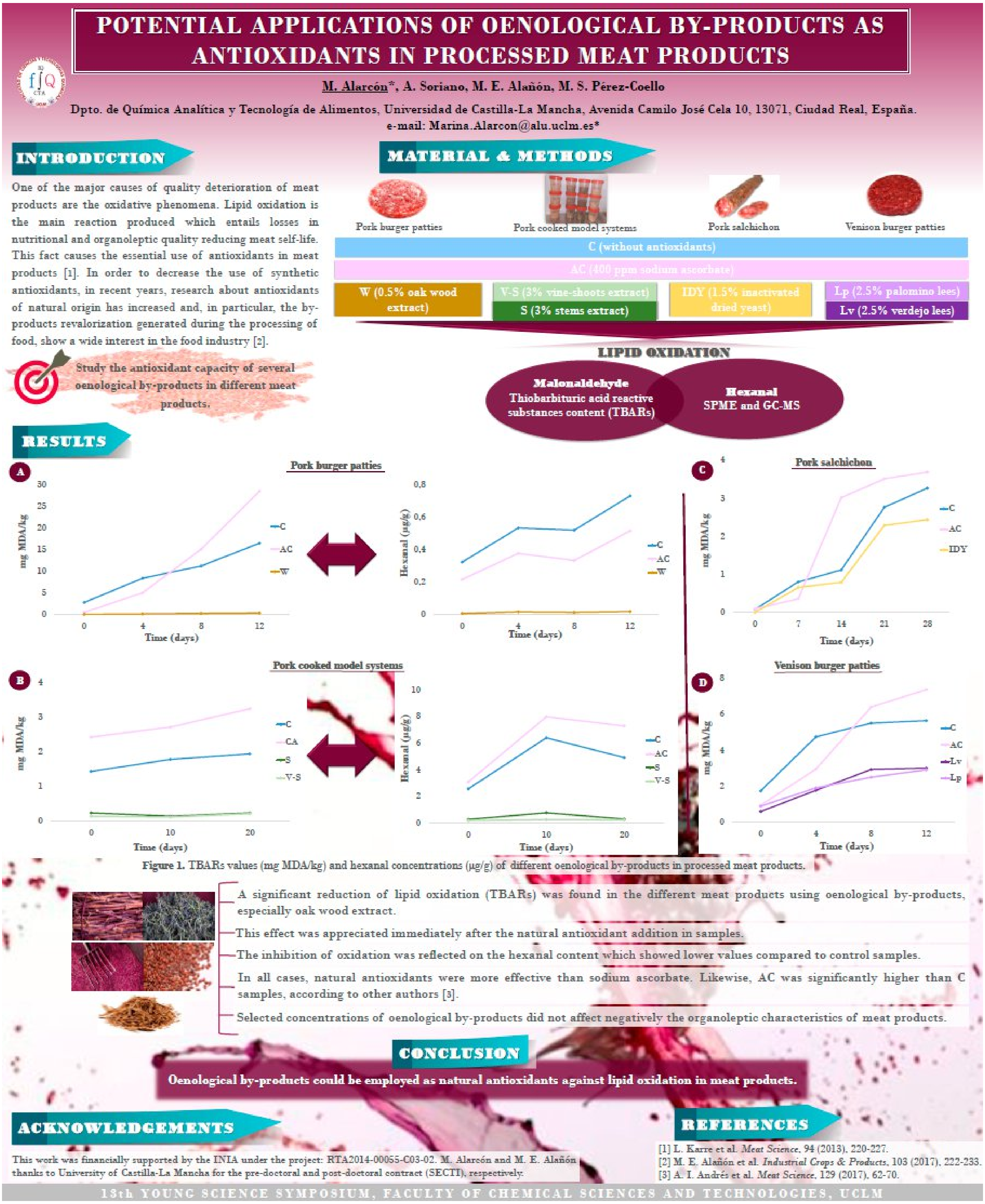
Acknowledgments

Authors appreciate the financial support from the Spanish Ministry of Economy, Industry and Competitiveness and European Union through project CTM2016-76197-R (AEI/FEDER, UE). G. Acosta-Santoyo would like to thank the National Council for Science and Technology (CVU: 264785, Mexico) for their financial support granted for a Postdoctoral Position at the UCLM and Centro de Investigación y Desarrollo Tecnológico en Electroquímica, S.C.



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

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INTRODUCTION

One of the major causes of quality deterioration of meat products are the oxidative phenomena. Lipid oxidation is the main reaction produced which entails losses in nutritional and organoleptic quality reducing meat self-life. This fact causes the essential use of antioxidants in meat products [1]. In order to decrease the use of synthetic antioxidants, in recent years, research about antioxidants of natural origin has increased and, in particular, the by-products revalorization generated during the processing of food, show a wide interest in the food industry [2].

Study the antioxidant capacity of several oenological by-products in different meat products.

MATERIAL & METHODS

Pork burger patties
Pork cooked model systems
Pork salchichon
Venison burger patties

C (without antioxidants)

AC (400 ppm sodium ascorbate)

W (0.5% oak wood extract)
V-S (3% vine-shoots extract)
S (3% stems extract)
IDY (1.5% inactivated dried yeast)
Lp (2.5% palomino lees)
Lv (2.5% verdejo lees)

LIPID OXIDATION

Malonaldehyde
Thiobarbituric acid reactive substances content (TBARs)

Hexanal
SPME and GC-MS

RESULTS

Figure 1. TBARs values (mg MDA/kg) and hexanal concentrations (µg/g) of different oenological by-products in processed meat products.

- A significant reduction of lipid oxidation (TBARs) was found in the different meat products using oenological by-products, especially oak wood extract.
- This effect was appreciated immediately after the natural antioxidant addition in samples.
- The inhibition of oxidation was reflected on the hexanal content which showed lower values compared to control samples.
- In all cases, natural antioxidants were more effective than sodium ascorbate. Likewise, AC was significantly higher than C samples, according to other authors [3].
- Selected concentrations of oenological by-products did not affect negatively the organoleptic characteristics of meat products.

CONCLUSION

Oenological by-products could be employed as natural antioxidants against lipid oxidation in meat products.

ACKNOWLEDGEMENTS

This work was financially supported by the INIA under the project: RTA2014-00055-C03-02. M. Alarcón and M. E. Alañón thanks to University of Castilla-La Mancha for the pre-doctoral and post-doctoral contract (SECTI), respectively.

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13th YOUNG SCIENCE SYMPOSIUM, FACULTY OF CHEMICAL SCIENCES AND TECHNOLOGIES, UCLM

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

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1. Abstract

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

2. Introduction

- ✓ Insecticide carbamates act as an inhibitor of acetylcholinesterase, the enzyme responsible for the hydrolysis of acetylcholine after transmission of information by this neurotransmitter. If this hydrolysis does not take place, the increase in acetylcholine concentration induces hyperactivity of nervous system resulting paralysis and death of the insect.

- ✓ The wide use of this carbamates causes the contamination of aquatic environments: rivers, lagoons, surface and underground water. Their trace-state determination, in various aqueous media, requires a preconcentration step followed by their analysis often conducted by HPLC-UV, HPLC LC-MS or CE-DAD.

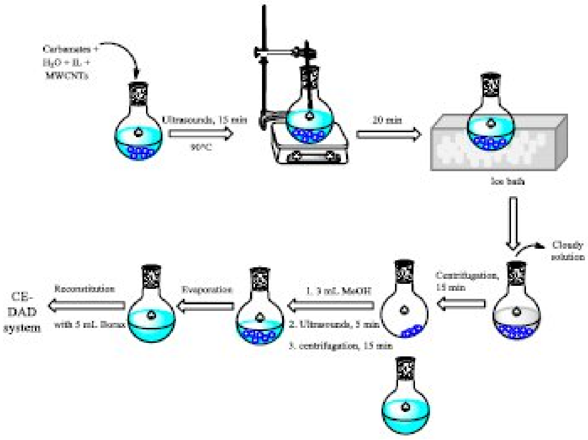
3. Aims

- ✓ The development of a novel methodology to extract N-methylcarbamate pesticides with ionic liquid and MWCNTs from water samples.

- ✓ The separation and the quantification of the carbamates in water samples by CE-DAD.

4. Materials and Methods

Extraction procedure



5. Results and Discussion

Extraction and CE-DAD parameters

Table 1. Operating conditions for extraction and separation of NMCs by CE-DAD

Parameter	Conditions
Extraction procedure	
Ionic liquid (IL)	1-hexyl-3-methylimidazolium hexafluorophosphate
IL volume	100µL
Sorbent material	MWCNTs
Sorbent mass	10 mg
Elution solvent	DCM
Elution solvent volume	3 mL
Sample volume	10 mL
Buffer composition	15mM borate solution
CE method	
Buffer pH	11,47
Separation voltage	20 kV
Capillary dimension	75 µm i.d. x 80 cm
Capillary temperature	25°C
Injection time	10 s
Injection pressure	50 mbar
Wavelength	209 nm

Detection of NMCs by CE-DAD

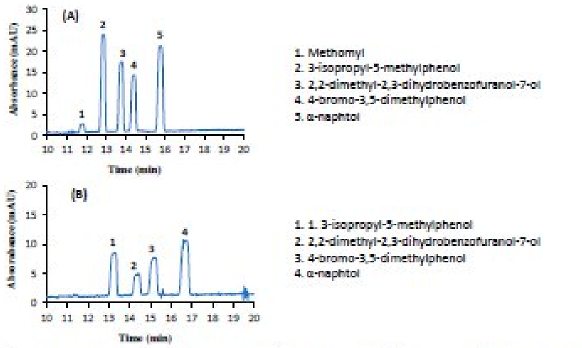


Figure 1: Electropherogram of: (A) Standard solution 20 µg.mL-1 and (B) Extracted, spiked water sample.

6. Conclusions

- ➢ In this work, the combination of IL and MWCNTs was used for the extraction of five N-methylcarbamate pesticides from water sample then determined by CE-DAD.

- ➢ The parameters that affected the extraction efficiency such as type and volume of extractant solvent, temperature, sorbent mass and type and volume of elution solvent were studied in order to found the optimal extraction conditions.

Acknowledgements

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

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AIMS

The main objective of this project is the synthesis and study of silica nanoparticles as a biomaterial for treatment of critical hemodialysis patients with dangerously high serum bilirubin levels. For that goal, we have synthesised one type of amino-functionalized silica nanoparticles. The functionalization of the particles with an amine organic group is necessary for bilirubing binding and removal from patients' blood stream. A reduction in bilirubin levels was observed in PBS solutions, but further analysis techniques are needed to confirm that the decreasing levels are due to the removal capacity of amino-modified nanoparticles.

SUMMARY

In critical patients with kidney failure, the development of simultaneous hepatic disease is especially dangerous, causing a rise in bilirubin serum levels that is not compatible with human life. Bilirubin builds up in skin, muscles and mucous membranes. It can even get into the brain and cause neurological damage (bilirubin encephalopathy).

In this study, we suggest the use of silica nanoparticles as a biomaterial for decreasing bilirubin levels in the blood of dialysed patients. The first step is the synthesis of nanosilica particles, functionalized with APTES as amine group donor for interaction with bilirubin carboxyl groups. Bilirubin adsorption assays are carried out in PBS solutions and human plasma to test the bilirubin removal capacity of the newly-synthesised biomaterial. If the results are promising, new sets of silica particles with other amino organic ligands will be produced and their bilirubin removal efficiencies will be compared.

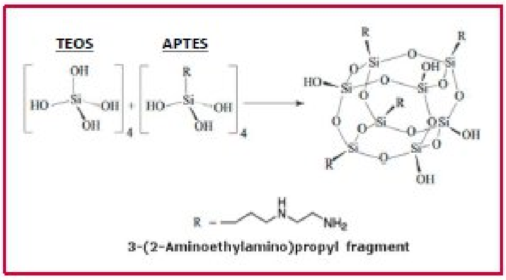


Fig 1. Diagram of the process of synthesis of silica nanoparticles modified with APTES.

RESULTS

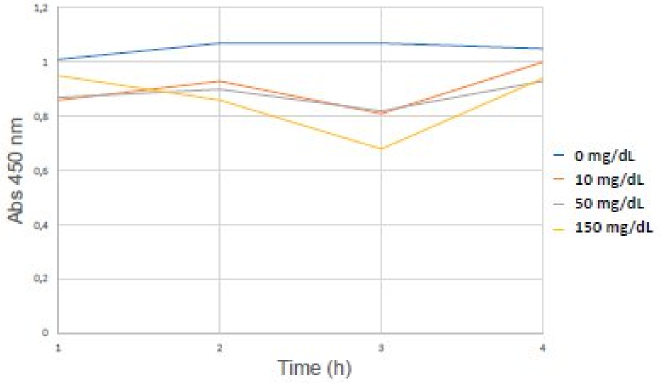
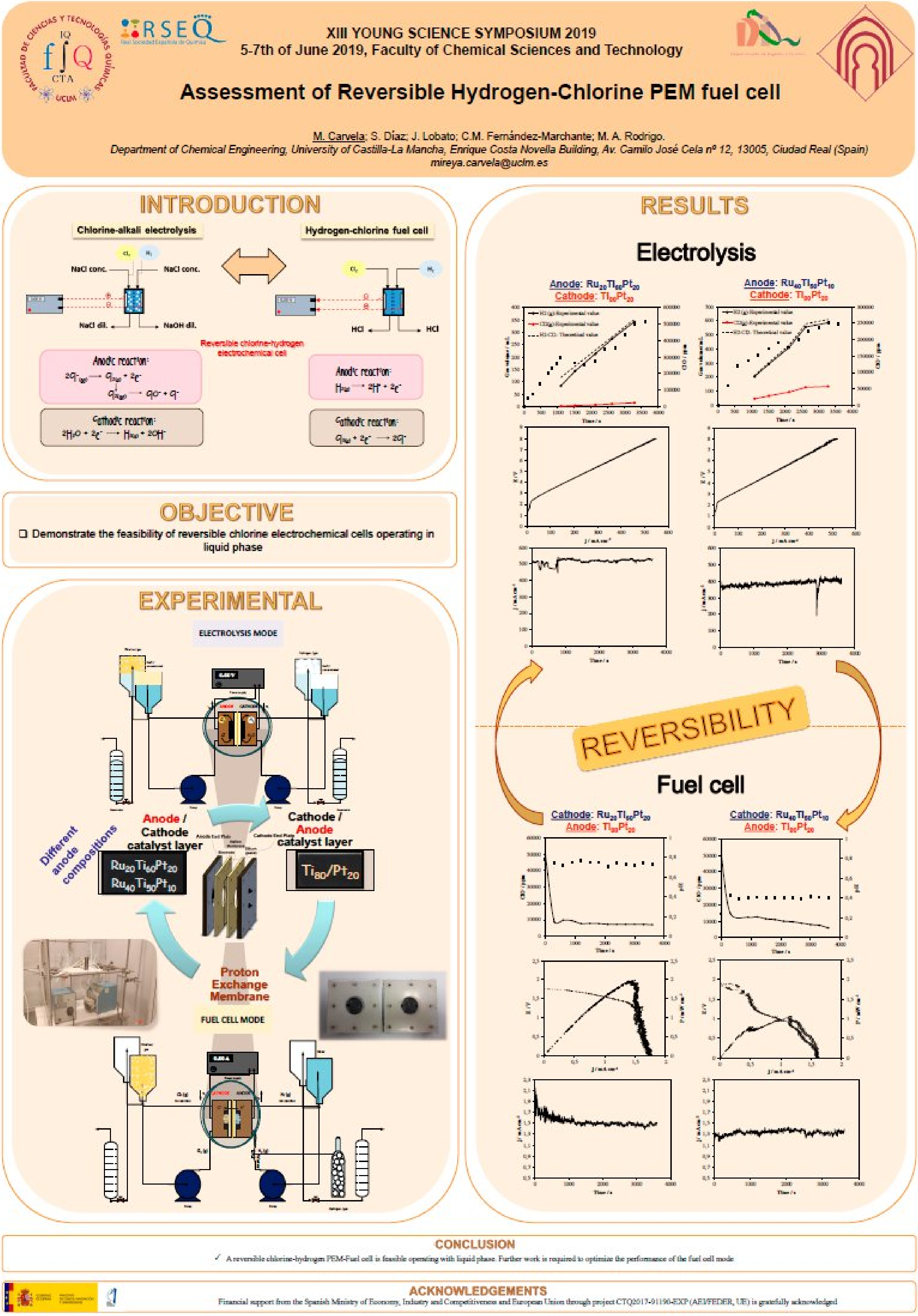


Fig 2. Bilirubin adsorption assays with different concentrations of amino-modified silica particles in bilirubin PBS solutions of 5 mg/dL. The reduction of bilirubin levels in the solutions over time were analysed by UV-visible spectroscopy, using the λmax of bilirubin (450 nm).

CONCLUSIONS

- A sufficient amount of amino-modified nanosilica particles were successfully synthesised for bilirubin adsorption assays.
- A slight reduction of bilirubin is observed at 3 hours, especially when using 150 mg/dL of particles.
- It is necessary to recover the particles from the solutions and analyse their composition by techniques like FTIR or TGA to confirm that the reduction in bilirubin levels is due to its interaction with silica particles.



XIII YOUNG SCIENCE SYMPOSIUM 2019
5-7th of June 2019, Faculty of Chemical Sciences and Technology

Assessment of Reversible Hydrogen-Chlorine PEM fuel cell

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INTRODUCTION

Chlorine-alkali electrolysis

Hydrogen-chlorine fuel cell

Reversible chlorine-hydrogen electrochemical cell

Anodic reaction:
$2Cl^-_{(aq)} \rightarrow Cl_{2(aq)} + 2e^-$
$Cl_{2(aq)} \rightarrow ClO^- + Cl^-$

Cathodic reaction:
$2H_2O + 2e^- \rightarrow H_{2(g)} + 2OH^-$

Anodic reaction:
$H_{2(g)} \rightarrow 2H^+ + 2e^-$

Cathodic reaction:
$Cl_{2(g)} + 2e^- \rightarrow 2Cl^-$

OBJECTIVE

☐ Demonstrate the feasibility of reversible chlorine electrochemical cells operating in liquid phase

EXPERIMENTAL

ELECTROLYSIS MODE

Anode / **Cathode catalyst layer**

Cathode / **Anode catalyst layer**

Different anode compositions

$Ru_{20}Ti_{60}Pt_{20}$
$Ru_{40}Ti_{50}Pt_{10}$

Ti_{80}/Pt_{20}

Proton Exchange Membrane

FUEL CELL MODE

RESULTS

Electrolysis

Anode: $Ru_{20}Ti_{60}Pt_{20}$
Cathode: $Ti_{80}Pt_{20}$

Anode: $Ru_{40}Ti_{50}Pt_{10}$
Cathode: $Ti_{80}Pt_{20}$

REVERSIBILITY

Fuel cell

Cathode: $Ru_{20}Ti_{60}Pt_{20}$
Anode: $Ti_{80}Pt_{20}$

Cathode: $Ru_{40}Ti_{50}Pt_{10}$
Anode: $Ti_{80}Pt_{20}$

CONCLUSION

✓ A reversible chlorine-hydrogen PEM-Fuel cell is feasible operating with liquid phase. Further work is required to optimize the performance of the fuel cell mode

ACKNOWLEDGEMENTS

Financial support from the Spanish Ministry of Economy, Industry and Competitiveness and European Union through project CTQ2017-91190-EXP (AEI/FEDER, UE) is gratefully acknowledged

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

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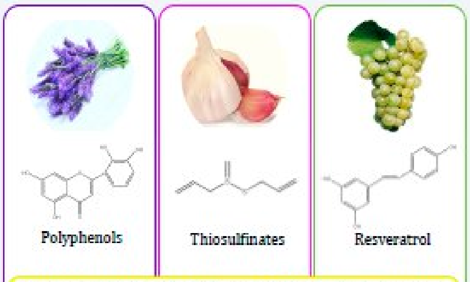
INTRODUCTION

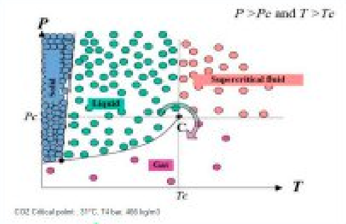
Nowadays, the increase in the demand of nutraceutical and pharmaceutical products of natural origin has led to the search of sources of bioactive compounds.

