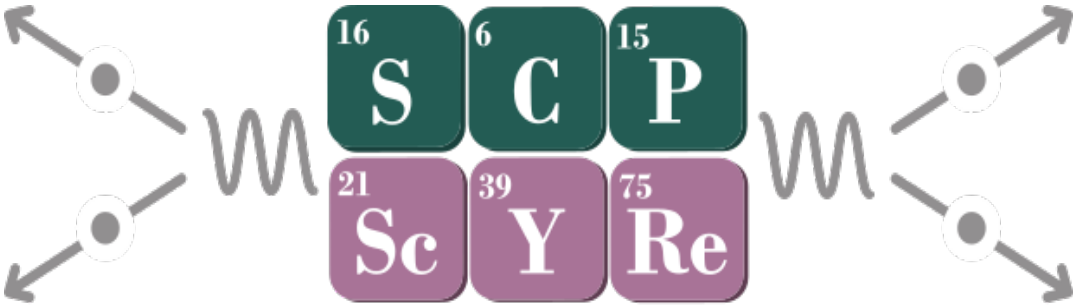
BOOK OF ABSTRACTS



I Symposium on Chemical and Physical Sciences for Young Researchers

ONLINE

Murcia, 22nd-23rd October 2020

ORGANIZER

Faculty of Chemistry

University of Murcia

BOOK OF ABSTRACTS I SYMPOSIUM ON CHEMICAL AND PHYSICAL SCIENCES FOR YOUNG RESEARCHERS

FACULTY OF CHEMISTRY, UNIVERSITY OF MURCIA 2020

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I Symposium on Chemical and Physical Sciences for Young Researchers

Murcia, 22nd-23rd October 2020

Welcome

On behalf of the organizing Committee of the I Symposium of Chemical and Physical Sciences for Young Researchers, we want to thank you for your participation. This conference provides an online forum to share scientific and technological knowledge produced around Faculty of Chemistry of the University of Murcia. The scientific program includes 2 plenary lectures given by national young scientists in the field of Chemistry and Physic and 66 communications, structured in 20 oral communications and 46 posters, 13 of which have been selected for presentation as "flash communication". The celebration of this congress was born aiming at connecting master and doctorate students with each other so that they can establish personal and scientific connections, as well as learn about the other research fields developed around them.

The situation due to the COVID-19 forced us to postpone the I Symposium of Chemical and Physical Sciences for Young Researchers in April 2020. For the new dates set in October 2020, our intention was to celebrate this Symposium in the facilities of Faculty of Chemistry but due to the current situation it was decided to celebrate it online. In this way, students would not miss out on the opportunity to learn about all the scientific research taking place in their environment and they can train the presentation of research results at scientific conferences.

From the organizing committee we would like to thank all the companies and institutions that have collaborated giving economic support to this Symposium. Five different prizes, 2 prizes for the best oral communications, 2 prizes for the best poster and 1 prize for the best flash poster presentation, will be awarded. These awards are sponsored by the UMU chairs of Hidrogea, Villapharma and Estrella de Levante and by Science Academy of the Region of Murcia.

On behalf of the organizing committee I want to give you a warm welcome to the online event, sincerely thanking you for your participation and wishing that these days are very profitable.

The Organizing Committee

I Symposium on Chemical and Physical Sciences for Young Researchers

Murcia, 22nd-23rd October 2020

Organizing Committee

José Juan Fernández Melgarejo (PhD in Physics)

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Ángela Molina Gómez (Physical Chemistry)

Juan Muñoz Madrid (Electromagnetism and Electronics)

Carmen Pérez Sirvent (Agricultural Chemistry, Geologý and Edaphology)

Invited speakers

Dr. Esperanza López

CSIC-UAM – Instituto de Física Teórica (IFT), Madrid

Tenured Scientist of the Spanish National Research Council (CSIC)

PhD in Physics at the Autonomous University of Madrid (1995)

Postdoctoral researcher at KITP (Santa Barbara), TU-Vienna, CERN, Max Planck Institute for Gravitational Physics and Ramón y Cajal" researcher at the Department of Theoretical Physics of the UAM (2002-2006)

Current research: Quantum field theory and gravity

Jesús Campos

CSIC-University of Seville, Sevilla

Tenured Scientist of the Spanish National Research Council (CSIC)

PhD in Chemistry at the University of Seville (2012)

Postdoctoral researcher at the Universities of Yale, Oxford, and Seville (Marie Curie IF fellowship)

Current research: New strategies in cooperative bond activation and catalysis within an ERC Starting Grant project (2017)

Schedule

Morning 22 October

9.30	**Opening ceremony** *Dr. Mª Senena Corbalán García (Vice-Rector for Research and Internationalization – UM)* *Dr. Pedro Lozano Rodríguez (Dean of the Faculty of Chemistry - UM)*
10.00	**Invited Talk** *"Living at the Frontier: An introduction to the Holographic Principle"* *Dr. Esperanza López (CSIC-UAM)*
11.00	**Oral communications** O-01 to O-04
Break	
12.30	**Oral communications** O-05 to O-08

Afternoon, 22 October

15.30	**Oral communications** O-09 to O-12
16.30	**Flash oral presentations** F-01 to F-06
17.00	**Poster exhibition** P-01 to P-17
Break	
18.00	**Poster exhibition** P-18 to P-33

Morning 23 October

9.00	**Invited Talk** *"Bimetallic Frustated Systems as Cooperative Entities for Bond activation"* *Dr. Jesús Campos (CSIC- Univ. Seville)*
10.00	**Oral communications** O-13 to O-16
Break	
11.30	**Oral communications** O-17 to O-20
12.30	**Flash oral presentations** F-07 to F-13
13.15	**Round Table: "Investigación y desarrollo en el mundo empresarial"** *Gustavo Calero (Head of Chairs of the Suez Water Spain Group)* *Sebastián Javaloy Pintado (Responsible for the technical department at LINASA)* *Juan Ignacio Cacho Aparicio (*Scientific & Regulatory Affairs at Health Tech Bioactives) *Rosa María Peñalver Soler (*Analytical Specialist at SABIC)
14.00	**Awards & Closing ceremony**

Scientific program

Thursday, 22nd October 2020

9.30-10.00 h: **Opening ceremony**

- Vice-Rector for Research and Internationalization (UM)
Dr. María Senena Corbalán García

- Dean of the Faculty of Chemistry (UM)
Dr. Pedro Lozano Rodríguez

10.00-11.00 h: **Invited talk (I)**

"Living at the Frontier: An Introduction to the Holographic Principle"
Dr. Esperanza López (CSIC-UAM - Instituto de Física Teórica (IFT), Madrid)

11.00-12.00 h: **Oral communications 1**

O-01 Biocatalytic synthesis of panthenyl monoesters in ionic liquids and deep eutectic solvents
E. Alvarez, R. Villa, S. Nieto,1 A. Donaire, and P. Lozano

O-02 D-brane Dynamics
Juan R. Balaguer

O-03 Towards novel photodynamic anticancer agents: cyclometalated Ru(II) complexes activated by green-light
F. J. Ballester, E. Ortega, M.D. Santana, J. Ruiz

O-04 Making computational chemistry based drug discovery accessible via web and improving its performance with HPC
Antonio-Jesús Banegas-Luna, Horacio Pérez-Sánchez

12.00-12.30: **Break**

12.30-13.30 h: **Oral communications 2**

O-05 Infrared study of the secondary structure of silk fibroin during nanoparticles production
G. Carissimi, M.G. Fuster, M.G. Montalbán, M. Chaala,1 G. Víllora and A. Barth

O-06 Stability of complex polysaccharide-based nanocomposites as a function of pH and ionic strength
M. Collado-González, M.C. Ferreri, A.R. Freitas, A.C. Santos2, N.R. Ferreira, G. Carissimi, J.A.D. Sequeira, F.G. Díaz Baños, G. Villora, F. Veiga and A. Ribeiro

O-07 Simulating the physical processes underlying proton therapy
Pablo de Vera, Isabel Abril, Rafael García-Molina,

O-08 Analytical theory for the square wave and cyclic voltammetric responses of electron transfers with non-unity stoichiometry
Gómez-Gil, J.M., Laborda, E., Molina, A.

13.30-15.30 h: **Lunch time**

15.30-16.30 h: **Oral communications 3**

0-09 Small molecular azaphenacene hole transporting materials in inverted hybrid perovskite solar cells.
P. Gómez, M. Más Montoya, D. Curiel.

O-10 Study of Carbamoyl phosphate synthase of E. coli regulation.
G. Lozano-Terol, J. Gallego-Jara, M. Cánovas and T. de Diego.

O-11 Design and validation of a method to measure laccase activity on methoxyphenolic food additives
J. Manzano-Nicolas, F. Marin-Iniesta, A. Taboada-Rodriguez, J. Tudela-Serrano, P. Garcia-Molina, J.L. Muñoz-Muñoz

O-12 Acoustic situation of the industrial noise in wastewater treatment plant
María del Mar Durán, Antonia Baeza, Mercedes Llorens and Miriam Sánchez

16.30-17.00 h: F**lash communications 1**

F-01 Design of a fluorescent α-glucosidase biosensor based on nanoparticles composed of lipid and conjugated polymer
Y. Alacid, M. Rubio, R. Mallavia, M.J. Martínez-Tomé, C.R. Mateo

F-02 Inversion barriers in σ3λ3-pnictogen compounds
A. García Alcaraz, A. Espinosa Ferao

F-03 Comparison of headspace gas chromatography – mass spectrometry and ion mobility spectrometry for the classification of virgin olive oils
M. García-Nicolás, N. Arroyo-Manzanares, L. Arce, M. Hernández-Córdoba, P. Viñas.

F-04 Bis-cyclometalated fluoro(aryl) Pt (IV) complexes
Juan Carlos López López, Delia Bautista, Pablo González Herrero

F-05 Development of co-poly-(methyl vinyl ether-alt- maleic anhydride) derivates nanocarriers to improve administration of different drugs
A.Mira, C.Sainz-Urruela, A.Falcó, R.Mallavia

F-06 Stability of Oxyresveratrol Encapsulated with Beta-cyclodextrin in Food Models
Silvia Navarro-Orcajada, Adrián Matencio, Irene Conesa, Iván Muñóz-Sánchez, Lorena Laveda-Cano, Desiré Cano-Yelo, Francisco García-Carmona, José Manuel López-Nicolás

17.00-17.45 h: **Poster communications 1**

P-01 Determination of cadmium in used engine oil, gasoline and diesel by electrothermal atomic absorption spectrometry using magnetic ionic liquid-based dispersive liquid-liquid microextraction
M. A. Aguirre, A. Canals, I. López-García, M. Hernández-Córdoba

P-02 Multi-emission fluorescent nanoplatforms based on lipid conjugated polymer complexes
Y. Alacid, M. Rubio, R. Mallavia, M.J. Martínez-Tomé, C.R. Mateo

P-03 Photocatalytic Degradation of Two Neonicotinoid Insecticides in Agro-Wastewater. Reuse for Irrigation of Pepper Crop
M. Aliste Fernández, J. Fenoll Serrano, S. Navarro García

P-04 Catechol biosensor based on lyophilised mushroom for the analytical determination of kojic acid.
Carmen M. Almagro, Maria S. Garcia,Joaquin A. Ortuño

P-05 Green copolymerization of carbazole-substituted epoxide with vinyl monomer by an eco-catalyst
F. Bekkar, F. Bettahar, R. Meghabar, M. Hamadouch2, L.Ruiz-Rubio

P-06 Effect of Degumming Methods on the Structure and Properties of Silk Fibroin Nanoparticles
G. Carissimi, A. A. Lozano-Pérez, M.G. Montalbán, S.D. Aznar-Cervantes, M.G. Fuster, J.L. Cenis and G. Víllora

P-07 Untargeted headspace gas chromatography – Ion mobility spectrometry analysis for detection of adulterated honey
A. Castell, N. Arroyo-Manzanares, M. García-Nicolás, N. Campillo, P. Viñas, I.López-García, M. Hernández-Córdoba

P-08 Study of the Reactivity of 2-Azidoisocyanobenzenes
G. Cutillas-Font, A. Pastor, M. Alajarín

P-09 Copolymerization of maleic anhydride with vinyl acetate by maghniteH+
F.Bettahar, F. Bekkar, M. Ferahi, L.Ruiz

P-10 Insertion reactions of insaturated molecules into the Pd–C bond of seven-member palladacycles
S. Fernández, I. Saura-Llamas

P-11 Improving anticancer therapy by Naringenin-Loaded Silk Fibroin Nanoparticles
M.G. Fuster, G. Carissimi, M.G. Montalbán, M.A. Pujante, M. Chaala and G. Víllora

P-12 Green synthesis of Naringenin-Loaded Silk FibroinNanoparticles
M.G. Fuster, G. Carissimi, M.G. Montalbán, M. Chaala, M. A. Pujante and G. Víllora

P-13 A green analytical method for the determination of nitrosamine impurities in pharmaceutical products
Claudia Giménez Campillo, Marta Pastor Belda, Natalia Campillo, Manuel Hernández-Córdoba and Pilar Viñas

P-14 Tea-derivated catechins with antitumor properties
Rebeca González Guerrero, Román Martí Díaz, Luis Sánchez del Campo Ferrer, Fernanda Montenegro Arce, J. Neptuno Rodríguez López.

P-15 New arene-complexes of Os(II) containing benzothiazole-based ligands. Study of its cytotoxic properties
A. Hernández-García, F.J. Ballester Hernández, M. D. Santana Lario, D. Bautista Cerezo, J. Ruiz López

P-16 Development of palladium-catalyzed coupling cascade reactions through intramolecular carbopalladation of alkenes
P. Herrera, J. A. García-López

P-17 Synthesis and characterization of Pt(IV) complexes with cyclometalated N-heterocyclic carbene and 2-arylpyridine ligands
A. Jiménez-García, Á. Vivancos, D. Bautista, P. González-Herrero.

18.00-18.45 h: **Poster communications 2**

P-18 Synthesis of novel, patentable scaffolds as potential highly selective Wee-1 kinase inhibitors
J. Jimenez-Bernad, JM. Villalgordo

P-19 New C^N cyclometalated platinum(II) complexes derived from N^O donor azo ligands as potential anticancer agents
Antonio Linero Artiaga, Venancio Rodríguez Hernández, Enrique Ortega Forte, José Ruiz López.

P-20 Reduction of air requirements and redesign of the biological aeration system, actions for energy optimization WWTP
Ana Belén Lozano Avilés, Francisco del Cerro Velázquez, Mercedes Llorens Pascual del Riquelme

P-21 Study of comparison between spatial distribution and personal exposure to urban air pollutants
María del Mar Durán, Antonia Baeza, Enrique González and Mercedes Llorens

P-22 Synthesis and characterization of new Ir(III) and Rh(III) halfs and wich complexes for cancer treatment.
A. Marco, G. Vigueras, N. Cutillas, J. Ruiz

P-23 Effect of metformin on melanoma cells
Román Martí Díaz, Rebeca González Guerrero, María Fernanda Montenegro Arce, Luis Sánchez del Campo Ferrer, José Neptuno Rodríguez López

P-24 Development of a potentiometric electronic tongue for the quality control of irrigation water
M. Miras, J. A. Ortuño, M. S. García

P-25 Analysis of the behavior of silk fibroin nanoparticles under DLVO theory
M.G. Montalbán, G. Carissimi, M G. Fuster, M. Chaala, F. Pedreño and G. Víllora

P-26 Effect of Ionic Strength on the Size of Silk Fibroin Nanoparticles
M.G. Montalbán, G. Carissimi, M G. Fuster, M. Chaala, C. Serrano and G. Víllora

P-27 Study of the metabolism of an anabolic steroid by combined approaches of ion mobility (LC-Q-TWIN-TOF MS) and molecular modelling
Tamara Moya Cavas, Jérôme Graton, Gaud Dervilly and Jean-Yves Le Questel

P-28 Speciation of low levels of thallium in waters using a magnetic nanocomposte and electrothermal atomic absorption spectrometry (ETAAS)
M.J. Muñoz Sandoval, M. Hernández Córdoba, I. López García

P-29 Determination of furvina® in medicated nail lacquers for onychomycosis treatment by direct UV/Vis spectrophotometry and liquid chromatography with diode array detection
Zenia Perez Rodriguez, Natalia Campillo, Pilar Viñas López-Pelegrín, Manuel Hernández-Córdoba, Yaset Rodríguez-Rodríguez, Orlando Álvarez, Zenaida Rodriguez Negrin,

P-30 Synthesis and study of [2] rotaxanes with geminal substituents in the benzylic positions of the macrocycle
J. Puigcerver, A. Martínez-Cuezva, M. Alajarín, J. Berná

P-31 Synthesis and characterization of polymeric nanostructures for drug delivery
M. Rubio-Camacho, Y. Alacid,1 A. Mira, A. Falcó,1 M.J. Martínez-Tomé, R. Mateo and R. Mallavia

P-32 Development of a platform to analyse human exhaled volatile organic compounds: workflow for biomarker discovery
R.A. Sola Martínez, G. Lozano Terol, J. Gallego-Jara, M. Cánovas Díaz and T. de Diego Puente.

P-33 Characterization of floral origin of honey samples using headspace gas chromatography – ion mobility spectrometry
F. Zafra, M. García -Nicolás, N. Arroyo-Manzanares, Pilar Viñas

Friday, 23rd October 2020

9.00-10.00 h: **Invited talk (II)**

"Bimetallic Frustrated Systems as Cooperative Entities for Bond Activation"
Dr. Jesús Campos (CSIC-University of Seville, Sevilla)

10.00-11.00 h: **Oral communications 4**

O-13 Improvement of Multiphoton Microscopy Images of the Living Human Eye through Deconvolution
R. M. Martínez-Ojeda, L. M. Mugnier, P. Artal and J. M. Bueno

O-14 Gold (I) and Gold (III) Complexes Containing Perfluoroalkyl and Perfluoroalkanediyl Ligands
A. Portugués, J. Gil-Rubio, I. López-García, J. Jiménez-Bernad, L.González-García, D. Bautista.

O-15 Dispersive liquid-liquid microextraction for capsaicinoid compounds preconcentration in human urine analysis by liquid chromatography and quadrupole time-of-flight mass spectrometry
María Consolación Rodríguez Palazón, Natalia Campillo, Natalia Arroyo Manzanares, Pilar Viñas and Manuel Hernández-Córdoba

O-16 Fluorescent and thermosensitive nanoparticles for drug delivery and bioimaging
M. Rubio-Camacho, Y. Alacid,1 R. Mallavia, M.J. Martínez-Tomé, and C.R. Mateo

11.00-11.30 h: **Break**

11.30-12.30 h: **Oral communications 5**

O-17 Design and Synthesis of β-Lactam Rotaxanes incorporating a Removable Macrocycle
A. Saura-Sanmartin, M. Tomas-Martinez, A. Martinez-Cuezva, M. Alajarin, J. Berna

O-18 Fine Particulate Matter impacts on Mortality in Europe-Present and Future mitigation renewables energy scenario
P. Tarín-Carrasco, U. Im, L. Palacios-Peña, P. Jiménez-Guerrero

O-19 In-situ measurements of collisionless plasmas, from the Earth's magnetosphere to the Solar corona
S. Toledo-Redondo

O-20 Synthesis and biological evaluation of new N-substituted 9- nitro-12,14-dioxo-9,10-dihydro-9,10-[3,4]epipyrroloanthracen- 13-yl derivatives
Maria Vera, James Mc Keown, Mary J. Meegan.

12.30-13.15 h: **Flash communications 2**

F-07 Novel osmium-based proteosynthesis inhibitor reduces in vivo tumor growth and extends C. Elegans lifespan.
Enrique Ortega, Francisco J. Ballester, Alba Hernández-García, Samanta Hernández-García, M. Alejandra Guerrero-Rubio, M. Dolores Santana Fernando Gandía-Herrero, and José Ruiz

F-08 Influence of biochar on soil C and N biogeochemical cycles
M.B. Pascual, M.A. Sánchez-Monedero, M.L. Cayuela

F-09 Photogeneration of Stable Bis-cyclometalated Platinum(IV) Hydrides and Alkyne Insertion Reactions
D. Poveda, A. Vivancos, D. Bautista, P. González-Herrero

F-10 Factors affecting ring strain in saturated three-membered heterocycles bearing one group 13-16 heteroatom
A. Rey Planells, A. Espinosa Ferao

F-11 Iridium (III) Anticancer Agents Generating Superoxide Anion Radicals: Overcoming the Achilles' Heel of Photodynamic Therapy
G. Vigueras, V. Novohradsky, J. Pracharova, N. Cutillas, C. Janiak,3 H. Kostrhunova, V. Brabec, J. Ruiz, J. Kasparkova.

