XVI EDICIÓN PREMIOS JOSÉ ANTONIO GARCÍA DOMÍNGUEZ

Dos años después de la última Reunión Científica de la Sociedad Española de Cromatografía y Técnicas Afines (SECyTA), celebrada de manera presencial en Santiago de Compostela en 2019, y dentro de la edición virtual XX SECyTA2021, se ha celebrado la "XVI Edición de los premios José Antonio García Domínguez". En esta ocasión se han concedido los premios a las mejores comunicaciones orales y a las mejores *web communication* (en sustitución de las presentadas habitualmente en formato de cartel), todas ellas presentadas en directo o mediante la grabación previa de los videos correspondientes. Como en años anteriores, Bruker ha patrocinado esta edición de los premios. Tras debatir los méritos científicos de las presentaciones, los jurados encargados de fallar los premios, tomaron por unanimidad los siguientes acuerdos:

1er Premio a la mejor Comunicación Oral (500 €):

Comunicación: OY-ND2

Título: EXPLORING GC-APCI-IMS-HRMS POSSIBILITIES FOR THE SCREENING OF ORGANIC-MICROPOLLUTANTS

Autores: *David Izquierdo-Sandoval[1]*, David Fabregat-Safont[1], Leticia Lacalle-Bergeron[1], Juan Vicente Sancho[1], Félix Hernández[1], Tania Portolés[1]*

[1] Environmental and Public Health Analytical Chemistry, Research Institute for Pesticides and Water (IUPA), University Jaume I, Castellón, Spain.

2º Premio a la mejor Comunicación Oral (400 €):

Comunicación OY-01

Título: THE ROLE OF OXIDIZED LIPIDS IN FUNGAL MEDIATED DISEASES USING ION MOBILITY-MASS SPECTROMETRY

Autores: *María Morán-Garrido[1]*, Jorge Sáiz[1], Coral Barbas[1]*

[1] CEMBIO, Facultad de Farmacia, Universidad San Pablo-CEU

1er Premio a la mejor Web Communication (300 €):

Communicación: WC-E11

Título: UHPLC-HRMS DETERMINATION OF AEROSOLIZED MARINE BIOTOXINS PRODUCED BY *OSTREOPSIS* cf. *OVATA*

Autores: *N.I. Medina-Pérez[1]*, E. Moyano[1], M. Dall'Osto[2], E. Berdalet[2]*

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2º Premio a la mejor Web Communication (200 €):

Comunicación: WC-CF5

Título: IN-DEPTH COMPARISON OF THE METABOLIC AND PHARMACOKINETIC BEHAVIOUR OF THE STRUCTURALLY RELATED SYNTHETIC CANNABINOIDS AMB-FUBINACA AND AMB-CHMICA IN RATS

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Los nombres de los ganadores fueron revelados tras la conferencia final, antes de la ceremonia de despedida de la reunión.

Juan Vicente Sancho
Secretario de la SECyTA

1er Premio a la mejor Comunicación Oral (OY-ND2)

EXPLORING GC-APCI-IMS-HRMS POSSIBILITIES FOR THE SCREENING OF ORGANIC-MICROPOLLUTANTS

David Izquierdo-Sandoval, David Fabregat-Safont, Leticia Lacalle-Bergeron, Juan Vicente Sancho, Félix Hernández, Tania Portolés

Ion mobility separation coupled to high resolution mass spectrometry (IMS-HRMS) provides extra valuable information in screening approaches of organic micropollutants in complex matrices. IMS allows to separate species of interest from co-eluting matrix interferences and/or resolve isomers based on their charge, shape and size being IMS-derived collision cross section (CCS) a robust parameter comparable between instruments [1].

Excellent separation power of gas chromatography (GC) combined with improved identification properties of HRMS is a powerful tool for identification and structure elucidation of unknown (semi)volatile compounds. Oppositely to electron ionization (EI), the soft ionization promoted by atmospheric pressure chemical ionization (APCI) source designed for GC allows a rapid and wide-scope non-target and suspect screening based on the investigation of the molecular ion and/or protonated molecule [2].

In the current study, the coupling between GC-APCI and IMS-HRMS has been used. A CCS library was built containing 264 relevant multi-class organic pollutants in environmental and food fields, comprising information regarding CCS for molecular ion and/or protonated molecules and some in-source fragments. Based on mobility data provided, the CCS values for both species were compared, and the possibility of separating isomers was explored, as well as the feasibility of employing CCS databases acquired by liquid chromatography-electrospray-IMS-HRMS. Moreover, the potential power of IMS was assessed in complex-matrix samples, such as feed fish extracts. The results reported in this work are of special interest for those researchers working on wide-scope screening of GC-amenable organic compounds.

Acknowledgements

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2º Premio a la mejor Comunicación Oral (OY-01)

THE ROLE OF OXIDIZED LIPIDS IN FUNGAL MEDIATED DISEASES USING ION MOBILITY-MASS SPECTROMETRY

María Morán-Garrido, Jorge Sáiz, Coral Barbas

Oxylipins are biologically active lipid mediators that play important roles in physio-pathological processes, like infections, cancer, and obesity. Recent findings from our research group have shown that several oxylipins are extremely altered in patients suffering from mucormycosis. These oxidized fatty acids have multiple isomers because of the double bonds and oxidation positions, which can be species-specific [1]. Therefore, its identification could reveal reliable diagnostic markers for the diseases they are involved in. Ion mobility (IM), which allows the separation of molecules based on their spatial configuration, stands out as an excellent tool to study different isomeric oxylipins [2]. In this research, ion mobility-mass spectrometry (IM-MS) was used to identify oxylipins related to mucormycosis.