These compounds can be obtained from raw materials or waste from the agro-industrial sector of Castilla-La Mancha.



ANTIOXIDANT AND ANTI-INFLAMMATORY POTENTIAL FOR TREATMENT OF SKIN DESEASES

SUPERCRITICAL FLUIDS EXTRACTION



$scCO_2$

- ✓ Tc=31°C, Pc=73 atm
- ✓ Easily separable
- ✓ Non-toxic
- ✓ Non-flammable
- ✓ Low cost

AIM OF THE PROJECT

- ✓ Getting natural nutraceuticals and pharmaceuticals product through a **green technology**.
- ✓ Valorization of raw materials allowing the **economic promotion of the** agro-industrial sector.

RESEARCH DEVELOPMENT

Evaluation of the solubility of raw materials in supercritical CO_2 → Extraction of valuable compounds → Modification of natural extracts → Determination of antioxidant and anti-iflammatory capacity → Economic review

EXPERIMENTAL SETUP

SOLUBILITY TEST → High pressure view cell

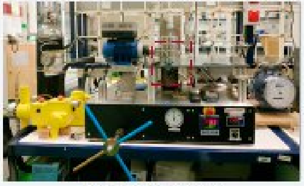


Figure 1. Experimental setup

MATERIALS AND METHODS

RAW MATERIALS

- Lavender essential oil
- Garlic oil
- Waste flows from wine

OPERATION CONDITIONS

- Pressure: 100-300 bar
- Temperature: 40-80 °C
- Contact time: 6-72 h

RESULTS

- ✓ After depressurization the solubility is calculated with the following equation:

$$Solubility = \left(\frac{kg\ lavender\ essential\ oil}{mCO_2\ in\ equilibrium}\right)$$

- ✓ The vapour phase was correlated using the semiempirical model of Chrastil:

$$\ln S = C_1 + \frac{C_2}{T} + C_3 \cdot \ln \rho$$

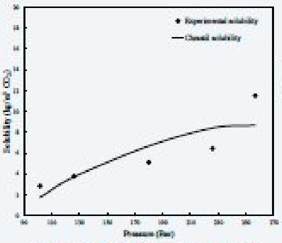


Figure 2. Influence of pressure in solubility of lavender essential oil in supercritical CO_2 (T=40 °C, contact time= 48 h)

Table 1. Optimised C_1, C_2 y C_3 values of carbon dioxide and essential lavender oil T=40 °C

C_1	C_2	C_3
-32,32	-0,004	5,091

↑ Pressure
↑ Solubility

CONCLUSIONS

- ☐ The use of $scCO_2$ avoids the handling of traditional organic solvents which are highly toxic and harmful to the environment.
- ☐ The samples obtained in liquid and vapor phases have to be analyzed by chromatography in order to determine the extracted compounds.
- ☐ An increase in pressure involves an increase in solubility of lavender oil in $scCO_2$.
- ☐ In Chrastil's equation, C_2 can be depreciated because, in this case, the experiments were carried out at isothermal conditions.

ACKNOWLEDGEMENTS

XII YOUNG SCIENCE SYMPOSIUM 2019
Castilla-La Mancha

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GLYCOLYSIS PROCESS FOR POLYURETHANE WASTE RECYCLING

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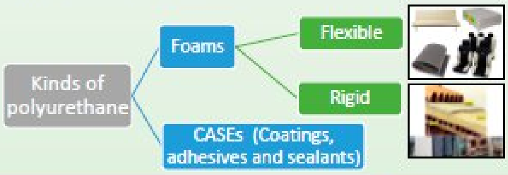
XIII YOUNG SCIENCE SYMPOSIUM 2019

INTRODUCTION

Polyurethanes (PUs) are generally thermostable polymers resulting from a series of additions between a multifunctional alcohol (polyol) and an isocyanate, resulting in a cross-linked structure. The characteristic functional group obtained by nucleophilic addition of the oxygen of the polyalcohol to the carbon of the cyano group is urethane.

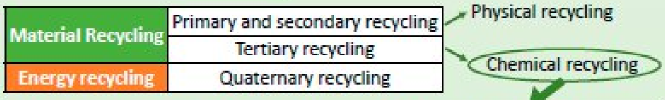
$$\underset{Polyol}{n\ HO\text{-}R\text{-}OH} + \underset{Isocyanate}{n\ O{=}C{=}N\text{-}R'\text{-}N{=}C{=}O} \rightarrow \underset{Urethane}{[\ \text{-}CO\text{-}NH\text{-}R'\text{-}NH\text{-}CO\text{-}O\text{-}R\text{-}O\text{-}\ ]_n}$$



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

POLYURETHANE WASTE RECYCLING

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



Material Recycling	Primary and secondary recycling
	Tertiary recycling
Energy recycling	Quaternary recycling

- *Hydrolysis* $\underset{Urethane}{\Phi\text{-}NH\text{-}CO\text{-}O\text{-}R'} + \underset{Water}{H_2O} \longrightarrow \underset{Amine}{\Phi\text{-}NH2} + CO_2 + \underset{Polyol}{HO\text{-}R'}$
- *Amynolysis* $\underset{Urethane}{\Phi\text{-}NH\text{-}CO\text{-}O\text{-}R'} + \underset{Amine}{NH_2\text{-}R''} \longrightarrow \underset{Urea}{\Phi\text{-}NH\text{-}CO\text{-}NH\text{-}R''} + \underset{Polyol}{HO\text{-}R'}$
- *Phosphorolysis*
- *Glycolysis* $\underset{Urethane}{\Phi\text{-}NH\text{-}CO\text{-}O\text{-}R'} + \underset{Glycol}{OH\text{-}R''\text{-}OH} \longrightarrow \underset{Carbamate}{\Phi\text{-}NH\text{-}CO\text{-}O\text{-}R''\text{-}OH} + \underset{Polyol}{HO\text{-}R'}$

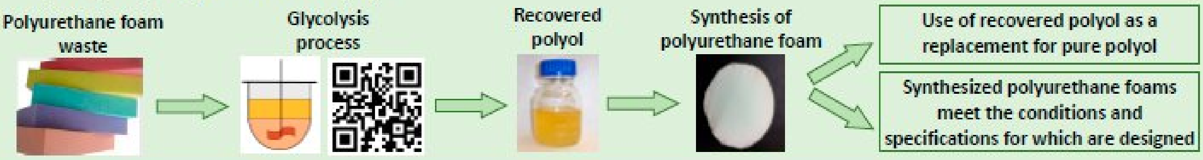
GLYCOLYSIS PROCESS

Glycolysis is the most widely used chemical recycling process for PUs and it is applied to elastomers, coatings, rigid foams, flexible foams and PU RIM (injection molding foams with reinforced reaction). In addition, with an excess of glycol in the reaction a biphasic product is obtained, where the upper phase is formed mainly by the recovered polyol and the bottom phase by the excess of glycolysis agent and by-products of the reaction; improving the quality of the recovered polyol.

Reaction conditions

- Temperature = 193 °C
- N = 300 rpm
- Catalyst concentration in the glycolysis agent = 1.3 – 2.0 %
- Mass ratio of glycolysis agent to PU foam = 1.5:1

Experimental unit



Use of recovered polyol as a replacement for pure polyol

Synthesized polyurethane foams meet the conditions and specifications for which are designed

CONCLUSIONS

One of the main advantages is the recovery of the raw materials (polyol) for the synthesis of new PUs foams, avoiding their deposit in landfills. In addition to the environmental benefits, it is worth highlighting the economic benefit. Previous studies have demonstrated that the glycolysis can be a profitable process, especially when it is carried out with crude glycerol as glycolysis agent since from two wastes, an added value product is obtained.

ACKNOWLEDGMENT

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EFFECT OF PROCESS PARAMETERS IN A SO_2 DEPOLARIZED ELECTROLYSIS CELL

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INTRODUCTION

Production of Hydrogen from alternative ways to carbon-based processes is one of the main concerns of researchers. Direct water electrolysis is the most obvious way to produce it. Unfortunately, high energy consumption is needed. So, new processes are being developed. Among them, the Westing-House cycle is of interest because of the low energy needed (equations 3 and 4).

$$2\,H_2O\,(g) \rightarrow O_2(g) + 4H^+ + 4\,e^- \quad (1)$$
$$4H^+ + 4\,e^- \rightarrow 2\,H_2\,(g) \quad (2)$$
$$E^0_{Cell} = 1.23\ V\ vs\ RHE$$

$$SO_2\,(g) + 2\,H_2O\,(g) \rightarrow H_2SO_4(aq) + 2H^+ + 2\,e^- \quad (3)$$
$$2H^+ + 2\,e^- \rightarrow H_2\,(g) \quad (4)$$
$$E^0_{Cell} = 0.16\ V\ vs\ RHE$$

For a high overall process efficiency, working temperatures in the electrolyzer above 100 °C are suggested. PBI based membranes are a promising material for working at those conditions because they do not need to be humidified as Nafion.

EXPERIMENTAL

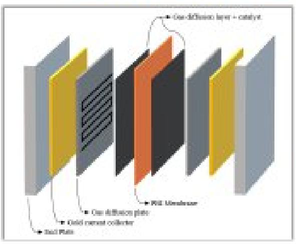


Figure 1. Electrolyzer scheme

25 cm² electrolyzer

Catalyst loading: **0.7 mgPt/cm²**

PBI acid doping level (H_3PO_4):
~11 mol H_3PO_4/mol PBI

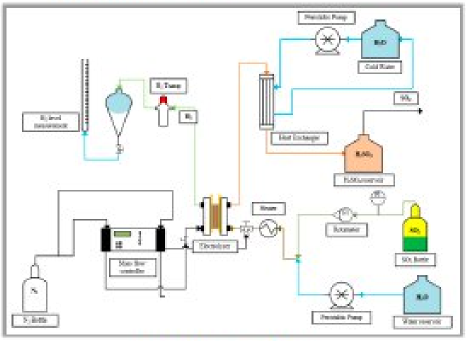


Figure 2. Experimental Set-Up

SO_2 and steam generated in a heater are introduced both in the gas phase into the anode side of the electrolyzer. The anode products are condensed and H_2SO_4 is collected in a recipient. H_2 level is measured in the cathode outlet with a water displacement column.

RESULTS

EFFECT OF SO_2 FLOW

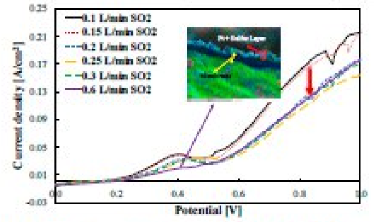


Figure 3. Polarization curves performed with different SO_2 flows. Voltage range: 0V – 1V; Scan rate: 10 mV s⁻¹. Temperature: 120 °C

- **Increasing SO_2 does not increase electrolyzer performance.**
- **Better performance at low SO_2 flows (0.1 – 0.15 L/min) under our operation conditions.**
- **Higher flow imply higher SO_2 crossover through the PBI membrane which causes sulfur layer formation.**

EFFECT OF TEMPERATURE

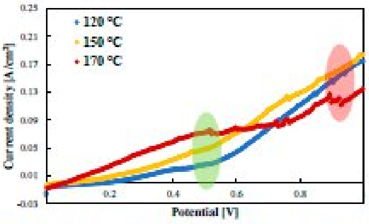
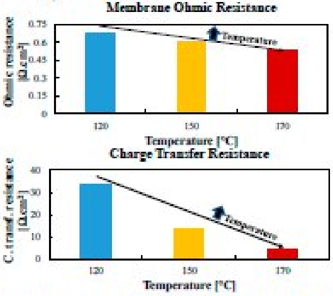


Figure 4. Polarization curves performed at different temperatures. Voltage range: 0V – 1V; Scan rate: 10 mV s⁻¹. SO_2 flow: 0.6L/min; H_2O flow: 0.9 mL/min

- **Higher current densities when increasing temperatures at low potentials**
- **Performance decrease for voltages above 0.6 V at temperatures higher than 150 °C**



- **Slight ohmic resistance decrease with temperature as expected.**
- **Considerable charge transfer resistance decrease with temperature. Reactions kinetics highly favoured when increasing temperature.**

Figure 5. Ohmic resistance and charge transfer resistance. Applied Voltage: 0.15 V; Amplitude: 15 mV; Frequency range: 0.1 - 10 kHz. SO_2 flow: 0.6L/min; H_2O flow: 0.9 mL/min

CONCLUSIONS

- **For this set-up, a SO_2 flow higher than 0.15 L/min is not benefitial for the system due to larger SO_2 crossover.**
- **For potentials lower than 0.6 V, increasing temperature allows to reach higher current densities.**
- **Increasing electrolyzer temperature decreases both ohmic and charge transfer resistance.**

Acknownledgements

Financial support from the Junta de Comunidades de Castilla-La Mancha and the FEDER –EU Program, Project ASEPHAM. Grant number "SBPLY/17/180501/000330" is gratefully acknowledged.

BIODIESEL PRODUCTION FROM WASTE OIL USING Fe/CaO AS BIFUNTCTIONAL CATALYST

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ABSTRACT

The aim of this study was to analyze the catalytic performance of Fe/CaO as bifunctional catalyst in the transesterification reaction using frying oil with methanol. Quicklime was used as a source of calcium oxide and three chemical precursors of iron (III) were studied (Fe_2O_3, $FeCl_3$ and $Fe(NO_3)_3{*}9H_2O$). Heterogeneous catalysts Fe/CaO were synthesized using impregnation method; followed by calcination at 800°C. The catalysts were characterized by: X-ray diffraction (XRD), thermal gravimetric analysis (TGA), nitrogen adsorption/desorption (BET). The produced biodiesel has 91% of fatty acid methyl esters (FAMEs) content under optimum reaction parameters; atmospheric pressure, reaction temperature of 60 °C, 12:1 methanol:oil ratio, catalyst amount of 5wt%, 10wt% of Fe and 3 h of reaction.

1. INTRODUCTION

Bifunctional heterogeneous catalysis is a novel trend that allows the transformation of waste oils into biodiesel in a one-step process [1]. It has been estimated that the use of this type of catalysts can reduce production costs derived from raw materials (refined oil) by up to 80%, additionally, eliminates separation processes with severe environmental effects and simplifies the process operations [2]. Essentially, a bifunctional catalyst is a material that contains in the same catalytic surface; acid sites to esterify free fatty acids and basic sites to transesterify triglycerides. In this work, a bifunctional catalyst of iron (III) supported in calcium oxide (CaO) was synthesized for the production of biodiesel from used frying oil with high content of free fatty acids.

2. EXPERIMENTAL

2.1 Characterization of used frying oil
2.2 Synthesis and characterization of Fe/CaO
Chemical precursors of iron (III): Fe_2O_3, $FeCl_3$ and $Fe(NO_3)_3{*}9H_2O$
2.3 Bifunctional heterogeneous catalytic evaluation
2.4 Optimization of reaction conditions
2.5 Characterization of biodiesel

3. RESULTS

3.1 Characterization of used frying oil

Acid value	Density at (15°C)	Kinematic viscosity at
1.53 mgKOH/g	926.021 kg/m^3	(40°C) 36.08 mm^2/s

3.2 Catalyst characterization

- *X-Ray Diffraction (XRD)*

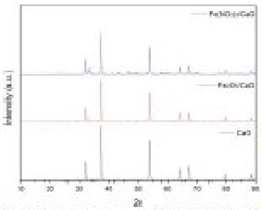


FIG 1. The XRD patterns of CaO, Fe_2O_3/CaO and $Fe(NO_3)_3$/CaO

- *Thermal Gravimetric Analysis (TGA)*

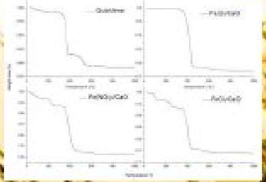


FIG 2. TGA analysis of Quicklime, Fe_2O_3/CaO, $Fe(NO_3)_3$/CaO and $FeCl_3$/CaO catalysts

- *Brunauer-Emmett-Teller method (BET)*

Catalysts	Surface area (m^2/g)	Pore volume (cc/g)
CaO	7.995	0.0683
Fe_2O_3/CaO	12.150	0.0754
$Fe(NO_3)_3$/CaO	6.714	0.0267

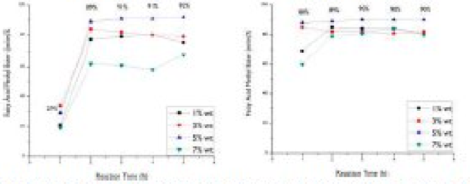
3.3 Conversion of used frying oil

- *Effect of percentage of iron (III)*

A) Fe_2O_3/CaO *B) $FeCl_3$/CaO* *C) $Fe(NO_3)_3$/CaO*

FIG 3. Influence of percentage of iron (III), reaction conditions: oil to methanol ratio 1:12, temperature 60°C

- *Effect of catalyst loading*



A) Fe_2O_3/CaO *B) $Fe(NO_3)_3$/CaO*

FIG 4. Effect of catalyst loading, reaction conditions: oil to methanol ratio 1:12, temperature 60°C, 10wt% Fe.

3.4 Biodiesel characterization

%FAMEs	Density at (15°C)	Kinematic viscosity at
91%	879.28 kg/m^3	(40°C) 4.6 mm^2/s

4. CONCLUSIONS

- Fe_2O_3/CaO catalyst has better performance with a high yield of methyl esters (91 % w/w).
- The best conditions were: 10 wt% of iron, alcohol: oil ratio 12:1, 5wt% of Fe_2O_3/CaO, reaction time= 3 hours and reaction temperature= 60 °C.

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[2] J. Gardy *et al.*, "A magnetically separable SO4/Fe-Al-TiO2solid acid catalyst for biodiesel production from waste cooking oil," *Appl. Catal. B Environ.*, vol. 234, no. 2010, pp. 268–278, 2018.

Acknowledgments

The authors are grateful for the help provided with the catalyst characterization to Dr. Uvaldo Hernández Balderas from Centro Conjunto de Investigación en Química Sustentable UAEM-UNAM. The financial support of Universidad Autónoma del Estado de México through Project 4754/2019 CIB is also acknowledged. V.E.G. wishes to thank Consejo Nacional de Ciencia y Tecnología (CONACYT) for scholarship No. 861011 to conduct postgraduate studies.

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

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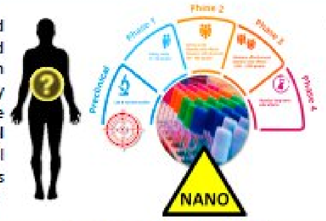
INTRODUCTION

Platinum nanoparticles (PtNPs) are being applied in clinical and biomedical domains nowadays due to their physicochemical and antibacterial properties [1]. However, the use of PtNPs has been accompanied by a growing concern about their potential toxicity on human health. In order to have an adequate control of these applications it is necessary the study of PtNPs in **complex clinical matrices**. These studies are challenging for current analytical methods and there are still important open questions that starts even from the **stability** of metallic NPs in the presence of biofluids.



OBJECTIVE

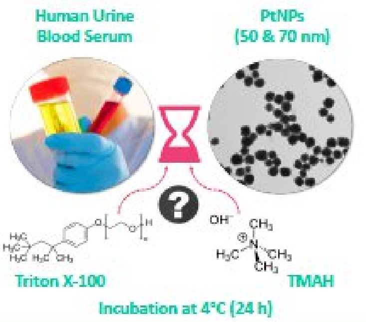
To evaluate the effect of several preservatives (tetramethylammonium (TMAH) and Triton X-100) to stabilize PtNPs in biofluids.

To test different concentrations of the most suitable preservative.

To achieve a correct characterization of various PtNPs sizes by Single Particle ICP-MS.