F-12 Enzymatic synthesis of Fatty Acid Solketal Esters using Sponge Like Ionic Liquids.
Rocio Villa, Elena Álvarez, Susana Nieto, Antonio Donaire, Pedro Lozano

F-13 Cascade carbopalladation reactions of skipped dienes for the synthesis of [4,5]-spirooxoindoles
M. Pérez-Gómez, H. Azizollahi, V. Mehta, J.-A. García-López

13.15-14.00 h: **Round table**

"Investigación y desarrollo en el mundo empresarial"

- Head of Chairs of the Suez Water Spain Group
Gustavo Calero
- Responsible for the technical department at LINASA
Sebastián Javaloy Pintado
- Scientific & Regulatory Affairs at Health Tech Bioactives.
Juan Ignacio Cacho Aparicio
- Analytical Specialist (Technology and Innovation Department) at SABIC
Rosa María Peñalver Soler

14.00-14.30 h: **Award & Closing ceremony**

- Dean of the Faculty of Chemistry (UM)
Dr. Pedro Lozano Rodríguez

Invited communications

Living at the Frontier:

An Introduction to the Holographic Principle

E. López

[1] *Instituto de Física Teórica, Universidad Autónoma de Madrid, Cantoblanco, Madrid,Spain*

esperanza.lopez@uam.es

Two conceptual revolutions redefined physics in the past century. The laws of Nature at small scales were uncovered, giving rise to quantum physics. Einstein stated the theory of general relativity, changing radically our understanding of space and time, and the universe itself. General relativity predicts the existence of black holes, fascinating objects whose existence has been beautifully confirmed by recent observations. Black holes hide in their interior a singularity. A full understanding of black holes, and thus also gravity, requires therefore the unification between general relativity and quantum physics.

The holographic principle arises as a direct consequence of the most basic principles in both theories. Although it does not provide a quantum theory of gravity, it is an important step towards it. It proposes that gravity in a space-time region can be fully described by a theory without gravity living on its boundary. In this way, the boundary theory acts as a hologram of the interior.

In this talk I will present an introduction to the holographic principle, its motivations and implications.

I Symposium on Chemical and Physical Sciences for Young Researchers

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Bimetallic Frustrated Systems as Cooperative Entities for Bond Activation

Jesús Campos[1]

[1] *Instituto de Investigaciones Químicas (IIQ). Consejo Superior de Investigaciones Científicas (CSIC) and University of Sevilla. Avenida Américo Vespucio 49, 41092 Sevilla (Spain).*

jesus.campos@iiq.csic.es

Keywords: bimetallic complexes • frustrated Lewis pair • bond activation

In the early 80s Chisholm proposed that "all the types of reactions which have been studied for mononuclear transition metal complexes will also occur for dinuclear transition metal complexes".[1] Almost 40 years later, continued research on the area of bimetallic systems has proven that claimed and gone beyond.[2] Regarding catalytic applications, there are many important transformations that require the concerted action of pairs of active metal sites, paralleling what is often found in metalloenzymes. We recently started to investigate late-transition bimetallic systems characterized by the use of sterically hindered phosphine ligands containing a terphenyl (2,6-C_6H_3-Ar_2) substituent.[3] In the last years we have analyzed the effect of the stereoelectronic properties of these terphenyl phosphine ligands in the competition between the formation of M-M bonds versus M···M frustration and investigated the reactivity derived from a variety of bimetallic systems, an example of which is depicted in the Figure 1.[4] Our results pertaining the reactivity and potential in catalysis of a number of bimetallic pairs based on late-transition metals and group 12 elements will be discussed.

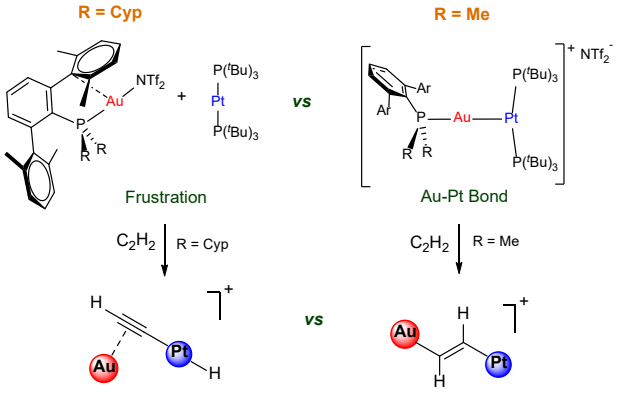

Figure 1. Example of bimetallic FLP-type reactivity

Acknowledgements

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References

[1] Chisholm, M. H. Ch. 2, Reactivity of Metal-Metal Bonds, *ACS Symposium Series*, **1981**, 155.
[2] Campos, J. *Nat. Rev. Chem.* **2020**, DOI: 10.1038/s41570-020-00226-5.
[3] (a) Moreno, J. J.; Espada, M. F.; Krüger, E.; López-Serrano, J.; Campos, J.; Carmona, E. *Eur. J. Inorg. Chem.* **2018**, 2309; (b) Moreno, J. J.; Espada, M. F.; Campos, J.; López-Serrano, J.; Macgregor, S. A.; Carmona, E. *J. Am. Chem. Soc.* **2019**, *141*, 2205.
[4] (a) Campos, J. *J. Am. Chem. Soc*. **2017**, 139, 2944; (b) Hidalgo, N.; Moreno, J. J.; Pérez-Jiménez, M.; Maya, C.; López-Serrano, J.; Campos, J. *Chem. Eur. J.* **2020**, *26*, 5982.

Oral communications

Biocatalytic synthesis of panthenyl monoesters in ionic liquids and deep eutectic solvents

E. Alvarez,[1] R. Villa,[1] S. Nieto,[1] A. Donaire,[2] and P. Lozano[1]

[1] *Department of Biochemistry and Molecular Biology B and Immunology, Faculty of Chemistry, University of Murcia. Murcia E-30100, Spain*
[2] *Department of Inorganic Chemistry, Faculty of Chemistry, University of Murcia. Murcia. E-30100, Spain.*

elena.alvarezg@um.es

Keywords: panthenol; biocatalysis; Ionic Liquids; Deep eutectic solvents.

Panthenol, also called pro-vitamin B5, exhibits therapeutic, cosmetic and cosmeceutical properties being usually present in cosmetic products (*e.g.* hair conditioners, body cream, etc.). However, due to its high hydrophilicity, its residence time in the skin and hair is very short. Panthenol esters (*e.g.* panthenyl triacetate) remain longer in the skin, improving its application as a cosmeceutical agent.

Biocatalysis is the most selective strategy for the synthesis of chemical compounds, being one of the pillars in the development of the Green Chemistry. In this context, it has been described a lot of applications with cosmetic and pharmaceutical interest.[1,2] However, to date panthenyl esters are produced using organic solvents, that compromise the sustainability of the processes. The aim of this work has been the development of sustainable approaches for integrate the selective biocatalytic synthesis and separation of panthenyl monoesters (PMEs). In this sense, two methodologies have been developed. The first one was based on the combination of a lipase with different ILs to carry out the selective synthesis of these compounds, allowing the full recuperation of the biocatalyst/IL system for further reuse. Alternatively, the suitability of panthenol to form deep eutectic solvents (DESs) with fatty acids has been described. Additionally, these mixtures showed to be excellent reaction media for the biocatalytic synthesis of PMEs, since high yields (>80%) and selectivities (>93%) were obtained and the enzyme was active and stable during seven operational cycles of reuse.

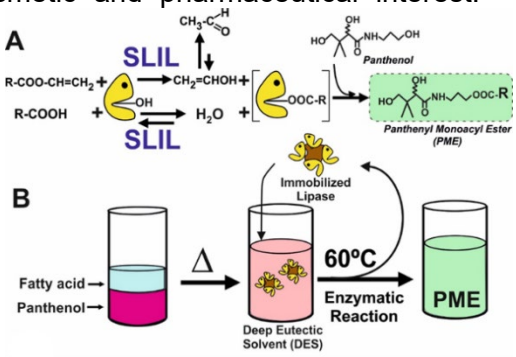

Figure 1. Scheme of the immobilized lipase-catalysed synthesis of PMEs by direct esterification of fatty acids with panthenol in **A)** SLIL. **B)** DESs.

Acknowledgements

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D-brane Dynamics

Juan R. Balaguer[1]

[1] Departamento de Física, Universidad de Murcia, Campus de Espinardo, 30100 Murcia, Spain

juanramon.balaguer@um.es

Keywords: • Quantum Field Theory • Particle Physics • Yang Mills • String Theory

Within the framework of string theory, Dp-branes are dynamical objects where open strings must end. A Dp-brane is extended along p spacetime dimensions and develops a (p+1)-dimensional volume in spacetime when time evolution is considered. For example, a D0-brane consists of a particle whose evolution is represented by a world-line in spacetime.

Firstly, as a generalization of the action of a relativistic particle, we will introduce the action that describes the motion of a Dp-brane in an arbitrary spacetime.

In this work, we will study the dynamics of a stack of N parallel D3-branes in a 10-dimensional spacetime. We will consider two cases: (i) D3-branes in a flat Minkowski background, and (ii) D3-branes in curved spacetime with non-vanishing electromagnetic fields. We will show that in the former case, the effective description of the brane dynamics is equivalent to 4-dimensional maximally supersymmetric Yang-Mills theory with U(N) gauge symmetry. On the other hand, in the latter case, the effective action corresponds to a deformation of super Yang-Mills theory. Such deformations, which consist of the presence of new terms in the Lagrangian (mass terms, Yukawa couplings, etc.) and coupling constants which are spacetime-dependent, only allow for the conservation of a partial amount of supersymmetry.

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I Symposium on Chemical and Physical Sciences for Young Researchers

Murcia, 22nd-23rd October 2020

O-03

Towards novel photodynamic anticancer agents: cyclometalated Ru(II) complexes activated by green-light

F. J. Ballester,[1] E. Ortega,[1] M.D. Santana,[1] J. Ruiz[1]

[1] *Department of Inorganic Chemistry, Faculty of Chemistry University of Murcia, 30100, Espinardo, Murcia, Spain*

franciscojose.ballester@um.es

Keywords: • Anticancer • PDT • Organometallic • Metallodrugs • Ruthenium

Photodynamic therapy (PDT) is an interesting alternative to traditional chemotherapy because it can reduce the side effects of the treatment. In this therapy, a photosensitizer (inactive in the dark) is activated under visible light irradiation generating reactive oxygen species (ROS) that cause cellular damage. One example of these kind of drugs is TLD1433, which is the first Ru(II)-based photosensitizer for PDT to enter a human clinical trial [1]. In this work, a series of eight new cyclometalated Ru(II) have been synthetized with stoichiometry $[Ru(C^N)(N^N)_2]PF_6$. The C^N ligands [2] are based on a benzimidazole core with a phenyl, biphenyl and naphthyl group in position two, and the N^N ligands are 1,10-phenantroline (phen), dipyrido[3,2-d:2',3'-f]quinoxaline (dpq) and dipyrido[3,2-a:2',3'-c]phenazine (dppz). All the compounds were characterised by ^1H and ^{13}C NMR experiments, HPLC-MS, IR and elemental analysis. UV-Vis and fluorescence spectra were also recorded. Preliminary biological experiments were carried out in the dark and under green light irradiation.

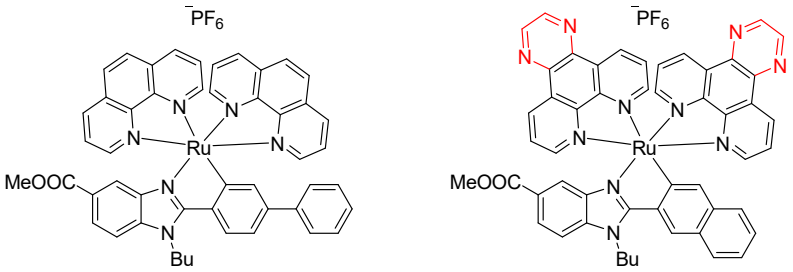

Figure 1. Examples of ruthenium complexes prepared in this work

Acknowledgements

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I Symposium on Chemical and Physical Sciences for Young Researchers

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O-04

Making computational chemistry based drug discovery accessible via web and improving its performance with HPC

Antonio-Jesús Banegas-Luna,[1] Horacio Pérez-Sánchez,[1]

[1] *Structural Bioinformatics and High Performance Computing Reseach Group (BIO-HPC), Universidad Católica San Antonio de Murcia, 30107, Spain*

ajbanegas@alu.ucam.edu

Keywords: computational chemistry • drug discovery • virtual screening • high performance computing • bioinformatics

Computational chemistry based drug discovery has progressed in the last decades helped by the evolution of high performance computing (HPC) [1] which has been proved successful to accelerate the development of new drugs in chemical sciences contexts. HPC is especially suitable to speed up those techniques that own a parallel nature, such as virtual screening (VS) which is a collection of computational techniques frequently used to screen large chemical datasets with the aim of predicting which compounds are most fitting to interact biologically with a given target. Several examples of VS running on HPC platforms can be found in literature, for instance, molecular dynamics simulations performed on grid computing systems and, more recently, docking tasks executed on graphical processing units (GPUs). An emerging approach that has gained importance in the last years is web servers providing ligand-based virtual screening (LBVS) services. LBVS methods are very useful at the early stages of the drug discovery process because of their ability to deal with huge chemical spaces and reduce them to others that only contain the most promising compounds. With the aim of providing a tool that contained the aforementioned features, BRUSELAS server has been developed.[2] BRUSELAS shows some novel quirks such as the implementation of shape and pharmacophore similarity and the usage of consensus scoring functions to improve predictions. The server is free of charge and is available at http://bio-hpc.eu/software/bruselas/. BRUSELAS has been applied in different contexts (e.g. search of blood anticoagulants) showing a good performance and promising results and we propose how it can be exploited in many other contexts related to chemical sciences.

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Infrared study of the secondary structure of silk fibroin during nanoparticles production

G. Carissimi,[1] M.G. Fuster,[1] M.G. Montalbán,[1] M. Chaala,[1] G. Víllora[1] and A. Barth[2]

[1] Department of Chemical Engineering, Faculty of Chemistry, Regional Campus of International Excellence "Campus Mare Nostrum", University of Murcia, 30071 Murcia, Spain.

[2] Department of Biochemistry and Biophysics Stockholm University. Stockholm, Sweden

guzmanaugusto.carissimin@um.es

Keywords: Silk fibroin • nanoparticles • infrared • secondary structure

Silk fibroin (SF) is an outstanding biocompatible polymer for the production of engineer nanodrug delivery systems. The encapsulation of drugs in nanoparticles (NP) can improve the bioavailability of drugs and prevent degradation[1]. The strength, elasticity and degradability of SF can be modulated through its secondary structure by tuning its β-sheet content. For this reason, a fast and reliable tool for SF secondary structure characterization is desirable. In this work, we produced SFNP by dissolving the protein in ionic liquids and subsequently precipitation in polar organic solvents [2]. By means of infrared spectroscopy and co-fitting of amide I band and its second derivative the secondary structure of silk fibroin was studied in its native state, dissolved in the ionic liquid 1-ethyl-3-methyl imidazolium acetate and after regeneration into nanoparticle form. Results indicated the content of 58% β-sheet, 9% of β-turns and 33% of unorder and/or turn like structures for the native silk fibroin. The fibroin solution in ionic liquids resembles that of silk I with a band pattern of higher complexity than just random coil structure. Silk fibroin nanoparticles regenerated from ionic liquid solution exhibited a reduction in β-sheet while an increase of the same magnitude of β-turns, suggesting an incomplete transition from the latter to the first.

Acknowledgments

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Stability of complex polysaccharide-based nanocomposites as a function of pH and ionic strength

M. Collado-González[1,2,3], M.C. Ferreri[2], A.R. Freitas[2], A.C. Santos[2], N.R. Ferreira[2], G. Carissimi[3], J.A.D. Sequeira[2], F.G. Díaz Baños[3], G. Villora[3], F. Veiga[2] and A. Ribeiro[2]

[1] *School of Food Science and Nutrition, University of Leeds, LS9 2JT UK*

[2] *Faculty of Pharmacy of the University of Coimbra, 3000-548 Coimbra, Portugal*

[3] *Faculty of Chemistry, University of Murcia, 30100 Murcia, Spain*

mdmcg1@um.es

Keywords: chitosan, alginate, polysaccharide nanocomposite, stability

Stability of nanocomposites (NC) is a crucial factor in developing drug delivery systems since their aggregation preclude their use in biomedical applications. We report the preparation of complex polysaccharide-based NC that contain several polyelectrolytes such as chitosan (CS), alginate and dextran sulphate, among other polymers [1]. We studied the effect of varying the molecular weight (MW) and the amount of CS in the final structures. According to the results (not shown), the amount of CS with no regard to its MW determines the size of the NC. NC containing 250 µg of CS showed a hydrodynamic size around 500 nm, while those containing 2.5 µg showed bigger size (around 900 nm). Increasing of ionic strength (I) up to 0.2 M (considering the I of the suspension as 0 M) resulted in the reduction of the hydrodynamic size (Table 1), indicating that NC became more compact. Changes in the hydrodynamic size of the NC resembles the change in the hydrodynamic size of polyelectrolytes after being exposed to an increment of I [2]. The change of the pH of the suspension, which was 4.6, to either pH 1 or pH 7.4 resulted in the aggregation of the NC immediately after the change in the pH (Table 1). The aggregation occurred after pH changes indicates changes in the conformation of the polyelectrolytes involved in NC.

Table 1. Hydrodynamic diameter of NC exposed to 0.2 M KNO_3 or different pH values. T0: time before changing the parameter, T1: immediately after the change, T24: after 24 h of the change.

Type of CS	Amount of CS (µg)	ΔI = 0.2 M		pH 1		pH 7.4	
		T0	T24	T0	T1	T0	T2
LMW	250	478 ± 132	271 ± 73	509 ± 121	2 ± 0	520 ± 119	1535 ± 93
MMW	250	600 ± 179	269 ± 49	389 ± 73	5404 ± 0	486 ± 141	48 ± 5

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Simulating the physical processes underlying proton therapy

Pablo de Vera,[1] Isabel Abril,[2] Rafael Garcia-Molina,[1]

[1]*Departamento de Física – Centro de Investigación en Óptica y Nanofísica, Univ. Murcia*
[2]*Departament de Física Aplicada, Universitat d'Alacant*

pablo.vera@um.es

Keywords: ion beams • cancer therapy • biological materials • computer simulation

The cutting-edge proton therapy for cancer treatment is starting to emerge in Spain, with the recent opening of the first treatment centre[1] and the clustering of the national scientific community in specialised meetings (e.g. WEP2018, Sevilla). Proton therapy features a dose distribution and tumour cell killing probability superior to conventional radiotherapy[2], due to the characteristic physico-chemical interactions between protons and tissue. These span over different space, time and energy scales, making their study a challenging task[2]: while the propagation of the primary ion beam happens in the macroscopic scale, the main processes behind clustered DNA damage and cell death (electronic excitations, generation of large numbers of secondary electrons and free radicals...) occur on nanometre distances around ions' tracks.

Besides presenting the state of the art of proton therapy, in this contribution we will review the simulation models we have developed in recent years for its physical description. We will focus on the simulation of the transport of primary ions and secondary electrons by means of the Monte Carlo codes SEICS (Simulation of Energetic Ions and Clusters through Solids)[3] and SEED (Secondary Electron Energy Deposition)[4]. These codes are fed by electronic interaction probabilities for ions and electrons moving through realistic biological materials in the condensed phase (liquid water, DNA and its molecular components, cell compartments, cortical bone…), obtained by a model that we have developed based on the dielectric formalism[5,6], which yields complete and reliable data. Simulation of effects produced in the biological medium, by means of molecular dynamics, will be also discussed: these include the hydrodynamic response of the liquid medium, together with its potential effects on the nascent radiation chemistry and thermo-mechanical damage of biomolecules[7]. The study of such physico-chemical processes is relevant for a better understanding (and exploitation) of the microscopic mechanisms underlying proton therapy.

Acknowledgements

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Analytical theory for the square wave and cyclic voltammetric responses of electron transfers with non-unity stoichiometry

Gómez-Gil, J.M.,[1] Laborda, E.,[1] Molina, A. [1]

[1] *Departamento de Química Física, Facultad de Química, Campus Regional de Excelencia Internacional "Campus Mare Nostrum", Universidad de Murcia, 30100, Murcia, España*

jm.gomezgil@um.es

Keywords: Non-unity stoichiometry• Analytical theory • Voltammetry • Macroelectrode

Key electrochemical processes show non-unity stoichiometry (see Scheme in Figure 1, a:b E-mechanism) such as the electro-reduction of some mercury complexes or the hydrogen evolution reaction (HER) [1], among others. In order to tackle the study of these systems, a general rigorous analytical treatment for the study of reversible electron transfer of complex stoichiometry is developed. A general formulation for the concentration profiles is obtained for any stoichiometry, deducing exact solutions for these profiles, the surface concentrations and the current-potential response of the 2:1 and 1:2 cases at macroelectrodes in any voltammetric technique. From the analytical solutions obtained, the particular features of the voltammetry of the 2:1 and 1:2 E mechanism, are analyzed for cyclic voltammetry (CV) and square wave voltammetry (SWV), comparing with 1:1 case. The value of SWV technique is proven to be very powerful in this context due to the additional working parameter as well as the experimental advantages for quantitative purposes.

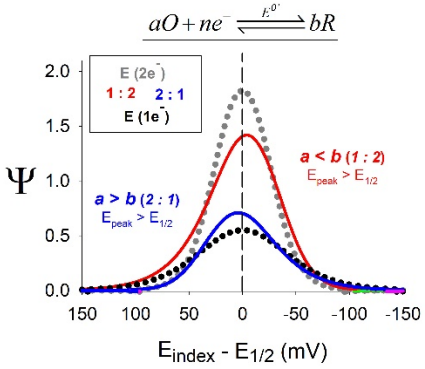

Figure 1. Dimensionless square wave voltammograms of the 1:2 (*red*) and 2:1 (*blue*), assuming 2 electrons transferred (*n*=2), comparing with those of the 1:1 case (*n=1*, gray; *n=2*, **black**).

