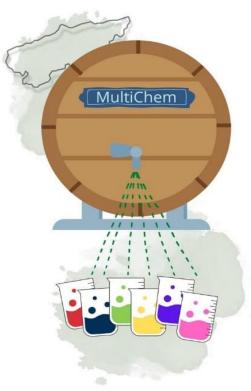
# I PhD Multidisciplinary Chemical Congress







January, 19-20, 2023 Escuela Politécnica de Ingeniería de Gijón (EPI) University of Oviedo



































## Thursday, January 19th

9:00-9:15	Opening Ceremony			
9:15-11:35	Morning session 1 Chairperson: Ma Jesús Lobo Castañón (University of Oviedo)			
9:15-10:15	Plenary Nanobiosensor Devices for Ultrasensitive Diagnostics at the Point-of-need Laura M. Lechuga Gómez Catalan Institute of Nanoscience and Nanotechnology (ICN2-CSIC)			
10:15-10:30	Scharlab			
10:30-10:50	Keynote A Using large 18-membered macrocycles for the complexation of metals with potential radiopharmaceutical applications Charlene María Harriswangler Harriswangler CICA-University of A Coruña			
10:50-11:05	Oral 1 Signal drift in electrochemical, aptamer-based (E-AB) sensors: understanding its mechanism and future challenges  Miguel Aller Pellitero Johns Hopkins University			
11:05-11:20	Oral 2  Main group mechanochemistry: challenges and opportunities for a sustainable society  Javier Fernández Reynes University of Oviedo			
11:20-11:35	Oral 3 Impact of chelate cooperativity on the supramolecular structure of self-assembled nanotubes  Marina González Sánchez  Autonomous University of Madrid			
11:35-12:20	Coffee break - Poster session			
12:20-13:40	Morning session 2 Chairperson: José Manuel Recio Muñiz (University of Oviedo)			
12:20-12:35	Oral 4 Understanding ruthenium-prompted amine fixation: deep insight on Bonding Evolution Theory Daniel Barrena Espés University of Oviedo			
12:35-12:50	Oral 5 Optimizing the process variables for microwave-induced synthesis of iron aerogels Judith González Lavín Institute of Carbon Science and Technology, INCAR-CSIC			
12:50-13:10	Keynote B Influence of vibronic instabilities on the geometry and properties of layered materials Inés Sánchez de Movellán Sáiz University of Cantabria			
13:10-13:25	Oral 6  Determination of methylmercury and inorganic mercury in human hair samples of individuals from Colombia by double spiking isotope dilution and GC-ICP-MS <u>Laura Suárez Criado</u> University of Oviedo			
13:25-13:40	Oral 7 Ruthenium(II) complexes as photosensitizers for photoactivated chemotherapy (PACT) with blue light activation: Photochemical properties and DNAbinding Piedad Herrera Ramírez NanoBIC. University of Barcelona			
13:40-15:30	Lunch			