MATERIAL & METHODS

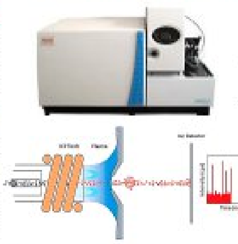
EXPERIMENTAL DESIGN

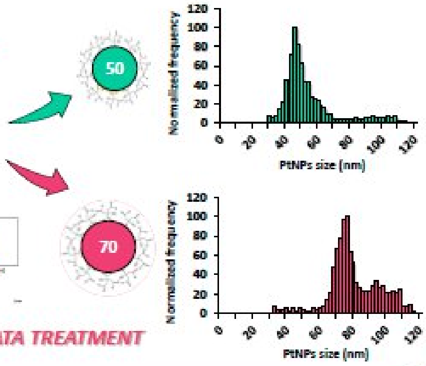


SP-ICP-MS optimized method

Instrument parameter	
RF-power	1400 W
Nebulizer	Meinhard
Gas flows	
Plasma gas	13 L min^{-1}
Nebulizer gas	0.9 L min^{-1}
Auxiliary gas	0.8 L min^{-1}
Data acquisition	Time Resolved Analysis
Ion monitoring	^{195}Pt
Spray chamber	Scott type
Cones	Sampler & Skimmer - Ni
Sample flow rate	0.8 mL min^{-1}
Transport Efficiency	2.0 %
Dwell Time	5 ms
Acquisition Time	60 s

Quadrupole ICP-MS X-Series®



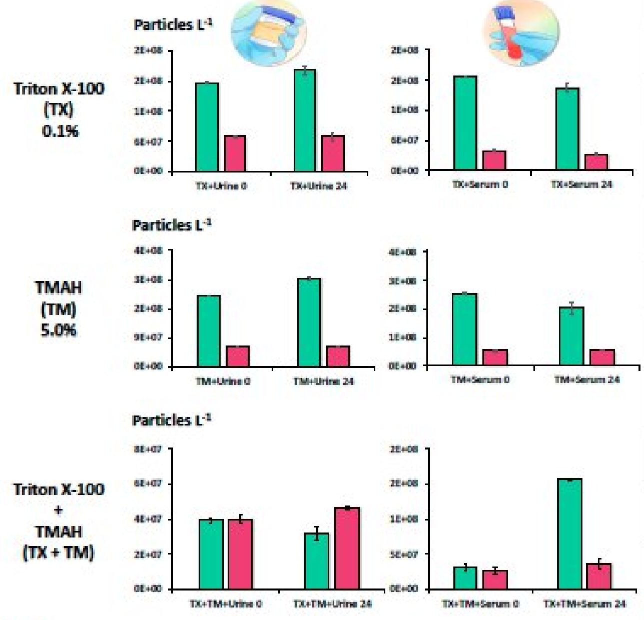


SINGLE PARTICLE ICP-MS ANALYSIS & DATA TREATMENT

RESULTS & DISCUSSION

1 COMPARISON OF PRESERVATIVES

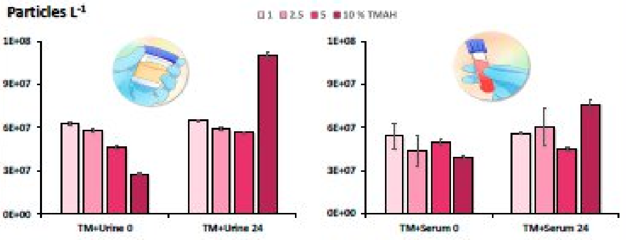
🟩 50 nm Nominal value (particles L^{-1}): 1.83E+08 🟥 70 nm Nominal value (particles L^{-1}): 6.92E+07



TMAH is the most suitable preservative to stabilize PtNPs in clinical matrices.

STUDY OF TMAH CONCENTRATIONS 2

Nominal value (particles L^{-1}): 6.92E+07 🟥 70 nm

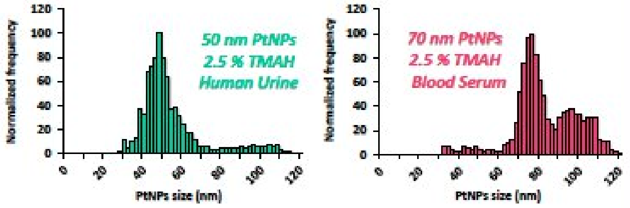


1.0 – 2.5 % TMAH

1.0 – 2.5 % TMAH

Results observed in particle mass concentration (ng L^{-1}) also confirm these TMAH intervals.

Particle size distribution (nm) at 24 h



24 h of incubation does not seem to induce a change in PtNPs sizes for both matrices.

CONCLUSIONS

TMAH concentrations up to 2.5 % are acceptable to stabilize complex clinical matrices.
Further studies will be useful to assess toxicological effects over time.

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Universidad de
Castilla-La Mancha

POLYMERIC NANOPARTICLES FOR CONTROLLED DASATINIB DELIVERY IN BREAST CANCER THERAPY

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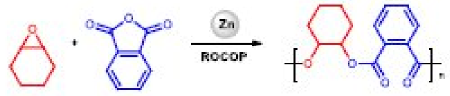
Email: *Erika.Garcia1@alu.uclm.es*

1. Introduction

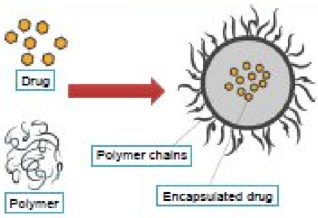
Dasatinib (DAS) is an inhibitor of several oncogenic kinases and the PDGFβ receptor. This mechanism of action makes it a great candidate for the treatment of breast cancer, but presents serious problems of solubility and primary metabolization by oral route.[1] In order to avoid these problems, in this work, we have carried out the encapsulation of DAS in poly(cyclohexene phthalate) (CHOPA) nanoparticles. Cytotoxicity and flow cytometry studies of the nanoparticles and the non-encapsulated drug in triple negative breast cancer cell lines were performed. The results showed a greater cytotoxic effect of the nanoparticles compared to the free drug.

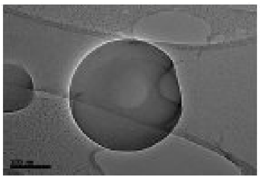
2. Synthesis of Polymeric Nanoparticles

Synthesis of CHOPA copolymer



Synthesis of nanoparticles by nanoprecipitation and evaporation solvent method



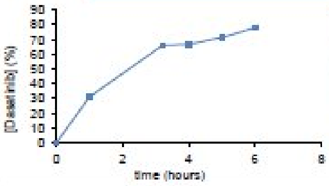


DLS measurements and Z Potential

Size	PDI	Z potential
134.7	0.267	25.1
130.4	0.390	28.9
145.6	0.353	31.8
131.5	0.345	30.7

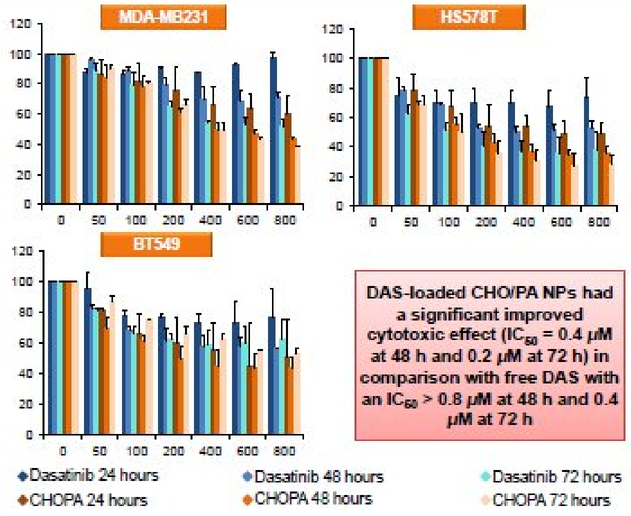
3. *In vitro* release profile at pH 7.4

Encapsulation Efficiency (%)	Loading Capacity (%)
97.7	15.5



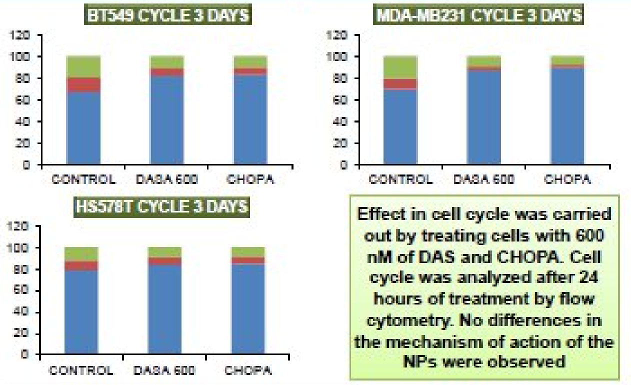
DAS release kinetics followed an exponential profile with a negligible burst and a sustained delivery over 6 hours for DAS-loaded CHOPA NPs at pH 7.4

4. Antiproliferative Studies *in Vitro*



DAS-loaded CHO/PA NPs had a significant improved cytotoxic effect (IC_{50} = 0.4 μM at 48 h and 0.2 μM at 72 h) in comparison with free DAS with an IC_{50} > 0.8 μM at 48 h and 0.4 μM at 72 h

5. Cell Cycle Arrest



Effect in cell cycle was carried out by treating cells with 600 nM of DAS and CHOPA. Cell cycle was analyzed after 24 hours of treatment by flow cytometry. No differences in the mechanism of action of the NPs were observed

6. Conclusions

A simple biodegradable and blood compatible copolymer has been developed as an alternative to FDA-approved polyesters for the generation of delivery nano-devices of DAS in breast cancer therapy. In vitro cytotoxicity in different breast tumor cell models demonstrated the superior efficacy of the NPs when comparable to free DAS.

7. References

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MECHANOCHEMISTRY IN THE SYNTHESIS OF NANOMATERIALS

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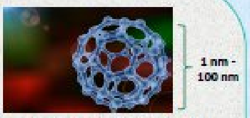
INTRODUCTION

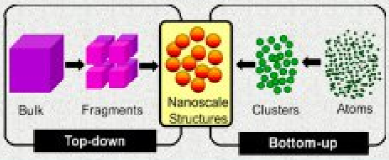
Nanomaterials:

Engineered particles with improved physical, chemical and biological properties.



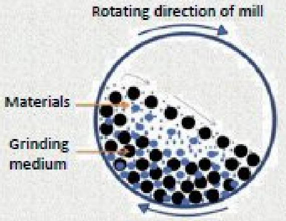
Nano-Zirconia (ZrO_2): Outstanding chemical stability, high strength and toughness, wear resistance, flexibility, good refractory properties and ionic conductivity.

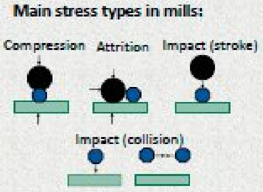
A typical classification of nanomaterials synthesis methods:



Mechano-chemical process:

Chemical and physico-chemical changes of substances due to the influence of mechanical energy.

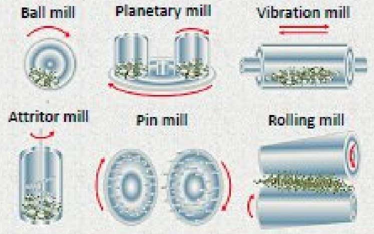




The less expensive, most simple and powerful way to produce nanoparticles at industrial scale.

The properties of the nanomaterial obtained in a milling process and its subsequent heat treatment are function of several **parameters**:

➡ Type of the Mill



➡ Milling Media Material

Agate, Nylon, PTFE, PU, Zirconia, Stainless Steel

➡ **Ball to powder ratio**

Weight ratio of the milling balls to the powder charge

➡ **Milling time**

➡ Milling operating conditions (temperature, pressure and frequency)

➡ **Subsequent calcination temperature**

RESULTS

"The ball milling induced transformation of α-Fe2O3 powder in air and oxygen atmosphere" by M.Zdujić et al.

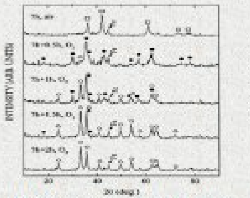


Fig 1. XDR patterns of powders pre-milled for 7 h in air and subsequently milled in oxygen at different times, (○) α-Fe_2O_3; (●) Fe_3O_4; (□) $Fe_{1-x}O$ (BPMR=40).

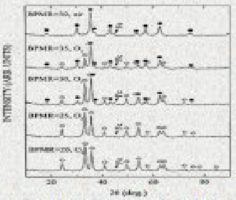


Fig 2. XDR patterns of powders milled for 5 h with various balls-to-powder mass ratio (BPMR), (○) α-Fe_2O_3; (●) Fe_3O_4.

"Effect of ball milling time on the thermoelectric properties of p-type (Bi, Sb)$_2$ Te$_3$" by J. H. Son et al.

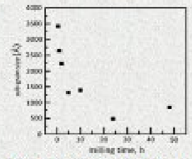


Fig 3. Estimated grain size of the p-type (Bi, Sb)$_2$Te$_3$ samples obtained in the milling process with Williamson–Hall equation.

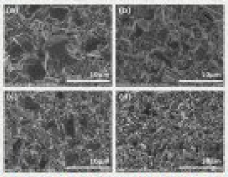
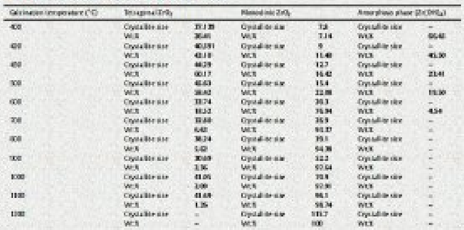


Fig 4. SEM images of fractured Surface of the bulk (Bi, Sb)$_2$Te$_3$ samples obtained from ball-milled powders from (a)0.5 h, (b) 5 h, (c) 10 h and (d) 48 h milling time.

"Mechanochemical synthesis of zirconia nanoparticles: Formation mechanism and phase transformation" by T. Dallali et al.

Table 1. Crystallite size and weight percent of the obtained zirconium hydroxide samples calcined at different temperatures for the corresponding phases.



These results are providing new ideas to produce nanomaterials, which have not been extensively considered so far.

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13th YOUNG SCIENCE SYMPOSIUM 2019

Gas-phase reactivity of acetone towards OH radicals at interstellar temperatures (11.7-64.4 K). Astrophysical Implications

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María Antiñolo,[2] José Albaladejo,[1,2] Elena Jiménez[1,2,(*)]

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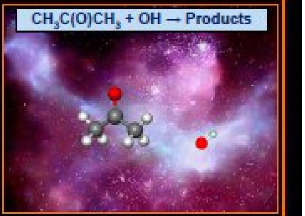
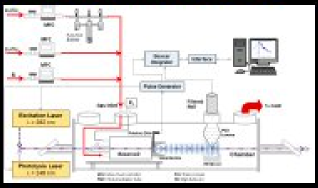
1. INTRODUCTION

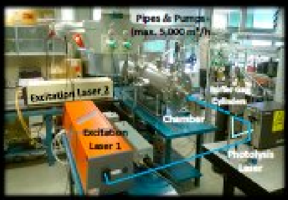
Acetone ($CH_3C(O)CH_3$) was detected for the first time in 1987 by Combes *et al.*[1] in the cold dense molecular cloud Sagittarius B2. More recently, its detection was confirmed by Snyder *et al.*[2] and acetone has been found in many other environments of the interstellar medium, such as Orion-KL hot core,[3] or Murchison meteorite.[4] **Hydroxyl radical (OH)** was detected for the first time in 1963 by Weinreb *et al.*[5] in Cassiopeia A, and later, in many other sources, such as Sagittarius B2.[6]

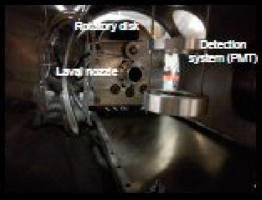
The purpose of our work is to determine **for the first time** the temperature dependence of the rate coefficient for the gas phase reactions of OH radicals with $CH_3C(O)CH_3$ at **very low temperatures**, between 11.7 and 64.4 K, and their potential pressure dependence at temperatures around 22, 50 and 64 K.



2. EXPERIMENTAL SET-UP

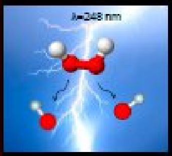






The **CRESU** (French acronym for *Cinétique de Réaction en Ecoulement Supersonique Uniforme* or *Reaction Kinetics in a Uniform Supersonic Flow*) technique was used to create a gas jet with a uniform temperature and gas density and the **pulsed laser photolysis/laser induced fluorescence** (PLP-LIF) technique was used to generate OH radicals and to monitor their temporal profile. The heart of the technique is the Laval Nozzle at the exit of which a uniform flow is formed.

3. THE PLP – LIF TECHNIQUE



For carrying out the kinetic experiment of the reaction, firstly the OH radicals have to be generated in situ. In this work, the **PLP** of **gaseous H_2O_2** at 248 nm was the **source of OH radicals**.

The **LIF from excited OH radicals** was detected at ca. 310 nm by a photomultiplier tube as a function of reaction time.

4. KINETICS OF THE $CH_3C(O)CH_3$ + OH REACTION

$$(I - I_{bck}) = (I_0 - I_{bck})e^{-k't}$$

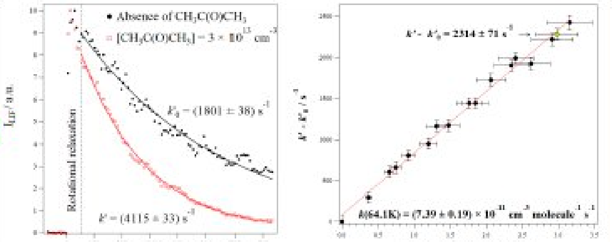
$$\ln(I - I_{bck}) = \ln(I_0 - I_{bck}) - k't$$

$OH + CH_3C(O)CH_3 \rightarrow Prod.\ k(T)$ $\quad k'$

$OH + H_2O_2 \rightarrow Prod. \quad k_{prec}$ $\quad k'_0$

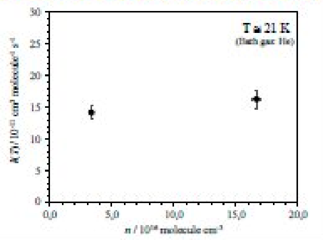
$OH \rightarrow$ Other losses $\quad k_{diff}$

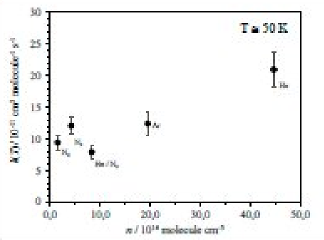
$$k' - k'_0 = k(T)\ [CH_3C(O)CH_3]$$

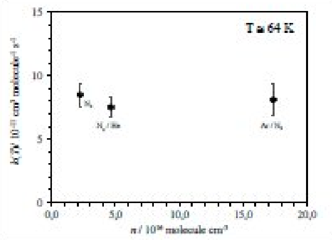


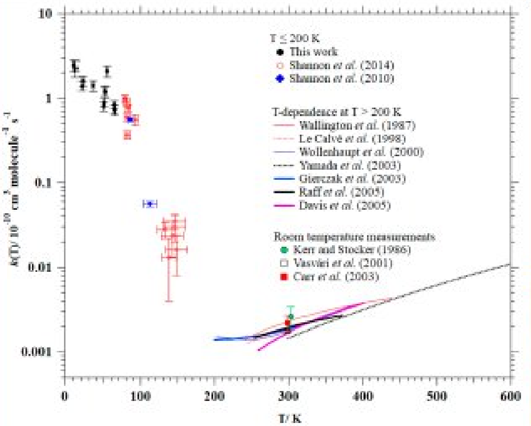
5. TEMPERATURE AND PRESSURE DEPENDENCE OF *k*(T)

T(K)	*k*(T) (10^{-11} cm³ molecule⁻¹ s⁻¹)
11.7 ± 0.7	24.5 ± 1.7
13.0 ± 0.7	22.7 ± 2.3
21.1 ± 0.6	13.9 ± 0.5
21.7 ± 1.4	16.1 ± 0.6
36.2 ± 1.2	14.1 ± 0.7
50.5 ± 1.6	9.01 ± 0.25
51.6 ± 1.7	12.1 ± 0.4
49.9 ± 1.4	8.04 ± 0.33
52.1 ± 0.5	11.8 ± 0.8
54.2 ± 0.5	20.9 ± 1.3
64.2 ± 1.7	8.44 ± 0.21
64.1 ± 1.6	7.39 ± 0.19
64.4 ± 0.6	7.27 ± 0.40









6. CONCLUSIONS AND ASTROPHYSICAL IMPACT

The rate coefficients obtained in this work at temperatures around 22 K and 64 K reveal no pressure dependence between 3.37×10^{16} and 16.7×10^{16} cm^{-3}, and between 2.24×10^{16} and 17.4×10^{16} cm^{-3} respectively, or bath gas dependence. At around 50 K, the rate coefficient at the largest density of 4.47×10^{17} cm^{-3}, is twice higher than the average values below that gas density, revealing a potential weak pressure dependence. This is somewhat surprising however because one would have expected finding a pressure dependence at 64 K as well since this has been observed by Shannon *et al.*[7] In the explored temperature range the experimental rate coefficient increases when decreasing temperature thus extending the trend observed by Shannon *et al.*[5] at temperatures higher than 79 K.