Acknowledgements

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Small molecular azaphenacene hole transporting materials in inverted hybrid perovskite solar cells.

P. Gómez[1], M. Más Montoya[1], D. Curiel[1].

[1] *Multifunctional Molecular Materials Group, Department of Organic Chemistry, Faculty of Chemistry, University of Murcia, Campus of Espinardo, 30100 Murcia, Spain.*

paula.gomez3@um.es

Keywords: heterocycles • self-assembly • organic semiconductors

The development of novel hole transporting materials, and its implementation as interfacial layers in organic-inorganic metal halide perovskite photovoltaics, is an area of intense research.[1, 2] Many interesting materials, whether small molecules or polymers, have been reported to accomplish this function. Some of the advantages of the molecular materials, when compared to polymers, are their easier synthesis and purification, well-defined structure, or the absence of variability between different batches. In this regard, simple azaphenacene-based systems, with hydrogen bond donor and acceptor binding centers directly incorporated in the polyheteroaromatic structure, have been designed and synthesized.[3, 4] The hydrogen bond-directed self-assembly of this molecular material governs its solid-state arrangement and, consequently, its charge transport properties.

The synthesis and characterization of a new molecular azaphenacene derivative will be presented, as well as its incorporation as non-doped hole transporting layer in inverted perovskite solar cells.[5]

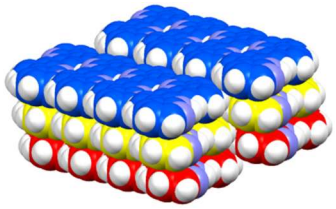

Figure 1. View of π-π stacking of azaphenacene system.

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Study of Carbamoyl phosphate synthase of *E. coli* regulation.

G. Lozano-Terol[1], J. Gallego-Jara[1], M. Cánovas[1] and T. de Diego[1].

[1] Department of Biochemistry and Molecular Biology (B) and Immunology, Faculty of Chemistry, University of Murcia, Campus of Espinardo, Regional Campus of International Excellence "Campus Mare Nostrum", P.O. Box 4021, Murcia E-30100.

gema.lozano@um.es

Keywords: Carbamoyl phosphate • *E. coli* • UMP • Regulation • Lysine acetylation

Carbamoyl phosphate (CP) is a key metabolite in the production of building blocks for the synthesis of proteins and nucleic acids, since CP is a common precursor in the biosynthesis of arginine and pyrimidines. Therefore the regulation of the production of this intermediate is essential to maintain the balance between these two pathways. In *E. coli* CP is synthetized by carbamoyl phosphate synthase (CPase), a heterodimer consisting in a synthetase subunit and an amidotransferase subunit. *E. coli* CPase synthetizes CP from Mg^{2+}ATP, bicarbonate and glutamine or ammonia [1]. Formation of CP is allosterically regulated by two activators, ornithine and IMP, and one inhibitor, UMP, which affect to Mg^{2+}ATP binding [2]. These regulators bind to the C-terminal region of synthetase subunit, specifically Lys993 is a crucial residue in UMP binding and inhibition [3].

Nε-lysine acetylation is a post-translational modification that could alter the activity of some proteins. This modification can occur in an enzymatic manner through acetyltransferase and deacetylase, or in a chemical way using acetyl-CoA and acetyl-P. In *E. coli* the best characterized deacetylase is CobB [4].

In this work we are going to study the level of intracellular metabolites from UMP biosynthesis under different culture conditions, employing *E. coli* wild type strain and *E. coli* Δ*cobB* strain. Moreover we are going to study if acetylation could have any effect in the activity of CPase.

Acknowledgements

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Design and validation of a method to measure laccase activity on methoxyphenolic food additives

J. Manzano-Nicolas,[1] F. Marin-Iniesta,[1] A. Taboada-Rodriguez, [1] J. Tudela-Serrano, [2] P. Garcia-Molina, [2] J.L. Muñoz-Muñoz, [3].

[1] *Group of Research Food Biotechnology-BTA, Department of Food Science, Nutrition and Bromatology, University of Murcia, E-30100 Espinardo, Murcia, Spain*.
[2] *GENZ-Group of Research on Enzymology, Department of Biochemistry and Molecular Biology-A, University of Murcia, E-30100 Espinardo, Murcia, Spain*.
[3] *Department of Applied Sciences, Northumbria University, Newcastle UponTyne NE1 8ST, Tyne & Wear, England, United Kingdom*.

jesus.manzano1@um.es

Keywords: Laccase • chronometric method • Guaiacol • 2,6-dimethoxyphenol • *Trametes versicolor*.

Laccase is a copper-protein[1] which presents different applications in food industry like: clarification of fruit juices through the fall of formation of phenol-protein complexes, bioremediation of phenolic residues from waste waters of agri-food industry or the improvement of antioxidant and antimicrobial ability of food additives and ingredients[2]. In this work, it has been studied the catalytic activity of laccase, oxidation, on methoxyphenolic food ingredients, such as 2-methoxyphenol (guaiacol) and 2,6-dimethoxyphenol (syringol), and isomers such as 3- and 4-methoxyphenol, 2,3-, 3,4- and 3,5-dimethoxyphenol. Normally, mistaken results of steady state rates are obtained by the production of unstable free radicals during the oxidation of methoxyphenols. In this sense, if it is added small quantities of ascorbic acid as coupling reagent during enzymatic measures assays, it produces a lag period for the regeneration of methoxyphenols (reduction of free radicals). So, quantification of lag period time allows to obtain a more accurate determination of true steady state rates, as it was described previously for peroxidase and tyrosinase[2]. In this work, we report the application and validation of this chronometric method to obtain the kinetic parameters (Km and Vm) of catalytic oxidation by *Trametes versicolor* laccase on methoxyphenols before listed. So, syringol presented the highest catalytic power (Vm/Km) respect to all substrates studied (142.20 ± 3.60 h^{-1}) according to its chemical displacements of the carbon atom that supports the hydroxyl group (128.5 ppm) [2].

Acknowledgements

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Acoustic situation of the industrial noise in a wastewater treatment plant

María del Mar Durán*, Antonia Baeza, Mercedes Llorens and Miriam Sánchez

Univ Murcia, Fac Química, Dept Ing. Química, Campus de Espinardo, Murcia 30071, Spain

*mariamar.duran@um.es

Keywords: noise pollution • WWTP • industrial noise • noise maps • spotlights

Noise pollution is an important problem nowadays, increased by the progress of the business activities made by humans. In recent years, noise as an acoustic pollutant has increased, establishing Spain as the noisiest country in Europe. This pollutant represents an important health damage because of it usually involves irreversible losses in the long term (the best known is the professional deafness). In addition, noise can produce harmful effects on the fauna of the environment or social and economic consequences decreasing significantly the quality of life.

This work studies the acoustic situation of the industrial noise in the Alcantarilla Waste Water Treatment Plant (WWTP) located in Murcia (SE Spain). Its water line treatment has the following parts: pretreatment, biological treatment and tertiary treatment. The removal of organic matter and the nitrification-denitrification process take place in two biological reactors with aeration and circular decanters. The tertiary treatment is composed by coagulation-flocculation, sand filters and UV disinfection. The sludge line consists of: gravity and flotation thickeners, anaerobic digester where biogas is generated for self-consumption in the plant, and centrifuge dewatering.

Continuous level of acoustic pressure equivalent [1] has been measured in 83 different points of the plant using an integrating sound level. From these values, noise maps are carried out, with which the greater sound impact places can be located. Measurements were made for low and high level of operation status. At low operation level, part of the pumps located in pretreatment, the blowers that supply air to the biological reactors and the centrifuge dewatering were stopped and these equipments were in the operational mode at high level (Figure 1).

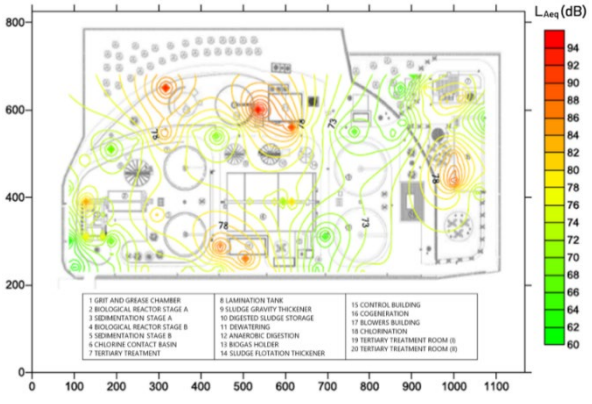

Figure 1. Noise map at high operation level

On other hand, for first time, a study of noise source apportionment has been developed applied to this case study. Some of the points that are part of the sampling are considered spotlights, by clearly being noise sources [2], which can be categorized and provide information about their contribution in the industrial noise in other points in the WWTP. Also, analysis of frequencies of some noise spotlights are carried out.

Acknowledgements

Authors gratefully acknowledge to Alcantarilla WWTP personnel and ESAMUR company.

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Improvement of Multiphoton Microscopy Images of the Living Human Eye through Deconvolution

R. M. Martínez-Ojeda,[1] L. M. Mugnier,[2] P. Artal[1] and J. M. Bueno[1]

[1] *Laboratorio de Óptica, Universidad de Murcia, 30100 Murcia, Spain*
[2] *ONERA / DOTA, Université Paris Saclay, F-92322 Châtillon, France*

rosamaria.martinez9@um.es

Keywords: Multiphoton Microscopy • Deconvolution

Multiphoton (MP) microscopy is limited by aberrations and scattering. Moreover, in living conditions, movements and non-controlled dynamics are an additional handicap. These factors make in vivo MP imaging challenging. Although adaptive optics[1] and deconvolution techniques[2] have been shown to improve MP microscopy, their use have been mainly restricted to static samples. Here, we present a deconvolution procedure based on a *marginal blind* approach[3] to improve the quality of MP microscopy images of the living human eye.

A compact clinically-adapted microscope developed at the Laboratorio de Óptica of the Universidad de Murcia[4] was used to acquired MP images of ocular tissues, both ex vivo (used a control tests) and in vivo. Imaged areas included different parts of the living cornea, as well as the sclera and the trabecular meshwork. The deconvolution technique was applied to the raw MP images (no frame averaging). The quality of the reconstructed images was compared to that of the original ones in terms of achieved resolution, contrast and feature visualization.

Unlike adaptive optics, deconvolution does not provide an increase in signal. However, our results show an improvement in the detection of sharp features, what leads to an image quality enhancement. In addition, an increase in contrast and resolution was also noticeable (Figure 1).

In conclusion, a deconvolution method to enhance MP microscopy images of the living human eye has been reported. Structures and morphological details that weren't visible in the original ones can be seen in the deconvolved ones.

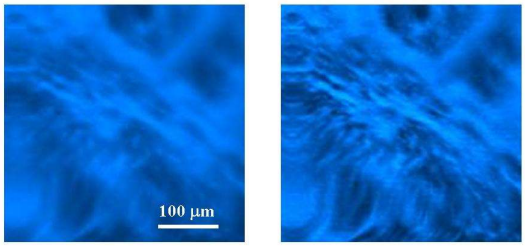

Figure 1. MP images of living human eye: original (left) and deconvolved (right).

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I Symposium on Chemical and Physical Sciences for Young Researchers

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O-14

Gold(I) and Gold(III) Complexes Containing Perfluoroalkyl and Perfluoroalkanediyl Ligands

A. Portugués,[1] J. Gil-Rubio,[1] I. López-García,[1] J. Jiménez-Bernad,[1] L. González-García,[1] D. Bautista.[2]

[1] *Grupo de Química Organometálica. Departamento de Química Inorgánica. Facultad de Química. Universidad de Murcia. Campus de Espinardo, 30100 Murcia. Spain.*
https://www.um.es/ggo/
[2] *ACTI, Universidad de Murcia, 30100 Murcia, Spain.*

alejandro.portugues@um.es

Keywords: Inorganic • Organometallic • Gold • Fluorine

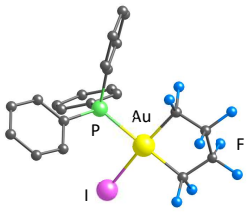
The knowledge of the chemistry of the transition metal perfluoroalkyl complexes is expected to contribute to the development of efficient metal-catalyzed or -mediated synthetic methods of highly fluorinated organic compounds. In contrast to the thoroughly studied trifluoromethyl complexes, metal complexes containing larger perfluoroalkyl ligands have received much less attention.[1,2,3]

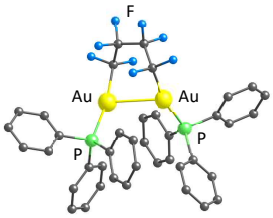
In this communication we report the first families of Au(I) and Au(III) complexes with (i) primary and secondary perfluoroalkyl ligands, and (ii) perfluoroalkanediyl ligands. These complexes have been prepared by photoinitiated reactions between Au(I) organometallic complexes and mono- and di-iodoperfluoroalkanes. Mechanistic studies, reductive elimination reactions from Au(III) perfluoroalkyl complexes and studies of the aurophilic interactions in these complexes are presented.

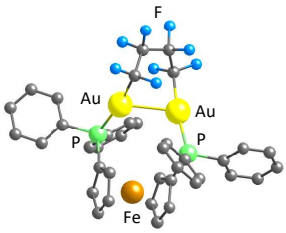
$L-Au-R_F$

L = PPh_3, NHC

R_F = $^nC_4F_9$, $^nC_6F_{13}$, $^iC_3F_7$, $^cC_6F_{11}$







Acknowledgements

This work has been financed by the Spanish Ministry of Science and Innovation/FEDER (Grants CTQ2015-69568-P and PGC2018-100719-B-100) and Séneca Foundation of the Region of Murcia (Grant 1980/GERM/15).

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Dispersive liquid-liquid microextraction for capsaicinoid compounds preconcentration in human urine analysis by liquid chromatography and quadrupole time-of-flight mass spectrometry

María Consolación Rodríguez Palazón, Natalia Campillo, Natalia Arroyo Manzanares, Pilar Viñas and Manuel Hernández-Córdoba

[1] Department of Analytical Chemistry, Faculty of Chemistry, Regional Campus of International Excellence "Campus Mare Nostrum", University of Murcia, E-30100 Murcia, Spain

mconsolacion.rodriguez@um.es

Keywords: human urine •microextraction techniques •liquid chromatography •high resolution mass spectrometry•capsaicinoids

Capsaicinoids are a group of alkaloid compounds (*Capsicum* family), commonly found in different varieties of pepper, and responsible of the characteristic sensation associated with spicy food ingestion. Among them, capsaicin (CAP) and dihydrocapsaicin (DCAP) are the most abundant and they differ only by the presence of a double bond on their lateral hydrocarbon chain[1]. Capsaicinoids are used as a flavoring agents and, because of their biological activity in the pharmaceutical industry[2]. N-Vanillylnonanamide, also known as pseudocapsaicin (PCAP), is sometimes used in pharmaceutical formulations as a cheaper alternative to CAP. Exposition to high concentration levels of capsaicinoids can caused different toxic side effects such as a local burning sensation, temporary blindness or even cardiovascular complications[3].

A new analytic method based on dispersive liquid-liquid microextraction (DLLME) for the determination of CAP, DCAP and PCAP in urine collected from patients treated with capsaicin-based topical drugs is presented. For DLLME, 7.5 mL of urine were preconcentrated in 600 µL of methyl isobutyl ketone using 1.5 mL of ethanol as dispersant agent. The extract, previously evaporated and reconstituted in 150 µL of acetonitrile, was analyzed by liquid chromatography with tandem mass spectrometry based on electrospray ionization, operating in positive mode, and quadrupole time-of-flight analyzer (LC-ESI-Q-TOF-MS^2). LC separation was carried out using a ZORBAX RRHD Eclipse Plus C18 (1.8 µm, 2.1 × 100 mm) column and a mobile phase consisting of ammonium formate/formic acid (50 mM, pH 4) (A) and acetonitrile containing 0.1% formic acid (B), in the proportion 50:50 A:B with 0.4 mL min^{-1} flow-rate. The analytes eluted with retention times in the 2.9-4.3 min range. Matrix-matched calibration was used for quantitation purposes. The method showed linearity in the 1-50 µg/L concentration range.

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Fluorescent and thermosensitive nanoparticles for drug delivery and bioimaging

M. Rubio-Camacho,[1] Y. Alacid,[1] R. Mallavia,[1] M.J. Martínez-Tomé, [1] and C.R. Mateo[1]

[1] Instituto de Investigación, Desarrollo e Innovación en Biotecnología Sanitaria de Elche (IDiBE). Universidad Miguel Hernández de Elche (UMHE). 03202 Elche, Alicante. Spain

marta.rubioc@umh.es

Keywords: Multifunctional nanoparticles • Drug delivery • Bioimaging •Thermosensitive liposomes • Fluorescent conjugated polyfluorenes (CPEs)

Drug delivery systems have attracted growing attention in recent years due to its capability to improve the efficiency of drugs and overcome some of its side effects. Nowadays, the integration of materials with different properties into a single entity has become the focus in order to develop more effective drug delivery systems which can integrate not only therapeutic but also diagnosis and imaging functionalities. At this regard, we have developed multifunctional nanoparticles with promising potential in drug delivery, controlled released and bioimaging by coupling thermosensitive liposomes and fluorescent conjugated polyfluorenes (CPEs).

In order to obtain these nanoparticles, thermosensitive liposomes (T_m ~ 40ºC) were coated with HTMA-PFP ($\lambda_{em.}$ 390-500 nm), HTMA-PFBT ($\lambda_{em.}$ 450-650 nm) or HTMA-PFNT ($\lambda_{em.}$ 550-750 nm) CPEs. Final nanoparticles were characterized by using transmission electronic microscopy, dynamic light scattering (DLS), zeta potential (ZP) and fluorescence spectroscopy techniques. The capability to be used as drug carriers and release their contents when triggered by temperature was assessed by using the model drug carboxyfluorescein (CF) and the chemotherapeutic drug temozolamide (TMZ). Whereas their ability to stain and visualize cells was proved with human embryonic cell line HEK293. Furthermore, in preliminary experiments, these nanoparticles were surrounded by metallic gold nanoparticles (AuNPs) which promising future applications in photothermal therapy.

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Design and Synthesis of β-Lactam Rotaxanes incorporating a Removable Macrocycle

A. Saura-Sanmartin, M. Tomas-Martinez, A. Martinez-Cuezva, M. Alajarin, J. Berna

Departamento de Química Orgánica, Facultad de Química, Regional Campus of International Excellence "Campus Mare Nostrum", Universidad de Murcia, E-30100, Murcia, Spain.

adrian.saura@um.es

Keywords: rotaxanes • β-lactams • cleavable group • removable macrocycle • MIMs

The intramolecular cyclization reaction of interlocked *N*-benzylfumaramide affords intertwined β-lactams in a diastereoselective manner (Figure 1).[1] A dethreading reaction[2] is possible when a kinetically stable pseudorotaxane is employed, furnishing the non-intertwined β-lactams.

In this communication, the synthesis of an intertwined β-lactam with a base-cleavable group in the macrocycle is described. The cleavable group excision would lead to increase the scope of this synthetic methodology.

Figure 1. Cartoon representation of the intramolecular cyclization reaction.

Acknowledgements

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Fine Particulate Matter impacts on Mortality in Europe-Present and Future mitigation renewables energy scenario

P. Tarín-Carrasco[1], U. Im[2], L. Palacios-Peña[1], P. Jiménez-Guerrero[1,3]

[1] *Dpt. of Physics, University of Murcia, 30100 Murcia, Spain.*
[2] *Aarhus Univ., Dpt. of Environmental Science, Frederiksborgvej 399, DK-4000, Roskilde, Denmark.*
[3] *Biomedical Research Institute of Murcia (IMIB-Arrixaca), 30120 Murcia, Spain*

patricia.tarin@um.es

Keywords: Climate Change • Air Pollution • Renewable Energy • Human Health

With the action of climate change, air quality on the future will become worse. There is evidence of the relation between air pollution and climate change and the impacts of both on human health. This study is focused on fine particles (particles with a diameter of 2.5 μm or less, $PM_{2.5}$). Bet on renewables energy can be a solution in the future for the air quality.

This study assesses the impacts of present (1991-2010) and future (RCP8.5,2031-2050) urban air pollution by fine particles on several Non-Communicable Diseases mortality causes. Two future scenarios under climate change action (RCP8.5) are proposed: (1) business-as-usual energy production system and emissions, and (2) an scenario in which 80% of the energy is obtained from renewables. Climate change scenarios were run by using the WRF-Chem online-coupled meteorological/chemistry model.

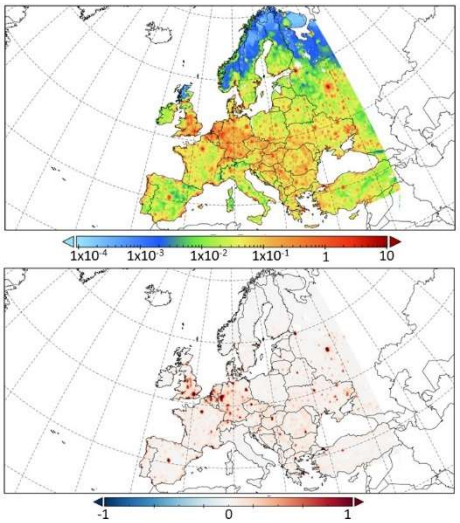

Figure 1*. Total mortality in Europe for present period (1991-2010) (up) and difference with future RCP8.5 scenario (2031-2050) (bottom)*

We estimated non-linear exposure-response functions following Burnett et al., (2018) and Lelieveld et al., (2019). The results obtained indicate that almost 900,000 deaths per year in Europe are caused by $PM_{2.5}$ for the present scenario *(Figure 1).* Generally, the mortality will increase for both future scenarios. Stroke is the cause which count with high of deaths in Europe.