### 15:30-16:15 Flash poster (FP1)

Chairperson: Marina Ramos Martín

Paula Gómez Meijide (University of Oviedo)	Prostate cancer diagnosis by PSA detection using new electrochemical aptasensors
Clara de Lorenzo González (University of Oviedo)	Hydrogels-based systems for the controlled release of therapeutic agents: an innovative treatment for osteoarthritis
Nayara Carral Sainz (University of Cantabria)	Second principles density functional theory models: a procedure to obtain their tight-binding parameters automatically
<u>Daniel Núñez Díaz</u> (University of Oviedo)	Effect of landfill leachate age on ultrafiltration performance
Ángela Arnosa Prieto (University of Santiago de Compostela)	Effect of Interleukin 4 loaded Citrate Coated Iron Oxide Nanoparticles on Macrophage Polarization for Bone Regeneration
Toraya Fernández Ruiz (University of Cantabria)	Modelling Optical Phenomena via Real-Time TD-DFT using Second-Principles: Measuring the effect of electron-hole interactions
Silvia Vázquez Díaz (Center for Cooperative Research in Biomaterials (CIC biomaGUNE) País Vasco)	Protein-nanoclusters as effective electrocatalyst for the production of inkjet printed paper analytical devices
Montserrat Redondo Velasco (University of Oviedo)	Determination of Chlorine-containing compounds by GC-ICP-MS/MS in plastic-based pyrolysis oil samples
Lucía Pola Fernández (University of Oviedo)	Kraft lignin as a source of carboxylic acids by wet oxidation
Miriam López García (Institute of Carbon Science and Technology, INCAR-CSIC)	A freeze-casted Ni/Fe graphene oxide aerogel as a catalyst for the electrolysis of water
Cristina Méndez López (University of Oviedo)	Halogen determination in liquid samples via optical emission spectroscopy: towards online analysis
Rubén García Soriano (University of Oviedo)	Phosphane and quinoline functionalized amidinato-type heavier tetrylenes: A new class of ligands
Raúl Llamas Unzueta (Institute of Carbon Science and Technology, INCAR-CSIC)	Stacked Archimedean spirals reactor with porous carbon walls, made from 3D printed sacrificial PLA moulds
Nieves García Ledesma (University of Salamanca)	One-Pot diastereoselective synthesis of indolizidine and pyrrolo-[1,2-a]azepine heterocycles

### 16:15-17:05 Afternoon session 1

Chairperson: Rosa Ma Sainz Menéndez (University of Oviedo)

#### 16:15-16:30 Oral 8

Development of a paste extruder system and production of Ni-electrodes by diw for water splitting

Pablo Rodríguez Lagar

Institute of Carbon Science and Technology, INCAR-CSIC

#### 16:30-16:45 Oral 9

Albumin-based nanomaterials: a novel treatment for triple-negative breast cancer <u>Victoria García Almodóvar</u> King Juan Carlos University

#### 16:45-17:05 Keynote C

Determination of endogenous proteins in individual cells from an in vitro model by elemental mass spectrometry

Paula Menero Valdés University of Oviedo

#### 17:05-17:50 Coffee break – Poster session

## 17:50-18:35 Afternoon session 2

Chairperson: Alejandro Presa Soto (University of Oviedo)

#### 17:50-18:05 Oral 10

Discrimination of TNT and its metabolites in the environment using voltammetric sensors, modified with molecularly imprinted polymers

Yohana López Aparicio

Autonomous University of Barcelona

#### 18:05-18:20 Oral 11

Scalable divergent synthesis of diterpenoid pyrones

Olaya García Pedrero University of Oviedo

#### 18:20-18:35 Oral 12

Perylene-based chromonic self-assemblies for the preparation of hierarchically porous silica and carbon nanofibers