This new experimental data at ultra-low temperature for this reaction could be added to astrophysical databases, so it will help to improve the existing models to make them closer to the real reactivity in the ISM.

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ACKNOWLEDGMENTS

All authors from UCLM wish to thank ERC Project (NANOCOSMOS) for supporting this work.

Mechanochemical synthesis of "Sweet Green Graphene" Part II

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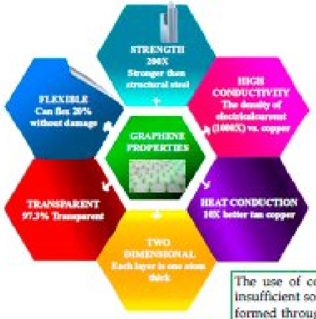
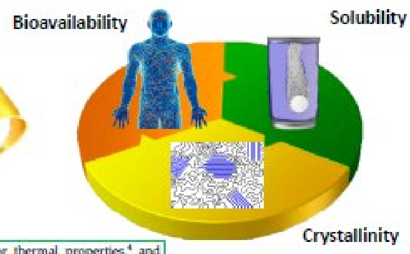
INTRODUCTION

Can we obtain Graphene Cocrystals?

Graphene

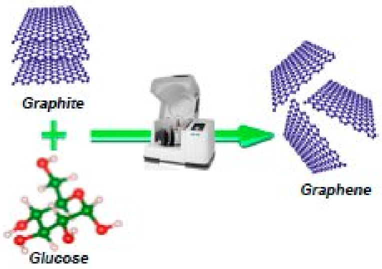


Cocrystals

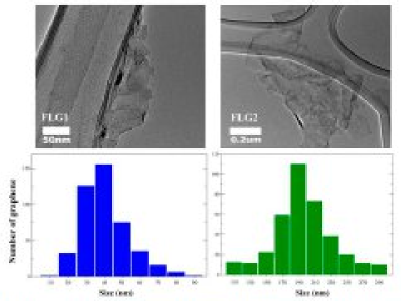


The use of cocrystals have solved problems in biology and chemistry,[1] including poor stability,[2] compressibility,[3] poor thermal properties,[4] and insufficient solubility.[5] Cocrystals are supramolecular structures of, at least, two neutral organic molecules via intermolecular interactions. These can be formed through mechanochemically treatments.[6] Mechanochemistry has also gained increasing importance in diverse fields of chemistry,[7] principally in the exfoliation and functionalization of nanomaterials like graphene.[8] We report the development of an environmentally friendly, cheap and simple approach for the synthesis of aqueous soluble few-layer graphene, useful for biological purposes, in the form of cocrystal with glucose.[9]

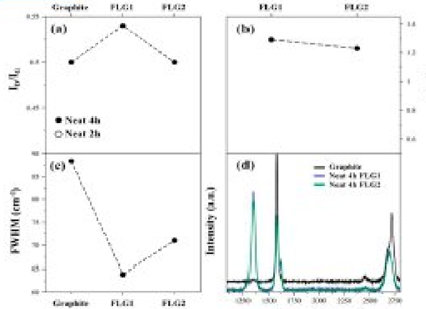
SYNTHESIS OF GRAPHENE



Neat 4 h (75 mg of graphite and 4.5g of glucose and 4 h of ball milling)



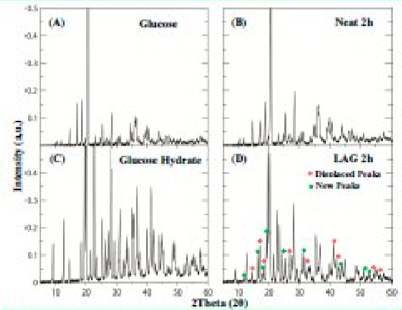
Neat 4 h, two different graphene batches, **FLG1** (50 nm) and **FLG2** (100-300 nm).



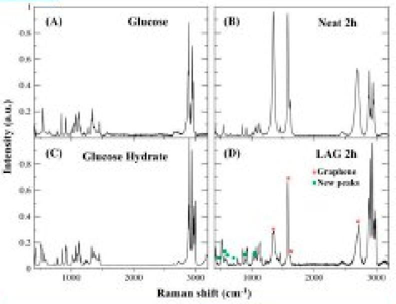
Raman of Neat 4h; (a) relation I_D/I_G and I_{2D}/I_G bands; (b) G and D band position; (c) FWHM of 2d band; and (d) Raman spectra for Graphite, FLG1 and FLG2.

SYNTHESIS OF GRAPHENE COCRYSTAL

Mechanochemical synthesis for graphene cocrystal under **LAG** (liquid assisted gridding) conditions.



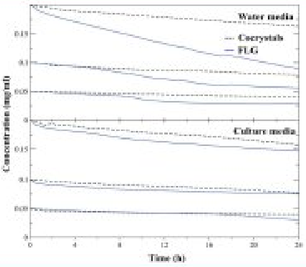
Powder X-Ray diffraction (PXRD) for glucose, glucose hydrate and Neat/LAG sample.



Raman for glucose, glucose hydrate and Neat /LAG conditions.

CONCLUSION

We successfully applied a mechanochemical treatment with carbohydrates to exfoliate graphite in a simple and green approach. The addition of molar equivalents of water to the ball milling treatment allowed the formation of glucose-graphene co-crystals. Analogously to what happens with drugs, glucose-graphene co-crystals display reasonably dispersion in water, with optimal colloidal stability.



Colloidal stability using UV-Vis absorption spectroscopy at 660 nm of Graphene (Neat 4h) and Graphene Cocrystals. We observe a higher stability in aqueous solutions in the Graphene Cocrystal.

THEORETICAL RESULTS

Ab initio studies of
"Sweet Green Graphene"
Part I
Dr. Antonio M. Rodríguez

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Universidad de Castilla-La Mancha

Unusual ligand rearrangement of a *N*-phosphinoguanidinato ligand

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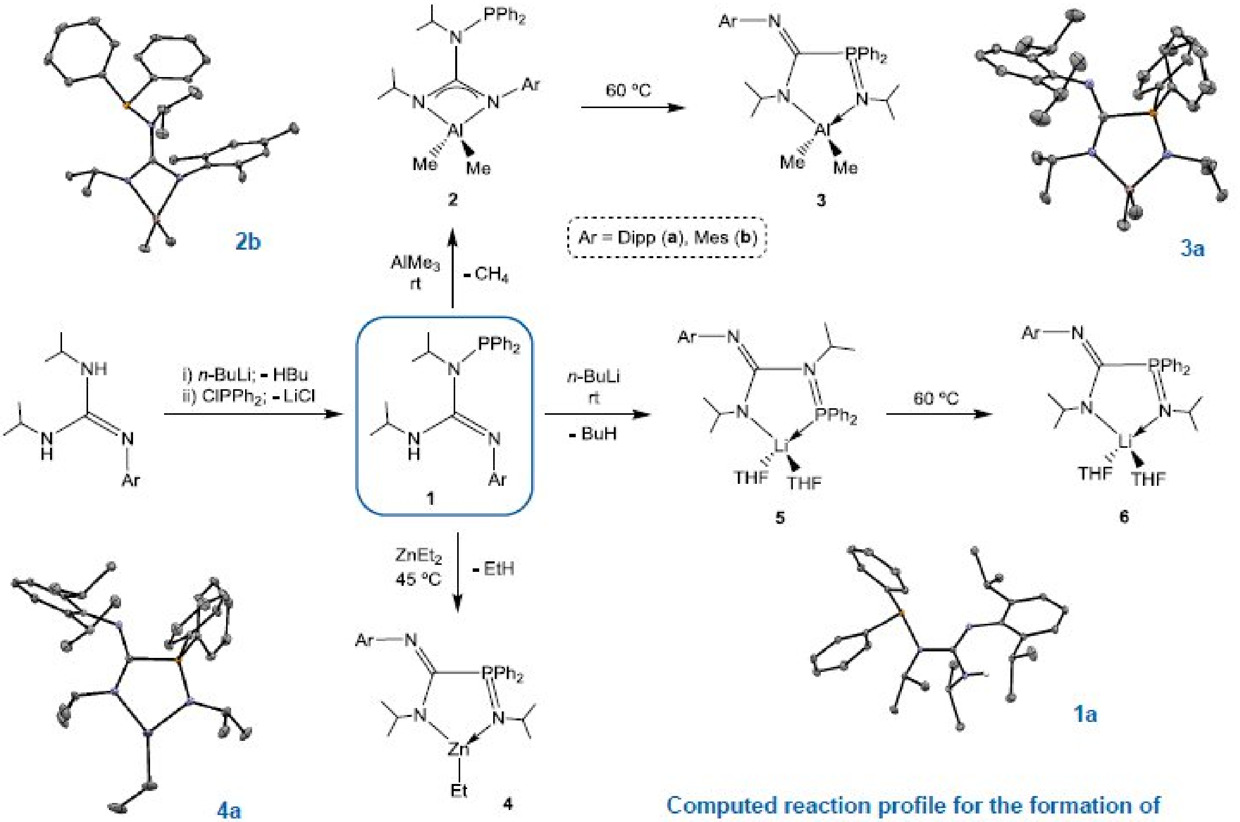
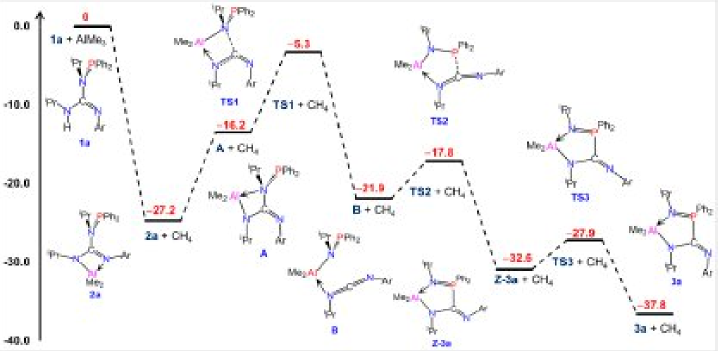
In the last years our group has focused on the development of catalytic methods to prepare guanidines and the coordination chemistry of guanidinato ligands with transition metals and main group elements.[1] As an extension of this work and encouraged by the lack of examples of anionic *N*-phosphinoguanidinato compounds, we aimed to prepare novel *N*-phosphinoguanidines from available trisubstituted guanidines to study their coordination chemistry through protonolysis reactions with different metal alkyls. Here we report the synthesis of *N*-phosphinoguanidines (**1**) and their reactivity towards metal alkyls.[2]



Unexpectedly, the reactions of **1** with metal alkyls lead to the formation of stable phosphinimine-amidinato compounds, after an unprecedented rearrangement under mild conditions of the initially formed *N*-phosphinoguanidinato intermediate.

We proposed a mechanism for this transformation in the reaction of **1a** with $AlMe_3$, supported by DFT calculations, involving cabodiimide de-insertion via a retro-[2,2] cycloaddition followed by a [3+2] dipolar regioselective cycloaddition.

Computed reaction profile for the formation of complex 3a, Gibbs free energies in kcal·mol^{-1}



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

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ABSTRACT

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 rich-sugar biomass, concretely Opuntia Ficus-Indica (OFI), aimed to develop an easy method to obtain 5-HMF and LA selectively from this starting material.

SUGAR EXTRACTION

1st extraction
Solvent: cyclohexane

Cyclohexane-soluble fraction

Cyclohexane extract (1% initial mass). Triacylglycerol fraction. Application in cosmetic or biodiesel synthesis

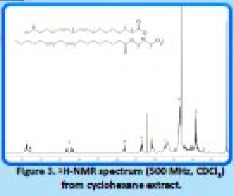


Figure 3. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) from cyclohexane extract.

Starting material

Cyclohexane-insoluble fraction

2nd extraction
Solvent: Ethanol

Ethanol-soluble fraction

Ethanol extract (52% initial mass). Sugar fraction (mainly glucose and fructose). Future transformation into platform chemicals

Ethanol-insoluble fraction

3rd extraction
Solvent: Water

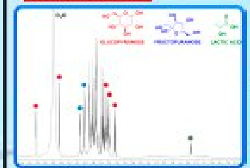


Figure 4. ^{1}H-NMR spectrum (500 MHz, D_2O) from ethanol extract.

Water-soluble fraction

Water extract (25% initial mass) Water-soluble molecules such as pectin or starch

Water-insoluble fraction

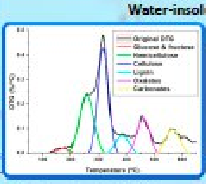
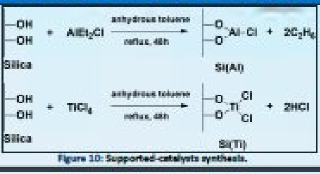


Figure 5. Final residue DTG deconvolution using Origin 9.1.

Final residue (22% initial mass). Insoluble fibres (cellulose, hemicellulose and lignin) and ashes

SUPPORTED-CATALYSTS SYNTHESIS[6]



$$\text{Silica}(-OH)_2 + AlEt_2Cl \xrightarrow[\text{reflux, 48h}]{\text{anhydrous toluene}} \text{Si(Al)} + 2C_2H_6$$

$$\text{Silica}(-OH)_2 + TiCl_4 \xrightarrow[\text{reflux, 48h}]{\text{anhydrous toluene}} \text{Si(Ti)} + 2HCl$$

Figure 10: Supported-catalysts synthesis.

FUTURE TRANSFORMATIONS

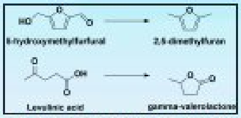


Figure 11: Transformations of 5-HMF and LA into biofuels.

CONCLUSIONS

- Two biofuel precursors, 5-HMF and LA, were obtained under environmentally friendly conditions, such as microwave heating or water as solvent.
- Catalysts employed were easily recoverable.
- Supported-catalysts inhibited humins formation, which is the main drawback of $AlCl_3{*}6H_2O$.
- Biphasic system emerged as a promising way to obtain 5-HMF, which tend to rehydrate into LA in acidic aqueous conditions.
- An easy method to separate soluble fractions of biomass was developed, in order to apply each fraction in an appropriate way, obtaining the maximum profit.

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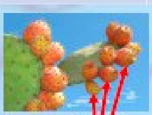
PRELIMINARY CHARACTERISATION

Table 1. Composition of OFI fruit (% w/w, dry matter).[5]

	PULP	SKIN	SEED
PROTEINS	5%	8%	12%
LIPIDS	1%	2%	7%
HEMICELLULOSE	3%	8%	5%
CELLULOSE	3%	29%	45%
PECTIN	14%	3%	4%
ASH	8%	12%	6%
GLUCOSE	35%	21%	0%
FRUCTOSE	26%	3%	0%
STARCH	5%	7%	5%

Pulp and skin were the starting material due to:
- High content in ethanol-soluble carbohydrates (glucose and fructose)
- Low content in fibers (hemicellulose and cellulose)



Fruits

Freeze-dryed, ground and sieved to remove seeds

Starting material

Thermogravimetric analysis

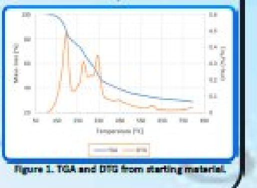


Figure 1. TGA and DTG from starting material.

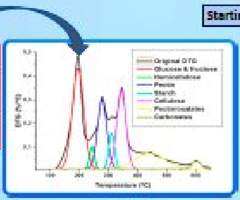


Figure 2. Starting material DTG deconvolution using Origin 9.1.

1st peak, which is the main mass loss, refers to glucose and frutose, corroborating that they are the major component

MICROWAVE-ASSISTED GLUCOSE DEHYDRATION

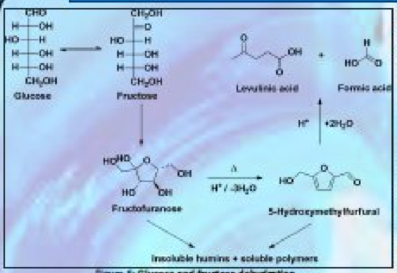


Figure 6: Glucose and fructose dehydration.

Table 2. Reaction conditions of microwave-assisted dehydration of glucose. Solvent: 2 mL of saturated water with inorganic salt.

Entry	Catalyst	Catalyst loading (w_{cat}/w_{gl})	Time (min)	Temperature (°C)
1	$AlCl_3{*}6H_2O$	0.5	10	160
2	$AlCl_3{*}6H_2O$	0.5	10	180
3	$AlCl_3{*}6H_2O$	0.5	10	200
4	$AlCl_3{*}6H_2O$	0.5	20	160
5	$AlCl_3{*}6H_2O$	0.5	30	160
6	SI(Al)	1	10	160
7	SI(Al)	1	10	170
8	SI(Al)	1	10	180
9	SI(Al)	1	20	170
10	SI(Al)	1	30	170
11	SI(Ti)	1	10	160
12	SI(Ti)	1	10	170
13	SI(Ti)	1	10	180
14	SI(Ti)	1	10	190

PRELIMINARY RESULTS

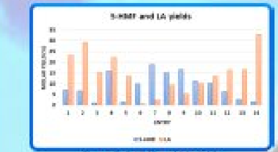


Figure 7: 5-HMF and LA yields.

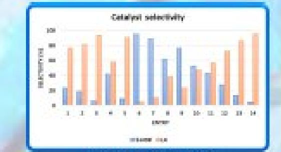


Figure 8: Catalyst selectivity.

Figure 9: Glucose conversion.