Acknowledgements

We acknowledge the project ACEX (CGL-2017-87921-R) of the Spanish Ministry of Economy and Competitiveness, the Fundación Biodiversidad of the Spanish Ministry for the Ecological Transition, and the FEDER European program, for support to conduct this research.

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In-situ measurements of collisionless plasmas, from the Earth's magnetosphere to the Solar corona

S. Toledo-Redondo[1]

[1] *Department of Electromagnetism and Electronics, University of Murcia, Murcia, Spain.*

sergio.toledo@um.es

Keywords: Space physics • Plasma physics • Magnetosphere • Solar wind • Ionosphere

In-situ space plasma measurements in the near-Earth environment are key for understanding the fundamental kinetic processes that occur in collisionless plasmas, e.g., magnetic reconnection, waves or turbulence. In such environments, like the Earth's magnetosphere or the Solar wind, the plasma is dominated by wave-particle interactions and their velocity distribution functions do not easily relax to gaussian distributions. Under this situation, the fundamental concept of plasma temperature loses its classical meaning and MHD theory fails to provide accurate predictions. I will provide a summary of recent discoveries using in-situ measurements made by the NASA Magnetospheric MultiScale (MMS) mission, with a focus on magnetic reconnection and multiple plasma populations. The understanding gained in the Earth's magnetosphere and its surroundings will help understanding these processes in the solar corona and the young solar wind. Parker Solar Probe is providing in-situ measurements in these regions for the first time since very recently, at only tens of Solar radii distance, and Solar Orbiter is expected to measure the Sun's polar regions at comparable distances within a few years. I plan to study magnetic reconnection and plasma turbulence using these missions to understand its role in particle acceleration and plasma heating in the solar wind.

Synthesis and biological evaluation of new N-substituted 9-nitro-12,14-dioxo-9,10-dihydro-9,10-[3,4]epipyrroloanthracen-13-yl derivatives

Maria Vera,[1] James Mc Keown,[2] Mary J. Meegan.[2]

[1] Departamento de Química Orgánica, Facultad de Química, Universidad de Murcia, Campus de Espinardo, 30100 Murcia, España
[2] Panoz Institute, Trinity College, Dublin 2, Ireland. Trinity Biomedical Sciences Institute (TBSI), 152-160 Pearse Street, Dublin 2, Ireland.

Maria.vera8@um.es

Keywords: Leukaemia • Breast cancer • epipyrroloanthracen-13-yl derivatives

Cancer is the second leading cause of death globally, and it was responsible for around 9.6 million deaths in 2018.[1] The majority of patients will need chemotherapy in conjunction with surgery or radiological treatments.

In this project we have developed a general procedure for the synthesis of N-substituted 9-nitro-12,14-dioxo-9,10-dihydro-9,10-[3,4]epipyrroloanthracen-13-yl derivatives in order to study their activity against leukaemia cell lines and breast cancer. [2]

The synthesis of these compounds involves the reaction between (E)-9-3-R-9,10-dihydro-9,10-[3,4]furanoanthracene-12,14-dione and N-substituted maleimides in acetic acid during 3h at 120ºC

The studies done in leukaemia cell lines (HG3 and PGA1) and breast cancer (MCF-7 and MDA MB 237) show that compound **6g** is the most active one, and it could be a good candidate for future experiments (Figure 1)

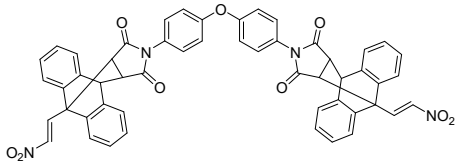

Figure 1. Structure of compound **6g**

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Flash communications

Design of a fluorescent α-glucosidase biosensor based on nanoparticles composed of lipid and conjugated polymer

Y. Alacid,[1] M. Rubio,[1] R. Mallavia, [1] M.J. Martínez-Tomé, [1] C.R. Mateo [1]

[1] *Instituto de Investigación, Desarrollo e Innovación en Biotecnología Sanitaria de Elche (IDiBE). Universidad Miguel Hernández. 03202 Elche, Alicante. Spain*

yalacid@umh.es

Keywords: fluorescent biosensor • conjugated polymers • nanoparticles • sol-gel

Diabetes mellitus type 2 (DMT2) is a common chronic metabolic condition with a high incidence that is a major public health problem worldwide. One of the therapeutic approaches used for DMT2 is to inhibit the activity of the α-glucosidase enzyme, but most of commercial glucosidase inhibitors (AGIs) have side effects after prolonged use. Consequently, the search for new therapeutic agents to treat type 2 DM has increased markedly in recent years.

The use of new devices such as biosensors can significantly improve the identification of new active agents, candidates to become antidiabetic drugs, through an exhaustive search/screening of a battery of compounds, both natural and synthetic, making these tests faster, cheaper and simpler.

In this respect, our group has designed a fluorescent biosensor based on blue-emitting nanoparticles composed by lipid and conjugated polymers (CPNs) that allows the screening of AGIs in a sensitive way. The operation of the biosensor is based on the strong deactivation of fluorescent CPNs induced by *p*-nitrophenol (PNP), a product resulting from the enzymatic hydrolysis of *p*-nitrophenyl-α-D-glucopyranoside (PNPG), catalyzed by α-glucosidase.

Both, the enzyme and the nanoparticles, have been successfully co-immobilized in a sol-gel matrix using 96-well microplates as holder, so that the developed biosensor can be reusable, easily manipulated and allows the simultaneous screening of a large number of samples.

The fluorescent biosensor was used to evaluate the inhibitory capacity of commercial antidiabetics drugs such as acarbose and miglitol, both known as competitive α-glucosidase inhibitors.

Acknowledgements

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I Symposium on Chemical and Physical Sciences for Young Researchers

Murcia, 22nd-23rd October 2020

F-02

The inversion mechanism in $\sigma^3\lambda^3$-pnictogen compounds: chemical bonding analysis and periodic trends

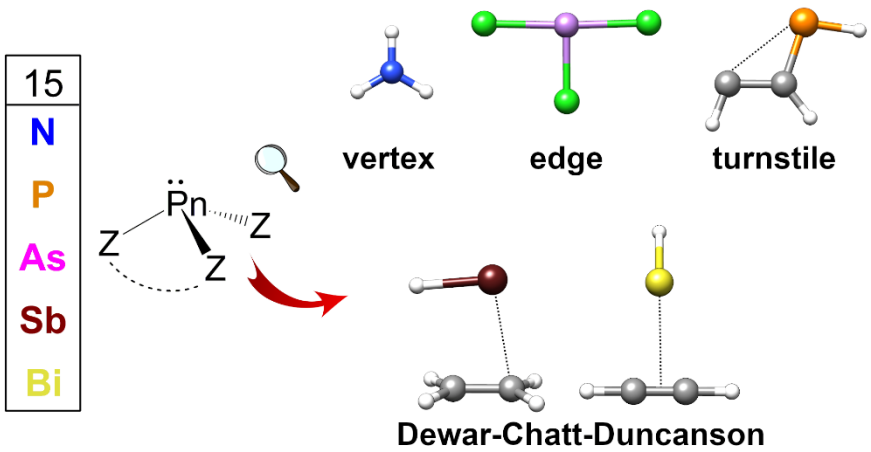
A. García Alcaraz,[1] A. Espinosa Ferao,[1]*

[1] *Departamento de Química Orgánica, Facultad de Química, Campus de Espinardo, Universidad de Murcia, 30100 Murcia (Spain)*

Email: antonio.garcia47@um.es

Keywords: pnictogen inversion, DFT calculations, dative bonding

$\sigma^3\lambda^3$-pnictogen compounds PnZ_3 (Pn = N to Bi) are of tremendous importance in many fields of chemistry such as catalysis, anion recognition or coordination chemistry.[1] The inversion at $\sigma^3\lambda^3$-pnictogen centres is a well-known process which has been studied in detail only for a limited set of compounds, using both experimental and theoretical methods.[2] Herein, a thorough computational examination of the inversion process in a wide set of both cyclic and acyclic Pn(III)-derivatives at the DFT level is presented, with special focus on the geometry of transition states (TS), the energy value of the inversion barriers and its possible relationship with structural or electronic parameters.



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Comparison of headspace gas chromatography - mass spectrometry and ion mobility spectrometry for the classification of virgin olive oils

M. García-Nicolás,[1] N. Arroyo-Manzanares,[1] L. Arce,[2] M. Hernández-Córdoba,[1] P. Viñas, [1].

[1] *Dept. Analytical Chemistry, Faculty of Chemistry, University of Murcia, Murcia, Spain*
[2] *Dept. Analytical Chemistry, Faculty of Science, University of Córdoba, Córdoba, Spain*

maria.garcia66@um.es

Keywords: Gas chromatography • ion mobility spectrometry • mass spectrometry • olive oil classification • chemometric models

According to its quality, the olive oil is classified into three different categories: extra virgin (EVOO), virgin (VOO) and lampante (LOO) olive oil. The official method to differentiate between these categories is based on Regulation (EC) 640/2008 of the European Commission and involves physico-chemical analysis together with a sensory assessment by a Panel Test. However, in the last years, researchers have moved their attention toward the search for alternative analytical methods to the Panel Test, due to the lack of accredited panels in some countries, the time required to analyse a sample, and the high number of tasters necessary.

In this work, headspace chromatography coupled to ion mobility spectrometry (HS-GC-IMS) or mass spectrometry (HS-GC-MS) are compared and proposed for differentiating olive oils according to their quality. Both methods were optimized and validated and, subsequently, they were used to analyse 160 olive oil samples (52 EVOO, 56 VOO and 52 LOO).

Firstly, some of the compounds detected in the olive oil samples were identified and quantified in order to establish relationships and differences between each analytical method and olive oil categories. However, this was not sufficient for the correct classification of samples due to variability within the same category. Therefore, all data obtained by HS-GC-IMS and HS-GC-MS were processed using different strategies. Chemometric models were constructed using 80% of the samples and validated with the remaining 20% for each strategy. The best results (96.8% validation success) in differentiating between EVOO, VOO and LOO were obtained by HS-GC-MS when chemometric models were constructed using the chromatographic peak areas.

Acknowledgements

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Bis-cyclometalated fluoro(aryl) Pt(IV) complexes

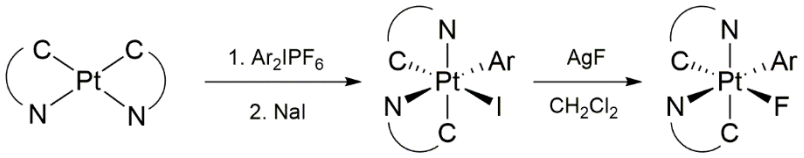
Juan Carlos López López,[1] Delia Bautista,[2] Pablo González Herrero[2,*]

[1] *Departamento de Química Inorgánica, Universidad de Murcia, 30071, Murcia, Spain.*
[2] *SAI, Universidad de Murcia, Spain.*
jc.lopezlopez@um.es

Keywords: Platinum • Cyclometalated ligands • Luminescence

Luminescent transition-metal complexes bearing heteroaromatic ligands have been studied for their long-lived and highly tunable excited states, which make them suitable for important light-based applications.[1] Most studies have focused on complexes of d^6 [Ir(III), Ru(II), Os(II)] or d^8 [Pt(II), Au(III)] ions. However, Pt(IV) complexes have received very little attention.

Pt(IV) complexes with cyclometalated 2-arylpyridines (C^N) may show efficient and long-lived emissions from triplet ligand-centered (^{3}LC) excited states with a very small metal-to-ligand charge-transfer (MLCT) character.[2] The MLCT contribution is crucial because it facilitates the formation of the emitting state and accelerates the radiative transition to the ground state due to the spin-orbit coupling effects induced by the metal. To develop Pt(IV) complexes with a higher MLCT admixture into the emitting state, we set out to synthesize complexes of the type $[Pt(C^N)_2(Ar)(F)]$. Both the aryl and fluoro ligands can be strong π-donors for the Pt(IV) ion, helping to increase the energy of the metal dπ orbitals and, hence, the MLCT contribution, which could lead to increased radiative rates and quantum yields. Complexes $[Pt(C^N)_2(Ar)(F)]$ with different C^N ligands were obtained via oxidative addition of Ar_2I^+ salts to *cis*-$[Pt(C^N)_2]$ followed by the addition of NaI to give $[Pt(C^N)_2(Ar)(I)]$ and substitution of the iodide ligand by fluoride with AgF (Scheme 1). A preliminary photophysical characterization will be presented.



Scheme 1. C^N: Cyclometalated 2-arylpyridine.

Acknowledgements

Ministerio de Ciencia, Innovación y Universidades (PGC2018-100719-B-I00) and Fundación Séneca (19890/GERM/15).

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Development of co-poly-(methyl vinyl ether-alt- maleic anhydride) derivates nanocarriers to improve administration of different drugs

A.Mira,[1]C.Sainz-Urruela,[1]A.Falcó,[1] R.Mallavia[1]

[1] *Institute of Research, Development and Innovation in Biotechnology of Elche (IDiBE), Miguel Hernández University (UMH), 03202, Elche (Alicante, Spain*).

a.mira@umh.es

Keywords: Biomaterials • polymers • nanofibers • nanoparticles • electrospinning

The relatively recent consortium created by polymer science with the medicine and biotechnology research fields has greatly boosted the development of nanotechnology with biological applications. This fact is largely due to the different properties that this technology confers to some compounds when they are nanoscopically structured. New advances based on these properties may facilitate the development of interesting monitoring tools and treatments in medicine.

In this study, we evaluate the ability to encapsulate into polymeric nanostructures a series of different drugs that differ in their properties, structure and therefore, in chemical property Two separate derivatives of poly(methyl vinyl ether-alt-maleic anhydride) (PMVE/MA), and acid (PMVE/MA-Ac) and a monoethyl ester (MPVE/MA-ES), were used as polymer source. One of nanostructure that we prepared by solvent displacement method. All of nanostructured were physico-chemical compatible systems, however, such efficiencies varied notably in nanoparticles depending on the tested compound (14-69 % with antibiotics). Finally, the mechanisms of action of encapsulated drugs are evaluated. On the other hand, the permeability and release of frugs in topical administration by Franz cells is evaluated.

Acknowledgements

Project ref MAT-2017-86805-R (Spanish Economy and Competitively Ministry) and Project ref. GVA-IDIFEDER_2018/020, “Una forma de hacer Europa”

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Stability of Oxyresveratrol Encapsulated with Beta-cyclodextrin in Food Models

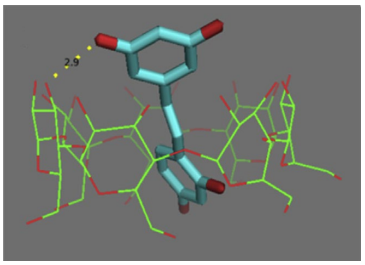
Silvia Navarro-Orcajada[1], Adrián Matencio[2], Irene Conesa[1], Iván Muñóz-Sánchez[1], Lorena Laveda-Cano[1], Desiré Cano-Yelo[1], Francisco García-Carmona[1], José Manuel López-Nicolás[1]

[1] Dpto. Bioquímica y Biología Molecular-A, Facultad de Biología, Universidad de Murcia - Regional Campus of International Excellence "Campus Mare Nostrum", E-30100 Murcia, Spain
[2] Dip. Di Chemica, Universitá di Torino, via P. Giuria 7, 10125, Torino, Italy
silvia.navarro6@um.es

Keywords: Oxyresveratrol • Cyclodextrin • Food Model • Stability • Industry

Society is increasingly demanding healthier food products, and one way to satisfy this request is the fortification of foods with bioactive compounds. Stilbenes are suitable candidates for this purpose because they have several bioactivities of interest: antioxidant, anticancer and antimicrobial. In the present study[1], food models of juice and milk enriched in oxyresveratrol inclusion complexes with β-cyclodextrin (β-CD) were designed and maintained under typical storage conditions (darkness and/or refrigeration) for one month. CD selection was made according to the characterization of the complexes with α-CD, β-CD and γ-CD by SEM, DSC, TGA and molecular docking (Figure 1). The stability of fortified food models was evaluated by measuring pH, ºBrix and UV-Vis spectrum. The effect of encapsulation on the solubility and antioxidant activity of oxyresveratrol was also analysed. The results showed that the food models were stable for five weeks and CD supplementation leads to a higher oxyresveratrol concentration and antioxidant capacity than when not used. These results may be interesting for industries to design functional food with oxyresveratrol.

Figure 1. Molecular docking of oxyresveratrol encapsulated with β-cyclodextrin



Acknowledgements

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Novel osmium-based proteosynthesis inhibitor reduces *in vivo* tumor growth and extends *C. Elegans* lifespan.

Enrique Ortega,[1] Francisco J. Ballester,[1] Alba Hernández-García,[1] Samanta Hernández-García,[2] M. Alejandra Guerrero-Rubio,[2] M. Dolores Santana[1] Fernando Gandía-Herrero,[2] and José Ruiz [1]

[1] *Departamento de Química Inorgánica, Universidad de Murcia and Institute for Bio-Health Research of Murcia (IMIB-Arrixaca). Campus de Espinardo, E-30071 Murcia, Spain.*

[2] *Departamento de Bioquímica y Biología Molecular A, Unidad Docente de Biología, Facultad de Veterinaria, Universidad de Murcia. Campus de Espinardo, E-30071 Murcia, Spain.*

enrique.ortega@um.es

Keywords: anticancer agents • cancer • drug design • *C. elegans* • osmium

Due to tumour growth demands, cancer cells require high protein synthesis rates. Therefore, targeting the protein synthesis process represents a therapeutic window to selectively eliminate cancer cells. Herein, we report the design and synthesis of three cyclometalated osmium(II) complexes of the type $[(\eta^6\text{-}p\text{-cym})Os(C\text{^}N)(X)]^{0/+}$ (C^N = deprotonated ppy-CHO) that have been tested *in vitro* an *in vivo*. Overall, complex **3** exhibited selective cytotoxicity to ovarian tumor cells. The mechanism of action underlying the anticancer effects *in vitro* showed a reduction of proteosynthesis up to 58 % and caspase-dependent apoptosis induction. Moreover, the model animal *Caenorhabditis elegans* was used to estimate the effects of osmium complex **3** *in vivo* (**Figure 1**). The compound was able to reduce tumor growth up to 19 % in the tumoral strain and was not toxic to the animals. Indeed, it induced an extension of a 17 % in the worm's lifespan both in the tumoral organisms and in the wild type ones. To the best of our knowledge, this is the first example of cost-effective identification and evaluation of new anticancer drug candidates through experimentation with a tumoral strain of *C. Elegans* coupled to *in vitro* studies.

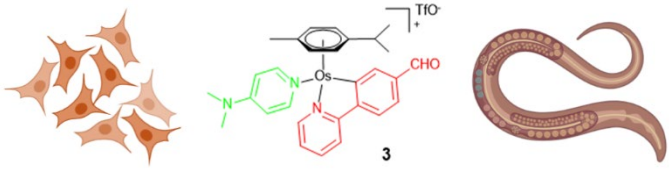

Figure 1. *In vitro* and *in vivo* studies with osmium-based photosynthesis inhibitor complex **3**.

Acknowledgements

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Influence of biochar on soil C and N biogeochemical cycles

M.B. Pascual, M.A. Sánchez-Monedero, M.L. Cayuela

Centro de Edafología y Biología Aplicada del Segura (CEBAS)-CSIC. Campus Universitario de Espinardo. 30100, Murcia.

blanca.pascualv@um.es

Keywords: C cycle • N cycle • greenhouse gas • pyrolysis • char

Biochar is a carbon-rich product obtained when biomass is subjected to thermal decomposition under the absence of oxygen and at relatively low temperatures (between 400 and 600°C). During this process, a series of reactions take place that lead biochar amorphous structure of carbon (C) arranged in recalcitrant aromatic functionalized rings. Among the possible benefits of biochar when applied to soil, it may influence C and nitrogen (N) cycles, potentially reducing the emission of CH_4 and N_2O. However, the mechanisms of interaction still remain unknown as well as which of biochar properties are determinant.

The study we present has the objective to cast light over how dissimilar biochars affect soil greenhouse gas emissions. A total of nine biochars produced from different feedstock and at two pyrolysis temperatures were synthetized and thoroughly analysed, physically and chemically. Afterwards, two soil incubation experiments were set in which the impact of the biochars over the CH_4 and N_2O emissions were investigated. The concentrations of both gases were monitored together with the measurement of other soil parameters. The modifications induced by biochar on the soil fluxes of CH_4 and N_2O were correlated to biochar physico-chemical properties through a multivariate statistical analysis.

The results showed soil CH_4 oxidation was favoured by woody biochars produced at high temperatures and with large total pore area. Soil N_2O emissions were not decreased by the biochars tested. Some biochars increased N_2O emissions by favouring the formation of N_2O through pathways different to denitrification. Therefore, we conclude that biochar impact differently C and N cycles depending on their characteristics, especially their biomass origin and pyrolysis temperature.