Oxylipin standards were used to identify those in plasma samples from patients with mucormycosis using an Agilent's 6560 ion mobility Q-TOF LC/MS. The identification was assisted by two features provided by the IM:

- The All-Ions working mode, which provides clean MS/MS spectra by filtering by the drift time (DT) of the precursor ion.

- The High Resolution demultiplexing (HRdm) tool, which improves the resolution in IM throughout a post-acquisition processing that allows the differentiation of unresolved for compounds with very similar collision cross section (CCS).

Elevated oxylipins in infected plasma samples were finally identified based on the comparison of their retention time (RT), drift time (DT), collision cross section (CCS) and fragmentation patterns. These values were used for the creation of an internal database.

Given the wide variety of isomers that comprise oxylipins, IM-MS has shown a great potential for as a further step in their identification. Combining retention time, exact mass, CCS values, highly resolved IM (HRdm) and clean MS/MS fragmentation spectrum (All-Ions) provides unprecedented levels of identification of oxylipin isomers. Moreover, the database is intended to be regularly updated with new oxylipin standards. Finally, applying this technique to samples such as mucormycosis patients allows for a higher identification level and provides new diagnostic approaches for a disease with limited diagnostic confidence.

Acknowledgements

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1er Premio a la mejor Web Communication (WC-E11)

UHPLC-HRMS DETERMINATION OF AEROSOLIZED MARINE BIOTOXINS PRODUCED BY OSTREOPSIS CF. OVATA

N.I. Medina-Pérez, E. Moyano, M. Dall'Osto, E. Berdalet

The proliferations of the benthic dinoflagellate Ostreopsis cf. ovata have been related to mild respiratory symptoms in people exposed to marine aerosols on some beaches in the Mediterranean Sea. These disorders have been attributed -but not yet fully demonstrated- to palytoxin analogues (PLTX) (ovatoxins -OVTX- and isobaric palytoxin -isoPLTX-) produced by Ostreopsis. To evaluate the risk to human health that these events represent, it is necessary to better understand the mechanisms of production of these toxins and their transfer to the atmosphere. Accordingly, in this work we run different laboratory experiments using an aerosol generation tank with microbial communities that were obtained during an Ostreopsis bloom in the summers of 2019 [1], 2020 and 2021.

The experiments were run weekly incubating in the laboratory natural microplanktonic communities obtained during Ostreopsis cf. ovata blooms (June-August). The experiments were run at a controlled temperature (24±1°C) using a high-quality stainless steel airtight cylindrical tank (75 L; internal dimensions: 50 cm high, 44 cm diameter) that allowed the generation and collection of aerosols. The concentration of palytoxin analogues in both particulate phase of the seawater and air (aerosols) samples were analyzed. The chromatographic separation of palytoxins analogues was achieved using a Hypersil GOLD C18 column (100 mm x 2.1 mm id., 1.9 µm particle size) packed with totally porous silica particles (Hypersil, Thermo Fisher Scientific) and using gradient elution mode (acetonitrile-water, 0.1% formic acid; 300 µL min–1). This chromatographic method was coupled to a high-resolution mass spectrometeter (Orbitrap) using a heated-electrospray ionization source (UHPLC-HESI-HRMS).

During the experiments in 2019 the cells content was 103-104 Ostreopsis cells·Lwater−1 and the toxins concentration in the particulate phase was in the range of 1.1x105 - 3.1x106 pgtox Lwater−1, while the toxin concentration in the aerosol was estimated at 12–54 pgtox·Lair−1. Then, when it was bubbled after enriching the seawater with a higher abundance of Ostreopsis cells (105 cells·Lwater−1) and a higher concentration of toxins in the particulate phase of the water (9.3x105 - 7.9x106 pgtox·Lwater−1) the toxin concentration in the aerosol remained in the same range (11–54 pgtox·Lair−1). Therefore, no direct relationship was observed between the concentration of Ostreopsis cells in the water and the toxin in the aerosol.

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2º Premio a la mejor Web Communication (WC-CF5)

IN-DEPTH COMPARISON OF THE METABOLIC AND PHARMACOKINETIC BEHAVIOUR OF THE STRUCTURALLY RELATED SYNTHETIC CANNABINOIDS AMB-FUBINACA AND AMB-CHMICA IN RATS

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The use of new psychoactive substances (NPS) has dramatically increased in the last years. Among the most consumed families are synthetic cannabinoid receptor agonists (SCRA). As these compounds are, in most cases, completely metabolised, the elucidation of their potential consumption biomarkers in biological samples is required for the detection of drugs intoxications. In this sense, in vivo metabolism studies using mice or rats, in combination with high resolution mass spectrometry (HRMS), has proven to be useful for the study and evaluation of the metabolic behaviour of NPS.

In this study, the in vivo metabolism and pharmacokinetics of two structurally related SCRAs, AMB-FUBINACA and AMB-CHMICA, were evaluated using male Sprague-Dawley rats. Brain, liver, kidney, blood (serum) and urine samples were collected at different times for assessing the differences in metabolism, metabolic reactions, tissue distribution and excretion. Both compounds experimented O-demethyl reaction, which occurred more rapidly for AMB-FUBINACA. The parent compounds and the O-demethyl metabolites were highly bioaccumulated in liver and they were still found in this tissue 48 h after injection. Due to the different N-functionalisation (indazole/indole), different urinary metabolites were formed, some of them being detected even 24h after the injection. Out of the two compounds, AMB-FUBINACA seemed to easily cross the blood-brain barrier, presenting higher brain/serum concentrations ratio than AMB-CHMICA.

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