Biphasic system was also tested using cyclopentil methyl eter (CPME) as organic phase

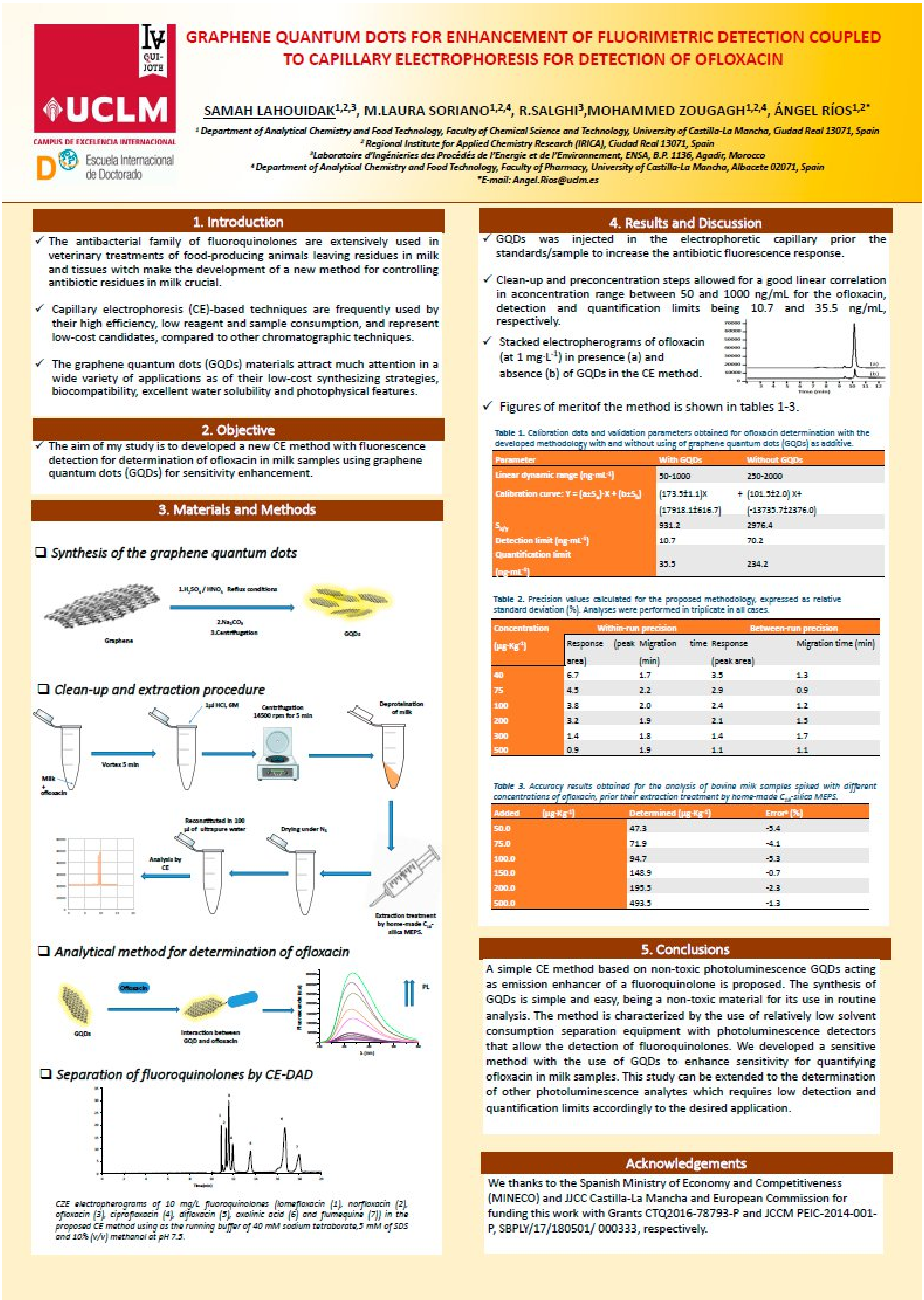
Table 3. Reaction conditions of microwave-assisted dehydration of glucose using biphasic system (1mL H_2O saturated with inorganic salt, 3mL CPME). Reaction conditions: 160 °C, 10 min.

Entry	Catalyst	Catalyst loading (w_{cat}/w_{gl})	5-HMF molar yield (%)	LA molar yield (%)	Selectivity 5-HMF (%)	Selectivity LA (%)	Glucose conversion (%)
15	$AlCl_3{*}6H_2O$	0.5	29	11	72.5	27.5	94.5
16	SI(Ti)	1	24	2	92.3	7.7	70.1

Biphasic system improves yields, selectivity and glucose conversion

ACKNOWLEDGEMENTS

Thanks to MINECO for financial support (Project Ref: CGL2014-57087-R) and Junta de Comunidades de Castilla-La Mancha (JCCM) (Project Ref: SBPLY/17/180501/000522) for financial support and JCCM, Fondo Social Europeo (FSE) and Iniciativa de Empleo Juvenil (IEP) for the AJHA grant.



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

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1. Introduction

- ✓ The antibacterial family of fluoroquinolones are extensively used in veterinary treatments of food-producing animals leaving residues in milk and tissues witch make the development of a new method for controlling antibiotic residues in milk crucial.
- ✓ Capillary electrophoresis (CE)-based techniques are frequently used by their high efficiency, low reagent and sample consumption, and represent low-cost candidates, compared to other chromatographic techniques.
- ✓ The graphene quantum dots (GQDs) materials attract much attention in a wide variety of applications as of their low-cost synthesizing strategies, biocompatibility, excellent water solubility and photophysical features.

2. Objective

- ✓ The aim of my study is to developed a new CE method with fluorescence detection for determination of ofloxacin in milk samples using graphene quantum dots (GQDs) for sensitivity enhancement.

3. Materials and Methods

❑ *Synthesis of the graphene quantum dots*

❑ *Clean-up and extraction procedure*

❑ *Analytical method for determination of ofloxacin*

❑ *Separation of fluoroquinolones by CE-DAD*

CZE electropherograms of 10 mg/L fluoroquinolones (lomefloxacin (1), norfloxacin (2), ofloxacin (3), ciprofloxacin (4), difloxacin (5), oxolinic acid (6) and flumequine (7)) in the proposed CE method using as the running buffer of 40 mM sodium tetraborate,5 mM of SDS and 10% (v/v) methanol at pH 7.5.

4. Results and Discussion

- ✓ GQDs was injected in the electrophoretic capillary prior the standards/sample to increase the antibiotic fluorescence response.
- ✓ Clean-up and preconcentration steps allowed for a good linear correlation in aconcentration range between 50 and 1000 ng/mL for the ofloxacin, detection and quantification limits being 10.7 and 35.5 ng/mL, respectively.
- ✓ Stacked electropherograms of ofloxacin (at 1 mg·L^{-1}) in presence (a) and absence (b) of GQDs in the CE method.

- ✓ Figures of meritof the method is shown in tables 1-3.

Table 1. Calibration data and validation parameters obtained for ofloxacin determination with the developed methodology with and without using of graphene quantum dots (GQDs) as additive.

Parameter	With GQDs	Without GQDs
Linear dynamic range (ng·mL^{-1})	50-1000	250-2000
Calibration curve: Y = (a±S$_a$)·X + (b±S$_b$)	(173.5±1.1)X + (17918.1±616.7)	(101.5±2.0) X+ (-13735.7±2376.0)
$S_{y/x}$	931.2	2976.4
Detection limit (ng·mL^{-1})	10.7	70.2
Quantification limit (ng·mL^{-1})	35.5	234.2

Table 2. Precision values calculated for the proposed methodology, expressed as relative standard deviation (%). Analyses were performed in triplicate in all cases.

Concentration (µg·Kg^{-1})	Within-run precision		Between-run precision	
	Response (peak area)	Migration time (min)	Response (peak area)	Migration time (min)
40	6.7	1.7	3.5	1.3
75	4.5	2.2	2.9	0.9
100	3.8	2.0	2.4	1.2
200	3.2	1.9	2.1	1.5
300	1.4	1.8	1.4	1.7
500	0.9	1.9	1.1	1.1

Table 3. Accuracy results obtained for the analysis of bovine milk samples spiked with different concentrations of ofloxacin, prior their extraction treatment by home-made C_{18}-silica MEPS.

Added (µg·Kg^{-1})	Determined (µg·Kg^{-1})	Error* (%)
50.0	47.3	-5.4
75.0	71.9	-4.1
100.0	94.7	-5.3
150.0	148.9	-0.7
200.0	195.5	-2.3
500.0	493.5	-1.3

5. Conclusions

A simple CE method based on non-toxic photoluminescence GQDs acting as emission enhancer of a fluoroquinolone is proposed. The synthesis of GQDs is simple and easy, being a non-toxic material for its use in routine analysis. The method is characterized by the use of relatively low solvent consumption separation equipment with photoluminescence detectors that allow the detection of fluoroquinolones. We developed a sensitive method with the use of GQDs to enhance sensitivity for quantifying ofloxacin in milk samples. This study can be extended to the determination of other photoluminescence analytes which requires low detection and quantification limits accordingly to the desired application.

Acknowledgements

We thanks to the Spanish Ministry of Economy and Competitiveness (MINECO) and JJCC Castilla-La Mancha and European Commission for funding this work with Grants CTQ2016-78793-P and JCCM PEIC-2014-001-P, SBPLY/17/180501/ 000333, respectively.

XIII YOUNG SCIENCE SYMPOSIUM 2019

STIMULI RESPONSIVE HYDROGELS FOR DRUG DELIVERY APPLICATIONS

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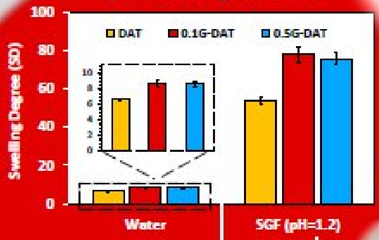
Diaminotriazines (DAT) are resourceful molecules that stand out for their ability to build supramolecular hydrophobic constructions. In addition, these structures respond to environmental changes, which has expanded the scope of DAT-based materials to the field of controlled delivery.[1,2]

In this work, we highlight triazine-based hydrogels as suitable responsive soft materials for drug delivery applications. By incorporating graphene (G) or magnetite nanoparticles (NPs) into the hydrogels, we have proven these materials successfully relase drugs in response to physiochemical stimuli such as magnetic fields, microwave radiation, or environmental pH.

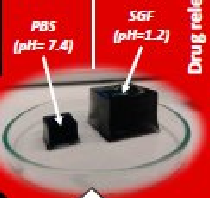
pH responsive

pH Swelling studies

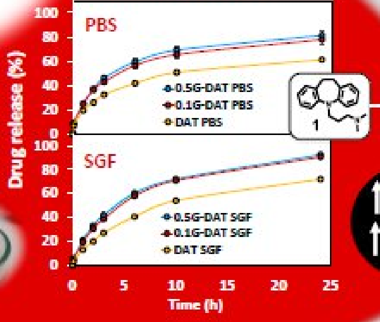


↑Graph ↑SD

↓pH ↑SD

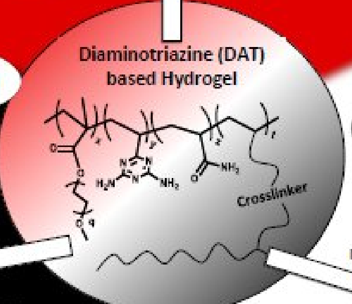


pH-responsive drug delivery

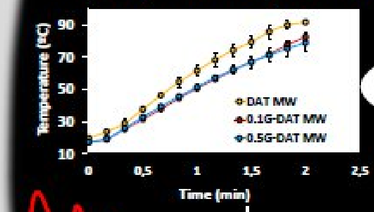


↑Graph ↑Release

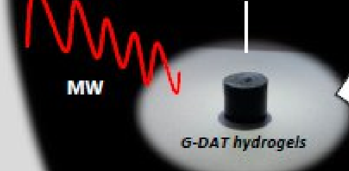
Graphene powder



MW-temperature dependence



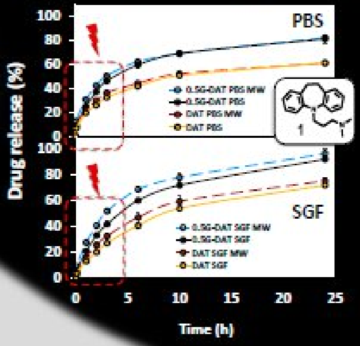
↑Graph ↓Tº(C)



Graphene powder

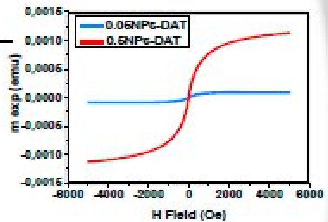
↑MW ↑Release

MW-responsive drug delivery



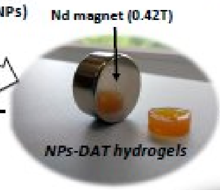
Microwave responsive

Magnetic hysteresis loop

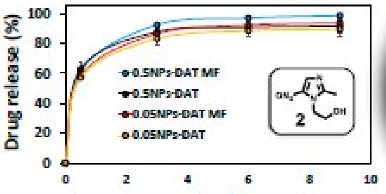


Magnetite NPs:
-Superparamagnetic

Magnetite Nanoparticles (NPs)



Magnetic-responsive drug delivery



↑MF ↑Release

Magnetically responsive

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[2] Wang P, Zhang J, Li Y, Wang N, Liu W.. *Mater Lett*. 2015;142:71-74.

Acknowledgements
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Project: CTQ 2017-88158-R

13 th Young Science Simposium

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

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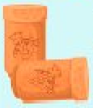
INTRODUCTION



The cork is the closure chosen for wine bottles, and will represent one of the multiple factors that influence its quality. Due to the development of instrumental analytical techniques, such as gas chromatography and mass spectrometry, several scientists attributed to the cork certain off-flavours that sometimes appear in wine, with aromas of moisture and mould[1],[2]. This aroma defect was called "cork taint".

GOAL

The objective of this work was to identify the corky off-flavour compounds in planks that will be used for producing wine stoppers.

MATERIAL AND METHODS

SAMPLING PLAN

- 6 months
- 9 months
- 12 months

CORK PLANKS
Gruart La Mancha, S.A.
(Valdepeñas, Ciudad Real)

EXTRACTION AND ANALYSIS OF VOLATILE COMPOUNDS

Dionex ASE 200
(Accelerated Solvent Extraction)

CH_2Cl_2 +

GC-MS
(Gas Chromatography-Mass Spectrometry)

SIM mode

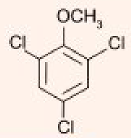
RESULTS AND DISCUSSION

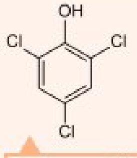
- Several compounds responsible for the sensory defect called "cork taint", as alkylmethoxypyrazines, chloroanisoles, chlorophenols, methylisoborneol and geosmin were detected in the newly harvested cork planks.
- "Cork taint" compounds concentration decreased during their storage (6, 9 and 12 months) outside the cork industry before processing.

Table 1. Off-flavour compounds identified in dichloromethane extracts of cork planks obtained by ASE. RI: retention index (DB-5).

Compound	RI	Nomenclature	Identifier ions (m/z)	Quantifier ion (m/z)
MDMP	1057	3,5-dimethyl-2-methoxypyrazine	109, 138	138
IPMP	1078	3-isopropyl-2-methoxypyrazine	124, 137, 152	137
IBMP	1170	3-isobutyl-2-methoxypyrazine	94, 124, 151	124
TCA	1319	2,4,6-trichloroanisole	169, 197, 212	197
TCP	1335	2,4,6-trichlorophenol	132, 160, 196	132
TeCA	1517	2,3,5,6-tetrachlorosanisole	203, 231, 246	203
TeCP	1552	2,3,4,6-tetrachlorophenol	131,230,232	232
TBA	1619	2,4,6-tribromoanisole	303, 331, 344	331
TBP	1624	2,4,6-tribromophenol	222, 330, 332	330
PCA	1721	pentachloroanisole	237, 265, 280	265
2-MIB	1158	2-methylisoborneol	95, 107, 168	95
Geosmin	1373	*t*-1,10-dimethyl-*t*-9-decalol	112, 125, 182	112

2,4,6-Trichloroanisole





2,4,6-Trichlorophenol

Geosmin

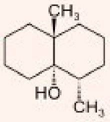
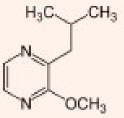
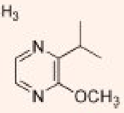


Table 2. Concentration (ng/g) of alkylmethoxypyrazines in cork planks during storage time before processing.

Storage time before proccessing	Samples	MDMP	IPMP	IBMP
6 months	S1	2.01	0.22	0.35
	S2	0.32		0.20
	S3	0.29		0.43
	S4	1.77	0.30	
	S5	0.55		0.67
9 months	S1	1.71		
	S2			
	S3			
	S4	0.73		
	S5			
12 months		-	-	-

3,5-dimethyl-2-methoxypyrazine





3-isopropyl-2-methoxypyrazine

Table 3. Evolution of the concentration (ng/g) of chloroanisoles and chlorophenols in cork planks during storage time before processing.

Storage time before proccessing	Samples	TCA	TCP	TeCA	TeCP	TBA	TBP	PCA
6 months	S1			1.80	0.44	0.62	0.59	6.27
	S2	0.28		0.45	0.12	0.50	0.41	2.08
	S3	0.19		0.39	0.14	0.33	0.33	0.45
	S4	0.30		0.24	0.19	0.47	0.49	4.27
	S5			0.36	0.28		0.37	0.19
9 months	S1			0.50	0.17		0.46	0.31
	S2	0.45						0.23
	S3				0.38		0.36	0.12
	S4				0.25		0.48	0.40
	S5			0.39			0.52	0.18
12 months	S1							0.13
	S2						0.43	0.17
	S3				0.24			0.16
	S4							
	S5						0.48	0.14

CONCLUSION

These results show the importance of storage stage of raw cork planks before their processing, because of the risk of contamination during these stage and as a result to control the formation of corky off-flavors compounds.

REFERENCES

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[2] Slabizki, P., Fischer, C., Legrum, C., Schmarr, H.G. (2015). Journal of Agricultural and Food Chemistry, 63: 7840-7848.

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

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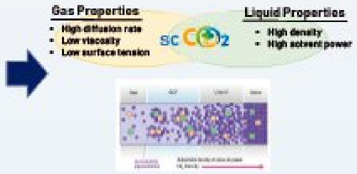
Introduction

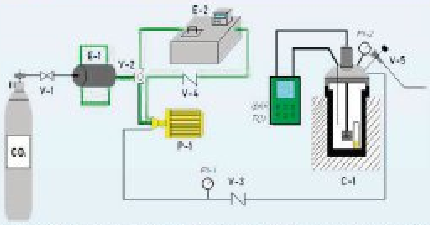
PEG-b-PLA In the last decade, amphiphilic block copolymers consisting of poly ethylene glycol (PEG) and poly lactide (PLA) have gained considerable attention in pharmaceutics and biomedical applications and furthermore have great potential for development drug delivery systems.

PLA PLA has been successfully implemented in many pharmaceutics applications, but its broader utilization as a biomaterial is limited due to its hydrophobicity and difficulties with encapsulation of significant loadings of polar drugs

PEG A common method to overcome these limitations and improve the hydrophilicity of the hydrophobic polymers is copolymerization with a hydrophilic block such as PEG.



Experimental Setup

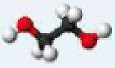


Schematic diagram of the experimental polymerization; V-1,V-3,V-4; check valves; PI-1, PI-2: manometer; TCI: temperature digital controller. Green lines represent the cooled pipes in order to avoid the cavitation of the pump.P-1: pump, E-2: cooler, C-1: batch reactor; V-5: regulator valves.

Materials

COUMARIN

PEG



PLA

- ✓ANTIOXIDANT
- ✓ANTICANCER
- ✓ANTIVIRAL
- ✓ANTI-INFLAMMATORY
- ✓ANTICOAGULANT

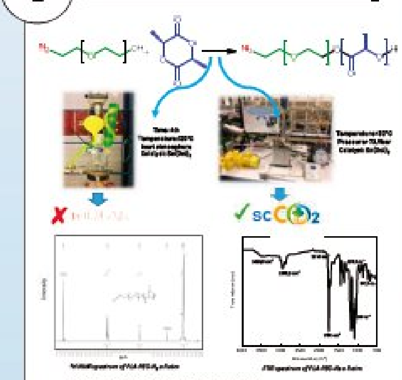
- ✓NON-TOXIC
- ✓AMPHIPHILIC
- ✓NON-IMMUNOGENIC
- ✓BIOCOMPATIBLE
- ✓APPROVED BY FDA

- ✓BIOCOMPATIBLE
- ✓BIODEGRADABLE
- ✓THERMOPLASTIC
- ✓VERSATILE
- ✓GREEN PRODUCT

Objetives and Results

1

1.1 COPOLYMERIZATION P ATM vs $scCO_2$



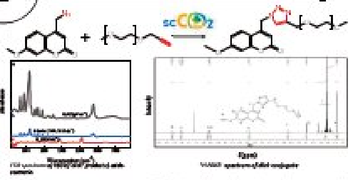
1.2 OPTIMIZATION IN $scCO_2$

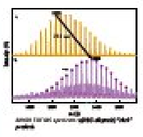
Factors studied in the DOE of the polymerization process and their levels

FACTOR	LOWER LEVEL(-)	HIGHER LEVEL(+)
Temperature(ºC)	130	150
Pressure(bar)	100	200
Polymerization time	7	24

2

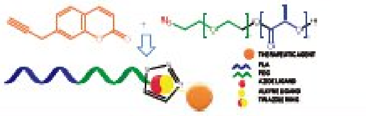
2.1. CONJUGATED PEG-DRUG in $scCO_2$





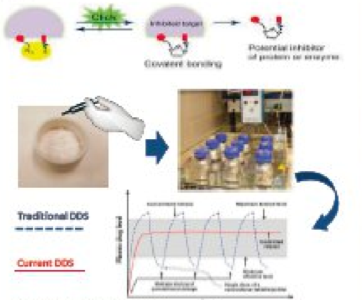
- FTIR it was found that the peak corresponding to the azide group (2110 cm⁻¹) observable in 4-azidomethyl-7-methoxycoumarin, disappears from the spectrum. This shows that the reaction has been carried out satisfactorily. In addition the triazole ring 862 cm⁻¹ formed.
- ¹H NMR the click product structure was determined for PEG 2000. The triazole ring signal (7.8 ppm) is clearly identified.
- MALDI mass spectroscopy, it was possible to determine the yield of the reaction.