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I Symposium on Chemical and Physical Sciences for Young Researchers

Murcia, 22nd-23rd October 2020

F-09

Photogeneration of Stable Bis-cyclometalated Platinum(IV) Hydrides and Alkyne Insertion Reactions

D. Poveda,[1] A. Vivancos,[1] D. Bautista,[2] P. González-Herrero[1]

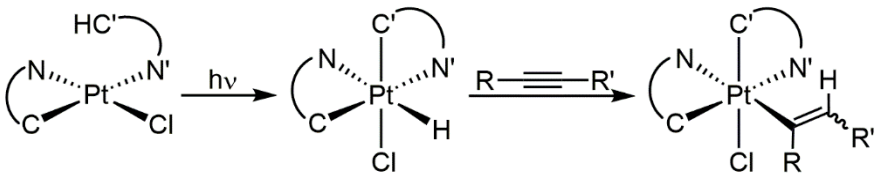
[1] *Departamento de Química Inorgánica, Facultad de Química, Universidad de Murcia, 30100, Murcia, Spain*

[2] *ACTI. Universidad de Murcia, Campus de Espinardo, 30100, Murcia, Spain*

dionisio.poveda@um.es

Keywords: Platinum • Cyclometalated ligands • Photochemistry • Hydrides

Platinum(II) complexes with cyclometalated 2-arylpyridines are well known for their luminescence properties.[1] However, there is still a long way to go in studying their photochemistry. A few years ago, our laboratory discovered a new photochemical reaction on methyl complexes of the type *cis-N,N*-[PtMe(C^N)(N^CH)], where N^CH represents an *N*-coordinated 2-arylpyridine and C^N is its cyclometalated form. The irradiation of these complexes with visible light induces the oxidative addition of the C-H bond from the N^CH ligand resulting in unstable platinum(IV) methyl hydride intermediates [PtCl(H)(C^N)$_2$] that eliminate methane to give *cis*-[PtC^N)$_2$] complexes.[2] Despite the significance of this reaction, the instability of the hydride intermediates is a disadvantage for developing a photochemical C-H activation/functionalization process. Our current work has been focused on designing alternative platforms for photooxidative C-H addition reactions with the main purpose of obtaining stable platinum(IV) bis-cyclometalated hydrides to study their reactivity. We have found that the chloride complexes *cis-N,N*-[PtCl(C^N)(N'^C'H)] are suitable for the photogeneration of bis-cyclometalated hydrido complexes [PtCl(H)(C^N)(C'^N')], which proved stable and could be isolated and structurally characterized. The reactions of the hydrides with different alkynes have been studied, which resulted in insertions into the Pt-H bond to give alkenyl derivatives.



Scheme 1. C^N: cyclometalated 2-arylpyridine

Acknowledgements

Ministerio de Ciencia, Innovación y Universidades (PGC2018-100719-B-I00) and Fundación Séneca (19890/GERM/15). DP thanks Fundación Séneca for a FPI grant (20725/FPI/18).

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I Symposium on Chemical and Physical Sciences for Young Researchers

Murcia, 22nd-23rd October 2020

F-10

Factors affecting ring strain in saturated three-membered heterocycles bearing one group 13-16 heteroatom

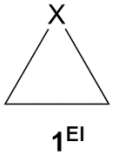
A. Rey Planells,[1] A. Espinosa Ferao [1]*

[1] *Department of Organic Chemistry, Faculty of Chemistry, University of Murcia, Espinardo Campus,30100 Murcia, Spain, artuesp@um.es*

alicia.rey@um.es

Keywords: RSE • ·3MRs • homodesmotic • hyperhomodesmotic

One of the most noteworthy aspects regarding the reactivity of three-membered rings (3MRs) is their high ring strain energy (RSE).[1] According to geometrical criteria, 3MRs should represent the group of molecules with the highest RSE, although actual values are lower than expected. To date, there are only partial or little accuracy theoretical studies covering RSE estimation for main three-membered heterocycles containing a single group 13-16 heteroatom.[2] Therefore, it is necessary to report reference RSE data for parent $(CH_2)_2X$ rings, where X is a groups 13-16 element (Figure 1) with its covalence completed by bonds to H and named as **1**^{El} ("El" referring to the heavy element of X). To this aim, energetics of appropriate hyperhomodesmotic (also homodesmotic) reactions[3] were computed at different levels of theory, thus providing a benchmark of high quality reference RSE values. Different geometric and electronic factors that can affect ring strain were also evaluated in order to explain the origin of the different observed RSE tendencies depending on the heteroelement group.



1^{El}

X			
BH	CH_2	NH	O
AlH	SiH_2	PH	S
GaH	GeH_2	AsH	Se
InH	SnH_2	SbH	Te
TlH	PbH_2	BiH	Po

Figure 1. Saturated three-membered heterocycles **1** studied.

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Iridium(III) Anticancer Agents Generating Superoxide Anion Radicals: Overcoming the Achilles' Heel of Photodynamic Therapy

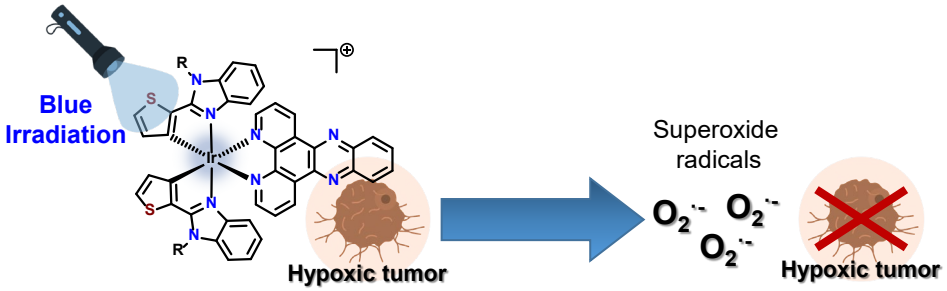
G. Vigueras,[1] V. Novohradsky,[2] J. Pracharova,[2] N. Cutillas,[1] C. Janiak,[3] H. Kostrhunova,[2] V. Brabec,[2] J. Ruiz,[1] J. Kasparkova.[2]

[1] *Departamento de Química Inorgánica, Universidad de Murcia*
[2] *Institute of Biophysics of the Czech Academy of Sciences, Czech Republic*
[3] *Institut für Anorganische Chemie und Strukturchemie, Germany*

gloria.vigueras@um.es

Keywords: anticancer • iridium • photodynamic therapy • hypoxia

Photodynamic therapy (PDT) represents a non-invasive medical approach that serves as a beneficial option or complementary treatment to other methods used to treat cancer, such as surgery chemotherapy, or radiotherapy.[1] It involves the accumulation of the drug in cancer cells, followed by its activation with light. However, the tumoricidal effect of traditional PDT is strongly oxygen dependent and the tumor hypoxia drastically decreases the anticancer outcome of this phototherapy. Herein, we will present our recent results on the synthesis and biological evaluation of three series of octahedral Ir(III) complexes of general formula $[Ir(C^N)_2(N^N)][PF_6]$. Their anticancer activity is activated by irradiation with blue light and they are able to overcome tumor hypoxia using a different mechanism than traditional PDT: generation of superoxide anion radicals.



Acknowledgements

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Enzymatic synthesis of Fatty Acid Solketal Esters using Sponge Like Ionic Liquids.

Rocio Villa,[1] Elena Álvarez,[1] Susana Nieto,[1] Antonio Donaire,[2] Pedro Lozano[1]

[1] Department of Biochemistry and Molecular Biology B and Immunology. Faculty of Chemistry, University of Murcia, E-30100, Murcia, Spain.
[2] Department of Inorganic Chemistry. Faculty of Chemistry, University of Murcia, E-30100, Murcia, Spain.

rocio.villa@um.es

Keywords: Fatty Acid Solketal Esters • Sponge Like Ionic Liquids.

Because of the increased production of biodiesel fuels (e.g. fatty acid methyl esters), there is an excess of the byproduct glycerol in the market, being necessary its valorization. Solketal (1,2-isopropylideneglycerol) is a glycerol derivative which has been successfully used in the production of new oxygenated fuels. For example, Fatty Acid Solketyl Esters (FASEs), are highly valued to enhance the octane number of gasolines. Biodiesel blends up to 20% volume fraction of FASEs, exhibiting excellent properties as liquid fuel (e.g. viscosity, cetane number, adiabatic flame temperature, etc.), as it was demonstrated by testing in an automotive engine. [1,2]

In this work, a green enzymatic synthesis of Fatty Acid Solketal Esters (FASEs) was carried out using Sponge Like Ionic Liquids. This biocatalytic reaction consists in the transesterification of different oils from natural resources with solketal at moderate temperatures, leading to a 100% product yield. Furthermore, it is important to highlight that this approach includes the full recovery of the enzyme/SLIL system for reuse (**Figure 1**).

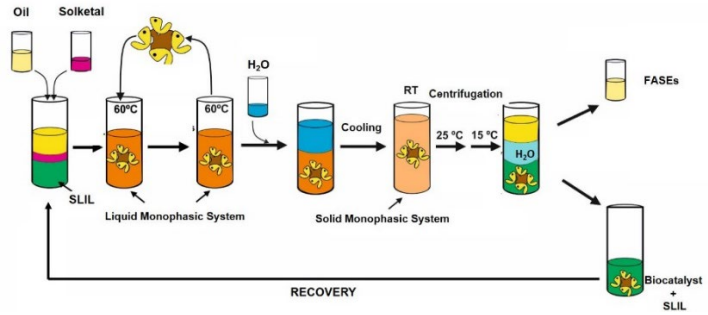

Figure 1. Experimental set-up of biocatalytic synthesis of FASEs using SLIL.

Acknowledgements Work partially supported by CICYT-MICINN (CTQ 2011-28903, CTQ2008-00877 and CTQ2008-04412), the SENECA Foundation (08616/PI/08) and Bancaixa-UJI (P1 2009-58) grants.

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Cascade carbopalladation reactions of skipped dienes for the synthesis of [4,5]-spirooxoindoles

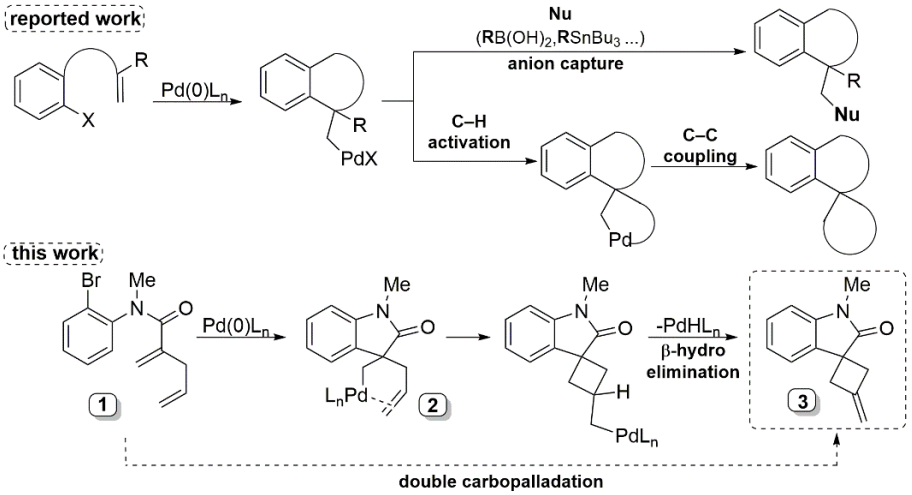
M. Pérez-Gómez,[1] H. Azizollahi,[1] V. Mehta,[1] J.-A. García-López[1*]

[1] *Grupo de Química Organometálica. Departamento de Química Inorgánica. Universidad de Murcia, Murcia-30100, Spain*

martapg@um.es

Keywords: spirooxoindole, Palladium, carbopalladation, cyclobutyl

Palladium-catalyzed cascade reactions are considered a powerful tool for the functionalization of remote C–H or even C–C bonds moieties,[1] giving rise to complex molecular structures from simple organic substrates, in a one-pot process. We present an efficient palladium-catalyzed cascade reaction arising from the double intramolecular carbopalladation of skipped diene chains tethered to an aryl group as starting material (**1**, Scheme 1). This synthetic process affords interesting [4,5]-spirooxoindol scaffolds containing four-membered rings, which are usually subject of study due to their biological properties.[2] The mechanism we propose is that a σ-alkyl-Pd(II) generated upon the intramolecular carbopalladation of the nearby C=C double bond, undergoes an insertion into the terminal olefin present in the tethered chain, giving rise to the intermediate **2**. Finally, a β-hydrogen elimination from **2** affords the corresponding spirocycles **3** in a selective way and in excellent yields.



Scheme 1. Pd-catalyzed cascade reactions applied to the synthesis of spirocycles.

Acknowledgements

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Poster communications

Determination of cadmium in used engine oil, gasoline and diesel by electrothermal atomic absorption spectrometry using magnetic ionic liquid-based dispersive liquid-liquid microextraction

M. A. Aguirre,[1] A. Canals,[1] I. López-García,[2] M. Hernández-Córdoba[2]

[1] Department of Analytical Chemistry and Food Science and University Institute of Materials, Faculty of Science, University of Alicante, P.O. Box 99, 03080 Alicante, Spain.
[2] Department of Analytical Chemistry, Faculty of Chemistry, Regional Campus of International Excellence "Campus Mare Nostrum", University of Murcia, 30071 Murcia, Spain.

aguirre.pastor@ua.es

Keywords: engine oil • fuel samples • electrothermal atomic absorption spectrometry • magnetic ionic liquid • dispersive liquid-liquid microextraction

In this work, an analytical methodology based on the combination of dispersive liquid-liquid microextraction (DLLME) with electrothermal atomic absorption spectrometry (ETAAS) was evaluated for sequential preconcentration and detection of Cd. The extractant solvent used for the microextraction procedure was a magnetic ionic liquid (MIL) (i.e., 1-hexyl-3-methylimidazolium 1-ethyl-3-methylimidazolium tetraisothiocyanato-cobaltate (II) $[Emim]_2[Co(NCS)_4]$), which presents a paramagnetic property, and allows an easy phase separation using a magnet. In order to eliminate the well-known drawbacks of direct introduction of MIL in the graphite furnace, a back-extraction procedure was performed to transfer the analyte into an aqueous phase. The main experimental factors affecting the extraction of Cd (i.e., amount of sample and MIL, extraction and back-extraction time and concentration and amount of nitric acid) were optimized using a multivariate analysis consisting in two steps: a Plackett-Burman design followed by a Circumscribed Central Composite Design (CCCD).

Under optimum conditions, the proposed analytical method was validated and successfully used to analyze three real-world samples (i.e., used engine oil, gasoline and diesel). The three samples were spiked at two levels (i.e., 10 and 20 μg kg^{-1} of Cd for used engine oil and 1 and 3 μg kg^{-1} of Cd for gasoline and diesel). RSD and recovery values were within the range of 6-10 % and 96-105 %, respectively.

Acknowledgements

The authors would like to thank the Spanish Government (projects n. CTQ2016-79991-R and PGC 2018-098363-100), Fundación Séneca (Project n. 19888/GERM/15) and European Union (FEDER funds) for the financial support.

Multi-emission fluorescent nanoplatforms based on lipid conjugated polymer complexes

Y. Alacid,[1] M. Rubio,[1] R. Mallavia, [1] M.J. Martínez-Tomé, [1] C.R. Mateo [1]

[1] *Instituto de Investigación, Desarrollo e Innovación en Biotecnología Sanitaria de Elche (IDiBE). Universidad Miguel Hernández. 03202 Elche, Alicante. Spain*

yalacid@umh.es

Keywords: Conjugated polymer • fluorescent nanoparticles • multi-emission

The development of new fluorescent materials is of great interest nowadays due to their optoelectronic and biological applications in labeling, biomedical imaging, sensing, etc. Multicolor fluorescent nanoparticles which show distinguishable emission bands when are excited at a single wavelength are especially attractive, because they reduce the complexity of fluorescence measurements, simplifying instrument requirements and allowing simultaneous excitation of all the fluorophores involved in the experiment.

Currently, multicolor emission is obtained by mixing quantum dots (QDs), which provide a controllable fluorescence emission and wide absorption bands. However, the potential cytotoxicity risk of QDs associated with their heavy metal components remains their major concern when used in biological studies. A promising solution to these problems is the incorporation into the device of complexes based on lipid systems coupled to biocompatible fluorophores, which emit at different wavelengths, to construct multicolored fluorescent nanoparticles. By varying the ratio of fluorophores, these fluorescent materials could exhibit distinguishable multicolored emission bands when excited on a single wavelength.

Conjugated polymers CPs seem to be interesting candidates for designing multicolour fluorescent devices. They offer the advantage of excellent thermal stability, photostability, high fluorescence efficiency, biocompatibility as well as a good synthetic accessibility which allows to extend the conjugation length. In this respect, our group has recently synthesized various blue-emitter polyfluorenes, a green polyfluorene and a red-emitter cationic polyfluorene.

In the present work we have explored the interaction of three synthesized polyfluorenes with different lipid systems in order to obtain stable nanoparticles emitting at different wavelengths. NPs were fabricated incorporating, one, two or three CPs simultaneously in the same lipid system and their size, morphology, stability and fluorescent properties were analyzed in detail. In order to facilitate the manipulation of the device and allow its reuse, NPs have been immobilized in sol-gel matrices. The success of the immobilization offers new opportunities in the development of biological and chemical sensors, through selective mechanisms of deactivation (quenching).

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Project ref. MAT-2017-86805-R (Spanish Economy and Competitively Ministry) and Project ref. GVA-IDIFEDER_2018/020, “Una forma de hacer Europa”

Photocatalytic Degradation of Two Neonicotinoid Insecticides in Agro-Wastewater. Reuse for Irrigation of Pepper Crop

M. Aliste Fernández,[1] J. Fenoll Serrano,[1] S. Navarro García,[2]

[1] *Murcia Institute of Agri-Food Research and Development, Murcia, Spain.*
[2] *University of Murcia, Murcia, Spain.*

marina.aliste@carm.es

Keywords: neonicotinoids • agro-wastewater • TiO_2 • pilot plant • pepper

Photocatalytic treatment has been researched in the last years as an effective method to remove pesticide residues from wastewater. Thus, different Advanced Oxidation Technologies (AOTs) are a hopeful solution to mitigate water pollution [1]. On account of environmental problems such as drought, the water used for agricultural purposes can be from different origins. Therefore, it is very important to know its effect on agricultural products and human health. The aim of this work was to evaluate and compare the pepper quality grown using non-polluted water (control) and polluted water with imidacloprid (IM) and thiamethoxam (TH), non-treated and treated by solar photocatalysis. In addition, the presence of the studied neonicotinoid insecticides and its transformation products in soil and pepper samples was also investigated. TiO_2 in tandem with $Na_2S_2O_8$ was used to treat 16,800 L of agro-wastewater at pilot plant scale under natural solar irradiation in Murcia (SE of Spain). At the end of the treatments, when 1,000 kJ m^{-2} were recovered, IM and TH were not detected in any case. Peppers were collected in three times during June and July, 2019. None of the insecticides and its metabolites were detected in soil and peppers when they were irrigated with control or treated water. When the plot was irrigated with polluted water, TH and IM were found in both, soil and harvest peppers. Besides, two metabolites of TH were identified: clothianidin (TH1) and thiamethoxam urea (TH2) in soil and peppers. In addition, hydroxy imidacloprid (IM1) was also detected as the only identified IM transformation product. Finally, quality of harvested peppers was not affected. In conclusion, photocatalysis could be considered as suitable strategy to reuse polluted water for agricultural irrigation.

Acknowledgements

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Catechol biosensor based on lyophilised mushroom for the analytical determination of kojic acid.

Carmen M. Almagro, María S. García,Joaquín A. Ortuño

Department of Analytical Chemistry, Faculty of Chemistry, University of Murcia

carmenmaria.almagro@um.es

Keywords: Biosensor•Kojic Acid•Lyophilised mushroom tissue•Tyrosinase

The main objective of this work is the development of an analytical method for the determination of kojic acid, a tyrosinase inhibitor, by using a catechol biosensor constructed with lyophilised mushroom.

Tyrosinase is an enzyme which catalyzes the oxidation of o-diphenols to o-quinones. The mushroom *Agaricus bisporus*is was directly used as tyrosinase source to its high content in enzyme. The biosensor was built by using lyophilised commercial mushroom which was grinded and sieved with a size of 60-250 µm, mineral oil and graphite, in a proportion vegetal tissue: graphite 1:5.

The substrate selected was catechol and the inhibitor effect of the kojic acid was studied using different concentrations of catechol. The catechol concentration chosen was $4x10^{-4}$ M. We checked the influence of the applied potential on the biosensor to best results. The selected working potential was -0.1 V.

The dynamic response of the biosensor to increasing kojic acid concentration in the presence of cathecol was obtained. A procedure for the signal treatment was developed that permits to considerably reduce the recording time by using recorded signals very far from steady-state currents. It also avoids the need of using a fixed recording time for the current after each analyte addition.

Calibration graph was obtained by plotting current change obtained with the signal treatment developed versus kojic acid concentration. In order to extent the linear response concentration range, a corrected inhibition parameter was proposed. This provides a linear range ($4x10^{-6}$-$7x10^{-5}$ M), which fits to the equation: *Inhibition* = 0.14 (± 0.03) +0.28 (± 0.009) x [kojic acid] x 10^5 (r^2= 0,994). The detection limit was $2,5x10^{-6}$ M.