Adrià Pérez Calm

Institute of Advanced Chemistry of Catalunya (IQAC)-CSIC

#### 18:35-19:20 Flash poster (FP2)

Chairperson: Daniel Núñez Díaz

Andrés Suárez Priede	ICP-MS based characterization of biogenic SeNPs and			
(University of Oviedo)	evaluation of their potential antibacterial activity			
Juan Rivas-Santisteban	Characterization of a chemical bias shaping microbial			
(National Biotechnology	functional evolution			
Center (CNB-CSIC))				
Leonardo Amaral	Magnetic MoS <sub>2</sub> based nanocomposites for the			
(King Juan Carlos University)	photodegradation of pesticides			
Ana da Lama Vázquez (CICA-	One-step synthesis of BODIPY dyes and analogues			
University of A Coruña)	under microwave irradiation			
Alejandro Rodríguez Penedo	Determination of GFAP biomarker in human serum using			
(University of Oviedo)	metal nanoclusters as label by elemental mass			
	spectrometry and cyclic voltammetry			
Raquel Pérez Guevara (CICA-	Synthesis of benzannulated spiroketals by indium-			
University of A Coruña)	catalyzed intramolecular double dihydroalkoxylation of			
	alkyne diols			
Helena Pérez del Pulgar	A three-pollutant simultaneous photodegradation.			
Villena (King Juan Carlos	$BiOX_xY_{1-x}$ (X=Br or CI; Y=I) as a photocatalytic solution			
University)	for water treatment			
<u>David Valero Calvo</u> (University of Oviedo)	Detection of MMP-9 biomarker using nanochannels			
Uxía Gómez Bouzó (University	The goal to create new vitamin D analogs with selective			
of Vigo)	biological activity			
Marcos López Aguilar	Design of a hybrid one-pot tandem combination of the			
(University of Oviedo)	Cu(II)-catalyzed oxidation of alcohols with an			
	enantioselective organocatalyzed aldol reaction			
David González Lizana (King	Very efficient organo-zinc scorpionates for the CO <sub>2</sub>			
Juan Carlos University)	fixation into a variety of cyclic carbonates			
Helena Fernández Piedra	Halogen-bonding assisted generation of vinyl radicals:			
(University of Oviedo)	stereoselective cross coupling between thiols and vinyl			
	halides			
Lourdes del Álamo Rodríguez	Supramolecular self-assembly of metal-metal bonded			
(Complutense University of	species			
Madrid)	Ostalistic malarara matica manatica (1)			
Dario Coto Menéndez	Catalytic cyclopropanation reactions with α-silyl-,			
(University of Oviedo)	germanyl- and stannyl carbenes generated from			
Datricia Caraía Martína-	cyclopropenes			
Patricia García Martínez	Synthesis of new phenethylamine-azulene conjugates			
(University of Oviedo)	via regioselective ring opening of 2-aryl- <i>N</i> -sulfonyl aziridines			
	L AZINONIES			

## Friday, January 20th

	Friday, January 20th					
9:00-10:50	Morning session 3					
	Francisco Calderón Celis (University of Oviedo)					
9:00-9:20	<b>Keynote D</b> Effect of H <sub>2</sub> S in biogas composition on the production of H <sub>2</sub> by sorption enhanced steam reforming (SESR) <u>Alma Capa Tamargo</u> Institute of Carbon Science and Technology, INCAR-CSIC					
9:20-9:35	Oral 13  Development of new pH-responsive delivery systems  Isabel Coloma Manjón-Cabeza  Complutense University of Madrid					
9:35-9:50	Oral 14  MD and DFT combined simulations  Jorge Suárez Recio  University of Oviedo					
9:50-10:05	Oral 15  Development of carbon materials for Na-ion capacitors  Sara Payá González  Institute of Carbon Science and Technology, INCAR-CSIC					
10:05-10:20	Oral 16 Graphene aerogels as nanomaterials for electrochemical detection of biomarkers  Mario Sánchez Suárez Institute of Carbon Science and Technology, INCAR-CSIC					
10:20-10:35	Oral 17 Compositional similarities and differences between North West Africa (NWA) 2975, 10628 and 1950 Martian Shergottites Iratxe Población Concejo University of País Vasco (EHU/UPV)					
10:35-11:35	Coffee break – Poster session					
11:35-13:40	Morning session 4					
	Chairperson: Félix Rodríguez Iglesias (University of Oviedo)					
11:35-11:55	Keynote E An original way to synthesize (Z)-β-silylenamides by silylium-catalyzed carbosilylation of ynamides Paz Yepes García University of Oviedo					
11:55-12:10	Oral 18  TiO <sub>2</sub> /SnO <sub>2</sub> – silver clusters hybrid nanomaterials for catalytic photodegradation of micropollutants  María Moreno Pérez  University of Santiago de Compostela					
12:10-12:25	Oral 19 Development of on-site sensors for quality control in agri-food Candela Melendreras García University of Oviedo					
12:25-12:40	Oral 20  "Vermellogens" and the development of CB[8]-based supramolecular switches using pH-responsive and non-toxic viologen analogues <u>Liliana Inés Barravecchia Prado</u> CICA-University of A Coruña					
12:40-12:55	Oral 21 The enhancing effect of iron on the activity of Ni and Ni/Fe graphene-based catalysts for the electrolysis of water  María González Ingelmo Institute of Carbon Science and Technology, INCAR-CSIC					
12:55-13:40	Plenary Chemistry facing the challenges of our era Amador Menéndez Velázquez Idonial					
13:40-14:00	Closing ceremony					