2.2 CONJUGATED PLA-b-PEG-DRUG in $scCO_2$



3

3.1. RELEASE IN VITRO STUDIES



3.2. RELEASE IN VIVO

Clinical trials

Conclusions

- We have successfully synthesized of PEG-b-PLA copolymers. Amphiphilic block copolymers consisting of poly (ethylene oxide) and poly(lactide) have great potential for formulating drug delivery systems.
- The biocompatibility and biodegradability of these copolymers makes them attractive, and they are used extensively in the pharmaceutical industry, in addition, these copolymers are good candidates for use in controlled delivery of anticancer drugs.
- The PEG-b-PLA copolymers provides steric stability and can possess targeting ligands on its end, and hydrophobic drugs can be incorporated. The incorporation of drugs will be carried out by click chemistry owing to the terminal group provided by the synthesized copolymer.

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5-7 de Junio de 2019 | Campus Ciudad Real, UCLM

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

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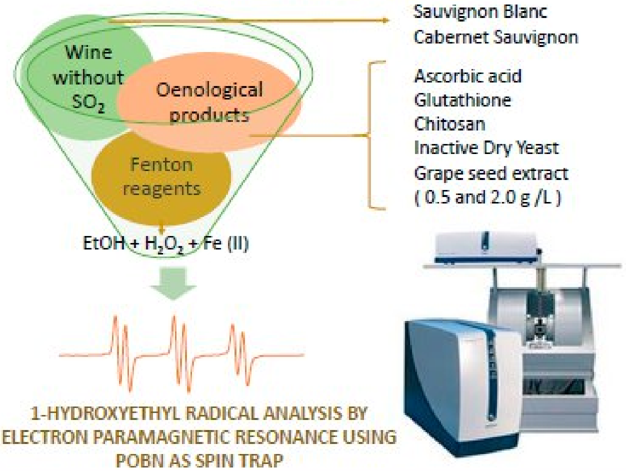
INTRODUCTION

The elaboration of wines without SO_2 is a complex challenge, since the free radicals produced in wine oxidation reactions can cause a great deterioration in its composition and organoleptic characteristics.

Among the free radicals formed during the oxidation of wine, it has been shown that the 1-hydroxyethyl radical is the most abundant and could be the main agent responsible for the oxidation of other organic substances in wine.

The objective of this work was to study the potential of different natural oenological products to inhibit 1-hydroxyethyl radical in wines without SO_2.

MATERIAL AND METHODS



Wine without SO_2

Oenological products

Fenton reagents

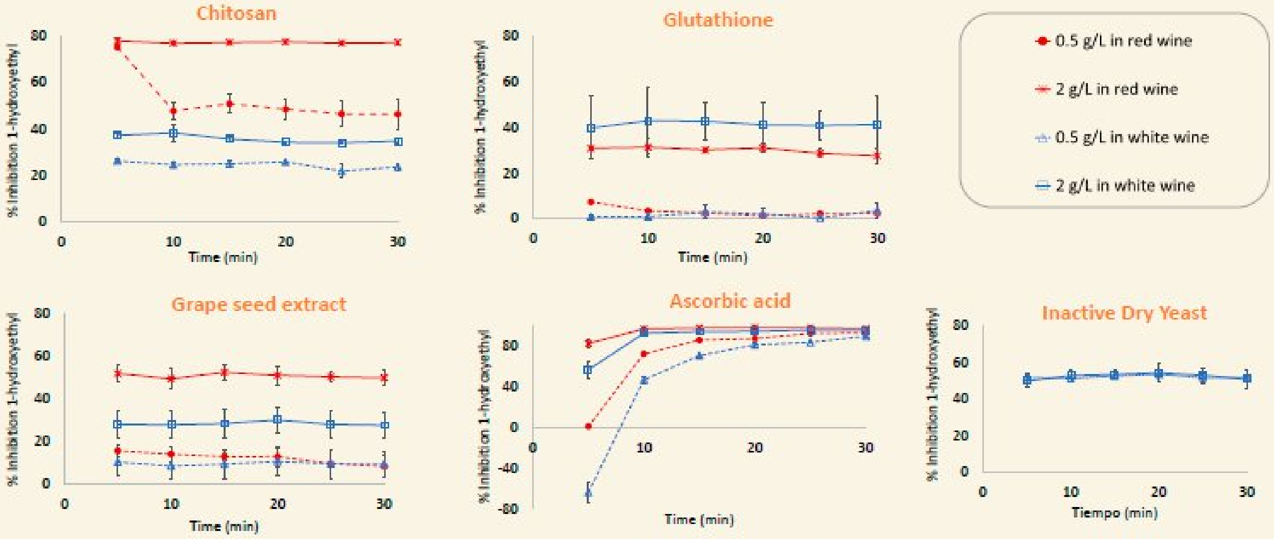
Sauvignon Blanc
Cabernet Sauvignon

Ascorbic acid
Glutathione
Chitosan
Inactive Dry Yeast
Grape seed extract
(0.5 and 2.0 g /L)

$EtOH + H_2O_2 + Fe (II)$

1-HYDROXYETHYL RADICAL ANALYSIS BY ELECTRON PARAMAGNETIC RESONANCE USING POBN AS SPIN TRAP

RESULTS AND DISCUSSION



- ➢ The addition of grape seed extract and chitosan offered higher percentages of radical inhibition in red wine.
- ➢ The ascorbic acid at 0.5 g/L showed a pro-oxidant effect at the beginning of the reaction in white wine.
- ➢ The effect of the inactive dry yeast to inhibit the radical was only observed in white wine.

❖ **The efficacy of the oenological products studied to inhibit the 1-hydroxyethyl radical in wines without SO_2 is influenced by both the concentration used and the type of wine.**

ACKNOWLEDGMENTS: This work has been carried out with the financing of INIA under the projects : RTA2014-00055-C03-01 y RTA2014-00055-C03-02.

Degradation of antibiotics by ElectroFenton process

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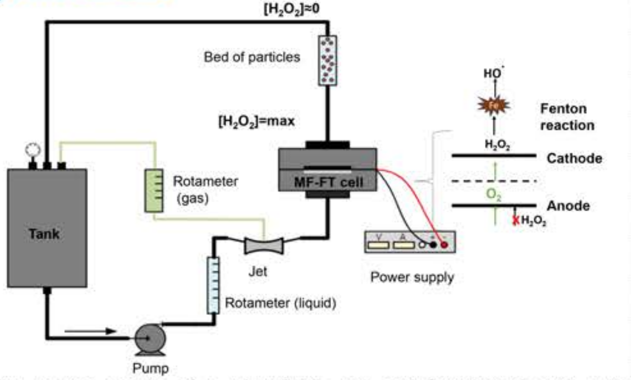
Introduction

Currently, there is a global environmental problem related to the presence of pharmaceutical compounds in wastewater. One of the main sources of these pollutants are hospitals, which generate a large volume of effluents every day. Among them stand out, not for the volume generated but for its concentration, the urine of the patients that presents a high content of antibiotics, antipyretics, hormones, etc. The conventional processes used in wastewater treatment plants have a low efficiency to eliminate this type of contaminants, causing the emergence of bacteria resistant to antibiotics. Therefore, hospital effluents must be adequately treated to protect both the environment and human health, since there is no legislation governing the concentration limits of drugs in water [5].

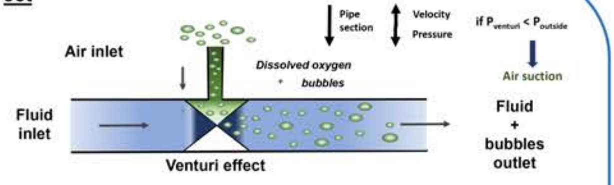
Based on this, in this work the heterogeneous electroFenton process has been chosen for the selective elimination of pharmaceutical compounds in urine medium. Urine is a very complex matrix, which contains organic components and inorganic salts that hinder the process.

Setup diagram

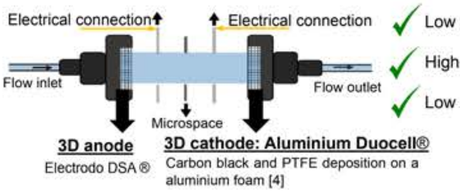


The system consits of a micro-fluidic cell and flow-through with a jet aeration, to supply large amounts of oxygen at low pressure to efficiently generate H_2O_2. In addition, it incorporates a fluidized-bed of iron particles (goethita) for catalyze the descomposition of H_2O_2 into oxidizing species.

Jet



Micro-fluidic cell and flow-through



- ✓ Low ohmic resistance
- ✓ High mass-transfer
- ✓ Low energy consumption

Results

Influence of the current densitie in the generation of H_2O_2

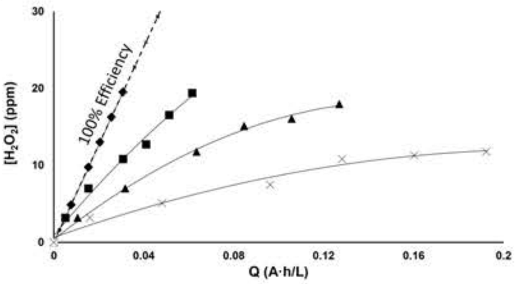


Figure 1. Hydrogen peroxide generation at different current densities in the MF-FT reactor. ◆ *j=5 mA/cm³* ■ *j= 10 mA/cm³* ▲ *j=20 mA/cm³* **X** *j=30 mA/cm³. Q_v=140 L/h. Q_{air}=100 NL/h. T=25ºC. pH 3. V=2.5 L. P=1 atm.*

Degradation of Chloramphenicol in urine. Generation of acids.

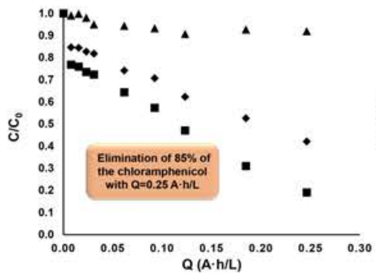


Figure 2. Chloramphenicol and compounds of the urin in heterogeneous EF. ◆ *Chloramphenicol* ■ *Uric acid* ▲ *Creatinine j=5 mA/cm³, [Goethita]= 4 g/L. Q_v=140 L/h. Q_{aire}=100 NL/h. T=25ºC. pH 3. V=2.5 L. P=1 atm. 50 ppm of $Chloramphenicol_0$.*

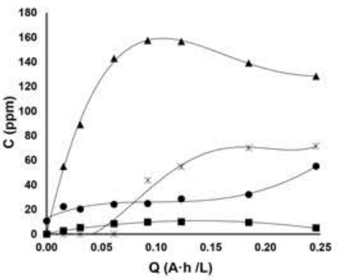


Figure 3. Carboxylic acid generated in the process. ▲ Formic acid ● Oxalic acid ■ Oxamic acid, Ж Propionic acid.

Conclusions

- El jet multiplies the aeration capacity at a given pressure and increases H_2O_2 production rate.
- Specific energy consumption of the MF-FT + Jet for the production of H_2O_2 is the lowest reported so far (4 kWh/kg H_2O_2).
- An excess of applied current density results counterproductive in terms of H_2O_2 generation (Figura 1).
- Heterogeneous ElectroFenton allows the elimination of chloramphenicol with a high selectivity, keeping most of the components of the urine unaltered. On the other hand, it is posible to degrade 58% of the chloramphenicol by applying load less than 0.3 A·h /L.

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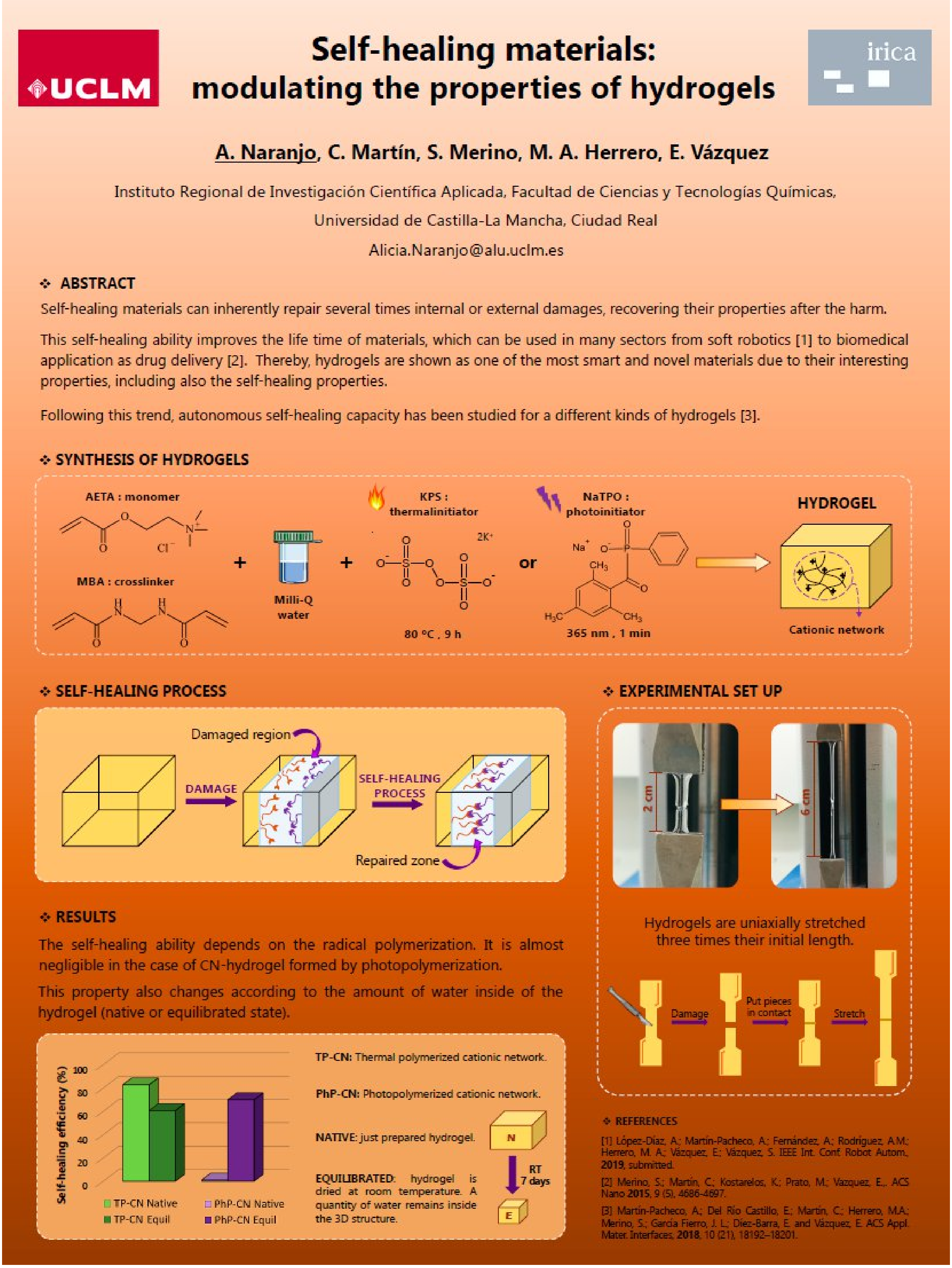

Self-healing materials: modulating the properties of hydrogels

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❖ ABSTRACT

Self-healing materials can inherently repair several times internal or external damages, recovering their properties after the harm.

This self-healing ability improves the life time of materials, which can be used in many sectors from soft robotics [1] to biomedical application as drug delivery [2]. Thereby, hydrogels are shown as one of the most smart and novel materials due to their interesting properties, including also the self-healing properties.

Following this trend, autonomous self-healing capacity has been studied for a different kinds of hydrogels [3].

❖ SYNTHESIS OF HYDROGELS

❖ SELF-HEALING PROCESS

❖ EXPERIMENTAL SET UP

Hydrogels are uniaxially stretched three times their initial length.

❖ RESULTS

The self-healing ability depends on the radical polymerization. It is almost negligible in the case of CN-hydrogel formed by photopolymerization.

This property also changes according to the amount of water inside of the hydrogel (native or equilibrated state).

TP-CN: Thermal polymerized cationic network.

PhP-CN: Photopolymerized cationic network.

NATIVE: just prepared hydrogel.

EQUILIBRATED: hydrogel is dried at room temperature. A quantity of water remains inside the 3D structure.

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Catalytic ammonia decomposition over Ru/SiC

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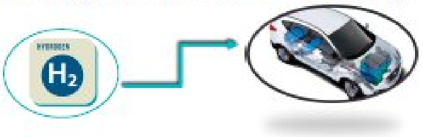
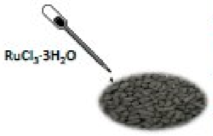
INTRODUCTION

Catalytic ammonia decomposition in order to generate hydrogen has been used for energy production. Different catalysts have been **synthesized**, using ruthenium (load 1-7.5% w/w) supported over silicon carbide (SiC).



EXPERIMENTAL

- **Catalysts synthesis:** incipient wetness impregnation and followed by overnight drying at 80 °C.

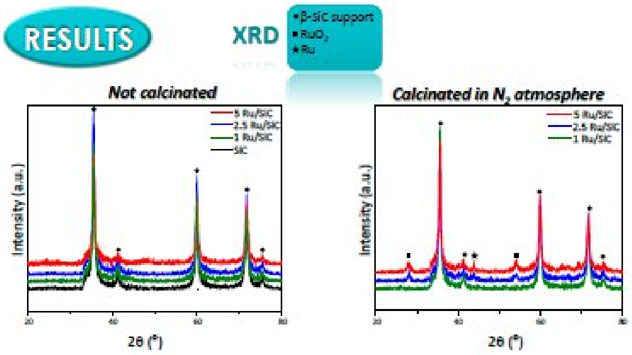


Calcination	
N_2-Ar (100ml·min^{-1}, 50:50)	500 °C x 2h, 10 °C·min^{-1}
Reduction	
H_2-Ar (100ml·min^{-1}, 50:50)	600 °C x 1h, 10 °C·min^{-1}
	400 °C x 1h, 10 °C·min^{-1}

- **Catalytic testing:**
  - -NH_3-Ar: 100 ml·min^{-1}, 10:90
  - -GHSV: 60000 ml/g·h
  - -Products analyse by Gas Chromatography (GC)

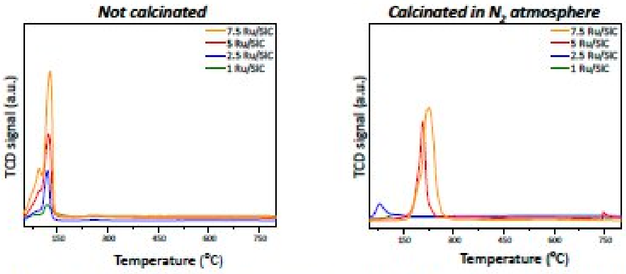
RESULTS

XRD



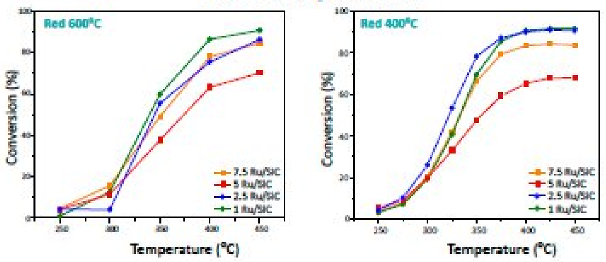
The characterization by XRD (X-Ray Power Diffraction) of the catalysts not calcinated shows that the Ru is very dispersed, only signals of silicon carbide are observed. However, Ru and RuO_2 are observed in catalysts calcinated in nitrogen atmosphere.