The proposed method shows a good repeatability of calibration parameters and a good reproducibility in the preparation of biosensors. The stability of the vegetal tissue kept in the fridge was checked during one year, from the same lyophilised mushroom but grinded at different moments. The results obtained from the corresponding biosensors prepared with the lyophilised tissue showed that it is very stable.

The biosensor developed was used to determine the bleaching capacity of a cosmetic ampoule expressed as kojic acid concentration.

Green copolymerization of carbazole-substituted epoxide with vinyl monomer by an eco-catalyst

F. Bekkar,[1] F. Bettahar,[1] R. Meghabar,[2] M. *Hamadouch[2], L.Ruiz-Rubio[3]*

[1]Laboratory of Polymer Chemistry, Department of Chemistry, Faculty of Science, University Oran1 Ahmed Ben bella. BP N°1524 El'Menouer, 31000 Oran, Algeria.

[2]Laboratory of Fine Chemistry, Department of Chemistry, Faculty of Science, University Oran1 Ahmed Benbella. BP N°1524 El'Menouer, 31000 Oran, Algeria.

[3] Macromolecular Chemistry Group (LABQUIMAC), Department of Physical Chemistry, Faculty of Science and Technology, University of the Basque Country, UPV/EHU, Barrio Sarriena, s/n 48940 Leioa, Spain

Bekkar31@outlook.com

Keywords: *Carbazole* • *Microwave* • *Copolymerization* • Clay

Green chemistry applies as well to the preparation of new products or more ecological processes as to the search for alternative solutions[1].

As part of this work, we sought to develop and characterize a synthesis of new classes of monomers, polymers and conductive nanocomposites based carbazole. The substitution of N-carbazole by epoxide group was obtained in two different ways, under microwave irradiation and conventional processes.

These monomers and copolymers are characterized and confirmed by infrared spectroscopy (FTIR), 1H and 13C nuclear magnetic resonance, Elemental Analysis, Thermogravimetric Analysis (TGA) .

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Direct Quantification of Drug Loading Content in Polymeric Nanoparticles by Infrared Spectroscopy

G. Carissimi,[1] M.G. Montalbán,[1] M.G. Fuster,[1] G. Víllora,[1] and Andreas Barth,[2]

[1] Department of Chemical Engineering,
Faculty of Chemistry, University of Murcia, 30071 Murcia, Spain.

[2] Department of Biochemistry and Biophysics, Stockholm University, Stockholm SE-106 91, Sweden

guzmanaugusto.carissimin@um.es

Keywords: Silk fibroin • nanoparticles • infrared spectroscopy • drug loading content

Nanotechnology has enabled the development of novel therapeutic strategies such as targeted nanodrug delivery systems, control and stimulus-responsive release mechanisms, and the production of theranostic agent.[1,2] As a prerequisite for the use of nanoparticles as drug delivery systems, the amount of loaded drug must be precisely quantified, a task for which two approaches are currently used. However, both approaches suffer from the inefficiencies of drug extraction and of the solid-liquid separation process, as well as from dilution errors. This work describes a new, reliable, and simple method for direct drug quantification in polymeric nanoparticles using attenuated total reflection Fourier transform infrared spectroscopy, which can be adapted for a wide variety of drug delivery systems. Silk fibroin nanoparticles and naringenin were used as model polymeric nanoparticle carrier and drug, respectively.[3] The specificity, linearity, detection limit, precision, and accuracy of the spectroscopic approach were determined in order to validate the method. The method's robustness is demonstrated by the notable similarities between the calibrations carried out using two different equipment setups at two different institutions.

Acknowledgements

This work has been partially supported from the European Commission (FEDER/ERDF) and the Spanish MINECO (Ref. CTQ2017-87708-R) and the programme of support to the research of the Seneca Foundation of Science and Technology of Murcia, Spain (Ref. 20977/PI/18). Marta G. Fuster acknowledges support from Spanish MINECO (FPI grant, PRE2018-086441).

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Untargeted headspace gas chromatography – Ion mobility spectrometry analysis for detection of adulterated honey

A. Castell,[1] N. Arroyo-Manzanares,[1] M. García-Nicolás,[1] N. Campillo,[1] P. Viñas,[1] I. López-García,[1] M. Hernández-Córdoba [1]

[1] *Department of Analytical Chemistry, Faculty of Chemistry, Regional Campus of International Excellence "Campus Mare Nostrum", University of Murcia, E-30100, Murcia, Spain*

ana.castell@um.es

Keywords: Ion mobility spectrometry • Headspace • Gas chromatography • Honey adulteration • Untargeted analysis

Honey is considered a natural high-quality product much appreciated for its nutritional and medicinal properties. Its worldwide use together with its price have, almost inevitably, led to economically motivated adulteration, which makes honey one of the most adulterated foods in the market [1]. In this work, headspace gas chromatography coupled to ion mobility spectrometry (HS-GC-IMS) is proposed for the differentiation of honey according to its purity and the level of adulteration by sugar cane or corn syrups. The IMS is characterized by a good sensitivity, minimal sample treatment, rapidity and low cost of analysis.

The proposed method consists of incubating 1 g of honey at 100 ºC for 15 min and then injecting 750 µL of the sample headspace into the GC-IMS system. A 3-dimensional data map is obtained in 32 min. In order to develop this methodology, 198 honey samples were analyzed (56 pure honeys of different botanical origins, 142 honeys adulterated with sugar cane and corn syrup). Data were processed selecting markers of the topographic plots, and chemometric models were created for the detection of adulterated honey samples. The differentiation between pure and adulterated honey had a validation success of 97.4%, and the assessment of adulterant content was obtained with a 93.8% validation success rate for both adulterant agents assayed. To check the applicability of the method, nine samples of commercial honey were analyzed using the proposed HS-GC-IMS methodology, and seven of them were classified as honey adulterated with corn molasses. These results support the importance to have an effective analytical tool to guarantee the quality of commercial honey.

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Study of the Reactivity of 2-Azidoisocyanobenzenes

G. Cutillas-Font,[1] A. Pastor,[1] M. Alajarín,[1]

[1] *Department of Organic Chemistry, Faculty of Chemistry, University of Murcia*

Campus de Espinardo, Murcia 30100

guillermo.cutillasf@um.es

Keywords: organic synthesis • azidoisocyanobenzenes • heterocyclic compounds

This project is focused on the exploration of the reactivity of azidoisocyanobenzenes directed to the synthesis of new nitrogen heterocycles. The novelty of this research relays on the scarcity of background information about this topic.

The starting 2-azidoisocyanobenzenes **1** have been prepared from the corresponding azidoanilines[1].

Delightfully, the treatment of 2-azidoisocyanobenzenes **1** with the α-ketophosphorane **2** leads to the chloromethyltriazoles **3**. Subsequently, triazoles **3** are transformed into azidomethyltriazoles **4** by reaction with sodium azide, under soft conditions and good yields. Interestingly, in the presence of substoichiometric amounts of sodium azide, the azidomethyltriazoles **4** furnish the heterocyclic cyanamides **5**. Mechanistic studies are currently in progress in order to rationalize this unprecedented transformation.

Furthermore, new reactions of the azidomethyltriazoles **4** are under studied.

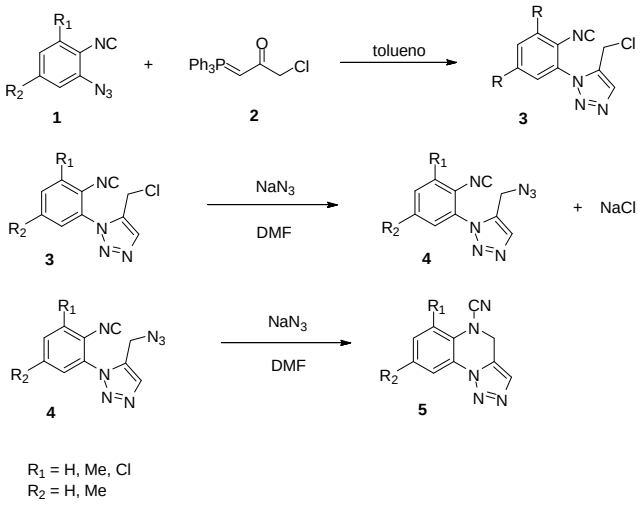

Figure 1. Synthetic pathway for the synthesis of heterocycles **5**.

Acknowledgements

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Copolymerization of maleic anhydride with vinyl acetate by maghniteH+

F.Bettahar 1 F. Bekkar2,[1] M. Ferahi3,[2] L.Ruiz…

[1] *Polymer Chemistry Laboratory, Department of Chemistry, Faculty of Exact and Applied Science,University of Oran 1. Ahmed Benbella.BP No. 1542 El'Menoeur, 31000 Oran, Algeria.*
[2] *a Laboratory of Macromolecular Chemistry (Labquimac), Department of Chemistry-Physics, Faculty of Science and Technology, University of the Basque Country (UPV / EHU), 48940 Leioa, Vizcaya, Spain*

faiza-bettahar@hotmail.com

Keywords: Synthesis of polymer• maleic anhydride • green chemistry, maghniteH+

Green chemistry aims to design products and chemical process that reduce or eliminate the use and synthesis of hazardous substances. We performed the copolymer synthesis of maleic anhydride with vinyl acetate catalyzed by maghnite H + under environmentally friendly conditions.

This copolymer is characterized, confirmed by transformation of IR quencher, H + NMR nuclear magnetic resonance, 13C NMR, DSC, GPC.

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I Symposium on Chemical and Physical Sciences for Young Researchers

Murcia, 22nd-23rd October 2020

P-10

Insertion reactions of insaturated molecules into the Pd–C bond of seven-member palladacycles

S. Fernández,[1] I. Saura-Llamas[1]

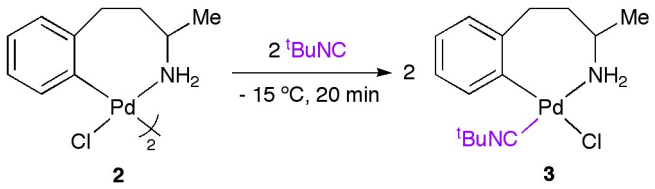
[1] *Department of Inorganic Chemistry, Faculty of Chemistry, Regional Campus of International Excellence "Campus Mare Nostrum", University of Murcia, E-30100, Murcia, Spain*

sara.fernandez4@gmail.com

Keywords: Palladacycles • Insertion reaction • arylalkylamines • orthometalation

Palladacycles are very versatile compounds that have aroused great interest due to their stability and reactivity. The most common palladacycles are those that contain *N*-donor ligands and five- or six-membered rings. Examples of seven- membered palladacycles are scarce in the bibliography. The synthesis of these compounds by C–H bond activation using a Pd(II) salt and the study of their reactivity are subject of great relevance because they provide information about the course of the catalytic cycles in which they are involved.

According to a general method previously described [1], the triflate of 1-methyl-3-phenylpropyl ammonium reacts with one equivalent of $Pd(OAc)_2$ in acetonitrile at 80 °C to afford, after the addition of NaCl, a dimeric seven-membered palladacycle containing chloro bridges. In this reaction, Pd(0) and a bis-amino complex of Pd(II) are also obtained, which decrease the yield of the desired product. In this research work, an experimental modification of the general method is described (changing time, temperature and "work up" of the reaction) that allows the synthesis of the palladacycle $[Pd_2\{\kappa^2(C,N)\text{-}C_6H_4(CH_2CH_2CH(Me)NH_2)\text{-}2\}_2(\mu\text{-}Cl)_2]$ (**2**) with a good yield. Complex **2** reacts with ^{t}BuNC to give the mononuclear derivative **3**.



2 **3**

Scheme. Reaction of complex **2** with ^{t}BuNC.

When 2,6-dimethylphenyl isocyanide is used in a similar reaction, an iminoacyl derivative (**4**) is obtained, which contains a coordinated isocyanide ligand and another one inserted. When **4** reacts with TlOTf and the reaction mixture is heated to 110 °C, the organometallic intermediate decomposes to give an amidinium salt (**5**), resulting from the C–N coupling, and Pd(0).

The reaction of **2** with styrene generates a nine-membered palladacycle containing hydrogen in β position to the metal center. This compound decomposes to give (*E,E*)-$[PdCl_2\{4\text{-}(2\text{-}(styrylphenyl)butan\text{-}2\text{-}amine\}_2]$ (**6**) and Pd(0). When $MeO_2CC{\equiv}CCO_2Me$ is used for the insertion reaction, a nine-membered alkenyl- palladacycle (**7**) is isolated.

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Improving anticancer therapy by Naringenin-Loaded Silk Fibroin Nanoparticles

M.G. Fuster, G. Carissimi, M.G. Montalbán, M.A. Pujante, M. Chaala and G. Víllora

Department of Chemical Engineering, Faculty of Chemistry, Regional Campus of International Excellence "Campus Mare Nostrum", University of Murcia, 30071 Murcia, Spain.

marta.g.f@um.es

Keywords: Anticancer activity • naringenin • silk fibroin • nanoparticle • cytotoxicity

The main goal of the present work was to assess the cytotoxicity effects of free NAR, silk fibroin nanoparticles (SFN) and naringenin-loaded silk fibroin nanoparticles (NAR-SFNs) on Human cervical cancer cells (HeLa) and human umbilical immortalized cells (EA.hy926). The cytotoxicity effects were evaluated with 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay after 48 h of exposure[1]. Results demonstrated the higher anticancer potential of synthesized NAR-SFNs than free NAR in HeLa cancer cell lines. However, cytotoxicity effects on EA.hy926 cell line were minimum in all cases (Figure 1).

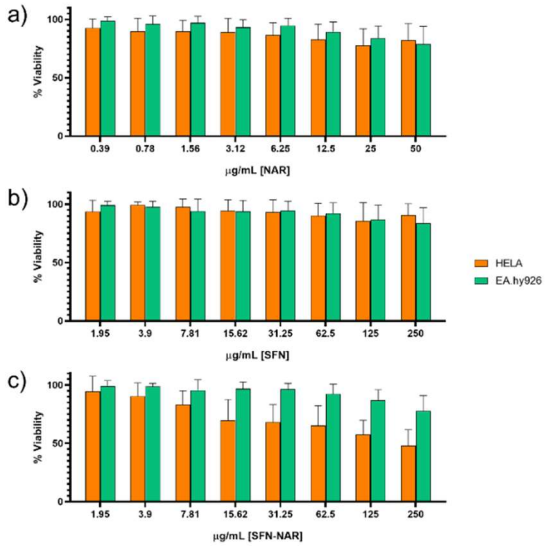

Figure 1. Cytotoxicity effect of free NAR (a), SFN (b) and NAR-SFNs (c) in Hela and in EA.hy926 cell lines. Data are expressed as percentage of cell viability ± SD versus concentration.

Acknowledgements

This work has been partially supported from (FEDER/ERDF) and the Spanish MINECO (Ref. CTQ2017-87708-R) and the Seneca Foundation (Ref. 20977/PI/18). Marta G. Fuster acknowledges support from Spanish MINECO (FPI grant, PRE2018-086441).

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Green synthesis of Naringenin-Loaded Silk Fibroin Nanoparticles

M.G. Fuster, G. Carissimi, M.G. Montalbán, M. Chaala, M. A. Pujante and G. Víllora

Department of Chemical Engineering,
Faculty of Chemistry, Regional Campus of International Excellence "Campus Mare Nostrum",
University of Murcia, 30071 Murcia, Spain.

marta.g.f@um.es

Keywords: Anticancer activity; naringenin; silk fibroin; nanoparticle

The aim of the present work was to synthesize naringenin-loaded silk fibroin nanoparticles (NAR-SFNs) by the dissolution of the silk fibroin in the ionic liquid, [emim$^+$][CH_3COO^-][1], using high-power ultrasound and rapid desolvation in methanol, followed by adsorption of naringenin[2]. The NAR-SFNs were characterized by dynamic light scattering (DLS) (Figure 1), Fourier transform infrared spectroscopy (FTIR) and differential scanning calorimetry (DSC). Drug Loading Content (DLC) and Encapsulation Efficiency (EE) were calculate.

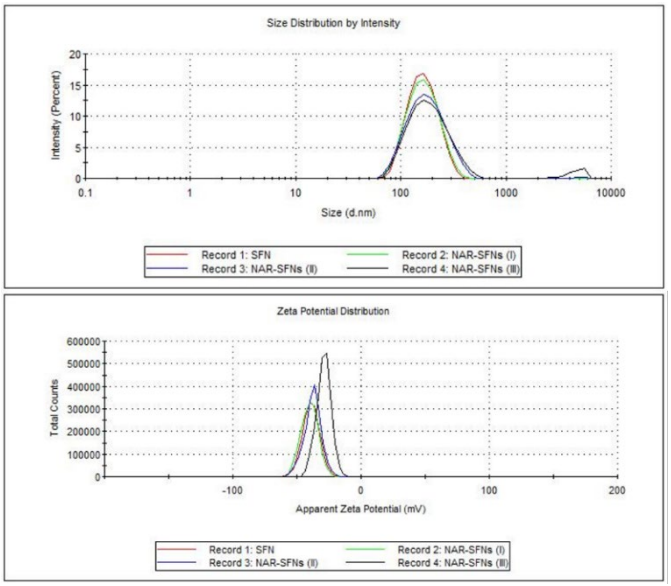

Figure 1. Size and Zeta Potential of silk fibroin nanoparticles and Naringenin-loaded silk fibroin nanoparticles for different concentrations.

Acknowledgements

This work has been partially supported from (FEDER/ERDF) and the Spanish MINECO (Ref. CTQ2017-87708-R) and the Seneca Foundation (Ref. 20977/PI/18). Marta G. Fuster acknowledges support from Spanish MINECO (FPI grant, PRE2018-086441).

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A green analytical method for the determination of nitrosamine impurities in pharmaceutical products

Claudia Giménez Campillo, Marta Pastor Belda, Natalia Campillo, Manuel Hernández-Córdoba and Pilar Viñas

Department of Analytical Chemistry, Faculty of Chemistry, Regional Campus of International Excellence "Campus Mare Nostrum", University of Murcia, E-30100 Murcia, Spain

claudia.gimenez@um.es

Keywords: nitrosamines • pharmaceutical products • dispersive liquid-liquid microextraction • gas chromatography-mass spectrometry

Nitrosamines (NAs) are chemicals including a nitro group attached to an amine in their chemical structure. A high number of NAs are known to be carcinogenic [1]. In particular, N-nitrosodimethylamine (NDMA) and N-nitrosodiethylamine (NDEA) have been catalogued as potential human carcinogens by the International Agency for Research on Cancer [2]. Recently, NAs impurities have been detected in some pharmaceutical products, such as those belonging to the sartan family and histamine-2 blockers as ranitidine. Thus, the medicines containing these active substances have been withdrawn. Gas and liquid chromatography coupled to mass spectrometry (GC-MS, LC-MS) are used as official methods in the determination of NAs in pharmaceutical products. In this study, a new analytical procedure based on a green sample treatment is proposed for the determination of nine nitrosamines in ranitidine pharmaceutical products. The crushed pills were dissolved in water (1 pill in 10 mL) and the insoluble excipients were removed by filtration using 0.45 µm Nylon filters. Because the NAs concentration level in the samples was very low, a microextraction step was applied for preconcentration purposes. For this, dispersive liquid-liquid microextraction (DLLME) was applied by rapidly injecting the mixture of chloroform (extractant solvent, 150 µL) and methanol (disperser solvent, 0.5 mL) into 10 mL of the pill solution containing 5% m/v NaCl. The analysis of the enriched organic extracts was carried out by GC-MS, providing high selectivity and unequivocal identification of the NAs, separated using a 20-min oven program with retention times ranging between 4.0 and 16.9 min, which corresponded to NDMA and N-nitrosodiphenylamine (NDPhA), respectively. The developed DLLME-GC-MS method was validated by obtaining the linearity, limits of detection and quantification, selectivity, precision and accuracy parameters.

Acknowledgements

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Tea-derivated catechins with antitumor properties

Rebeca González Guerrero[1], Román Martí Díaz[1], Luis Sánchez del Campo Ferrer[1], Fernanda Montenegro Arce[1], J. Neptuno Rodríguez López[1].

[1] *Dpto. Bioquímica y Biología Molecular A. Universidad de Murcia.*

rebeca.gonzalez4@um.es

Keywords: tea catechins, protein methylation, cancer.

Epidemiological studies have long shown that tea consumption has numerous beneficial effects on human health and illness prevention, including cancer and coronary disease [1]. These effects have been generally attributed to a family of polyphenolic compounds known as catechins.

In order to increase the bioavailability of catechins and make them more suitable for a potential therapeutic use, two methoxylated derivatives of catechins, TMCG and TMECG, with increased stability and lipophilicity, were obtained.

Through the inhibition of DHFR, these drugs act as antifolates and have the ability to block the methionine cycle. Methionine cycle is a key cycle in metabolism. Amongst other functions, it participates in protein synthesis and provides the methyl groups for protein and DNA methylation reactions. Compared with normal cells, cancer cells are greatly sensitive to methionine restriction, which makes the use of these drugs an interesting approach for cancer treatment [2].