TPR-H_2

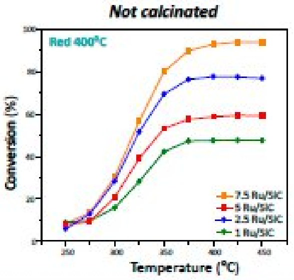


As it can be observed, Ru is very easily reduced ($Ru^{3+} \rightarrow Ru^0$) at 120 °C if it was not calcinated. On the other hand, the catalysts calcinated in N_2 show a peak related with reduction of Ru^{3+} at higher temperature (245 °C).

Reactivity



The decrease in reduction temperature improves the catalytic activity in the catalysts with low loading of ruthenium. Nevertheless, if the catalysts were not calcinated, the 7.5% Ru/SiC catalysts presents the best behaviour.



CONCLUSION

In this context, taking into account the Ru content, the most favourable catalyst is the one that presents lower load of metal, one step of calcination and reduction at 400 °C. So the best performance was achieved by the 1%Ru/SiC catalyst calcinated in N_2. In this case, 95% of conversion was reached at 400 °C.

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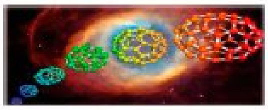
FEDER
Fondo Europeo de Desarrollo Regional



2-(2-HYDROXYPHENYL)-4,6-STYRYLPYRIMIDINES. SYNTHESIS AND OPTICAL PROPERTIES

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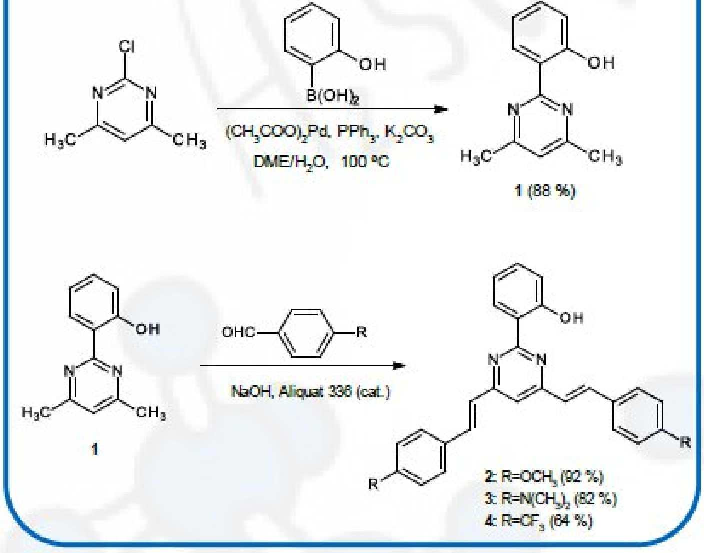
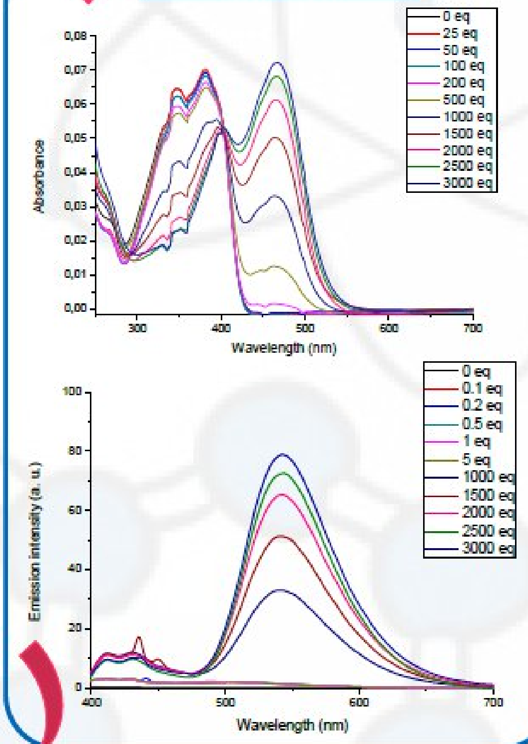
ABSTRACT

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

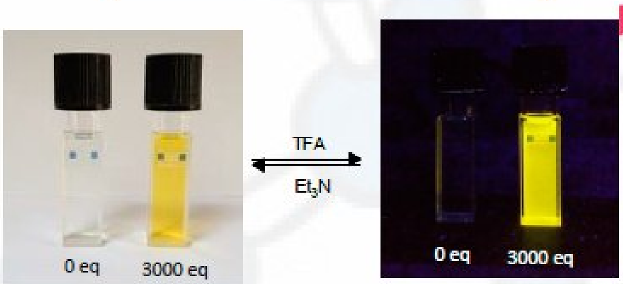
SYNTHESIS



TITRATION CURVES OF A CH_2Cl_2 SOLUTION OF 3 WITH TFA



CHANGES IN THE COLOR OF A CH_2Cl_2 SOLUTION OF 3 AFTER ADDITION OF TFA UNDER VISIBLE (LEFT) AND UV LIGHT (RIGHT)



Visible

Uv (λ_{em}= 365 nm)

CONCLUSIONS

The route of synthesis was straightforward. The compounds display reversible color changes and luminescence switching upon addition of acid that could enable the development of new colorimetric and luminescence pH sensors.

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Membrane-less electrolyzer: a new concept for H_2 production via alcohol electrochemical reforming

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INTRODUCTION

The increasing demand of worldwide energy joint to the environmental problems encourages the development of clean and renewable energy such as hydrogen.

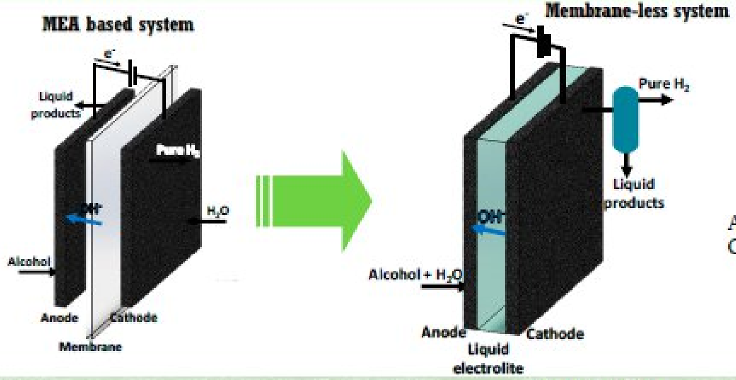
WATER ELECTROLYSIS

✓ Most stablished technology
✗ High cell voltages → high energy consumption [1]

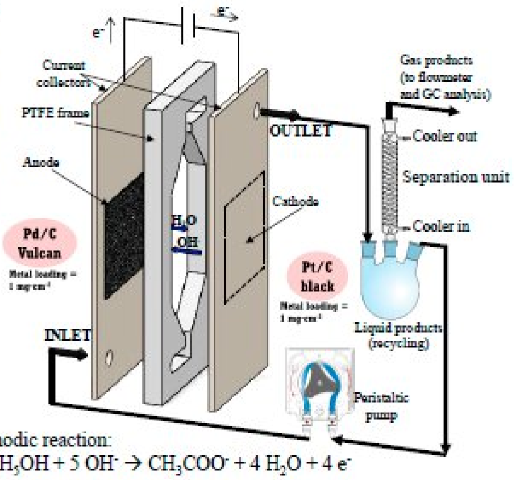
ALCOHOL ELECTROCHEMICAL REFORMING

✓ High energy contained → lower energy consumption

SIMPLE AND INTEGRATED FREE CARBONACEOUS H_2 PRODUCTION SYSTEM



EXPERIMENTAL



Anodic reaction:

$$C_2H_5OH + 5\ OH^- \rightarrow CH_3COO^- + 4\ H_2O + 4\ e^-$$

Cathodic reaction:

$$2\ H_2O + 2\ e^- \rightarrow H_2 + 2\ OH^-$$

RESULTS

Proof of concept

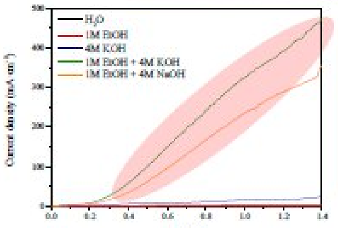


Figure 2. Linear sweep voltammetry measurements in a 0-1.4 V range. Scanrate = 10 mV·s-1, T = 85 °C.

ELECTROCATALYTIC ACTIVITY
⬇
ETHANOL ELECTRO-OXIDATION CONTRIBUTION
+
LIQUID ELECTROLYTE
- OH- TRANSPORTATION PATHWAY
- HIGH IONIC CONDUCTIVITY

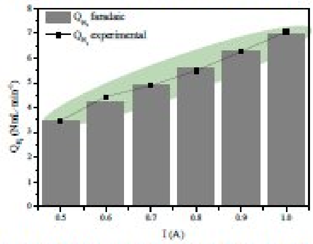


Figure 3. Galvanostatic transients: H_2 production rates vs current applied. T = 25 °C

PURE AND FARADAIC HYDROGEN

Figure 4. Gas chromatograph of the outlet gas phase from measurement obtained at 1 A galvanostatic transient (Figure 3).

Influence of the membrane-less electrolyzer conditions

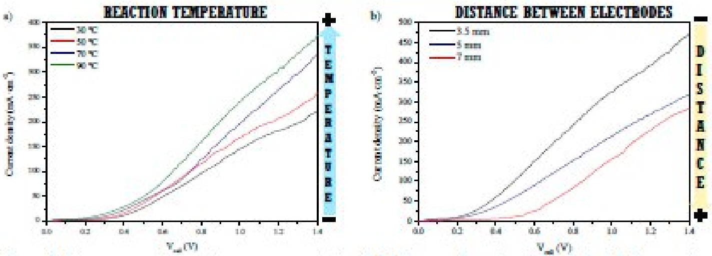


Figure 3. Linear sweep voltammetry measurements in a 0-1.4 V range. Scanrate = 10 mV·s-1. a) Influence of the temperature. b) Influence of the chamber width.

⬆ TEMPERATURE ⬆ ELECTROCATALYTIC ACTIVITY
- INCREASE OF THE IONIC CONDUCTIVITY OF THE ELECTROLYTE
- ENHANCEMENT OF THE KINETICS OF THE ELECTROCHEMICAL REACTIONS

⬇ DISTANCE ⬆ ELECTROCATALYTIC ACTIVITY
- DECREASE OF THE OHMIC LOSSES OF THE SYSTEM

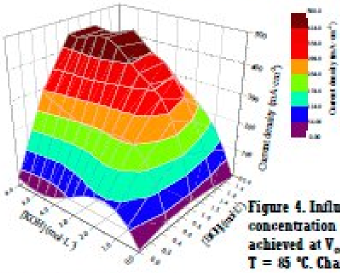


Figure 4. Influence of EtOH and KOH concentration vs. current density achieved at V_{cell} = 1.4 V. T = 85 °C. Chamber width = 3.5 mm.

0 mol·L-1 → ETHANOL CONCENTRATION → 2 mol·L-1
INSUFFICIENT FUEL SUPPLY
MASS TRANSFER LIMITATIONS
LOW IONIC CONDUCTIVITY OF THE SOLUTION
UNAVAILABILITY OF OH- IONS AT CATALYST SITES

6 mol·L-1 ← KOH CONCENTRATION ← 0 mol·L-1
HIGH SOLUTION VISCOSITY
LARGE OH- COVERAGE OF THE ACTIVE SITES
LOW IONIC CONDUCTIVITY OF THE SOLUTION

OPTIMIZED EXPERIMENTAL CONDITIONS
1 mol·L-1 EtOH + 4 mol·L-1 KOH
TEMPERATURE = 85 °C
CHAMBER WIDTH = 3.5 mm

CONCLUSIONS

This membrane-less configuration may simplify the further scale up, enhancing the stability of the system due the lack of a polymer electrolyte membrane. Under optimized conditions, pure hydrogen can be obtained with a lower energy consumption (16.9 kWh·kg$^{-1}_{H2}$) than reported in previous studies.

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ACKNOWLEDGMENTS

GOBIERNO DE ESPAÑA
MINISTERIO DE ECONOMÍA Y EMPRESA

Organogels from 2*H*-benzo[*d*]1,2,3-triazole derivatives. Application in crystallization of drugs.

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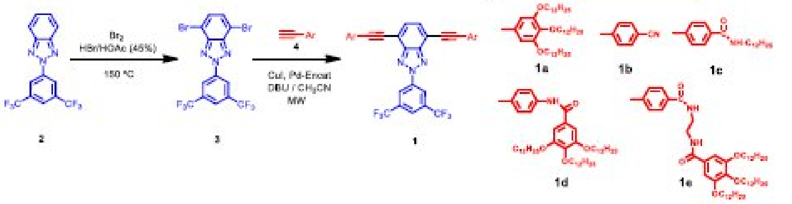
Abstract



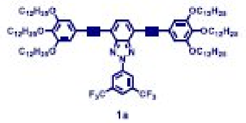
Scheme 1. Synthesis of 2-(3,5-bis(trifluoromethyl)phenyl)-4,7-bis(phenylethynyl)-2*H*-benzo[*d*]1,2,3-triazole derivatives (1) by a Sonogashira cross-coupling reaction between 3 and 4.

2*H*-Benzo[*d*]1,2,3-triazole derivatives have been previously tested as **optical waveguides**[1], **OFETs**[2], and **polymers in bioimaging**[3]. In this work, benzotriazole derivatives with a range of chemical functionalities **form organogels.** Noteworthy, bis-amide derivative **1e** gave robust thermally stable gels in a range of solvents down to 0.1 wt%.

The gels have also been showed to be useful **vehicles to crystallize pharmaceutical drugs**, resulting in a change in the polymorphism in the case of sulfathiazole.

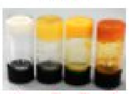
Results and discussion

Gelation tests



1a

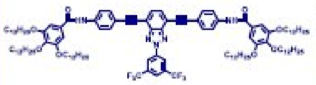
2% wt



1. **1,4-butanediol**
2. **2-propanol**
3. **1-pentanol**
4. **Methanol**

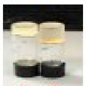
1% wt

1. **1-pentanol**
2. **1,4-butanediol**

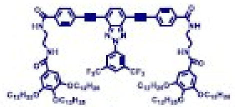


1d

2% wt



1. **DMF**
2. **Diethylene glycol**



1e

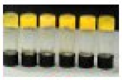
2% wt

1. **DMF**
2. **Ethanol**
3. **Methanol**
4. **1-butanol**
5. **1-propanol**

1% wt

1. **Ethanol**
2. **Methanol**
3. **Hexane**
4. **2-butanol**
5. **1-propanol**
6. **1-butanol**
7. **2-propanol**
8. **1,4-butanediol**

0.5% wt



1. **Ethanol**
2. **1-propanol**
3. **1-butanol**
4. **2-butanol**
5. **2-propanol**
6. **1,4-butanediol**

Gelation tests were carried out for compounds **1** using **thirty different** solvents and at **different concentrations** (2% wt, 1% wt and 0.5% wt). Gelators were dissolved in 0.5 mL of the respective solvent through gentle heating followed by sonication for 1 min until complete dissolution. The vials were then kept undisturbed at room temperature and were checked after 4, 24, 48 and 72 hours using **the simple tube inversion test** to assess the flow properties of the resulting mixture.

CGC

The critical gelation concentration (CGC) is the minimum amount of gelator which is needed to obtain a gel in a specific solvent.

1a → **0.7-1.7 % wt**

1d → **1.5-1.8 % wt**

1e → **0.1-1.8 % wt** **SUPERGELATOR**

T_{sol}

The gel to sol phase transition temperature, (Tsol) is the temperature when the gel breaks down, becoming solution again.

1a → **62-105 °C**

1d → **45-53 °C**

1e → **70-178 °C**

The strong hydrogen bonds between the protons of N–H groups and interdigitation between the long alkyl chains may explain the strength of these gels and the high values of T_{sol} in **1e**.

IR experiments

In **1e**, the **C=O stretching frequency** of the amide group appears at 1682 cm^{-1}, **increasing** highly **the intensity** in the case of the gel. **N-H amide stretching** appears at 3256 cm^{-1} in the compound in the solid state, but in the dried xerogel it can be observed a surprising **change**, not only of **the intensity**, but also in **the morphology** in the band (Figure 1). This can be attributed for **the strong hydrogen bonds** between amide groups responsible of the gel formation.

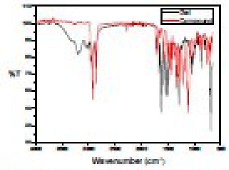


Figure 1. Spectra for compound **1e** (red) and the dry xerogel (black)

Rheology experiments

Gels of **1a** and **1e** proved to be particularly robust by rheology experiments with **high mechanical resistance**. The additional amide groups in **1e** apparently results in more robust fiber formation. In the case of **1a** the gels are opaque suggesting larger, more crystalline particles and the high yield stress may indicate the presence of large solid particles rather than an elastic gel network. This difference is also reflected in the **higher σ values** for **1e** compared to **1a** in 1,4-butanediol (1585 vs 914 Pa)

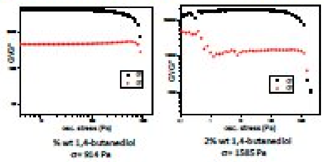


Figure 2. Stress sweep experiments for **1a** (left) and **1e** (right).

Drug crystallization

Sulfathiazole crystals undergo a morphological change when crystallized in the absence or presence of **1e** gel. Thus, when sulfathiazole crystallizes in solution of 1-propanol, needle-shaped crystals corresponding to polymorph II are observed. On the other hand, when crystallization is performed in the presence of organogel **1e**, block shaped crystals corresponding to polymorph I are observed. This **change in the polymorphism**[4] is able to change the drug properties and its possible pharmacological application.

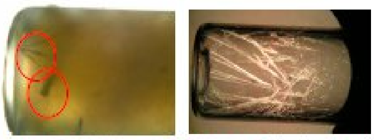


Figure 3. Crystals of sulfathiazole grown in **1e** gel in 1-propanol (left) and by solution evaporation (right).

Conclusions

- ✓ **2*H*-benzo[*d*]1,2,3-triazole derivatives 1a, 1d,** and **1e form organogels** in specific solvents.
- ✓ Compound **1e** proved to be an effective gelator of a wide range of solvents even at low concentrations, in some cases acting as a **supergelator** (e.g. ethanol, critical gelation concentration 0.1% wt).
- ✓ These gels also displayed **high thermal stability** and **significant mechanical resistance**, especially **1e**.
- ✓ Gels of **1e** were used in the crystallization of the pharmaceutical drugs. In the case of **sulfathiazole** the gel induces **a change in the polymorphism**. These gels offer significant scope for expanding the rage of current polymorph discovery methods particularly in the pharmaceutical industry.

References

[1] I. Torres-Moya, J. R. Carrillo, A. Díaz-Ortiz, J. Orduna, M. J. Blesa, L. Sánchez, P. Prieto. Dyes and pigments, 2017, *142*, 212-225.

[2] I. Torres-Moya, I. Arrechea-Marcos, C. Tardío, J. R. Carrillo, A. Díaz-Ortiz, J. T. López Navarrete, M. C. Ruiz Delgado, P. Prieto, R. Ponce. RSC Advances, 2018, *8*, 21879-21888.

[3] R. Vázquez, M. J. Martinez-Tomé, Z. Kahveci, I. Torres-Moya, A. Falco, R. Mallavia, C. Reyes. Polymers, 2018, *10*, 938.