The antitumor activity of these drugs has been assessed in *in vitro* and *in vivo* studies, showing the induction of apoptosis in different cancer cell lines and the reduction of tumour size and the increase in overall survival in mice. The combined use with other drugs and treatments as radiation therapy has also been studied.

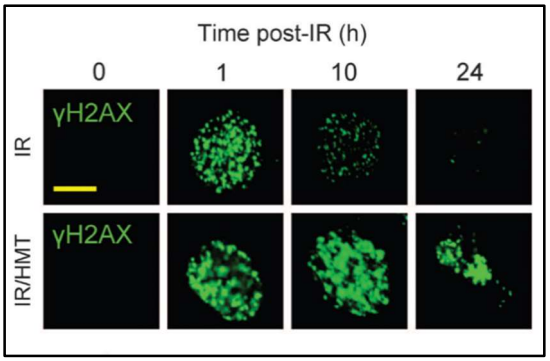

Figure 1. HMT treatment (TMCG+DIPY) impedes the repair of double strand breaks in DNA caused by ionizing radiation.

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New arene-complexes of Os(II) containing benzothiazole-based ligands. Study of its cytotoxic properties

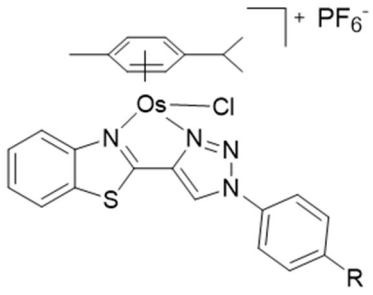
A. Hernández-García[1], F.J. Ballester Hernández[1], M. D. Santana Lario[1], D. Bautista Cerezo[2], J. Ruiz López[1]

[1]*Departamento Química Inorgánica, Universidad de Murcia, 30100 Murcia, España*
[2] *SAI, Universidad de Murcia, 30100 Murcia, España*

alba.hernandezg@um.es, jruiz@um.es

Keywords: arene-complex • benzothiazole • triazole

Cisplatin, carboplatin and oxaliplatin are three platinum-based compounds used clinically worldwide. The first osmium-based compounds to be studied as anticancer agents were analogs of ruthenium complexes: RAPTA-C[1], RM175[2] and NAMI-A[3] and the most studied arene-complexes are those with structure type $[Os(arene)(N^N)X]^+$, where N^N is a bidentate ligand N,N-donor and X is a halide[4]. In this proyect, we have synthesized new arene-complexes with structure type $[Os(\eta^6\text{-p-cymene})(N^N)Cl]PF_6$, where N^N is a bidentate ligand based on a benzothiazole to which a triazole fragment is attached. The triazole fragment contains a benzene substituent with a variable group, R. The variable group can be: $-CH_3$ (L1), -F (L2), $-CF_3$ (L3), $-NO_2$ (L4), $-OCH_3$ (L5) or $-NMe_2$ (L6). To characterize them, the spectroscopic technique of nuclear magnetic resonance, mass spectrometry (ESI-MS), infrared spectroscopy, analysis of C, H, N and S were carried out, and the UV-Visible and emission spectra were recorded. Furthermore, the crystalline structure of various compounds has been resolved by X-ray diffraction. Likewise, preliminary studies of cytotoxicity have been carried out.



R= $-CH_3$ (1), -F (2), $-CF_3$ (3), $-NO_2$ (4), $-OCH_3$ (5), NMe_2 (6)

Figure 1. General structure of the synthesized compounds.

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P-16

Development of palladium-catalyzed coupling cascade reactions through intramolecular carbopalladation of alkenes

P. Herrera,[1] J. A. García-López[1]

[1] *Grupo de Química Organometálica, Departamento de Q. Inorgánica, Facultad de Química, Campus de Espinardo, Universidad de Murcia, 30100.*

piedad.herrerar@um.es

Keywords: cascade • coupling • palladium • catalysis • heterocycles

Cascade reactions represent a straightforward synthetic strategy to obtain complex molecular structures from simple substrates. Different palladium-catalyzed cascade processes have been developed by trapping σ-alkyl Pd^{II} intermediates generated *in situ* with diverse coupling partners, showcasing the exceptional versatility of Pd catalysts in organic synthesis.[1]

In this work, an optimization process was carried out by analyzing different catalytic conditions that favour the formation of phosphorylated heterocycles, which were generated from the coupling of halogenated starting materials with dimethylphosphite. It has been proven that ether- as well as amide-type substrates were particularly well suited for an efficient development of these reactions.[2] Moreover, organometallic σ-alkyl Pd^{II} intermediates were isolated stoichiometrically in order to verify that the initially proposed reaction mechanism for the synthesis of the new coupling products obtained was compatible with the cascade processes outlined above.

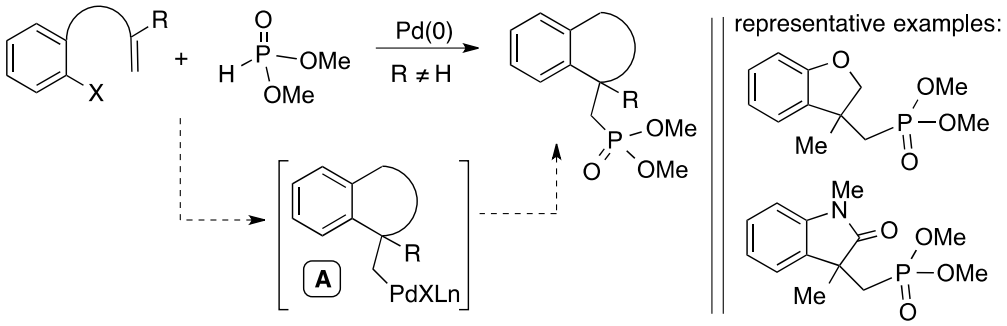

Figure 1. Pd-catalyzed synthesis of phosphorylated heterocycles.

Acknowledgements

Financial support from MICINN (grant PGC2018-100719-B-I00-with FEDER funding) and Fundación Séneca-Agencia de Ciencia y Tecnología de la Región de Murcia (grant 19890/GERM/15) is gratefully acknowledged.

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Synthesis and characterization of Pt(IV) complexes with cyclometalated *N*-heterocyclic carbene and 2-arylpyridine ligands

A. Jiménez-García,[1] Á. Vivancos,[1] D. Bautista,[2] P. González-Herrero.[1]

[1]*Departamento de Química Inorgánica, Facultad de Química, Universidad de Murcia, Apdo. 4021, 30071, Murcia, Spain*
[2]*SAI, Universidad de Murcia, Apdo. 4021, 30071, Murcia, Spain*

adrianjose.jimenez@um.es

Keywords: Platinum • Cyclometalation • NHC ligands • Luminescence

Cyclometalated Pt(II) complexes have been extensively studied for their luminescence and, therefore, numerous applications have been found for this type of compounds. The reported cyclometalated Pt(IV) complexes are much scarcer, although they have potential to present equally interesting photophysical properties.[1] Recently, the organometallic chemistry group at the University of Murcia has described the first Pt(IV) complexes that contain cyclometalated aryl-*N*-heterocyclic carbene and 2-arylpyridine ligands,[2] demonstrating that the carbene ligand benefits the luminescence properties of this type of complexes.

Based on this precedent, we have synthesized new bis-cyclometalated Pt(IV) complexes using different cyclometalated ligands of type 2-arylpyridine and maintaining the same *N*-heterocyclic carbene ligand to study their characteristics, including their photophysical properties.

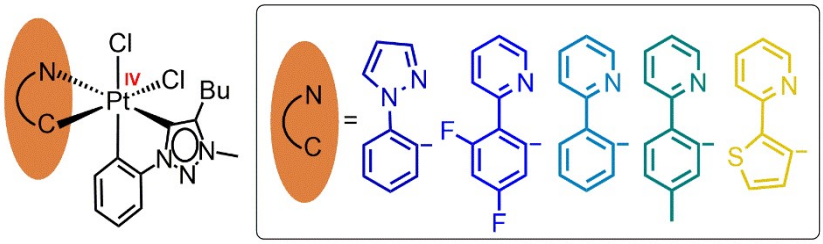

Figure 1. Bis-cyclometalated platinum(IV) complexes.

Acknowledgements

We gratefully acknowledge the financial support from Ministerio de Economía y Competitividad (PGC2018-100719-B-I00) and Fundación Séneca (19890/GERM/15). A.V. thanks Fundación Séneca for a Saavedra Fajardo Fellowship (20398/SF/17).

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Synthesis of novel, patentable scaffolds as potential highly selective Wee-1 kinase inhibitors

J. Jimenez-Bernad, JM. Villalgordo

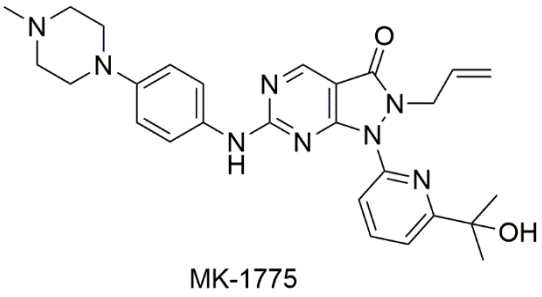
Eurofins-Villapharma Research. Parque Tecnológico de Fuente Álamo. C/ El Estrecho-Lobosillo, Km. 2,5. E-30320, Fuente Álamo (Murcia).

Facultad de Química de la Universidad de Murcia. C/ Campus Universitario, 5, 30100 (Murcia).

j.jimenezbernad@um.es

Keywords: Wee-1 • inhibitors • Oncology • SAR

We are developing the synthesis of novel, patentable and highly selective scaffolds as new inhibitors of Wee-1 kinase, with potential applications in Oncology. Selecting MK-1775 as reference and model compound, and through the use of pharmacophoric models and docking techniques, we have designed small libraries based on the above mentioned scaffolds. Screening of these libraries against Wee-1 allows the establishment of SAR tables and the selection of the best compounds for kinase selectivity, some ADME properties and the possible nomination of a new lead.[1,2]



MK-1775

Figure 1. MK-1775

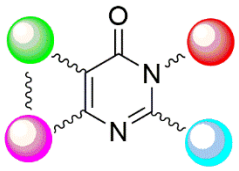


Figure 2. Scaffold.

Acknowledgements

Eurofins Villapharma-Research.

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New C^N cyclometalated platinum(II) complexes derived from N^O donor azo ligands as potential anticancer agents

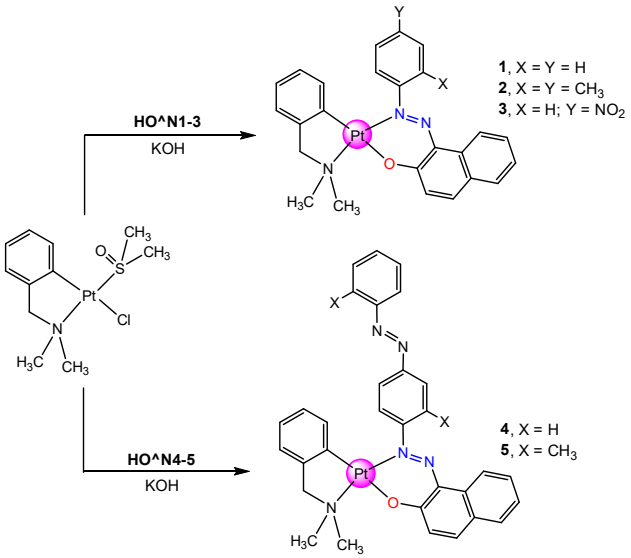
Antonio Linero Artiaga,[1] Venancio Rodríguez Hernández,[1] Enrique Ortega Forte,[1] José Ruiz López.[1]

[1]Departamento de Química Inorgánica, Facultad de Química, Universidad de Murcia, 30071 Murcia, Spain

antonio.linero@um.es

Keywords: azo compounds • platinum • antitumoral • cytotoxicity

Cisplatin is the most common platinum(II) complex used as an antitumoral agent in chemotherapy of testicular and ovarian tumors and colorectal carcinomas.[1] Nevertheless, several side effects related to its administration and acquired resistances of cancerous cells have been discovered. These facts have led the investigation to focus on the search of other platinum and metal transition-based complexes. In addition, organometallic compounds exhibit unique properties regarding to their diversity in structures.[2] In this work we report the synthesis and characterization of some new cyclometalated platinum(II) complexes derived from azo compounds, largely employed as drug carriers.[3] Cytotoxic tests of new complexes have been carried out against cellular lines of A2780 ovarian carcinoma and CHO health ovarian cells.



Acknowledgements

This work was supported by funds of the Spanish Ministerio de Economía y Competitividad and FEDER (RTI2018-096891-B-I00) and Fundación Séneca-CARM (Project 20857/PI/18).

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Reduction of air requirements and redesign of the biological aeration system, actions for energy optimization WWTP

Ana Belén Lozano Avilés,[1] Francisco del Cerro Velázquez,[2] Mercedes Llorens Pascual del Riquelme,[3]

[1] *Water Department, VECTORIS, S.L., 30100 Espinardo, Murcia, Spain*
[2] *Department of Electromagnetism and Electronics. Faculty of Chemistry, Campus of Espinardo*
[3] *Department of Chemical Engineering, Faculty of Chemistry, Campus of Espinardo*

ala71225@um.es

Keywords: WWTP • Oxygen requirements • Air transfer efficiency • Flow modelling and simulation techniques • Control strategy

Urban wastewater treatment involves a series of energy-intensive processes with significant room for improvement in terms of energy footprint. The biological aeration stage alone at the San Pedro del Pinatar wastewater treatment plant (WWTP), equipped with an activated sludge biological treatment system and a membrane biological reactor, accounts for more than 65% of operating costs. This study focuses on the analysis of the available aeration facility and the changes that must be incorporated to reduce load losses and increase oxygen transfer, with the aim of reducing the air needs for the biological process. For this purpose, flow modelling and simulation techniques are used [1], methods for determining and calculating the efficiency of air transfer [2-5] and the implementation of specific instrumentation for equipment control [6-7]. The actions carried out involve reductions in energy consumption of over 35%, in addition to contributing to the reduction of CO_2 emissions into the atmosphere.

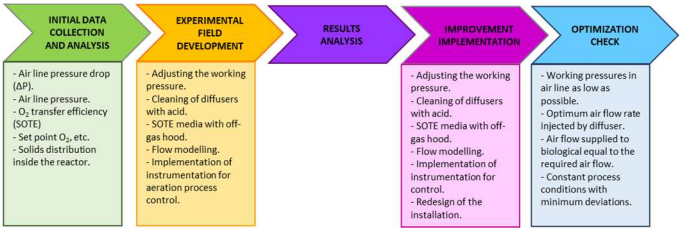

Figure 1. Figure 1. Steps followed for the energy optimization of an aeration system in WWTP.

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Study of comparison between spatial distribution and personal exposure to urban air pollutants

María del Mar Durán*, Antonia Baeza, Enrique González and Mercedes Llorens

Univ Murcia, Fac Química, Dept Ing. Química, Campus de Espinardo, Murcia 30071, Spain

*mariamar.duran@um.es

Keywords: environmental impact • spatial distribution • air pollution • personal exposure • risk analysis

Legislation 96/62/EC, 2000/69/EC, RD 102/2011 and RD 39/2017 established a new strategy for the assessment and management of ambient air quality in Spanish zones. They describe strategies and techniques of measurement to carry out action plans in all the zones that could overpass limit values.

During this study, air concentration values of benzene are represented by isoconcentration maps using Surfer 11.0 program. This representation provides with an overall vision of the environmental situation, indicates the most affected zones and lets to know the population exposure to air pollutants into the city. It also serves as a base to evaluate surface and population distributions of concentrations and enables to calculate the spatial mean concentration of the area analysed and the average personal exposure in Murcia.

Figure 1 represents personal exposure and spatial distribution to the whole city of Murcia. The comparison shows that the average concentration for benzene in the city is 5.08 μg/m^3 in function of area, while it is 5.21 μg/m^3 in function of population. This demonstrates that the personal exposure in cities can´t be represented only by the spatial mean concentration, but population distribution has also to be considered. This personal exposure could even be higher than spatial distribution, mainly when the distribution of population in the area is not homogeneous.

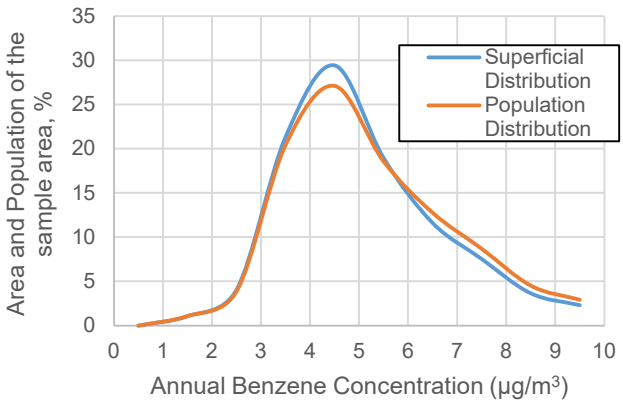

Figure 1. Annual Values for distribution of benzene concentrations in air in function of population (personal exposure) and area (spatial distribution).

Finally, the main results of this work stablish the most sensible areas where the exposure of population living there is higher and it will provide information for local authorities to take the measures necessary to control sources that contribute to air pollution, such as traffic flow, in order to improve air quality and to reduce the citizen exposure.

Acknowledgements: Authors acknowledge the financial support received from the Murcia Council and the favor from University of Murcia.

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Synthesis and characterization of new Ir(III) and Rh(III) half-sandwich complexes for cancer treatment.

A. Marco,[1] G. Vigueras,[1] N. Cutillas,[1] J. Ruiz.[1]

[1] *Departamento de Química Inorgánica. Facultad de Química. Universidad de Murcia. Murcia. Spain.*

alicia.marco@um.es

Keywords: rhodium • iridium • complexes • functionalization • cancer.

In the last few years iridium and rhodium compounds have emerged as potential alternatives to platinum-based drugs due to the advantages they offer over platinum. They have less side effects and important pharmacological properties.[1]
We have synthetized six new Ir(III) and Rh(III) complexes with three different benzimidazole based ligands (two of them functionalized, one with a valproate group and the other one with valproate and a fluorophore). The complexes have been characterized by elemental analysis, mass spectrometry and NMR techniques. Their purity has been confirmed by RP-HPLC. Furthermore, we have studied their stability in solution by NMR and their stability in cell culture medium by UV-Visible spectrometry. Biological studies are currently being carried out to test their anti-cancer action.

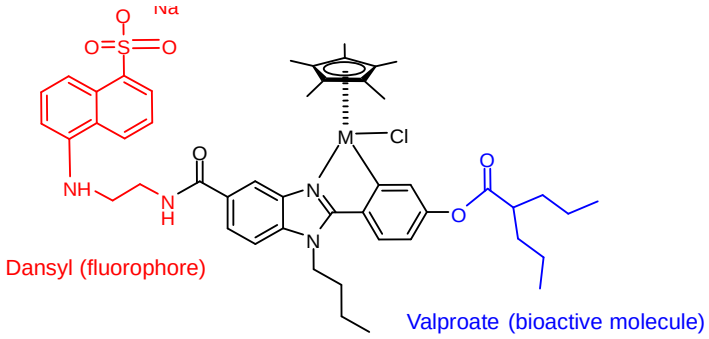

Figure 1. General structure of the complexes synthetized.

Acknowledgements

This work was supported by funds of the Spanish Ministerio de Economía y Competitividad and FEDER (CTQ2015-64319-R, RTI2018-096891-B-I00) and Fundación Séneca-CARM (Project 20857/PI/18). A. Marco thanks Fundación Séneca-CARM for a FPI grant (21234/FPI/19).

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Effect of metformin on melanoma cells

Román Martí Díaz[1], Rebeca González Guerrero[1], María Fernanda Montenegro Arce[1], Luis Sánchez del Campo Ferrer[1], José Neptuno Rodríguez López[1].

[1] *Dpto. Bioquímica y Biología Molecular A, Universidad de Murcia.*

roman.marti@um.es

Keywords: Cancer • melanoma • metformin • apoptosis • MITF

Melanoma is a type of cancer with a high capacity for invasion that can often lead to death. Although the molecular mechanisms involved in carcinogenesis are not well understood, knowledge of certain genes that act as master regulators in the development, differentiation, proliferation and cell survival offers an alternative in future therapies for the treatment of cancer. An example of this type of master gene in melanoma is the microphthalmia-associated transcription factor (MITF) [1].

Currently, metformin (1,1-dimethylbiguanide) is the most used therapy in patients with type 2 diabetes. Several studies have identified an association between the use of metformin and a beneficial effect on the prevention and treatment of many types of tumors, including those of the breast, liver, colon, pancreas and skin; this has generated a growing interest in the potential use of this drug as an anticancer agent [2].

This experimental work has mainly focused on evaluating the effect of metformin on melanoma cells. For this, proliferation, cytotoxicity and apoptosis assays were performed where differences in growth rate were observed as well as a phenotypic change in the cells. Interestingly, after exposure to high concentrations of metformin, there was also a significant decrease in MITF expressions levels, suggesting that this transcription factor may be involved in the morphological changes associated with apoptosis that take place in melanoma cells.

Overall, the results showed that, in the presence of metformin along with a significant decrease in MITF expression levels, there was a pronounced apoptosis in melanoma cells. In this sense, the results obtained could be of interest in order to design new therapeutic strategies based for the treatment of melanoma skin cancer, where metformin could be used as an adjuvant substance.

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Development of a potentiometric electronic tongue for the quality control of irrigation water

M. Miras, J. A. Ortuño, M. S. García

Group of Automatic Methods of Analysis: Chemical Sensors, Department of Analytical Chemistry, University of Murcia, Faculty of Chemistry, Spain

marina.mirasl@um.es

Keywords: electronic tongue • potentiometry • irrigation water • quality control

The objectives of this study are the development and application of a potentiometric electronic tongue to the quality control of irrigation water.

For this, six electrodes were built with plasticized membranes differing in the plasticizer and ion exchanger class. The selected plasticizers had different dielectrics constants: DOS (bis-[2-ethylhexyl] sebacate), TCP (tricresyl phosphate) and NPOE (2-nitrophenylotyl ether), which slightly change electrodes selectivity. With regards to ions exchangers, an anionic exchanger (tridodecylmethylamonium chloride: TDMACl) and a cationic one (potassium tetrakis [4-chlorophenyl] borate: KTFB) were used.

The irrigation waters which were studied were analyzed by ionic chromatography, ICP-OES (inductively coupled plasma atomic emission spectroscopy), potentiometric titration and conductivity measurement.

An exhaustive study of each electrode potentiometric responses to irrigation waters was performed for the selection of the analysis experimental conditions. As a result, the following conditions were selected: a 5-ml sample volume was injected on 100-ml of KCl $1x10^{-5}$M solution. The potential was meased after the 50-second sample injection. The different samples were measured from lowest to highest conductivity.

The potentiometric electronic tongue provides multivariate data related to the irrigation waters analyzed. By using a Radar plot to represent this data, a difference in the electrodes selectivity profile (crossed selectivity) was observed, which is a sufficient requirement for the subsequent sample differentiation. The principal components analysis (PCA) of these same data showed that the proposed potentiometric tongue allows the differentiation between most of the analyzed samples.

Moreover, the electronic tongue was applied to the quantitative analysis of irrigation waters. A mathematical treatment based on a lineal multivariate regression from the potentials of each electrode and the ion concentration in references samples. The results showed that the proposed method satisfactorily predicts Mg^{2+}, Na^{+} and Cl^{-} concentrations and, to a lower extent, the concentration of the rest of tested ions.

In conclusion, the proposed electronic tongue is suitable for the quality control of irrigation waters.

Analysis of the behavior of silk fibroin nanoparticles under DLVO theory

M.G. Montalbán, G. Carissimi, M G. Fuster, M. Chaala, F. Pedreño and G. Víllora

Department of Chemical Engineering,Faculty of Chemistry, Regional Campus of International Excellence "Campus Mare Nostrum", University of Murcia, 30071 Murcia, Spain.

mercedes.garcia@um.es

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Keywords: Silk Fibroin Nanoparticles • Stability • DLVO theory • Aggregation.

Derjaguin – Landau – Verwey – Overbeek (DLVO) theory is a well-known method to evaluate the stability of particles in aqueous solutions by analyzing the interaction energy between particles. Classical DLVO theory mainly considered two terms to represent the forces between the particles, van der Waals attraction (V_{vdW}) and electrical double layer repulsion (V_{elec}) [1]. The sum of these two forces determines if the net interaction between particles is repulsive or attractive, which is expressed by equation (1).

$$V_{total} = V_{vdW} + V_{elec} \quad (1)$$

The influence of variables in stabilization of silk fibroin nanoaparticles (SFNs) have been checked with aggregation studies by DLVO theory of Bian[2]. An example is shown in Figure 1.

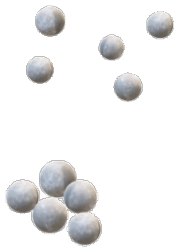

Figure 1. Calculated DLVO interaction energy between SFNs in 2.10^{-4}M of $Ca(NO_3)_2$

Acknowledgements

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Effect of Ionic Strength on the Size of Silk Fibroin Nanoparticles

M.G. Montalbán, G. Carissimi, M G. Fuster, M. Chaala, C. Serrano and G. Víllora

Department of Chemical Engineering, Faculty of Chemistry, Regional Campus of International Excellence "Campus Mare Nostrum", University of Murcia, 30071 Murcia, Spain.

mercedes.garcia@um.es

Keywords: Silk Fibroin Nanoparticles •Stability • Ionic Strength • Aggregation.

Drug delivery vehicle based on silk fibroin nanoparticles (SFNs) has been proved as an effective system for the release of drugs and other bioactive substances, because of its biocompatibility and controlled degradation. However, its applications are limited due to its tendency for aggregation in biological media. In this way, it is relevant to study their aggregation behavior to describe the health risks and the environmental transport. Stability of nanoparticles under different environmental conditions is a key factor on the development of their applications and, even more, when they are going to be used in the field of biomedicine[1]. In this work, the effect of monovalent versus divalent cations on SFNs aggregation in media with different ionic strength was examined.

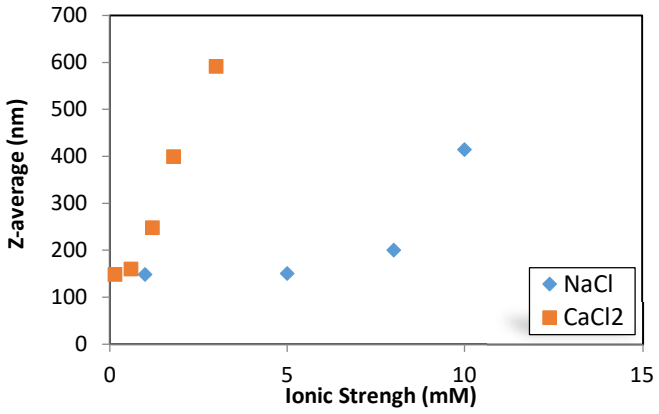

Figure 1. Effect of monovalent versus divalent cations on SFNs with ionic strength at 10min. of incubation.

As can be seen in Figure 1, in 10 min, the size of aggregates of SFNs in 3.10^{-3}M $CaCl_2$ suspension reached about 600nm, while much higher ionic strength (8.10^{-3}M) was necessary to observe aggregation in the NaCl suspension.

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Study of the metabolism of an anabolic steroid by combined approaches of ion mobility (LC-Q-TWIN-TOF MS) and molecular modelling

Tamara Moya Cavas, Jérôme Graton, Gaud Dervilly and Jean-Yves Le Questel

[1] Department of Modelling and Spectroscopy, CEISAM UMR CNRS 6230, University of Nantes, 44322 Nantes, France
[2] Laboratory for the Study of Residues and Contaminants in Foods, INRA UMR 1329, University of Nantes, Oniris, 44307 Nantes, France

td.moyacavas@um.es

Keywords: Stanozolol • Ion Mobility Spectrometry • Cross Collisional Section • The Density Functional Theory

The study of steroid metabolism faces the diversity of chemical structures and the existence of many isomeric forms, which are difficult to separate and identify with the usual analytical techniques. However, ion mobility spectrometry (TWIM)[1], coupled with liquid chromatography, quadrupole-time of flight with mass spectrometry (LC-Q-TOF MS), enables the determination of the collision cross section (CCS). This new parameter allows an improved characterization of the analytes, besides of being able to be calculated using molecular modelling tools.

The aim of this study is to detect the anabolic drug stanozolol[2,3], and its metabolites in a bovine urine sample. These compounds are difficult to detect experimentally because of their fast metabolism which leads to trace concentrations in complex matrices. First, we identified, through theoretical calculations (DFT and empirical), the exclusive protonation site of stanozolol and eight of its metabolites, the N1 nitrogen. Then, we estimated their respective theoretical CCS. Very good agreement was attained between both values measured experimentally in simple model matrices.

Unfortunately, we were not able to detect the analytes in the biological matrix because of the phenomenon of ion suppression. Finally, the experimental detection of glucuronide derivatives has been faced and the theoretical calculation of CCS of stanozolol glucuronides has been performed as a consequence.

Acknowledgements. *Erasmus Program 2018-2019*

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Speciation of low levels of thallium in waters using a magnetic nanocomposte and electrothermal atomic absorption spectrometry (ETAAS)

M.J. Muñoz Sandoval[1], M. Hernández Córdoba[1], I. López García[1].

[1]*Department of Analytical Chemistry, Faculty of Chemistry, Regional Campus of International Excellence "Campus Mare Nostrum", University of Murcia, E-30100 Murcia, Spain*

mariajose.munoz11@um.es

Keywords: ETAAS • Thallium • Nanoparticles • Ferrite • Graphene Oxide

Thallium species have a large number of applications in high-tech and chemical industries. Thallium compounds are very toxic to humans and other forms of life causing chronic and acute poisoning. Consequently, thallium poisoning is recognized as a risk, and its monitoring is of paramount importance.

In this work, a new analytical procedure for the determination of the two inorganic species of thallium, Tl(I) and Tl(III), is proposed. The procedure has been outlined following the criteria of Green Chemistry by minimizing the consumption of reagent, and so the production of wastes at the laboratory, and has enough sensitivity to achieve a reliable determination of these species in drinking water at the level established in the most demanding regulations.

The procedure is based in a dispersive micro-solid extraction step using Fe3O4@GO nanoparticles as the adsorbent material. In a slightly acidic medium and in the presence of potassium iodide, thallium is retained irrespectively of its oxidation state. The analyte is then released form the solid micro-phase and next measured by means ETAAS. Speciation is even possible provided that both forms of the element are previously separated. For such a purpose, the sample, in the presence of a large excess of bromide ions, is treated with cetylpyridinium chloride, and the neutral Tl(III) complex thus formed is extracted in a small amount of organic solvent. After eliminating the solvent, the ETAAS measurement is repeated, which permits both forms of the analyte to be discriminated. It is of note that the use of such a preconcentration stage results in an enrichment factor of 110, which, together with the sensitivity of ETAAS allows a very low detection limit (0.5 μg · L^{-1}) to be achieved.

Acknowledgements

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Determination of furvina® in medicated nail lacquers for onychomycosis treatment by direct UV/Vis spectrophotometry and liquid chromatography with diode array detection

Zenia Perez Rodriguez,[1] Natalia Campillo, [2] Pilar Viñas López-Pelegrín, [2] Manuel Hernández-Córdoba,[2] Yaset Rodríguez-Rodríguez, [3] Orlando Álvarez, [1] Zenaida Rodriguez Negrin,[1]

[1] Centro de Bioactivos Químicos (CBQ). Universidad Central "Marta Abreu" de las Villas. Carretera a Camajuaní km 51/2. Santa Clara, Villa Clara, Cuba. CP. 54830
[2] Department of Analytical Chemistry, Faculty of Chemistry, Regional Campus of International Excellence "Campus Mare Nostrum", University of Murcia, E-30100 Murcia, Spain
[3] Instituto Tecnológico de Santo Domingo (INTEC). Avenida de Los Próceres #49, Los Jardines del Norte 10602, Santo Domingo, República Dominicana

zperez@uclv.edu.cu; zenia.perezr@um.es

Keywords: furvina(R) • onychomycosis • UV/Vis spectrophotometry • HPLC-DAD • medicated nail lacquer

Fungal infections of the hands and feet are one of the most common infections in humans. Dermatophytes, yeasts, and molds are the three main fungi affecting the skin, and can cause onychomycosis, which affects around 4% of the world's population. Today, there are many commercially available oral antifungal agents used for nail treatment, but these have several disadvantages such as toxicity and large treatment periods. 2-Bromo-5-(2-bromo-2-nitrovinyl)furan (Furvina, active pharmaceutical ingredient (API)) is an efficient antimicrobial agent with broad-spectrum activity against Gram-positive and Gram-negative bacteria, yeasts and filamentous fungi. Furvina is currently in medical use in Cuba, being marketed as Dermofural ointment for human skin treatment and as Furvinol for veterinary use.[1,2]

In this research, a medicated nail lacquer is developed for the treatment of fungal infections, with less toxicity than oral treatments. A spectrophotometric method is developed and validated for the quantification of API furvina in the lacquer, using a blank matrix spiked at 0.25% level. This method was precise, accurate and linear in the range of 1-5 mg L^{-1}. On the other hand, capillary liquid chromatography with diode array detection (LC-DAD) has been proposed for the same purpose, with the possibility of detect impurities usually found in the API. LC separation was carried out using a Zorbax C18 (5 µm, 0.5 × 150 mm) column and a mobile phase consisting of 0.1% formic acid in wather and acetonitrile, in the 20:80 proportion with 20 µL min^{-1} flow-rate. The analyte eluted with a retention time of 1.9 min.

Acknowledgements

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Synthesis and study of [2]rotaxanes with geminal substituents in the benzylic positions of the macrocycle

J. Puigcerver, A. Martínez-Cuezva, M. Alajarín, J. Berná

Department of Organic Chemistry, Faculty of Chemistry, Regional Campus of Internacional Excellence "Campus Mare Nostrum", University of Murcia, E-30100, Murcia, Spain.

julio.puigcervera@um.es

Keywords: hydrogen bond • rotaxane • non-covalent interaction • macrocycle

Rotaxanes are a type of molecules formed by a linear component (thread) with two bulky ends, and one or more cyclic components (macrocycle) which are threaded in the linear component. The interaction that keeps the different component together is called mechanical bond. Importantly in the last decades these molecules have been employed as artificial molecular machines, finding new excited applications.[1]

Herein we described the design and synthesis of Leigh-type [2]rotaxanes[2] with significant variations on the structure of the macrocyclic counterpart. By following a clipping methodology, a five-component reaction was carried, employing a fumaramide axis as template. The establishment of hydrogen bonds between the thread and the macrocyclic precursor allows a facile formation of the interlocked systems, which were fully characterized. Moreover, NMR dynamic studies were carried out in order to estimate the rotation energy of the new functionalized macrocycles around the thread.[3]

Acknowledgements

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Synthesis and characterization of polymeric nanostructures for drug delivery

M. Rubio-Camacho,[1] Y. Alacid,[1] A. Mira,[1] A. Falcó,[1] M.J. Martínez-Tomé, [1] R. Mateo[1] and R. Mallavia[1]

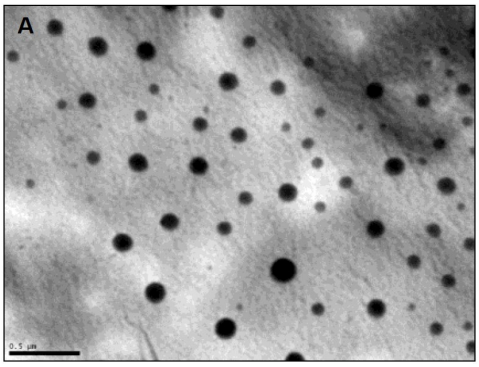
[1] *Instituto de Investigación, Desarrollo e Innovación en Biotecnología Sanitaria de Elche (IDiBE). Universidad Miguel Hernández de Elche (UMHE). 03202 Elche, Alicante. Spain*

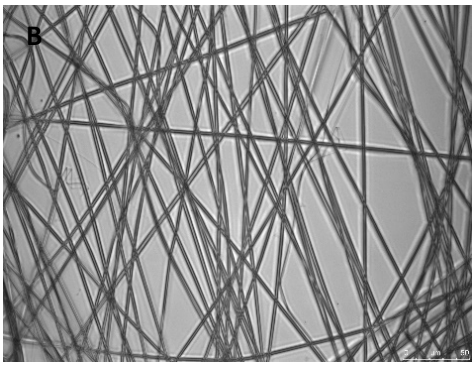
marta.rubioc@umh.es

Keywords: Polymers • poly [methyl vinyl ether-alt-(maleic anhydride)] (PMVEMA) • Nanoparticles • Nanofibers • Drug delivery

Nanotechnology has acquired great role in biomedicine due to the solutions it offers in order to improve the efficacy and security of conventional drugs. When it comes to developing nanostructures, polymers offer a wide range of biodegradable and biocompatible molecules with high bioavailability, adaptability and ease of handling. At this regard, we have developed several types of nanostructures –nanoparticles and nanofibers– based on synthetic derivatives of poly [methyl vinyl ether-alt-(maleic anhydride)] (PMVEMA) which are characterized by their high biocompatibility and low toxicity.

Polymeric nanoparticles were prepared with the ester derivative (PMVEMA-ES) through solvent displacement method while polymeric nanofibers were prepared with the anhydride derivative (PMVEMA-An) by electrospinning. Nanoparticles have been employed to treat tumors by loading them with different chemotherapeutic drugs such as temozolamide (TMZ) or doxorubicine (DOX). Nanofibers, on the contrary, have been applied to treat superficial inflammatory diseases such as Fascitis Plantar by loading them with natural analgesic compounds such as menthol. Both structures have been, properly, characterized by using physicochemical techniques.





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Development of a platform to analyse human exhaled volatile organic compounds: workflow for biomarker discovery

R.A. Sola Martínez,[1] G. Lozano Terol,[1] J. Gallego-Jara,[1] M. Cánovas Díaz[1] and T. de Diego Puente[1].

[1] Department of Biochemistry and Molecular Biology (B) and Immunology, Faculty of Chemistry, University of Murcia and Murcian Institute of Biosanitary Research Virgen de la Arrixaca (IMIB), Campus of Espinardo, Regional Campus of International Excellence "Campus Mare Nostrum", P.O. Box 4021, 30100, Murcia, Spain

rosaalba.sola@um.es

Keywords: Volatile organic compounds • Mass Spectrometry • Data pre-processing

The scientific community aims to achieve non-invasive detection of high prevalent diseases such as asthma or different types of cancer. Thus, analysis of volatile organic compounds (VOCs) in exhaled breath has been proposed as promising tool in therapeutic monitoring and diagnosis of certain pathologies. Currently, this strategy is in exploratory phase (biomarker discovery)[1]. This phase involves steps below: subject selection, breath sampling, analysis of exhaled breath, data pre-processing, statistical analysis, identification of interesting and validation of putative biomarkers in another study population[2] . For this phase to be successfully completed, all steps must be carried out following a reproducible protocol. In this sense, our group has developed a workflow for searching of biomarkers in exhaled air by a coupled system of thermal desorption and gas chromatography-single quadrupole mass spectrometry (TD-GC/q-MS). Here, special attention has been paid to steps such as sample collection and data pre-processing. So, open sources have been used for data pre-processing. Concretely, three different packages of R: xcms[3] , erah[4] and cliqueMS[5] .

Acknowledgements

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Characterization of floral origin of honey samples using headspace gas chromatography – ion mobility spectrometry

F. Zafra, M. García -Nicolás, N. Arroyo-Manzanares, Pilar Viñas

Department of Analytical Chemistry, Faculty of Chemistry, Regional Campus of International Excellence "Campus Mare Nostrum", University of Murcia, E-30100, Murcia, Spain
fa.zafranavarro@um.es

Keywords: Honey characterization • Ion mobility spectrometry • Headspace • Gas chromatography • Chemometric models

Nowadays, many types of honey from different botanical origin are available in the market. They differ in their organoleptic properties such as color, flavor or smell, thereby the interest in honey characterization relating to floral origin is increasing. In this work, the instrumental technique headspace gas chromatography coupled to ion mobility spectrometry (HS-GC-IMS) is used for monitoring honey volatile compounds that allow the differentiation and characterization of honey samples according to their floral origin. IMS is a state-of-the-art analytical technique that is based on the gas phase separation of ions in a drift tube under the influence of a constant electric field at atmospheric pressure. This separation is based on the charge, mass, size, and shape of the ions. However, the coupling GC-IMS generates complex multi-dimensional data, whose interpretation is a challenge requiring an exhaustive chemometric processing.

The analytical procedure consists on the incubation of 1g of honey sample at 100 ºC for 15 minutes and the injection of 750 µL of the headspace in the GC-IMS equipment. Compounds are ionized by a Tritium source in positive ion mode, and separated in a drift tube of 98 mm length operating with a constant voltage (500 V cm^{-1}) at 80 °C. For development of the chemometric model a total of 96 samples from ten different floral origin (orange blossom, albaid, rosemary, thousand flowers, thyme, broom, cantueso, melon, oak and heather) were analyzed.

The data processing is based on a non-targeted strategy using peak-region features (markers). A total of 275 markers was manually selected. Orthogonal partial least squares analysis (OPLS-DA) chemometric model was constructed using the 80% of the samples and the remaining 20% were used for method validation, the intensity of the reactant ion peak (RIP) being used for normalization. This chemometric model allowed the classification of honey sample into five groups named, albaid, thousand flowers, rosemary, orange blossom and other floral origins (including the rest of investigated floral origins, which due to the number of available samples could not build an individual group) with success validation rate of 100%.

Finally, in order to demonstrate the suitability of the proposed methodology, a total of 14 unknown honey samples were analyzed and classified attending to their floral origin. Two of them were classified as orange blossom, seven samples as thousand flowers, one sample as albaid and the rest belonged to another floral origin.

Acknowledgements

The authors acknowledge the financial support of Fundación Séneca (Project 19888/GERM/15) and the Spanish MICINN (Project PGC2018-098363-B-100).

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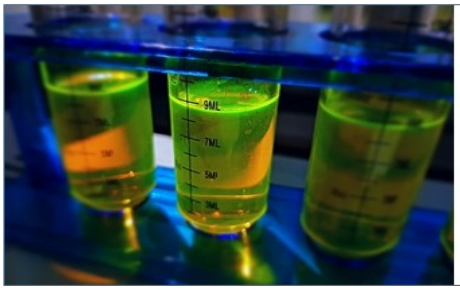

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