[4] I. Torres-Moya, B. Saikia, P. Prieto, J. R. Carrillo, B, J. W. Steed. CrystEngComm. 2019, *21*, 2135-2143.

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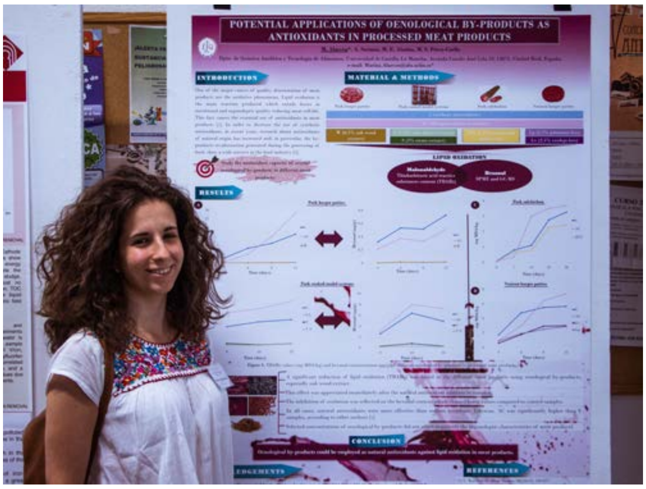

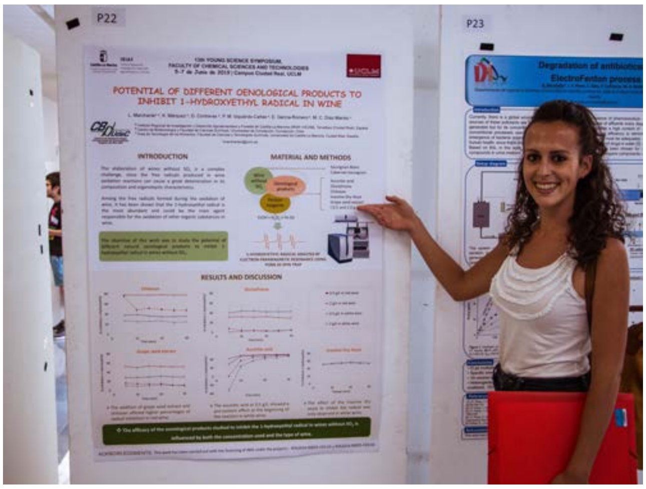

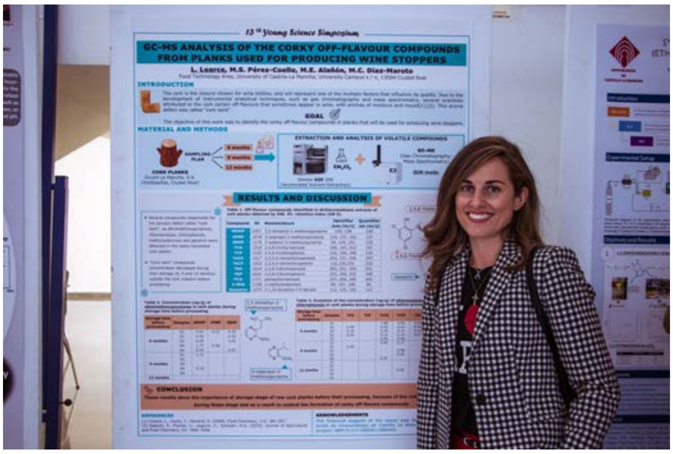

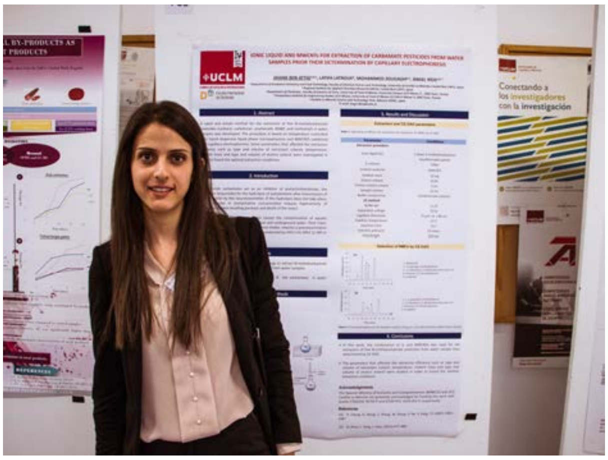

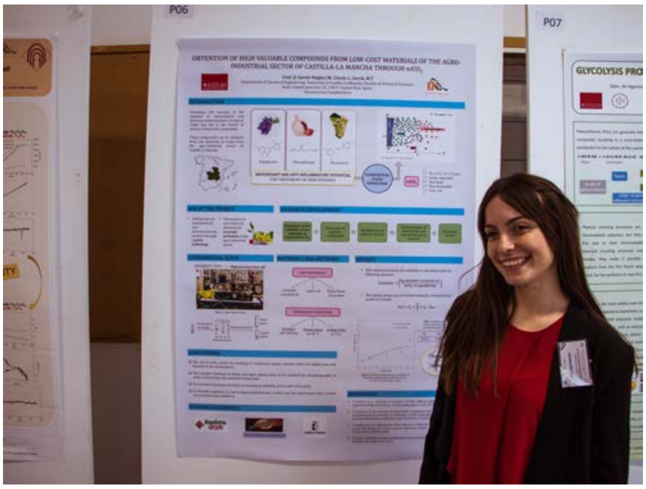

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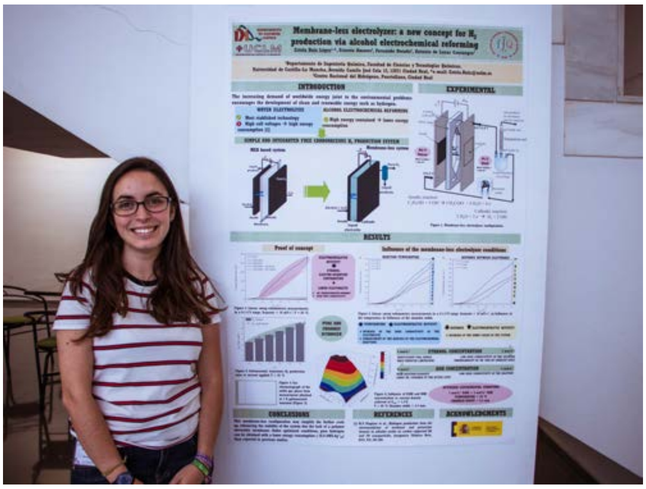

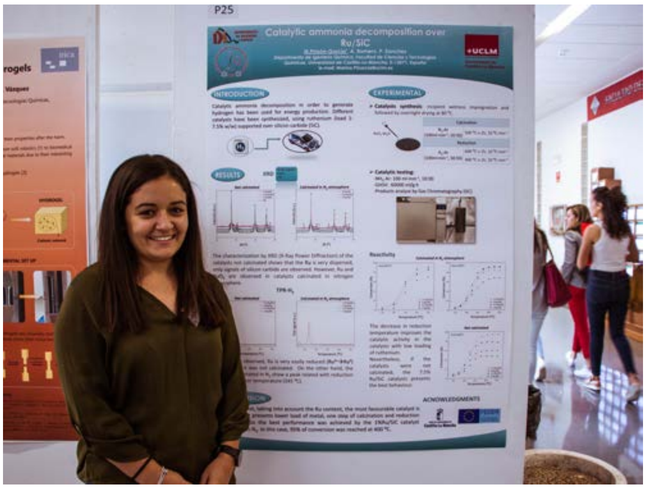

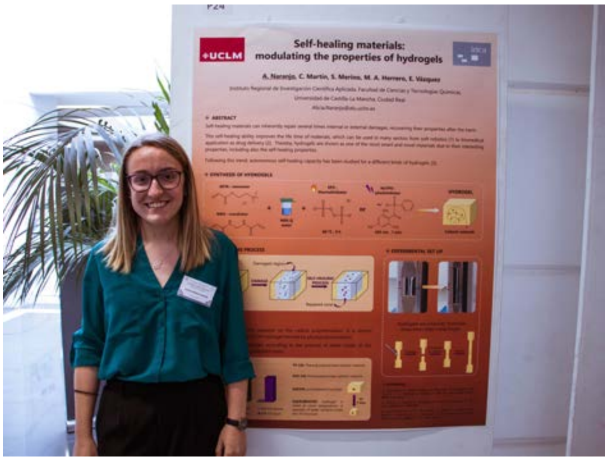

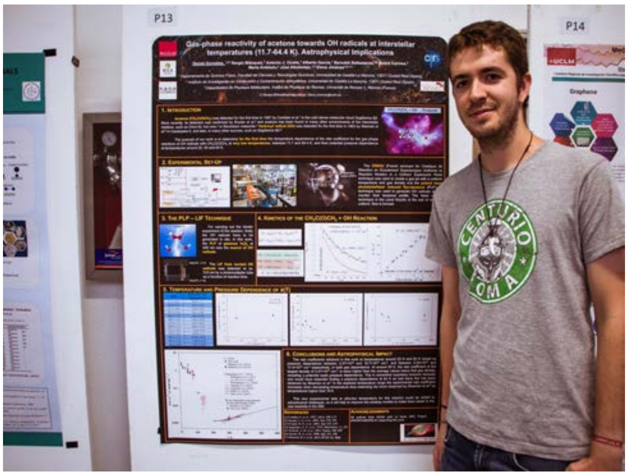

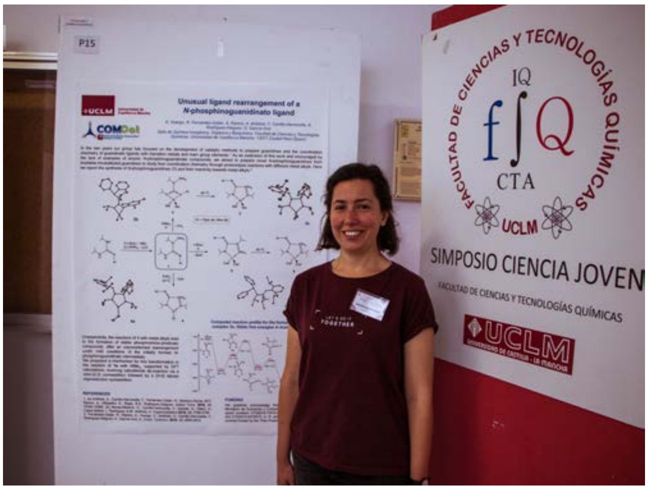

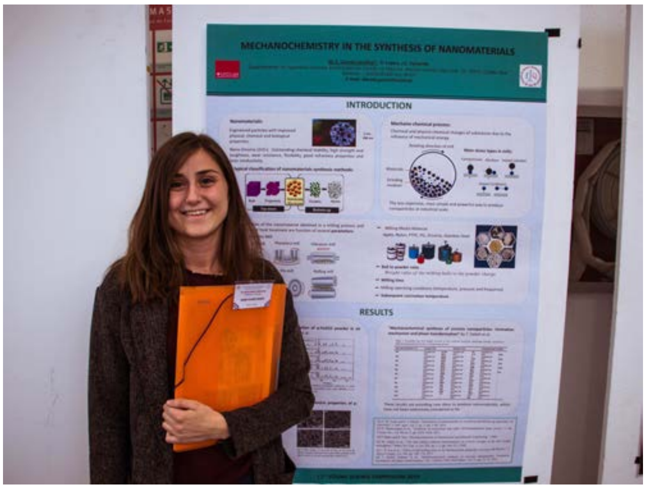

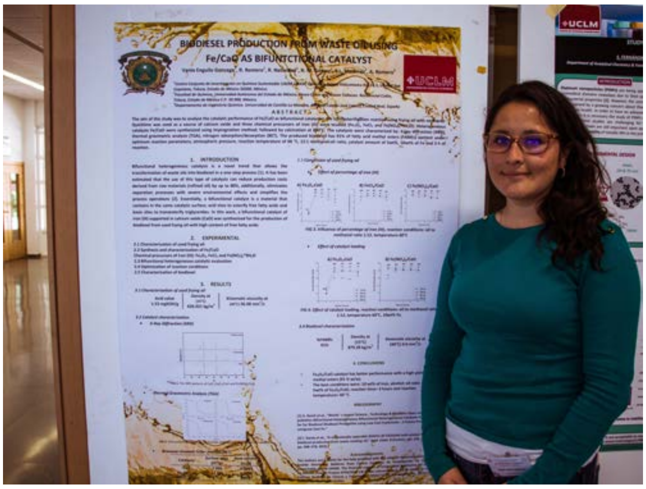
BIODIESEL PRODUCTION FROM WASTE OIL USING
Fe/CaO AS BIFUNCTIONAL CATALYST
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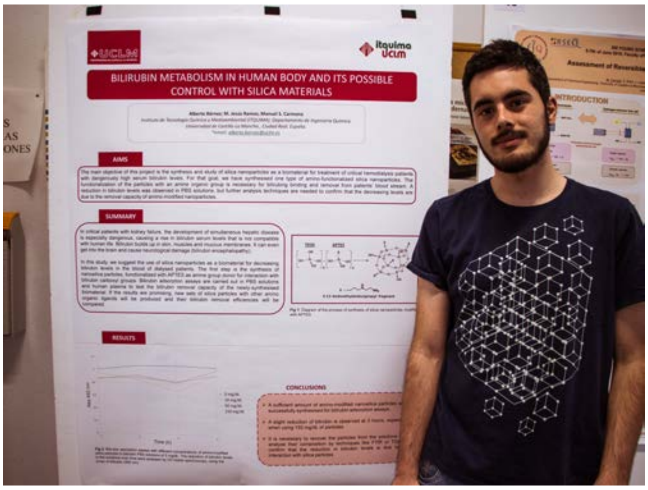
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BILIRUBIN METABOLISM IN HUMAN BODY AND ITS POSSIBLE
CONTROL WITH SILICA MATERIALS
AIMS
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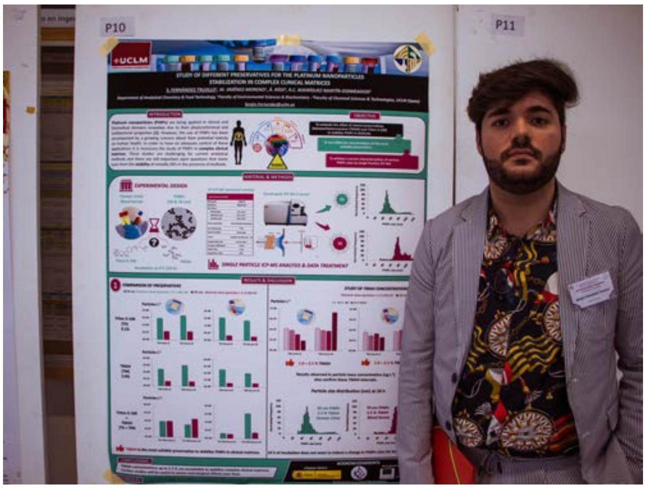
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STUDY OF DIFFERENT PRESERVATIVES FOR THE PLATINUM NANOPARTICLES
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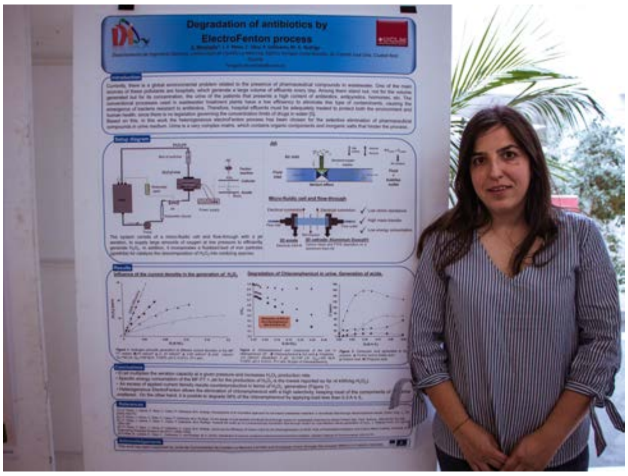
17-β ESTRADIOL DEGRADATION IN AQUEOUS MEDIUM
USING BORON DOPED DIAMOND ELECTRODES
UCLM
Introduction
Results
Aims
Conclusion


Degradation of antibiotics by
ElectroFenton process
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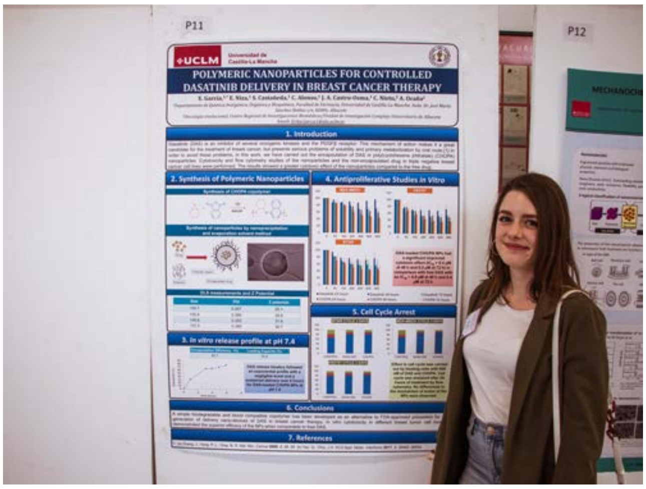
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DASATINIB DELIVERY IN BREAST CANCER THERAPY
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2. Synthesis of Polymeric Nanoparticles
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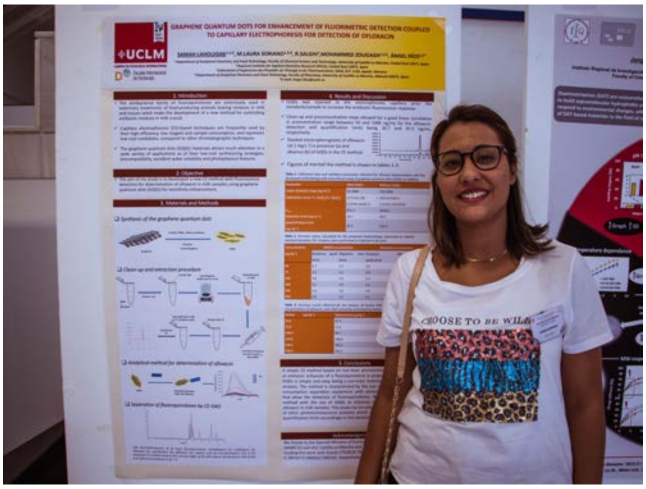
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GRAPHENE QUANTUM DOTS FOR ENHANCEMENT OF FLUORIMETRIC DETECTION COUPLED
TO CAPILLARY ELECTROPHORESIS FOR DETECTION OF OFLOXACIN

ACTO CONMEMORACIÓN SISTEMA PERIÓDICO

Durante el segundo día del XIII Simposio de Ciencia Joven, tuvo lugar un acto de conmemoración del Sistema Periódico moderado por D. Ángel Ríos, decano de a Facultad de Ciencias y Tecnológías Químicas, y con la participación de:

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

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

- María Antonia Herrero Chamorro (RSEQ): "Reseña de la Jornada de la RSEQ"

IV PREMIO CIENCIA JOVEN
II PREMIO CIENCIA JOVEN POSTER

Como en ediciones anteriores, el comité organizador del XIII Simposio de Ciencia Joven hizo entrega del IV Premio Ciencia Joven en el acto de clausura del evento. En esta edición, el premio ha sido otorgado a José Fernando Pérez con el trabajo titulado "New electroFenton reactors for wastewater treatment". También se hizo entrega del II Premio Ciencia Joven al mejor póster a Jorge Leganés Bayón, con el póster titulado "Stimuli responsive hydrogels for drug delivery applications".

¡Enhorabuena a los premiados!

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Javier Toledano Villar "Simbiosis Producciones"

En el próximo número de Molécula...

El próximo número de MOLÉCULA recogerá distintas actividades de la Facultad durante el mes de Julio, conferencias, noticias y curiosidades del Año Internacional del Sistema Periódico.

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